# NUMERICAL SOLUTION METHODS FOR FRACTIONAL PARTIAL DIFFERENTIAL EQUATIONS

A Thesis submitted by

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# Abstract

Fractional partial differential equations have been developed in many different fields such as physics, finance, fluid mechanics, viscoelasticity, engineering and biology. These models are used to describe anomalous diffusion. The main feature of these equations is their nonlocal property, due to the fractional derivative, which makes their solution challenging. However, analytic solutions of the fractional partial differential equations either do not exist or involve special functions, such as the Fox (H–function) function (Mathai & Saxena 1978) and the Mittag–Leffler function (Podlubny 1998) which are difficult to evaluate. Consequently, numerical techniques are required to find the solution of fractional partial differential equations.

This thesis can be considered as two parts, the first part considers the approximation of the Riemann–Liouville fractional derivative and the second part develops numerical techniques for the solution of linear and nonlinear fractional partial differential equations where the fractional derivative is defined as a Riemann–Liouville derivative.

In the first part we modify the L1 scheme, developed initially by Oldham & Spanier (1974), to develop the three schemes which will be defined as the C1, C2 and C3 schemes. The accuracy of each method is considered. Then the memory effect of the fractional derivative due to nonlocal property is discussed. Methods of reduction of the computation L1 scheme are proposed using regression approximations.

In the second part of this study, we consider numerical solution schemes for linear fractional partial differential equations. Here the numerical approximation schemes are developed using an approximation of the fractional derivative and a spatial discretisation scheme. In this thesis the L1, C1, C2, C3 fractional derivative approximation schemes, de-

veloped in the first part of the thesis, are used in conjunction with either the Centred–finite difference scheme, the Dufort–Frankel scheme or the Keller Box scheme. The stability of these numerical schemes are investigated via the technique of the Fourier analysis (Von Neumann stability analysis). The convergence of each the numerical schemes is also discussed. Numerical tests were used to confirm the accuracy and stability of each proposed method.

In the last part of the thesis numerical schemes are developed to handle nonlinear partial differential equations and systems of nonlinear fractional partial differential equations. We considered two models of a reversible reaction in the presence of anomalous subdiffusion. The Centred–finite difference scheme and the Keller Box methods are used to spatially discretise the spatial domain in these schemes. Here the L1 scheme and a modification of the L1 scheme are used to approximate the fractional derivative. The accuracy of the methods are discussed and the convergence of the scheme are demonstrated by numerical experiments. We also give numerical examples to illustrate the efficiency of the proposed scheme.

**Keywords:** Riemann-Liouville fractional derivative, Caputo fractional derivative, Grünwald-Letnikov fractional derivative, fractional subdiffusion equation, fractional advection-diffusion equation, accuracy, stability and convergence, L1 approximation, numerical method.

# Certification of Thesis

This thesis is entirely the work of *Sheelan Abdulkader Osman* except where otherwise acknowledged. The work is original and has not previously been submitted for any other award, except where acknowledged.

Student and supervisors signatures of endorsement are held at USQ.

Dr Trevor Langlands

Principal Supervisor

Professor Yury Stepanyants

Associate Supervisor

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Sheelan Abdulkader Osman

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# Notation

Notation used in this thesis.

## Chapter 1

| | |
|---|---|
| $\gamma$ | The anomalous diffusion exponent. |
| $K_\gamma$ | Anomalous diffusion coefficient. |
| $D, K_{1,\gamma}$ | Diffusion coefficient. |
| $f(x,t)$ | Source function. |
| $g(x)$ | Initial condition. |
| $\varphi_1(t)$, $\varphi_2(t)$ | Fixed (Dirchlet) boundary conditions. |
| $k_1$ | Forward reaction rate. |
| $k_{-1}$ | Reverse reaction rate. |
| $A(x,t)$, $B(x,t)$, $C(x,t)$ | Concentrations of each chemical species. |
| $L_t^{1-\gamma}$ | Non-standard/modified fractional derivative operator. |

## Chapter 2

| | |
|---|---|
| $p$ | The fractional derivative order. |
| $\nu_l$ | Scaled weights for the L1 scheme. |
| $A_l(p)$, $B_l(p)$, $\alpha_j(p)$, $\beta_j^*(p)$, $\mu_j^*(p)$, | Scaled weights for the C1 scheme. |
| $\widetilde{\beta}_j(p)$, $\widetilde{\mu}_j(p)$, $\widetilde{\nu}_l$ | Scaled weights for the C2 scheme. |
| $\widehat{\alpha}_j(p)$, $\widehat{\beta}_j(p)$, $\widehat{\mu}_j(p)$, $\widehat{\nu}_l$ | Scaled weights for the C3 scheme. |
| $\vartheta(j,p)$ | Error bound coefficient for the L1 scheme. |
| $\Upsilon(j,p)$ | Error bound coefficient for the C1 scheme. |
| $\hat{\vartheta}(j,p)$ | Error bound coefficient for the C2 scheme. |
| $K(j,p)$ | Error bound coefficient for the C3 scheme. |
| $\widehat{R}$ | Approximate order of convergence in $\Delta t$. |
| $\zeta(s,a)$ | The Hurwitz Zeta function. |
| $M_n$ | Maximum absolute value of the second derivative. |
| $\aleph_j(p)$ | Scaled weights for the $L1^*$ scheme. |
| $\hbar_j(p)$, $\aleph_j(p)$ | Scaled weights for the RL1 scheme. |
| $k(j,n,p)$ | Error bound coefficient for the $L1^*$ scheme. |
| $\widehat{k}(j,n,p)$ | Error bound coefficient for the RL1 scheme. |
| $C$, $C^*$ | Accuracy coefficients. |
| $\beta_0$, $\beta_1$, $\beta_2$ | Fitting parameters of the regression line. |
| $I_s(p,q)$ | The Incomplete Beta function. |
| $B(p,q)$ | The Beta function. |

## Chapter 3

| | |
|---|---|
| $\gamma$ | Anomalous diffusion exponent. |
| $\rho$ | Diffusion coefficient. |
| $x_i$ | Spatial grid points. |
| $t_j$ | Temporal grid points. |
| $a_j$, $\beta_j^*(\gamma)$, $\mu_j^*(\gamma)$ | Scaled weights for the IMC1 scheme. |
| $u_i$ | Approximate solution. |
| $U_i$ | Exact solution. |
| $\mathbf{A}^*$ | Tridiagonal matrix. |
| $\tau_{i,j}$ | Scaled truncation error. |
| $\zeta_j$ | Von Neumann stability variable. |
| $\epsilon_i$ | Numerical error. |
| $\lambda_q$ | Stability constant. |
| $\varpi_j(\gamma)$ | Stability weight. |
| $R1$ | Approximate order of convergence in $\Delta x$. |
| $R2$ | Approximate order of convergence in $\Delta t$. |

## Chapter 4

| | |
|---|---|
| $\gamma$ | Anomalous diffusion exponent. |
| $\sigma$ | Diffusion coefficient. |
| $x_i$ | Spatial grid points. |
| $t_j$ | Temporal grid points. |
| $\mathbf{A}$ | Tridiagonal matrix. |
| $a_j$, $\beta_j(\gamma)$, $\mu_j(\gamma)$ | Scaled weights. |
| $u_i$ | Approximate solution. |
| $U_i$ | Exact solution. |
| $\tau_{i,j}$ | Scaled truncation error. |
| $\zeta_j$ | Von Neumann stability variable. |
| $\epsilon_i$ | Numerical error. |
| $V_q$ | Stability constant. |

# Chapter 5

| | |
|---|---|
| $\gamma$ | Anomalous diffusion exponent. |
| $d$, $d_1$, $d_2$ | Diffusion coefficients. |
| $x_i$ | Spatial grid points. |
| $t_j$ | Temporal grid points. |
| $u_i$ | Approximate solution. |
| $U_i$, $V_i$ | Exact solution. |
| $\widetilde{\beta}_j(\gamma)$, $\widetilde{\mu}_j(\gamma)$ | Scaled weights for the KBMC2 scheme. |
| $\kappa_j(\gamma)$, $\widehat{\alpha}_j(\gamma)$, $\widehat{\beta}_j(\gamma)$, $\widehat{\mu}_j(\gamma)$ | Scaled weights for the KBMC3 scheme. |
| $\beta_j(\gamma)$, $\mu_j(\gamma)$ | Scaled weights for the KBML1 scheme. |
| $\tau_{i,j}^{(1)}$, $\tau_{i,j}^{(2)}$, $\tau_{i,j}^{(3)}$ | Scaled truncation errors. |
| $M(t)$ | Maximum absolute value of the fourth derivative in space. |
| $\zeta_j$, $\xi_j$ | Von Neumann stability variables. |
| $\epsilon_i$, $\varepsilon_i$ | Numerical errors. |
| $\Lambda_q$, $\breve{\Lambda}_q$, $\hat{\Lambda}_q$, $U_q$ | Stability constants. |
| $\rho(\gamma, k, \Lambda_q)$, $\breve{\rho}(\gamma, k, \breve{\Lambda}_q)$ | Stability bound. |
| $\widetilde{\alpha}_j(\gamma)$, $\widetilde{\omega}_l(\gamma)$ | Stability weights for the KBMC2 scheme. |
| $\varphi_{kj}(\gamma)$, $k = 1, 2, 3$ | Stability weights for the KBMC3 scheme. |
| $\alpha_j(\gamma)$, $\omega_l(\gamma)$ | Stability weights for the KBML1 scheme. |

## Chapter 6

| | |
|---|---|
| $\gamma$ | Anomalous diffusion exponent. |
| $A(x,t)$, $B(x,t)$, $C(x,t)$ | Concentration Chemical species. |
| $k_1$ | Forward reaction rate. |
| $k_{-1}$ | Reverse reaction rate. |
| $L_t^{1-\gamma}$ | Non-standard/modified fractional derivative operator. |
| $d$, $\hat{d}$ | Diffusion coefficients. |
| $y_k(x,t)$, $k = 1, 2, 3$ | Auxiliary functions for Model Type 2. |
| $\widetilde{\beta}_j(\gamma)$, $\widetilde{\mu}_j(\gamma)$ | Scaled weights for the KBMC2 scheme. |
| $\beta_j(\gamma)$, $\mu_j(\gamma)$ | Scaled weights for the IML1 scheme. |
| $\tau_{i,j}$ | Truncation error. |

# Acronyms & Abbreviations

| | |
|---|---|
| $L1$ | L1 approximation scheme. |
| $GL$ | Grünwald-Letnikov approximation scheme. |
| $C1$ | First modified L1 approximation scheme. |
| $C2$ | Second modified L1 approximation scheme. |
| $C3$ | Third modified L1 approximation scheme. |
| $RInt$ | Romberg Integration scheme. |
| $RL1$ | Reduction of the L1 approximation scheme. |
| $LRA$ | Linear Regression Approximation scheme. |
| $QRA$ | Quadratic Regression Approximation scheme. |
| $NLRA$ | Nonlinear Regression Approximation scheme. |
| $IMC1$ | Implicit finite difference method with the C1 scheme. |
| $IML1$ | Implicit finite difference method with the L1 scheme. |
| $DFL1$ | Dufort–Frankel method with the L1 scheme. |
| $KBMC2$ | Keller Box method with the C2 scheme. |
| $KBMC3$ | Keller Box method with the C3 scheme. |
| $KBML1$ | Keller Box method with the L1 scheme. |
| $KBMC2 - FADE$ | KBMC2 scheme for the fractional advection-diffusion equation. |

# Chapter 1

# Introduction and Literature Review

## 1.1 Background

Anomalous subdiffusion is a physical phenomenon which is observed in many systems which involving trapping, binding or macromolecular crowding. In recent years, examples of anomalous diffusion have been discovered in many different fields such as fluid mechanics (Chen, Wei, Sui, Zhang & Zheng 2011, Elbeleze, Kılıçman & Taib 2013), physics (Metzler & Klafter 2000*b*), engineering, and biology (Atangana & Alabaraoye 2013, Roul 2013). Anomalous diffusion is characterised by the asymptotic long-time behaviour of the mean-squared displacement of the form

$$\langle \Delta x^2(t) \rangle \sim \frac{2K_\gamma}{\Gamma(1+\gamma)} \Delta t^\gamma \tag{1.1}$$

where $\gamma$ is the anomalous diffusion exponent and $K_\gamma$ is the anomalous diffusion coefficient. For standard diffusion (ordinary or Brownian motion) the exponent is $\gamma = 1$, whilst in anomalous subdiffusion $0 < \gamma < 1$, and in superdiffusion $1 < \gamma < 2$. If the exponent is $\gamma = 2$, we have ballistic diffusion. Anomalous subdiffusion can be modelled using a number of methods including Continuous Time Random Walks (CTRWs) (Metzler & Klafter 2000*b*), Monte Carlo simulations (Marseguerra & Zoia 2006), Langevin equations (Porrà, Wang & Masoliver 1996, Mura 2008), Stochastic differential equations (Metzler & Klafter 2000*b*, Mura 2008) and by using Fractional Partial Differential Equations (FPDEs) (Metzler & Klafter 2000*b*).

A Fractional Partial Differential Equation is a partial differential equation, which involves a temporal fractional derivative or spatial fractional derivative. For example one of the well-known FPDEs is the fractional subdiffusion equation, which has the form

$$\frac{\partial f(x,t)}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 f(x,t)}{\partial x^2} \right) , \tag{1.2}$$

where the anomalous exponent $\gamma$ lies in the interval $0 < \gamma < 1$.

Another example is the fractional superdiffusion equation, which has the form:

$$\frac{\partial f(x,t)}{\partial t} = K \frac{\partial^{\beta} f(x,t)}{\partial |x|^{\beta}} , \tag{1.3}$$

where the exponent $\beta$ lies in the range $1 < \beta < 2$. In Equations (1.2) and (1.3), $\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}$ and $\frac{\partial^{\beta}}{\partial |x|^{\beta}}$ are fractional partial derivatives of temporal and spatial type respectively. Baeumer, Kovács & Meerschaert (2007) considered the fractional superdiffusion equation by extending the Reproduction–Dispersal equations, where the second derivative in a diffusion or dispersion model is replaced by a fractional derivative of order $1 < \beta < 2$.

A fractional derivative is an extension of the familiar derivative operator $\frac{\partial^n f(t)}{\partial t^n}$ by replacing the integer value $n$ with a non-integer parameter $p$ which can also be denoted as $\frac{\partial^p f(t)}{\partial t^p}$ or $D_t^p f(t)$ (Samko, Kilbas & Marichev 1993, Podlubny 1998). Definitions of several common fractional derivatives are given in the next section.

## 1.2 Different types of Fractional Derivatives

There are several definitions of fractional derivatives of the order $p$, the Riemann–Liouville fractional derivative, the Caputo fractional derivative, the Grünwald–Letnikov fractional derivative and the Riesz fractional derivative (Gorenflo & Mainardi 1998, Podlubny 1998, Li & Zeng 2015). Note $p$ can also defined as a complex number or variable, but in this research we focus on $p$ being a real number. In the following some definitions are introduced.

**Definition 1.2.1.** The left and right Riemann–Liouville fractional derivatives of order

$p > 0$ of the given function $f(t)$, $t \in (a, b)$ are defined respectively as (Li & Zeng 2015);

$$_{RL}D^p_{a,t}f(t) = \frac{1}{\Gamma(n-p)} \frac{d^n}{dt^n} \int_a^t \frac{f(\tau)}{(t-\tau)^{p-n+1}} d\tau \ , \tag{1.4}$$

and

$$_{RL}D^p_{t,b}f(t) = \frac{(-1)^n}{\Gamma(n-p)} \frac{d^n}{dt^n} \int_t^b \frac{f(\tau)}{(\tau-t)^{p-n+1}} d\tau \ , \tag{1.5}$$

where $\Gamma(.)$ is the Euler's Gamma function, with $n \in \mathbb{Z}^+$ satisfies $n-1 < p < n$.

**Definition 1.2.2.** The left and right Caputo fractional derivatives of order $p > 0$ of the given function $f(t)$, $t \in (a, b)$ are defined respectively as (Li & Zeng 2015);

$$_{C}D^p_{a,t}f(t) = \frac{1}{\Gamma(n-p)} \int_a^t \frac{f^{(n)}(\tau)}{(t-\tau)^{p-n+1}} d\tau \ , \tag{1.6}$$

and

$$_{C}D^p_{t,b}f(t) = \frac{(-1)^n}{\Gamma(n-p)} \int_t^b \frac{f^{(n)}(\tau)}{(\tau-t)^{p-n+1}} d\tau \ , \tag{1.7}$$

where $n \in \mathbb{Z}^+$ satisfies $n-1 < p < n$.

**Definition 1.2.3.** The left and right Grünwald–Letnikov fractional derivatives of order $p > 0$ of the given function $f(t)$, $t \in (a, b)$ are defined respectively as (Li & Zeng 2015);

$$_{GL}D^p_{a,t}f(t) = \lim_{\substack{h\to 0\\ Nh=t-a}} h^{-p} \sum_{k=0}^{N} (-1)^k \binom{p}{k} f(t-kh) \ , \tag{1.8}$$

and

$$_{GL}D^p_{t,b}f(t) = \lim_{\substack{h\to 0\\ Nh=b-t}} h^{-p} \sum_{k=0}^{N} (-1)^k \binom{p}{k} f(t+kh) \ . \tag{1.9}$$

**Definition 1.2.4.** The left and right fractional integrals (or left and right Riemann–Liouville integrals) with order $p > 0$ of the given function $f(t)$, $t \in (a, b)$ are defined respectively as (Li & Zeng 2015);

$$D^{-p}_{a,t}f(t) = {}_{RL}D^{-p}_{a,t}f(t) = \frac{1}{\Gamma(p)} \int_a^t f(\tau)(t-\tau)^{p-1} d\tau \ , \tag{1.10}$$

and

$$D^{-p}_{b,t}f(t) = {}_{RL}D^{p}_{t,b}f(t) = \frac{1}{\Gamma(p)} \int_t^b f(\tau)(\tau-t)^{p-1} d\tau \ . \tag{1.11}$$

**Definition 1.2.5.** The Riesz derivative with order $p > 0$ of the given function $f(t)$, $t \in (a, b)$ is defined as (Li & Zeng 2015)

$$ {}_{RZ}D^p f(t) = -\frac{1}{2\cos\left(\frac{p\pi}{2}\right)} \left( {}_{RL}D^p_{a,t} f(t) + {}_{RL}D^p_{t,b} f(t) \right) , \tag{1.12} $$

where $p \neq 2n+1$, $n = 0, 1, ....$ The Riesz derivative is sometimes denoted by $\frac{\partial^p f(t)}{\partial |t|^p}$.

It should be noted that the definition of the Riemann–Liouville fractional derivative in Equation (1.4) and the definition of the Caputo fractional derivative in Equation (1.6) are different but they are related in Laplace space. For example the fractional derivative of a constant function $f(t) = 1$, using the Caputo definition is zero, but using the Riemann–Liouville definition is not zero, that is

$$ {}_{C}D^p_{a,t}(1) = 0, \text{ and } {}_{RL}D^p_{a,t}(1) = \frac{t^{-p}}{\Gamma(1-p)} . \tag{1.13} $$

However, the Grünwald-Letnikov and Riemann–Liouville definitions have been shown to be equivalent (Podlubny 1998).

The Riemann–Liouville derivative and the Caputo derivative of the function $f(t)$ have the following relation

$$ {}_{RL}D^p_{a,t} f(t) = {}_{C}D^p_{a,t} f(t) + \sum_{k=0}^{n-1} \frac{f^{(k)}(a)(t-a)^{k-p}}{\Gamma(k+1-p)} , \tag{1.14} $$

where $n \in \mathbb{Z}^+$ satisfies $n-1 < p < n$ and $f(t)$ is integrable on $[a, t]$.

## 1.3 Focus of the Research

The focus of this research is to find the numerical solution of partial differential equation of fractional order such as:

$$ \frac{\partial u(x,t)}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( D \frac{\partial^2 u(x,t)}{\partial x^2} + K_\gamma \frac{\partial u(x,t)}{\partial x} \right) + f(x,t) \tag{1.15} $$

along with the initial and boundary conditions

$$ u(x,0) = g(x), \qquad 0 \le x \le L, \tag{1.16} $$

$$ u(0,t) = \varphi_1(t) \quad \text{and} \quad u(L,t) = \varphi_2(t), \qquad 0 \le t \le T, \tag{1.17} $$

where $D > 0$, $K_\gamma > 0$, the fractional order $0 < \gamma \leq 1$, and $f(x,t)$ is a given source function. The fractional derivative in Equation (1.15) can be discretised by using the L1 scheme (Oldham & Spanier 1974) or by using a modification of L1 scheme (given in Chapter 2). The centred finite difference scheme, the Dufort–Frankel, or the Keller Box methods will be used to discretise the second spatial derivative (or diffusion term) respectively in Chapters 3, 4, and 5.

In this work we develop an alternative numerical method based upon the Keller Box Method for Equation (1.15). This scheme extends the standard approach to the fractional case where the Riemann-Liouville definition of the fractional derivative is used instead of the Caputo definition used by Al-Shibani, Ismail & Abdullah (2012). We also use a modification of the L1 scheme to approximate the fractional derivative instead of the Grünwald–Letnikov approximation used by Al-Shibani et al. (2012).

Other examples to be considered in this research, in Chapter 6, are models of reversible reactions. Let $A$, $B$ and $C$ be three chemical species undergoing a reversible reaction, $A+B \rightleftharpoons C$ ( the double arrow symbol $\rightleftharpoons$ indicates that the reaction is reversible). In the absence of diffusion, the governing equations for $A$ and $B$ reduce to the reaction kinetic equations

$$\frac{dA}{dt} = -k_1 AB + k_{-1} C \ , \tag{1.18}$$

$$\frac{dB}{dt} = -k_1 AB + k_{-1} C \ , \tag{1.19}$$

and

$$\frac{dC}{dt} = k_1 AB - k_{-1} C \ , \tag{1.20}$$

where $k_1$ is the forward reaction rate constant and $k_{-1}$ is the reverse reaction rate. These equations correspond to the reaction, $A$ and $B$ reacting together to form species $C$, $A + B \rightarrow C$, if $k_{-1} = 0$.

Reversible reactions, in the presence of subdiffusion can be modelled by the system of fractional reaction–diffusion equations by using the CTRW model in Henry & Wearne (2000), which we will denote as Model Type 1,

$$\frac{\partial A(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma} A(x,t)}{\partial t^{1-\gamma}}\right) - k_1 A(x,t)B(x,t) + k_{-1}C(x,t) \ , \tag{1.21}$$

$$\frac{\partial B(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}B(x,t)}{\partial t^{1-\gamma}}\right) - k_1 A(x,t)B(x,t) + k_{-1}C(x,t) \ , \tag{1.22}$$

and

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}C(x,t)}{\partial t^{1-\gamma}}\right) + k_1 A(x,t)B(x,t) - k_{-1}C(x,t) \ . \tag{1.23}$$

Another model, which we call Model Type 2, has been derived by Angstmann, Donnelly & Henry (2013*a*) is of the form

$$\begin{aligned}\frac{\partial A(x,t)}{\partial t} &= D\frac{\partial^2}{\partial x^2}\left[e^{-k_1\int_0^t B(x,s)ds}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_1\int_0^t B(x,s)ds}A(x,t)\right)\right] \\ &\quad - k_1 A(x,t)B(x,t) + k_{-1}C(x,t) \ ,\end{aligned} \tag{1.24}$$

$$\begin{aligned}\frac{\partial B(x,t)}{\partial t} &= D\frac{\partial^2}{\partial x^2}\left[e^{-k_1\int_0^t A(x,s)ds}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_1\int_0^t A(x,s)ds}B(x,t)\right)\right] \\ &\quad - k_1 A(x,t)B(x,t) + k_{-1}C(x,t) \ ,\end{aligned} \tag{1.25}$$

and

$$\begin{aligned}\frac{\partial C(x,t)}{\partial t} &= D\frac{\partial^2}{\partial x^2}\left[e^{-k_{-1}t}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_{-1}t}C(x,t)\right)\right] \\ &\quad + k_1 A(x,t)B(x,t) - k_{-1}C(x,t) \ .\end{aligned} \tag{1.26}$$

This equation involves the non–standard fractional derivative operator $L_t^{1-\gamma}f(t)$

$$L_t^{1-\gamma}f(t) = e^{-k_1\int_0^t B(x,s)ds}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_1\int_0^t B(x,s)ds}f(t)\right) \ . \tag{1.27}$$

The current methods for approximating fractional derivatives will need to be modified to approximate the operator in Equation (1.27). We consider numerical solutions for Equations (1.21) – (1.23) and Equations (1.24) – (1.26), by applying the Keller Box method with the modification of the L1 scheme (developed in Chapter 5) and the Implicit finite difference with the L1 scheme (IML1) in Chapter 6.

One of the major issues in evaluating fractional derivatives numerically is the cost of the evaluation of the convolution sum. This computational cost increases as the number of time steps increases, which becomes significant for a large number of time steps. This is not as significant for problems involving only space–fractional derivatives, on a finite domain, as the computational domain is not normally growing and so the computational cost does not increase. We do acknowledge that if it is on infinite domain the computational cost is significant. One way to reduce this computational cost is to eliminate the

tail of the integral known as the short memory principle (Deng 2007*b*). This takes advantage of the fact that the integral in the fractional derivative is weighted mainly around the time $t$, that is the most recent history of the function $f(t)$, with the earlier history near $t = 0$ being weighted less.
In Chapter 2, we consider methods such as the short memory principle, the reduction of the computation of L1 scheme, and regression methods (the Linear regression method, the Quadratic regression method and the Nonlinear regression method) to reduce the cost of the evaluation of the convolution sum.

## 1.4 The Aim and Thesis Objectives

Recently fractional differential equations have attracted attention in the areas of science and engineering. The main feature of these types of equations is their nonlocal property in time or space. It is known that the integer order of the differential operator is a local operator, however the fractional operator is a non-local operator (Podlubny 1998, Diethelm, Ford & Freed 2004). The non-locality of the fractional derivative is quite attractive from the physical aspect as it allows us to model phenomena with memory effects. However, there is a fundamental problem related with all fractional differential operators, not only the Riemann–Liouville in Equation (1.4), in contrast with the differential operators of integer order which is its non-locality. Computationally, this non-locality leads to higher computational effort and storage requirements.

This research proposes developing numerical techniques to solve FPDEs. It will help develop more efficient (less computationally expensive) methods to approximate the Riemann–Liouville fractional derivatives whilst maintaining accuracy of their approximation. These approximation methods will be combined with finite–difference spatial discretisation methods to help more efficiently solve FPDEs. The advantages of such an approach are:

1. The numerical approximation is more useful where the analytical method is either unavailable or difficult to evaluate such as those that require the evaluation of the Fox or H-function.

2. It will enable the development of flexible and more accurate computational methods

to solve a variety of fractional partial differential equations.

3. It will help determine more computationally efficient methods and help reduce the computational effort and slow down involved in evaluating the memory sum.

## Thesis Objectives

In the present research, using numerical analysis for linear and nonlinear fractional partial differential equation, the objectives of this thesis are given below.

1. To develop a numerical scheme to find the approximate solution of Equation (1.15), Equations (1.21) - (1.23) and Equations (1.24) - (1.26).
2. To develop new accurate numerical methods for solving linear and nonlinear fractional partial differential equations.
3. To investigate a more efficient way to approximate fractional derivative whilst maintaining accuracy.
4. To discover the accuracy, convergence, and stability of these numerical schemes.

## 1.5 Previous Work

Fractional differential equations have acquired popularity in the area of science and engineering and have increasingly been used to model problems in physical processes, biology, finance, fluid mechanics and many other processes. In fluid mechanics for example Chen et al. (2011) demonstrated the feasibility and efficiency in the approximate solutions of the time–fractional diffusion and wave equation by using the generalised differential transform method. Elbeleze et al. (2013) investigated the unsteady flows of viscoelastic fluids through a channel tube and solutions for velocity field using a fractional Burgers model and a fractional generalised Burgers model.

There are also several types of the fractional partial differential equation which are interesting in the area of physics such as the fractional diffusion-advection equation, the fractional kinetic equation, and the fractional Fokker–Planck equation. The fractional Fokker–Planck equation takes into account the effect of an external force (Metzler & Klafter 2000*b*) which is given by

$$\frac{\partial P}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( K_\gamma \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\gamma} \frac{\partial}{\partial x} F(x,t) \right) P(x,t) \ , \tag{1.28}$$

where the fractional derivative operates on the forcing term $F(x,t)$. An alternative model, where the fractional derivative does not act on the forcing term is given by (i.e. as in Equation (1.24) with $A = P$ and $k_1 = 0$)

$$\frac{\partial P(x,t)}{\partial t} = \left( D \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} F(x,t) \right) \left[ \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} P(x,t) \right] \ . \tag{1.29}$$

In the area of biology, Roul (2013) considered the analytical and numerical solutions for the time-fractional biological population model

$$\frac{\partial^\alpha u(x,y,t)}{\partial t^\alpha} = \frac{\partial^2 u^2(x,y,t)}{\partial x^2} + \frac{\partial^2 u^2(x,y,t)}{\partial y^2} + g(u(x,y,t)) \ , \tag{1.30}$$

where the fractional derivative were described by the definition of Caputo derivative and $0 < \alpha \leq 1$. The homotopy perturbation method was applied to the model given in Equation (1.30) with, in the special case of $\alpha = 1$ the general solution reduces to the diffusion solution. Roul (2013) concluded that the homotopy–perturbation method is an effective and very powerful method for obtaining analytical solutions of a wide class of problems involving fractional derivatives. Atangana & Alabaraoye (2013) similarly demonstrated that the homotopy decomposition method (HDM) is a powerful and efficient tool for a solution of system of fractional partial differential equations that arose in the model for HIV (Human Immune Virus) infection of CD4+T cells.

Cable equations with fractional order temporal operators have been introduced to model electrotonic properties of spiny neuronal dendrites (Henry, Langlands & Wearne 2008, Langlands, Henry & Wearne 2009). These equations were derived from Nernst–Planck equations with fractional order operators to model the anomalous subdiffusion that arises from trapping properties of dendritic spines (Henry et al. 2008). The solution of the fractional cable equations are given as a functions of scaling parameters for infinite cables and semi-infinite cables with instantaneous current injections (Langlands et al. 2009). The authors show that electrotonic properties and firing rates of nerve cells are altered by anomalous subdiffusion, and they suggest electrophysiological experiments to calibrate and validate such models.

Langlands, Henry & Wearne (2011) modeled the subdiffusion by using two different approaches leading to two different fractional cable equations

$$\text{Model I} \qquad \frac{\partial V}{\partial T} = \gamma \, \frac{\partial^{\gamma-1}}{\partial T^{\gamma-1}} \left( \frac{\partial^2 V}{\partial x^2} \right) - \mu^2 k \frac{\partial^{k-1}(V)}{\partial T^{k-1}} \ , \tag{1.31}$$

and

$$\text{Model II} \qquad \frac{\partial V}{\partial T} = \frac{\partial^{1-\gamma}}{\partial T^{1-\gamma}} \left( \frac{\partial^2 V}{\partial X^2} \right) - \mu^2 \frac{\partial^{1-k}(V)}{\partial T^{1-k}} \ . \tag{1.32}$$

They also presented the fundamental solutions on finite and semi-finite domains.

The fractional chemotaxis equation was developed by Langlands & Henry (2010). They provided a new class of models for biological transport influenced by chemotactic forcing, macro–molecular crowding and traps. In this research they considered two separate equations which are similar to the fractional Fokker–Planck equation in Equation (1.28),

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( D_\gamma \frac{\partial^2}{\partial x^2} u(x,t) - \chi_\gamma \frac{\partial}{\partial x} \left( \frac{\partial c(x,t)}{\partial x} u(x,t) \right) \right) \ , \tag{1.33}$$

and

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} D_\gamma \frac{\partial^2 u(x,t)}{\partial x^2} - \chi_\gamma \frac{\partial}{\partial x} \left( \frac{\partial c(x,t)}{\partial x} \, \frac{\partial^{1-\gamma} u(x,t)}{\partial t^{1-\gamma}} \right) \ , \tag{1.34}$$

where the motion is influenced by the chemotactic forcing term

$$F(x,t) = -\chi_\gamma \frac{\partial c(x,t)}{\partial x} \ . \tag{1.35}$$

The fractional Fokker-Planck equation with space-time dependent forcing was derived by Henry, Langlands & Straka (2010). Angstmann, Donnelly & Henry (2013*a*) present a derivation of the generalized master equation for an ensemble of particles undergoing reactions whilst being subject to an external force field. They show reductions to a range of well–known models such as the fractional reaction diffusion equation and the fractional Fokker–Planck equation.

The CTRW model has also been extended to the networks including the effects of reaction (Angstmann, Donnelly & Henry 2013*b*) and forces (Angstmann, Donnelly, Henry & Langlands 2013). Recently Angstmann, Donnelly, Henry & Langlands (2016) introduced a mathematical network model to simulate a pathogenic protein neurodegenerative disease in the brain taking into account the anomalous transport. The set of reaction kinetics equations on the nodes of a network was used to model the proliferation and accumulation of the pathogenic proteins. The model predicts the disease extends as a propagating front over the brain and the anomalous behavior leads to the difference in the concentration of pathogenic proteins.

### 1.5.1 Analytical Solution of FPDEs

The analytic solutions of FPDEs have been considered recently by a number of researchers. These include the fractional diffusion equation (Mainardi 1996, Wyss 1986, Metzler & Klafter 2000*a*, Agrawal 2002, Jiang, Liu, Turner & Burrage 2012), the fractional reaction–diffusion equation (Henry & Wearne 2000, Langlands, Henry & Wearne 2008), the fractional time-space differential equation (Duan 2005, Huang & Liu 2005, Zhang & Zhang 2011), and space fractional diffusion equations (Zhang & Liu 2007, Shen, Liu, Anh & Turner 2008, Muslih & Agrawal 2010).

The solution of the fractional diffusion equation can be written in terms of Fox's H-function (Mainardi, Pagnini & Saxena 2005). Wyss (1986) applied the Mellin transform to the fractional diffusion equation, with the solution given in terms of Fox's H-function diffusion. Later Metzler & Klafter (2000*b*) found the solution for the fractional time and space equation in terms of Fox's H-function by using Mellin and Laplace transforms. Liu, Anh, Turner & Zhuang (2003) derived the solution of the time fractional advection–dispersion equation

$$\frac{\partial^\gamma u(x,t)}{\partial t^\gamma} = -v\frac{\partial u(x,t)}{\partial x} + D\frac{\partial^2 u(x,t)}{\partial x^2}\ , \tag{1.36}$$

where $(x,t) \in \mathbb{R}^+ \times \mathbb{R}^+$ and $0 < \gamma \leq 1$, by using a variable transformation, Mellin and Laplace transforms, and the properties of Fox's H-function (Mathai, Saxena & Haubold 2010). The Green's solution of space–time fractional advection–dispersion equation was derived by Huang & Liu (2005). The method of characteristics can also be applied to solving fractional partial differential equations as in Wu (2011).

The fractional diffusion–wave equation can be expressed in term of an auxiliary function by using Laplaces method which was based on Cauchy and Signalling problems (Mainardi 1996). Anh & Leonenko (2000) applied Gaussian and non-Gaussian scenarios to find the rescaled solutions to the equation given singular random initial data.

In 2001, Anh and Leonenko used a similar method to solve fractional diffusion and fractional kinetic equations. Agrawal (2002) considered a time fractional diffusion-wave equation in a bounded spatial domain. The space-time Riesz fractional partial differential equation with periodic conditions

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^\beta u(x,t)}{\partial |x|^\beta} \ , \text{ where } (x,t) \in \mathbb{R}^+ \times \mathbb{R}^+ \ , \tag{1.37}$$

was considered by Zhang & Liu (2007). They found the fundamental solution of the equation using a Fourier and Laplace transforms. Shen et al. (2008) considered a Riesz Fractional Advection–Dispersion Equation (RFADE),

$$\frac{\partial u(x,t)}{\partial t} = A\frac{\partial^\alpha u(x,t)}{\partial |x|^\alpha} + B\frac{\partial^\beta u(x,t)}{\partial |x|^\beta} \ , \text{ where } (x,t) \in \mathbb{R}^+ \times \mathbb{R}^+ \ , \tag{1.38}$$

where $0 < \alpha < 1$, and $1 < \beta < 2$, which is derived from the kinetics of chaotic dynamics. Shen et al. (2008) derived the fundamental solution for the RFADE and generated a discrete random walk model for this RFADE.

Muslih & Agrawal (2010) used the Fourier transform method to solve the fractional Poisson equation with Riesz fractional derivative of order $\alpha$,

$$(-\triangle)^{\frac{\alpha}{2}} = \frac{\rho}{\varepsilon_0}, \quad \text{where} \quad 1 < \alpha \leq 2 \ . \tag{1.39}$$

Recently, Momani & Odibat (2007) proposed the homotopy perturbation method for linear inhomogeneous fractional partial differential equations and compared this method with the variational iteration method. The authors found that the homotopy methods were more effective and convenient. The linear and nonlinear problem can be solved by using the homotopy analysis method (Xu, Liao & You 2009). The same method has been achieved for computing the approximate analytical solution of nonlinear partial differential equations of fractional order (Roul 2013).

Most fractional differential equations do not have exact solutions, so numerical techniques are required to approximate the solution of fractional partial differential equations because the closed form analytic solutions either do not exist or involve special functions, such as the Fox (H-function) function and the Mittag–Leffler function (Podlubny 1998), which are difficult to evaluate. For instance the solution of the fractional diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = K_\gamma \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u(x,t)}{\partial x^2} \right) \ , \tag{1.40}$$

by using the separation of variables, can be written as

$$u(x,t) = \sum_{n=0}^{\infty} c_n X_n(x) E_\gamma(-K_\gamma \lambda_n^2 t^\gamma), \tag{1.41}$$

where $X_n(x)$ and $\lambda_n$ are the eigenfunction and eigenvalue of the problem and $E_\gamma(z)$ is the Mittag–Leffler function (Klafter & Sokolov 2011). As a consequence many researchers have developed numerical schemes to approximate the solution of fractional partial differential equations. In the next subsection we give a review of the numerical methods used to approximate the solution of fractional partial differential equations.

### 1.5.2 Numerical Solution for Linear and Nonlinear FPDEs

The numerical solution of fractional partial differential equations has been developed in several ways by using the Finite Difference method (Chen, Liu & Burrage 2008, Murio 2008, Hu & Zhang 2012, Sweilam, Khader & Mahdy 2012, Tadjeran 2007, Tadjeran & Meerschaert 2007), the Adomian Decomposition method (Dhaigude & Birajdar 2012, Diethelm & Ford 2002), the Predictor–Corrector method (Diethelm & Ford 2002), the Finite Element method (Deng 2008, Jiang & Ma 2013), and Numerical Quadrature (Diethelm 1997, Murio 2008). The majority of these numerical methods either use the Grünwald–Letnikov approximation or the L1 scheme to approximate the fractional derivative. However, there are other techniques used to approximate the fractional derivative such as the Spline method (Pedas & Tamme 2011, Li 2012) and the Collocation method (Rawashdeh 2006, Hesameddini & Asadollahifard 2016).

The finite difference method can be used to numerically approximate the second spatial derivative. This method has been used to develop both explicit numerical methods (Yuste & Acedo 2005, Shen & Liu 2005, Liu, Zhuang, Anh, Turner & Burrage 2007, Chen, Liu, Anh & Turner 2012, Liu, Dong, Lewis & He 2015) and implicit numerical methods (Langlands & Henry 2005, Liu et al. 2007, Chen et al. 2008, Murio 2008, Chen et al. 2012). Explicit methods require less computation per time-step compared to implicit methods due to their requirement to solve systems of equations in the implicit case especially in two or three dimensions. However there is a stability problem when explicit methods are used to approximate the solution of the fractional partial differential equations.
For instance Yuste & Acedo (2005) proposed an explicit numerical scheme based on the finite difference method for the fractional diffusion equation, given by Equation (1.40), where the fractional derivative is a Riemann–Liouville derivative, defined previously given in Equation (1.4), and where the Grünwald-Letnikov approximation scheme (given in

Chapter 2), was used to approximate the fractional derivative. The numerical method was only conditionally stable for the equation, and they did not give the convergence of the method. Later Langlands & Henry (2005) considered an implicit numerical method for the fractional diffusion equation, Equation (1.40), developed using the L1 approximation (Oldham & Spanier 1974) for the fractional derivative: here they discussed the accuracy and stability of the numerical method and showed the method was stable and the accuracy of the fractional derivative was of the order $1+\gamma$ in time. Stability was later proven by Chen, Liu, Turner & Anh (2007) using the Energy 2–norm approach.

Murio (2008) developed the implicit method for the fractional diffusion equation, in Equation (1.40). The proposed method incorporated the Caputo derivative, Equation (1.6), and the fractional derivative was approximated by using a quadrature formula. The Fourier analysis method was used to show the method was unconditionally stable, and that it was first–order in time and second–order in space. Zhuang, Liu, Anh & Turner (2008) also proposed an implicit numerical method for the anomalous subdiffusion equation. The stability analysis was investigated by the Energy method and the convergence order was $O(\tau + h^2)$, that is first–order in time and second–order in space.
Liu et al. (2007) developed implicit and explicit methods for the space-and time-fractional advection dispersion equation on a finite domain and considered the stability and convergence of these methods. They proved the implicit method was unconditionally stable, but the explicit method was only conditionally stable. The convergence order for both implicit and explicit methods was first–order in time and first–order in space. Chen et al. (2008) applied the finite difference method for the fractional reaction subdiffusion equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( k_\gamma \frac{\partial^2}{\partial x^2} u(x,t) - k u(x,t) \right) + f(x,t) \ , \tag{1.42}$$

where $0 < \gamma \leq 1$, and $k > 0$. The relationship between the Riemann–Liouville and the Grünwald–Letnikov definitions of fractional derivatives was used to evaluate the fractional derivative with the Grünwald–Letnikov approximation. The discrete Fourier method was used to show the method is unconditionally stable and the accuracy of the proposed method was discussed and the convergence order was found to be $O(\tau + h^2)$. Chen et al. (2012) also used explicit and implicit methods to solve the two-dimensional fractional order anomalous subdiffusion equation. In this work they considered the case where the anomalous exponent $\alpha$ varied with $x$ and $t$ and also investigated the convergence and stability for these methods.

The semi–implicit numerical scheme, which is a modification of the Euler method, was used by Yu, Deng & Wu (2013) for a fractional reaction-diffusion equation. The stability and convergence of the method were investigated and the method was found to be first order accurate in time and second–order accurate in space. Ding & Li (2013) also developed two classes of finite difference schemes for the reaction subdiffusion equation by using a mixed spline function in space. The stability analysis was investigated, showing that the method is unconditionally stable and convergent of order $O(\tau + h^2)$.
Cao, Li & Chen (2015) derived a high–order compact finite difference scheme for solving the fractional reaction subdiffusion equation

$$ {}_C D_t^{\alpha} u(x,t) = K_\alpha \frac{\partial^2}{\partial x^2} u(x,t) - C_\alpha u(u,x,t) + f(x,t) \ , \tag{1.43} $$

with a Neumann boundary condition, $0 < \alpha < 1$, $K_\alpha > 0$ is the diffusion coefficient, $C_\alpha > 0$ is the constant reaction rate, and ${}_C D_t^{\alpha}$ is Caputo derivative. The compact finite difference method through the L2–norm was unconditionally stable and convergent with order $O(\tau^{2-\alpha} + h^4)$, where $\tau$ is the temporal step size, and $h$ is the spatial step size.

Recently, Mustapha, Abdallah, Furati & Nour (2016) considered a piecewise-linear time stepping discontinuous Galerkin method to solve the fractional diffusion equation with variable coefficients numerically. The fractional derivative was defined as a Caputo fractional derivative of order $\mu$ where $\mu \in (0, 1)$. The stability and convergence of the method was investigated and the method was found to be second–order in time and second–order in space.
Dehghan, Abbaszadeh & Mohebbi (2016) developed a numerical technique for solving time fractional diffusion wave equation by using a meshless Galerkin method to approximate the spatial derivative with Robin boundary conditions. The fractional derivative was defined by Caputo fractional derivative of order $\alpha$ where $\alpha \in (1, 2)$. The numerical method was unconditionally stable by using Energy method and the convergence of the method is first–order in space and order $3 - \alpha$ in time.

Al-Shibani, Ismail & Abdullah (2013) used the compact Dufort–Frankel method for solving time fractional diffusion equation

$$ \frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t) \ , \tag{1.44} $$

where $f(x,t)$ is a source term and $0 < \alpha < 1$ in which the fractional derivative was approximated by Grünwald–Letnikov approximation. Liao, Zhang, Zhao & Shi (2014) also constructed a new explicit Dufort–Frankel method for the fractional subdiffusion equation

$$\frac{\partial u(x,t)}{\partial t} = K_\gamma \, {}_0D_t^{1-\gamma} \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t) \ , \tag{1.45}$$

where $K_\gamma > 0$ and ${}_0D_t^{1-\gamma}$ is Jumarie's modified Riemann–Liouville form of the fractional derivative (Jumarie 2006) given by

$${}_0D_t^{1-\gamma} u(x,t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t \frac{u(x,\tau) - u(x,0)}{(t-\tau)^{1-\gamma}} d\tau \ , \qquad 0 < \gamma < 1 \ . \tag{1.46}$$

To approximate the fractional derivative, the Grünwald–Letnikov approximation was applied for the first time step and then the L1 approximation was used for the subsequent time steps. The method was found to be convergent under the same time–step, consistency condition, required by the classical Dufort–Frankel scheme. In addition, the stability of the method was established in the sense of a discrete Energy method. In Chapter 4, we develop a Dufort–Frankel-based scheme for Equation (1.15). In this equation the fractional derivative is defined by Riemann–Liouville derivative given in Equation (1.4) instead of the modified Riemann–Liouville derivative in Equation (1.46) as in Liao et al. (2014) or Caputo derivative as in Al-Shibani et al. (2013). In this work the fractional derivative is approximated using the L1 scheme instead of the Grünwald-Letnikov approximation.

The Keller Box method is an implicit numerical scheme with second order accuracy in both space and time for the heat conduction equation, or diffusion equation (Pletcher, Tannehill & Anderson 2012), which is also referred to as the Preissman Box scheme. This method was developed by Keller in 1971 (Keller 1971). Al–Shibani (Al-Shibani et al. 2012) proposed using the Keller Box method for the one dimensional time fractional diffusion equation, where the fractional derivative was replaced by a Caputo derivative and the Grünwald-Letnikov approximation was applied to approximate the fractional derivative.

In Chapter 5 we develop a Keller Box method for Equation (1.15). This scheme extends the standard approach to the fractional case where the Riemann–Liouville definition of the fractional derivative is used instead of the Caputo definition used by Al-Shibani (Al-Shibani et al. 2012). In addition, we use a modification of the L1 scheme to approximate the fractional derivative instead of the Grünwald–Letnikov approximation used by Al–Shibani.

Angstmann, Donnelly, Henry, Jacobs, Langlands & Nichols (2016) introduced an explicit numerical method for a class of fractional reaction–subdiffusion equation of the form

$$\frac{\partial u(x,t)}{\partial t} = D_\alpha \frac{\partial^2}{\partial x^2}\left[e^{-\int_0^t a(u,x,s)ds}\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(e^{\int_0^t a(u,x,s)ds}u(x,t)\right)\right] + c(u,x,t) - a(u,x,t)u \ , \tag{1.47}$$

where $c(u,x,t) > 0$, $a(u,x,t) > 0$, and the fractional derivative is defined by Riemann–Liouville definition. In Chapter 6 we consider the implicit Keller Box method with the modification of the L1 scheme to develop a numerical scheme to solve systems of fractional reaction–subdiffusion equations, Model Type 1 given in Equations (1.21) to (1.23) and Model Type 2 given in Equations (1.24) to (1.26). The latter system is of the form given in Equation (1.47).

The Crank–Nicolson method is a finite difference method, which is second–order accurate in time and in space, developed by Crank & Nicolson (1947). Tadjeran (2007) presented the Crank–Nicolson method for the fractional diffusion equation, when the diffusion coefficient was dependent on time and space, which was based upon a shifted Grünwald-Letnikov derivative approximation. Tadjeran (2007) showed by investigating stability, this method failed if the diffusion coefficient was evaluated at the time grid points instead of at the mid points of the temporal subinterval, that is if the diffusion coefficient was evaluated at the two endpoints of each time subinterval during the integration process. Tadjeran & Meerschaert (2007) obtained an unconditionally stable second–order accurate method for the two–dimensional fractional diffusion equation in both time and space

$$\frac{\partial u(x,y,t)}{\partial t} = d(x,y)\frac{\partial^\alpha u(x,y,t)}{\partial x^\alpha} + e(x,y)\frac{\partial^\beta u(x,y,t)}{\partial y^\beta} + q(x,y,t) \ , \tag{1.48}$$

where $d(x,y) > 0$ and $e(x,y) > 0$ are diffusion coefficients and $1 < \alpha \leq 2$ and $1 < \beta \leq 2$ are fractional orders. They combined the alternating directions implicit approach with a Crank–Nicolson discretisation and with a Richardson extrapolation scheme. The right–shifted Grünwald–Letnikov approximation was used to approximate the fractional derivative. The stability and convergence of these methods were discussed, and both methods were shown to be unconditionally stable: furthermore, the convergence order was $O(\Delta t^2 + \Delta x + \Delta y)$ by using the Crank–Nicolson method, while it was of the order $O(\Delta t^2 + \Delta x^2 + \Delta y^2)$ with the Richardson extrapolation scheme.

Hu & Zhang (2012) proposed a similar scheme for the fourth order fractional wave equation.

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} + b^2 \frac{\partial^4 u(x,t)}{\partial x^4} = f(x,t) \ , \qquad x \in (0,L), \quad t \in (0,T), \tag{1.49}$$

where $1 < \alpha < 2$ is a fractional exponent and $b$ is a constant coefficient with a source term $f(x,t)$. The method was unconditionally stable in the $l_2$–norm and the convergence order was $O(\tau^{2-\alpha} + h^2)$. Sweilam et al. (2012) also developed the Crank–Nicolson method to solve linear time fractional diffusion equations involving a Caputo fractional derivative. To study the stability, they used the standard Von Neumann stability analysis and showed the method was unconditionally stable. They also showed the convergence order was $O(\tau + h^2)$, that is first–order in time and second–order in space.

The Adomian Decomposition method (Adomian 1988) is an analytical/numerical approximation method for solving partial differential equations. Diethelm & Ford (2002) used the Adomian decomposition method for the Bagley-Torvik equation of fractional order as

$$Ay''(t) + BD_*^{\frac{3}{2}} y(t) + Cy(t) = f(t) \ , \tag{1.50}$$

where $D_*^q$ denotes the fractional differential operator of order $q \in \mathbb{N}$, defined through the Caputo derivative, and the convergence order was found to be $O(h^{\frac{3}{2}})$. Wang (2006) used a similar method for the fractional KdV–Burgers equation with time and spatial fractional derivatives

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} + \varepsilon u \frac{\partial^\beta u(x,t)}{\partial x^\beta} + \eta \frac{\partial^2 u(x,t)}{\partial x^2} + \vartheta \frac{\partial^3 u(x,t)}{\partial x^3} = 0 \ , \qquad t > 0 \ , \tag{1.51}$$

where $\varepsilon$, $\eta$ and $\vartheta$ are parameters, $\alpha > 0$ and $\beta \leq 1$. The fractional derivatives were described in the sense of the Caputo derivative. The method was shown to generate more realistic series solutions that generally converge rapidly in real physical problems. Yu, Liu, Anh & Turner (2008) have also used the Adomian Decomposition method to construct explicit solutions of the linear and non-linear time-space fractional reaction-diffusion equations.

Finite element methods are numerical schemes for solving an integral or differential equations. Deng (2008) developed a finite element method for solving the space and time fractional Fokker–Planck equation, the stability and error were also discussed. Deng (2008) showed the accuracy of this method was of order $2 - \alpha$ in time and $\mu$ in space i.e., $O(k^{2-\alpha} + h^\mu)$ where $\alpha \in (0,1)$ and $\mu \in (1,2)$. Recently, a moving finite element method was employed for the time fractional partial differential equation which was based on non-uniform meshes in both time and space (Jiang & Ma 2013). This method was proven to be unconditionally stable and accurate to order $2 - \alpha$ in time and order $r$ in space, where $0 < \alpha < 1$ and $r \geq 2$.

A quadrature formula (numerical integration formula) can also be used to evaluate the approximation of an integral defining the fractional derivative. Diethelm (1997) proposed the implicit algorithm based on a quadrature formula for solving the fractional differential equation. Murio (2008) investigated a similar quadrature formula for the definition of the Caputo derivative for the fractional diffusion equation.
Diethelm, Ford & Freed (2002) successfully constructed a Predictor–Corrector method for a fractional differential equation through the definition of the Caputo derivative. The way to use this method is to first rewrite the fractional ordinary differential equation as a Volterra Integral Equation and then use the Rectangle rule for the Predictor step, and the Trapezoid rule for the Corrector step. The convergence order of the predictor-corrector approach was $\min(2, 1 + \alpha)$, where $\alpha > 1$. They also discussed the accuracy and reduction of the computation cost where some techniques presented such as the Richardson extrapolation and the short memory principle.

Deng (2007*a*) presented an improved version of the Predictor–Corrector algorithm with the accuracy increased to $\min(2, 1 + 2\alpha)$, where $\alpha > 1$, and half of the computational cost when compared to the algorithm in Diethelm et al. (2004). Deng (2007*b*) proposed the short memory principle after using the nested meshes in Ford & Simpson (2001). By combining the short memory principle and the Predictor–Corrector approach, the computational cost was minimized to $O(h^{-1} \log(h^{-1}))$. In this work we investigate the short-memory approach for the fractional derivative by reduction of the computation of the L1 scheme, the fractional derivative is defined by the Riemann–Liouville derivative. We also used a new approach to reduce the computation cost by using regression methods in Chapter 2.

Other numerical methods are proposed by several researchers. Liu, Anh & Turner (2004) used the Method of Lines technique for discretising the space–fractional Fokker–Planck equations by using backward differentiation formulas. Similarly, Deng (2007*a*) applied this method for time fractional Fokker–Planck equations involving the Caputo fractional derivatives. A numerical scheme was proposed by Chen, Liu, Turner, Anh & Chen (2013) for a variable-order nonlinear reaction subdiffusion equation with a Riemann–Liouville derivative of variable-order. The stability of this method was investigated using Fourier analysis and shown to be unconditionally stable. The method was also found to be accurate of order two in time and in space.

Baeumer, Kovács & Sankaranarayanan (2015) recently considered the approximate solution of the space fractional partial differential equation

$$\frac{\partial u(x,t)}{\partial t} = (-1)^{q+1}\frac{\partial^\alpha u(x,t)}{\partial x^\alpha}\ , \tag{1.52}$$

with $2q - 1\alpha < 2q + 1$, $q \in \mathbb{N}$ where the shifted Grünwald–Letnikov approximation was used to approximate the fractional derivative. The stability and convergence of the method were discussed and the method was shown to be unconditionally stable.

Recently, Hesameddini & Asadollahifard (2016) considered a new method based on the sinc function for the time fractional diffusion equation Equation (1.44) without source term. The Energy method was used to show the method is stable and the method was found to be convergent under the time-step $O(\tau^{2-\alpha})$.

## 1.6 Overview of the Thesis

This thesis is organized as follows:

**Chapter 1** presents a description of the problem, a literature review, the motivation for the present study, and a concise review on the analytical and numerical solution methods for fractional partial differential equations including their application areas. The objectives of the present research are also summarised in this chapter.

**Chapter 2** describes approximation methods for the fractional derivative. In this chapter we focus on the L1 approximation scheme (Oldham & Spanier 1974). From the L1 scheme we develop three schemes that we use in the present research, denoted as the C1, C2, and C3 schemes. Another method considered to approximate the fractional derivative was Romberg Integration. We also discuss the short memory principle for the numerical evaluation of fractional derivatives.

**Chapter 3** develops a numerical scheme to solve the fractional subdiffusion equation with a source term using the C1 approximation and the centred finite difference scheme. In this chapter the accuracy analysis, consistency and convergence of the method are presented with the stability analysis conducted using Von Neumann stability analysis. Numerical tests are also used to confirm the accuracy and stability of the proposed method with examples being given.

**Chapter 4** develops a numerical scheme for the fractional subdiffusion equation with a source term using the L1 scheme with the Dufort–Frankel method. Here the accuracy analysis is presented and the stability analysis is again determined using the Von Neumann stability analysis. The convergence of the method is also discussed. Numerical tests are used of the proposed method with examples being given.

**Chapter 5** uses the Keller Box method to develop a numerical solution scheme for the fractional subdiffusion equation with a source term. Here we consider the use of three approximation schemes of the L1, C2, and C3 schemes to evaluate the fractional derivative. A numerical scheme for the fractional advection equation with source term is also developed by using the Keller Box method along with the C2 scheme. The stability analysis of each proposed method was investigated by Von-Neumann stability analysis. The accuracy and the convergence of each of the proposed methods were also tested. In addition, numerical tests are also used to confirm the accuracy and stability results of the proposed methods.

**Chapter 6** develops two numerical schemes for solving a nonlinear fractional reaction diffusion equation by using two methods; the finite difference discretisation scheme with the L1 scheme and the Keller Box method with the C2 scheme. The accuracy analysis and the convergence of the proposed methods are tested. Results from the proposed numerical methods for both models are determined by using numerical simulations.

**Chapter 7** discusses the conclusions of the thesis work, and gives some recommendations for future work.

# Chapter 2

# Approximation Methods of the Fractional Derivative

## 2.1 Introduction

In this chapter, we consider approximation methods to evaluate fractional derivative numerically. In particular we look for approximations for the Riemann–Liouville fractional derivative definition

$$ {}_{RL}D^{p}_{0,t}f(t) = \frac{1}{\Gamma(n-p)}\frac{d^n}{dt^n}\int_0^t \frac{f(\tau)}{(t-\tau)^{p-n+1}}d\tau. \tag{2.1}$$

The fractional derivative of $f(t)$ in the definition of Riemann–Liouville fractional derivative, Equation (2.1), depends upon $f(t)$ at the times $[0, t]$, which means that the fractional derivative of function $f(t)$ depends on the historical behavior of $f(t)$ (Podlubny 1998). One of the main approximations of the Riemann–Liouville fractional derivative is L1 scheme (Oldham & Spanier 1974). We give definition of the function $f(t)$ which is used further in this chapter.

**Definition 2.1.1.** A real function $f(t)$, $t > 0$, is said to be in the space $C_l$, $l \in \mathbb{R}$, if there exists a real number $p > l$, such that $f(t) = t^p f^*(t)$, where $f^*(t) \in C(0, \infty)$, and it is said to be in the space $C_l^k$ iff $f^{(k)}(t) \in C_l$, $k \in \mathbb{N}$ (Podlubny 1998, Momani 2006).

In this chapter, we develop three schemes based upon the L1 scheme (Oldham & Spanier

1974), the C1, C2, and C3 schemes. We also consider the accuracy of the L1 scheme as well as for the three modifications is investigated and numerical results are given. We also consider Romberg Integration to approximate the fractional derivative, again based on the Riemann–Liouville fractional derivative definition. In addition, we study the short–memory principle in two different ways; reduction of the L1 scheme and using regression approximation. There are more recent methods used to approximate the fractional derivative which is Spline method as in (Pedas & Tamme 2011, Li 2012) and Collocation method, based on the sinc function, as in (Hesameddini & Asadollahifard 2016). Another method to approximate the fractional derivative is the Grünwald-Letnikov approximation based upon the Grünwald-Letnikov definition, given by Equation (1.8) in Chapter 1.

## 2.2 Grünwald–Letnikov Scheme

As mentioned in the introduction, one method to approximate the fractional derivatives numerically is the Grünwald–Letnikov approximation. The approximation of Grünwald–Letnikov fractional derivative given in Definition 1.2.3 can be written as (Lubich 1986, Podlubny 1998, Yuste & Acedo 2005)

$$ {}_{GL}D_t^p f(t) = \Delta t^{-p} \sum_{k=0}^{[t/\Delta t]} w_k^p f(t - k\Delta t) + O(\Delta t^r), \tag{2.2} $$

where $\Delta t$ is the time step and $r$ is the order of the approximation which depends on the weight $w_k^p$ chosen. If $r = 1$, we have the first order approximation and $w_k^p$ is the $k^{th}$ coefficient of $z^k$ in the power series expansion of $(1 - z)^p$, that is

$$ (1 - z)^p = \sum_{k=0}^{\infty} w_k^p z^k, \tag{2.3} $$

or in particular

$$ w_k^p = (-1)^k \binom{p}{k}, \tag{2.4} $$

where

$$ w_0^p = 1. \tag{2.5} $$

Higher order approximations are available, such as the second–order approximation where the weights, $w_k^p$, are found from the power series (Lubich 1986)

$$\left(\frac{3}{2} - 2z + \frac{1}{2}z^2\right)^p = \sum_{k=0}^{\infty} w_k^p z^k. \tag{2.6}$$

The coefficients $w_k^p$ in Equation (2.6) can be computed by using Fourier Transforms (Podlubny 1998). The Grünwald–Letnikov derivative (GL scheme), given in Chapter 1 by Definition 1.2.3, was modified by (Meerschaert & Tadjeran 2004) for the case of right–hand and left–hand fractional derivatives which are given in Equations (1.8) and (1.9) respectively.

The estimate of the accuracy of the GL scheme, using the weights $w_k^p$ given by Equation (2.3), was tested on the functions

$$f(t) = \begin{cases} t^k, & \text{where } t > 0, \text{ and } k = 2,3,4 \\ 1 - e^t + t^3, & \text{where } t > 0 \\ 1 + t^\gamma, & \text{where } t > 0 \end{cases} \tag{2.7}$$

to approximate the fractional derivative of order $p = 1 - \gamma$ at time $t = 1$ and the value $\gamma = 0.1, \ldots, 0.9$. Note the function $f(t) = 1 + t^\gamma$ was chosen here to represent the first two terms of a Mittag–Leffler function which occur in the separation of variables solution Equation (1.41), where the derivatives become singular near $t = 0$ for this function.

The error is plotted as a function of $\Delta t$ on double logarithmic scale plot given in Figures 2.1 – 2.5. From these results which we see, as $\Delta t$ is decreased, the error decreases for each value of $\gamma$. We also note the error decreases in magnitude as the value of $\gamma$ increases for a fixed $\Delta t$ value. This is also reflected in the results shown in Table 2.1, for example in case $f(t) = t^2$ the maximum error occurs where $\gamma = 0.1$ which is $8.598 \times 10^{-3}$, and the minimum error occurs where $\gamma = 0.9$ which is $9.444 \times 10^{-4}$. Also for the functions $f(t) = t^3$, $t^4$, and $1 - e^t + t^3$ the maximum error occurs for $\gamma = 0.1$ and the minimum error occurs for $\gamma = 0.9$. But for function $f(t) = 1 + t^\gamma$ we see the minimum error occurs for $\gamma = 0.9$ and the maximum error occurs for $\gamma = 0.4$. As shown in the Figures 2.1 – 2.5, the slope of the lines matches asymptotically the slope of 1 of the dashed lines shown in each figure indicating a first order approximation.

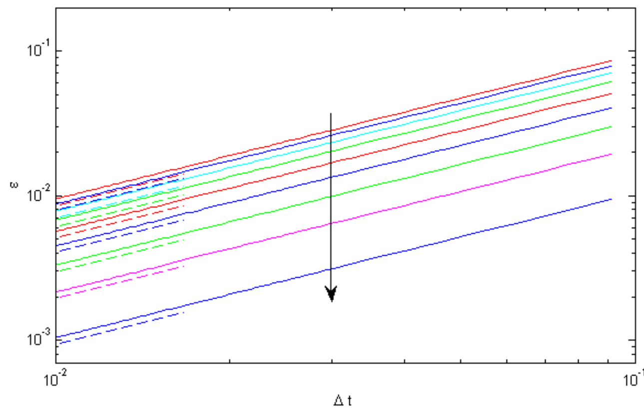



Figure 2.1: (Color online) The absolute error in using the GL scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = t^2$ at time $t = 1.0$. Results are shown for $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow and dashed lines show lines of slop $\gamma$ for comparison.

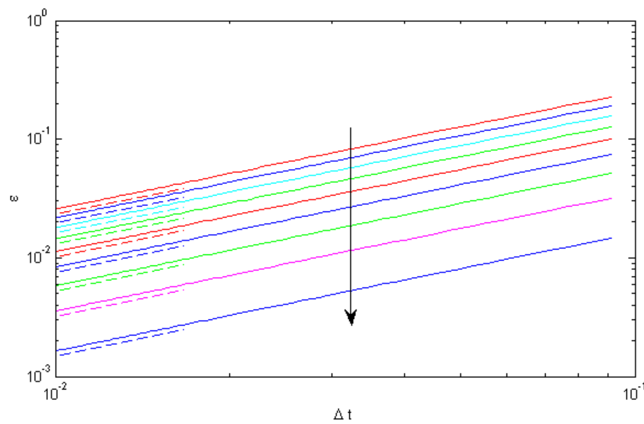



Figure 2.2: (Color online) The absolute error in using the GL scheme for the fractional derivative of order $1-\gamma$ of the function $f(t) = t^3$ at time $t = 1.0$. Results are shown for $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow, and dashed lines show lines of slop $\gamma$ for comparison.

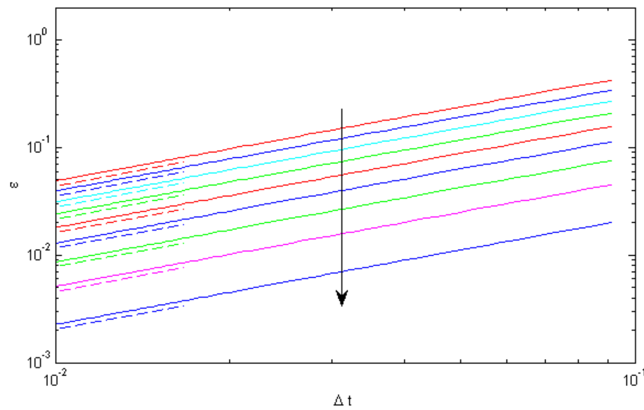



Figure 2.3: (Color online) The absolute error in using the GL scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = t^4$ at the time $t = 1.0$. Results are shown for $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow and dashed lines show lines of slop $\gamma$ for comparison.

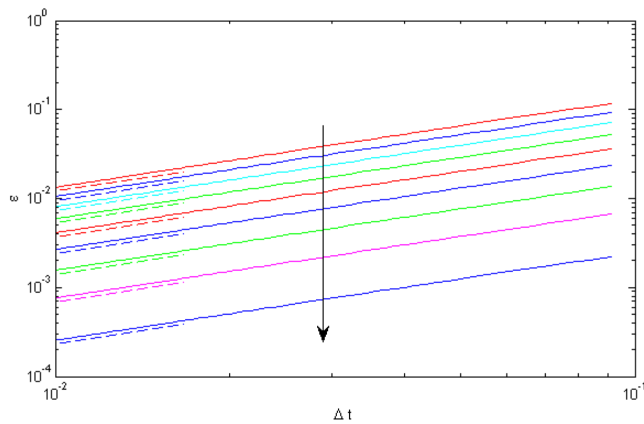



Figure 2.4: (Color online) The absolute error in using the GL scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 - e^t + t^3$, where $\gamma = 0.1, \ldots, 0.9$ and time $t = 1.0$. The value $\gamma$ increases in the direction of the arrow and dashed lines show lines of slop $\gamma$ for comparison.

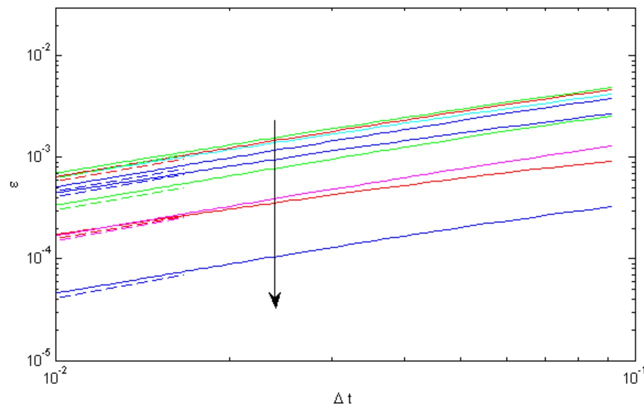



Figure 2.5: (Color online) The absolute error in using the GL scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 + t^\gamma$ at the time $t = 1.0$ for $\gamma = 0.1, \ldots, 0.9$, where $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slop $\gamma$ for comparison.

Table 2.1: The comparison of the absolute error in evaluating the fractional derivative of order $1-\gamma$ for the functions $f(t)$, Equation (2.7), at time $t = 1.0$ by using the GL scheme where $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^3$ | $f(t) = t^4$ | $f(t) = 1 - e^t + t^3$ | $f(t) = 1 + t^\gamma$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 8.598e–03 | 2.338e–02 | 4.441e–02 | 1.213e–02 | 1.600e–04 |
| $\gamma = 0.2$ | 7.917e–03 | 1.974e–02 | 3.580e–02 | 9.608e–03 | 4.100e–04 |
| $\gamma = 0.3$ | 7.086e–03 | 1.631e–02 | 2.830e–02 | 7.351e–03 | 5.833e–04 |
| $\gamma = 0.4$ | 6.142e–03 | 1.313e–02 | 2.184e–02 | 5.394e–03 | 6.395e–04 |
| $\gamma = 0.5$ | 5.124e–03 | 1.023e–02 | 1.634e–02 | 3.754e–03 | 5.900e–04 |
| $\gamma = 0.6$ | 4.066e–03 | 7.610e–03 | 1.169e–02 | 2.432e–03 | 4.660e–04 |
| $\gamma = 0.7$ | 2.999e–03 | 5.284e–03 | 7.817e–03 | 1.419e–03 | 3.075e–04 |
| $\gamma = 0.8$ | 1.950e–03 | 3.247e–03 | 4.632e–03 | 6.940e–04 | 1.530e–04 |
| $\gamma = 0.9$ | 9.444e–04 | 1.490e–03 | 2.053e–03 | 2.317e–04 | 4.177e–05 |

In this thesis we have concentrated on the L1 approximation scheme (Oldham & Spanier 1974) as this scheme is exact for the linear function whereas the Grünwald–Letnikov approximation scheme is not exact. In the next sections we will give the L1 approximation and discuss its accuracy.

## 2.3 L1 Scheme

The L1 scheme can be used to approximate the fractional derivative of order $p$ with $0 < p \leq 1$. This scheme was originally developed by Oldham & Spanier (1974). In this method the function $f(t)$ is defined as a piecewise linear, and the Riemann–Liouville derivative given in Equation (2.1) with $n = 1$ is written as

$$\frac{d^p f(t)}{dt^p} = \frac{1}{\Gamma(1-p)} \frac{d}{dt} \int_0^t \frac{f(\tau)}{(t-\tau)^p} d\tau. \tag{2.8}$$

The L1 approximation scheme (Oldham & Spanier 1974) is found, after rewriting Equation (2.8) as

$$\frac{d^p f(t)}{dt^p} = \frac{t^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \int_0^t \frac{df(\tau)}{d\tau} \frac{d\tau}{(t-\tau)^p}. \tag{2.9}$$

The integral is then split into equally–spaced time points, $t_k = k\Delta t \, (1 \leq k \leq j)$, to give

$$\left[ \frac{d^p f(t)}{dt^p} \right|_{t=t_j} = \frac{t_j^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \sum_{k=0}^{j-1} \int_{k\Delta t}^{(k+1)\Delta t} \frac{df(\tau)}{d\tau} \frac{d\tau}{(t_j-\tau)^p}, \tag{2.10}$$

where in each interval, $k\Delta t \leq \tau \leq (k+1)\Delta t$ the derivative is then assumed to be constant and is approximated by a first order finite difference approximation. The approximation is then given as

$$\left[ \frac{d^p f(t)}{dt^p} \right|_{t=t_j} \approx \frac{t_j^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \sum_{k=0}^{j-1} \frac{(f_{k+1} - f_k)}{\Delta t} \int_{k\Delta t}^{(k+1)\Delta t} (t_j - \tau)^p, \tag{2.11}$$

which after evaluation of the integral, gives the L1 approximation scheme

$$\left[ \frac{d^p f(t)}{dt^p} \right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)} \left\{ \frac{(1-p)}{j^p} f_0 + \sum_{k=0}^{j-1} (f_k - f_{k+1}) \left[ (j-(k+1))^{1-p} - (j-k)^{1-p} \right] \right\}. \tag{2.12}$$

Langlands & Henry (2005) used the L1 scheme to approximate the fractional derivative to develop the implicit method to solve fractional subdiffusion equation. We will follow their approach to evaluate the accuracy of the L1 scheme in Section 2.4.

The L1 scheme in Equation (2.12) can be rewritten as

$$\left[ \frac{d^p f(t)}{dt^p} \right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)} \left[ \frac{(1-p)}{j^p} f_0 + \sum_{k=0}^{j} \nu_{j-k} f(k\Delta t) \right], \tag{2.13}$$

where the weight $\nu_l$ is defined by

$$\nu_l = \begin{cases} 1 & \text{if} \quad l = 0, \\ (j-1)^{1-p} - j^{1-p} & \text{if} \quad l = j, \\ (l-1)^{1-p} - 2l^{1-p} + (l+1))^{1-p} & \text{if} \quad 1 \leq l \leq j-1. \end{cases} \tag{2.14}$$

To evaluate the L1 approximation of the functions $f(t) = 1$ and $f(t) = t$ at time $t_j$, we need the following Lemmas to show the accuracy of the L1 scheme.

**Lemma 2.3.1.** Given the weights $\nu_{j-k}$ defined in Equation (2.14), and $j \geq n$, we have

1. $\sum_{k=n}^{j} \nu_{j-k} = (j-(n-1))^{1-p} - (j-n)^{1-p}$, if $n \geq 1$, and
2. $\sum_{k=n}^{j} \nu_{j-k} = 0$, if $n = 0$.

*Proof.* For $n \geq 1$ using the definition of the weights in Equation (2.14), we have

$$\begin{aligned}
\sum_{k=n}^{j} \nu_{j-k} &= \sum_{k=n}^{j-1} \nu_{j-k} + \nu_0 \\
&= \sum_{k=n}^{j-1} \left[ (j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p} \right] + 1 \\
&= \sum_{k=n+1}^{j} (j-k)^{1-p} - 2\sum_{k=n}^{j-1} (j-k)^{1-p} + \sum_{k=n-1}^{j-2} (j-k)^{1-p} + 1 \\
&= 1 + \sum_{k=n+1}^{j-2} (j-k)^{1-p} - 2(j-n)^{1-p} - 2 - 2\sum_{k=n+1}^{j-2} (j-k)^{1-p} \\
&\qquad + (j-(n-1))^{1-p} + (j-n)^{1-p} + \sum_{k=n+1}^{j-2} (j-k)^{1-p} + 1 \\
&= (j-(n-1))^{1-p} - (j-n)^{1-p}.
\end{aligned} \tag{2.15}$$

Hence result (1) holds.

For $n = 0$ and using Equation (2.15) with $n = 1$ we have

$$\begin{aligned}
\sum_{k=0}^{j} \nu_{j-k} &= (j-1)^{1-p} - j^{1-p} + \sum_{k=1}^{j} \nu_{j-k} \\
&= (j-1)^{1-p} - j^{1-p} + \left( j^{1-p} - (j-1)^{1-p} \right) \\
&= 0.
\end{aligned} \tag{2.16}$$

There for the second result (2) also holds. ∎

**Lemma 2.3.2.** Given the weights $\nu_{j-k}$ defined in Equation (2.14), with $j \geq n$, we have

1. $\sum\limits_{k=n}^{j} k\nu_{j-k} = n(j-(n-1))^{1-p} - (n-1)(j-n))^{1-p}$, if $n \geq 1$, and

2. $\sum\limits_{k=n}^{j} k\nu_{j-k} = j^{1-p}$, if $n = 0$.

*Proof.* For $n \geq 1$ using the definition of the weights in Equation (2.14), we have

$$
\begin{aligned}
\sum_{k=n}^{j} k\nu_{j-k} &= \sum_{k=n}^{j-1} k\nu_{j-k} + j\nu_0 \\
&= \sum_{k=n}^{j-1} k(j-(k+1))^{1-p} - 2\sum_{k=n}^{j-1} k(j-k)^{1-p} + \sum_{k=n}^{j-1} k(j-(k-1))^{1-p} + j \\
&= \sum_{k=n+1}^{j} (k-1)(j-k)^{1-p} - 2\sum_{k=n}^{j-1} k(j-k)^{1-p} + \sum_{k=n-1}^{j-2} (k+1)(j-k)^{1-p} + j \\
&= \sum_{k=n+1}^{j} k(j-k)^{1-p} - 2\sum_{k=n}^{j-1} k(j-k)^{1-p} + \sum_{k=n-1}^{j-2} k(j-k)^{1-p} \\
&+ \sum_{k=n-1}^{j-2} (j-k)^{1-p} - \sum_{k=n+1}^{j} (j-k)^{1-p} + j \\
&= (j-1) + \sum_{k=n+1}^{j-2} k(j-k)^{1-p} - 2n(j-n)^{1-p} - 2(j-1) - 2\sum_{k=n+1}^{j-2} k(j-k)^{1-p} \\
&+ (n-1)(j-(n-1))^{1-p} + n(j-n)^{1-p} + \sum_{k=n+1}^{j-2} k(j-k)^{1-p} + (j-(n-1))^{1-p} \\
&+ (j-n)^{1-p} + \sum_{k=n+1}^{j-2} (j-k)^{1-p} - \sum_{k=n+1}^{j-2} (j-k)^{1-p} - 1 + j \\
&= -n(j-n)^{1-p} + (n-1)(j-(n-1))^{1-p} + (j-(n-1))^{1-p} + (j-n)^{1-p} \\
&= n(j-(n-1))^{1-p} - (n-1)(j-n)^{1-p}. \qquad (2.17)
\end{aligned}
$$

Hence result (1) holds. To show the second result we have

$$\sum_{k=0}^{j} k\nu_{j-k} = 0 + \sum_{k=1}^{j} k\nu_{j-k}. \qquad (2.18)$$

By using Equation (2.17) with $n = 1$ gives

$$\sum_{k=0}^{j} k\nu_{j-k} = j^{1-p}, \qquad (2.19)$$

and so result (2) also holds. □

## 2.4 Accuracy of the L1 Scheme

In this section the accuracy of L1 scheme, in Equation (2.12), is estimated at $t = t_j$. To do this we follow the approach of Langlands & Henry (2005) by assuming $f(t)$ can be expanded in Taylor series around $t = 0$ with an integral remainder term, that is

$$f(t) = f(0) + tf'(0) + \int_0^t f''(\tau)(t-\tau)d\tau. \tag{2.20}$$

Now taking the fractional derivative of Equation (2.20) with respect to the $t$, and then evaluating at time $t = t_j$ we find

$$\begin{aligned}\left[\frac{d^p f(t)}{dt^p}\right|_{t=t_j} &= f(0)\left[\frac{d^p(1)}{dt^p}\right|_{t=t_j} + f'(0)\left[\frac{d^p(t)}{dt^p}\right|_{t=t_j} + \left[\frac{d^p}{dt^p}\left(\int_0^t f''(\tau)(t-\tau)d\tau\right)\right|_{t=t_j} \\ &= f(0)\frac{t_j^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} + \frac{d^p}{dt^p}\left(\int_0^{t_j} f''(\tau)(t_j-\tau)d\tau\right). \end{aligned} \tag{2.21}$$

To evaluate the last term in Equation (2.21) we use the following result in Podlubny (1998), for the fractional derivative of a convolution

$$\frac{d^p}{dt^p}\int_0^t K(t-\tau)f(\tau)d\tau = \int_0^t \frac{d^p K(\tau)}{d\tau^p} f(t-\tau)d\tau + \lim_{\tau\to+0} f(t-\tau)\frac{d^{p-1}K(\tau)}{d\tau^{p-1}}. \tag{2.22}$$

Then the fractional derivative of the last term in Equation (2.21) takes the form

$$\left[\frac{d^p}{dt^p}\left(\int_0^t f''(\tau)(t-\tau)d\tau\right)\right|_{t=t_j} = \int_0^{t_j} \frac{d^p(\tau)}{d\tau^p} f''(t_j-\tau)d\tau + \lim_{\tau\to+0} f''(t_j-\tau)\frac{d^{p-1}(\tau)}{d\tau^{p-1}}. \tag{2.23}$$

The limit in the last term on the right of Equation (2.23) is zero if $0 < p < 1$. Changing the integration variable in the integral on the right hand side by setting $s = t_j - \tau$, and so $ds = -d\tau$, we then find

$$\begin{aligned}\left[\frac{d^p}{dt^p}\left(\int_0^t f''(\tau)(t-\tau)d\tau\right)\right|_{t=t_j} &= \int_0^{t_j} \frac{d^p(t_j-s)}{ds^p} f''(s)\, ds \\ &= \int_0^{t_j} f''(s)\frac{(t_j-s)^{1-p}}{\Gamma(2-p)}ds. \end{aligned} \tag{2.24}$$

The exact value of the fractional derivative of $f(t)$ in Equation (2.21) is then given by

$$\left[\frac{d^p f(t)}{dt^p}\right|_{t=t_j} = f_0 \frac{t_j^{-p}}{\Gamma\left(1-p\right)} + f'(0)\frac{t_j^{1-p}}{\Gamma\left(2-p\right)} + \int\limits_0^{t_j} f''(s)\frac{(t_j-s)^{1-p}}{\Gamma(2-p)}ds. \tag{2.25}$$

The accuracy of the L1 scheme can now be determined by comparing the exact value with the value obtained from the L1 approximation. Thus we need to evaluate the L1 fractional approximation operating on the functions 1, $t$, and the convolution integral in Equation (2.20). Now we evaluate the L1 approximation of the function $f(t) = 1$ at time $t_j$, which is given by

$$\left[\frac{d^p(1)}{dt^p}\right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left[\frac{(1-p)}{j^p}(1) + \sum_{k=0}^{j}\nu_{j-k}(1)\right], \tag{2.26}$$

which, using Lemma 2.3.1 with $n = 0$, simplifies to

$$\left[\frac{d^p(1)}{dt^p}\right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}(1-p)j^{-p} = \frac{(j\Delta t)^{-p}}{\Gamma(1-p)} = \frac{t_j^{-p}}{\Gamma(1-p)}. \tag{2.27}$$

The L1 approximation for function $f(t) = t$ at time $t_j$ is

$$\left[\frac{d^p(t)}{dt^p}\right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left[\frac{(1-p)}{j^p}(0) + \sum_{k=0}^{j}\nu_{j-k}k\Delta t\right] = \frac{\Delta t^{1-p}}{\Gamma(2-p)}\sum_{k=0}^{j}k\nu_{j-k}. \tag{2.28}$$

Using Lemma 2.3.2 with $n = 0$, we then have the result

$$\left[\frac{d^p(t)}{dt^p}\right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}j^{1-p} = \frac{(j\Delta t)^{1-p}}{\Gamma\left(2-p\right)} = \frac{t_j^{1-p}}{\Gamma\left(2-p\right)}. \tag{2.29}$$

We note here the results for $f(t) = 1$ and $f(t) = t$ are exact for the L1 scheme.

Now applying the L1 approximation to the convolution integral in Equation (2.20) gives

$$\left[\frac{d^p}{dt^p}\left(\int_0^t f''(s)(t-s)ds\right)\right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{(1-p)j^{-p}\lim_{t\to 0}\int\limits_0^t f''(s)(t-s)ds \right.$$
$$\left. + \sum_{k=0}^{j}\nu_{j-k}\int\limits_0^{k\Delta t} f''(s)(k\Delta t - s)ds\right\}. \tag{2.30}$$

The limit in the first term on the right of Equation (2.30) is zero if $f''(t)$ is a well–behaved function of $t$. Now by dividing the interval into equal $\Delta t$ steps, we then have

$$\left[\frac{d^p}{dt^p}\left(\int_0^t f''(s)(t-s)ds\right)\right|_{L1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=1}^{j}\nu_{j-k}\sum_{l=0}^{k-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)(k\Delta t - s)ds. \tag{2.31}$$

Interchanging the order of summation and simplifying, we then have the L1 approximation of fractional derivative of the convolution integral

$$\left[\frac{d^p}{dt^p}\left(\int_0^t f''(s)(t-s)ds\right)\right|_{L1}^j = \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{l=0}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\nu_{j-k}(k\Delta t-s)ds. \quad (2.32)$$

Now using Lemmas 2.3.1 and 2.3.2 with $n = l+1$, we can evaluate the summation

$$\sum_{k=l+1}^{j}\nu_{j-k}\left(k\Delta t-s\right) = (j-l)^{1-p}((l+1)\Delta t-s)-(j-(l+1))^{1-p}(l\Delta t-s). \quad (2.33)$$

Letting

$$L_{j,l,p}(s) = (j-l)^{1-p}((l+1)\Delta t-s)-(j-(l+1))^{1-p}(l\Delta t-s), \quad (2.34)$$

then the L1 approximation of $f(t)$ in Equation (2.20) becomes

$$\left[\frac{d^p f(t)}{dt^p}\right|_{L1}^j = f_0\frac{t_j^{-p}}{\Gamma(1-p)}+f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)}+\frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{l=0}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)L_{j,l,p}(s)ds. \quad (2.35)$$

The value of the L1 approximation in Equation (2.35) can now be compared with the exact value of the fractional derivative given by Equation (2.21). The absolute error can now be evaluated as

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|_{L1}^j\right| = \left|f_0\frac{t_j^{-p}}{\Gamma(1-p)}+f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)}+\left[\int\limits_0^t f''(s)\frac{(t-s)^{1-p}}{\Gamma(2-p)}ds\right|_{t=t_j}\right.$$
$$\left. -f_0\frac{t_j^{-p}}{\Gamma(1-p)}-f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)}-\frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{l=0}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)L_{j,l,p}(s)ds\right|, \quad (2.36)$$

which simplifies to

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|_{L1}^j\right| = \frac{1}{\Gamma(2-p)}\left|\sum_{l=0}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t_j-s)^{1-p}-\Delta t^{-p}L_{j,l,p}(s)\right]ds\right|. \quad (2.37)$$

Then Equation (2.37) can be written as follows

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|_{L1}^j\right| \le \frac{1}{\Gamma(2-p)}\sum_{l=0}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} \left|f''(s)\right|\left|(t_j-s)^{1-p}-\Delta t^{-p}L_{j,l,p}(s)\right|ds, \quad (2.38)$$

since

$$\left| \int_a^b f(x)g(x)dx \right| \leq \int_a^b |f(x)|\,|g(x)|\,dx. \tag{2.39}$$

Now we let the maximum absolute value of the second derivative in the interval $[l\Delta t, (l+1)\Delta t]$ be given by

$$M_l = \max_{l\Delta t \leq s \leq (l+1)\Delta t} \left| f''(s) \right|, \tag{2.40}$$

then Equation (2.38) becomes

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1} \right| \leq \frac{1}{\Gamma(2-p)} \sum_{l=0}^{j-1} M_l \int_{l\Delta t}^{(l+1)\Delta t} \left| (t_j - s)^{1-p} - \Delta t^{-p} L_{j,l,p}(s) \right| ds. \tag{2.41}$$

It is shown in Appendix B.1 that the term $(t_j - s)^{1-p} - \Delta t^{-p} L_{j,l,p}(s)$ is positive and so we can drop the absolute sign. Evaluating the integral in Equation (2.41), we have

$$\int_{l\Delta t}^{(l+1)\Delta t} (t_j - s)^{1-p}\, ds = \frac{\Delta t^{2-p}}{2-p} \left[ (j-l)^{2-p} - (j-(l+1))^{2-p} \right], \tag{2.42}$$

and

$$\begin{aligned} \int_{l\Delta t}^{(l+1)\Delta t} L_{j,l,s}(p) ds &= \int_{l\Delta t}^{(l+1)\Delta t} \left[ (j-l)^{1-p} ((l+1)\Delta t - s) - (j-(l+1))^{1-p} (l\Delta t - s) \right] ds \\ &= \int_{l\Delta t}^{(l+1)\Delta t} \left[ (j-l)^{1-p} (l+1)\Delta t - (j-(l+1))^{1-p} (l\Delta t) \right] ds \\ &\quad - \int_{l\Delta t}^{(l+1)\Delta t} \left[ (j-l)^{1-p} - (j-(l+1))^{1-p} \right] s\; ds \\ &= \frac{\Delta t^2}{2} \left[ (j-l)^{1-p} - (j-(l+1))^{1-p} \right]. \end{aligned} \tag{2.43}$$

Inserting these results in Equation (2.41), we obtain

$$\begin{aligned} \left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1} \right| \leq \frac{\Delta t^{2-p}}{(2-p)\Gamma(2-p)} \sum_{l=0}^{j-1} M_l \Big[ (j-l)^{2-p} - (j-(l+1))^{2-p} \\ - \frac{2-p}{2} \left[ (j-l)^{1-p} - (j-(l+1))^{1-p} \right] \Big]. \end{aligned} \tag{2.44}$$

Let $M = \max(\{M_i; i = 0, 1, 2, ..., j\})$, and then simplifying Equation (2.44) gives

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1} \right| \tag{2.45}$$
$$\leq \frac{M\Delta t^{2-p}}{\Gamma(3-p)} \sum_{l=0}^{j-1} \left[ (j-l)^{1-p} \left( j - l - \frac{2-p}{2} \right) - (j-(l+1))^{1-p} \left( j - l - 1 + \frac{2-p}{2} \right) \right],$$

which can be rewritten as

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1} \right| \leq \frac{M\Delta t^{2-p}}{\Gamma(3-p)} \sum_{l=1}^{j} \left[ l^{1-p} \left( l - 1 + \frac{p}{2} \right) - (l-1)^{1-p} \left( l - \frac{p}{2} \right) \right]. \tag{2.46}$$

We then evaluate the summation as

$$\begin{aligned} &\sum_{l=1}^{j} \left[ l^{1-p} \left( l - 1 + \frac{p}{2} \right) - (l-1)^{1-p} \left( l - \frac{p}{2} \right) \right] \\ &= \sum_{l=1}^{j} l^{1-p} \left( l - 1 + \frac{p}{2} \right) - \sum_{l=0}^{j-1} l^{1-p} \left( l + 1 - \frac{p}{2} \right) \\ &= j^{1-p} \left( j - 1 + \frac{p}{2} \right) + \sum_{l=1}^{j-1} l^{1-p} \left( l - 1 + \frac{p}{2} \right) - \sum_{l=1}^{j-1} l^{1-p} \left( l + 1 - \frac{p}{2} \right) \\ &= j^{1-p} \left( j - 1 + \frac{p}{2} \right) + (p-2) \sum_{l=1}^{j-1} l^{1-p} \\ &= \frac{1}{2} \left[ j^{1-p} (2j - (2-p)) - 2(2-p) \sum_{l=1}^{j-1} l^{1-p} \right]. \end{aligned} \tag{2.47}$$

The estimate error is then given by

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1} \right| \leq C\Delta t^{2-p}, \tag{2.48}$$

where $C$ is constant

$$C = \frac{M\vartheta(j,p)}{2\Gamma(3-p)} \tag{2.49}$$

and $\vartheta(j,p)$ is defined by

$$\vartheta(j,p) = j^{1-p} (2j - (2-p)) - 2(2-p) \sum_{l=1}^{j-1} l^{1-p}. \tag{2.50}$$

In Equation (2.50), we have $\vartheta(j,0) = 0$ and $\vartheta(j,1) = 1$. If $0 < p \leq 1$ then $\vartheta(j,p)$ is bounded $0 \leq \vartheta(j,p) \leq 1$ as shown in Figure. 2.6. Furthermore in Appendix B.3 it can be shown the sum in Equation (2.46) is bounded. Using Equation (B.26) we find $\vartheta(j,p)$ is bounded above by

$$\vartheta(j,p) \leq \frac{p}{2} \zeta(1+p,1), \tag{2.51}$$

where $\zeta(1+p,1)$ is the Hurwitz Zeta function (Apostol et al. 1951). This is the same bound given by Langlands & Henry (2005). Hence the error is bounded by a constant independent of $t$ and so shows the L1 approximation scheme is of order $O(\Delta t^{2-p})$ for function that can be expanded as in Equation (2.20).

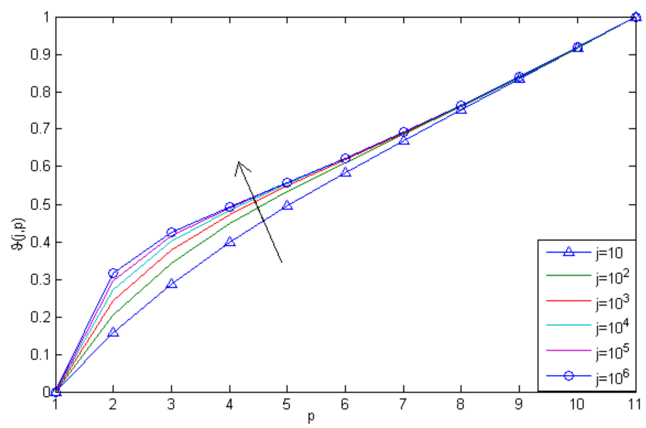



Figure 2.6: (Color online) The value of $\vartheta(j,p)$ in Equation (2.50) is shown versus $p$ for varying number of time steps $j = 10, 10^2, \ldots, 10^6$, where $j$ increases in the direction of the arrow. These results show $\vartheta(j,p)$ is bounded above by 1.

The estimate of the accuracy of the L1 scheme was tested on the functions given by Equation (2.7), with $p = 1-\gamma$ with $\gamma = 0.1, \ldots, 0.9$. The error is plotted as a function of $\Delta t$ on double logarithmic scale plot given in Figures 2.7 – 2.11. We see as $\Delta t$ is decreased the error decreases for each value of $p$ as expected. In these figures we note the error decreases in magnitude as $\gamma$ increases for a fixed $\Delta t$ value. This is also seen in the results shown in Table 2.2.

As shown in the Figures 2.7 – 2.11, the slope of the lines match asymptotically the slope of $1+\gamma$ of the dashed lines shown in the figure as expected.

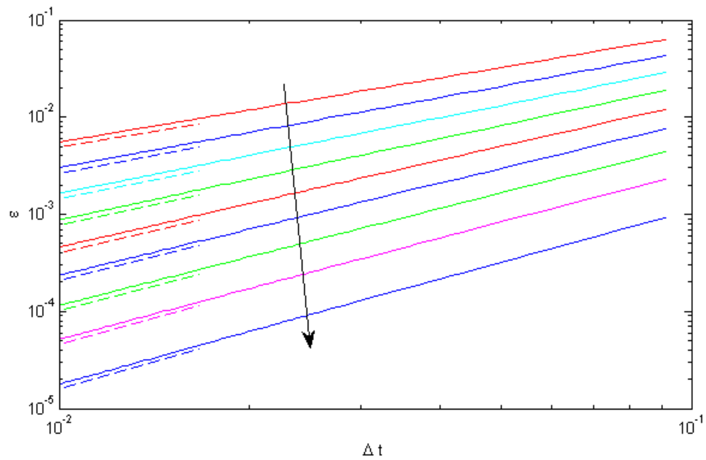



Figure 2.7: (Color online) The absolute error in using the L1 scheme to evaluate the fractional derivative of order $1-\gamma$ on the function $f(t) = t^2$ at time $t = 1.0$ given for $\gamma = 0.1, \ldots, 0.9$. Note $\gamma$ increases in the direction of the arrow and the dashed lines show lines of slope $1+\gamma$ for comparison.

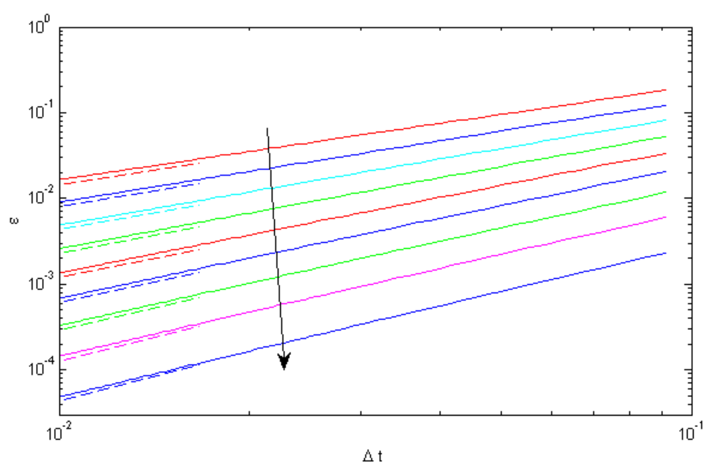



Figure 2.8: (Color online) The absolute error, $\varepsilon$, in the L1 approximation of the fractional derivative of order $1-\gamma$ on the function $f(t) = t^3$ at time $t = 1.0$ given for $\gamma = 0.1, \ldots, 0.9$. Note $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

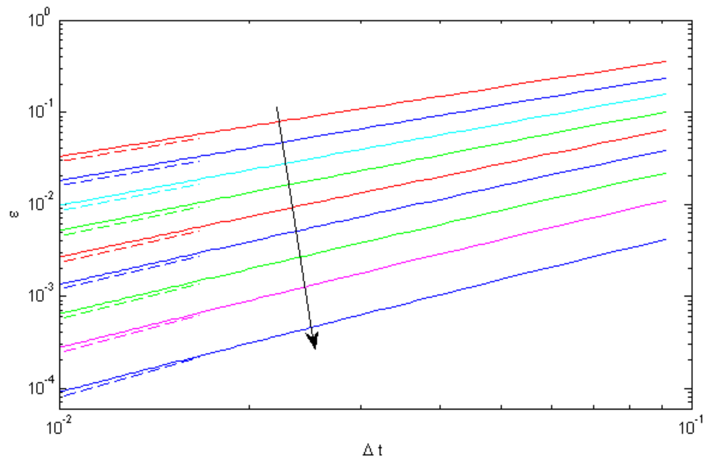



Figure 2.9: (Color online) The absolute error in using the L1 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t)=t^4$. Results are shown for $\gamma=0.1,\ldots,0.9$ at the time $t=1.0$ and $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

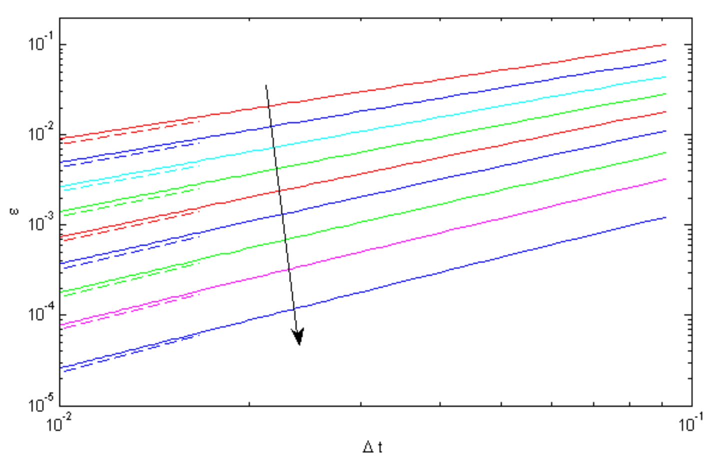



Figure 2.10: (Color online) The absolute error in using the L1 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t)=1-e^t+t^3$, where $\gamma=0.1,\ldots,0.9$ and time $t=1.0$. Note $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison.

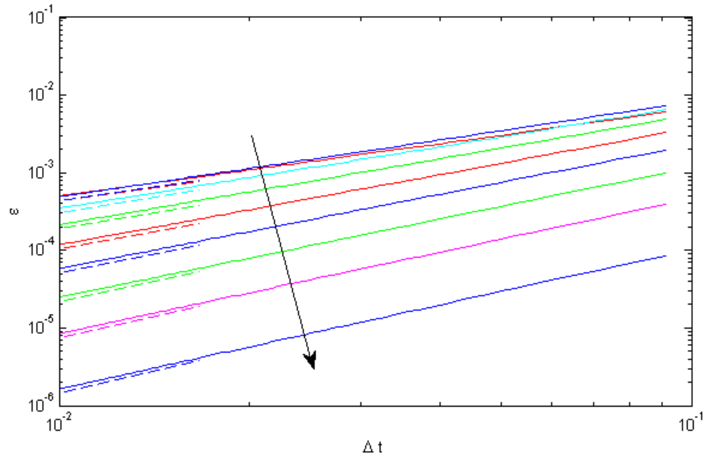



Figure 2.11: (Color online) The absolute error in using the L1 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 + t^\gamma$ at the time $t = 1.0$. The results are shown for $\gamma = 0.1, \ldots, 0.9$, and $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

In Table 2.2 we see that the maximum error occurs where $\gamma = 0.1$ for $f(t) = t^2$ of magnitude $4.98 \times 10^{-3}$ and the minimum error occurs when $\gamma = 0.9$ which is $1.4 \times 10^{-5}$. Also, for the functions $f(t) = t^3$, $t^4$, $1-e^t+t^3$ and $1+t^\gamma$ the maximum error again occurs where $\gamma = 0.1$ and the minimum error occurs where $\gamma = 0.9$.

Table 2.2: The comparison of the absolute error in the L1 approximation of the fractional derivative of order $p = 1-\gamma$ of the function $f(t)$, given by Equation (2.7), at time $t = 1.0$ where $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^3$ | $f(t) = t^4$ | $f(t) = 1 - e^t + t^3$ | $f(t) = 1 + t^\gamma$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 4.982e–03 | 1.489e–02 | 2.966e–02 | 8.141e–03 | 4.519e–04 |
| $\gamma = 0.2$ | 2.702e–03 | 8.057e–03 | 1.603e–02 | 4.406e–03 | 4.366e–04 |
| $\gamma = 0.3$ | 1.448e–03 | 4.307e–03 | 8.553e–03 | 2.354e–03 | 3.082e–04 |
| $\gamma = 0.4$ | 7.665e–04 | 2.269e–03 | 4.492e–03 | 1.239e–03 | 1.871e–04 |
| $\gamma = 0.5$ | 3.989e–04 | 1.172e–03 | 2.310e–03 | 6.396e–04 | 1.018e–04 |
| $\gamma = 0.6$ | 2.025e–04 | 5.883e–04 | 1.152e–03 | 3.205e–04 | 4.980e–05 |
| $\gamma = 0.7$ | 9.836e–05 | 2.812e–04 | 5.458e–04 | 1.528e–04 | 2.120e–05 |
| $\gamma = 0.8$ | 4.359e–05 | 1.218e–04 | 2.336e–04 | 6.590e–05 | 7.150e–06 |
| $\gamma = 0.9$ | 1.494e–05 | 4.049e–05 | 7.641e–05 | 2.180e–05 | 1.370e–06 |

We verify the accuracy of the approximate scheme by computing the absolute error between the exact value of the fractional derivative and the estimate value of the fractional derivative by using

$$e_\infty(\Delta t) = \left| \left[ \frac{d^p}{dt^p} f(t) \right|^M - \left[ \frac{d^p}{dt^p} f(t) \right|^M_{A_p} \right|. \tag{2.52}$$

Numerical accuracy is studied for $\gamma = 0.1, \dots, 0.9$, and the approximate order of convergence in $\Delta t$, $\widehat{R}$, was estimated by computing

$$\widehat{R} = \log_2[e_\infty(2\Delta t)/e_\infty(\Delta t)]. \tag{2.53}$$

In Table 2.3, the error and order of convergence estimate are given for the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 + t^\gamma$ by using Equations (2.52) and (2.53) for the L1 scheme. The results are shown for time $t = 1.0$, it can be seen numerically that the L1 scheme is of order $O(\Delta t^{1+\gamma})$.

Table 2.3: Numerical accuracy in $\Delta t$ of the L1 scheme applied to the function $f(t) = 1 + t^\gamma$, and $\widehat{R}$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.2$ | | $\gamma = 0.3$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $\widehat{R}$ | $e_\infty(\Delta t)$ | $\widehat{R}$ | $e_\infty(\Delta t)$ | $\widehat{R}$ |
| 1/1000 | 3.960e–05 | – | 3.065e–05 | – | 1.734e–05 | – |
| 1/2000 | 1.847e–05 | 1.1 | 1.334e–05 | 1.2 | 7.038e–06 | 1.3 |
| 1/4000 | 8.613e–06 | 1.1 | 5.802e–06 | 1.2 | 2.857e–06 | 1.3 |
| 1/8000 | 4.018e–06 | 1.1 | 2.525e–06 | 1.2 | 1.160e–06 | 1.3 |
| 1/16000 | 1.874e–06 | 1.1 | 1.099e–06 | 1.2 | 4.710e–07 | 1.3 |
| | $\gamma = 0.4$ | | $\gamma = 0.5$ | | $\gamma = 0.6$ | |
| 1/1000 | 8.454e–06 | – | 3.710e–05 | – | 1.474e–06 | – |
| 1/2000 | 3.201e–06 | 1.4 | 1.311e–06 | 1.5 | 4.872e–07 | 1.6 |
| 1/4000 | 1.212e–06 | 1.4 | 4.636e–07 | 1.5 | 1.610e–07 | 1.6 |
| 1/8000 | 4.593e–07 | 1.4 | 1.639e–07 | 1.5 | 5.316e–08 | 1.6 |
| 1/16000 | 1.740e–07 | 1.4 | 5.795e–08 | 1.5 | 1.755e–08 | 1.6 |
| | $\gamma = 0.7$ | | $\gamma = 0.8$ | | $\gamma = 0.9$ | |
| 1/1000 | 5.165e–07 | – | 1.460e–07 | – | 2.402e–08 | – |
| 1/2000 | 1.601e–07 | 1.7 | 4.271e–08 | 1.8 | 6.683e–09 | 1.9 |
| 1/4000 | 4.959e–08 | 1.7 | 1.246e–08 | 1.8 | 1.853e–09 | 1.9 |
| 1/8000 | 1.534e–08 | 1.7 | 3.66e–09 | 1.8 | 5.115e–10 | 1.9 |
| 1/16000 | 4.739e–09 | 1.7 | 1.054e–09 | 1.8 | 1.412e–10 | 1.9 |

## 2.5 Modification of the L1 Scheme

In this section, we consider three modifications of the L1 scheme: the C1 scheme, the C2 scheme, and the C3 scheme. We will discuss the development of these schemes in the next sections and we will show the accuracy of each of these methods.

### 2.5.1 C1 Scheme

In this subsection, we modify the L1 scheme given by Equation (2.9) to estimate the fractional derivative at time $t = t_j$. We will refer to this method as the C1 scheme. The Riemann–Liouville derivative is first rewritten as given in Equation (2.9)

$$\frac{d^p f(t)}{dt^p} = \frac{t^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \int_0^t \frac{df(\tau)}{d\tau} \frac{d\tau}{(t-\tau)^p}. \tag{2.54}$$

Then the integral is split into equally–spaced time points, $t_k = k\Delta t\,(1 \leq k \leq j)$. As in Figure 2.12 where, in each interval, the integral over $(k-1)\Delta t \leq \tau \leq (k+1)\Delta t$ is repeated twice, except for the integral over the intervals $[0, \Delta t]$ and $[(j-1)\Delta t, j\Delta t]$. We add the integral over these two regions and then take half of the integral to approximate the integral in Equation (2.54).

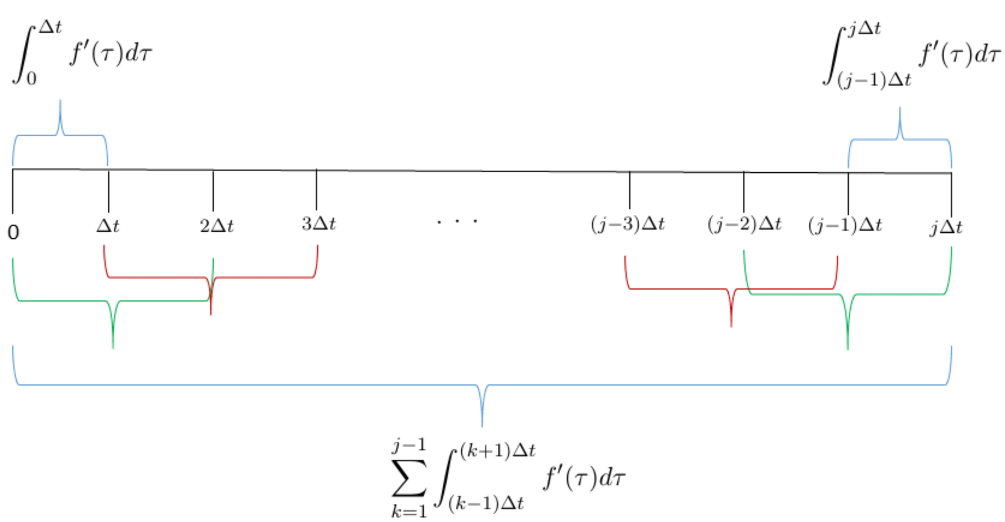



Figure 2.12: Intervals used to evaluate the integral in Equation (2.54).

Then the first modification of the L1 approximation, the C1 approximation scheme, is then given by

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C1} = \frac{t_j^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{2\Gamma(1-p)} \left\{ \sum_{k=1}^{j-1} \int_{(k-1)\Delta t}^{(k+1)\Delta t} \frac{df(\tau)}{d\tau} \frac{d\tau}{(t_j-\tau)^p} \right.$$
$$\left. + \int_0^{\Delta t} \frac{df(\tau)}{d\tau} \frac{d\tau}{(t_j-\tau)^p} + \int_{(j-1)\Delta t}^{j\Delta t} \frac{df(\tau)}{d\tau} \frac{d\tau}{(t_j-\tau)^p} \right\}. \tag{2.55}$$

In the L1 scheme the approximation of the first derivative was based on first order difference scheme. However it should be noted the approximation

$$f'(\tau) \approx \frac{f_{k+1} - f_k}{\Delta\tau}, \tag{2.56}$$

is second–order accurate if considered at the midpoint $\tau = t_{k-1/2} = \frac{1}{2}(t_k + t_{k-1})$ and an approximation of the form

$$\int_0^1 f'(\tau) w(\tau) d\tau \approx \sum_{k=1}^{M} \frac{f_k - f_{k-1}}{\Delta\tau} \int_{t_{k-1}}^{t_k} w(\tau) d\tau, \tag{2.57}$$

will also be second–order accurate if $f'''(t)$ is bounded.

In our modification we use a second–order accurate finite difference approximation over the intervals $(k-1)\Delta t \leq \tau \leq (k+1)\Delta t$ and the first–order accurate finite difference approximation over the intervals $[0, \Delta t]$ and $[(j-1)\Delta t, j\Delta t]$. The approximation is then given by

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C1} = \frac{t_j^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{2\Gamma(1-p)} \left\{ \left( \frac{f(\Delta t) - f_0}{\Delta t} \right) \int_0^{\Delta t} \frac{d\tau}{(t_j-\tau)^p} \right. \tag{2.58}$$
$$+ \sum_{k=1}^{j-1} \left( \frac{f((k+1)\Delta t) - f((k-1)\Delta t)}{2\Delta t} \right) \int_{(k-1)\Delta t}^{(k+1)\Delta t} \frac{d\tau}{(t_j-\tau)^p}$$
$$\left. + \left( \frac{f(j\Delta t) - f((j-1)\Delta t)}{\Delta t} \right) \int_{(j-1)\Delta t}^{j\Delta t} \frac{d\tau}{(t_j-\tau)^p} \right\}.$$

Evaluating the integrals, we then have

$$\left[\frac{d^p}{dt^p} f(t)\right|_{C1}^{j} = \frac{t_j^{-p}}{\Gamma(1-p)} f(0) + \frac{1}{2\Gamma(1-p)} \left\{ \right. \tag{2.59}$$
$$\frac{\Delta t^{-p}}{2(1-p)} \sum_{k=1}^{j-1} \left[ f((k+1)\Delta t) - f((k-1)\Delta t) \right] \left[ (j-(k-1))^{1-p} - (j-(k+1)\Delta t)^{1-p} \right]$$
$$\left. + \frac{\Delta t^{-p}}{(1-p)} \left[ f(\Delta t) - f(0) \right] \left[ j^{1-p} - (j-1)^{1-p} \right] + \frac{\Delta t^{-p}}{1-p} \left[ f(j\Delta t) - f((j-1)\Delta t) \right] \right\},$$

which can be rewritten in the form

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C1}^{j} = \frac{(\Delta t)^{-p}}{2\Gamma(2-p)}\left\{\beta_j^*(p)f_0 + \alpha_j(p)f_1 + (f_j - f_{j-1}) + \sum_{k=1}^{j-1}\mu_{j-k}^*(p)\left(f_{k+1} - f_{k-1}\right)\right\}. \tag{2.60}$$

For $j > 1$, Equation (2.60) becomes

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C1}^{j} = \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left[\beta_j^*(p)f_0 + \sum_{k=0}^{j-1}A_{j-k}(p)f_{k+1} + \sum_{k=1}^{j}B_{j-k}(p)f_{k-1}\right], \tag{2.61}$$

where the weights are defined by

$$A_{j-k}(p) = \begin{cases} \alpha_j(p) & \text{if} \quad k = 0, \\ 1 + \frac{1}{2}2^{1-p} & \text{if} \quad k = j-1, \\ \frac{1}{2}\left[(j-k+1)^{1-p} - (j-k-1)^{1-p}\right] & \text{if} \quad 1 \leq k \leq j-2, \end{cases} \tag{2.62}$$

$$B_{j-k}(p) = \begin{cases} -1 & \text{if} \quad k = j, \\ -\frac{1}{2}\left[(j-k+1)^{1-p} - (j-k-1)^{1-p}\right] & \text{if} \quad 1 \leq k \leq j-1, \end{cases} \tag{2.63}$$

$$\alpha_j(p) = j^{1-p} - (j-1)^{1-p}, \tag{2.64}$$

and

$$\beta_j^*(p) = 2(1-p)j^{-p} - \alpha_j. \tag{2.65}$$

As before we denote the function value at $t = k\Delta t$ as

$$f_k = f\left(k\Delta t\right). \tag{2.66}$$

In Section 2.6.1, the accuracy of the C1 approximation scheme will be evaluated, before that though we need the following Lemmas.

**Lemma 2.5.1.** Given the weights $A_{j-k}(p)$ defined in Equation (2.62) and for $j \geq n \geq 1$, we have

1. $\sum\limits_{k=n}^{j-1} A_{j-k}(p) = \frac{1}{2}\left[(j-(n-1)^{1-p} + (j-n)^{1-p} + 1\right]$,
2. $\sum\limits_{k=n}^{j-1} kA_{j-k}(p) = -1 + \frac{1}{2}\left[n(j-(n-1))^{1-p} + (n-1)(j-n)^{1-p} + j + 2\sum_{k=n}^{j-1}(j-k)^{1-p}\right]$.

*Proof.* Using the definition in Equation (2.62), we have

$$\begin{aligned}
\sum_{k=n}^{j-1} A_{j-k}(p) &= 1 + \frac{1}{2}2^{1-p} + \frac{1}{2}\sum_{k=n}^{j-2}\left[(j-(k-1))^{1-p} - (j-(k+1))^{1-p}\right] \\
&= 1 + \frac{1}{2}2^{1-p} + \frac{1}{2}\left[\sum_{k=n-1}^{j-3}(j-k)^{1-p} - \sum_{k=n+1}^{j-1}(j-k)^{1-p}\right] \\
&= 1 + \frac{1}{2}2^{1-p} + \frac{1}{2}\left[(j-(n-1))^{1-p} + (j-n)^{1-p} - 1 - 2^{1-p}\right] \\
&= \frac{1}{2}\left[(j-(n-1))^{1-p} + (j-n)^{1-p} + 1\right]. \qquad (2.67)
\end{aligned}$$

Then the first result (1) holds.

To show the second result, with Equation (2.62), we have

$$\begin{aligned}
\sum_{k=n}^{j-1} kA_{j-k}(p) &= (j-1)\left(1 + \frac{1}{2}2^{1-p}\right) + \frac{1}{2}\sum_{k=n}^{j-2} k\left[(j-(k-1))^{1-p} - (j-(k+1))^{1-p}\right] \\
&= (j-1)\left(1 + 2^{-p}\right) + \frac{1}{2}\left[\sum_{k=n-1}^{j-3}(k+1)(j-k)^{1-p} - \sum_{k=n+1}^{j-1}(k-1)(j-k)^{1-p}\right] \\
&= (j-1)\left(1 + 2^{-p}\right) + \frac{1}{2}\Bigg[n(j-(n-1))^{1-p} + (n+1)(j-n)^{1-p} \\
&\qquad -(j-2) - (j-3)2^{1-p} + 2\sum_{k=n+1}^{j-3}(j-k)^{1-p}\Bigg] \\
&= -1 + \frac{1}{2}\left[n(j-(n-1))^{1-p} + (n-1)(j-n)^{1-p} + j + 2\sum_{k=n}^{j-1}(j-k)^{1-p}\right]. \qquad (2.68)
\end{aligned}$$

Hence the second result (2) also holds. □

**Lemma 2.5.2.** Given the weight $B_{j-k}(p)$ defined in Equation (2.63) and for $j \geq n \geq 1$, we have

1. $\sum_{k=n}^{j} B_{j-k}(p) = -\frac{1}{2}\left[(j-(n-1))^{1-p} + (j-n)^{1-p} + 1\right]$, and
2. $\sum_{k=n}^{j} kB_{j-k}(p) = -\frac{1}{2}\left[n(j-(n-1))^{1-p} + (n-1)(j-n)^{1-p} + j + 2\sum_{k=n}^{j-1}(j-k)^{1-p}\right]$.

*Proof.* Similar to Lemma 2.5.1, using the definition in Equation (2.63), we have

$$\begin{aligned}\sum_{k=n}^{j} B_{j-k}(p) &= -1 - \frac{1}{2}\sum_{k=n}^{j-1}\left[(j-(k-1))^{1-p} - (j-(k+1))^{1-p}\right]\\ &= -1 - \frac{1}{2}\left[\sum_{k=n-1}^{j-2}(j-k)^{1-p} - \sum_{k=n+1}^{j}(j-k)^{1-p}\right]\\ &= -1 - \frac{1}{2}\left[(j-(n-1))^{1-p} + (j-n)^{1-p} - 1\right]\\ &= -\frac{1}{2}\left[(j-(n-1))^{1-p} + (j-n)^{1-p} + 1\right]. \end{aligned} \tag{2.69}$$

Then the first result (1) holds.

Likewise using Equation (2.63), we have

$$\sum_{k=n}^{j} kB_{j-k}(p) = j(-1) - \frac{1}{2}\sum_{k=n}^{j-1} k\left[(j-(k-1))^{1-p} - (j-(k+1))^{1-p}\right] \tag{2.70}$$

$$\begin{aligned}&= -j - \frac{1}{2}\left[\sum_{k=n-1}^{j-2}(k+1)(j-k)^{1-p} - \sum_{k=n+1}^{j}(k-1)(j-k)^{1-p}\right]\\ &= -j - \frac{1}{2}\left[n(j-(n-1))^{1-p} + (n+1)(j-n)^{1-p} - (j-2) + 2\sum_{k=n+1}^{j-2}(j-k)^{1-p}\right]\\ &= -\frac{1}{2}\left[n(j-(n-1))^{1-p} + (n-1)(j-n)^{1-p} + j + 2\sum_{k=n}^{j-1}(j-k)^{1-p}\right],\end{aligned}$$

and so the second result (2) also holds. □

**Corollary 2.5.3.** From Lemmas 2.5.1 and 2.5.2, $1 \le n \le j-1$, we have the following results

1. $\sum\limits_{k=n}^{j-1} A_{j-k}(p) + \sum\limits_{k=n}^{j} B_{j-k}(p) = 0,$
2. $\sum\limits_{k=n}^{j-1} A_{j-k}(p) - \sum\limits_{k=n}^{j} B_{j-k}(p) = (j-(n-1))^{1-p} + (j-n)^{1-p},$
3. $\sum\limits_{k=n}^{j-1} kA_{j-k}(p) + \sum\limits_{k=n}^{j} kB_{j-k}(p) = -1$, and
4. $\sum\limits_{k=n}^{j-1} kA_{j-k}(p) - \sum\limits_{k=n}^{j} kB_{j-k}(p) = -1 + n(j-(n-1))^{1-p} + (n-1)(j-n)^{1-p}$
$+j + 2\sum\limits_{k=n}^{j-1}(j-k)^{1-p}.$

### 2.5.2 C2 Scheme

In this subsection, we modify the L1 approximation in Equation (2.12), to approximate the fractional derivative at $t = t_{j+\frac{1}{2}}$ instead of at the time $t = t_j$. Recently a similar scheme was given by Liu, Li & Liu (2016). As in L1 scheme we begin by rewriting the Riemann–Liouville derivative, given by Equation (2.1) with $n = 1$, in the form

$$\left[\frac{d^p}{dt^p} f(t)\right|_{t=t_{j+\frac{1}{2}}} = \left[\frac{t^{-p}}{\Gamma(1-p)} f_0\right|_{t=t_{j+\frac{1}{2}}} + \frac{1}{\Gamma(1-p)} \left[\int_0^t \frac{df(\tau)}{d\tau}(t-\tau)^{-p} d\tau\right|_{t=t_{j+\frac{1}{2}}}. \quad (2.71)$$

Next we split the integral into two with one integral over the interval $\tau \in [0, t_j]$ and the other over the interval $\tau \in [t_j, t_{j+\frac{1}{2}}]$

$$\begin{aligned}\left[\frac{d^p}{dt^p} f(t)\right|_{t=t_{j+\frac{1}{2}}} &= \frac{(t_{j+\frac{1}{2}})^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \int_0^{t_j} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}} - \tau)^{-p} d\tau \\ &+ \frac{1}{\Gamma(1-p)} \int_{t_j}^{t_{j+\frac{1}{2}}} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}} - \tau)^{-p} d\tau. \quad (2.72)\end{aligned}$$

We then further split the integral interval $\tau \in [0, t_j]$ into equally–spaced time steps with $t_j = j\Delta t$ $(1 \leq j \leq M)$ to give

$$\begin{aligned}\left[\frac{d^p}{dt^p} f(t)\right|_{t=t_{j+\frac{1}{2}}} &= \frac{(t_{j+\frac{1}{2}})^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \sum_{k=1}^{j} \int_{(k-1)\Delta t}^{k\Delta t} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}} - \tau)^{-p} d\tau \quad (2.73) \\ &+ \frac{1}{\Gamma(1-p)} \int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}} - \tau)^{-p} d\tau.\end{aligned}$$

In each interval, the integer–order time derivative, as in Oldham & Spanier (1974), is then approximated using a first-order finite difference approximation

$$\begin{aligned}\left[\frac{d^p}{dt^p} f(t)\right|_{t=t_{j+\frac{1}{2}}} &\approx \frac{(t_{j+\frac{1}{2}})^{-p}}{\Gamma(1-p)} f_0 + \left(\frac{f\left(t_{j+\frac{1}{2}}\right) - f(t_j)}{\Gamma(1-p)\frac{1}{2}\Delta t}\right) \int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} \left(t_{j+\frac{1}{2}} - \tau\right)^{-p} d\tau \\ &+ \frac{1}{\Gamma(1-p)} \sum_{k=1}^{j} \left(\frac{f(t_k) - f(t_{k-1})}{\Delta t}\right) \int_{(k-1)\Delta t}^{k\Delta t} \left(t_{j+\frac{1}{2}} - \tau\right)^{-p} d\tau, \quad (2.74)\end{aligned}$$

which after simplifying can be written in the form

$$\begin{aligned}\left[\frac{d^p f(t)}{dt^p}\right|_{C2}^{j+\frac{1}{2}} &= \frac{\Delta t^{-p}}{\Gamma(2-p)} \left\{\widetilde{\beta}_j(p) f_0 + 2\left(\frac{1}{2}\right)^{1-p} \left(f\left(t_{j+\frac{1}{2}}\right) - f(t_j)\right)\right. \\ &\left. + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(p) \left(f(t_k) - f(t_{k-1})\right)\right\}, \quad (2.75)\end{aligned}$$

where the weights are defined by

$$\widetilde{\beta}_j(p) = (1-p)\left(j+\frac{1}{2}\right)^{-p}, \tag{2.76}$$

and

$$\widetilde{\mu}_j(p) = \left(j+\frac{3}{2}\right)^{1-p} - \left(j+\frac{1}{2}\right)^{1-p}. \tag{2.77}$$

We refer to the modified method given in Equations (2.75) – (2.77) as the C2 scheme. The scheme can be written as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C2}^{j+\frac{1}{2}} = \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} f_0 + \frac{\Delta t^{-p}}{\Gamma(2-p)} \sum_{k=0}^{j} \widetilde{\nu}_{j-k} f_k + \frac{2\left(\frac{1}{2}\right)^{1-p}\Delta t^{-p}}{\Gamma(2-p)} f_{j+\frac{1}{2}}, \tag{2.78}$$

with the weights $\widetilde{\nu}_l$ is defined by

$$\widetilde{\nu}_l = \begin{cases} \left(l-\frac{1}{2}\right)^{1-p} - \left(l+\frac{1}{2}\right)^{1-p} & \text{if} \quad l = j, \\ \left(\frac{3}{2}\right)^{1-p} - 3\left(\frac{1}{2}\right)^{1-p} & \text{if} \quad l = 0, \\ \left(l+\frac{3}{2}\right)^{1-p} - 2\left(l+\frac{1}{2}\right)^{1-p} + \left(l-\frac{1}{2}\right)^{1-p} & \text{if} \quad 1 \le l \le j-1. \end{cases} \tag{2.79}$$

In Section 2.6.2, the accuracy of the C2 approximation scheme will be evaluated. The following Lemmas will be used in that process.

**Lemma 2.5.4.** Given the weights $\widetilde{\nu}_l$ defined in Equation (2.79), and $j \ge n$, we have

1. $\sum\limits_{k=0}^{j} \widetilde{\nu}_{j-k} = -2\left(\frac{1}{2}\right)^{1-p}$, and
2. $\sum\limits_{k=n}^{j} \widetilde{\nu}_{j-k} = -2\left(\frac{1}{2}\right)^{1-p} + \left(j-(n-1)+\frac{1}{2}\right)^{1-p} - \left(j-(n-1)-\frac{1}{2}\right)^{1-p}$, if $n \ge 1$ .

*Proof.* For the case $n \ge 1$, using the definition of the weights in Equation (2.79), we have

$$\begin{aligned}
&\sum_{k=n}^{j} \widetilde{\nu}_{j-k} = \sum_{k=n}^{j-1} \widetilde{\nu}_{j-k} + \widetilde{\nu}_0 \\
&= \sum_{k=n}^{j-1}\left[\left(j-k+\frac{3}{2}\right)^{1-p} - 2\left(j-k+\frac{1}{2}\right)^{1-p} + \left(j-k-\frac{1}{2}\right)^{1-p}\right] + \left(\frac{3}{2}\right)^{1-p} - 3\left(\frac{1}{2}\right)^{1-p} \\
&= \sum_{k=n}^{j-1}\left(j-(k-1)+\frac{1}{2}\right)^{1-p} - \sum_{k=n}^{j-1}\left(j-k+\frac{1}{2}\right)^{1-p} \\
&\qquad - \left[\sum_{k=n}^{j-1}\left(j-(k-1)-\frac{1}{2}\right)^{1-p} - \sum_{k=n}^{j-1}\left(j-k-\frac{1}{2}\right)^{1-p}\right] + \left(\frac{3}{2}\right)^{1-p} - 3\left(\frac{1}{2}\right)^{1-p} \\
&= -2\left(\frac{1}{2}\right)^{1-p} + \left(j-(n-1)+\frac{1}{2}\right)^{1-p} - \left(j-(n-1)-\frac{1}{2}\right)^{1-p}.
\end{aligned} \tag{2.80}$$

Hence the second result (2) holds.

To show the first result also holds we have, from Equation (2.79),

$$\begin{aligned}\sum_{k=0}^{j} \widetilde{\nu}_{j-k} &= \widetilde{\nu}_0 + \sum_{k=1}^{j} \widetilde{\nu}_{j-k} \\ &= \left(j - \frac{1}{2}\right)^{1-p} - \left(j + \frac{1}{2}\right)^{1-p} + \sum_{k=1}^{j} \widetilde{\nu}_{j-k}, \qquad (2.81)\end{aligned}$$

which by using Equation (2.80) with $n = 1$, gives

$$\begin{aligned}\sum_{k=0}^{j} \widetilde{\nu}_{j-k} &= \left(j - \frac{1}{2}\right)^{1-p} - \left(j + \frac{1}{2}\right)^{1-p} - 2\left(\frac{1}{2}\right)^{1-p} + \left(j + \frac{1}{2}\right)^{1-p} - \left(j - \frac{1}{2}\right)^{1-p} \\ &= -2\left(\frac{1}{2}\right)^{1-p}. \qquad (2.82)\end{aligned}$$

Hence the first result (1) also holds. □

**Lemma 2.5.5.** Given the weights $\widetilde{\nu}_{j-k}$ defined in Equation (2.79), with $j \geq n$, we have

1. $\sum_{k=0}^{j} k\widetilde{\nu}_{j-k} = \left(j + \frac{1}{2}\right)^{1-p} - 2\left(j + \frac{1}{2}\right)\left(\frac{1}{2}\right)^{1-p}$, and

2. $\sum_{k=n}^{j} k\widetilde{\nu}_{j-k} = n\left(j - (n-1) + \frac{1}{2}\right)^{1-p} - (n-1)\left(j - n + \frac{1}{2}\right)^{1-p} - 2\left(j + \frac{1}{2}\right)\left(\frac{1}{2}\right)^{1-p}$,
   if $n \geq 1$.

*Proof.* For $n \geq 1$, using the definition of the weights in Equation (2.79), we have

$$\begin{aligned}\sum_{k=n}^{j} k\widetilde{\nu}_{j-k} &= \sum_{k=n}^{j-1} k\widetilde{\nu}_{j-k} + j\widetilde{\nu}_0 \\ &= \sum_{k=n}^{j-1} k\left(j - (k-1) + \frac{1}{2}\right)^{1-p} - 2\sum_{k=n}^{j-1} k\left(j - k + \frac{1}{2}\right)^{1-p} + \sum_{k=n}^{j-1} k\left(j - (k+1) + \frac{1}{2}\right)^{1-p} \\ &\quad + j\left[\left(\frac{3}{2}\right)^{1-p} - 3\left(\frac{1}{2}\right)^{1-p}\right] \\ &= \sum_{k=n-1}^{j-2} (k+1)\left(j - k + \frac{1}{2}\right)^{1-p} - 2\sum_{k=n}^{j-1} k\left(j - k + \frac{1}{2}\right)^{1-p} + \sum_{k=n+1}^{j} (k-1)\left(j - k + \frac{1}{2}\right)^{1-p} \\ &\quad + j\left[\left(\frac{3}{2}\right)^{1-p} - 3\left(\frac{1}{2}\right)^{1-p}\right] \\ &= n\left(j - (n-1) + \frac{1}{2}\right)^{1-p} - (n-1)\left(j - n + \frac{1}{2}\right)^{1-p} - 2\left(j + \frac{1}{2}\right)\left(\frac{1}{2}\right)^{1-p}, \qquad (2.83)\end{aligned}$$

then result (2) holds.

The first result can also be shown to be true, by using Equation (2.83) with $n = 1$, to obtain

$$\sum_{k=0}^{j} k\widetilde{\nu}_{j-k} = 0 + \sum_{k=1}^{j} \widetilde{\nu}_{j-k} = \left(j+\frac{1}{2}\right)^{1-p} - 2\left(j+\frac{1}{2}\right)\left(\frac{1}{2}\right)^{1-p} \tag{2.84}$$

and so result (1) also holds. □

### 2.5.3 C3 Scheme

In this section another modification of the L1 approximation will be considered by estimating the fractional derivative at time $t_{j+\frac{1}{2}}$. In similar manner, as in Oldham & Spanier (1974), we begin by rewriting the Riemann–Liouville derivative in the form given in Equation (2.71). Unlike the C2 scheme we first split the integral domain in Equation (2.71) into the two intervals $[0, t_{\frac{1}{2}}]$ and $[t_{\frac{1}{2}}, t_{j+\frac{1}{2}}]$ instead which gives

$$\begin{aligned}\left[\frac{d^p f(t)}{dt^p}\right|_{t=t_{j+\frac{1}{2}}} &= \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \int_0^{t_{j+\frac{1}{2}}} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}}-\tau)^{-p} d\tau \\ &= \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \int_0^{t_{\frac{1}{2}}} \frac{df(\tau)}{d\tau}\left(t_{j+\frac{1}{2}}-\tau\right)^{-p} d\tau \\ &+ \frac{1}{\Gamma(1-p)} \int_{t_{\frac{1}{2}}}^{t_{j+\frac{1}{2}}} \frac{df(\tau)}{d\tau}\left(t_{j+\frac{1}{2}}-\tau\right)^{-p} d\tau.\end{aligned} \tag{2.85}$$

We then further split the integral interval $\tau \in [t_{\frac{1}{2}}, t_{j+\frac{1}{2}}]$ into equally-spaced time steps with $t_{j+\frac{1}{2}} = \left(j+\frac{1}{2}\right)\Delta t$ $(1 \le j \le M)$ to give

$$\begin{aligned}\left[\frac{d^p}{dt^p} f(t)\right|_{t=t_{j+\frac{1}{2}}} &= \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \sum_{k=1}^{j} \int_{(k-\frac{1}{2})\Delta t}^{(k+\frac{1}{2})\Delta t} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}}-\tau)^{-p} d\tau \\ &+ \frac{1}{\Gamma(1-p)} \int_0^{\frac{1}{2}\Delta t} \frac{df(\tau)}{d\tau}(t_{j+\frac{1}{2}}-\tau)^{-p} d\tau.\end{aligned} \tag{2.86}$$

Again in each interval the integer–order time derivative is then approximated using first and second–order finite difference approximations

$$\begin{aligned}\left[\frac{d^p}{dt^p} f(t)\right|_{t=t_{j+\frac{1}{2}}} &\approx \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} f_0 + \frac{f\left(t_{\frac{1}{2}}\right) - f(t_0)}{\Gamma(1-p)\frac{1}{2}\Delta t} \int_0^{\frac{1}{2}\Delta t} \left(t_{j+\frac{1}{2}}-\tau\right)^{-p} d\tau \\ &+ \frac{1}{\Gamma(1-p)} \sum_{k=1}^{j} \frac{f\left(t_{k+\frac{1}{2}}\right) - f\left(t_{k-\frac{1}{2}}\right)}{\Delta t} \int_{(k-\frac{1}{2})\Delta t}^{(k+\frac{1}{2})\Delta t} \left(t_{j+\frac{1}{2}}-\tau\right)^{-p} d\tau,\end{aligned} \tag{2.87}$$

which after simplifying can be written in the form

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C3}^{j+\frac{1}{2}} = \frac{\Delta t^{-p}}{\Gamma(2-p)} \left\{ \widehat{\beta}_j(p) f_0 + 2\widehat{\alpha}_j(p) f_{\frac{1}{2}} + \sum_{k=1}^{j} \widehat{\mu}_{j-k}(p) \left( f_{k+\frac{1}{2}} - f_{k-\frac{1}{2}} \right) \right\}, \quad (2.88)$$

where the weights are defined by

$$\widehat{\alpha}_j(p) = \left(j + \frac{1}{2}\right)^{1-p} - j^{1-p}, \quad (2.89)$$

$$\widehat{\beta}_j(p) = (1-p)\left(j + \frac{1}{2}\right)^{-p} - 2\widehat{\alpha}_j, \quad (2.90)$$

and

$$\widehat{\mu}_j(p) = (j+1)^{1-p} - j^{1-p}. \quad (2.91)$$

We refer to this modified method, given in Equations (2.88) – (2.91), as the C3 scheme. The scheme can be written as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C3} = \frac{\Delta t^{-p}}{\Gamma(2-p)} \left[ \widehat{\beta}_j f_0 + \sum_{k=0}^{j} \widehat{\nu}_{j-k} f_{k+\frac{1}{2}} \right], \quad (2.92)$$

where the weights $\widehat{\nu}_l$ are defined by

$$\widehat{\nu}_l = \begin{cases} 1 & \text{if} \quad l = j, \\ 2\widehat{\alpha}_j - (j^{1-p} - (j-1)^{1-p} & \text{if} \quad l = 0, \\ (l+1)^{1-p} - 2l^{1-p} + (l-1)^{1-p} & \text{if} \quad 1 \le l \le j-1, \end{cases} \quad (2.93)$$

and $\widehat{\alpha}_j$ and $\widehat{\beta}_j$ are as defined in Equations (2.89) and (2.90) respectively. In Section 2.6.3 the accuracy of the C3 approximation scheme will be evaluated, in which we will need the following two Lemmas.

**Lemma 2.5.6.** Given the weights $\widehat{\nu}_{j-k}$ defined in Equation (2.93), and $j \ge n$, we have

1. $\sum\limits_{k=0}^{j} \widehat{\nu}_{j-k} = 2\widehat{\alpha}_j$, and
2. $\sum\limits_{k=n}^{j} \widehat{\nu}_{j-k} = (j-(n-1))^{1-p} - (j-n)^{1-p}$, if $n \ge 1$ .

*Proof.* For $n \geq 1$ using the definition of the weights in Equation (2.93), we have

$$\begin{aligned}
\sum_{k=n}^{j} \widehat{\nu}_{j-k} &= \sum_{k=n}^{j-1} \widehat{\nu}_{j-k} + 1 \\
&= \sum_{k=n}^{j-1} \left[ (j-(k-1))^{1-p} - 2\,(j-k)^{1-p} + (j-(k+1))^{1-p} \right] + 1 \\
&= \sum_{k=n-1}^{j-2} (j-k)^{1-p} - \sum_{k=n}^{j-1} (j-k)^{1-p} - \left[ \sum_{k=n}^{j-1} (j-k)^{1-p} - \sum_{k=n+1}^{j} (j-k)^{1-p} \right] + 1 \\
&= (j-(n-1))^{1-p} - 1 - (j-n)^{1-p} + 1 \\
&= (j-(n-1))^{1-p} - (j-n)^{1-p}\,. \qquad (2.94)
\end{aligned}$$

Hence result (2) holds. To show the first result, we have

$$\sum_{k=0}^{j} \widehat{\nu}_{j-k} = 2\widehat{\alpha}_j - \left(j^{1-p} - (j-1)^{1-p}\right) + \sum_{k=1}^{j} \widehat{\nu}_{j-k}, \qquad (2.95)$$

which, by using Equation (2.94) with $n = 1$, we find

$$\sum_{k=0}^{j} \widehat{\nu}_{j-k} = 2\widehat{\alpha}_j - \left(j^{1-p} - (j-1)^{1-p}\right) + j^{1-p} - (j-1)^{1-p}\,. \qquad (2.96)$$

Then result (1) also holds. □

**Lemma 2.5.7.** Given the weights $\widehat{\nu}_{j-k}$ defined in Equation (2.93), with $j \geq n$, we have

1. $\sum\limits_{k=0}^{j} k\widehat{\nu}_{j-k} = j^{1-p}$, and
2. $\sum\limits_{k=n}^{j} k\widehat{\nu}_{j-k} = n\,(j-(n-1))^{1-p} - (n-1)\,(j-n)^{1-p}$, if $n \geq 1$.

*Proof.* For $n \geq 1$ using the definition of the weights in Equation (2.93), we have

$$\begin{aligned}
&\sum_{k=n}^{j} k\widehat{\nu}_{j-k} = \sum_{k=n}^{j-1} k\widehat{\nu}_{j-k} + j(1) \\
&= \sum_{k=n}^{j-1} k\left(j-(k-1)\right)^{1-p} - 2\sum_{k=n}^{j-1} k\left(j-k\right)^{1-p} + \sum_{k=n}^{j-1} k\left(j-(k+1)\right)^{1-p} + j \\
&= \sum_{k=n-1}^{j-2} (k+1)\left(j-k\right)^{1-p} - 2\sum_{k=n}^{j-1} k\left(j-k\right)^{1-p} + \sum_{k=n+1}^{j} (k-1)\left(j-k\right)^{1-p} + j \\
&= \sum_{k=n-1}^{j-2} (k+1)\left(j-k\right)^{1-p} - 2\sum_{k=n}^{j-1} (k+1)\left(j-k\right)^{1-p} + 2\sum_{k=n}^{j-1} \left(j-k\right)^{1-p} \\
&\qquad + \sum_{k=n+1}^{j} (k+1)\left(j-k\right)^{1-p} - 2\sum_{k=n+1}^{j} \left(j-k\right)^{1-p} + j \\
&= n\left(j-(n-1)\right)^{1-p} + (n+1)\left(j-n\right)^{1-p} - 2(n+1)\left(j-n\right)^{1-p} - 2j + 2j + 2\left(j-n\right)^{1-p} \\
&= n\left(j-(n-1)\right)^{1-p} - (n-1)\left(j-n\right)^{1-p}. \qquad (2.97)
\end{aligned}$$

The result (2) holds. Using the previous result with $n = 1$ to show first part of the lemma, we have

$$\sum_{k=0}^{j} k\widehat{\nu}_{j-k} = 0 + \sum_{k=1}^{j} \widehat{\nu}_{j-k} = j^{1-p}. \qquad (2.98)$$

and so we see result (1) also holds. □

## 2.6 Accuracy of the Modified L1 Schemes

In this section, we consider the accuracy of the modified L1 schemes: the C1 scheme given in Equations (2.61) – (2.63), the C2 scheme in Equations (2.75) – (2.77), and the C3 scheme in Equations (2.88) – (2.91). We will discuss the accuracy of each scheme in the following sections. In each section we assume that $f(t)$, $f \in C^2[0,\infty)$, can be expanded in Taylor series around $t = 0$ with an integral remainder term, that is

$$f(t) = f_0 + tf'(0) + \int_0^t f''(\tau)(t-\tau)d\tau. \qquad (2.99)$$

### 2.6.1 Accuracy of the C1 Scheme

In this subsection, we consider the accuracy of the C1 scheme given in Equations (2.61) – (2.63), where $t_j = j\Delta t$, and $0 < p < 1$. The value of fractional derivative of (2.99) is given by

$$\frac{d^p f(t_j)}{dt^p} = f_0 \frac{t_j^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} + \int_0^{t_j} f''(s)\frac{(t_j - s)^{1-p}}{\Gamma(2-p)} ds, \tag{2.100}$$

as shown previously in Equation (2.25). The accuracy of the C1 scheme can now be determined by comparing the exact value in Equation (2.100) with the value obtained using the C1 scheme. Thus we need to evaluate the C1 fractional approximation operating on the functions 1, $t$, and the convolution integral in Equation (2.99).

The C1 approximation scheme given by Equations (2.61) – (2.63) of the function $f(t) = 1$ at time $t_j$, is

$$\begin{aligned}\left[\frac{d^p(1)}{dt^p}\right|_{C1}^{j} &= \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left[\big(2(1-p)j^{-p} - \alpha_j(p)\big)(1) + \sum_{k=0}^{j-1} A_{j-k}(p)(1) + \sum_{k=1}^{j} B_{j-k}(p)(1)\right] \\ &= \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left[\big(2(1-p)j^{-p} - \alpha_j(p)\big) + \alpha_j(p) + \sum_{k=1}^{j-1} A_{j-k}(p) + \sum_{k=1}^{j} B_{j-k}(p)\right],\end{aligned} \tag{2.101}$$

which upon using Corollary 2.5.3 with $n = 1$, we then have

$$\begin{aligned}\left[\frac{d^p(1)}{dt^p}\right|_{C1}^{j} &= \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left\{2(1-p)j^{-p} - \alpha_j(p) + \alpha_j(p) + 0\right\} \\ &= \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left[2(1-p)j^{-p}\right] \\ &= \frac{(j\Delta t)^{-p}}{\Gamma(1-p)} \\ &= \frac{t_j{}^{-p}}{\Gamma(1-p)}.\end{aligned} \tag{2.102}$$

The C1 scheme's approximation for function $f(t) = t$ at time $t_j$ is

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{C1}^{j} &= \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left[\beta_j^*(p)(0) + \sum_{k=0}^{j-1} A_{j-k}(p)\,(k+1)\,\Delta t + \sum_{k=1}^{j} B_{j-k}(p)\,(k-1)\,\Delta t\right] \\ &= \frac{\Delta t^{1-p}}{2\Gamma(2-p)}\left[\alpha_j(p) + \sum_{k=1}^{j-1} kA_{j-k}(p) + \sum_{k=1}^{j} kB_{j-k}(p) + \sum_{k=1}^{j-1} A_{j-k}(p) - \sum_{k=1}^{j} B_{j-k}(p)\right],\end{aligned} \tag{2.103}$$

using Corollary 2.5.3 with $n = 1$ and Equation (2.64), we obtain

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{C1}^{j} &= \frac{\Delta t^{1-p}}{2\Gamma(2-p)}\left\{\left(j^{1-p}-(j-1)^{1-p}\right)-1+j^{1-p}+(j-1)^{1-p}+1\right\} \\ &= \frac{\Delta t^{1-p}}{2\Gamma(2-p)}\left(2j^{1-p}\right) \\ &= \frac{(j\Delta t)^{1-p}}{\Gamma(2-p)} \\ &= \frac{{t_j}^{1-p}}{\Gamma(2-p)}. \qquad (2.104)\end{aligned}$$

Now we apply the C1 scheme's approximation to the convolution integral $\int_0^t f''(s)(t-s)ds$ in Equation (2.99) which gives

$$\left[\frac{d^p}{dt^p}\int_0^t f''(s)\,(t-s)\,ds\right|_{C1}^{j} = \frac{\Delta t^{-p}}{2\Gamma\left(2-p\right)}\left\{\beta_j^*(p)\lim_{t\to 0}\int_0^t f''(s)(t-s)ds \right. \qquad (2.105)$$

$$\left. +\sum_{k=0}^{j-1}A_{j-k}(p)\int_0^{(k+1)\Delta t} f''(s)((k+1)\Delta t-s)ds+\sum_{k=1}^{j}B_{j-k}(p)\int_0^{(k-1)\Delta t} f''(s)((k-1)\Delta t-s)ds\right\}.$$

Note the limit in the first term on the right is zero if $f''(t)$ is a well–behaved function of $t$ and so we have

$$\begin{aligned}\left[\frac{d^p}{dt^p}\int_0^t f''(s)\,(t-s)\,ds\right|_{C1}^{j} = \frac{\Delta t^{-p}}{2\Gamma\left(2-p\right)}&\left\{\sum_{k=0}^{j-1}A_{j-k}(p)\int_0^{(k+1)\Delta t} f''(s)((k+1)\Delta t-s)ds\right. \\ &\left.+\sum_{k=2}^{j}B_{j-k}(p)\int_0^{(k-1)\Delta t} f''(s)((k-1)\Delta t-s)ds\right\}. \qquad (2.106)\end{aligned}$$

Now by dividing the integration interval into equal $\Delta t$ steps, we then have

$$\begin{aligned}\left[\frac{d^p}{dt^p}\int_0^t f''(s)\,(t-s)\,ds\right|_{C1}^{j} = \frac{\Delta t^{-p}}{2\Gamma\left(2-p\right)}&\left\{\sum_{k=0}^{j-1}A_{j-k}(p)\sum_{l=0}^{k}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)((k+1)\Delta t-s)ds\right. \\ &\left.+\sum_{k=2}^{j}B_{j-k}(p)\sum_{l=0}^{k-2}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)((k-1)\Delta t-s)ds\right\}, \qquad (2.107)\end{aligned}$$

and then by changing the order of summation and simplifying, we obtain

$$\begin{aligned}\left[\frac{d^p}{dt^p}\int_0^t f''(s)\,(t-s)\,ds\right|_{C1}^{j} = \frac{\Delta t^{-p}}{2\Gamma\left(2-p\right)}&\left\{\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l}^{j-1}A_{j-k}(p)((k+1)\Delta t-s)ds\right. \\ &\left.+\sum_{l=0}^{j-2}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+2}^{j}B_{j-k}(p)((k-1)\Delta t-s)ds\right\}. \qquad (2.108)\end{aligned}$$

Equation (2.108) becomes

$$\left[\frac{d^p}{dt^p}\int_0^t f''(s)\,(t-s)\,ds\right|_{C1}^{j}$$

$$= \frac{\Delta t^{-p}}{2\Gamma\,(2-p)}\left\{\left(1+2^{-p}\right)\int\limits_{(j-1)\Delta t}^{j\Delta t} f''(s)(j\Delta t - s)ds + \sum_{l=0}^{j-2}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\psi_l(s)ds\right\}, \quad (2.109)$$

where $\psi_l(s)$ is defined as

$$\psi_l(s) = \sum_{k=l}^{j-1} A_{j-k}(p)((k+1)\Delta t - s) + \sum_{k=l+2}^{j} B_{j-k}(p)((k-1)\Delta t - s). \quad (2.110)$$

Evaluating $\psi_l(s)$ we have

$$\begin{aligned}
\psi_l(s) = &\left[\sum_{k=l}^{j-1} kA_{j-k}(p) + \sum_{k=l+2}^{j} kB_{j-k}(p)\right]\Delta t + \left[\sum_{k=l}^{j-1} A_{j-k}(p) - \sum_{k=l+2}^{j} B_{j-k}(p)\right]\Delta t \\
&- \left[\sum_{k=l}^{j-1} A_{j-k}(p) + \sum_{k=l+2}^{j} B_{j-k}(p)\right] s \\
= &\frac{\Delta t}{2}\left[l\left((j-(l-1))^{1-p} - (j-(l+1))^{1-p}\right) + (l+1)\left((j-l)^{1-p} - (j-(l+2))^{1-p}\right)\right] \\
&+ \frac{\Delta t - s}{2}\left[\left((j-(l-1))^{1-p} - (j-(l+1))^{1-p}\right) + \left((j-l)^{1-p} - (j-(l+2))^{1-p}\right)\right] \\
&+ \left[\sum_{k=l+2}^{j-1} kA_{j-k}(p) + \sum_{k=l+2}^{j} kB_{j-k}(p)\right]\Delta t + \left[\sum_{k=l+2}^{j-1} A_{j-k}(p) - \sum_{k=l+2}^{j} B_{j-k}(p)\right]\Delta t \\
&- \left[\sum_{k=l+2}^{j-1} A_{j-k}(p) + \sum_{k=l+2}^{j} B_{j-k}(p)\right] s. \qquad (2.111)
\end{aligned}$$

Using Corollary 2.5.3 with $n = l + 2$, we have

$$\begin{aligned}
\psi_l(s) = &\frac{\Delta t}{2}\left[l\left((j-(l-1))^{1-p} - (j-(l+1))^{1-p}\right) + (l+1)\left((j-l)^{1-p} - (j-(l+2))^{1-p}\right)\right] \\
&+ \frac{\Delta t - s}{2}\left[\left((j-(l-1))^{1-p} - (j-(l+1))^{1-p}\right) + \left((j-l)^{1-p} - (j-(l+2))^{1-p}\right)\right] \\
&+ [-1]\Delta t + \left[(j-(l+1))^{1-p} + (j-(l+2))^{1-p} + 1\right]\Delta t - [0]s, \qquad (2.112)
\end{aligned}$$

which after simplifying becomes

$$\begin{aligned}
\psi_l(s) = &\frac{l\Delta t - s}{2}\left[(j-l)^{1-p} + (j-(l-1))^{1-p} - (j-(l+1))^{1-p} - (j-(l+2))^{1-p}\right] \\
&+ \frac{\Delta t}{2}\left[2(j-l)^{1-p} + (j-(l-1))^{1-p} + (j-(l+1))^{1-p}\right]. \qquad (2.113)
\end{aligned}$$

The value of the C1 scheme's approximation in Equation (2.61) can now be compared with the value of exact value of the fractional derivative in Equation (2.100). The error can be evaluated as follows

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{C1}\right| = \left| f_0\frac{t_j^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} + \int\limits_0^{j\Delta t} f''(s)\frac{(t_j-s)^{1-p}}{\Gamma(2-p)}ds \right.$$

$$- f_0\frac{t_j^{-p}}{\Gamma(1-p)} - f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} - \frac{\Delta t^{-p}}{2\Gamma(2-p)}\left\{\left(1+2^{-p}\right)\int\limits_{(j-1)\Delta t}^{j\Delta t} f''(s)(j\Delta t - s)ds\right.$$

$$\left.\left. + \sum_{l=0}^{j-2}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\psi_l(s)ds\right\}\right|, \tag{2.114}$$

where the first terms cancel, we then have

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{C1}\right|$$

$$= \frac{1}{\Gamma(2-p)}\left|\int\limits_{(j-1)\Delta t}^{j\Delta t} f''(s)\left[(t_j-s)^{1-p} - \frac{\Delta t^{-p}}{2}\left(1+2^{-p}\right)(j\Delta t - s)\right]ds\right.$$

$$\left. + \sum_{l=0}^{j-2}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t_j-s)^{1-p} - \frac{\Delta t^{-p}}{2}\psi_l(s)\right]ds\right|. \tag{2.115}$$

Using Equation (2.39) in Equation (2.115) we then have

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{L1}\right|$$

$$\leq \frac{1}{\Gamma(2-p)}\int\limits_{(j-1)\Delta t}^{j\Delta t} |f''(s)|\left|(t_j-s)^{1-p} - \frac{\Delta t^{-p}}{2}\left(1+2^{-p}\right)(j\Delta t - s)\right|ds$$

$$+ \sum_{l=0}^{j-2}\int\limits_{l\Delta t}^{(l+1)\Delta t} |f''(s)|\left|(t_j-s)^{1-p} - \frac{\Delta t^{-p}}{2}\psi_l(s)\right|ds. \tag{2.116}$$

We now let the maximum absolute value of the second derivative in the interval $[l\Delta t, (l+1)\Delta t]$ be given by

$$M_l = \max_{l\Delta t \leq s \leq (l+1)\Delta t}\left|f''(s)\right|, \tag{2.117}$$

then Equation (2.116) becomes

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{L1}\right| \leq \frac{M_j}{\Gamma(2-p)}\int\limits_{(j-1)\Delta t}^{j\Delta t}\left|(t-s)^{1-p} - \frac{\Delta t^{-p}}{2}\left(1+2^{-p}\right)(j\Delta t - s)\right|ds$$

$$+ \sum_{l=0}^{j-2} M_l \int\limits_{l\Delta t}^{(l+1)\Delta t}\left|(t-s)^{1-p} - \frac{\Delta t^{-p}}{2}\psi_l(s)\right|ds. \tag{2.118}$$

We know from Appendix B.4 that both terms in the absolute value functions are nonnegative. Dropping the absolute value and then evaluating the integrals in Equation (2.118), we then have

$$\int_{(j-1)\Delta t}^{j\Delta t} (t_j - s)^{1-p}\, ds = \frac{\Delta t^{2-p}}{2-p}, \text{ and } \int_{(j-1)\Delta t}^{j\Delta t} (t_j - s)\, ds = \frac{\Delta t^2}{2}, \tag{2.119}$$

$$\int_{l\Delta t}^{(l+1)\Delta t} (t_j - s)^{1-p}\, ds = \frac{\Delta t^{2-p}}{2-p}\left[(j-l)^{2-p} - (j-(l+1))^{2-p}\right], \tag{2.120}$$

and

$$\begin{aligned}
&\int_{l\Delta t}^{(l+1)\Delta t} \psi_l(s)\, ds \\
&= \int_{l\Delta t}^{(l+1)\Delta t} \frac{l\Delta t - s}{2}\left[(j-l)^{1-p} + (j-(l-1))^{1-p} - (j-(l+1))^{1-p} - (j-(l+2))^{1-p}\right] ds \\
&\quad + \int_{l\Delta t}^{(l+1)\Delta t} \frac{\Delta t}{2}\left[2(j-l)^{1-p} + (j-(l-1))^{1-p} + (j-(l+1))^{1-p}\right] ds \\
&= -\frac{\Delta t^2}{4}\left[(j-l)^{1-p} + (j-(l-1))^{1-p} - (j-(l+1))^{1-p} - (j-(l+2))^{1-p}\right] \\
&\quad + \frac{\Delta t^2}{2}\left[2(j-l)^{1-p} + (j-(l-1))^{1-p} + (j-(l+1))^{1-p}\right] \\
&= \frac{\Delta t^2}{4}\left[3(j-l)^{1-p} + (j-(l-1))^{1-p} + 3(j-(l+1))^{1-p} + (j-(l+2))^{1-p}\right].
\end{aligned} \tag{2.121}$$

If we now let $M = \max\left(\{M_i; i = 0, 1, 2, ..., j\}\right)$, and then use the value of the above integrals in Equation (2.118), we then have

$$\begin{aligned}
&\left|\left[\frac{d^p}{dt^p} f(t)\right|^j - \left[\frac{d^p}{dt^p} f(t)\right|^j_{C1}\right| \\
&= \frac{M\Delta t^{2-p}}{(2-p)\Gamma(2-p)}\left\{\left[1 - \frac{2-p}{4}\left(1 + 2^{-p}\right)\right] + \sum_{l=0}^{j-2}\left[(j-l)^{2-p} - (j-(l+1))^{2-p}\right.\right. \\
&\left.\left. -\frac{2-p}{8}\left[3(j-l)^{1-p} + (j-(l-1))^{1-p} + 3(j-(l+1))^{1-p} + (j-(l+2))^{1-p}\right]\right]\right\} \\
&= \frac{M\Delta t^{2-p}}{(2-p)\Gamma(2-p)}\left\{\left[1 - \frac{2-p}{4}\left(1 + 2^{-p}\right)\right] + \sum_{k=2}^{j}\left[k^{2-p} - (k-1)^{2-p}\right.\right. \\
&\left.\left. -\frac{2-p}{8}\left[3k^{1-p} + (k+1)^{1-p} + 3(k-1)^{1-p} + (k-2)^{1-p}\right]\right]\right\}.
\end{aligned} \tag{2.122}$$

Evaluating the summations

$$\sum_{k=2}^{j}\left(k^{2-p}-(k-1)^{2-p}\right)=\sum_{k=2}^{j}k^{2-p}-\sum_{k=1}^{j-1}k^{2-p}=j^{2-p}-1, \tag{2.123}$$

and

$$\begin{aligned}\sum_{k=2}^{j}\big[3k^{1-p} &+(k+1)^{1-p}+3(k-1)^{1-p}+(k-2)^{1-p}\big]\\ &=3\sum_{k=2}^{j}k^{1-p}+\sum_{k=3}^{j+1}k^{1-p}+3\sum_{k=1}^{j-1}k^{1-p}+\sum_{k=0}^{j-2}k^{1-p}\\ &=3\left(2^{1-p}+j^{1-p}+(j-1)^{1-p}\right)+(j+1)^{1-p}+j^{1-p}+(j-1)^{1-p}\\ &\quad+3\left(1+2^{1-p}+(j-1)^{1-p}\right)+1+2^{1-p}+8\sum_{3}^{j-2}k^{1-p}\\ &=4j^{1-p}+(j+1)^{1-p}-(j-1)^{1-p}-4-2^{1-p}+8\sum_{1}^{j-1}k^{1-p},\end{aligned} \tag{2.124}$$

we then find

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j}-\left[\frac{d^p}{dt^p}f(t)\right|^{j}_{C1}\right|\leq C\Delta t^{2-p}, \tag{2.125}$$

where $C=\frac{M\Upsilon(j,p)}{\Gamma(3-p)}$, and $\Upsilon(j,p)$ is given by

$$\begin{aligned}\Upsilon(j,p)=&\left[1-\frac{2-p}{4}\left(1+2^{-p}\right)\right]+j^{2-p}-1 \qquad (2.126)\\ &-\frac{(2-p)}{8}\left[4j^{1-p}+(j+1)^{1-p}-(j-1)^{1-p}-4-2^{1-p}+8\sum_{k=1}^{j-1}k^{1-p}\right]\\ =&\left(j^{1-p}\left[j-\frac{2-p}{2}\right]-(2-p)\sum_{k=1}^{j-1}k^{1-p}\right)+\frac{2-p}{8}\left((j-1)^{1-p}-(j+1)^{1-p}\right)+\frac{2-p}{4},\end{aligned}$$

or

$$\Upsilon(j,p)=\frac{1}{2}\left[\vartheta(j,p)+\frac{2-p}{4}\left((j-1)^{1-p}-(j+1)^{1-p}\right)+\frac{2-p}{2}\right]. \tag{2.127}$$

In Equation (2.127), we have $\Upsilon(j,0)=0$, and $\Upsilon(j,1)=\frac{3}{4}$. If $0<p\leq 1$ then $\Upsilon(j,p)$ is bounded $0\leq\Upsilon(j,p)\leq\frac{3}{4}$ as shown in Figure 2.13. Compared with the L1 scheme we see the first term in Equation (2.127) is bounded by

$$\vartheta(j,p)\leq\frac{p}{2}\zeta\left(1+p,1\right). \tag{2.128}$$

After using this result and since the term $\left((j-1)^{1-p}-(j+1)^{1-p}\right)$, as shown in Appendix B.5, is bounded by $-2^{1-p}$, we obtain the bound of $\Upsilon(j,p)$, of

$$\Upsilon(j,p)\leq\frac{p}{4}\zeta\left(1+p,1\right)+\frac{2-p}{4}\left(1-2^{-p}\right). \tag{2.129}$$

This verifies this scheme is of order $O(\Delta t^{2-p})$ for any function that can be expanded as a Taylor series around $t = 0$ as in Equation (2.99).

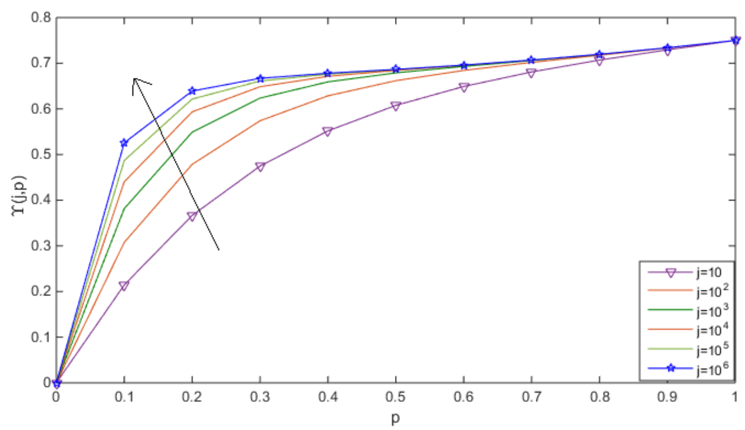



Figure 2.13: (Color online) The value of $\Upsilon(j,p)$ in Equation (2.127) as shown versus $p$ for varying number of time steps $j = 10, 10^2, 10^3, \ldots, 10^6$, where $j$ increases in the direction of the arrow. These results show $\Upsilon(j,p)$ is bounded above by $\frac{3}{4}$ for all $0 \leq p \leq 1$.

The estimate of the accuracy of the C1 scheme was tested on the functions given in Equation (2.7). The error is plotted as a function of $\Delta t$ on double logarithmic scale plot as given in Figures 2.14 – 2.18. We see the error decreases for each value of $\gamma$ as $\Delta t$ is decreased, and the slope of the lines match asymptotically the slope of $1+\gamma$ of the dashed lines.

In Table 2.4, we see that the maximum error occurs when $\gamma = 0.1$ and the minimum error occurs when $\gamma = 0.9$, except for the function $f(t) = 1 + t^\gamma$ where the maximum error occurs when $\gamma = 0.2$. For small $\Delta t$ the error is of order $O(\Delta t^{2-p})$.

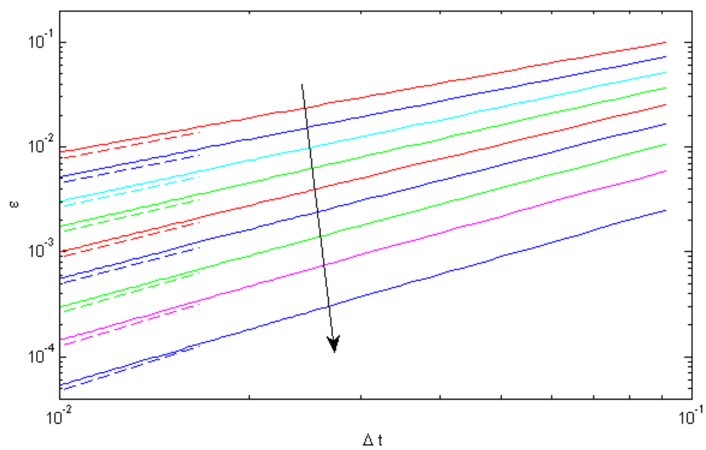



Figure 2.14: (Color online) The absolute error found by using the C1 scheme to evaluate the fractional derivative of order $p = 1 - \gamma$, where $0 < \gamma \leq 1$, of function $f(t) = t^2$ at time $t = 1.0$. The error is given for $\gamma = 0.1, \ldots, 0.9$, where $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1 + \gamma$ for comparison.

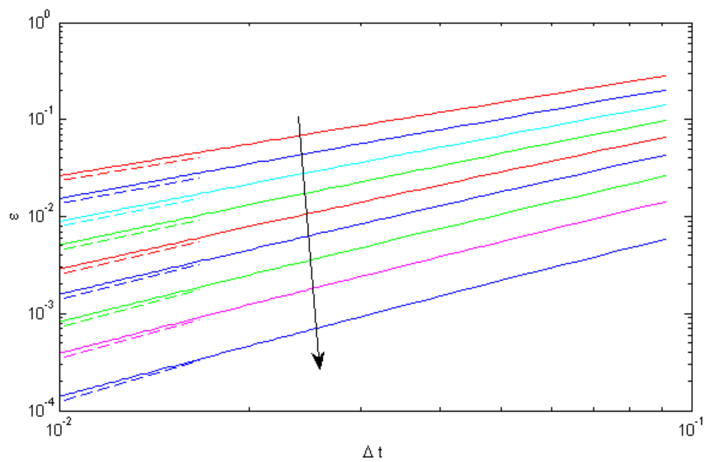



Figure 2.15: (Color online) The value of the absolute error in using C1 scheme to approximate the fractional derivative of order $1 - \gamma$ for the function $f(t) = t^3$ at the time $t = 1.0$, with $\gamma = 0.1, \ldots, 0.9$. The value of $\gamma$ increases in the direction of the arrow and the dashed lines show lines of slope $1 + \gamma$ for comparison.

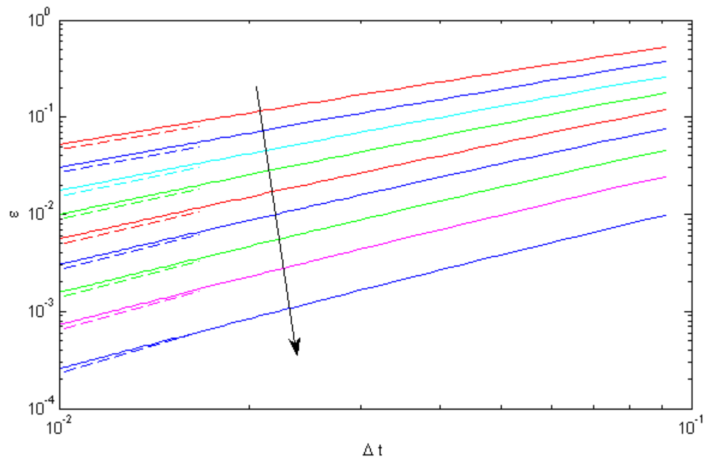



Figure 2.16: (Color online) The absolute error in using the C1 scheme to estimate the fractional derivative of order $1-\gamma$ for the function $f(t) = t^4$ shown at the time $t = 1.0$, for $\gamma = 0.1, \ldots, 0.9$. The value of $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

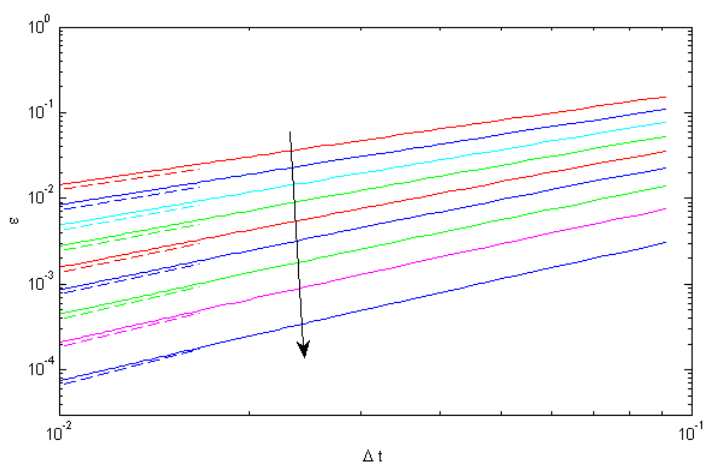



Figure 2.17: (Color online) The absolute error in using the C1 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 - e^t + t^3$, where $\gamma = 0.1, \ldots, 0.9$ and time $t = 1.0$. Note $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison.

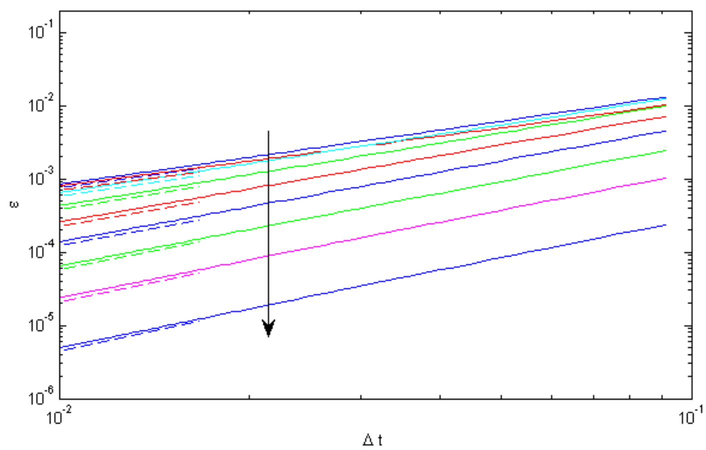



Figure 2.18: (Color online) The absolute error in using the C1 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 + t^{\gamma}$ at the time $t = 1.0$. The results are shown for $\gamma = 0.1, \ldots, 0.9$, and $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

Table 2.4: The comparison of the absolute error in the C1 scheme estimate of the fractional derivative of order $p = 1 - \gamma$ of the functions $f(t)$ in Equation (2.7) at the time $t = 1.0$ with $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^3$ | $f(t) = t^4$ | $f(t) = 1 - e^t + t^3$ | $f(t) = 1 + t^{\gamma}$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 7.964e–03 | 2.371e–02 | 4.710e–02 | 1.297e–02 | 7.268e–04 |
| $\gamma = 0.2$ | 4.626e–03 | 1.372e–02 | 2.718e–02 | 7.501e–03 | 7.542e–04 |
| $\gamma = 0.3$ | 2.671e–03 | 7.878e–03 | 1.555e–02 | 4.303e–03 | 5.748e–04 |
| $\gamma = 0.4$ | 1.529e–03 | 4.474e–03 | 8.782e–03 | 2.441e–03 | 3.785e–04 |
| $\gamma = 0.5$ | 8.645e–04 | 2.499e–03 | 4.872e–03 | 1.361e–03 | 2.241e–04 |
| $\gamma = 0.6$ | 4.778e–04 | 1.359e–03 | 2.624e–03 | 7.381e–04 | 1.194e–04 |
| $\gamma = 0.7$ | 2.528e–04 | 7.037e–04 | 1.343e–03 | 3.807e–04 | 5.530e–05 |
| $\gamma = 0.8$ | 1.217e–04 | 3.295e–04 | 6.194e–04 | 1.773e–04 | 2.020e–05 |
| $\gamma = 0.9$ | 4.500e–05 | 1.178e–04 | 2.175e–04 | 6.300e–05 | 4.140e–06 |

The approximate order of convergence in $\Delta t$ given in Table 2.5, we give the error and order of convergence estimate for the fractional derivative of order $1-\gamma$ of the function $f(t) = 1 + t^{\gamma}$. The results are shown for $\gamma = 0.1, \ldots, 0.9$ with time $t = 1.0$, we see the C1 scheme is also of order $O(\Delta t^{1+\gamma})$.

Table 2.5: Numerical accuracy in $\Delta t$ of the C1 scheme applied to the function $f(t) = 1 + t^{\gamma}$, where $\widehat{R}$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.2$ | | $\gamma = 0.3$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_{\infty}(\Delta t)$ | $\widehat{R}$ | $e_{\infty}(\Delta t)$ | $\widehat{R}$ | $e_{\infty}(\Delta t)$ | $\widehat{R}$ |
| 1/1000 | 6.338e–05 | – | 5.264e–05 | – | 3.216e–05 | – |
| 1/2000 | 2.955e–05 | 1.1 | 2.289e–05 | 1.2 | 1.304e–06 | 1.3 |
| 1/4000 | 1.378e–05 | 1.1 | 9.955e–06 | 1.2 | 5.292e–06 | 1.3 |
| 1/8000 | 6.426e–06 | 1.1 | 4.332e–06 | 1.2 | 2.148e–06 | 1.3 |
| 1/16000 | 2.997e–06 | 1.1 | 1.885e–06 | 1.2 | 8.721e–07 | 1.3 |
| | $\gamma = 0.4$ | | $\gamma = 0.5$ | | $\gamma = 0.6$ | |
| 1/1000 | 1.703e–05 | – | 8.170e–06 | – | 3.563e–06 | – |
| 1/2000 | 6.446e–06 | 1.4 | 2.888e–06 | 1.5 | 1.180e–06 | 1.6 |
| 1/4000 | 2.441e–06 | 1.4 | 1.021e–06 | 1.5 | 3.902e–07 | 1.6 |
| 1/8000 | 9.243e–07 | 1.4 | 3.610e–07 | 1.5 | 1.290e–07 | 1.6 |
| 1/16000 | 3.501e–07 | 1.4 | 1.277e–07 | 1.5 | 4.261e–08 | 1.6 |
| | $\gamma = 0.7$ | | $\gamma = 0.8$ | | $\gamma = 0.9$ | |
| 1/1000 | 1.373e–06 | – | 4.254e–07 | – | 7.607e–08 | – |
| 1/2000 | 4.273e–07 | 1.7 | 1.253e–07 | 1.8 | 2.137e–08 | 1.9 |
| 1/4000 | 1.327e–07 | 1.7 | 3.675e–08 | 1.8 | 5.973e–09 | 1.9 |
| 1/8000 | 4.114e–08 | 1.7 | 1.075e–08 | 1.8 | 1.662e–09 | 1.9 |
| 1/16000 | 1.274e–08 | 1.7 | 3.135e–09 | 1.8 | 4.611e–10 | 1.9 |

### 2.6.2 Accuracy of the C2 Scheme

Here we determine the accuracy of the fractional derivative approximation at $t = t_{j+\frac{1}{2}}$ given by the C2 scheme in Equations (2.75) – (2.77). To do this we follow a similar approach to that used for the C1 scheme.

To estimate the accuracy we compare the results of taking the Riemann–Liouville fractional derivative of the function $f(t)$ in Equation (2.99) with the approximate result obtained by applying the C2 scheme, in Equations (2.78) – (2.79), to the same function. The exact expression of the of the fractional derivative in Equation (2.99) is given by

Equation (2.25), by replacing $t_j$ by $t_{j+\frac{1}{2}}$ we then have

$$\left[\frac{d^p f(t)}{dt^p}\right|^{j+\frac{1}{2}} = f_0\frac{t_{j+1/2}^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_{j+\frac{1}{2}}^{1-p}}{\Gamma(2-p)} + \int_0^{t_{j+\frac{1}{2}}} f''(s)\frac{(t_{j+\frac{1}{2}}-s)^{1-p}}{\Gamma(2-p)}ds. \tag{2.130}$$

Next we apply the C2 fractional approximation scheme on the functions 1, $t$, and the convolution integrals in Equation (2.99) at the time $t = t_{j+\frac{1}{2}}$.

The C2 approximation of the function $f(t) = 1$ at time $t_{j+\frac{1}{2}}$, is given by

$$\left[\frac{d^p(1)}{dt^p}\right|_{C2} = \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)}(1) + \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=0}^{j}\widetilde{\nu}_{j-k}(1) + \frac{2\left(\frac{1}{2}\right)^{1-p}\Delta t^{-p}}{\Gamma(2-p)}(1), \tag{2.131}$$

which simplifies, after using the first result of Lemma 2.5.4, to

$$\left[\frac{d^p(1)}{dt^p}\right|_{C2} = \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} + \frac{\Delta t^{-p}}{\Gamma(2-p)}\left[-2\left(\frac{1}{2}\right)^{1-p} + 2\left(\frac{1}{2}\right)^{1-p}\right] = \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)}. \tag{2.132}$$

The C2 approximation for function $f(t) = t$ at time $t_{j+\frac{1}{2}}$ is

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{C2} &= 0 + \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=0}^{j}\widetilde{\nu}_{j-k}(\gamma)(k\Delta t) + \frac{2\left(\frac{1}{2}\right)^{1-p}\Delta t^{-p}}{\Gamma(2-p)}\left(\left(j+\frac{1}{2}\right)\Delta t\right)\\ &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left\{\sum_{k=0}^{j}k\widetilde{\nu}_{j-k}(\gamma) + 2\left(\frac{1}{2}\right)^{1-p}\left(j+\frac{1}{2}\right)\right\}.\end{aligned} \tag{2.133}$$

Using the first result of Lemma 2.5.5, we then have the result

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right| &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left[\left(j+\frac{1}{2}\right)^{1-p} - 2\left(j+\frac{1}{2}\right)\left(\frac{1}{2}\right)^{1-p} + 2\left(j+\frac{1}{2}\right)\left(\frac{1}{2}\right)^{1-p}\right]\\ &= \frac{t_{j+\frac{1}{2}}^{1-p}}{\Gamma(2-p)}.\end{aligned} \tag{2.134}$$

Applying the C2 approximation to the convolution in Equation (2.99) gives

$$\begin{aligned}\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C2} &= \frac{(\Delta t)^{-p}}{\Gamma(2-p)}\left\{(1-p)\left(j+\frac{1}{2}\right)^{-p}\lim_{t\to 0}\int_0^t f''(\tau)(t-\tau)d\tau\right.\\ +2\left(\frac{1}{2}\right)^{1-p}&\left.\int_0^{(j+\frac{1}{2})\Delta t} f''(\tau)\left(t_{j+\frac{1}{2}}-\tau\right)d\tau + \sum_{k=0}^{j}\widetilde{\nu}_{j-k}\int_0^{k\Delta t} f''(\tau)\left(k\Delta t-\tau\right)d\tau\right\}.\end{aligned} \tag{2.135}$$

The limit in the first term on the right in (2.135) is zero if $f''(t)$ is a well–behaved function as mentioned earlier. Now dividing the integration interval, $[0, j\Delta t]$, into equal $\Delta t$ steps and the integral interval from $\tau = j\Delta t$ to $\tau = \left(j+\frac{1}{2}\right)\Delta t$, we then have

$$\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C2}^{j+\frac{1}{2}} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{2\left(\frac{1}{2}\right)^{1-p}\int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} f''(\tau)\left(\left(j+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right.$$
$$\left.+2\left(\frac{1}{2}\right)^{1-p}\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(\tau)\left(\left(j+\frac{1}{2}\right)\Delta t-\tau\right)d\tau+\sum_{k=0}^{j}\widetilde{\nu}_{j-k}\sum_{l=0}^{k-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(\tau)\left(k\Delta t-\tau\right)d\tau\right\}. \tag{2.136}$$

Upon simplifying this expression we have

$$\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C2}^{j+\frac{1}{2}} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{2\left(\frac{1}{2}\right)^{1-p}\int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} f''(\tau)\left(t_{j+\frac{1}{2}}-\tau\right)d\tau\right.$$
$$\left.+\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(\tau)\left[\sum_{k=l+1}^{j}\widetilde{\nu}_{j-k}\left(k\Delta t-\tau\right)+2\left(\frac{1}{2}\right)^{1-p}\left(t_{j+\frac{1}{2}}-\tau\right)\right]d\tau\right\}. \tag{2.137}$$

Now using Lemmas 2.5.4 and 2.5.5, with $n = l+1$, we evaluate the summation to find

$$\sum_{k=l+1}^{j}\widetilde{\nu}_{j-k}(\gamma)\left(k\Delta t-\tau\right) = 2\left(\frac{1}{2}\right)^{1-p}\left(\tau-t_{j+\frac{1}{2}}\right)+\left(j-l+\frac{1}{2}\right)^{1-p}\left((l+1)\Delta t-\tau\right)$$
$$-\left(j-l-\frac{1}{2}\right)^{1-p}(l\Delta t-\tau). \tag{2.138}$$

The C2 approximation of the fractional derivative of $f(t)$, in Equation (2.99), is then given by

$$\left[\frac{d^p f(t)}{dt^p}\right|_{C2} = f_0\frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)}+f'(0)\frac{t_{j+\frac{1}{2}}^{1-p}}{\Gamma(2-p)} \tag{2.139}$$
$$+\frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{2\left(\frac{1}{2}\right)^{1-p}\int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} f''(\tau)\left(t_{j+\frac{1}{2}}-\tau\right)d\tau+\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(\tau)\right.$$
$$\left.\left[\left(j-l+\frac{1}{2}\right)^{1-p}\left((l+1)\Delta t-\tau\right)-\left(j-l-\frac{1}{2}\right)^{1-p}(l\Delta t-\tau)\right]d\tau\right\}.$$

The value of the C2 approximation in Equation (2.139) can now compared with the exact value of the fractional derivative in Equation (2.130). The absolute error is given by

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}-\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C2}\right| \tag{2.140}$$

$$=\Bigg|\frac{t_{j+1/2}^{-p}}{\Gamma(1-p)}f_0+\frac{t_{j+1/2}^{1-p}}{\Gamma(2-p)}f'(0)+\int_0^{t_{j+\frac{1}{2}}} f''(\tau)\frac{(t_{j+\frac{1}{2}}-\tau)^{1-p}}{\Gamma(2-p)}d\tau-\frac{t_{j+1/2}^{-p}}{\Gamma(1-p)}f_0$$

$$-\frac{t_{j+1/2}^{1-p}}{\Gamma(2-p)}f'(0)-\frac{\Delta t^{-p}}{\Gamma(2-p)}\Bigg\{2\left(\frac{1}{2}\right)^{1-p}\int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} f''(\tau)\left(\left(j+\frac{1}{2}\right)\Delta t-\tau\right)d\tau$$

$$+\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(\tau)\left[\left(j-l+\frac{1}{2}\right)^{1-p}((l+1)\Delta t-\tau)-\left(j-l-\frac{1}{2}\right)^{1-p}(l\Delta t-\tau)\right]\Bigg\}\Bigg|,$$

which reduces to

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}-\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C2}\right| \tag{2.141}$$

$$=\Bigg|\frac{1}{\Gamma(2-p)}\Bigg\{\int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} f''(\tau)\left[(t_{j+\frac{1}{2}}-\tau)^{1-p}-\left(\frac{\Delta t}{2}\right)^{-p}\left(t_{j+\frac{1}{2}}-\tau\right)\right]d\tau$$

$$+\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(\tau)\Bigg((t_{j+\frac{1}{2}}-\tau)^{1-p}-\Delta t^{-p}\Bigg[\left(j-l+\frac{1}{2}\right)^{1-p}((l+1)\Delta t-\tau)$$

$$-\left(j-l-\frac{1}{2}\right)^{1-p}(l\Delta t-\tau)\Bigg]\Bigg)ds\Bigg\}\Bigg|.$$

Now using the inequality Equation (2.39) we then have

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}-\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C2}\right| \tag{2.142}$$

$$\leq\frac{1}{\Gamma(2-p)}\Bigg\{\int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} |f''(\tau)|\left|(t_{j+\frac{1}{2}}-\tau)^{1-p}-\left(\frac{\Delta t}{2}\right)^{-p}\left(t_{j+\frac{1}{2}}-\tau\right)\right|d\tau$$

$$+\sum_{l=0}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} |f''(\tau)|\Bigg|(t_{j+\frac{1}{2}}-\tau)^{1-p}-\Delta t^{-p}\Bigg[\left(j-l+\frac{1}{2}\right)^{1-p}((l+1)\Delta t-\tau)$$

$$-\left(j-l-\frac{1}{2}\right)^{1-p}(l\Delta t-\tau)\Bigg]\Bigg|ds\Bigg\}.$$

Now we let the maximum absolute value of the second derivative in the interval $[j\Delta t,(j+1/2)\Delta t]$ be denoted by

$$M^*_{j+\frac{1}{2}}=\max_{j\Delta t\leq s\leq(j+\frac{1}{2})\Delta t}\left|f''(s)\right|, \tag{2.143}$$

and in the intervals $[l\Delta t, (l+1)\Delta t]$ by

$$M_l = \max_{l\Delta t \le s \le (l+1)\Delta t} \left| f''(s) \right| . \tag{2.144}$$

Then from Equation (2.142) we have the inequality

$$\begin{aligned} &\left| \left[ \frac{d^p}{dt^p} f(t) \right|^{j+\frac{1}{2}} - \left[ \frac{d^p}{dt^p} f(t) \right|^{j+\frac{1}{2}}_{C2} \right| \qquad (2.145) \\ &\le \frac{M^*_{j+\frac{1}{2}}}{\Gamma(2-p)} \int_{j\Delta t}^{(j+\frac{1}{2})\Delta t} \left| (t_{j+\frac{1}{2}} - \tau)^{1-p} - \left( \frac{\Delta t}{2} \right)^{-p} \left( t_{j+\frac{1}{2}} - \tau \right) \right| d\tau \\ &+ \frac{1}{\Gamma(2-p)} \sum_{l=0}^{j-1} M_l \int_{l\Delta t}^{(l+1)\Delta t} \left| (t_{j+\frac{1}{2}} - \tau)^{1-p} - \Delta t^{-p} \left[ \left( j - l + \frac{1}{2} \right)^{1-p} ((l+1)\Delta t - \tau) \right. \right. \\ &\qquad \left. \left. - \left( j - l - \frac{1}{2} \right)^{1-p} (l\Delta t - \tau) \right] \right| ds. \end{aligned}$$

Now we know, from Appendix B.6, each term in the absolute value functions is positive and so we can drop the absolute value sign. Evaluating the integrals in Equation (2.145), we obtain the bound on the error

$$\begin{aligned} &\left| \left[ \frac{d^p}{dt^p} f(t) \right|^{j+\frac{1}{2}} - \left[ \frac{d^p}{dt^p} f(t) \right|^{j+\frac{1}{2}}_{C2} \right| \le \frac{M^*_{j+\frac{1}{2}} \Delta t^{2-p}}{(2-p)\Gamma(2-p)} \left[ \left( \frac{1}{2} \right)^{2-p} - \frac{2-p}{4} \left( \frac{1}{2} \right)^{1-p} \right] \\ &\qquad + \frac{\Delta t^{2-p}}{(2-p)\Gamma(2-p)} \sum_{l=0}^{j-1} M_l \left[ \left( j - l + \frac{1}{2} \right)^{2-p} - \left( j - l - \frac{1}{2} \right)^{2-p} \right. \\ &\qquad \left. - \frac{(2-p)}{2} \left[ \left( j - l + \frac{1}{2} \right)^{1-p} + \left( j - l - \frac{1}{2} \right)^{1-p} \right] \right]. \end{aligned} \tag{2.146}$$

If we further let $M = \max\left( \{M_i; i = 0, 1, 2, ..., j\} \bigcup \{M^*_{j+\frac{1}{2}}\} \right)$, and then simplifying we obtain

$$\begin{aligned} &\left| \left[ \frac{d^p}{dt^p} f(t) \right|^{j+\frac{1}{2}} - \left[ \frac{d^p}{dt^p} f(t) \right|^{j+\frac{1}{2}}_{C2} \right| \le \frac{M \Delta t^{2-p}}{\Gamma(3-p)} \left\{ \left( \frac{1}{2} \right)^{1-p} \left| \frac{p}{4} \right| \right. \qquad (2.147) \\ &+ \left. \sum_{l=0}^{j-1} \left| \left( j - l + \frac{1}{2} \right)^{1-p} \left( j - l - \frac{1-p}{2} \right) - \left( j - l - \frac{1}{2} \right)^{1-p} \left( j - l + \frac{1-p}{2} \right) \right| \right\}. \end{aligned}$$

Evaluating the sum in Equation (2.147) we find

$$\begin{aligned} &\sum_{l=0}^{j-1} \left[ \left( j - l + \frac{1}{2} \right)^{1-p} \left( j - l - \frac{1-p}{2} \right) - \left( j - l - \frac{1}{2} \right)^{1-p} \left( j - l + \frac{1-p}{2} \right) \right] \qquad (2.148) \\ &= \left( j + \frac{1}{2} \right)^{1-p} \left( j - \frac{1-p}{2} \right) - \left( \frac{3-p}{2} \right) \left( \frac{1}{2} \right)^{1-p} - (2-p) \sum_{k=1}^{j-1} \left( k + \frac{1}{2} \right)^{1-p}. \end{aligned}$$

The estimate error is then given by

$$\left| \left[\frac{d^p}{dt^p} f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p} f(t)\right|^{j+\frac{1}{2}}_{C2} \right| \leq C\Delta t^{2-p}, \tag{2.149}$$

where $C$ is constant

$$C = \frac{M\hat{\vartheta}(j,p)}{\Gamma(3-p)}, \tag{2.150}$$

and $\hat{\vartheta}(j,p)$ is defined by

$$\begin{aligned}\hat{\vartheta}(j,p) = \frac{p}{4}\left(\frac{1}{2}\right)^{1-p} + \left(j+\frac{1}{2}\right)^{1-p}\left(j - \frac{1-p}{2}\right) - \left(\frac{3-p}{2}\right)\left(\frac{1}{2}\right)^{1-p} \\ - (2-p)\sum_{k=1}^{j-1}\left(k+\frac{1}{2}\right)^{1-p}.\end{aligned} \tag{2.151}$$

In Equation (2.151), we have $\hat{\vartheta}(j,0) = \frac{1}{4}$, and $\hat{\vartheta}(j,1) = 0$. If $0 \leq p \leq 1$ then $\hat{\vartheta}(j,p)$ is bounded $0 \leq \hat{\vartheta}(j,p) \leq \frac{1}{4}$ as shown in Figure 2.19. Furthermore in Appendix B.7 it can be shown this sum in Equation (2.148) is bounded and $\hat{\vartheta}(j,p)$ is bounded above by

$$\hat{\vartheta}(j,p) \leq \frac{p}{4}\left(\frac{1}{2}\right)^{1-p} + \frac{p}{2}\zeta\left(1+p, \frac{3}{2}\right), \tag{2.152}$$

after using the bound given by Equation (B.72).

Hence the error is bounded by a constant independent of $t$ and so demonstrates that the approximation scheme is of order $O(\Delta t^{2-p})$ assuming the scheme is applied to a function that can be expanded as in Equation (2.99).

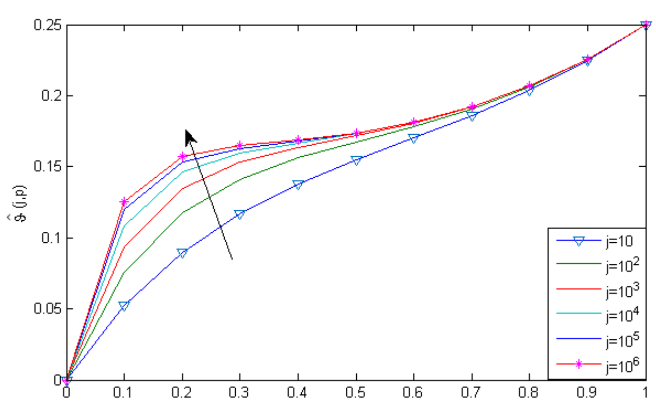



Figure 2.19: (Color online) The value of $\hat{\vartheta}(j,\gamma)$ in Equation (2.151) is shown versus $p$ for varying number of time steps $j = 10, 10^2, 10^3, \ldots, 10^6$, where $j$ increases in the direction of the arrow. These results show $\hat{\vartheta}(j,\gamma)$ is bounded above by $\frac{1}{4}$ for all $0 \leq p \leq 1$.

The estimate of the accuracy of the C2 scheme was tested on the functions given in Equation (2.7). The error in the value of the fractional derivative, for each function, is again shown in the double logarithmic scale plots given in Figures 2.20 – 2.24. We also see the error is decreases for each value of $\gamma$ as the value of $\Delta t$ is decreased, and we see the slope of the lines match asymptotically the slope of $1 + \gamma$ of the dashed lines shown in the figure as expected.

From Table 2.6, for the function $f(t) = t^2$, we see that the maximum error of $2.45 \times 10^{-3}$ occurs for $\gamma = 0.1$ and the minimum error of $1.10 \times 10^{-5}$ occurs for $\gamma = 0.9$. Also, for the functions $f(t) = t^3$, $t^4$, $1 - e^t + t^3$ and $1 + t^\gamma$ the minimum error again occurs for $\gamma = 0.9$ and the maximum error occurs for $\gamma = 0.1$.

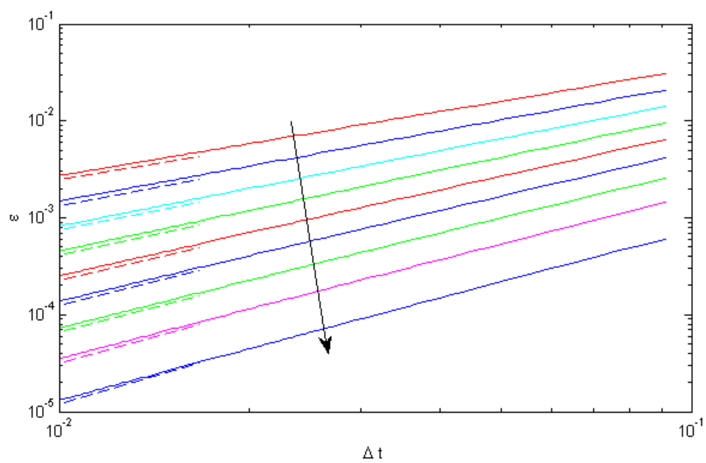



Figure 2.20: (Color online) The absolute error, $\varepsilon$, in the C2 approximation of the fractional derivative of order $1 - \gamma$ on the function $f(t) = t^2$ at the time $t = 1.0$ given for $\gamma = 0.1, 0.2, 0.3 \ldots, 0.8, 0.9$. Note $\gamma$ increases in the direction of the arrow, and dashed lines show lines of slope $1 + \gamma$ for comparison.

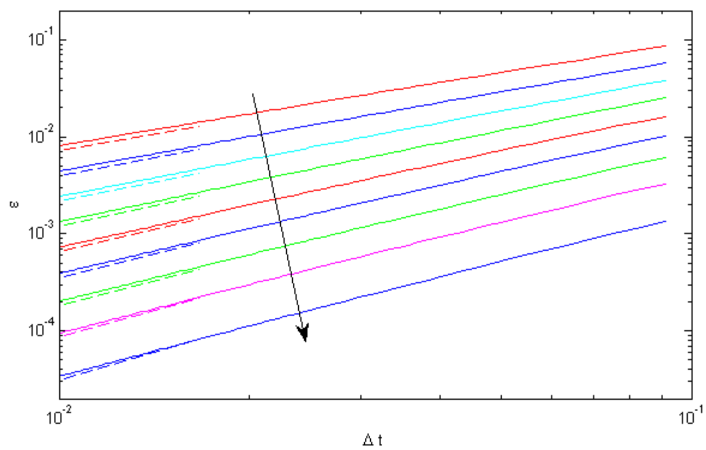



Figure 2.21: (Color online) The absolute error in the C2 scheme approximation of the order $1-\gamma$ fractional derivative of the function $f(t) = t^3$ shown at the time $t = 1.0$ with $\gamma = 0.1, \ldots, 0.9$. The value of $\gamma$ increases in the direction of the arrow, and for comparison we show lines of slope $1+\gamma$ as a dashed lines.

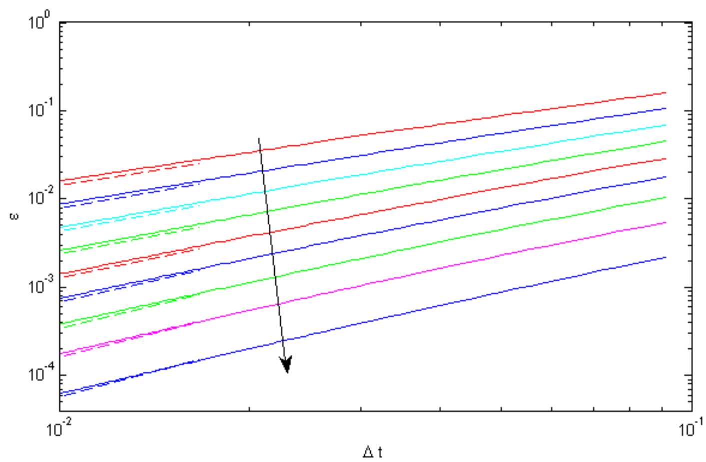



Figure 2.22: (Color online) The absolute error found by using the C2 scheme approximation of the fractional derivative of order $1-\gamma$ on the function $f(t) = t^4$ at the time $t = 1.0$, and for $\gamma = 0.1, \ldots, 0.9$. The value of $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

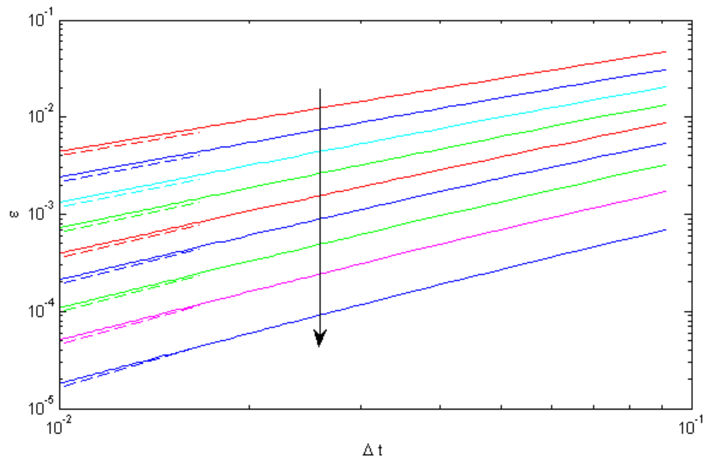



Figure 2.23: (Color online) The absolute error in using the C2 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 - e^t + t^3$, where $\gamma = 0.1, \ldots, 0.9$ and time $t = 1.0$. Note $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison.

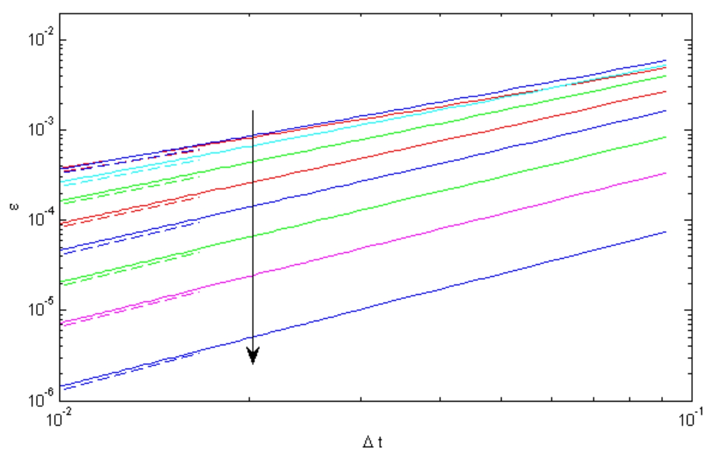



Figure 2.24: (Color online) The absolute error in using the C2 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 + t^\gamma$ at the time $t = 1.0$. The results are shown for $\gamma = 0.1, \ldots, 0.9$, and $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

Table 2.6: The comparison of the absolute error in the estimate of the fractional derivative of order $p = 1 - \gamma$ by using the C2 scheme on the functions $f(t)$ in Equation (2.7) at the time $t = 1.0$ where $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| Operator | $f(t) = t^2$ | $f(t) = t^3$ | $f(t) = t^4$ | $f(t) = 1 - e^t + t^3$ | $f(t) = 1 + t^\gamma$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 2.451e–03 | 7.292e–03 | 1.447e–02 | 3.988e–03 | 3.399e–04 |
| $\gamma = 0.2$ | 1.330e–03 | 3.943e–03 | 7.804e–03 | 2.156e–03 | 3.287e–04 |
| $\gamma = 0.3$ | 7.268e–04 | 2.142e–03 | 4.222e–03 | 1.170e–03 | 2.337e–04 |
| $\gamma = 0.4$ | 3.990e–04 | 1.165e–03 | 2.284e–03 | 6.359e–04 | 1.437e–04 |
| $\gamma = 0.5$ | 2.189e–04 | 6.313e–04 | 1.228e–03 | 3.438e–04 | 7.970e–05 |
| $\gamma = 0.6$ | 1.187e–04 | 3.364e–04 | 6.477e–04 | 1.827e–04 | 4.000e–05 |
| $\gamma = 0.7$ | 6.216e–05 | 1.722e–04 | 3.273e–04 | 9.310e–05 | 1.750e–05 |
| $\gamma = 0.8$ | 2.981e–05 | 8.024e–05 | 1.501e–04 | 4.310e–05 | 6.080e–06 |
| $\gamma = 0.9$ | 1.103e–05 | 2.868e–05 | 5.265e–05 | 1.530e–05 | 1.200e–06 |

The approximate order of convergence in $\Delta t$ was estimated by using Equation (2.53). The error and order of convergence estimate was used for function $f(t) = 1 + t^\gamma$. The results are shown in Table 2.7 for $\gamma = 0.1, \ldots, 0.9$ with time $t = 1.0$, it can be seen that the C2 scheme is of order $O(\Delta t^{1+\gamma})$.

Table 2.7: Numerical accuracy in $\Delta t$ of the C2 scheme used for the function $f(t) = 1 + t^{\gamma}$, and $\widehat{R}$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.2$ | | $\gamma = 0.3$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_{\infty}(\Delta t)$ | $\widehat{R}$ | $e_{\infty}(\Delta t)$ | $\widehat{R}$ | $e_{\infty}(\Delta t)$ | $\widehat{R}$ |
| 1/1000 | 2.957e–05 | – | 2.291e–05 | – | 1.305e–05 | – |
| 1/2000 | 1.378e–05 | 1.1 | 9.960e–06 | 1.2 | 5.294e–06 | 1.3 |
| 1/4000 | 6.427e–06 | 1.1 | 4.333e–06 | 1.2 | 2.148e–06 | 1.3 |
| 1/8000 | 2.998e–06 | 1.1 | 1.885e–06 | 1.2 | 8.722e–07 | 1.3 |
| 1/16000 | 1.398e–06 | 1.1 | 8.205e–07 | 1.2 | 3.541e–07 | 1.3 |
| | $\gamma = 0.4$ | | $\gamma = 0.5$ | | $\gamma = 0.6$ | |
| 1/1000 | 6.451e–06 | – | 2.891e–06 | – | 1.180e–06 | – |
| 1/2000 | 2.442e–06 | 1.4 | 1.022e–06 | 1.5 | 3.903e–07 | 1.6 |
| 1/4000 | 9.245e–07 | 1.4 | 3.611e–07 | 1.5 | 1.290e–07 | 1.6 |
| 1/8000 | 3.502e–07 | 1.4 | 1.277e–07 | 1.5 | 4.261e–08 | 1.6 |
| 1/16000 | 1.327e–07 | 1.4 | 4.513e–08 | 1.5 | 1.407e–08 | 1.6 |
| | $\gamma = 0.7$ | | $\gamma = 0.8$ | | $\gamma = 0.9$ | |
| 1/1000 | 4.276e–07 | – | 1.253e–07 | – | 2.138e–08 | – |
| 1/2000 | 1.327e–07 | 1.7 | 3.676e–08 | 1.8 | 5.975e–09 | 1.9 |
| 1/4000 | 4.115e–08 | 1.7 | 1.075e–08 | 1.8 | 1.663e–09 | 1.9 |
| 1/8000 | 1.274e–08 | 1.7 | 3.135e–09 | 1.8 | 4.609e–10 | 1.9 |
| 1/16000 | 3.939e–09 | 1.7 | 9.124e–10 | 1.8 | 1.274e–10 | 1.9 |

### 2.6.3 Accuracy of the C3 Scheme

In this subsection, we determine the accuracy of the fractional derivative approximation at $t = t_{j+\frac{1}{2}}$ given by the C3 scheme in Equations (2.88) – (2.91). We again follow the approach of Langlands & Henry (2005) by assuming $f(t)$, $f \in C^2[0, \infty)$, can be expanded as in Equation (2.99). We likewise compare the results of taking the exact fractional derivative of $f(t)$ given in Equation (2.130) with the approximate result obtained by applying the C3 scheme in Equation (2.88) to the same function.

Similar to before we apply the C3 fractional approximation scheme on the functions 1, $t$, and the convolution integral in Equation (2.99) at the time $t = t_{j+\frac{1}{2}}$.

The C3 approximation of the function $f(t) = 1$ in Equation (2.99) is.

$$\left[\frac{d^p(1)}{dt^p}\right|_{C3}^{j+\frac{1}{2}} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left[\widehat{\beta}_j(1) + \sum_{k=0}^{j}\widehat{\nu}_{j-k}(1)\right], \tag{2.153}$$

which, upon simplifying, after using Lemma 2.5.6, reduces to

$$\begin{aligned}\left[\frac{d^p(1)}{dt^p}\right|_{C3}^{j+\frac{1}{2}} &= \frac{\Delta t^{-p}}{\Gamma(2-p)}\left[(1-p)\left(j+\frac{1}{2}\right)^{-p} - 2\widehat{\alpha}_j + 2\widehat{\alpha}_j\right] \\ &= \frac{\Delta t^{-p}}{\Gamma(2-p)}(1-p)\left(j+\frac{1}{2}\right)^{-p} \\ &= \frac{\left(\left(j+\frac{1}{2}\right)\Delta t\right)^{-p}}{\Gamma(1-p)} \\ &= \frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)}.\end{aligned} \tag{2.154}$$

The C3 approximation acting upon $f(t) = t$ is

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{C3}^{j+\frac{1}{2}} &= 0 + \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=0}^{j}\widehat{\nu}_{j-k}\left(k+\frac{1}{2}\right)\Delta t \\ &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left\{\sum_{k=0}^{j}k\widehat{\nu}_{j-k} + \frac{1}{2}\sum_{k=0}^{j}\widehat{\nu}_{j-k}\right\}.\end{aligned} \tag{2.155}$$

Using Lemma 2.5.6 and 2.5.7, we then have the result

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{C3}^{j+\frac{1}{2}} &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left\{j^{1-p} + \frac{1}{2}(2\widehat{\alpha}_j)\right\} \\ &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left\{j^{1-p} + \left(j+\frac{1}{2}\right)^{1-p} - j^{1-p}\right\} \\ &= \frac{\left(\left(j+\frac{1}{2}\right)\Delta t\right)^{1-p}}{\Gamma(2-p)} \\ &= \frac{t_{j+\frac{1}{2}}^{1-p}}{\Gamma\left(2-p\right)}.\end{aligned} \tag{2.156}$$

Finally applying the C3 approximation to the convolution in Equation (2.99) gives

$$\begin{aligned}\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C3}^{j+\frac{1}{2}} &= \frac{\Delta t^{-p}}{\Gamma\left(2-p\right)}\left\{\widehat{\beta}_j \lim_{t\to 0}\int_0^t f''(\tau)(t-\tau)d\tau\right. \\ &\left. + \sum_{k=0}^{j}\widehat{\nu}_{j-k}\int_0^{\left(k+\frac{1}{2}\right)\Delta t} f''(\tau)\left(\left(k+\frac{1}{2}\right)\Delta t - \tau\right)d\tau\right\}.\end{aligned} \tag{2.157}$$

The limit is again zero if $f''(t)$ is a well–behaved function of $t$, and so the C3 approximation of the convolution is then

$$\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C3}^{j+\frac{1}{2}} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=0}^{j}\widehat{\nu}_{j-k}\int_0^{\left(k+\frac{1}{2}\right)\Delta t} f''(\tau)\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau. \tag{2.158}$$

Now by dividing the integration interval into equal $\Delta t$ steps and simplifying and we then have

$$\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C3}^{j+\frac{1}{2}} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{k=0}^{j}\widehat{\nu}_{j-k}\sum_{l=1}^{k}\int_{\left(l-\frac{1}{2}\right)\Delta t}^{\left(l+\frac{1}{2}\right)\Delta t} f''(\tau)\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right.$$
$$\left.+\sum_{k=0}^{j}\widehat{\nu}_{j-k}\int_0^{\frac{1}{2}\Delta t} f''(\tau)\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right\}. \tag{2.159}$$

Changing the order of summation, Equation (2.159) becomes

$$\frac{d^p}{dt^p}\left[\int_0^t f''(\tau)(t-\tau)d\tau\right|_{C3} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{l=1}^{j}\int_{\left(l-\frac{1}{2}\right)\Delta t}^{\left(l+\frac{1}{2}\right)\Delta t} f''(\tau)\sum_{k=l}^{j}\widehat{\nu}_{j-k}\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right.$$
$$\left.+\sum_{k=0}^{j}\widehat{\nu}_{j-k}\int_0^{\frac{1}{2}\Delta t} f''(\tau)\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right\}. \tag{2.160}$$

The C3 approximation of $f(t)$ in Equation (2.99) is then given by

$$\left[\frac{d^p}{dt^p}f(t)\right|_{C3}^{j+\frac{1}{2}} = f_0\frac{t_{j+\frac{1}{2}}^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_{j+\frac{1}{2}}^{1-p}}{\Gamma(2-p)} \tag{2.161}$$
$$+\frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{l=1}^{j}\int_{\left(l-\frac{1}{2}\right)\Delta t}^{\left(l+\frac{1}{2}\right)\Delta t} f''(\tau)\sum_{k=l}^{j}\widehat{\nu}_{j-k}\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right.$$
$$\left.+\int_0^{\frac{1}{2}\Delta t} f''(\tau)\sum_{k=0}^{j}\widehat{\nu}_{j-k}\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right)d\tau\right\}.$$

Now using Lemmas 2.5.6 and 2.5.7, with $n=l$, we have

$$\sum_{k=l}^{j}\widehat{\nu}_{j-k}\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right) = (j-(l-1))^{1-p}\left(\left(l+\frac{1}{2}\right)-\tau\right)-(j-l)^{1-p}\left(\left(l-\frac{1}{2}\right)-\tau\right)$$
$$= L_{C3,p}(j,l,\tau), \tag{2.162}$$

and

$$\sum_{k=0}^{j}\widehat{\nu}_{j-k}\left(\left(k+\frac{1}{2}\right)\Delta t-\tau\right) = \Delta t(j^{1-p}+\widehat{\alpha}_j)-2\widehat{\alpha}_j\tau. \tag{2.163}$$

The value of the C3 approximation, in Equation (2.161), is now compared with the exact value of the fractional derivative given by Equation (2.130). The absolute error is then

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right| \tag{2.164}$$

$$= \left|\frac{t_{j+1/2}^{-p}}{\Gamma(1-p)}f_0 + \frac{t_{j+1/2}^{1-p}}{\Gamma(2-p)}f'(0) + \int_0^{t_{j+\frac{1}{2}}} f''(\tau)\frac{(t_{j+\frac{1}{2}}-\tau)^{1-p}}{\Gamma(2-p)}d\tau - \frac{t_{j+1/2}^{-p}}{\Gamma(1-p)}f_0 - \frac{t_{j+1/2}^{1-p}}{\Gamma(2-p)}f'(0)\right.$$

$$\left. -\frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{l=1}^{j}\int_{(l-\frac{1}{2})\Delta t}^{(l+\frac{1}{2})\Delta t} f''(\tau)L_{C3,p}(j,l,\tau)d\tau + \int_0^{\frac{1}{2}\Delta t} f''(\tau)\left[\Delta t(j^{1-p}+\widehat{\alpha}_j) - 2\widehat{\alpha}_j\tau\right]d\tau\right\}\right|,$$

Which can be written as

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right| \tag{2.165}$$

$$= \frac{1}{\Gamma(2-p)}\left|\sum_{l=1}^{j}\int_{(l-\frac{1}{2})\Delta t}^{(l+\frac{1}{2})\Delta t} f''(\tau)\left[(t-\tau)^{1-p} - \Delta t^{-p}L_{C3,p}(j,l,\tau)\right]d\tau\right.$$

$$\left. + \int_0^{\frac{1}{2}\Delta t} f''(\tau)\left[(t-\tau)^{1-p} - \Delta t^{-p}\Big(\Delta t(j^{1-p}+\widehat{\alpha}_j) - 2\widehat{\alpha}_j\tau\Big)\right]d\tau\right|.$$

Using Equation (2.39), we then have the inequality

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right| \tag{2.166}$$

$$\leq \frac{1}{\Gamma(2-p)}\left\{\sum_{l=1}^{j}\int_{(l-\frac{1}{2})\Delta t}^{(l+\frac{1}{2})\Delta t} |f''(\tau)|\left|(t-\tau)^{1-p} - \Delta t^{-p}L_{C3,p}(j,l,\tau)\right|d\tau\right.$$

$$\left. + \int_0^{\frac{1}{2}\Delta t} |f''(\tau)|\left|(t-\tau)^{1-p} - \Delta t^{-p}\Big(\Delta t(j^{1-p}+\widehat{\alpha}_j) - 2\widehat{\alpha}_j\tau\Big)\right|d\tau\right\}.$$

Similar to before we let the maximum absolute value of the second derivative in the intervals $[0, \frac{1}{2}\Delta t]$ and $[\left(l-\frac{1}{2}\right)\Delta t, \left(l+\frac{1}{2}\right)\Delta t]$ be denoted respectively by

$$M_{l+\frac{1}{2}} = \max_{(l-\frac{1}{2})\Delta t \leq s \leq (l+\frac{1}{2})\Delta t} \left|f''(s)\right|, \tag{2.167}$$

and

$$M_{\frac{1}{2}} = \max_{0 \leq s \leq \frac{1}{2}\Delta t} \left|f''(s)\right|. \tag{2.168}$$

Then the bound of the absolute error becomes

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right| \tag{2.169}$$

$$\leq \frac{1}{\Gamma(2-p)}\left\{\sum_{l=1}^{j} M_{l+\frac{1}{2}} \int_{(l-\frac{1}{2})\Delta t}^{(l+\frac{1}{2})\Delta t} \left|(t-\tau)^{1-p} - \Delta t^{-p} L_{C3,p}(j,l,\tau)\right| d\tau \right.$$

$$\left. + M_{\frac{1}{2}} \int_0^{\frac{1}{2}\Delta t} \left|(t-\tau)^{1-p} - \Delta t^{-p}\Big(\Delta t(j^{1-p} + \widehat{\alpha}_j) - 2\widehat{\alpha}_j \tau\Big)\right| d\tau \right\}.$$

We know, from Appendix B.8, that each term in the absolute value functions in Equation (2.169) is positive, then by evaluating the integrals in (2.169) and letting $M = \max\{M_i; i = 0, 1, 2, ..., j+\frac{1}{2}\}$, we obtain the result

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right| \leq \frac{M\Delta t^{1-p}}{\Gamma(3-p)}\left\{\sum_{l=1}^{j}\big[(j-l+1)^{2-p} - (j-l)^{2-p}\right.$$

$$-(2-p)\left[\left[l(j-(l-1))^{1-p} - (l-1)(j-l)^{1-p}\right] - \left(l - \frac{1}{2}\right)\left[(j-(l-1))^{1-p} - (j-l)^{1-p}\right]\right]\Big]$$

$$\left. + \left[\left(j+\frac{1}{2}\right)^{2-p} - j^{2-p} - \frac{2-p}{4}\left(j^{1-p} + \left(j+\frac{1}{2}\right)^{1-p}\right)\right]\right\}, \tag{2.170}$$

or upon simplifying

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right|$$

$$\leq \frac{M\Delta t^{1-p}}{(2-p)\Gamma(2-p)}\left\{\sum_{l=1}^{j}\left[(j-l+1)^{1-p}\left(j-l+1-\frac{2-p}{2}\right) - (j-l)^{1-p}\left(j-l+\frac{2-p}{2}\right)\right]\right.$$

$$\left. + \left[\left(j+\frac{1}{2}\right)^{1-p}\left(j+\frac{1}{2}-\frac{2-p}{4}\right) - j^{1-p}\left(j+\frac{2-p}{4}\right)\right]\right\}$$

$$\leq \frac{M\Delta t^{1-p}}{(2-p)\Gamma(2-p)}\left\{\sum_{l=1}^{j}\left[(j-l+1)^{1-p}\left(j-l+\frac{p}{2}\right) - (j-l)^{1-p}\left(j-l+1-\frac{p}{2}\right)\right]\right.$$

$$\left. + \left[\left(j+\frac{1}{2}\right)^{1-p}\left(j+\frac{p}{4}\right) - j^{1-p}\left(j+\frac{1}{2}-\frac{p}{4}\right)\right]\right\}. \tag{2.171}$$

After simplifying, the estimate of the error becomes

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}} - \left[\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}_{C3}\right|$$

$$\leq \frac{M\Delta t^{1-p}}{(2-p)\Gamma(2-p)}\left\{\sum_{l=0}^{j-1}\left[(l+1)^{1-p}\left(l+\frac{p}{2}\right) - l^{1-p}\left(l+1-\frac{p}{2}\right)\right]\right.$$

$$\left. + \left[\left(j+\frac{1}{2}\right)^{1-p}\left(j+\frac{p}{4}\right) - j^{1-p}\left(j+\frac{1}{2}-\frac{p}{4}\right)\right]\right\}. \tag{2.172}$$

Now we evaluate the sum in Equation (2.172) to give

$$\begin{aligned}
&\sum_{l=0}^{j-1}\left[(l+1)^{1-p}\left(l+\frac{p}{2}\right)-l^{1-p}\left(l+1-\frac{p}{2}\right)\right] \\
&\qquad= \sum_{l=1}^{j} l^{1-p}\left(l-1+\frac{p}{2}\right)-\sum_{l=0}^{j-1} l^{1-p}\left(l+1-\frac{p}{2}\right) \\
&\qquad= j^{1-p}\left(j-1+\frac{p}{2}\right)+\sum_{l=1}^{j-1} l^{1-p}\left(l-1+\frac{p}{2}\right)-\sum_{l=1}^{j-1} l^{1-p}\left(l+1-\frac{p}{2}\right) \\
&\qquad= j^{1-p}\left(j-1+\frac{p}{2}\right)+(p-2)\sum_{l=1}^{j-1} l^{1-p}. \qquad (2.173)
\end{aligned}$$

The estimate error is then given by

$$\left|\left.\frac{d^p}{dt^p}f(t)\right|^{j+\frac{1}{2}}-\left.\frac{d^p}{dt^p}f(t)\right|_{C3}^{j+\frac{1}{2}}\right|\leq C\Delta t^{2-p}, \qquad (2.174)$$

where $C$ is the constant

$$C=\frac{MK(j,p)}{\Gamma(3-p)}, \qquad (2.175)$$

and $K(j,p)$ is defined by

$$\begin{aligned}
K(j,p) &= j^{1-p}\left(j-1+\frac{p}{2}\right)+(p-2)\sum_{l=1}^{j-1} l^{1-p} \\
&\quad+\left(j+\frac{1}{2}\right)^{1-p}\left(j+\frac{1}{2}-\frac{2-p}{4}\right)-j^{1-p}\left(j+\frac{2-p}{4}\right). \qquad (2.176)
\end{aligned}$$

In Equation (2.176), we have $K(j,0)=0$, and $K(j,1)=\frac{1}{2}$. For $0<p\leq 1$ the constant $K(j,p)$ is bounded by $0\leq K(j,p)\leq\frac{1}{2}$ as shown in Figure 2.25. In Appendix B.9 we show this sum, in Equation (2.176), is bounded and hence $K(j,p)$ is bounded above by

$$K(j,p)\leq\frac{p-4}{4}\left(\frac{1}{2}\right)^{1-p}+\frac{p-2}{4}+\frac{p}{2}\zeta\left(1+p,1\right), \qquad (2.177)$$

after using Equations (B.91) and (B.105). Hence the error is bounded by a constant independent of $t$ and so demonstrates that the approximation scheme is of order $O(\Delta t^{2-p})$.

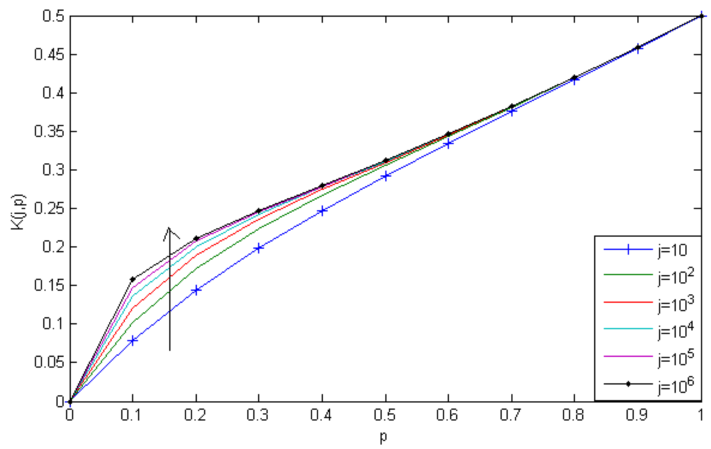



Figure 2.25: (Color online) The value of $K(j,p)$ in Equation (2.176) as shown versus $p$ for varying number of time steps are $j = 10, 10^2, 10^3, \ldots, 10^6$, where $j$ increases in the direction of the arrow. These results show $K(j,p)$ is bounded by $\frac{1}{2}$ for all $0 \leq p \leq 1$.

The estimate of the accuracy of the C3 scheme was tested on the functions $f(t)$, given in Equation (2.7), at the time $t = 1.0$ and $p = 1 - \gamma$ when $\gamma = 0.1, \ldots, 0.9$. We again see the error appears to be linear on a log-log plot which shows error behaves as

$$\varepsilon \sim C\Delta t^{1+\gamma}$$

for some constant $C$. In Figures 2.26 – 2.30, we see as $\Delta t$ is decreased the error also decreases for each value of $\gamma$, and the slope of the lines match asymptotically the slope of $1 + \gamma$ of the dashed lines as shown in the figure. In Table 2.8, we see that the maximum error occurs where $\gamma = 0.1$ for all functions $f(t)$ and the minimum error occurs for $\gamma = 0.9$.

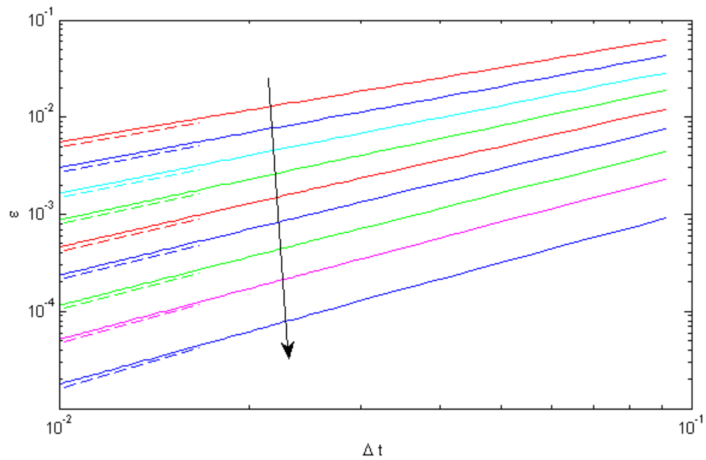



Figure 2.26: (Color online) The value of the absolute error found by using the C3 scheme to approximate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^2$ at time $t = 1.0$. The error is shown for $\gamma = 0.1, \ldots, 0.9$, where the value of $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison. For small $\Delta t$ the error is of order $O(\Delta t^{1+\gamma})$.

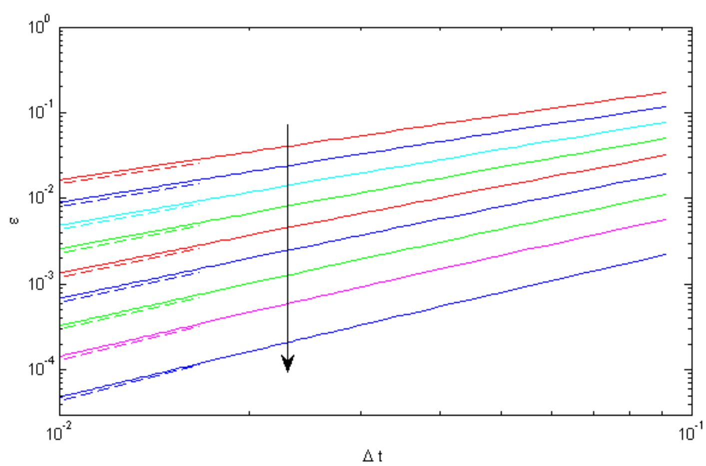



Figure 2.27: (Color online) The absolute error in the estimate of the C3 approximation of the fractional derivative of order $1-\gamma$ of the function $f(t) = t^3$ shown at $t = 1.0$. The error is shown for $\gamma = 0.1, \ldots, 0.9$ with $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

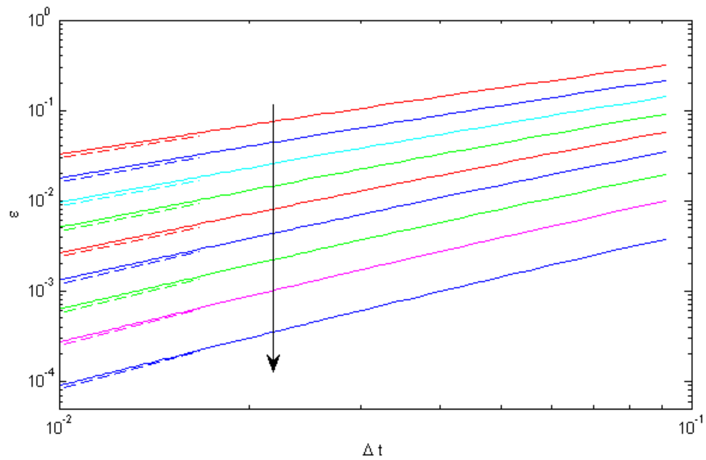



Figure 2.28: (Color online) The value of the absolute error in the estimate of the fractional derivative of order $1-\gamma$ for the function $f(t) = t^4$ found by using the C3 approximation at the time $t = 1.0$, and for $\gamma = 0.1, \ldots, 0.9$. Note the value of $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

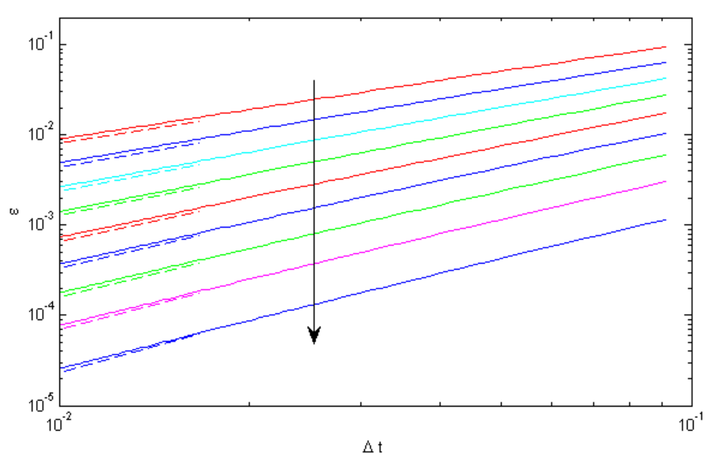



Figure 2.29: (Color online) The absolute error in using the C3 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 - e^t + t^3$, where $\gamma = 0.1, \ldots, 0.9$ and time $t = 1.0$. Note $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison.

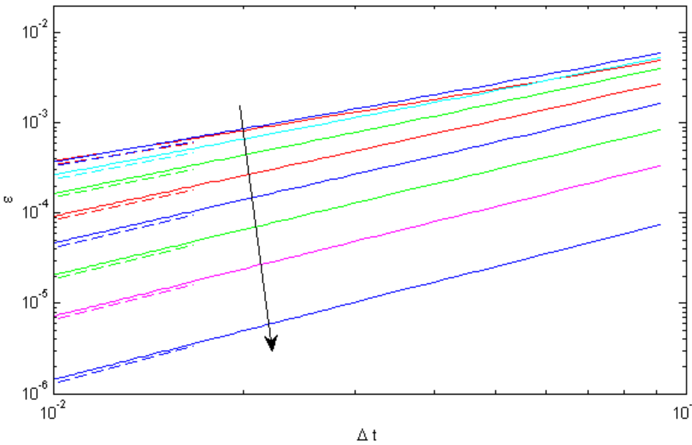



Figure 2.30: (Color online) The absolute error in using the C3 scheme to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1+t^{\gamma}$ at the time $t = 1.0$ with $\gamma = 0.1, \ldots, 0.9$, and $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1 + \gamma$ for comparison.

Table 2.8: The comparison of the absolute error in the estimate of the order $1 - \gamma$ fractional derivative of the functions $f(t)$, Equation (2.7), at time $t = 1.0$ where $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$ by using the C3 approximation.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^3$ | $f(t) = t^4$ | $f(t) = 1 - e^t + t^3$ | $f(t) = 1 + t^{\gamma}$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 4.982e–03 | 1.481e–02 | 2.985e–02 | 8.103e–03 | 3.399e–04 |
| $\gamma = 0.2$ | 2.701e–03 | 8.020e–03 | 1.585e–02 | 4.385e–03 | 3.287e–04 |
| $\gamma = 0.3$ | 1.448e–03 | 4.287e–03 | 8.475e–03 | 2.344e–03 | 2.337e–04 |
| $\gamma = 0.4$ | 7.665e–04 | 2.258e–03 | 4.451e–03 | 1.234e–03 | 1.437e–04 |
| $\gamma = 0.5$ | 3.989e–04 | 1.166e–03 | 2.288e–03 | 6.365e–04 | 7.970e–05 |
| $\gamma = 0.6$ | 2.024e–04 | 5.855e–04 | 1.141e–03 | 3.189e–04 | 4.000e–05 |
| $\gamma = 0.7$ | 9.830e–05 | 2.798e–04 | 5.407e–04 | 1.520e–04 | 1.750e–05 |
| $\gamma = 0.8$ | 4.360e–05 | 1.212e–04 | 2.314e–04 | 6.560e–05 | 6.080e–06 |
| $\gamma = 0.9$ | 1.490e–05 | 4.030e–05 | 7.570e–05 | 2.170e–05 | 1.200e–06 |

The absolute error and order of convergence estimated of the fractional derivative of order $1 - \gamma$ for the function $f(t) = 1 + t^{\gamma}$ are shown in Table 2.9. To estimate the convergence we used Equation (2.53), from the results given in Table 2.9 for $\gamma = 0.1, \ldots, 0.9$ with time $t = 1.0$, we see that the C3 scheme is of order $O(\Delta t^{1+\gamma})$.

Table 2.9: Numerical accuracy in $\Delta t$ of the C3 scheme applied to the function $f(t) = 1 + t^\gamma$, and $\widehat{R}$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.2$ | | $\gamma = 0.3$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $\widehat{R}$ | $e_\infty(\Delta t)$ | $\widehat{R}$ | $e_\infty(\Delta t)$ | $\widehat{R}$ |
| 1/1000 | 2.957e–05 | – | 2.291e–05 | – | 1.305e–05 | – |
| 1/2000 | 1.378e–05 | 1.1 | 9.960e–06 | 1.2 | 5.294e–06 | 1.3 |
| 1/4000 | 6.427e–06 | 1.1 | 4.333e–06 | 1.2 | 2.148e–06 | 1.3 |
| 1/8000 | 4.484e–06 | 1.1 | 1.885e–06 | 1.2 | 8.723e–07 | 1.3 |
| 1/16000 | 1.398e–06 | 1.1 | 8.205e–07 | 1.2 | 3.541e–07 | 1.3 |
| | $\gamma = 0.4$ | | $\gamma = 0.5$ | | $\gamma = 0.6$ | |
| 1/1000 | 6.451e–06 | – | 2.891e–06 | – | 1.180e–06 | – |
| 1/2000 | 2.442e–06 | 1.4 | 1.022e–06 | 1.5 | 3.903e–07 | 1.6 |
| 1/4000 | 9.245e–07 | 1.4 | 3.611e–07 | 1.5 | 1.290e–07 | 1.6 |
| 1/8000 | 3.502e–07 | 1.4 | 1.277e–07 | 1.5 | 4.261e–08 | 1.6 |
| 1/16000 | 1.327e–07 | 1.4 | 4.513e–08 | 1.5 | 1.407e–08 | 1.6 |
| | $\gamma = 0.7$ | | $\gamma = 0.8$ | | $\gamma = 0.9$ | |
| 1/1000 | 4.276e–07 | – | 1.253e–07 | – | 2.138e–08 | – |
| 1/2000 | 1.327e–07 | 1.7 | 3.676e–08 | 1.8 | 5.975e–09 | 1.9 |
| 1/4000 | 4.115e–08 | 1.7 | 1.075e–08 | 1.8 | 1.662e–09 | 1.9 |
| 1/8000 | 1.274e–08 | 1.7 | 3.135e–09 | 1.8 | 4.609e–10 | 1.9 |
| 1/16000 | 3.939e–09 | 1.7 | 9.124e–10 | 1.8 | 1.274e–10 | 1.9 |

We conclude that from these results that the accuracy of the L1 scheme, C1 scheme, C2 scheme and C3 scheme approximations are the same order of $1 + \gamma$, where $p = 1 - \gamma$. We see in the Tables 2.2, 2.4, 2.6, and 2.8 the minimum error occurs for $\gamma = 0.9$ and the maximum error occurs for $\gamma = 0.1$. We also note that, from Figures 2.7 – 2.11, 2.14 – 2.18, 2.20 – 2.24, and 2.26 – 2.30, the error decreases as the value of $\Delta t$ is decreased for each value of $\gamma$. We also see, from these results, that the C2 scheme is a better approximation as it is more accurate in magnitude than the other schemes.

## 2.7 Romberg Integration

In this section, we use Romberg Integration (Mathews & Fink 1999) to help approximate the integral in Equation (2.9) to evaluate the fractional derivative. We consider the use of Romberg Integration because it may give a higher order accuracy and the other benefit is that we can evaluate the estimates iteratively. Because of the singularity of the function $f'(\tau)(t-\tau)^{-p}$ we need to rewrite the integral as

$$\begin{aligned}\int_0^t f'(\tau)(t-\tau)^{-p}d\tau &= \int_0^t \big(f'(\tau)-f'(t)\big)(t-\tau)^{-p}ds + \int_0^t f'(t)(t-\tau)^{-p}d\tau \\ &= \int_0^t \big(f'(\tau)-f'(t)\big)(t-\tau)^{-p}d\tau + f'(t)\int_0^t (t-\tau)^{-p}d\tau. \end{aligned} \tag{2.178}$$

The last integral can be evaluated as

$$\int_0^t (t-\tau)^{-p}d\tau = -\left[\frac{(t-\tau)^{1-p}}{1-p}\right|_0^t = \frac{t^{1-p}}{1-p}. \tag{2.179}$$

Equation (2.178) is then given by

$$\int_0^t f'(\tau)(t-\tau)^{-p}d\tau = \int_0^t \big(f'(\tau)-f'(t)\big)(t-\tau)^{-p}d\tau + f'(t)\frac{t^{1-p}}{1-p}. \tag{2.180}$$

Let

$$g(\tau,t) = \big(f'(\tau)-f'(t)\big)(t-\tau)^{-p}, \tag{2.181}$$

then we have

$$\int_0^t f'(\tau)(t-\tau)^{-p}d\tau = \int_0^{\Delta t} g(\tau,t)d\tau + \int_{\Delta t}^{(j-1)\Delta t} g(\tau,t)d\tau + \int_{(j-1)\Delta t}^{j\Delta t} g(\tau,t)d\tau + f'(t)\frac{t^{1-p}}{1-p}. \tag{2.182}$$

To evaluate the integral from $\tau = (j-1)\Delta t$ to $\tau = j\Delta t$, we use the finite difference approximation of $f'(\tau)$, to find

$$\begin{aligned}\int_{(j-1)\Delta t}^{j\Delta t} g(\tau,t)d\tau &= \int_{(j-1)\Delta t}^{j\Delta t} \big(f'(\tau)-f'(t)\big)(t-\tau)^{-p}d\tau \\ &\approx \left(\frac{f(j\Delta t)-f((j-1)\Delta t)}{\Delta t} - f'(t)\right)\left[-\frac{(t-\tau)^{1-p}}{1-p}\right|_{(j-1)\Delta t}^{j\Delta t} \\ &= \left(\frac{f(j\Delta t)-f((j-1)\Delta t)}{\Delta t} - f'(t)\right)\frac{\Delta t^{1-p}}{1-p} \\ &= \frac{\Delta t^{-p}}{1-p}\left(f(j\Delta t)-f((j-1)\Delta t)\right) - \frac{\Delta t^{1-p}}{1-p}f'(t), \end{aligned} \tag{2.183}$$

and the integral from $\tau = 0$ to $\tau = \Delta t$, gives

$$\int_0^{\Delta t} g(\tau,t)d\tau = \int_0^{\Delta t} \left(f'(\tau) - f'(t)\right)(t-\tau)^{-p}d\tau$$
$$\approx \left(\frac{f(\Delta t) - f(0)}{\Delta t}\right)\left[\frac{t^{1-p} - (t-\Delta t)^{1-p}}{1-p}\right] - f'(t)\left[\frac{t^{1-p} - (t-\Delta t)^{1-p}}{1-p}\right]. \tag{2.184}$$

To evaluate the second integral in Equation (2.182) from $\tau = \Delta t$ to $\tau = (j-1)\Delta t$, we use Romberg integration (Mathews & Fink 1999) by setting $a = \Delta t$, $b = (j-1)\Delta t$, and with $h_n = (b-a)/2^{n-1}$. We then have

$$\int_a^b g(\tau,t)d\tau \approx I_{n,k} + \epsilon, \tag{2.185}$$

The one and two-interval Composite Trapezoidal approximations of this integral are

$$I_{1,1} = \frac{b-a}{2}\left[g(a,t) + g(b,t)\right], \tag{2.186}$$

for one interval, and

$$I_{2,1} = \frac{b-a}{4}\left[g(a,t) + 2g\left(\frac{a+b}{2},t\right) + g(b,t)\right], \tag{2.187}$$

for two intervals. The Composite Trapezoidal rule of subinterval $n$ is given by

$$I_{n,1} = \frac{h_n}{2}\left[g(a,t) + 2\sum_{i=1}^{2^{n-1}-1} g(\tau_i,t) + g(b,t)\right], \tag{2.188}$$

where $\tau_i = a + ih$. For $n > 1$ we split the summation into two summations containing odd numbered terms and containing even numbered terms like so

$$I_{n,1} = \frac{h_n}{2}\left[g(a,t) + 2\sum_{i=1}^{2^{n-2}} g(a+(2i-1)h,t) + 2\sum_{i=1}^{2^{n-2}-1} g(a+2ih,t) + g(b,t)\right]$$
$$= \frac{h_n}{2}\left[g(a,t) + 2\sum_{i=1}^{2^{n-2}-1} g(a+2ih,t) + g(b,t)\right] + h_i\sum_{i=1}^{2^{n-2}} g(a+(2i-1)h,t)$$
$$= \frac{1}{2}I_{n-1,1} + h_n\sum_{i=1}^{2^{n-2}-1} g(a+(2i-1)h,t). \tag{2.189}$$

For $2 \le k \le n$, we can use Richardson Extrapolation (Richardson 1911, Mathews & Fink 1999)

$$I_{n,k} = I_{n,k-1} + \frac{I_{n,k-1} - I_{n-1,k-1}}{4^{k-1} - 1}. \tag{2.190}$$

For instance, to obtain $I_{3,2}$ we can apply Richardson Extrapolation in Equation (2.190) using $I_{2,1}$ and $I_{3,1}$. There is a significant decrease in error in using the estimate $I_{n,2}$

as it has fourth-order accuracy and $I_{n,2}$ is computed using half the step size of $I_{n-1,2}$. This follows from the error term in the Composite Trapezoidal Rule is $O(h^2)$, and in the Richardson is $O(h^6)$ (Kress 1998).

In using Romberg Integration to approximate the integral in Equation (2.185) we currently use a set number of subintervals $n$ and order $k$.

Using Equations (2.183), (2.184) and $I_{n,k}$ in Equation (2.190) into Equation (2.9), we then have the $RInt$ approximation at $t = t_j$

$$\left[\frac{d^p f(t)}{dt^p}\right|_{RInt} = \frac{1}{\Gamma(2-p)}\left\{\left[(1-p)t_j^{-p} - \left(\frac{t_j^{1-p} - (t_j - \Delta t)^{1-p}}{\Delta t}\right)\right] f_0 + \left[\frac{t_j^{1-p} - (t_j - \Delta t)^{1-p}}{\Delta t}\right] f_1 + \left((t_j - \Delta t)^{1-p} - \Delta t^{1-p}\right) f'(t_j) + \Delta t^{-p}\left(f_j - f_{j-1}\right)\right\} + \frac{1}{\Gamma(1-p)} I_{n,k} \, . \tag{2.191}$$

Using the finite difference method to approximate the first order derivative, we then obtain the approximation

$$\left[\frac{d^p f(t)}{dt^p}\right|_{RInt} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\left[(1-p)j^{-p} - \left(j^{1-p} - (j-1)^{1-p}\right)\right] f_0 + \left[j^{1-p} - (j-1)^{1-p}\right] f_1 + (j-1)^{1-p}\left(f_j - f_{j-1}\right)\right\} + \frac{1}{\Gamma(1-p)} I_{n,k} \, . \tag{2.192}$$

where $f_j = f(j\Delta t)$. The $RInt$ scheme (given in Equation (2.191)) was tested on the function $f(t)$ given in Equation (2.7) at time $t = 1.0$ with $p = 1-\gamma$ when $\gamma = 0.1, \ldots, 0.9$. The error of the approximation is plotted as a function of $\Delta t$ on double logarithmic scale plot given in Figures 2.31 – 2.35. Here the $I_{10,2}$ estimate of the integral was used.
We see in Figures 2.31 – 2.35, the error decreases as $\Delta t$ decreases and for small $\Delta t$ the error is of order $O(\Delta t^{1+\gamma})$. We also see the slope of the lines match asymptotically the slope of $1 + \gamma$ of the dashed lines. The comparison of the absolute error for each function given in Table 2.10. We see in Table 2.10, the maximum error occurs where $\gamma = 0.1$ for all functions $f(t)$ and the minimum error occurs for $\gamma = 0.9$.

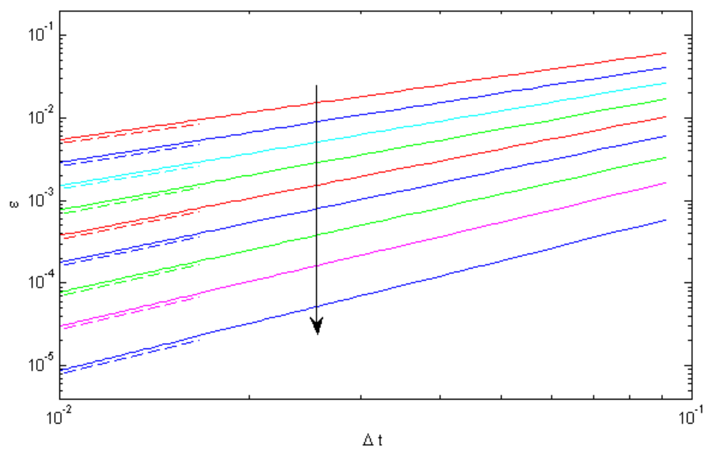



Figure 2.31: (Color online) The value of the absolute error found by using the *RInt* scheme, Equation (2.191), to approximate the order $1-\gamma$ fractional derivative of the function $f(t) = t^2$ at $t = 1.0$. Results are shown for $\gamma = 0.1, \ldots, 0.9$, and the value of $\gamma$ increases in the direction of the arrow. For comparison we show lines of slope $1 + \gamma$ as the dashed lines.

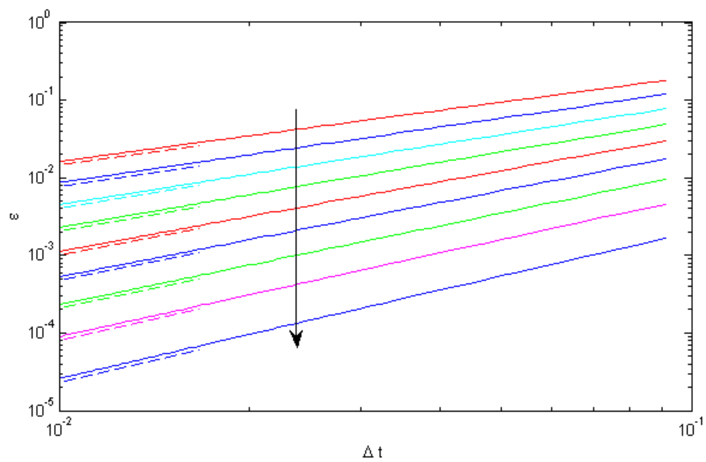



Figure 2.32: (Color online) The absolute error in the estimate of the *RInt* approximation, Equation (2.191), found for the fractional derivative of the function $f(t) = t^3$ of order $1-\gamma$ at $t = 1.0$. The error is shown for $\gamma = 0.1, \ldots, 0.9$ with $\gamma$ increases in the direction of the arrow and the dashed lines show lines of slope $1 + \gamma$ for comparison.

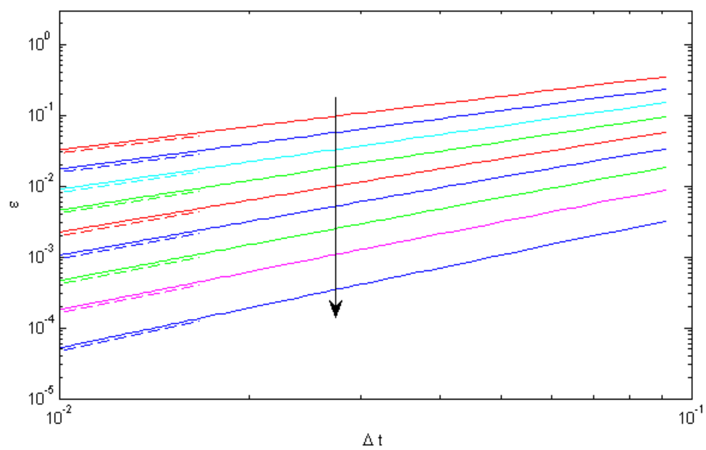



Figure 2.33: (Color online) The value of the absolute error of the fractional derivative of order $1-\gamma$ for the function $f(t) = t^4$ found by using the *RInt* approximation, Equations (2.191), at the time $t = 1.0$, and for $\gamma = 0.1, \ldots, 0.9$. Note the value of $\gamma$ increases in the direction of the arrow. Dashed lines show lines of slope $1+\gamma$ for comparison.

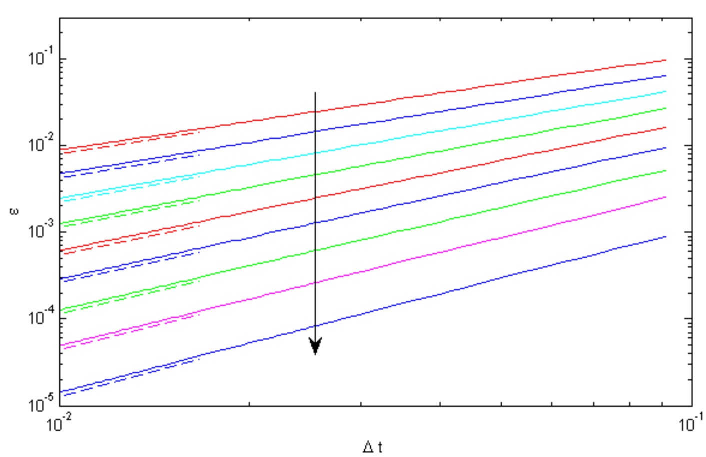



Figure 2.34: (Color online) The absolute error in using the *RInt* approximation, Equations (2.191), to evaluate the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 - e^t + t^3$, where $\gamma = 0.1, \ldots, 0.9$ and time $t = 1.0$. Note $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison.

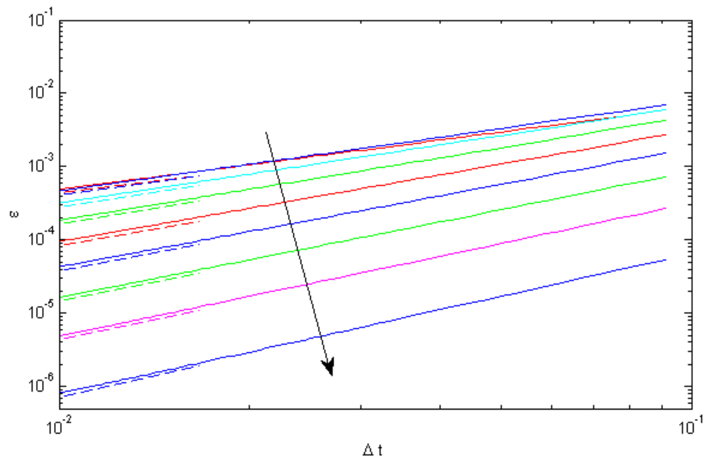



Figure 2.35: (Color online) The absolute error in using the *RInt* approximation, Equations (2.191), to evaluate the fractional derivative of order $1-\gamma$, where $\gamma = 0.1, \ldots, 0.9$, for the function $f(t) = 1 + t^{\gamma}$ at the time $t = 1.0$. Note $\gamma$ increases in the direction of the arrow, and the dashed lines show lines of slope $1+\gamma$ for comparison.

Table 2.10: The comparison of the absolute error in the estimate of the fractional derivative of order $1-\gamma$ on the functions $f(t)$, Equation (2.7), at the time $t = 1.0$ with $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$ by using the *RInt* scheme approximation.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^3$ | $f(t) = t^4$ | $f(t) = 1 - e^t + t^3$ | $f(t) = 1 + t^{\gamma}$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 4.886e–03 | 1.461e–02 | 2.913e–02 | 7.992e–03 | 4.428e–04 |
| $\gamma = 0.2$ | 2.578e–03 | 7.709e–03 | 1.537e–02 | 4.216e–03 | 4.157e–04 |
| $\gamma = 0.3$ | 1.331e–03 | 3.981e–03 | 7.934e–03 | 2.177e–03 | 2.820e–04 |
| $\gamma = 0.4$ | 6.699e–04 | 2.003e–03 | 3.991e–03 | 1.095e–03 | 1.624e–04 |
| $\gamma = 0.5$ | 3.260e–04 | 9.745e–04 | 1.942e–03 | 5.330e–04 | 8.250e–05 |
| $\gamma = 0.6$ | 1.516e–04 | 4.530e–04 | 9.026e–04 | 2.478e–04 | 3.691e–05 |
| $\gamma = 0.7$ | 6.575e–05 | 1.965e–04 | 3.915e–04 | 1.075e–04 | 1.413e–05 |
| $\gamma = 0.8$ | 2.524e–05 | 7.543e–05 | 1.503e–04 | 4.124e–05 | 4.142e–06 |
| $\gamma = 0.9$ | 7.246e–06 | 2.162e–05 | 4.307e–05 | 1.181e–05 | 6.831e–07 |

In Table 2.11, we show the convergence result in $\Delta t$ of the fractional derivative of order $1-\gamma$ for the function $f(t) = 1 + t^{\gamma}$, where $\gamma = 0.1, \ldots, 0.9$ and the $I_{20,2}$ estimate of the integral was used with time $t = 1.0$. From the results given in Table 2.11, we obtain the prediction accuracy of $1+\gamma$ in time.

Table 2.11: Numerical accuracy in $\Delta t$ of the $RInt$ scheme applied to the function $f(t) = 1+t^{\gamma}$, where $\widehat{R}$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.2$ | | $\gamma = 0.3$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $\widehat{R}$ | $e_\infty(\Delta t)$ | $\widehat{R}$ | $e_\infty(\Delta t)$ | $\widehat{R}$ |
| 1/1000 | 3.882e–05 | – | 2.920e–05 | – | 1.587e–05 | – |
| 1/2000 | 1.810e–05 | 1.1 | 1.271e–05 | 1.2 | 6.444e–06 | 1.3 |
| 1/4000 | 8.444e–06 | 1.1 | 5.530e–06 | 1.2 | 2.617e–06 | 1.3 |
| 1/8000 | 3.939e–06 | 1.1 | 2.407e–06 | 1.2 | 1.063e–06 | 1.3 |
| 1/16000 | 1.838e–06 | 1.1 | 1.048e–06 | 1.2 | 4.316e–07 | 1.3 |
| | $\gamma = 0.4$ | | $\gamma = 0.5$ | | $\gamma = 0.6$ | |
| 1/1000 | 7.319e–06 | – | 2.975e–05 | – | 1.065e–06 | – |
| 1/2000 | 2.773e–06 | 1.4 | 1.052e–06 | 1.5 | 3.513e–07 | 1.6 |
| 1/4000 | 1.050e–06 | 1.4 | 3.717e–07 | 1.5 | 1.158e–07 | 1.6 |
| 1/8000 | 3.980e–07 | 1.4 | 1.314e–07 | 1.5 | 3.821e–08 | 1.6 |
| 1/16000 | 1.509e–07 | 1.4 | 4.648e–08 | 1.5 | 1.261e–08 | 1.6 |
| | $\gamma = 0.7$ | | $\gamma = 0.8$ | | $\gamma = 0.9$ | |
| 1/1000 | 3.241e–07 | – | 7.603e–07 | – | 9.832e–09 | – |
| 1/2000 | 9.974e–08 | 1.7 | 2.183e–08 | 1.8 | 2.634e–09 | 1.9 |
| 1/4000 | 3.069e–08 | 1.7 | 6.268e–09 | 1.8 | 7.056e–10 | 1.9 |
| 1/8000 | 9.447e–09 | 1.7 | 1.800e–09 | 1.8 | 1.891e–10 | 1.9 |
| 1/16000 | 2.910e–09 | 1.7 | 5.176e–10 | 1.8 | 5.081e–11 | 1.9 |

## 2.8 The Short Memory Principle

The value of a fractional derivative of a given function $f(t)$, see Definitions 1.2.1 – 1.2.3, depends on the function values in the interval $0 \le \tau \le t$ and so the fractional derivative of function $f(t)$ depends on the historical behavior of the function $f(t)$ (Podlubny 1998). It should be noted that to use the fractional derivative approximations, as in Equations (2.12), (2.60), (2.75) and (2.88), the history of the function $f(t)$ needs to be stored and the convolution sum needs to be evaluated. One of the major issues in evaluating fractional derivatives numerically is the cost of the evaluation of this convolution sum. This computational cost increases as the number of time steps increases, becoming significant for a large number of time steps. This is not as significant for problems involving space-fractional derivatives as the domain does not grow and so the computational cost does not increase. One way to reduce this computational cost is to eliminate the tail of the integral, known as the short memory principle (Podlubny 1998). This takes advantage of the fact that the integral in the fractional derivative is weighted mainly around the time $t$, that is the most recent history of the function $f(t)$, with earlier history near $t = 0$ contributing less to the value of the fractional derivative.

The idea behind the short memory principle is to consider only the most recent history of the $f(t)$ when evaluating the fractional derivative. That is only in the interval $[t-T, t]$ where $T$ is the memory length

$$ {}_aD_t^p f(t) \approx {}_{t-T}D_t^p f(t), \ (t > a + T). \tag{2.193} $$

Podlubny (1998) shows that the truncation error is given by

$$ \epsilon \leq \frac{MT^p}{\Gamma(1-p)}, $$

with a fixed integral length $T$, if $|f(t)| \leq M$ for $a < t < b$ and where $p$ is the fractional derivative order.

Ford & Simpson (2001) introduce a short-memory principle for the Caputo derivative, and show that the truncation error is given by

$$ \epsilon \leq \frac{M}{\Gamma(2-p)} \left(t^{1-p} - T^{1-p}\right), $$

where $p \in (n-1, n)$, $n \in \mathbb{N}$. Deng (2007*b*) extended the effective range of short memory principle from $p \in (0, 1)$ to $p \in (0, 2)$, where the integral interval $[0, t_n]$ split as follows

$$ [0, t_n] = [0, t_n - q^m\tau] \cup [t_n - q^m\tau, t_n - q^{m-1}\tau] \cup ... \cup [t_n - q^2\tau, t_n - q\tau] \cup [t_n - q\tau, t_n], $$

where $\tau = h$, $h \in \mathbb{R}^+$, $m, , q \in \mathbb{N}$ and $q^m\tau \leq t_n < q^{m+1}\tau$. Deng (2007*b*) implemented the numerical computation by using the Predictor–Corrector approach, as in Diethelm et al. (2002), where $0 < p < 1$. The convergent order was found to be order $1 + p$ in time.

In this section, we introduce a short-memory principle for the Riemann–Liouville fractional derivative in Equation (2.8) by using Equation (2.12). We also consider regression methods to approximate the early history given in Equation (2.9) instead of ignoring this early history. We will discuss this in the next sections.

## 2.9 Reduction of the Computation of the L1 Scheme

In this section, we consider reduction of the computation of the L1 scheme following the short memory principle approach. To do this we suppose that the summation in Equation (2.12) starts from $k = n$ instead of $k = 0$. We refer to this approximation as the $L1^*$ scheme and it is given, for $n < j$, as follows

$$\left[\frac{d^p f(t)}{dt^p}\right|_{L1^*}^{j} = \frac{{t_j}^{-p}}{\Gamma(1-p)} f_0 + \frac{\Delta t^{-p}}{\Gamma(2-p)} \sum_{k=n}^{j-1} (f_k - f_{k+1}) \left[(j-(k+1))^{1-p} - (j-k)^{1-p}\right], \tag{2.194}$$

again we denote $f_j = f(j\Delta t)$. We can rewrite $L1^*$ scheme, if $1 \le n < j$, as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{L1^*}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)} \left\{(1-p) j^{-p} f_0 + \sum_{k=n}^{j} \aleph_{j-k}(p) f_k \right\}, \tag{2.195}$$

where the weights $\aleph_l(p)$ are defined by

$$\aleph_l(p) = \begin{cases} (j-(n+1))^{1-p} - (j-n)^{1-p} & \text{if} \quad l = j-n, \\ (l-1)^{1-p} - 2l^{1-p} + (l+1)^{1-p} & \text{if} \quad 1 \le l \le j-(n+1), \\ 1 & \text{if} \quad l = 0. \end{cases} \tag{2.196}$$

To evaluate the $L1^*$ at the functions 1 and $t$ we need the following lemma.

**Lemma 2.9.1.** Given the weights $\aleph_{j-k}(p)$ defined in Equation (2.196), and $n < j$, we have

1. $\sum_{k=n}^{j} \aleph_{j-k}(p) = 0$, and
2. $\sum_{k=n}^{j} k\aleph_{j-k}(p) = (j-n)^{1-p}$.

*Proof.* Using the definition of the weights in Equation (2.196), we then have

$$\begin{aligned}
\sum_{k=n}^{j} \aleph_{j-k}(p) &= (j-(n+1))^{1-p} - (j-n)^{1-p} + 1 \\
&\quad + \sum_{k=n+1}^{j-1} \left[ (j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p} \right] \\
&= (j-(n+1))^{1-p} - (j-n)^{1-p} + 1 \\
&\quad + \sum_{r_1=n+2}^{j} (j-r_1)^{1-p} - \sum_{k=n+1}^{j-1} (j-k)^{1-p} - \left[ \sum_{k=n+1}^{j-1} (j-k)^{1-p} - \sum_{r_2=n}^{j-2} (j-r_2)^{1-p} \right] \\
&= (j-(n+1))^{1-p} - (j-n)^{1-p} + 1 + 0 + \sum_{r_1=n+2}^{j-1} (j-r_1)^{1-p} - (j-(n+1))^{1-p} \\
&\quad - \sum_{k=n+2}^{j-1} (j-k)^{1-p} - \left[ 1 + \sum_{k=n+1}^{j-2} (j-k)^{1-p} - (j-n)^{1-p} - \sum_{r_2=n+1}^{j-2} (j-r_2)^{1-p} \right] \\
&= 0.
\end{aligned} \tag{2.197}$$

Hence the first result holds. We now show the second result also holds

$$\begin{aligned}
\sum_{k=n}^{j} k\aleph_{j-k}(p) &= n\left[ (j-(n+1))^{1-p} - (j-n)^{1-p} \right] + j \\
&\quad + \sum_{k=n+1}^{j-1} k\left[ (j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p} \right] \\
&= n\left[ (j-(n+1))^{1-p} - (j-n)^{1-p} \right] + j + \sum_{k=n+1}^{j-1} k\,(j-(k+1))^{1-p} \\
&\quad - 2\sum_{k=n+1}^{j-1} k\,(j-k)^{1-p} + \sum_{k=n+1}^{j-1} k\,(j-(k-1))^{1-p},
\end{aligned} \tag{2.198}$$

and rewriting the first and last sums, we find

$$\begin{aligned}
\sum_{k=n}^{j} k\aleph_{j-k}(p) &= n\left[(j-(n+1))^{1-p}-(j-n)^{1-p}\right]+j+\sum_{r_1=n+2}^{j}(r_1-1)\,(j-r_1)^{1-p}\\
&\quad -2\sum_{k=n+1}^{j-1}k(j-k)^{1-p}+\sum_{r_2=n}^{j-2}(r_2+1)\,(j-r_2)^{1-p}\\
&= n\left[(j-(n+1))^{1-p}-(j-n)^{1-p}\right]+j+\sum_{r_1=n+2}^{j}r_1(j-r_1)^{1-p}\\
&\quad -\sum_{k=n+1}^{j-1}k(j-k)^{1-p}-\left[\sum_{k=n+1}^{j-1}k(j-k)^{1-p}-\sum_{r_2=n}^{j-2}r_2(j-r_2)^{1-p}\right]\\
&\quad -\sum_{r_1=n+2}^{j}(j-r_1)^{1-p}+\sum_{r_2=n}^{j-2}(j-r_2)^{1-p}\\
&= n\left[(j-(n+1))^{1-p}-(j-n)^{1-p}\right]+j-(n+1)\,(j-(n+1))^{1-p}-(j-1)\\
&\quad +n(j-n)^{1-p}-1+(j-n)^{1-p}+(j-(n+1))^{1-p}\\
&= (j-n)^{1-p}. \qquad (2.199)
\end{aligned}$$

Hence result (2) also holds. □

We note there is a problem with the $L1^*$ approximation. We note it is exact for $f(t)=1$, i.e.

$$\left[\frac{d^p(1)}{dt^p}\right|_{L1^*}^{j} = \frac{{t_j}^{-p}}{\Gamma(1-p)}(1)+\frac{\Delta t^{1-p}}{\Gamma(2-p)}\sum_{k=n}^{j-1}\aleph_{j-k}(p), \qquad (2.200)$$

and by using first result in Lemma 2.9.1, we have the exact value of the derivative

$$\left[\frac{d^p(1)}{dt^p}\right|_{L1^*}^{j} = \frac{t_j^{-p}}{\Gamma(1-p)}. \qquad (2.201)$$

But for $f(t)=t$ we have the approximation

$$\begin{aligned}
\left[\frac{d^p(t)}{dt^p}\right|_{L1^*}^{j} &= \frac{{t_j}^{-p}}{\Gamma(1-p)}(0)+\frac{\Delta t^{1-p}}{\Gamma(2-p)}\sum_{k=n}^{j-1}k\aleph_{j-k}(p)\\
&= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\sum_{k=n}^{j-1}k\aleph_{j-k}(p). \qquad (2.202)
\end{aligned}$$

Now evaluating the summation, by using the second result in Lemma 2.9.1, we find

$$\left[\frac{d^p(t)}{dt^p}\right|_{L1^*}^{j} = \frac{\Delta t^{1-p}}{\Gamma(2-p)}(j-n)^{1-p} = \frac{(j\Delta t - n\Delta t)^{1-p}}{\Gamma(2-p)} = \frac{(t_j - t_n)^{1-p}}{\Gamma(2-p)}. \tag{2.203}$$

When we compare this result with the exact fractional derivative of the function $f(t) = t$, $\frac{d^p f(t)}{dt^p} = \frac{t^{1-p}}{\Gamma(2-p)}$, we have an error unlike when the full L1 scheme is used. To remedy this we add an extra term

$$\frac{1}{\Gamma(2-p)}\left[{t_j}^{1-p} - (t_j - t_n)^{1-p}\right] f'(0)$$

to Equation (2.194). We then have the approximation

$$\left[\frac{d^p f(t)}{dt^p}\right| = \frac{{t_j}^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(2-p)}\left[{t_j}^{1-p} - (t_j - t_n)^{1-p}\right] f'(0) + \frac{\Delta t^{-p}}{\Gamma(2-p)} \sum_{k=n}^{j-1} (f_k - f_{k+1}) \left[(j-(k+1))^{1-p} - (j-k)^{1-p}\right], \tag{2.204}$$

which we will refer to as the RL1 scheme. Equation (2.204) can be rewritten as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{RL1}^{j} = \frac{{t_j}^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(2-p)}\left[{t_j}^{1-p} - (t_j - t_n)^{1-p}\right] f'(0) + \frac{\Delta t^{-p}}{\Gamma(2-p)}\Bigg\{ f_j + \left[(j-(n+1))^{1-p} - (j-n)^{1-p}\right] f_n + \sum_{k=n+1}^{j-1} f_k \left[(j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p}\right] \Bigg\}, \tag{2.205}$$

or, upon using the first order finite difference approximation for $f'(0)$, as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{RL1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\Bigg\{ \left[(1-p)j^{-p} - j^{1-p} + (j-n)^{1-p}\right] f_0 + \left[j^{1-p} - (j-n)^{1-p}\right] f_1 + f_j + \left[(j-(n+1))^{1-p} - (j-n)^{1-p}\right] f_n + \sum_{k=n+1}^{j-1} f_k \left[(j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p}\right] \Bigg\}. \tag{2.206}$$

If $n > 0$ the RL1 scheme can be rewritten as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{RL1}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{ \hbar(p) f_0 + \left[j^{1-p} - (j-n)^{1-p}\right] f_1 + \sum_{k=n}^{j} \aleph_{j-k}(p) f_k \right\}, \tag{2.207}$$

where $\hbar(p)$

$$\hbar(p) = (1-p)j^{-p} - j^{1-p} + (j-n)^{1-p}, \tag{2.208}$$

and the weights $\aleph_{j-k}(p)$ are given in Equation (2.196). In the next section we give the accuracy of the RL1 scheme and the $L1^*$ scheme.

## 2.10 Accuracy of the RL1 and $L1^*$ Schemes

In this section, we determine the accuracy of the fractional approximation RL1 and $L1^*$ schemes given by Equations (2.204) and (2.195) at time $t = t_j$ and $0 < p < 1$. We again follow the approach of Langlands & Henry (2005) by assuming $f(t)$ can be expanded as in Equation (2.20). The value of the fractional derivative of Equation (2.20) is given by Equation (2.25).

### 2.10.1 Accuracy of the $L1^*$ Scheme

In this section, we consider the accuracy of $L1^*$ scheme given in Equations (2.195) and (2.196). As shown previously in Section 2.6, the accuracy of $L1^*$ can now be determined by comparing the exact value in Equation (2.25) with the value obtained using the $L1^*$ scheme. Now we need to evaluate the $L1^*$ fractional approximation operating on the functions 1, $t$ and the convolution integral in Equation (2.20).
In Equations (2.201) and (2.203) we found the $L1^*$ fractional approximation operating on the functions 1 and $t$.

We now apply the $L1^*$ fractional approximation on the convolution integral, to find

$$\left[\frac{d^p}{dt^p}\left(\int_0^t f''(s)(t-s)ds\right)\right|_{L1^*}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{(1-p)j^{-p}\lim_{t\to 0}\int\limits_0^t f''(s)(t-s)ds + \sum_{k=n}^{j}\aleph_{j-k}(p)\int\limits_0^{k\Delta t} f''(s)(k\Delta t - s)ds\right\}. \tag{2.209}$$

Note the limit in the first term on the right is zero if $f(t)$ is a well–behaved function of $t$. By dividing the integration interval into equal $\Delta t$ steps, we have

$$\frac{d^p}{dt^p}\left[\int_0^t f''(s)(t-s)ds\right|_{L1^*}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=n}^{j}\aleph_{j-k}(p)\sum_{l=0}^{k-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)(k\Delta t - s)ds, \tag{2.210}$$

and then by changing the order of summation, we obtain the expression

$$\frac{d^p}{dt^p}\left[\int_0^t f''(s)(t-s)ds\right|_{L1^*}^{j} = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{l=0}^{n-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t-s)ds\right.$$
$$\left.+\sum_{l=n}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t-s)ds\right\}. \quad (2.211)$$

Then the $L1^*$ scheme approximation for the function $f(t)$ is then given

$$\left[\frac{d^p f(t)}{dt^p}\right|_{L1^*} = \frac{t_j^{-p}}{\Gamma(1-p)}f_0 + \frac{(t_j-t_n)^{1-p}}{\Gamma(2-p)}f'(0)$$
$$+\frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{l=0}^{n-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t-s)ds\right.$$
$$\left.+\sum_{l=n}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t-s)ds\right\}. \quad (2.212)$$

The value of the $L1^*$ approximation scheme in Equation (2.212) can now be compared with the value of exact of the fractional derivative in Equation (2.25). The error can be evaluated as follows

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j} - \left[\frac{d^p}{dt^p}f(t)\right|_{L1^*}^{j}\right| = \left|f_0\frac{t_j^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} + \int\limits_0^{t_j} f''(s)\frac{(t_j-s)^{1-p}}{\Gamma(2-p)}ds\right.$$
$$-f_0\frac{t_j^{-p}}{\Gamma(1-p)} - f'(0)\frac{(t_j-t_n)^{1-p}}{\Gamma(2-p)} - \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\sum_{l=0}^{n-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t-s)ds\right.$$
$$\left.\left.+\sum_{l=n}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t-s)ds\right\}\right|, \quad (2.213)$$

which, after simplifying, becomes

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^{j} - \left[\frac{d^p}{dt^p}f(t)\right|_{L1^*}^{j}\right| = \left|\frac{1}{\Gamma(2-p)}\left(t_j^{1-p}-(t_j-t_n)^{1-p}\right)f'(0)\right.$$
$$\frac{1}{\Gamma(2-p)}\left\{\sum_{l=0}^{n-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t_j-s)^{1-p}-\Delta t^{-p}\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t-s)\right]ds\right.$$
$$\left.\left.+\sum_{l=n}^{j-1}\int\limits_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t_j-s)^{1-p}-\Delta t^{-p}\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t-s)\right]ds\right\}\right|. \quad (2.214)$$

To evaluate the summations $\sum_{k=l+1}^{j} \aleph_{j-k}(p)$ and $\sum_{k=l+1}^{j} k\aleph_{j-k}(p)$ we need the following two Lemmas.

**Lemma 2.10.1.** Given the weights $\aleph_{j-k}(p)$ defined in Equation (2.196), and $n \leq l+1 \leq j$, we then have

$$\sum_{k=l+1}^{j} \aleph_{j-k}(p) = (j-l)^{1-p} - (j-(l+1))^{1-p} . \tag{2.215}$$

*Proof.* By using Equation (2.196), we have

$$\begin{aligned} \sum_{k=l+1}^{j} \aleph_{j-k}(p) &= 1 + \sum_{k=l+1}^{j-1} \left[ (j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p} \right] \\ &= 1 + \sum_{k=l+1}^{j-1} (j-(k+1))^{1-p} - 2\sum_{k=l+1}^{j-1} (j-k)^{1-p} + \sum_{k=l+1}^{j-1} (j-(k-1))^{1-p} , \end{aligned} \tag{2.216}$$

and, after rewriting the first and last sums, we find

$$\begin{aligned} \sum_{k=l+1}^{j} \aleph_{j-k}(p) &= 1 + \sum_{r_1=l+2}^{j} (j-r_1)^{1-p} - \sum_{k=l+1}^{j-1} (j-k)^{1-p} - \left[ \sum_{k=l+1}^{j-1} (j-k)^{1-p} - \sum_{r_2=l}^{j-2} (j-r_2)^{1-p} \right] \\ &= 1 + 0 + \sum_{r_1=l+2}^{j-1} (j-r_1)^{1-p} - (j-(l+1))^{1-p} - \sum_{k=l+2}^{j-1} (j-k)^{1-p} \\ &\quad - \left[ 1 + \sum_{k=l+1}^{j-2} (j-k)^{1-p} - (j-l)^{1-p} - \sum_{r_2=l+1}^{j-2} (j-r_2)^{1-p} \right] \\ &= (j-l)^{1-p} - (j-(l+1))^{1-p} . \end{aligned} \tag{2.217}$$

Hence the result in Equation (2.215) is correct. □

**Lemma 2.10.2.** Given the weights $\aleph_{j-k}(p)$ defined in Equation (2.196), and $k < j$, then

$$\sum_{k=l+1}^{j} k\aleph_{j-k}(p) = (l+1)(j-l)^{1-p} - l\,(j-(l+1))^{1-p} . \tag{2.218}$$

*Proof.* By using Equation (2.196), we have

$$\begin{aligned}\sum_{k=l+1}^{j} k\aleph_{j-k}(p) &= j + \sum_{k=l+1}^{j-1} k\left[(j-(k+1))^{1-p} - 2(j-k)^{1-p} + (j-(k-1))^{1-p}\right] \\ &= j + \sum_{k=l+1}^{j-1} k\,(j-(k+1))^{1-p} - 2\sum_{k=l+1}^{j-1} k\,(j-k)^{1-p} \\ &\quad + \sum_{k=l+1}^{j-1} k\,(j-(k-1))^{1-p}, \end{aligned} \tag{2.219}$$

then, after rewriting the first and last sums, we find

$$\begin{aligned}\sum_{k=l+1}^{j} k\aleph_{j-k}(p) &= j + \sum_{r_1=l+2}^{j} (r_1-1)\,(j-r_1)^{1-p} - 2\sum_{k=l+1}^{j-1} k(j-k)^{1-p} \\ &\quad + \sum_{r_2=l}^{j-2} (r_2+1)\,(j-r_2)^{1-p} \\ &= j + \sum_{r_1=l+2}^{j} r_1(j-r_1)^{1-p} - \sum_{k=l+1}^{j-1} k(j-k)^{1-p} - \left[\sum_{k=l+1}^{j-1} k(j-k)^{1-p}\right. \\ &\quad \left. - \sum_{r_2=l}^{j-2} r_2(j-r_2)^{1-p}\right] - \sum_{r_1=l+2}^{j} (j-r_1)^{1-p} + \sum_{r_2=l}^{j-2}(j-r_2)^{1-p} \\ &= j - (l+1)\,(j-(l+1))^{1-p} - (j-1) + l(j-l)^{1-p} - 1 \\ &\quad + (j-l)^{1-p} + (j-(l+1))^{1-p} \\ &= (l+1)(j-l)^{1-p} - l\,(j-(l+1))^{1-p}. \end{aligned} \tag{2.220}$$

Hence the result in Equation (2.218) is true. □

Now using Lemmas 2.9.1, 2.10.1, and 2.10.2, then the summations in Equation (2.214) are given by

$$\sum_{k=n}^{j} \aleph_{j-k}(p)(k\Delta t - s) = \Delta t(j-n)^{1-p}, \tag{2.221}$$

and

$$\sum_{k=l+1}^{j} \aleph_{j-k}(p)(k\Delta t - s) = (j-l)^{1-p}((l+1)\Delta t - s) - (j-(l+1))^{1-p}(l\Delta t - s). \tag{2.222}$$

Using the inequality

$$\left|\int f(x)dx\right| \le \int |f(x)|\,dx \tag{2.223}$$

Equation (2.214) then becomes

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1^*} \right| \leq \frac{1}{\Gamma(2-p)} \left| t_j^{1-p} - (t_j - t_n)^{1-p} \right| |f'(0)| \tag{2.224}$$

$$+ \frac{1}{\Gamma(2-p)} \sum_{l=0}^{n-1} \int_{l\Delta t}^{(l+1)\Delta t} \left| f''(s) \right| \left| (t_j - s)^{1-p} - \Delta t^{1-p} (j-n)^{1-p} \right| ds$$

$$+ \frac{1}{\Gamma(2-p)} \sum_{l=n}^{j-1} \int_{l\Delta t}^{(l+1)\Delta t} \left| f''(s) \right| \Big| (t_j - s)^{1-p} - \Delta t^{-p} \Big[ (j-l)^{1-p} ((l+1)\Delta t - s)$$

$$- (j-(l+1))^{1-p} (l\Delta t - s) \Big] \Big| \, ds.$$

Let the maximum absolute value of the second derivative in each interval $[l\Delta t, (l+1)\Delta t]$ where $l = 0, \ldots, j-1$, by

$$M_l = \max_{l\Delta t \leq s \leq (l+1)\Delta t} \left| f''(s) \right|. \tag{2.225}$$

The bound then becomes

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1^*} \right| \leq \frac{1}{\Gamma(2-p)} \left| t_j^{1-p} - (t_j - t_n)^{1-p} \right| |f'(0)| \tag{2.226}$$

$$+ \frac{1}{\Gamma(2-p)} \sum_{l=0}^{n-1} M_l \int_{l\Delta t}^{(l+1)\Delta t} \left| (t_j - s)^{1-p} - \Delta t^{1-p} (j-n)^{1-p} \right| ds$$

$$+ \frac{1}{\Gamma(2-p)} \sum_{l=n}^{j-1} M_l \int_{l\Delta t}^{(l+1)\Delta t} \Big| (t_j - s)^{1-p} - \Delta t^{-p} \Big[ (j-l)^{1-p} ((l+1)\Delta t - s)$$

$$- (j-(l+1))^{1-p} (l\Delta t - s) \Big] \Big| \, ds.$$

We conclude that the term

$$(t_j - s)^{1-p} - \Delta t^{1-p} (j-n)^{1-p} = (t_j - s)^{1-p} - (t_j - t_n)^{1-p},$$

is positive since $f(x) = x^{1-p}$ is an increasing function of $x$ and for $0 \leq l \leq n-1$ and $l\Delta t < s < (l+1)\Delta t$ we have $0 < s < t_n < t_j$ and so $t_j > t_j - s > t_j - t_n > 0$. Also it is shown in Appendix B, Section B.1, that the term in the absolute value function in the second integrand is positive and so we can drop the absolute sign in both integrals.

Evaluating the integrals in Equation (2.226), we have

$$\int_{l\Delta t}^{(l+1)\Delta t} (t_j - s)^{1-p} \, ds = \left[ \frac{-(t_j - s)^{2-p}}{2-p} \right|_{l\Delta t}^{(l+1)\Delta t}$$

$$= \frac{(\Delta t)^{2-p}}{2-p} \left[ (j-l)^{2-p} - (j-l-1)^{2-p} \right], \tag{2.227}$$

$$\int_{l\Delta t}^{(l+1)\Delta t} [l\Delta t - s]\, ds = \left[ l\Delta t s - \frac{s^2}{2} \right|_{l\Delta t}^{(l+1)\Delta t}$$
$$= \left[ l(\Delta t)^2 - \frac{2l+1}{2}(\Delta t)^2 \right]$$
$$= -\frac{\Delta t^2}{2}, \tag{2.228}$$

and

$$\int_{l\Delta t}^{(l+1)\Delta t} [(l+1)\Delta t - s]\, ds = \left[ (l+1)\Delta t s - \frac{s^2}{2} \right|_{l\Delta t}^{(l+1)\Delta t}$$
$$= \left[ (l+1)(\Delta t)^2 - \frac{2l+1}{2}(\Delta t)^2 \right]$$
$$= \frac{\Delta t^2}{2}. \tag{2.229}$$

Inserting the value of the integrals into Equation (2.226) and then letting $M = \max\{M_l;\ l = 0, 1, 2, ..., j\}$, we have

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|^j_{L1^*} \right| \leq \frac{1}{\Gamma(2-p)} \left| t_j^{1-p} - (t_j - t_n)^{1-p} \right| |f'(0)| \tag{2.230}$$
$$+ \frac{\Delta t^{2-p} M}{(2-p)\Gamma(2-p)} \left\{ \sum_{l=0}^{n-1} \left[ (j-l)^{2-p} - (j-l-1)^{2-p} - (2-p)(j-n)^{1-p} \right] \right.$$
$$\left. + \sum_{l=n}^{j-1} \left[ (j-l)^{2-p} - (j-(l+1))^{2-p} - \frac{2-p}{2} \left[ (j-l)^{1-p} + (j-(l+1))^{1-p} \right] \right] \right\}.$$

Evaluating the summations

$$\sum_{l=0}^{n-1} \left[ (j-l)^{2-p} - (j-(l+1))^{2-p} \right] = \sum_{l=0}^{n-1} (j-l)^{2-p} - \sum_{l=1}^{n} (j-l)^{2-p}$$
$$= j^{2-p} - (j-n)^{2-p}, \tag{2.231}$$

$$\sum_{l=n}^{j-1} \left[ (j-l)^{2-p} - (j-(l+1))^{2-p} \right] = \sum_{l=n}^{j-1} (j-l)^{2-p} - \sum_{l=n+1}^{j} (j-l)^{2-p}$$
$$= (j-n)^{2-p}, \tag{2.232}$$

$$\sum_{l=n}^{j-1} \left[ (j-l)^{1-p} + (j-(l+1))^{1-p} \right] = \sum_{l=n}^{j-1} (j-l)^{1-p} + \sum_{l=n+1}^{j} (j-l)^{1-p}$$
$$= (j-n)^{1-p} + 2 \sum_{l=n+1}^{j-1} (j-l)^{1-p}, \tag{2.233}$$

and using these results in Equation (2.230), we then have

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{L1^*}\right| \leq \frac{1}{\Gamma(2-p)}\left|t_j^{1-p} - (t_j - t_n)^{1-p}\right| |f'(0)| \tag{2.234}$$
$$+\frac{\Delta t^{2-p}M}{(2-p)\Gamma(2-p)}\Bigg\{ j^{2-p} - (j-n)^{2-p} - (2-p)n(j-n)^{1-p} + (j-n)^{2-p}$$
$$-\frac{2-p}{2}\left[(j-n)^{1-p} + 2\sum_{l=n+1}^{j-1}(j-l)^{1-p}\right]\Bigg\}.$$

Equation (2.234) simplifies to

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{L1^*}\right| \leq \frac{1}{\Gamma(2-p)}\left|t_j^{1-p} - (t_j - t_n)^{1-p}\right| |f'(0)| \tag{2.235}$$
$$+\frac{\Delta t^{2-p}M}{\Gamma(3-p)}\left[j^{2-p} - \frac{2-p}{2}(j-n)^{1-p}(2n+1) - (2-p)\sum_{k=1}^{j-(n+1)}k^{1-p}\right]$$
$$= \frac{1}{\Gamma(2-p)}\left|t_j^{1-p} - (t_j - t_n)^{1-p}\right| |f'(0)| + \frac{\Delta t^{2-p}M}{2\Gamma(3-p)}\left[j^{1-p}(2j-(2-p)) - 2(2-p)\sum_{k=1}^{j-1}k^{1-p}\right]$$
$$+\frac{\Delta t^{2-p}M}{2\Gamma(2-p)}\left[j^{1-p} - (j-n)^{1-p}(2n+1) + 2\sum_{k=j-n}^{j-1}k^{1-p}\right]. \tag{2.236}$$

The estimate error is then given by

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{L1^*}\right| \leq \frac{1}{\Gamma(2-p)}\left|t_j^{1-p} - (t_j - t_n)^{1-p}\right| |f'(0)| + C\Delta t^{2-p} + C_n^*\Delta t^{2-p}, \tag{2.237}$$

where $C$ is defined by

$$C = \frac{M\vartheta(j,p)}{2\Gamma(3-p)}, \tag{2.238}$$

and $\vartheta(j,p)$ is given by Equation (2.50). The bound of $C$ is given by Equations (2.49) and (2.51). The value of $C_n^*$ is given by

$$C_n^* = \frac{M\kappa(j,n,p)}{2\Gamma(2-p)}, \tag{2.239}$$

where $\kappa(j,n,p)$ is

$$\kappa(j,n,p) = j^{1-p} - (j-n)^{1-p}(2n+1) + 2\sum_{k=j-n}^{j-1}k^{1-p}. \tag{2.240}$$

In Equation (2.240), we have $\kappa(j,n,0) = n^2$ and $\kappa(j,n,1) = 0$. For $0 \leq p \leq 1$ the constant $\kappa(j,n,p)$ is bounded by $0 \leq \kappa(j,n,p) \leq n^2$ as shown in Figure 2.36. Another bound can be found by sitting $j = n$, which gives

$$\begin{aligned}\kappa(j,j,p) &= j^{1-p} + 2\sum_{k=0}^{j-1} k^{1-p} \\ &\leq j^{1-p} + 2\sum_{k=1}^{j-1} (j-1)^{1-p} \\ &\leq j^{1-p} + 2(j-1)^{2-p}. \end{aligned} \tag{2.241}$$

This shows the term $C_n^* \Delta t^{2-p}$ is of order $t^{2-p}$ as an upper bound. We see the error increases in Equation (2.237), so this suggests that just by adding the extra term in Equation (2.204) does not improve the accuracy even though makes it exact for linear functions of time.

In Figures 2.36 – 2.38, we show the value of $\kappa(j,n,p)$ given in Equation (2.240) against $p$, where $p = 0, \ldots, 1$. In Figure 2.36 we set $j = 1000$ and varied $n = 50l$, where $l = 1, 2, \ldots, 8$. We see the value of $\kappa(j,n,p)$ increases as $n$ increases in the direction of the arrow. Whilst in Figure 2.37 when $n$ is fixed and varying $j = 10^k$ where $k = 2, 3, 4, 5$ and 6, the value of $\kappa(j,n,p)$ decreases as $j$ increases in the direction of the arrow. We also note that the value of $\kappa(j,n,p)$ increases as $p$ decreases, we see that the maximum value of $\kappa(j,n,p)$ occurs for $p = 0$ and the minimum value of $\kappa(j,n,p)$ occurs for $p = 1$. We show the maximum value of the $\kappa(j,n,p)$ in Figure 2.38 for $n = j = 1, \ldots, 10$. We note the value of $\kappa(j,n,p)$ increases as $j$ increases in the direction of arrow, as suggested by the upper bound in Equation (2.241).

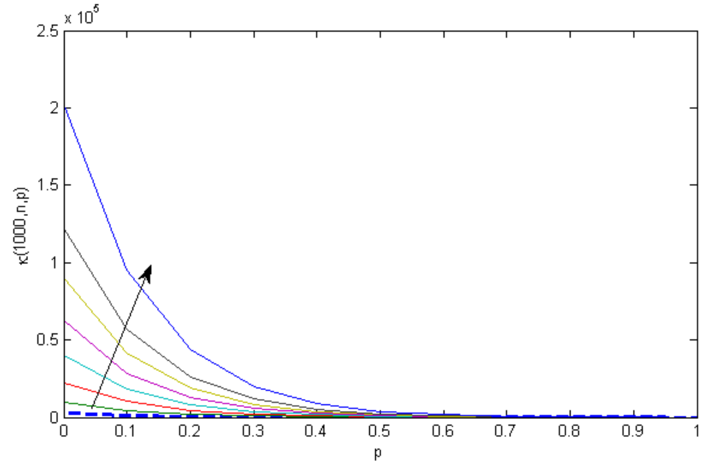



Figure 2.36: The value of $\kappa(1000, n, p)$ in Equation (2.240) is shown against $p$ for varying values of $n = 50l$, where $l = 1, 2, \ldots, 8$. The value of $n$ increases in the direction of the arrow. Note the value of $\kappa(1000, n, p)$ increases as $p$, $0 \le p \le 1$, decreases.

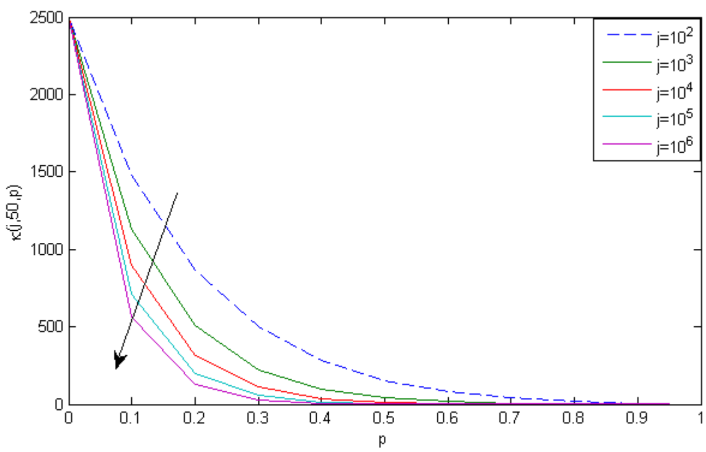



Figure 2.37: The value of $\kappa(j, 50, p)$ in Equation (2.240) is shown against $p$ for $0 \le p \le 1$ for fixed $n = 50$ and $j = 10^k$ where $k = 2, 3, 4, 5$ and 6. The value of $\kappa(j, 50, p)$ decreases as $j$ increases in the direction of the arrow.

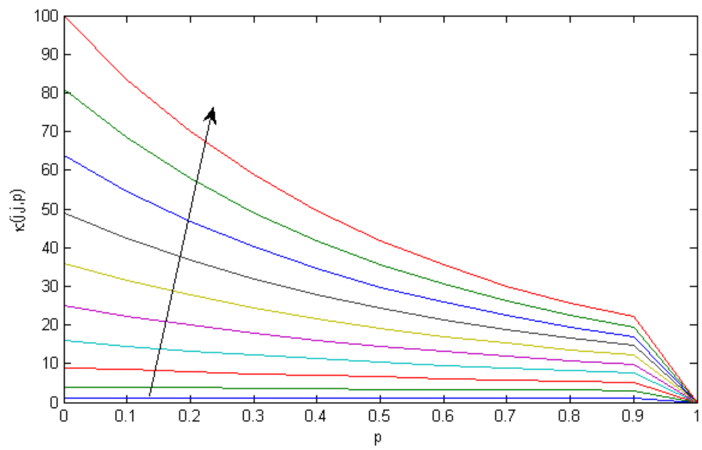



Figure 2.38: The maximum value of $\kappa(j, j, p)$ in Equation (2.240) is shown against $p$ for $0 \le p \le 1$ for $n = j = 1, \ldots, 10$. The value of $\kappa(j, j, p)$ increases as $j$ increases in the direction of the arrow.

The accuracy of the $L1^*$ scheme was estimated by comparing the fractional derivative of order $p = 1 - \gamma$, for $\gamma = 0.1, \ldots, 0.9$, of the function $f(t) = t^k$, for exponents $k = 2, 2.5, 3, 3.5$, and 4, at the time $t = 1.0$. The error is plotted as a function of $n$ for each function in Figures 2.39 through to 2.43. Also the comparison of the absolute error is given in Table 2.12, where we have set $j = 100$ and $n = 100$. We see that the maximum error occurs for $\gamma = 0.5$ for functions $f(t) = t^2$ and $f(t) = t^{2.5}$, and the minimum error occurs for $\gamma = 0.1$. Whilst the maximum error occurs for $\gamma = 0.4$ for functions $f(t) = t^3$, $f(t) = t^{3.5}$, and $f(t) = t^4$.

In Figure 2.39, we see the error does not increase immediately for all $\gamma$ values when $n$ is small. For example for $\gamma = 0.1$ the error only begins to increase when $n = 20$. Thus suggests we can use the $L1^*$ scheme with $n = 1, \ldots, 20$ without introducing a large error for $n > 20$. Whilst for $\gamma = 0.9$ the error begins to increase for $n > 2$, which is not as good as $\gamma = 0.1$. We also see in Figure 2.43 for the value $\gamma = 0.1$ the error only begins to increase when $n > 70$, so we can use the $L1^*$ scheme with $n = 1, \ldots, 70$, to still maintain the same level of error. But for the case $\gamma = 0.9$ the error begins to increase for $n > 6$, so we can only ignore a smaller number of terms for case $\gamma = 0.9$ compared with the number that can be ignored for $\gamma = 0.1$. We see similar behaviour in Figures 2.40 and 2.41.

From these figures it appears we can ignore more terms as the power of $t$ increases. This is most likely due to the fact the value of $M = \max(f''(x))$ and $f'(0)$ being smaller as the power increases. From Table 2.12 and the Figures 2.39 – 2.43, we conclude that the error increases as $n$ increases (as we ignore more history), and the minimum error occurs for $n$ is near zero. This is to be expected as $n = 0$ is similar to the L1 scheme.

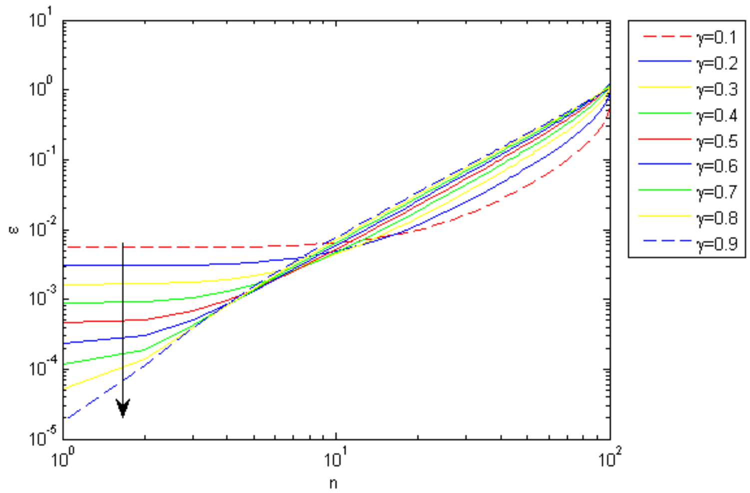



Figure 2.39: The absolute error in using the $L1^*$ scheme, Equation (2.194), for the fractional derivative of order $1-\gamma$ of the function $f(t) = t^2$, at time $t = 1.0$, with $j = 100$ and $n = 1, \ldots, j$. Results are shown for $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

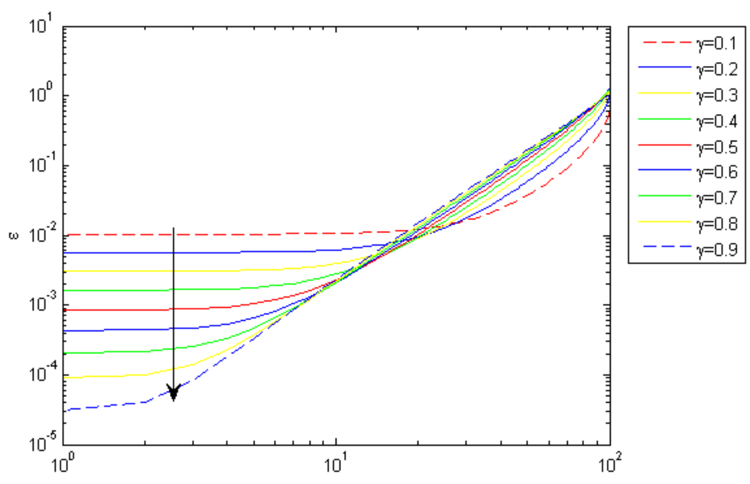



Figure 2.40: The absolute error in using the $L1^*$ scheme, Equation (2.194), for the fractional derivative of order $1-\gamma$ of the function $f(t) = t^{2.5}$, at time $t = 1.0$, with $j = 100$ with $n = 1, \ldots, 100$. Results are shown for $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

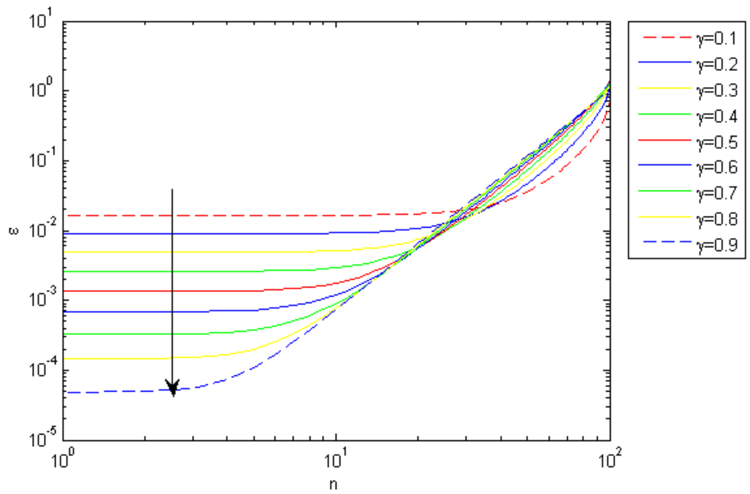



Figure 2.41: The absolute error in using the $L1^*$ scheme, Equation (2.194), to evaluate the fractional derivative of order $1-\gamma$ for function $f(t)=t^3$, at time $t=1.0$. Results shown for $j=100$, with $n=1,\ldots,100$ for $\gamma=0.1,\ldots,0.9$ where $\gamma$ increases in the direction of the arrow.

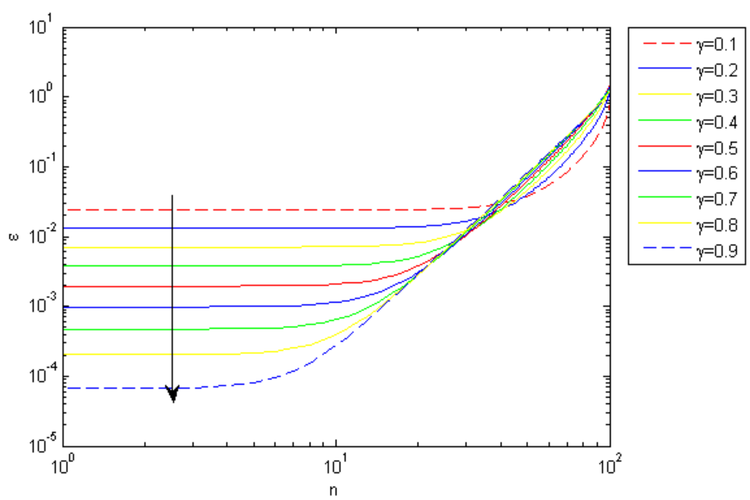



Figure 2.42: The absolute error in using the $L1^*$ scheme, Equation (2.194), for the fractional derivative of order $1-\gamma$ of the function $f(t)=t^{3.5}$, at time $t=1.0$, with the time step $j=100$ where $n=1,\ldots,100$. Results are shown for $\gamma=0.1,\ldots,0.9$ where $\gamma$ increases in the direction of the arrow.

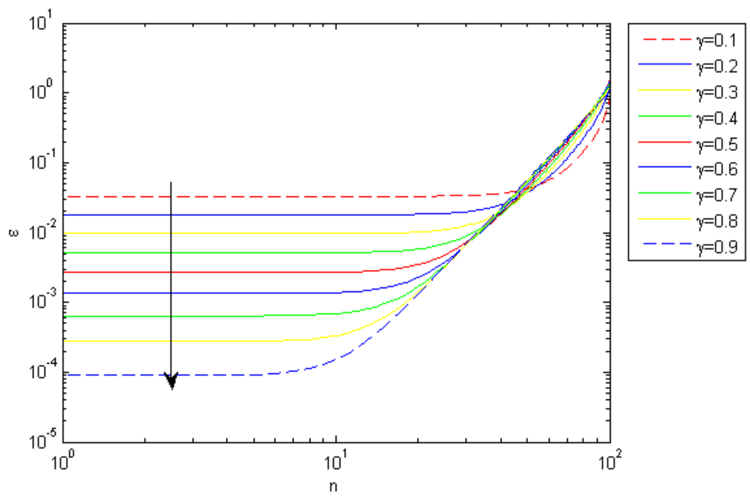



Figure 2.43: The absolute error in using the $L1^*$ scheme, Equation (2.194), to evaluate the fractional derivative of order $1-\gamma$ for function $f(t)=t^4$, at time $t=1.0$. Results shown for $j=100$, $n=1,\dots,100$, and for value $\gamma=0.1,\dots,0.9$ where $\gamma$ increases in the direction of the arrow.

Table 2.12: The comparison of the absolute error for functions $f(t)=t^k$, $k=2,2.5,3,3.5,$ and 4 at time $t=1.0$ with $n=100$, $j=100$, and $\Delta t=0.01$ using the $L1^*$ scheme to evaluate the $1-\gamma$ order fractional derivative, where $\gamma=0.1,...,0.9$.

| $\gamma$ | $f(t)=t^2$ | $f(t)=t^{2.5}$ | $f(t)=t^3$ | $f(t)=t^{3.5}$ | $f(t)=t^4$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 5.914e–01 | 6.790e–01 | 7.604e–01 | 8.369e–01 | 9.0951e–01 |
| $\gamma=0.2$ | 9.524e–01 | 1.076e–00 | 1.188e–00 | 1.290e–00 | 1.386e–00 |
| $\gamma=0.3$ | 1.157e–00 | 1.288e–00 | 1.405e–00 | 1.510e–00 | 1.607e–00 |
| $\gamma=0.4$ | 1.255e–00 | 1.375e–00 | 1.482e–00 | 1.578e–00 | 1.664e–00 |
| $\gamma=0.5$ | 1.280e–00 | 1.382e–00 | 1.470e–00 | 1.549e–00 | 1.619e–00 |
| $\gamma=0.6$ | 1.259e–00 | 1.337e–00 | 1.405e–00 | 1.463e–00 | 1.515e–00 |
| $\gamma=0.7$ | 1.208e–00 | 1.262e–00 | 1.309e–00 | 1.348e–00 | 1.383e–00 |
| $\gamma=0.8$ | 1.139e–00 | 1.172e–00 | 1.198e–00 | 1.220e–00 | 1.239e–00 |
| $\gamma=0.9$ | 1.062e–00 | 1.074e–00 | 1.0836e–00 | 1.091e–00 | 1.096e–00 |

### 2.10.2 Accuracy of the RL1 Scheme

In this section, we determine the accuracy of the fractional derivative at time $t=t_j$ and $0<p<1$ given by the RL1 scheme in Equation (2.207). We again compare the result of taking the exact fractional derivative of $f(t)$ given in Equation (2.25) with approximate result obtained by RL1 scheme in Equation (2.207). Similar to before we apply the RL1 approximation scheme on the functions 1, $t$ and the convolution integrals in Equation (2.20) at time $t = t_j$.

The RL1 approximation of the function $f(t) = 1$ at time $t = t_j$, is given by

$$\begin{aligned}\left[\frac{d^p(1)}{dt^p}\right|_{RL1} &= \frac{\Delta t^{-p}}{\Gamma(2-p)}\Bigg\{ \left[(1-p)j^{-p} - j^{1-p} + (j-n)^{1-p}\right](1) \\ &\quad + \left[j^{1-p} - (j-n)^{1-p}\right](1) + \sum_{k=n}^{j} \aleph_{j-k}(p)(1)\Bigg\} \\ &= \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{(1-p)j^{-p} + \sum_{k=n}^{j} \aleph_{j-k}(p)\right\}. \qquad (2.242)\end{aligned}$$

Using the first result of Lemma 2.9.1, Equation (2.242) becomes

$$\begin{aligned}\left[\frac{d^p(1)}{dt^p}\right|_{RL1}^{j} &= \frac{\Delta t^{-p}}{\Gamma(2-p)}(1-p)j^{-p} \\ &= \frac{t_j^{-p}}{\Gamma(1-p)}, \qquad (2.243)\end{aligned}$$

which is exact for $f(t) = 1$.

We next use the RL1 approximation on $f(t) = t$

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{RL1} &= \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{0 + \left[j^{1-p} - (j-n)^{1-p}\right](\Delta t) + \sum_{k=n}^{j}(k\Delta t)\aleph_{j-k}(p)\right\} \\ &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left\{j^{1-p} - (j-n)^{1-p} + \sum_{k=n}^{j} k\aleph_{j-k}(p)\right\}, \qquad (2.244)\end{aligned}$$

which after using Lemma 2.9.1, we then have the result

$$\begin{aligned}\left[\frac{d^p(t)}{dt^p}\right|_{RL1}^{j} &= \frac{\Delta t^{1-p}}{\Gamma(2-p)}\left\{j^{1-p} - (j-n)^{1-p} + (j-n)^{1-p}\right\} \\ &= \frac{(j\Delta t)^{1-p}}{\Gamma(2-p)} \\ &= \frac{t_j^{1-p}}{\Gamma(2-p)}, \qquad (2.245)\end{aligned}$$

which is also exact for $f(t) = t$.

We now we apply the RL1 approximation on the convolution integral

$$\frac{d^p}{dt^p}\left[\int_0^t f''(s)(t-s)ds\right|_{RL1}^j$$
$$= \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\left[(1-p)j^{-p} - j^{1-p} + (j-n)^{1-p}\right]\lim_{t\to 0}\int_0^t f''(s)(t-s)ds\right.$$
$$\left. + \left[j^{1-p} - (j-n)^{1-p}\right]\int_0^{\Delta t} f''(s)(\Delta t - s)ds + \sum_{k=n}^{j}\aleph_{j-k}(p)\int_0^{k\Delta t} f''(s)(k\Delta t - s)ds\right\}. \quad (2.246)$$

The limit is again zero if $f''(t)$ is a well behaved function of $t$. Now by dividing the integration interval into equal $\Delta t$ steps, we then have

$$\frac{d^p}{dt^p}\left[\int_0^t f''(s)(t-s)ds\right|_{RL1}^j = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\left[j^{1-p} - (j-n)^{1-p}\right]\int_0^{\Delta t} f''(s)(\Delta t - s)ds\right.$$
$$\left. + \sum_{k=n}^{j}\aleph_{j-k}(p)\sum_{l=0}^{k-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)(k\Delta t - s)ds\right\}. \quad (2.247)$$

Then by changing the order of summation, we obtain

$$\frac{d^p}{dt^p}\left[\int_0^t f''(s)(t-s)ds\right|_{RL1}^j = \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\left[j^{1-p} - (j-n)^{1-p}\right]\int_0^{\Delta t} f''(s)(\Delta t - s)ds\right.$$
$$+ \sum_{l=0}^{n-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t - s)ds$$
$$\left. + \sum_{l=n}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t - s)ds\right\}. \quad (2.248)$$

The RL1 approximation of function $f(t)$ in Equation (2.20) then becomes

$$\left[\frac{d^p f(t)}{dt^p}\right|_{RL1}^j = \frac{t_j^{-p}f_0}{\Gamma(1-p)} + \frac{t_j^{1-p}f'(0)}{\Gamma(2-p)} + \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\left[j^{1-p} - (j-n)^{1-p}\right]\int_0^{\Delta t} f''(s)(\Delta t - s)ds\right.$$
$$\left. + \sum_{l=0}^{n-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t - s)ds + \sum_{l=n}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t - s)ds\right\}. \quad (2.249)$$

The value of the RL1 approximation in Equation (2.249) will be now compared with the exact value of the fractional derivative given by Equation (2.25). The absolute error is then given by

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{RL1}\right| = \left| f_0\frac{t_j^{-p}}{\Gamma(1-p)} + f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} + \int_0^{j\Delta t} f''(s)\frac{(t-s)^{1-p}}{\Gamma(2-p)}ds \right.$$

$$- f_0\frac{t_j^{-p}}{\Gamma(1-p)} - f'(0)\frac{t_j^{1-p}}{\Gamma(2-p)} - \frac{\Delta t^{-p}}{\Gamma(2-p)}\left\{\left[j^{1-p}-(j-n)^{1-p}\right]\int_0^{\Delta t} f''(s)(\Delta t - s)ds \right.$$

$$\left.\left. + \sum_{l=0}^{n-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t - s)ds + \sum_{l=n}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t - s)ds\right\}\right|, \tag{2.250}$$

or by

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{RL1}\right| = \frac{1}{\Gamma(2-p)}\left|\left\{\Delta t^{-p}\left[(j-n)^{1-p} - j^{1-p}\right]\int_0^{\Delta t} f''(s)(\Delta t - s)ds\right.\right.$$

$$+ \sum_{l=0}^{n-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t-s)^{1-p} - \Delta t^{-p}\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t - s)\right]ds$$

$$\left.\left. + \sum_{l=n}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t-s)^{1-p} - \Delta t^{-p}\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t - s)\right]ds\right\}\right|. \tag{2.251}$$

Now using Lemmas 2.9.1, 2.10.1 and 2.10.2, the summations simplify to

$$\sum_{k=n}^{j}\aleph_{j-k}(p)(k\Delta t - s) = \Delta t(j-n)^{1-p}, \tag{2.252}$$

and

$$\sum_{k=l+1}^{j}\aleph_{j-k}(p)(k\Delta t - s) = (j-l)^{1-p}((l+1)\Delta t - s) - (j-(l+1))^{1-p}(l\Delta t - s). \tag{2.253}$$

The absolute error of the RL1 scheme is then

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j - \left[\frac{d^p}{dt^p}f(t)\right|^j_{RL1}\right| \tag{2.254}$$

$$= \frac{1}{\Gamma(2-p)}\left|\int_0^{\Delta t} f''(s)\left[(t-s)^{1-p} - \Delta t^{-p}\left(\Delta t j^{1-p} + \left((j-n)^{1-p} - j^{1-p}\right)s\right)\right]ds\right.$$

$$+ \sum_{l=1}^{n-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t-s)^{1-p} - \Delta t^{1-p}(j-n)^{1-p}\right]ds$$

$$\left. + \sum_{l=n}^{j-1}\int_{l\Delta t}^{(l+1)\Delta t} f''(s)\left[(t-s)^{1-p} - \Delta t^{-p}\left[(j-l)^{1-p}((l+1)\Delta t - s) - (j-(l+1))^{1-p}(l\Delta t - s)\right]\right]ds\right|.$$

Noting

$$\left| \int_a^b f(x)g(x)dx \right| \leq \int_a^b |f(x)| \, |g(x)| \, dx, \tag{2.255}$$

we then have

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|_{RL1}^j \right| \tag{2.256}$$

$$\leq \frac{1}{\Gamma(2-p)} \left\{ \int_0^{\Delta t} |f''(s)| \left| (t-s)^{1-p} - \Delta t^{-p} \left( \Delta t j^{1-p} + \left( (j-n)^{1-p} - j^{1-p} \right) s \right) \right| ds \right.$$

$$+ \sum_{l=1}^{n-1} \int_{l\Delta t}^{(l+1)\Delta t} |f''(s)| \left| (t-s)^{1-p} - \Delta t^{1-p} (j-n)^{1-p} \right| ds$$

$$\left. + \sum_{l=n}^{j-1} \int_{l\Delta t}^{(l+1)\Delta t} |f''(s)| \left| (t-s)^{1-p} - \Delta t^{-p} \left[ (j-l)^{1-p} ((l+1)\Delta t - s) - (j-(l+1))^{1-p} (l\Delta t - s) \right] \right| ds \right\}.$$

Let the maximum absolute value of the second derivative in each interval $[l\Delta t, (l+1)\Delta t]$ and $[0, \Delta t]$ by

$$M_l = \max_{l\Delta t \leq s \leq (l+1)\Delta t} \left| f''(s) \right|, \tag{2.257}$$

and

$$M_1 = \max_{0 \leq s \leq \Delta t} \left| f''(s) \right|. \tag{2.258}$$

Then from Equation (2.256) we have

$$\left| \left[ \frac{d^p}{dt^p} f(t) \right|^j - \left[ \frac{d^p}{dt^p} f(t) \right|_{RL1}^j \right| \tag{2.259}$$

$$\leq \frac{1}{\Gamma(2-p)} \left\{ M_1 \int_0^{\Delta t} \left| (t-s)^{1-p} - \Delta t^{-p} \left( \Delta t j^{1-p} + \left( (j-n)^{1-p} - j^{1-p} \right) s \right) \right| ds \right.$$

$$+ \sum_{l=1}^{n-1} M_l \int_{l\Delta t}^{(l+1)\Delta t} \left| (t-s)^{1-p} - \Delta t^{1-p} (j-n)^{1-p} \right| ds$$

$$\left. + \sum_{l=n}^{j-1} M_l \int_{l\Delta t}^{(l+1)\Delta t} \left| (t-s)^{1-p} - \Delta t^{-p} \left[ (j-l)^{1-p} ((l+1)\Delta t - s) - (j-(l+1))^{1-p} (l\Delta t - s) \right] \right| ds \right\}.$$

By Appendix B.1, the term in the absolute value sign in each integrand is positive, and so evaluating these integrals gives

$$\int_{l\Delta t}^{(l+1)\Delta t} \left[(t_j - s)^{1-p} - \Delta t^{1-p}(j-n)^{1-p}\right] ds = \left[\frac{-(t_j - s)^{2-p}}{2-p} - \Delta t^{1-p}(j-n)^{1-p} s\right|_{l\Delta t}^{(l+1)\Delta t}$$
$$= \frac{(\Delta t)^{2-p}}{2-p}\left[(j-l)^{2-p} - (j-(l+1))^{2-p}\right] - \Delta t^{2-p}(j-n)^{1-p}, \tag{2.260}$$

$$\int_{l\Delta t}^{(l+1)\Delta t} [l\Delta t - s]\, ds = \left[l\Delta t s - \frac{s^2}{2}\right|_{l\Delta t}^{(l+1)\Delta t} = \left[l - \frac{2l+1}{2}\right](\Delta t)^2 = -\frac{\Delta t^2}{2}, \tag{2.261}$$

$$\int_{l\Delta t}^{(l+1)\Delta t} [(l+1)\Delta t - s]\, ds = \left[(l+1)\Delta t s - \frac{s^2}{2}\right|_{l\Delta t}^{(l+1)\Delta t} = \left[(l+1) - \frac{2l+1}{2}\right](\Delta t)^2 = \frac{\Delta t^2}{2}, \tag{2.262}$$

$$\int_0^{\Delta t} (t_j - s)^{1-p}\, ds = \left[\frac{-(t_j - s)^{2-p}}{2-p}\right|_0^{\Delta t} = \frac{(\Delta t)^{2-p}}{2-p}\left[j^{2-p} - (j-1)^{2-p}\right], \tag{2.263}$$

and

$$\int_0^{\Delta t} \left[\Delta t j^{1-p} + \left((j-n)^{1-p} - j^{1-p}\right) s\right] ds = \frac{\Delta t^2}{2}\left(j^{1-p} + (j-n)^{1-p}\right). \tag{2.264}$$

Now we let $M = \max\{M_i;\ l = 0, 1, 2, ..., j\}$, and using Equations (2.260) – (2.264) in Equation (2.259), we then have

$$\left|\left[\frac{d^p}{dt^p} f(t)\right|^j - \left[\frac{d^p}{dt^p} f(t)\right|_{RL1}^j\right| \tag{2.265}$$
$$\leq \frac{M\Delta t^{2-p}}{(2-p)\Gamma(2-p)}\left\{j^{2-p} - (j-1)^{2-p} - \frac{2-p}{2}\left(j^{1-p} + (j-n)^{1-p}\right)\right.$$
$$+ \sum_{l=1}^{n-1}\left((j-l)^{2-p} - (j-(l+1))^{2-p} - (2-p)(j-n)^{1-p}\right)$$
$$\left.+ \sum_{l=n}^{j-1}\left[(j-l)^{2-p} - (j-(l+1))^{2-p} - \frac{2-p}{2}\left[(j-l)^{1-p} + (j-(l+1))^{1-p}\right]\right]\right\}.$$

Evaluating the summations, we find

$$\sum_{l=1}^{n-1}\left[(j-l)^{2-p} - (j-(l+1))^{2-p}\right] = \sum_{l=1}^{n-1}(j-l)^{2-p} - \sum_{l=2}^{n}(j-l)^{2-p}$$
$$= (j-1)^{2-p} - (j-n)^{2-p}, \tag{2.266}$$

$$\sum_{l=n}^{j-1}\left[(j-l)^{2-p}-(j-(l+1))^{2-p}\right]=\sum_{l=n}^{j-1}(j-l)^{2-p}-\sum_{r=n+1}^{j}(j-r)^{2-p}$$
$$=(j-n)^{2-p}, \tag{2.267}$$

and

$$\sum_{l=n}^{j-1}\left[(j-l)^{1-p}+(j-(l+1))^{1-p}\right]=(j-n)^{1-p}+2\sum_{l=n+1}^{j-1}(j-l)^{1-p}. \tag{2.268}$$

Substituting these in Equation (2.265), we then have the bound

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j-\left[\frac{d^p}{dt^p}f(t)\right|^j_{RL1}\right|\le\frac{M\Delta t^{2-p}}{(2-p)\Gamma(2-p)}\left\{\left[j^{1-p}\left(j-\frac{2-p}{2}\right)-(2-p)\sum_{k=1}^{j-1)}k^{1-p}\right]\right.$$
$$\left.-(2-p)n\,(j-n)^{1-p}+(2-p)\sum_{k=j-n}^{j-1}k^{1-p}\right\}$$
$$=\frac{M\Delta t^{2-p}}{2\Gamma(3-p)}\left[j^{1-p}\,(2j-(2-p))-2(2-p)\sum_{k=1}^{j-1)}k^{1-p}\right]$$
$$+\frac{M\Delta t^{2-p}}{\Gamma(2-p)}\left[\sum_{k=j-n}^{j-1}k^{1-p}-n\,(j-n)^{1-p}\right]. \tag{2.269}$$

Equation (2.269) becomes

$$\left|\left[\frac{d^p}{dt^p}f(t)\right|^j-\left[\frac{d^p}{dt^p}f(t)\right|^j_{RL1}\right|\le C\Delta t^{2-p}+Ç_n^*\Delta t^{2-p}, \tag{2.270}$$

where $C$ is a constant and defined by

$$C=\frac{M\vartheta(j,p)}{2\Gamma(3-p)}, \tag{2.271}$$

where $\vartheta(j,p)$ is given by Equation (2.50). The bound for value of $C$ is given by Equations (2.49) to (2.51). $Ç_n^*$ is defined by

$$Ç_n^*=\frac{M\widehat{\kappa}(j,n,p)}{\Gamma(2-p)}, \tag{2.272}$$

where $\widehat{\kappa}(j,n,p)$

$$\widehat{\kappa}(j,n,p)=\sum_{k=j-n}^{j-1}k^{1-p}-n\,(j-n)^{1-p}. \tag{2.273}$$

In Equation (2.273), we have $\widehat{\kappa}(j,n,0) = \frac{n}{2}(2j-n-1)$, and $\widehat{\kappa}(j,n,1) = 0$, as shown in Figure 2.44. Another bound can be found by sitting $j = n$, which gives

$$\begin{aligned}\widehat{\kappa}(j,j,p) &= \sum_{k=0}^{j-1} k^{1-p} \\ &\leq \sum_{k=1}^{j-1} (j-1)^{1-p} \\ &\leq (j-1)^{2-p}. \end{aligned} \tag{2.274}$$

This shows the term $\c{C}_n^* \Delta t^{2-p}$ is of order $t^{2-p}$ as an upper bound. Again we see the error increases in Equation (2.270), so this suggests that reduction of the computation of the L1 scheme does not improve the accuracy.

In Figures 2.44 – 2.46, we show the value of $\widehat{\kappa}(j,n,p)$ given in Equation (2.273) against $p$, for $0 \leq p \leq 1$. In Figure 2.44 the number of time steps is fixed to $j = 1000$ and the value of $n$ is varied with $n = 50l$, where $l = 1, 2, \ldots, 8$. We note that the maximum value occurs where $n$ near the value of $j$, we also see the value of $\widehat{\kappa}(j,n,p)$ increases as $n$ increases, and the minimum value occurs for $n$ is near zero. In Figure 2.45, we show the value of the $\widehat{\kappa}(j,n,p)$ against $p$, for fixed $n = 50$ and $j = 10^k$ where $k = 2, 3, 4, 5$ and 6. The value of $\widehat{\kappa}(j,n,p)$ decreases as $j$ increases for fixed $n$. In addition, the magnitude of the value of $\widehat{\kappa}(j,n,p)$ increases as $p$ decreases. We also show in Figure 2.46 the maximum value of the $\widehat{\kappa}(j,n,p)$ occurs when $n = j$. We note the value of $\widehat{\kappa}(j,n,p)$ increases as $j$ increases as suggested by the upper bound in Equation (2.274).

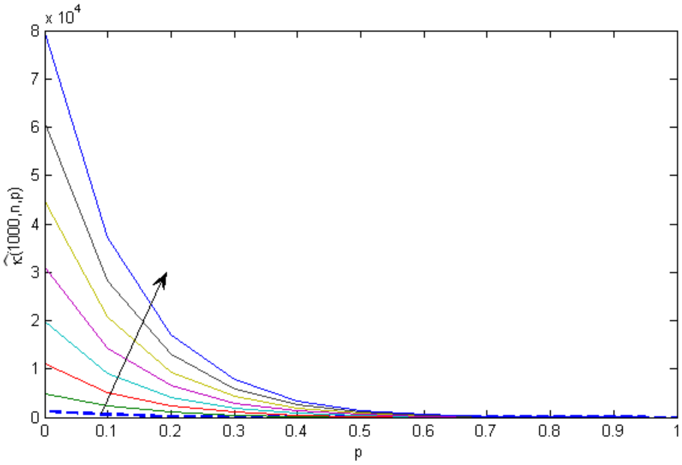



Figure 2.44: The value of $\widehat{\kappa}(j, n, p)$ in Equation (2.273) is shown against $p$, for $0 \leq p \leq 1$, for varying number of $n = 50l$, where $l = 1, 2, \ldots, 8$ and $j = 1000$. Note $n$ increases in the direction of the arrow.

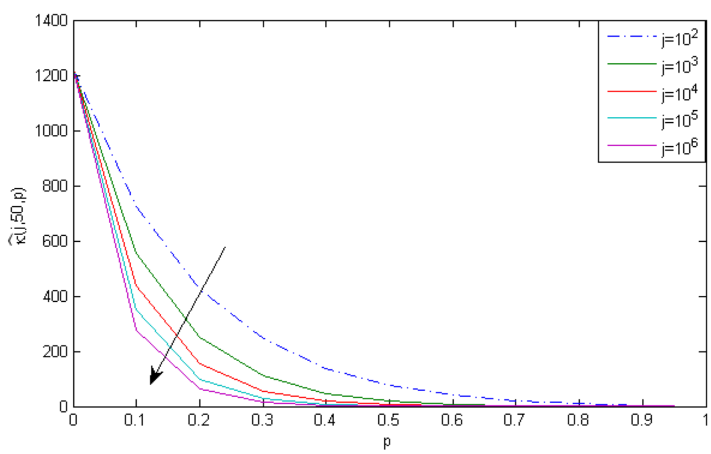



Figure 2.45: The value of $\widehat{\kappa}(j, n, p)$ in Equation (2.273) is shown against $p$, for $0 \leq p \leq 1$, for fixed $n = 50$ and $j = 10^k$ where $k = 2, 3, 4, 5$ and 6. The value of $\widehat{\kappa}(j, n, p)$ decreases as $j$ increases in the direction of the arrow for fixed $n$.

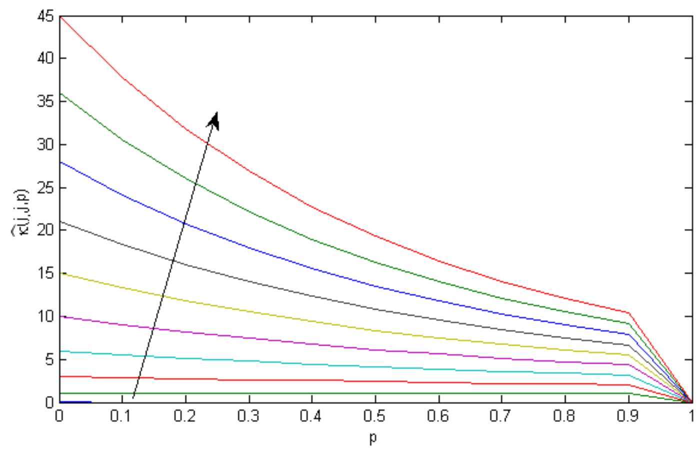



Figure 2.46: The value of $\widehat{\kappa}(j,n,p)$ in Equation (2.273) is shown against $p$, for $0 \le p \le 1$, for $n = j = 1, \ldots, 10$. The value of $\widehat{\kappa}(j,j,p)$ increases as $j$ increases in the direction of the arrow.

The accuracy of the RL1 scheme was estimated by comparing the fractional derivative of order $p = 1-\gamma$ of the functions $f(t) = t^k$, ($k = 2, 2.5, 3, 3.5,$ and 4) evaluated at the time $t = 1.0$. Results are shown for varying exponents $\gamma = 0.1, \ldots, 0.9$.

In Figure 2.47, the error does not increase immediately for small $n$. We see for $\gamma = 0.1$ the error starts increase when $n > 20$, so for this case we could start at $n = 20$, if we use the RL1 scheme as the error does not change dramatically for $n = 1, 2, \ldots, 20$. Whilst in Figure 2.48, we see the error only begins to increase, for $\gamma = 0.1$, when $n > 70$ which is better and so we can ignore the first 70 terms in this case. But for the value $\gamma = 0.9$ the error begins to increase sooner for $n > 2$ which is not good as $\gamma = 0.1$. We also see the similar behaviour in Figures 2.49 –2.51. That is as the power of $t$ increases we can ignore more terms as mentioned for the $L1^*$ scheme.

The absolute error for given functions are compared in Table 2.13, where $j = 100$. From Table 2.13 and the Figures 2.47 and 2.51, we obtained similar error estimate results found by using the $L1^*$ approximation scheme.

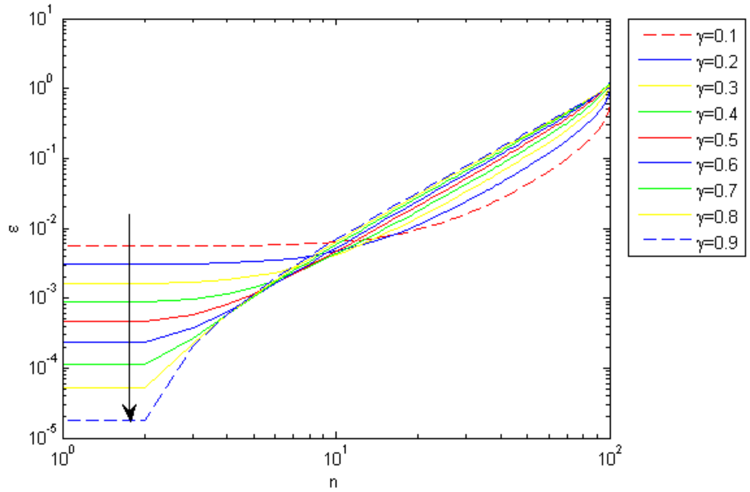



Figure 2.47: The absolute error in using the RL1 scheme, in Equation (2.270), to approximate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^2$, at the time $t = 1.0$, using $j = 100$ time steps, $n = 1, \dots, 100$ and $\gamma = 0.1, \dots, 0.9$. In the figure $\gamma$ increases in the direction of the arrow.

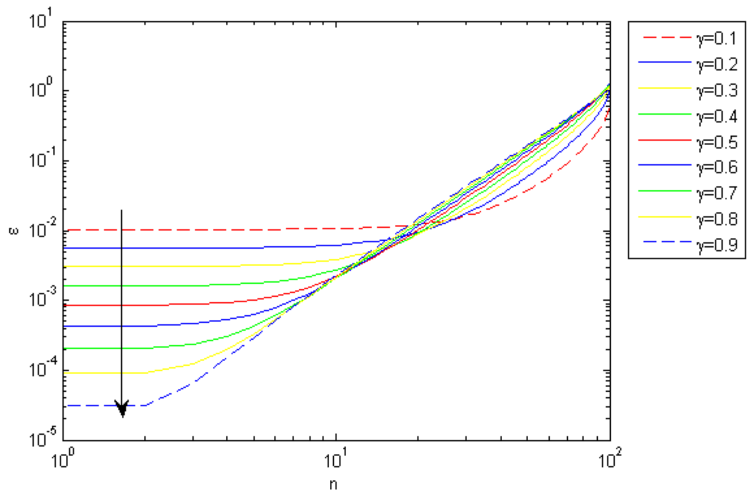



Figure 2.48: The absolute error in using the RL1 scheme, Equation (2.270), to approximate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^{2.5}$, at the time $t = 1.0$, using 100 time steps for $n = 1, \dots, 100$ and $\gamma = 0.1, \dots, 0.9$. The value $\gamma$ increases in the direction of the arrow.

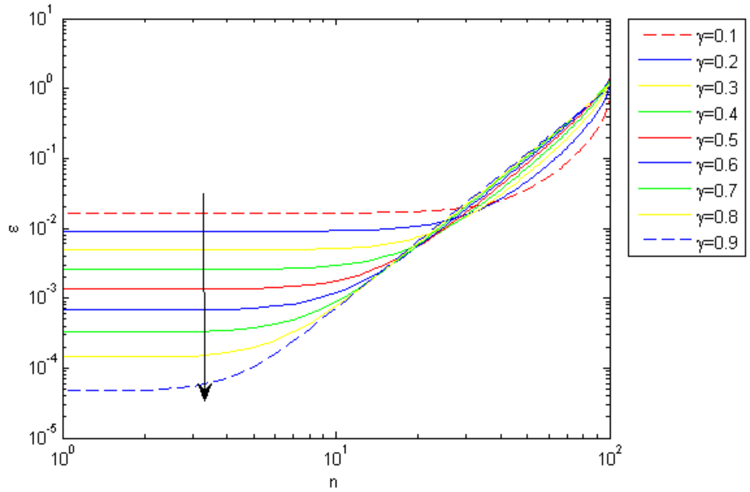



Figure 2.49: The absolute error in using the RL1 scheme, in Equation (2.270), to evaluate the fractional derivative of order $1-\gamma$ for function $f(t) = t^3$, at the time $t = 1.0$. Results are shown for $j = 100$, $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

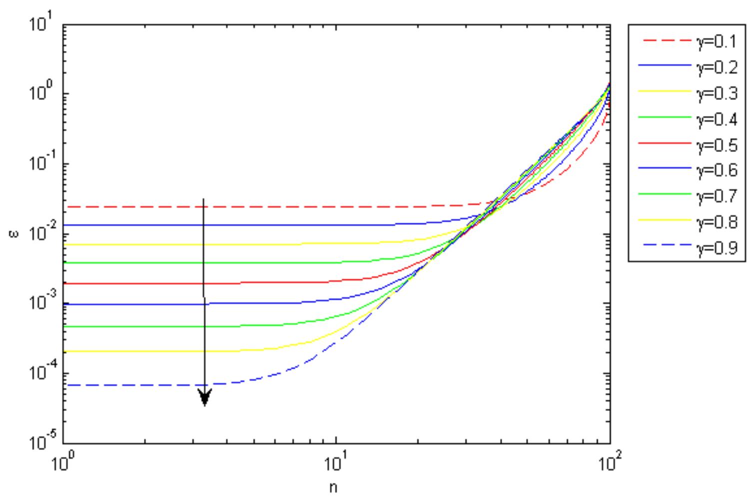



Figure 2.50: The absolute error in using the RL1 scheme, Equation (2.270), to approximate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^{3.5}$, at time $t = 1.0$, using 100 time steps and for $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

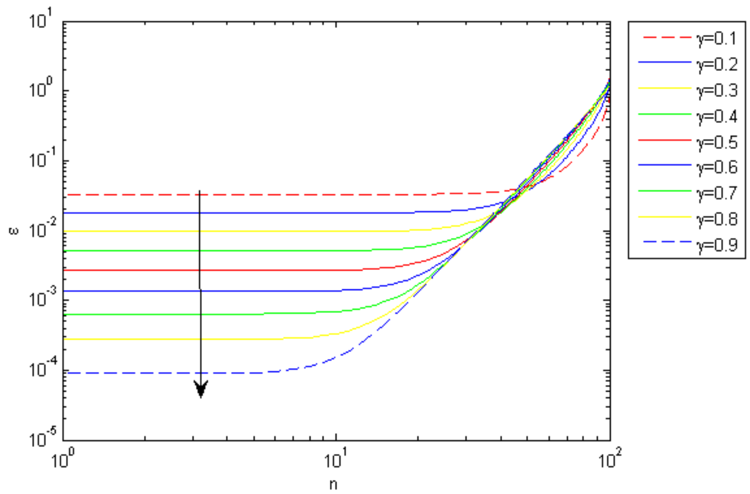



Figure 2.51: The absolute error in using the RL1 scheme, in Equation (2.270), to evaluate the fractional derivative of order $1-\gamma$ for function $f(t)=t^4$, at time $t=1.0$. Results are shown for $j=100$, $n=1,\ldots,j$ and $\gamma=0.1,\ldots,0.9$ where $\gamma$ increases in the direction of the arrow.

Table 2.13: The comparison of the absolute error in the RL1 approximate estimate of the fractional derivative of order $1-\gamma$ of the functions $f(t)=t^k$, $k=2,2.5,3,3.5$, and 4 at time $t=1.0$ where $\gamma=0.1,...,0.9$, $n=100$, $j=100$ and $\Delta t=0.01$.

| $\gamma$ | $f(t)=t^2$ | $f(t)=t^{2.5}$ | $f(t)=t^3$ | $f(t)=t^{3.5}$ | $f(t)=t^4$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 5.914e–01 | 6.790e–01 | 7.604e–01 | 8.369e–01 | 9.0951e–01 |
| $\gamma=0.2$ | 9.524e–01 | 1.076e–00 | 1.188e–00 | 1.290e–00 | 1.386e–00 |
| $\gamma=0.3$ | 1.157e–00 | 1.288e–00 | 1.405e–00 | 1.510e–00 | 1.607e–00 |
| $\gamma=0.4$ | 1.255e–00 | 1.375e–00 | 1.482e–00 | 1.578e–00 | 1.664e–00 |
| $\gamma=0.5$ | 1.280e–00 | 1.382e–00 | 1.470e–00 | 1.549e–00 | 1.619e–00 |
| $\gamma=0.6$ | 1.258e–00 | 1.337e–00 | 1.405e–00 | 1.463e–00 | 1.515e–00 |
| $\gamma=0.7$ | 1.208e–00 | 1.262e–00 | 1.309e–00 | 1.348 e–00 | 1.383e–00 |
| $\gamma=0.8$ | 1.139e–00 | 1.172e–00 | 1.198e–00 | 1.220e–00 | 1.239e–00 |
| $\gamma=0.9$ | 1.062e–00 | 1.074e–00 | 1.0836e–00 | 1.091e–00 | 1.096e–00 |

From the results given in Tables 2.12 and 2.13 and Figures 2.39 – 2.43, and Figures 2.47 – 2.51, we see that the $L1^*$ scheme and RL1 scheme are not good approximations, since the error increases as the value of $n$ increases for each value of $\gamma$.

In the next sections, we consider the regression approximation to approximate the early history. We also estimate the error given by these approximations.

## 2.11 Regression Methods

In this section, we consider regression methods to approximate the early history given in Equation (2.9). Now we use regression to approximate $f'(\tau)$ in Equation (2.9) in the interval $\tau = 0$ to $\tau = T$ instead of ignoring this contribution to the integral as in short memory approach. We begin by rewriting the integral in Equation (2.9) as

$$\int_0^t f'(\tau)(t-\tau)^{-p} d\tau = \int_0^T f'(\tau)(t-\tau)^{-p} d\tau + \int_T^t f'(\tau)(t-\tau)^{-p} d\tau, \tag{2.275}$$

where $T = n\Delta t$ and $t = j\Delta t$. We then have

$$\frac{d^p f(t)}{dt^p} = \frac{t^{-p}}{\Gamma(1-p)} f_0 + \frac{1}{\Gamma(1-p)} \int_0^T f'(\tau)(t-\tau)^{-p} d\tau + \frac{1}{\Gamma(1-p)} \int_T^t f'(\tau)(t-\tau)^{-p} d\tau. \tag{2.276}$$

In the following analysis we introduce three different functions to approximate the function $f(\tau)$ in the first integral in this equation.

### 2.11.1 Linear Regression Approximation

To evaluate the first integral in Equation (2.275) we first used the Linear Regression to approximate the function $f(\tau)$ for $0 \leq \tau \leq T$, that is with

$$f(\tau) = \beta_0 + \beta_1 \tau, \tag{2.277}$$

where $\beta_1$ is the slope and $\beta_0$ is the intercept point of the regression line. We used a piecewise linear approximation for the second integral as in the L1 approximation. We then have

$$\begin{aligned}\int_0^t f'(\tau)(t-\tau)^{-p} d\tau &= \beta_1 \int_0^T (t-\tau)^{-p} d\tau + \sum_{k=n}^{j-1} \int_{k\Delta t}^{(k+1)\Delta t} f'(\tau)(t-\tau)^{-p} d\tau \\ &= \frac{\beta_1}{1-p}\left[t^{1-p} - (t-T)^{1-p}\right] + \frac{\Delta t^{-p}}{1-p} \sum_{k=n}^{j-1} (f_k - f_{k+1}) \left[(j-(k+1))^{1-p} - (j-k)^{1-p}\right].\end{aligned} \tag{2.278}$$

The approximation of the fractional derivative, which will be denoted as LRA, is then given by

$$\left[\frac{d^p f(t)}{dt^p}\right|_{LRA} = \frac{t^{-p}}{\Gamma(1-p)} f_0 + \frac{\beta_1}{\Gamma(2-p)} \left(t^{1-p} - (t-T)^{1-p}\right) + \frac{\Delta t^{-p}}{\Gamma(2-p)} \sum_{k=n}^{j-1} (f_k - f_{k+1}) \left[(j-(k+1))^{1-p} - (j-k)^{1-p}\right]. \tag{2.279}$$

Using Equation (2.195), then Equation (2.279) can be rewritten as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{LRA}^{j} = \left[\frac{d^p f(t)}{dt^p}\right|_{L1^*}^{j} + \frac{\Delta t^{1-p} \beta_1}{\Gamma(2-p)} \left(j^{1-p} - (j-n)^{1-p}\right). \tag{2.280}$$

The accuracy of the LRA scheme was tested by comparing the exact value of the fractional derivative of the function $f(t) = t^k$, for $k = 2, 2.5, 3, 3.5$, and 4, with the value from the LRA approximation. The exact and approximate value of fractional derivative was estimated at time $t = 1$. The error in the fractional derivative estimate using $j = 100$ time steps is shown in Figures 2.52, 2.53, ..., and 2.56 against the value $n$, where $1 \leq n \leq j$, for various values of $\gamma = 0.1, \ldots, 0.9$.

From Table 2.14, and Figures 2.52 – 2.56, we conclude that the maximum error occurs when $n$ approaches $j$. That is as we approximate more history, using regression, the error increases.

From the results shown in Figures 2.52 – 2.56, we conclude that if we do ignore some terms for small $n$ the error does not increase immediately. For example in Figure 2.52 the error only begins to increase for $n > 51$ when $\gamma = 0.1$ and for $n > 47$ when $\gamma = 0.2, 0.3, 0.4$. But in the case $\gamma = 0.5$ the error increases earlier for $n > 9$ and increases for $n > 12$ in the cases of $\gamma = 0.6$ and 0.7. Whilst for the cases $\gamma = 0.8$ and 0.9 the error increases from $n = 0$.

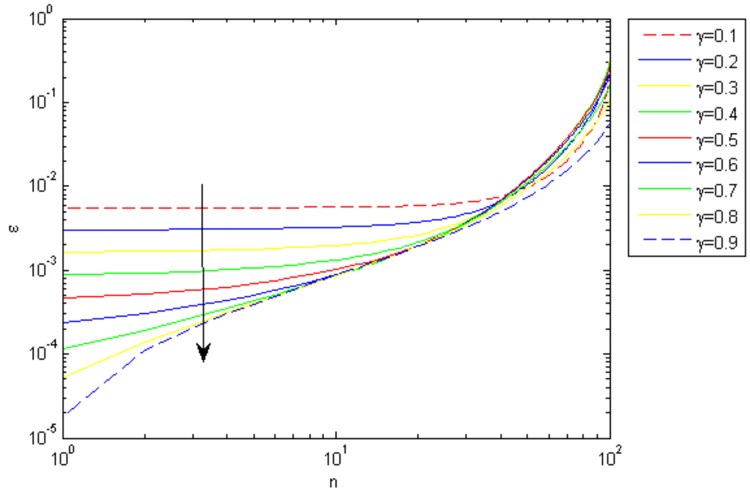



Figure 2.52: The value of the absolute error in using the LRA scheme, Equation (2.279), to approximate the fractional derivative of order $1-\gamma$ of function $f(t) = t^2$, at time $t = 1.0$. The results are shown $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

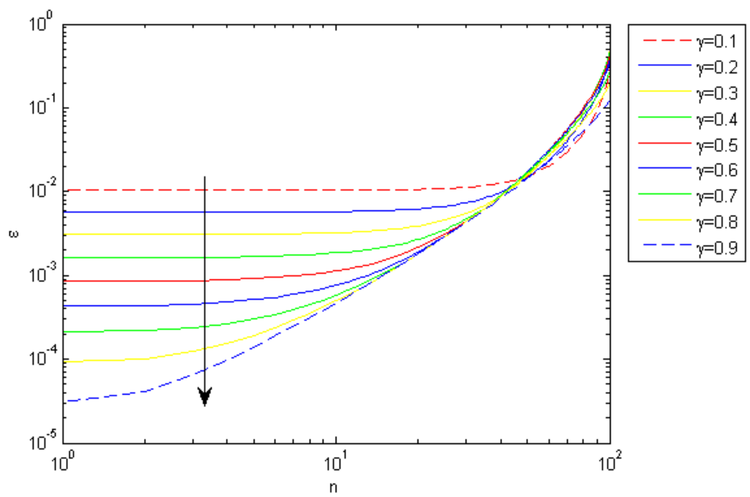



Figure 2.53: The value of the absolute error in using the LRA scheme, Equation (2.279), to estimate the fractional derivative of order $1-\gamma$ of function $f(t) = t^{2.5}$, at time $t = 1.0$. The results are shown for $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

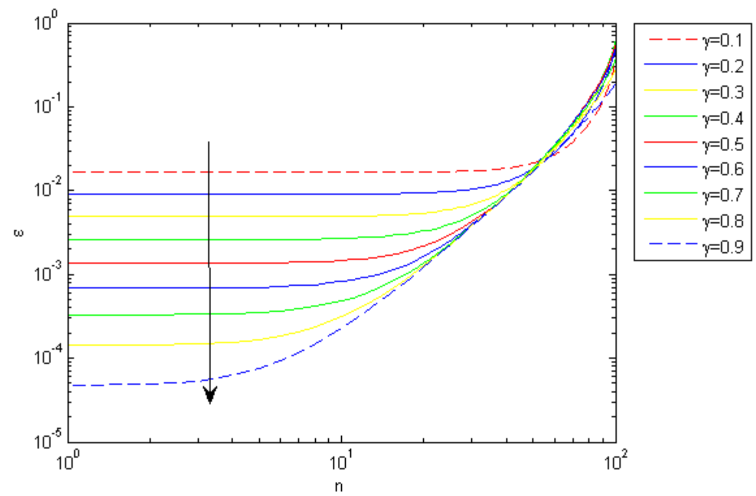



Figure 2.54: The value of the absolute error by using Equation (2.279), to evaluate the fractional derivative of order $1-\gamma$ of function $f(t) = t^3$, at time $t = 1.0$, $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

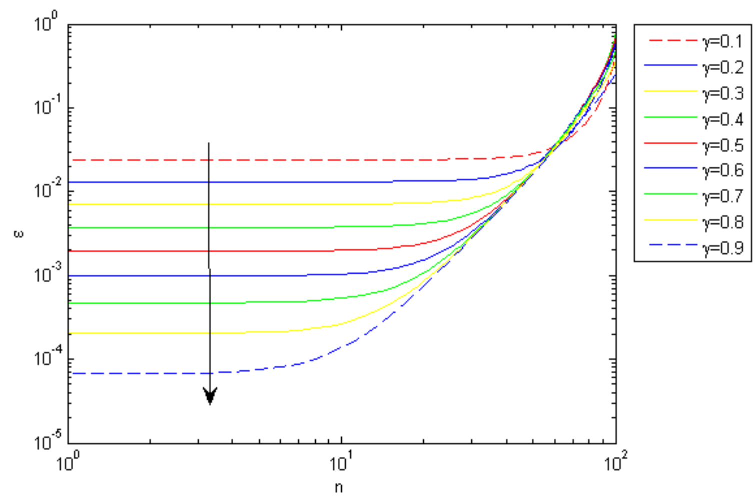



Figure 2.55: The value of the absolute error by using Equation (2.279), to evaluate the fractional derivative of order $1-\gamma$ of function $f(t) = t^{3.5}$, at time $t = 1.0$, $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

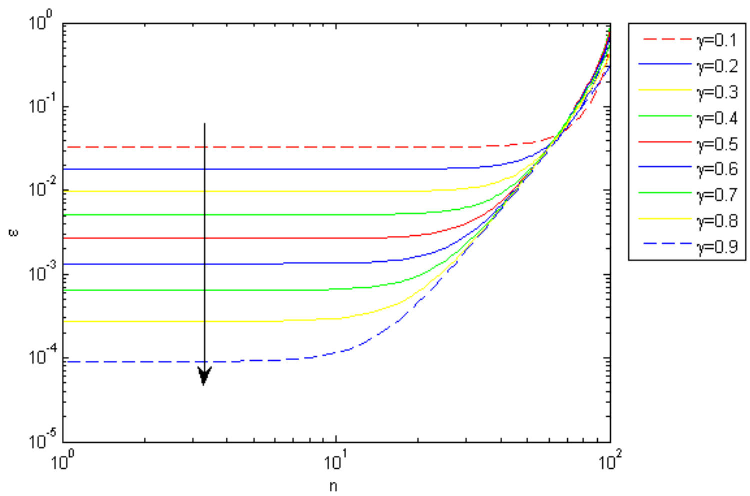



Figure 2.56: The value of the absolute error in using the LRA scheme, Equation (2.279), to evaluate the fractional derivative of order $1-\gamma$ of function $f(t) = t^4$, at time $t = 1.0$, $n = 1, \ldots, 100$. Results are shown for $\gamma = 0.1, \ldots, 0.9$ where $\gamma$ increases in the direction of the arrow.

Table 2.14: The comparison of the absolute error in the LRA scheme estimate of the fractional derivative of order $1-\gamma$ of the functions $f(t) = t^k$, $k = 2, 2.5, 3, 3.5$, and 4 at the time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 100$, $j = 100$, and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^{2.5}$ | $f(t) = t^3$ | $f(t) = t^{3.5}$ | $f(t) = t^4$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 2.112e–01 | 3.200e–01 | 4.240e–01 | 5.223e–01 | 6.152e–01 |
| $\gamma = 0.2$ | 3.099e–01 | 4.690e–01 | 6.190e–01 | 7.586e–01 | 8.883e–01 |
| $\gamma = 0.3$ | 3.396e–01 | 5.158e–01 | 6.810e–01 | 8.338e–01 | 9.744e–01 |
| $\gamma = 0.4$ | 3.253e–01 | 4.978e–01 | 6.595e–01 | 8.083e–01 | 9.444e–01 |
| $\gamma = 0.5$ | 2.847e–01 | 4.420e–01 | 5.895e–01 | 7.249e–01 | 8.482e–01 |
| $\gamma = 0.6$ | 2.309e–01 | 3.667e–01 | 4.951e–01 | 6.128e–01 | 7.198e–01 |
| $\gamma = 0.7$ | 1.720e–01 | 2.845e–01 | 3.920e–01 | 4.910e–01 | 5.809e–01 |
| $\gamma = 0.8$ | 1.135e–01 | 2.030e–01 | 2.903e–01 | 3.714e–01 | 4.451e–01 |
| $\gamma = 0.9$ | 5.888e–02 | 1.270e–01 | 1.958e–01 | 2.606e–01 | 3.200e–01 |

### 2.11.2 Quadratic Regression Approximation

Another way to approximate the first integral in Equation (2.275) is to use the Quadratic Regression to fit the function $f(\tau)$ by

$$f(\tau) = \beta_0 + \beta_1\tau + \beta_2\tau^2, \tag{2.281}$$

in the interval $\tau \in [0, T]$ where $\beta_1$, $\beta_2$ and $\beta_0$ are fitting parameters of the regression line. We again use piecewise linear approximation, as per the L1 scheme, for the integral over $\tau \in [T, t]$.

$$\begin{aligned}\int_0^t f'(\tau)(t-\tau)^{-p}d\tau = \beta_1 \int_0^T (t-\tau)^{-p}d\tau + 2\beta_2 \int_0^T \tau(t-\tau)^{-p}d\tau \\ + \sum_{k=n}^{j-1} \int_{k\Delta t}^{(k+1)\Delta t} f'(\tau)(t-\tau)^{-p}d\tau.\end{aligned} \tag{2.282}$$

Now evaluating the integral, setting $u = t - \tau$, we then have

$$\begin{aligned}\int_0^T \tau(t-\tau)^{-p}d\tau &= -\int_t^{t-T} (t-u)u^{-p}du \\ &= \int_{t-T}^{t} (t-u)u^{-p}du \\ &= \left[ t\frac{u^{1-p}}{1-p} - \frac{u^{2-p}}{2-p} \right|_{t-T}^{t} \\ &= t\frac{t^{1-p}}{1-p} - \frac{t^{2-p}}{2-p} - t\frac{(t-T)^{1-p}}{1-p} + \frac{(t-T)^{2-p}}{2-p} \\ &= \frac{t^{2-p}}{(1-p)(2-p)} + \frac{(t-T)^{1-p}}{(1-p)(2-p)}\left((1-p)(t-T) - (2-p)t\right) \\ &= \frac{1}{(1-p)(2-p)}\left[t^{2-p} - \left(t + (1-p)T\right)(t-T)^{1-p}\right].\end{aligned} \tag{2.283}$$

Using this approximation in Equation (2.9) we have the approximation for the fractional derivative

$$\begin{aligned}\left[\frac{d^p f(t)}{dt^p}\right| &= \frac{t^{-p}}{\Gamma(1-p)}f_0 + \frac{\beta_1}{\Gamma(2-p)}\left[t^{1-p} - (t-T)^{1-p}\right] \\ &+ \frac{2\beta_2}{(1-p)(2-p)\Gamma(2-p)}\left[t^{2-p} - (t+(1-p)T)(t-T)^{1-p}\right] \\ &+ \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=n}^{j-1}(f_k - f_{k+1})\left[(j-(k+1))^{1-p} - (j-k)^{1-p}\right].\end{aligned} \tag{2.284}$$

Using Equation (2.195), then Equation (2.284) can be rewritten in terms of the $L1^*$ scheme as

$$\left[\frac{d^p f(t)}{dt^p}\right|_{QRA} = \left[\frac{d^p f(t)}{dt^p}\right|_{L1^*}^{j} + \frac{\beta_1}{\Gamma(2-p)}\left[t^{1-p} - (t-T)^{1-p}\right] + \frac{2\beta_2}{(1-p)\Gamma(3-p)}\left[(t+(1-p)T)(t-T)^{1-p} - t^{2-p}\right]. \qquad (2.285)$$

We denote this approximation as the QRA scheme. Similar to the LRA scheme, the accuracy of the QRA scheme is estimated by comparing the exact value of the fractional derivative of order $1-\gamma$ of the functions $f(t) = t^k$, where $k = 2, 2.5, 3, 3.5$, and 4, with the value obtained from the QRA approximation. The error is plotted as a function of $n$ on log-log plot in Figures 2.57, 2.58, 2.59, 2.60, and 2.61.

The approximation and the exact values are evaluated for time $t = 1.0$ using 100 time steps, for $n$ changing from 1 to 100, and $\gamma = 0.1, \ldots, 0.9$. In Figures 2.57, 2.58, 2.59, 2.60, and 2.61, we can see the error increases as $n$ increases. For instance we note for $\gamma = 0.3$ the minimum error of $1.72 \times 10^{-5}$ occurs in Figure 2.57. While in Figure 2.61 the minimum error is $1.84 \times 10^{-5}$ for $n = 21$ when $\gamma = 0.8$. From these figures we expect similar behaviour to the LRA scheme except, unlike the LRA scheme, there are for larger $n$ values where the error is smaller than when $n = 0$ as seen in Table 2.16.

The comparison of the absolute errors is also shown in Table 2.15. We note that the maximum error occurs where $\gamma = 0.9$ for functions $f(t) = t^k$ and the minimum error occurs where $\gamma = 0.1$. From the results shown in Figures 2.57 – 2.61, we note that if we ignore some terms for $n$ small, then the error does not increase immediately as $n$ is increased. For example in Figure 2.57 the error increases only when $n > 10$ for $\gamma = 0.1$, and for case $\gamma = 0.9$ the error also only increases when $n > 2$. We note though that the optimal choice $n$ (where the error is smallest) may occur for $n = 0$, as in the $L1^*$, RL1, LRA, but for an intermediate value $n$.

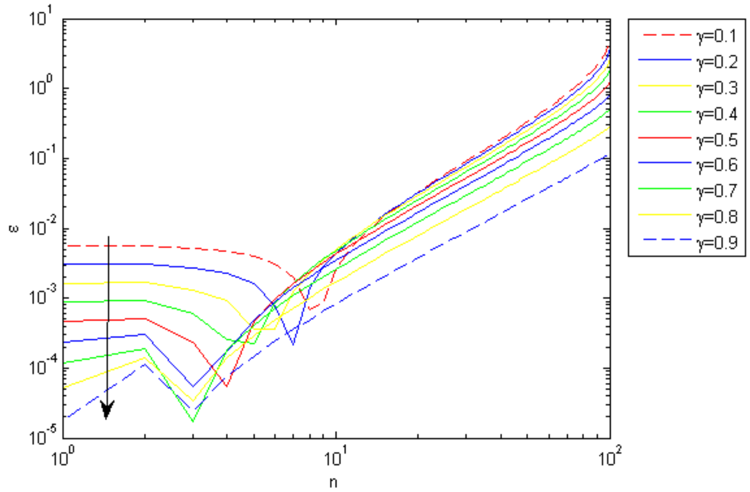



Figure 2.57: The value of the absolute error in using Equation (2.284) to evaluate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^2$ at time $t = 1$. The error increases as $n$ increases for large $n$ and the value of $\gamma$ increases in the direction of the arrow.

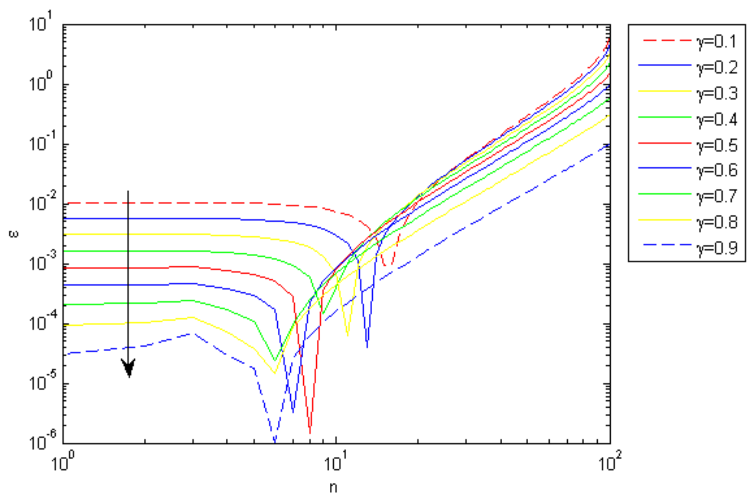



Figure 2.58: The value of the absolute error in evaluating the fractional derivative of order $1-\gamma$ of the function $f(t) = t^{2.5}$ at $t = 1$ by using Equation (2.284). Note as $n$ increases the error increases for large $n$ and the value of $\gamma$ increases in the direction of the arrow.

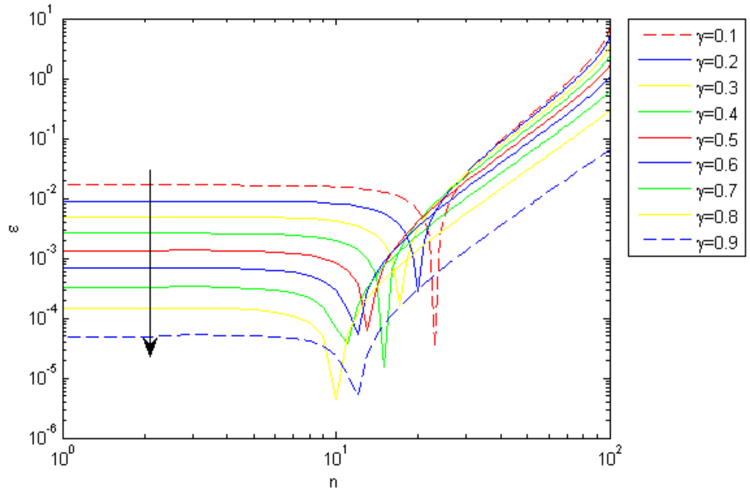



Figure 2.59: The value of the absolute error in evaluating the fractional derivative of order $1-\gamma$ of the function $f(t) = t^3$ at $t = 1$ by using Equation (2.284). Note as $n$ increases the error increases for large $n$ and $\gamma$ increases in the direction of the arrow.

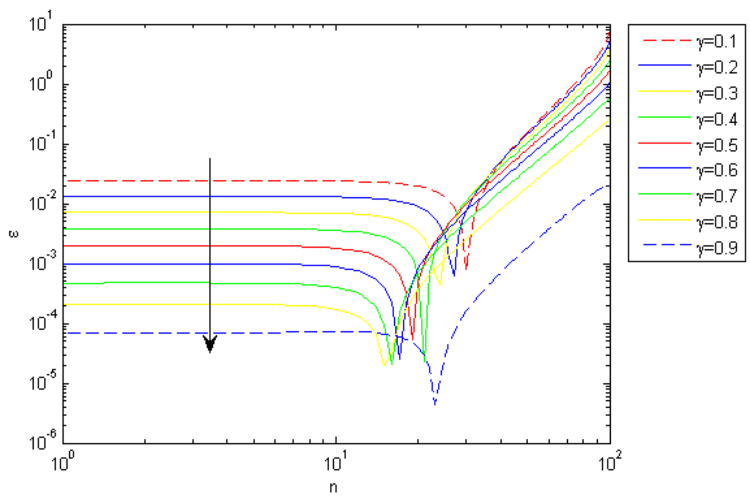



Figure 2.60: The value of the absolute error in evaluating the fractional derivative of order $1-\gamma$ of the function $f(t) = t^{3.5}$ at $t = 1$ by using Equation (2.284). Note as $n$ increases the error increases for large $n$ and the value of $\gamma$ increases in the direction of the arrow.

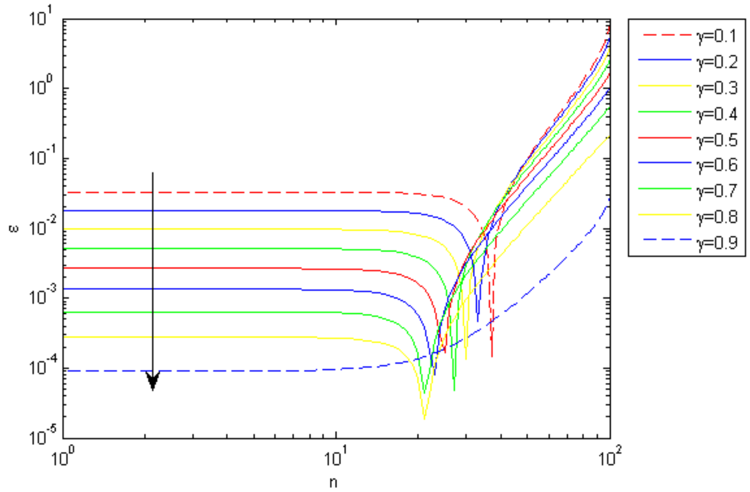



Figure 2.61: The value of the absolute error in using Equation (2.284) to evaluate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^4$ at time $t = 1$, for large $n$ the error increases as $n$ increases. Note $\gamma$ increases in the direction of the arrow.

Table 2.15: The comparison of the absolute error in the QRA scheme estimate of the fractional derivative of order $1-\gamma$ of the functions $f(t) = t^k$, $k = 2, 2.5, 3, 3.5$, and 4 at the time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 100$, $j = 100$, and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^{2.5}$ | $f(t) = t^3$ | $f(t) = t^{3.5}$ | $f(t) = t^4$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 5.268e–00 | 6.721e–00 | 7.630e–00 | 8.160e–00 | 8.428e–00 |
| $\gamma = 0.2$ | 3.795e–00 | 4.806e–00 | 5.415e–00 | 5.747e–00 | 5.887e–00 |
| $\gamma = 0.3$ | 2.695e–00 | 3.384e–00 | 3.780e–00 | 3.976e–00 | 4.035e–00 |
| $\gamma = 0.4$ | 1.880e–00 | 2.336e–00 | 2.582e–00 | 2.686e–00 | 2.695e–00 |
| $\gamma = 0.5$ | 1.279e–00 | 1.568e–00 | 1.710e–00 | 1.753e–00 | 1.733e–00 |
| $\gamma = 0.6$ | 8.387e–01 | 1.008e–00 | 1.077e–00 | 1.082e–00 | 1.046e–00 |
| $\gamma = 0.7$ | 5.174e–01 | 6.014e–01 | 6.214e–01 | 6.014e–01 | 5.570e–01 |
| $\gamma = 0.8$ | 2.848e–01 | 3.089e–01 | 2.952e–01 | 2.599e–01 | 2.124e–01 |
| $\gamma = 0.9$ | 1.180e–01 | 1.003e–01 | 6.413e–02 | 1.958e–02 | 2.812e–02 |

Table 2.16: The comparison minimum absolute error in the QRA scheme estimate of the fractional derivative of order $1-\gamma$ of the functions $f(t)=t^k$, $k=2,2.5,3,3.5$, and 4 at the time $t=1.0$ for $\gamma=0.1,...,0.9$, $j=100$, and $\Delta t=0.01$.

| $\gamma$ | $f(t)=t^2$ | $f(t)=t^{2.5}$ | $f(t)=t^3$ | $f(t)=t^{3.5}$ | $f(t)=t^4$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 6.920e–04 | 9.302e–04 | 3.220e–05 | 7.455e–04 | 1.458e–04 |
| $\gamma=0.2$ | 2.129e–04 | 4.040e–05 | 2.825e–04 | 6.164e–04 | 4.713e–04 |
| $\gamma=0.3$ | 2.695e–04 | 6.070e–05 | 1.589e–04 | 4.404e–04 | 1.368e–04 |
| $\gamma=0.4$ | 3.580e–04 | 1.458e–04 | 1.500e–05 | 2.280e–05 | 4.750e–05 |
| $\gamma=0.5$ | 5.330e–05 | 1.430e–06 | 6.080e–05 | 5.480e–05 | 1.697e–04 |
| $\gamma=0.6$ | 5.530e–05 | 3.240e–06 | 5.410e–05 | 2.500e–05 | 7.900e–05 |
| $\gamma=0.7$ | 1.740e–05 | 2.390e–05 | 3.860e–05 | 2.020e–05 | 4.480e–05 |
| $\gamma=0.8$ | 3.470e–05 | 1.470e–05 | 4.350e–06 | 2.010e–05 | 1.840e–05 |
| $\gamma=0.9$ | 1.780e–05 | 1.050e–06 | 5.160e–06 | 4.400e–06 | 9.050e–05 |

### 2.11.3 Nonlinear Regression Approximation

To evaluate the first integral in Equation (2.275) we use the Nonlinear Regression model to approximate the function $f(\tau)$

$$y=\beta_0+\beta_1\tau^{1-p}, \tag{2.286}$$

for $0\le\tau\le T$. Here $\beta_1$ and $\beta_0$ are constant parameters. The solution of the fractional subdiffusion equation is in term Mittag–Leffler function which is the power series of $t^{1-p}$, so we choose the same type of function as in Equation (2.286) to approximate the function $f(\tau)$. As in the other schemes in this section we again use the piecewise linear approximation for the integral over $T\le\tau\le t$. Splitting the integrals into two, we have

$$\int_0^t f'(\tau)(t-\tau)^{-p}d\tau=(1-p)\beta_1\int_0^T \tau^{-p}(t-\tau)^{-p}d\tau+\sum_{k=n}^{j-1}\int_{k\Delta t}^{(k+1)\Delta t} f'(\tau)(t-\tau)^{-p}d\tau. \tag{2.287}$$

We now evaluate the integral $\int_0^T \tau^{-p}(t-\tau)^{-p}d\tau$, by setting $\tau = tu$ and simplifying

$$\begin{aligned}\int_0^T \tau^{-p}(t-\tau)^{-p}d\tau &= \int_0^{T/t} t^{-p}u^{-p}(t-tu)^{-p}t du \\ &= t^{1-2p}\int_0^{T/t} u^{-p}(1-u)^{-p}du \\ &= t^{1-2p}B(1-p,1-p)I_{\frac{T}{t}}(1-p,1-p),\end{aligned} \tag{2.288}$$

where $I_{\frac{T}{t}}(1-p,1-p)$ is the Incomplete Beta function (Thompson, Pearson, Comrie & Hartley 1941, Temme 1975)

$$I_{\frac{T}{t}}(1-p,1-p) = \frac{1}{B(1-p,1-p)}\int_0^{T/t} u^{-p}(1-u)^{-p}du, \tag{2.289}$$

and the Beta function (Abramowitz, Stegun et al. 1966) is given by

$$B(1-p,1-p) = \int_0^1 u^{-p}(1-u)^{-p}du = \frac{(\Gamma(1-p))^2}{\Gamma(2-2p)}. \tag{2.290}$$

Using Equation (2.288), in Equation (2.9), we then have the approximation

$$\begin{aligned}\left[\frac{d^p f(t)}{dt^p}\right| &= \frac{t^{-p}}{\Gamma(1-p)}f_0 + \frac{\beta_1}{\Gamma(2-p)}t^{1-2p}B(1-p,1-p)I_{\frac{T}{t}}(1-p,1-p) \\ &+ \frac{\Delta t^{-p}}{\Gamma(2-p)}\sum_{k=n}^{j-1}(f_k - f_{k+1})\left[(j-(k+1))^{1-p} - (j-k)^{1-p}\right].\end{aligned} \tag{2.291}$$

Now using Equation (2.195), Equation (2.291) simplifies to

$$\left[\frac{d^p f(t)}{dt^p}\right|_{NLRA} = \left[\frac{d^p f(t)}{dt^p}\right|_{L1^*}^{j} + \frac{\beta_1}{\Gamma(2-p)}t^{1-2p}B(1-p,1-p)I_{\frac{T}{t}}(1-p,1-p). \tag{2.292}$$

We denote this approximation as the NLRA scheme. Similar to the LRA scheme and the QRA scheme, the estimate of the error was found by comparing the exact value of the fractional derivative of order $1-\gamma$ for functions $f(t) = t^k$, where $k = 2, 2.5, 3, 3.5$, and 4, with the value obtained from the NLRA approximation scheme. The error is plotted as a function of $n$ on log-log plot in Figures 2.62 – 2.66. The approximation and the exact value are evaluated for time $t = 1.0$ using 100 time steps with $n$ changing from 1 to 100 for $\gamma = 0.1, \ldots, 0.9$. We can see in Figures 2.62, 2.63, 2.64, 2.65, and 2.66 the error increases as $n$ increases, for large $n$. We also note in Table 2.17 that the maximum error occurs when $\gamma = 0.9$ for each function and the minimum error occurs when $\gamma = 0.1$.

In Figure 2.62 the error is still the same where $n$ is small, we see for the value $\gamma = 0.1, \ldots, 0.6$ the error increases where $n > 3$. Similar to the QRA scheme, we see there are some values of $n$ which give smaller errors than if we use the full L1 scheme. The smaller error of $5.001 \times 10^{-4}$ occurs for $n = 26$ when $\gamma = 0.6$ and when $n = 96$ for $\gamma = 0.4$ and is $8.042 \times 10^{-3}$. We also see the error increases where $n > 7$ for $\gamma = 0.7$ and for $\gamma = 0.8, 0.9$ when $n > 2$.

From results shown in Figures 2.62 through to 2.66 and Table 2.18, we see for some values of $\gamma$ there is a smaller error than when intermediate values of $n$ are used rather than $n = 0$. For example in Figure 2.66 the smallest error occurs when $n = 26$ and $\gamma = 0.5$ which is $1.563 \times 10^{-6}$.

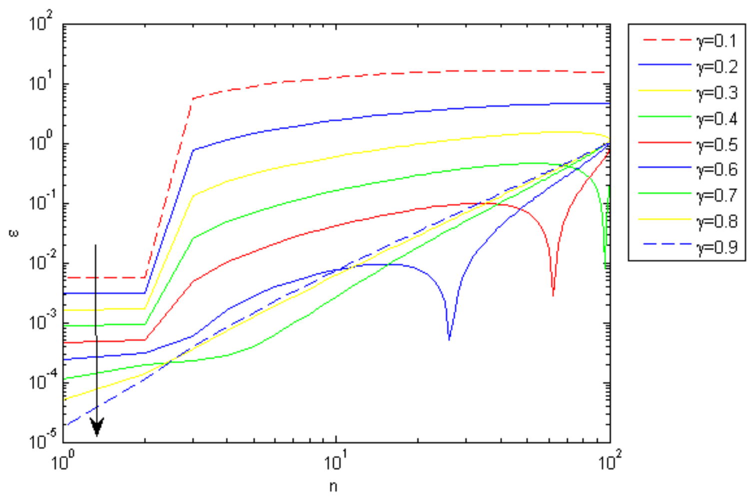



Figure 2.62: The value of the absolute error in using the NLRA scheme, Equation (2.291), to approximate the fractional derivative of order $1 - \gamma$ of the function $f(t) = t^2$ at time $t = 1.0$. Here 100 time steps were taken with $n$ varying from 1 to 100 and $\gamma = 0.1, \ldots, 0.9$. The error increases as $n$ increases and the value of $\gamma$ increases in the direction of the arrow.

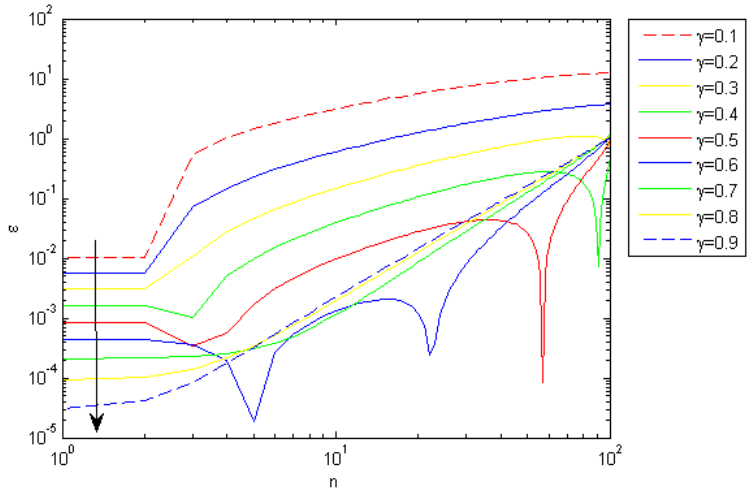



Figure 2.63: The value of the absolute error in evaluating the fractional derivative of order $1-\gamma$ of the function $f(t)=t^{2.5}$, at time $t=1.0$ by using Equation (2.291). The results are shown for $j=100$, $n=1,\ldots,j$ and $\gamma=0.1,\ldots,0.9$, and the error increase as $n$ increases and the value of $\gamma$ increases in the direction of the arrow.

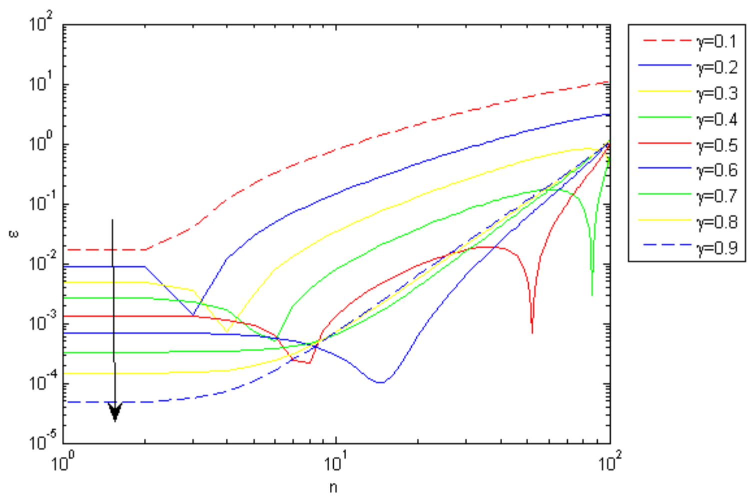



Figure 2.64: The value of the absolute error in evaluating the fractional derivative of order $1-\gamma$ of the function $f(t)=t^{3}$, at time $t=1.0$ by using Equation (2.291). The results are shown for $j=100$, $n=1,\ldots,j$ and $\gamma=0.1,\ldots,0.9$, and the error increase as $n$ increases and the value of $\gamma$ increases in the direction of the arrow.

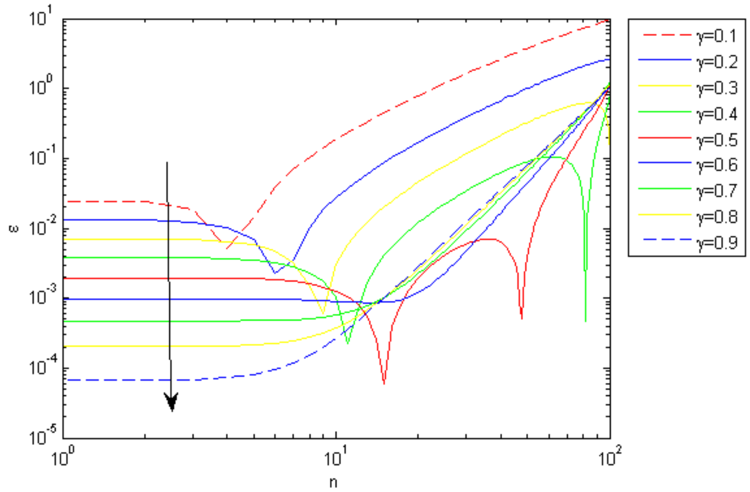



Figure 2.65: The value of the absolute error in evaluating the fractional derivative of order $1-\gamma$ of the function $f(t) = t^{3.5}$, at time $t = 1.0$ by using Equation (2.291). The results are shown for $j = 100$, $n = 1, \ldots, j$ and $\gamma = 0.1, \ldots, 0.9$, and the error increase as $n$ increases. Note $\gamma$ increases in the direction of the arrow.

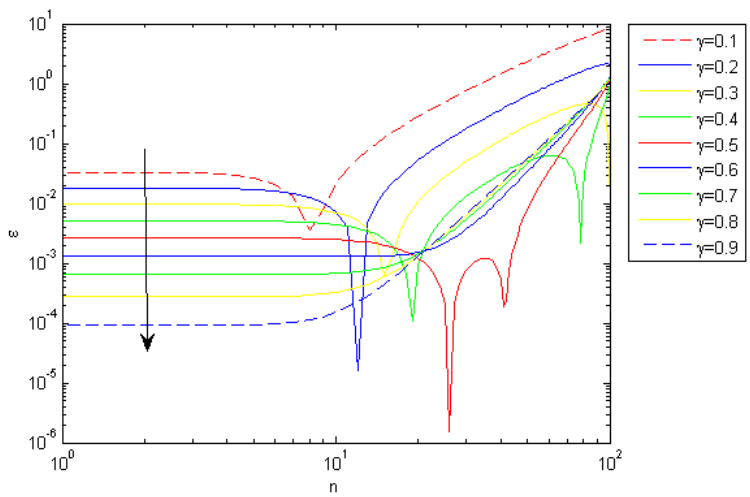



Figure 2.66: The value of the absolute error in using Equation (2.291) to evaluate the fractional derivative of order $1-\gamma$ of the function $f(t) = t^4$, at time $t = 1.0$. Results shown for 100 time steps, $n = 1, \ldots, 100$ and $\gamma = 0.1, \ldots, 0.9$ and $\gamma$ increases in the direction of the arrow.

Table 2.17: The comparison of the absolute error in the estimate of the fractional derivative of order $1-\gamma$ using the NLRA scheme on the functions $f(t) = t^k$, $k = 2, 2.5, 3, 3.5$, and 4 at the time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 100$, $j = 100$, and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^{2.5}$ | $f(t) = t^3$ | $f(t) = t^{3.5}$ | $f(t) = t^4$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 15.74e–00 | 13.34e–00 | 11.50e–00 | 10.04e–00 | 8.852e–00 |
| $\gamma = 0.2$ | 4.623e–00 | 3.759e–00 | 3.072e–00 | 2.509e–00 | 2.039e–00 |
| $\gamma = 0.3$ | 1.152e–00 | 7.344e–01 | 3.899e–01 | 9.952e–02 | 1.498e–01 |
| $\gamma = 0.4$ | 2.385e–01 | 4.767e–01 | 6.786e–01 | 8.525e–01 | 1.005e–00 |
| $\gamma = 0.5$ | 8.214e–01 | 9.719e–01 | 1.101e–00 | 1.214e–00 | 1.313e–00 |
| $\gamma = 0.6$ | 1.049 e–00 | 1.148e–00 | 1.233e–00 | 1.307e–00 | 1.371e–00 |
| $\gamma = 0.7$ | 1.112e–00 | 1.175e–00 | 1.228e–00 | 1.274e–00 | 1.315e–00 |
| $\gamma = 0.8$ | 1.095e–00 | 1.131e–00 | 1.160e–00 | 1.186e–00 | 1.207e–00 |
| $\gamma = 0.9$ | 1.041e–00 | 1.055e–00 | 1.066e–00 | 1.074e–00 | 1.081e–00 |

Table 2.18: The comparison minimum absolute error in the NLRA scheme estimate of the fractional derivative of order $1-\gamma$ of the functions $f(t) = t^k$, $k = 2, 2.5, 3, 3.5$, and 4 at the time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $j = 100$, and $\Delta t = 0.01$.

| $\gamma$ | $f(t) = t^2$ | $f(t) = t^{2.5}$ | $f(t) = t^3$ | $f(t) = t^{3.5}$ | $f(t) = t^4$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 5.533e–03 | 1.304e–02 | 1.652e–02 | 5.234e–03 | 3.607e–04 |
| $\gamma = 0.2$ | 3.029e–03 | 5.660e–03 | 1.413e–03 | 2.297e–03 | 1.640e–05 |
| $\gamma = 0.3$ | 1.639e–03 | 3.058e–03 | 7.133e–04 | 6.099e–04 | 6.175e–04 |
| $\gamma = 0.4$ | 8.755e–04 | 1.035e–03 | 4.974e–04 | 2.274e–04 | 1.051e–04 |
| $\gamma = 0.5$ | 4.598e–04 | 8.360e–05 | 2.200e–04 | 5.950e–05 | 1.560e–06 |
| $\gamma = 0.6$ | 2.354e–04 | 1.890e–05 | 1.021e–04 | 8.611e–04 | 1.314e–03 |
| $\gamma = 0.7$ | 1.153e–04 | 2.100e–04 | 3.291e–04 | 4.719e–04 | 6.381e–04 |
| $\gamma = 0.8$ | 5.150e–05 | 9.250e–05 | 1.436e–04 | 2.045e–04 | 2.750e–04 |
| $\gamma = 0.9$ | 1.780e–05 | 3.130e–05 | 4.800e–05 | 6.780e–05 | 9.050e–05 |

In Tables 2.14, 2.15 and 2.17 we obtained results for the estimate of the fractional derivative of the functions $f(t) = t^k$, $k = 2, 2.5, 3, 3.5$, and 4 at time $t = 1.0$, if we set $n = j$. We see the minimum error occurs for $\gamma = 0.9$ and the maximum error occurs for $\gamma = 0.1$. From the results given in Figures 2.52 – 2.56, Figures 2.57 – 2.61, and Figures 2.62 – 2.66, we see that the LRA scheme is a better approximation as overall it introduces less error as the value of $n$ increases for each value of $\gamma$. However, in the NLRA and QRA schemes for some values of $n$ a smaller error occurs when a specific intermediate value of $n$ is used, as shown in Tables 2.16 and 2.18.

## 2.12 Results and Discussion

In this section, we compare the results from the modifications of L1 scheme with the L1 scheme and Romberg integration, and also we compare the results from the memory principle effect scheme with Regression methods. Each scheme was compared by looking at the error in their approximations of the fractional derivative of order $1-\gamma$ of the function $f(t)$ given in Equation (2.7), for $\gamma = 0.1, ..., 0.9$ at the time $t = 1.0$.

### The L1, C1, C2, C3 and Romberg Integration Schemes

The fractional derivative approximations given by Equations (2.2), (2.12), (2.60), (2.75), (2.88), and (2.191), were compared. From Tables 2.19 through to 2.22 we see that the C2 approximation introduces the smallest error in most cases, for $0 < \gamma < 1$, when compared with the L1, C1, C3 and Romberg integration (where $k = 2$) schemes. It was only in the cases $\gamma = 0.8$, and $\gamma = 0.9$, for all functions where Romberg integration performed better. In Table 2.23 we see the smallest error appear for the C2 scheme where $\gamma = 0.1, \ldots, 0.5$, whilst for $\gamma = 0.6, \ldots, 0.9$ the smallest error occurs for the Romberg integration scheme.

Improvement in these results my be made if we use higher order Romberg approximation ($k > 2$) but this is left to future work.

Table 2.19: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of function $f(t) = t^2$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| $\gamma$ | GL | L1 | C1 | C2 | C3 | RInt (k=2) |
|---|---|---|---|---|---|---|
| $\gamma = 0.1$ | 8.60e–03 | 4.98e–03 | 7.96e–03 | 2.45e–03 | 4.98e–03 | 4.89e–03 |
| $\gamma = 0.2$ | 7.92e–03 | 2.70e–03 | 4.63e–03 | 1.33e–03 | 2.70e–03 | 2.58e–03 |
| $\gamma = 0.3$ | 7.09e–03 | 1.45e–03 | 2.67e–03 | 7.27e–04 | 1.45e–03 | 1.33e–03 |
| $\gamma = 0.4$ | 6.14e–03 | 7.67e–04 | 1.53e–03 | 3.99e–04 | 7.67e–04 | 6.70e–04 |
| $\gamma = 0.5$ | 5.12e–03 | 3.99e–04 | 8.65e–04 | 2.19e–04 | 3.99e–04 | 3.26e–04 |
| $\gamma = 0.6$ | 4.07e–03 | 2.03e–04 | 4.78e–04 | 1.19e–04 | 2.02e–04 | 1.52e–04 |
| $\gamma = 0.7$ | 3.00e–03 | 9.84e–05 | 2.53e–04 | 6.22e–05 | 9.83e–05 | 6.58e–05 |
| $\gamma = 0.8$ | 1.95e–03 | 4.36e–05 | 1.22e–04 | 2.98e–05 | 4.36e–05 | 2.52e–05 |
| $\gamma = 0.9$ | 9.44e–04 | 1.49e–05 | 4.50e–05 | 1.10e–05 | 1.49e–05 | 7.24e–06 |

Table 2.20: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of function $f(t) = t^3$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| $\gamma$ | GL | L1 | C1 | C2 | C3 | RInt (k=2) |
|---|---|---|---|---|---|---|
| $\gamma = 0.1$ | 2.34e–02 | 1.49e–02 | 2.37e–02 | 7.29e–03 | 1.48e–02 | 1.46e–02 |
| $\gamma = 0.2$ | 1.97e–02 | 8.06e–03 | 1.37e–02 | 3.94e–03 | 8.02e–03 | 7.71e–03 |
| $\gamma = 0.3$ | 1.63e–02 | 4.31e–03 | 7.88e–03 | 2.14e–03 | 4.29e–03 | 3.98e–03 |
| $\gamma = 0.4$ | 1.31e–02 | 2.27e–03 | 4.47e–03 | 1.17e–03 | 2.26e–03 | 2.00e–03 |
| $\gamma = 0.5$ | 1.02e–02 | 1.17e–03 | 2.50e–03 | 6.31e–04 | 1.17e–03 | 9.75e–04 |
| $\gamma = 0.6$ | 7.61e–03 | 5.88e–04 | 1.36e–03 | 3.36e–04 | 5.86e–04 | 4.53e–04 |
| $\gamma = 0.7$ | 5.28e–03 | 2.81e–04 | 7.04e–04 | 1.72e–04 | 2.80e–04 | 1.97e–04 |
| $\gamma = 0.8$ | 3.25e–03 | 1.22e–04 | 3.30e–04 | 8.02e–05 | 1.21e–04 | 7.54e–05 |
| $\gamma = 0.9$ | 1.49e–03 | 4.05e–05 | 1.18e–04 | 2.87e–05 | 4.03e–05 | 2.16e–05 |

Table 2.21: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of function $f(t)=t^4$ at time $t=1.0$ for $\gamma=0.1,...,0.9$ and $\Delta t=0.01$.

| $\gamma$ | GL | L1 | C1 | C2 | C3 | RInt (k=2) |
|---|---|---|---|---|---|---|
| $\gamma=0.1$ | 4.44e–02 | 2.97e–02 | 4.71e–02 | 1.45e–02 | 2.94e–02 | 2.91e–02 |
| $\gamma=0.2$ | 3.58e–02 | 1.60e–02 | 2.72e–02 | 7.80e–03 | 1.59e–02 | 1.54e–02 |
| $\gamma=0.3$ | 2.83e–02 | 8.55e–03 | 1.56e–02 | 4.22e–03 | 8.48e–03 | 7.93e–03 |
| $\gamma=0.4$ | 2.18e–02 | 4.49e–03 | 8.78e–03 | 2.28e–03 | 4.45e–03 | 3.99e–03 |
| $\gamma=0.5$ | 1.63e–02 | 2.31e–03 | 4.87e–03 | 1.23e–03 | 2.29e–03 | 1.94e–03 |
| $\gamma=0.6$ | 1.17e–02 | 1.15e–03 | 2.62e–03 | 6.48e–04 | 1.14e–03 | 9.03e–04 |
| $\gamma=0.7$ | 7.82e–03 | 5.46e–04 | 1.34e–03 | 3.27e–04 | 5.41e–04 | 3.92e–04 |
| $\gamma=0.8$ | 4.63e–03 | 2.34e–04 | 6.19e–04 | 1.50e–04 | 2.31e–04 | 1.50e–04 |
| $\gamma=0.9$ | 2.05e–03 | 7.64e–05 | 2.18e–04 | 5.27e–05 | 7.57e–05 | 4.31e–05 |

Table 2.22: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of function $f(t)=1-e^t+t^3$ at time $t=1.0$ for $\gamma=0.1,...,0.9$ and $\Delta t=0.01$.

| $\gamma$ | GL | L1 | C1 | C2 | C3 | RInt (k=2) |
|---|---|---|---|---|---|---|
| $\gamma=0.1$ | 1.21e–02 | 8.14e–03 | 1.30e–02 | 3.99e–03 | 8.10e–03 | 7.992e–03 |
| $\gamma=0.2$ | 9.61e–03 | 4.41e–03 | 7.50e–03 | 2.16e–03 | 4.39e–03 | 4.216e–03 |
| $\gamma=0.3$ | 7.35e–03 | 2.35e–03 | 4.30e–03 | 1.17e–03 | 2.34e–03 | 2.177e–03 |
| $\gamma=0.4$ | 5.39e–03 | 1.24e–03 | 2.44e–03 | 6.36e–04 | 1.23e–03 | 1.095e–03 |
| $\gamma=0.5$ | 3.75e–03 | 6.40e–04 | 1.36e–03 | 3.44e–04 | 6.37e–04 | 5.330e–04 |
| $\gamma=0.6$ | 2.43e–03 | 3.21e–04 | 7.38e–04 | 1.83e–04 | 3.19e–04 | 2.478e–04 |
| $\gamma=0.7$ | 1.42e–03 | 1.53e–04 | 3.81e–04 | 9.31e–05 | 1.52e–04 | 1.075e–04 |
| $\gamma=0.8$ | 6.94e–04 | 6.59e–05 | 1.77e–04 | 4.31e–05 | 6.56e–05 | 4.124e–05 |
| $\gamma=0.9$ | 2.32e–04 | 2.18e–05 | 6.30e–05 | 1.53e–05 | 2.17e–05 | 1.181e–05 |

Table 2.23: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of function $f(t) = 1 + t^{\gamma}$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$ and $\Delta t = 0.01$.

| $\gamma$ | GL | L1 | C1 | C2 | C3 | RInt (k=2) |
|---|---|---|---|---|---|---|
| $\gamma = 0.1$ | 1.60e–04 | 4.52e–04 | 7.27e–04 | 3.40e–04 | 3.40e–04 | 4.428e–04 |
| $\gamma = 0.2$ | 4.10e–04 | 4.37e–04 | 7.54e–04 | 3.29e–04 | 3.29e–04 | 4.157e–04 |
| $\gamma = 0.3$ | 5.83e–04 | 3.08e–04 | 5.75e–04 | 2.34e–04 | 2.34e–04 | 2.820e–04 |
| $\gamma = 0.4$ | 6.40e–04 | 1.87e–04 | 3.79e–04 | 1.44e–04 | 1.44e–04 | 1.624e–04 |
| $\gamma = 0.5$ | 5.90e–04 | 1.02e–04 | 2.24e–04 | 7.97e–05 | 7.97e–05 | 8.250e–05 |
| $\gamma = 0.6$ | 4.66e–04 | 4.98e–05 | 1.19e–04 | 4.00e–05 | 4.00e–05 | 3.691e–05 |
| $\gamma = 0.7$ | 3.08e–04 | 2.12e–05 | 5.53e–05 | 1.75e–05 | 1.75e–05 | 1.413e–05 |
| $\gamma = 0.8$ | 1.53e–04 | 7.15e–06 | 2.02e–05 | 6.08e–06 | 6.08e–06 | 4.142e–06 |
| $\gamma = 0.9$ | 4.18e–04 | 1.37e–06 | 4.14e–06 | 1.20e–06 | 1.20e–06 | 6.831e–07 |

### Short Memory and Regression Schemes

Here we compare the results found in the fractional derivative approximations, given by the $L1^{*}$, RL1, LRA, QRA, NLRA schemes in Equations (2.194), (2.206), (2.279), (2.284) and (2.291) respectively. In Tables 2.24 – 2.26, and Tables 2.27 – 2.29, it can be seen that, if we approximate the first part of the integral by regression, as given by Equation (2.276), the errors are smaller rather than ignoring the early history of $f(t)$.

Note by choosing $j = n = 100$ we are attempting to approximate all the early history. However, if we choose to only approximate half of the integration interval (by setting $n = 50$) we see the estimates are better, as seen by comparing the $n = 50$ and $n = 100$ cases.

We also see that if the function $f(t)$ is linear, and if we do not ignore the first part in the integral, there is no error in the approximation, whilst if we do ignore the early history (of the linear function) then error is introduced. We also note, if linear regression is used to approximate the early history, that there is less error in the estimate then the other regression methods or by ignoring the early history as shown in Tables 2.24, 2.25, and 2.26.

However for all methods the error, in the approximation, increases as more of the history of $f(t)$ is ignored (i.e. as $n$ increases). But using regression was found to be better than if we ignore the early history.

If we choose the value of $n$ where the error is smallest, as given in Tables 2.30 – 2.32, we see that the $QRA$ scheme performs better when compared with the $L1^*$, RL1, LRA, and NLRA schemes, instead.

Table 2.24: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t) = t^2$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 100$, $j = 100$, and $\Delta t = 0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 5.91e–01 | 5.91e–01 | 2.11e–01 | 5.27e–00 | 1.57e+01 |
| $\gamma = 0.2$ | 9.52e–01 | 9.52e–01 | 3.10e–01 | 3.80e–00 | 4.62e–00 |
| $\gamma = 0.3$ | 1.16e–00 | 1.16e–00 | 3.40e–01 | 2.70e–00 | 1.15e–00 |
| $\gamma = 0.4$ | 1.26e–00 | 1.26e–00 | 3.25e–01 | 1.88e–00 | 2.39e–01 |
| $\gamma = 0.5$ | 1.28e–00 | 1.28e–00 | 2.85e–01 | 1.28e–00 | 8.21e–01 |
| $\gamma = 0.6$ | 1.26e–00 | 1.26e–00 | 2.31e–01 | 8.39e–01 | 1.05e–00 |
| $\gamma = 0.7$ | 1.21e–00 | 1.21e–00 | 1.72e–01 | 5.17e–01 | 1.11e–00 |
| $\gamma = 0.8$ | 1.14e–00 | 1.14e–00 | 1.14e–01 | 2.85e–01 | 1.10e–00 |
| $\gamma = 0.9$ | 1.06e–00 | 1.06e–00 | 5.89e–02 | 1.18e–01 | 1.04e–00 |

Table 2.25: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t) = t^3$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 100$, $j = 100$ and $\Delta t = 0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 7.60e–01 | 7.60e–01 | 4.24e–01 | 7.63e–00 | 1.15e+01 |
| $\gamma = 0.2$ | 1.19e–00 | 1.19e–00 | 6.19e–01 | 5.42e–00 | 3.07e–00 |
| $\gamma = 0.3$ | 1.41e–00 | 1.41e–00 | 6.81e–01 | 3.78e–00 | 3.90e–01 |
| $\gamma = 0.4$ | 1.48e–00 | 1.48e–00 | 6.60e–01 | 2.58e–00 | 6.79e–01 |
| $\gamma = 0.5$ | 1.47e–00 | 1.47e–00 | 5.90e–01 | 1.71e–00 | 1.10e–00 |
| $\gamma = 0.6$ | 1.41e–00 | 1.41e–00 | 4.95e–01 | 1.08e–00 | 1.23e–00 |
| $\gamma = 0.7$ | 1.31e–00 | 1.31e–00 | 3.92e–01 | 6.21e–01 | 1.23e–00 |
| $\gamma = 0.8$ | 1.20e–00 | 1.20e–00 | 2.90e–01 | 2.95e–01 | 1.16e–00 |
| $\gamma = 0.9$ | 1.08e–00 | 1.08e–00 | 1.96e–01 | 6.41e–02 | 1.07e–00 |

Table 2.26: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t)=t^4$ at time $t=1$ for $\gamma=0.1,...,0.9$, $n=100$, $j=100$ and $\Delta t=0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 9.10e–01 | 9.10e–01 | 6.15e–01 | 8.43e–00 | 8.85e–00 |
| $\gamma=0.2$ | 1.39e–00 | 1.39e–00 | 8.88e–01 | 5.89e–00 | 2.04e–00 |
| $\gamma=0.3$ | 1.61e–00 | 1.61e–00 | 9.74e–01 | 4.04e–00 | 1.50e–01 |
| $\gamma=0.4$ | 1.66e–00 | 1.66e–00 | 9.44e–01 | 2.70e–00 | 1.01e–00 |
| $\gamma=0.5$ | 1.62e–00 | 1.62e–00 | 8.48e–01 | 1.73e–00 | 1.31e–00 |
| $\gamma=0.6$ | 1.52e–00 | 1.52e–00 | 7.20e–01 | 1.05e–00 | 1.37e–00 |
| $\gamma=0.7$ | 1.38e–00 | 1.38e–00 | 5.81e–01 | 5.57e–01 | 1.32e–00 |
| $\gamma=0.8$ | 1.24e–00 | 1.24e–00 | 4.45e–01 | 2.12e–01 | 1.21e–00 |
| $\gamma=0.9$ | 1.20e–00 | 1.10e–00 | 3.20e–01 | 2.81e–02 | 1.08e–00 |

Table 2.27: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t)=t^2$ at time $t=1.0$ for $\gamma=0.1,...,0.9$, $n=50$, $j=100$, and $\Delta t=0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 4.24e–02 | 4.18e–02 | 9.58e–03 | 4.11e–01 | 1.64e+01 |
| $\gamma=0.2$ | 7.63e–02 | 7.49e–02 | 1.04e–02 | 4.42e–01 | 4.38e–00 |
| $\gamma=0.3$ | 1.09e–01 | 1.07e–01 | 1.15e–02 | 4.68e–01 | 1.45e–00 |
| $\gamma=0.4$ | 1.40e–01 | 1.37e–01 | 1.22e–02 | 4.88e–01 | 4.55e–01 |
| $\gamma=0.5$ | 1.67e–01 | 1.64e–01 | 1.25e–02 | 5.01e–01 | 6.82e–02 |
| $\gamma=0.6$ | 1.91e–01 | 1.87e–01 | 1.21e–02 | 5.08e–01 | 9.61e–02 |
| $\gamma=0.7$ | 2.10e–01 | 2.05e–01 | 1.10e–02 | 5.09e–01 | 1.72e–01 |
| $\gamma=0.8$ | 2.24e–01 | 2.20e–01 | 9.38e–03 | 5.04e–01 | 2.09e–01 |
| $\gamma=0.9$ | 2.34e–01 | 2.29e–01 | 7.31e–03 | 4.94e–01 | 2.28e–01 |

Table 2.28: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t) = t^3$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 50$, $j = 100$ and $\Delta t = 0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 3.55e–02 | 3.55e–02 | 2.12e–02 | 3.11e–01 | 6.00e–00 |
| $\gamma = 0.2$ | 4.66e–02 | 4.65e–02 | 1.79e–02 | 3.29e–01 | 1.61e–01 |
| $\gamma = 0.3$ | 5.97e–02 | 5.97e–02 | 1.72e–02 | 3.46e–01 | 5.27e–01 |
| $\gamma = 0.4$ | 7.31e–02 | 7.31e–02 | 1.76e–02 | 3.60e–01 | 1.54e–01 |
| $\gamma = 0.5$ | 8.55e–02 | 8.54e–02 | 1.81e–02 | 3.70e–01 | 5.66e–03 |
| $\gamma = 0.6$ | 9.61e–02 | 9.61e–02 | 1.85e–02 | 3.76e–01 | 5.90e–02 |
| $\gamma = 0.7$ | 1.05e–01 | 1.05e–01 | 1.84e–02 | 3.77e–01 | 8.96e–02 |
| $\gamma = 0.8$ | 1.11e–01 | 1.11e–01 | 1.78e–02 | 3.74e–01 | 1.05e–01 |
| $\gamma = 0.9$ | 1.15e–01 | 1.15e–01 | 1.68e–02 | 3.67e–01 | 1.13e–01 |

Table 2.29: The comparison absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t) = t^4$ at time $t = 1.0$ for $\gamma = 0.1, ..., 0.9$, $n = 50$, $j = 100$ and $\Delta t = 0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma = 0.1$ | 4.25e–02 | 4.25e–02 | 3.64e–02 | 1.96e–01 | 2.32e–00 |
| $\gamma = 0.2$ | 3.69e–02 | 3.69e–02 | 2.45e–02 | 1.96e–01 | 6.15e–01 |
| $\gamma = 0.3$ | 3.72e–02 | 3.72e–02 | 1.89e–02 | 2.00e–01 | 1.95e–01 |
| $\gamma = 0.4$ | 4.04e–02 | 4.04e–02 | 1.65e–02 | 2.05e–01 | 5.02e–02 |
| $\gamma = 0.5$ | 4.46e–02 | 4.46e–02 | 1.56e–02 | 2.10e–01 | 7.92e–03 |
| $\gamma = 0.6$ | 4.88e–02 | 4.88e–02 | 1.54e–02 | 2.12e–01 | 3.37e–02 |
| $\gamma = 0.7$ | 5.24e–02 | 5.24e–02 | 1.52e–03 | 2.13e–01 | 4.61e–02 |
| $\gamma = 0.8$ | 5.51e–02 | 5.51e–02 | 1.49e–02 | 2.11e–01 | 5.25e–02 |
| $\gamma = 0.9$ | 5.68e–02 | 5.68e–02 | 1.44e–02 | 2.08e–01 | 5.58e–02 |

Table 2.30: The comparison minimum absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t)=t^2$ at time $t=1.0$ for $\gamma=0.1,...,0.9$, $j=100$, and $\Delta t=0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 5.53e–03 | 5.53e–03 | 5.53e–03 | 6.92e–04 | 5.53e–03 |
| $\gamma=0.2$ | 3.03e–03 | 3.03e–03 | 3.03e–03 | 2.13e–04 | 3.03e–03 |
| $\gamma=0.3$ | 1.64e–03 | 1.64e–03 | 1.64e–03 | 3.58e–04 | 1.64e–03 |
| $\gamma=0.4$ | 8.76e–04 | 8.76e–04 | 8.76e–04 | 2.24e–04 | 8.76e–04 |
| $\gamma=0.5$ | 4.60e–04 | 4.60e–04 | 4.60e–04 | 5.33e–05 | 4.60e–04 |
| $\gamma=0.6$ | 2.35e–04 | 2.35e–04 | 2.35e–04 | 5.53e–05 | 2.35e–04 |
| $\gamma=0.7$ | 1.15e–04 | 1.15e–04 | 1.15e–04 | 1.74e–05 | 1.15e–04 |
| $\gamma=0.8$ | 5.15e–05 | 5.15e–05 | 5.15e–05 | 3.47e–05 | 5.15e–05 |
| $\gamma=0.9$ | 1.78e–05 | 1.78e–05 | 1.78e–05 | 1.78e–05 | 1.78e–05 |

Table 2.31: The comparison minimum absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t)=t^3$ at time $t=1.0$ for $\gamma=0.1,...,0.9$, $j=100$ and $\Delta t=0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 1.65e–02 | 1.65e–02 | 1.65e–02 | 3.22e–05 | 1.65e–02 |
| $\gamma=0.2$ | 9.03e–03 | 9.03e–03 | 9.03e–01 | 2.83e–04 | 1.41e–03 |
| $\gamma=0.3$ | 4.87e–03 | 4.87e–03 | 4.87e–03 | 1.59e–04 | 7.13e–04 |
| $\gamma=0.4$ | 2.59e–03 | 2.59e–03 | 2.59e–03 | 1.50e–05 | 4.97e–04 |
| $\gamma=0.5$ | 1.35e–03 | 1.35e–03 | 1.35e–03 | 6.08e–05 | 2.20e–04 |
| $\gamma=0.6$ | 6.83e–04 | 6.83e–04 | 6.83e–04 | 5.41e–05 | 1.02e–04 |
| $\gamma=0.7$ | 3.29e–04 | 3.29e–04 | 3.29e–04 | 3.86e–05 | 3.29e–04 |
| $\gamma=0.8$ | 1.44e–04 | 1.44e–04 | 1.44e–04 | 4.35e–06 | 1.44e–04 |
| $\gamma=0.9$ | 4.80e–05 | 4.80e–05 | 4.80e–05 | 5.16e–06 | 4.80e–05 |

Table 2.32: The comparison minimum absolute error of the fractional derivative approximation of order $1-\gamma$ of the function $f(t)=t^4$ at time $t=1.0$ for $\gamma=0.1,...,0.9$, $j=100$ and $\Delta t=0.01$.

| $\gamma$ | $L1^*$ | $RL1$ | $LRA$ | $QRA$ | $NLRA$ |
|---|---|---|---|---|---|
| $\gamma=0.1$ | 3.29e–02 | 3.29e–02 | 3.29e–02 | 1.46e–04 | 3.61e–03 |
| $\gamma=0.2$ | 1.80e–02 | 1.80e–02 | 1.80e–02 | 4.71e–04 | 1.64e–04 |
| $\gamma=0.3$ | 9.67e–03 | 9.67e–03 | 9.67e–03 | 1.37e–04 | 6.18e–04 |
| $\gamma=0.4$ | 5.12e–03 | 5.12e–03 | 5.12e–03 | 4.75e–05 | 1.05e–04 |
| $\gamma=0.5$ | 2.66e–03 | 2.66e–03 | 2.68e–03 | 1.70e–04 | 1.56e–06 |
| $\gamma=0.6$ | 1.34e–03 | 1.34e–03 | 1.34e–03 | 7.90e–05 | 1.31e–03 |
| $\gamma=0.7$ | 6.38e–04 | 6.38e–04 | 6.38e–04 | 4.48e–05 | 6.38e–04 |
| $\gamma=0.8$ | 2.75e–04 | 2.75 e–04 | 2.75e–04 | 1.84e–05 | 2.75e–04 |
| $\gamma=0.9$ | 9.05e–05 | 9.05e–05 | 9.05e–05 | 9.05e–05 | 9.05e–05 |

## 2.13 Conclusion

In this chapter, we described the approximation of the fractional derivative and we focused on the L1 scheme (Oldham & Spanier 1974). We modified the L1 scheme to develop the C1, C2, and C3 schemes. The accuracy of each of these approximations for the order $p$ fractional derivative was found to be of order $O(\Delta t^{2-p})$. The numerical tests on powers of $t$ verified the accuracy of each of these approximations. From these results we conclude that the C2 scheme is more accurate when compared with the L1, C1, C3 and Romberge integration ($k=2$) schemes. We also considered short memory based approximate fractional derivatives of order $p$, the $L1^*$ and RL1 schemes. The accuracy of each these approximations was discussed, and the numerical tests on powers of $t$ compared with the exact fractional derivative to verify the accuracy of each of these methods.

In future work a stopping criterion based upon the convergence of integral estimates will be used to shorten the number of the steps, $n$, required. We will analyse the accuracy of the Romberg Integration analytically and this method also needs to be incorporated into a full numerical method.

In addition, the Regression methods, $LRA$, $QRA$ and $NLR$ schemes, are used to approximate the fractional derivative by using regressions to approximate the early history in the integral in Equation (2.276) instead of ignoring this history. We conclude that using linear regression is a better approximation to reduce the error that accrues if we ignore the early history. It is also easier to determine what value of $n$ should be used.

These approximations can be potentially implemented in the full numerical solution. The advantage of using LRA over using the full L1 scheme is that we no longer need to evaluate the complete convolution sum but rather need only update the estimate of the slope parameter. This can be done iteratively whilst the full convolution sum cannot. The QRA method outperforms the LRA scheme when the optimal value $n$ is used. However the LRA is more predictable in deciding when to truncate the sum.

# Chapter 3

# Implicit Numerical Method: IMC1 Scheme

## 3.1 Introduction

Many researchers have investigated ways of finding the solution of fractional partial differential equations (FPDEs) such as analytical solutions (Wyss 1986, Mainardi 1996, Henry & Wearne 2000, Metzler & Klafter 2000*b*, Langlands et al. 2008) and numerical solutions (Diethelm & Ford 2002, Langlands & Henry 2005, Deng 2008, Murio 2008, Dhaigude & Birajdar 2012, Chen et al. 2013). Some analytic solutions are known but they are difficult to evaluate. Most fractional partial differential equations do not have exact solutions and so consequently numerical techniques must be used to obtain their approximate solutions.

In this chapter, we consider a finite difference solution scheme for the fractional subdiffusion equation with a source term given by Equation (1.15), where $K_\gamma = 0$, which we repeat here as

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u(x,t)}{\partial x^2}\right) + f(x,t) \tag{3.1}$$

with the initial condition

$$u(x,0) = g(x), \qquad 0 \le x \le L, \tag{3.2}$$

and the boundary conditions

$$u(0,t) = \varphi_1(t) \quad \text{and} \quad u(L,t) = \varphi_2(t), \qquad 0 \le t \le T, \tag{3.3}$$

where $D > 0$, $0 < \gamma \le 1$ and $f(x,t)$ is a given source function. We also suppose that $u(x,t) \in U(\Omega)$ is the exact solution for the fractional subdiffusion equation (3.1), where

$$\Omega = \{(x,t) | 0 \le x \le L, 0 \le t \le T\}, \tag{3.4}$$

and

$$U(\Omega) = \left\{ u(x,t) \middle| \frac{\partial^4 u(x,t)}{\partial x^4}, \frac{\partial^3 u(x,t)}{\partial x^2 \partial t}, \frac{\partial^2 u(x,t)}{\partial t^2} \in C(\Omega) \right\}. \tag{3.5}$$

We approximate the second-order spatial derivative by using second-order centred finite difference approximation. The centred difference at time step $j$ around the point $i$ is

$$\left[ \frac{\partial^2 u}{\partial x^2} \right|_i^j \approx \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}. \tag{3.6}$$

The time derivative on the left of Equation (3.1), can be approximated using a Centred–finite difference, as in Figure 3.1,

$$\left[ \frac{\partial u}{\partial t} \right|_i^j \approx \frac{u_i^{j+1} - u_i^{j-1}}{2\Delta t}, \qquad \text{(Central Method)} \tag{3.7}$$

a forward finite difference

$$\left[ \frac{\partial u}{\partial t} \right|_i^j \approx \frac{u_i^{j+1} - u_i^j}{\Delta t}, \qquad \text{(Explicit)} \tag{3.8}$$

or a backward finite difference

$$\left[ \frac{\partial u}{\partial t} \right|_i^j \approx \frac{u_i^j - u_i^{j-1}}{\Delta t}, \qquad \text{(Implicit).} \tag{3.9}$$

Both explicit or implicit numerical schemes can be derived using these approximations similar to the standard (non-fractional) partial differential equation. Explicit methods evaluate the right hand of Equation (3.1) at the current time, whilst implicit methods evaluate the right hand side at the new time level. Implicit methods require the solution of systems of equations to update their solution.

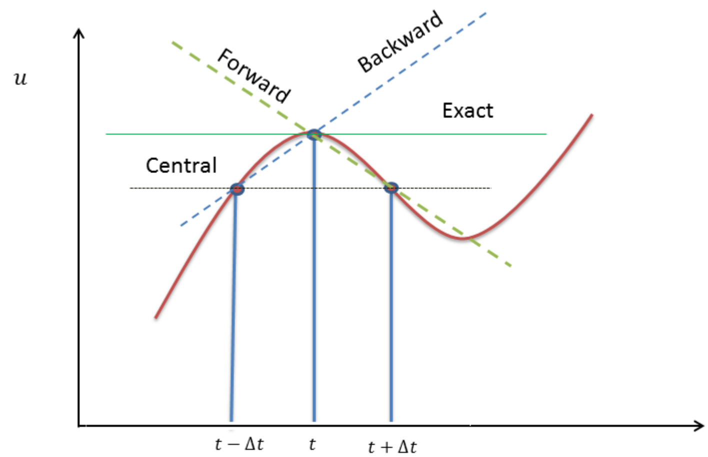



Figure 3.1: Geometric interpretation of the finite difference approximation of the time derivative.

## 3.2 Derivation of the Numerical Method (IMC1 Method)

An implicit numerical method for the fractional diffusion equation was derived by Langlands & Henry (2005), where the fractional derivative was approximated by using the L1 approximation (Oldham & Spanier 1974). In this section, we describe the derivation of a modified implicit method for the fractional subdiffusion equation.

In this modified method the finite difference scheme is used to approximate the second spatial derivative. Instead of the L1 scheme, the C1 scheme, given in Chapter 2 by Equation (2.60), is used to approximate the fractional derivative of order $p = 1-\gamma$ at the time $t_j = j\Delta t$. Using the approximation in Equation (3.6) for the second spatial derivative and Equation (3.9) to approximate the first temporal derivative in Equation (3.1), we arrive at the scheme

$$\frac{u_i^j - u_i^{j-1}}{\Delta t} = \frac{D\Delta t^{\gamma-1}}{2\Delta x^2\Gamma(1+\gamma)}\Bigg\{ \beta_j^*(\gamma)\left(u_{i+1}^0 - 2u_i^0 + u_{i-1}^0\right) \tag{3.10}$$
$$+ a_j(\gamma)\left(u_{i+1}^1 - 2u_i^1 + u_{i-1}^1\right) + \left[\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) - \left(u_{i+1}^{j-1} - 2u_i^{j-1} + u_{i-1}^{j-1}\right)\right]$$
$$+\frac{1}{2}\sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\left(u_{i+1}^{k+1} - 2u_i^{k+1} + u_{i-1}^{k+1}\right) - \left(u_{i+1}^{k-1} - 2u_i^{k-1} + u_{i-1}^{k-1}\right)\right]\Bigg\} + f_i^j,$$

Equation (3.10) can be written as

$$u_i^j = u_i^{j-1} + \frac{D\Delta t^\gamma}{2\Gamma(1+\gamma)} \Bigg\{ \beta_j^*(\gamma)\delta_x^2 u_i^0 + a_j(\gamma)\delta_x^2 u_i^1 + \delta_x^2 u_i^j - \delta_x^2 u_i^{j-1} + \sum_{k=1}^{j-1} \mu_{j-k}^*(\gamma) \left[\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^{k-1}\right] \Bigg\} + f_i^j, \tag{3.11}$$

where $\delta_x^2 u_i^j$ is defined as

$$\delta_x^2 u_i^j = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}, \tag{3.12}$$

which $u_i^j$ is the numerical approximation of the solution $U_i^j = u(x_i, t_j)$ at the discrete grid point $(x_i, t_j)$, $\Delta x$ is the spatial grid-step size, $\Delta t$ is the time-step size, and $f_i^j = f(x_i, t_j)$ is the numerical approximation of the source term. We refer to this approximation as IMC1 scheme. Equation (3.10) can be rewritten in matrix form as

$$\boldsymbol{A}^* \boldsymbol{u}^j = \boldsymbol{A}^* \boldsymbol{u}^{j-1} + \boldsymbol{c} + \Delta t\, \boldsymbol{f}^j, \tag{3.13}$$

where

$$\boldsymbol{A}^* = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ -\rho & 1+2\rho & -\rho & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\rho & 1+2\rho & -\rho \\ 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{pmatrix}, \tag{3.14}$$

and

$$\boldsymbol{c} = \rho\beta_j^*(\gamma)\boldsymbol{u}^0 + \rho a_j(\gamma)\boldsymbol{u}^1 + \rho \sum_{k=1}^{j-1} \mu_{j-k}^*(\gamma) \left(\boldsymbol{u}^{k+1} - \boldsymbol{u}^{k-1}\right). \tag{3.15}$$

In Equations (3.14) and (3.15) the term $\rho$ is given by

$$\rho = \frac{D\Delta t^\gamma}{2\Delta x^2 \Gamma(1+\gamma)}, \tag{3.16}$$

where the weights $a_j(\gamma)$, $\beta_j^*(\gamma)$ and $\mu_j^*(\gamma)$ are given by

$$a_j(\gamma) = j^\gamma - (j-1)^\gamma, \tag{3.17}$$

$$\beta_j^*(\gamma) = 2\gamma j^{\gamma-1} - a_j(\gamma), \tag{3.18}$$

and

$$\mu_j^*(\gamma) = \frac{1}{2}\left[(j+1)^\gamma - (j-1)^\gamma\right]. \tag{3.19}$$

## 3.3 Accuracy of the IMC1 Method

Here we determine the truncation error accuracy of IMC1 numerical scheme. Now from Equation (3.11) we have

$$\frac{1}{\Delta t}\left[u_i^j - u_i^{j-1}\right] = \frac{D\Delta t^{\gamma-1}}{2\Gamma(1+\gamma)}\Bigg\{ \beta_j^*(\gamma)\delta_x^2 u_i^0 + a_j(\gamma)\delta_x^2 u_i^1 + \delta_x^2 u_i^j - \delta_x^2 u_i^{j-1} + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^{k-1}\right]\Bigg\} + f(x_i,t_j). \tag{3.20}$$

The first term on the right hand side of Equation (3.20) is the C1 approximation, Equation (2.60), with $u(t)$ replaced by $\delta_x^2 u_i(t)$

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u\right)\right|_{i,C1}^{j} = \frac{D\Delta t^{\gamma-1}}{2\Gamma(1+\gamma)}\Bigg\{ \beta_j^*(\gamma)\delta_x^2 u_i^0 + a_j(\gamma)\delta_x^2 u_i^1 + \delta_x^2 u_i^j - \delta_x^2 u_i^{j-1} + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^{k-1}\right]\Bigg\}, \tag{3.21}$$

and so Equation (3.20) can be written

$$\frac{1}{\Delta t}\left[u_i^j - u_i^{j-1}\right] = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u\right)\right|_{i,C1}^{j} + f(x_i,t_j). \tag{3.22}$$

Now taking the Taylor series expansion around the point $x_i = i\Delta x$ in space, we then have

$$\delta_x^2 U_i^j \simeq \left[\frac{\partial^2 U}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 U}{\partial x^4}\right|_i^j + O(\Delta x^4). \tag{3.23}$$

Also taking the Taylor series expansion around the point $t_j = j\Delta t$ gives

$$\frac{U_i^j - U_i^{j-1}}{\Delta t} \simeq \left[\frac{\partial U}{\partial t}\right|_i^j + O(\Delta t), \tag{3.24}$$

and so we have

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^j + O(\Delta t) &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\Delta x^2}{12}\left[\frac{\partial^4 U}{\partial x^4}\right|_i^j + O(\Delta x^4)\right)\right|_{i,C1}^{j} + f(x_i,t_j) \\ &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i,C1}^{j} + \frac{D\Delta x^2}{12}\left[\frac{\partial^{1-\gamma}M(t)}{\partial t^{1-\gamma}}\right|_{i,C1}^{j} + f(x_i,t_j),\end{aligned} \tag{3.25}$$

where

$$M(t) = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left|\frac{\partial^4 U}{\partial x^4}\right|. \tag{3.26}$$

Adding and subtracting the exact fractional derivative, we find

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^j &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j + f(x_i,t_j) + O(\Delta t) + O(\Delta x^2) \\ &\quad + D\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i,C1}^{j} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j\right].\end{aligned} \tag{3.27}$$

From Equation (2.125) the last term

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i,C1}^{j} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i}^{j} \tag{3.28}$$

is $O(\Delta t^{1+\gamma})$ but the Equation (3.27) also includes $O(\Delta t)$ terms, and so we then find the truncation error, $\tau_{i,j}$, is first order in time and second order in space, that is

$$\tau_{i,j} = O(\Delta t) + O(\Delta x^2). \tag{3.29}$$

## 3.4 Consistency

The numerical approximation for the fractional subdiffusion equation is consistent, if we can show that the truncation approaches zero as $\Delta x \to 0$ and $\Delta t \to 0$, that is we let $u_i^j \approx U_i^j = u(x_i, t_j)$, then

$$\lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} (u_i^j - U_i^j) = \lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} \tau_{i,j} = 0. \tag{3.30}$$

From Equation (3.29), we have

$$\lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} \tau_{i,j} = 0. \tag{3.31}$$

This shows that the IMC1 method is consistent with the original fractional partial differential equation.

## 3.5 Stability Analysis

In this section, the stability of the modified implicit numerical method (IMC1) in Equation (3.10) is considered by using Von Neumann stability analysis. Before this we first rewrite Equations (3.10) – (3.19) as

$$\begin{aligned} u_i^j = {} & u_i^{j-1} + \rho \beta_j^*(\gamma)\left(u_{i+1}^0 - 2u_i^0 + u_{i-1}^0\right) + \rho a_j(\gamma)\left(u_{i+1}^1 - 2u_i^1 + u_{i-1}^1\right) \\ & + \rho\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) - \rho\left(u_{i+1}^{j-1} - 2u_i^{j-1} + u_{i-1}^{j-1}\right) \\ & + \rho \sum_{r=2}^{j} \mu_{j-r+1}^*(\gamma)\left(u_{i+1}^r - 2u_i^r + u_{i-1}^r\right) - \rho \sum_{p=0}^{j-2} \mu_{j-p-1}^*(\gamma)\left(u_{i+1}^p - 2u_i^p + u_{i-1}^p\right) + \Delta t f_i^j. \end{aligned} \tag{3.32}$$

Now let $U_i^j$ be the exact solution of the Equation (3.1) and satisfying Equation (3.32), we then have

$$U_i^j = U_i^{j-1} + \rho\beta_j^*(\gamma)\left(U_{i+1}^0 - 2U_i^0 + U_{i-1}^0\right) + \rho a_j(\gamma)\left(U_{i+1}^1 - 2U_i^1 + U_{i-1}^1\right) \tag{3.33}$$
$$+ \rho\left(U_{i+1}^j - 2U_i^j + U_{i-1}^j\right) - \rho\left(U_{i+1}^{j-1} - 2U_i^{j-1} + U_{i-1}^{j-1}\right) + \rho\sum_{r=2}^{j}\mu_{j-r+1}^*(\gamma)\left(U_{i+1}^r - 2U_i^r + U_{i-1}^r\right)$$
$$- \rho\sum_{p=0}^{j-2}\mu_{j-p-1}^*(\gamma)\left(U_{i+1}^p - 2U_i^p + U_{i-1}^p\right) + \Delta t f_i^j + \Delta t R_i^j.$$

The error is then given by

$$\epsilon_i^j = U_i^j - u_i^j, \tag{3.34}$$

and so the error satisfies the equation

$$\begin{aligned}\epsilon_i^j &= \epsilon_i^{j-1} + \rho\beta_j^*(\gamma)\left(\epsilon_{i+1}^0 - 2\epsilon_i^0 + \epsilon_{i-1}^0\right) + \rho a_j(\gamma)\left(\epsilon_{i+1}^1 - 2\epsilon_i^1 + \epsilon_{i-1}^1\right) \\ &+ \rho\left(\epsilon_{i+1}^j - 2\epsilon_i^j + \epsilon_{i-1}^j\right) - \rho\left(\epsilon_{i+1}^{j-1} - 2\epsilon_i^{j-1} + \epsilon_{i-1}^{j-1}\right) \\ &+ \rho\sum_{r=2}^{j}\mu_{j-r+1}^*(\gamma)\left(\epsilon_{i+1}^r - 2\epsilon_i^r + \epsilon_{i-1}^r\right) - \rho\sum_{p=0}^{j-2}\mu_{j-p-1}^*(\gamma)\left(\epsilon_{i+1}^p - 2\epsilon_i^p + \epsilon_{i-1}^p\right).\end{aligned} \tag{3.35}$$

In Equation (3.35) we set the truncation error to zero (in stability analysis the truncation error is not required), but later in Section 3.6 we will use the truncation error to show the convergence rate of the numerical method.

To investigate the stability by Von Neumann stability analysis, we let

$$\epsilon_i^j = \zeta_j e^{i' q i \Delta x}, \tag{3.36}$$

where $i'$ is the imaginary number, $\sqrt{-1}$, $q$ is a real spatial wave number and

$$e^{i' q \Delta x} = \cos(q\Delta x) + i' \sin(q\Delta x). \tag{3.37}$$

Using Equation (3.36) in Equation (3.35) gives the equation for $\zeta_j$

$$\zeta_j e^{i'qi\Delta x} = \zeta_{j-1} e^{i'qi\Delta x} + \rho\Big\{\beta_j^*(\gamma)\left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_0 \tag{3.38}$$
$$+ a_j\left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_1 + \left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_j$$
$$- \left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_{j-1} + \sum_{r=2}^{j}\mu_{j-r+1}^*(\gamma)\left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x}\right.$$
$$\left.+ e^{i'q(i-1)\Delta x}\right)\zeta_r - \sum_{p=0}^{j-2}\mu_{j-p-1}^*(\gamma)\left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_p\Big\},$$

which can be rewritten as

$$\begin{aligned}\zeta_j = \zeta_{j-1} + \rho\Big\{&\beta_j^*(\gamma)\left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_0 + a_j(\gamma)\left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_1 \\ &+ \left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_j - \left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_{j-1} \\ &+ \sum_{r=2}^{j}\mu_{j-r+1}^*(\gamma)\left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_r - \sum_{p=0}^{j-2}\mu_{j-p-1}^*(\gamma)\left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_p\Big\}.\end{aligned} \tag{3.39}$$

Noting

$$e^{i'q\Delta x} - 2 + e^{-i'q\Delta x} = -2\left(1 - \cos(q\Delta x)\right) = -4\sin^2\left(\frac{q\Delta x}{2}\right). \tag{3.40}$$

Equation (3.39) can then be rewritten as

$$\begin{aligned}\zeta_j = \zeta_{j-1} -4\sin^2\left(\frac{q\Delta x}{2}\right)\rho\Big\{&\beta_j^*(\gamma)\zeta_0 + a_j\zeta_1 + \zeta_j - \zeta_{j-1} \\ &+ \sum_{r=2}^{j}\mu_{j-r+1}^*(\gamma)\zeta_r - \sum_{p=0}^{j-2}\mu_{j-p-1}^*(\gamma)\zeta_p\Big\}.\end{aligned} \tag{3.41}$$

Setting

$$v_q = 4\sin^2\left(\frac{q\Delta x}{2}\right)\rho, \tag{3.42}$$

for $j \geq 1$, Equation (3.41) becomes

$$\zeta_j = \zeta_{j-1} - \lambda_q\Big\{\beta_j^*(\gamma)\zeta_0 + a_j(\gamma)\zeta_1 + \sum_{r=2}^{j}\mu_{j-r+1}^*(\gamma)\zeta_r - \sum_{p=0}^{j-2}\mu_{j-p-1}^*(\gamma)\zeta_p\Big\}, \tag{3.43}$$

where

$$\lambda_q = \frac{v_q}{1+v_q}. \tag{3.44}$$

For $0 \leq v_q < \infty$, $\lambda_q$ satisfies the inequality $0 \leq \lambda_q \leq 1$.

For $j \geq 3$, Equation (3.43) can be rewritten as

$$\begin{aligned}\zeta_j = \frac{1}{1+2^{\gamma-1}\lambda_q}\Big\{&\left(1 + \frac{1}{2}\left(1 - 3^\gamma\right)\lambda_q\right)\zeta_{j-1} + \lambda_q\left(\frac{1}{2}\left(j^\gamma - (j-2)^\gamma\right) - \beta_j^*(\gamma)\right)\zeta_0 \\ &+\lambda_q\left(\frac{1}{2}\left((j-1)^\gamma - (j-3)^\gamma\right) - a_j(\gamma)\right)\zeta_1 - \lambda_q\sum_{2}^{j-2}\varpi_{j-r}(\gamma)\zeta_r\Big\},\end{aligned} \tag{3.45}$$

where the weight $\varpi_j(\gamma)$ is defined as

$$\varpi_j(\gamma) = \frac{1}{2}\left[(j+2)^\gamma - 2j^\gamma + (j-2)^\gamma\right]. \tag{3.46}$$

We next consider the following lemmas which will aid in showing the stability of our numerical method.

**Lemma 3.5.1.** Let $a_j(\gamma) = j^\gamma - (j-1)^\gamma$, where $j \geq 1$ and $0 < \gamma < 1$ then $a_j$ satisfies:

1. $a_j(\gamma) > 0$, and,
2. $a_j(\gamma) > a_{j+1}(\gamma)$.

*Proof.* To show $a_j(\gamma) > 0$, we have

$$a_j(\gamma) = j^\gamma - (j-1)^\gamma = j^\gamma \left[1 - \left(\frac{j-1}{j}\right)^\gamma\right], \tag{3.47}$$

but

$$0 \leq \frac{j-1}{j} < 1, \tag{3.48}$$

when $j \geq 1$ and so

$$0 \leq \left(\frac{j-1}{j}\right)^\gamma < 1, \tag{3.49}$$

and

$$0 < 1 - \left(\frac{j-1}{j}\right)^\gamma \leq 1. \tag{3.50}$$

Hence from Equation (3.47) we have $0 < a_j(\gamma) \leq j^\gamma$ since $j^\gamma > 0$ and so $a_j(\gamma) > 0$.
To prove the second result we let $f_1(y) = (y-1)^\gamma$ and $f_2(y) = y^\gamma - (y-1)^\gamma$. We will show these functions, $f_1(y)$ and $f_2(y)$, are monotonically increasing and decreasing functions respectively of $y$, for $\gamma \in (0,1)$.
Since

$$\begin{aligned} \frac{df_1(y)}{dy} &= \gamma\,(y-1)^{\gamma-1} \\ &= \frac{\gamma}{(y-1)^{1-\gamma}} > 0, \end{aligned} \tag{3.51}$$

we can conclude, for $y \geq 1$ and $0 < \gamma < 1$, that the function $f_1(y)$ is a monotonically increasing function in $y$.
Finding the derivative of $f_2(y)$ we have

$$\frac{df_2(y)}{dy} = \gamma y^{\gamma-1} - \gamma\,(y-1)^{\gamma-1}. \tag{3.52}$$

Now since

$$y^{1-\gamma} > (y-1)^{1-\gamma},$$

as $f_1(y)$ is an increasing function for $0 < \gamma < 1$, then

$$\frac{1}{y^{1-\gamma}} < \frac{1}{(y-1)^{1-\gamma}}. \tag{3.53}$$

Hence

$$\frac{df_2(y)}{dy} \leq \frac{\gamma}{(y-1)^{1-\gamma}} - \frac{\gamma}{(y-1)^{1-\gamma}} < 0 \tag{3.54}$$

and so the function $f_2(y)$ is a monotonically decreasing function of $y$, for $0 < \gamma < 1$.
Setting $y = j$ we then have

$$\begin{aligned} a_j(\gamma) &= j^\gamma - (j-1)^\gamma \\ &> (j+1)^\gamma - ((j+1)-1)^\gamma \\ &> a_{j+1}(\gamma). \end{aligned} \tag{3.55}$$

Hence results (1) and (2) hold for $0 < \gamma < 1$. □

**Lemma 3.5.2.** The coefficients $\varpi_j(\gamma)$, defined in Equation (3.46) for $0 < \gamma \leq 1$ and $j \geq 2$, obey the constraint $\varpi_j(\gamma) \leq 0$.

*Proof.* First we can write $\varpi_j(\gamma)$ in terms of $a_j(\gamma)$ (defined in Lemma 3.5.1)

$$\begin{aligned} \varpi_j(\gamma) &= \frac{1}{2}\left[\left((j+2)^\gamma - (j+1)^\gamma + (j+1)^\gamma - j^\gamma\right) - \left(j^\gamma - (j-1)^\gamma + (j-1)^\gamma - (j-2)^\gamma\right)\right] \\ &= \frac{1}{2}\left[a_{j+2}(\gamma) + a_{j+1}(\gamma) - \left(a_j(\gamma) + a_{j-1}(\gamma)\right)\right]. \end{aligned} \tag{3.56}$$

By Lemma 3.5.1 we have $a_{j+2}(\gamma) < a_{j+1}(\gamma) < a_j(\gamma)$, and so

$$\begin{aligned} \varpi_j(\gamma) &< \frac{1}{2}\left[2a_{j+1}(\gamma) - a_j(\gamma) - a_{j-1}(\gamma)\right] \\ &< \frac{1}{2}\left[a_j(\gamma) - a_{j-1}(\gamma)\right]. \end{aligned} \tag{3.57}$$

Since $a_j(\gamma) < a_{j-1}(\gamma)$, then we have the result $\varpi_j(\gamma) < 0$.
If $\gamma = 1$, then $\varpi_j(\gamma) = 0$, for $j \geq 2$ by direct substitution. □

**Lemma 3.5.3.** If $\hat{b}_j = \frac{1}{2}\left(j^\gamma - (j-2)^\gamma\right) - \beta_j^*(\gamma)$, where $\beta_j^*(\gamma)$ is defined in Equation (3.18) and $0 < \gamma \leq 1$, then $\hat{b}_j > 0$, for $j \geq 2$.

*Proof.* By using Equation (3.18), we then rewrite $\hat{b}_j$ as follows

$$\begin{aligned} \hat{b}_j &= \frac{1}{2}\left(a_j(\gamma) + a_{j-1}(\gamma)\right) - \left(2\gamma j^{\gamma-1} - a_j(\gamma)\right) \\ &= \frac{1}{2}\left(a_j(\gamma) + a_{j-1}(\gamma)\right) - 2\gamma j^{\gamma-1} + a_j(\gamma). \end{aligned} \tag{3.58}$$

By using Lemma 3.5.1, we have $a_{j-1}(\gamma) > a_j(\gamma)$, and so

$$\hat{b}_j > 2a_j(\gamma) - 2\gamma j^{\gamma-1} = 2\left(a_j - \gamma j^{\gamma-1}\right). \tag{3.59}$$

From Appendix B.10, we have $\gamma j^{\gamma-1} - a_j(\gamma) < 0$ then $a_j(\gamma) - \gamma j^{\gamma-1} > 0$, and we conclude that $\hat{b}_j > 0$, $\forall j \geq 2$. □

**Lemma 3.5.4.** Given $b_j = \frac{1}{2}\left[(j-1)^\gamma - (j-3)^\gamma\right] - a_j(\gamma)$ where $a_j(\gamma)$ defined in Equation (3.17) and $0 < \gamma < 1$, then $b_j > 0$, $\forall j \geq 3$.

*Proof.* Rewrite $b_j$ as follows

$$b_j = \frac{1}{2}\left(a_{j-1}(\gamma) + a_{j-2}(\gamma)\right) - a_j(\gamma) \tag{3.60}$$

and using the result $a_{j-2}(\gamma) > a_{j-1}(\gamma)$ from Lemma 3.5.1 twice we then have

$$\begin{aligned} b_j &> \frac{1}{2}\left(a_{j-1}(\gamma) + a_{j-1}(\gamma)\right) - a_j(\gamma) \\ &= a_{j-1}(\gamma) - a_j(\gamma) > 0. \end{aligned} \tag{3.61}$$

We then conclude that $b_j > 0$, $\forall j \geq 3$. □

We now consider the stability of our scheme.

**Proposition 3.5.5.** Let $\zeta_j$, where $j = 1, 2, ..., M$ be the solutions of Equation (3.43), then

$$|\zeta_j| \leq |\zeta_0|. \tag{3.62}$$

*Proof.* We use mathematical induction method to prove the relation in Equation (3.62). We assume $\zeta_0 > 0$, and first consider the case $j = 1$. From Equation (3.43) we have

$$\zeta_1 = \zeta_0 - \lambda_q(\beta_1^*(\gamma)\zeta_0 + a_1(\gamma)\zeta_1). \tag{3.63}$$

Using $\beta_1^*(\gamma) = 2\gamma - 1$ and $a_1(\gamma) = 1$, gives

$$(1 + \lambda_q)\zeta_1 = [1 - \lambda_q(2\gamma - 1)]\zeta_0, \tag{3.64}$$

which can be simplified to

$$\zeta_1 = \left(1 - \frac{2\gamma\lambda_q}{1 + \lambda_q}\right)\zeta_0. \tag{3.65}$$

Since the second term in the bracket is positive then $\zeta_1$ is bounded above by $\zeta_0$, that is

$$\zeta_1 = \left(1 - \frac{2\gamma\lambda_q}{1+\lambda_q}\right)\zeta_0 \le \zeta_0. \tag{3.66}$$

In addition, for $0 \le \lambda_q \le 1$, we have

$$0 \le \frac{2\gamma\lambda_q}{1+\lambda_q} \le \gamma, \tag{3.67}$$

so

$$1 \ge 1 - \frac{2\gamma\lambda_q}{1+\lambda_q} \ge 1-\gamma \ge 0 \ge -1, \tag{3.68}$$

and we conclude that

$$\zeta_1 = \left(1 - \frac{2\gamma\lambda_q}{1+\lambda_q}\right)\zeta_0 \ge -\zeta_0, \tag{3.69}$$

hence

$$-\zeta_0 \le \zeta_1 \le \zeta_0, \tag{3.70}$$

or

$$|\zeta_1| < |\zeta_0|. \tag{3.71}$$

So Equation (3.62) is true for $j = 1$.

In the case $j = 2$, from Equation (3.43), we have

$$\zeta_2 = \zeta_1 - \lambda_q\left[\beta_2^*(\gamma)\zeta_0 + a_2(\gamma)\zeta_1 + 2^{\gamma-1}\zeta_2 - 2^{\gamma-1}\zeta_0\right]. \tag{3.72}$$

Then using Equations (3.17) – (3.19), we find

$$\zeta_2 = \frac{1}{1+2^{\gamma-1}\lambda_q}\left\{\left[1-\lambda_q(2^\gamma-1)\right]\zeta_1 - \lambda_q\left(2\gamma 2^{\gamma-1} - 2^\gamma + 1 - 2^{\gamma-1}\right)\zeta_0\right\}. \tag{3.73}$$

Since for $0 \le \lambda_q \le 1$ and $0 < \gamma \le 1$, we have $2^\gamma - 1 > 0$, we see the coefficient of $\zeta_1$ obeys the inequality

$$0 \le 2 - 2^\gamma \le 1 - \lambda_q(2^\gamma - 1) \le 1. \tag{3.74}$$

In addition since $\zeta_1 \le \zeta_0$ we have

$$\zeta_2 \le \frac{1}{1+2^{\gamma-1}\lambda_q}\left\{\left[1+\lambda_q(1-2^\gamma)\right] - \lambda_q\left(2\gamma 2^{\gamma-1} - 2^\gamma + 1 - 2^{\gamma-1}\right)\right\}\zeta_0 \tag{3.75}$$

$$\le \left(1 - \frac{\gamma 2^\gamma\lambda_q}{1+2^{\gamma-1}\lambda_q}\right)\zeta_0. \tag{3.76}$$

Since the second term in the brackets is positive then $\zeta_2$ is bounded above by $\zeta_0$

$$\zeta_2 = \left(1 - \frac{\gamma 2^\gamma\lambda_q}{1+2^{\gamma-1}\lambda_q}\right)\zeta_0 < \zeta_0. \tag{3.77}$$

Since we also have $-\zeta_0 \leq \zeta_1$, then from Equation (3.73)

$$\zeta_2 \geq \frac{1}{1+2^{\gamma-1}\lambda_q}\left\{1+\lambda_q(1-2^\gamma)+\lambda_q\left(2\gamma 2^{\gamma-1}-2^\gamma+1-2^{\gamma-1}\right)\right\}(-\zeta_0), \tag{3.78}$$

which simplifies to

$$\zeta_2 \geq -\left(1+\frac{\lambda_q\left(2+2^\gamma(\gamma-3)\right)}{1+2^{\gamma-1}\lambda_q}\right)\zeta_0. \tag{3.79}$$

For $0 \leq \lambda_q \leq 1$ and since $-2 < 2^\gamma(\gamma-3) < -1$ for $0 < \gamma < 1$, we have

$$\frac{\lambda_q\left(2+2^\gamma(\gamma-3)\right)}{1+2^{\gamma-1}\lambda_q} \leq \frac{2+2^\gamma(\gamma-3)}{1+2^{\gamma-1}}, \tag{3.80}$$

and for $0 < \gamma \leq 1$

$$-1 \leq \frac{2+2^\gamma(\gamma-3)}{1+2^{\gamma-1}} \leq -2/3 < 0. \tag{3.81}$$

So we then have

$$0 \leq 1+\frac{\lambda_q(2+2^\gamma(\gamma-3))}{1+2^{\gamma-1}\lambda_q} \leq 1, \tag{3.82}$$

which gives the bound

$$\zeta_2 \geq -\left(1+\frac{\lambda_q\left(2+2^\gamma(\gamma-3)\right)}{1+2^{\gamma-1}\lambda_q}\right)\zeta_0 \geq -\zeta_0. \tag{3.83}$$

We then conclude that

$$-\zeta_0 \leq \zeta_2 \leq \zeta_0, \tag{3.84}$$

or

$$|\zeta_2| \leq |\zeta_0|. \tag{3.85}$$

So Equation (3.62) is also true for $j = 2$.

We now assume that

$$-\zeta_0 \leq \zeta_n \leq \zeta_0, \qquad \text{for} \qquad n = 1, 2, ..., k, \tag{3.86}$$

and then need to show that

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0. \tag{3.87}$$

From Equation (3.45) we have

$$\begin{aligned}\zeta_{k+1} = \frac{1}{1+2^{\gamma-1}\lambda_q}\Bigg\{&\left[1+\frac{1}{2}\left(1-3^\gamma\right)\lambda_q\right]\zeta_k+\lambda_q\left[\frac{1}{2}\left(k^\gamma-(k-2)^\gamma\right)-\beta_k^*(\gamma)\right]\zeta_0\\ &+\lambda_q\left[\frac{1}{2}\left((k-1)^\gamma-(k-3)^\gamma\right)-a_k(\gamma)\right]\zeta_1+\lambda_q\sum_{l=2}^{k-2}(-\varpi_{k-l}(\gamma))\zeta_l\Bigg\}.\end{aligned} \tag{3.88}$$

In Lemma 3.5.2 we have shown $\varpi_l(\gamma) < 0$ therefore $-\varpi_l(\gamma) > 0$, and for $0 \le \lambda_q \le 1$ and $0 < \gamma \le 1$ the coefficient of $\zeta_k$ satisfies

$$0 < \frac{1}{2}\left(3 - 3^{\gamma}\right) \le 1 + \frac{1}{2}\left(1 - 3^{\gamma}\right)\lambda_q \le 1.$$

By using Lemmas 3.5.3 and 3.5.4 with Equation (3.86), where $\zeta_n \le \zeta_0$, then Equation (3.88) becomes

$$\zeta_{k+1} \le \frac{1}{1 + 2^{\gamma-1}\lambda_q}\left\{ 1 + \frac{1}{2}\left(1 - 3^{\gamma}\right)\lambda_q + \lambda_q\left[\frac{1}{2}\left(k^{\gamma} - (k-2)^{\gamma}\right) - \beta_k^*(\gamma)\right] \right.$$
$$\left. + \lambda_q\left[\frac{1}{2}\left((k-1)^{\gamma} - (k-3)^{\gamma}\right) - a_k(\gamma)\right] + \lambda_q\sum_{l=2}^{k-2}(-\varpi_{k-l}(\gamma))\right\}\zeta_0. \tag{3.89}$$

Now evaluating the summation in Equation (3.89), gives

$$\begin{aligned}\sum_{l=2}^{k-2}(-\varpi_{k-l}(\gamma)) &= \frac{1}{2}\sum_{l=2}^{k-2}\left[-(k-l+2)^{\gamma} + 2(k-l)^{\gamma} - (k-l-2)^{\gamma}\right] \\ &= \frac{1}{2}\left[-\sum_{l=0}^{k-4}(k-l)^{\gamma} + \sum_{l=2}^{k-2}(k-l)^{\gamma} + \left(\sum_{l=2}^{k-2}(k-l)^{\gamma} - \sum_{l=4}^{k}(k-l)^{\gamma}\right)\right] \\ &= \frac{1}{2}\left[-k^{\gamma} - (k-1)^{\gamma} + (k-2)^{\gamma} + (k-3)^{\gamma} + 2^{\gamma} + 3^{\gamma} - 1\right].\end{aligned} \tag{3.90}$$

Using this result in Equation (3.89), we find

$$\zeta_{k+1} \le \frac{1}{1 + 2^{\gamma-1}\lambda_q}\left\{ 1 + \frac{1}{2}\left(1 - 3^{\gamma}\right)\lambda_q + \lambda_q\left[\frac{1}{2}\left(k^{\gamma} - (k-2)^{\gamma}\right) - \beta_k^*(\gamma)\right] \right.$$
$$+ \lambda_q\left[\frac{1}{2}\left((k-1)^{\gamma} - (k-3)^{\gamma}\right) - a_k(\gamma)\right]$$
$$\left. + \frac{\lambda_q}{2}\left[3^{\gamma} + 2^{\gamma} - 1 - k^{\gamma} - (k-1)^{\gamma} + (k-2)^{\gamma} + (k-3)^{\gamma}\right]\right\}\zeta_0, \tag{3.91}$$

which can be simplified to

$$\zeta_{k+1} \le \left(1 - \frac{2\gamma k^{\gamma-1}\lambda_q}{1 + 2^{\gamma-1}\lambda_q}\right)\zeta_0. \tag{3.92}$$

Since the second term is positive then $\zeta_{j+1}$ is bounded above by $\zeta_0$

$$\zeta_{k+1} < \left(1 - \frac{2\gamma k^{\gamma-1}\lambda_q}{1 + 2^{\gamma-1}\lambda_q}\right)\zeta_0 < \zeta_0. \tag{3.93}$$

Since $-\zeta_0 \le \zeta_n$ then Equation (3.88) becomes

$$\zeta_{k+1} \ge \frac{1}{1 + 2^{\gamma-1}\lambda_q}\left\{ 1 + \frac{1}{2}\left(1 - 3^{\gamma}\right)\lambda_q + \lambda_q\left[\frac{1}{2}\left(k^{\gamma} - (k-2)^{\gamma}\right) - \beta_k^*(\gamma)\right] \right.$$
$$\left. + \lambda_q\left[\frac{1}{2}\left((k-1)^{\gamma} - (k-3)^{\gamma}\right) - a_k(\gamma)\right] - \lambda_q\sum_{l=2}^{k-2}\varpi_{k-l}(\gamma)\right\}(-\zeta_0), \tag{3.94}$$

which can be simplified to

$$\zeta_{k+1} \geq -\left(1 - \frac{2\gamma k^{\gamma-1}\lambda_q}{1+2^{\gamma-1}\lambda_q}\right)\zeta_0, \tag{3.95}$$

we then have

$$\zeta_{k+1} \geq -\left(1 - \frac{2\gamma k^{\gamma-1}\lambda_q}{1+2^{\gamma-1}\lambda_q}\right)\zeta_0 \geq -\zeta_0. \tag{3.96}$$

So Equation (3.62) is true for $n = k+1$ that is

$$-\zeta_0 < \zeta_{k+1} < \zeta_0, \tag{3.97}$$

or

$$|\zeta_{k+1}| < |\zeta_0|. \tag{3.98}$$

Then for all $n \in \mathbb{N}$ Equation (3.62) is true. Hence according to Von Neumann stability analysis the numerical method is unconditionally stable. □

### 3.5.1 Numerical Solution of the Recurrence Relationship

In this section we investigate the solution of the recurrence relationship in Equation (3.43) by direct evaluation, where $0 < \gamma < 1$. The ratio $\zeta_j/\zeta_0$ is shown in Figure 3.2 against $j$ (where $j = 1, \ldots, 100$) for various values of $\gamma = 0.1, \ldots, 0.9$ when $\lambda_q = 1$. Also the ratio $\zeta_j/\zeta_{j-1}$ is plotted as a loglog plot given in Figure 3.3. From these results this method is stable as the ratio is less than 1, as predicted.

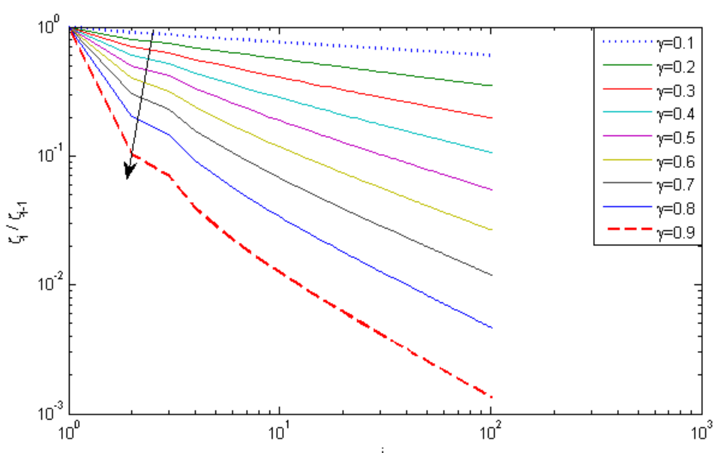



Figure 3.2: Prediction of $\zeta_j/\zeta_0$ found from numerically evaluating the recurrence relation in Equation (3.43). Results are shown for 100 time steps, $\lambda_q = 1$ and $\gamma = 0.1, \ldots, 0.9$. In this figure $\gamma$ increases in the direction of the arrow.

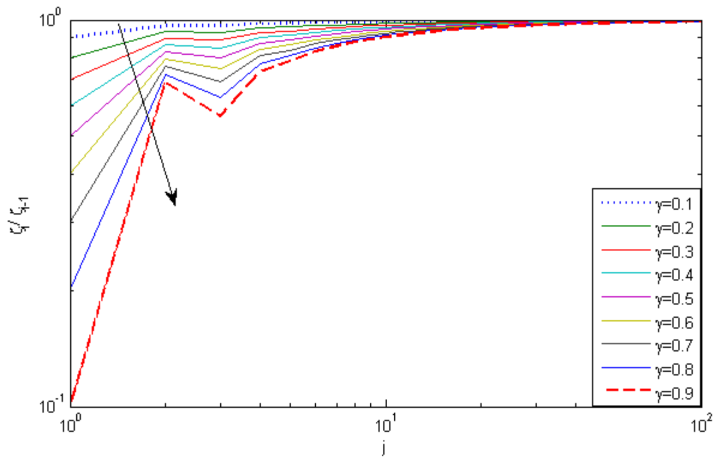



Figure 3.3: Results of $\zeta_j/\zeta_{j-1}$ found from Equation (3.43) for $j = 1, \ldots, 100$, $\lambda_q = 1$ and $\gamma = 0.1, \ldots, 0.9$. In this figure $\gamma$ increases in the direction of the arrow.

## 3.6 Convergence of the IMC1 Method

In this section, we consider the the convergence of the IMC1 scheme, we follow the approach as in Chen, Liu, Anh & Turner (2010) by defining

$$R_i^j = \frac{U_i^j - U_i^{j-1}}{\Delta t} - \frac{D\Delta t^{\gamma-1}}{2\Gamma(1+\gamma)}\Bigg\{ \beta_j^*(\gamma)\delta_x^2 U_i^0 + a_j(\gamma)\delta_x^2 U_i^1 + \delta_x^2 U_i^j - \delta_x^2 U_i^{j-1} + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^{k-1}\right]\Bigg\} - f_i^j, \tag{3.99}$$

where $\delta_x^2 U_i^j$ is defined as in Equation (3.12), from the C1 scheme we note that

$$\left[\frac{d^{1-\gamma} f(t)}{dt^{1-\gamma}}\right|_{C1}^{j} = \frac{\Delta t^{\gamma-1}}{2\Gamma(1+\gamma)}\Bigg\{ \beta_j^*(\gamma) f_0 + a_j(\gamma) f_1 + f_j - f_{j-1} + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[f_{k+1} - f_{k-1}\right]\Bigg\} + O(\Delta t^{1+\gamma}). \tag{3.100}$$

Now using Equations (3.23), (3.24) and (3.100) in to Equation (3.99), we then have

$$\begin{aligned} R_i^j &= \frac{\partial U_i^j}{\partial t} - f_i^j + O(\Delta t) - D\frac{\Delta t^{\gamma-1}}{2\Gamma(1+\gamma)}\Bigg\{ \beta_j^*(\gamma)\frac{\partial^2 U_i^0}{\partial x^2} + a_j(\gamma)\frac{\partial^2 U_i^1}{\partial x^2} + \frac{\partial^2 U_i^j}{\partial x^2} - \frac{\partial^2 U_i^{j-1}}{\partial x^2} \\ &\quad + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\frac{\partial^2 U_i^{k+1}}{\partial x^2} - \frac{\partial^2 U_i^{k-1}}{\partial x^2}\right] + O(\Delta x^2)\Bigg\} + O(\Delta t^{1+\gamma}) \\ &= \left[\frac{\partial U}{\partial t}\right|_i^j - D\left[\frac{\partial^{1-\gamma}}{\partial^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j - f_i^j + O(\Delta t + \Delta x^2). \end{aligned} \tag{3.101}$$

According to the Equation (3.101), we have

$$R_i^j = O(\Delta t + \Delta x^2)\ , \tag{3.102}$$

where $i = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, M$, since $i, j$ are finite, there is a positive constant $c_1$ for all $i, j$ such that

$$|R_i^j| \leq c_1(\Delta t + \Delta x^2). \tag{3.103}$$

Let

$$E_i^j = U_i^j - u_i^j \tag{3.104}$$

where $i = 1, 2, \ldots, N$ and $j = 0, 1, 2, \ldots, M$. From Equation (3.99) we have

$$\begin{aligned} U_i^j &= U_i^{j-1} + \frac{\Delta t^\gamma}{2\Gamma(1+\gamma)}\Bigg\{\beta_j^*(\gamma)\delta_x^2 U_i^0 + a_j(\gamma)\delta_x^2 U_i^1 + \delta_x^2 U_i^j - \delta_x^2 U_i^{j-1} \\ &\quad + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^{k-1}\right]\Bigg\} + \Delta t f_i^j + \Delta t R_i^j. \end{aligned} \tag{3.105}$$

Subtracting (3.11) from (3.105), we then have the following error equation

$$\begin{aligned} E_i^j &= E_i^{j-1} + \frac{\Delta t^\gamma}{2\Gamma(1+\gamma)}\Bigg\{\beta_j^*(\gamma)\delta_x^2 E_i^0 + a_j(\gamma)\delta_x^2 E_i^1 + \delta_x^2 E_i^j - \delta_x^2 E_i^{j-1} \\ &\quad + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\delta_x^2 E_i^{k+1} - \delta_x^2 E_i^{k-1}\right]\Bigg\} + \Delta t R_i^j. \end{aligned} \tag{3.106}$$

For $i = 1, 2, \ldots, N$ we define the following grid function

$$E^j(x) = \begin{cases} E_i^j & \text{if } x \in \left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right],\ i = 1, 2, \ldots, N \\ 0 & \text{if } x \in \left[0, \frac{\Delta x}{2}\right] \bigcup \left(L - \frac{\Delta x}{2}, L\right], \end{cases} \tag{3.107}$$

and

$$R^j(x) = \begin{cases} R_i^j & \text{if } x \in \left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right],\ i = 1, 2, \ldots, N \\ 0 & \text{if } x \in \left[0, \frac{\Delta x}{2}\right] \bigcup \left(L - \frac{\Delta x}{2}, L\right] \end{cases} \tag{3.108}$$

respectively and then $E_i^j$ and $R_i^j$ can be expanded in Fourier series as

$$E^j(x) = \sum_{l=-\infty}^{\infty} \xi_j(l) e^{i' 2\pi l x/L}, \qquad j = 0, 1, 2, \ldots, M \tag{3.109}$$

and

$$R^j(x) = \sum_{l=-\infty}^{\infty} \eta_j(l) e^{i' 2\pi l x/L}, \qquad j = 0, 1, 2, \ldots, M \tag{3.110}$$

where

$$\xi_j(l) = \frac{1}{L}\int_0^L E^j(x)e^{-i'2\pi lx/L}dx, \tag{3.111}$$

and

$$\eta_j(l) = \frac{1}{L}\int_0^L R^j(x)e^{-i'2\pi lx/L}dx. \tag{3.112}$$

Next we applying the Parseval identity (Spiegel 1965, Spiegel 1991), we then have

$$\|E^j\|_2 = \left(\sum_{i=1}^{N-1}\Delta x|E_i^j|^2\right)^{\frac{1}{2}} = \left(\sum_{l=-\infty}^{\infty}|\xi_j(l)|^2\right)^{\frac{1}{2}}, \qquad j = 0,1,2,\ldots,M \tag{3.113}$$

and

$$\|R^j\|_2 = \left(\sum_{i=1}^{N-1}\Delta x|R_i^j|^2\right)^{\frac{1}{2}} = \left(\sum_{l=-\infty}^{\infty}|\eta_j(l)|^2\right)^{\frac{1}{2}}, \qquad j = 0,1,2,\ldots,M. \tag{3.114}$$

Now we assume that

$$E_i^j = \xi_j e^{i'qi\Delta x}, \tag{3.115}$$

and

$$R_i^j = \eta_j e^{i'qi\Delta x}, \tag{3.116}$$

where $q = 2\pi l/L$ and $i' = \sqrt{-1}$. Using Equations (3.115) and (3.116) in (3.106) gives

$$\xi_j = \xi_{j-1} - v_q\left\{\beta_j^*(\gamma)\xi_0 + a_j(\gamma)\xi_1 + \xi_j - \xi_{j-1} + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\xi_{k+1} - \xi_{k-1}\right]\right\} + \Delta t\eta_j, \tag{3.117}$$

where $v_q$ is defined as in Equation (3.42). Equation (3.117) becomes

$$\xi_j = \xi_{j-1} - \frac{v_q}{1+v_q}\left\{\beta_j^*(\gamma)\xi_0 + a_j(\gamma)\xi_1 + \sum_{k=1}^{j-1}\mu_{j-k}^*(\gamma)\left[\xi_{k+1} - \xi_{k-1}\right]\right\} + \frac{\Delta t\eta_j}{1+v_q}. \tag{3.118}$$

For $j \geq 3$, Equation (3.117) can be rewritten as

$$\begin{aligned}\xi_j = \frac{1}{1+2^{\gamma-1}\lambda_q}\Bigg\{&\left(1+\frac{1}{2}\left(1-3^\gamma\right)\lambda_q\right)\xi_{j-1} + \lambda_q\left(\frac{1}{2}\left(j^\gamma - (j-2)^\gamma\right) - \beta_j^*(\gamma)\right)\xi_0 \\ &+\lambda_q\left(\frac{1}{2}\left((j-1)^\gamma - (j-3)^\gamma\right) - a_j(\gamma)\right)\xi_1 - \lambda_q\sum_{2}^{j-2}\varpi_{j-r}(\gamma)\xi_r + \Delta t\eta_j\Bigg\},\end{aligned} \tag{3.119}$$

where the weight $\varpi_j(\gamma)$ is defined as in Equation (3.46), and also $\lambda_q$ is defined as in Equation (3.44).

**Proposition 3.6.1.** Let $\xi_j$ be the solution of Equation (3.118). Then there exists a positive constant $c_2$ such that

$$|\xi_j| \le c_2 j \Delta t |\eta_1|, \tag{3.120}$$

where $j = 1, 2, \ldots, M$.

*Proof.* From Equation (3.104), we note that $E^0 = 0$, we then have.

$$\xi_0 = \xi_0(l) = 0. \tag{3.121}$$

From Equations (3.103) and (3.114), we obtain

$$\|R^j\|_2 \le c_2 \sqrt{N\Delta x}(\Delta t + \Delta x^2) = c_2\sqrt{L}(\Delta t + \Delta x^2), \tag{3.122}$$

where $j = 1, 2, \ldots, M$, and on the right hand side (3.114) by the convergence of the series there is a positive constant $c_j$ such that

$$|\eta_j| \equiv |\eta_j(l)| \le c_j|\eta_1| \equiv c_j|\eta_1(l)|, \qquad j = 1, 2, \ldots, M. \tag{3.123}$$

We then obtain

$$|\eta_j| \le c_2|\eta_1(l)|, \qquad j = 1, 2, \ldots, M, \tag{3.124}$$

where

$$c_2 = \max_{1\le j\le M}\{c_j\}. \tag{3.125}$$

Now using mathematical induction, starting with $j = 1$, from Equation (3.118), we have

$$\left(1 + \frac{v_q}{1+v_q}\right)\xi_1 = \frac{\Delta t \eta_j}{1+v_q}, \tag{3.126}$$

Equation (3.126) becomes

$$\xi_1 = \frac{1}{1+2v_q}\Delta t \eta_1, \tag{3.127}$$

since $1 + 2v_q > 0$, we obtain

$$|\xi_1| \le \frac{1}{1+2v_q}\Delta t|\eta_1| \le \Delta t|\eta_1| \le c_2\Delta t|\eta_1|. \tag{3.128}$$

For $j = 2$, from Equation (3.118), we have

$$\xi_2 = \xi_1 - \frac{v_q}{1+v_q}\left[\beta_2^*(\gamma)\xi_0 + a_2(\gamma)\xi_1 + 2^{\gamma-1}\xi_2 - 2^{\gamma-1}\xi_0\right] + \frac{\Delta t \eta_2}{1+v_q}, \tag{3.129}$$

which upon using Equation (3.127) in Equation (3.129), is then given by

$$\begin{aligned}\xi_2 &= \frac{\Delta t}{(1+2v_q)(1+v_q+v_q 2^{\gamma-1})}\left[(1+v_q(2-2^{\gamma}))\eta_1+(1+2v_q)\eta_2\right]\\ &= \frac{\Delta t}{1+v_q+v_q 2^{\gamma-1}}\left[\left(1-\frac{v_q 2^{\gamma}}{1+2v_q}\right)\eta_1+\eta_2\right],\end{aligned} \tag{3.130}$$

since $|\eta_2| \le c_2|\eta_1|$, we then obtain

$$\begin{aligned}|\xi_2| &\le \frac{\Delta t}{1+v_q+v_q 2^{\gamma-1}}\left[\left|1-\frac{v_q 2^{\gamma}}{1+2v_q}\right|+c_2\right]|\eta_1|\\ &\le \frac{(1+c_2)}{1+v_q+v_q 2^{\gamma-1}}\Delta t|\eta_1|\\ &\le 2c_2\Delta t|\eta_1|.\end{aligned} \tag{3.131}$$

Suppose that

$$|\xi_n| \le c_2 n\Delta t|\eta_1|, \qquad n=1,2,\ldots,k-1. \tag{3.132}$$

For $0<\gamma<1$ and $v_q>0$, from Equation (3.119), we have

$$\begin{aligned}|\xi_k| \le \frac{1}{1+2^{\gamma-1}\lambda_q}\Bigg\{&\left|1+\frac{1}{2}\left(1-3^{\gamma}\right)\lambda_q\right||\xi_{k-1}|+\lambda_q\left|\frac{1}{2}\left(k^{\gamma}-(k-2)^{\gamma}\right)-\beta_k^*(\gamma)\right||\xi_0|\\ &+\lambda_q\left|\frac{1}{2}\left((k-1)^{\gamma}-(k-3)^{\gamma}\right)-a_k(\gamma)\right||\xi_1|+\lambda_q\sum_{l=2}^{k-2}|-\varpi_{k-l}(\gamma)||\xi_l|+\Delta t|\eta_k|\Bigg\}.\end{aligned} \tag{3.133}$$

In Lemma 3.5.2 we have shown $\varpi_l(\gamma)<0$ therefore $-\varpi_l(\gamma)>0$, and in Lemma 3.5.4 the coefficient $\frac{1}{2}\left[(k-1)^{\gamma}-(k-3)^{\gamma}\right]-a_k(\gamma)$ is positive. For $0\le\lambda_q\le 1$ and $0<\gamma\le 1$ the coefficient of $\xi_{k-1}$ satisfies

$$0<\frac{1}{2}\left(3-3^{\gamma}\right)\le 1+\frac{1}{2}\left(1-3^{\gamma}\right)\lambda_q\le 1.$$

Equation (3.133) becomes after using Equation (3.132)

$$\begin{aligned}|\xi_k| \le \frac{c_2\Delta t}{1+2^{\gamma-1}\lambda_q}\Bigg\{&\left[1+\frac{1}{2}\left(1-3^{\gamma}\right)\lambda_q\right](k-1)+\lambda_q\left(\frac{1}{2}\left((k-1)^{\gamma}-(k-3)^{\gamma}\right)-a_k(\gamma)\right)\\ &+\lambda_q\sum_{l=2}^{k-2}(-l\varpi_{k-l}(\gamma))+1\Bigg\}|\eta_1|.\end{aligned} \tag{3.134}$$

Now evaluating the summation in Equation (3.134), gives

$$\begin{aligned}\sum_{l=2}^{k-2}(-l\varpi_{k-l}(\gamma)) &= \frac{1}{2}\sum_{l=2}^{k-2} l\left[-(k-l+2)^{\gamma}+2(k-l)^{\gamma}-(k-l-2)^{\gamma}\right]\\ &= \frac{1}{2}\left[-\sum_{l=0}^{k-4}(l+2)(k-l)^{\gamma}+\sum_{l=2}^{k-2} l\,(k-l)^{\gamma}+\left[\sum_{l=2}^{k-2} l\,(k-l)^{\gamma}-\sum_{l=4}^{k}(l-2)(k-l)^{\gamma}\right]\right]\\ &= \frac{1}{2}\left[-2k^{\gamma}-3(k-1)^{\gamma}+(k-3)^{\gamma}+k(2^{\gamma}+3^{\gamma}-1)-(3^{\gamma}-3)\right].\end{aligned} \tag{3.135}$$

Using this result in Equation (3.134), we then have

$$
\begin{aligned}
|\xi_k| \leq & \frac{c_2\Delta t}{1+2^{\gamma-1}\lambda_q}\left\{\left[1+\frac{1}{2}\left(1-3^\gamma\right)\lambda_q\right](k-1)+\lambda_q\left(\frac{1}{2}\left((k-1)^\gamma-(k-3)^\gamma\right)-\left(k^\gamma-(k-1)^\gamma\right)\right)\right.\\
& \left.+\frac{\lambda_q}{2}\left[-2k^\gamma-3(k-1)^\gamma+(k-3)^\gamma+k(3^\gamma+2^\gamma-1)-(3^\gamma-3)\right]+1\right\}|\eta_1|\\
& = \frac{c_2\Delta t}{1+2^{\gamma-1}\lambda_q}\left\{\left[1+\frac{1}{2}\left(1-3^\gamma\right)\lambda_q\right](k-1)+\lambda_q\left(-2k^\gamma+\frac{1}{2}\left[(3^\gamma+2^\gamma-1)k+(3-3^\gamma)\right]\right)+1\right\}|\eta_1|\\
& = \frac{c_2\Delta t}{1+2^{\gamma-1}\lambda_q}\left\{k(1+\lambda_q 2^{\gamma-1})+\lambda_q\left(1-2k^\gamma\right)\right\}|\eta_1|\\
& = c_2\Delta t k|\eta_1| - \frac{c_2\Delta t\lambda_q\left(2k^\gamma-1\right)}{1+2^{\gamma-1}\lambda_q}|\eta_1|\\
& \leq c_2\Delta t k|\eta_1|.
\end{aligned}
\tag{3.136}
$$

We then conclude that for $n = k$

$$
|\xi_k| \leq c_2 k\Delta t|\eta_1| \tag{3.137}
$$

and hence for all $n \in \mathbb{N}$ we have $|\xi_n| \leq c_2 n\Delta t|\eta_1|$. The proof of the proposition is completed. □

**Theorem 3.6.2.** Let $u(x,t) \in U(\Omega)$ be the exact solution for the fractional subdiffusion equation. Then the numerical scheme (3.10) – (3.19) is convergent with the convergence order $O(\Delta t + \Delta x^2)$.

*Proof.* Using Equations (3.103), (3.113), (3.114), Proposition 3.6.1, and $j\Delta t \leq T$, we then have

$$
\|E^j\|_2 \leq c_2 j\Delta t\|R_1\| \leq c_1c_2 j\Delta t\sqrt{L}(\Delta t+\Delta x^2) \leq C(\Delta t+\Delta x^2) \tag{3.138}
$$

where $C = c_1c_2T\sqrt{L}$. □

## 3.7 Numerical Examples and Results

In this section, we provide three examples of the implementation the implicit scheme, IMC1, where the analytic solution is known. For each example we compare graphically the numerical prediction against the exact solution. We also verify the accuracy of the implicit scheme by computing the maximum norm of the error between the numerical estimate $u_i^M$ and the exact solution $u(x_i, t_M)$ using the infinity norm

$$e_\infty(\Delta t, \Delta x) = \max_{1 \le i \le N} \mid u_i^M - u(x_i, t_M) \mid . \tag{3.139}$$

Numerical accuracy is studied for varying time and spatial steps sizes in the cases of $\gamma = 0.1$, 0.5, 0.9, and 1. The approximate order of convergence in $\Delta x$, $R1$, was estimated by computing the term

$$R1 = \log_2 \left[ e_\infty(\Delta t, 2\Delta x)/e_\infty(\Delta t, \Delta x) \right], \tag{3.140}$$

and the approximate order of convergence in $\Delta t$, $R2$, was estimated by computing the term

$$R2 = \log_2 \left[ e_\infty(2\Delta t, \Delta x)/e_\infty(\Delta t, \Delta x) \right]. \tag{3.141}$$

This scheme was implemented in MATLAB R2014a (see Appendix C.2) using the linsolve subroutine to solve the system of linear equations.

**Example 3.7.1.** Consider the following fractional subdiffusion equation with a source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} \right) + \sin(\pi x) \left[ 2t + \pi^2 \left( \frac{t^{\gamma-1}}{\Gamma(\gamma)} + \frac{2t^{\gamma+1}}{\Gamma(2+\gamma)} \right) \right], \tag{3.142}$$

with $0 < \gamma \le 1$ and the initial and fixed boundary conditions

$$u(x, 0) = \sin(\pi x), \ u(0, t) = 0, \ u(L, t) = 0, \tag{3.143}$$

where $0 < x < L$, $t > 0$, $L = 1$. The exact solution of Equation (3.142) given the conditions in Equation (3.143), is

$$u(x, t) = \left(1 + t^2\right) \sin(\pi x). \tag{3.144}$$

In Tables 3.1 and 3.2 we give the error and order of convergence estimates for this example. To estimate the convergence in space we kept $\Delta t$ fixed at $10^{-3}$ whilst varying the value of $\Delta x$. To estimate the convergence in time we kept $\Delta x$ fixed at $10^{-3}$ whilst varying $\Delta t$. From the results shown in Tables 3.1 and 3.2 it can be seen that the implicit method IMC1 is of order $O(\Delta x^2)$ and $O(\Delta t)$.

Table 3.1: Numerical accuracy in $\Delta x$ of the IMC1 scheme applied to Example 3.7.1 with $\Delta t = 10^{-3}$ and $R1$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.32 e–00 | – | 0.41e–00 | – | 0.42e–00 | – | 0.42e–00 | – |
| 1/4 | 0.75e–01 | 2.11 | 0.95e–01 | 2.11 | 0.99e–01 | 2.12 | 0.96e–02 | 2.12 |
| 1/8 | 0.19e–01 | 2.01 | 0.23 e–01 | 2.03 | 0.24e–01 | 2.03 | 0.24e–01 | 2.03 |
| 1/16 | 0.49e–02 | 1.93 | 0.59e–02 | 2.00 | 0.59e–02 | 2.00 | 0.59e–02 | 2.00 |
| 1/32 | 0.15e–02 | 1.72 | 0.15e–02 | 1.96 | 0.15e–02 | 1.97 | 0.15e–02 | 1.97 |

Table 3.2: Numerical accuracy in $\Delta t$ of the IMC1 scheme applied to Example 3.7.1 with $\Delta x = 10^{-3}$ and $R2$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.11e–00 | – | 0.37e–01 | – | 0.13e–01 | – | 0.10e–01 | – |
| 1/20 | 0.52e–01 | 1.06 | 0.15e–01 | 1.26 | 0.61e–02 | 1.11 | 0.51e–02 | 1.00 |
| 1/40 | 0.25e–01 | 1.07 | 0.64e–02 | 1.27 | 0.29e–02 | 1.08 | 0.25e–02 | 1.00 |
| 1/80 | 0.12e–01 | 1.08 | 0.27e–02 | 1.25 | 0.14e–02 | 1.05 | 0.13e–02 | 1.00 |
| 1/160 | 0.55e–02 | 1.08 | 0.12e–02 | 1.22 | 0.67e–03 | 1.03 | 0.64e–03 | 1.00 |

A comparison of the exact solution and the numerical solution of Equation (3.10) in the case of the fractional exponent $\gamma = 0.5$ at the times $t = 0.25$, 0.5, 0.75 and 1.0 is shown in Figure 3.4. It can be seen that, the approximate solution obtained from the numerical scheme is in good agreement with the exact solution. Results are not shown here for other values of $\gamma$, but the exact solution is the same for all $\gamma$ in this and in the next example.

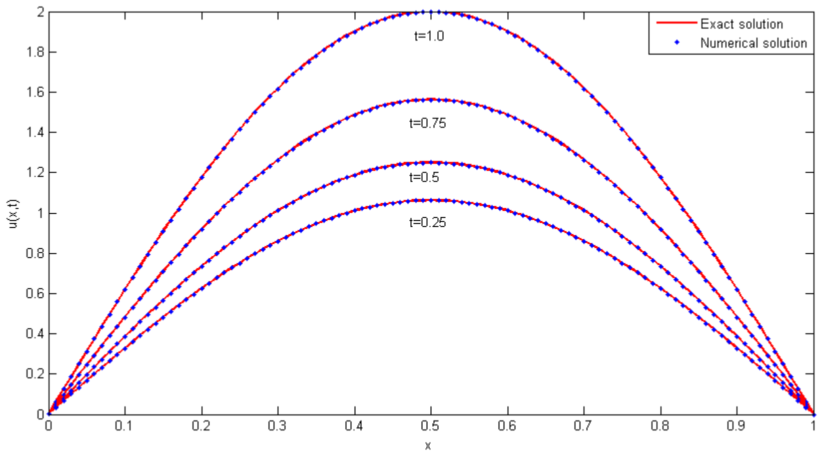



Figure 3.4: A comparison of the exact solution and the numerical solution of Equation (3.142) shown at the times $t = 0.25, 0.5, 0.7$ and $1.0$, for $\gamma = 0.5$, and time step $\Delta t = 10^{-3}$.

The numerical solution of Equation (3.142) for fractional exponent $\gamma = 0.5$, time $t = 1.0$ and $\Delta t = 10^{-2}$ is shown in Figure 3.5.

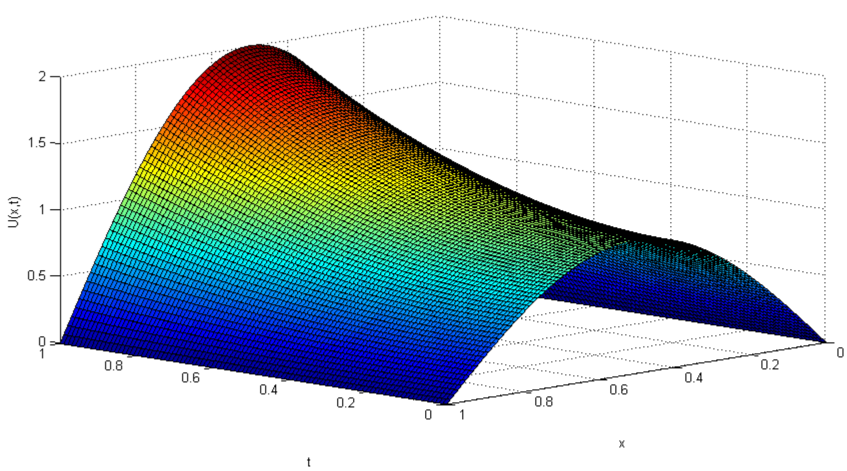



Figure 3.5: The numerical solution by the IMC1 scheme for Equation (3.142) shown for $0 \le t \le 1$, and $0 \le x \le 1$ in the case $\gamma = 0.5$.

**Example 3.7.2.** Consider the following fractional subdiffusion equation with the source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} \right) + 2e^x t \left[ 1 - \frac{t^\gamma}{\Gamma(2+\gamma)} \right], \tag{3.145}$$

with $0 < \gamma \le 1$ and the initial and fixed boundary conditions

$$u(x, 0) = 0,\ 0 < x < L,\ u(0, t) = t^2,\ u(L, t) = et^2, \tag{3.146}$$

where $t > 0$ and $L = 1$. The exact solution of Equations (3.145) and (3.146) is

$$u(x,t) = e^x t^2. \tag{3.147}$$

The absolute error and order of convergence estimated for this example are shown in Tables 3.3 and 3.4. To estimate the convergence in space we again kept $\Delta t$ fixed at $10^{-3}$ whilst varying $\Delta x$ and kept $\Delta x$ fixed at $10^{-3}$ whilst varying $\Delta t$ to estimate the convergence in time. From the results given in Tables 3.3 and 3.4, we see again that the approximate truncation order of the IMC1 scheme, given in Equation (3.10), is of order in space $O(\Delta x^2)$ and $O(\Delta t)$ in time.

Table 3.3: Numerical accuracy in $\Delta x$ of the IMC1 scheme applied to Example 3.7.2 with $\Delta t = 10^{-3}$ and $R1$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.38e–02 | – | 0.36e–02 | – | 0.34e–02 | – | 0.34e–02 | – |
| 1/4 | 0.98e–03 | 1.96 | 0.94e–03 | 1.95 | 0.90e–03 | 1.94 | 0.89e–03 | 1.94 |
| 1/8 | 0.25e–03 | 1.98 | 0.24e–03 | 1.96 | 0.23e–03 | 1.95 | 0.23e–03 | 1.95 |
| 1/16 | 0.65e–04 | 1.93 | 0.67e–04 | 1.86 | 0.64e–04 | 1.86 | 0.63e–04 | 1.86 |
| 1/32 | 0.19e–04 | 1.79 | 0.22e–04 | 1.59 | 0.21e–04 | 1.58 | 0.21e–04 | 1.58 |

Table 3.4: Numerical accuracy in $\Delta t$ of the IMC1 scheme applied to Example 3.7.2 with $\Delta x = 10^{-3}$ and $R2$ is order of convergence.

| | $\gamma = 0.2$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.45e–02 | – | 0.15e–01 | – | 0.21e–01 | – | 0.21e–01 | – |
| 1/20 | 0.31e–02 | 0.53 | 0.86e–02 | 0.85 | 0.11e–01 | 0.98 | 0.11e–01 | 1.00 |
| 1/40 | 0.20e–02 | 0.65 | 0.46e–02 | 0.89 | 0.54e–02 | 0.99 | 0.53e–02 | 1.00 |
| 1/80 | 0.12e–02 | 0.74 | 0.24e–02 | 0.93 | 0.27e–02 | 0.99 | 0.27e–02 | 1.00 |
| 1/160 | 0.68e–03 | 0.80 | 0.13e–02 | 0.95 | 0.14e–02 | 1.00 | 0.13e–02 | 1.00 |

In Figure 3.6 we show the comparison of the exact solution and the numerical solution at the times $t = 0.25$, 0.5, 0.75 and 1.0, and for the fractional exponent $\gamma = 0.5$. Again we see the numerical estimate is in agreement with the exact solution.

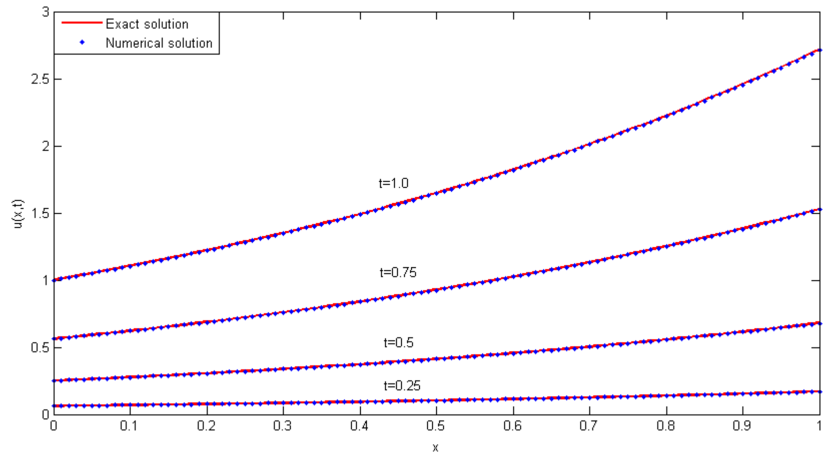



Figure 3.6: A comparison of the exact solution and the numerical solution for Equation (3.145) at different times $t = 0.25$, 0.5, 0.75, and 1.0 with $\gamma = 0.5$ and $\Delta t = 10^{-3}$.

The numerical solution of Equation (3.145) for fractional exponent $\gamma = 0.5$, for $0 \leq t \leq 1$, and $0 \leq x \leq 1$ with $\Delta t = 10^{-2}$ is shown in Figure 3.7.

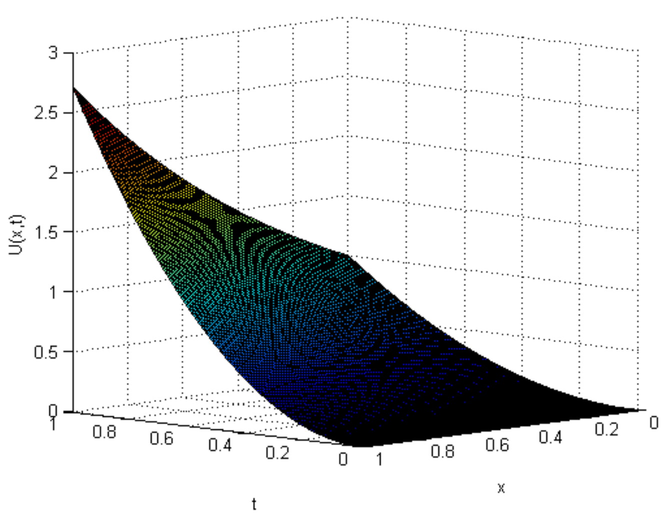



Figure 3.7: The numerical solution by the IMC1 scheme for Equation (3.145) for $0 \leq t \leq 1$, and $0 \leq x \leq 1$ in case $\gamma = 0.5$ and $\Delta t = 10^{-2}$.

**Example 3.7.3.** Consider the following fractional subdiffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} \right), \tag{3.148}$$

with the initial and fixed boundary conditions

$$u(x, 0) = \sin(\pi x), \; u(0, t) = 0, \; u(L, t) = 0 \tag{3.149}$$

where $0 < x < L$, $t > 0$, $L = 1$. The exact solution of Equation (3.148) subject to the initial and boundary condition is

$$u(x,t) = \sin(\pi x) E_\gamma(-\pi^2 t^\gamma). \tag{3.150}$$

In this example we need to evaluate the Mittag–Leffler function, $E_\gamma(z)$, (Podlubny 1998) with $\gamma = 0.5$ and $\gamma = 1.0$. To do this we rewrite the Mittag–Leffler function $E_{1/2}(z)$ in terms of known functions in MATLAB. The exact solution for $\gamma = 0.5$ then is given by

$$u(x,t) = \sin(\pi x)\exp(\pi^4 t)\,\mathrm{erfc}(\pi^2 t^\gamma) \tag{3.151}$$

and for $\gamma = 1.0$ by

$$u(x,t) = \sin(\pi x)\exp(-\pi^2 t), \tag{3.152}$$

which can be evaluated in MATLAB.

In Figure 3.8 we show the comparison of the exact solution and the numerical solution at the time $t = 0.25$, $0.5$, $0.75$ and $1.0$ with $\Delta t = 10^{-4}$. We also give a comparison at $x = 0.5$, $u(0.5,t)$ for $0 \le t \le 1$ in Figure 3.9. We see the numerical estimate lags behind the exact solution as evidenced in Figures 3.8 and 3.9.

In this example we also give the error and order of convergence estimates; For the convergence in space we kept $\Delta t$ fixed at $10^{-7}$ whilst varying $\Delta x$ and for the convergence in time we kept $\Delta x$ fixed at $10^{-3}$ whilst varying $\Delta t$. From the results shown in Table 3.5 it can be seen that, where $\gamma = 0.5$, we are not able to get the order of accuracy predicted in Section 3.3. A potential reason for this (and the lag seen in Figures 3.8 and 3.9) is that the first and second derivatives at $t = 0$ are not bounded in this example. Therefore the assumption in Section 2.6.1 in Chapter 2, that we can expanded the solution as a Taylor series around $t = 0$ is not satisfied. By decreasing $\Delta t$ we are in fact trying to approximate this singularity at $t = 0$ more closely but this is difficult to do numerically.

In Table 3.6 we show the convergence results in $\Delta x$, keeping $\Delta t = 10^{-5}$ fixed, and in $\Delta t$ keeping $\Delta x = 10^{-3}$ fixed, in the case $\gamma = 1$. From the results given in Table 3.6, we obtain the predicted accuracy of second order in space and first order in time. This is because the singularity in the derivative at $t = 0$ does not occur in the case $\gamma = 1$.

The numerical solution of Equation (3.148) by using the IMC1 scheme for fractional exponent $\gamma = 0.1, 0.5, 0.9$, and $1.0$, and $\Delta t = 10^{-4}$ are shown in Figures 3.10 and 3.11

respectively. From the results shown in these figures we see the numerical solution of Equation (3.148) changes with the value of the exponent $\gamma$. It can be seen that the solution, in the long term, decays faster to zero for larger values of $\gamma$ compared to smaller values of $\gamma$. However, it should be noted that the initial decay is faster for smaller values of $\gamma$. This behavior is consistent with the behavior of the Mittag–Leffler function.

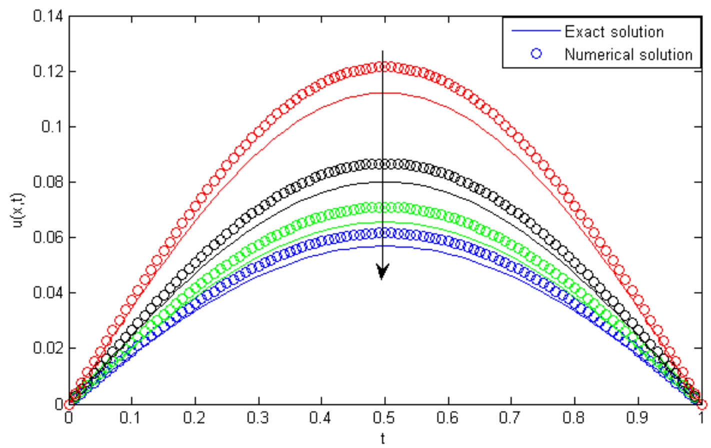



Figure 3.8: A comparison of the exact solution and the numerical solution for Equation (3.148) at times $t = 0.25$, 0.5, 0.75, and 1.0 in the case $\gamma = 0.5$ and $\Delta t = 10^{-4}$.

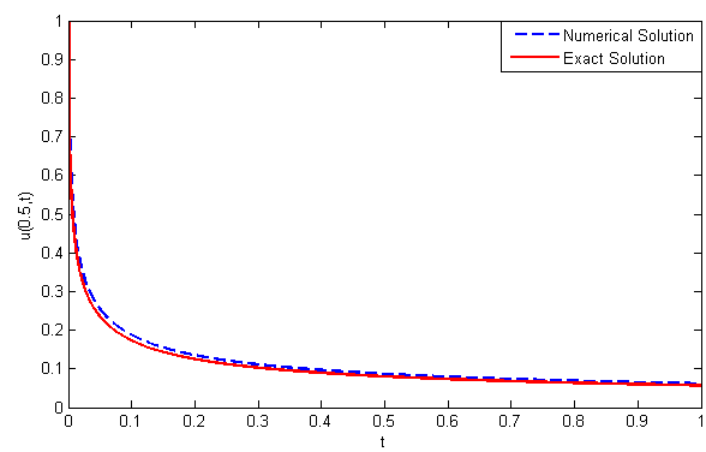
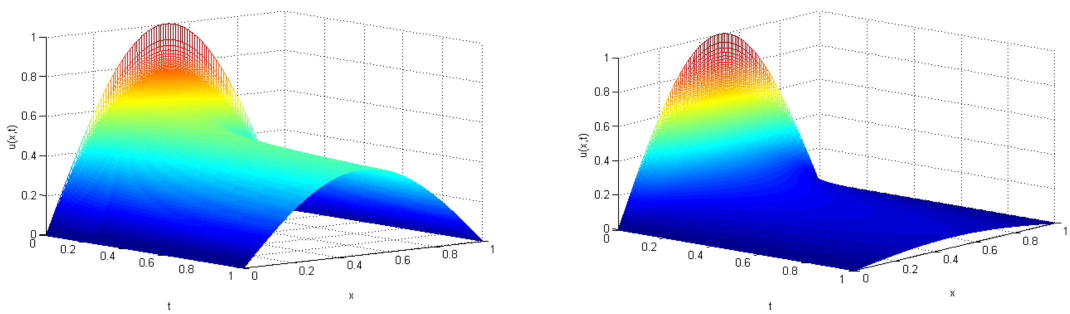
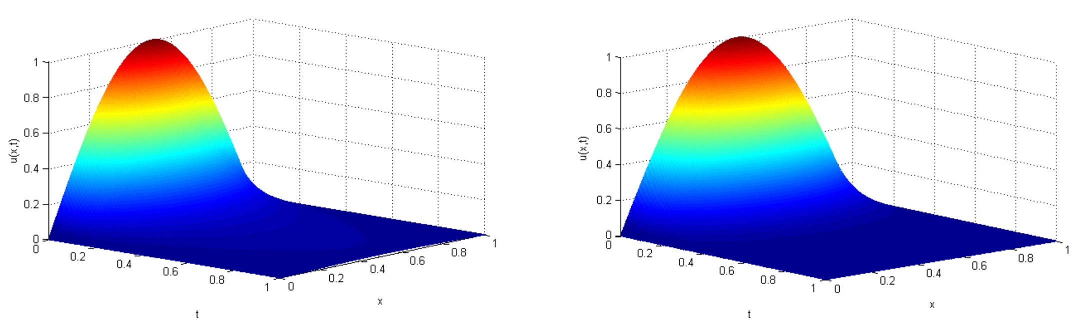



Figure 3.9: A comparison of the exact solution and the numerical solution present at the mid point $x = 0.5$ for Equation (3.148) with $\gamma = 0.5$ and time step $\Delta t = 10^{-4}$.




(a) (b)

Figure 3.10: The numerical solution of Equation (3.148), using the IMC1 scheme, shown in the case of the fractional exponent (a) $\gamma = 0.1$, and (b) $\gamma = 0.5$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ with $\Delta t = 10^{-4}$.




(a) (b)

Figure 3.11: The numerical solution of Equation (3.148), using the IMC1 scheme, shown in the case of the fractional exponent (a) $\gamma = 0.9$, and (b) $\gamma = 1$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ with $\Delta t = 10^{-4}$.

Table 3.5: Numerical accuracy in $\Delta t$ and $\Delta x$ applied to Example 3.7.3 with $\gamma = 0.5$.

| | $O(\Delta t)$ | | | $O(\Delta x)$ | |
|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/1000 | 0.11e–00 | – | 1/2 | 0.43e–00 | – |
| 1/2000 | 0.81e–01 | 0.5 | 1/4 | 0.13e–01 | 1.8 |
| 1/4000 | 0.57e–01 | 0.5 | 1/8 | 0.46e–02 | 1.5 |
| 1/8000 | 0.40e–01 | 0.5 | 1/16 | 0.25e–02 | 0.8 |
| 1/16000 | 0.28e–01 | 0.5 | 1/32 | 0.20e–02 | 0.3 |

Table 3.6: Numerical accuracy in $\Delta t$ and $\Delta x$ applied to Example 3.7.3 with $\gamma = 1$.

| $O(\Delta t)$ | | | $O(\Delta x)$ | | |
|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/1000 | 0.44e–03 | – | 1/2 | 0.17e–01 | – |
| 1/2000 | 0.22e–03 | 1.0 | 1/4 | 0.45e–02 | 1.9 |
| 1/4000 | 0.11e–03 | 1.0 | 1/8 | 0.12e–02 | 2.0 |
| 1/8000 | 0.55e–04 | 1.0 | 1/16 | 0.29e–03 | 2.0 |
| 1/16000 | 0.28 e–04 | 1.0 | 1/32 | 0.76e–04 | 2.0 |

## 3.8 Conclusion

In this chapter, we constructed the implicit method, IMC1, for the solution of the fractional subdiffusion equation, where the C1 scheme was used to approximate the fractional derivative. We have shown that the unconditional stability of the proposed method by using Von Neumann stability analysis. The order of convergence of the method is first–order in time and second–order in space. The numerical experiments have verified these results, where the known solution can be expanded as a Taylor series in time around $t = 0$.

# Chapter 4

# The Dufort–Frankel Method

## 4.1 Introduction

The Du Fort–Frankel method is an alternative approximation method, in which the value at the central grid point $u_i^j$ at time step $j$, in the centred–finite difference scheme for the second derivative, is replaced with the average of $u_i^{j+1}$ and $u_i^{j-1}$. Al-Shibani et al. (2013) applied the compact Dufort–Frankel method to solve the time-fractional diffusion equation given in Equation (1.44), in which the fractional derivative was defined by the Caputo derivative and the Grünwald-Letnikov approximation was applied to approximate the fractional derivative. Liao et al. (2014) developed the explicit Dufort–Frankel method for a fractional subdiffusion equation, where the fractional derivative was defined as Jumarie's modified Riemann–Liouville derivative (Jumarie 2006) given by Equation (1.46).

In this chapter, the Dufort–Frankel method is developed for the fractional subdiffusion equation with the inclusion of a source term $f(x,t)$, given by Equation (1.15), with $K_\gamma = 0$, which we repeat here as

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u(x,t)}{\partial x^2}\right) + f(x,t), \tag{4.1}$$

along with the initial and boundary conditions

$$u(x,0) = g(x), \qquad 0 \le x \le L, \tag{4.2}$$

$$u(0,t) = \varphi_1(t) \quad \text{and} \quad u(L,t) = \varphi_2(t), \qquad 0 \le t \le T, \tag{4.3}$$

where $D > 0$, $0 < \gamma \leq 1$ and $f(x,t)$ is a given source function. In this chapter, we suppose that $u(x,t) \in U(\Omega)$ is the exact solution for the fractional subdiffusion equation, where

$$\Omega = \{(x,t)|0 \leq x \leq L, 0 \leq t \leq T\}, \tag{4.4}$$

and

$$U(\Omega) = \left\{ u(x,t) \middle| \frac{\partial^4 u(x,t)}{\partial x^4}, \frac{\partial^2 u(x,t)}{\partial x^2 \partial t}, \frac{\partial^2 u(x,t)}{\partial t^2} \in C(\Omega) \right\}. \tag{4.5}$$

This scheme is applied to the fractional partial differential equation where the fractional derivative is given by the Riemann–Liouville definition, instead of the Caputo definition used by Al-Shibani et al. (2013).

To find the Dufort–Frankel scheme for Equation (4.1) we need to approximate the second order spatial derivative and the first order time derivative. The second order spatial derivative can be discretised using the Dufort–Frankel scheme as

$$\frac{\partial^2 u(x_i, t_j)}{\partial x^2} \approx \frac{u_{i+1}^j - u_i^{j+1} - u_i^{j-1} + u_{i-1}^j}{\Delta x^2}. \tag{4.6}$$

The time derivative on the left of Equation (4.1) can be approximated using the backward difference given by Equation (3.9) as

$$\frac{\partial u(x_i, t_j)}{\partial t} \approx \frac{u_i^j - u_i^{j-1}}{\Delta t}. \tag{4.7}$$

In the next section we develop the numerical method and in later sections we will investigate the stability, convergence and the accuracy of the numerical method and provide examples of its use.

## 4.2 Dufort–Frankel Method with the L1 Scheme: DFL1 Scheme

In this section, we describe the derivation of the Dufort–Frankel method using the L1 approximation in Equation (2.12) to evaluate the fractional derivative of order $1 - \gamma$ at time $t_j = j\Delta t$. In evaluating the L1 fractional derivative approximation of the second order spatial derivative, we use the centred difference approximation in Equation (3.6) at

$t = 0$ and $t = t_j$ and the approximation in Equation (4.6) for all other times. Together with the approximation in Equation (4.7), we then have the scheme

$$\frac{u_i^j - u_i^{j-1}}{\Delta t} = \frac{D\Delta t^{\gamma-1}}{\Delta x^2 \Gamma(1+\gamma)} \Bigg\{ \beta_j(\gamma) \left(u_{i+1}^0 - 2u_i^0 + u_{i-1}^0\right) + \left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left(u_{i+1}^k - u_i^{k+1} - u_i^{k-1} + u_{i-1}^k\right) \Bigg\} + f_i^j, \tag{4.8}$$

where $u_i^j$ is the numerical approximation of the solution $U_i^j = u(x_i, t_j)$ at the discrete grid point $(x_i, t_j)$, $\Delta x$ is the spatial grid-step size, $\Delta t$ is the time-step size and $f_i^j = f(x_i, t_j)$ is the numerical approximation of the source term. The weights $\beta_j(\gamma)$ and $\mu_j(\gamma)$ in Equation (4.8) are defined by

$$\beta_j(\gamma) = \gamma j^{\gamma-1} - \left[j^\gamma - (j-1)^\gamma\right], \tag{4.9}$$

and

$$\mu_j(\gamma) = (j+1)^\gamma - 2j^\gamma + (j-1)^\gamma \ , \tag{4.10}$$

and the term $\sigma$ is defined by

$$\sigma = \frac{D\Delta t^\gamma}{\Delta x^2 \Gamma(1+\gamma)}. \tag{4.11}$$

We denote this approximation, in Equations (4.8) – (4.11), as the DFL1 scheme. For each grid point $i$ and time step $j$, the approximations of the second derivative need to be stored for the summation in Equation (4.8). The evaluation of the summation in the Equation (4.8) is a major contributor to the computational cost that increases with each time step.

We consider the following lemma which will use later to show the stability of our numerical method.

**Lemma 4.2.1.** The coefficients $\beta_j(\gamma)$ and $\mu_j(\gamma)$ are given in Equations (4.9) and (4.10) respectively for $j \geq 1$, then $\beta_j(\gamma)$ and $\mu_j(\gamma)$ satisfy the following:

1. $\beta_j(\gamma) < 0$, where $j = 1, 2, ...,$
2. $\mu_j(\gamma) < 0$, where $j = 1, 2, ....$

*Proof.* By the result in Appendix B.10, the first result is true, that is $\beta_j(\gamma) < 0$.

To show the second result, we can rewrite $\mu_j(\gamma)$ as

$$\mu_j(\gamma) = a_{j+1} - a_j, \tag{4.12}$$

where

$$a_j = j^\gamma - (j-1)^\gamma, \tag{4.13}$$

then by Lemma 3.5.1 we have $a_{j+1} < a_j$. Then we obtain the result $\mu_{j-k} < 0$.

Hence the results (1) and (2) hold for $0 < \gamma < 1$. □

## 4.3 The Accuracy of the Dufort–Frankel Method

In this section we consider the accuracy of the numerical scheme the Dufort–Frankel method in Equation (4.8). We let

$$\delta_x^2 u_i^j = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}, \tag{4.14}$$

and then rewrite Equation (4.8), noting $\mu_{j-k}(\gamma) = a_{j-k+1} - a_{j-k}$, as

$$\begin{aligned} \frac{u_i^j - u_i^{j-1}}{\Delta t} &= \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{ \beta_j \delta_x^2 u_i^0 + \delta_x^2 u_i^j + \sum_{k=1}^{j-1} (a_{j-k+1} - a_{j-k})\, \delta_x^2 u_i^k \right. \\ &\left. + \sum_{k=1}^{j-1} (a_{j-k+1} - a_{j-k}) \left( \frac{2u_i^k - u_i^{k+1} - u_i^{k-1}}{\Delta x^2} \right) \right\} + f_i^j. \end{aligned} \tag{4.15}$$

Identifying the first term on the right hand side of Equation (4.15) as the L1 approximation, Equation (2.12), with $u(t)$ replaced by $\delta_x^2 u_i(t)$, we then have

$$\begin{aligned} \frac{u_i^j - u_i^{j-1}}{\Delta t} &= D \left[ \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left(\delta_x^2 u\right) \right|_{i,L1}^{j} + f_i^j \\ &+ \frac{D\Delta t^{\gamma-1}}{\Delta x^2 \Gamma(1+\gamma)} \sum_{k=1}^{j-1} [a_{j-k+1} - a_{j-k}] \left( 2u_i^k - u_i^{k+1} - u_i^{k-1} \right). \end{aligned} \tag{4.16}$$

Taking the Taylor series expansion around the point $x_i = i\Delta x$ and $t_j = j\Delta t$ in time, we then have

$$\frac{U_i^j - U_i^{j-1}}{\Delta t} \approx \left[ \frac{\partial U}{\partial t} \right|_i^j + \frac{\Delta t}{2!} \left[ \frac{\partial^2 U}{\partial t^2} \right|_i^j + O(\Delta t^2), \tag{4.17}$$

$$U_i^{j+1} \approx U_i^j + \Delta t \left[\frac{\partial U}{\partial t}\right|_i^j + \frac{\Delta t^2}{2!}\left[\frac{\partial^2 U}{\partial t^2}\right|_i^j + \frac{\Delta t^3}{3!}\left[\frac{\partial^3 U}{\partial t^3}\right|_i^j + O(\Delta t^4), \tag{4.18}$$

and

$$U_i^{j-1} \approx U_i^j - \Delta t \left[\frac{\partial U}{\partial t}\right|_i^j + \frac{\Delta t^2}{2!}\left[\frac{\partial^2 U}{\partial t^2}\right|_i^j - \frac{\Delta t^3}{3!}\left[\frac{\partial^3 U}{\partial t^3}\right|_i^j + O(\Delta t^4), \tag{4.19}$$

then we have

$$2U_i^j - U_i^{j+1} - U_i^{j-1} = -2\left(\left[\frac{\Delta t^2}{2!}\frac{\partial^2 U}{\partial t^2}\right|_i^j + \frac{\Delta t^4}{4!}\left[\frac{\partial^4 U}{\partial t^4}\right|_i^j + O(\Delta t^6)\right). \tag{4.20}$$

Likewise expanding around the point $x_i = i\Delta x$ and $t_j = j\Delta t$ gives

$$\delta_x^2 U_i^j \approx \left[\frac{\partial^2 U}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 U}{\partial x^4}\right|_i^j + O(\Delta x^4). \tag{4.21}$$

Using Equations (4.17), (4.20), and (4.21) in Equation (4.16)

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^j + \frac{\Delta t}{2!}\left[\frac{\partial^2 U}{\partial t^2}\right|_i^j + O(\Delta t^3) = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\left[\frac{\partial^2 U}{\partial x^2}\right|_{i,L1}^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 U}{\partial x^4}\right|_{i,L1}^j + O(\Delta x^6)\right) + f_i^j \\ - \frac{2D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\sum_{k=1}^{j-1}(a_{j-k+1} - a_{j-k})\left(\frac{\Delta t^2}{2!}\left[\frac{\partial^2 U}{\partial t^2}\right|_i^k + \frac{\Delta t^4}{4!}\left[\frac{\partial^4 U}{\partial t^4}\right|_i^k + O(\Delta t^6)\right),\end{aligned} \tag{4.22}$$

and simplifying gives

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^j + O(\Delta t) = \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i,L1}^j + \frac{\Delta x^2}{12}\left[\frac{\partial^{1-\gamma} M(t)}{\partial t^{1-\gamma}}\right|_{i,L1}^j + O(\Delta x^6) + f_i^j \\ - \frac{2D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\sum_{k=1}^{j-1}[a_{j-k+1} - a_{j-k}]\left[\frac{\Delta t^2}{2!}\frac{\partial^2 U}{\partial t^2} + \frac{\Delta t^4}{4!}\frac{\partial^4 U}{\partial t^4} + O(\Delta t^6)\right|_i^k,\end{aligned} \tag{4.23}$$

where

$$M(t) = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left[\frac{\partial^4 U}{\partial x^4}\right]. \tag{4.24}$$

The order of the last term in Equation (4.23) is given by

$$\begin{aligned}&\frac{2D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\sum_{k=1}^{j-1}(a_{j-k+1} - a_{j-k})\left(\frac{\Delta t^2}{2!}\left[\frac{\partial^2 U}{\partial t^2}\right|_i^k + \frac{\Delta t^4}{4!}\left[\frac{\partial^4 U}{\partial t^4}\right|_i^k + O(\Delta t^6)\right) \\ &\quad = \frac{2D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\sum_{k=1}^{j-1}(a_{j-k+1} - a_{j-k})\,O(\Delta t^2) \\ &\quad = O\left(\frac{\Delta t^{1+\gamma}}{\Delta x^2}\right).\end{aligned} \tag{4.25}$$

Adding and subtracting the exact fractional derivative, we then find

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^j = \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j + f_i^j + O(\Delta t) + O(\Delta x^2) + O\left(\frac{\Delta t^{1+\gamma}}{\Delta x^2}\right) \\ - \left\{\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i,L1}^j\right\}.\end{aligned} \tag{4.26}$$

By Equation (2.48) the term

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{i,L1}^j \tag{4.27}$$

is $O(\Delta t^{1+\gamma})$ and so we obtain the truncation error for Equation (4.16) as

$$\tau_{i,j} = O(\Delta t) + O(\Delta x^2) + O\left(\frac{\Delta t^{1+\gamma}}{\Delta x^2}\right). \tag{4.28}$$

The error term $O\left(\frac{\Delta t^{1+\gamma}}{\Delta x^2}\right)$ gives the following consistency condition

$$\frac{\Delta t^{1+\gamma}}{\Delta x^2} \to 0, \qquad \text{as} \qquad \Delta x \to 0 \text{ and } \Delta t \to 0. \tag{4.29}$$

The numerical approximation for the fractional diffusion equation is consistent, if the truncation error approaches zero as $\frac{\Delta t^{1+\gamma}}{\Delta x^2} \to 0$. The proposed scheme, Equation (4.8), is similar to the original Du Fort–Frankel scheme. That is why we had to use a small $\Delta t^{1+\gamma}/\Delta x^2$ in order to keep the numerical solution stable. The impact of the consistency problem of the Du Fort–Frankel method can be seen in the case of the standard diffusion equation. When $\Delta t = \Delta x$ then the solution converges to the wave equation, but if $\frac{\Delta t}{\Delta x} \to 0$, i.e consistency influences a restriction on $\Delta t$ in relation to $\Delta x$, then the solution converges to the diffusion equation (Gottlieb & Gustafsson 1976).

## 4.4 Stability Analysis

In this section, we investigate the stability of the Dufort–Frankel method by using standard Von Neumann stability analysis. Using a similar approach, as in Section 3.5 (Chapter 3), we let $U_i^j$ be the exact solution of the Equation (4.1) and satisfies Equation (4.8). The error is then given by

$$\epsilon_i^j = U_i^j - u_i^j \tag{4.30}$$

and so the error satisfies the equation

$$\begin{aligned}\epsilon_i^j = \epsilon_i^{j-1} &+ \sigma\beta_j\left(\epsilon_{i+1}^0 - 2\epsilon_i^0 + \epsilon_{i-1}^0\right) + \sigma\left(\epsilon_{i+1}^j - 2\epsilon_i^j + \epsilon_{i-1}^j\right)\\ &+ \sigma\sum_{k=1}^{j-1}\left[a_{j-k+1} - a_{j-k}\right]\left(\epsilon_{i+1}^k - \epsilon_i^{k+1} - \epsilon_i^{k-1} + \epsilon_{i-1}^k\right),\end{aligned} \tag{4.31}$$

where the coefficient $\sigma$, $\beta_j(\gamma)$ and $a_j$ were defined previously in Equations (4.9), (4.11) and (4.13) respectively. In Equation (4.31) we set the truncation error to zero, as in stability analysis the truncation error is not required, but later in Section 4.5 we include the truncation error to show the convergence of the numerical method.

To investigate the stability by Von Neumann stability analysis, similar to Chapter 3 we let $\epsilon_i^j = \zeta_j e^{i' q i \Delta x}$, where $i'$ is the imaginary number, $\sqrt{-1}$, $q$ is a real spatial wave number and $e^{i' q \Delta x}$ is defined in Equation (3.36).

Now using Equation (3.36) in Equation (4.31) gives

$$\begin{aligned}\zeta_j e^{i'qi\Delta x} &= \zeta_{j-1} e^{i'qi\Delta x} + \sigma\beta_j \left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_0 \\ &+ \sigma\left(e^{i'q(i+1)\Delta x} - 2e^{i'qi\Delta x} + e^{i'q(i-1)\Delta x}\right)\zeta_j \\ &+ \sigma\sum_{r=1}^{j-1}\left[a_{j-r+1} - a_{j-r}\right]\left(\zeta_r e^{i'q(i+1)\Delta x} - (\zeta_{r+1} + \zeta_{r-1})e^{i'qi\Delta x} + \zeta_r e^{i'q(i-1)\Delta x}\right),\end{aligned} \tag{4.32}$$

which simplifies to

$$\begin{aligned}\zeta_j &= \zeta_{j-1} + \sigma\beta_j\left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_0 + \sigma\left(e^{i'q\Delta x} - 2 + e^{-i'q\Delta x}\right)\zeta_j \\ &+ \sigma\sum_{r=1}^{j-1}\left[a_{j-r+1} - a_{j-r}\right]\left(\zeta_r\left(e^{i'q\Delta x} + e^{-i'q\Delta x}\right) - (\zeta_{r+1} + \zeta_{r-1})\right).\end{aligned} \tag{4.33}$$

Noting

$$e^{i'q\Delta x} - 2 + e^{-i'q\Delta x} = -2\left(1 - \cos(q\Delta x)\right) = -4\sin^2\left(\frac{q\Delta x}{2}\right), \tag{4.34}$$

$$e^{i'q\Delta x} + e^{-i'q\Delta x} = 2\cos(q\Delta x) = 2 - 4\sin^2\left(\frac{q\Delta x}{2}\right), \tag{4.35}$$

and letting

$$V_q = 4\sin^2\left(\frac{q\Delta x}{2}\right), \tag{4.36}$$

where $0 \le V_q \le 4$, we then have

$$(1 + V_q\sigma)\zeta_j = \zeta_{j-1} - V_q\sigma\beta_j\zeta_0 + \sigma\sum_{r=1}^{j-1}\left[a_{j-r+1} - a_{j-r}\right]\left(\zeta_r\left(2 - V_q\right) - (\zeta_{r+1} + \zeta_{r-1})\right), \tag{4.37}$$

where $0 \le V_q\sigma < \infty$.

For $j \geq 2$, Equation (4.37) is then given by

$$\zeta_j = \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Bigg\{(1+(2^\gamma-2)(2-V_q)\sigma)\zeta_{j-1} - V_q\sigma\beta_j\zeta_0 - (2^\gamma-2)\sigma\zeta_{j-2}$$
$$+\sigma\sum_{r=1}^{j-2}\left[a_{j-r+1}-a_{j-r}\right]\left(\zeta_r\left(2-V_q\right)-\left(\zeta_{r+1}+\zeta_{r-1}\right)\right)\Bigg\}$$
$$= \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Bigg\{(1+(2^\gamma-2)(2-V_q)\sigma)\zeta_{j-1} - V_q\sigma\beta_j\zeta_0 - (2^\gamma-2)\sigma\zeta_{j-2}$$
$$+\sigma(2-V_q)\sum_{r=1}^{j-2}\left[a_{j-r+1}-a_{j-r}\right]\zeta_r - \sigma\sum_{r=1}^{j-2}\left[a_{j-r+1}-a_{j-r}\right]\left(\zeta_{r+1}+\zeta_{r-1}\right)\Bigg\}. \quad (4.38)$$

In the following proposition we prove the stability of the Dufort–Frankel scheme given in Equation (4.8).

**Proposition 4.4.1.** Let $\zeta_j$, where $j = 1, 2, ..., M$, be the solutions of Equation (4.39) then

$$|\zeta_j| \leq |\zeta_0|, \quad (4.39)$$

if $2 \leq V_q \leq 4$ and $0 < \gamma \leq 1$.

*Proof.* We use mathematical induction method to prove the relation in Equation (4.39). We assume $\zeta_0 > 0$ in this analysis. In the case $j = 1$, Equation (4.37) gives

$$(1+V_q\sigma)\zeta_1 = \zeta_0 - V_q\sigma\beta_1(\gamma)\zeta_0. \quad (4.40)$$

Noting $\beta_1(\gamma) = \gamma - 1$, then Equation (4.40) becomes

$$\zeta_1 = \left(1 - \frac{V_q\sigma\gamma}{1+V_q\sigma}\right)\zeta_0. \quad (4.41)$$

Since the second term is positive, we find $\zeta_1$ is bounded above by $\zeta_0$, that is

$$\zeta_1 = \left(1 - \frac{V_q\sigma\gamma}{1+V_q\sigma}\right)\zeta_0 \leq \zeta_0. \quad (4.42)$$

For $0 \leq V_q\sigma < \infty$, since the term

$$0 \leq \frac{V_q\sigma\gamma}{1+V_q\sigma} \leq \gamma, \quad (4.43)$$

then

$$0 \geq -\frac{V_q\sigma\gamma}{1+V_q\sigma} \geq -\gamma, \quad (4.44)$$

we then have

$$1 \geq 1 - \frac{V_q\sigma\gamma}{1+V_q\sigma} \geq 1-\gamma \geq 0. \quad (4.45)$$

We then conclude that

$$\zeta_1 = \left(1 - \frac{V_q\sigma\gamma}{1+V_q\sigma}\right)\zeta_0 \geq 0 \geq -\zeta_0, \tag{4.46}$$

and so

$$-\zeta_0 \leq \zeta_1 \leq \zeta_0, \tag{4.47}$$

or

$$|\zeta_1| < |\zeta_0|. \tag{4.48}$$

Hence Equation (4.39) is true for $j = 1$.

We now assume that

$$-\zeta_0 \leq \zeta_n \leq \zeta_0, \qquad \text{where} \qquad n = 1, 2, ..., k, \tag{4.49}$$

and then need to show that

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0. \tag{4.50}$$

From Equation (4.38) we have

$$\zeta_{k+1} = \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Bigg\{(1+(2-2^\gamma)(V_q-2)\sigma)\zeta_k + V_q\sigma(-\beta_{k+1}(\gamma))\zeta_0 + (2-2^\gamma)\sigma\zeta_{k-1}$$
$$+\sigma(V_q-2)\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right]\zeta_r + \sigma\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right](\zeta_{r+1}+\zeta_{r-1})\Bigg\}. \tag{4.51}$$

From Lemma 4.2.1 we have $-\beta_j(\gamma) > 0$, and from Lemma 3.5.1 we have $a_j - a_{j+1} > 0$, and the term $2 - 2^\gamma > 0$. Also for $2 \leq V_q \leq 4$ the terms satisfies $(V_q - 2) \geq 0$,

$$\frac{1}{1+(V_q+2^\gamma-2)\sigma} > 0, \tag{4.52}$$

and

$$1+(2-2^\gamma)(V_q-2)\sigma > 0. \tag{4.53}$$

Equation (4.51) then becomes

$$\zeta_{k+1} \leq \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Bigg\{(1+(2-2^\gamma)(V_q-2)\sigma) + V_q\sigma(-\beta_{k+1}(\gamma)) + (2-2^\gamma)\sigma$$
$$+\sigma(V_q-2)\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right] + 2\sigma\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right]\Bigg\}\zeta_0. \tag{4.54}$$

Now evaluating the summation in Equation (4.54), gives

$$\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right] = \sum_{r=1}^{k-1}a_{k-r+1} - \sum_{r=0}^{k-2}a_{k-r+1} = a_2 - a_{k+1}, \tag{4.55}$$

where $a_2 = 2^\gamma - 1$ and $a_{k+1} = (k+1)^\gamma - k^\gamma$. Using this result in Equation (4.54), we then obtain the inequality

$$\zeta_{k+1} \leq \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Big\{(1+(2-2^\gamma)V_q\sigma - 2(2-2^\gamma)\sigma) + V_q\sigma(a_{k+1}-\gamma(k+1)^{\gamma-1}) + (2-2^\gamma)\sigma + \sigma(V_q-2)\left[a_2-a_{k+1}\right] + 2\sigma\left[a_2-a_{k+1}\right]\Big\}\zeta_0, \tag{4.56}$$

which can be simplified to

$$\zeta_{k+1} \leq \left(1 - \frac{V_q\sigma\gamma(k+1)^{\gamma-1}}{1+(V_q+2^\gamma-2)\sigma}\right)\zeta_0. \tag{4.57}$$

Since the second term is positive, the value of $\zeta_{j+1}$ is bounded above by $\zeta_0$

$$\zeta_{k+1} \leq \left(1 - \frac{V_q\sigma\gamma(k+1)^{\gamma-1}}{1+(V_q+2^\gamma-2)\sigma}\right)\zeta_0 \leq \zeta_0. \tag{4.58}$$

From Equation (4.49) we have $-\zeta_0 \leq \zeta_n$, then Equation (4.51) becomes

$$\begin{aligned}\zeta_{k+1} &= \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Big\{(1+(2-2^\gamma)(V_q-2)\sigma)\zeta_k + V_q\sigma(-\beta_{k+1}(\gamma))\zeta_0 + (2-2^\gamma)\sigma\zeta_{k-1} \\ &\quad +\sigma(V_q-2)\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right]\zeta_r + \sigma\sum_{r=1}^{k-1}\left[a_{k-r+1}-a_{k-r+2}\right](\zeta_{r+1}+\zeta_{r-1})\Big\} \\ &\geq \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Big\{(1+(2-2^\gamma)V_q\sigma - 2(2-2^\gamma)\sigma) + V_q\sigma(a_{k+1}-\gamma(k+1)^{\gamma-1}) \\ &\quad + (2-2^\gamma)\sigma + \sigma(V_q-2)\left[a_2-a_{k+1}\right] + 2\sigma\left[a_2-a_{k+1}\right]\Big\}(-\zeta_0).\end{aligned} \tag{4.59}$$

which can be simplified to

$$\zeta_{k+1} \geq -\left(1 - \frac{V_q\sigma\gamma(k+1)^{\gamma-1}}{1+(V_q+2^\gamma-2)\sigma}\right)\zeta_0. \tag{4.60}$$

Now for $2 \leq V_q \leq 4$ we have

$$0 \leq \frac{V_q\sigma\gamma(k+1)^{\gamma-1}}{1+(V_q+2^\gamma-2)\sigma} \leq \frac{4\sigma\gamma(k+1)^{\gamma-1}}{1+(2+2^\gamma)\sigma}, \tag{4.61}$$

and for $0 < \gamma \leq 1$ and $k \geq 0$, we also have $0 \leq (k+1)^{\gamma-1} \leq 1$. We then have

$$0 < \frac{4\sigma\gamma(k+1)^{\gamma-1}}{1+(2+2^\gamma)\sigma} \leq \frac{4\sigma\gamma}{1+(2+2^\gamma)\sigma}, \tag{4.62}$$

which gives the inequality

$$1 \geq 1 - \frac{4\sigma\gamma(k+1)^{\gamma-1}}{1+(2+2^\gamma)\sigma} \geq 1 - \frac{4\sigma\gamma}{1+(2+2^\gamma)\sigma} \geq 1 - \frac{4\gamma}{2+2^\gamma} \geq 0. \tag{4.63}$$

Then the bound for $\zeta_{k+1}$ becomes

$$\zeta_{k+1} \geq -\left(1 - \frac{V_q\sigma\gamma(k+1)^{\gamma-1}}{1+(V_q+2^\gamma-2)\sigma}\right)\zeta_0 \geq -\zeta_0, \tag{4.64}$$

and so

$$-\zeta_0 < \zeta_{k+1} < \zeta_0, \tag{4.65}$$

or

$$|\zeta_{k+1}| < |\zeta_0|. \tag{4.66}$$

Hence if $2 \leq V_q \leq 4$ then Equation (4.39) is satisfied which means the numerical method is stable. This method is only conditionally stable as evidenced by the results of the next section. □

### 4.4.1 Numerical Solution of the Recurrence Relationship

In this section, we investigate the solution of the recurrence relationship in Equation (4.37) by direct evaluation, where $0 < \gamma < 1$. The ratio $\zeta_j/\zeta_0$ is plotted on a double logarithmic scale. These results are shown in Figures 4.1 to 4.4 against $j$, where we have taken $j = 1, 2, ..., 100$ time steps, with the value of $V_q = 1$, 1.5, 2 and 4. The value of $\sigma$ used is given by Equation (4.11) with $\Delta t = 10^{-2}$ and $\Delta x = 10^{-2}$.

From the results shown, for the cases of $V_q = 2$ and 4 in Figures 4.1 and 4.2, this method is stable as the ratio remains less than 1. Consequently, these results suggest this method is stable, where $2 \leq V_q \leq 4$, as the ratio remains less than 1.
Whilst we see in Figure 4.3 for the case $V_q = 1.5$ and $0.5 \leq \gamma \leq 0.9$ the ratio is less than 1 but for $0.1 \leq \gamma < 0.5$ the ratio is bigger than 1. We also note in Figure 4.4, for the case $V_q = 1$ and $0.7 \leq \gamma \leq 0.9$, the ratio is less than 1 but for $0.1 \leq \gamma < 0.7$ the ratio is bigger than 1. We conclude that for $0 \leq V_q < 2$ this method is stable for some values of $\gamma$ only.

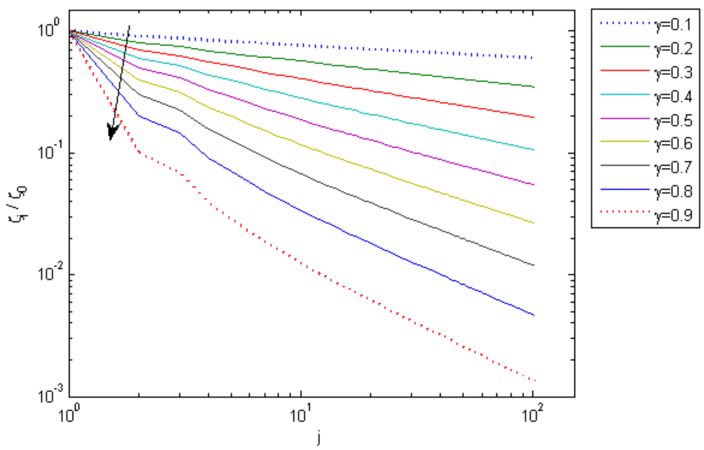



Figure 4.1: The value of the ratio $\zeta_j/\zeta_0$ predicted by evaluating Equation (4.33). Results are shown for 100 time steps, $V_q = 4$, and $\gamma = 0.1, \ldots, 0.9$. Note the value of $\gamma$ increases in the direction of the arrow.

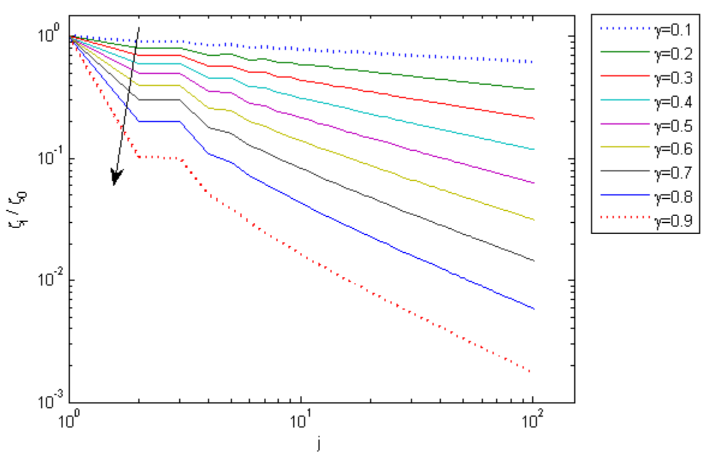



Figure 4.2: The value of the ratio $\zeta_j/\zeta_0$ found from recurrence relation in Equation (4.33). Results are shown for 100 time steps, $V_q = 2$, and $\gamma = 0.1, \ldots, 0.9$. Note the value of $\gamma$ increases in the direction of the arrow.

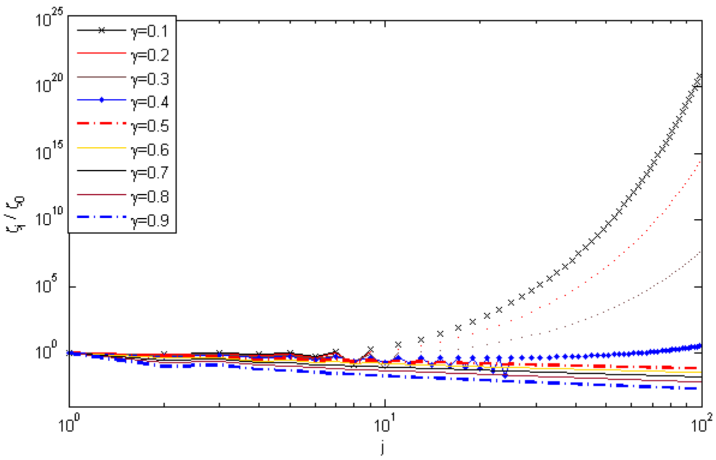



Figure 4.3: The value of the ratio $\zeta_j/\zeta_0$ predicted by evaluating Equation (4.33). Results are shown for 100 time steps, $V_q = 1.5$, and $\gamma = 0.1, \ldots, 0.9$.

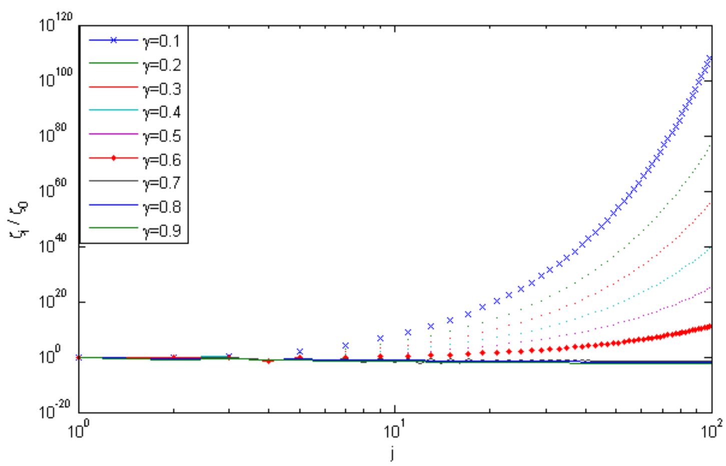



Figure 4.4: The value of the ratio $\zeta_j/\zeta_0$ found from recurrence relation in Equation (4.33). Results are shown for 100 time steps, $V_q = 1$, and $\gamma = 0.1, \ldots, 0.9$.

## 4.5 Convergence of the DFL1 Method

In this section, we consider the convergence of the DFL1 scheme. Following the approach of Chen et al. (2010), in Equation (4.8) we let

$$R_i^j = \frac{U_i^j - U_i^{j-1}}{\Delta t} - \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\delta_x^2 U_i^0 + \delta_x^2 U_i^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\delta_x^2 U_i^k\right\}$$
$$- \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\sum_{k=1}^{j-1}\left[a_{j-k+1} - a_{j-k}\right]\left(2U_i^k - U_i^{k+1} - U_i^{k-1}\right) - f_i^j, \quad (4.67)$$

where $\delta_x^2 U_i^j$ is as defined in Equation (4.14). Noting that

$$\frac{U_i^j - U_i^{j-1}}{\Delta t} = \frac{\partial U_i^j}{\partial t} + O(\Delta t), \quad (4.68)$$

$$\frac{\delta_x^2 U_i^j}{\Delta x^2} = \frac{\partial^2 U_i^j}{\partial x^2} + O(\Delta x^2), \quad (4.69)$$

and we also have

$$2U_i^j - U_i^{j+1} - U_i^{j-1} = -2\left(\left[\frac{\Delta t^2}{2!}\frac{\partial^2 U}{\partial t^2}\right|_i^j + O(\Delta t^4)\right), \quad (4.70)$$

and from the L1 scheme we note that

$$\left[\frac{d^{1-\gamma}f(t)}{dt^{1-\gamma}}\right|_{L1}^j = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)f_0 + f_j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)f_k\right\}. \quad (4.71)$$

Now applying Equation (4.67) – (4.71), we then have

$$R_i^j = \left[\frac{\partial U}{\partial t}\right|_i^j - D\left[\frac{\partial^{1-\gamma}}{\partial^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j + \frac{D\Delta t^{\gamma+1}}{\Delta x^2\Gamma(1+\gamma)}\sum_{k=1}^{j-1}\left[a_{j-k+1} - a_{j-k}\right] - f_i^j + O(\Delta t + \Delta x^2)$$
$$= \left[\frac{\partial U}{\partial t}\right|_i^j - D\left[\frac{\partial^{1-\gamma}}{\partial^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j + \frac{D\left[a_j - a_1\right]}{\Gamma(1+\gamma)}\left(\frac{\Delta t^{\gamma+1}}{\Delta x^2}\right) - f_i^j + O(\Delta t + \Delta x^2). \quad (4.72)$$

According to the Equation (4.72), we have

$$R_i^j = O\left(\Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2}\right), \qquad i = 1, 2, \ldots, N,\ j = 1, 2, \ldots, M, \quad (4.73)$$

since $i, j$ are finite, there is a positive constant $c_1$ for all $i, j$ such that

$$|R_i^j| \le c_1\left(\Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2}\right). \quad (4.74)$$

Let the error

$$E_i^j = U_i^j - u_i^j, \quad (4.75)$$

where $i = 1, 2, \ldots, N$ and $j = 0, 1, 2, \ldots, M$. In Equation (4.67) we have

$$U_i^j = U_i^{j-1} + \frac{D\Delta t^\gamma}{\Gamma(1+\gamma)} \left\{ \beta_j(\gamma)\delta_x^2 U_i^0 + \delta_x^2 U_i^j + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma)\delta_x^{2*} U_i^k \right\} + \Delta t f_i^j + \Delta t R_i^j, \tag{4.76}$$

where

$$\delta_x^{2*} U_i^j = \frac{U_{i+1}^j - U_i^{j+1} - U_i^{j-1} + U_{i-1}^j}{\Delta x^2}. \tag{4.77}$$

Subtracting (4.8) from (4.76) gives

$$E_i^j = E_i^{j-1} + \frac{D\Delta t^\gamma}{\Gamma(1+\gamma)} \left\{ \beta_j(\gamma)\delta_x^2 E_i^0 + \delta_x^2 E_i^j + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma)\delta_x^{2*} E_i^k \right\} + \Delta t R_i^j. \tag{4.78}$$

For $i = 1, 2, \ldots, N$ using a similar grid function as given in Chapter 3, Section 3.6, by Equations (3.107) and (3.108) respectively, and then $E_i^j$ and $R_i^j$ can be expanded in Fourier series as in Equations (3.109) and (3.110). Again the Parseval identity can be used to give Equations (3.113) and (3.114).

Now with $q = 2\pi l/L$, we assume that

$$E_i^j = \xi_j e^{i' q i \Delta x}, \tag{4.79}$$

and

$$R_i^j = \eta_j e^{i' q i \Delta x}. \tag{4.80}$$

Using Equations (4.79) and (4.80) in (4.78) gives

$$(1 + V_q\sigma)\xi_j = \xi_{j-1} - V_q\sigma\beta_j\xi_0 + \sigma \sum_{l=1}^{j-1} \left[a_{j-l+1} - a_{j-l}\right] \left(\xi_l \left(2 - V_q\right) - \left(\xi_{l+1} + \xi_{l-1}\right)\right) + \Delta t \eta_j, \tag{4.81}$$

where $V_q = 4\sin^2(q\Delta x/2) \geq 0$.

For $j \geq 2$, Equation (4.81) can be rewritten as

$$\xi_j = \frac{1}{1 + (V_q + 2^\gamma - 2)\sigma} \Bigg\{ (1 + (2^\gamma - 2)(2 - V_q)\sigma)\xi_{j-1} - V_q\sigma\beta_j\xi_0 - (2^\gamma - 2)\sigma\xi_{j-2}$$
$$+ \sigma(2 - V_q) \sum_{r=1}^{j-2} \left[a_{j-r+1} - a_{j-r}\right] \xi_r - \sigma \sum_{r=1}^{j-2} \left[a_{j-r+1} - a_{j-r}\right] \left(\xi_{r+1} + \xi_{r-1}\right) + \Delta t \eta_j \Bigg\}, \tag{4.82}$$

where the weights $a_j(\gamma)$ and $a_{j+1}(\gamma)$ are given in Equation (4.13).

**Proposition 4.5.1.** Let $\xi_j$ be the solution of Equation (4.81). Then there exists a positive constant $c_2$ such that

$$|\xi_j| \leq c_2 j \Delta t |\eta_1|, \text{ where } j = 1, 2, \ldots, M \tag{4.83}$$

if $2 \leq V_q \leq 4$ and $0 < \gamma \leq 1$.

*Proof.* From Equation (4.75), noting that $E^0 = 0$, we then have $\xi_0 = \xi_0(l) = 0$. From the Equations (4.74) and (3.114), we obtain

$$\|R^j\|_2 \leq c_2 \sqrt{N \Delta x} \left( \Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2} \right) = c_2 \sqrt{L} \left( \Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2} \right), \tag{4.84}$$

where $j = 1, 2, \ldots, M$, and by the convergence of the series on the right hand side Equation (3.114) there is a positive constant $c_j$ such that

$$|\eta_j| \equiv |\eta_j(l)| \leq c_j |\eta_1| \equiv c_j |\eta_1(l)|, \qquad j = 1, 2, \ldots, M. \tag{4.85}$$

We then obtain

$$|\eta_j| \leq c_2 |\eta_1(l)|, \qquad j = 1, 2, \ldots, M, \tag{4.86}$$

where

$$c_2 = \max_{1 \leq j \leq M} \{c_j\}. \tag{4.87}$$

Now using the mathematical induction. In Equation (4.81) for $j = 1$ we have

$$(1 + V_q \sigma) \, \xi_1 = \Delta t \eta_j, \tag{4.88}$$

Equation (4.88) becomes

$$\xi_1 = \frac{1}{1 + V_q \sigma} \Delta t \eta_1, \tag{4.89}$$

since $0 < \frac{1}{1+V_q\sigma} \leq 1$, we obtain

$$|\xi_1| \leq \frac{1}{1 + V_q \sigma} \Delta t |\eta_1| \leq \Delta t |\eta_1| \leq c_2 \Delta t |\eta_1|. \tag{4.90}$$

Suppose that

$$|\xi_n| \leq c_2 n \Delta t |\eta_1|, \qquad n = 1, 2, \ldots, k - 1. \tag{4.91}$$

For $0 < \gamma < 1$, $2 \leq V_q \leq 4$ and $V_q\sigma > 0$, from Equation (4.82), we have

$$|\xi_k| \leq \frac{1}{1+(V_q+2^\gamma-2)\sigma}\Bigg\{|1+(2^\gamma-2)(2-V_q)\sigma||\xi_{k-1}| + |-V_q\sigma\beta_k||\xi_0| + (2-2^\gamma)\sigma|\xi_{k-2}| + |\sigma(2-V_q)|\sum_{l=1}^{k-2}|a_{k-l+1}-a_{k-l}|\,|\xi_l| + \sigma\sum_{l=1}^{k-2}|a_{k-l}-a_{k-l+1}|\,(|\xi_{l+1}|+|\xi_{l-1}|) + \Delta t|\eta_k|\Bigg\}. \tag{4.92}$$

For $2 \leq V_q \leq 4$, $\sigma > 0$, and $0 < \gamma \leq 1$, then the first term in the brackets satisfies

$$\frac{1+(2-2^\gamma)(V_q-2)\sigma}{1+(V_q+2^\gamma-2)\sigma} > 0,$$

and for $0 < \gamma \leq 1$, the term $2 - 2^\gamma > 0$. By Lemma 3.5.1 we also have $a_{j+1} < a_j$. Applying Equation (4.91) in Equation (4.92), gives

$$|\xi_k| \leq \frac{c_2\Delta t}{1+(V_q+2^\gamma-2)\sigma}\Bigg\{(1+(2-2^\gamma)(V_q-2)\sigma)\,(k-1) + (2-2^\gamma)\sigma(k-2) \tag{4.93}$$

$$+\sigma(V_q-2)\sum_{l=1}^{k-2} l\,[a_{k-l}-a_{k-l+1}] + \sigma\sum_{l=1}^{k-2}2l\,[a_{k-l}-a_{k-l+1}] + 1\Bigg\}|\eta_1|$$

$$= \frac{c_2\Delta t}{1+(V_q+2^\gamma-2)\sigma}\left\{k + (2^\gamma-2)\sigma k + V_q\sigma\left[(2-2^\gamma)(k-1) + \sum_{l=1}^{k-2} l\,(a_{k-l}-a_{k-l+1})\right]\right\}|\eta_1|.$$

Evaluating the summation in Equation (4.92) gives

$$\sum_{l=1}^{k-2} l\,[a_{k-l}-a_{k-l+1}] = \sum_{l=1}^{k-2} la_{k-l} - \sum_{l=1}^{k-2} la_{k-l+1}$$

$$= a_2(k-1) - \sum_{l=2}^{k} a_l. \tag{4.94}$$

Using this results, where $a_2 = 2^\gamma - 1$, in Equation (4.92), we then have

$$|\xi_k| \leq \frac{c_2\Delta t}{1+(V_q+2^\gamma-2)\sigma}\left\{k + (2^\gamma-2)\sigma k + V_q\sigma\left[(2-2^\gamma)(k-1) + a_2(k-1) - \sum_{l=2}^{k} a_l\right]\right\}|\eta_1|$$

$$\leq \frac{c_2\Delta t}{1+(V_q+2^\gamma-2)\sigma}\left\{k + (2^\gamma-2)\sigma k + V_q\sigma(k-1) - \sigma V_q\sum_{l=2}^{k} a_l\right\}|\eta_1|. \tag{4.95}$$

We note that $\sum_{l=2}^{k} a_l = k^\gamma - 1$ and so Equation (4.95) becomes

$$|\xi_k| \leq c_2\Delta t k|\eta_1| - \frac{c_2\Delta t V_q\sigma k^\gamma}{1+(V_q+2^\gamma-2)\sigma}|\eta_1|$$

$$\leq c_2\Delta t k|\eta_1|. \tag{4.96}$$

We then conclude that, for $n = k$

$$|\xi_k| \leq c_2\Delta t k|\eta_1|. \tag{4.97}$$

Hence for all $n \in \mathbb{N}$, and if $2 \leq V_q \leq 4$ and $0 < \gamma \leq 1$, we have $|\xi_n| \leq c_2 n\Delta t|\eta_1|$. □

**Theorem 4.5.2.** Let $u(x,t) \in U(\Omega)$ be the exact solution for the fractional subdiffusion equation. Then the numerical scheme (4.8) – (4.11) is convergent with the converge order $O\left(\Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2}\right)$, if $2 \le V_q \le 4$ and $0 < \gamma \le 1$.

*Proof.* Using Equations (4.74), (3.113), (3.114), Proposition 4.5.1, and $j\Delta t \le T$, we then have

$$\|E^j\|_2 \le c_2 j\Delta t\|R_1\| \le c_1c_2 j\Delta t\sqrt{L}\left(\Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2}\right) \le C\left(\Delta t + \Delta x^2 + \frac{\Delta t^{\gamma+1}}{\Delta x^2}\right) \tag{4.98}$$

where $C = c_1c_2T\sqrt{L}$. □

## 4.6 Numerical Examples and Results

To verify the accuracy of our scheme, we compute the maximum norm of the error between the numerical estimate, given by Equation (4.8), and the exact solution

$$e_\infty(\Delta t, \Delta x) = \max_{1\le i\le N}\left|u_i^M - u(x_i, t_M)\right|, \tag{4.99}$$

for two examples where the exact solution is known. Numerical accuracy is tested for various time and spatial steps sizes in the cases $\gamma = 0.3$, 0.5, 0.7, 0.9, and 1. The estimated convergence order, $R1$, recorded as order of convergence in $\Delta x$, is estimated by computing

$$R1 = \log_2\left[e_\infty(\Delta t, 2\Delta x)/e_\infty(\Delta t, \Delta x)\right].$$

This scheme is implemented in MATLAB R2014a (see Appendix C.3) using the linsolve subroutine to solve the system of algebraic equations.

**Example 4.6.1.** Consider the following fractional subdiffusion equation with a source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right) + \sin(\pi x)\left[2t + \pi^2\left(\frac{t^{\gamma-1}}{\Gamma(\gamma)} + \frac{2t^{\gamma+1}}{\Gamma(2+\gamma)}\right)\right], \tag{4.100}$$

with $0 < \gamma \le 1$ and the initial and fixed boundary conditions

$$u(x,0) = \sin(\pi x), \qquad u(0,t) = 0, \quad u(L,t) = 0. \tag{4.101}$$

The exact solution of (4.100) given the conditions (4.101) is

$$u(x,t) = \left(1 + t^2\right)\sin(\pi x). \tag{4.102}$$

Numerical accuracy of the DFL1 methods in Equation (4.8) is tested for different time steps that is $\Delta t = O(\Delta x)$, $\Delta t = O(\Delta x^2)$ and $\Delta t = O(\Delta x^3)$ for the fractional exponent values $\gamma = 0.3$, 0.5, 0.7, 0.9, and 1.0. In Tables 4.2 and 4.3 we see the consistency condition, $\frac{\Delta t^{1+\gamma}}{\Delta x^2} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$, is satisfied and so the expected second order is obtained. However when $\Delta t = 10^{-5}\Delta x$ the consistency condition is not satisfied and here the expected second order result is not obtained as seen in Table 4.1. Note the negative order appear in Table 4.1 for $\gamma = 0.3$ and $\Delta x = 1/16$ where the error is very large. Also the results for $\gamma = 0.3$ where $\Delta x = 1/32$ and $\Delta x^2 = 1/32$ could not be obtained in Tables 4.1 and 4.2.

A comparison of the exact solution and the numerical solution at $t = 0.25$, 0.5, 0.75, and 1.0 for $\gamma = 0.9$ with the time steps $j = 1000$, is shown in Figure 4.5. We see the numerical method, DFL1, estimate is in agreement with the exact solution, with respect to the consistency condition in DFL1 scheme (we have taken $\Delta t^{1+\gamma}/\Delta x^2 = 0.8$).

Table 4.1: Numerical accuracy in $\Delta x$ of the Dufort–Frankel scheme, Equation (4.8), with $\Delta t = 10^{-5}\Delta x$ and $R1$ is order of convergence.

| | $\gamma = 0.3$ | | $\gamma = 0.5$ | | $\gamma = 0.7$ | | $\gamma = 0.9$ | | $\gamma = 1.0$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 1.14e–02 | – | 1.26e–03 | – | 1.01e–04 | – | 7.22e–05 | – | 1.87e–06 | – |
| 1/4 | 3.57e–03 | 1.67 | 3.87e–04 | 1.70 | 2.92e–05 | 1.80 | 1.97e–05 | 1.88 | 4.97e–07 | 1.91 |
| 1/8 | 9.78e–04 | 1.87 | 1.09e–04 | 1.83 | 7.85e–06 | 1.90 | 5.08e–06 | 1.95 | 1.26e–07 | 1.98 |
| 1/16 | 2.27e+03 | -21.1 | 2.93e–05 | 1.89 | 2.04e–06 | 1.94 | 1.29e–06 | 1.98 | 3.17e–08 | 2.00 |
| 1/32 | – | – | 7.67e–06 | 1.93 | 5.25e–07 | 1.97 | 3.25e–07 | 1.99 | 7.92e–09 | 2.00 |

Table 4.2: Numerical accuracy in $\Delta x$ of the Dufort–Frankel scheme, Equation (4.8), with $\Delta t = 10^{-5}\Delta x^2$ and $R1$ is order of convergence.

| | $\gamma = 0.3$ | | $\gamma = 0.5$ | | $\gamma = 0.7$ | | $\gamma = 0.9$ | | $\gamma = 1.0$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 1.41e–02 | – | 1.46e–03 | – | 1.10e–04 | – | 7.40e–06 | – | 1.87e–06 | – |
| 1/4 | 4.86e–03 | 1.54 | 4.63e–04 | 1.65 | 3.21e–05 | 1.77 | 2.02e–06 | 1.87 | 4.97e–07 | 1.91 |
| 1/8 | 1.43e–03 | 1.77 | 1.29e–04 | 1.85 | 8.50e–06 | 1.92 | 5.19e–07 | 1.96 | 1.26e–07 | 1.98 |
| 1/16 | 4.04e–04 | 1.86 | 3.38e–05 | 1.93 | 2.17e–06 | 1.97 | 1.31e–07 | 1.99 | 3.17e–08 | 2.00 |
| 1/32 | – | – | 8.66e–06 | 1.97 | 5.48e–07 | 1.99 | 3.28e–08 | 2.00 | 7.91e–09 | 2.00 |

Table 4.3: Numerical accuracy in $\Delta x$ of the Dufort–Frankel scheme, Equation (4.8), with $\Delta t = 10^{-5}\Delta x^3$ and $R1$ is order of convergence.

| | $\gamma = 0.3$ | | $\gamma = 0.5$ | | $\gamma = 0.7$ | | $\gamma = 0.9$ | | $\gamma = 1.0$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 1.67e–02 | – | 1.62e–03 | – | 1.62e–04 | – | 7.53e–05 | – | 1.87e–05 | – |
| 1/4 | 5.80e–03 | 1.51 | 5.08e–04 | 1.67 | 3.35e–05 | 1.80 | 2.05e–05 | 1.88 | 4.97e–06 | 1.91 |
| 1/8 | 1.67e–03 | 1.79 | 1.37e–04 | 1.89 | 8.69e–06 | 1.95 | 5.22e–06 | 1.97 | 1.26e–06 | 1.98 |
| 1/16 | 4.46e–04 | 1.90 | 3.50e–05 | 1.96 | 2.19e–06 | 1.99 | 1.31e–06 | 1.99 | 3.17e–07 | 2.00 |
| 1/32 | 1.23e–04 | 1.95 | 8.82e–06 | 1.99 | 5.50e–07 | 2.00 | 3.28e–07 | 2.00 | 7.93e–08 | 2.00 |

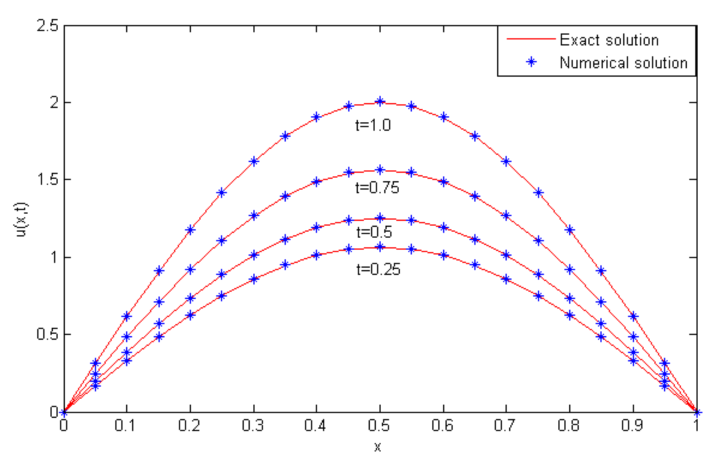



Figure 4.5: A comparison of the exact solution and the numerical solution present for equation (4.100) at different time $t = 1.0$, 0.25, 0.5, and 0.75, for $\gamma = 0.9$ with the time steps $j = 1000$, and $\Delta t^{1+\gamma}/\Delta x^2 = 0.8$.

**Example 4.6.2.** Consider the following fractional subdiffusion equation with the source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right) + 2e^x t\left[1 - \frac{t^\gamma}{\Gamma(2+\gamma)}\right], \tag{4.103}$$

with $0 < \gamma \leq 1$ and the initial and fixed boundary conditions

$$u(x,0) = 0, \qquad u(0,t) = t^2, \quad u(L,t) = et^2. \tag{4.104}$$

The exact solution of Equation (4.103) given the conditions (4.104) is

$$u(x,t) = e^x t^2. \tag{4.105}$$

Numerical accuracy of the Dufort–Frankel method is again tested for different time steps that is $\Delta t = O(\Delta x)$, $\Delta t = O(\Delta x^2)$ and $\Delta t = O(\Delta x^3)$ for $\gamma = 0.3$, 0.5, 0.7, 0.9 and 1.0. The results are given in Tables 4.4 and 4.6, we see the DFL1 scheme is of order one in space when $\Delta t = O(\Delta x)$, of order two when $\Delta t = O(\Delta x^2)$, and of order three when $\Delta t = O(\Delta x^3)$.

Table 4.4: Numerical accuracy in $\Delta x$ of the Dufort–Frankel scheme, Equation (4.8), with $\Delta t = 10^{-6}\Delta x$ and $R1$ is order of convergence.

| | $\gamma = 0.3$ | | $\gamma = 0.5$ | | $\gamma = 0.7$ | | $\gamma = 0.9$ | | $\gamma = 1.0$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 8.20e–21 | – | 8.24e–21 | – | 8.24e–21 | – | 8.24e–21 | – | 8.24e–21 | – |
| 1/4 | 5.27e–21 | 0.64 | 5.29e–21 | 0.64 | 5.29e–21 | 0.64 | 5.29e–21 | 0.64 | 5.29e–21 | 0.64 |
| 1/8 | 2.99e–21 | 0.82 | 3.00e–21 | 0.82 | 3.00e–21 | 0.82 | 3.00e–21 | 0.82 | 3.00e–21 | 0.82 |
| 1/16 | 1.77e–21 | 0.76 | 1.59e–21 | 0.91 | 1.60e–21 | 0.91 | 1.60e–21 | 0.91 | 1.60e–21 | 0.91 |
| 1/32 | 1.28e–21 | 0.46 | 8.20e–22 | 0.96 | 8.23e–22 | 0.96 | 8.23e–22 | 0.96 | 8.23e–22 | 0.96 |

Table 4.5: Numerical accuracy in $\Delta x$ of the Dufort–Frankel scheme, Equation (4.8), with $\Delta t = 10^{-6}\Delta x^2$ and $R1$ is order of convergence.

| | $\gamma = 0.3$ | | $\gamma = 0.5$ | | $\gamma = 0.7$ | | $\gamma = 0.9$ | | $\gamma = 1.0$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 4.10e–21 | – | 4.12e–21 | – | 4.12e–21 | – | 4.12e–21 | – | 4.12e–21 | – |
| 1/4 | 1.32e–21 | 1.64 | 1.32e–21 | 1.64 | 1.32e–21 | 1.64 | 1.32e–21 | 1.64 | 1.32e–21 | 1.64 |
| 1/8 | 3.68e–22 | 1.84 | 3.75e–22 | 1.82 | 3.75e–22 | 1.82 | 3.75e–22 | 1.82 | 3.75e–22 | 1.82 |
| 1/16 | 1.00e–22 | 1.87 | 9.96e–23 | 1.91 | 9.98e–23 | 1.91 | 9.98e–23 | 1.91 | 9.98e–23 | 1.91 |
| 1/32 | 2.95e–23 | 1.87 | 2.56e–23 | 1.96 | 2.57e–23 | 1.96 | 2.57e–23 | 1.96 | 2.57e–23 | 1.96 |

Table 4.6: Numerical accuracy in $\Delta x$ of the Dufort–Frankel scheme, Equation (4.8), with $\Delta t = 10^{-6}\Delta x^3$ and $R1$ is order of convergence.

| | $\gamma = 0.3$ | | $\gamma = 0.5$ | | $\gamma = 0.7$ | | $\gamma = 0.9$ | | $\gamma = 1.0$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 2.05e–21 | – | 2.06e–21 | – | 2.06e–21 | – | 2.06e–21 | – | 2.06e–21 | – |
| 1/4 | 3.29e–22 | 2.64 | 3.31e–22 | 2.64 | 3.31e–22 | 2.64 | 3.31e–22 | 2.64 | 3.31e–22 | 2.64 |
| 1/8 | 4.52e–23 | 2.86 | 4.68e–23 | 2.82 | 4.69e–23 | 2.82 | 4.69e–23 | 2.82 | 4.69e–23 | 2.82 |
| 1/16 | 5.98e–24 | 2.92 | 6.22e–24 | 2.91 | 6.23e–24 | 2.91 | 6.23e–24 | 2.91 | 6.23e–24 | 2.91 |
| 1/32 | 7.93e–25 | 2.91 | 7.98e–25 | 2.96 | 8.04e–25 | 2.96 | 8.04e–25 | 2.96 | 8.04e–25 | 2.96 |

A comparison of the exact solution and the numerical solution at $t = 10^{-6}$, $7.5 \times 10^{-7}$, $5 \times 10^{-7}$, and $2.5 \times 10^{-7}$, $\gamma = 0.5$ is shown in Figure 4.6, it is apparent that the numerical method, DFL1, estimate is in agreement with the exact solution, with respect to the consistency condition in DFL1 scheme, we have taken $\Delta t^{1+\gamma}/\Delta x^2 = 10^{-10}$.

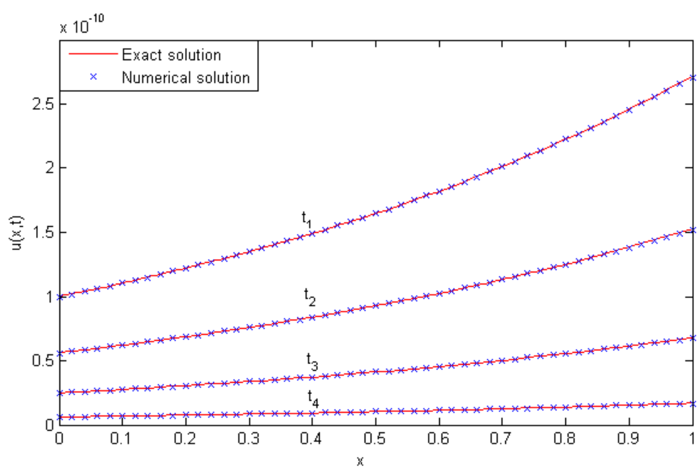



Figure 4.6: A comparison of the exact solution and the numerical solution present for equation (4.103) at the times $t_1 = 10^{-6}$, $t_2 = 0.75 \times 10^{-6}$, $t_3 = 0.5 \times 10^{-6}$, and $t_4 = 0.25 \times 10^{-6}$, with $\gamma = 0.5$ and $\Delta t^{1+\gamma}/\Delta x^2 = 10^{-10}$.

## 4.7 Conclusion

In this chapter, we constructed an implicit method based upon the Dufort–Frankel discretisation scheme for the solution of the fractional subdiffusion equation with a source term, where the L1 scheme was used to approximate the fractional derivative. We have proved the stability of the DFL1 scheme by using Von Neumann stability analysis, if $2 \leq V_q \leq 4$ but the scheme appears to be unstable if $0 \leq V_q < 2$. The DFL1 scheme is also shown only to be conditionally consistent, that is we to ensure the ratio $\Delta t^{1+\gamma}/\Delta x^2$ is small to be consistent with the original equation. The numerical experiments have verified our results.

We conclude that the method that we considered in Chapter 3, IMC1 scheme, is better than DFL1 scheme. The DFL1 method is only conditionally consistent and these consistency problems affect the stability and the convergence of the method. We see in Chapter 5 we will obtain a better method than the IMC1 scheme and the DFL1 scheme.

# Chapter 5

# Keller Box Method

## 5.1 Introduction

The Keller Box method is an implicit numerical scheme which is second order accurate in both space and time for the Heat conduction equation or the Diffusion equation (Pletcher et al. 2012)

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2}. \tag{5.1}$$

It is sometimes referred to as the Preissman Box scheme and was developed by Keller in 1971 (Keller 1971). The idea of Keller Box method is to replace the higher derivatives by first derivatives via the introduction of an additional variable. Following the Keller Box approach, as in Pletcher et al. (2012), Equation (5.1) can be written as a system of first order equations

$$\frac{\partial u(x,t)}{\partial x} = v(x,t), \tag{5.2}$$

and

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial v(x,t)}{\partial x}. \tag{5.3}$$

To approximate these equations by using the central difference method at the point $x = x_{i-\frac{1}{2}}$ and at the time $t = t_{j+\frac{1}{2}}$. The resulting equations are

$$\frac{u_i^j - u_{i-1}^j}{\Delta x_i} = v_{i-\frac{1}{2}}^j, \tag{5.4}$$

and

$$\frac{u_{i-\frac{1}{2}}^{j+1} - u_{i-\frac{1}{2}}^{j}}{\Delta t_{j+1}} = D \frac{v_i^{j+\frac{1}{2}} - v_{i-1}^{j+\frac{1}{2}}}{\Delta x_i}. \tag{5.5}$$

The grid points used in the Keller Box scheme for Equations (5.4) and (5.5) are shown in Figure 5.1.

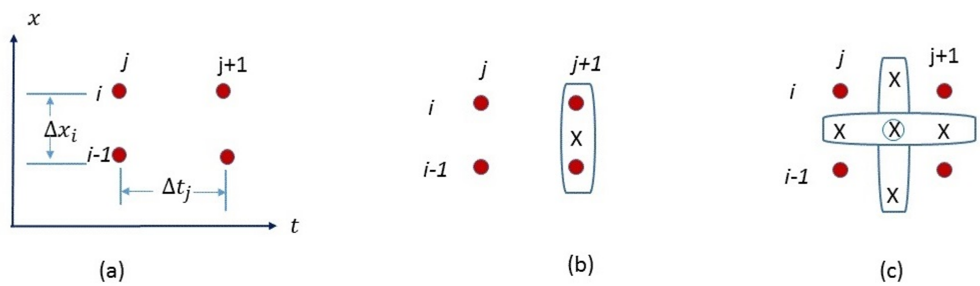



Figure 5.1: The grid points used in the Keller Box method (a) shows the grid points for the Box scheme, (b) the difference molecule for evaluation $v_{i-\frac{1}{2}}^{j}$ in equation (5.4), and (c) the difference molecule for equation (5.5).

After replacing the values $v_i^{j+\frac{1}{2}}$ and $v_{i-\frac{1}{2}}^{j}$ terms by their corresponding temporal and spatial averages, we have

$$\frac{u_i^j - u_{i-1}^j}{\Delta x_i} = \frac{v_i^j + v_{i-1}^j}{2}, \tag{5.6}$$

and

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{\Delta t_{j+1}} = D \frac{v_i^{j+1} - v_{i-1}^{j+1}}{\Delta x_i} + \frac{u_i^j + u_{i-1}^j}{\Delta t_{j+1}} + D \frac{v_i^j - v_{i-1}^j}{\Delta x_i}. \tag{5.7}$$

The strategy of the modified method is to express $v$'s in the term $u$'s. Then the term $v_{i-1}^j$ can be eliminated by using Equation (5.6) into Equation (5.7), becomes

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{\Delta t_{j+1}} = 2D \frac{v_i^{j+1}}{\Delta x_i} - 2D \frac{u_i^{j+1} - u_{i-1}^{j+1}}{\Delta x_i^2} + \frac{u_i^j + u_{i-1}^j}{\Delta t_{j+1}} + 2D \frac{v_i^j}{\Delta x_i} - 2D \frac{u_i^j - u_{i-1}^j}{\Delta x_i^2}. \tag{5.8}$$

In a similar way by replacing $i$ with $i+1$ in Equations (5.6) and (5.7), we then have equation

$$\frac{u_{i+1}^{j+1} + u_i^{j+1}}{\Delta t_{j+1}} = 2D \frac{u_{i+1}^{j+1} - u_i^{j+1}}{\Delta x_{i+1}^2} - 2D \frac{v_i^{j+1}}{\Delta x_{i+1}} + \frac{u_{i+1}^j + u_i^j}{\Delta t_{j+1}} + 2D \frac{u_{i+1}^j - u_i^j}{\Delta x_{i+1}^2} - 2D \frac{v_i^j}{\Delta x_{i+1}}. \tag{5.9}$$

Multiplying Equation (5.8) by $\Delta x_i$ and Equation (5.9) by $\Delta x_{i+1}$, then the terms $v_i^{j+1}$ and $v_i^j$ can be eliminated. After adding the two, the resulting equations

$$A_i u_{i+1}^{j+1} + B_i u_i^{j+1} + C_i u_{i-1}^{j+1} = D_i, \tag{5.10}$$

where

$$A_i = \frac{\Delta x_{i+1}}{\Delta t_{j+1}} - \frac{2D}{\Delta x_{i+1}}, \qquad C_i = \frac{\Delta x_i}{\Delta t_{j+1}} - \frac{2D}{\Delta x_i}, \tag{5.11}$$

$$B_i = \frac{\Delta x_{i+1}}{\Delta t_{j+1}} + \frac{\Delta x_i}{\Delta t_{j+1}} + \frac{2D}{\Delta x_{i+1}} + \frac{2D}{\Delta x_i}, \tag{5.12}$$

$$D_i = \frac{\Delta x_{i+1}}{\Delta t_{j+1}}(u_{i+1}^j + u_i^j) + \frac{\Delta x_i}{\Delta t_{j+1}}(u_i^j + u_{i-1}^j) + 2D\frac{u_{i-1}^j - u_i^j}{\Delta x_i} + 2D\frac{u_{i+1}^j - u_i^j}{\Delta x_{i+1}}. \tag{5.13}$$

In the case of constant grid spacing $\Delta x_i = \Delta x$ and time spacing $\Delta t_j = \Delta t$, Equations (5.10) – (5.13), after multiplying both side by $\Delta t/\Delta x$, we then have

$$\begin{aligned}\left(u_{i+1}^{j+1} + 2u_i^{j+1} + u_{i-1}^{j+1}\right) - \frac{2D\Delta t}{\Delta x^2}\left(u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right)& \\ = \left(u_{i+1}^{j} + 2u_i^{j} + u_{i-1}^{j}\right) + \frac{2D\Delta t}{\Delta x^2}\left(u_{i+1}^{j} - 2u_i^{j} + u_{i-1}^{j}\right).&\end{aligned} \tag{5.14}$$

Al-Shibani (Al-Shibani et al. 2013) proposed a Keller Box method for the one dimensional time fractional diffusion equation

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \tag{5.15}$$

where $0 < \alpha < 1$ in which the fractional derivative was replaced by a Caputo derivative, and the Grünwald-Letnikov approximation was applied to approximate the fractional derivative.

In this chapter we develop an alternative numerical method to Al-Shibani using the Keller Box method for the modified version of the fractional subdiffusion equation, Equation (1.15) with the inclusion of a source term $f(x,t)$

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u(x,t)}{\partial x^2}\right) + f(x,t), \tag{5.16}$$

and for the fractional advection-diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(D\frac{\partial^2 u(x,t)}{\partial x^2} + K_\gamma\frac{\partial u(x,t)}{\partial x}\right) + f(x,t), \tag{5.17}$$

where $D > 0$, $K_\gamma > 0$, and $0 < \gamma \leq 1$. Both equations are to be solved on the finite spatial domain $0 \leq x \leq L$ and for times $0 \leq t \leq T$ subject to the following the initial and Dirchlet boundary conditions

$$u(x,0) = g(x), \qquad 0 \leq x \leq L, \tag{5.18}$$

$$u(0,t) = \varphi_1(t) \quad \text{and} \quad u(L,t) = \varphi_2(t), \qquad 0 \leq t \leq T. \tag{5.19}$$

We suppose that $u(x,t) \in U(\Omega)$ is the exact solution for the fractional subdiffusion equation and the fractional advection-diffusion equation, where

$$\Omega = \{(x,t)|0 \leq x \leq L, 0 \leq t \leq T\}, \tag{5.20}$$

and

$$U(\Omega) = \left\{ u(x,t) \middle| \frac{\partial^4 u(x,t)}{\partial x^4}, \frac{\partial^3 u(x,t)}{\partial x^2 \partial t}, \frac{\partial^2 u(x,t)}{\partial t^2} \in C(\Omega) \right\}. \tag{5.21}$$

This scheme is applied to the fractional case where the Riemann-Liouville definition of the fractional derivative is used instead of Caputo definition used by Al-Shibani (Al-Shibani et al. 2013). In addition, we use a modification of the L1 scheme (Oldham & Spanier 1974) to approximate the fractional derivative instead of the Grünwald-Letnikov approximation used by Al-Shibani et al. (2013). In Section 5.2, we derive the numerical solution schemes for Equation (5.16) and in later sections we investigate the stability, convergence, and the accuracy of these implicit numerical methods and give examples of their implementation.

In Section 5.7, we also develop the modified scheme for the fractional advection-diffusion equation in Equation (5.17), which again is based upon the Keller Box method for the standard diffusion equation but extended to the fractional case. We also investigate the accuracy of this numerical method and provide examples of its application.

## 5.2 Derivation of the Numerical Method for the Fractional Subdiffusion Equation

In this section, we develop an implicit numerical scheme using the Keller Box method to spatially discretise Equation (5.16) and a modification of the L1 scheme to approximate the Riemann-Liouville fractional derivative. For positive integers $M$ and $N$, we define the spatial grid points, $x_i$ as $\{x_i | \, 0 = x_1 < x_2 < x_3 < \cdots < x_{N-1} < x_N = L\}$, denote the spatial grid spacing as $\Delta x_i = x_i - x_{i-1}$, and the equally spaced temporal points as $t_j = j\Delta t$, for $j = 0, 1, ..., M$ with $\Delta t = T/M$ which denotes the time step.

To approximate the fractional derivative in the following numerical method we either use the L1 scheme (Oldham & Spanier 1974), the C2 scheme or the C3 scheme (which were developed earlier in Chapter 2) instead of the Grünwald–Letnikov approximation used in Al-Shibani et al. (2013). In Section 5.2.1, we develop a scheme using the C2 scheme (KBMC2), in Section 5.2.2 we develop a scheme using the C3 scheme (KBMC3), and in Section 5.2.3 we use the L1 scheme (KBML1).

An alternative to the Keller Box method is the Crank–Nicolson scheme; both methods are second-order accurate in space and time. In the fractional case, a generalised Crank–Nicolson scheme could be constructed using the C2 or C3 approximation scheme for the fractional derivative. One advantage of the Keller Box method is that it can more easily accommodate non-uniform spatial grid points. Another advantage of Keller Box scheme is that it can be constructed using the L1 scheme, whilst we cannot use the Crank–Nicolson scheme with L1 scheme. In the Crank–Nicolson method we will need to evaluate the average of the fractional derivative on the right hand side of Equation (5.16) at the current and previous time steps. But the L1 scheme is not bounded at $t = 0$ and so we cannot take the average $t = 0$ and $t = \Delta t$ using the fractional derivative values.

In the KBMC2 and KBMC3 schemes, following the Keller Box approach, we approximate Equation (5.16) at the point $x = x_{i-\frac{1}{2}}$ and time $t = t_{j+\frac{1}{2}}$

$$\left[\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f\left(x_{i-\frac{1}{2}}, t_{j+\frac{1}{2}}\right). \tag{5.22}$$

First we define the first spatial derivative in Equation (5.22) by similar to the standard diffusion case

$$v = \frac{\partial u}{\partial x}. \tag{5.23}$$

We then obtain a system of two first order equations

$$\left[\frac{\partial u}{\partial x}\right|_{i-\frac{1}{2}}^{j} = [v|_{i-\frac{1}{2}}^{j}, \tag{5.24}$$

and

$$\left[\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial v}{\partial x}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f\left(x_{i-\frac{1}{2}}, t_{j+\frac{1}{2}}\right). \tag{5.25}$$

The grid points for Equations (5.23) and (5.25) are shown in Figure 5.1. We will discuss the discretisation of the fractional partial differential equations using the Keller Box method in the next sections.

### 5.2.1 Keller Box Method with the C2 Scheme: the KBMC2 Scheme

In this section, the numerical scheme for solving Equation (5.16) will be developed using the Keller Box method combined with the C2 approximation scheme for the fractional derivative given earlier in Equation (2.75) in Chapter 2, with $p = 1-\gamma$, which we repeat here as

$$\begin{aligned}\left[\frac{d^{1-\gamma}u(t)}{dt^{1-\gamma}}\right|_{C2}^{j+\frac{1}{2}} = \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\Bigg\{&\widetilde{\beta}_j(\gamma)u(0) + 2\left(\frac{1}{2}\right)^{\gamma}\left(u\left(t_{j+\frac{1}{2}}\right) - u\left(t_j\right)\right) \\ &+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u\left(t_k\right) - u\left(t_{k-1}\right)\right]\Bigg\},\end{aligned} \tag{5.26}$$

with the weights

$$\widetilde{\beta}_j(\gamma) = \gamma\left(j+\frac{1}{2}\right)^{\gamma-1}, \tag{5.27}$$

and

$$\widetilde{\mu}_j(\gamma) = \left(j+\frac{3}{2}\right)^{\gamma} - \left(j+\frac{1}{2}\right)^{\gamma}. \tag{5.28}$$

We will refer to this scheme as the KBMC2 scheme. We now use Equation (5.26) to approximate the fractional derivative in Equation (5.25) to give

$$\begin{aligned}\left[\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\Bigg\{&\widetilde{\beta}_j(\gamma)\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{0} + 2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - \left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{j}\right) \\ &+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{k} - \left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{k-1}\right)\Bigg\} + \left[f\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}.\end{aligned} \tag{5.29}$$

Now we use the centred-finite difference scheme to approximate the first order spatial derivatives in Equations (5.24) and (5.29)

$$v_{i-\frac{1}{2}}^{j+1} = \left[\frac{\partial u}{\partial x}\right|_{i-\frac{1}{2}}^{j+1} \approx \frac{u_i^{j+1} - u_{i-1}^{j+1}}{\Delta x_i}, \tag{5.30}$$

and

$$\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{j} \approx \frac{v_i^j - v_{i-1}^j}{\Delta x_i}. \tag{5.31}$$

We also use a centred-finite difference for the first order time derivative in Equation (5.25)

$$\left[\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} \approx \frac{u_{i-\frac{1}{2}}^{j+1} - u_{i-\frac{1}{2}}^{j}}{\Delta t}. \tag{5.32}$$

Using these approximations in Equations (5.24) and (5.25) gives

$$\frac{u_i^{j+1} - u_{i-1}^{j+1}}{\Delta x_i} = [v|_{i-\frac{1}{2}}^{j+1}, \tag{5.33}$$

and

$$\frac{u_{i-\frac{1}{2}}^{j+1} - u_{i-\frac{1}{2}}^{j}}{\Delta t} = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)} \left\{ \widetilde{\beta}_j(\gamma)\left(\frac{v_i^0 - v_{i-1}^0}{\Delta x_i}\right) + 2\left(\frac{1}{2}\right)^{\gamma}\left(\frac{v_i^{j+\frac{1}{2}} - v_{i-1}^{j+\frac{1}{2}}}{\Delta x_i}\right) \right. \tag{5.34}$$
$$\left. -2\left(\frac{1}{2}\right)^{\gamma}\left(\frac{v_i^j - v_{i-1}^j}{\Delta x_i}\right) + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left(\frac{v_i^k - v_{i-1}^k}{\Delta x_i} - \frac{v_i^{k-1} - v_{i-1}^{k-1}}{\Delta x_i}\right)\right\} + [f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}.$$

Now replacing the values $v_i^{j+\frac{1}{2}}$ and $v_{i-\frac{1}{2}}^{j}$ terms, in Equations (5.33) and (5.34), by their corresponding temporal and spatial averages

$$v_i^{j+\frac{1}{2}} = \frac{v_i^j + v_i^{j+1}}{2}, \qquad \text{and} \qquad v_{i-\frac{1}{2}}^{j} = \frac{v_i^j + v_{i-1}^j}{2}, \tag{5.35}$$

we then have

$$\frac{u_i^{j+1} - u_{i-1}^{j+1}}{\Delta x_i} = \frac{v_i^{j+1} + v_{i-1}^{j+1}}{2}, \tag{5.36}$$

and

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} - \frac{u_i^j + u_{i-1}^j}{2\Delta t} \tag{5.37}$$
$$= \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \left\{ \widetilde{\beta}_j(\gamma)\left(v_i^0 - v_{i-1}^0\right) + 2\left(\frac{1}{2}\right)^{\gamma}\left(\frac{v_i^j + v_i^{j+1}}{2} - \frac{v_{i-1}^j + v_{i-1}^{j+1}}{2}\right) \right.$$
$$\left. -2\left(\frac{1}{2}\right)^{\gamma}\left(v_i^j - v_{i-1}^j\right) + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left(v_i^k - v_{i-1}^k - \left(v_i^{k-1} - v_{i-1}^{k-1}\right)\right)\right\} + [f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}.$$

Equation (5.37) can then be simplified to

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} = \frac{u_i^j + u_{i-1}^j}{2\Delta t} + \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \left\{ \widetilde{\beta}_j(\gamma)\left(v_i^0 - v_{i-1}^0\right) + \left(\frac{1}{2}\right)^{\gamma}\left[\left(v_i^{j+1} - v_{i-1}^{j+1}\right)\right.\right.$$
$$\left.\left. - \left(v_i^j - v_{i-1}^j\right)\right] + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left[v_i^k - v_{i-1}^k - \left(v_i^{k-1} - v_{i-1}^{k-1}\right)\right]\right\} + [f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{5.38}$$

Using Equation (5.36) we have

$$v_{i-1}^{j}=\frac{2}{\Delta x_i}\left(u_i^j-u_{i-1}^j\right)-v_i^j, \tag{5.39}$$

which, when combined with Equation (5.38), gives an equation between $u_i^j$ and $v_i^j$

$$\begin{aligned}\frac{u_i^{j+1}+u_{i-1}^{j+1}}{2\Delta t}&=\frac{u_i^j+u_{i-1}^j}{2\Delta t}+\frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{-\frac{\widetilde{\beta}_j(\gamma)}{\Delta x_i}\left(u_i^0-u_{i-1}^0\right)+\widetilde{\beta}_j v_i^0 \\ &-\frac{1}{\Delta x_i}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j+1}-u_{i-1}^{j+1}\right)+\left(\frac{1}{2}\right)^{\gamma}v_i^{j+1}+\frac{1}{\Delta x_i}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^j-u_{i-1}^j\right)-\left(\frac{1}{2}\right)^{\gamma}v_i^j \\ &-\frac{1}{\Delta x_i}\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k-u_{i-1}^k-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_i^k-v_i^{k-1}\right)\Bigg\}+[f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}\,.\end{aligned} \tag{5.40}$$

In a similar manner, by replacing $i$ with $i+1$ in Equations (5.36) and (5.37), we have the equations

$$\frac{u_{i+1}^{j+1}-u_i^{j+1}}{\Delta x_{i+1}}=\frac{v_{i+1}^{j+1}+v_i^{j+1}}{2}, \tag{5.41}$$

and

$$\begin{aligned}&\frac{u_{i+1}^{j+1}+u_i^{j+1}}{2\Delta t}-\frac{u_{i+1}^j+u_i^j}{2\Delta t} \\ &\quad=\frac{D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\widetilde{\beta}_j(\gamma)\left(v_{i+1}^0-v_i^0\right)+2\left(\frac{1}{2}\right)^{\gamma}\left(\frac{v_{i+1}^j+v_{i+1}^{j+1}}{2}-\frac{v_i^j+v_i^{j+1}}{2}\right) \\ &\quad-2\left(\frac{1}{2}\right)^{\gamma}\left(v_{i+1}^j-v_i^j\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_{i+1}^k-v_i^k-\left(v_{i+1}^{k-1}-v_i^{k-1}\right)\right)\Bigg\}+[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,.\end{aligned} \tag{5.42}$$

As before we solve Equation (5.41) to find $v_{i+1}^j$

$$v_{i+1}^{j}=\frac{2}{\Delta x_{i+1}}\left(u_{i+1}^j-u_i^j\right)-v_i^j, \tag{5.43}$$

and use this result in Equation (5.42) to give a second equation between $u_i^j$ and $v_i^j$

$$\begin{aligned}\frac{u_{i+1}^{j+1}+u_i^{j+1}}{2\Delta t}&=\frac{u_{i+1}^j+u_i^j}{2\Delta t}+\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\frac{\widetilde{\beta}_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^0-u_i^0\right)-\widetilde{\beta}_j(\gamma)v_i^0 \\ &+\frac{1}{\Delta x_{i+1}}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j+1}-u_i^{j+1}\right)-\left(\frac{1}{2}\right)^{\gamma}v_i^{j+1}-\frac{1}{\Delta x_{i+1}}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^j-u_i^j\right)+\left(\frac{1}{2}\right)^{\gamma}v_i^j \\ &+\frac{1}{\Delta x_{i+1}}\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^k-u_i^k-\left(u_{i+1}^{k-1}-u_i^{k-1}\right)\right]-\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_i^k-v_i^{k-1}\right)\Bigg\}+[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,.\end{aligned} \tag{5.44}$$

Now multiplying Equation (5.40) by $\Delta x_i$ and Equation (5.44) by $\Delta x_{i+1}$ and then adding the two, we obtain the equation

$$\begin{aligned}
&\frac{\Delta x_i}{2\Delta t}\left(u_i^{j+1}+u_{i-1}^{j+1}\right)+\frac{\Delta x_{i+1}}{2\Delta t}\left(u_{i+1}^{j+1}+u_i^{j+1}\right) \qquad (5.45)\\
&=\frac{\Delta x_i}{2\Delta t}\left(u_i^{j}+u_{i-1}^{j}\right)+\frac{\Delta x_{i+1}}{2\Delta t}\left(u_{i+1}^{j}+u_i^{j}\right)+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\Bigg\{-\frac{\widetilde{\beta}_j(\gamma)}{\Delta x_i}\left(u_i^0-u_{i-1}^0\right)+\widetilde{\beta}_j(\gamma)v_i^0\\
&-\frac{1}{\Delta x_i}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j+1}-u_{i-1}^{j+1}\right)+\left(\frac{1}{2}\right)^{\gamma}v_i^{j+1}+\frac{1}{\Delta x_i}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j}-u_{i-1}^{j}\right)-\left(\frac{1}{2}\right)^{\gamma}v_i^{j}\\
&-\frac{1}{\Delta x_i}\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k-u_{i-1}^k-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_i^k-v_i^{k-1}\right)\Bigg\}+\Delta x_i\,[f]\Big|_{i-\frac{1}{2}}^{j+\frac{1}{2}}\\
&+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\Bigg\{\frac{\widetilde{\beta}_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^0-u_i^0\right)-\widetilde{\beta}_j(\gamma)v_i^0+\frac{1}{\Delta x_{i+1}}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j+1}-u_i^{j+1}\right)-\left(\frac{1}{2}\right)^{\gamma}v_i^{j+1}\\
&-\frac{1}{\Delta x_{i+1}}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j}-u_i^{j}\right)+\left(\frac{1}{2}\right)^{\gamma}v_i^{j}-\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_i^k-v_i^{k-1}\right)\\
&+\frac{1}{\Delta x_{i+1}}\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^k-u_i^k-\left(u_{i+1}^{k-1}-u_i^{k-1}\right)\right]\Bigg\}+\Delta x_{i+1}\,[f]\Big|_{i+\frac{1}{2}}^{j+\frac{1}{2}}.
\end{aligned}$$

This equation can then be simplified to give the equation for $u_i^j$ at each grid point $x_i$ and time step $t_j$

$$\begin{aligned}
&\frac{\Delta x_i}{2\Delta t}\left(u_i^{j+1}+u_{i-1}^{j+1}\right)+\frac{\Delta x_{i+1}}{2\Delta t}\left(u_{i+1}^{j+1}+u_i^{j+1}\right) \qquad (5.46)\\
&=\frac{\Delta x_i}{2\Delta t}\left(u_i^{j}+u_{i-1}^{j}\right)+\frac{\Delta x_{i+1}}{2\Delta t}\left(u_{i+1}^{j}+u_i^{j}\right)+\frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{-\widetilde{\beta}_j(\gamma)\left(u_i^0-u_{i-1}^0\right)\\
&-\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j+1}-u_{i-1}^{j+1}\right)+\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j}-u_{i-1}^{j}\right)-\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k-u_{i-1}^k-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]\Bigg\}\\
&+\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\widetilde{\beta}_j(\gamma)\left(u_{i+1}^0-u_i^0\right)+\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j+1}-u_i^{j+1}\right)-\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j}-u_i^{j}\right)\\
&+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^k-u_i^k-\left(u_{i+1}^{k-1}-u_i^{k-1}\right)\right]\Bigg\}+\Delta x_i\,[f]\Big|_{i-\frac{1}{2}}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[f]\Big|_{i+\frac{1}{2}}^{j+\frac{1}{2}}.
\end{aligned}$$

Equation (5.46) can also be written as a system of equations

$$A_i u_{i+1}^{j+1}+E_i u_i^{j+1}+B_i u_{i-1}^{j+1}=C_i+\Delta x_i\,[f]\Big|_{i-\frac{1}{2}}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[f]\Big|_{i+\frac{1}{2}}^{j+\frac{1}{2}}, \qquad (5.47)$$

with the coefficients

$$A_i=\frac{\Delta x_{i+1}}{2\Delta t}-\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}, \qquad (5.48)$$

$$B_i=\frac{\Delta x_i}{2\Delta t}-\frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}, \qquad (5.49)$$

$$E_i = \frac{\Delta x_i + \Delta x_{i+1}}{2\Delta t} + \frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left[\frac{1}{\Delta x_i} + \frac{1}{\Delta x_{i+1}}\right], \tag{5.50}$$

and

$$\begin{aligned} C_i &= A_i u_{i+1}^j + E_i u_i^j + B_i u_{i-1}^j \\ &+ \frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i+1}^0 - u_i^0\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^k - u_i^k - \left(u_{i+1}^{k-1} - u_i^{k-1}\right)\right]\right\} \\ &- \frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_i^0 - u_{i-1}^0\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k - u_{i-1}^k - \left(u_i^{k-1} - u_{i-1}^{k-1}\right)\right]\right\}. \end{aligned} \tag{5.51}$$

In the case of constant grid spacing $\Delta x_i = \Delta x$, Equations (5.47) – (5.51), after multiplying both sides by $2\Delta t/\Delta x$, reduces to

$$\begin{aligned} &\left(u_{i+1}^{j+1} + 2u_i^{j+1} + u_{i-1}^{j+1}\right) - \left(\frac{1}{2}\right)^{\gamma} d\left(u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right) \\ &= \left(u_{i+1}^{j} + 2u_i^{j} + u_{i-1}^{j}\right) - \left(\frac{1}{2}\right)^{\gamma} d\left(u_{i+1}^{j} - 2u_i^{j} + u_{i-1}^{j}\right) + d\,\widetilde{\beta}_j(\gamma)\left(u_{i+1}^0 - 2u_i^0 + u_{i-1}^0\right) \\ &+ d\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^k - 2u_i^k + u_{i-1}^k - \left(u_{i+1}^{k-1} - 2u_i^{k-1} + u_{i-1}^{k-1}\right)\right] + 2\Delta t\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right], \end{aligned} \tag{5.52}$$

where

$$d = \frac{4D\Delta t^{\gamma}}{\Delta x^2\Gamma(1+\gamma)}. \tag{5.53}$$

If we set $\gamma = 1$, noting $\widetilde{\beta}_j(1) = 1$ and $\widetilde{\mu}_{j-k}(1) = 1$, Equation (5.52) simplifies to the Equation (5.14), which is the Keller Box method (Pletcher et al. 2012) when applied to the diffusion equation with a source term.

### 5.2.2 Keller Box Method with the C3 Scheme: the KBMC3 Scheme

In this section, we now use the C3 scheme approximation instead for the fractional derivative given in Chapter 2 by Equations (2.88) – (2.91), where $p = 1-\gamma$,

$$\left[\frac{d^{1-\gamma}u(t)}{dt^{1-\gamma}}\right|_{C3}^{j+\frac{1}{2}} = \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widehat{\beta}_j(\gamma)u(0) + 2\widehat{\alpha}_j(\gamma)u\left(t_{\frac{1}{2}}\right) + \sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[u\left(t_{k+\frac{1}{2}}\right) - u\left(t_{k-\frac{1}{2}}\right)\right]\right\}, \tag{5.54}$$

where the weights are defined by

$$\widehat{\alpha}_j(\gamma) = \left(j + \frac{1}{2}\right)^{\gamma} - j^{\gamma}, \tag{5.55}$$

$$\widehat{\beta}_j(\gamma) = \gamma \left( j + \frac{1}{2} \right)^{\gamma - 1} - 2\widehat{\alpha}_j, \tag{5.56}$$

and

$$\widehat{\mu}_j(\gamma) = (j+1)^{\gamma} - j^{\gamma}. \tag{5.57}$$

We will refer to this method as the KBMC3 scheme. Using a similar process, as given in the previous section, we approximate the fractional derivative in Equation (5.25) using Equations (5.54) – (5.57), and Equation (5.25) is replaced by the equations

$$\frac{u_i^j - u_{i-1}^j}{\Delta x_i} = \frac{v_i^j + v_{i-1}^j}{2}, \tag{5.58}$$

and

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} - \frac{u_i^j + u_{i-1}^j}{2\Delta t} = \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \left\{ \widehat{\beta}_j(\gamma) \left( v_i^0 - v_{i-1}^0 \right) + 2\widehat{\alpha}_j(\gamma) \left[ \frac{v_i^0 + v_i^1}{2} - \frac{v_{i-1}^0 + v_{i-1}^1}{2} \right] \right.$$
$$\left. + \frac{1}{2} \sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma) \left( \left[ v_i^k + v_i^{k+1} - \left( v_{i-1}^k + v_{i-1}^{k+1} \right) \right] - \left[ v_i^k + v_i^{k-1} - \left( v_{i-1}^k + v_{i-1}^{k-1} \right) \right] \right) \right\} + [f]_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{5.59}$$

Equation (5.59) is then simplified to give

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} = \frac{u_i^j + u_{i-1}^j}{2\Delta t} + \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \left\{ \kappa_j(\gamma) \left( v_i^0 - v_{i-1}^0 \right) + \widehat{\alpha}_j(\gamma) \left( v_i^1 - v_{i-1}^1 \right) \right.$$
$$\left. + \frac{1}{2} \sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma) \left[ v_i^{k+1} - v_{i-1}^{k+1} - \left( v_i^{k-1} - v_{i-1}^{k-1} \right) \right] \right\} + [f]_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \tag{5.60}$$

where the weight is defined as

$$\begin{aligned} \kappa_j(\gamma) &= \widehat{\beta}_j(\gamma) + \widehat{\alpha}_j(\gamma) \\ &= \gamma \left( j + \frac{1}{2} \right)^{\gamma-1} - \left( j + \frac{1}{2} \right)^{\gamma} + j^{\gamma}. \end{aligned} \tag{5.61}$$

Solving Equation (5.58) to find $v_{i-1}^j$ and combining with Equation (5.60) gives

$$\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} = \frac{u_i^j + u_{i-1}^j}{2\Delta t} + \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \left\{ \kappa_j(\gamma) \left[ v_i^0 - \left( 2\frac{u_i^0 - u_{i-1}^0}{\Delta x_i} - v_i^0 \right) \right] \right. \tag{5.62}$$
$$+ \widehat{\alpha}_j(\gamma) \left[ v_i^1 - \left( 2\frac{u_i^1 - u_{i-1}^1}{\Delta x_i} - v_i^1 \right) \right] + \frac{1}{2} \sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma) \left[ v_i^{k+1} - \left( 2\frac{u_i^{k+1} - u_{i-1}^{k+1}}{\Delta x_i} - v_i^{k+1} \right) \right.$$
$$\left. \left. - \left( v_i^{k-1} - \left( 2\frac{u_i^{k-1} - u_{i-1}^{k-1}}{\Delta x_i} - v_i^{k-1} \right) \right) \right] \right\} + f_{i-\frac{1}{2}}^{j+\frac{1}{2}},$$

which can be further simplified to

$$\frac{u_i^{j+1}+u_{i-1}^{j+1}}{2\Delta t}=\frac{u_i^j+u_{i-1}^j}{2\Delta t}+\frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\kappa_j(\gamma)v_i^0-\frac{\kappa_j(\gamma)}{\Delta x_i}\left(u_i^0-u_{i-1}^0\right)$$
$$+\widehat{\alpha}_j(\gamma)v_i^1-\frac{\widehat{\alpha}_j(\gamma)}{\Delta x_i}\left(u_i^1-u_{i-1}^1\right)+\frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[v_i^{k+1}-v_i^{k-1}\right]$$
$$-\frac{1}{2\Delta x_i}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\left(u_i^{k+1}-u_{i-1}^{k+1}\right)-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]\Bigg\}+[f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}\,. \tag{5.63}$$

In a similar manner, by replacing $i$ by $i+1$ in Equations (5.58) and (5.60) we then have

$$\frac{u_{i+1}^j-u_i^j}{\Delta x_{i+1}}=\frac{v_{i+1}^j+v_i^j}{2}, \tag{5.64}$$

and

$$\frac{u_{i+1}^{j+1}+u_i^{j+1}}{2\Delta t}=\frac{u_{i+1}^j+u_i^j}{2\Delta t}+\frac{D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\kappa_j(\gamma)\left(v_{i+1}^0-v_i^0\right)$$
$$+\widehat{\alpha}_j(\gamma)\left(v_{i+1}^1-v_i^1\right)+\frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[v_{i+1}^{k+1}-v_i^{k+1}-(v_{i+1}^{k-1}-v_i^{k-1})\right]\Bigg\}+[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,. \tag{5.65}$$

Solving Equation (5.64) to find $v_{i+1}^j$ and then using in Equation (5.65) gives

$$\frac{u_{i+1}^{j+1}+u_i^{j+1}}{2\Delta t}=\frac{u_{i+1}^j+u_i^j}{2\Delta t}+\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\frac{\kappa_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^0-u_i^0\right)-\kappa_j(\gamma)v_i^0$$
$$+\frac{\widehat{\alpha}_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^1-u_i^1\right)-\widehat{\alpha}_j(\gamma)v_i^1-\frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[v_i^{k+1}-v_i^{k-1}\right]$$
$$+\frac{1}{2\Delta x_{i+1}}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k+1}-u_i^{k+1}-\left(u_{i+1}^{k-1}-u_i^{k-1}\right)\right]\Bigg\}+[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,. \tag{5.66}$$

Multiplying Equation (5.63) by $\Delta x_i$ and Equation (5.66) by $\Delta x_{i+1}$, and then adding the two, we then obtain the equation

$$\frac{\Delta x_i}{2\Delta t}\left[u_i^{j+1}+u_{i-1}^{j+1}\right]+\frac{\Delta x_{i+1}}{2\Delta t}\left[u_{i+1}^{j+1}+u_i^{j+1}\right]=\frac{\Delta x_i}{2\Delta t}\left[u_i^j+u_{i-1}^j\right]+\frac{\Delta x_{i+1}}{2\Delta t}\left[u_{i+1}^j+u_i^j\right]$$
$$+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\Bigg\{\kappa_j(\gamma)v_i^0-\frac{\kappa_j}{\Delta x_i}\left(u_i^0-u_{i-1}^0\right)+\widehat{\alpha}_j(\gamma)v_i^1-\frac{\widehat{\alpha}_j(\gamma)}{\Delta x_i}\left(u_i^1-u_{i-1}^1\right)$$
$$+\frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[v_i^{k+1}-v_i^{k-1}\right]-\frac{1}{2\Delta x_i}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\left(u_i^{k+1}-u_{i-1}^{k+1}\right)-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]\Bigg\}$$
$$+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\Bigg\{\frac{\kappa_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^0-u_i^0\right)-\kappa_j(\gamma)v_i^0+\frac{\widehat{\alpha}_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^1-u_i^1\right)-\widehat{\alpha}_j(\gamma)v_i^1$$
$$-\frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[v_i^{k+1}-v_i^{k-1}\right]+\frac{1}{2\Delta x_{i+1}}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k+1}-u_i^{k+1}-\left(u_{i+1}^{k-1}-u_i^{k-1}\right)\right]\Bigg\}$$
$$+\Delta x_i\,[f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,. \tag{5.67}$$

Multiplying both sides of Equation (5.67) by $2\Delta t$ and simplifying, we then obtain the system of equations

$$\Delta x_i u_{i-1}^{j+1} + \left(\Delta x_i + \Delta x_{i+1}\right) u_i^{j+1} + \Delta x_{i+1} u_{i+1}^{j+1} = C_i + 2\Delta t \left[\Delta x_i f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + \Delta x_{i+1} f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right], \tag{5.68}$$

where

$$\begin{aligned} C_i = {} & \Delta x_i u_{i-1}^{j} + \left(\Delta x_i + \Delta x_{i+1}\right) u_i^{j} + \Delta x_{i+1} u_{i+1}^{j} - \frac{4D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \Bigg\{ \kappa_j \left(u_i^0 - u_{i-1}^0\right) \\ & + \widehat{\alpha}_j(\gamma)\left(u_i^1 - u_{i-1}^1\right) + \frac{1}{2}\sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma)\left[\left(u_i^{k+1} - u_{i-1}^{k+1}\right) - \left(u_i^{k-1} - u_{i-1}^{k-1}\right)\right]\Bigg\} \\ & + \frac{4D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)} \Bigg\{ \kappa_j(\gamma)\left(u_{i+1}^0 - u_i^0\right) + \widehat{\alpha}_j(\gamma)\left(u_{i+1}^1 - u_i^1\right) \\ & + \frac{1}{2}\sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k+1} - u_i^{k+1} - \left(u_{i+1}^{k-1} - u_i^{k-1}\right)\right]\Bigg\}. \end{aligned} \tag{5.69}$$

In the case of constant grid spacing $\Delta x_i = \Delta x$, Equations (5.68) – (5.69) after multiplying both sides by $1/\Delta x$, reduces to

$$\begin{aligned} \left(u_{i-1}^{j+1} + 2u_i^{j+1} + u_{i+1}^{j+1}\right) = {} & \left(u_{i-1}^{j} + 2u_i^{j} + u_{i+1}^{j}\right) + d\kappa_j(\gamma)\left(u_{i-1}^0 - 2u_i^0 + u_{i+1}^0\right) \\ & + d\widehat{\alpha}_j(\gamma)\left(u_{i-1}^1 - 2u_i^1 + u_{i+1}^1\right) + \frac{d}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\left(u_{i-1}^{k+1} - 2u_i^{k+1} + u_{i+1}^{k+1}\right)\right. \\ & \left. - \left(u_{i-1}^{k-1} - 2u_i^{k-1} + u_{i+1}^{k-1}\right)\right] + 2\Delta t\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right], \end{aligned} \tag{5.70}$$

where $d$ is as defined in Equation (5.53). In the standard diffusion case, $\gamma = 1$, we again get a similar equation to that given by Equation (5.14) with the source term.

### 5.2.3 Keller Box Method with the L1 Scheme: the KBML1 Scheme

In this section, the numerical scheme for solving Equation (5.16) will be developed by applying the Keller Box method together with the L1 scheme approximation for the fractional derivative. We refer to this implicit method as the KBML1 scheme. Here we approximate Equation (5.16) at the point $x = x_{i-\frac{1}{2}}$ and time $t = t_j$ that is

$$\left[\left.\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j}\right] = D\left[\left.\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_{i-\frac{1}{2}}^{j}\right] + f\left(x_{i-\frac{1}{2}}, t_j\right). \tag{5.71}$$

The L1 scheme (given in Chapter 2 by Equation (2.12) for $p = 1 - \gamma$), is

$$\left[\frac{d^{1-\gamma}u(t)}{dt^{1-\gamma}}\right|_{L1}^{j} = \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)u(0) + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[u(t_{k+1}) - u(t_k)\right]\right\}, \tag{5.72}$$

where the weights are defined by

$$\beta_j(\gamma) = \gamma j^{\gamma-1}, \tag{5.73}$$

and

$$\mu_j(\gamma) = j^{\gamma} - (j-1)^{\gamma}. \tag{5.74}$$

Similar to Sections 5.2.1 and 5.2.2, we again define the first spatial derivative by

$$\left[\frac{\partial u}{\partial x}\right|_{i-\frac{1}{2}}^{j} = [v|_{i-\frac{1}{2}}^{j}. \tag{5.75}$$

Approximating the fractional derivative using Equations (5.72) – (5.74), we then have

$$\left[\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j} = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{0} + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{k+1} - \left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{k}\right)\right\} + f_{i-\frac{1}{2}}^{j}. \tag{5.76}$$

Note instead of evaluating at time $t = t_{j+\frac{1}{2}}$ we evaluate the equation at the time $t = t_j$. Approximating the first order spatial and time derivative in Equations (5.75) and (5.76) by using the finite difference scheme, in Chapter 3 given by Equation (3.9), and applying the spatial averages, given by Equation (5.35), we then obtain the algebraic equations for $u_i^j$ and $v_i^j$

$$\frac{u_i^j - u_{i-1}^j}{\Delta x_i} = \frac{v_i^j + v_{i-1}^j}{2}, \tag{5.77}$$

and

$$\begin{aligned}\frac{u_i^j + u_{i-1}^j}{2\Delta t} - \frac{u_i^{j-1} + u_{i-1}^{j-1}}{2\Delta t} = \frac{D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{&\beta_j(\gamma)\left(v_i^0 - v_{i-1}^0\right) \\ &+ \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(v_i^{k+1} - v_{i-1}^{k+1}\right) - \left(v_i^k - v_{i-1}^k\right)\right]\Bigg\} + [f|_{i-\frac{1}{2}}^{j}.\end{aligned} \tag{5.78}$$

Combining Equation (5.77) with Equation (5.78), gives

$$\begin{aligned}\frac{u_i^j + u_{i-1}^j}{2\Delta t} &= \frac{u_i^{j-1} + u_{i-1}^{j-1}}{2\Delta t} + \frac{D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\beta_j(\gamma)\left(v_i^0 - \left[2\frac{u_i^0 - u_{i-1}^0}{\Delta x_i} - v_i^0\right]\right) \\ &+ \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(v_i^{k+1} - \left[2\frac{u_i^{k+1} - u_{i-1}^{k+1}}{\Delta x_i} - v_i^{k+1}\right]\right) - \left(v_i^k - \left[2\frac{u_i^k - u_{i-1}^k}{\Delta x_i} - v_i^k\right]\right)\right]\Bigg\} + [f|_{i-\frac{1}{2}}^{j}\end{aligned} \tag{5.79}$$

which can be simplified to

$$\frac{u_i^j + u_{i-1}^j}{2\Delta t} = \frac{u_i^{j-1} + u_{i-1}^{j-1}}{2\Delta t} + \frac{2D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)} \Bigg\{ -\frac{\beta_j(\gamma)}{\Delta x_i}\left(u_i^0 - u_{i-1}^0\right) + \beta_j v_i^0 \tag{5.80}$$
$$-\frac{1}{\Delta x_i}\sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_i^{k+1} - u_{i-1}^{k+1}\right) - \left(u_i^k - u_{i-1}^k\right)\right] + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(v_i^{k+1} - v_i^k\right)\Bigg\} + [f|_{i-\frac{1}{2}}^j .$$

In similar manner, by replacing $i$ with $i+1$ in Equations (5.77) and (5.78), we have

$$\frac{u_{i+1}^j - u_i^j}{\Delta x_{i+1}} = \frac{v_{i+1}^j + v_i^j}{2}, \tag{5.81}$$

and

$$\frac{u_{i+1}^j + u_i^j}{2\Delta t} - \frac{u_{i+1}^{j-1} + u_i^{j-1}}{2\Delta t} = \frac{D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\beta_j(\gamma)\left(v_{i+1}^0 - v_i^0\right) \tag{5.82}$$
$$+\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(v_{i+1}^{k+1} - v_i^{k+1}\right) - \left(v_{i+1}^k - v_i^k\right)\right]\Bigg\} + [f|_{i+\frac{1}{2}}^j .$$

Combining Equation (5.81) with Equation (5.82) gives another equation involving $u_i^j$ and $v_i^j$

$$\frac{u_{i+1}^j + u_i^j}{2\Delta t} = \frac{u_{i+1}^{j-1} + u_i^{j-1}}{2\Delta t} + \frac{D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\beta_j(\gamma)\left(\left[2\frac{u_{i+1}^0 - u_i^0}{\Delta x_{i+1}} - v_i^0\right] - v_i^0\right)$$
$$+\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(\left[2\frac{u_{i+1}^{k+1} - u_i^{k+1}}{\Delta x_{i+1}} - v_i^{k+1}\right] - v_i^{k+1}\right) - \left(\left[2\frac{u_{i+1}^k - u_i^k}{\Delta x_{i+1}} - v_i^k\right] - v_j^k\right)\right]\Bigg\}$$
$$+ [f|_{i+\frac{1}{2}}^j . \tag{5.83}$$

This equation is then simplified to

$$\frac{u_{i+1}^j + u_i^j}{2\Delta t} = \frac{u_{i+1}^{j-1} + u_i^{j-1}}{2\Delta t} + \frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\Bigg\{\frac{\beta_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^0 - u_i^0\right) - \beta_j(\gamma)v_i^0$$
$$+\frac{1}{\Delta x_{i+1}}\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_{i+1}^{k+1} - u_i^{k+1}\right) - \left(u_{i+1}^k - u_i^k\right)\right] - \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(v_i^{k+1} - v_i^k\right)\Bigg\}$$
$$+ [f|_{i+\frac{1}{2}}^j . \tag{5.84}$$

Now multiplying Equation (5.80) by $\Delta x_i$ and Equation (5.84) by $\Delta x_{i+1}$ and then adding the two gives the equation for $u_i^j$ at each grid point $i$ and time step $j$

$$\begin{aligned}
&\frac{\Delta x_i}{2\Delta t}\left(u_i^j+u_{i-1}^j\right)+\frac{\Delta x_{i+1}}{2\Delta t}\left(u_{i+1}^j+u_i^j\right)=\frac{\Delta x_i}{2\Delta t}\left(u_i^{j-1}+u_{i-1}^{j-1}\right)+\frac{\Delta x_{i+1}}{2\Delta t}\left(u_{i+1}^{j-1}+u_i^{j-1}\right)\\
&-\frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\left(u_i^0-u_{i-1}^0\right)+\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_i^{k+1}-u_{i-1}^{k+1}\right)-\left(u_i^k-u_{i-1}^k\right)\right]\right\}\\
&+\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\left(u_{i+1}^0-u_i^0\right)+\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_{i+1}^{k+1}-u_i^{k+1}\right)-\left(u_{i+1}^k-u_i^k\right)\right]\right\}\\
&+\Delta x_i\,[f|_{i-\frac{1}{2}}^j+\Delta x_{i+1}\,[f|_{i+\frac{1}{2}}^j\,. \qquad (5.85)
\end{aligned}$$

Multiplying both sides by $2\Delta t$, Equation (5.85) is then given by system of equations

$$\Delta x_i u_{i-1}^j+\left(\Delta x_{i+1}+\Delta x_{i+1}\right)u_i^j+\Delta x_{i+1}u_{i+1}^j=C_i+2\Delta t\left(\Delta x_{i+1}\,[f|_{i+\frac{1}{2}}^j+\Delta x_i\,[f|_{i-\frac{1}{2}}^j\right), \qquad (5.86)$$

where

$$\begin{aligned}
C_i&=\Delta x_i u_{i-1}^{j-1}+\left(\Delta x_{i+1}+\Delta x_{i+1}\right)u_i^{j-1}+\Delta x_{i+1}u_{i+1}^{j-1} \qquad (5.87)\\
&-\frac{4D\Delta t^{\gamma}}{\Delta x_i\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\left(u_i^0-u_{i-1}^0\right)+\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_i^{k+1}-u_{i-1}^{k+1}\right)-\left(u_i^k-u_{i-1}^k\right)\right]\right\}\\
&+\frac{4D\Delta t^{\gamma}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\left(u_{i+1}^0-u_i^0\right)+\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_{i+1}^{k+1}-u_i^{k+1}\right)-\left(u_{i+1}^k-u_i^k\right)\right]\right\}.
\end{aligned}$$

In the case of constant grid spacing $\Delta x_i=\Delta x$, Equations (5.86) and (5.87) reduce to the equation

$$\begin{aligned}
&(u_{i-1}^j+2u_i^j+u_{i+1}^j)=(u_{i+1}^{j-1}+2u_i^{j-1}+u_{i-1}^{j-1})+d\beta_j(\gamma)(u_{i+1}^0-2u_i^0+u_{i-1}^0) \qquad (5.88)\\
&+d\sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\left(u_{i+1}^{k+1}-2u_i^{k+1}+u_{i-1}^{k+1}\right)-\left(u_{i+1}^k-2u_i^k+u_{i-1}^k\right)\right]+2\Delta t\left(f_{i+\frac{1}{2}}^j+f_{i-\frac{1}{2}}^j\right),
\end{aligned}$$

where $d$ is as defined previously by Equation (5.53).

If we set $\gamma=1$, Equation (5.88) reduces to

$$\begin{aligned}
\left(u_{i+1}^j+2u_i^j+u_{i-1}^j\right)-\frac{2D\Delta t}{\Delta x^2}\left(u_{i+1}^j-2u_i^j+u_{i-1}^j\right)&=\left(u_{i+1}^{j-1}+2u_i^{j-1}+u_{i-1}^{j-1}\right) \qquad (5.89)\\
&+2\Delta t\left[f\left(x_{i-\frac{1}{2}},t_j\right)+f\left(x_{i+\frac{1}{2}},t_j\right)\right],
\end{aligned}$$

since $\beta_j(1)=1$ and $\mu_{j-k}(1)=1$. Equation (5.89) is the Keller Box method (Pletcher et al. 2012) for the non–fractional diffusion equation with a source term.

## 5.3 The Accuracy of the Numerical Methods

In this section, we consider the consistency and the order of accuracy of the three numerical schemes KBMC2, KBMC3, and KBML1 methods given by Equations (5.52), (5.70) and (5.88) respectively. Similar to Chapter 3, we let

$$\delta_x^2 u_i^j = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}, \tag{5.90}$$

to aid in the analysis of each scheme.

### 5.3.1 Accuracy of the KBMC2 Scheme

We now determine the truncation error of the KBMC2 scheme. First using Equation (5.90) in Equation (5.52) we then have

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] \qquad (5.91)\\
&= \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right) - 2\left(\delta_x^2 u_i^{j+\frac{1}{2}} - \delta_x^2 u_i^j\right)\right]\right\} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right]\\
&+ \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 u_i^0 + 2\left(\frac{1}{2}\right)^\gamma\left(\delta_x^2 u_i^{j+\frac{1}{2}} - \delta_x^2 u_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 u_i^k - \delta_x^2 u_i^{k-1}\right]\right\}.
\end{aligned}$$

Next we identify the term in the third line of Equation (5.91) as the C2 approximation, Equation (5.26), with $u(t)$ replaced by $\delta_x^2 u(t)$. We can then further rewrite Equation (5.91) as

$$\begin{aligned}
\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u\right)\right|_{C2,i}^{j+\frac{1}{2}} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right]\\
&+ \frac{\left(\frac{1}{2}\right)^\gamma D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\delta_x^2 u_i^{j+1} + \delta_x^2 u_i^j - 2\delta_x^2 u_i^{j+\frac{1}{2}}\right].
\end{aligned} \tag{5.92}$$

Adding and subtracting the exact value of the fractional derivative, Equation (5.92) then becomes

$$\begin{aligned}
\frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] - \frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right]\\
&+ D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u\right)\right|_{C2,i}^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\partial^2 u}{\partial x^2}\right|_i^{j+\frac{1}{2}} + \left(\frac{1}{2}\right)^\gamma\frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\delta_x^2 u_i^{j+1} + \delta_x^2 u_i^j - 2\delta_x^2 u_i^{j+\frac{1}{2}}\right].
\end{aligned} \tag{5.93}$$

Now taking the Taylor series expansion around the point $(x_i, t_j)$, we have

$$\delta_x^2 U_i^j \simeq \left[\frac{\partial^2 U}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 U}{\partial x^4}\right|_i^j + O(\Delta x^4). \tag{5.94}$$

Expanding the Taylor series around the point $(x_i, t_{j+\frac{1}{2}})$, we find

$$\frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] \simeq f_i^{j+\frac{1}{2}} + \frac{\Delta x^2}{8}\left[\frac{\partial^2 f}{\partial x^2}\right|_i^{j+\frac{1}{2}} + O(\Delta x^4), \tag{5.95}$$

$$\delta_x^2 U_i^{j+1} + \delta_x^2 U_i^j - 2\delta_x^2 U_i^{j+\frac{1}{2}} \simeq \frac{\Delta t^2}{4}\left[\frac{\partial^4 U}{\partial x^2 \partial t^2}\right|_i^{j+\frac{1}{2}} + \frac{\Delta x^2 \Delta t^2}{48}\left[\frac{\partial^6 U}{\partial x^4 \partial t^2}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4), \tag{5.96}$$

and

$$\frac{U_i^{j+1} - U_i^j}{\Delta t} \simeq \left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} + \frac{\Delta t^2}{24}\left[\frac{\partial^3 U}{\partial t^3}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4). \tag{5.97}$$

We also have

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right] \simeq \frac{\Delta x^2}{4}\left[\frac{\partial^3 U}{\partial x^2 \partial t}\right|_i^{j+\frac{1}{2}} + \frac{\Delta x^2 \Delta t^2}{96}\left[\frac{\partial^5 U}{\partial x^2 \partial t^3}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4) + O(\Delta x^4). \tag{5.98}$$

Combining these approximations with Equation (5.93) gives

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + f(x_i, t_{j+\frac{1}{2}}) + O(\Delta t^{1+\gamma}) + O(\Delta x^2)\\ &+ D\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{C2,i}^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}}\right] + \frac{D\Delta x^2}{12}\left[\frac{\partial^{1-\gamma} M(t)}{\partial t^{1-\gamma}}\right|_i^{j+\frac{1}{2}},\end{aligned} \tag{5.99}$$

where $M(t)$ is defined by

$$M(t) = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left|\frac{\partial^4 U}{\partial x^4}\right|. \tag{5.100}$$

By Equation (2.149) the term

$$\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{C2,i}^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}}\right] \tag{5.101}$$

is $O(\Delta t^{1+\gamma})$, we then get the truncation error, $\tau_{i,j}^{(1)}$, of Equation (5.52), is order $1+\gamma$ in time and second order in space, that is

$$\tau_{i,j}^{(1)} = O(\Delta t^{1+\gamma}) + O(\Delta x^2). \tag{5.102}$$

### 5.3.2 Accuracy of the KBMC3 Scheme

We now also determine the truncation error of the KBMC3 scheme. First using Equation (5.90) in Equation (5.70) we then have

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] = \frac{D\Delta t^{\gamma-1}\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}\left[\delta_x^2 u_i^1 + \delta_x^2 u_i^0 - 2\delta_x^2 u_i^{\frac{1}{2}}\right]$$
$$+\frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{1}{2}\left(\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^{k-1}\right) - \left(\delta_x^2 u_i^{k+\frac{1}{2}} - \delta_x^2 u_i^{k-\frac{1}{2}}\right)\right]$$
$$+\frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widehat{\beta}_j(\gamma)\delta_x^2 u_i^0 + 2\widehat{\alpha}_j(\gamma)\delta_x^2 u_i^{\frac{1}{2}} + \sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left(\delta_x^2 u_i^{k+\frac{1}{2}} - \delta_x^2 u_i^{k-\frac{1}{2}}\right)\right\}$$
$$+\frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right]. \tag{5.103}$$

Next recognising the terms on the third line in Equation (5.103) as the C3 approximation, Equation (5.54), with $u(t)$ replaced by $\delta_x^2 u(t)$, we can then rewrite Equation (5.103) as

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] = \frac{D\Delta t^{\gamma-1}\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}\left[\delta_x^2 u_i^1 + \delta_x^2 u_i^0 - 2\delta_x^2 u_i^{\frac{1}{2}}\right]$$
$$+\frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{1}{2}\left(\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^{k-1}\right) - \left(\delta_x^2 u_i^{k+\frac{1}{2}} - \delta_x^2 u_i^{k-\frac{1}{2}}\right)\right]$$
$$+D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u_i\right)\Big|_{C3}^{j+\frac{1}{2}} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right]\right]. \tag{5.104}$$

Adding and subtracting the value of the exact fractional derivative then gives

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right]$$
$$= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\Big|_i^{j+\frac{1}{2}} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right]\right] + \frac{D\Delta t^{\gamma-1}\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}\left[\delta_x^2 u_i^1 + \delta_x^2 u_i^0 - 2\delta_x^2 u_i^{\frac{1}{2}}\right]$$
$$+\frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{1}{2}\left(\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^{k-1}\right) - \left(\delta_x^2 u_i^{k+\frac{1}{2}} - \delta_x^2 u_i^{k-\frac{1}{2}}\right)\right]$$
$$+D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u_i\right)\Big|_{C3}^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\Big|_i^{j+\frac{1}{2}}\right.\right.. \tag{5.105}$$

Now taking the Taylor series expansion around the point $(x_i, t_k)$ using Equations (5.94) gives

$$\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^{k-1} \simeq 2\Delta t\left[\frac{\partial(\delta_x^2 U)}{\partial t}\Big|_i^k + 2\frac{\Delta t^3}{3!}\left[\frac{\partial^3(\delta_x^2 U)}{\partial t^3}\Big|_i^k + O(\Delta t^5),\right.\right. \tag{5.106}$$

$$\delta_x^2 U_i^{k+\frac{1}{2}} - \delta_x^2 U_i^{k-\frac{1}{2}} \simeq \Delta t\left[\frac{\partial(\delta_x^2 U)}{\partial t}\Big|_i^k + \frac{2}{3!}\left(\frac{\Delta t}{2}\right)^3\left[\frac{\partial^3(\delta_x^2 U)}{\partial t^3}\Big|_i^k + O(\Delta t^5),\right.\right. \tag{5.107}$$

and so

$$\frac{1}{2}\left[\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^{k-1}\right] - \left[\delta_x^2 U_i^{k+\frac{1}{2}} - \delta_x^2 U_i^{k-\frac{1}{2}}\right] = \frac{\Delta t^3}{8}\left[\frac{\partial^3(\delta_x^2 U)}{\partial t^3}\right|_i^k + O(\Delta t^5). \tag{5.108}$$

Using these expansions, along with those in Equations (5.94) – (5.98) and Equation (5.96) with $j = 0$, Equation (5.105) then becomes

$$\begin{aligned}
&\frac{\Delta x^2}{4}\left[\frac{\partial^3 U}{\partial x^2 \partial t}\right|_i^{j+\frac{1}{2}} + \left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} \qquad (5.109)\\
&\quad + f_i^{j+\frac{1}{2}} + O(\Delta x^2) + \frac{D\Delta t^{\gamma-1}\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}\left[\frac{\Delta t^2}{4}\left[\frac{\partial^2}{\partial t^2}\left(\delta_x^2 U\right)\right|_i^{\frac{1}{2}} + O(\Delta t^4)\right]\\
&\quad + \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{\Delta t^3}{8}\left[\frac{\partial^3(\delta_x^2 U)}{\partial t^3}\right|_i^k + O(\Delta t^5)\right]\\
&\quad + D\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left[\frac{\partial^2 U}{\partial x^2}\right|_{C3,i}^{j+\frac{1}{2}} + \frac{\Delta x^2}{12}D\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left[\frac{\partial^4 U}{\partial x^4}\right|_{C3,i}^{j+\frac{1}{2}} + O(\Delta x^4) - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}}.
\end{aligned}$$

We note the term

$$\begin{aligned}
\frac{D\Delta t^{\gamma-1}\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}\left[\frac{\Delta t^2}{4}\left[\frac{\partial^2}{\partial t^2}\left(\delta_x^2 U\right)\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right] &= \frac{D\Delta t^{1+\gamma}\widehat{\alpha}_j(\gamma)}{4\Gamma(1+\gamma)}\left[\frac{\partial^2}{\partial t^2}\left(\delta_x^2 U\right)\right|_i^{j+\frac{1}{2}}\\
&\quad + \frac{D\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}O(\Delta t^{3+\gamma}), \qquad (5.110)
\end{aligned}$$

is of order $O(\Delta t^{1+\gamma})$, and the term

$$\begin{aligned}
&\frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{\Delta t^3}{8}\left[\frac{\partial^3(\delta_x^2 U)}{\partial t^3}\right|_i^k + O(\Delta t^5)\right] \qquad (5.111)\\
&\qquad = \frac{D\Delta t^{2+\gamma}}{8\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{\partial^3(\delta_x^2 U)}{\partial t^3}\right|_i^k + \frac{D}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)O(\Delta t^{4+\gamma}),
\end{aligned}$$

is of order $O(\Delta t^{2+\gamma})$. Then Equation (5.109) can be simplified to

$$\begin{aligned}
&\left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + f_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}) \qquad (5.112)\\
&+ D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{C3,i}^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + \frac{D\Delta x^2}{12}\left[\frac{\partial^{1-\gamma}M(t)}{\partial t^{1-\gamma}}\right|_{C3,i}^{j+\frac{1}{2}},
\end{aligned}$$

where

$$M(t) = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left|\frac{\partial^4 U}{\partial x^4}\right|. \tag{5.113}$$

By Equation (2.174) we note

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{C3,i}^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} \tag{5.114}$$

is $O(\Delta t^{1+\gamma})$ we then get the truncation error is of order $1+\gamma$ in time and second order in space i.e.

$$\tau_{i,j}^{(2)} = O(\Delta t^{1+\gamma}) + O(\Delta x^2), \tag{5.115}$$

where $\tau_{i,j}^{(2)}$ is the truncation error of Equation (5.70).

### 5.3.3 Accuracy of the KBML1 Scheme

Here we determine the truncation error of the KBML1 scheme. Rewriting Equation (5.88) using Equation (5.90), we have

$$\begin{aligned} &\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^j - \delta_x^2 u_i^{j-1}\right] + \frac{1}{\Delta t}\left[u_i^j - u_i^{j-1}\right] \\ &= \frac{D\Delta t^\gamma}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\delta_x^2 u_i^0 + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(\delta_x^2 u_i^{k+1} - \delta_x^2 u_i^k\right)\right\} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^j + f_{i+\frac{1}{2}}^j\right]. \end{aligned} \tag{5.116}$$

Recognising the first term in the right–hand side as the L1 approximation given by Equation (5.72) with $u(t)$ replaced by $\delta_x^2 u(t)$. Equation (5.116) becomes

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^j - \delta_x^2 u_i^{j-1}\right] + \frac{1}{\Delta t}\left[u_i^j - u_i^{j-1}\right] = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u\right)\Big|_{L1,i}^j + \frac{1}{2}\left[f_{i-\frac{1}{2}}^j + f_{i+\frac{1}{2}}^j\right]\right]. \tag{5.117}$$

Now adding and subtracting the exact fractional derivative we then have

$$\begin{aligned} &\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^j - \delta_x^2 u_i^{j-1}\right] + \frac{1}{\Delta t}\left[u_i^j - u_i^{j-1}\right] \qquad (5.118) \\ &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\Big|_i^j + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u\right)\Big|_{L1,i}^j - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\Big|_i^j + \frac{1}{2}\left[f_{i-\frac{1}{2}}^j + f_{i+\frac{1}{2}}^j\right]\right.\right.\right. . \end{aligned}$$

Expanding the Taylor series around the point $(x_i, t_j)$, we have

$$U_i^j - U_i^{j-1} \simeq \Delta t\left[\frac{\partial U}{\partial t}\Big|_i^j - \frac{\Delta t^2}{12}\left[\frac{\partial^2 U}{\partial t^2}\Big|_i^j + O(\Delta t^3).\right.\right. \tag{5.119}$$

We also have

$$\delta_x^2 U_i^{j-1} \simeq \delta_x^2 U_i^j - \Delta t\left[\frac{\partial}{\partial t}(\delta_x^2 U)\Big|_i^j + \frac{\Delta t^2}{12}\left[\frac{\partial^2}{\partial t^2}(\delta_x^2 U)\Big|_i^j + O(\Delta t^3),\right.\right. \tag{5.120}$$

and so

$$\delta_x^2 U_i^j - \delta_x^2 U_i^{j-1} \simeq \Delta t\left[\frac{\partial}{\partial t}(\delta_x^2 U)\Big|_i^j - \frac{\Delta t^2}{12}\left[\frac{\partial^2}{\partial t^2}(\delta_x^2 U)\Big|_i^j + O(\Delta t^3).\right.\right. \tag{5.121}$$

Using Equations (5.94), (5.95), (5.119) and (5.121) in Equation (5.118), we then have

$$\frac{\Delta x^2}{4\Delta t}\left[\Delta t\left[\frac{\partial(\delta_x^2 U)}{\partial t}\right|_i^j + O(\Delta t^2)\right] + \frac{1}{\Delta t}\left[\Delta t\left[\frac{\partial U}{\partial t}\right|_i^j + O(\Delta t^2)\right]$$
$$= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j + f_i^j + \frac{1}{4}\frac{\Delta x^2}{2!}\left[\frac{\partial^2 f}{\partial x^2}\right|_i^j + O(\Delta x^4)$$
$$+ D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 U}{\partial x^4} + O(\Delta x^4)\right)\right|_{L1,i}^j - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j. \tag{5.122}$$

This equation is then simplified to

$$\left[\frac{\partial U}{\partial t}\right|_i^j = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j + f_i^j + \frac{D\Delta x^2}{12}\left[\frac{\partial^{1-\gamma} M(t)}{\partial t^{1-\gamma}}\right|_{L1,i}^j$$
$$+ D\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{L1,i}^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j\right] + O(\Delta x^2) + O(\Delta t), \tag{5.123}$$

where

$$M(t) = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left|\frac{\partial^4 U}{\partial x^4}\right|. \tag{5.124}$$

By Equation (2.48) in Chapter 2 we note that the term

$$\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{L1,i}^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j\right] \tag{5.125}$$

is $O(\Delta t^{1+\gamma})$, we then get the truncation error is first order in time and second order in space i.e.

$$\tau_{i,j}^{(3)} = O(\Delta t) + O(\Delta x^2), \tag{5.126}$$

where $\tau_{i,j}^{(3)}$ is the truncation error of Equation (5.88).

## 5.4 Consistency of the Numerical Methods

A numerical approximation scheme for the fractional diffusion equation is consistent, if we can show the truncation approaches zero as $\Delta t \to 0$ and $\Delta x \to 0$. Let $u_i^j \approx U_i^j = u(x_i, t_j)$ then

$$\lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}} (u_i^j - U_i^j) = \lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}} \tau_{i,j} = 0. \tag{5.127}$$

From Equations (5.102), (5.115), and (5.126) we see this condition is satisfied, that is

$$\lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}} \tau_{i,j} = 0. \tag{5.128}$$

This means the KBMC2, KBMC3, and KBML1 numerical methods are consistent with the original fractional partial differential equation.

## 5.5 Stability Analysis of the Numerical Methods

In this section, the stability of the numerical methods in Equations (5.52), (5.70) and (5.88) is considered by using Von Neumann stability analysis. We will discuss the stability of each scheme in the following sections.

### 5.5.1 Stability Analysis of the KBMC2 Scheme

To investigate the stability by Von Neumann stability analysis, we let $u_i^j$ and $v_i^j$ be the approximate solution of the Equations (5.36) and (5.37), and so we have

$$\left(u_i^{j+1} - u_{i-1}^{j+1}\right) = \frac{\Delta x_i}{2}\left(v_i^{j+1} + v_{i-1}^{j+1}\right), \tag{5.129}$$

and

$$\begin{aligned}\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} - \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left(v_i^{j+1} - v_{i-1}^{j+1}\right) = \frac{u_i^j + u_{i-1}^j}{2\Delta t} \\ + \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left\{ \widetilde{\beta}_j(\gamma)\left(v_i^0 - v_{i-1}^0\right) - \left(\frac{1}{2}\right)^{\gamma}\left(v_i^j - v_{i-1}^j\right)\right. \\ \left. + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left[v_i^k - v_{i-1}^k - \left(v_i^{k-1} - v_{i-1}^{k-1}\right)\right]\right\} + [f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}.\end{aligned} \tag{5.130}$$

The errors then are given by

$$\epsilon_i^j = U_i^j - u_i^j, \qquad \text{and} \qquad \varepsilon_i^j = V_i^j - v_i^j, \tag{5.131}$$

where $U_i^j$ and $V_i^j$ are the exact solution of Equations (5.24) and (5.25). These errors satisfy the equations

$$\left(\epsilon_i^{j+1} - \epsilon_{i-1}^{j+1}\right) - \frac{\Delta x_i}{2}\left(\varepsilon_i^{j+1} + \varepsilon_{i-1}^{j+1}\right) = 0, \tag{5.132}$$

and

$$\begin{aligned}\frac{\epsilon_i^{j+1} + \epsilon_{i-1}^{j+1}}{2\Delta t} - \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left(\varepsilon_i^{j+1} - \varepsilon_{i-1}^{j+1}\right) = \frac{\epsilon_i^j + \epsilon_{i-1}^j}{2\Delta t} \\ + \frac{D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left\{ \widetilde{\beta}_j(\gamma)\left(\varepsilon_i^0 - \varepsilon_{i-1}^0\right) - \left(\frac{1}{2}\right)^{\gamma}\left(\varepsilon_i^j - \varepsilon_{i-1}^j\right)\right. \\ \left. + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left[\varepsilon_i^k - \varepsilon_{i-1}^k - \left(\varepsilon_i^{k-1} - \varepsilon_{i-1}^{k-1}\right)\right]\right\}\end{aligned} \tag{5.133}$$

with zero boundary conditions. In Equations (5.132) and (5.133) we set the truncation error to zero, but later in the convergence section, we will use the truncation error to find the convergence rate of the numerical method.

Let $\epsilon_i^j = \zeta_j e^{i' q x_i}$, and $\varepsilon_i^j = \xi_j e^{i' q x_i}$, where $i'$ is the imaginary number, $\sqrt{-1}$, $q$ is a real spatial wave number. Equations (5.132) and (5.133) can then be rewritten as

$$\left(\zeta_{j+1} e^{i' q x_i} - \zeta_{j+1} e^{i' q (x_i - \Delta x_i)}\right) = \frac{\Delta x_i}{2}\left(\xi_{j+1} e^{i' q x_i} + \xi_{j+1} e^{i' q (x_i - \Delta x_i)}\right), \tag{5.134}$$

and

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(\zeta_{j+1} e^{i' q x_i} + \zeta_{j+1} e^{i' q (x_i - \Delta x_i)}\right) - \frac{D \Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left(\xi_{j+1} e^{i' q x_i} - \xi_{j+1} e^{i' q (x_i - \Delta x_i)}\right) \\
&= \frac{1}{2\Delta t}\left(\zeta_j e^{i' q x_i} + \zeta_j e^{i' q (x_i - \Delta x_i)}\right) + \frac{D \Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\Bigg\{ \widetilde{\beta}_j(\gamma)\left(\xi_0 e^{i' q x_i} - \xi_0 e^{i' q (x_i - \Delta x_i)}\right) \\
&\quad - \left(\frac{1}{2}\right)^{\gamma}\left(\xi_j e^{i' q x_i} - \xi_j e^{i' q (x_i - \Delta x_i)}\right) + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\Big[\xi_k e^{i' q x_i} - \xi_k e^{i' q (x_i - \Delta x_i)} \\
&\quad - \left(\xi_{k-1} e^{i' q x_i} - \xi_{k-1} e^{i' q (x_i - \Delta x_i)}\right)\Big]\Bigg\}.
\end{aligned} \tag{5.135}$$

Using Equation (5.134) in Equation (5.135), and simplifying, we obtain the recursive equation for $\zeta_{j+1}$

$$\begin{aligned}
&\zeta_{j+1} - \widehat{\rho}\left(\frac{1}{2}\right)^{\gamma}\left(\frac{1 - e^{-i' w \Delta x_i}}{1 + e^{-i' w \Delta x_i}}\right)^2 \zeta_{j+1} = \zeta_j - \widehat{\rho}\left(\frac{1}{2}\right)^{\gamma}\left(\frac{1 - e^{-i' w \Delta x_i}}{1 + e^{-i' w \Delta x_i}}\right)^2 \zeta_j \\
&\quad + \widehat{\rho}\left(\frac{1 - e^{-i' w \Delta x_i}}{1 + e^{-i' w \Delta x_i}}\right)^2 \widetilde{\beta}_j(\gamma)\zeta_0 + \widehat{\rho}\left(\frac{1 - e^{-i' w \Delta x_i}}{1 + e^{-i' w \Delta x_i}}\right)^2 \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left[\zeta_k - \zeta_{k-1}\right],
\end{aligned} \tag{5.136}$$

where

$$\widehat{\rho} = \frac{4 \Delta t^{\gamma}}{\Gamma(1+\gamma)(\Delta x_i)^2}\ . \tag{5.137}$$

Noting

$$\left(\frac{1 - e^{-i' q \Delta x_i}}{1 + e^{-i' q \Delta x_i}}\right)^2 = \frac{-\sin^2(q \Delta x_i)}{\left(1 + \cos(q \Delta x_i)\right)^2} = -\tan^2\left(\frac{q \Delta x_i}{2}\right), \tag{5.138}$$

Equation (5.136) then becomes

$$\zeta_{j+1} = \zeta_j - \Lambda_q \left\{ \widetilde{\beta}_j(\gamma)\zeta_0 + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\left[\zeta_k - \zeta_{k-1}\right] \right\}. \tag{5.139}$$

Here the coefficient $\Lambda_q$ is defined by

$$\Lambda_q = \frac{\Upsilon_q}{1 + \left(\frac{1}{2}\right)^{\gamma} \Upsilon_q}\ , \tag{5.140}$$

and $Ų_q$ is defined by

$$Ų_q = \widehat{\rho} \tan^2 \left( \frac{q \Delta x_i}{2} \right), \tag{5.141}$$

where $0 \leq Ų_q < \infty$.

When $j \geq 1$, the recurrence relation in Equation (5.139) can be rewritten as

$$\zeta_{j+1} = \left[1 - \Lambda_q \widetilde{\mu}_0(\gamma)\right] \zeta_j - \Lambda_q \left\{ \widetilde{\alpha}_j(\gamma)\zeta_0 + \sum_{k=1}^{j-1} \widetilde{\omega}_{j-k}(\gamma)\zeta_k \right\}, \tag{5.142}$$

with the weights

$$\widetilde{\alpha}_j(\gamma) = \widetilde{\beta}_j(\gamma) - \widetilde{\mu}_{j-1}(\gamma), \tag{5.143}$$

and

$$\widetilde{\omega}_j(\gamma) = \widetilde{\mu}_j(\gamma) - \widetilde{\mu}_{j-1}(\gamma), \tag{5.144}$$

where $\widetilde{\beta}_j(\gamma)$ and $\widetilde{\mu}_j(\gamma)$ are defined earlier in Equations (5.27) and (5.28) respectively.

We consider the following lemmas which will help in showing the stability of our numerical method.

**Lemma 5.5.1.** Given $0 < \gamma \leq 1$ and $0 \leq Ų_q < \infty$ then the parameter $\Lambda_q$ given in Equation (5.146) is bounded by

$$0 \leq \Lambda_q \leq 2^\gamma. \tag{5.145}$$

*Proof.* Note Equation (5.140) can be written as

$$\Lambda_q = 2^\gamma \left( 1 - \frac{2^\gamma}{2^\gamma + Ų_q} \right) . \tag{5.146}$$

The second term $2^\gamma / [2^\gamma + Ų_q]$ is always positive and it is bounded between 0 and 1 as $0 \leq Ų_q < 1$. Consequently, we have the bound $0 \leq \Lambda_q \leq 2^\gamma$. □

**Lemma 5.5.2.** (adapted from Zhuang et al. (2008))

Let $f(x) = x^\gamma - (x-1)^\gamma$, where $x \geq 1$, then $f(x)$ satisfies:

1. $f(x) > 0$, and

2. $f(x) > f(x+1)$.

*Proof.* To show $f(x) > 0$, we have

$$f(x) = x^\gamma - (x-1)^\gamma = x^\gamma \left[1 - \left(\frac{x-1}{x}\right)^\gamma\right], \tag{5.147}$$

but

$$0 \leq \frac{x-1}{x} < 1, \tag{5.148}$$

when $x \geq 1$ and so

$$0 \leq \left(\frac{x-1}{x}\right)^\gamma < 1, \tag{5.149}$$

or

$$0 < 1 - \left(\frac{x-1}{x}\right)^\gamma \leq 1. \tag{5.150}$$

Hence from Equation (5.147) we have $0 < f(x) \leq x^\gamma$ since $x^\gamma > 0$ and so $f(x) > 0$.

To prove the second result, we let $f_1(x) = x^\gamma$ and $f_2(x) = x^\gamma - (x-1)^\gamma$. We will show the functions $f_1(x)$ and $f_2(x)$ are monotonically increasing and decreasing functions respectively, when $\gamma \in (0,1)$.

Since

$$\frac{df_1(x)}{dx} = \gamma x^{\gamma-1} = \frac{\gamma}{x^{1-\gamma}} > 0, \tag{5.151}$$

we can conclude, for $x \geq 0$ and $0 < \gamma < 1$, that the function $f_1(x)$ is monotonically increasing function in $x$.

Differentiating $f_2(x)$ with respect to $x$ we find

$$\frac{df_2(x)}{dx} = \gamma x^{\gamma-1} - \gamma\,(x-1)^{\gamma-1}\,. \tag{5.152}$$

Now since

$$x^{1-\gamma} > (x-1)^{1-\gamma}\,,$$

as $f_1(x)$ is an increasing function for $0 < \gamma < 1$, then

$$\frac{1}{x^{1-\gamma}} < \frac{1}{(x-1)^{1-\gamma}}. \tag{5.153}$$

Hence

$$\begin{aligned} \frac{df_2(x)}{dx} &= \gamma x^{\gamma-1} - \gamma\,(x-1)^{\gamma-1} \\ &\leq \frac{\gamma}{(x-1)^{1-\gamma}} - \frac{\gamma}{(x-1)^{1-\gamma}} < 0 \end{aligned} \tag{5.154}$$

and so the function $f_2(x)$ is a monotonically decreasing function of $x$, for $0 < \gamma < 1$. Now we have, for $x \geq 1$,

$$f(x) = x^{\gamma} - (x-1)^{\gamma} > (x+1)^{\gamma} - ((x+1)-1)^{\gamma} = f(x+1). \tag{5.155}$$

Hence results (1) and (2) hold for $0 < \gamma < 1$. □

**Lemma 5.5.3.** Let $g_1(x) = \gamma x^{\gamma-1} - x^{\gamma} + (x-1)^{\gamma}$, and $g_2(x) = (x+1)^{\gamma} - 2x^{\gamma} + (x-1)^{\gamma}$ where $x \geq 1$ and $0 < \gamma < 1$, then $g_1(x)$ and $g_2(x)$ satisfy the following:

1. $g_1(x) < 0$, where $x \geq 1$, and
2. $g_2(x) < 0$, where $x \geq 1$.

*Proof.* First apply the binomial expansion to $(x-1)^{\gamma}$ then $g_1(x)$ becomes

$$\begin{aligned} g_1(x) &= \gamma x^{\gamma-1} - x^{\gamma} + \sum_{k=0}^{\infty} \begin{pmatrix} \gamma \\ n \end{pmatrix} (-1)^n x^{\gamma-n} \\ &= \sum_{n=2}^{\infty} \begin{pmatrix} \gamma \\ n \end{pmatrix} (-1)^n x^{\gamma-n}. \end{aligned} \tag{5.156}$$

Now by rewriting the binomial coefficient, using the result in Appendix B.2, we then find

$$\begin{aligned} g_1(x) &= \sum_{n=2}^{\infty} \frac{\gamma\Gamma(n-\gamma)}{n!\Gamma(1-\gamma)} (-1)^{2n-1} x^{\gamma-n} \\ &= -\sum_{n=2}^{\infty} \frac{\gamma\Gamma(n-\gamma)}{n!\Gamma(1-\gamma)} x^{\gamma-n}, \end{aligned} \tag{5.157}$$

since $(-1)^{2n-1} = -1$.

For $n \geq 2$ and $0 < \gamma \leq 1$ the term

$$\frac{\gamma\Gamma(n-\gamma)}{n!\Gamma(1-\gamma)} > 0,$$

is positive since the Gamma function is positive for positive arguments. Also the term $x^{\gamma-n} > 0$ is positive and so we then conclude that $g_1(x) < 0$.

By the second result of Lemma 5.5.2

$$g_2(x) = f(x+1) - f(x) < f(x) - f(x) = 0, \tag{5.158}$$

then $g_2(x) < 0$. Hence results (1) and (2) hold for $0 < \gamma < 1$. □

**Lemma 5.5.4.** For $0 < \gamma < 1$ given the weights $\mu_j(\gamma) = j^\gamma - (j-1)^\gamma$, for $j \geq 1$, and $\widetilde{\mu}_j(\gamma) = \left(j + \frac{3}{2}\right)^\gamma - \left(j + \frac{1}{2}\right)^\gamma$, for $j \geq 0$, then $\mu_j(\gamma)$ and $\widetilde{\mu}_j(\gamma)$ satisfy:

1. $\mu_j(\gamma) > 0$, where $j \geq 1$,
2. $\mu_j(\gamma) > \mu_{j+1}(\gamma)$, where $j \geq 1$,
3. $\widetilde{\mu}_j(\gamma) > 0$, where $j \geq 0$, and
4. $\widetilde{\mu}_j(\gamma) > \tilde{\mu}_{j+1}(\gamma)$, where $j \geq 0$.

*Proof.* Using results (1) and (2) from Lemma 5.5.2 with $x = j$, we find results (1) and (2) above hold. Similarly setting $x = j + \frac{3}{2}$ we find results (3) and (4) above hold from results (1) and (2) in Lemma 5.5.2. □

**Lemma 5.5.5.** For $j \geq 1$ and $0 < \gamma \leq 1$ given

$$\begin{aligned}
\widetilde{\alpha}_j(\gamma) &= \gamma\left(j + \frac{1}{2}\right)^{\gamma-1} - \left(j + \frac{1}{2}\right)^\gamma + \left(j - \frac{1}{2}\right)^\gamma, \\
\alpha_j(\gamma) &= \gamma j^{\gamma-1} - j^\gamma + (j-1)^\gamma, \\
\widetilde{\omega}_j(\gamma) &= \left(j + \frac{3}{2}\right)^\gamma - 2\left(j + \frac{1}{2}\right)^\gamma + \left(j - \frac{1}{2}\right)^\gamma,
\end{aligned}$$

and

$$\omega_j(\gamma) = (j+1)^\gamma - 2j^\gamma + (j-1)^\gamma$$

then the weights $\alpha_j(\gamma)$, $\widetilde{\alpha}_j(\gamma)$, $\omega_j(\gamma)$ and $\widetilde{\omega}_j(\gamma)$ are negative if $0 < \gamma < 1$ and zero otherwise.

*Proof.* Setting $x = j + \frac{1}{2}$ in results (1) and (2) of Lemma 5.5.3 we see $\alpha_j(\gamma) < 0$, and $\widetilde{\alpha}_j(\gamma) < 0$. Similarly by using Lemma 5.5.3 with $x = j$, we have from results (1), $\widetilde{\omega}_j(\gamma) < 0$ and from (2) $\omega_j(\gamma) < 0$.
If $\gamma = 1$ we have $\alpha_j(\gamma) = 0$, $\widetilde{\alpha}_j(\gamma) = 0$, $\widetilde{\omega}_j(\gamma) = 0$ and $\omega_j(\gamma) = 0$. □

**Proposition 5.5.6.** Let $\zeta_j$, where $j = 0, 1, 2, ..., M$, be the solution of Equation (5.139), then we have

$$\mid \zeta_j \mid \leq \mid \zeta_0 \mid, \tag{5.159}$$

if $0 \leq \Lambda_q \leq \min(1/\widetilde{\mu}_0(\gamma), 2^\gamma)$ and $0 < \gamma \leq 1$.

*Proof.* We use the mathematical induction method to prove the relation in Equation (5.159). For simplicity we assume $\zeta_0 > 0$. The case $\zeta_0 < 0$ can be handled in analogous manner to the method below.

Consider the case $j = 1$ in Equation (5.139), where we have

$$\begin{aligned}\zeta_1 &= \zeta_0 - \Lambda_q \gamma \left(\frac{1}{2}\right)^{\gamma-1} \zeta_0 \\ &= \left(1 - \Lambda_q \gamma \left(\frac{1}{2}\right)^{\gamma-1}\right) \zeta_0. \end{aligned} \tag{5.160}$$

First we note

$$1 - \Lambda_q \gamma \left(\frac{1}{2}\right)^{\gamma-1} \leq 1, \tag{5.161}$$

is automatically satisfied as the second term on the left is positive and so

$$\zeta_1 = \left(1 - \Lambda_q \gamma \left(\frac{1}{2}\right)^{\gamma-1}\right) \zeta_0 \leq \zeta_0. \tag{5.162}$$

We now consider the inequality

$$1 - \Lambda_q \gamma \left(\frac{1}{2}\right)^{\gamma-1} \geq -1, \tag{5.163}$$

which is satisfied if

$$\frac{2^\gamma}{\gamma} \geq \Lambda_q.$$

However since $0 < \gamma < 1$ and using Lemma 5.5.1 then Equation (5.163) is satisfied. We then have

$$\zeta_1 = \left(1 - \Lambda_q \gamma \left(\frac{1}{2}\right)^{\gamma-1}\right) \zeta_0 \geq -\zeta_0. \tag{5.164}$$

Hence for $0 < \gamma < 1$,

$$-\zeta_0 \leq \zeta_1 \leq \zeta_0, \tag{5.165}$$

or

$$| \zeta_1 | \leq | \zeta_0 | \tag{5.166}$$

and so Equation (5.159) is true for $j = 1$.

We now assume

$$-\zeta_0 \leq \zeta_n \leq \zeta_0, \text{ for } n = 1, 2, \ldots, k \tag{5.167}$$

and then need to show that

$$-\zeta_0 < \zeta_{k+1} < \zeta_0. \tag{5.168}$$

From Equation (5.142), we have

$$\zeta_{k+1} = [1 - \Lambda_q \widetilde{\mu}_0(\gamma)]\,\zeta_k - \Lambda_q \left\{ \widetilde{\alpha}_k(\gamma)\zeta_0 + \sum_{l=1}^{k-1} \widetilde{\omega}_{k-l}(\gamma)\zeta_l \right\}. \tag{5.169}$$

Note by using Lemma 5.5.5, we have $-\widetilde{\omega}_{j-k}(\gamma) > 0$ and $-\tilde{\alpha}_k(\gamma) > 0$. However the sign of the first term $(1 - \Lambda_q \widetilde{\mu}_0(\gamma))$ may be positive or negative and so we need to consider two cases when checking the stability.

These cases are

1. $(1 - \Lambda_q \widetilde{\mu}_0(\gamma)) \geq 0$, and $0 \leq \Lambda_q \leq 2^\gamma$, and
2. $(1 - \Lambda_q \widetilde{\mu}_0(\gamma)) \leq 0$, and $0 \leq \Lambda_q \leq 2^\gamma$.

The range of values of $\Lambda_q$ and $\gamma$ which satisfy each case is shown in Figure 5.2.

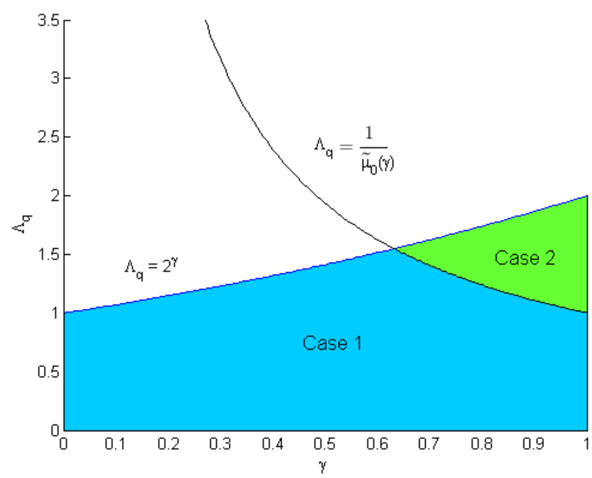



Figure 5.2: The range of values of $\Lambda_q$ and $\gamma$ for both cases to be considered when testing the stability of the KBMC2 scheme.

### Case 1

Case 1 occurs if the first term satisfies

$$(1 - \Lambda_q \widetilde{\mu}_0(\gamma)) \geq 0 \tag{5.170}$$

then we have, from Equations (5.167) and (5.169),

$$(1-\Lambda_q\widetilde{\mu}_0(\gamma))\,(-\zeta_0) \leq (1-\Lambda_q\widetilde{\mu}_0(\gamma))\,\zeta_k \leq (1-\Lambda_q\widetilde{\mu}_0(\gamma))\,\zeta_0, \tag{5.171}$$

$$\Lambda_q\,(-\widetilde{\alpha}_k(\gamma))\,(-\zeta_0) \leq \Lambda_q\,(-\widetilde{\alpha}_k(\gamma))\,\zeta_0 \leq \Lambda_q\,(-\widetilde{\alpha}_k(\gamma))\,\zeta_0, \tag{5.172}$$

and

$$\Lambda_q\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\,(-\zeta_0) \leq \Lambda_q\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\,\zeta_l \leq \Lambda_q\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\,\zeta_0. \tag{5.173}$$

Using these results, we have the expression for the upper bound for $\zeta_{k+1}$

$$\begin{aligned}\zeta_{k+1} &= (1-\Lambda_q\widetilde{\mu}_0(\gamma))\,\zeta_k - \Lambda_q\left\{\widetilde{\alpha}_k(\gamma)\zeta_0 + \sum_{l=1}^{k-1}\widetilde{\omega}_{k-l}(\gamma)\zeta_l\right\}\\ &\leq \left(1-\Lambda_q\widetilde{\mu}_0(\gamma)+\Lambda_q\,(-\widetilde{\alpha}_k(\gamma))+\Lambda_q\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\right)\zeta_0.\end{aligned} \tag{5.174}$$

Next we evaluate the summation, where $\widetilde{\omega}_j(\gamma)$ is given in Equation (5.144), to find

$$\begin{aligned}\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma)) &= \sum_{l=1}^{k-1}\left[\widetilde{\mu}_{k-l-1}(\gamma)-\widetilde{\mu}_{k-l}(\gamma)\right]\\ &= \sum_{n=1}^{k-1}\left[\widetilde{\mu}_{n-1}(\gamma)-\widetilde{\mu}_{n}(\gamma)\right]\\ &= \widetilde{\mu}_0(\gamma)-\widetilde{\mu}_{k-1}(\gamma).\end{aligned} \tag{5.175}$$

Using Equation (5.143) with the result in Equation (5.175), Equation (5.174) becomes

$$\zeta_{k+1} \leq \left(1-\Lambda_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}\right)\zeta_0. \tag{5.176}$$

Since the second term, in the brackets, is positive then $\zeta_{k+1}$ is bounded above by $\zeta_0$

$$\zeta_{k+1} \leq \left(1-\frac{\Lambda_q\gamma}{\left(k+\frac{1}{2}\right)^{1-\gamma}}\right)\zeta_0 \leq \zeta_0. \tag{5.177}$$

Considering the lower bound we have, after using Equations (5.171) – (5.173),

$$\begin{aligned}\zeta_{k+1} &= (1-\Lambda_q\widetilde{\mu}_0(\gamma))\,\zeta_k - \Lambda_q\left\{\widetilde{\alpha}_k(\gamma)\zeta_0 + \sum_{l=1}^{k-1}\widetilde{\omega}_{k-l}(\gamma)\zeta_l\right\}\\ &\geq \left(1-\Lambda_q\widetilde{\mu}_0(\gamma)+\Lambda_q\,(-\widetilde{\alpha}_k(\gamma))+\Lambda_q\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\right)(-\zeta_0).\end{aligned} \tag{5.178}$$

In a similar way, we obtain the inequality

$$\zeta_{k+1} \geq \left(1 - \Lambda_q \gamma \left(k + \frac{1}{2}\right)^{\gamma-1}\right)(-\zeta_0) = \left(\Lambda_q \gamma \left(k + \frac{1}{2}\right)^{\gamma-1} - 1\right)\zeta_0. \tag{5.179}$$

Since $0 < \gamma < 1$ and $\left(k + \frac{1}{2}\right)^{1-\gamma} > 0$ for $k \geq 0$ then

$$0 \leq \frac{\Lambda_q \gamma}{\left(k + \frac{1}{2}\right)^{1-\gamma}} \leq 2^{\gamma-1}\Lambda_q \gamma, \tag{5.180}$$

which satisfies

$$-1 \leq \frac{\Lambda_q \gamma}{\left(k + \frac{1}{2}\right)^{1-\gamma}} - 1 \leq 2^{\gamma-1}\Lambda_q \gamma - 1, \tag{5.181}$$

as $0 \leq \Lambda_q \leq 2$ and $0 < \gamma < 1$. We then have

$$\zeta_{k+1} \geq \left(\frac{\Lambda_q \gamma}{\left(k + \frac{1}{2}\right)^{1-\gamma}} - 1\right)\zeta_0 \geq -\zeta_0, \tag{5.182}$$

and so

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0 \quad \text{or} \quad |\zeta_{k+1}| \leq |\zeta_0|, \tag{5.183}$$

which shows Equation (5.159) is true for $j = k + 1$.

Hence if $0 \leq \Lambda_q \leq 2^\gamma$ and $(1 - \Lambda_q \widetilde{\mu}_0(\gamma)) > 0$ then Equation (5.159) is satisfied, for all $j \geq 0$ which means the numerical method is stable for this range of parameters.

**Case 2**

Case 2 occurs if

$$(1 - \Lambda_q \widetilde{\mu}_0(\gamma)) < 0. \tag{5.184}$$

We then have from Equations (5.167) and (5.169)

$$(1 - \Lambda_q \widetilde{\mu}_0(\gamma))\,\zeta_0 \leq (1 - \Lambda_q \widetilde{\mu}_0(\gamma))\,\zeta_k \leq (1 - \Lambda_q \widetilde{\mu}_0(\gamma))\,(-\zeta_0), \tag{5.185}$$

$$\Lambda_q\,(-\widetilde{\alpha}_k(\gamma))\,(-\zeta_0) \leq \Lambda_q\,(-\widetilde{\alpha}_k(\gamma))\,\zeta_0 \leq \Lambda_q\,(-\widetilde{\alpha}_k(\gamma))\,\zeta_0, \tag{5.186}$$

and

$$\Lambda_q \sum_{l=1}^{k-1} (-\widetilde{\omega}_{k-l}(\gamma))\,(-\zeta_0) \leq \Lambda_q \sum_{l=1}^{k-1} (-\widetilde{\omega}_{k-l}(\gamma))\,\zeta_l \leq \Lambda_q \sum_{l=1}^{k-1} (-\widetilde{\omega}_{k-l}(\gamma))\,\zeta_0. \tag{5.187}$$

Adding these equations we find

$$\zeta_{k+1} \leq (1 - \Lambda_q \widetilde{\mu}_0(\gamma))(-\zeta_0) + \Lambda_q (-\widetilde{\alpha}_k(\gamma))\zeta_0 + \Lambda_q \sum_{l=1}^{k-1} (-\widetilde{\omega}_{k-l}(\gamma))\zeta_0. \tag{5.188}$$

Then using the value of $\widetilde{\alpha}_k$, given in Equation (5.143), and the summation, given in Equation (5.175), in Equation (5.174) we obtain the inequality

$$\zeta_{k+1} \leq \left(2\Lambda_q \widetilde{\mu}_0(\gamma) - 1 - \Lambda_q \gamma \left(k + \frac{1}{2}\right)^{\gamma-1}\right)\zeta_0. \tag{5.189}$$

Considering the lower bound, we have

$$\zeta_{k+1} \geq (1 - \Lambda_q \widetilde{\mu}_0(\gamma))(\zeta_0) + \Lambda_q (-\widetilde{\alpha}_k(\gamma))(-\zeta_0) + \Lambda_q \sum_{l=1}^{k-1} (-\widetilde{\omega}_{k-l}(\gamma))(-\zeta_0). \tag{5.190}$$

Then, again using Equations (5.143) and (5.175), Equation (5.174) becomes

$$\zeta_{k+1} \geq \left(2\Lambda_q \widetilde{\mu}_0(\gamma) - 1 - \Lambda_q \gamma \left(k + \frac{1}{2}\right)^{\gamma-1}\right)(-\zeta_0). \tag{5.191}$$

Therefore $\zeta_{k+1}$ is bounded by

$$-\rho(\gamma, k, \Lambda_q)\zeta_0 \leq \zeta_{k+1} \leq \rho(\gamma, k, \Lambda_q)\zeta_0, \tag{5.192}$$

where

$$\rho(\gamma, k, \Lambda_q) = 2\Lambda_q \widetilde{\mu}_0(\gamma) - 1 - \Lambda_q \gamma \left(k + \frac{1}{2}\right)^{\gamma-1}. \tag{5.193}$$

Unlike Case 1, the value of $\rho(\gamma, k, \Lambda_q)$ is not bounded by 1 for all values of $\Lambda_q$, $k$ and $\gamma$, see Figure 5.3. As a result we cannot conclude from this analysis that the method is stable. However these bounds are lower and upper bounds on the actual values of $\zeta_k$ and the actual values of $\zeta_k$ may be indeed still satisfy Proposition 5.5.6.

In the next section we demonstrate the method is stable by evaluating the solution of the recurrence relationship in Equation (5.169) numerically.

Note if $\gamma = 1$ the solution of Equation (5.169) is

$$\zeta_k = (1 - \Lambda_q)^k \zeta_0, \tag{5.194}$$

which is bounded if $0 \leq \Lambda_q < 2$ for both Case 1 and Case 2. So proposition 5.5.6 is true if $\gamma = 1$. □

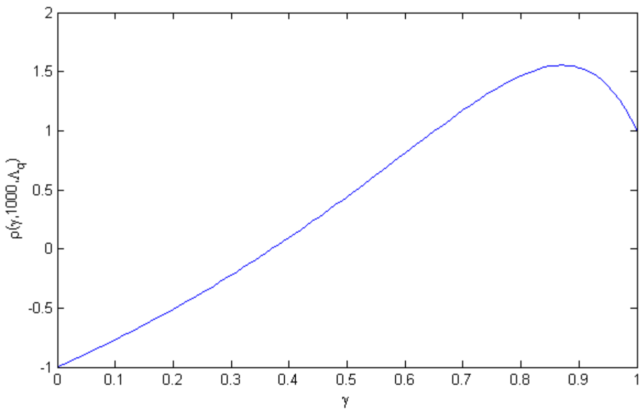



Figure 5.3: The predicted of $\rho(\gamma, k, \Lambda_q)$ for $\gamma = 0, 0.1, 0.2, \ldots, 1$, $k = 1000$ and $\Lambda_q = 2^\gamma$.

### 5.5.2 Numerical Solution of the Recurrence Relationship

In this section, we investigate the solution of the recurrence relationship in Equation (5.169) by numerical evaluation for both Case 1 and Case 2.

For Case 2 the value of $\gamma$ lies in the range $\log_3 2 \leq \gamma \leq 1$ where $\gamma = \log_3 2$ is the $\gamma$ value at the intersection of $\Lambda_q = 2^\gamma$ and $\Lambda_q = 1/\widetilde{\mu}_0(\gamma)$ curves. Figures 5.4, 5.5, and 5.6 show the results of simulating Equation (5.169) against $j$ for $0 \leq \gamma \leq 1$ with $\Lambda_q = 1/\widetilde{\mu}_0(\gamma)$, $\Lambda_q = 2^\gamma$, and $\Lambda_q = 2^{\log_3 2}$ respectively. We see from Figure 5.4 the value of the ratio $\zeta_j/\zeta_0$ decays quickly to zero but does undergo some initial oscillations. Meanwhile in Figure 5.5 we see the values of $\zeta_j/\zeta_0$ also oscillates but decays to zero if $0 < \gamma < 1$. We also see similar behavior when we choose $\Lambda_q = 2^{\log_3 2}$ as shown in Figure 5.6. Note though that in the case of $\gamma = 1$ we have the solution $\zeta_j/\zeta_0 = (1 - \Lambda_q)^j$, which for $\Lambda_q = 2$ will oscillate between $-1$ and 1 without decaying as shown in Figure 5.5.

For Case 1, shown in Figure 5.7, we give the results for $\Lambda_q = 1$ with $\gamma$ in the range $0 < \gamma \leq 1$ and $j = 0, \ldots, 100$. We see from Figure 5.7 the value of the ratio $\zeta_j/\zeta_0$ decays quickly to zero. We conclude that this method for $\Lambda_q = 1$ is stable as the ratio is positive and is less than 1, as expected.

The results in Figures 5.4, 5.5, 5.6 and 5.7 demonstrate this method is stable for both Case 1 and Case 2 as the values of $\zeta_j/\zeta_0$ do not grow but instead remain bounded above and below by 1 and $-1$ respectively.

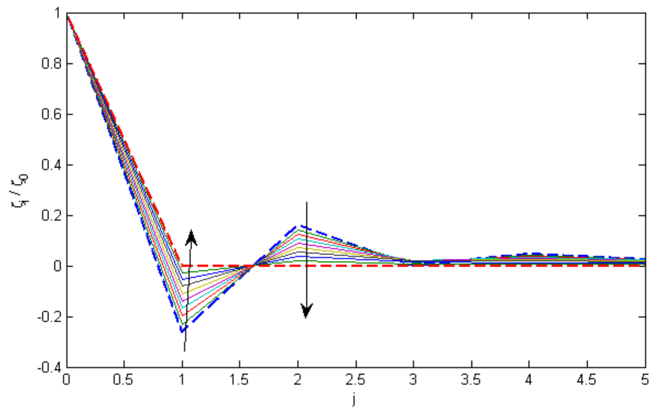



Figure 5.4: Case 2 the predicted ratios $\zeta_j/\zeta_0$ from Equation (5.169), with $\zeta_0 = 1$, for various of $\gamma$ is shown for $\Lambda_q = 1/\widetilde{\mu}_0(\gamma)$. Note the ratios $\zeta_j/\zeta_0$ for $j = 1, \ldots, 5$ and $\log_3 2 \leq \gamma \leq 1$ are bounded above by 1 and below by $-1$. The ratios for $\gamma = 0.1, 0.2, \ldots, 1$ decay to zero. Arrows show the direction of increasing $\gamma$.

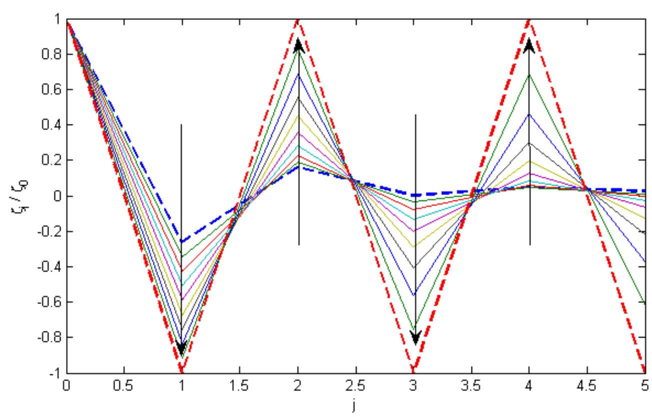



Figure 5.5: Case 2 the predicted ratios $\zeta_j/\zeta_0$ from Equation (5.169), with $\zeta_0 = 1$ for various of $\gamma$ is shown for $\Lambda_q = 2^\gamma$. Note the ratios $\zeta_j/\zeta_0$ for $j = 1, \ldots, 5$ and $\log_3 2 \leq \gamma \leq 1$ are bounded above by 1 and below by $-1$. The ratios for $\gamma = 0.1, 0.2, \ldots, 1$ decay to zero. Arrows show the direction of increasing $\gamma$.

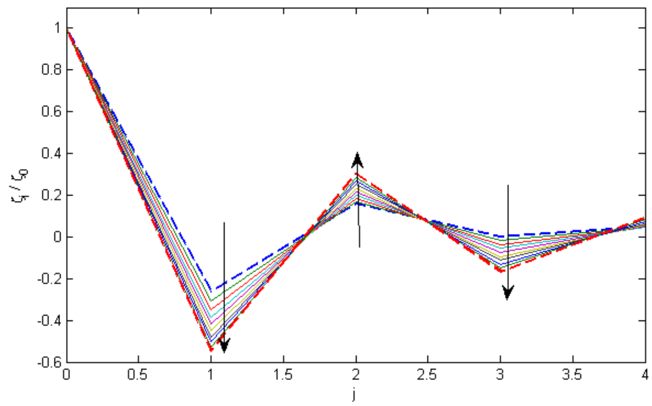



Figure 5.6: Ratios $\zeta_j/\zeta_0$ predicted by Equation (5.169) with $\zeta_0 = 1$ for various of $\gamma$ in Case 2 where $\Lambda_q = 2^{\log_3 2}$, $j = 1, \ldots, 4$ and $\log_3 2 \leq \gamma \leq 1$, the magnitude of the ratios is less than 1. The arrows show the direction of increasing $\gamma$.

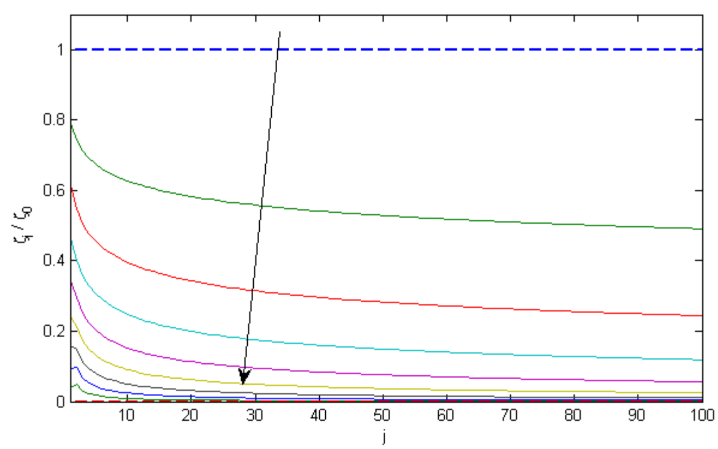



Figure 5.7: The predictions from Equation (5.169) of the ratio $\zeta_j/\zeta_0$ with $\zeta_0 = 1$ for various of $\gamma$ is shown for Case 1 where $\Lambda_q = 1$, $j = 1, \ldots, 100$ and $\gamma = 0, 0.1, 0.2, \ldots, 1$ . The arrow shows the direction of increasing $\gamma$.

### 5.5.3 Stability Analysis of the KBMC3 Scheme

In this section we investigate the stability of the KBMC3 scheme by using Von Neumann stability analysis. Similar to Section 5.5.1, we again let $u_i^j$ and $v_i^j$ be the approximate solution of the Equations (5.58) and (5.60), we then have

$$\left(u_i^j - u_{i-1}^j\right) = \frac{\Delta x_i}{2}\left(v_i^j + v_{i-1}^j\right), \tag{5.195}$$

and

$$\frac{u_i^{j+1}+u_{i-1}^{j+1}}{2\Delta t}=\frac{u_i^{j}+u_{i-1}^{j}}{2\Delta t}+\frac{D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\kappa_j(\gamma)\left(v_i^0-v_{i-1}^0\right)+\widehat{\alpha}_j(\gamma)\left(v_i^1-v_{i-1}^1\right)$$
$$+\frac{1}{2\Delta x_i}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[v_i^{k+1}-v_{i-1}^{k+1}-(v_i^{k-1}-v_{i-1}^{k-1})\right]\Bigg\}+[f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \qquad (5.196)$$

The errors, using Equations (5.24), (5.25), (5.131) as well as Equations (5.195) and (5.196) satisfy the equations

$$\left(\epsilon_i^j-\epsilon_{i-1}^j\right)-\frac{\Delta x_i}{2}\left(\varepsilon_i^j+\varepsilon_{i-1}^j\right)=0, \qquad (5.197)$$

and

$$\frac{\epsilon_i^{j+1}+\epsilon_{i-1}^{j+1}}{2\Delta t}=\frac{\epsilon_i^{j}+\epsilon_{i-1}^{j}}{2\Delta t}+\frac{D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\kappa_j(\gamma)\left(\varepsilon_i^0-\varepsilon_{i-1}^0\right)+\widehat{\alpha}_j(\gamma)\left(\varepsilon_i^1-\varepsilon_{i-1}^1\right)$$
$$+\frac{\sigma}{2\Delta x_i}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\varepsilon_i^{k+1}-\varepsilon_{i-1}^{k+1}-\left(\varepsilon_i^{k-1}-\varepsilon_{i-1}^{k-1}\right)\right]\Bigg\}, \qquad (5.198)$$

again with zero boundary conditions. We again omit the truncation errors (in Equations (5.197) and (5.198), however in the later section we will include them to show the convergence rate of the numerical method.

As before we let $\epsilon_i^j=\zeta_j e^{i'qx_i}$, and $\varepsilon_i^j=\xi_j e^{i'qx_i}$, where $i'$ is the imaginary number, $\sqrt{-1}$, $q$ is a real spatial wave number, Equations (5.197) and (5.198) can then be rewritten as

$$\left(\zeta_{j+1}e^{i'qx_i}-\zeta_{j+1}e^{i'q(x_i-\Delta x_i)}\right)=\frac{\Delta x_i}{2}\left(\xi_{j+1}e^{i'qx_i}+\xi_{j+1}e^{i'q(x_i-\Delta x_i)}\right), \qquad (5.199)$$

and

$$\frac{1}{2\Delta t}\left(\zeta_{j+1}e^{i'qx_i}+\zeta_{j+1}e^{i'q(x_i-\Delta x_i)}\right)=\frac{1}{2\Delta t}\left(\zeta_{j}e^{i'qx_i}+\zeta_{j}e^{i'q(x_i-\Delta x_i)}\right)$$
$$+\frac{D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\kappa_j(\gamma)\left(\xi_0e^{i'qx_i}-\xi_0e^{i'q(x_i-\Delta x_i)}\right)+\widehat{\alpha}_j(\gamma)\left(\xi_1e^{i'qx_i}-\xi_1e^{i'q(x_i-\Delta x_i)}\right)$$
$$+\frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\xi_{k+1}e^{i'qx_i}-\xi_{k+1}e^{i'q(x_i-\Delta x_i)}-\left(\xi_{k-1}e^{i'qx_i}-\xi_{k-1}e^{i'q(x_i-\Delta x_i)}\right)\right]\Bigg\}. \qquad (5.200)$$

Using Equation (5.199) and simplifying, we obtain the recursive equation for $\zeta_{j+1}$

$$\zeta_{j+1}=\zeta_j+\widehat{\rho}\left(\frac{1-e^{-i'w\Delta x_i}}{1+e^{-i'w\Delta x_i}}\right)^2\kappa_j(\gamma)\zeta_0+\widehat{\rho}\left(\frac{1-e^{-i'w\Delta x_i}}{1+e^{-i'w\Delta x_i}}\right)^2\widehat{\alpha}_j(\gamma)\zeta_1$$
$$+\frac{\widehat{\rho}}{2}\left(\frac{1-e^{-i'w\Delta x_i}}{1+e^{-i'w\Delta x_i}}\right)^2\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\zeta_{k+1}-\zeta_{k-1}\right], \qquad (5.201)$$

where $\widehat{\rho}$ is defined in Equation (5.137). Now using Equation (5.138) in Equation (5.201) gives the recurrence relation for $\zeta_{j+1}$

$$\zeta_{j+1} = \zeta_j - \text{Ų}_q \left[ \kappa_j(\gamma)\zeta_0 + \widehat{\alpha}_j(\gamma)\zeta_1 + \frac{1}{2}\sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma)\left(\zeta_{k+1} - \zeta_{k-1}\right) \right], \tag{5.202}$$

where the coefficient $\text{Ų}_q$ is defined in Equation (5.141), and the weights $\widehat{\alpha}_j(\gamma)$, $\widehat{\mu}_j(\gamma)$, and $\kappa_j(\gamma)$ are given earlier by Equations (5.55), (5.57), and (5.61) respectively.

When $j \geq 2$, the recurrence relation in Equation (5.202) can be rewritten as

$$\zeta_{j+1} = \frac{1}{1 + \frac{1}{2}\text{Ų}_q} \left\{ \left( 1 - \text{Ų}_q \left( \frac{2^\gamma - 1}{2} \right) \right) \zeta_j - \text{Ų}_q \left[ \varphi_{1_j}(\gamma)\zeta_0 + \varphi_{2_j}(\gamma)\zeta_1 + \sum_{k=2}^{j-1} \varphi_{3_{j-k}}(\gamma)\zeta_k \right] \right\}, \tag{5.203}$$

or

$$\zeta_{j+1} = \left( 1 - 2^{\gamma-1}\breve{\Lambda}_q \right) \zeta_j - \breve{\Lambda}_q \left[ \varphi_{1_j}(\gamma)\zeta_0 + \varphi_{2_j}(\gamma)\zeta_1 + \sum_{k=2}^{j-1} \varphi_{3_{j-k}}(\gamma)\zeta_k \right], \tag{5.204}$$

where the coefficient $\breve{\Lambda}_q$ is defined by

$$\breve{\Lambda}_q = \frac{\text{Ų}_q}{1 + \frac{1}{2}\text{Ų}_q}, \tag{5.205}$$

and the weights are defined as

$$\begin{aligned} \varphi_{1_j}(\gamma) &= \kappa_j(\gamma) - \frac{1}{2}\left(j^\gamma - (j-1)^\gamma\right) \\ &= \gamma\left(j + \frac{1}{2}\right)^{\gamma-1} - \left(j + \frac{1}{2}\right)^{\gamma} + j^\gamma - \frac{1}{2}\left(j^\gamma - (j-1)^\gamma\right), \end{aligned} \tag{5.206}$$

$$\begin{aligned} \varphi_{2_j}(\gamma) &= \widehat{\alpha}_j(\gamma) - \frac{1}{2}\left((j-1)^\gamma - (j-2)^\gamma\right) \\ &= \left(j + \frac{1}{2}\right)^{\gamma} - j^\gamma - \frac{1}{2}\left((j-1)^\gamma - (j-2)^\gamma\right), \end{aligned} \tag{5.207}$$

and

$$\varphi_{3_j}(\gamma) = \frac{1}{2}\left[(j+2)^\gamma - (j+1)^\gamma - j^\gamma + (j-1)^\gamma\right]. \tag{5.208}$$

Note for $0 \leq \text{Ų}_q < \infty$ then $\breve{\Lambda}_q$ in Equation (5.205) satisfies the inequality $0 \leq \breve{\Lambda}_q \leq 2$. We next consider lemma which will help in showing the stability of the KBMC3 method.

**Lemma 5.5.7.** The weights $\varphi_{1_j}(\gamma)$, $\varphi_{2_j}(\gamma)$ and $\varphi_{3_j}(\gamma)$ defined earlier in Equations (5.206), (5.207) and (5.208) respectively are negative if $0 < \gamma < 1$ or zero if $\gamma = 1$.

*Proof.* To show $\varphi_{1_j} < 0$, we first rewrite Equation (5.206) as

$$\begin{aligned}\varphi_{1_j}(\gamma) &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} - \left(j+\frac{1}{2}\right)^{\gamma} + j^{\gamma} - \frac{1}{2}\left(j^{\gamma}-(j-1)^{\gamma}\right)\\ &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} - \left(j+\frac{1}{2}\right)^{\gamma} + \left(\left(j+\frac{1}{2}\right)-\frac{1}{2}\right)^{\gamma} - \frac{1}{2}j^{\gamma} + \frac{1}{2}(j-1)^{\gamma}. \qquad (5.209)\end{aligned}$$

Now using the binomial expansion and simplifying, we have

$$\begin{aligned}\varphi_{1_j}(\gamma) &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} - \left(j+\frac{1}{2}\right)^{\gamma} + \left(j+\frac{1}{2}\right)^{\gamma} + \sum_{k=1}^{\infty}\binom{\gamma}{k}\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k}\\ &\qquad - \frac{1}{2}j^{\gamma} + \frac{1}{2}j^{\gamma} + \frac{1}{2}\sum_{k=1}^{\infty}\binom{\gamma}{k}(-1)^{k}j^{\gamma-k}\\ &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} + \sum_{k=1}^{\infty}\binom{\gamma}{k}\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}\sum_{k=1}^{\infty}\binom{\gamma}{k}(-1)^{k}j^{\gamma-k}\\ &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} + \sum_{k=1}^{\infty}\binom{\gamma}{k}\left[\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}(-1)^{k}j^{\gamma-k}\right]. \qquad (5.210)\end{aligned}$$

Using the result from Appendix B.2, we then have

$$\begin{aligned}\varphi_{1_j}(\gamma) &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} + \sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}(-1)^{k-1}\left[\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}(-1)^{k}j^{\gamma-k}\right]\\ &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} - \sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}\left[\left(\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}(-1)^{2k}j^{\gamma-k}\right]\\ &= \gamma\left(j+\frac{1}{2}\right)^{\gamma-1} - \frac{\gamma}{2}\left(j+\frac{1}{2}\right)^{\gamma-1} - \frac{\gamma}{2}j^{\gamma-1}\\ &\qquad - \sum_{k=2}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}\left[\left(\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}(-1)^{2k}j^{\gamma-k}\right]. \qquad (5.211)\end{aligned}$$

Now for $0 < \gamma \leq 1$ the term $\gamma\left(j+\frac{1}{2}\right)^{\gamma-1} \leq \gamma j^{\gamma-1}$, we then obtain the upper bound for the weight $\varphi_{1_j}(\gamma)$

$$\varphi_{1_j}(\gamma) < -\sum_{k=2}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}\left[\left(\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}(-1)^{2k}j^{\gamma-k}\right]. \qquad (5.212)$$

For $0 < \gamma \leq 1$ the binomial coefficient

$$\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)} > 0, \qquad (5.213)$$

is positive since the Gamma function for positive argument is positive.

The term $\left[\left(\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}(-1)^{2k}j^{\gamma-k}\right]$ is also positive $\forall k \geq 2$, we then conclude that for $0 < \gamma < 1$ $\varphi_{1_j}(\gamma) < 0$. If $\gamma = 1$ then $\varphi_{1_j}(\gamma) = 0$.

To show second, $\varphi_{2_j}(\gamma)$ is also negative, we rewrite Equation (5.207) as

$$\begin{aligned}\varphi_{2_j}(\gamma) &= \left(j+\frac{1}{2}\right)^{\gamma} - j^{\gamma} - \frac{1}{2}\left((j-1)^{\gamma} - (j-2)^{\gamma}\right)\\ &= \left(j+\frac{1}{2}\right)^{\gamma} - \left(\left(j+\frac{1}{2}\right)-\frac{1}{2}\right)^{\gamma} - \frac{1}{2}(j-1)^{\gamma} + \frac{1}{2}((j-1)-1)^{\gamma}\end{aligned} \tag{5.214}$$

and then use the binomial expansion of the second and fourth terms to find

$$\begin{aligned}\varphi_{2_j}(\gamma) &= \left(j+\frac{1}{2}\right)^{\gamma} - \left(j+\frac{1}{2}\right)^{\gamma} - \sum_{k=1}^{\infty}\binom{\gamma}{k}\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k}\\ &\qquad - \frac{1}{2}(j-1)^{\gamma} + \frac{1}{2}\sum_{k=1}^{\infty}\binom{\gamma}{k}(-1)^{k}(j-1)^{\gamma-k}\\ &= -\sum_{k=1}^{\infty}\binom{\gamma}{k}\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}\sum_{k=1}^{\infty}\binom{\gamma}{k}(-1)^{k}(j-1)^{\gamma-k}.\end{aligned} \tag{5.215}$$

Using Equation (B.7) in Equation (5.215), we then obtain

$$\begin{aligned}\varphi_{2_j}(\gamma) &= -\sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}(-1)^{k-1}\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} \qquad (5.216)\\ &\qquad + \frac{1}{2}\sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}(-1)^{2k-1}(j-1)^{\gamma-k}\\ &= \sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}(-1)^{k}\left(-\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} + \frac{1}{2}\sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}(-1)^{2k-1}(j-1)^{\gamma-k}\\ &= \sum_{k=1}^{\infty}\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)}\left[\left(\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} - (-1)^{2k}(j-1)^{\gamma-k}\right].\end{aligned}$$

For $j \geq 2$, the term

$$\begin{aligned}\left(\frac{1}{2}\right)^{k}\left(j+\frac{1}{2}\right)^{\gamma-k} - (-1)^{2k}(j-1)^{\gamma-k} &< \left(\frac{1}{2}\right)^{k}(j-1)^{\gamma-k} - (-1)^{2k}(j-1)^{\gamma-k}\\ &< (j-1)^{\gamma-k}\left(\left(\frac{1}{2}\right)^{k}-1\right),\end{aligned} \tag{5.217}$$

is bounded and since for $k \geq 1$, the term $\left(\frac{1}{2}\right)^{k} - 1 < 0$, we then conclude that the weight $\varphi_{2_j}(\gamma)$ for $0 < \gamma < 1$ is also negative. If $\gamma = 1$ then $\varphi_{2_j}(\gamma) = 0$.

Finally, by the second result in Lemma 5.5.4, we have

$$\mu_j(\gamma) > \mu_{j+1}(\gamma) > \mu_{j+2}(\gamma), \tag{5.218}$$

and then rewriting $\varphi_{3_j}(\gamma)$ in terms of $\mu_j(\gamma)$ we have

$$\varphi_{3_j}(\gamma) = \frac{1}{2}\left[\mu_{j+2}(\gamma) - \mu_j(\gamma)\right] < \frac{1}{2}\left[\mu_j(\gamma) - \mu_j(\gamma)\right] < 0, \tag{5.219}$$

which shows $\varphi_{3_j}(\gamma) < 0$ if $0 < \gamma < 1$. If $\gamma = 1$, then $\varphi_{3_j}(\gamma) = 0$. □

**Proposition 5.5.8.** Let $\zeta_j$, where $j = 1, 2, 3, ..., M$, be the solution of Equation (5.202), then we have

$$|\zeta_j| \leq |\zeta_0|, \tag{5.220}$$

if $0 \leq \breve{\Lambda}_q \leq 1$ and $0 < \gamma \leq 1$.

*Proof.* We use the mathematical induction method to prove the relation in Equation (5.220). For simplicity we assume $\zeta_0 > 0$. The case $\zeta_0 < 0$ can be handled in analogous manner to the method below.

Setting $j = 1$ in Equation (5.202), we find the value for $\zeta_1$

$$\begin{aligned}\zeta_1 &= \frac{1}{1 + \text{Ų}_q \left(\frac{1}{2}\right)^\gamma} \left[1 - \text{Ų}_q \left(\gamma \left(\frac{1}{2}\right)^{\gamma-1} - \left(\frac{1}{2}\right)^\gamma\right)\right] \zeta_0 \\ &= \left(1 - \frac{\text{Ų}_q \gamma \left(\frac{1}{2}\right)^{\gamma-1}}{1 + \text{Ų}_q \left(\frac{1}{2}\right)^\gamma}\right) \zeta_0 \\ &= \left(1 - \frac{2\gamma}{\frac{1}{\text{Ų}_q \left(\frac{1}{2}\right)^\gamma} + 1}\right) \zeta_0.\end{aligned} \tag{5.221}$$

The second term is positive and so $\zeta_1$ is bounded above by $\zeta_0$

$$\zeta_1 = \left(1 - \frac{2\gamma}{\frac{1}{\text{Ų}_q \left(\frac{1}{2}\right)^\gamma} + 1}\right) \zeta_0 \leq \zeta_0. \tag{5.222}$$

Since for $0 < \gamma \leq 1$ and $0 \leq \text{Ų}_q < \infty$, we also have

$$1 - \frac{2\gamma}{\frac{1}{\text{Ų}_q \left(\frac{1}{2}\right)^\gamma} + 1} \geq 1 - 2\gamma \geq -1, \tag{5.223}$$

and so

$$\zeta_1 = \left(1 - \frac{2\gamma}{\frac{1}{\text{Ų}_q \left(\frac{1}{2}\right)^\gamma} + 1}\right) \zeta_0 \geq -\zeta_0. \tag{5.224}$$

Combining the results in Equations (5.222) and (5.224), we have

$$-\zeta_0 \leq \left(1 - \frac{2\gamma}{\frac{1}{\text{Ų}_q \left(\frac{1}{2}\right)^\gamma} + 1}\right) \zeta_0 \leq \zeta_0, \tag{5.225}$$

and so $\zeta_1$ is bounded by

$$-\zeta_0 \leq \zeta_1 \leq \zeta_0, \tag{5.226}$$

or

$$|\zeta_1| \leq |\zeta_0|. \tag{5.227}$$

Hence Equation (5.220) is true for $j = 1$.

For $j = 2$, we have from Equation (5.202)

$$\zeta_2 = \zeta_1 - \text{Ų}_q \left\{ \left[ \gamma \left(\frac{3}{2}\right)^{\gamma-1} - \left(\frac{3}{2}\right)^{\gamma} + 1 \right] \zeta_0 + \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right) \zeta_1 + \frac{1}{2} \left[\zeta_2 - \zeta_0\right] \right\}, \tag{5.228}$$

which after simplifying becomes

$$\zeta_2 = \frac{1}{(1 + \frac{1}{2}\text{Ų}_q)} \left\{ \left[ 1 - \text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right) \right] \zeta_1 + \text{Ų}_q \left[ \left(\frac{3}{2}\right)^{\gamma} - \frac{1}{2} - \gamma \left(\frac{3}{2}\right)^{\gamma-1} \right] \zeta_0 \right\}. \tag{5.229}$$

For $0 \leq \text{Ų}_q < \infty$ and $0 < \gamma \leq 1$ the coefficient term of $\zeta_0$ obeys

$$0 \leq \frac{\text{Ų}_q}{1 + \frac{1}{2}\text{Ų}_q} \left[ \left(\frac{3}{2}\right)^{\gamma} - \frac{1}{2} - \gamma \left(\frac{3}{2}\right)^{\gamma-1} \right] \leq 1. \tag{5.230}$$

We also have

$$0 \leq \left( \frac{\text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right)}{1 + \frac{1}{2}\text{Ų}_q} \right) \leq 2 \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right) \leq 1, \tag{5.231}$$

and

$$0 \leq \frac{1}{1 + \frac{1}{2}\text{Ų}_q} \leq 1. \tag{5.232}$$

The coefficient of $\zeta_1$ then satisfies

$$1 \geq \frac{1 - \text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right)}{1 + \frac{1}{2}\text{Ų}_q} \geq 1 - 2 \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right) \geq 0. \tag{5.233}$$

From Equations (5.232) and (5.233), we conclude that

$$0 \leq \frac{1 - \text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right)}{1 + \frac{1}{2}\text{Ų}_q} \leq 1. \tag{5.234}$$

Now using Equation (5.226), the first term in Equation (5.229) satisfies

$$\left( \frac{1 - \text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right)}{1 + \frac{1}{2}\text{Ų}_q} \right) (-\zeta_0) \leq \left( \frac{1 - \text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right)}{1 + \frac{1}{2}\text{Ų}_q} \right) \zeta_1 \leq \left( \frac{1 - \text{Ų}_q \left( \left(\frac{3}{2}\right)^{\gamma} - 1 \right)}{1 + \frac{1}{2}\text{Ų}_q} \right) \zeta_0. \tag{5.235}$$

Equation (5.229) then becomes

$$\zeta_2 \leq \frac{1}{(1+\frac{1}{2}\text{Ų}_q)}\left\{1-\text{Ų}_q\left(\left(\frac{3}{2}\right)^{\gamma}-1\right)+\text{Ų}_q\left(\left(\frac{3}{2}\right)^{\gamma}-\frac{1}{2}-\gamma\left(\frac{3}{2}\right)^{\gamma-1}\right)\right\}\zeta_0, \quad (5.236)$$

which then simplifies to

$$\zeta_2 \leq \left(1-\frac{\text{Ų}_q\gamma\left(\frac{3}{2}\right)^{\gamma-1}}{(1+\frac{1}{2}\text{Ų}_q)}\right)\zeta_0. \quad (5.237)$$

The second term is positive and so $\zeta_2$ is bounded above by $\zeta_0$

$$\zeta_2 \leq \left(1-\frac{\text{Ų}_q\gamma\left(\frac{3}{2}\right)^{\gamma-1}}{(1+\frac{1}{2}\text{Ų}_q)}\right)\zeta_0 \leq \zeta_0. \quad (5.238)$$

Considering the lower bound, we have

$$\zeta_2 \geq \frac{1}{(1+\frac{1}{2}\text{Ų}_q)}\left\{1-\text{Ų}_q\left(\left(\frac{3}{2}\right)^{\gamma}-1\right)+\text{Ų}_q\left(\left(\frac{3}{2}\right)^{\gamma}-\frac{1}{2}-\gamma\left(\frac{3}{2}\right)^{\gamma-1}\right)\right\}(-\zeta_0). \quad (5.239)$$

In similar way, we obtain the inequality

$$\zeta_2 \geq \left(1-\frac{\text{Ų}_q\gamma\left(\frac{3}{2}\right)^{\gamma-1}}{(1+\frac{1}{2}\text{Ų}_q)}\right)(-\zeta_0) = \left(\frac{\text{Ų}_q\gamma\left(\frac{3}{2}\right)^{\gamma-1}}{(1+\frac{1}{2}\text{Ų}_q)}-1\right)\zeta_0. \quad (5.240)$$

Since $0 \leq \text{Ų}_q < \infty$, $0 < \gamma \leq 1$ and $\left(\frac{3}{2}\right)^{1-\gamma} > 0$ then

$$0 \leq \frac{\text{Ų}_q\gamma}{(1+\frac{1}{2}\text{Ų}_q)\left(\frac{3}{2}\right)^{1-\gamma}} \leq \frac{2\gamma}{\left(\frac{3}{2}\right)^{1-\gamma}} \leq 2, \quad (5.241)$$

and so we have

$$-1 \leq \frac{\text{Ų}_q\gamma\left(\frac{3}{2}\right)^{\gamma-1}}{(1+\frac{1}{2}\text{Ų}_q)}-1 \leq 1, \quad (5.242)$$

as $0 \leq \text{Ų}_q < \infty$, $0 < \gamma \leq 1$. We then have

$$\zeta_2 \geq \left(\frac{\text{Ų}_q\gamma\left(\frac{3}{2}\right)^{\gamma-1}}{(1+\frac{1}{2}\text{Ų}_q)}-1\right)\zeta_0 \geq -\zeta_0, \quad (5.243)$$

and so

$$-\zeta_0 \leq \zeta_2 \leq \zeta_0 \quad \text{or} \quad |\zeta_2| \leq |\zeta_0|, \quad (5.244)$$

and so Equation (5.220) is true for $j = 2$.

We now assume that

$$-\zeta_0 \leq \zeta_n \leq \zeta_0 \qquad \text{for} \qquad n = 1, 2, ..., k \quad (5.245)$$

and then need to show that

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0. \tag{5.246}$$

From (5.204) we have

$$\zeta_{k+1} = \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)\zeta_k - \breve{\Lambda}_q\left[\varphi_{1k}(\gamma)\zeta_0 + \varphi_{2k}(\gamma)\zeta_1 + \sum_{l=2}^{k-1}\varphi_{3k-l}(\gamma)\zeta_l\right]. \tag{5.247}$$

By using Lemma 5.5.7, we know $-\varphi_{1k}(\gamma) > 0$, $-\varphi_{2k}(\gamma) > 0$, and $-\varphi_{3k}(\gamma) > 0$, but the sign of the first term $\left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)$ may be positive or negative and so we consider two cases to check the stability, which are

1. $\left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) \geq 0$, and $0 \leq \breve{\Lambda}_q \leq 1$,
2. $\left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) \leq 0$, and $1 < \breve{\Lambda}_q \leq 2$.

**Case 1**

For $0 < \gamma \leq 1$ and $0 \leq \breve{\Lambda}_q \leq 1$ occurs when $1 - 2^{\gamma-1}\breve{\Lambda}_q > 0$. From Equations (5.245) and (5.247), we have

$$\left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)(-\zeta_0) \leq \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)\zeta_k \leq \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)\zeta_0, \tag{5.248}$$

$$\breve{\Lambda}_q\left(-\varphi_{1k}(\gamma)\right)(-\zeta_0) \leq \breve{\Lambda}_q\left(-\varphi_{1k}(\gamma)\right)\zeta_0 \leq \breve{\Lambda}_q\left(-\varphi_{1k}(\gamma)\right)\zeta_0, \tag{5.249}$$

$$\breve{\Lambda}_q\left(-\varphi_{2k}(\gamma)\right)(-\zeta_0) \leq \breve{\Lambda}_q\left(-\varphi_{2k}(\gamma)\right)\zeta_1 \leq \breve{\Lambda}_q\left(-\varphi_{2k}(\gamma)\right)\zeta_0, \tag{5.250}$$

and

$$\breve{\Lambda}_q\sum_{l=2}^{k-1}\left(-\varphi_{3k-l}(\gamma)\right)(-\zeta_0) \leq \breve{\Lambda}_q\sum_{l=2}^{k-1}\left(-\varphi_{3k-l}(\gamma)\right)\zeta_l \leq \breve{\Lambda}_q\sum_{l=2}^{k-1}\left(-\varphi_{3k-l}(\gamma)\right)\zeta_0. \tag{5.251}$$

Adding these equations, we then have

$$\begin{aligned}\zeta_{k+1} &= \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)\zeta_k - \breve{\Lambda}_q\left[\varphi_{1k}(\gamma)\zeta_0 + \varphi_{2k}(\gamma)\zeta_1 + \sum_{l=2}^{k-1}\varphi_{3k-l}(\gamma)\zeta_l\right] \\ &\leq \left\{1 - 2^{\gamma-1}\breve{\Lambda}_q + \breve{\Lambda}_q(-\varphi_{1k}(\gamma)) + \breve{\Lambda}_q(-\varphi_{2k}(\gamma)) + \breve{\Lambda}_q\sum_{l=2}^{k-1}\varphi_{3k-l}(\gamma)\right\}\zeta_0. \end{aligned} \tag{5.252}$$

Next we evaluate the summation, where $\varphi_{3_j}(\gamma)$ is given in Equation (5.208), we then find

$$\sum_{l=2}^{k-1}\left(-\varphi_{3_{k-l}}(\gamma)\right) = \frac{1}{2}\sum_{l=2}^{k-1}\left[(k-l)^{\gamma}-(k-l-1)^{\gamma}-(k-l+2)^{\gamma}+(k-l+1)^{\gamma}\right]$$
$$= \frac{1}{2}\left[(k-2)^{\gamma}-k^{\gamma}+2^{\gamma}\right]. \tag{5.253}$$

Then using Equations (5.206) and (5.207) with the result in Equation (5.253), Equation (5.252) becomes

$$\zeta_{k+1} \leq \Bigg\{1-2^{\gamma-1}\breve{\Lambda}_q+\breve{\Lambda}_q\left(\frac{1}{2}\left[k^{\gamma}-(k-1)^{\gamma}\right]+\left(k+\frac{1}{2}\right)^{\gamma}-k^{\gamma}-\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}\right)$$
$$+\breve{\Lambda}_q\left(\frac{1}{2}\left[(k-1)^{\gamma}-(k-2)^{\gamma}+k^{\gamma}-\left(k+\frac{1}{2}\right)^{\gamma}\right]\right)+\frac{1}{2}\left[(k-2)^{\gamma}-k^{\gamma}+2^{\gamma}\right]\breve{\Lambda}_q\Bigg\}\zeta_0. \tag{5.254}$$

Equation (5.254) simplifies to

$$\zeta_{k+1} \leq \left(1-\breve{\Lambda}_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}\right)\zeta_0. \tag{5.255}$$

Since the second term is positive then $\zeta_{k+1}$ is bounded above by $\zeta_0$

$$\zeta_{k+1} \leq \left(1-\breve{\Lambda}_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}\right)\zeta_0 \leq \zeta_0. \tag{5.256}$$

Considering the lower bound we have

$$\zeta_{k+1} = \left(1-2^{\gamma-1}\breve{\Lambda}_q\right)\zeta_k-\breve{\Lambda}_q\left[\varphi_{1_k}(\gamma)\zeta_0+\varphi_{2_k}(\gamma)\zeta_1+\sum_{l=2}^{k-1}\varphi_{3_{k-l}}(\gamma)\zeta_l\right]$$
$$\geq \left\{1-2^{\gamma-1}\breve{\Lambda}_q+\breve{\Lambda}_q(-\varphi_{1_k}(\gamma))+\breve{\Lambda}_q(-\varphi_{2_k}(\gamma))+\breve{\Lambda}_q\sum_{l=2}^{k-1}\varphi_{3_{k-l}}(\gamma)\right\}(-\zeta_0), \tag{5.257}$$

which simplifies to

$$\zeta_{k+1} \geq \left(1-\breve{\Lambda}_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}\right)(-\zeta_0) = \left(\breve{\Lambda}_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}-1\right)\zeta_0. \tag{5.258}$$

Since, for $0<\gamma<1$, $0\leq\breve{\Lambda}_q\leq 1$, and $k\geq 0$ we have $0<\left(k+\frac{1}{2}\right)^{1-\gamma}\leq 1$ then we have inequality

$$0 \leq \breve{\Lambda}_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1} \leq 1, \tag{5.259}$$

or

$$-1 \leq \breve{\Lambda}_q\gamma\left(k+\frac{1}{2}\right)^{\gamma-1}-1 \leq 0. \tag{5.260}$$

The lower bound of $\zeta_{k+1}$ is then

$$\zeta_{k+1} \geq \left( \breve{\Lambda}_q \gamma \left( k + \frac{1}{2} \right)^{\gamma - 1} - 1 \right) \zeta_0 \geq -\zeta_0 \tag{5.261}$$

and so

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0 \quad \text{or} \quad |\zeta_{k+1}| \leq |\zeta_0|. \tag{5.262}$$

Hence, if $0 \leq \breve{\Lambda}_q \leq 1$ and $\left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) \geq 0$, Equation (5.220) is satisfied for $j = k+1$, and hence for all $j \in \mathbb{N}$, which shows the numerical method is stable for this range of parameters.

**Case 2**

Case 2 occurs when $1 - 2^{\gamma-1}\breve{\Lambda}_q \leq 0$ given $0 < \gamma \leq 1$ and $1 < \breve{\Lambda}_q \leq 2$. Using Equations (5.245) and (5.247), we have the bounds

$$\left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) \zeta_0 \leq \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) \zeta_k \leq \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) (-\zeta_0), \tag{5.263}$$

$$\breve{\Lambda}_q \left(-\varphi_{1k}(\gamma)\right) (-\zeta_0) \leq \breve{\Lambda}_q \left(-\varphi_{1k}(\gamma)\right) \zeta_0 \leq \breve{\Lambda}_q \left(-\varphi_{1k}(\gamma)\right) \zeta_0, \tag{5.264}$$

$$\breve{\Lambda}_q \left(-\varphi_{2k}(\gamma)\right) (-\zeta_0) \leq \breve{\Lambda}_q \left(-\varphi_{2k}(\gamma)\right) \zeta_1 \leq \breve{\Lambda}_q \left(-\varphi_{2k}(\gamma)\right) \zeta_0, \tag{5.265}$$

and

$$\breve{\Lambda}_q \sum_{l=2}^{k-1} \left(-\varphi_{3k-l}(\gamma)\right) (-\zeta_0) \leq \breve{\Lambda}_q \sum_{l=2}^{k-1} \left(-\varphi_{3k-l}(\gamma)\right) \zeta_l \leq \breve{\Lambda}_q \sum_{l=2}^{k-1} \left(-\varphi_{3k-l}(\gamma)\right) \zeta_0. \tag{5.266}$$

Using these results, we find the upper bound for $\zeta_{k+1}$

$$\begin{aligned} \zeta_{k+1} &= \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right) \zeta_k - \breve{\Lambda}_q \left[ \varphi_{1k}(\gamma)\zeta_0 + \varphi_{2k}(\gamma)\zeta_1 + \sum_{l=2}^{k-1} \varphi_{3k-l}(\gamma)\zeta_l \right] \\ &\leq \left\{ 2^{\gamma-1}\breve{\Lambda}_q - 1 + \breve{\Lambda}_q(-\varphi_{1k}(\gamma)) + \breve{\Lambda}_q(-\varphi_{2k}(\gamma)) + \breve{\Lambda}_q \sum_{l=2}^{k-1} \varphi_{3k-l}(\gamma) \right\} \zeta_0. \end{aligned} \tag{5.267}$$

Using the weights in Equations (5.206) and (5.207), with the result in Equation (5.253), Equation (5.267) then becomes

$$\begin{aligned} \zeta_{k+1} \leq \Bigg\{ & 2^{\gamma-1}\breve{\Lambda}_q - 1 + \breve{\Lambda}_q \left( \frac{1}{2} \left[ k^\gamma - (k-1)^\gamma \right] + \left( k + \frac{1}{2} \right)^\gamma - k^\gamma - \gamma \left( k + \frac{1}{2} \right)^{\gamma-1} \right) \\ & + \breve{\Lambda}_q \left( \frac{1}{2} \left[ (k-1)^\gamma - (k-2)^\gamma + k^\gamma - \left( k + \frac{1}{2} \right)^\gamma \right] \right) + \frac{1}{2} \left[ (k-2)^\gamma - k^\gamma + 2^\gamma \right] \breve{\Lambda}_q \Bigg\} \zeta_0, \end{aligned} \tag{5.268}$$

which after simplifying becomes

$$\zeta_{k+1} \leq \left( \breve{\Lambda}_q 2^{\gamma} - 1 - \breve{\Lambda}_q \gamma \left( k + \frac{1}{2} \right)^{\gamma - 1} \right) \zeta_0. \tag{5.269}$$

Considering the lower bound we have

$$\begin{aligned} \zeta_{k+1} &= \left(1 - 2^{\gamma-1}\breve{\Lambda}_q\right)\zeta_k - \breve{\Lambda}_q \left[ \varphi_{1k}(\gamma)\zeta_0 + \varphi_{2k}(\gamma)\zeta_1 + \sum_{l=2}^{k-1} \varphi_{3k-l}(\gamma)\zeta_l \right] \\ &\geq \left\{ 2^{\gamma-1}\breve{\Lambda}_q - 1 + \breve{\Lambda}_q(-\varphi_{1k}(\gamma)) + \breve{\Lambda}_q(-\varphi_{2k}(\gamma)) + \breve{\Lambda}_q \sum_{l=2}^{k-1} \varphi_{3k-l}(\gamma) \right\} (-\zeta_0), \end{aligned} \tag{5.270}$$

which reduces to

$$\zeta_{k+1} \geq \left( \breve{\Lambda}_q 2^{\gamma} - 1 - \breve{\Lambda}_q \gamma \left( k + \frac{1}{2} \right)^{\gamma - 1} \right) (-\zeta_0). \tag{5.271}$$

Then $\zeta_{k+1}$ is bounded by

$$-\breve{\rho}_q(\gamma, k, \breve{\Lambda}_q)\zeta_0 \leq \zeta_{k+1} \leq \breve{\rho}(\gamma, k, \breve{\Lambda}_q)\zeta_0 \tag{5.272}$$

where

$$\breve{\rho}_q(\gamma, k, \breve{\Lambda}_q) = \breve{\Lambda}_q 2^{\gamma} - 1 - \breve{\Lambda}_q \gamma \left( k + \frac{1}{2} \right)^{\gamma - 1}. \tag{5.273}$$

The value of $\breve{\rho}(\gamma, k, \breve{\Lambda}_q)$ is not bounded by 1 for all values of $\breve{\Lambda}_q$, $k$ and $\gamma$ as shown in Figure 5.8. Unlike Case 1, we cannot conclude from this analysis that the method is stable. However these bounds are lower and upper bounds on the actual values of $\zeta_k$ and the actual values of $\zeta_k$ may be indeed still satisfy Proposition 5.5.8. In the next section we demonstrate the method is stable by evaluating the solution of the recurrence relationship in Equation (5.247) numerically. □

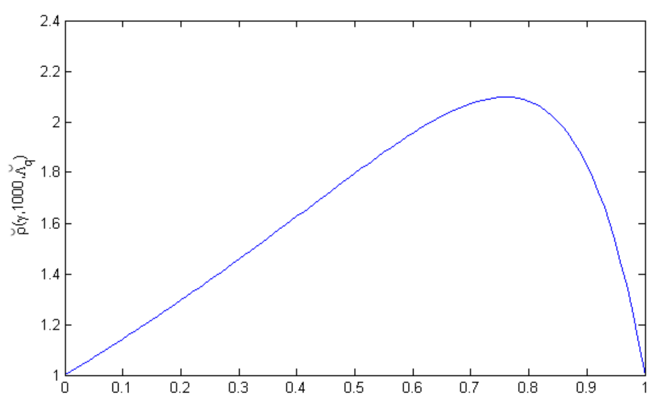



Figure 5.8: The predicted of $\breve{\rho}(\gamma, k, \breve{\Lambda}_q)$ for $\gamma = 0, 0.1, 0.2, \ldots, 1$, $k = 1000$ and $\breve{\Lambda}_q = 2$.

### 5.5.4 Numerical Solution of the Recurrence Relationship

Similar to method the KBMC2, we investigate the solution of the recurrence relationship in Equation (5.247) by numerical evaluation for both Case 1 and Case 2, where the value of $\gamma$ lies in the range $0 < \gamma \leq 1$ and the $0 < \breve{\Lambda}_q \leq 2$. For Case 1, these results are shown in Figure 5.9 for $j = 1, \ldots, 6$, $\gamma = 0.1, \ldots, 1$ and $\breve{\Lambda}_q = 1$. Similar results for Case 2 with $\breve{\Lambda}_q = 2$ and $\breve{\Lambda}_q = 2^{1-\gamma}$ are shown in Figures 5.10 and 5.11 respectively. From these results the KBMC3 method is stable for both Case 1 and Case 2 as the values of $\zeta_j/\zeta_0$ do not grow but instead remain bounded above and below by 1 and $-1$ respectively. Comparing Figures 5.9 and 5.10 we see if $\breve{\Lambda}_q = 1$ the ratios decay faster than if $\breve{\Lambda}_q = 2$.

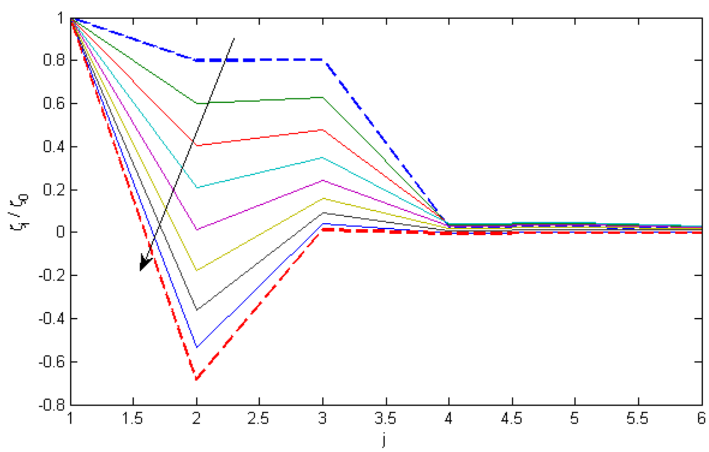



Figure 5.9: The predictions of the ratio $\zeta_j/\zeta_0$ found from Equation (5.247), with $\zeta_0 = 1$. Results are shown for Case 1, where $j = 1, \ldots, 6$, $\gamma = 0.1, \ldots, 0.9$ and $\breve{\Lambda}_q = 1$. Note the ratios $\zeta_j/\zeta_0$ is less than 1 where the value of $\gamma$ decreases in the direction of the arrow.

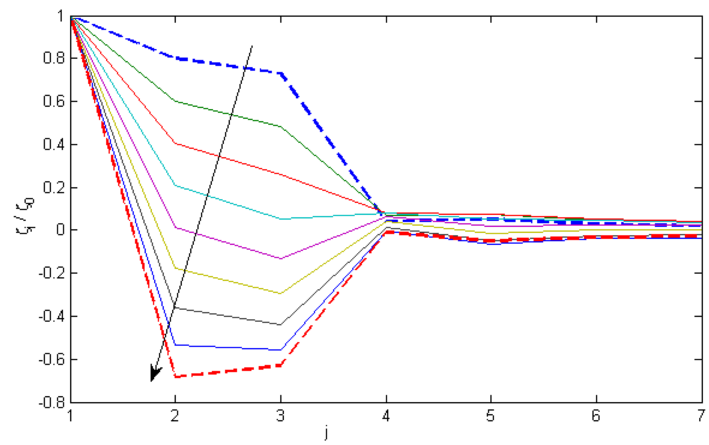



Figure 5.10: The predictions from Equation (5.247) of the ratio $\zeta_j/\zeta_0$ with $\zeta_0 = 1$ is shown for Case 2, where $\breve{\Lambda}_q = 2$. Note the ratios $\zeta_j/\zeta_0$ for $j = 1, \ldots, 7$, and $\gamma = 0.1, \ldots, 0.9$ is less than 1 and the value of $\gamma$ decreases in the direction of the arrow.

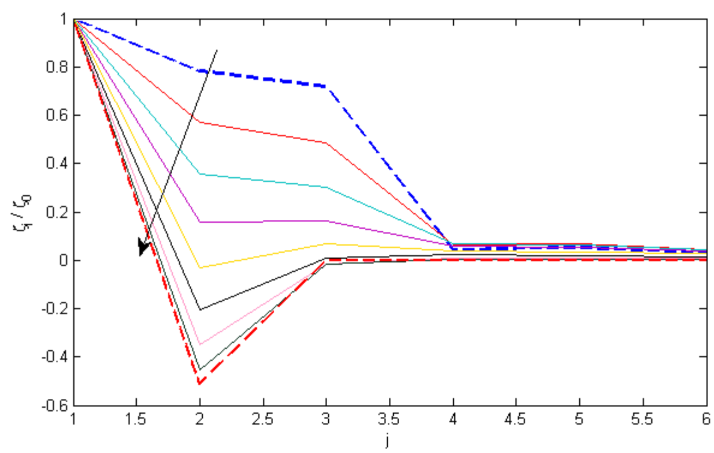



Figure 5.11: The predictions from Equation (5.247) of the ratio $\zeta_j/\zeta_0$ with $\zeta_0 = 1$ is shown for Case 2, where $\breve{\Lambda}_q = 2^{1-\gamma}$. Note the ratios $\zeta_j/\zeta_0$ for $j = 1, \ldots, 6$, and $\gamma = 0.1, \ldots, 0.9$. The value of $\gamma$ decreases in the direction of the arrow.

### 5.5.5 Stability Analysis of the KBML1 Scheme

In similar manner to Sections 5.5.1 and 5.5.3, we again use Von Neumann stability analysis to assess the stability of the KBML1 scheme. The recurrence equation for $\zeta_j$ using

Equation (5.71) is

$$\zeta_j = \zeta_{j-1} - Ų_q \left\{ \beta_j(\gamma)\zeta_0 + \sum_{k=0}^{j-1} \mu_{j-k}(\gamma) \left[\zeta_{k+1} - \zeta_k\right] \right\}, \tag{5.274}$$

which can be rewritten as

$$\zeta_j = \left(1 - \hat{\Lambda}_q\right) \zeta_{j-1} - \hat{\Lambda}_q \left[ \alpha_j(\gamma)\zeta_0 + \sum_{k=1}^{j-1} \omega_{j-k}(\gamma)\zeta_k \right], \tag{5.275}$$

where

$$\hat{\Lambda}_q = \frac{Ų_q}{1 + Ų_q}, \tag{5.276}$$

$0 \leq \hat{\Lambda}_q \leq 1$, and $Ų_q$ as defined in Equation (5.141). The weights are defined as

$$\alpha_j(\gamma) = \gamma j^{\gamma-1} - \mu_j(\gamma), \tag{5.277}$$

and

$$\omega_j(\gamma) = \mu_{j+1}(\gamma) - \mu_j(\gamma). \tag{5.278}$$

We now show the recurrence relationship in Equation (5.275) is stable.

**Proposition 5.5.9.** Let $\zeta_j$, where $j = 1, 2, 3, ..., M$, be the solution of Equation (5.275) then

$$|\zeta_j| \leq |\zeta_0|, \tag{5.279}$$

for all $0 < \hat{\Lambda}_q < 1$.

*Proof.* We use the mathematical induction to prove the relation in Equation (5.279). For simplicity we assume $\zeta_0 > 0$. Consider the case $j = 1$, we have from Equation (5.275)

$$\zeta_1 = \left(1 - \hat{\Lambda}_q \gamma\right) \zeta_0. \tag{5.280}$$

First we note the term in the bracket satisfies

$$1 - \hat{\Lambda}_q \gamma \leq 1, \tag{5.281}$$

as the second term is positive and so $\zeta_1$ is bounded above by $\zeta_0$

$$\zeta_1 = \left(1 - \hat{\Lambda}_q \gamma\right) \zeta_0 \leq \zeta_0. \tag{5.282}$$

Since $0 < \gamma \leq 1$ and $0 \leq \hat{\Lambda}_q \leq 1$ then

$$1 - \hat{\Lambda}_q \gamma \geq 1 - \gamma \geq 0 > -1, \tag{5.283}$$

and so

$$\zeta_1 = \left(1 - \hat{\Lambda}_q \gamma\right) \zeta_0 \geq -\zeta_0. \tag{5.284}$$

Hence for $0 \leq \gamma \leq 1$ we have

$$-\zeta_0 \leq \left(1 - \hat{\Lambda}_q \gamma\right) \zeta_0 \leq \zeta_0, \tag{5.285}$$

and so

$$-\zeta_0 \leq \zeta_1 \leq \zeta_0, \tag{5.286}$$

or

$$|\zeta_1| \leq |\zeta_0|. \tag{5.287}$$

Hence Equation (5.279) is satisfied for $j = 1$.

We now assume that

$$-\zeta_0 \leq \zeta_n \leq \zeta_0 \qquad \text{for} \qquad n = 1, 2, ..., k \tag{5.288}$$

and then need to show that

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0. \tag{5.289}$$

From Equation (5.275), we have

$$\zeta_{k+1} = \left(1 - \hat{\Lambda}_q\right) \zeta_k - \hat{\Lambda}_q \hat{\alpha}_{k+1}(\gamma)\zeta_0 - \hat{\Lambda}_q \sum_{l=1}^{k} \omega_{k-l+1}(\gamma)\zeta_l. \tag{5.290}$$

Note from Lemma 5.5.5 we have $-\alpha_{k+1} > 0$ and $-\omega_{j-k+1}(\gamma) > 0$. In addition for $0 \leq \hat{\Lambda}_q \leq 1$ the term $1 - \hat{\Lambda}_q \geq 0$. Using Equation (5.288), we then obtain the upper bound

$$\zeta_{k+1} \leq \left(1 - \hat{\Lambda}_q - \hat{\Lambda}_q \alpha_{k+1}(\gamma) - \hat{\Lambda}_q \sum_{l=1}^{k-1} \omega_{j-k+1}(\gamma)\right) \zeta_0. \tag{5.291}$$

Evaluating the summation of weights $\omega_{j-k+1}(\gamma)$ defined in Equation (5.278), we find

$$\sum_{l=1}^{k} \omega_{j-k+1}(\gamma) = (k+1)^\gamma - k^\gamma - 1. \tag{5.292}$$

Using this result and Equation (5.277) in Equation (5.291), we then find

$$\zeta_{k+1} \leq \left(1 - \hat{\Lambda}_q \gamma (k+1)^{\gamma-1}\right) \zeta_0. \tag{5.293}$$

Since the second term is positive then $\zeta_{k+1}$ is bounded above by $\zeta_0$

$$\zeta_{k+1} \leq \left(1 - \hat{\Lambda}_q \gamma (k+1)^{\gamma-1}\right) \zeta_0 \leq \zeta_0. \tag{5.294}$$

We now consider the lower bound. Since $-\zeta_0 \leq \zeta_n$ for $n = 1, \ldots, k$ then we also have

$$\zeta_{k+1} \geq \left(1 - \hat{\Lambda}_q - \hat{\Lambda}_q \alpha_{k+1}(\gamma) - \hat{\Lambda}_q \sum_{l=1}^{k-1} \omega_{j-k+1}(\gamma)\right) (-\zeta_0), \tag{5.295}$$

which, after simplifying, becomes

$$\zeta_{k+1} \geq -\left(1 - \hat{\Lambda}_q \gamma (k+1)^{\gamma-1}\right) \zeta_0. \tag{5.296}$$

Noting $0 \leq \hat{\Lambda}_q \leq 1$, $0 \leq \gamma \leq 1$ and $0 < (k+1)^{1-\gamma} \leq 1$ for $k \geq 1$, we have

$$0 \leq 1 - \hat{\Lambda}_q \gamma (k+1)^{\gamma-1} \leq 1. \tag{5.297}$$

We then have the lower bound

$$\zeta_{k+1} \geq -\left(1 - \hat{\Lambda}_q \gamma (k+1)^{\gamma-1}\right) \zeta_0 \geq -\zeta_0. \tag{5.298}$$

Therefore combining Equations (5.294) and (5.298), we then have

$$-\zeta_0 \leq \left(1 - \hat{\Lambda}_q \gamma (k+1)^{\gamma-1}\right) \zeta_0 \leq \zeta_0, \tag{5.299}$$

and so we obtain

$$-\zeta_0 \leq \zeta_{k+1} \leq \zeta_0. \tag{5.300}$$

Equation (5.279) is then true for $j = k + 1$ and hence for all $j \geq 1$. According to Von Neumann stability analysis the numerical method KBML1 is then unconditionally stable. □

### 5.5.6 Numerical Solution of the Recurrence Relationship

In this section again, by direct evaluation, we investigate the solution of the recurrence relationship in Equation (5.275), for the parameter values $\hat{\Lambda}_q = 1$ and $\hat{\Lambda}_q = 1/2$. Calculations were performed for $\gamma = 0.1, \ldots, 0.9$ and $j = 100$ time steps. These results are shown in Figures 5.12 and 5.13 for $\hat{\Lambda}_q = 1$ and $\hat{\Lambda}_q = 1/2$ respectively. From these results this method is stable as the ratio remains less than 1, as expected, and also remains positive, unlike the previous methods in this chapter. Comparing Figures 5.12 and 5.13 we see if $\hat{\Lambda}_q = 1$ the ratios decay faster than if $\hat{\Lambda}_q = 1/2$.

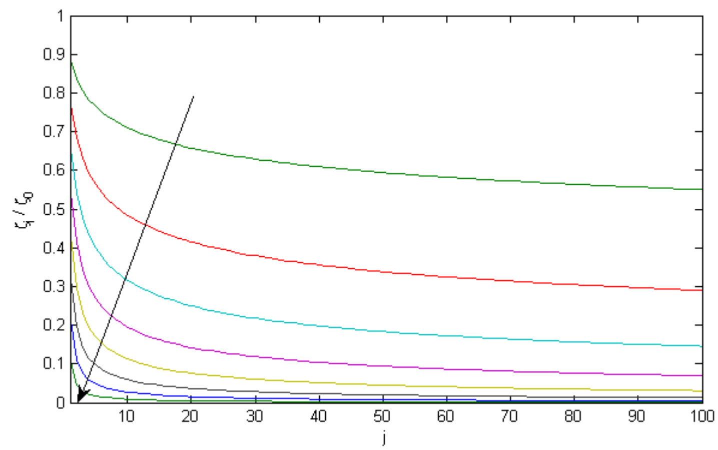



Figure 5.12: The ratio $\zeta_j/\zeta_0$ predictions from Equation (5.275) with $\zeta_0 = 1$ for $\gamma = 0.1, \ldots, 0.9$ and $\hat{\Lambda}_q = 1$. Note the ratios $\zeta_j/\zeta_0$ remain less than 1. The value of $\gamma$ decreases in the direction of the arrow.

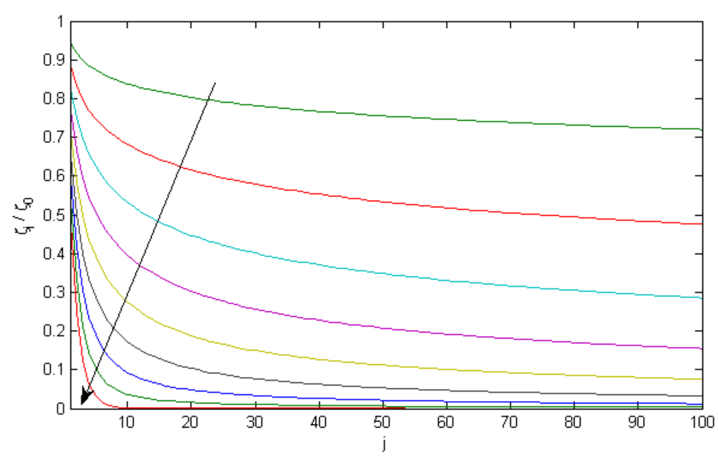



Figure 5.13: The ratio $\zeta_j/\zeta_0$ predictions from Equation (5.275), with $\zeta_0 = 1$, for $\gamma = 0.1, \ldots, 0.9$ and $\hat{\Lambda}_q = 1/2$. Note the ratios $\zeta_j/\zeta_0$, for $j = 1, \ldots, 100$ and $0 < \gamma \leq 1$, remain less than 1. The value of $\gamma$ decreases in the direction of the arrow.

## 5.6 Convergence of the Numerical Methods

In this section, the convergence of the numerical methods given by Equations (5.52), (5.70) and (5.88) is considered similar to Chapters 3 and 4. First we let the error

$$E_i^j = U_i^j - u_i^j, \tag{5.301}$$

where $i = 1, 2, \ldots, N$ and $j = 0, 1, 2, \ldots, M$, again we define the following grid functions

$$E^j(x) = \begin{cases} E_i^j & \text{if } x \in \left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right], \; i = 1, 2, \ldots, N, \\ 0 & \text{if } x \in \left[0, \frac{\Delta x}{2}\right] \bigcup \left(L - \frac{\Delta x}{2}, L\right], \end{cases} \tag{5.302}$$

and

$$R^j(x) = \begin{cases} R_i^j & \text{if } x \in \left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right], \; i = 1, 2, \ldots, N, \\ 0 & \text{if } x \in \left[0, \frac{\Delta x}{2}\right] \bigcup \left(L - \frac{\Delta x}{2}, L\right], \end{cases} \tag{5.303}$$

where $i = 1, 2, \ldots, N$. Then expanding $E_i^j$ and $R_i^j$ in Fourier series we have

$$E^j(x) = \sum_{l=-\infty}^{\infty} \xi_j(l) e^{i' 2\pi l x/L}, \qquad j = 0, 1, 2, \ldots, M, \tag{5.304}$$

and

$$R^j(x) = \sum_{l=-\infty}^{\infty} \eta_j(l) e^{i' 2\pi l x/L}, \qquad j = 0, 1, 2, \ldots, M, \tag{5.305}$$

where

$$\xi_j(l) = \frac{1}{L} \int_0^L E^j(x) e^{-i' 2\pi l x/L} dx, \tag{5.306}$$

and

$$\eta_j(l) = \frac{1}{L} \int_0^L R^j(x) e^{-i' 2\pi l x/L} dx. \tag{5.307}$$

Next we applied the Parseval identity (Spiegel 1965, Spiegel 1991), we then have

$$\|E^j\|_2 = \left( \sum_{i=1}^{N-1} \Delta x |E_i^j|^2 \right)^{\frac{1}{2}} = \left( \sum_{l=-\infty}^{\infty} |\xi_j(l)|^2 \right)^{\frac{1}{2}}, \qquad j = 0, 1, 2, \ldots, M, \tag{5.308}$$

and

$$\|R^j\|_2 = \left( \sum_{i=1}^{N-1} \Delta x |R_i^j|^2 \right)^{\frac{1}{2}} = \left( \sum_{l=-\infty}^{\infty} |\eta_j(l)|^2 \right)^{\frac{1}{2}}, \qquad j = 0, 1, 2, \ldots, M. \tag{5.309}$$

Now we assume that

$$E_i^j = \xi_j e^{i' q i \Delta x}, \tag{5.310}$$

and

$$R_i^j = \eta_j e^{i' q i \Delta x}, \tag{5.311}$$

where $q = 2\pi l/L$ is a real spatial wave number and $i'$ is the imaginary number, $i' = \sqrt{-1}$.

From Equation (5.301), we note that $E^0 = 0$, which satisfies the equation

$$\xi_0 = \xi_0(l) = 0. \tag{5.312}$$

By the convergence of the series on the right hand side (5.309) there is a positive constant $c_j$ such that

$$|\eta_j| \equiv |\eta_j(l)| \leq c_j |\eta_1| \equiv c_j |\eta_1(l)|, \qquad j = 1, 2, \ldots, M. \tag{5.313}$$

We then obtain

$$|\eta_j| \leq c|\eta_1(l)|, \qquad j = 1, 2, \ldots, M, \tag{5.314}$$

where

$$c = \max_{1 \leq j \leq M} \{c_j\}. \tag{5.315}$$

We will discuss the convergence of each scheme in the following sections.

### 5.6.1 Convergence of the KBMC2 Scheme

In this section, we will discuss the convergence of the KBMC2 scheme. In Equation (5.52) we define

$$\begin{aligned} R_i^{j+1} = {} & \frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right] + \frac{1}{\Delta t}\left[U_i^{j+1} - U_i^j\right] - \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] \\ & - \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^{\gamma}\left[\left(\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right) - 2\left(\delta_x^2 U_i^{j+\frac{1}{2}} - \delta_x^2 U_i^j\right)\right]\right\} \\ & - \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 U_i^0 + 2\left(\frac{1}{2}\right)^{\gamma}\left(\delta_x^2 U_i^{j+\frac{1}{2}} - \delta_x^2 U_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 U_i^k - \delta_x^2 U_i^{k-1}\right]\right\}. \end{aligned} \tag{5.316}$$

where $\delta_x^2 U_i^j$ is defined as in Equation (5.90), and according to C2 scheme, we note that

$$\left[\frac{d^{1-\gamma}f(t)}{dt^{1-\gamma}}\right|_{C2}^{j+\frac{1}{2}} = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)f_0 + 2\left(\frac{1}{2}\right)^{\gamma}\left(f_{j+\frac{1}{2}} - f_j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(f_k - f_{k-1}\right)\right\} + O(\Delta t^{1+\gamma}). \tag{5.317}$$

Now applying Equations (5.94) – (5.98) and (5.317), we then have

$$R_i^{j+1} = \left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - [f|_i^{j+\frac{1}{2}} + O(\Delta t^{1+\gamma} + \Delta x^2). \tag{5.318}$$

From Equation (5.318), we have

$$R_i^{j+1} = O(\Delta t^{1+\gamma} + \Delta x^2)\ , \tag{5.319}$$

where $i = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, M$, since $i, j$ are finite, there is a positive constant $c_1$ for all $i, j$ such that

$$|R_i^{j+1}| \le c_1(\Delta t^{1+\gamma} + \Delta x^2). \tag{5.320}$$

In Equation (5.316) we have

$$\Delta x^2\delta_x^2 U_i^{j+1} + 4U_i^{j+1} = \Delta x^2\delta_x^2 U_i^j + 4U_i^j + 2\Delta t\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] + 4\Delta t R_i^{j+1} \tag{5.321}$$
$$+ \frac{4D\Delta t^{\gamma}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 U_i^0 + \left(\frac{1}{2}\right)^{\gamma}\left(\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 U_i^k - \delta_x^2 U_i^{k-1}\right]\right\},$$

Subtracting Equation (5.52) from Equation (5.321), gives

$$\Delta x^2\delta_x^2 E_i^{j+1} + 4E_i^{j+1} = \Delta x^2\delta_x^2 E_i^j + 4E_i^j + 4\Delta t R_i^{j+1} \tag{5.322}$$
$$+ \frac{4D\Delta t^{\gamma}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 E_i^0 + \left(\frac{1}{2}\right)^{\gamma}\left(\delta_x^2 E_i^{j+1} - \delta_x^2 E_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 E_i^k - \delta_x^2 E_i^{k-1}\right]\right\}.$$

Using Equations (5.310) and (5.311) in (5.322), we then obtain

$$\xi_{j+1} = \xi_j - \widetilde{\lambda}_q\left\{\widetilde{\beta}_j(\gamma)\xi_0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\xi_k - \xi_{k-1}\right]\right\} + \frac{\Delta t\eta_{j+1}}{1 - V_q + V_q\left(\frac{1}{2}\right)^{\gamma}d}. \tag{5.323}$$

The coefficient $\widetilde{\lambda}_q$ is given by

$$\widetilde{\lambda}_q = \frac{V_q d}{1 - V_q + V_q\left(\frac{1}{2}\right)^{\gamma}d}, \tag{5.324}$$

where $d$ is as defined in Equation (5.53), and

$$V_q = \sin^2\left(\frac{q\Delta x}{2}\right). \tag{5.325}$$

When $j \geq 1$, Equation (5.323) can be rewritten as

$$\xi_{j+1} = \left[1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right] \xi_j - \widetilde{\lambda}_q \left\{ \widetilde{\alpha}_j(\gamma)\xi_0 + \sum_{k=1}^{j-1} \widetilde{\omega}_{j-k}(\gamma)\xi_k \right\} + \frac{\Delta t \eta_{j+1}}{1 - V_q + dV_q \left(\frac{1}{2}\right)^\gamma}, \quad (5.326)$$

where the weights $\widetilde{\alpha}_j(\gamma)$ and $\widetilde{\omega}_j(\gamma)$ are given in Equations (5.143) and (5.144) respectively.

**Lemma 5.6.1.** Given $0 < \gamma \leq 1$ and $0 \leq V_q d < \infty$ then the parameter $\widetilde{\lambda}_q$ given in Equation (5.324) is bounded by

$$0 \leq \widetilde{\lambda}_q \leq 2^\gamma. \quad (5.327)$$

*Proof.* From Equation (5.324), the term $\widetilde{\lambda}_q$ can be rewritten as

$$\widetilde{\lambda}_q = \frac{1}{\frac{1-V_q}{V_q d} + \left(\frac{1}{2}\right)^\gamma}. \quad (5.328)$$

For $0 < V_q \leq 1$ and $0 < V_q d < \infty$, we then have $0 < \frac{1-V_q}{V_q d} < \infty$. Consequently, we have the bound $0 \leq \widetilde{\lambda}_q \leq 2^\gamma$. □

**Proposition 5.6.2.** Let $\xi_j$ be the solution of Equation (5.323). Then there exists a positive constant $c_2$ such that

$$|\xi_j| \leq c_2 j \Delta t |\eta_1|, \qquad j = 1, 2, \ldots, M, \quad (5.329)$$

if $0 \leq \widetilde{\lambda}_q \leq \min(1/\widetilde{\mu}_0(\gamma), 2^\gamma)$ and $0 < \gamma \leq 1$.

*Proof.* From Equations (5.309) and (5.320), we obtain

$$\|R^j\|_2 \leq c_2 \sqrt{N\Delta x}(\Delta t^{1+\gamma} + \Delta x^2) = c_2\sqrt{L}(\Delta t^{1+\gamma} + \Delta x^2), \quad (5.330)$$

where $j = 1, 2, \ldots, M$. We use mathematical induction to prove the relation in Equation (5.329), and consider the case $j = 0$. From Equation (5.323) and using Equation (5.312), we have

$$\xi_1 = \frac{\Delta t}{1 - V_q + V_q d \left(\frac{1}{2}\right)^\gamma} \eta_1. \quad (5.331)$$

since $0 \leq V_q \leq 1$ and $d > 0$, we obtain

$$|\xi_1| \leq \frac{\Delta t}{1 - V_q + V_q d \left(\frac{1}{2}\right)^\gamma} |\eta_1| \leq \Delta t |\eta_1| \leq c_2 \Delta t |\eta_1|. \quad (5.332)$$

Suppose that

$$|\xi_n| \leq c_2 n\Delta t|\eta_1|, \qquad n = 1, 2, \ldots, k. \tag{5.333}$$

For $0 < \gamma < 1$ and $dV_q > 0$, from Equation (5.326), we have

$$\begin{aligned} |\xi_{k+1}| \leq & \left|1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right| |\xi_k| + \widetilde{\lambda}_q \left|-\widetilde{\alpha}_k(\gamma)\right| |\xi_0| + \widetilde{\lambda}_q \sum_{l=1}^{k-1} \left|-\widetilde{\omega}_{k-l}(\gamma)\right| |\xi_l| \\ & + \left|\frac{\Delta t}{1 - V_q + V_q d\left(\frac{1}{2}\right)^{\gamma}}\right| |\eta_{k+1}|. \end{aligned} \tag{5.334}$$

Now using Equations (5.312) and (5.333) into Equation (5.334), gives

$$|\xi_{k+1}| \leq c_2 \Delta t \left\{\left|1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right| k + \widetilde{\lambda}_q \sum_{l=1}^{k-1} l \left|-\widetilde{\omega}_{k-l}(\gamma)\right| + \left|\frac{1}{1 - V_q + V_q \left(\frac{1}{2}\right)^{\gamma} d}\right|\right\} |\eta_1|. \tag{5.335}$$

The sign of the first term $\left(1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right)$ may be positive or negative. Also for $0 < \gamma < 1$ and $V_q d > 0$, which is satisfied since

$$0 \leq \frac{1}{1 - V_q + V_q \left(\frac{1}{2}\right)^{\gamma} d} \leq 1. \tag{5.336}$$

By Lemma 5.5.5 the weight $\widetilde{\omega}_j(\gamma)$ is negative then $-\widetilde{\omega}_j(\gamma) > 0$, we then evaluate the summation in Equation (5.335) by

$$\begin{aligned} \sum_{l=1}^{k-1} l \left(-\widetilde{\omega}_{k-l}(\gamma)\right) &= \sum_{l=1}^{k-1} l \left[\widetilde{\mu}_{k-l-1}(\gamma) - \widetilde{\mu}_{k-l}(\gamma)\right] \\ &= \sum_{n=1}^{k-1} (k-n) \left[\widetilde{\mu}_{n-1}(\gamma) - \widetilde{\mu}_n(\gamma)\right] \\ &= k\left(\widetilde{\mu}_0(\gamma) - \widetilde{\mu}_{k-1}(\gamma)\right) - \left[\sum_{l=0}^{k-2} \widetilde{\mu}_l(\gamma) - (k-1)\widetilde{\mu}_{k-1}(\gamma)\right] \\ &= k\widetilde{\mu}_0(\gamma) - \left(k + \frac{1}{2}\right)^{\gamma} + \left(\frac{1}{2}\right)^{\gamma}. \end{aligned} \tag{5.337}$$

We need to consider two cases.

**Case 1**

Case 1 occurs if the first term satisfies

$$\left(1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right) \geq 0. \tag{5.338}$$

Using Equation (5.337) into Equation (5.335), we then have

$$|\xi_{k+1}| \leq c_2\Delta t \left\{ \left[1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right] k + \widetilde{\lambda}_q \left[k\widetilde{\mu}_0(\gamma) - \left(k + \frac{1}{2}\right)^\gamma + \left(\frac{1}{2}\right)^\gamma\right] + \frac{1}{1 - V_q + V_q d\left(\frac{1}{2}\right)^\gamma} \right\} |\eta_1|$$
$$\leq c_2\Delta t \left[k + \frac{1}{1 - V_q + V_q d\left(\frac{1}{2}\right)^\gamma}\right] |\eta_1| - c_2\Delta t \widetilde{\lambda}_q \left[\left(k + \frac{1}{2}\right)^\gamma - \left(\frac{1}{2}\right)^\gamma\right] |\eta_1|. \quad (5.339)$$

Since for $0 < \gamma \leq 1$ we have $\left(k + \frac{1}{2}\right)^\gamma - \left(\frac{1}{2}\right)^\gamma > 0$, and by using Equation (5.336), we then conclude that for $n = k + 1$

$$|\xi_{k+1}| \leq c_2\Delta t(k + 1)|\eta_1|. \quad (5.340)$$

Hence if $0 \leq \widetilde{\lambda}_q \leq 2^\gamma$ and $\left(1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right) \geq 0$ then Equation (5.329) is satisfied for all $j \geq 0$. The proof of the proposition is completed for case 1.

**Case 2**

Case 2 occurs if the first term satisfies

$$\left(1 - \widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)\right) \leq 0. \quad (5.341)$$

From Lemma 5.6.1 we have $0 \leq \widetilde{\lambda}_q \leq 2^\gamma$ and $0 < \gamma < 1$, then using Equation (5.337) in Equation (5.335), we then have

$$|\xi_{k+1}| \leq c_2\Delta t \left\{ \left[\widetilde{\lambda}_q \widetilde{\mu}_0(\gamma) - 1\right] k + \widetilde{\lambda}_q \left[k\widetilde{\mu}_0(\gamma) - \left(k + \frac{1}{2}\right)^\gamma + \left(\frac{1}{2}\right)^\gamma\right] + \frac{1}{1 - V_q + V_q d\left(\frac{1}{2}\right)^\gamma} \right\} |\eta_1|$$
$$\leq c_2\Delta t \left[2\widetilde{\lambda}_q \widetilde{\mu}_0(\gamma)k + \frac{1}{1 - V_q + V_q d\left(\frac{1}{2}\right)^\gamma}\right] |\eta_1| - c_2\Delta t \widetilde{\lambda}_q \left[\left(k + \frac{1}{2}\right)^\gamma - \left(\frac{1}{2}\right)^\gamma\right] |\eta_1|$$
$$\leq c_2\Delta t(2^{\gamma+1}\widetilde{\mu}_0(\gamma)k + 1)|\eta_1|, \quad (5.342)$$

since for $0 < \gamma \leq 1$ and $0 \leq \widetilde{\lambda}_q \leq 2^\gamma$, the term $0 < 2^{\gamma+1}\widetilde{\mu}_0(\gamma) \leq 4$. We then conclude that for $n = k + 1$

$$|\xi_{k+1}| \leq 4c_2\Delta t(k + 1)|\eta_1|, \quad (5.343)$$

but this does not satisfy the assumption in Equation (5.333) and so convergence in this case cannot be confirmed. □

### 5.6.2 Convergence of the KBMC3 Scheme

In this section similar to Section 5.6.1, we will discuss the convergence of the KBMC3 scheme, in Equation (5.70) we assume that

$$\begin{aligned} R_i^{j+1} &= \frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right] + \frac{1}{\Delta t}\left[U_i^{j+1} - U_i^j\right] - \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] \\ &- \frac{D\Delta t^{\gamma-1}\widehat{\alpha}_j(\gamma)}{\Gamma(1+\gamma)}\left[\delta_x^2 U_i^1 + \delta_x^2 U_i^0 - 2\delta_x^2 U_i^{\frac{1}{2}}\right] \\ &- \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\frac{1}{2}\left(\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^{k-1}\right) - \left(\delta_x^2 U_i^{k+\frac{1}{2}} - \delta_x^2 U_i^{k-\frac{1}{2}}\right)\right] \\ &- \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widehat{\beta}_j(\gamma)\delta_x^2 U_i^0 + 2\widehat{\alpha}_j(\gamma)\delta_x^2 U_i^{\frac{1}{2}} + \sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left(\delta_x^2 U_i^{k+\frac{1}{2}} - \delta_x^2 U_i^{k-\frac{1}{2}}\right)\right\}, \end{aligned} \tag{5.344}$$

where $\delta_x^2 U_i^j$ is given by Equation (5.90), and according to the C3 scheme, we have

$$\left[\frac{d^{1-\gamma}f(t)}{dt^{1-\gamma}}\right|_{C3}^{j+\frac{1}{2}} = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widehat{\beta}_j(\gamma)f_0 + 2\widehat{\alpha}_j(\gamma)f_{\frac{1}{2}} + \sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left(f_{k+\frac{1}{2}} - f_{k-\frac{1}{2}}\right)\right\} + O(\Delta t^{1+\gamma}). \tag{5.345}$$

Now using Equations (5.94) – (5.98) and (5.345), Equation (5.344) becomes

$$R_i^{j+1} = \left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - [f|_i^{j+\frac{1}{2}} + O(\Delta t^{1+\gamma} + \Delta x^2). \tag{5.346}$$

We then have

$$R_i^{j+1} = O(\Delta t^{1+\gamma} + \Delta x^2)\ , \tag{5.347}$$

where $i = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, M$, since $i, j$ are finite, there is a positive constant $c_1$ for all $i, j$ such that

$$|R_i^{j+1}| \le c_1(\Delta t^{1+\gamma} + \Delta x^2). \tag{5.348}$$

In Equation (5.344) we have

$$\begin{aligned} \Delta x^2\delta_x^2 U_i^{j+1} + 4U_i^{j+1} &= \Delta x^2\delta_x^2 U_i^j + 4U_i^j + 2\Delta t\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] \\ + \frac{4D\Delta t^\gamma}{\Gamma(1+\gamma)}&\left\{\kappa_j(\gamma)\delta_x^2 U_i^0 + \widehat{\alpha}_j(\gamma)\delta_x^2 U_i^1 + \frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^{k-1}\right]\right\} + 4\Delta t R_i^{j+1}, \end{aligned} \tag{5.349}$$

subtracting (5.70) from (5.349), gives

$$\begin{aligned} \Delta x^2\delta_x^2 E_i^{j+1} + 4E_i^{j+1} &= \Delta x^2\delta_x^2 E_i^j + 4E_i^j \\ + \frac{4D\Delta t^\gamma}{\Gamma(1+\gamma)}&\left\{\kappa_j(\gamma)\delta_x^2 E_i^0 + \widehat{\alpha}_j(\gamma)\delta_x^2 E_i^1 + \frac{1}{2}\sum_{k=1}^{j}\widehat{\mu}_{j-k}(\gamma)\left[\delta_x^2 E_i^{k+1} - \delta_x^2 E_i^{k-1}\right]\right\} + 4\Delta t R_i^{j+1}. \end{aligned} \tag{5.350}$$

Using Equations (5.310) and (5.311) in (5.350) gives

$$\xi_{j+1} = \xi_j - \widehat{\lambda}_q \left\{ \kappa_j(\gamma)\xi_0 + \widehat{\alpha}_j(\gamma)\xi_1 + \frac{1}{2}\sum_{k=1}^{j} \widehat{\mu}_{j-k}(\gamma)\left[\xi_{k+1} - \xi_{k-1}\right] \right\} + \frac{\Delta t \eta_{j+1}}{1 - V_q}, \quad (5.351)$$

where $V_q$ is given in Equation (5.325), and $\widehat{\lambda}_q$ is defined as

$$\widehat{\lambda}_q = \frac{V_q d}{1 - V_q}, \quad (5.352)$$

where $d$ is as define in Equation (5.53), for $V_q d > 0$ and $0 < V_q \leq 1$, then $\widehat{\lambda}_q > 0$. When $j \geq 2$, Equation (5.351) can be written as

$$\begin{aligned} \xi_{j+1} = & \frac{1}{1 + \widehat{\lambda}_q \widehat{\mu}_0(\gamma)/2} \Bigg\{ \left(1 - \widehat{\lambda}_q \widehat{\mu}_1(\gamma)/2\right) \xi_j - \widehat{\lambda}_q \Bigg[ \left(\kappa_j(\gamma) - \widehat{\mu}_{j-1}(\gamma)/2\right) \xi_0 \\ & + \left(\widehat{\alpha}_j(\gamma) - \widehat{\mu}_{j-2}(\gamma)/2\right) \xi_1 + \sum_{k=2}^{j-1} \varphi_{j-k}(\gamma)\xi_k \Bigg] + \Delta t \eta_{j+1} \Bigg\}, \end{aligned} \quad (5.353)$$

where the weights $\widehat{\alpha}_j(\gamma)$, $\widehat{\mu}_j(\gamma)$ and $\kappa_j(\gamma)$ are given in Equations (5.55), (5.57) and (5.61), and $\varphi_j(\gamma)$ is given in Equation (5.208).

**Proposition 5.6.3.** Let $\xi_j$ be the solution of Equation (5.351). Then there exists a positive constant $c_2$ such that

$$|\xi_j| \leq c_2 j \Delta t |\eta_1|, \qquad j = 1, 2, \ldots, M. \quad (5.354)$$

if $\widehat{\lambda}_q \leq 2/\widehat{\mu}_1(\gamma)$ and $0 < \gamma \leq 1$.

*Proof.* From Equations (5.309) and (5.348), we conclude that

$$\|R^j\|_2 \leq c_2 \sqrt{N \Delta x}(\Delta t + \Delta x^2) = c_2 \sqrt{L}(\Delta t + \Delta x^2), \quad (5.355)$$

where $j = 1, 2, \ldots, M$. We use mathematical induction to prove Equation (5.354). First start with $j = 0$, and then using Equation (5.312), Equation (5.351) becomes

$$\xi_1 = \frac{\Delta t}{(1 - V_q)(1 + \widehat{\lambda}_q \widehat{\alpha}_0(\gamma))} \eta_1. \quad (5.356)$$

since $\widehat{\alpha}_0(\gamma) = \left(\frac{1}{2}\right)^\gamma$, $0 \leq V_q < 1$ and $\widehat{\lambda}_q > 0$, we obtain

$$|\xi_1| \leq \frac{\Delta t}{(1 - V_q)\left(1 + \widehat{\lambda}_q \left(\frac{1}{2}\right)^\gamma\right)} |\eta_1| \leq \Delta t |\eta_1| \leq c_2 \Delta t |\eta_1|. \quad (5.357)$$

For $j = 1$, from Equation (5.351) and using Equation (5.356), we have

$$\begin{aligned}
\xi_2 &= \xi_1 - \widehat{\lambda}_q \left\{ \kappa_1(\gamma)\xi_0 + \widehat{\alpha}_1(\gamma)\xi_1 + \frac{1}{2}\sum_{k=1}^{1} \widehat{\mu}_{j-k}(\gamma)\left[\xi_{k+1} - \xi_{k-1}\right] \right\} + \frac{\Delta t}{1-V_q}\eta_2 \\
&= \left(1 - \widehat{\lambda}_q\widehat{\alpha}_1(\gamma)\right)\xi_1 - \frac{1}{2}\widehat{\lambda}_q\xi_2 + \frac{\Delta t}{1-V_q}\eta_2 \\
&= \left(1 - \widehat{\lambda}_q\widehat{\alpha}_1(\gamma)\right)\left(\frac{\Delta t}{(1-V_q)(1+\widehat{\lambda}_q\widehat{\alpha}_0(\gamma))}\right)\eta_1 - \frac{1}{2}\widehat{\lambda}_q\xi_2 + \frac{\Delta t}{1-V_q}\eta_2. \qquad (5.358)
\end{aligned}$$

Equation (5.358) simplifies to

$$|\xi_2| \leq \frac{\Delta t}{(1-V_q)\left(1+\frac{1}{2}\widehat{\lambda}_q\right)}\left\{\left|\frac{1-\widehat{\lambda}_q\widehat{\alpha}_1(\gamma)}{1+\widehat{\lambda}_q\widehat{\alpha}_0(\gamma))}\right| + c_2\right\}|\eta_1|. \qquad (5.359)$$

Now rewrite the term as

$$\frac{1-\widehat{\lambda}_q\widehat{\alpha}_1(\gamma)}{1+\widehat{\lambda}_q\widehat{\alpha}_0(\gamma))} = 1 - \frac{\widehat{\alpha}_1(\gamma)+\widehat{\alpha}_0(\gamma)}{\frac{1}{\widehat{\lambda}_q}+\widehat{\alpha}_0(\gamma)}, \qquad (5.360)$$

since $0 < \widehat{\lambda}_q < \infty$, then we have

$$0 < \frac{\widehat{\alpha}_1(\gamma)+\widehat{\alpha}_0(\gamma)}{\frac{1}{\widehat{\lambda}_q}+\widehat{\alpha}_0(\gamma)} < \frac{\widehat{\alpha}_1(\gamma)+\widehat{\alpha}_0(\gamma)}{\widehat{\alpha}_0(\gamma)}.$$

Now for $0 < \gamma \leq 1$, we have

$$\frac{\widehat{\alpha}_1(\gamma)+\widehat{\alpha}_0(\gamma)}{\widehat{\alpha}_0(\gamma)} = 1 + \frac{\widehat{\alpha}_1(\gamma)}{\widehat{\alpha}_0(\gamma)} < 2, \qquad (5.361)$$

where $\widehat{\alpha}_1(\gamma) = \left(\frac{3}{2}\right)^{\gamma} - 1$ and $\widehat{\alpha}_0(\gamma) = \left(\frac{1}{2}\right)^{\gamma}$, which is satisfies

$$1 > 1 - \frac{\widehat{\alpha}_1(\gamma)+\widehat{\alpha}_0(\gamma)}{\frac{1}{U_q}+\widehat{\alpha}_0(\gamma)} > -1,$$

we then obtain the bound of $\left|1 - \frac{\widehat{\alpha}_1(\gamma)+\widehat{\alpha}_0(\gamma)}{\frac{1}{U_q}+\widehat{\alpha}_0(\gamma)}\right| \leq 1$, and then we conclude that

$$|\xi_2| \leq \frac{(1+c_2)\Delta t}{(1-V_q)\left(1+\frac{1}{2}\widehat{\lambda}_q\right)}|\eta_1| \leq 2c_2\Delta t|\eta_1|, \qquad (5.362)$$

where for $0 < \widehat{\lambda}_q < \infty$ and $0 < V_q < 1$, we have $0 < \frac{1}{(1-V_q)\left(1+\frac{1}{2}\widehat{\lambda}_q\right)} < 1$.
Hence for $n = 2$ we have $|\xi_2| \leq 2c_2\Delta t|\eta_1|$.

Suppose that

$$|\xi_n| \leq c_2 n\Delta t|\eta_1|, \qquad n = 1, 2, \ldots, k. \qquad (5.363)$$

For $0 < \gamma < 1$ and $\widehat{\lambda}_q > 0$, from Equation (5.353) we then have

$$|\xi_{k+1}| \leq \frac{1}{1+\widehat{\lambda}_q\widehat{\mu}_0(\gamma)/2}\Bigg\{ \left|1-\widehat{\lambda}_q\widehat{\mu}_1(\gamma)/2\right| |\xi_k| + \widehat{\lambda}_q\,|\widehat{\mu}_{k-1}(\gamma)/2-\kappa_k(\gamma)|\,|\xi_0| + \widehat{\lambda}_q\,|\widehat{\mu}_{k-2}(\gamma)/2-\widehat{\alpha}_k(\gamma)|\,|\xi_1| + \widehat{\lambda}_q\sum_{l=2}^{k-1}|-\varphi_{k-l}(\gamma)||\xi_l| + \Delta t|\eta_{k+1}|\Bigg\}. \tag{5.364}$$

Now using Equations (5.312) and (5.363), we then have

$$|\xi_{k+1}| \leq \frac{c_2\Delta t}{1+\widehat{\lambda}_q\widehat{\mu}_0(\gamma)/2}\Bigg\{ \left|1-\widehat{\lambda}_q\widehat{\mu}_1(\gamma)/2\right| k + \widehat{\lambda}_q\,|\widehat{\mu}_{k-2}(\gamma)/2-\widehat{\alpha}_k(\gamma)| + \widehat{\lambda}_q\sum_{l=2}^{k-1} l|-\varphi_{k-l}(\gamma)| + 1\Bigg\}|\eta_1|. \tag{5.365}$$

The sign of the first term $1-\widehat{\lambda}_q\widehat{\mu}_1(\gamma)/2$ may be positive or negative. Also for $0<\gamma<1$ and $\widehat{\lambda}_q > 0$, we have $0 \leq \frac{1}{1+\widehat{\lambda}_q\widehat{\mu}_0(\gamma)/2} \leq 1$. From Lemma 5.5.7 we have $[\widehat{\mu}_{k-2}(\gamma)/2-\widehat{\alpha}_k(\gamma)] > 0$ and $\varphi_j(\gamma) < 0$, then $-\varphi_j(\gamma) > 0$, we then evaluate the summation to find

$$\begin{aligned}
\sum_{l=2}^{k-1} l\left(-\varphi_{k-l}(\gamma)\right) &= \frac{1}{2}\sum_{l=2}^{k-1} l\left[-(k-l+2)^\gamma + (k-l+1)^\gamma + (k-l)^\gamma - (k-l-1)^\gamma\right] \\
&= \frac{1}{2}\left[-\sum_{l=2}^{k-1} l(k-l+2)^\gamma + \sum_{l=2}^{k-1} l(k-l+1)^\gamma + \sum_{l=2}^{k-1} l(k-l)^\gamma - \sum_{l=2}^{k-1} l(k-l-1)^\gamma\right] \\
&= \frac{1}{2}\left[-\sum_{l=1}^{k-2}(k-l+1)^\gamma - k^\gamma + (k-1)2^\gamma + \sum_{l=3}^{k}(k-l)^\gamma + 2(k-2)^\gamma\right] \\
&= \frac{1}{2}\left[-2k^\gamma - (k-1)^\gamma + (k-2)^\gamma + 1 + 2^\gamma k\right].
\end{aligned} \tag{5.366}$$

We need to consider two cases.

### Case 1

Case 1 occurs if the first term satisfies

$$\left(1-\widehat{\lambda}_q\widehat{\mu}_1(\gamma)/2\right) \geq 0. \tag{5.367}$$

Using Equation (5.366) in Equation (5.365), we then have

$$
\begin{aligned}
|\xi_{k+1}| &\leq \frac{c_2\Delta t}{1+\widehat{\lambda}_q\frac{1}{2}}\left\{\left(1-\widehat{\lambda}_q\frac{1}{2}\left(2^\gamma-1\right)\right)k+\widehat{\lambda}_q\left[\frac{1}{2}\left((k-1)^\gamma-(k-2)^\gamma\right)-\left(\left(k+\frac{1}{2}\right)^\gamma-k^\gamma\right)\right]\right.\\
&\left.+\widehat{\lambda}_q\frac{1}{2}\left[-2k^\gamma-(k-1)^\gamma+(k-2)^\gamma+1+2^\gamma k\right]+1\right\}|\eta_1|\\
&= \frac{c_2\Delta t}{1+\widehat{\lambda}_q\frac{1}{2}}\left[k-\widehat{\lambda}_q\frac{1}{2}k-\widehat{\lambda}_q\left(k+\frac{1}{2}\right)^\gamma+\widehat{\lambda}_q\frac{1}{2}+1\right]|\eta_1|\\
&= \frac{c_2\Delta t}{1+\widehat{\lambda}_q\frac{1}{2}}\left[(k+1)\left(1+\widehat{\lambda}_q\frac{1}{2}\right)-\widehat{\lambda}_q\left(k+\left(k+\frac{1}{2}\right)^\gamma\right)\right]|\eta_1|\\
&\leq c_2\Delta t(k+1)|\eta_1|. \qquad (5.368)
\end{aligned}
$$

We then conclude that for $n=k+1$

$$|\xi_{k+1}| \leq c_2\Delta t(k+1)|\eta_1|, \qquad (5.369)$$

Hence all $j \geq 0$ if $\left(1-\widehat{\lambda}_q\widehat{\mu}_1(\gamma)/2\right) \geq 0$ then Equation (5.354) is satisfied. The proof of the proposition is completed for case 1.

**Case 2**

Case 2 occurs if the first term satisfies

$$\left(1-\widehat{\lambda}_q\widehat{\mu}_1(\gamma)/2)\right) \leq 0. \qquad (5.370)$$

As $0 \leq \widehat{\lambda}_q \leq 2^\gamma$ and $0<\gamma<1$, then using Equation (5.366) in Equation (5.365), we then have

$$
\begin{aligned}
|\xi_{k+1}| &\leq \frac{c_2\Delta t}{1+\widehat{\lambda}_q\frac{1}{2}}\left\{\left(\widehat{\lambda}_q\frac{1}{2}\left(2^\gamma-1\right)-1\right)k+\widehat{\lambda}_q\left[\frac{1}{2}\left((k-1)^\gamma-(k-2)^\gamma\right)-\left(\left(k+\frac{1}{2}\right)^\gamma-k^\gamma\right)\right]\right.\\
&\quad\left.+\widehat{\lambda}_q\frac{1}{2}\left[-2k^\gamma-(k-1)^\gamma+(k-2)^\gamma+1+2^\gamma k\right]+1\right\}|\eta_1|\\
&= \frac{c_2\Delta t}{1+\widehat{\lambda}_q\frac{1}{2}}\left[\widehat{\lambda}_q 2^\gamma k-\left(\widehat{\lambda}_q\frac{1}{2}+1\right)k-\widehat{\lambda}_q\left(k+\frac{1}{2}\right)^\gamma+\widehat{\lambda}_q\frac{1}{2}+1\right]|\eta_1|\\
&\leq c_2\Delta t\left[\left(\frac{\widehat{\lambda}_q 2^\gamma}{1+\widehat{\lambda}_q\frac{1}{2}}-1\right)k+1\right]|\eta_1|-c_2\Delta t\frac{\widehat{\lambda}_q\left(k+\frac{1}{2}\right)^\gamma}{1+\widehat{\lambda}_q\frac{1}{2}}|\eta_1|, \qquad (5.371)
\end{aligned}
$$

since for $0<\gamma\leq 1$ and $\widehat{\lambda}_q>0$ then the term $1 \leq \left(\frac{\widehat{\lambda}_q 2^\gamma}{1+\widehat{\lambda}_q\frac{1}{2}}-1\right) \leq 3$. We then conclude that

$$|\xi_{k+1}| \leq 2^{\gamma+1}c_2\Delta t(k+1)|\eta_1|. \qquad (5.372)$$

The result for the second case cannot satisfy Equation (5.354), since we obtain a constant which is bigger than the constant given in Equation (5.363). □

### 5.6.3 Convergence of the KBML1 Scheme

In this section similar to Sections 5.6.1 and 5.6.2, we will discuss the convergence of the KBMC3 scheme, in Equation (5.88) we assume that

$$R_i^j = \frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 U_i^j - \delta_x^2 U_i^{j-1}\right] + \frac{1}{\Delta t}\left[U_i^j - U_i^{j-1}\right] \tag{5.373}$$
$$- \frac{D\Delta t^\gamma}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\delta_x^2 U_i^0 + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^k\right)\right\} - \frac{1}{2}\left[f_{i-\frac{1}{2}}^j + f_{i+\frac{1}{2}}^j\right],$$

where $\delta_x^2 U_i^j$ is given by Equation (5.90), and according to the L1 scheme, we have

$$\left[\frac{d^{1-\gamma}f(t)}{dt^{1-\gamma}}\right|_{L1}^j = \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)f_0 + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[f_{k+1} - f_k\right]\right\} + O(\Delta t^{1+\gamma}). \tag{5.374}$$

Now using Equations (5.94), (5.95), (5.119) and (5.121), Equation (5.373) becomes

$$R_i^j = \left[\frac{\partial U}{\partial t}\right|_i^j - D\left[\frac{\partial^{1-\gamma}}{\partial^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^j - [f|_i^j + O(\Delta t + \Delta x^2). \tag{5.375}$$

We then have

$$R_i^j = O(\Delta t + \Delta x^2), \qquad i = 1, 2, \ldots, N, \qquad j = 1, 2, \ldots, M, \tag{5.376}$$

since $i, j$ are finite, there is a positive constant $c_1$ for all $i, j$ such that

$$|R_i^j| \leq c_1(\Delta t + \Delta x^2). \tag{5.377}$$

In Equation (5.373) we have

$$\Delta x^2\delta_x^2 U_i^j + 4U_i^j = \Delta x^2\delta_x^2 U_i^{j-1} + 4U_i^{j-1} + 2\Delta t\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] \tag{5.378}$$
$$+ \frac{4D\Delta t^\gamma}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\delta_x^2 U_i^0 + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(\delta_x^2 U_i^{k+1} - \delta_x^2 U_i^k\right)\right\} + 4\Delta t R_i^j.$$

Subtracting (5.88) from (5.378) gives

$$\Delta x^2\delta_x^2 E_i^j + 4E_i^j = \Delta x^2\delta_x^2 E_i^{j-1} + 4E_i^{j-1} \tag{5.379}$$
$$+ \frac{4D\Delta t^\gamma}{\Gamma(1+\gamma)}\left\{\beta_j(\gamma)\delta_x^2 E_i^0 + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left(\delta_x^2 E_i^{k+1} - \delta_x^2 E_i^k\right)\right\} + 4\Delta t R_i^j.$$

Using Equations (5.310) and (5.311) in (5.379), we then have

$$(1 - V_q)\xi_j = (1 - V_q)\xi_{j-1} - V_q d\left\{\beta_j(\gamma)\xi_0 + \sum_{k=0}^{j-1}\mu_{j-k}(\gamma)\left[\xi_{k+1} - \xi_k\right]\right\} + \Delta t\eta_j, \tag{5.380}$$

where $V_q$ is given by Equations (5.325). Equation (5.381) can be written as

$$\xi_j = \frac{1}{1 - V_q + V_q d}\left\{(1 - V_q)\xi_{j-1} - V_q d\left[\alpha_j(\gamma)\xi_0 + \sum_{k=1}^{j-1}\omega_{j-k}(\gamma)\xi_k\right] + \Delta t\eta_j\right\}, \quad (5.381)$$

where $j = 1, 2, \ldots, M$, and the weights $\alpha_j(\gamma)$, and $\omega_j(\gamma)$ are given in Equations (5.277) and (5.278) respectively.

**Proposition 5.6.4.** Let $\xi_j$ be the solution of Equation (5.381). Then there exists a positive constant $c_2$ such that

$$|\xi_j| \leq c_2 j\Delta t|\eta_1|, \qquad j = 1, 2, \ldots, M. \quad (5.382)$$

*Proof.* From Equations (5.309) and (5.377), we get

$$\|R^j\|_2 \leq c_2\sqrt{N\Delta x}(\Delta t + \Delta x^2) = c_2\sqrt{L}(\Delta t + \Delta x^2), \qquad j = 1, 2, \ldots, M. \quad (5.383)$$

We apply the mathematical induction to prove the relation given in (5.382). For $j = 0$, using Equation (5.312) in Equation (5.381), we then have

$$\xi_1 = \frac{\Delta t}{1 - V_q + V_q d}\eta_1, \quad (5.384)$$

since $0 < V_q < 1$ and $U_q > 0$, Equation (5.443) becomes

$$|\xi_1| \leq \frac{\Delta t}{1 - V_q + V_q d}|\eta_1| \leq \Delta t|\eta_1| \leq c_2\Delta t|\eta_1|. \quad (5.385)$$

Now suppose that

$$|\xi_n| \leq c_2 n\Delta t|\eta_1|, \qquad n = 1, 2, \ldots, k - 1. \quad (5.386)$$

For $0 < \gamma < 1$ and $U_q > 0$, from Equation (5.381), we have

$$|\xi_k| \leq \frac{1}{|1 - V_q + V_q d|}\left\{|1 - V_q||\xi_{k-1}| + V_q d\left[| - \alpha_k(\gamma)||\xi_0| + \sum_{l=1}^{k-1}| - \omega_{k-l}(\gamma)||\xi_l|\right] + \Delta t|\eta_k|\right\}. \quad (5.387)$$

Now using Equations (5.312) and (5.448), we then have

$$|\xi_k| \leq \frac{c_2\Delta t}{|1 - V_q + V_q d|}\left\{|1 - V_q|(k - 1) + V_q d\sum_{l=1}^{k-1} l| - \omega_{k-l}(\gamma)| + 1|\right\}|\eta_1|. \quad (5.388)$$

For $0 < \gamma < 1$, $0 < V_q < 1$ the term $0 < 1 - V_q \leq 1$, and for $V_q d > 0$, the term

$$0 \leq \frac{1}{1 - V_q + V_q d} \leq 1. \quad (5.389)$$

By Lemma 5.5.5 the weight $\omega_j(\gamma)$ is negative then $-\omega_j(\gamma) > 0$. Now evaluate the summation to find

$$\begin{aligned}\sum_{l=1}^{k-1} l\left(-\omega_{k-l}(\gamma)\right) &= \sum_{l=1}^{k-1} l\left[-(k-l+1)^{\gamma} + 2(k-l)^{\gamma} - (k-l-1)^{\gamma}\right] \\ &= 2\sum_{l=1}^{k-1}(k-l)l^{\gamma} - \sum_{l=2}^{k}(k-l+1)l^{\gamma} - \sum_{l=0}^{k-2}(k-l-1)l^{\gamma} \\ &= k - k^{\gamma}. \end{aligned} \tag{5.390}$$

Using Equation (5.390) in Equation (5.388), we then have

$$\begin{aligned}|\xi_k| &\le \frac{c_2\Delta t}{1 - V_q + V_q d}\left[(1-V_q)(k-1) + V_q d\,(k - k^{\gamma}) + 1\right]|\eta_1| \\ &= c_2\Delta t k|\eta_1| + \frac{r_1\Delta t\,(V_q - V_q d k^{\gamma})}{1 - V_q + V_q d}|\eta_1| \\ &\le c_2\Delta t k|\eta_1|. \end{aligned} \tag{5.391}$$

Since for $0 < \gamma < 1$, $0 < V_q \le 1$ and $V_q d > 0$, we have $-k^{\gamma} \le \frac{(V_q - V_q d\ k^{\gamma})}{1 - V_q + V_q d} < 0$. We then conclude that for $n = k$

$$|\xi_k| \le c_2 k\Delta t|\eta_1|. \tag{5.392}$$

Hence for all $n \in \mathbb{N}$ we have $|\xi_n| \le c_2 n\Delta t|\eta_1|$. The proof of the proposition is completed.

□

**Theorem 5.6.5.** Let $u(x,t) \in U(\Omega)$ be the exact solution for the fractional subdiffusion equation. Then the numerical scheme given by Equations (5.52), if $\widetilde{\lambda}_q = \min(\widetilde{\mu}_0(\gamma), 2^{\gamma})$, and (5.70), if $\widehat{\lambda}_q \le 2/\widehat{\mu}_1(\gamma)$, are convergent with order $O(\Delta t^{1+\gamma} + \Delta x^2)$ and Equation (5.88) is convergent with order $O(\Delta t + \Delta x^2)$.

*Proof.* Using Equations (5.308) and (5.309) with Equation (5.320) and Proposition 5.6.2 or with Equation (5.348) and Proposition 5.6.3, $j\Delta t \le T$, we then obtain

$$\|E^j\|_2 \le c_2\Delta t k\|R_1\| \le c_1c_2 j\Delta t\sqrt{L}(\Delta t^{1+\gamma} + \Delta x^2) \le C(\Delta t^{1+\gamma} + \Delta x^2), \tag{5.393}$$

but with Equation (5.377) and Proposition 5.6.4, $j\Delta t \le T$, gives the order

$$\|E^j\|_2 \le c_2 j\Delta t\|R_1\| \le c_1c_2 j\Delta t\sqrt{L}(\Delta t + \Delta x^2) \le C(\Delta t + \Delta x^2), \tag{5.394}$$

where $C = c_1c_2T\sqrt{L}$. □

## 5.7 Solution of Fractional Advection-Diffusion Equation (FADE) by the KBMC2 Scheme

### 5.7.1 Derivation of the Numerical Method for FADE

In this section a numerical scheme for solving Equation (5.17) will be developed based upon the Keller Box method and the C2 scheme approximation for the fractional derivative given in Equation (5.26). We refer to this approximation as the KBMC2-FADE scheme. Similar to the KBMC2 scheme in Section 5.2.1, we approximate Equation (5.17) at the point $\left(x_{i-\frac{1}{2}}, t_{j+\frac{1}{2}}\right)$ as

$$\left[\frac{\partial u}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial u}{\partial x}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f\left(x_{i-\frac{1}{2}}, t_{j+\frac{1}{2}}\right). \quad (5.395)$$

Using a similar process, as given in Section 5.2.1, we approximate the fractional derivative in Equation (5.395) using Equations (5.26) – (5.28), and then Equation (5.395) is replaced by the equation

$$\frac{u_i^j - u_{i-1}^j}{\Delta x_i} = \frac{v_i^j + v_{i-1}^j}{2}, \quad (5.396)$$

and

$$\begin{aligned}
\frac{u_i^{j+1} + u_{i-1}^{j+1}}{2\Delta t} - \frac{u_i^j + u_{i-1}^j}{2\Delta t} &= \frac{D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\widetilde{\beta}_j(\gamma)\left(v_i^0 - v_{i-1}^0\right) \\
&+ 2\left(\frac{1}{2}\right)^\gamma\left(\frac{v_i^j + v_i^{j+1}}{2} - \frac{v_{i-1}^j + v_{i-1}^{j+1}}{2}\right) - 2\left(\frac{1}{2}\right)^\gamma\left(v_i^j - v_{i-1}^j\right) \\
&+ \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[v_i^k - v_{i-1}^k - \left(v_i^{k-1} - v_{i-1}^{k-1}\right)\right]\Bigg\} + \frac{K_\gamma\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\Bigg\{\widetilde{\beta}_j(\gamma)\left(u_i^0 - u_{i-1}^0\right) \\
&+ 2\left(\frac{1}{2}\right)^\gamma\left(\frac{u_i^j + u_i^{j+1}}{2} - \frac{u_{i-1}^j + u_{i-1}^{j+1}}{2}\right) - 2\left(\frac{1}{2}\right)^\gamma\left(u_i^j - u_{i-1}^j\right) \\
&+ \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k - u_{i-1}^k - \left(u_i^{k-1} - u_{i-1}^{k-1}\right)\right]\Bigg\} + [f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \quad (5.397)
\end{aligned}$$

where the weights, $\widetilde{\beta}_j(\gamma)$ and $\widetilde{\mu}_{j-k}(\gamma)$, are as defined previously in Equations (5.27) and (5.28). Using Equation (5.396) in Equation (5.397) then gives an equation between $u_i$

and $v_i$

$$\frac{u_i^{j+1}+u_{i-1}^{j+1}}{2\Delta t}-\frac{K_\gamma \Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j+1}-u_{i-1}^{j+1}\right)=\frac{u_i^j+u_{i-1}^j}{2\Delta t}$$
$$+\frac{2D\Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left\{\frac{-\widetilde{\beta}_j(\gamma)}{\Delta x_i}\left(u_i^0-u_{i-1}^0\right)+\widetilde{\beta}_j(\gamma)v_i^0-\frac{1}{\Delta x_i}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^{j+1}-u_{i-1}^{j+1}\right)\right.$$
$$+\left(\frac{1}{2}\right)^{\gamma}v_i^{j+1}+\frac{1}{\Delta x_i}\left(\frac{1}{2}\right)^{\gamma}\left(u_i^j-u_{i-1}^j\right)-\left(\frac{1}{2}\right)^{\gamma}v_i^j+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_i^k-v_i^{k-1}\right)$$
$$\left.-\frac{1}{\Delta x_i}\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k-u_{i-1}^k-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]\right\}$$
$$+\frac{K_\gamma \Delta t^{\gamma-1}}{\Delta x_i \Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_i^0-u_{i-1}^0\right)-\left(\frac{1}{2}\right)^{\gamma}\left(u_i^j-u_{i-1}^j\right)\right.$$
$$\left.+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_i^k-u_{i-1}^k-\left(u_i^{k-1}-u_{i-1}^{k-1}\right)\right]\right\}+[f]\big|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{5.398}$$

Similarly by replacing $i$ by $i+1$ in Equation (5.396) and (5.397), we have the equations

$$\frac{u_{i+1}^j-u_i^j}{\Delta x_{i+1}}=\frac{v_{i+1}^j+v_i^j}{2}, \tag{5.399}$$

and

$$\frac{u_{i+1}^{j+1}+u_i^{j+1}}{2\Delta t}-\frac{u_{i+1}^j+u_i^j}{2\Delta t}=\frac{D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(v_{i+1}^0-v_i^0\right)\right.$$
$$+2\left(\frac{1}{2}\right)^{\gamma}\left(\frac{v_{i+1}^j+v_{i+1}^{j+1}}{2}-\frac{v_i^j+v_i^{j+1}}{2}\right)-2\left(\frac{1}{2}\right)^{\gamma}\left(v_{i+1}^j-v_i^j\right)$$
$$\left.+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[v_{i+1}^k-v_i^k-\left(v_{i+1}^{k-1}-v_i^{k-1}\right)\right]\right\}+\frac{K_\gamma \Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i+1}^0-u_i^0\right)\right.$$
$$+2\left(\frac{1}{2}\right)^{\gamma}\left(\frac{u_{i+1}^j+u_{i+1}^{j+1}}{2}-\frac{u_i^j+u_i^{j+1}}{2}\right)-2\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^j-u_i^j\right)$$
$$\left.+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^k-u_i^k-\left(u_{i+1}^{k-1}-u_i^{k-1}\right)\right]\right\}+[f]\big|_{i+\frac{1}{2}}^{j+\frac{1}{2}}. \tag{5.400}$$

Solving Equation (5.399) to find $v_{j+1}^{j}$ and then combining with Equation (5.400) gives a second equation involving $u_i$ and $v_i$

$$\frac{u_{i+1}^{j+1}+u_{i}^{j+1}}{2\Delta t}-\frac{2K_\gamma\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j+1}-u_{i}^{j+1}\right)=\frac{u_{i+1}^{j}+u_{i}^{j}}{2\Delta t}$$
$$+\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\frac{\widetilde{\beta}_j(\gamma)}{\Delta x_{i+1}}\left(u_{i+1}^{0}-u_{i}^{0}\right)-\widetilde{\beta}_j(\gamma)v_i^0+\frac{1}{\Delta x_{i+1}}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j+1}-u_{i}^{j+1}\right)\right.$$
$$-\left(\frac{1}{2}\right)^{\gamma}v_i^{j+1}-\frac{1}{\Delta x_{i+1}}\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j}-u_{i}^{j}\right)+\left(\frac{1}{2}\right)^{\gamma}v_i^j-\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(v_i^k-v_i^{k-1}\right)$$
$$\left.+\frac{1}{\Delta x_{i+1}}\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k}-u_{i}^{k}-\left(u_{i+1}^{k-1}-u_{i}^{k-1}\right)\right]\right\}+\frac{K_\gamma\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i+1}^{0}-u_{i}^{0}\right)\right.$$
$$\left.-\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j}-u_{i}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k}-u_{i}^{k}-\left(u_{i+1}^{k-1}-u_{i}^{k-1}\right)\right]\right\}+[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,. \tag{5.401}$$

Now multiplying Equation (5.398) by $\Delta x_i$ and Equation (5.401) by $\Delta x_{i+1}$, and adding the two gives the equation for $u_i^j$ at each grid point $i$ and time step $j$

$$\frac{\Delta x_i}{2\Delta t}\left[u_{i}^{j+1}+u_{i-1}^{j+1}\right]+\frac{\Delta x_{i+1}}{2\Delta t}\left[u_{i+1}^{j+1}+u_{i}^{j+1}\right]-\frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left[\left(u_{i+1}^{j+1}-u_{i}^{j+1}\right)\right.$$
$$\left.+\left(u_{i}^{j+1}-u_{i-1}^{j+1}\right)\right]+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left[\frac{1}{\Delta x_i}\left(u_{i}^{j+1}-u_{i-1}^{j+1}\right)-\frac{1}{\Delta x_{i+1}}\left(u_{i+1}^{j+1}-u_{i}^{j+1}\right)\right]$$
$$=\frac{\Delta x_i}{2\Delta t}\left[u_{i}^{j}+u_{i-1}^{j}\right]+\frac{\Delta x_{i+1}}{2\Delta t}\left[u_{i+1}^{j}+u_{i}^{j}\right]-\frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i}^{0}-u_{i-1}^{0}\right)\right.$$
$$\left.-\left(\frac{1}{2}\right)^{\gamma}\left(u_{i}^{j}-u_{i-1}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i}^{k}-u_{i-1}^{k}-\left(u_{i}^{k-1}-u_{i-1}^{k-1}\right)\right]\right\}$$
$$+\frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i}^{0}-u_{i-1}^{0}\right)-\left(\frac{1}{2}\right)^{\gamma}\left(u_{i}^{j}-u_{i-1}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i}^{k}-u_{i-1}^{k}\right.\right.$$
$$\left.\left.-\left(u_{i}^{k-1}-u_{i-1}^{k-1}\right)\right]\right\}+\frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i+1}^{0}-u_{i}^{0}\right)-\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j}-u_{i}^{j}\right)\right.$$
$$\left.+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k}-u_{i}^{k}-\left(u_{i+1}^{k-1}-u_{i}^{k-1}\right)\right]\right\}+\frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\left(u_{i+1}^{0}-u_{i}^{0}\right)\right.$$
$$\left.-\left(\frac{1}{2}\right)^{\gamma}\left(u_{i+1}^{j}-u_{i}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[u_{i+1}^{k}-u_{i}^{k}-\left(u_{i+1}^{k-1}-u_{i}^{k-1}\right)\right]\right\}$$
$$+\Delta x_i\,[f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,. \tag{5.402}$$

Equation (5.402) can be rewritten as

$$A_i u_{i+1}^{j+1}+D_i u_{i}^{j+1}+B_i u_{i-1}^{j+1}=C_i+\Delta x_i\,[f|_{i-\frac{1}{2}}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[f|_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,, \tag{5.403}$$

where

$$A_i = \frac{\Delta x_{i+1}}{2\Delta t} - \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)} \left(\frac{1}{2}\right)^\gamma - \frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)} \left(\frac{1}{2}\right)^\gamma, \tag{5.404}$$

$$B_i = \frac{\Delta x_i}{2\Delta t} - \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)} \left(\frac{1}{2}\right)^\gamma + \frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)} \left(\frac{1}{2}\right)^\gamma, \tag{5.405}$$

$$D_i = \frac{\Delta x_i + \Delta x_{i+1}}{2\Delta t} + \frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)} \left(\frac{1}{2}\right)^\gamma \left[\frac{1}{\Delta x_i} + \frac{1}{\Delta x_{i+1}}\right], \tag{5.406}$$

and

$$\begin{aligned} C_i &= A_i u_{i+1}^j + D_i u_i^j + B_i u_{i-1}^j + \widetilde{\beta}_j(\gamma)\left(a_i u_{i+1}^0 - c_i u_i^0 + b_i u_{i-1}^0\right) \\ &+ \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)(\gamma)\left[a_i u_{i+1}^k - c_i u_i^k + b_i u_{i-1}^k - \left(a_i u_{i+1}^{k-1} - c_i u_i^{k-1} + b_i u_{i-1}^{k-1}\right)\right]. \end{aligned} \tag{5.407}$$

In Equation (5.407) the constants, $a_i, b_i$, and $c_i$, are given by

$$a_i = \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)} + \frac{2D\Delta t^{\gamma-1}}{\Delta x_{i+1}\Gamma(1+\gamma)}, \tag{5.408}$$

$$b_i = \frac{2D\Delta t^{\gamma-1}}{\Delta x_i\Gamma(1+\gamma)} - \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)}, \tag{5.409}$$

and

$$c_i = \frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)} \left[\frac{1}{\Delta x_i} + \frac{1}{\Delta x_{i+1}}\right]. \tag{5.410}$$

In the case of constant grid spacing $\Delta x_i = \Delta x$, Equations (5.403) – (5.410) after simplifying, reduce to the equation

$$\begin{aligned} &\left(u_{i+1}^{j+1} + 2u_i^{j+1} + u_{i-1}^{j+1}\right) - \left(\frac{1}{2}\right)^\gamma \left[(d_1+d_2)\, u_{i+1}^{j+1} - 2d_1 u_i^{j+1} + (d_1-d_2)u_{i-1}^{j+1}\right] \\ &= \left(u_{i+1}^{j} + 2u_i^{j} + u_{i-1}^{j}\right) - \left(\frac{1}{2}\right)^\gamma \left[(d_1+d_2)\, u_{i+1}^{j} - 2d_1 u_i^{j} + (d_1-d_2)u_{i-1}^{j}\right] \\ &+ \widetilde{\beta}_j(\gamma)\left((d_1+d_2)u_{i+1}^0 - 2d_1 u_i^0 + (d_1-d_2)u_{i-1}^0\right) \\ &+ \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma)\Big[(d_1+d_2)u_{i+1}^k - 2d_1 u_i^k + (d_1-d_2)u_{i-1}^k \\ &- \left((d_1+d_2)u_{i+1}^{k-1} - 2d_1 u_i^{k-1} + (d_1-d_2)u_{i-1}^{k-1}\right)\Big] + 2\Delta t\left(f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right), \end{aligned} \tag{5.411}$$

where

$$d_1 = \frac{4D\Delta t^\gamma}{\Delta x^2\Gamma(1+\gamma)}, \qquad \text{and} \qquad d_2 = \frac{2K_\gamma \Delta t^\gamma}{\Delta x\Gamma(1+\gamma)}. \tag{5.412}$$

### 5.7.2 Accuracy of the Numerical Method

In this section, we consider the accuracy of the numerical scheme KBMC2-FADE method given by Equation (5.411). First we let

$$\triangle_x u_i^j = \frac{u_{i+1}^j - u_{i-1}^j}{2\Delta x}, \tag{5.413}$$

and then rewrite Equation (5.411) as

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] \\
&= \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right) - 2\left(\delta_x^2 u_i^{j+\frac{1}{2}} - \delta_x^2 u_i^j\right)\right]\right\} \\
&+ \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\triangle_x u_i^{j+1} - \triangle_x u_i^j\right) - 2\left(\triangle_x u_i^{j+\frac{1}{2}} - \triangle_x u_i^j\right)\right]\right\} \\
&+ \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 u_i^0 + 2\left(\frac{1}{2}\right)^\gamma\left(\delta_x^2 u_i^{j+\frac{1}{2}} - \delta_x^2 u_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 u_i^k - \delta_x^2 u_i^{k-1}\right]\right\} \\
&+ \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\triangle_x u_i^0 + 2\left(\frac{1}{2}\right)^\gamma\left(\triangle_x u_i^{j+\frac{1}{2}} - \triangle_x u_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\triangle_x u_i^k - \triangle_x u_i^{k-1}\right]\right\} \\
&+ \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right],
\end{aligned} \tag{5.414}$$

where $\delta_x^2 u_i^j$ is defined in Equation (5.90). Noting the terms on the fourth and fifth lines in Equation (5.414) as the C2 approximation (5.26) with $u(t)$ replaced by $\delta_x^2 u(t)$ and by $\triangle_x u(t)$ respectively, we can further rewrite Equation (5.414) as

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] = \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right)\right.\right. \\
&\left.\left.- 2\left(\delta_x^2 u_i^{j+\frac{1}{2}} - \delta_x^2 u_i^j\right)\right]\right\} + \frac{K_\gamma \Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\triangle_x u_i^{j+1} - \triangle_x u_i^j\right) - 2\left(\triangle_x u_i^{j+\frac{1}{2}} - \triangle_x u_i^j\right)\right]\right\} \\
&+ D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u_i\right)\Big|_{C2,i}^{j+\frac{1}{2}} + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\triangle_x u_i\right)\Big|_{C2,i}^{j+\frac{1}{2}} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right].\right.\right.
\end{aligned} \tag{5.415}$$

Adding and subtracting the exact fractional derivative, Equation (5.415) becomes

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right] + \frac{1}{\Delta t}\left[u_i^{j+1} - u_i^j\right] = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial u}{\partial x}\right)\right|_i^{j+\frac{1}{2}} \\
&\quad + \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\delta_x^2 u_i^{j+1} - \delta_x^2 u_i^j\right) - 2\left(\delta_x^2 u_i^{j+\frac{1}{2}} - \delta_x^2 u_i^j\right)\right]\right\} \\
&\quad + \frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\triangle_x u_i^{j+1} - \triangle_x u_i^j\right) - 2\left(\triangle_x u_i^{j+\frac{1}{2}} - \triangle_x u_i^j\right)\right]\right\} \\
&\quad + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 u_i\right)\right|_{C2,i}^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} \\
&\quad + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\triangle_x u_i\right)\right|_{C2,i}^{j+\frac{1}{2}} - K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial u}{\partial x}\right)\right|_i^{j+\frac{1}{2}} + \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right]. \qquad (5.416)
\end{aligned}$$

Taking the Taylor series expansion around the point $x_i = i\Delta x$ in space, we have

$$\triangle_x U_i^j \simeq \left[\frac{\partial U}{\partial x}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^3 U}{\partial x^3}\right|_i^j + O(\Delta x^4). \qquad (5.417)$$

Also expanding the Taylor series around the point $(x_i, t_{j+\frac{1}{2}})$, we find

$$\triangle_x U_i^{j+1} + \triangle_x U_i^j - 2\triangle_x U_i^{j+\frac{1}{2}} \simeq \frac{\Delta t^2}{4}\left[\frac{\partial^3 U}{\partial x \partial t^2}\right|_i^{j+\frac{1}{2}} + \frac{\Delta x^2 \Delta t^2}{48}\left[\frac{\partial^5 U}{\partial x^3 \partial t^2}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4). \qquad (5.418)$$

Using Equations (5.94) – (5.98), and Equations (5.417) and (5.418) in Equation (5.416), we then have

$$\begin{aligned}
\left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) + O(\Delta x^2) \\
&\quad + \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^\gamma\left[\frac{\Delta t^2}{4}\left[\frac{\partial^4 U}{\partial x^2 \partial t^2}\right|_i^{j+\frac{1}{2}} + \frac{\Delta x^2 \Delta t^2}{48}\left[\frac{\partial^6 U}{\partial x^4 \partial t^2}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right] \\
&\quad + \frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^\gamma\left[\frac{\Delta t^2}{4}\left[\frac{\partial^3 U}{\partial x \partial t^2}\right|_i^{j+\frac{1}{2}} + \frac{\Delta x^2 \Delta t^2}{48}\left[\frac{\partial^5 U}{\partial x^3 \partial t^2}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right] \\
&\quad + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 U}{\partial x^4} + O(\Delta x^4)\right)\right|_{C2,i}^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} \\
&\quad + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x} + \frac{\Delta x^2}{12}\frac{\partial^3 U}{\partial x^3} + O(\Delta x^3)\right)\right|_{C2,i}^{j+\frac{1}{2}} - K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_i^{j+\frac{1}{2}} \\
&\quad + f_i^{j+\frac{1}{2}} + \frac{\Delta x^2}{8}\left[\frac{\partial^2 f}{\partial x^2}\right|_i^{j+\frac{1}{2}} + O(\Delta x^4). \qquad (5.419)
\end{aligned}$$

This equation is then simplified to

$$\begin{aligned}\left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_i^{j+\frac{1}{2}} + f_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^{1+\gamma}) \\ &+ D\left\{\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{C2,i}^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}}\right\} + K_\gamma\left\{\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_{C2,i}^{j+\frac{1}{2}} \right. \\ &\left. - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_i^{j+\frac{1}{2}}\right\} + \frac{D\Delta x^2}{2}\left(\frac{\partial^{1-\gamma}M(t)}{\partial t^{1-\gamma}}\right) + \frac{K_\gamma\Delta x^2}{2}\left(\frac{\partial^{1-\gamma}M^*(t)}{\partial t^{1-\gamma}}\right),\end{aligned} \tag{5.420}$$

where

$$M = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left|\frac{\partial^4 U}{\partial x^4}\right|, \text{ and } M^* = \max_{(i-1)\Delta x \le x \le (i+1)\Delta x}\left|\frac{\partial^3 U}{\partial x^3}\right|. \tag{5.421}$$

By Equation (2.149) we note the terms

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_{C2,i}^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}}, \tag{5.422}$$

and

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_{C2,i}^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_i^{j+\frac{1}{2}}, \tag{5.423}$$

are both $O(\Delta t^{1+\gamma})$. Consequently the truncation error, $\tau_{i,j}$, is then of order $1+\gamma$ in time and second order in space, i.e.

$$\tau_{i,j} = O(\Delta t^{1+\gamma}) + O(\Delta x^2). \tag{5.424}$$

### 5.7.3 Consistency of the Numerical Method

The numerical approximation for the fractional advection–differential equation is consistent, since as in previous sections, the truncation error in Equation (5.424) obeys the limit

$$\lim_{\substack{\Delta t \to 0 \\ \Delta x \to 0}} \tau_{i,j} = 0. \tag{5.425}$$

This means that the KBMC2-FADE method is consistent with the original fractional partial differential equation, in Equation (5.17) .

### 5.7.4 Convergence of the KBMC2-FADE Scheme

In this section similar Sections 5.6.1 – 5.6.3, we will discuss the convergence of the KBMC2-FADE scheme, in Equation (5.411) we assume that

$$R_i^{j+1} = \frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right] + \frac{1}{\Delta t}\left[U_i^{j+1} - U_i^j\right] - \frac{1}{2}\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] \tag{5.426}$$
$$- \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\delta_x^2 U_i^{j+1} - \delta_x^2 U_i^j\right) - 2\left(\delta_x^2 U_i^{j+\frac{1}{2}} - \delta_x^2 U_i^j\right)\right]\right\}$$
$$- \frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma\left[\left(\triangle_x U_i^{j+1} - \triangle_x U_i^j\right) - 2\left(\triangle_x U_i^{j+\frac{1}{2}} - \triangle_x U_i^j\right)\right]\right\}$$
$$- \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 U_i^0 + 2\left(\frac{1}{2}\right)^\gamma\left(\delta_x^2 U_i^{j+\frac{1}{2}} - \delta_x^2 U_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 U_i^k - \delta_x^2 U_i^{k-1}\right]\right\}$$
$$- \frac{K_\gamma\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\triangle_x U_i^0 + 2\left(\frac{1}{2}\right)^\gamma\left(\triangle_x U_i^{j+\frac{1}{2}} - \triangle_x U_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\triangle_x U_i^k - \triangle_x U_i^{k-1}\right]\right\},$$

where $\delta_x^2 U_i^j$ and $\triangle_x U_i^j$ are given by Equation (5.90) and (5.413) respectively. The last two terms in the right hand represent the C2 approximation (5.26) with $U(t)$ replaced by $\delta_x^2 U(t)$ and $\triangle_x U(t)$. Using Equations (5.94) – (5.98), and Equations (5.417) and (5.418), Equation (5.426) becomes

$$R_i^{j+1} = \left[\frac{\partial U}{\partial t}\right|_i^{j+\frac{1}{2}} - D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 U}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - K_\gamma\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial U}{\partial x}\right)\right|_i^{j+\frac{1}{2}} - f_i^{j+\frac{1}{2}} + O(\Delta t^{1+\gamma} + \Delta x^2). \tag{5.427}$$

We then have

$$R_i^{j+1} = O(\Delta t^{1+\gamma} + \Delta x^2), \qquad i = 1, 2, \ldots, N, \qquad j = 1, 2, \ldots, M, \tag{5.428}$$

since $i, j$ are finite, there is a positive constant $c_1$ for all $i, j$ such that

$$|R_i^{j+1}| \le c_1(\Delta t^{1+\gamma} + \Delta x^2). \tag{5.429}$$

From Equation (5.426) we have

$$\left(\Delta x^2 - \sigma_1\left(\frac{1}{2}\right)^\gamma\right)\delta_x^2 U_i^{j+1} + 4U_i^{j+1} - \sigma_2\left(\frac{1}{2}\right)^\gamma \triangle_x U_i^{j+1}$$
$$= \left(\Delta x^2 - \sigma_1\left(\frac{1}{2}\right)^\gamma\right)\delta_x^2 U_i^j + 4U_i^j - \sigma_2\left(\frac{1}{2}\right)^\gamma \triangle_x U_i^j + \sigma_1\Big\{\widetilde{\beta}_j(\gamma)\delta_x^2 U_i^0$$
$$+ \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 U_i^k - \delta_x^2 U_i^{k-1}\right]\Big\} + \sigma_2\left\{\widetilde{\beta}_j(\gamma)\triangle_x U_i^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\triangle_x U_i^k - \triangle_x U_i^{k-1}\right]\right\}$$
$$+ 2\Delta t\left[f_{i-\frac{1}{2}}^{j+\frac{1}{2}} + f_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right] + 4\Delta t R_i^{j+1}, \tag{5.430}$$

where $\sigma_1$ and $\sigma_2$ are given by

$$\sigma_1 = \frac{4D\Delta t^{\gamma}}{\Gamma(1+\gamma)}, \qquad \text{and} \qquad \sigma_2 = \frac{4K_{\gamma}\Delta t^{\gamma}}{\Gamma(1+\gamma)}. \tag{5.431}$$

Subtracting (5.411) from (5.430) gives

$$\begin{aligned}
&\left(\Delta x^2 - \sigma_1 \left(\frac{1}{2}\right)^{\gamma}\right) \delta_x^2 E_i^{j+1} + 4E_i^{j+1} - \sigma_2 \left(\frac{1}{2}\right)^{\gamma} \triangle_x E_i^{j+1} \\
&\quad = \left(\Delta x^2 - \sigma_1 \left(\frac{1}{2}\right)^{\gamma}\right) \delta_x^2 E_i^{j} + 4E_i^{j} - \sigma_2 \left(\frac{1}{2}\right)^{\gamma} \triangle_x E_i^{j} \\
&\qquad + \sigma_1 \left\{ \widetilde{\beta}_j(\gamma)\delta_x^2 E_i^0 + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma) \left[\delta_x^2 E_i^k - \delta_x^2 E_i^{k-1}\right] \right\} \\
&\qquad + \sigma_2 \left\{ \widetilde{\beta}_j(\gamma)\triangle_x E_i^0 + \sum_{k=1}^{j} \widetilde{\mu}_{j-k}(\gamma) \left[\triangle_x E_i^k - \triangle_x E_i^{k-1}\right] \right\} + 4\Delta t R_i^{j+1}.
\end{aligned} \tag{5.432}$$

Using Equations (5.310) and (5.311) in (5.432), we then have

$$\left[\left(1 - d_1 \left(\frac{1}{2}\right)^{\gamma}\right)\left(-\sin^2\left(\frac{q\Delta x}{2}\right)\right) + 1 - \frac{d_2}{2}\left(\frac{1}{2}\right)^{\gamma} i\sin(q\Delta x)\right]\xi_{j+1} \tag{5.433}$$

$$\begin{aligned}
&= \left[\left(1 - d_1 \left(\frac{1}{2}\right)^{\gamma}\right)\left(-\sin^2\left(\frac{q\Delta x}{2}\right)\right) + 1 - \frac{d_2}{2}\left(\frac{1}{2}\right)^{\gamma} i\sin(q\Delta x)\right]\xi_{j} \\
&+ \left(\frac{d_2}{2} i\sin(q\Delta x) - d_1\sin^2\left(\frac{q\Delta x}{2}\right)\right)\left\{\widetilde{\beta}_j(\gamma)\xi_0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\xi_k - \xi_{k-1}\right]\right\} + \Delta t\eta_{j+1},
\end{aligned}$$

where $d_1$ and $d_2$ are defined in Equation (5.412), and

$$\delta_x^2 E_i^j = \frac{1}{\Delta x^2}\left(-4\sin^2\left(\frac{q\Delta x}{2}\right)\right)e^{i'qi\Delta x}\xi_j \tag{5.434}$$

and

$$\triangle_x E_i^j = \frac{1}{2\Delta x}\left(2i\sin\left(q\Delta x\right)\right)e^{i'qi\Delta x}\xi_j \tag{5.435}$$

Equation (5.433) simplifies to

$$\xi_{j+1} = \xi_j - \widetilde{U_q}\left\{\widetilde{\beta}_j(\gamma)\xi_0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\xi_k - \xi_{k-1}\right]\right\} + \frac{\Delta t}{1+z}\eta_{j+1}, \tag{5.436}$$

where

$$z = \sin^2\left(\frac{q\Delta x}{2}\right)\left(\left(\frac{1}{2}\right)^{\gamma} d_1 - 1\right) - \frac{d_2}{2}\left(\frac{1}{2}\right)^{\gamma}\sin(q\Delta x)i, \tag{5.437}$$

where $0 < \sin^2\left(\frac{q\Delta x}{2}\right) < 1$ and $-1 < \sin(q\Delta x) < 1$. The coefficient $\widetilde{U_q}$ is given by

$$\begin{aligned}
\widetilde{U_q} &= \frac{d_1\sin^2(q\Delta x/2) - \frac{d_2}{2}\sin(q\Delta x)i}{1 + \sin^2(q\Delta x/2)\left(\left(\frac{1}{2}\right)^{\gamma} d_1 - 1\right) - \frac{d_2}{2}\left(\frac{1}{2}\right)^{\gamma}\sin(q\Delta x)i} \\
&= 2^{\gamma}\frac{\left(\frac{1}{2}\right)^{\gamma}\left[d_1\sin^2(q\Delta x/2) - \frac{d_2}{2}\sin(q\Delta x)i\right]}{1 + \sin^2(q\Delta x/2)\left(\left(\frac{1}{2}\right)^{\gamma} d_1 - 1\right) - \frac{d_2}{2}\left(\frac{1}{2}\right)^{\gamma}\sin(q\Delta x)i},
\end{aligned} \tag{5.438}$$

Equation (5.438) simplifies to

$$\widetilde{U_q} = 2^\gamma \left[\frac{x+z}{1+z}\right], \tag{5.439}$$

where $z$ is given in Equation (5.437), $x = \sin^2(q\Delta x/2)$ and $0 \le x \le 1$. Equation (5.436) can be written as

$$\xi_{j+1} = \left[1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right]\xi_j - \widetilde{U_q}\left\{\widetilde{\alpha}_j(\gamma)\xi_0 + \sum_{l=1}^{j-1}\widetilde{\omega}_{j-l}(\gamma)\xi_l\right\} + \frac{\Delta t}{1+z}\eta_{j+1}, \tag{5.440}$$

where the weights $\widetilde{\mu}_0(\gamma)$, $\widetilde{\alpha}_j(\gamma)$ and $\widetilde{\omega}_j(\gamma)$ are given in Equations (5.28), (5.143) and (5.144) respectively.

**Conjecture 5.7.1.** Let $\xi_j$ be the solution of Equation (5.440). Then there exist a positive constant $c_2$ such that

$$|\xi_j| \le c_2 j\Delta t|\eta_1|, \qquad j = 1, 2, \ldots, M, \tag{5.441}$$

if $\mathrm{Re}(z) > 0$ $(d_1 \ge 2^\gamma)$, where $z$ is given by Equation (5.437).

*Proof.* From Equations (5.309) and (5.429), we obtain

$$\|R^j\|_2 \le c_2\sqrt{N\Delta x}(\Delta t^{1+\gamma} + \Delta x^2) = c_2\sqrt{L}(\Delta t^{1+\gamma} + \Delta x^2), \tag{5.442}$$

where $j = 1, 2, \ldots, M$. We use mathematical induction to prove the relation in Equation (5.441), consider the case $j = 0$. From Equation (5.440) and using Equation (5.312), we have

$$\xi_1 = \frac{\Delta t}{1+z}\eta_1, \tag{5.443}$$

by using Lemma B.11.1, we have

$$|\xi_1| \le \left|\frac{\Delta t}{1+z}\right| |\eta_1| \le \Delta t|\eta_1| \le c_2\Delta t|\eta_1|. \tag{5.444}$$

Hence Equation (5.441) is true for $j = 0$.

Now for case $j = 1$, from Equation (5.440) we then have

$$\xi_2 = \left[1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right]\xi_1 + \frac{\Delta t}{1+z}\eta_2, \tag{5.445}$$

by using Lemma B.11.1 and Equation (5.444) gives

$$|\xi_2| \leq \left|1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| |\xi_1| + \left|\frac{\Delta t}{1+z}\right| |\eta_1|$$
$$\leq c_2 \Delta t \left[\left|1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| + 1\right] |\eta_1|. \tag{5.446}$$

From Lemma B.11.3 the term $\left|1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| \leq 1$, we then conclude that

$$|\xi_2| \leq c_2 2\Delta t |\eta_1|. \tag{5.447}$$

Hence for $j = 1$ Equation (5.440) is satisfied.

Suppose that

$$|\xi_n| \leq c_2 n \Delta t |\eta_1|, \qquad n = 1, 2, \ldots, k. \tag{5.448}$$

From Equation (5.440), we have

$$|\xi_{k+1}| \leq \left|1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| |\xi_k| + \left|\widetilde{U_q}\right| \left|\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\right| |\xi_l| + \left|\frac{\Delta t}{1+z}\right| |\eta_{k+1}|. \tag{5.449}$$

Now using Equations (5.312) and (5.448) in to Equation (5.449), gives

$$|\xi_{k+1}| \leq c_2 \Delta t \left\{ \left|1 - \widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| k + \left|\widetilde{U_q}\right| \left|\sum_{l=1}^{k-1}(-\widetilde{\omega}_{k-l}(\gamma))\right| l + \left|\frac{1}{1+z}\right| \right\} |\eta_1|. \tag{5.450}$$

Since the weight $-\widetilde{\omega}_{k-l}(\gamma)$ is positive, and using Lemmas B.11.1, B.11.2 and B.11.3, Equation (5.450) becomes

$$|\xi_{k+1}| \leq c_2 \Delta t (k+1) |\eta_1| + c_2 \Delta t |\eta_1| 2^\gamma \sum_{l=1}^{k-1} l(-\widetilde{\omega}_{k-l}(\gamma)), \tag{5.451}$$

after evaluating the summation, we then have

$$|\xi_{k+1}| \leq c_2 \Delta t (k+1) |\eta_1| + c_2 \Delta t \left[k(3^\gamma - 1) - (2k+1)^\gamma + 1\right] |\eta_1|, \tag{5.452}$$

From the analysis, it can be seen that through the mathematical induction the relation given in Equation (5.441) may not be satisfied, but in later Section 5.8 we have estimated the convergence order numerically.

□

## 5.8 Numerical Examples and Results

In this section, we provide three examples of the implementation of the four Keller Box based schemes, KBMC2, KBMC3, KBML1, and KBMC2-FADE on problems where the analytic solution is known. For each example we compare graphically the numerical predictions against the exact solution. We also verify the accuracy of our scheme by computing the maximum norm of the error between the numerical estimate and the exact solution at the time $t = t_M$.

These schemes are implemented in MATLAB R2014a (see Appendix C.4) using the linsolve subroutine to solve the system of algebraic equations.

**Example 5.8.1.** Consider the following fractional subdiffusion equation with a source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2}\right) + \sin(\pi x)\left[2t + \pi^2\left(\frac{t^{\gamma-1}}{\Gamma(\gamma)} + \frac{2t^{\gamma+1}}{\Gamma(2+\gamma)}\right)\right], \tag{5.453}$$

and the fractional advection–diffusion equation with source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x}\right) + 2t\sin(\pi x) + \left(\pi^2\sin(\pi x) - \pi\cos(\pi x)\right)\left(\frac{t^{\gamma-1}}{\Gamma(\gamma)} + \frac{2t^{\gamma+1}}{\Gamma(2+\gamma)}\right), \tag{5.454}$$

which will be solved on the domain $0 \le x \le 1$ and $0 \le t \le 1$ subject to the initial and fixed boundary conditions

$$u(x,0) = \sin(\pi x), \qquad u(0,t) = 0, \quad u(1,t) = 0. \tag{5.455}$$

The exact solution of Equations (5.453) and (5.454) given the conditions (5.455) is

$$u(x,t) = \left(1 + t^2\right)\sin(\pi x). \tag{5.456}$$

The error and order of convergence estimates found from applying the KBMC2, KBMC3 and KBML1 schemes on Equations (5.453) subject to Equation (5.455) are given in Tables 5.1 – 5.6 respectively. Results for Equation (5.454) are given in Tables 5.7 and 5.8. To estimate the convergence in space we kept $\Delta t$ fixed at $10^{-3}$ whilst varying $\Delta x$. To estimate the convergence in time we kept $\Delta x$ fixed at $10^{-3}$ whilst varying $\Delta t$.

From the results shown in Tables 5.1 – 5.4, 5.7 and 5.8, it can be seen that the KBMC2, KBMC3 and KBMC2-FADE schemes appear to be of order $O(\Delta x^2)$ and $O(\Delta t^{1+\gamma})$. Whilst the KBML1 method is appears to be of order $O(\Delta x^2)$ and $O(\Delta t)$, as shown by the results in Tables 5.5 and 5.6.

Table 5.1: Numerical accuracy in $\Delta x$ of the KBMC2 scheme applied to Example 5.8.1 with $\Delta t = 10^{-3}$, where $R1$ is the order of convergence in $\Delta x$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.17e–00 | – | 0.20e–00 | – | 0.19e–00 | – | 0.19e–00 | – |
| 1/4 | 0.32e–01 | 2.36 | 0.39e–01 | 2.37 | 0.37e–01 | 2.40 | 0.36e–01 | 2.41 |
| 1/8 | 0.76 e–02 | 2.09 | 0.92e–02 | 2.10 | 0.86e–02 | 2.11 | 0.84e–02 | 2.11 |
| 1/16 | 0.19e–02 | 2.01 | 0.23e–02 | 2.02 | 0.21e–02 | 2.03 | 0.21e–02 | 2.03 |
| 1/32 | 0.49e–03 | 1.94 | 0.57e–03 | 2.00 | 0.52e–03 | 2.01 | 0.51e–03 | 2.01 |

Table 5.2: Numerical accuracy in $\Delta t$ of the KBMC2 scheme applied to Example 5.8.1 with $\Delta x = 10^{-3}$, where $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.49e–02 | – | 0.60e–02 | – | 0.29e–02 | – | 0.25e–02 | – |
| 1/20 | 0.22e–02 | 1.16 | 0.20e–02 | 1.60 | 0.75e–03 | 1.96 | 0.63e–03 | 2.00 |
| 1/40 | 0.10e–03 | 1.14 | 0.66e–03 | 1.58 | 0.19e–03 | 1.95 | 0.16 e–03 | 2.00 |
| 1/80 | 0.46e–03 | 1.12 | 0.22e–03 | 1.56 | 0.51e–04 | 1.94 | 0.40e–04 | 1.99 |
| 1/160 | 0.21e–03 | 1.11 | 0.77e–04 | 1.54 | 0.13e–04 | 1.91 | 0.10e–04 | 1.94 |

Table 5.3: Numerical accuracy in $\Delta x$ of the KBMC3 scheme applied to Example 5.8.1 with $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.17e–00 | – | 0.20e–00 | – | 0.19e–00 | – | 0.19e–00 | – |
| 1/4 | 0.32e–01 | 2.36 | 0.39e–01 | 2.37 | 0.37e–01 | 2.40 | 0.36e–01 | 2.41 |
| 1/8 | 0.75e–02 | 2.11 | 0.92e–02 | 2.10 | 0.86e–02 | 2.11 | 0.84e–02 | 2.11 |
| 1/16 | 0.17e–02 | 2.10 | 0.23e–02 | 2.03 | 0.21e–02 | 2.03 | 0.21e–02 | 2.03 |
| 1/32 | 0.34e–03 | 2.35 | 0.56e–03 | 2.01 | 0.52e–03 | 2.01 | 0.51e–03 | 2.01 |

Table 5.4: Numerical accuracy in $\Delta t$ of the KBMC3 scheme applied to Example 5.8.1 with $\Delta x = 10^{-3}$, where $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.61e–01 | – | 0.11e–01 | – | 0.14e–02 | – | 0.25e–02 | – |
| 1/20 | 0.29e–01 | 1.05 | 0.44e–02 | 1.33 | 0.30e–03 | 2.22 | 0.63e–03 | 2.00 |
| 1/40 | 0.14e–01 | 1.07 | 0.17e–02 | 1.40 | 0.62e–04 | 2.28 | 0.16e–03 | 2.00 |
| 1/80 | 0.66e–02 | 1.08 | 0.61e–03 | 1.43 | 0.12e–04 | 2.36 | 0.39e–04 | 2.00 |
| 1/160 | 0.31 e–02 | 1.09 | 0.223e–03 | 1.46 | 0.20e–05 | 2.47 | 0.10e–04 | 1.99 |

Table 5.5: Numerical accuracy in $\Delta x$ of the KBML1 scheme applied to Example 5.8.1 where $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.16e–00 | – | 0.20e–00 | – | 0.19e–00 | – | 0.19e–00 | – |
| 1/4 | 0.29e–01 | 2.40 | 0.39e–01 | 2.37 | 0.37e–01 | 2.40 | 0.36e–01 | 2.41 |
| 1/8 | 0.63e–02 | 2.22 | 0.90e–02 | 2.12 | 0.84e–02 | 2.13 | 0.82e–02 | 2.13 |
| 1/16 | 0.97e–03 | 2.68 | 0.21e–02 | 2.11 | 0.20e–02 | 2.11 | 0.19e–02 | 2.11 |
| 1/32 | 0.32e–03 | 1.64 | 0.38e–03 | 2.43 | 0.37e–03 | 2.39 | 0.37e–03 | 2.38 |

Table 5.6: Numerical accuracy in $\Delta t$ of the KBML1 scheme applied to Example 5.8.1 with $\Delta x = 10^{-3}$, where $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.74e–01 | – | 0.24e–01 | – | 0.11e–01 | – | 0.10e–01 | - |
| 1/20 | 0.35e–01 | 1.08 | 0.10e–01 | 1.23 | 0.55e–02 | 1.05 | 0.51e–02 | 1.00 |
| 1/40 | 0.17e–01 | 1.08 | 0.44e–02 | 1.20 | 0.27e–02 | 1.03 | 0.25e–02 | 1.00 |
| 1/80 | 0.78e–02 | 1.08 | 0.20e–02 | 1.18 | 0.13e–02 | 1.02 | 0.13e–02 | 1.00 |
| 1/160 | 0.37e–02 | 1.08 | 0.88e–03 | 1.14 | 0.66e–03 | 1.01 | 0.63e–03 | 1.00 |

Table 5.7: Numerical accuracy in $\Delta x$ of the KBMC2-FADE scheme applied to Example 5.8.1 with $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.17e–00 | – | 0.20e–00 | – | 0.19e–00 | – | 0.19e–00 | – |
| 1/4 | 0.31e–01 | 2.41 | 0.38e–01 | 2.42 | 0.36e–01 | 2.45 | 0.35e–01 | 2.46 |
| 1/8 | 0.74e–02 | 2.07 | 0.91e–02 | 2.07 | 0.84e–02 | 2.08 | 0.83e–02 | 2.08 |
| 1/16 | 0.19e–02 | 2.00 | 0.22e–02 | 2.01 | 0.21e–02 | 2.02 | 0.20e–02 | 2.02 |
| 1/32 | 0.48e–03 | 1.94 | 0.56e–03 | 2.00 | 0.52e–03 | 2.00 | 0.51e–03 | 2.00 |

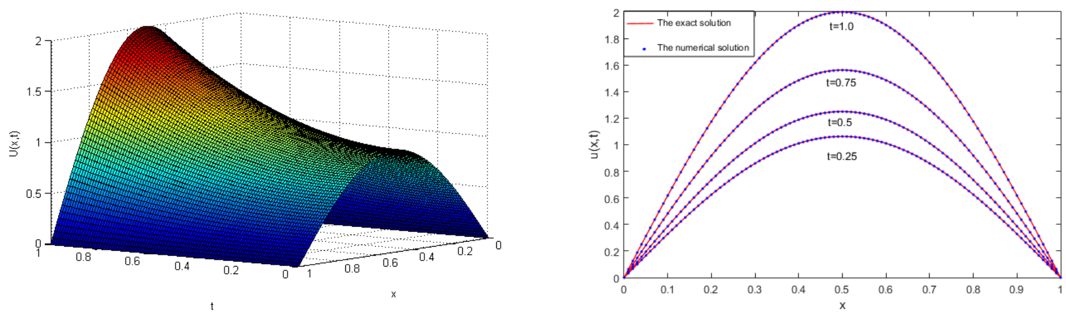
Table 5.8: Numerical accuracy in $\Delta t$ of the KBMC2-FADE scheme applied to Example 5.8.1, where $\Delta x = 10^{-3}$, and $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/20 | 0.22e–02 | – | 0.20e–02 | – | 0.75e–03 | – | 0.63e–03 | – |
| 1/40 | 0.10e–02 | 1.14 | 0.66e–03 | 1.58 | 0.19e–03 | 1.95 | 0.16e–03 | 2.00 |
| 1/80 | 0.46e–03 | 1.12 | 0.22e–03 | 1.56 | 0.50e–04 | 1.94 | 0.40e–04 | 1.99 |
| 1/160 | 0.21e–03 | 1.11 | 0.77e–04 | 1.54 | 0.13e–04 | 1.91 | 0.10e–04 | 1.95 |
| 1/320 | 0.98e–04 | 1.11 | 0.27e–04 | 1.51 | 0.40e–05 | 1.80 | 0.30e–05 | 1.80 |

The results of the solution of Equation (5.453) for the fractional exponent $\gamma = 0.5$, and $0 \le x \le 1$, time $0 \le t \le 1$ and $\Delta t = 10^{-3}$, by using the KBMC2, KBMC3, and KBML1 schemes are shown in Figures 5.14(a), 5.16(a) and 5.18(a) respectively, and for $\gamma = 1$ are shown in Figures 5.15(a), 5.17(a) and 5.19(a) respectively. The numerical solution for Equation (5.454), found using the KBMC2-FADE scheme, is shown in Figure 5.20(a) for $\gamma = 0.5$ and in Figure 5.21(a) for $\gamma = 1$.

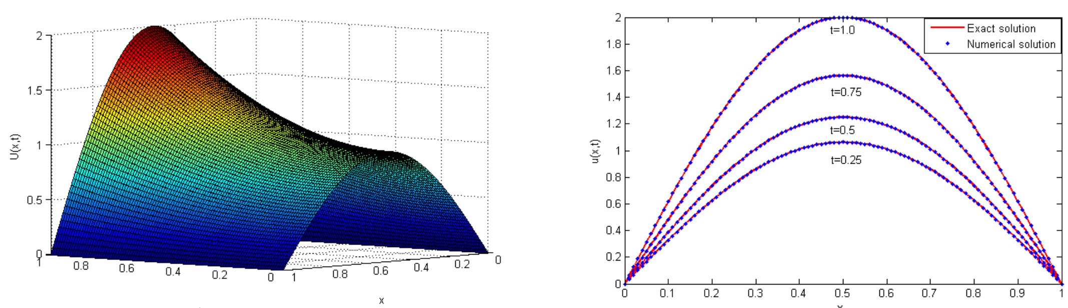
A comparison of the exact solution (shown as solid red lines) and the numerical solution (shown as blue dots) of Equation (5.453), using the KBMC2 scheme, in the case the fractional exponent $\gamma = 0.5$ at the times $t = 0.25$, $0.50$, $0.75$, and $1.00$, is shown in Figure 5.14(b), and for $\gamma = 1$ is shown in Figure 5.15(b). Similarly in Figures 5.16(b), 5.18(b) and 5.20(b), the results of applying the KBMC3, KBML1 and KBMC2-FADE schemes are compared with the exact solution for $\gamma = 0.5$ at the same time. Figures 5.17(b), 5.19(b) and 5.21(b) show the results for $\gamma = 1$. It can be seen that the approximate solutions obtained from all numerical schemes are in good agreement with the exact solution.

Results are not shown here for other values of $\gamma$. However the exact solution is the same for all values of $\gamma$ for both fractional partial differential equations in this example. Due to the order of accuracy we don't see much of a difference between the predicted values and the exact solution, when they are compared in the case of different $\gamma$ values.



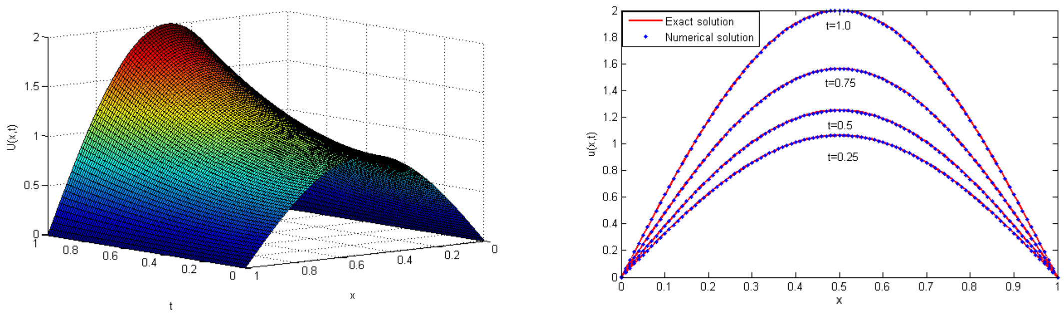

(a) (b)

Figure 5.14: Numerical results of applying the KBMC2 method to solve Equation (5.453) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution(blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.



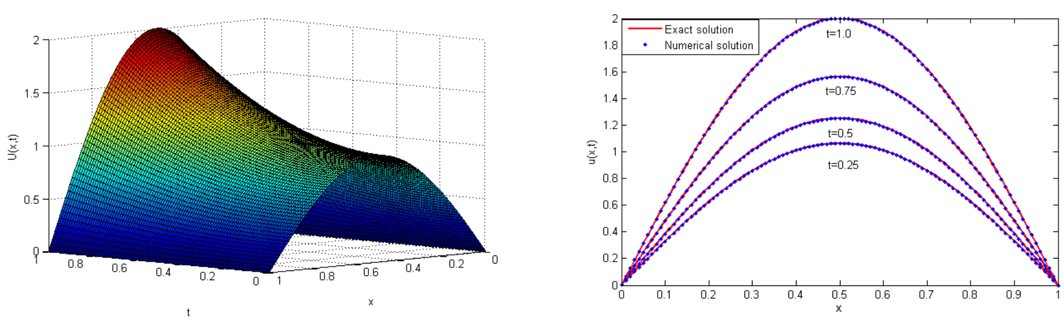

(a) (b)

Figure 5.15: Numerical results of applying the KBMC2 method to solve Equation (5.453) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.



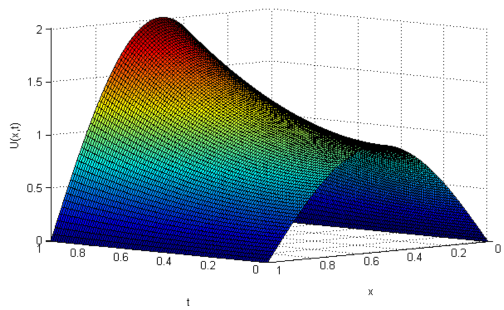

(a) (b)

Figure 5.16: Numerical results of applying the KBMC3 method to solve Equation (5.453) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.

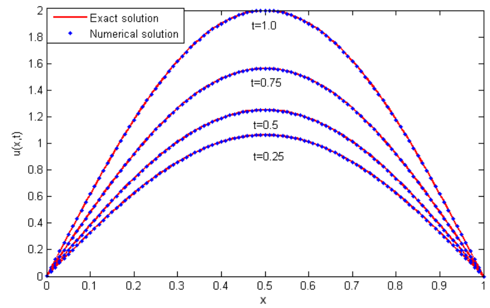



(a) (b)

Figure 5.17: Numerical results of applying the KBMC3 method to solve Equation (5.453) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.

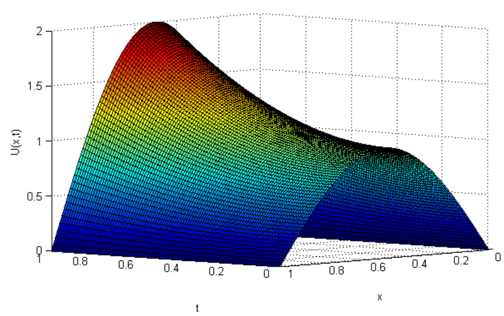



(a)

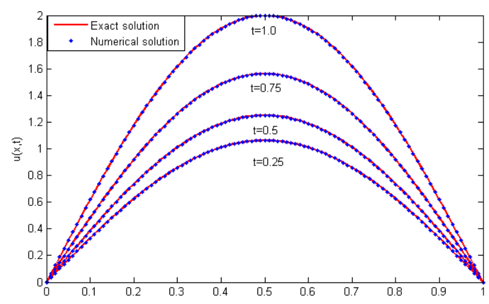



(b)

Figure 5.18: Numerical results of applying the KBML1 method to solve Equation (5.453) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.

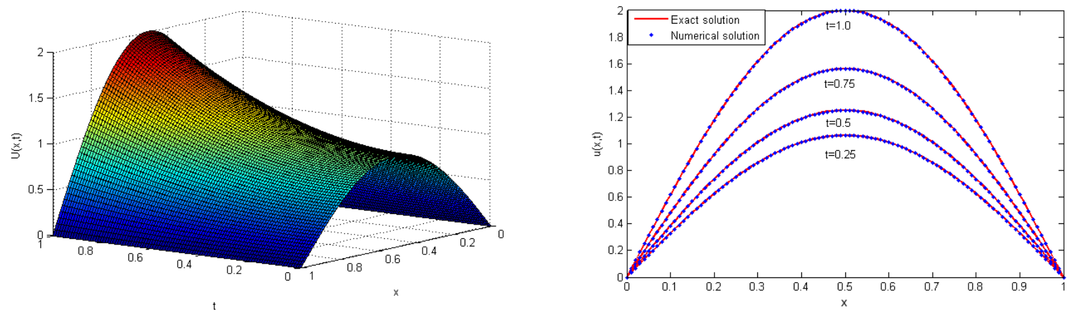



(a)



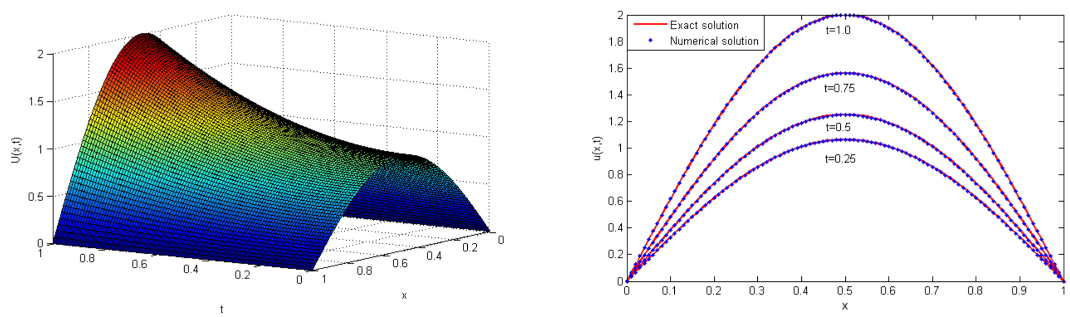

(b)

Figure 5.19: Numerical results of applying the KBML1 method to solve Equation (5.453) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.




(a) (b)

Figure 5.20: Numerical results of applying the KBMC2-FADE method to solve Equation (5.454) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.




(a) (b)

Figure 5.21: Numerical results of applying the KBMC2-FADE method to solve Equation (5.454) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.

**Example 5.8.2.** Consider the following fractional subdiffusion equation with the source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} \right) + 2e^x t \left[ 1 - \frac{t^\gamma}{\Gamma(2+\gamma)} \right], \tag{5.457}$$

and fractional advection–differential equation with a source term

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} \right) + 2e^x t \left[ 1 - \frac{2t^\gamma}{\Gamma(2+\gamma)} \right], \tag{5.458}$$

with $0 < \gamma \leq 1$ and the initial and fixed boundary conditions

$$u(x,0) = 0, \qquad u(0,t) = t^2, \quad u(L,t) = et^2, \tag{5.459}$$

where $0 \le x \le L$, $0 \le t \le 1$ and $L = 1$.

The exact solution of Equations (5.457) subject to the condition (5.459) is

$$u(x,t) = e^x t^2. \tag{5.460}$$

The error and order of convergence estimates for this example, by using the KBMC2, KBMC3, and KBML1 methods for Equation (5.457) and the KBMC2–FADE method for Equation (5.458), are shown in Tables 5.9 – 5.16. To estimate the convergence in space, we again kept $\Delta t$ fixed at $10^{-3}$ whilst varying $\Delta x$, and to estimate the convergence in time we kept $\Delta x$ fixed at $10^{-3}$ whilst varying $\Delta t$. From the results given in Tables 5.13 and 5.14, we see the approximate truncation order of the KBML1 scheme is again of order $O(\Delta x^2)$, and $O(\Delta t)$. The results in Tables 5.9 – 5.12 show the truncation order of the KBMC2 and KBMC3 schemes are of order $O(\Delta x^2)$ and $O(\Delta t^{1+\gamma})$. Likewise in Tables 5.15 and 5.16, we see that the KBMC2-FADE scheme has the same order of $O(\Delta x^2)$ and $O(\Delta t^{1+\gamma})$.

Table 5.9: Numerical accuracy in $\Delta x$ of the KBMC2 scheme applied to Example 5.8.2 where $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$ .

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.88e–02 | – | 0.11e–01 | – | 0.15e–01 | – | 0.14e–01 | – |
| 1/4 | 0.21e–02 | 2.06 | 0.27e–02 | 2.07 | 0.33e–02 | 2.07 | 0.34e–02 | 2.07 |
| 1/8 | 0.52e–03 | 2.03 | 0.66e–03 | 2.02 | 0.81e–03 | 2.02 | 0.85e–03 | 2.02 |
| 1/16 | 0.13e–03 | 2.04 | 0.17e–03 | 2.00 | 0.20e–03 | 1.99 | 0.21e–03 | 1.99 |
| 1/32 | 0.27e–04 | 2.22 | 0.41e–04 | 2.03 | 0.51e–04 | 2.00 | 0.53e–04 | 2.00 |

Table 5.10: Numerical accuracy in $\Delta t$ of the KBMC2 scheme applied to Example 5.8.2 with $\Delta x = 10^{-3}$, where $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.10e–02 | – | 0.13e–02 | – | 0.62e–03 | – | 0.53e–03 | – |
| 1/20 | 0.46e–03 | 1.16 | 0.42e–03 | 1.60 | 0.16e–03 | 1.96 | 0.132e–03 | 2.00 |
| 1/40 | 0.21e–03 | 1.14 | 0.14e–03 | 1.58 | 0.41e–04 | 1.96 | 0.33e–04 | 2.00 |
| 1/80 | 0.97e–04 | 1.13 | 0.47e–04 | 1.56 | 0.11e–04 | 1.96 | 0.80e–05 | 2.01 |
| 1/160 | 0.45e–04 | 1.12 | 0.16e–04 | 1.55 | 0.30e–05 | 1.97 | 0.20e–05 | 2.03 |

Table 5.11: Numerical accuracy in $\Delta x$ of the KBMC3 scheme applied to Example 5.8.2 with $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.89e–02 | – | 0.11e–01 | – | 0.14e–01 | – | 0.14e–01 | – |
| 1/4 | 0.22e–02 | 2.04 | 0.27e–02 | 2.08 | 0.33e–02 | 2.07 | 0.34e–02 | 2.07 |
| 1/8 | 0.55e–03 | 1.98 | 0.27e–02 | 2.07 | 0.81e–03 | 2.02 | 0.85e–03 | 2.02 |
| 1/16 | 0.15e–03 | 1.85 | 0.17e–03 | 1.99 | 0.20e–03 | 1.99 | 0.21e–03 | 2.00 |
| 1/32 | 0.52e–04 | 1.54 | 0.42e–04 | 1.99 | 0.51e–04 | 2.00 | 0.53e–04 | 2.00 |

Table 5.12: Numerical accuracy in $\Delta t$ of the KBMC3 scheme applied to Example 5.8.2 with $\Delta x = 10^{-3}$, and $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.13e–01 | – | 0.23e–02 | – | 0.30e–03 | – | 0.53e–03 | – |
| 1/20 | 0.62e–02 | 1.05 | 0.92e–03 | 1.33 | 0.64e–04 | 2.23 | 0.13e–03 | 2.00 |
| 1/40 | 0.30e–02 | 1.07 | 0.35e–03 | 1.39 | 0.13e–04 | 2.28 | 0.33e–04 | 2.00 |
| 1/80 | 0.14e–02 | 1.08 | 0.13e–03 | 1.43 | 0.30e–05 | 2.38 | 0.80e–05 | 2.00 |
| 1/160 | 0.65e–03 | 1.10 | 0.47e–04 | 1.46 | 0.10e–06 | 2.58 | 0.20e–05 | 2.01 |

Table 5.13: Numerical accuracy in $\Delta x$ of the KBML1 scheme applied to Example 5.8.2, where $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.94e–02 | – | 0.16e–01 | – | 0.19e–01 | – | 0.21e–01 | – |
| 1/4 | 0.22e–02 | 2.08 | 0.36e–02 | 2.09 | 0.46e–02 | 2.08 | 0.50e–02 | 2.07 |
| 1/8 | 0.51e–03 | 2.13 | 0.82e–03 | 2.15 | 0.11e–02 | 2.12 | 0.12e–02 | 2.11 |
| 1/16 | 0.83e–04 | 2.61 | 0.12e–03 | 2.73 | 0.19e–03 | 2.52 | 0.21e–03 | 2.46 |
| 1/32 | 0.23e–04 | 1.83 | 0.52e–04 | 1.52 | 0.35e–04 | 2.39 | 0.27e–04 | 2.94 |

Table 5.14: Numerical accuracy in $\Delta t$ of the KBML1 scheme applied to Example 5.8.2 with $\Delta x = 10^{-3}$, and $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/10 | 0.60e–02 | – | 0.18e–01 | – | 0.21e–01 | – | 0.21e–01 | – |
| 1/20 | 0.35e–02 | 0.79 | 0.97e–02 | 0.92 | 0.11e-01 | 0.99 | 0.11e–01 | 1.00 |
| 1/40 | 0.20e–02 | 0.83 | 0.50e–02 | 0.95 | 0.54e–02 | 0.99 | 0.53e–02 | 1.00 |
| 1/80 | 0.11e–02 | 0.86 | 0.26e–02 | 0.97 | 0.27e–02 | 1.00 | 0.27e–02 | 1.00 |
| 1/160 | 0.59e–03 | 0.88 | 0.13e–02 | 0.98 | 0.14e–02 | 1.00 | 0.13e–02 | 1.00 |

Table 5.15: Numerical accuracy in $\Delta x$ of the KBMC2-FADE scheme applied to Example 5.8.2 with $\Delta t = 10^{-3}$, and $R1$ is the order of convergence in $\Delta x$.

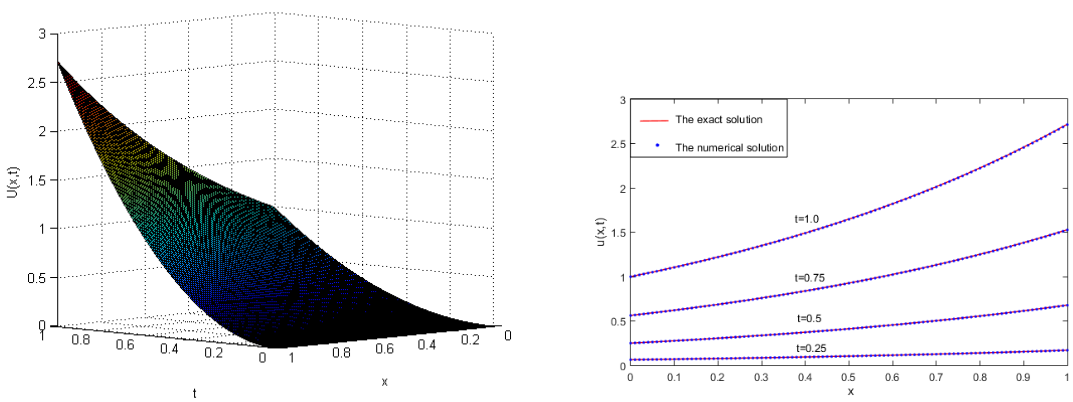
| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ | $e_\infty(\Delta t, \Delta x)$ | $R1$ |
| 1/2 | 0.68e–02 | – | 0.92e–02 | – | 0.12e–01 | – | 0.13e–01 | – |
| 1/4 | 0.16e–02 | 2.06 | 0.22e–02 | 2.06 | 0.28e–02 | 2.06 | 0.30e–02 | 2.06 |
| 1/8 | 0.39e–03 | 2.04 | 0.54e–03 | 2.02 | 0.70e–03 | 2.02 | 0.74e–03 | 2.01 |
| 1/16 | 0.90e–04 | 2.14 | 0.13e–03 | 2.02 | 0.17e–03 | 2.01 | 0.19e–03 | 2.00 |
| 1/32 | 0.14e–04 | 2.72 | 0.32e–04 | 2.07 | 0.43e–04 | 2.01 | 0.46e–04 | 2.00 |

Table 5.16: Numerical accuracy in $\Delta t$ of the KBMC2-FADE scheme applied to Example 5.8.2 with $\Delta x = 10^{-3}$, and $R2$ is the order of convergence in $\Delta t$.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | | $\gamma = 1$ | |
|---|---|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ | $e_\infty(\Delta t, \Delta x)$ | $R2$ |
| 1/20 | 0.92e–03 | – | 0.82e–03 | – | 0.32e–03 | – | 0.26e–03 | – |
| 1/40 | 0.42e–03 | 1.14 | 0.28e–03 | 1.58 | 0.81e–04 | 1.96 | 0.66e–04 | 2.00 |
| 1/80 | 0.19e–03 | 1.13 | 0.93e–04 | 1.56 | 0.21e–04 | 1.96 | 0.16e–04 | 2.00 |
| 1/160 | 0.89e–04 | 1.12 | 0.32e–04 | 1.55 | 0.50e–05 | 1.96 | 0.40e–05 | 2.01 |
| 1/320 | 0.41e–04 | 1.11 | 0.11e–04 | 1.54 | 0.10e–05 | 1.98 | 0.10e–05 | 2.05 |

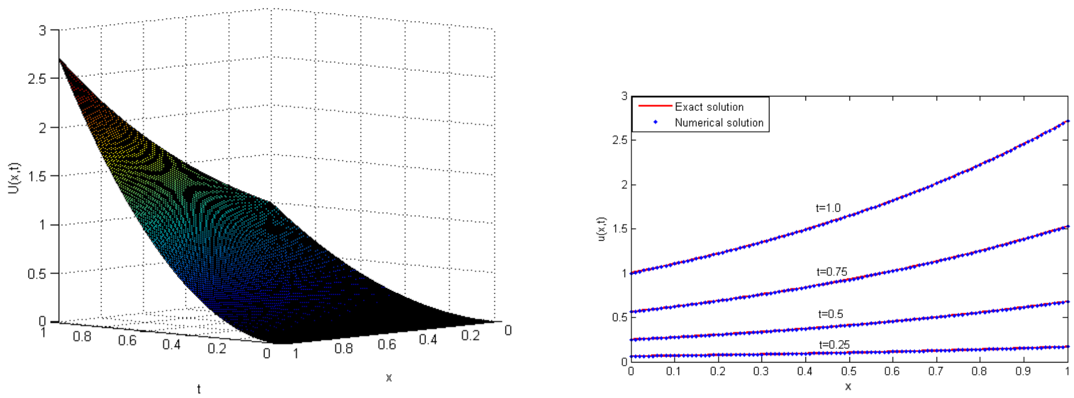
The numerical solution of Equation (5.457) versus $0 \le x \le 1$, time $0 \le t \le 1$ in the case $\gamma = 0.5$ by using the KBMC2, KBMC3 and KBML1 schemes, are shown part (a) of Figures 5.22, 5.24, and 5.26 respectively and in the case $\gamma = 1$ are shown in part (a) of Figures 5.23, 5.25, and 5.27 respectively, where $\Delta t = 10^{-3}$. The numerical solution of Equation (5.458) for $\gamma = 0.5$ by using the KBMC2-FADE scheme is shown in Figure 5.28(a) and for $\gamma = 1$ is shown in Figure 5.29(a).

In part (b) of Figures 5.22, 5.24, 5.26, and 5.28, for $\gamma = 0.5$, and Figures 5.23, 5.25, 5.27 and 5.29, for $\gamma = 1$, we show the comparison of the exact solution (shown as solid red lines) and the numerical estimate found using the KBMC2, KBMC3, KBML1 and KBMC2-FADE methods (shown as blue dots) at the times $t = 0.25$, 0.5, 0.75, and 1.00. Again we see the numerical estimates from all schemes are in agreement with the exact solution.



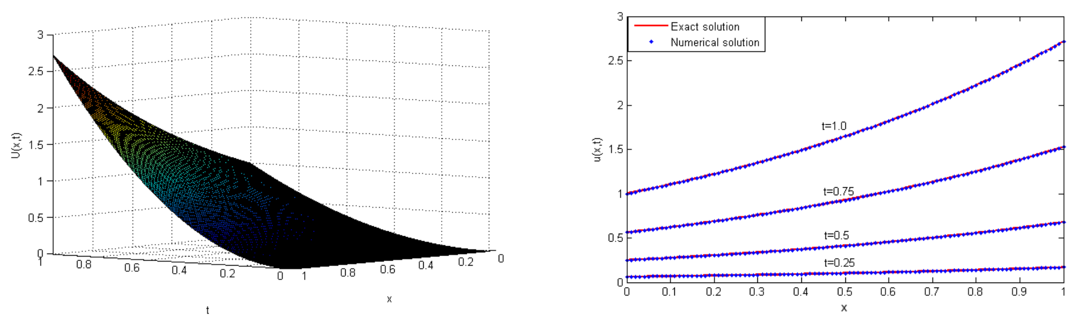

(a) (b)

Figure 5.22: Numerical results of applying the KBMC2 method to solve Equation (5.457) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.



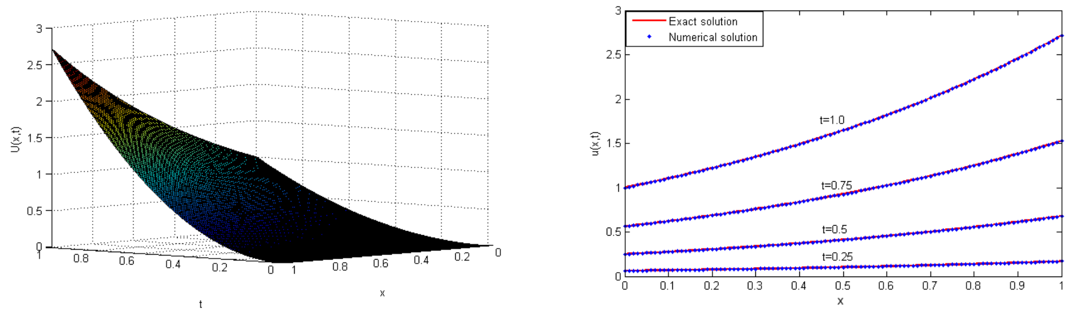

(a) (b)

Figure 5.23: Numerical results of applying the KBMC2 method to solve Equation (5.457) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.



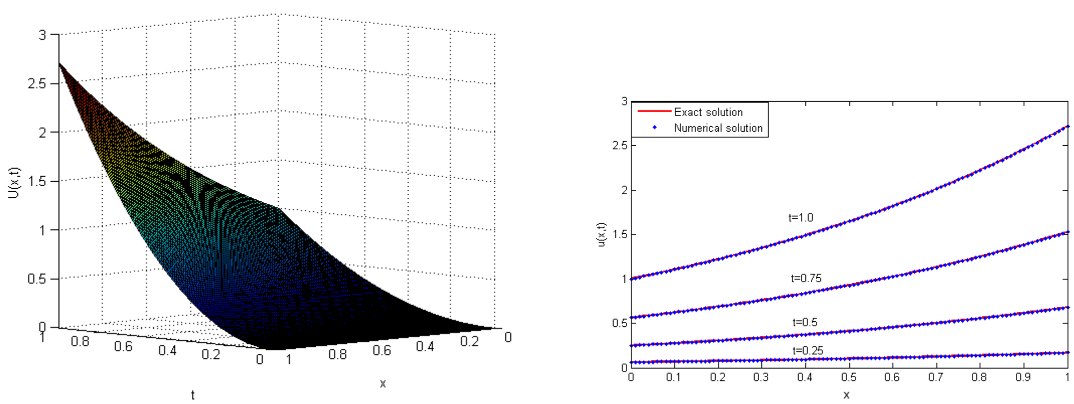

(a) (b)

Figure 5.24: Numerical results of applying the KBMC3 method to solve Equation (5.457) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.



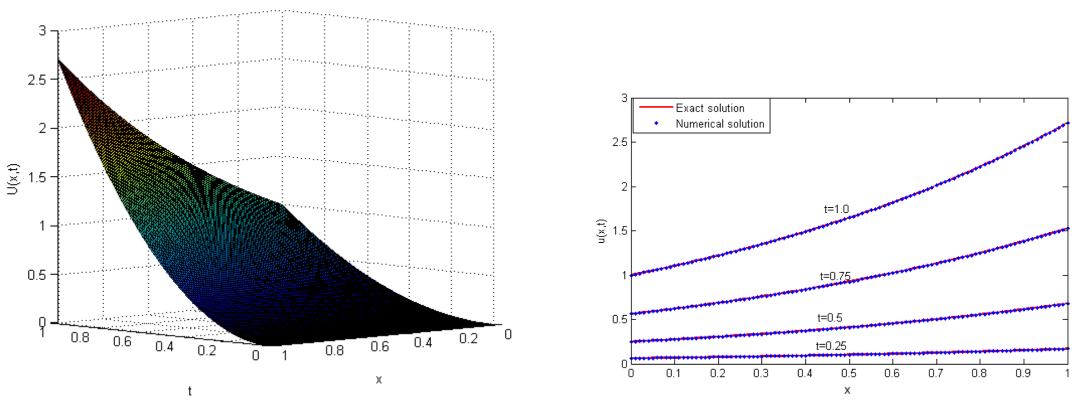

(a) (b)

Figure 5.25: Numerical results of applying the KBMC3 method to solve Equation (5.457) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.



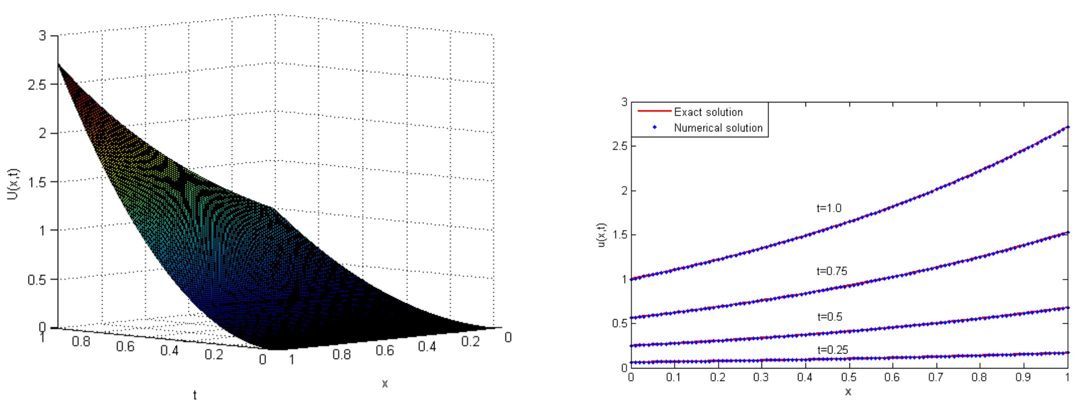

(a) (b)

Figure 5.26: Numerical results of applying the KBML1 method to solve Equation (5.457) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.



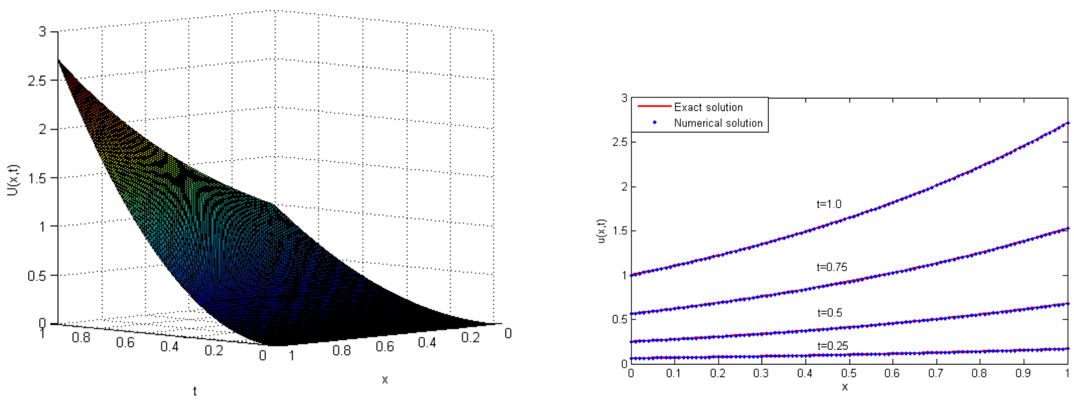

(a) (b)

Figure 5.27: Numerical results of applying the KBML1 method to solve Equation (5.457) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.




(a) (b)

Figure 5.28: Numerical results of applying the KBMC2-FADE method to solve Equation (5.458) in the case $\gamma = 0.5$. In (a) the numerical solution $u(x,t)$ is given for $0 \leq t \leq 1$ and $0 \leq x \leq 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, 0.50, 0.75, and 1.




(a) (b)

Figure 5.29: Numerical results of applying the KBMC2-FADE method to solve Equation (5.458) in the case $\gamma = 1$. In (a) the numerical solution $u(x,t)$ is given for $0 \le t \le 1$ and $0 \le x \le 1$, and in (b) the exact solution (red line) is compared with the approximation solution (blue dots) at the times $t = 0.25$, $0.50$, $0.75$, and $1$.

**Example 5.8.3.** Consider the following fractional subdiffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} \right), \tag{5.461}$$

with the initial and fixed boundary conditions

$$u(x,0) = \sin(\pi x), \;\; u(0,t) = 0, \;\; u(1,t) = 0 \tag{5.462}$$

where $0 \le x \le 1$, $0 \le t$. The exact solution of Equations (5.461) is

$$u(x,t) = \sin(\pi x) E_\gamma(-\pi^2 t^\gamma). \tag{5.463}$$

The exact solution for the case $\gamma = 0.5$ and $1.0$ are given in Chapter 3 by Equations (3.151) and (3.152) respectively.

In Figures 5.30 – 5.32, we show the comparison of the exact solution and the numerical solution at the times $t = 0.25$, $0.5$, $0.75$, and $1.0$ with $\Delta t = 10^{-4}$ by using the KBMC2, KBMC3, and KBML1 schemes. Also the comparison of the solution at $x = 0.5$, $u(0.5, t)$, at time $t = 1.0$ are shown in Figures 5.33 – 5.35. We see the numerical estimate in Figures 5.33 – 5.35 lags behind the exact solution. The KBMC2 scheme appears to better predict these values though when compared with the KBML1 scheme.

The numerical solutions of Equation (5.461) for fractional exponent $\gamma = 0.1, 0.5, 0.9$, and 1.0, with $\Delta t = 10^{-4}$, found by using the KBMC2, KBMC3, and KBML1 schemes are shown in Figures 5.37, 5.39 and 5.41 respectively. From the results shown in these figures we see the numerical solution of Equation (5.461) changes with the value of the exponent $\gamma$. It can be seen that the solution, in the long term, decays faster to zero for larger values of $\gamma$ compared to smaller values of $\gamma$. However, it should be noted that the initial decay is faster for smaller values of $\gamma$. This behavior is consistent with the behavior of the Mittag–Leffler function as mentioned earlier in Chapter 3.

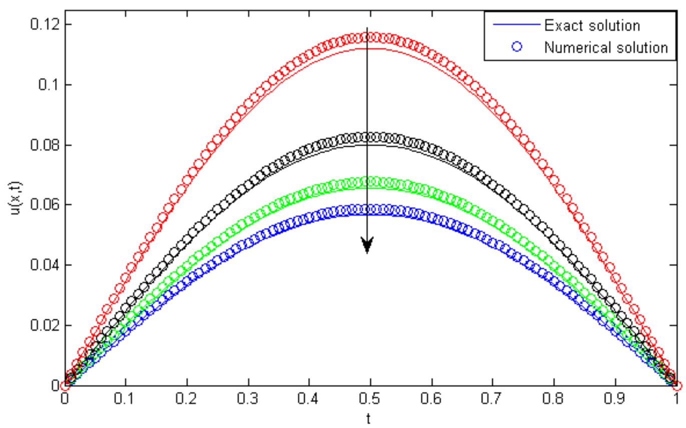



Figure 5.30: A comparison of the exact solution and the numerical solution, using the KBMC2 scheme, for Equation (5.461) shown at times $t = 0.25$, 0.5, 0.75, and 1.0 in the case $\gamma = 0.5$ and $\Delta t = 10^{-4}$. Time increases in the direction of arrow.

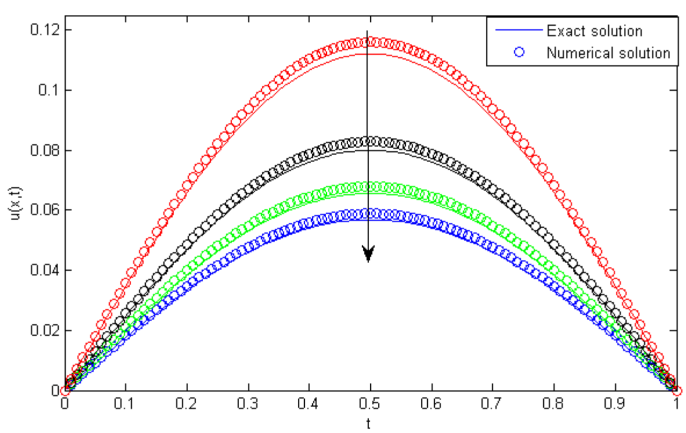



Figure 5.31: A comparison of the exact solution and the numerical solution, using the KBMC3 scheme, for Equation (5.461) shown at times $t = 0.25$, 0.5, 0.75, and 1.0 in the case $\gamma = 0.5$ and $\Delta t = 10^{-4}$. Time increases in the direction of arrow.

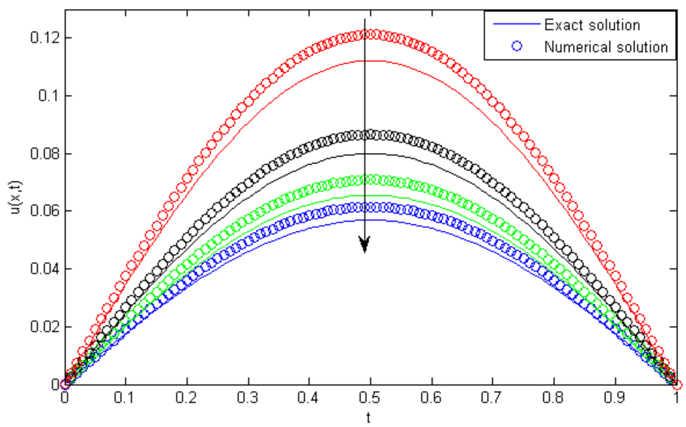



Figure 5.32: A comparison of the exact solution and the numerical solution, using the KBML1 scheme, for Equation (5.461) shown at times $t = 0.25$, 0.5, 0.75, and 1.0 in the case $\gamma = 0.5$ and $\Delta t = 10^{-4}$. Time increases in the direction of arrow.

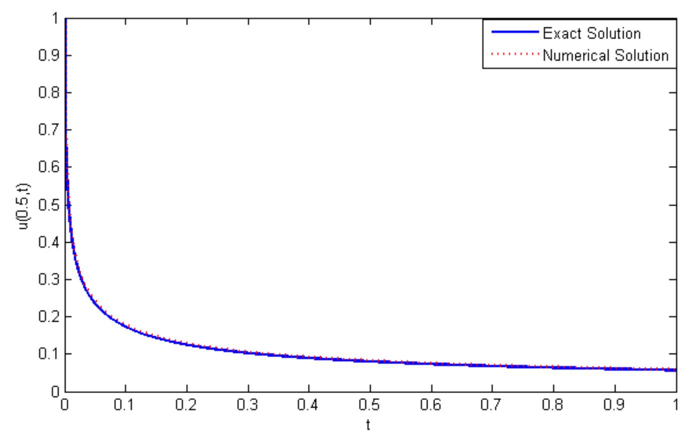



Figure 5.33: A comparison of the exact solution and the numerical solution, using the KBMC2 scheme, present at the mid point $x = 0.5$ for Equation (5.461) with $\gamma = 0.5$ and time step $\Delta t = 10^{-4}$.

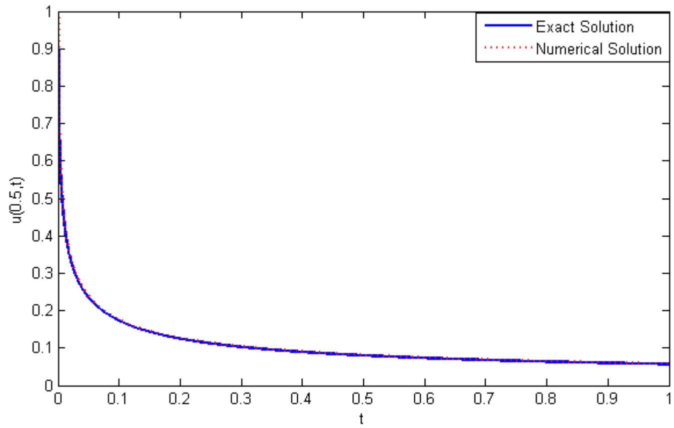



Figure 5.34: A comparison of the exact solution and the numerical solution, using the KBMC3 scheme, present at the mid point $x = 0.5$ for Equation (5.461) with $\gamma = 0.5$ and time step $\Delta t = 10^{-4}$.

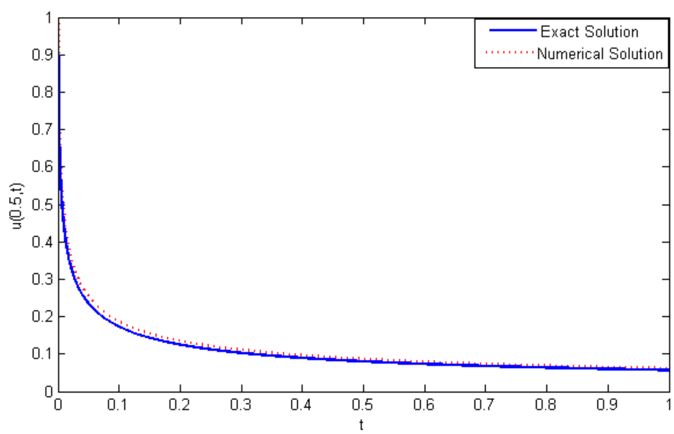
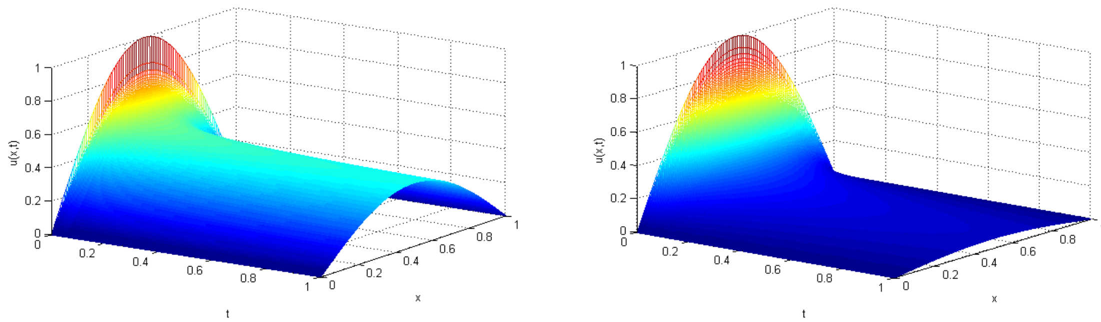
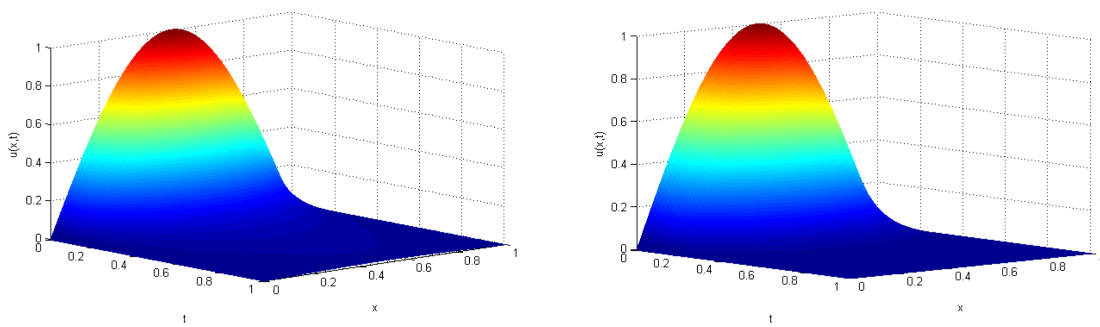



Figure 5.35: A comparison of the exact solution and the numerical solution, using the KBML1 scheme, present at the mid point $x = 0.5$ for Equation (5.461) with $\gamma = 0.5$ and time step $\Delta t = 10^{-4}$.




(a) (b)

Figure 5.36: The numerical solution of Equation (5.461) using the KBMC2 scheme shown here in the case of the fractional exponent (a) $\gamma = 0.1$, and (b) $\gamma = 0.5$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ using with $\Delta t = 10^{-4}$.




(a) (b)

Figure 5.37: The numerical solution of Equation (5.461) using the KBMC2 scheme shown here in the case of the fractional exponent (a) $\gamma = 0.9$, and (b) $\gamma = 1$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ using with $\Delta t = 10^{-4}$.

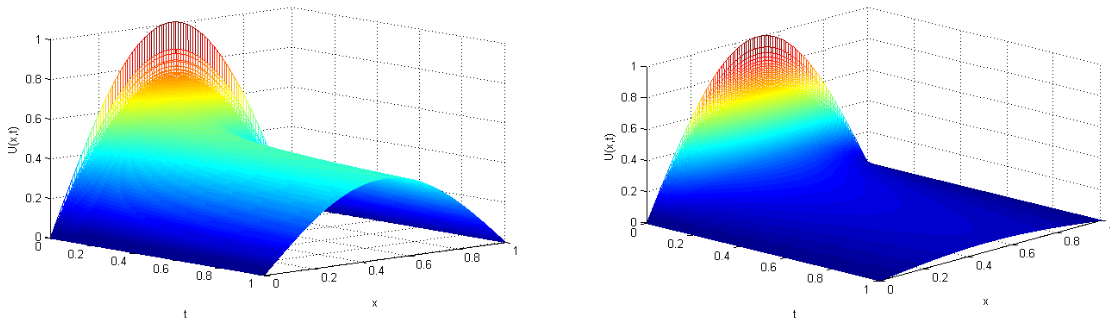



Figure 5.38: The numerical solution of Equation (5.461) using the KBMC3 scheme shown here in the case of the fractional exponent (a) $\gamma = 0.1$, and (b) $\gamma = 0.5$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ using with $\Delta t = 10^{-4}$.

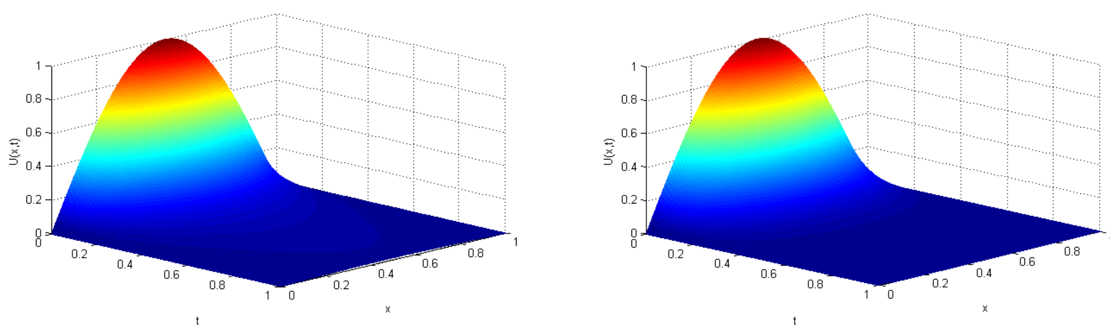
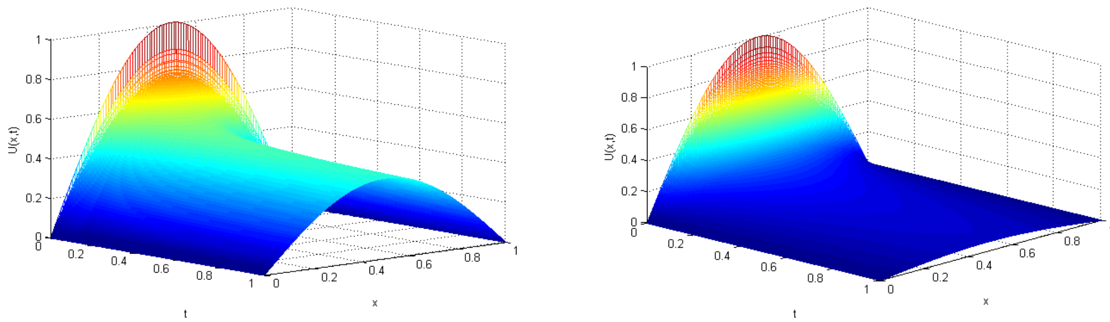
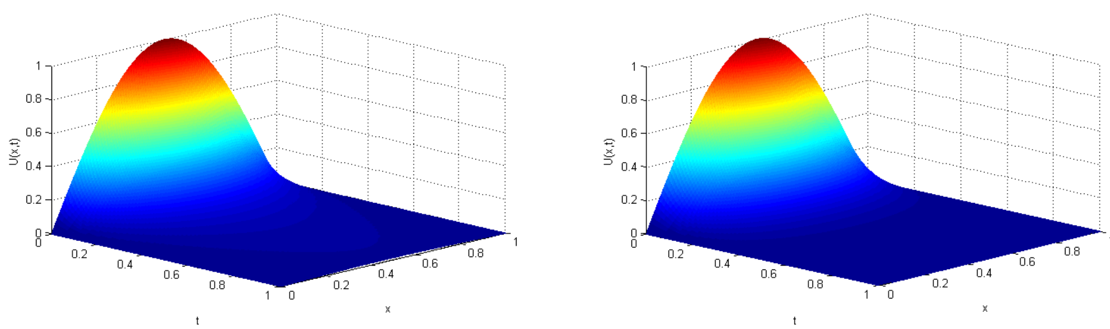



Figure 5.39: The numerical solution of Equation (5.461) using the KBMC3 scheme shown here in the case of the fractional exponent (a) $\gamma = 0.9$, and (b) $\gamma = 1$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ using with $\Delta t = 10^{-4}$.




(a) (b)

Figure 5.40: The numerical solution of Equation (5.461) using the KBML1 scheme shown here in the case of the fractional exponent (a) $\gamma = 0.1$, and (b) $\gamma = 0.5$ on the domain $0 \le t \le 1$, and $0 \le x \le 1$ using with $\Delta t = 10^{-4}$.




(a) (b)

Figure 5.41: The numerical solution of Equation (5.461) using the KBML1 scheme shown here in the case of the fractional exponent (a) $\gamma = 0.9$, and (b) $\gamma = 1$ on the domain $0 \le t \le 1$, and $0 \le x \le 1$ using with $\Delta t = 10^{-4}$.

**Example 5.8.4.** Consider the following fractional advection–diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} \right), \tag{5.464}$$

with the initial and fixed boundary conditions

$$u(x,0) = e^{-x/2} \sin(n\pi x),\ u(0,t) = 0,\ u(1,t) = 0 \tag{5.465}$$

where $0 \le x \le 1$, $0 \le t$. The exact solution of Equations (5.464), given (5.465), is

$$u(x,t) = e^{-x/2} \sin(n\pi x) E_\gamma(-\lambda_n^2 t^\gamma), \tag{5.466}$$

where $\lambda_n^2 = (1+4n^2\pi^2)/4$ with $n = 1$ and $E_\gamma(z)$ is the Mittag–Leffler function (Podlubny 1998).

We show the comparison of the exact solution and the numerical solution at the time $t = 0.25$, $0.5$, $0.75$ and $1.0$ with $\Delta t = 10^{-4}$ by using the KBMC2–FADE scheme, in Figure 5.42. The comparison at $x = 0.5$, $u(0.5, t)$ at time $t = 10^{-4}$ is given in Figure 5.43; we see the numerical estimate again lags behind the exact solution. This difference is more prominent than the difference seen in the previous example for the subdiffusion equation.

As we mentioned before in Chapter 3, a potential reason for this (and the lag seen in Figures 5.42) is that the first and second derivatives at $t = 0$ are not bounded in this example. Thus the assumption in Section 2.6.1 (in Chapter 2) that we can expand the solution as a Taylor series around $t = 0$ is not satisfied. When $\Delta t$ is decreased, we are in fact trying to approximate this singularity more closely but this is difficult to do numerically.

The results from the KBMC2–FADE scheme for Equation (5.464) given $\gamma = 0.1, 0.5, 0.9$, and 1, and $\Delta t = 10^{-4}$ are shown in Figures 5.44 and 5.45 respectively. Similar to Example 5.8.3 again we see the numerical solution of Equation (5.464) changes with the value of the exponent $\gamma$. From the results shown in Figures 5.44 and 5.45 again the solution decays faster to zero for larger values of $\gamma$ compared to smaller values of $\gamma$.

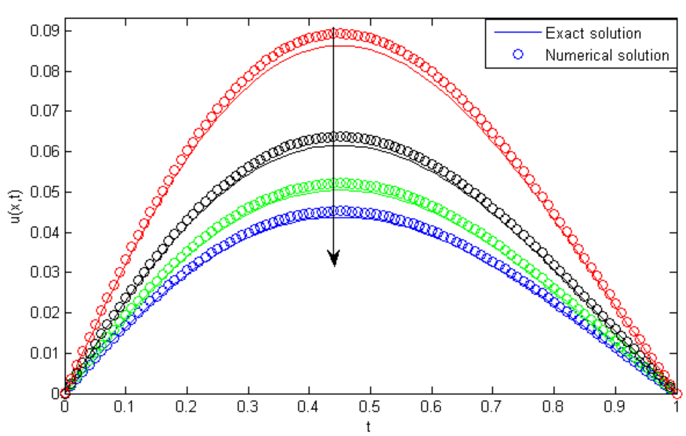



Figure 5.42: A comparison of the exact solution and the numerical solution for Equation (5.464), using the KBMC2–FADE scheme, shown at times $t = 0.25$, $0.5$, $0.75$, and $1.0$ in the case $\gamma = 0.5$ and $\Delta t = 10^{-4}$. Time increases in the direction of arrow.

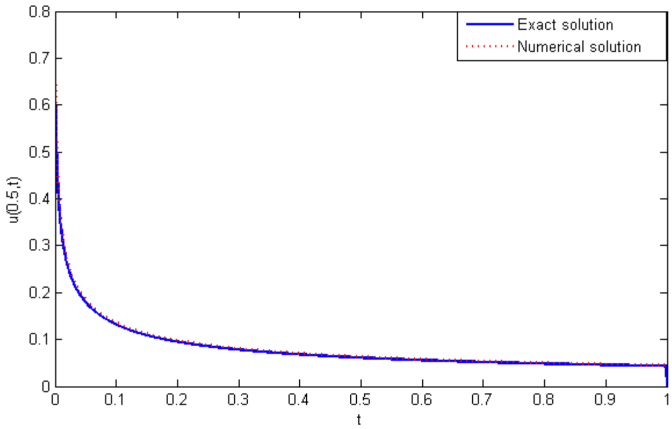
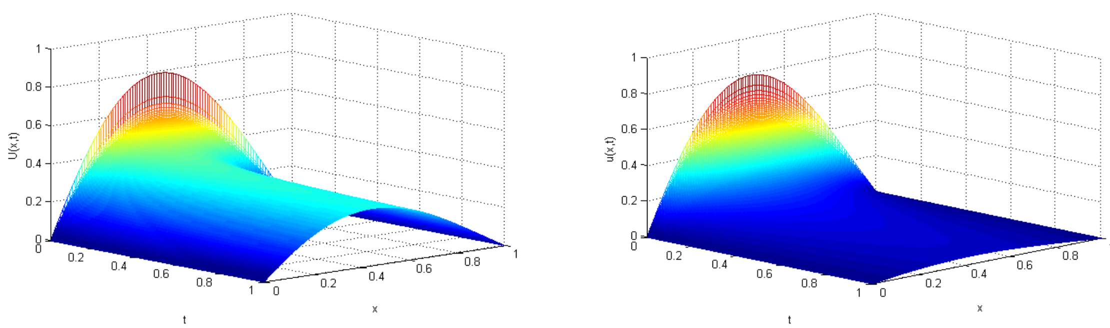



Figure 5.43: A comparison of the exact solution and the numerical solution present at the mid point $x = 0.5$ for Equation (5.464), using the KBMC2-FADE scheme, with $\gamma = 0.5$ and time step $\Delta t = 10^{-4}$.




(a) (b)

Figure 5.44: The numerical solution of Equation (5.464) using the KBMC2–FADE scheme shown here in the case of the fractional exponent (a) $\gamma = 0.1$, and (b) $\gamma = 0.5$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ using with $\Delta t = 10^{-4}$.

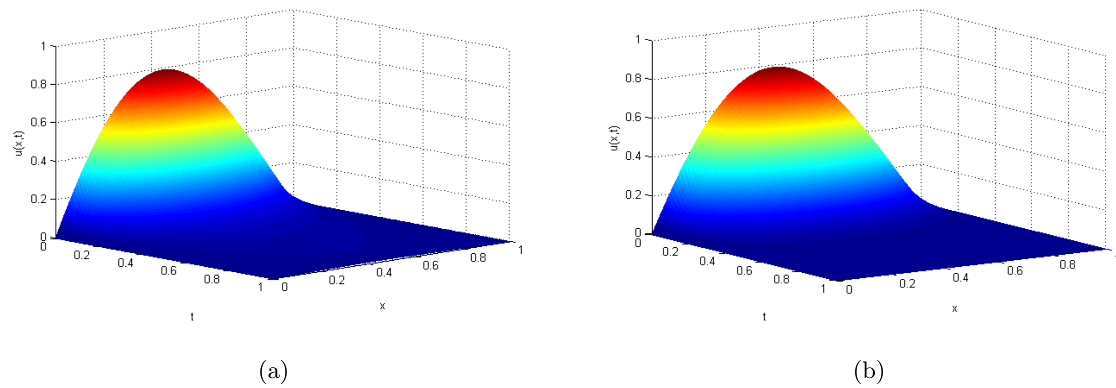



Figure 5.45: The numerical solution of Equation (5.464) using the KBMC2–FADE scheme shown here in the case of the fractional exponent (a) $\gamma = 0.9$, and (b) $\gamma = 1$ on the domain $0 \leq t \leq 1$, and $0 \leq x \leq 1$ using with $\Delta t = 10^{-4}$.

## 5.9 Conclusion

In this work, we constructed three Keller Box numerical schemes; the KBMC2, KBMC3 and KBML1 schemes for the solution of fractional subdiffusion equation. These schemes used the C2, C3, and the L1 approximation to estimate the Riemann–Liouville fractional derivative at the time $t = t_j$ for the KBML1 scheme and $t = t_{j+\frac{1}{2}}$ for the KBMC2 and KBMC3 schemes. The accuracy of KBMC2 and KBMC3 methods were found to be order $1 + \gamma$ in time and second order in space, whilst the accuracy of the KBML1 method was found again to be second order in space but only first order in time.

The stability of the KBMC2 method has been proved when $0 < \Lambda_q < \min(\frac{1}{\tilde{\mu}_0(\gamma)}, 2^\gamma)$ and $0 \leq \gamma \leq 1$ and demonstrated numerically when $\frac{1}{\tilde{\mu}_0(\gamma)} < \Lambda_q \leq 2^\gamma$ and $\log_3 2 \leq \gamma \leq 1$. We have also proved the stability of the KBMC3 method in the case where $0 < \breve{\Lambda}_q \leq 1$ and $0 < \gamma \leq 1$, and demonstrated the method is also stable numerically in case when $1 < \breve{\Lambda}_q \leq 2$. We have shown the KBML1 method is unconditionally stable using Von Neumann stability analysis. The convergence analysis of these methods are discussed. We show that the KBMC2 scheme, if $\widetilde{\lambda}_q = \min(\widetilde{\mu}_0(\gamma), 2^\gamma)$, and the KBMC3 scheme, if $0 < \widehat{\lambda}_q \leq 2/\widehat{\mu}_1(\gamma)$, are both convergent with order $1+\gamma$ in time and second order in space. But for the KBMC2–FADE schemes the convergence order, $1+\gamma$ in time and second order, was confirmed numerically. We also show the KBML1 method is convergent with first order in time and second order in space.

We conclude that the KBMC2 and KBMC3 method is more accurate in $\Delta t$ than KBML1 method especially when applied to the subdiffusion equation with no source term. The KBMC2 was also used for the fractional advection–diffusion equation and, similar to the KBMC2 and KBMC3 schemes, it was found to be second order in space and $1 + \gamma$ in time. The convergence orders were confirmed in the test examples for these methods where there was a source term and the exact solution is known and can be evaluated in MATLAB R2014a.

In addition, the numerical schemes, KBMC2, KBMC3, KBML1, and KBMC2–FADE schemes, for fractional subdiffusion and subdiffusion advection equations, where the source term is zero, are compared with the exact solution. We see the numerical estimate lags behind the exact solution. The numerical solutions in these cases decay faster to zero for larger values of $\gamma$ compared to smaller values of $\gamma$ as predicted by the behaviour of the Mittag–Leffler function for $0 < \gamma < 1$. We conclude that using the KBMC2 scheme is better method than the KBMC3 and KBML1 methods for all the examples given. Although both the KBMC2 and KBMC3 schemes perform better than the KBML1 scheme when applied to the subdiffusion equation.

# Chapter 6

# Solving a System of Nonlinear Fractional Differential Equation

## 6.1 Introduction

Fractional reaction subdiffusion equations have been found from Continuous Time Random Walk models which take into account the effect of long–tailed waiting time densities (i.e anomalous subdiffusion) on the reaction process (Henry & Wearne 2000, Seki, Wojcik & Tachiya 2003, Angstmann, Donnelly & Henry 2013*a*, Angstmann, Donnelly & Henry 2013*b*, Angstmann, Donnelly, Henry & Langlands 2016). Reaction diffusion equation provide a description of pattern formation in-homogeneous media since few realistic physical and biological systems are spatially homogeneous (Henry & Wearne 2002). The study of the solution of a fractional reaction–subdiffusion equations has become more prominent and important since there is growing estimation that anomalous diffusion is in fact ubiquitous in nature (Eliazar & Klafter 2011). But analytic solution of such equations are seldom available and so numerical techniques are needed.

In this chapter, we extend the Keller Box scheme, KBMC2 in Chapter 5, Section 5.2.1, to find the solution of systems of nonlinear fractional reaction–subdiffusion equations. We also develop another scheme, based upon the implicit scheme of Langlands & Henry (2005) to solve the same equations. These schemes were used to solve two fractional reaction–subdiffusion equation models. The first model, which we will denote as Model Type 1, is based upon the model by Henry & Wearne (2000) which is given by

$$\frac{\partial A(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}A(x,t)}{\partial t^{1-\gamma}}\right) - k_1A(x,t)B(x,t) + k_{-1}C(x,t), \tag{6.1}$$

$$\frac{\partial B(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}B(x,t)}{\partial t^{1-\gamma}}\right) - k_1A(x,t)B(x,t) + k_{-1}C(x,t), \tag{6.2}$$

and

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}C(x,t)}{\partial t^{1-\gamma}}\right) + k_1A(x,t)B(x,t) - k_{-1}C(x,t). \tag{6.3}$$

Here the reaction term is simply added to the subdiffusion equation (given by Equations (1.21) – (1.23) in Chapter 1). The solution of the Model Type 1 in the case $C \to A + B$ was found by Langlands et al. (2009) in the infinite domain, the result of a negative value was predicted which is physically unrealistic. From this we consider the second model, which we will denote as Model Type 2, is based upon a more recent model from Angstmann, Donnelly & Henry (2013*a*) which has a modified fractional operator (given by Equations (1.24) – (1.26) in Chapter 1)

$$\begin{aligned}\frac{\partial A(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}&\left[e^{-k_1\int_0^t B(x,s)ds}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_1\int_0^t B(x,s)ds}A(x,t)\right)\right]\\ &- k_1A(x,t)B(x,t) + k_{-1}C(x,t),\end{aligned} \tag{6.4}$$

$$\begin{aligned}\frac{\partial B(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}&\left[e^{-k_1\int_0^t A(x,s)ds}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_1\int_0^t A(x,s)ds}B(x,t)\right)\right]\\ &- k_1A(x,t)B(x,t) + k_{-1}C(x,t),\end{aligned} \tag{6.5}$$

and

$$\begin{aligned}\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}&\left[e^{-k_{-1}t}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(e^{k_{-1}t}C(x,t)\right)\right]\\ &+ k_1A(x,t)B(x,t) - k_{-1}C(x,t).\end{aligned} \tag{6.6}$$

Both of these models attempt to model the reversible reaction

$$A + B \rightleftharpoons C \tag{6.7}$$

in the presence of anomalous subdiffusion where $A$, $B$, and $C$ are three chemical species. In the absence of diffusion (a homogeneous environment) the governing equations for the concentrations of $A$, $B$, and $C$ for both models reduce to the reaction kinetic equations

$$\frac{dA}{dt} = -k_1AB + k_{-1}C, \tag{6.8}$$

$$\frac{dB}{dt} = -k_1 AB + k_{-1} C, \tag{6.9}$$

and

$$\frac{dC}{dt} = -k_{-1} C + k_1 AB, \tag{6.10}$$

where $k_1$ is reaction rate constant (forward rate), $k_{-1}$ is reverse reaction rate (backward rate). If $k_{-1} = 0$ then $A$ and $B$ react together to form species $C$ with no reverse reaction i.e. $A + B \to C$.

In Sections 6.2 and 6.5, the numerical schemes are developed for Model Type 1 and Model Type 2. We investigate the accuracy of these schemes, respectively, in Sections 6.4 and 6.7 for both models. We note the method in Cuesta, Lubich & Palencia (2006) could be used to discretise the equations for Model Type 1 by integrating both sides first. However, for Model Type 2, it is difficult to integrate both sides of equation because of the modified fractional operator and so this method will not work for this model.

## 6.2 Model Type 1

The fractional reaction–subdiffusion equation model in the case of a reversible reaction, in the presence of anomalous subdiffusion, is given by Equations (6.1) – (6.3). We refer to this model as a Model Type 1, which is based upon the reaction–subdiffusion model proposed by Henry & Wearne (2000).

## 6.3 Numerical Solution of Model Type 1

In this section, we develop two numerical schemes to solve Model Type 1. The first uses the Keller Box method with the C2 scheme, KBMC2, and the second uses the implicit method with the L1 scheme.

### 6.3.1 The Keller Box Scheme: KBMC2 Scheme

In this section, the numerical scheme for solving Model Type 1 will be developed based upon the Keller Box method with the C2 scheme approximation for the fractional derivative given in Chapter 2 by Equation (2.75). Similar to the KBMC2 scheme in Section 5.2.1, Chapter 5, we approximate each equation of Model Type 1 at the point $\left(x_{i-\frac{1}{2}}, t_{j+\frac{1}{2}}\right)$ as

$$\left[\frac{\partial A}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma} A}{\partial t^{1-\gamma}}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_1 \left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \tag{6.11}$$

$$\left[\frac{\partial B}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma} B}{\partial t^{1-\gamma}}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_1 \left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \tag{6.12}$$

$$\left[\frac{\partial C}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma} C}{\partial t^{1-\gamma}}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_1 \left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{6.13}$$

Following the approach in Chapter 5 Section 5.2.1, we have found the following equation for constant grid spacing for $A$

$$\begin{aligned}
&\left[2A_i^{j+1} + A_{i-1}^{j+1} + A_{i+1}^{j+1}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[A_{i-1}^{j+1} - 2A_i^{j+1} + A_{i+1}^{j+1}\right] \\
&= \left[2A_i^{j} + A_{i-1}^{j} + A_{i+1}^{j}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[A_{i-1}^{j} - 2A_i^{j} + A_{i+1}^{j}\right] + d\widetilde{\beta}_j(\gamma)\left(A_{i-1}^0 - 2A_i^0 + A_{i+1}^0\right) \\
&+ d\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\left(A_{i-1}^k - 2A_i^k + A_{i+1}^k\right) - \left(A_{i-1}^{k-1} - 2A_i^{k-1} + A_{i+1}^{k-1}\right)\right] \\
&- \frac{\Delta t k_1}{2}\left(\left[AB\right|_{i+1}^{j+1} + 2\left[AB\right|_i^{j+1} + \left[AB\right|_{i-1}^{j+1} + \left[AB\right|_{i+1}^{j} + 2\left[AB\right|_i^{j} + \left[AB\right|_{i-1}^{j}\right) \\
&+ \frac{\Delta t k_{-1}}{2}\left(\left[C\right|_{i+1}^{j+1} + 2\left[C\right|_i^{j+1} + \left[C\right|_{i-1}^{j+1} + \left[C\right|_{i+1}^{j} + 2\left[C\right|_i^{j} + \left[C\right|_{i-1}^{j}\right).
\end{aligned} \tag{6.14}$$

We find the corresponding discretised equation for $B$ in Equation (6.2) in a similar manner, swapping $A$ and $B$, to find

$$\begin{aligned}
&\left[2B_i^{j+1} + B_{i-1}^{j+1} + B_{i+1}^{j+1}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[B_{i-1}^{j+1} - 2B_i^{j+1} + B_{i+1}^{j+1}\right] \\
&= \left[2B_i^{j} + B_{i-1}^{j} + B_{i+1}^{j}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[B_{i-1}^{j} - 2B_i^{j} + B_{i+1}^{j}\right] + d\widetilde{\beta}_j(\gamma)\left(B_{i-1}^0 - 2B_i^0 + B_{i+1}^0\right) \\
&+ d\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\left(B_{i-1}^k - 2B_i^k + B_{i+1}^k\right) - \left(B_{i-1}^{k-1} - 2B_i^{k-1} + B_{i+1}^{k-1}\right)\right] \\
&- \frac{\Delta t k_1}{2}\left[2\left[AB\right|_i^{j+1} + \left[AB\right|_{i-1}^{j+1} + \left[AB\right|_{i+1}^{j+1} + 2\left[AB\right|_i^{j} + \left[AB\right|_{i-1}^{j} + \left[AB\right|_{i+1}^{j}\right] \\
&+ \frac{\Delta t k_{-1}}{2}\left[2\left[C\right|_i^{j+1} + \left[C\right|_{i-1}^{j+1} + \left[C\right|_{i+1}^{j+1} + 2\left[C\right|_i^{j} + \left[C\right|_{i-1}^{j} + \left[C\right|_{i+1}^{j}\right].
\end{aligned} \tag{6.15}$$

Finally we find the approximation of the last equation in Equation (6.3) for $C$, as

$$\begin{aligned}
&\left[2C_i^{j+1} + C_{i-1}^{j+1} + C_{i+1}^{j+1}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[C_{i-1}^{j+1} - 2C_i^{j+1} + C_{i+1}^{j+1}\right] \\
&= \left[2C_i^{j} + C_{i-1}^{j} + C_{i+1}^{j}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[C_{i-1}^{j} - 2C_i^{j} + C_{i+1}^{j}\right] + d\widetilde{\beta}_j(\gamma)\left(C_{i-1}^{0} - 2C_i^{0} + C_{i+1}^{0}\right) \\
&+ d\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\left(C_{i-1}^{k} - 2C_i^{k} + C_{i+1}^{k}\right) - \left(C_{i-1}^{k-1} - 2C_i^{k-1} + C_{i+1}^{k-1}\right)\right] \\
&+ \frac{\Delta t k_1}{2}\left[2\left[AB\right|_i^{j+1} + \left[AB\right|_{i-1}^{j+1} + \left[AB\right|_{i+1}^{j+1} + 2\left[AB\right|_i^{j} + \left[AB\right|_{i-1}^{j} + \left[AB\right|_{i+1}^{j}\right] \\
&- \frac{\Delta t k_{-1}}{2}\left[2\left[C\right|_i^{j+1} + \left[C\right|_{i-1}^{j+1} + \left[C\right|_{i+1}^{j+1} + 2\left[C\right|_i^{j} + \left[C\right|_{i-1}^{j} + \left[C\right|_{i+1}^{j}\right],
\end{aligned} \tag{6.16}$$

with

$$d = \frac{4D\Delta t^{\gamma}}{\Delta x^2\Gamma(1+\gamma)}. \tag{6.17}$$

### 6.3.2 The Implicit Finite Difference Scheme: IML1 Scheme

In this section, we develop the implicit finite difference scheme with the L1 scheme, in Chapter 2 Equation (2.12), where $p = 1-\gamma$. Using a similar approach to that used in Langlands & Henry (2005), for the subdiffusion equation, we approximate the derivatives in Equations (6.1) – (6.3) at the point $(x_i, t_j)$ as

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_i^j, \tag{6.18}$$

$$\left[\frac{\partial B}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma}B}{\partial t^{1-\gamma}}\right|_i^j, \tag{6.19}$$

and

$$\left[\frac{\partial C}{\partial t}\right|_i^j = k_1\left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma}C}{\partial t^{1-\gamma}}\right|_i^j. \tag{6.20}$$

We refer to this approximation as the IML1 scheme. We now approximate the second order spatial derivative in Equations (6.18), (6.19) and (6.20) by using the centred finite difference scheme (Equation (3.6) for the second spatial derivative), and the backward finite difference (Equation (3.9) for the first temporal), so we have

$$\frac{A_i^j - A_i^{j-1}}{\Delta t} = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + \frac{D}{\Delta x^2}\left\{\left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_{i+1}^j - 2\left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_i^j + \left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_{i-1}^j\right\}, \tag{6.21}$$

$$\frac{B_i^j - B_i^{j-1}}{\Delta t} = -k_1 \left[AB\right|_i^j + k_{-1} \left[C\right|_i^j + \frac{D}{\Delta x^2} \left\{ \left[ \frac{\partial^{1-\gamma} B}{\partial t^{1-\gamma}} \right|_{i+1}^j - 2 \left[ \frac{\partial^{1-\gamma} B}{\partial t^{1-\gamma}} \right|_i^j + \left[ \frac{\partial^{1-\gamma} B}{\partial t^{1-\gamma}} \right|_{i-1}^j \right\}, \tag{6.22}$$

and

$$\frac{C_i^j - C_i^{j-1}}{\Delta t} = k_1 AB - k_{-1} C + \frac{D}{\Delta x^2} \left\{ \left[ \frac{\partial^{1-\gamma} C}{\partial t^{1-\gamma}} \right|_{i+1}^j - 2 \left[ \frac{\partial^{1-\gamma} C}{\partial t^{1-\gamma}} \right|_i^j + \left[ \frac{\partial^{1-\gamma} C}{\partial t^{1-\gamma}} \right|_{i-1}^j \right\}. \tag{6.23}$$

After approximating the fractional derivative using the L1 scheme (in Chapter 2 Equation (2.12)), Equations (6.21) – (6.23) reduce to

$$\begin{aligned} A_i^j - \hat{d}\left(A_{i+1}^j - 2A_i^j + A_{i-1}^j\right) &= A_i^{j-1} - \Delta t k_1 \left[AB\right|_i^j + \Delta t k_{-1} \left[C\right|_i^j \\ + \hat{d}\left\{ \beta_j(\gamma)\left(A_{i+1}^0 - 2A_i^0 + A_{i-1}^0\right) \right. &+ \left. \sum_{k=1}^{j-1} \mu_{j-k}(\gamma)\left(A_{i+1}^k - 2A_i^k + A_{i-1}^k\right) \right\}, \end{aligned} \tag{6.24}$$

$$\begin{aligned} B_i^j - \hat{d}\left(B_{i+1}^j - 2B_i^j + B_{i-1}^j\right) &= B_i^{j-1} - \Delta t k_1 \left[AB\right|_i^j + \Delta t k_{-1} \left[C\right|_i^j \\ + \hat{d}\left\{ \beta_j(\gamma)\left(B_{i+1}^0 - 2B_i^0 + B_{i-1}^0\right) \right. &+ \left. \sum_{k=1}^{j-1} \mu_{j-k}(\gamma)\left(B_{i+1}^k - 2B_i^k + B_{i-1}^k\right) \right\}, \end{aligned} \tag{6.25}$$

and

$$\begin{aligned} (1 + \Delta t k_{-1}) C_i^j - \hat{d}\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right) &= C_i^{j-1} + \Delta t k_1 \left[AB\right|_i^j \\ + \hat{d}\left[ \beta_j(\gamma)\left(C_{i+1}^0 - 2C_i^0 + C_{i-1}^0\right) \right. &+ \left. \sum_{k=1}^{j-1} \mu_{j-k}(\gamma)\left(C_{i+1}^k - 2C_i^k + C_{i-1}^k\right) \right\}, \end{aligned} \tag{6.26}$$

where

$$\hat{d} = \frac{D \Delta t^\gamma}{\Delta x^2 \Gamma(1+\gamma)}, \tag{6.27}$$

and the weights $\beta_j(\gamma)$ and $\mu_j(\gamma)$ are given by

$$\beta_j(\gamma) = \gamma j^{\gamma-1} + (j-1)^\gamma - j^\gamma, \tag{6.28}$$

and

$$\mu_j(\gamma) = (j-1)^\gamma - 2j^\gamma + (j+1)^\gamma. \tag{6.29}$$

## 6.4 Accuracy of the Numerical Methods for Model Type 1

In this section, we consider the order of accuracy of the numerical schemes developed in Sections 6.3.1 and 6.3.2. In the following we denote the centred–finite difference approximation by the symbol $\delta_x^2 Z$

$$\delta_x^2 Z_i^j = \frac{Z_{i+1}^j - 2Z_i^j + Z_{i-1}^j}{\Delta x^2} \tag{6.30}$$

for $Z(x,t)$.

### 6.4.1 Accuracy of the Keller Box Method

We now determine the truncation error of KBMC2 scheme for Model 1, first by using Equation (6.30) with $Z = A$ to rewrite Equation (6.14) as

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right] + \frac{1}{\Delta t}\left[A_i^{j+1} - A_i^j\right] \\
&= \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^{\gamma}\left[\left(\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right) - 2\left(\delta_x^2 A_i^{j+\frac{1}{2}} - \delta_x^2 A_i^j\right)\right]\right\} \\
&+ \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 A_i^0 + 2\left(\frac{1}{2}\right)^{\gamma}\left(\delta_x^2 A_i^{j+\frac{1}{2}} - \delta_x^2 A_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left[\delta_x^2 A_i^k - \delta_x^2 A_i^{k-1}\right]\right\} \\
&- \frac{k_1}{8}\left[\Delta x^2\left(\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^j\right) + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^j\right)\right] \\
&+ \frac{k_{-1}}{8}\left[\Delta x^2\left(\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^j\right) + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^j\right)\right].
\end{aligned} \tag{6.31}$$

Identifying the second line on the right hand side of Equation (6.31) as the C2 approximation with $A(t)$ replaced by $\delta_x^2 A(t)$. We can rewrite Equation (6.31) as

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right] + \frac{1}{\Delta t}\left[A_i^{j+1} - A_i^j\right] \\
&= \frac{\left(\frac{1}{2}\right)^{\gamma} D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\delta_x^2 A_i^{j+1} + \delta_x^2 A_i^j - 2\delta_x^2 A_i^{j+\frac{1}{2}}\right] + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 A\right)\right|_{i,C2}^{j+\frac{1}{2}} \\
&- \frac{k_1}{8}\left[\Delta x^2\left(\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^j\right) + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^j\right)\right] \\
&+ \frac{k_{-1}}{8}\left[\Delta x^2\left(\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^j\right) + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^j\right)\right].
\end{aligned} \tag{6.32}$$

Taking the Taylor series expansion around the point $x_i = i\Delta x$ in space, we then have

$$\delta_x^2 A_i^j \simeq \left[\frac{\partial^2 A}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 A}{\partial x^4}\right|_i^j + O(\Delta x^6). \tag{6.33}$$

Likewise taking the Taylor series expansion around the point $\left(x_i, t_{j+\frac{1}{2}}\right)$ we have

$$\Delta t^{\gamma-1}\left(\delta_x^2 A_i^{j+1} + \delta_x^2 A_i^j - 2\delta_x^2 A_i^{j+\frac{1}{2}}\right) \simeq \Delta t^{\gamma-1}\left(\frac{\Delta t^2}{4}\left[\frac{\partial^2}{\partial t^2}\delta_x^2 A\right|_i^{j+\frac{1}{2}} + O(\Delta x^2 \Delta t^2)\right)$$
$$= O(\Delta t^{1+\gamma}), \tag{6.34}$$

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right] \simeq \frac{\Delta x^2}{4\Delta t}\left(\Delta t\left[\frac{\partial^3 A}{\partial x^2 \partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta x^2 \Delta t)\right)$$
$$= O(\Delta x^2), \tag{6.35}$$

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 A\right)\right|_{i,C2}^{j+\frac{1}{2}} \simeq \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}} + O(\Delta x^2), \tag{6.36}$$

$$[AB]_i^{j+1} + [AB]_i^j \simeq 2\,[AB]_i^{j+\frac{1}{2}} + O(\Delta t^2), \tag{6.37}$$

$$\left[\delta_x^2 AB\right]_i^{j+1} + \left[\delta_x^2 AB\right]_i^j \simeq 2\left[\frac{\partial^2 (AB)}{\partial x^2}\right]_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^2), \tag{6.38}$$

$$\left[\delta_x^2 C\right]_i^{j+1} + \left[\delta_x^2 C\right]_i^j \simeq 2\left[\frac{\partial^2 C}{\partial x^2}\right]_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^2), \tag{6.39}$$

$$C_i^{j+1} + C_i^j \simeq 2\,[C|_i^{j+\frac{1}{2}} + O(\Delta t^2), \tag{6.40}$$

and

$$\frac{A_i^{j+1} - A_i^j}{\Delta t} \simeq \left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2). \tag{6.41}$$

We also have

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right] \simeq \Delta x^2\left[\frac{1}{4}\frac{\partial}{\partial t}\delta_x^2 A_i^{j+\frac{1}{2}} + O(\Delta t^2)\right] = \frac{\Delta x^2}{4}\left[\frac{\partial^3 A}{\partial x^2 \partial t}\right|_i^{j+\frac{1}{2}}. \tag{6.42}$$

Using these expansions in Equation (6.32) we find

$$\left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^{1+\gamma}) - k_1\,[AB]_i^{j+\frac{1}{2}} + k_{-1} C_i^{j+\frac{1}{2}}. \tag{6.43}$$

Now adding and subtracting the exact value of the fractional derivative, we then have

$$\left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} = \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - k_1 \left[AB\right|_i^{j+\frac{1}{2}} + k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^{1+\gamma})$$
$$- D\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right]. \tag{6.44}$$

By (2.149) in Chapter 2 the term

$$\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 A}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right] \tag{6.45}$$

is $O(\Delta t^{1+\gamma})$, we then find the truncation error is of the order $1+\gamma$ in time and second order in space, similar to that which was found in Chapter 5. Following a similar process, swapping $A$ and $B$ we see the truncation error for Equation (6.15) is also the same.

In a similar manner, to find the truncation error accuracy of Equation (6.16), we again use Equation (6.30), with $Z = C$, to find

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 C_i^{j+1} - \delta_x^2 C_i^j\right] + \frac{1}{\Delta t}\left[C_i^{j+1} - C_i^j\right]$$
$$= \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\left(\frac{1}{2}\right)^\gamma \left[\left(\delta_x^2 C_i^{j+1} - \delta_x^2 C_i^j\right) - 2\left(\delta_x^2 C_i^{j+\frac{1}{2}} - \delta_x^2 C_i^j\right)\right]\right\}$$
$$+ \frac{D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\widetilde{\beta}_j(\gamma)\delta_x^2 C_i^0 + 2\left(\frac{1}{2}\right)^\gamma\left(\delta_x^2 C_i^{j+\frac{1}{2}} - \delta_x^2 C_i^j\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}\left[\delta_x^2 C_i^k - \delta_x^2 C_i^{k-1}\right]\right\}$$
$$+ \frac{k_1}{8}\left[\Delta x^2\left(\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^j\right) + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^j\right)\right]$$
$$- \frac{k_{-1}}{8}\left[\Delta x^2\left(\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^j\right) + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^j\right)\right]. \tag{6.46}$$

Note the second term on the right hand side in Equation (6.46) is the C2 approximation with $C(t)$ replaced by $\delta_x^2 C(t)$. We can then rewrite Equation (6.46) as

$$\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 C_i^{j+1} - \delta_x^2 C_i^j\right] + \frac{1}{\Delta t}\left[C_i^{j+1} - C_i^j\right]$$
$$= \frac{\left(\frac{1}{2}\right)^\gamma D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\delta_x^2 C_i^{j+1} + \delta_x^2 C_i^j - 2\delta_x^2 C_i^{j+\frac{1}{2}}\right] + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 C\right)\right|_{i,C2}^{j+\frac{1}{2}}$$
$$+ \frac{k_1}{8}\left[\Delta x^2\left(\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^j\right) + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^j\right)\right]$$
$$- \frac{k_{-1}}{8}\left[\Delta x^2\left(\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^j\right) + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^j\right)\right]. \tag{6.47}$$

In a similar manner to earlier, expanding the Taylor series around the point $\left(x_i, t_{j+\frac{1}{2}}\right)$

by using Equations (6.33) – (6.42), we then have

$$\left[\frac{\partial C}{\partial t}\right|_i^{j+\frac{1}{2}} = D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^{1+\gamma}) + k_1\left[AB\right]_i^{j+\frac{1}{2}} - k_{-1}C_i^{j+\frac{1}{2}}. \tag{6.48}$$

Adding and subtracting the exact fractional derivative, we then have

$$\begin{aligned}\left[\frac{\partial C}{\partial t}\right|_i^{j+\frac{1}{2}} &= D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} + k_1\left[AB\right|_i^{j+\frac{1}{2}} - k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^{1+\gamma}) \\ &\quad - D\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right].\end{aligned} \tag{6.49}$$

By Equation (2.149) we know the term

$$\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right] \tag{6.50}$$

is $O(\Delta t^{1+\gamma})$, and hence the truncation error, $\tau_{i,j}$, for Equation (6.16) (and Equations (6.14) and (6.15)) is of the order $1+\gamma$ in time and second order in space i.e.

$$\tau_{i,j} = O(\Delta t^{1+\gamma}) + O(\Delta x^2). \tag{6.51}$$

### 6.4.2 Accuracy of the Implicit Finite Difference Scheme (IML1)

To find the truncation error accuracy of the IML1 scheme in Section 6.3.2, we first rewrite Equation (6.24), using the notation in Equation (6.30), with $Z = A$, as

$$\frac{A_i^j - A_i^{j-1}}{\Delta t} = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\beta_j(\gamma)\delta_x^2 A_i^0 + \delta_x^2 A_i^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\delta_x^2 A_i^k\right]. \tag{6.52}$$

Note the last term in the brackets in Equation (6.52) is the L1 approximation, Equation (2.12), with $A(t)$ replaced by $\delta_x^2 A(t)$. Therefore we can rewrite Equation (6.60) as

$$\frac{A_i^j - A_i^{j-1}}{\Delta t} = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\delta_x^2 A\right)\right|_{i,L1}^j. \tag{6.53}$$

Now taking the Taylor series expansion around the point $t_j = j\Delta t$ gives

$$\frac{A_i^{j+1} - A_i^j}{\Delta t} \simeq \left[\frac{\partial A}{\partial t}\right|_i^j + \frac{\Delta t}{2!}\left[\frac{\partial^2 A}{\partial t^2}\right|_i^j + O(\Delta t^2), \tag{6.54}$$

$$\delta_x^2 A_i^j \simeq \left[\frac{\partial^2 A}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 A}{\partial x^4}\right|_i^j + O(\Delta x^6), \tag{6.55}$$

and using these results in Equation (6.53) we find

$$\begin{aligned}\left[\frac{\partial A}{\partial t}\right|_i^j + \frac{\Delta t}{2!}\left[\frac{\partial^2 A}{\partial t^2}\right|_i^j + O(\Delta t^2) = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j \\ + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\left[\frac{\partial^2 A}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 A}{\partial x^4}\right|_i^j + O(\Delta x^6)\right)\right|_{L1}.\end{aligned} \tag{6.56}$$

Adding and subtracting the exact value of the fractional derivative, then gives

$$\begin{aligned}\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_i^j + O(\Delta x^2) + O(\Delta t) \\ - D\left[\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right)\right|_i^j - \left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right)\right|_{i,L1}^j\right].\end{aligned} \tag{6.57}$$

Note by Equation (2.48) the term

$$\left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_i^j - \left[\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right|_{i,L1}^j \tag{6.58}$$

is $O(\Delta t^{1+\gamma})$, and so we have

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}A}{\partial t^{1-\gamma}}\right)\right|_i^j + O(\Delta x^2) + O(\Delta t). \tag{6.59}$$

Hence the truncation error is first order in time and second order in space. Using similar steps the truncation error of Equation (6.25) again is first order in time and second order in space.

We now will consider the truncation error of Equation (6.26). Again using Equation (6.30), with $Z = C$, we have

$$\frac{C_i^j - C_i^{j-1}}{\Delta t} = k_1\left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\beta_j(\gamma)\delta_x^2 C_i^0 + \delta_x^2 C_i^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\delta_x^2 C_i^k\right]. \tag{6.60}$$

Identifying the last term in the brackets in Equations (6.60) as the L1 approximation with $C(t)$ replaced by $\delta_x^2 C(t)$, we can then rewrite Equation (6.60) as

$$\frac{C_i^j - C_i^{j-1}}{\Delta t} = k_1\left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\delta_x^2 C\right|_{i,L1}^j. \tag{6.61}$$

Expanding the Taylor series around the point $(x_i, t_j)$, using Equations (6.54) and (6.55) with $A = C$, then Equation (6.61) becomes

$$\left[\frac{\partial C}{\partial t}\right|_i^j + \frac{\Delta t}{2!}\left[\frac{\partial^2 C}{\partial t^2}\right|_i^j + O(\Delta t^2) = k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\left[\frac{\partial^2 C}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 C}{\partial x^4}\right|_i^j + O(\Delta x^6)\right)\right|_{L1}. \tag{6.62}$$

Adding and subtracting the exact value of the fractional derivative, we then obtain

$$\begin{aligned}\left[\frac{\partial C}{\partial t}\right|_i^j &= k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left[\frac{\partial^2 C}{\partial x^2}\right|_i^j + O(\Delta x^2) + O(\Delta t) \\ &\quad - D\left[\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_{i,L1}^j\right].\end{aligned} \tag{6.63}$$

Note by Equation (2.48) the term

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{\partial^2 C}{\partial x^2}\right)\right|_{i,L1}^j \simeq O(\Delta t^{1+\gamma}), \tag{6.64}$$

therefore we have

$$\left[\frac{\partial C}{\partial t}\right|_i^j = k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma} C}{\partial t^{1-\gamma}}\right)\right|_i^j + O(\Delta x^2) + O(\Delta t). \tag{6.65}$$

Hence the truncation error, $\tau_{i,j}$, for Equations (6.24) – (6.26) is first order in time and second order in space, that is

$$\tau_{i,j} = O(\Delta x^2) + O(\Delta t). \tag{6.66}$$

## 6.5 Model Type 2

In this section, we consider another model, Model Type 2, of the reversible reaction $A + B \rightleftarrows C$ given by Equations (6.4) – (6.6), based upon the model by Angstmann, Donnelly & Henry (2013*a*). These equations include the non-standard fractional derivative operator $L_t^{1-\gamma}$

$$L_t^{1-\gamma} = e^{-k_1 \int_0^t B(x,s)ds}\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}e^{k_1 \int_0^t B(x,s)ds}, \tag{6.67}$$

which takes into account that reactants may be removed before diffusing. The current methods for approximating fractional derivatives will need to be modified to approximate the operator in Equation (6.67).

To do this we also define the auxiliary variables

$$y_1(x,t) = e^{-k_1 \int_0^t B(x,s)ds}, \tag{6.68}$$

$$y_2(x,t) = e^{-k_1 \int_0^t A(x,s)ds}, \tag{6.69}$$

and

$$y_3(x,t) = e^{-k_{-1}t}, \tag{6.70}$$

which will be used to evaluate the non–standard fractional operator in Equation (6.67). Taking the derivative of $y_r$, where $r = 1, 2, 3$ with respect to $t$ we then get

$$\frac{\partial y_1}{\partial t} = e^{-k_1 \int_0^t B(x,s)ds}\left[-k_1 B(x,t)\right] = -k_1 B(x,t) y_1(x,t), \tag{6.71}$$

$$\frac{\partial y_2}{\partial t} = e^{-k_1 \int_0^t A(x,s)ds}\left[-k_1 A(x,t)\right] = -k_1 A(x,t) y_2(x,t), \tag{6.72}$$

and

$$\frac{\partial y_3}{\partial t} = -k_{-1} e^{-k_{-1}t} = -k_{-1} y_3(x,t). \tag{6.73}$$

The differential equations in Equations (6.71), (6.72), and (6.73) are supplemented by the initial conditions $y_r(x,0) = 1$, where $r = 1, 2, 3$.

## 6.6 Numerical Solution of Model Type 2

In this section, we develops two numerical schemes to solve the equations for Model Type 2. As in Section 6.3, the first scheme is based upon the Keller Box method and the C2 scheme while the second uses the implicit method with the L1 scheme.

### 6.6.1 The Keller Box Scheme: KBMC2 Scheme

In this section, the numerical scheme for solving the equations for Model Type 2 will be developed based on the Keller Box method with the C2 scheme as given in Section 5.2.1

of Chapter 5. Here, similar to Section 6.3.1, we approximate Equations (6.4) – (6.6) and Equations (6.71) – (6.73) at the point $\left(x_{i-\frac{1}{2}}, t_{j+\frac{1}{2}}\right)$ as

$$\left[\frac{\partial A}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\frac{\partial^2}{\partial x^2}\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_1\left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \tag{6.74}$$

$$\left[\frac{\partial B}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\frac{\partial^2}{\partial x^2}\left[y_2\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{B}{y_2}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_1\left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \tag{6.75}$$

$$\left[\frac{\partial C}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\frac{\partial^2}{\partial x^2}\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_1\left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}, \tag{6.76}$$

$$\left[\frac{\partial y_1}{\partial t}\right|_{i}^{j+\frac{1}{2}} = -k_1\left[By_1\right|_{i}^{j+\frac{1}{2}}, \tag{6.77}$$

$$\left[\frac{\partial y_2}{\partial t}\right|_{i}^{j+\frac{1}{2}} = -k_1\left[Ay_2\right|_{i}^{j+\frac{1}{2}}, \tag{6.78}$$

and

$$\left[\frac{\partial y_3}{\partial t}\right|_{i}^{j+\frac{1}{2}} = -k_{-1}\left[y_3\right|_{i}^{j+\frac{1}{2}}. \tag{6.79}$$

We now consider the discretisation of Equation (6.74) first. We define first the spatial derivative in Equation (6.74) by

$$v = \frac{\partial}{\partial x}\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right]. \tag{6.80}$$

Using Equation (6.80) in Equation (6.74) we get the system of equations

$$\left[\frac{\partial}{\partial x}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_{i-\frac{1}{2}}^{j} = \left[v\right|_{i-\frac{1}{2}}^{j}, \tag{6.81}$$

and

$$\left[\frac{\partial A}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_1\left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{6.82}$$

Approximating the first order spatial and time derivatives in Equations (6.81) and (6.82) by using the centred finite difference scheme (as in Chapter 3 given by Equations (3.8) and (3.9)), we then obtain the equations

$$\frac{1}{\Delta x_i}\left(\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i}^{j} - \left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^{j}\right) = \left[v\right|_{i-\frac{1}{2}}^{j}, \tag{6.83}$$

and

$$\left[\frac{A_{i-\frac{1}{2}}^{j+1} - A_{i-\frac{1}{2}}^{j}}{\Delta t}\right] = \frac{D}{\Delta x_i}\left(v_i^{j+\frac{1}{2}} - v_{i-1}^{j+\frac{1}{2}}\right) - k_1 \left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{6.84}$$

We also approximate the terms $A_{i-\frac{1}{2}}^{j}$, $[AB|_{i-\frac{1}{2}}^{j}$ and $C_{i-\frac{1}{2}}^{j}$ by the corresponding spatial averages

$$A_{i-\frac{1}{2}}^{j} = \frac{A_i^j + A_{i-1}^j}{2},\ [AB|_{i-\frac{1}{2}}^{j} = \frac{[AB|_i^j + [AB|_{i-1}^j}{2},\ \text{and } C_{i-\frac{1}{2}}^{j} = \frac{C_i^j + C_{i-1}^j}{2}. \tag{6.85}$$

Using these averages in Equations (6.83) and (6.84), gives

$$\frac{1}{\Delta x_i}\left(\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^j - \left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^j\right) = \frac{1}{2}\left(v_i^j + v_{i-1}^j\right), \tag{6.86}$$

and

$$\begin{aligned}\frac{1}{2\Delta t}\left[\left(A_i^{j+1} + A_{i-1}^{j+1}\right) - \left(A_i^j + A_{i-1}^j\right)\right] &= \frac{D}{\Delta x_i}\left(v_i^{j+\frac{1}{2}} - v_{i-1}^{j+\frac{1}{2}}\right) \\ &- \frac{k_1}{2}\left([AB|_i^{j+\frac{1}{2}} + [AB|_{i-1}^{j+\frac{1}{2}}\right) + \frac{k_{-1}}{2}\left([C|_i^{j+\frac{1}{2}} + [C|_{i-1}^{j+\frac{1}{2}}\right).\end{aligned} \tag{6.87}$$

Solving Equation (6.86) for $v_{i-1}^j$, we find

$$v_{i-1}^j = \frac{2}{\Delta x_i}\left(\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^j - \left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^j\right) - v_i^j, \tag{6.88}$$

and then combining with Equation (6.87), gives

$$\begin{aligned}&\frac{1}{2\Delta t}\left[\left(A_i^{j+1} + A_{i-1}^{j+1}\right) - \left(A_i^j + A_{i-1}^j\right)\right] \\ &= \frac{D}{\Delta x_i}\left\{v_i^{j+\frac{1}{2}} - \left[\frac{2}{\Delta x_i}\left(\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}} - \left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^{j+\frac{1}{2}}\right) - v_i^{j+\frac{1}{2}}\right]\right\} \\ &- \frac{k_1}{2}\left([AB|_i^{j+\frac{1}{2}} + [AB|_{i-1}^{j+\frac{1}{2}}\right) + \frac{k_{-1}}{2}\left([C|_i^{j+\frac{1}{2}} + [C|_{i-1}^{j+\frac{1}{2}}\right),\end{aligned} \tag{6.89}$$

or

$$\begin{aligned}&\frac{1}{2\Delta t}\left[\left(A_i^{j+1} + A_{i-1}^{j+1}\right) - \left(A_i^j + A_{i-1}^j\right)\right] \\ &\quad = \frac{2D}{\Delta x_i}v_i^{j+\frac{1}{2}} - \frac{2D}{\Delta x_i^2}\left(\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}} - \left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^{j+\frac{1}{2}}\right) \\ &\quad - \frac{k_1}{2}\left([AB|_i^{j+\frac{1}{2}} + [AB|_{i-1}^{j+\frac{1}{2}}\right) + \frac{k_{-1}}{2}\left([C|_i^{j+\frac{1}{2}} + [C|_{i-1}^{j+\frac{1}{2}}\right).\end{aligned} \tag{6.90}$$

Using a similar process to the above, except now replacing $i$ with $i+1$ in Equations (6.81) and (6.82) and eliminating $v_{i+1}^{j}$, we have the equation

$$\frac{1}{2\Delta t}\left[\left(A_{i+1}^{j+1}+A_{i}^{j+1}\right)-\left(A_{i+1}^{j}+A_{i}^{j}\right)\right] \tag{6.91}$$
$$=\frac{2D}{\Delta x_{i+1}^{2}}\left(\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1}^{j+\frac{1}{2}}-\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i}^{j+\frac{1}{2}}\right)$$
$$-\frac{2D}{\Delta x_{i+1}}v_i^{j+\frac{1}{2}}-\frac{k_1}{2}\left([AB|_{i+1}^{j+\frac{1}{2}}+[AB|_{i}^{j+\frac{1}{2}}\right)+\frac{k_{-1}}{2}\left([C|_{i+1}^{j+\frac{1}{2}}+[C|_{i}^{j+\frac{1}{2}}\right).$$

Now multiplying Equation (6.90) by $\Delta x_i$ and Equation (6.91) by $\Delta x_{i+1}$, and adding the two gives the equation for species $A$

$$\frac{1}{2\Delta t}\left[\Delta x_i\left(A_i^{j+1}+A_{i-1}^{j+1}\right)+\Delta x_{i+1}\left(A_{i+1}^{j+1}+A_i^{j+1}\right)\right] \tag{6.92}$$
$$=\frac{1}{2\Delta t}\left[\Delta x_i\left(A_i^{j}+A_{i-1}^{j}\right)+\Delta x_{i+1}\left(A_{i+1}^{j}+A_i^{j}\right)\right]$$
$$-D\left[\frac{2}{\Delta x_{i+1}}+\frac{2}{\Delta x_i}\right]y_{1}{}_i^{j+\frac{1}{2}}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}}+\frac{2D}{\Delta x_{i+1}}y_{1}{}_{i+1}^{j+\frac{1}{2}}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1}^{j+\frac{1}{2}}$$
$$+\frac{2D}{\Delta x_i}y_{1}{}_{i-1}^{j+\frac{1}{2}}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^{j+\frac{1}{2}}-\frac{k_1}{2}\left[(\Delta x_i+\Delta x_{i+1})\,[AB|_i^{j+\frac{1}{2}}+\Delta x_i\,[AB|_{i-1}^{j+\frac{1}{2}}\right.$$
$$\left.+\Delta x_{i+1}\,[AB|_{i+1}^{j+\frac{1}{2}}\right]+\frac{k_{-1}}{2}\left[(\Delta x_i+\Delta x_{i+1})\,[C|_i^{j+\frac{1}{2}}+\Delta x_i\,[C|_{i-1}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[C|_{i+1}^{j+\frac{1}{2}}\right].$$

Now using the C2 approximation, Equation (2.75), of the fractional derivative in Equation (6.92) we then have

$$\frac{1}{2\Delta t}\left[\Delta x_i\left(A_i^{j+1}+A_{i-1}^{j+1}\right)+\Delta x_{i+1}\left(A_{i+1}^{j+1}+A_i^{j+1}\right)\right]=\frac{1}{2\Delta t}\left[\Delta x_i\left(A_i^{j}+A_{i-1}^{j}\right)\right.$$
$$\left.+\Delta x_{i+1}\left(A_{i+1}^{j}+A_i^{j}\right)\right]+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{-\left(\frac{1}{\Delta x_{i+1}}+\frac{1}{\Delta x_i}\right)y_{1}{}_i^{j+\frac{1}{2}}\left[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y_1}\right|_i^{0}\right.\right.$$
$$\left.+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y_1}\right|_i^{j+\frac{1}{2}}-\left[\frac{A}{y_1}\right|_i^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_i^{k}-\left[\frac{A}{y_1}\right|_i^{k-1}\right)\right]$$
$$+\frac{1}{\Delta x_{i+1}}y_{1}{}_{i+1}^{j+\frac{1}{2}}\left[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y_1}\right|_{i+1}^{0}+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y_1}\right|_{i+1}^{j+\frac{1}{2}}-\left[\frac{A}{y_1}\right|_{i+1}^{j}\right)\right.$$
$$\left.+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i+1}^{k}-\left[\frac{A}{y_1}\right|_{i+1}^{k-1}\right)\right]+\frac{1}{\Delta x_i}y_{1}{}_{i-1}^{j+\frac{1}{2}}\left[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y_1}\right|_{i-1}^{0}\right.$$
$$\left.\left.+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y_1}\right|_{i-1}^{j+\frac{1}{2}}-\left[\frac{A}{y_1}\right|_{i-1}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i-1}^{k}-\left[\frac{A}{y_1}\right|_{i-1}^{k-1}\right)\right]\right\}$$
$$-\frac{k_1}{2}\left[(\Delta x_i+\Delta x_{i+1})\,[AB|_i^{j+\frac{1}{2}}+\Delta x_i\,[AB|_{i-1}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[AB|_{i+1}^{j+\frac{1}{2}}\right]$$
$$+\frac{k_{-1}}{2}\left[(\Delta x_i+\Delta x_{i+1})\,[C|_i^{j+\frac{1}{2}}+\Delta x_i\,[C|_{i-1}^{j+\frac{1}{2}}+\Delta x_{i+1}\,[C|_{i+1}^{j+\frac{1}{2}}\right]. \tag{6.93}$$

Now upon replacing the terms at $t = t_{j+\frac{1}{2}}$ by their corresponding temporal averages

$$u_i^{j+\frac{1}{2}} = \frac{u_i^j + u_i^{j+1}}{2}, \tag{6.94}$$

we then have the following equation given in the case of constant grid spacing $\Delta x_i = \Delta x$, as

$$\begin{aligned}
&\left[2A_i^{j+1} + A_{i-1}^{j+1} + A_{i+1}^{j+1}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[A_{i-1}^{j+1} - 2A_i^{j+1} + A_{i+1}^{j+1}\right] \\
&= \left[2A_i^{j} + A_{i-1}^{j} + A_{i+1}^{j}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[A_{i-1}^{j} - 2A_i^{j} + A_{i+1}^{j}\right] + d\left(\frac{1}{2}\right)^{\gamma}\left\{ y_1{}_{i+1}^{j}\left[\frac{A}{y_1}\right|_{i+1}^{j+1}\right. \\
&\quad \left. - y_1{}_{i+1}^{j+1}\left[\frac{A}{y_1}\right|_{i+1}^{j} - 2y_1{}_i^j\left[\frac{A}{y_1}\right|_{i}^{j+1} + 2y_1{}_i^{j+1}\left[\frac{A}{y_1}\right|_{i}^{j} + y_1{}_{i-1}^{j}\left[\frac{A}{y_1}\right|_{i-1}^{j+1} - y_1{}_{i-1}^{j+1}\left[\frac{A}{y_1}\right|_{i-1}^{j}\right\} \\
&\quad - 2d\left(y_1{}_i^{j+1} + y_1{}_i^{j}\right)\left[\widetilde{\beta}_j(\gamma)A_i^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_i^k - \left[\frac{A}{y_1}\right|_i^{k-1}\right)\right] \\
&\quad + d\left(y_1{}_{i+1}^{j+1} + y_1{}_{i+1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)A_{i+1}^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i+1}^k - \left[\frac{A}{y_1}\right|_{i+1}^{k-1}\right)\right] \\
&\quad + d\left(y_1{}_{i-1}^{j+1} + y_1{}_{i-1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)A_{i-1}^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i-1}^k - \left[\frac{A}{y_1}\right|_{i-1}^{k-1}\right)\right] \\
&\quad - \frac{\Delta t k_1}{2}\left([AB|_{i+1}^{j+1} + 2\,[AB|_i^{j+1} + [AB|_{i-1}^{j+1} + [AB|_{i+1}^{j} + 2\,[AB|_i^{j} + [AB|_{i-1}^{j}\right) \\
&\quad + \frac{\Delta t k_{-1}}{2}\left([C|_{i+1}^{j+1} + 2\,[C|_i^{j+1} + [C|_{i-1}^{j+1} + [C|_{i+1}^{j} + 2\,[C|_i^{j} + [C|_{i-1}^{j}\right),
\end{aligned} \tag{6.95}$$

where we have noted $y_1(x, 0) = y_1^0 = 1$ and $d$ is as defined earlier in Equation (6.17).

We find the corresponding equation for species $B$ in Equation (6.75) in a similar manner swapping $A$ with $B$ and $y_1$ with $y_2$. The corresponding equation for species $B$ is given by

$$\begin{aligned}
&\left[2B_i^{j+1} + B_{i-1}^{j+1} + B_{i+1}^{j+1}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[B_{i-1}^{j+1} - 2B_i^{j+1} + B_{i+1}^{j+1}\right] \\
&= \left[2B_i^{j} + B_{i-1}^{j} + B_{i+1}^{j}\right] - d\left(\frac{1}{2}\right)^{\gamma}\left[B_{i-1}^{j} - 2B_i^{j} + B_{i+1}^{j}\right] + d\left(\frac{1}{2}\right)^{\gamma}\left[y_2{}_{i+1}^{j}\left[\frac{B}{y_2}\right|_{i+1}^{j+1}\right. \\
&\left. -y_2{}_{i+1}^{j+1}\left[\frac{B}{y_2}\right|_{i+1}^{j} - 2y_2{}_i^{j}\left[\frac{B}{y_2}\right|_{i}^{j+1} + 2y_2{}_i^{j+1}\left[\frac{B}{y_2}\right|_{i}^{j} + y_2{}_{i-1}^{j}\left[\frac{B}{y_2}\right|_{i-1}^{j+1} - y_2{}_{i-1}^{j+1}\left[\frac{B}{y_2}\right|_{i-1}^{j}\right] \\
&- 2d\left(y_2{}_i^{j+1} + y_2{}_i^{j}\right)\left[\widetilde{\beta}_j(\gamma)B_i^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{B}{y_2}\right|_i^{k} - \left[\frac{B}{y_2}\right|_i^{k-1}\right)\right] \\
&+ d\left(y_2{}_{i+1}^{j+1} + y_2{}_{i+1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)B_{i+1}^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{B}{y_2}\right|_{i+1}^{k} - \left[\frac{B}{y_2}\right|_{i+1}^{k-1}\right)\right] \\
&+ d\left(y_2{}_{i-1}^{j+1} + y_2{}_{i-1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)B_{i-1}^0 + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{B}{y_2}\right|_{i-1}^{k} - \left[\frac{B}{y_2}\right|_{i-1}^{k-1}\right)\right] \\
&- \frac{\Delta t k_1}{2}\left[2\left[AB\right|_i^{j+1} + \left[AB\right|_{i-1}^{j+1} + \left[AB\right|_{i+1}^{j+1} + 2\left[AB\right|_i^{j} + \left[AB\right|_{i-1}^{j} + \left[AB\right|_{i+1}^{j}\right] \\
&+ \frac{\Delta t k_{-1}}{2}\left[2\left[C\right|_i^{j+1} + \left[C\right|_{i-1}^{j+1} + \left[C\right|_{i+1}^{j+1} + 2\left[C\right|_i^{j} + \left[C\right|_{i-1}^{j} + \left[C\right|_{i+1}^{j}\right],
\end{aligned} \tag{6.96}$$

for a uniform mesh, noting $y_2(x,0)=1$, and $d$ is as given earlier in Equation (6.17).

We now find the approximation for Equation (6.76), using a similar process to that used for approximating Equation (6.74). We first define the spatial derivative by

$$v = \frac{\partial}{\partial x}\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right] \tag{6.97}$$

and then use this in Equation (6.76) to give the equations

$$\left[\frac{\partial}{\partial x}\left(y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_{i-\frac{1}{2}}^{j} = \left[v\right|_{i-\frac{1}{2}}^{j}, \tag{6.98}$$

and

$$\left[\frac{\partial C}{\partial t}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} = D\left[\frac{\partial v}{\partial x}\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} + k_1\left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}} - k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{6.99}$$

Now approximating the first order spatial and time derivatives in Equation (6.98) and (6.99) by using centred finite difference method (as in Chapter 3 Equations (3.8) and (3.9)), we then have

$$\frac{1}{\Delta x_i}\left(\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^{j} - \left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1}^{j}\right) = \left[v\right|_{i-\frac{1}{2}}^{j}, \tag{6.100}$$

and

$$\left[\frac{C_{i-\frac{1}{2}}^{j+1}-C_{i-\frac{1}{2}}^{j}}{\Delta t}\right]=\frac{D}{\Delta x_i}\left(v_i^{j+\frac{1}{2}}-v_{i-1}^{j+\frac{1}{2}}\right)+k_1\left[AB\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}-k_{-1}\left[C\right|_{i-\frac{1}{2}}^{j+\frac{1}{2}}. \tag{6.101}$$

Now replacing the term at the point $x_{i-\frac{1}{2}}^{j}$ by their corresponding spatial averages at $i-1$ and $i$, gives

$$\frac{1}{\Delta x_i}\left(\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^j-\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1}^j\right)=\frac{1}{2}\left(v_i^j+v_{i-1}^j\right), \tag{6.102}$$

and

$$\begin{aligned}\frac{1}{2\Delta t}\left[\left(C_i^{j+1}+C_{i-1}^{j+1}\right)-\left(C_i^j+C_{i-1}^j\right)\right]&=\frac{D}{\Delta x_i}\left(v_i^{j+\frac{1}{2}}-v_{i-1}^{j+\frac{1}{2}}\right)\\&+\frac{k_1}{2}\left[\left[AB\right|_i^{j+\frac{1}{2}}+\left[AB\right|_{i-1}^{j+\frac{1}{2}}\right]-\frac{k_{-1}}{2}\left[\left[C\right|_i^{j+\frac{1}{2}}+\left[C\right|_{i-1}^{j+\frac{1}{2}}\right].\end{aligned} \tag{6.103}$$

Eliminating $v_{i-1}^j$ from Equations (6.102) and (6.103), we obtain the equation

$$\begin{aligned}&\frac{1}{2\Delta t}\left[\left(C_i^{j+1}+C_{i-1}^{j+1}\right)-\left(C_i^j+C_{i-1}^j\right)\right]\\&=\frac{2D}{\Delta x_i}v_i^{j+\frac{1}{2}}-\frac{2D}{\Delta x_i^2}\left(\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^{j+\frac{1}{2}}-\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1}^{j+\frac{1}{2}}\right)\\&+\frac{k_1}{2}\left[\left[AB\right|_i^{j+\frac{1}{2}}+\left[AB\right|_{i-1}^{j+\frac{1}{2}}\right]-\frac{k_{-1}}{2}\left[\left[C\right|_i^{j+\frac{1}{2}}+\left[C\right|_{i-1}^{j+\frac{1}{2}}\right].\end{aligned} \tag{6.104}$$

Similarly replacing $i$ with $i+1$ in Equations (6.98) and (6.99), we then get the equations

$$\left[\frac{\partial}{\partial x}\left(y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_{i+\frac{1}{2}}^j=\left[v\right|_{i+\frac{1}{2}}^j, \tag{6.105}$$

and

$$\left[\frac{\partial C}{\partial t}\right|_{i+\frac{1}{2}}^{j+\frac{1}{2}}=D\left[\frac{\partial v}{\partial x}\right|_{i+\frac{1}{2}}^{j+\frac{1}{2}}+k_1\left[AB\right|_{i+\frac{1}{2}}^{j+\frac{1}{2}}-k_{-1}\left[C\right|_{i+\frac{1}{2}}^{j+\frac{1}{2}}. \tag{6.106}$$

Replacing the terms evaluated at the point $x_{i+\frac{1}{2}}$ by their corresponding spatial average at $i$ and $i+1$, we then have

$$\frac{1}{\Delta x_{i+1}}\left(\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i+1}^j-\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^j\right)=\frac{1}{2}\left(v_{i+1}^j+v_i^j\right), \tag{6.107}$$

and

$$\begin{aligned}\frac{1}{2\Delta t}\left[\left(C_{i+1}^{j+1}+C_i^{j+1}\right)-\left(C_{i+1}^j+C_i^j\right)\right]&=\frac{D}{\Delta x_{i+1}}\left(v_{i+1}^{j+\frac{1}{2}}-v_i^{j+\frac{1}{2}}\right)\\&+\frac{k_1}{2}\left[\left[AB\right|_{i+1}^{j+\frac{1}{2}}+\left[AB\right|_i^{j+\frac{1}{2}}\right]-\frac{k_{-1}}{2}\left[\left[C\right|_{i+1}^{j+\frac{1}{2}}+\left[C\right|_i^{j+\frac{1}{2}}\right].\end{aligned} \tag{6.108}$$

Solving Equation (6.107) for $v_{i+1}^{j}$ and then combining (replacing $j$ with $j+\frac{1}{2}$) with Equation (6.108), gives

$$\begin{aligned}
&\frac{1}{2\Delta t}\left[\left(C_{i+1}^{j+1}+C_{i}^{j+1}\right)-\left(C_{i+1}^{j}+C_{i}^{j}\right)\right] \\
&=\frac{2D}{\Delta x_{i+1}^{2}}\left(\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i+1}^{j+\frac{1}{2}}-\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i}^{j+\frac{1}{2}}\right) \\
&-\frac{2D}{\Delta x_{i+1}}v_i^{j+\frac{1}{2}}+\frac{k_1}{2}\left[[AB|_{i+1}^{j+\frac{1}{2}}+[AB|_{i}^{j+\frac{1}{2}}\right]-\frac{k_{-1}}{2}\left[[C|_{i+1}^{j+\frac{1}{2}}+[C|_{i}^{j+\frac{1}{2}}\right].
\end{aligned} \tag{6.109}$$

Now multiplying Equation (6.104) by $\Delta x_i$ and Equation (6.109) by $\Delta x_{i+1}$, and adding the two, we have

$$\begin{aligned}
&\frac{1}{2\Delta t}\left[\Delta x_i\left(C_{i}^{j+1}+C_{i-1}^{j+1}\right)+\Delta x_{i+1}\left(C_{i+1}^{j+1}+C_{i}^{j+1}\right)\right]=\frac{1}{2\Delta t}\left[\Delta x_i\left(C_{i}^{j}+C_{i-1}^{j}\right)\right. \\
&\left.+\Delta x_{i+1}\left(C_{i+1}^{j}+C_{i}^{j}\right)\right]-\left[\frac{2}{\Delta x_{i+1}}+\frac{2}{\Delta x_i}\right][y_3|_{i}^{j+\frac{1}{2}}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i}^{j+\frac{1}{2}} \\
&+\frac{2}{\Delta x_{i+1}}[y_3|_{i+1}^{j+\frac{1}{2}}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i+1}^{j+\frac{1}{2}}+\frac{2}{\Delta x_i}[y_3|_{i-1}^{j+\frac{1}{2}}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1}^{j+\frac{1}{2}} \\
&+\frac{k_1}{2}\left[\Delta x_i\left([AB|_{i}^{j+\frac{1}{2}}+[AB|_{i-1}^{j+\frac{1}{2}}\right)+\Delta x_{i+1}\left([AB|_{i+1}^{j+\frac{1}{2}}+[AB|_{i}^{j+\frac{1}{2}}\right)\right] \\
&-\frac{k_{-1}}{2}\left[\Delta x_i\left([C|_{i}^{j+\frac{1}{2}}+[C|_{i-1}^{j+\frac{1}{2}}\right)+\Delta x_{i+1}\left([C|_{i+1}^{j+\frac{1}{2}}+[C|_{i}^{j+\frac{1}{2}}\right)\right].
\end{aligned} \tag{6.110}$$

Using the fractional derivative approximation in Equation (6.110), we then find

$$\begin{aligned}
&\frac{1}{2\Delta t}\left[\Delta x_i\left(C_{i}^{j+1}+C_{i-1}^{j+1}\right)+\Delta x_{i+1}\left(C_{i+1}^{j+1}+C_{i}^{j+1}\right)\right]=\frac{1}{2\Delta t}\left[\Delta x_i\left(C_{i}^{j}+C_{i-1}^{j}\right)\right. \\
&\left.+\Delta x_{i+1}\left(C_{i+1}^{j}+C_{i}^{j}\right)\right]+\frac{2D\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{-\left[\frac{1}{\Delta x_{i+1}}+\frac{1}{\Delta x_i}\right][y_3|_{i}^{j+\frac{1}{2}}\left[\widetilde{\beta}_j(\gamma)\left[\frac{C}{y_3}\right|_{i}^{0}\right.\right. \\
&\left.+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{C}{y_3}\right|_{i}^{j+\frac{1}{2}}-\left[\frac{C}{y_3}\right|_{i}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y_3}\right|_{i}^{k}-\left[\frac{C}{y_3}\right|_{i}^{k-1}\right)\right] \\
&+\frac{1}{\Delta x_{i+1}}[y_3|_{i+1}^{j+\frac{1}{2}}\left[\widetilde{\beta}_j(\gamma)\left[\frac{C}{y_3}\right|_{i+1}^{0}+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{C}{y_3}\right|_{i+1}^{j+\frac{1}{2}}-\left[\frac{C}{y_3}\right|_{i+1}^{j}\right)\right. \\
&\left.+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y_3}\right|_{i+1}^{k}-\left[\frac{C}{y_3}\right|_{i+1}^{k-1}\right)\right]+\frac{1}{\Delta x_i}[y_3|_{i-1}^{j+\frac{1}{2}}\left[\widetilde{\beta}_j(\gamma)\left[\frac{C}{y_3}\right|_{i-1}^{0}\right. \\
&\left.\left.+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{C}{y_3}\right|_{i-1}^{j+\frac{1}{2}}-\left[\frac{C}{y_3}\right|_{i-1}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y_3}\right|_{i-1}^{k}-\left[\frac{C}{y_3}\right|_{i-1}^{k-1}\right)\right]\right\} \\
&+\frac{k_1}{2}\left[\Delta x_i\left([AB|_{i}^{j+\frac{1}{2}}+[AB|_{i-1}^{j+\frac{1}{2}}\right)+\Delta x_{i+1}\left([AB|_{i+1}^{j+\frac{1}{2}}+[AB|_{i}^{j+\frac{1}{2}}\right)\right] \\
&-\frac{k_{-1}}{2}\left[\Delta x_i\left([C|_{i}^{j+\frac{1}{2}}+[C|_{i-1}^{j+\frac{1}{2}}\right)+\Delta x_{i+1}\left([C|_{i+1}^{j+\frac{1}{2}}+[C|_{i}^{j+\frac{1}{2}}\right)\right].
\end{aligned} \tag{6.111}$$

Replacing the terms evaluated at the point $t_{j+\frac{1}{2}}$ by their corresponding temporal average at $j$ and $j+1$, and then Equation (6.111), with the case of constant grid spacing $\Delta x_i = \Delta x$ and noting $y_3(x,0) = {y_3}^0 = 1$, reduces to

$$
\begin{aligned}
&\left(1+\frac{\Delta t k_{-1}}{2}\right)\left[C_{i-1}^{j+1}+2C_i^{j+1}+C_{i+1}^{j+1}\right]-d\left(\frac{1}{2}\right)^{\gamma}\left[C_{i-1}^{j+1}-2C_i^{j+1}+C_{i+1}^{j+1}\right]\\
&=\left(1-\frac{\Delta t k_{-1}}{2}\right)\left[C_{i-1}^{j}+2C_i^{j}+C_{i+1}^{j}\right]-d\left(\frac{1}{2}\right)^{\gamma}\left[C_{i-1}^{j}-2C_i^{j}+C_{i+1}^{j}\right]\\
&+d\left(\frac{1}{2}\right)^{\gamma}\left\{ {y_3}_{i+1}^{j}\left[\frac{C}{y_3}\right|_{i+1}^{j+1}-{y_3}_{i+1}^{j+1}\left[\frac{C}{y_3}\right|_{i+1}^{j}-2{y_3}_i^{j}\left[\frac{C}{y_3}\right|_{i}^{j+1}+2{y_3}_i^{j+1}\left[\frac{C}{y_3}\right|_{i}^{j}\right.\\
&\qquad\qquad\left.+{y_3}_{i-1}^{j}\left[\frac{C}{y_3}\right|_{i-1}^{j+1}-{y_3}_{i-1}^{j+1}\left[\frac{C}{y_3}\right|_{i-1}^{j}\right\}\\
&-2d\left({y_3}_i^{j+1}+{y_3}_i^{j}\right)\left[\widetilde{\beta}_j(\gamma)\left[C\right|_i^0+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y_3}\right|_i^k-\left[\frac{C}{y_3}\right|_i^{k-1}\right)\right]\\
&+d\left({y_3}_{i+1}^{j+1}+{y_3}_{i+1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)\left[C\right|_{i+1}^0+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y_3}\right|_{i+1}^k-\left[\frac{C}{y_3}\right|_{i+1}^{k-1}\right)\right]\\
&+d\left({y_3}_{i-1}^{j+1}+{y_3}_{i-1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)\left[C\right|_{i-1}^0+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y_3}\right|_{i-1}^k-\left[\frac{C}{y_3}\right|_{i-1}^{k-1}\right)\right]\\
&+\frac{\Delta t k_1}{2}\left[\left[AB\right|_{i+1}^{j+1}+2\left[AB\right|_{i}^{j+1}+\left[AB\right|_{i-1}^{j+1}+\left[AB\right|_{i+1}^{j}+2\left[AB\right|_{i}^{j}+\left[AB\right|_{i-1}^{j}\right],
\end{aligned}
\tag{6.112}
$$

where $d$ is given in Equation (6.17).

Finally we find the approximation for the auxiliary variables $y_k(x,t)$, where $k = 1, 2, 3$, in Equations (6.77) – (6.79). Approximating the first order time derivatives by a centred finite difference (as in Chapter 3 Equation (3.9)), and approximating the values at $t = t_{j+\frac{1}{2}}$ by their temporal average (Equation (6.94)), we then obtain the equations

$$ {y_1}_i^{j+1} = {y_1}_i^{j} - \frac{\Delta t k_1}{2}\left(\left[By_1\right|_i^{j+1}+\left[By_1\right|_i^{j}\right), \tag{6.113}$$

$$ {y_2}_i^{j+1} = {y_2}_i^{j} - \frac{\Delta t k_1}{2}\left(\left[Ay_2\right|_i^{j+1}+\left[Ay_2\right|_i^{j}\right), \tag{6.114}$$

and

$$ {y_3}_i^{j+1} = {y_3}_i^{j} - \frac{\Delta t k_{-1}}{2}\left({y_3}_i^{j+1}+{y_3}_i^{j}\right). \tag{6.115}$$

Equations (6.95), (6.96), and (6.112) along with Equations (6.113) – (6.115) form the equations for the Keller Box method for Model Type 2.

### 6.6.2 The Implicit Finite Difference Scheme: IML1 Scheme

In this section, we develop the implicit finite difference scheme using the L1 scheme given by Equation (2.12), where $p = 1 - \gamma$. We approximate the derivatives in Equations (6.4) – (6.6) at the point $(x_i, t_j)$

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1 \left[AB\right|_i^j + k_{-1} \left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[y_1 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^j, \tag{6.116}$$

$$\left[\frac{\partial B}{\partial t}\right|_i^j = -k_1 \left[AB\right|_i^j + k_{-1} \left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[y_2 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{B}{y_2}\right)\right|_i^j, \tag{6.117}$$

$$\left[\frac{\partial C}{\partial t}\right|_i^j = k_1 \left[AB\right|_i^j - k_{-1} \left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[y_3 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^j, \tag{6.118}$$

and likewise for Equations (6.71) – (6.73)

$$\left[\frac{\partial y_1}{\partial t}\right|_i^j = -k_1 \left[By_1\right|_i^j, \tag{6.119}$$

$$\left[\frac{\partial y_2}{\partial t}\right|_i^j = -k_1 \left[Ay_2\right|_i^j, \tag{6.120}$$

and

$$\left[\frac{\partial y_3}{\partial t}\right|_i^j = -k_{-1} \left[y_3\right|_i^j. \tag{6.121}$$

We approximate the second order spatial derivative and the first order time derivative in Equations (6.116) by using the centred finite difference scheme and the backward difference scheme (given in Chapter 3 by Equations (3.6) and (3.9)), to find

$$\frac{A_i^j - A_i^{j-1}}{\Delta t} = -k_1 \left[AB\right|_i^j + k_{-1} \left[C\right|_i^j + \frac{D}{\Delta x^2}\left\{\left[y_1 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1}^j - 2\left[y_1 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^j + \left[y_1 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1}^j\right\}. \tag{6.122}$$

Now using the L1 approximation, given by Equation (2.12), and simplifying, Equation (6.122) then reduces to

$$\begin{aligned} A_i^j &= A_i^{j-1} - \Delta t k_1 \left[AB\right|_i^j + \Delta t k_{-1} \left[C\right|_i^j \\ &+ \frac{D\Delta t^\gamma}{\Delta x^2 \Gamma(1+\gamma)} \left\{ [y_1|_{i+1}^j \left[ \beta_j(\gamma) \left[\frac{A}{y_1}\right|_{i+1}^0 + \left[\frac{A}{y_1}\right|_{i+1}^j + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{A}{y_1}\right|_{i+1}^k \right] \right. \\ &\qquad - 2[y_1|_i^j \left[ \beta_j(\gamma) \left[\frac{A}{y_1}\right|_i^0 + \left[\frac{A}{y_1}\right|_i^j + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{A}{y_1}\right|_i^k \right] \\ &\qquad \left. + [y_1|_{i-1}^j \left[ \beta_j(\gamma) \left[\frac{A}{y_1}\right|_{i-1}^0 + \left[\frac{A}{y_1}\right|_{i-1}^j + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{A}{y_1}\right|_{i-1}^k \right] \right\}. \end{aligned} \tag{6.123}$$

After simplifying we have the following equation for $A$

$$\begin{aligned} A_i^j - \hat{d}\left(A_{i+1}^j - 2A_i^j + A_{i-1}^j\right) &= A_i^{j-1} - \Delta t k_1 \left[AB\right|_i^j + \Delta t k_{-1} \left[C\right|_i^j \\ &+ \hat{d}[y_1|_{i+1}^j \left[ \beta_j(\gamma) \left[A\right|_{i+1}^0 + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{A}{y_1}\right|_{i+1}^k \right] \\ &- 2\hat{d}[y_1|_i^j \left[ \beta_j(\gamma) \left[A\right|_i^0 + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{A}{y_1}\right|_i^k \right] \\ &+ \hat{d}[y_1|_{i-1}^j \left[ \beta_j(\gamma) \left[A\right|_{i-1}^0 + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{A}{y_1}\right|_{i-1}^k \right], \end{aligned} \tag{6.124}$$

where $\hat{d}$ is given earlier in Equation (6.27). Note in the above we have used the condition $y_1(x,0) = {y_1}^0 = 1$ to simplify the equation.

We find the corresponding equation for $B$ from Equation (6.117) by repeating similar steps but now with $B$ replacing $A$ and $y_2$ replacing $y_1$, and so we have

$$\begin{aligned} B_i^j - \hat{d}\left(B_{i+1}^j - 2B_i^j + B_{i-1}^j\right) &= B_i^{j-1} - \Delta t k_1 \left[AB\right|_i^j + \Delta t k_{-1} \left[C\right|_i^j \\ &+ \hat{d}[y_2|_{i+1}^j \left[ \beta_j(\gamma) \left[B\right|_{i+1}^0 + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[B\right|_{i+1}^k \right] \\ &- 2\hat{d}[y_2|_i^j \left[ \beta_j(\gamma) \left[B\right|_i^0 + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{B}{y_2}\right|_i^k \right] \\ &+ \hat{d}[y_2|_{i-1}^j \left[ \beta_j(\gamma) \left[B\right|_{i-1}^0 + \sum_{k=1}^{j-1} \mu_{j-k}(\gamma) \left[\frac{B}{y_2}\right|_{i-1}^k \right], \end{aligned} \tag{6.125}$$

where again we have used the fact $y_2(x,0) = {y_2}^0 = 1$.

We next find the approximation of Equation (6.118) in a similar way by first approximating the integer–order derivatives

$$\frac{C_i^j - C_i^{j-1}}{\Delta t} = k_1 AB - k_{-1}C + \frac{D}{\Delta x^2}\left\{\left[y_3 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i+1}^{j} - 2\left[y_3 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i}^{j} + \left[y_3 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1}^{j}\right\}, \tag{6.126}$$

and then the fractional derivative, using the L1 approximation in Equation (2.12), to find

$$\begin{aligned} C_i^j &= C_i^{j-1} + \Delta t k_1 \left[AB\right|_i^j - \Delta t k_{-1}\left[C\right|_i^j \\ &+ \frac{D\Delta t^\gamma}{\Delta x^2 \Gamma(1+\gamma)}\left\{[y_3|_{i+1}^j \left[\beta_j(\gamma)\left[\frac{C}{y_3}\right|_{i+1}^0 + \left[\frac{C}{y_3}\right|_{i+1}^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{C}{y_3}\right|_{i+1}^k\right]\right. \\ &- 2[y_3|_i^j \left[\beta_j(\gamma)\left[\frac{C}{y_3}\right|_i^0 + \left[\frac{C}{y_3}\right|_i^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{C}{y_3}\right|_i^k\right] \\ &\left. + [y_3|_{i-1}^j \left[\beta_j(\gamma)\left[\frac{C}{y_3}\right|_{i-1}^0 + \left[\frac{C}{y_3}\right|_{i-1}^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{C}{y_3}\right|_{i-1}^k\right]\right\}. \end{aligned} \tag{6.127}$$

Using $\hat{d}$ defined in Equation (6.27) and simplifying, we have the equation for $C$

$$\begin{aligned} &(1+\Delta t k_{-1})C_i^j - \hat{d}\left(C_{i+1}^j - 2C_i^j + C_{i-1}^j\right) = C_i^{j-1} + \Delta t k_1 \left[AB\right|_i^j \\ &+ \hat{d}[y_3|_{i+1}^j \left[\beta_j(\gamma)\left[C\right|_{i+1}^0 + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{C}{y_3}\right|_{i+1}^k\right] - 2\hat{d}[y_3|_i^j \left[\beta_j(\gamma)\left[C\right|_i^0 + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{C}{y_3}\right|_i^k\right] \\ &+ \hat{d}[y_3|_{i-1}^j \left[\beta_j(\gamma)\left[C\right|_{i-1}^0 + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{C}{y_3}\right|_{i-1}^k\right]. \end{aligned} \tag{6.128}$$

Finally we find the approximations for the auxiliary variables $y_k(x,t)$, where $k = 1, 2, 3$, given in Equations (6.119) – (6.121). Now approximating the first order time derivatives by using the backward difference method (as in Chapter 3 Equation (3.9)), and rearranging we then obtain

$$y_1{}_i^j = y_1{}_i^{j-1} - \Delta t k_1 \left[B y_1\right|_i^j, \tag{6.129}$$

$$y_2{}_i^j = y_2{}_i^{j-1} - \Delta t k_1 \left[A y_2\right|_i^j, \tag{6.130}$$

and

$$y_3{}_i^j = y_3{}_i^{j-1} - \Delta t k_{-1} \left[y_3\right|_i^j. \tag{6.131}$$

Equations (6.124), (6.125), and (6.128) along with Equations (6.129) – (6.131) form the equations for the IML1 method for Model Type 2.

## 6.7 Accuracy of the Numerical Methods for Model Type 2

In this section, we consider the truncation error accuracy of the numerical schemes KBMC2 and the IML1 method given in Section 6.6. Similar to Section 6.4 we use the notation in Equation (6.30) to aid in the analysis of each scheme.

### 6.7.1 The Accuracy of the Keller Box Scheme

We now determine the truncation error of KBMC2 scheme for Model Type 2. Using the notation in Equation (6.30), with $Z = A$. Equation (6.95) after rewriting becomes

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right] + \frac{1}{\Delta t}\left[A_i^{j+1} - A_i^j\right] \\
&= \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left\{\left({y_1}_{i+1}^{j+1} + {y_1}_{i+1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i+1}^{j+1} - \left[\frac{A}{y_1}\right|_{i+1}^{j}\right)\right. \\
&\left.-2\left({y_1}_{i}^{j+1} + {y_1}_{i}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i}^{j+1} - \left[\frac{A}{y_1}\right|_{i}^{j}\right) + \left({y_1}_{i-1}^{j+1} + {y_1}_{i-1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i-1}^{j+1} - \left[\frac{A}{y_1}\right|_{i-1}^{j}\right)\right\} \\
&+ \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left\{\left({y_1}_{i+1}^{j+1} + {y_1}_{i+1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y_1}\right|_{i+1}^{0} + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i+1}^{k} - \left[\frac{A}{y_1}\right|_{i+1}^{k-1}\right)\right]\right. \\
&- 2\left({y_1}_{i}^{j+1} + {y_1}_{i}^{j}\right)\left[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y_1}\right|_{i}^{0} + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i}^{k} - \left[\frac{A}{y_1}\right|_{i}^{k-1}\right)\right] \\
&\left.+\left({y_1}_{i-1}^{j+1} + {y_1}_{i-1}^{j}\right)\left[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y_1}\right|_{i-1}^{0} + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y_1}\right|_{i-1}^{k} - \left[\frac{A}{y_1}\right|_{i-1}^{k-1}\right)\right]\right\} \\
&- \frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^{j} + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^{j}\right)\right\} \\
&+ \frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^{j} + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^{j}\right)\right\}. \qquad (6.132)
\end{aligned}$$

Note in the above we used the identity

$$
\begin{aligned}
&\left[\left(A_{i-1}^{j+1} - 2A_i^{j+1} + A_{i+1}^{j+1}\right) - \left(A_{i-1}^{j} - 2A_i^{j} + A_{i+1}^{j}\right)\right] + \left[{y_1}_{i+1}^{j}\left[\frac{A}{y_1}\right|_{i+1}^{j+1} - {y_1}_{i+1}^{j+1}\left[\frac{A}{y_1}\right|_{i+1}^{j}\right. \\
&\left. -2{y_1}_{i}^{j}\left[\frac{A}{y_1}\right|_{i}^{j+1} + 2{y_1}_{i}^{j+1}\left[\frac{A}{y_1}\right|_{i}^{j} + {y_1}_{i-1}^{j}\left[\frac{A}{y_1}\right|_{i-1}^{j+1} - {y_1}_{i-1}^{j+1}\left[\frac{A}{y_1}\right|_{i-1}^{j}\right] \\
&= \left[\frac{A}{y_1}\right|_{i+1}^{j+1}\left({y_1}_{i+1}^{j+1} + {y_1}_{i+1}^{j}\right) - \left[\frac{A}{y_1}\right|_{i+1}^{j}\left({y_1}_{i+1}^{j+1} + {y_1}_{i+1}^{j}\right) - 2\left[\frac{A}{y_1}\right|_{i}^{j+1}\left({y_1}_{i}^{j+1} + {y_1}_{i}^{j}\right) \\
&\quad + 2\left[\frac{A}{y_1}\right|_{i}^{j}\left({y_1}_{i}^{j+1} + {y_1}_{i}^{j}\right) + \left[\frac{A}{y_1}\right|_{i-1}^{j+1}\left({y_1}_{i-1}^{j+1} + {y_1}_{i-1}^{j}\right) - \left[\frac{A}{y_1}\right|_{i-1}^{j}\left({y_1}_{i-1}^{j+1} + {y_1}_{i-1}^{j}\right) \\
&= \left({y_1}_{i+1}^{j+1} + {y_1}_{i+1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i+1}^{j+1} - \left[\frac{A}{y_1}\right|_{i+1}^{j}\right) - 2\left({y_1}_{i}^{j+1} + {y_1}_{i}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i}^{j+1} - \left[\frac{A}{y_1}\right|_{i}^{j}\right) \\
&\quad + \left({y_1}_{i-1}^{j+1} + {y_1}_{i-1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i-1}^{j+1} - \left[\frac{A}{y_1}\right|_{i-1}^{j}\right). \qquad (6.133)
\end{aligned}
$$

After adding and subtracting the terms of the form

$$
\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left[2\left(\frac{1}{2}\right)^{\gamma}\left({y_1}_{p}^{j+1} + {y_1}_{p}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{p}^{j+\frac{1}{2}} - \left[\frac{A}{y_1}\right|_{p}^{j}\right)\right] \qquad (6.134)
$$

with $p = i, i+1, i-1$, Equation (6.132) then becomes

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1} - \delta_x^2 A_i^j\right] + \frac{1}{\Delta t}\left[A_i^{j+1} - A_i^j\right] \\
&= \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\Bigg\{\left(y1_{i+1}^{j+1} + y1_{i+1}^{j}\right)\left(\left[\frac{A}{y1}\right|_{i+1}^{j+1} - \left[\frac{A}{y1}\right|_{i+1}^{j}\right) \\
&\quad -2\left(y1_i^{j+1} + y1_i^j\right)\left(\left[\frac{A}{y1}\right|_{i}^{j+1} - \left[\frac{A}{y1}\right|_{i}^{j}\right) + \left(y1_{i-1}^{j+1} + y1_{i-1}^{j}\right)\left(\left[\frac{A}{y1}\right|_{i-1}^{j+1} - \left[\frac{A}{y1}\right|_{i-1}^{j}\right)\Bigg\} \\
&- \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}2\left(\frac{1}{2}\right)^{\gamma}\Bigg\{\left(y1_{i+1}^{j+1} + y1_{i+1}^{j}\right)\left(\left[\frac{A}{y1}\right|_{i+1}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{i+1}^{j}\right) \\
&\quad -2\left(y1_i^{j+1} + y1_i^j\right)\left(\left[\frac{A}{y1}\right|_{i}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{i}^{j}\right) + \left(y1_{i-1}^{j+1} + y1_{i-1}^{j}\right)\left(\left[\frac{A}{y1}\right|_{i-1}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{i-1}^{j}\right)\Bigg\} \\
&+ \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\Bigg\{\left(y1_{i+1}^{j+1} + y1_{i+1}^{j}\right)\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y1}\right|_{i+1}^{0} + 2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y1}\right|_{i+1}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{i+1}^{j}\right) \\
&\quad + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y1}\right|_{i+1}^{k} - \left[\frac{A}{y1}\right|_{i+1}^{k-1}\right)\Bigg] - 2\left(y1_i^{j+1} + y1_i^j\right)\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y1}\right|_{i}^{0} \\
&\quad +2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y1}\right|_{i}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{i}^{j}\right) + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y1}\right|_{i}^{k} - \left[\frac{A}{y1}\right|_{i}^{k-1}\right)\Bigg] \\
&\quad + \left(y1_{i-1}^{j+1} + y1_{i-1}^{j}\right)\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y1}\right|_{i-1}^{0} + 2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y1}\right|_{i-1}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{i-1}^{j}\right) \\
&\quad + \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y1}\right|_{i-1}^{k} - \left[\frac{A}{y1}\right|_{i-1}^{k-1}\right)\Bigg]\Bigg\} \\
&- \frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^{j} + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^{j}\right)\right\} \\
&+ \frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^{j} + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^{j}\right)\right\}. \qquad (6.135)
\end{aligned}$$

We note the terms

$$\begin{aligned}
g_p(t) = \frac{\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}&\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{A}{y1}\right|_{p}^{0} + 2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{A}{y1}\right|_{p}^{j+\frac{1}{2}} - \left[\frac{A}{y1}\right|_{p}^{j}\right) \\
&+ \sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{A}{y1}\right|_{p}^{k} - \left[\frac{A}{y1}\right|_{p}^{k-1}\right)\Bigg], \qquad (6.136)
\end{aligned}$$

are the C2 fractional derivative approximation at the point $p$, when compared with Equation (2.75), we can then rewrite the last equation in terms of the C2 fractional derivative approximation, i.e.

$$
\begin{aligned}
&\frac{A_i^{j+1}-A_i^j}{\Delta t}+\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1}-\delta_x^2 A_i^j\right] \\
&=\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left\{\left({y_1}_{i+1}^{j+1}+{y_1}_{i+1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i+1}^{j+1}-2\left[\frac{A}{y_1}\right|_{i+1}^{j+\frac{1}{2}}+\left[\frac{A}{y_1}\right|_{i+1}^{j}\right)\right. \\
&\qquad -2\left({y_1}_{i}^{j+1}+{y_1}_{i}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i}^{j+1}-2\left[\frac{A}{y_1}\right|_{i}^{j+\frac{1}{2}}+\left[\frac{A}{y_1}\right|_{i}^{j}\right) \\
&\qquad \left.+\left({y_1}_{i-1}^{j+1}+{y_1}_{i-1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i-1}^{j+1}-2\left[\frac{A}{y_1}\right|_{i-1}^{j+\frac{1}{2}}+\left[\frac{A}{y_1}\right|_{i-1}^{j}\right)\right\} \\
&+\frac{D}{\Delta x^2}\left\{\left({y_1}_{i+1}^{j+1}+{y_1}_{i+1}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1,C2}^{j+\frac{1}{2}}-2\left({y_1}_{i}^{j+1}+{y_1}_{i}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right. \\
&\qquad \left.+\left({y_1}_{i-1}^{j+1}+{y_1}_{i-1}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1,C2}^{j+\frac{1}{2}}\right\} \\
&-\frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1}+\left[\delta_x^2 AB\right|_i^{j}+4\left(\left[AB\right|_i^{j+1}+\left[AB\right|_i^{j}\right)\right\} \\
&+\frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1}+\left[\delta_x^2 C\right|_i^{j}+4\left(\left[C\right|_i^{j+1}+\left[C\right|_i^{j}\right)\right\}. \qquad (6.137)
\end{aligned}
$$

We now let

$$
\begin{aligned}
Q(y_1,A)=&\left({y_1}_{i+1}^{j+1}+{y_1}_{i+1}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1,C2}^{j+\frac{1}{2}}-2\left({y_1}_{i}^{j+1}+{y_1}_{i}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,C2}^{j+\frac{1}{2}} \\
&+\left({y_1}_{i-1}^{j+1}+{y_1}_{i-1}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1,C2}^{j+\frac{1}{2}}, \qquad (6.138)
\end{aligned}
$$

and

$$
\begin{aligned}
G(y_1,A)=&\left({y_1}_{i+1}^{j+1}+{y_1}_{i+1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i+1}^{j+1}-2\left[\frac{A}{y_1}\right|_{i+1}^{j+\frac{1}{2}}+\left[\frac{A}{y_1}\right|_{i+1}^{j}\right) \\
&-2\left({y_1}_{i}^{j+1}+{y_1}_{i}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i}^{j+1}-2\left[\frac{A}{y_1}\right|_{i}^{j+\frac{1}{2}}+\left[\frac{A}{y_1}\right|_{i}^{j}\right) \\
&+\left({y_1}_{i-1}^{j+1}+{y_1}_{i-1}^{j}\right)\left(\left[\frac{A}{y_1}\right|_{i-1}^{j+1}-2\left[\frac{A}{y_1}\right|_{i-1}^{j+\frac{1}{2}}+\left[\frac{A}{y_1}\right|_{i-1}^{j}\right). \qquad (6.139)
\end{aligned}
$$

Then Equation (6.137) can be more simply rewritten as

$$
\begin{aligned}
\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 A_i^{j+1}-\delta_x^2 A_i^j\right]+\frac{A_i^{j+1}-A_i^j}{\Delta t}=&\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}G(y_1,A)+\frac{D}{\Delta x^2}Q(y_1,A) \\
&-\frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1}+\left[\delta_x^2 AB\right|_i^{j}+4\left(\left[AB\right|_i^{j+1}+\left[AB\right|_i^{j}\right)\right\} \\
&+\frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1}+\left[\delta_x^2 C\right|_i^{j}+4\left(\left[C\right|_i^{j+1}+\left[C\right|_i^{j}\right)\right\}. \qquad (6.140)
\end{aligned}
$$

Now taking the Taylor series expansion around the point $x_i = i\Delta x$ in space we have

$$\delta_x^2 A_i^j \simeq \left[\frac{\partial^2 A}{\partial x^2}\right|_i^j + \frac{\Delta x^2}{12}\left[\frac{\partial^4 A}{\partial x^4}\right|_i^j + O(\Delta x^6), \tag{6.141}$$

and

$$\frac{D}{\Delta x^2} Q(y_1, A) \simeq 2D\left[\frac{\partial^2}{\partial x^2}\left(y_1 \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_{i,C2}^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^2). \tag{6.142}$$

Taking the Taylor series expansion around the point $\left(x_i, t_{j+\frac{1}{2}}\right)$ in time, we have

$$\begin{aligned} &\frac{D\Delta t^{\gamma-1}}{\Delta x^2 \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^\gamma G(y_1, A) \\ &\simeq \frac{D\Delta t^{\gamma-1}}{\Delta x^2 \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^\gamma \left(\Delta t^2 \Delta x^2 \left[\frac{\partial^2}{\partial x^2}\left(y_1 \frac{\partial^2}{\partial t^2}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}} + O(\Delta x^2 \Delta t^2) + O(\Delta t^4)\right) \\ &\simeq O(\Delta t^{1+\gamma}), \end{aligned} \tag{6.143}$$

$$y_{1_i}^{j+1} + y_{1_i}^{j} \simeq 2\left[y_{1_i}^{j+\frac{1}{2}} + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2\left[\frac{\partial^2 y_1}{\partial t^2}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right], \tag{6.144}$$

$$\begin{aligned} \frac{\Delta x^2}{4\Delta t}\left(\left[\delta_x^2 A\right|_i^{j+1} - \left[\delta_x^2 A\right|_i^{j}\right) &\simeq \frac{\Delta x^2}{4}\left[\frac{\partial^3 A}{\partial x^2 \partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta x^4) + O(\Delta x^2 \Delta t^2) \\ &\simeq O(\Delta x^2), \end{aligned} \tag{6.145}$$

$$\frac{k_1}{8}\left[\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^{j} + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^{j}\right)\right] \simeq k_1\left[AB\right|_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^2), \tag{6.146}$$

$$\frac{k_{-1}}{8}\left[\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^{j} + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^{j}\right)\right] \simeq k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + O(\Delta x^2) + O(\Delta t^2), \tag{6.147}$$

and

$$\frac{A_i^{j+1} - A_i^j}{\Delta t} \simeq \left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2). \tag{6.148}$$

Using Equations (6.141) – (6.148), we then have

$$\begin{aligned} \left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) + O(\Delta x^2) = &-k_1\left[AB\right|_i^{j+\frac{1}{2}} + k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + O(\Delta t^{1+\gamma}) + O(\Delta x^2) \\ &+ D\left[\frac{\partial^2}{\partial x^2}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}. \end{aligned} \tag{6.149}$$

Now adding and subtracting the exact value of the fractional derivative, we then get

$$\left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} = -k_1\left[AB\right|_i^{j+\frac{1}{2}} + k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + D\frac{\partial^2}{\partial x^2}\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}}$$
$$- D\left\{\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^2}{\partial x^2}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}\right\}$$
$$+ O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}). \tag{6.150}$$

Now evaluating the spatial derivatives as

$$\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}} = \left[y_1\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}} + 2\left[\frac{\partial y_1}{\partial x}\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}}$$
$$+ \left[\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\left(\frac{\partial^2 y_1}{\partial x^2}\right)\right|_i^{j+\frac{1}{2}}, \tag{6.151}$$

Equation (6.150) becomes

$$\left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} = -k_1\left[AB\right|_i^{j+\frac{1}{2}} + k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + D\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}}$$
$$- D\left\{\left[y_1\right|_i^{j+\frac{1}{2}}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}} + 2\left[\frac{\partial y_1}{\partial x}\right|_i^{j+\frac{1}{2}}\left[\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^{j+\frac{1}{2}}\right.$$
$$+ \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}}\left[\frac{\partial^2 y_1}{\partial x^2}\right|_i^{j+\frac{1}{2}} - \left[\left[y_1\right|_i^{j+\frac{1}{2}}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_{i,C2}^{j+\frac{1}{2}}\right.$$
$$\left.\left. +2\left[\frac{\partial y_1}{\partial x}\right|_i^{j+\frac{1}{2}}\left[\frac{\partial}{\partial x}\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{C2}\right|_i^{j+\frac{1}{2}} + \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,C2}^{j+\frac{1}{2}}\left[\frac{\partial^2 y_1}{\partial x^2}\right|_i^{j+\frac{1}{2}}\right]\right\}$$
$$+ O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}), \tag{6.152}$$

and then combining the common terms we find

$$\left[\frac{\partial A}{\partial t}\right|_i^{j+\frac{1}{2}} = -k_1\left[AB\right|_i^{j+\frac{1}{2}} + k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + D\frac{\partial^2}{\partial x^2}\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}}$$
$$- D\left\{\left[y_1\right|_i^{j+\frac{1}{2}}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}\right.$$
$$+ 2\left[\frac{\partial y_1}{\partial x}\right|_i^{j+\frac{1}{2}}\left[\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}$$
$$\left. + \left[\frac{\partial^2 y_1}{\partial x^2}\right|_i^{j+\frac{1}{2}}\left(\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right)\right\}$$
$$+ O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}). \tag{6.153}$$

The terms

$$\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,C2}^{j+\frac{1}{2}} \tag{6.154}$$

are each of $O(\Delta t^{1+\gamma})$, as shown in Chapter 2 by Equation (2.149). We then see the truncation error from Equations (6.153) and (6.154) is order $1+\gamma$ in time and second order in space.

Using similar process, we find the truncation error of Equation (6.96) is again of order $1+\gamma$ in time and second order in space.

We now find the truncation error for Equation (6.112), where we again use the notation in Equation (6.30) with $Z = C$, and then add and subtract the terms of the form

$$\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left[2\left(\frac{1}{2}\right)^{\gamma}\left(y3_p^{j+1}+y3_p^j\right)\left(\left[\frac{C}{y3}\right|_p^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_p^{j}\right)\right] \tag{6.155}$$

for $p = i, i+1$, and $i-1$. Equation (6.112) then becomes

$$\begin{aligned}
&\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 C_i^{j+1}-\delta_x^2 C_i^j\right]+\frac{1}{\Delta t}\left[C_i^{j+1}-C_i^j\right]\\
&=\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\Bigg\{\left(y3_{i+1}^{j+1}+y3_{i+1}^j\right)\left(\left[\frac{C}{y3}\right|_{i+1}^{j+1}-\left[\frac{C}{y3}\right|_{i+1}^{j}\right)\\
&\qquad -2\left(y3_i^{j+1}+y3_i^j\right)\left(\left[\frac{C}{y3}\right|_{i}^{j+1}-\left[\frac{C}{y3}\right|_{i}^{j}\right)+\left(y3_{i-1}^{j+1}+y3_{i-1}^j\right)\left(\left[\frac{C}{y3}\right|_{i-1}^{j+1}-\left[\frac{C}{y3}\right|_{i-1}^{j}\right)\Bigg\}\\
&-\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}2\left(\frac{1}{2}\right)^{\gamma}\Bigg\{\left(y3_{i+1}^{j+1}+y3_{i+1}^j\right)\left(\left[\frac{C}{y3}\right|_{i+1}^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_{i+1}^{j}\right)\\
&\qquad -2\left(y3_i^{j+1}+y3_i^j\right)\left(\left[\frac{C}{y3}\right|_{i}^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_{i}^{j}\right)+\left(y3_{i-1}^{j+1}+y3_{i-1}^j\right)\left(\left[\frac{C}{y3}\right|_{i-1}^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_{i-1}^{j}\right)\Bigg\}\\
&+\frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\Bigg\{\left(y3_{i+1}^{j+1}+y3_{i+1}^j\right)\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{C}{y3}\right|_{i+1}^{0}+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{C}{y3}\right|_{i+1}^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_{i+1}^{j}\right)\\
&\qquad +\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y3}\right|_{i+1}^{k}-\left[\frac{C}{y3}\right|_{i+1}^{k-1}\right)\Bigg]-2\left(y3_i^{j+1}+y3_i^j\right)\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{C}{y3}\right|_{i}^{0}\\
&\qquad +2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{C}{y3}\right|_{i}^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_{i}^{j}\right)+\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y3}\right|_{i}^{k}-\left[\frac{C}{y3}\right|_{i}^{k-1}\right)\Bigg]\\
&\qquad +\left(y3_{i-1}^{j+1}+y3_{i-1}^j\right)\Bigg[\widetilde{\beta}_j(\gamma)\left[\frac{C}{y3}\right|_{i-1}^{0}+2\left(\frac{1}{2}\right)^{\gamma}\left(\left[\frac{C}{y3}\right|_{i-1}^{j+\frac{1}{2}}-\left[\frac{C}{y3}\right|_{i-1}^{j}\right)\\
&\qquad +\sum_{k=1}^{j}\widetilde{\mu}_{j-k}(\gamma)\left(\left[\frac{C}{y3}\right|_{i-1}^{k}-\left[\frac{C}{y3}\right|_{i-1}^{k-1}\right)\Bigg]\Bigg\}\\
&+\frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1}+\left[\delta_x^2 AB\right|_i^{j}+4\left(\left[AB\right|_i^{j+1}+\left[AB\right|_i^{j}\right)\right\}\\
&-\frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1}+\left[\delta_x^2 C\right|_i^{j}+4\left(\left[C\right|_i^{j+1}+\left[C\right|_i^{j}\right)\right\}.
\end{aligned} \tag{6.156}$$

Note the term in the third square brackets, highlighted in blue, in Equation (6.156) is the

C2 approximation acting upon the function $g_p(t) = \left[\frac{C}{y_3}\right|_p$, where $p = i, i+1$, and $i-1$. Equation (6.156) can then be written as

$$\begin{aligned}
&\frac{C_i^{j+1} - C_i^j}{\Delta t} + \frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 C_i^{j+1} - \delta_x^2 C_i^j\right] \\
&= \frac{D\Delta t^{\gamma-1}}{\Delta x^2 \Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma}\left\{\left(y_3{}_{i+1}^{j+1} + y_3{}_{i+1}^{j}\right)\left(\left[\frac{C}{y_3}\right|_{i+1}^{j+1} - 2\left[\frac{C}{y_3}\right|_{i+1}^{j+\frac{1}{2}} + \left[\frac{C}{y_3}\right|_{i+1}^{j}\right)\right. \\
&\qquad - 2\left(y_3{}_i^{j+1} + y_3{}_i^{j}\right)\left(\left[\frac{C}{y_3}\right|_{i}^{j+1} - 2\left[\frac{C}{y_3}\right|_{i}^{j+\frac{1}{2}} + \left[\frac{C}{y_3}\right|_{i}^{j}\right) \\
&\qquad \left. + \left(y_3{}_{i-1}^{j+1} + y_3{}_{i-1}^{j}\right)\left(\left[\frac{C}{y_3}\right|_{i-1}^{j+1} - 2\left[\frac{C}{y_3}\right|_{i-1}^{j+\frac{1}{2}} + \left[\frac{C}{y_3}\right|_{i-1}^{j}\right)\right\} \\
&+ \frac{D}{\Delta x^2}\left\{\left(y_3{}_{i+1}^{j+1} + y_3{}_{i+1}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i+1,C2}^{j+\frac{1}{2}} - 2\left(y_3{}_i^{j+1} + y_3{}_i^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right. \\
&\qquad \left. + \left(y_3{}_{i-1}^{j+1} + y_3{}_{i-1}^{j}\right)\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1,C2}^{j+\frac{1}{2}}\right\} \\
&+ \frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^{j} + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^{j}\right)\right\} \\
&- \frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^{j} + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^{j}\right)\right\}. \qquad (6.157)
\end{aligned}$$

Using Equations (6.138) and (6.139), with $C$ replacing $A$ and $y_3$ replacing $y_1$, we then have

$$\begin{aligned}
\frac{\Delta x^2}{4\Delta t}\left[\delta_x^2 C_i^{j+1} - \delta_x^2 C_i^j\right] + \frac{C_i^{j+1} - C_i^j}{\Delta t} &= \frac{D\Delta t^{\gamma-1}}{\Delta x^2\Gamma(1+\gamma)}\left(\frac{1}{2}\right)^{\gamma} G(y_3, C) + \frac{D}{\Delta x^2} Q(y_3, C) \\
&+ \frac{k_1}{8}\left\{\left[\delta_x^2 AB\right|_i^{j+1} + \left[\delta_x^2 AB\right|_i^{j} + 4\left(\left[AB\right|_i^{j+1} + \left[AB\right|_i^{j}\right)\right\} \\
&- \frac{k_{-1}}{8}\left\{\left[\delta_x^2 C\right|_i^{j+1} + \left[\delta_x^2 C\right|_i^{j} + 4\left(\left[C\right|_i^{j+1} + \left[C\right|_i^{j}\right)\right\}. \qquad (6.158)
\end{aligned}$$

Taking the Taylor series expansion around the point $\left(x_i, t_{j+\frac{1}{2}}\right)$, using Equations (6.141) – (6.148) with $C$ replacing $A$ and $y_3$ replacing $y_1$, we then have

$$\begin{aligned}
&\left[\frac{\partial C}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) + O(\Delta x^2\Delta t^2) + O(\Delta x^2) = k_1\left[AB\right|_i^{j+\frac{1}{2}} - k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) + O(\Delta x^2) \\
&+ \frac{\Delta t^{\gamma+1} D}{2\Gamma(1+\gamma)}\left[\frac{\partial^2 y_3}{\partial x^2}\left(\frac{\partial^2}{\partial t^2}\left(\frac{C}{y_3}\right)\right)\right|_i^{j+\frac{1}{2}} + D\left[\frac{\partial^2}{\partial x^2}\left(y_3\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}. \qquad (6.159)
\end{aligned}$$

Now adding and subtracting the exact value of the fractional derivative then we have

$$\begin{aligned}
\left[\frac{\partial C}{\partial t}\right|_i^{j+\frac{1}{2}} &= k_1\left[AB\right|_i^{j+\frac{1}{2}} - k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + D\left[\frac{\partial^2}{\partial x^2}\left(y_3\,\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_i^{j+\frac{1}{2}} \\
&- D\left\{\left[\frac{\partial^2}{\partial x^2}\left(y_3\,\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^2}{\partial x^2}\left(y_3\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}\right\} \\
&+ O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}). \qquad (6.160)
\end{aligned}$$

Now evaluating the spatial derivatives using Equation(6.151) for $\left[\frac{\partial^2}{\partial x^2}\left(y_3\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}$, we find the equation

$$\begin{aligned}\left[\frac{\partial C}{\partial t}\right|_i^{j+\frac{1}{2}} &= k_1\left[AB\right|_i^{j+\frac{1}{2}} - k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + D\frac{\partial^2}{\partial x^2}\left[y_3\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{C}{y_3}\right)\right|_i^{j+\frac{1}{2}} \\ &- D\left\{\left[y_3\right|_i^{j+\frac{1}{2}}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{C}{y_3}\right|_{C2}\right)\right|_i^{j+\frac{1}{2}}\right. \\ &+ 2\left[\frac{\partial y_3}{\partial x}\right|_i^{j+\frac{1}{2}}\left[\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{C2}\right)\right|_i^{j+\frac{1}{2}} \\ &+ \left.\left[\frac{\partial^2 y_3}{\partial x^2}\right|_i^{j+\frac{1}{2}}\left(\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^{j+\frac{1}{2}} - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i,C2}^{j+\frac{1}{2}}\right)\right\} \\ &+ O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}). \end{aligned} \tag{6.161}$$

The difference between the exact and C2 approximation of the fractional derivatives in the braces are each of $O(\Delta t^{1+\gamma})$ as seen in Chapter 2 Equation (2.149), then we have

$$\begin{aligned}\left[\frac{\partial C}{\partial t}\right|_i^{j+\frac{1}{2}} &= k_1\left[AB\right|_i^{j+\frac{1}{2}} - k_{-1}\left[C\right|_i^{j+\frac{1}{2}} + D\frac{\partial^2}{\partial x^2}\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^{j+\frac{1}{2}} \\ &+ O(\Delta x^2) + O(\Delta t^2) + O(\Delta t^{1+\gamma}). \end{aligned} \tag{6.162}$$

We then get the truncation error, $\tau_{i,j}$, of this equation is of order $1+\gamma$ in time and second order in space i.e

$$\tau_{i,j} = O(\Delta x^2) + O(\Delta t^{1+\gamma}). \tag{6.163}$$

Now to find the accuracy order of ${y_r}_i^j$, where $r = 1, 2, 3$, in Equations (6.113) – (6.115), we now rewrite the equations as

$$\frac{{y_1}_i^{j+1} - {y_1}_i^j}{\Delta t} = -\frac{k_1}{2}\left(\left[By_1\right|_i^{j+1} + \left[By_1\right|_i^j\right), \tag{6.164}$$

$$\frac{{y_2}_i^{j+1} - {y_2}_i^j}{\Delta t} = -\frac{k_1}{2}\left(\left[Ay_2\right|_i^{j+1} + \left[Ay_2\right|_i^j\right), \tag{6.165}$$

and

$$\frac{{y_3}_i^{j+1} - {y_3}_i^j}{\Delta t} = -\frac{k_{-1}}{2}\left({y_3}_i^{j+1} + {y_3}_i^j\right). \tag{6.166}$$

Now expanding the Taylor series around the point $\left(x_i, t_{j+\frac{1}{2}}\right)$ in time by using Equation (6.144) with $By_1$ and $Ay_1$ respectively replacing $y_1$, and Equation (6.148) with $y_r$

replacing $A$, we then have the equations

$$\left[\frac{\partial y_1}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) = -\frac{k_1}{2}2\left[[By_1|_i^{j+\frac{1}{2}} + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2\left[\frac{\partial^2}{\partial t^2}(By_1)\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right], \tag{6.167}$$

$$\left[\frac{\partial y_2}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) = -\frac{k_1}{2}2\left[[Ay_2|_i^{j+\frac{1}{2}} + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2\left[\frac{\partial^2}{\partial t^2}(Ay_2)\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right], \tag{6.168}$$

and

$$\left[\frac{\partial y_3}{\partial t}\right|_i^{j+\frac{1}{2}} + O(\Delta t^2) = -\frac{k_{-1}}{2}2\left[{y_3}_i^{j+\frac{1}{2}} + \frac{1}{2!}\left(\frac{\Delta t}{2}\right)^2\left[\frac{\partial^2 y_3}{\partial t^2}\right|_i^{j+\frac{1}{2}} + O(\Delta t^4)\right]. \tag{6.169}$$

These equations can be rewritten as

$$\left[\frac{\partial y_1}{\partial t}\right|_i^{j+\frac{1}{2}} = -k_1\,[By_1|_i^{j+\frac{1}{2}} + O(\Delta t^2), \tag{6.170}$$

$$\left[\frac{\partial y_2}{\partial t}\right|_i^{j+\frac{1}{2}} = -k_1\,[Ay_2|_i^{j+\frac{1}{2}} + O(\Delta t^2), \tag{6.171}$$

and

$$\left[\frac{\partial y_3}{\partial t}\right|_i^{j+\frac{1}{2}} = -k_{-1}{y_3}_i^{j+\frac{1}{2}} + O(\Delta t^2), \tag{6.172}$$

which are all of second order in time.

### 6.7.2 Accuracy of the Implicit Finite Difference Method (IML1)

In this subsection, we consider the accuracy of the implicit numerical method given in Section 6.6.2. We begin by first rewriting Equation (6.124) as

$$\begin{aligned}\frac{A_i^j - A_i^{j-1}}{\Delta t} &= -k_1\,[AB|_i^j + k_{-1}\,[C|_i^j \\ &+ \frac{D}{\Delta x^2}[y_1|_{i+1}^j\left\{\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\beta_j(\gamma)\left[\frac{A}{y_1}\right|_{i+1}^0 + \left[\frac{A}{y_1}\right|_{i+1}^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{A}{y_1}\right|_{i+1}^k\right]\right\} \\ &- 2\frac{D}{\Delta x^2}[y_1|_i^j\left\{\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\beta_j(\gamma)\left[\frac{A}{y_1}\right|_i^0 + \left[\frac{A}{y_1}\right|_i^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{A}{y_1}\right|_i^k\right]\right\} \\ &+ \frac{D}{\Delta x^2}[y_1|_{i-1}^j\left\{\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left[\beta_j(\gamma)\left[\frac{A}{y_1}\right|_{i-1}^0 + \left[\frac{A}{y_1}\right|_{i-1}^j + \sum_{k=1}^{j-1}\mu_{j-k}(\gamma)\left[\frac{A}{y_1}\right|_{i-1}^k\right]\right\}.\end{aligned} \tag{6.173}$$

Identifying the last three terms in Equation (6.173) as the L1 approximation acting upon the function $g(t) = \frac{A}{y_1}$, at the points $i+1$, $i$ and $i-1$, we can rewrite Equation (6.173) as

$$\frac{A_i^j - A_i^{j-1}}{\Delta t} = -k_1 \left[AB\right|_i^j + k_{-1} \left[C\right|_i^j$$
$$+ \frac{D}{\Delta x^2}\left\{ {y_1}_{i+1}^j \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1,L1}^j - 2{y_1}_i^j \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,L1}^j + {y_1}_{i-1}^j \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1,L1}^j \right\}. \tag{6.174}$$

Taking the Taylor series expansion around the point $t_j = j\Delta t$ for the term on the left-hand side, gives

$$\begin{aligned}\frac{A_i^{j+1} - A_i^j}{\Delta t} &= \left[\frac{\partial A}{\partial t}\right|_i^j + \frac{\Delta t}{2!}\left[\frac{\partial^2 A}{\partial t^2}\right|_i^j + O(\Delta t^2) \\ &= \left[\frac{\partial A}{\partial t}\right|_i^j + O(\Delta t). \end{aligned} \tag{6.175}$$

Furthermore taking the Taylor series expansion around the point $x_i = i\Delta x$ in space for the last term on the right of Equation (6.174), we have

$$\begin{aligned}&{y_1}_{i+1}^j \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i+1,L1}^j - 2{y_1}_i^j \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,L1}^j + {y_1}_{i-1}^j \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i-1,L1}^j \\ &= 2\left\{\frac{(\Delta x)^2}{2!}\left[\frac{\partial^2}{\partial x^2}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j + \frac{(\Delta x)^4}{4!}\left[\frac{\partial^4}{\partial x^4}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j + O(\Delta x^6)\right\} \\ &= \Delta x^2\left[\frac{\partial^2}{\partial x^2}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j + O(\Delta x^4).\end{aligned} \tag{6.176}$$

Equation (6.174) then becomes

$$\left[\frac{\partial A}{\partial t}\right|_i^j + O(\Delta t) = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j + O(\Delta x^2). \tag{6.177}$$

Adding and subtracting the term $D\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j$ we find

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j \tag{6.178}$$
$$- D\left\{\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j - \left[\frac{\partial^2}{\partial x^2}\left(y_1\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j\right\} + O(\Delta x^2) + O(\Delta t),$$

which after using Equation (6.151) becomes

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j + O(\Delta x^2) + O(\Delta t)$$
$$- D\left\{y_1{}_i^j\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j + 2\left[\frac{\partial y_1}{\partial x}\right|_i^j\left[\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j\right.$$
$$+ \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^j\left[\frac{\partial^2 y_1}{\partial x^2}\right|_i^j - \left(y_1{}_i^j\left[\frac{\partial^2}{\partial x^2}\left(\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j\right.$$
$$\left.\left. +2\left[\frac{\partial y_1}{\partial x}\right|_i^j\left[\frac{\partial}{\partial x}\left(\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j + \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,L1}^j\left[\frac{\partial^2 y_1}{\partial x^2}\right|_i^j\right)\right\}. \tag{6.179}$$

Simplifying we then find

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right]_i^j + O(\Delta x^2) + O(\Delta t)$$
$$- D\left\{y_1{}_i^j\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{A}{y_1}\right|_{L1}\right)\right|_i^j\right.$$
$$+ 2\left[\frac{\partial y_1}{\partial x}\right|_i^j\left[\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{L1}\right)\right|_i^j$$
$$\left. + \left[\frac{\partial^2 y_1}{\partial x^2}\right|_i^j\left(\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right|_{i,L1}^j\right)\right\}. \tag{6.180}$$

Now by Equation (2.48) the terms of the form $\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}(g)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}(g)\right|_{i,L1}^j$ are of $O(\Delta t^{1+\gamma})$, then we have

$$\left[\frac{\partial A}{\partial t}\right|_i^j = -k_1\left[AB\right|_i^j + k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(y_1\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{A}{y_1}\right)\right)\right|_i^j$$
$$+ O(\Delta x^2) + O(\Delta t) + O(\Delta t^{1+\gamma}). \tag{6.181}$$

We now see the truncation error for this equation is first order in time and second order in space.

In a similar manner, swapping $A$ with $B$ and $y_1$ with $y_2$, we see the truncation error of Equation (6.125) is again first order in time and second order in space.

Using a similar process, we can find the truncation error accuracy of Equation (6.127). We begin by rewriting Equation (6.127) as

$$\frac{C_i^j - C_i^{j-1}}{\Delta t} = k_1\left[AB\right|_i^j - k_{-1}\left[C\right|_i^j \tag{6.182}$$
$$+ \frac{D}{\Delta x^2}\left\{y_3{}_{i+1}^j\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i+1,L1}^j - 2y_3{}_i^j\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i,L1}^j + y_3{}_{i-1}^j\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i-1,L1}^j\right\}.$$

Expanding the Taylor series around the point $(x_i, t_j)$ and then using Equations (6.175) and (6.176) with $C$ replacing $A$ and $y_3$ replacing $y_1$, we then have

$$\left[\frac{\partial C}{\partial t}\right|_i^j + O(\Delta t) = k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(y_3\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{L1}\right)\right|_i^j + O(\Delta x^2). \tag{6.183}$$

Adding and subtracting the term $\left[\frac{\partial^2}{\partial x^2}\left(y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_i^j$ we then find

$$\begin{aligned}\left[\frac{\partial C}{\partial t}\right|_i^j &= k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right]_i^j \\ &- D\left\{\left[\frac{\partial^2}{\partial x^2}\left(y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_i^j - \left[\frac{\partial^2}{\partial x^2}\left(y_3\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{L1}\right)\right|_i^j\right\} + O(\Delta x^2) + O(\Delta t).\end{aligned} \tag{6.184}$$

After evaluating the second spatial derivative, using Equation (6.151), and simplifying, gives

$$\begin{aligned}\left[\frac{\partial C}{\partial t}\right|_i^j &= k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\frac{\partial^2}{\partial x^2}\left[y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right]_i^j + O(\Delta x^2) + O(\Delta t) \\ &- D\left\{y_{3\,i}^{\,j}\left[\frac{\partial^2}{\partial x^2}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{L1}\right)\right|_i^j\right. \\ &+ 2\left[\frac{\partial y_3}{\partial x}\right|_i^j\left[\frac{\partial}{\partial x}\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right) - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{L1}\right)\right|_i^j \\ &\left.+\left[\frac{\partial^2 y_3}{\partial x^2}\right|_i^j\left(\left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_i^j - \left[\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right|_{i,L1}^j\right)\right\}.\end{aligned} \tag{6.185}$$

Note by Equation (2.48) the difference between the exact and the L1 approximation is $O(\Delta t^{1+\gamma})$ as mentioned earlier. We then have

$$\left[\frac{\partial C}{\partial t}\right|_i^j = k_1 \left[AB\right|_i^j - k_{-1}\left[C\right|_i^j + D\left[\frac{\partial^2}{\partial x^2}\left(y_3\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\left(\frac{C}{y_3}\right)\right)\right|_i^j + O(\Delta x^2) + O(\Delta t) + O(\Delta t^{1+\gamma}) \tag{6.186}$$

which shows the truncation error, $\tau_{i,j}$, for this equation is first order in time and second order in space i.e.

$$\tau_{i,j} = O(\Delta x^2) + O(\Delta t). \tag{6.187}$$

Now to find the accuracy order of ${y_r}_i^j$, where $r = 1, 2, 3$, in Equations (6.129) – (6.131), now rewrite the equations as

$$\frac{{y_1}_i^j - {y_1}_i^{j-1}}{\Delta t} = -k_1\left[By_1\right|_i^j, \tag{6.188}$$

$$\frac{y2_i^j - y2_i^{j-1}}{\Delta t} = -k_1 \left[Ay_2\right|_i^j, \tag{6.189}$$

and

$$\frac{y3_i^j - y3_i^{j-1}}{\Delta t} = -k_{-1} \left[y_3\right|_i^j, \tag{6.190}$$

and then taking the Taylor series expansion around the point $x_i = i\Delta x$ in space, by using Equation (6.175) with ${y_r}_i^j$ replacing $A_i^j$, we then have

$$\left[\frac{\partial y_1}{\partial t}\right|_i^j = -k_1 \left[By_1\right|_i^j + O(\Delta t), \tag{6.191}$$

$$\left[\frac{\partial y_2}{\partial t}\right|_i^j = -k_1 \left[Ay_2\right|_i^j + O(\Delta t), \tag{6.192}$$

and

$$\left[\frac{\partial y_3}{\partial t}\right|_i^j = -k_{-1} \left[y_3\right|_i^j + O(\Delta t), \tag{6.193}$$

which shows each is first order in time.

## 6.8 Consistency of the Numerical Methods for Model 1 and Model 2

The numerical schemes for solving Model Type 1 and Model Type 2 are consistent, as the truncation error approaches zero as $\Delta t \to 0$ and $\Delta x \to 0$. Hence the KBMC2 and the IML1 methods are both consistent with the original fractional reaction diffusion equations.

## 6.9 Numerical Examples and Results

In this section, three examples considered of the implementation for Model type 1 and Model Type 2 based on the KBMC2 and the IML1 schemes. For each example, the numerical predictions of each model are shown. These schemes are implemented in MATLAB R2014a (see Appendix C.5) using the fsolve subroutine to solve the system of nonlinear equations.

We estimate the order of convergence numerically for the KBMC2 method by computing the maximum norm of the error between the numerical estimate and the approximate "exact solution" at the time $t = 1$, by using a large number of grid points and time steps.

**Example 6.9.1.** In this Example we consider the solution of the ordinary differential equation (ODE) models of the reversible reaction given by Equations (6.8) – (6.10) with the initial conditions $A(0) = 0$, $B(0) = 1$ and $C(0) = 2$. We use $k_1 = 1$, and $k_{-1} = 1$ and we take time $t \in [0, 10]$. In Figure 6.1, we see the chemical species $A$ and $B$ react together to form the reactant $C$ and $C$ reacts to form $A$ and $B$. In Figure 6.2 we use $k_1 = 1$, and $k_{-1} = 3$, the results shown that the chemical species $C$ reacts faster to form $A$ and $B$. Whilst in Figure 6.3 with $k_1 = 3$, and $k_{-1} = 1$, we see the chemical species $A$ and $B$ react together faster to form $C$. In each case the solution for each species quickly approaches a steady state. Note in each case the solution for each species remains positive.

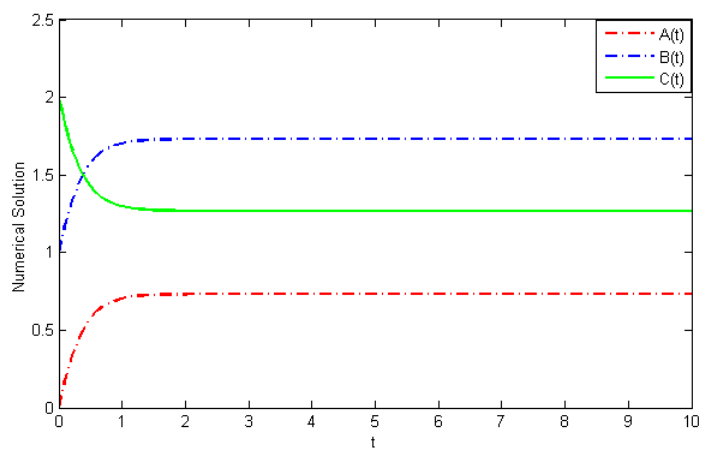



Figure 6.1: Numerical solution for ODE, where $k_1 = 1$, $k_{-1} = 1$ and time $t \in [0, 10]$.

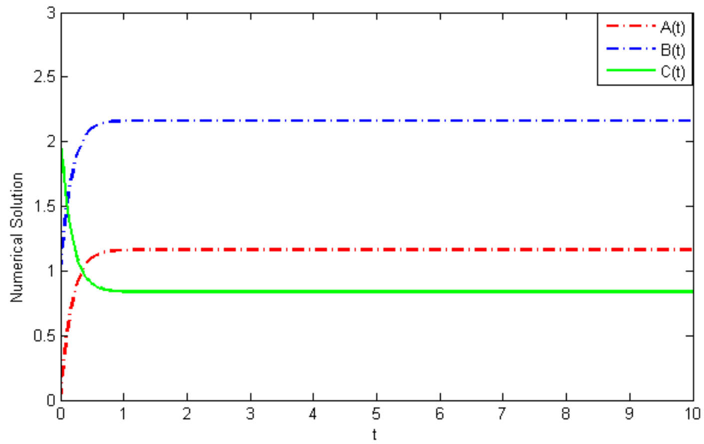



Figure 6.2: Numerical solution for ODE, where $k_1 = 1$, $k_{-1} = 3$ and time $t \in [0, 10]$.

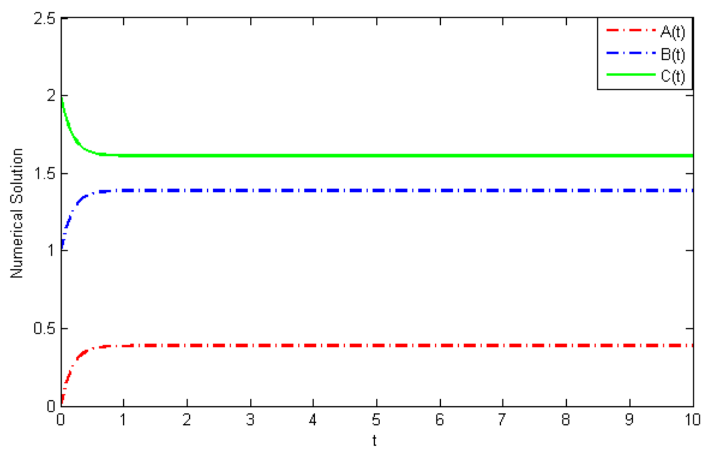



Figure 6.3: Numerical solution for ODE, where $k_1 = 3$, $k_{-1} = 1$ and time $t \in [0, 10]$.

**Example 6.9.2.** In this Example we consider the solution of the two fractional partial differential equation models of the reversible reaction

$$A + B \rightleftharpoons C \tag{6.194}$$

in the presence of anomalous subdiffusion as given in Sections 6.2 and 6.5 for $0 \le x \le 1$ and $0 \le t \le 1$. For both models we use the initial conditions

$$\begin{aligned} A(x, 0) &= (1 - \cos(2\pi x))/2, \\ B(x, 0) &= (1 - \cos(2\pi x))/2, \\ C(x, 0) &= 1, \end{aligned} \tag{6.195}$$

along with the no-flux boundary conditions

$$\frac{\partial A(0,t)}{\partial x} = 0,$$
$$\frac{\partial B(0,t)}{\partial x} = 0, \tag{6.196}$$
$$\frac{\partial C(0,t)}{\partial x} = 0.$$

For Model Type 2 we also need the initial conditions

$$y_i(0) = 1, \;\; i = 1, 2, 3. \tag{6.197}$$

For both models we set the fractional exponent $\gamma = 1/2$, the forward reaction rate $k_1 = 1$, the backward reaction rate $k_{-1} = 1$, and the diffusion coefficient $D = 1$.

### 6.9.1 KBMC2 Predictions

Here we compare the numerical solution of Model Type 1 and Model Type 2 using the KBMC2 scheme in Sections 6.3 and 6.6. We first use the KBMC2 scheme for Model Type 1 given by Equations (6.14), (6.15) and (6.16), with $\Delta t = 0.001$ and $\Delta x = 0.02$. To include the no-flux boundary condition in both schemes we approximate the derivative by centred finite difference at the boundary point. When we set this to zero requires we replace the value of species $A$ at $x = -\Delta x$ with the value of $A$ at $x = \Delta x$. Similarly we also replace the value of $A$ at $x = L - \Delta x$ with $x = L + \Delta x$. We also use same approximation for species $B$ and $C$.

The results are shown in Figures 6.4 – 6.6, similar to the preview example it can be seen that the chemical species $A$ and $B$ react together to form the reactant $C$ and $C$ reacts to form $A$ and $B$. We also see that $C$ decays to a homogeneous steady state, whilst $A$ and $B$ increase to a homogeneous steady state. This is similar to the behaviour of the homogeneous solution in Example 6.9.1 in Figure 6.1 at longer times.

We also show the numerical solution KBMC2 scheme for Model Type 2, Equations (6.95), (6.96) and (6.112), under the same initial and boundary conditions for the chemical species used for Model Type 1 in Figures 6.7 – 6.9. It can be seen that the chemical species $A$ and $B$ react together to form $C(x,t)$ and vice versa. Once again the solution behaves similar to ODE system in Figure 6.1 for long times.

In Figure 6.10 we give a comparison of the predicted values of $A(x,t)$ using Model Type 1 and Model Type 2 at $x = 0.5$ and $x = 0.9$. From this figure we see similar asymptotic behaviour from both models (Model Type 1 and Model Type 2). We also see in Figure 6.11 the difference for species $A$ between the two models, $\epsilon = A_1(0.5,t) - A_2(0.5,t)$ at $x = 0.5$. From this we see the results from Model Type 1 predicts a higher value than Model Type 2.

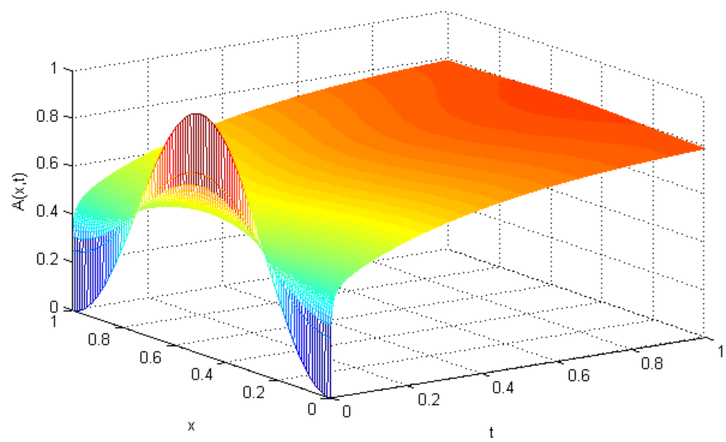



Figure 6.4: The predictions of $A(x,t)$ given by the KBMC2 scheme, Section 6.3.1, for Model Type 1.

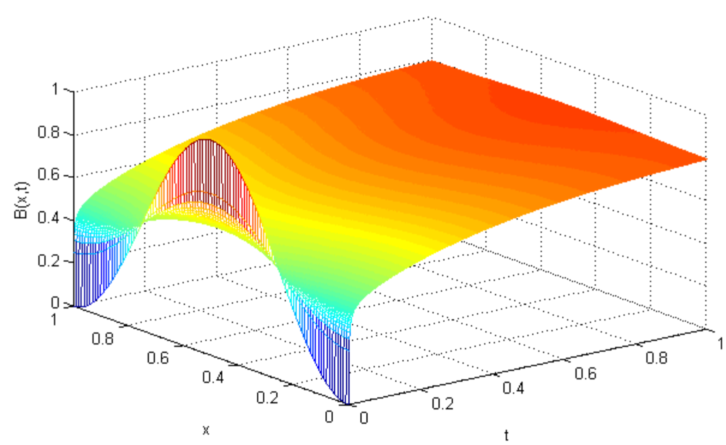



Figure 6.5: The Model Type 1 predictions of $B(x,t)$ using the KBMC2 scheme in Section 6.3.1.

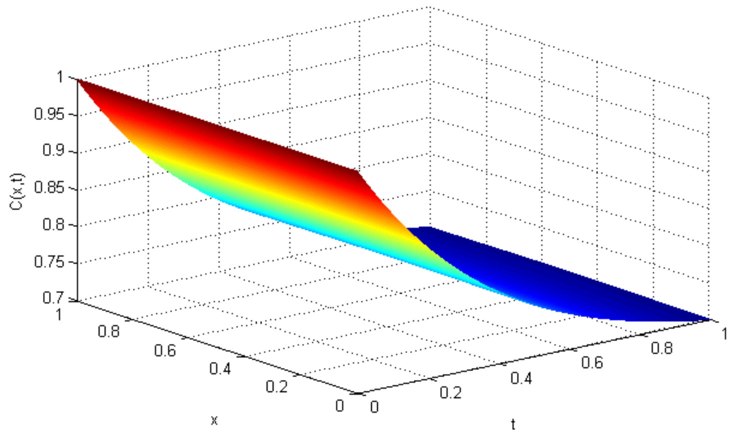



Figure 6.6: The Model Type 1 predictions of $C(x,t)$ using the KBMC2 scheme, Section 6.3.1.

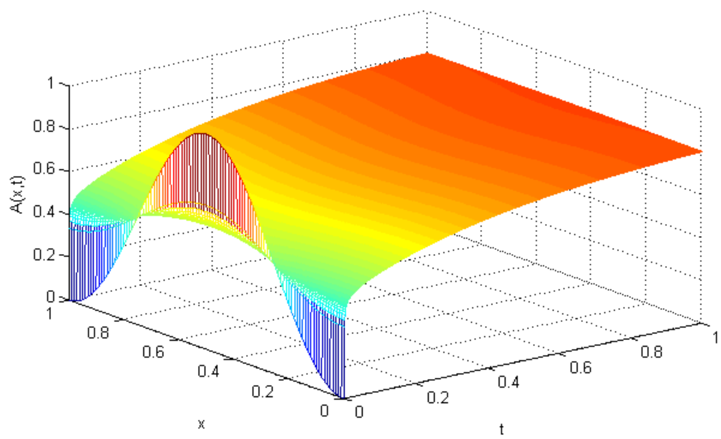



Figure 6.7: The Model Type 2 predictions of $A(x,t)$ using the KBMC2 scheme, Section 6.6.1.

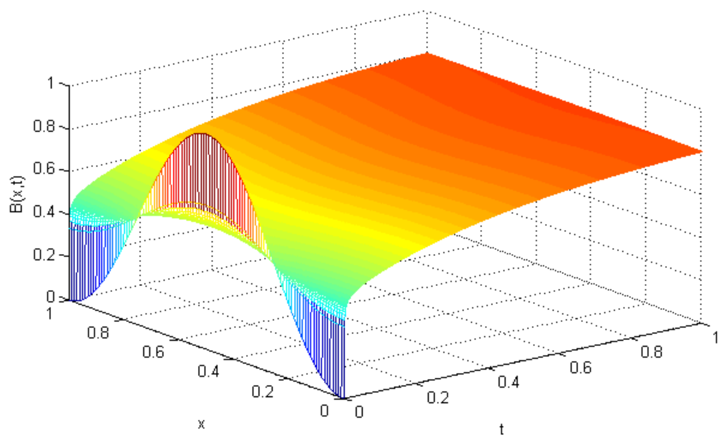



Figure 6.8: The predictions of $B(x,t)$ using the KBMC2 scheme in Section 6.6.1 for Model Type 2.

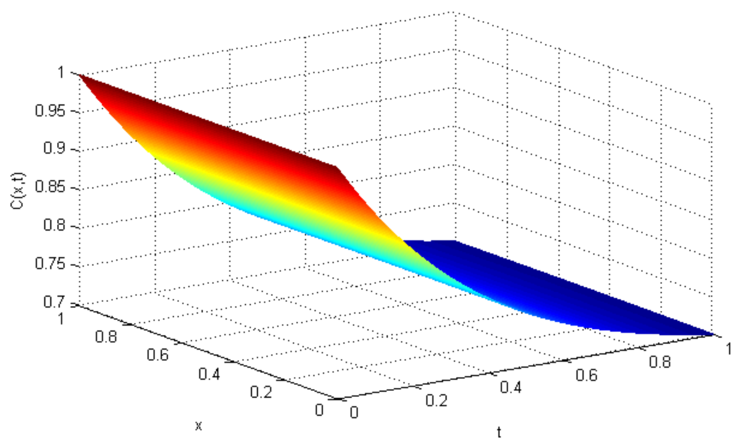



Figure 6.9: The Model Type 2 predictions of $C(x,t)$ using the KBMC2 scheme, Section 6.6.1.

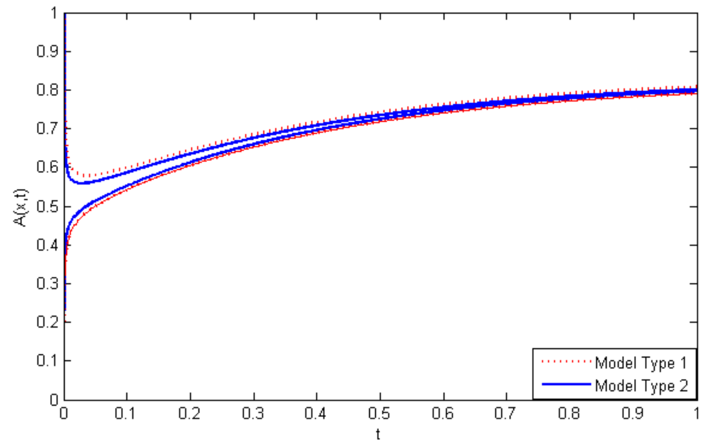



Figure 6.10: The comparison between Model Type 1 and Model Type 2 by using KBMC2 for species $A$ in Equations (6.14) and (6.95) at $x = 0.5$ (upper two lines) and 0.9 (lower two lines).

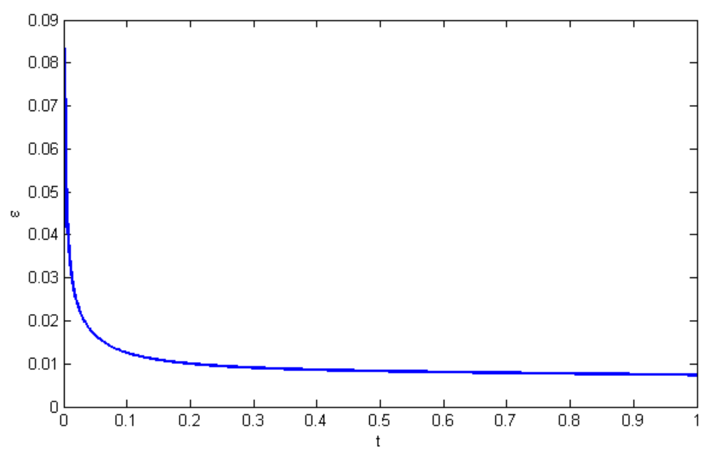



Figure 6.11: The estimate of the difference, $\epsilon$, in the prediction for $A(0.5, t)$ given by Model Type 1, and Model Type 2 by using KBMC2 for Equations (6.14) and (6.95) where $\epsilon = A_1(0.5, t) - A_2(0.5, t)$.

### 6.9.2 IML1 Predictions

Here we again compare the numerical solution of Model Type 1 and Model Type 2 using the IML1 scheme in Sections 6.3 and 6.6. We use the IML1 scheme for Model Type 1 given by Equations (6.24), (6.25), and (6.26), with $\Delta t = 0.001$ and $\Delta x = 0.01$, also we use the same initial conditions as in previous examples. The results are shown in Figures 6.12

– 6.14, it can be seen again that the chemical species $A$ and $B$ react together to form the reactant $C$ and vice versa. We also see that $C$ decays to a homogeneous steady state, whilst $A$ and $B$ increase to a homogeneous steady state. Again this is similar to the ODE prediction in Example 6.9.1 after $A$, $B$, and $C$ here reacted a homogeneous state.

The numerical solution IML1 scheme for Model Type 2 (Equations (6.124), (6.125) and (6.128)) was also obtained under the same initial and boundary conditions for the chemical species. Again in Figures 6.15 – 6.17, it can be seen that the chemical species $A$ and $B$ are react together to form $C(x,t)$ and we also see the species $A$ and $B$ increase to a homogeneous steady state, whilst $C$ decays to a homogeneous steady state. This behaviour is similar to the KBMC2 method predictions.

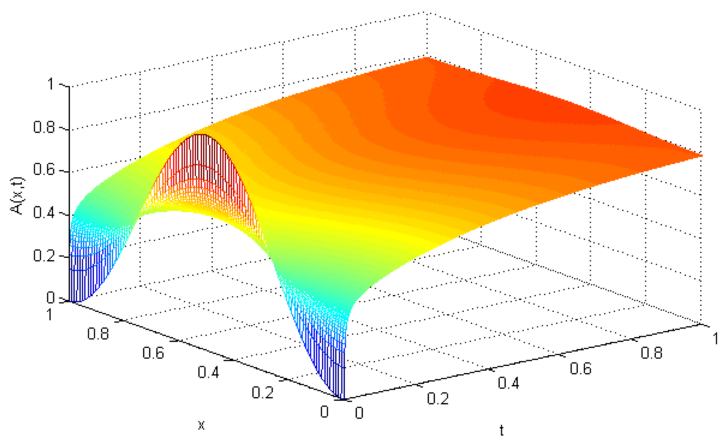



Figure 6.12: The Model Type 1 predictions of $A(x,t)$ using the IML1 scheme.

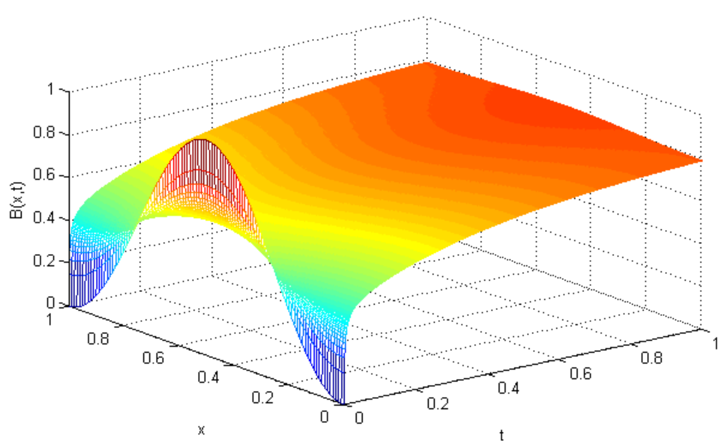



Figure 6.13: The Model Type 1 predictions of $B(x,t)$ using the IML1 scheme.

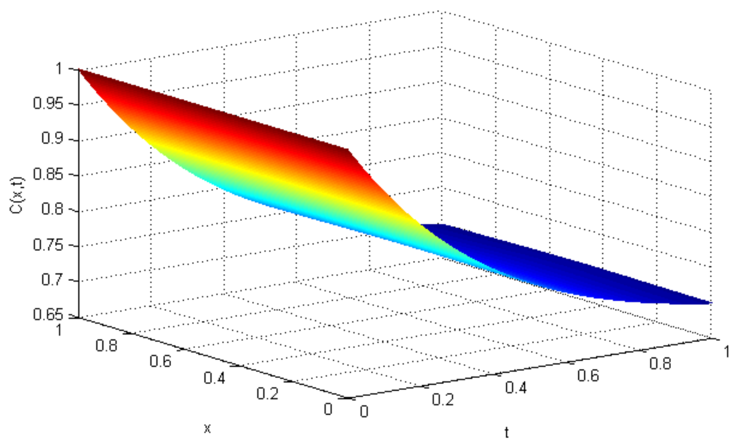



Figure 6.14: The Model Type 1 predictions of $C(x, t)$ using the IML1 scheme.

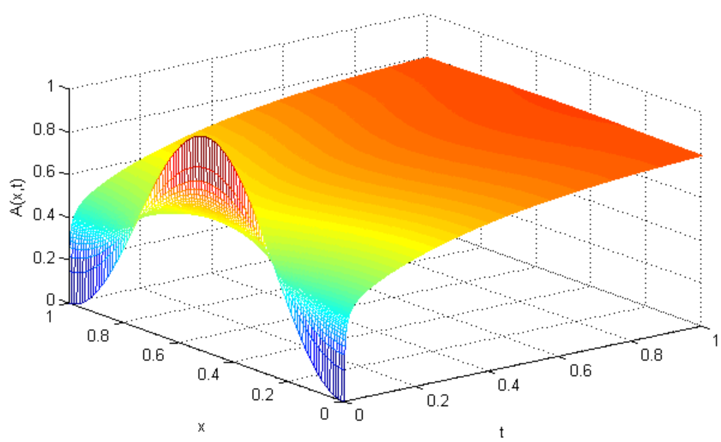



Figure 6.15: The Model Type 2 predictions of $A(x, t)$ using the IML1 scheme.

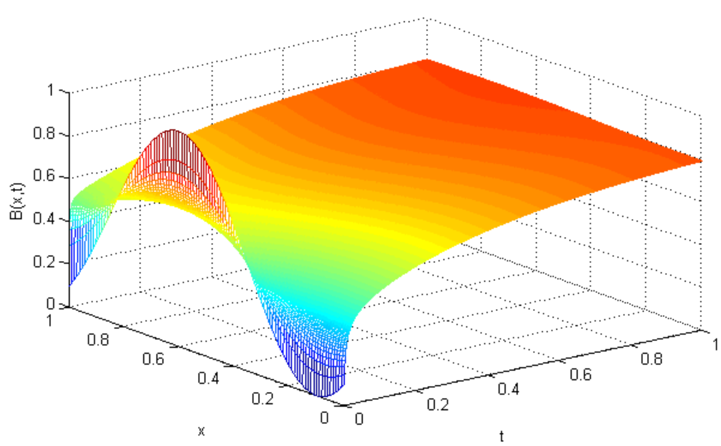



Figure 6.16: The Model Type 2 predictions of $B(x, t)$ using the IML1 scheme.

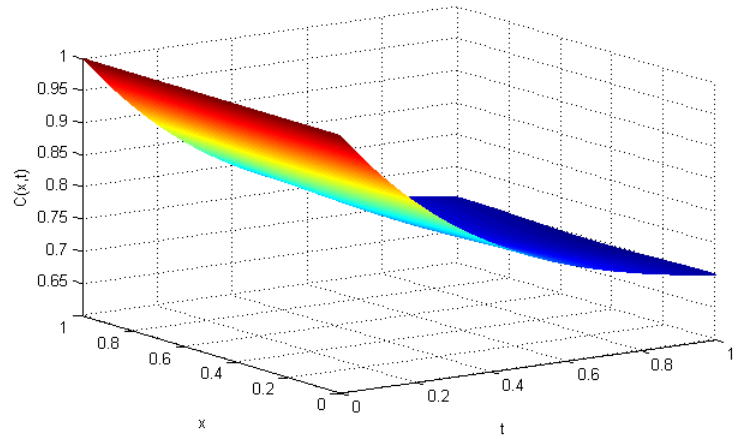



Figure 6.17: The Model Type 2 predictions of $C(x,t)$ using the IML1 scheme.

## Estimation of the order of Convergence

In Figures 6.18 – 6.21 we give the difference between predictions for species $A$ and $C$ at the mid point when different time steps are used for Model Type 2 and Model Type 1 respectively at time $t = 1$. In Figure 6.18 the value $\epsilon_1$ is the difference between the estimates if $\Delta t = 10^{-2}$ (100 time steps) with when the time step is $\Delta t = 10^{-3}$ is used (1000 time steps). The value $\epsilon_2$ is the difference between when $\Delta t = 10^{-3}$ and $\Delta t = 10^{-4}$ time steps are used, also the value $\epsilon_3$ is the difference between when $\Delta t = 10^{-4}$ and $\Delta t = 10^{-5}$ time steps are used. We see the difference between the numerical predictions for species $A$ decreases as the time step is decreased and appear to converge to zero as shown by the arrows in each figure. We also see similar behaviour in Figures 6.19 – 6.21.

The error and order of convergence estimates found from applying the KBMC2 on Model Type 2 and Model Type 1 for species $A$ and $C$. The error approximated in using a long run with a large number of time steps, with $\Delta t = 1.25 \times 10^{-4}$ and a large number of grid points, with $\Delta x = 5 \times 10^{-4}$, to approximate the "exact solution" because we do not have the exact solution for both models. The results are given in Tables 6.1–6.8 for species $A(x,t)$ and $C(x,t)$ respectively where $\gamma = 0.1, 0.5, 0.9$ and time $t = 1.0$. To estimate the convergence in space we kept $\Delta t$ fixed at $10^{-3}$ whilst varying $\Delta x$. To estimate the convergence in time we kept $\Delta x$ fixed at $10^{-3}$ whilst varying $\Delta t$.

For both species $A(x,t)$ and $C(x,t)$, Model Type 2, in Tables 6.2 and 6.6 we see the numerical scheme appears to be of order $O(\Delta x^2)$ which compares well with the accuracy analysis. However for Model Type 1 in Tables 6.4 and 6.8, the numerical scheme does not appear to be second order in space.

The obtained numerical convergence order estimates do not appear to match up with the expected order of $1+\gamma$ in time, but the errors do decrease as $\Delta t$ is decreased showing convergence. Note the computational time and memory requirement prohibited the run of a very large simulation with a larger number of time and spatial points, and hence smaller $\Delta x$ and $\Delta t$. Therefore, the numerical predictions used to approximate the "exact solution" to find the error may still include an error which may influence the results. Another reason could be the spatial truncation error may not be small enough and may also still affect the estimate of the convergence order in time. Increasing the number of grid points may alleviate this at the expense of a large computational time. We may not able to obtain the convergence order $1+\gamma$ in time, since we have a system of nonlinear equations unlike in Chapters 3,4 and 5.

We know the stability and convergence are very important requirements for a robust numerical scheme. These models involve a very complicated set of equations and so it is not possible to obtain exact analytical conditions for the stability and convergence. However, we tested our scheme under different time and grid steps and found the solutions appear to be converge. Hence we believe that our scheme does converge at least for the range of parameters tested. We have not tested the estimate of convergence for the IML1 scheme since we are not expecting to obtain a better convergence order result given the accuracy analysis.

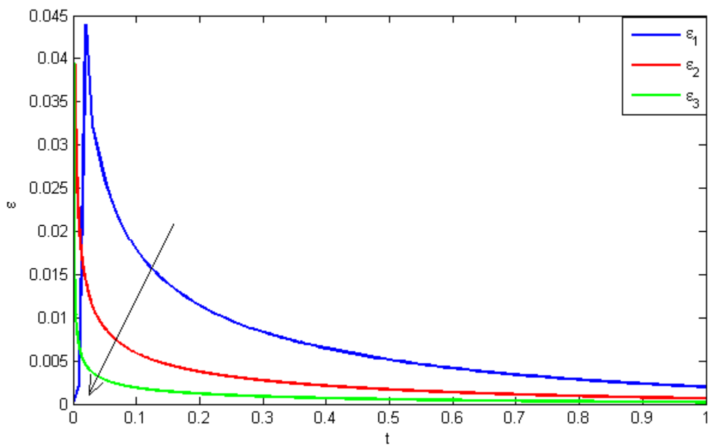



Figure 6.18: The estimate of the difference, $\epsilon$, in the prediction for $A(0.5, t)$ given by Model Type 2 with KBMC2, where $\epsilon_1$ is the difference between when $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$ time steps, $\epsilon_2$ is the difference between $\Delta t = 10^{-3}$ and $\Delta t = 10^{-4}$ time steps. The value $\epsilon_3$ is the difference between $\Delta t = 10^{-4}$ and $\Delta t = 10^{-5}$ time steps.

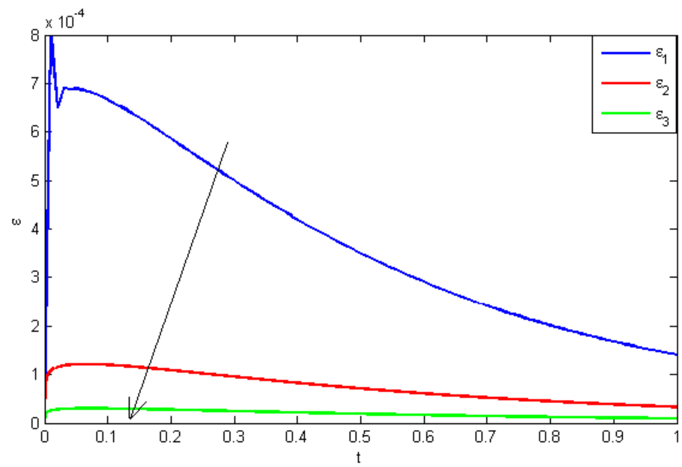



Figure 6.19: The estimate of the difference, $\epsilon$, in the prediction for $C(0.5, t)$ given by Model Type 2 with KBMC2, where $\epsilon_1$ is the difference between when $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$ time steps, $\epsilon_2$ is the difference between $\Delta t = 10^{-3}$ and $\Delta t = 10^{-4}$ time steps. The value $\epsilon_3$ is the difference between $\Delta t = 10^{-4}$ and $\Delta t = 10^{-5}$ time steps.

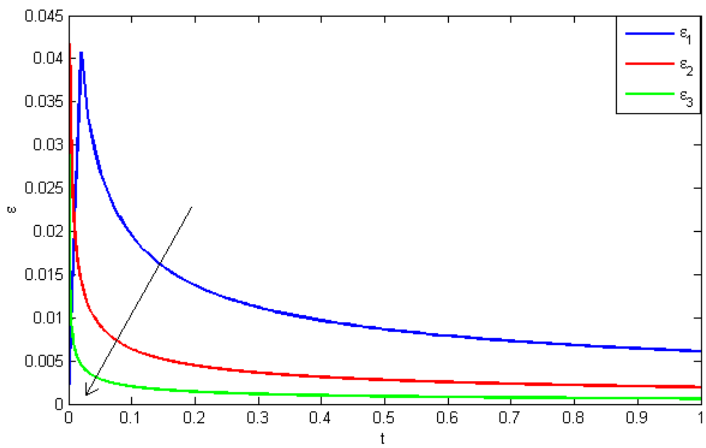



Figure 6.20: The estimate of the difference, $\epsilon$, in the prediction for $A(0.5, t)$ given by Model Type 1 with KBMC2, where $\epsilon_1$ is the difference between when $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$ time steps, $\epsilon_2$ is the difference between $\Delta t = 10^{-3}$ and $\Delta t = 10^{-4}$ time steps. The value $\epsilon_3$ is the difference between $\Delta t = 10^{-4}$ and $\Delta t = 10^{-5}$ time steps.

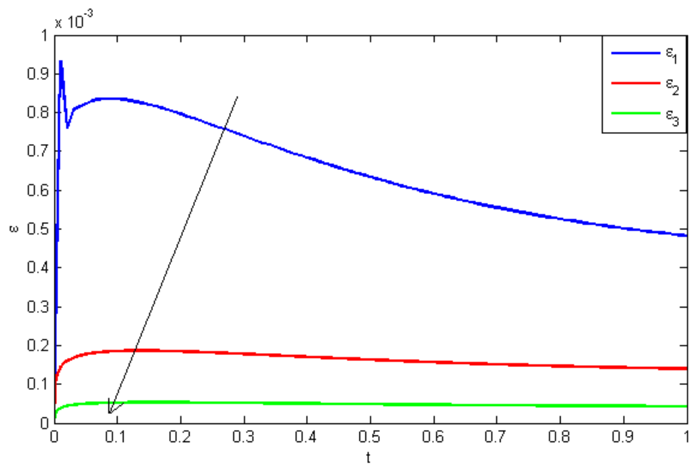



Figure 6.21: The estimate of the difference, $\epsilon$, in the prediction for $C(0.5, t)$ given by Model Type 1 with KBMC2, where $\epsilon_1$ is the difference between when $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$ time steps, $\epsilon_2$ is the difference between $\Delta t = 10^{-3}$ and $\Delta t = 10^{-4}$ time steps. The value $\epsilon_3$ is the difference between $\Delta t = 10^{-4}$ and $\Delta t = 10^{-5}$ time steps.

Table 6.1: Numerical convergence order in $\Delta t$ for Model Type 2 based of the KBMC2 scheme for species $A(x,t)$, and $R1$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ |
| 1/125 | 2.800e–02 | – | 2.455e–03 | – | 1.351e–04 | – |
| 1/250 | 2.247e–02 | 0.3 | 1.623e–03 | 0.6 | 4.646e–05 | 1.5 |
| 1/500 | 1.742e–02 | 0.4 | 1.041e–03 | 0.6 | 1.705e–06 | 1.5 |
| 1/1000 | 1.279e–02 | 0.5 | 6.320e–04 | 0.7 | 6.341e–07 | 1.6 |
| 1/2000 | 8.552e–03 | 0.6 | 3.448e–04 | 0.9 | 1.974e–07 | 1.7 |

Table 6.2: Numerical convergence order in $\Delta x$ for Model Type 2 based of the KBMC2 scheme for species $A(x,t)$, and $R2$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ |
| 1/125 | 1.482e–06 | – | 3.513e–05 | – | 7.189e–05 | – |
| 1/250 | 3.663e–07 | 2.0 | 8.781e–06 | 2.0 | 1.776e–05 | 2.0 |
| 1/500 | 8.722e–08 | 2.1 | 2.195e–06 | 2.0 | 4.228e–06 | 2.1 |
| 1/1000 | 1.746e–08 | 2.3 | 5.488e–07 | 2.0 | 8.457e–07 | 2.3 |

Table 6.3: Numerical convergence order in $\Delta t$ for Model Type 1 based of the KBMC2 scheme for species $A(x,t)$, and $R1$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ |
| 1/125 | 6.173e–02 | – | 7.211e–03 | – | 3.359e–05 | – |
| 1/250 | 4.451e–02 | 0.5 | 4.791e–03 | 0.6 | 1.642e–05 | 1.0 |
| 1/500 | 2.855e–02 | 0.6 | 3.083e–03 | 0.6 | 7.895e–06 | 1.1 |
| 1/1000 | 1.374e–02 | 1.1 | 1.878e–03 | 0.7 | 3.511e–06 | 1.2 |

Table 6.4: Numerical convergence order in $\Delta x$ for Model Type 1 based of the KBMC2 scheme for species $A(x,t)$ , and $R2$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ |
| 1/125 | 8.762e–04 | – | 1.352e–03 | – | 1.389e–03 | – |
| 1/250 | 4.084e–04 | 1.1 | 6.295e–04 | 1.1 | 6.470e–04 | 1.1 |
| 1/500 | 1.749e–04 | 1.2 | 2.695e–04 | 1.2 | 2.77e–04 | 1.2 |
| 1/1000 | 5.828e–05 | 1.6 | 8.976e–05 | 1.6 | 9.230e–05 | 1.6 |

Table 6.5: Numerical convergence order in $\Delta t$ for Model Type 2 based of the KBMC2 scheme for species $C(x,t)$, and $R1$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ |
| 1/125 | 2.418e–03 | – | 1.466e–04 | – | 1.351e–05 | – |
| 1/250 | 1.898e–03 | 0.4 | 8.961e–05 | 0.7 | 4.646e–06 | 1.5 |
| 1/500 | 1.439e–03 | 0.4 | 5.400e–05 | 0.7 | 1.705e–06 | 1.5 |
| 1/1000 | 1.035e–03 | 0.5 | 3.129e–05 | 0.8 | 6.341e–07 | 1.6 |
| 1/2000 | 6.780e–04 | 0.6 | 1.649e–05 | 0.9 | 1.974e–07 | 1.7 |

Table 6.6: Numerical convergence order in $\Delta x$ for Model Type 2 based of the KBMC2 scheme for species $C(x,t)$, and $R2$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ |
| 1/125 | 2.157e–06 | – | 3.762e–08 | – | 2.028e–06 | – |
| 1/250 | 5.331e–07 | 2.0 | 9.407e–09 | 2.0 | 5.012e–07 | 2.0 |
| 1/500 | 1.270e–07 | 2.1 | 2.355e–09 | 2.0 | 1.193e–07 | 2.1 |
| 1/1000 | 2.551e–08 | 2.3 | 5.885e–10 | 2.0 | 2.387e–08 | 2.3 |

Table 6.7: Numerical convergence order in $\Delta t$ for Model Type 1 based of the KBMC2 scheme for species $C(x,t)$, and $R1$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta t$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ | $e_\infty(\Delta t)$ | $R1$ |
| 1/125 | 7.400e–03 | – | 5.389e–04 | – | 9.962e–06 | – |
| 1/250 | 5.219e–03 | 0.5 | 3.494e–04 | 0.6 | 4.166e–06 | 1.3 |
| 1/500 | 3.277e–03 | 0.7 | 2.208e–04 | 0.7 | 1.814e–06 | 1.3 |
| 1/1000 | 1.545e–03 | 1.1 | 1.328e–04 | 0.7 | 7.600e–07 | 1.3 |

Table 6.8: Numerical convergence order in $\Delta x$ for Model Type 1 based of the KBMC2 scheme for species $C(x,t)$ , and $R2$ is order of convergence.

| | $\gamma = 0.1$ | | $\gamma = 0.5$ | | $\gamma = 0.9$ | |
|---|---|---|---|---|---|---|
| $\Delta x$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ | $e_\infty(\Delta t)$ | $R2$ |
| 1/125 | 8.734e–04 | – | 1.349e–03 | – | 1.388e–03 | – |
| 1/250 | 4.077e–04 | 1.1 | 6.288e–04 | 1.1 | 6.468e–04 | 1.1 |
| 1/500 | 1.747e–04 | 1.2 | 2.693e–04 | 1.2 | 2.770e–04 | 1.2 |
| 1/1000 | 5.825e–05 | 1.6 | 8.973e–05 | 1.6 | 9.230e–05 | 1.6 |

### 6.9.3 Comparison between the KBMC2 Scheme and the IML1 Scheme

Here we compare the numerical solution of Model Type 2 using the KBMC2 and the IML1 scheme, with $\Delta t = 0.001$, $\Delta x = 0.01$ and $\gamma = \frac{1}{2}$ for $0 \leq t \leq 1$. We also use the same initial conditions as in the previous example. In Figures 6.22 and 6.23 we give a comparison at $x = 0.3$, 0.5 and $x = 0.9$ for species $A(x,t)$. We see the KBMC2 predictions for the concentration of chemical species $A$ appear to be lower than the predictions from the IML1 scheme at $x = 0.3$ and $x = 0.5$ whilst being slightly higher at $x = 0.9$. The numerical predictions are different, and this could be due to the order of accuracy where the KBMC2 is of order $1+\gamma$ in time whilst the IML1 is only first order in time. However the asymptotic of behaviour of Model Type 2 is similar for both methods.

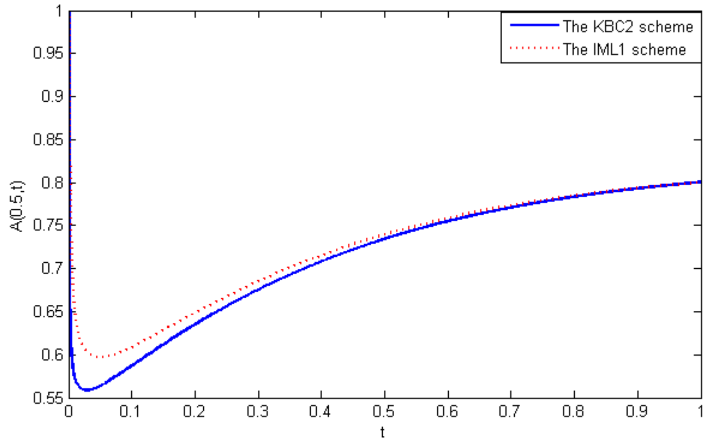



Figure 6.22: The comparison between the KBMC2 scheme and the IML1 scheme for Model Type 2 (species $A$) at $x = 0.5$ with $0 \leq t \leq 1$.

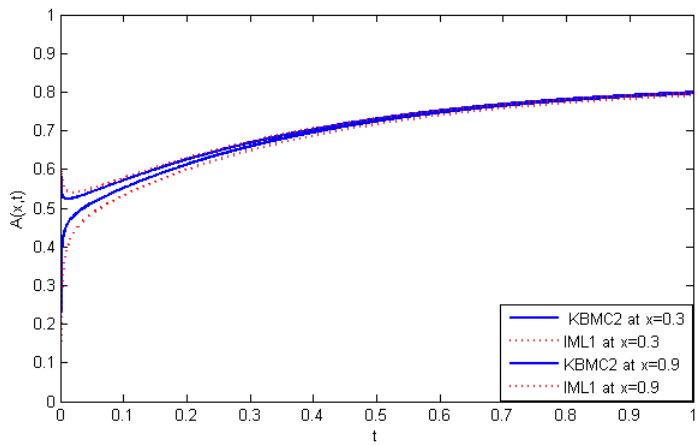



Figure 6.23: The comparison between the KBMC2 scheme and the IML1 scheme for Model Type 2 (species $A$) at $x = 0.3$ (upper two lines) and 0.9 (lower two lines), with $0 \leq t \leq 1$.

**Example 6.9.3.** In this Example we consider the solution of the two fractional partial differential equation models of the backward reaction only, as given in Sections 6.2 and 6.5 for $0 \leq x \leq 1$ and $0 \leq t \leq 1$, with $k_1 = 0$ and $k_{-1} = 2$. For both models we use the initial condition

$$C(x, 0) = (1 - \cos(2\pi x))/2 \tag{6.198}$$

along with boundary condition given by Equation (6.196). For Model Type 2 we also need the initial condition

$$y_3(0) = 1. \tag{6.199}$$

The exact solution of Model Type 1 and Model Type 2, where $k_1 = 0$ is given in Henry, Langlands & Wearne (2006) and Langlands et al. (2011). The exact solution for Equation (6.3), with $k_1 = 0$, is

$$C(x,t) = \sum_{n=0}^{\infty} a_n \cos(\lambda_n x) \sum_{m=0}^{\infty} \frac{(-k_{-1}t)^m}{m!} E_{\gamma,1+(1-\gamma)m}^{(m)}(-\lambda_n^2 t^\gamma), \tag{6.200}$$

and for Equation (6.6), is

$$C(x,t) = \sum_{n=0}^{\infty} a_n \cos(\lambda_n x) \exp(-k_{-1}t) E_\gamma(-\lambda_n^2 t^\gamma), \tag{6.201}$$

where $\lambda_n = \frac{n\pi}{L}$.

For the initial condition in Equation (6.198) we have $a_0 = \frac{1}{2}$, $a_1 = -\frac{1}{2}$ and $a_n = 0$ otherwise. For Model Type 1 we use the KBMC2 scheme needing only Equation (6.16) and for Model Type 2 we only need Equation (6.112) with $y_3^j = \exp(-k_{-1}t_j)$.

For both models we have found the solution at $t = 5$ using $\Delta t = 0.001$, $\gamma = 0.5$, $k_{-1} = 2$, $D = 1$ and $\Delta x = 0.01$. In Figures 6.24 and 6.25, we show the numerical solution of Model Type 1 and Model Type 2 by using KBMC2 scheme under the same boundary and initial conditions. The solution evolves to homogeneous state, for both models, and then decays to zero.

A comparison of the value of $C$ for Model Type 1 and Model Type 2 using the KBMC2 scheme, with the same boundary and initial conditions and $\gamma = \frac{1}{2}$ is shown in Figures 6.26 and 6.27 at the points $x = 0.1$ and $x = 0.9$. We see in both figures that the predicted solution of Model Type 1 becomes negative whilst Model Type 2 remains positive. The result of a negative value was predicted in Langlands et al. (2009) in the infinite domain case for Model Type 1. The negative prediction is physically unrealistic showing Model Type 2 with the modified operator is the better model to use.

Results for comparison between the two models are not shown here for IML1 scheme, because the order of accuracy the KBMC2 method is more accurate in $\Delta t$ than IML1 method and the focus of this chapter was the KBMC2 scheme.

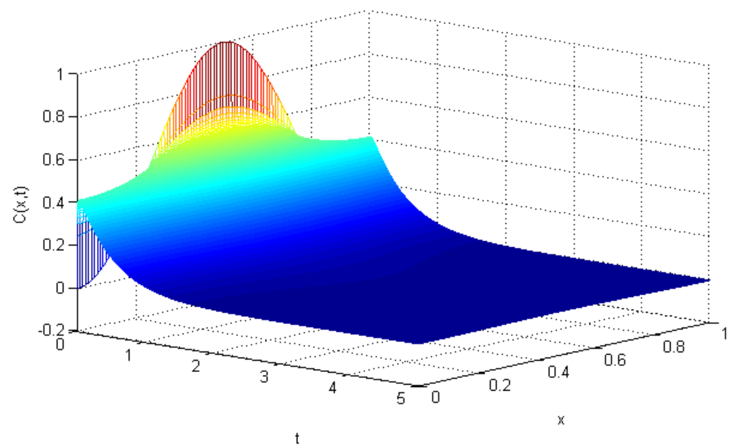



Figure 6.24: The Model Type 1 predictions of $C(x,t)$ using the KBMC2 scheme, Section 6.6.1, where $k_1 = 0$, and $k_{-1} = 2$.

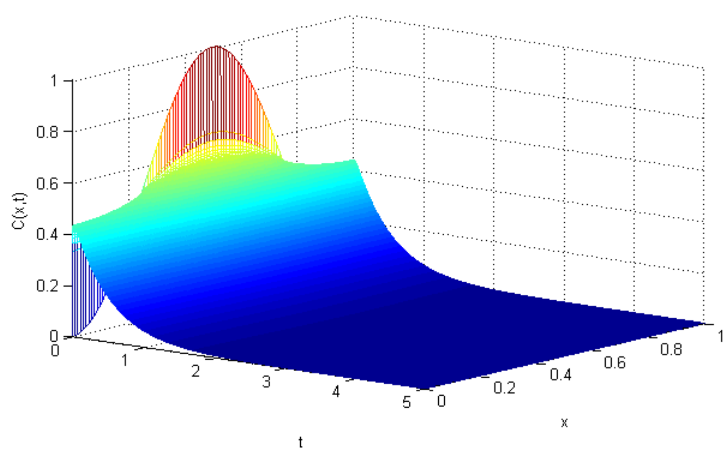



Figure 6.25: The Model Type 2 predictions of $C(x,t)$ using the the KBMC2 scheme, Section 6.3.1, where $k_1 = 0$, and $k_{-1} = 2$.

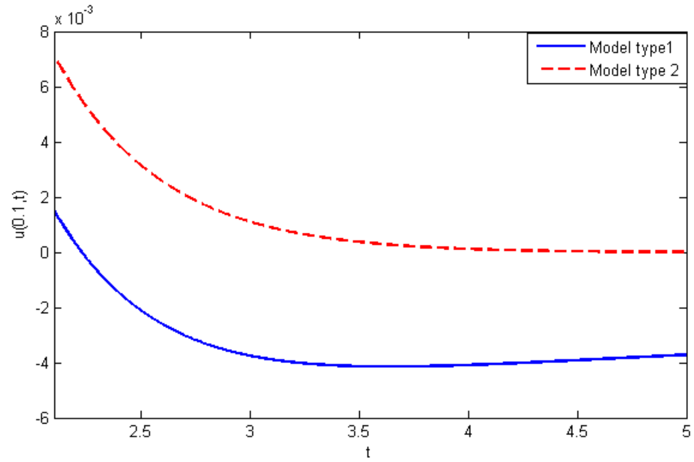



Figure 6.26: Comparison between Model Type 1 and Model Type 2 predictions for $C(0.1, t)$ by using the KBMC2 scheme for $\gamma = 0.5$, with $\Delta t = 0.001$, $k_1 = 0$, and $k_{-1} = 2$.

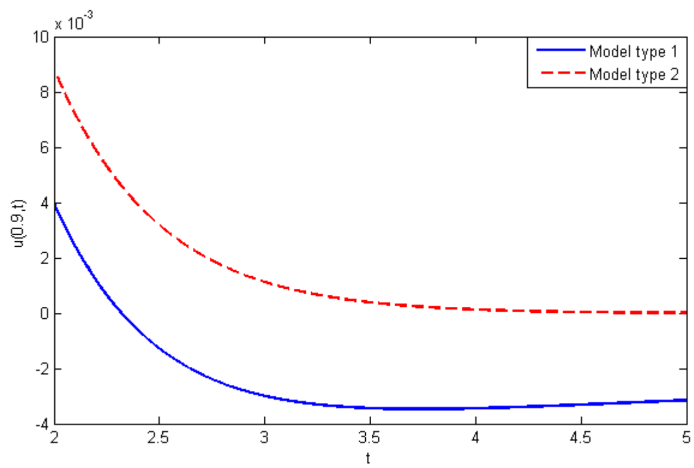



Figure 6.27: Comparison between Model Type 1 and Model Type 2 predictions for $C(0.9, t)$ by using the KBMC2 scheme for $\gamma = 0.5$, with $\Delta t = 0.001$, $k_1 = 0$, and $k_{-1} = 2$.

## 6.10 Conclusion

In this work, we extended the KBMC2 scheme and the IML1 scheme to the case of systems of nonlinear fractional partial differential equations. We considered two models of a reversible reaction in the case of anomalous subdiffusion: Model Type 1 (Henry & Wearne 2000) and Model Type 2 (Angstmann, Donnelly & Henry 2013$a$). The accuracy of the KBMC2 method was found to be order $1+\gamma$ in time and second order in space, whilst for the IML1 method was first order in time and second order in space. In this chapter we conclude that the KBMC2 method is more accurate than IML1 method, given the higher order truncation error in $\Delta t$. The convergence of the KBMC2 scheme for both models are demonstrated numerically, we found the difference between the numerical predictions for species $A$ and $C$ decreases as the time step decreases and appear to converge to zero. However, the expected $1 + \gamma$ order of convergence was not found. But the spatial convergence order of two was found for Model Type 2 but not for Model Type 1.

The two models were compared for two examples given the same initial and boundary conditions and the same anomalous exponent. From the results, similar behaviour for both models was predicted by using the KBMC2 and IML1 schemes for short times. We note that the Model Type 2 takes longer to run computationally when compared to Model Type 1. This is most likely due to the need to solve a system of six differential equations in Model Type 2 rather than three in Model Type 1. However we see for long times the solution of Model Type 2 remains positive whilst the Model Type 1 predictions may become negative as shown for the case of the reaction $C \rightarrow A + B$ which is physically unrealistic.

We also compared the two numerical methods, the KBMC2 scheme and the IML1 scheme, for solving Model Type 2. The numerical predictions were slightly different. This is likely due to the difference in order of accuracy of both methods, as mentioned earlier. We also note the asymptotic behaviour of the Model Type 2 is similar for both methods. We conclude that using Model Type 2 with the modified operator is the better model than using Model Type 1 if we require the solution to remain positive to remain realistic.

# Chapter 7

# Conclusions and Further Work

## 7.1 Research Outcomes

The main objective of this thesis is to developing numerical methods for solving fractional partial differential equations. The fractional derivative is a nonlocal operator which has memory-like effect which makes numerical solution of the fractional diffusion equation challenging. Computationally this non-locality leads to higher computational effort and storage requirements.

In Chapter 2, we considered the approximation of the Riemann–Liouville fractional derivative. There are different techniques for approximating the fractional derivative such as the L1 scheme approximation and the Grünwald–Letnikov approximation (Oldham & Spanier 1974, Podlubny 1998). In this thesis we have concentrated on L1 scheme as this scheme is exact for linear function whereas the Grünwald–Letnikov approximation is not exact. One of the significant contributions made in this chapter was the development of the C1, C2, and C3 fractional derivative approximation schemes. These schemes were based on the Riemann–Liouville definition assuming a piecewise linear approximation as in the L1 scheme in Oldham & Spanier (1974). The accuracy of each these methods was considered. It was found that the C2 and the C3 schemes have a smaller asymptotic coefficient in the truncation error, although they have the same order as the L1 scheme.

Another method also considered in Chapter 2 was to approximate the fractional derivative using Romberg Integration. Here we estimated numerically the accuracy of the Romberg Integration (where $k = 2$) (in future work we will analyse the approximation error analytically). The comparisons were tested for the fractional derivative approximations at functions given by Equation (2.7) from these compression we conclude that the C2 approximation has less error for $0 < \gamma < 1$ than the L1, C1, C3, and Romberg Integration approximation schemes.

One of the major issues in evaluating fractional derivatives numerically is the cost of the evaluation of the convolution sum common to all fractional derivative approximations. The computational cost increases as the number of time steps increases when the full history is used. In this thesis we investigated the short–memory principle approach to evaluate fractional derivatives (Diethelm 1997, Podlubny 1998, Murio 2008). In this approach only the most recent history is used and the tail of the integral $0 \leq t \leq T$ (or convolution sum) is ignored.
Here we investigated the effect of ignoring the early history on the predictions by the L1 scheme. We considered short memory-based approximations of the fractional derivative of order $p$, namely the $L1^*$ and RL1 schemes. The $L1^*$ approximation was not exact for linear functions. To improve this approximation, the RL1 scheme was developed where we added an extra term $\frac{1}{\Gamma(2-p)}\left[{t_j}^{1-p} - (t_j - T)^{1-p}\right] f'(0)$, which then made the approximate value of the fractional derivative exact in the case of linear function similar to the L1 approximation. We compared the error for each of these methods and we saw that as more history is ignored the error increases.
Another method we considered was to use regression methods to approximate the early history for $0 \leq t \leq T$ and then use the piecewise linear approximation of the L1 method for the more recent history. We used three different approaches to approximate the early history including linear, quadratic and nonlinear regression. We again compared the error for each of these methods. We note that the smallest error occurs when we do not ignore the early history in these schemes (occurs for $n$ near zero). We also saw the error increases as more of the early history is ignored or approximated using regression. We conclude that using linear regression was more accurate than using quadratic or nonlinear regression.

In Chapter 3, we developed a numerical scheme for fractional subdiffusion equation with a source term. Here the implicit method was created by combining the C1 scheme (a modification of the L1 scheme) for the fractional derivative with the centred finite difference schemes for the spatial derivative. Thus the scheme is similar to the implicit scheme in Langlands & Henry (2005) for the fractional diffusion equation. In this thesis, the stability (using Von Neumann stability analysis) and the convergence of the numerical method was investigated theoretically. The accuracy of the method was found to be first order in time and second order in space. The numerical experiments conducted have confirmed these results.

In Chapter 4, we extended the implicit Dufort–Frankel method to solve the fractional subdiffusion equation. The L1 approximation was used here to approximate the fractional derivative. The proposed schemes were shown to be convergent, with an order $O\left(\Delta t, \Delta x^2, \frac{\Delta t^{1+\gamma}}{\Delta x^2}\right)$ but only if the consistency condition $\frac{\Delta t^{1+\gamma}}{\Delta x^2} \rightarrow 0$ is satisfied will the scheme be consistent with the original equation. The stability of the Dufort–Frankel method was investigated by using Von Neumann stability analysis, and we have shown the method is unconditionally stable for the parameter range $2 \leq V_q \leq 4$. We also demonstrated the method becomes unstable numerically when $0 < V_q < 2$ and $0 < \gamma \leq 1$. The convergence for the numerical method demonstrated theoretically for $2 \leq V_q \leq 4$. Numerical results were also conducted to verify the accuracy of the method. These results confined the earlier results. To get the order of the convergence though we had to choose a very small $\Delta t/\Delta x$ ratio to ensure the consistency condition was satisfied. We conclude that this method is severely limited because the method is only conditionally consistent.

In Chapter 5, we constructed three implicit Keller Box–based numerical schemes, the KBMC2, the KBMC3, and the KBML1 schemes for the solution of the fractional subdiffusion equation and the KBMC2–FADE scheme for solving the fractional advection–diffusion equation. The L1 scheme and the modified L1 schemes, i.e. the C2 and the C3 schemes, were used to estimate the Riemann–Liouville fractional derivative at the times $t_j$ and $t_{j+\frac{1}{2}}$ respectively. The accuracy of the KBMC2, the KBMC3 and the KBMC2–FADE methods proved to be order $1+\gamma$ in time and second order in space. The stability of these methods was investigated by using Von Neumann stability analysis. The stability of the KBMC2 method was proven in the case $0 \leq \Lambda_q \leq \min(\frac{1}{\tilde{\mu}_0}, 2^\gamma)$ when $0 < \gamma \leq 1$ and demonstrated numerically in case $\frac{1}{\tilde{\mu}_0} < \Lambda_q \leq 2^\gamma$ and $\log_3 2 \leq \gamma \leq 1$. We have also proved the stability of the KBMC3 method in case $0 < \breve{\Lambda}_q \leq 2$ and $0 < \gamma \leq 1$ and demonstrated the method is also stable numerically when $1 < \breve{\Lambda}_q \leq 2$ and $0 < \gamma \leq 1$. We have shown the KBML1 method is unconditionally stable using Von Neumann stability analysis. The convergence analysis was discussed, we have proved the KBMC2 scheme, in the case $\widetilde{\lambda}_q = \min(\widetilde{\mu}_0(\gamma), 2^\gamma)$, and the KBMC3 scheme, in the case if $0 < \widehat{\lambda}_q \leq 2/\widehat{\mu}_1(\gamma)$, are convergent with order $1+\gamma$ in time and second order in space, but the KBML1 method was shown to be second order in space and only first order in time. The convergence orders for KBMC2–FADE scheme by using the mathematical induction was unsuccessful, but we demonstrated the order of convergence numerically. We conclude that the KBMC2 method is more accurate than KBML1 method. The convergence orders of the KBMC2, KBMC3, KBML1 and KBMC2–FADE schemes were confirmed when applied to three test examples.

In Chapter 6, we extended the numerical methods in Chapter 5 to systems of nonlinear fractional partial differential equations. The first, the KBMC2 scheme, was based upon the Keller Box method and the second, the IML1 scheme, was based on the implicit method in Langlands & Henry (2005). We tested these schemes on two models of the reversible reactions, $A + B \rightleftharpoons C$, extended to the case of anomalous subdiffusion. The accuracy of the KBMC2 method was found to be $1+\gamma$ in time and second order in space, whilst the IML1 method was found to be only first order in time but also second order in space. We also investigated examples for the Models Type 1 and Model Type 2, and we saw that the chemical species $A$ and $B$ react together to form the reactant $C$, and $C$ reacts to form $A$ and $B$. We also see that $C$ decays to a homogeneous steady state, whilst $A$ and $B$ increase to a homogeneous steady state.

The error and order of convergence estimates found from applying the KBMC2 on Model Type 2 and Model Type 1 for species $A$ and $C$. The error approximated in using a long run with a large number of time steps with $\Delta t = 1.25 \times 10^{-4}$, and a large number of grid points, with $\Delta x = 5 \times 10^{-4}$, to approximate the exact solution because we do not have the exact solution for both models. From the difference between the numerical predictions for species $A$ and $C$ decreases as the time step is decreased and so appear to converge to zero. We also found the numerical scheme on Model Type 2 appears to be second order in space, but for Model Type 1 the numerical scheme does not appear to be second order in space. The obtained results do not appear to match up with the order that we expected $1+\gamma$ in time, but the errors do decrease as $\Delta t$ is decreased showing convergence. Note the amount of computational time and memory required prohibited the run of a very large simulations with a larger number of time steps and spatial points. We may not able to obtain the convergence order $1+\gamma$ in time since we have a system of nonlinear equation. The numerical predictions used to approximate the exact solution to find the error may still include an error which may influence the results.

A comparison of the results for both models given the same initial and boundary conditions and the same anomalous exponent, show similar behaviour. However we see for long times the solution of Model Type 2 remains positive whilst Model Type 1 becomes negative for the case of the reaction $C \to A + B$. The negative prediction is physically unrealistic showing Model Type 2 with the modified operator is the better model to use. However we note that Model Type 2 takes longer to run compared to Model Type 1.

## 7.2 Future Work

There are a number of areas in this thesis that could be pursued in the future. In particular, the accuracy analysis of the Romberg Integration and Regression approximation schemes in Chapter 2 has been left as future work. These methods also need to be incorporated into the full numerical method, which will allow testing of the convergence and stability of full methods. It could be interesting to consider higher order Romberg Integration approximation, i.e. $k \geq 2$, to obtain more accurate approximations but with less computation.

The problem of the computational cost of the memory sum though is still an open problem. The Regression and Romberg approximations may aid in reducing the computation if implemented carefully. The computational cost of using Regression methods versus the full convolution sum is somewhat mitigated by the iterative nature of the regression predictions versus the cost of using the full summation.

As mentioned earlier in Chapter 2 there are higher order approximations for the fractional derivative, which could be combined with the Keller Box method to give a more accurate scheme. Combining such approximations with the Keller Box method will give higher order methods for both linear and nonlinear partial differential equations.

We have also only considered the solution in one spatial dimension in this thesis but this work can be extended to the two or three dimensions. However extending to the multi-dimensional case will increase the impact of evaluating the convolution sum. So it is important to reduce the cost of this sum using the regression method or Romberg integration scheme developed in this thesis.

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# Appendix A

# Conference Presentation in Connection with this Research

Sh. A. Osman, (2014). Solution of Fractional Diffusion Equation, presented at 8th Australia New Zealand Mathematics Convention, Melbourne, Australia, Dec 8–11, 2014.

**Abstract**

Anomalous subdiffusion is a physical phenomenon which observed in many systems that involving trapping, binding or macromolecular crowding. In recent years, the examples of anomalous diffusion have been discovered in many fields such as fluid mechanics, physics, engineering and biology. Anomalous diffusion can be modelled using fractional subdiffusion equation which involve a fractional derivative. The fractional derivative is a nonlocal operator which has memory-like effect which makes numerical solution of fractional subdiffusion equation challenging. In this work, we present the numerical solution for the fractional diffusion equations. We use the Riemann-Liouville definition for the fractional derivative. We approximate the fractional differential equation using a combination of either the using piecewise linear approximation (L1 scheme) and the Dufort-Frankel method, or the L1 scheme and the Keller Box method. The stability analysis of the proposed methods are investigated by Von-Neumann stability analysis and the Energy method. Numerical tests are given to show the accuracy and stability of the proposed methods.

# Appendix B

# Some Supporting Information

In this appendix we evaluate some supporting information for this thesis.

## B.1 Sign of the integrand in Equation (2.41)

We show the term in the first integrand of Equation (2.41)

$$(t_j - \tau)^{1-p} - \Delta t^{-p} \left[ (j-l)^{1-p} (t_{l+1} - \tau) - (j-(l+1))^{1-p} (t_l - \tau) \right]$$

is positive. We first let

$$f_1(\tau) = (t_j - \tau)^{1-p} \ , \tag{B.1}$$

and

$$f_2(\tau) = \Delta t^{-p} \left[ (j-l)^{1-p} (t_{l+1} - \tau) - (j-(l+1))^{1-p} (t_l - \tau) \right] \ , \tag{B.2}$$

where $t_l = l\Delta t$ and $\tau \in [t_l, t_{l+1}]$. Now taking the difference between $f_1(\tau)$ and $f_2(\tau)$ we then have

$$g(\tau) = f_1(\tau) - f_2(\tau) \ , \tag{B.3}$$

where by direction substitution we have

$$g(t_l) = (t_j - t_l)^{\gamma} - \Delta t^{-p} \left[ (j-l)^{1-p} (t_{l+1} - t_l) - (j-(l+1))^{1-p} (t_l - t_l) \right] = 0, \tag{B.4}$$

and

$$g(t_{l+1}) = (t_j - t_{l+1})^{\gamma} - \Delta t^{-p}\left[(j-l)^{1-p}(t_{l+1} - t_{l+1}) - (j-(l+1))^{1-p}(t_l - t_{l+1})\right] = 0. \tag{B.5}$$

The second derivative of the function $g(\tau)$ with respect to $\tau$ is then given by

$$\begin{aligned}\frac{d^2 g(\tau)}{d\tau^2} &= (1-p)(-p)(t_j - \tau)^{-p-1} \\ &= -p(1-p)(t_j - \tau)^{-p-1} \ .\end{aligned} \tag{B.6}$$

The value of the second derivative of $g(\tau)$ is negative, where $0 < p < 1$, we conclude that $g(\tau)$ is a concave down function of $\tau$. Since $g(t_l) = g(t_{l+1})$ and $g(\tau)$ is concave down then $g(\tau) > 0$ for $\tau \in (t_l, t_{l+1})$, i.e. $g(\tau) = f_1(\tau) - f_2(\tau) \geq 0$ and hence $f_1(\tau) \geq f_2(\tau)$ which we can see clearly in Figure B.1.

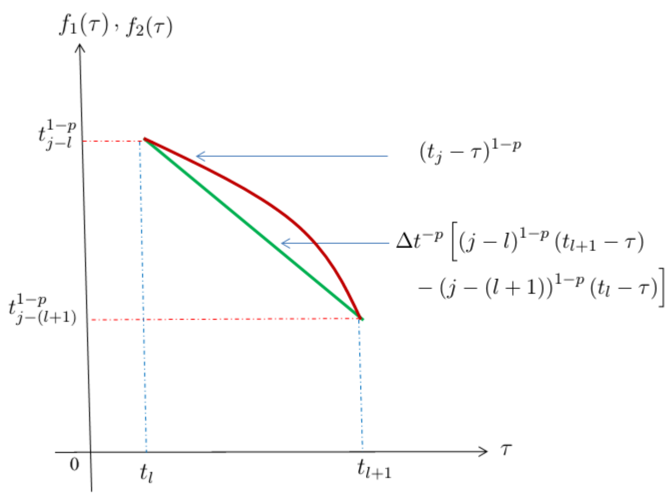



Figure B.1: Plot of functions $f_1(\tau)$ and $f_2(\tau)$ showing $f_1(\tau) \geq f_2(\tau)$ over the range $\tau \in [t_l, t_{l+1}]$.

## B.2 Binomial coefficient identity

Evaluating the identity of binomial coefficient, we then have

$$\begin{aligned}
\begin{pmatrix} \gamma \\ k \end{pmatrix} &= (-1)^k \binom{k}{k-\gamma-1} \\
&= (-1)^k \frac{(k-\gamma-1)!}{k!(-\gamma-1)!} \\
&= (-1)^k \frac{\Gamma(k-\gamma)}{k!\,\Gamma(-\gamma)} \\
&= \frac{(-\gamma)(-1)^k}{k!} \; \frac{\Gamma(k-\gamma)}{(-\gamma)\Gamma(-\gamma)} \\
&= \frac{\gamma\Gamma(k-\gamma)}{\Gamma(1-\gamma)} \; \frac{(-1)^{k-1}}{k!} \; .
\end{aligned} \tag{B.7}$$

## B.3 Bound for Equation (2.46) summation

In this section we obtain a bound for the summation in Equation (2.46), first from Equation (2.46) we have

$$S = \sum_{l=1}^{j} \left[ l^{1-p} \left( l - 1 + \frac{p}{2} \right) - (l-1)^{1-p} \left( l - \frac{p}{2} \right) \right] . \tag{B.8}$$

Expanding $(l-1)^{1-p}$ if $l \geq 1$, we find

$$(l-1)^{1-p} = \sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} l^{1-p-n} (-1)^n. \tag{B.9}$$

Then the summation term becomes

$$\begin{aligned}
l^{1-p}\left(l-1+\frac{p}{2}\right)-(l-1)^{1-p}\left(l-\frac{p}{2}\right) \\
&= l^{1-p}\left(l-1+\frac{p}{2}\right)-\left(l-\frac{p}{2}\right)\sum_{n=0}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{1-p-n}(-1)^n \\
&= l^{1-p}\left[\left(l-1+\frac{p}{2}\right)-\left(l-\frac{p}{2}\right)\right]-\left(l-\frac{p}{2}\right)\sum_{n=1}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{1-p-n}(-1)^n \\
&= (p-1)l^{1-p}-\left(l-\frac{p}{2}\right)\sum_{n=1}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{1-p-n}(-1)^n \\
&= (p-1)l^{1-p}-\sum_{n=1}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{2-p-n}(-1)^n+\frac{p}{2}\sum_{n=1}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{1-p-n}(-1)^n \\
&= -\sum_{n=2}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{2-p-n}(-1)^n+\frac{p}{2}\sum_{n=1}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{1-p-n}(-1)^n\ .
\end{aligned} \tag{B.10}$$

Rewriting the first summation as

$$-\sum_{n=2}^{\infty}\begin{pmatrix}1-p\\ n\end{pmatrix}l^{2-p-n}(-1)^n=\sum_{n=1}^{\infty}l^{1-p-n}(-1)^n\begin{pmatrix}1-p\\ n+1\end{pmatrix}\ , \tag{B.11}$$

and then combining the second we obtain

$$l^{1-p}\left(l-1+\frac{p}{2}\right)-(l-1)^{1-p}\left(l-\frac{p}{2}\right)=\sum_{n=1}^{\infty}l^{1-p-n}(-1)^n\left[\begin{pmatrix}1-p\\ n+1\end{pmatrix}+\frac{p}{2}\begin{pmatrix}1-p\\ n\end{pmatrix}\right]\ . \tag{B.12}$$

Note if $n=1$

$$\left[\begin{pmatrix}1-p\\ 2\end{pmatrix}+\frac{p}{2}\begin{pmatrix}1-p\\ 1\end{pmatrix}\right]=\frac{(1-p)(-p)}{2}+\frac{p(1-p)}{2}=0, \tag{B.13}$$

and so we have if $l\geq 1$

$$l^{1-p}\left(l-1+\frac{p}{2}\right)-(l-1)^{1-p}\left(l-\frac{p}{2}\right)=\sum_{n=2}^{\infty}l^{1-p-n}(-1)^n\left[\begin{pmatrix}1-p\\ n+1\end{pmatrix}+\frac{p}{2}\begin{pmatrix}1-p\\ n\end{pmatrix}\right]. \tag{B.14}$$

Note the coefficient

$$(-1)^n\left[\begin{pmatrix}1-p\\ n+1\end{pmatrix}+\frac{p}{2}\begin{pmatrix}1-p\\ n\end{pmatrix}\right] \tag{B.15}$$

can be shown to be positive for $0 < 1-p < 1$ and $n \geq 2$ as follows. We note from Equation (B.7)

$$\begin{pmatrix} 1-p \\ r \end{pmatrix} = \frac{(1-p)\Gamma(r-(1-p))}{\Gamma(p)} \frac{(-1)^{r-1}}{r!} \ . \tag{B.16}$$

Now using Equation (B.16) with $r = n+1$ and with $r = n$, we find

$$\begin{aligned}
&(-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \\
&\quad = (-1)^n \left[ \frac{(1-p)\Gamma(n+1-(1-p))}{(n+1)!\,\Gamma(p)} (-1)^n + \frac{p(1-p)\Gamma(n-(1-p))}{2n!\,\Gamma(p)} (-1)^{n-1} \right] \\
&\quad = \frac{(-1)^{2n}(1-p)}{2\Gamma(p)(n+1)!} \left[ 2\Gamma(n+p) - p\Gamma(n-(1-p))(n+1) \right] \\
&\quad = \frac{(1-p)}{2\Gamma(p)(n+1)!} \left[ 2(n+p-1)\Gamma(n+p-1) - p\Gamma(n+p-1)(n+1) \right] \\
&\quad = \frac{(1-p)\Gamma(n+p-1)}{2\Gamma(p)(n+1)!} \left[ 2(n+p-1) - p(n+1) \right] \\
&\quad = \frac{(1-p)\Gamma(n+p-1)}{2\Gamma(p)(n+1)!} \left[ (2-p)(n-1) \right] \\
&\quad = \frac{(1-p)(2-p)}{2} \frac{\Gamma(n+p-1)}{\Gamma(p)} \frac{(n-1)}{(n+1)!}.
\end{aligned} \tag{B.17}$$

Since $n \geq 2$ and $0 < p < 1$ then all terms, including the Gamma function, are positive and hence the coefficient in Equation (B.15) is positive. So the sum $S$ in Equation (B.8), after using Equation (B.14), is given by

$$\begin{aligned}
S &= \sum_{l=1}^{j} \left[ l^{1-p} \left( l - 1 + \frac{p}{2} \right) - (l-1)^{1-p} \left( l - \frac{p}{2} \right) \right] \\
&= \sum_{l=1}^{j} \sum_{n=2}^{\infty} l^{1-p-n} (-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \\
&= \sum_{n=2}^{\infty} (-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \sum_{l=1}^{j} l^{1-p-n}.
\end{aligned} \tag{B.18}$$

Now

$$\begin{aligned}
\sum_{l=1}^{j} l^{1-p-n} &= \sum_{l=0}^{j-1} (l+1)^{1-p-n} \\
&= \sum_{l=0}^{\infty} (l+1)^{1-p-n} - \sum_{l=j-1}^{\infty} (l+1)^{1-p-n} \\
&= \sum_{l=0}^{\infty} (l+1)^{1-p-n} - \sum_{l=0}^{\infty} (l+j)^{1-p-n} \\
&= \zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right),
\end{aligned} \tag{B.19}$$

where $\zeta(s,a)$ is the Hurwitz Zeta function (Apostol et al. 1951). So we need to evaluate

$$S = \sum_{n=2}^{\infty}(-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \left\{ \zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right) \right\} \ . \tag{B.20}$$

As shown earlier, the coefficient is positive. In addition for $s > 1$ and $a > 1$, the Hurwitz Zeta function is a monotonically decaying function, in both $s$ and $a$, so

$$\zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right) > 0, \tag{B.21}$$

and so

$$\begin{aligned}
S &= \sum_{n=2}^{\infty}(-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \left\{ \zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right) \right\} \\
&\leq \sum_{n=2}^{\infty}(-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \zeta\left(n-(1-p),1\right) \\
&\leq \sum_{n=2}^{\infty}(-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] \zeta\left(1+p,1\right).
\end{aligned} \tag{B.22}$$

Evaluating the summations we find

$$\begin{aligned}
\sum_{n=2}^{\infty}(-1)^n \binom{1-p}{n+1} &= -\sum_{n=2}^{\infty}(-1)^{n+1} \binom{1-p}{n+1} \\
&= -\sum_{n=3}^{\infty}(-1)^n \binom{1-p}{n} \\
&= -\left[\sum_{n=0}^{\infty}(-1)^n \binom{1-p}{n} - \binom{1-p}{0} + \binom{1-p}{1} - \binom{1-p}{2}\right] \\
&= -\left[0 - 1 + (1-p) - \frac{(1-p)(-p)}{2}\right] \\
&= \frac{p\,(1+p)}{2}, \qquad \text{(B.23)}
\end{aligned}$$

and

$$\begin{aligned}
\sum_{n=2}^{\infty}(-1)^n \binom{1-p}{n} &= \sum_{n=0}^{\infty}(-1)^n \binom{1-p}{n} - \binom{1-p}{0} + \binom{1-p}{1} \\
&= 0 - 1 + (1-p) \\
&= -p, \qquad \text{(B.24)}
\end{aligned}$$

where we have used the identity

$$\sum_{n=0}^{\infty}(-1)^n \binom{1-p}{n} = 0. \qquad \text{(B.25)}$$

We now have

$$\begin{aligned}
S &\leq \sum_{n=2}^{\infty}(-1)^n \left[\binom{1-p}{n+1} + \frac{p}{2}\binom{1-p}{n}\right] \zeta\,(1+p,1) \\
&\leq \left[\frac{p(1+p)}{2} + \frac{p}{2}(-p)\right] \zeta\,(1+p,1) \\
&\leq \frac{p}{2}\,\zeta\,(1+p,1)\,, \qquad \text{(B.26)}
\end{aligned}$$

which is finite for all $0 < p < 1$ and hence $S$ is bounded.

In the case of $p = 0$ and $p = 1$ the summation reduces to zero. In particular if $p = 0$ we find

$$S = \sum_{l=1}^{j}\left[l^{1-p}\left(l - 1 + \frac{p}{2}\right) - (l-1)^{1-p}\left(l - \frac{p}{2}\right)\right] = 0, \qquad \text{(B.27)}$$

and if $p = 1$ we obtain the result

$$S = \sum_{l=1}^{j} \left[ l^{1-p} \left( l - 1 + \frac{p}{2} \right) - (l-1)^{1-p} \left( l - \frac{p}{2} \right) \right] = 0.$$

So is $S$ is bounded for all $0 \leq p \leq 1$.

## B.4 The sign of the integrands in (2.116) is positive

We show the term in the first integrand of Equation (2.116)

$$(t_j - s)^{1-p} - \frac{\Delta t^{-p}}{2} \left(1 + 2^{-p}\right)(j\Delta t - s)$$

is positive for $0 < p < 1$. We first note

$$\frac{\Delta t^{-p}}{2} \left(1 + 2^{-p}\right)(j\Delta t - s) < \Delta t^{-p}(j\Delta t - s),$$

as $0 \leq \frac{1+2^{-p}}{2} \leq \frac{1}{4}$ for $0 < p < 1$. So we have

$$(t_j - s)^{1-p} - \frac{\Delta t^{-p}}{2} \left(1 + 2^{-p}\right)(j\Delta t - s) \geq (t_j - s)^{1-p} - \Delta t^{-p}(j\Delta t - s).$$

We now define

$$f(s) = (t_j - s)^{1-p} - \Delta t^{-p}(j\Delta t - s),$$

and show this function is positive. We note $f(j\Delta t) = 0$ and $f((j-1)\Delta t) = 0$ by direction evaluation. We also note

$$\frac{d^2 f}{ds^2} = -p(1-p)(t_j - s)^{-p-1} < 0,$$

and so $f(s)$ is a concave down function of $s$ in the interval $s \in ((j-1)\Delta t, j\Delta t)$. Hence $f(s) \geq 0$ and so the term

$$(t_j - s)^{1-p} - \frac{\Delta t^{-p}}{2} \left(1 + 2^{-p}\right)(j\Delta t - s) > f(s) \geq 0,$$

is positive as required. We also need to show the term

$$G(s) = (t_j - s)^{1-p} - \frac{\Delta t^{-p}}{2} \psi_l(s), \tag{B.28}$$

is also positive for $l\Delta t \leq s \leq (l+1)\Delta t$. From Equation (2.115) we have

$$\begin{aligned} \psi_l(s) = {} & \frac{1}{2}(l\Delta t - s)\left[(j-l)^{1-p} + (j-(l-1))^{1-p} - (j-(l+1))^{1-p} - (j-(l+2))^{1-p}\right] \\ & + \frac{\Delta t}{2}\left[2(j-l)^{1-p} + (j-(l-1))^{1-p} + (j-(l+1))^{1-p}\right] . \end{aligned} \tag{B.29}$$

We note at $s = l\Delta t$, we have

$$\frac{\Delta t^{-p}}{2}\psi_l(l\Delta t) = \frac{\Delta t^{1-p}}{4}\left[2(j-l)^{1-p} + (j-(l-1))^{1-p} + (j-(l+1))^{1-p}\right] . \quad \text{(B.30)}$$

Now expanding $(j-(l-1))^{1-p}$ and $(j-(l+1))^{1-p}$, we have

$$(j-(l-1))^{1-p} = \sum_{r=0}^{\infty} \begin{pmatrix} 1-p \\ r \end{pmatrix} (j-l)^{1-p-r}, \quad \text{(B.31)}$$

and

$$(j-(l+1))^{1-p} = \sum_{r=0}^{\infty} \begin{pmatrix} 1-p \\ r \end{pmatrix} (j-l)^{1-p-r}(-1)^r. \quad \text{(B.32)}$$

Using these results in Equation (B.30), we find

$$\frac{\Delta t^{-p}}{2}\psi_l(l\Delta t) = \frac{\Delta t^{1-p}}{4}\left[2(j-l)^{1-p} + \sum_{r=0}^{\infty} \begin{pmatrix} 1-p \\ r \end{pmatrix} (j-l)^{1-p-r}\left(1+(-1)^r\right)\right] . \quad \text{(B.33)}$$

which simplifies to

$$\begin{aligned} \frac{\Delta t^{-p}}{2}\psi_l(l\Delta t) &= \frac{\Delta t^{1-p}}{4}\left[4(j-l)^{1-p} + 2\sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ 2n \end{pmatrix} (j-l)^{1-p-2n}\right] \\ &= (j-l)^{1-p}\Delta t^{1-p} + \frac{\Delta t^{1-p}}{2}\sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ 2r \end{pmatrix} (j-l)^{1-p-2n}. \end{aligned} \quad \text{(B.34)}$$

Here we note the coefficient $\begin{pmatrix} 1-p \\ 2n \end{pmatrix}$ is negative since

$$\begin{aligned} \begin{pmatrix} 1-p \\ 2n \end{pmatrix} &= (-1)^{2n}\frac{\Gamma(2n-(1-p))}{(2n)!\,\Gamma(p-1)} \\ &= \frac{(p-1)(-1)^{2n}}{(2n)!}\frac{\Gamma(n-(1-p))}{(p-1)\Gamma(p-1)} \\ &= \frac{(p-1)\Gamma(n-(1-p))}{(2n)!\Gamma(p)}. \end{aligned} \quad \text{(B.35)}$$

Therefore we have

$$\frac{\Delta t^{-p}}{2}\psi_l(l\Delta t) < (j-l)^{1-p}\Delta t^{1-p} = (t_j - l\Delta t)^{1-p}$$

and so at $s = l\Delta t$ the term in Equation (B.28) is positive, i.e. $G(l\Delta t) > 0$.

Likewise at $s = (l+1)\Delta t$, we have

$$\frac{\Delta t^{-p}}{2}\psi_l((l+1)\Delta t) = \frac{\Delta t^{1-p}}{4}\left[(j-l)^{1-p} + 2(j-(l+1))^{1-p} + (j-(l+2))^{1-p}\right], \quad \text{(B.36)}$$

which after using the expansions

$$\begin{aligned}(j-l))^{1-p} &= (j-(l+1)+1)^{1-p} \\ &= \sum_{r=0}^{\infty}\begin{pmatrix}1-p\\ r\end{pmatrix}(j-(l+1))^{1-p-r},\end{aligned} \quad \text{(B.37)}$$

and

$$\begin{aligned}(j-(l+2))^{1-p} &= (j-(l+1)-1)^{1-p} \\ &= \sum_{r=0}^{\infty}\begin{pmatrix}1-p\\ r\end{pmatrix}(j-(l+1))^{1-p-r}(-1)^r,\end{aligned} \quad \text{(B.38)}$$

we then have

$$\begin{aligned}\frac{\Delta t^{-p}}{2}\psi_l((l+1)\Delta t) &= \frac{\Delta t^{1-p}}{4}\left[4(j-(l+1))^{1-p} + \sum_{r=0}^{\infty}\begin{pmatrix}1-p\\ r\end{pmatrix}(j-(l+1))^{1-p-r}\left(1+(-1)^r\right)\right] \\ &= (j-(l+1))^{1-p}\Delta t^{1-p} + \frac{\Delta t^{1-p}}{2}\sum_{n=0}^{\infty}\begin{pmatrix}1-p\\ 2r\end{pmatrix}(j-(l+1))^{1-p-2n}.\end{aligned} \quad \text{(B.39)}$$

Since $\begin{pmatrix}1-p\\ 2r\end{pmatrix}$ is negative, we then have

$$\frac{\Delta t^{-p}}{2}\psi_l((l+1)\Delta t) < (j-(l+1))^{1-p}\Delta t^{1-p} = (t_j-(l+1)\Delta t)^{1-p}, \quad \text{(B.40)}$$

and so at $s = (l+1)\Delta t$ the term in Equation (B.28) is also positive, i.e. $G((l+1)\Delta t) > 0$. So we have shown that $G(s)$ is positive at the ends of the interval $l\Delta t \le s \le (l+1)\Delta t$. Furthermore taking the second derivative, we have

$$\frac{d^2G}{ds^2} = -p(1-p)(t_j-s)^{-p-1}, \quad \text{(B.41)}$$

which is negative which shows the function $G(s)$ is concave down for $l\Delta t \le s \le (l+1)\Delta t$ and so $G(s) > 0$ for all $s \in [l\Delta t, (l+1)\Delta t]$ as required.

## B.5 Bound for Equation (2.127)

Here we find the bound for $(k-1)^{1-p} - (k+1)^{1-p}$. To show this we first use Equations (B.31) and (B.32), to find

$$\begin{aligned}(k-1)^{1-p} - (k+1)^{1-p} &= \sum_{n=0}^{\infty} \binom{1-p}{n} k^{1-p-n}(-1)^n - \sum_{n=0}^{\infty} \binom{1-p}{n} k^{1-p-n}(1)^n \\ &= \sum_{n=1}^{\infty} \binom{1-p}{n} k^{1-p-n} \left((-1)^n - 1\right) \ . \end{aligned} \tag{B.42}$$

Note we have

$$1 - (-1)^n = \begin{cases} 0 & \text{if} \quad n \text{ is even,} \\ 2 & \text{if} \quad n \text{ is odd.} \end{cases} \tag{B.43}$$

Then, using the result in Equation (B.43), we have

$$(k-1)^{1-p} - (k+1)^{1-p} = -2\sum_{n=0}^{\infty} \binom{1-p}{2n+1} k^{-(p+2n)} \ . \tag{B.44}$$

Since for $k \geq 1$, $n \geq 0$ and $0 < p \leq 1$ the term $2 \leq 2k^{-(p+2n)}$ then $-2 \geq -2k^{-(p+2n)}$ and so we obtain

$$(k-1)^{1-p} - (k+1)^{1-p} \geq -2\sum_{n=0}^{\infty} \binom{1-p}{2n+1} = -2(2)^{1-p-1} = -2^{1-p}.$$

But if $k \to \infty$ then the term $(k-1)^{1-p} - (k+1)^{1-p} \to 0$, so we then conclude that

$$-2^{1-p} \leq (k-1)^{1-p} - (k+1)^{1-p} \leq 0 \ .$$

## B.6 Sign of the integrands in Equation (2.145)

We show the following term the first integral of Equation (2.145)

$$(t_{j+\frac{1}{2}} - \tau)^{\gamma} - \left(\frac{\Delta t}{2}\right)^{\gamma-1} \left(t_{j+\frac{1}{2}} - \tau\right)$$

is positive. We let

$$f_1(\tau) = (t_{j+\frac{1}{2}} - \tau)^{\gamma} \ , \tag{B.45}$$

and

$$f_2(\tau) = \left(\frac{\Delta t}{2}\right)^{\gamma-1} \left(t_{j+\frac{1}{2}} - \tau\right) \ , \tag{B.46}$$

where $\tau \in [t_j, t_{j+\frac{1}{2}}]$. Now taking the difference between $f_1(\tau)$ and $f_2(\tau)$ we then have

$$g(\tau) = f_1(\tau) - f_2(\tau) \ , \tag{B.47}$$

where by direct substitution

$$g(t_j) = \left(t_{j+\frac{1}{2}} - t_j\right)^{\gamma} - \left(\frac{\Delta t}{2}\right)^{\gamma-1} \left(t_{j+\frac{1}{2}} - t_j\right) = 0, \tag{B.48}$$

and

$$g(t_{j+\frac{1}{2}}) = \left(t_{j+\frac{1}{2}} - t_{j+\frac{1}{2}}\right)^{\gamma} - \left(\frac{\Delta t}{2}\right)^{\gamma-1} \left(t_{j+\frac{1}{2}} - t_{j+\frac{1}{2}}\right) = 0, \tag{B.49}$$

The second derivative of the function $g(\tau)$ with respect to $\tau$ is then given by

$$\frac{d^2 g(\tau)}{d\tau^2} = \gamma(\gamma-1) \left(t_{j+\frac{1}{2}} - \tau\right)^{\gamma-2} \ . \tag{B.50}$$

The value of the second derivative of $g(\tau)$ is negative, where $0 < \gamma < 1$, we conclude that $g(\tau)$ is a concave down function of $\tau$. Since $g(t_j) = g(t_{j+\frac{1}{2}})$ and $g(\tau)$ is a concave down then $g(\tau) > 0$ for $\tau \in (t_j, t_{j+\frac{1}{2}})$, and we can see this clearly in the Figure B.2(a), which shows $g(\tau)$ is positive.

Also in similar manner we want to show the term in the second integral in Equation (2.145), i.e.

$$(t_{j+\frac{1}{2}} - \tau)^{\gamma} - \Delta t^{\gamma-1} \left[\left(j-l+\frac{1}{2}\right)^{\gamma} (t_{l+1} - \tau) - \left(j-l-\frac{1}{2}\right)^{\gamma} (t_l - \tau)\right]$$

is also positive. We let

$$f_3(\tau) = \Delta t^{\gamma-1} \left[\left(j-l+\frac{1}{2}\right)^{\gamma} (t_{l+1} - \tau) - \left(j-l-\frac{1}{2}\right)^{\gamma} (t_l - \tau)\right] \ , \tag{B.51}$$

where $\tau \in [t_l, t_{l+1}]$ and then we take the difference between the two functions $f_1(\tau)$ given in Equation (B.45) and $f_3(\tau)$

$$G(\tau) = f_1(\tau) - f_3(\tau), \tag{B.52}$$

where by direct substitution

$$G(t_l) = \left(t_{j+\frac{1}{2}} - t_l\right)^{\gamma} - \Delta t^{\gamma-1} \left[\left(j-l+\frac{1}{2}\right)^{\gamma} (t_{l+1} - t_l) - \left(j-l-\frac{1}{2}\right)^{\gamma} (t_l - t_l)\right] = 0, \tag{B.53}$$

and

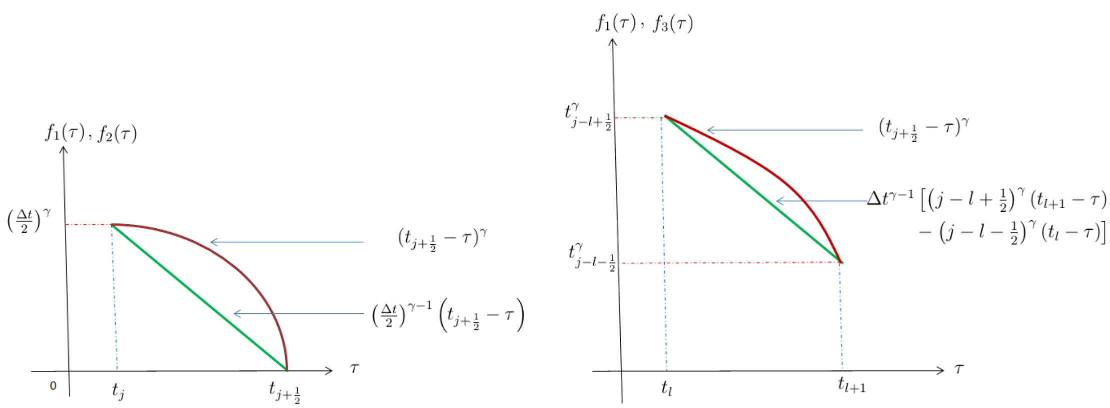
$$G(t_{l+1}) = \left(t_{j+\frac{1}{2}} - t_{l+1}\right)^{\gamma} - \Delta t^{\gamma-1}\left[\left(j-l+\frac{1}{2}\right)^{\gamma}(t_{l+1}-t_{l+1}) - \left(j-l-\frac{1}{2}\right)^{\gamma}(t_l - t_{l+1})\right]$$
$$= 0\ . \tag{B.54}$$

The second derivative of the function $G(\tau)$ with respect to $\tau$ is

$$\frac{d^2G(\tau)}{d\tau^2} = \gamma(\gamma-1)\left(t_{j+\frac{1}{2}} - \tau\right)^{\gamma-2}\ .$$

For $0 < \gamma < 1$ the second derivative of $G(\tau)$ is negative, hence $G(\tau)$ is also a concave down function of $\tau$. Since $G(t_l) = G(t_{l+1})$ and $G(\tau)$ is concave down then $G(\tau) > 0$ for $\tau \in (t_l, t_{l+1})$, and we can see from Figure B.2(b).

Hence the difference $g(\tau) = f_1(\tau) - f_2(\tau)$ and $G(\tau) = f_1(\tau) - f_3(\tau)$ are both positive. The terms in the integrands are therefore positive.




(a) (b)

Figure B.2: Plot of functions in the terms in the first integrand (a) $f_1(\tau)$ and $f_2(\tau)$, and the term in the second integrand (b) $f_1(\tau)$ and $f_3(\tau)$ of Equation (2.145). Note $f_1(\tau) \geq f_2(\tau)$ and $f_1(\tau) \geq f_3(\tau)$ over the range of $\tau$ plotted.

## B.7 Bound for Equation (2.149) summation

In similar way to section B.3, we obtain a bound for the summation in Equation (2.149)

$$S = \sum_{l=0}^{j-1}\left[\left(j-l+\frac{1}{2}\right)^{1-p}\left(j-l-\frac{1-p}{2}\right) - \left(j-l-\frac{1}{2}\right)^{1-p}\left(j-l+\frac{1-p}{2}\right)\right], \tag{B.55}$$

which can be rewritten as

$$S = \sum_{l=1}^{j} \left[ \left(l + \frac{1}{2}\right)^{1-p} \left(l - \frac{1-p}{2}\right) - \left(l - \frac{1}{2}\right)^{1-p} \left(l + \frac{1-p}{2}\right) \right]. \tag{B.56}$$

Expanding $\left(l - \frac{1}{2}\right)^{1-p}$ if $l \geq 1$ we find

$$\begin{aligned} \left(l - \frac{1}{2}\right)^{1-p} &= \left(\left(l + \frac{1}{2}\right) - 1\right)^{1-p} \\ &= \sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{1-p-n} (-1)^n \ . \end{aligned} \tag{B.57}$$

Then the summation term becomes

$$\begin{aligned} &\left(l + \frac{1}{2}\right)^{1-p} \left(l - \frac{1-p}{2}\right) - \left(l - \frac{1}{2}\right)^{1-p} \left(l + \frac{1-p}{2}\right) \\ =&\left(l + \frac{1}{2}\right)^{1-p} \left(l - \frac{1-p}{2}\right) - \left(l + \frac{1-p}{2}\right) \sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{1-p-n} (-1)^n \\ =&\left(l + \frac{1}{2}\right)^{1-p} \left[\left(l - \frac{1-p}{2}\right) - \left(l + \frac{1-p}{2}\right)\right] - \left(l + \frac{1-p}{2}\right) \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{1-p-n} (-1)^n \\ =&(p-1) \left(l + \frac{1}{2}\right)^{1-p} - \left(l + \frac{1}{2} - \frac{1}{2} + \frac{1-p}{2}\right) \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{1-p-n} (-1)^n \ . \end{aligned} \tag{B.58}$$

Simplifying further gives

$$\begin{aligned} &\left(l + \frac{1}{2}\right)^{1-p} \left(l - \frac{1-p}{2}\right) - \left(l - \frac{1}{2}\right)^{1-p} \left(l + \frac{1-p}{2}\right) \\ &\quad =(p-1) \left(l + \frac{1}{2}\right)^{1-p} - \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{2-p-n} (-1)^n \\ &\quad\quad + \frac{p}{2} \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{1-p-n} (-1)^n \\ &\quad = - \sum_{n=2}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{2-p-n} (-1)^n \\ &\quad\quad + \frac{p}{2} \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left(l + \frac{1}{2}\right)^{1-p-n} (-1)^n. \end{aligned} \tag{B.59}$$

Combining the summations we then obtain

$$\left(l+\frac{1}{2}\right)^{1-p}\left(l-\frac{1-p}{2}\right)-\left(l-\frac{1}{2}\right)^{1-p}\left(l+\frac{1-p}{2}\right)$$
$$=\sum_{n=1}^{\infty}\left(l+\frac{1}{2}\right)^{1-p-n}(-1)^{n}\left[\binom{1-p}{n+1}+\frac{p}{2}\binom{1-p}{n}\right]. \tag{B.60}$$

Note if $n=1$, the first term in the summation is zero

$$\left[\binom{1-p}{2}+\frac{p}{2}\binom{1-p}{1}\right]=\frac{(1-p)(-p)}{2}+\frac{p(1-p)}{2}=0, \tag{B.61}$$

and so we have if $l \geq 1$

$$\left(l+\frac{1}{2}\right)^{1-p}\left(l-\frac{1-p}{2}\right)-\left(l-\frac{1}{2}\right)^{1-p}\left(l+\frac{1-p}{2}\right)$$
$$=\sum_{n=2}^{\infty}\left(l+\frac{1}{2}\right)^{1-p-n}(-1)^{n}\left[\binom{1-p}{n+1}+\frac{p}{2}\binom{1-p}{n}\right]. \tag{B.62}$$

So the sum $S$ in Equation (B.56), after using Equation (B.62), becomes

$$S=\sum_{l=1}^{j}\left[\left(l+\frac{1}{2}\right)^{1-p}\left(l-\frac{1-p}{2}\right)-\left(l-\frac{1}{2}\right)^{1-p}\left(l+\frac{1-p}{2}\right)\right]$$
$$=\sum_{l=1}^{j}\sum_{n=2}^{\infty}\left(l+\frac{1}{2}\right)^{1-p-n}(-1)^{n}\left[\binom{1-p}{n+1}+\frac{p}{2}\binom{1-p}{n}\right]$$
$$=\sum_{n=2}^{\infty}(-1)^{n}\left[\binom{1-p}{n+1}+\frac{p}{2}\binom{1-p}{n}\right]\sum_{l=1}^{j}\left(l+\frac{1}{2}\right)^{1-p-n}. \tag{B.63}$$

Now

$$\sum_{l=1}^{j}\left(l+\frac{1}{2}\right)^{1-p-n}=\sum_{l=0}^{j-1}\left(l+\frac{3}{2}\right)^{1-p-n}$$
$$=\sum_{l=0}^{\infty}\left(l+\frac{3}{2}\right)^{1-p-n}-\sum_{l=j}^{\infty}\left(l+\frac{3}{2}\right)^{1-p-n}$$
$$=\sum_{l=0}^{\infty}\left(l+\frac{3}{2}\right)^{1-p-n}-\sum_{l=0}^{\infty}\left(l+j+\frac{3}{2}\right)^{1-p-n}$$
$$=\zeta\left(n-(1-p),\frac{3}{2}\right)-\zeta\left(n-(1-p),j+\frac{3}{2}\right), \tag{B.64}$$

where $\zeta(s,a)$ is the Hurwitz Zeta function (Apostol et al. 1951). So we need to evaluate the sum

$$S=\sum_{n=2}^{\infty}(-1)^{n}\left[\binom{1-p}{n+1}+\frac{p}{2}\binom{1-p}{n}\right]\left\{\zeta\left(n-(1-p),\frac{3}{2}\right)-\zeta\left(n-(1-p),j+\frac{3}{2}\right)\right\}. \tag{B.65}$$

Note the coefficient

$$(-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \tag{B.66}$$

can be shown to be positive for $0 < 1-p < 1$ and $n \geq 2$ as shown earlier in Section B.3. Since $n \geq 2$ and $0 < p < 1$ then all terms including the Gamma function are positive and hence the coefficient in Eq. (B.66) is positive.

In addition for $s > 1$ and $a > \frac{3}{2}$, the Hurwitz Zeta function $\zeta(s,a)$ is a monotonically decaying function in both $s$ and $a$ so

$$\zeta\left(n-(1-p), \frac{3}{2}\right) - \zeta\left(n-(1-p), j+\frac{3}{2}\right) > 0,$$

and so

$$\begin{aligned} S &= \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \left\{ \zeta\left(n-(1-p), \frac{3}{2}\right) - \zeta\left(n-(1-p), j+\frac{3}{2}\right) \right\} \\ &\leq \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \zeta\left(n-(1-p), \frac{3}{2}\right) \\ &\leq \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \zeta\left(1+p, \frac{3}{2}\right). \end{aligned} \tag{B.67}$$

Evaluating the summations we find

$$\begin{aligned} \sum_{n=2}^{\infty} (-1)^n \binom{1-p}{n+1} &= -\sum_{n=2}^{\infty} (-1)^{n+1} \binom{1-p}{n+1} \\ &= -\sum_{n=3}^{\infty} (-1)^n \binom{1-p}{n} \\ &= -\left[ \sum_{n=0}^{\infty} (-1)^n \binom{1-p}{n} - \binom{1-p}{0} + \binom{1-p}{1} - \binom{1-p}{2} \right] \\ &= -\left[ 0 - 1 + (1-p) - \frac{(1-p)(-p)}{2} \right] \\ &= \frac{p\,(1+p)}{2}, \end{aligned} \tag{B.68}$$

and

$$\sum_{n=2}^{\infty}(-1)^n \begin{pmatrix} 1-p \\ n \end{pmatrix} = \sum_{n=0}^{\infty}(-1)^n \begin{pmatrix} 1-p \\ n \end{pmatrix} - \begin{pmatrix} 1-p \\ 0 \end{pmatrix} + \begin{pmatrix} 1-p \\ 1 \end{pmatrix}$$
$$= 0 - 1 + (1-p)$$
$$= -p, \tag{B.69}$$

where we have used the identity

$$\sum_{n=0}^{\infty}(-1)^n \begin{pmatrix} 1-p \\ n \end{pmatrix} = 0. \tag{B.70}$$

Using Equations (B.68) and (B.70) gives

$$\sum_{n=2}^{\infty}(-1)^n \left[\begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2}\begin{pmatrix} 1-p \\ n \end{pmatrix}\right] = \left[\frac{p(1+p)}{2} + \frac{p}{2}(-p)\right] = \frac{p}{2}\,. \tag{B.71}$$

We now have

$$S \le \sum_{n=2}^{\infty}(-1)^n \left[\begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2}\begin{pmatrix} 1-p \\ n \end{pmatrix}\right] \zeta\left(1+p, \frac{3}{2}\right)$$
$$\le \frac{p}{2}\zeta\left(1+p, \frac{3}{2}\right) \tag{B.72}$$

which is finite for all $0 < p < 1$ and hence $S$ is bounded.

In the case of $p = 0$ and $p = 1$ the summation reduces to zero. In particular if $p = 0$ we find

$$S = \sum_{l=1}^{j}\left[\left(l+\frac{1}{2}\right)^{1-p}\left(l-\frac{1-p}{2}\right) - \left(l-\frac{1}{2}\right)^{1-p}\left(l+\frac{1-p}{2}\right)\right] = 0,$$

and if $p = 1$ we obtain the result

$$S = \sum_{l=1}^{j}\left[\left(l+\frac{1}{2}\right)^{1-p}\left(l-\frac{1-p}{2}\right) - \left(l-\frac{1}{2}\right)^{1-p}\left(l+\frac{1-p}{2}\right)\right] = 0.$$

So is the sum $S$ is bounded for all $0 \le p \le 1$.

## B.8 Sign of the integrand in Equation (2.169)

We show the term in the integrand of the first integral in Equation (2.169), with $p = 1-\gamma$

$$(t_{j+\frac{1}{2}} - \tau)^{\gamma} - \Delta t^{\gamma-1}\left[(j-(l-1))^{\gamma}\left(t_{l+\frac{1}{2}} - \tau\right) - (j-l)^{\gamma}\left(t_{l-\frac{1}{2}} - \tau\right)\right]$$

is positive. We let

$$f_1(\tau) = (t_{j+\frac{1}{2}} - \tau)^\gamma \ , \tag{B.73}$$

and

$$f_2(\tau) = \Delta t^{\gamma-1}\left[(j-(l-1))^\gamma \left(t_{l+\frac{1}{2}} - \tau\right) - (j-l)^\gamma \left(t_{l-\frac{1}{2}} - \tau\right)\right] \tag{B.74}$$

where $\tau \in [t_{l-\frac{1}{2}}, t_{l+\frac{1}{2}}]$. Now taking the difference between $f_1(\tau)$ and $f_2(\tau)$ we then have

$$g(\tau) = f_1(\tau) - f_2(\tau) \ , \tag{B.75}$$

where by direct substitution we have

$$\begin{aligned} g\left(t_{l-\frac{1}{2}}\right) &= \left(t_{j+\frac{1}{2}} - t_{l-\frac{1}{2}}\right)^\gamma - \Delta t^{\gamma-1}\left[(j-(l-1))^\gamma \left(t_{l+\frac{1}{2}} - t_{l-\frac{1}{2}}\right) - (j-l)^\gamma \left(t_{l-\frac{1}{2}} - t_{l-\frac{1}{2}}\right)\right] \\ &= 0 \ , \end{aligned} \tag{B.76}$$

and

$$\begin{aligned} g\left(t_{l+\frac{1}{2}}\right) &= \left(t_{j+\frac{1}{2}} - t_{l+\frac{1}{2}}\right)^\gamma - \Delta t^{\gamma-1}\left[(j-(l-1))^\gamma \left(t_{l+\frac{1}{2}} - t_{l+\frac{1}{2}}\right) - (j-l)^\gamma \left(t_{l-\frac{1}{2}} - t_{l+\frac{1}{2}}\right)\right] \\ &= 0 \ . \end{aligned} \tag{B.77}$$

The second derivative of the function $g(\tau)$ with respect to $\tau$ is then given by

$$\frac{d^2 g(\tau)}{d\tau^2} = \gamma(\gamma-1)\left(t_{j+\frac{1}{2}} - \tau\right)^{\gamma-2} \ . \tag{B.78}$$

The value of the second derivative of $g(\tau)$ is negative, where $0 < \gamma < 1$, we conclude that $g(\tau)$ is a concave down function of $\tau$. Since $g\left(t_{l-\frac{1}{2}}\right) = g\left(t_{l+\frac{1}{2}}\right) = 0$ and $g(\tau)$ is concave down then $g(\tau) > 0$ for $\tau \in \left(t_{l-\frac{1}{2}}, t_{l+\frac{1}{2}}\right)$, i.e. $g(\tau) = f_1(\tau) - f_2(\tau) > 0$ and so $f_1(\tau) > f_2(\tau)$. Hence the term

$$\left(t_{j+\frac{1}{2}} - \tau\right)^\gamma - \Delta t^{\gamma-1}\left[(j-(l-1))^\gamma \left(t_{l+\frac{1}{2}} - \tau\right) - (j-l)^\gamma \left(t_{l-\frac{1}{2}} - \tau\right)\right]$$

is positive.

Also in similar manner we want to show the term in the second integral Equation (2.169), i.e.

$$\left(t_{j+\frac{1}{2}} - \tau\right)^\gamma - \Delta t^{\gamma-1}\Big(\Delta t(j^\gamma + \widehat{\alpha}_j) - 2\widehat{\alpha}_j \tau\Big) \ ,$$

is also positive. We let

$$f_3(\tau) = \Delta t^{\gamma-1}\Big(\Delta t(j^\gamma + \widehat{\alpha}_j) - 2\widehat{\alpha}_j \tau\Big) \ , \tag{B.79}$$

where $\tau \in \left[0, t_{\frac{1}{2}}\right]$ and $\widehat{\alpha}_j$ is given by Equation (2.89), then we take the difference between the two functions $f_1(\tau)$, given in Equation (B.73), and $f_3(\tau)$

$$G(\tau) = f_1(\tau) - f_3(\tau), \tag{B.80}$$

where

$$G(0) = \left(t_{j+\frac{1}{2}} - 0\right)^{\gamma} - \Delta t^{\gamma-1}\left(\Delta t(j^{\gamma} + \widehat{\alpha}_j) - 2\widehat{\alpha}_j(0)\right) = 0, \tag{B.81}$$

and

$$G\left(t_{\frac{1}{2}}\right) = \left(t_{j+\frac{1}{2}} - t_{\frac{1}{2}}\right)^{\gamma} - \Delta t^{\gamma-1}\left(\Delta t(j^{\gamma} + \widehat{\alpha}_j) - 2\widehat{\alpha}_j t_{\frac{1}{2}}\right) = 0. \tag{B.82}$$

The second derivative of the function $G(\tau)$ with respect to $\tau$ gives

$$\frac{d^2G(\tau)}{d\tau^2} = \gamma(\gamma-1)\left(t_{j+\frac{1}{2}} - \tau\right)^{\gamma-2}.$$

For $0 < \gamma < 1$ the second derivative of $G(\tau)$ is negative, hence $G(\tau)$ is concave down function of $\tau$. Since $G(0) = G\left(t_{\frac{1}{2}}\right)$ and $G(\tau)$ is a concave down then $G(\tau) > 0$ for $\tau \in \left(0, t_{\frac{1}{2}}\right)$, i.e. $G(\tau) = f_1(\tau) - f_3(\tau) = 0$ and so $f_1(\tau) > f_3(\tau)$.
Hence the term

$$\left(t_{j+\frac{1}{2}} - \tau\right)^{\gamma} - \Delta t^{\gamma-1}\left(\Delta t(j^{\gamma} + \widehat{\alpha}_j) - 2\widehat{\alpha}_j\tau\right)$$

is also positive.

## B.9 Bound for Equation (2.172) summation

In this section we obtain a bound for the summation in Equation (2.172), first we have

$$S = \sum_{l=0}^{j-1}\left[(l+1)^{1-p}\left(l + \frac{p}{2}\right) - l^{1-p}\left(l + 1 - \frac{p}{2}\right)\right]. \tag{B.83}$$

Expanding $l^{1-p}$ if $l \geq 1$ we find

$$(l+1-1)^{1-p} = \sum_{n=0}^{\infty}\begin{pmatrix} 1-p \\ n \end{pmatrix}(l+1)^{1-p-n}(-1)^n. \tag{B.84}$$

Then the $l^{th}$ term in the summation in Equation (B.83) can be rewritten as

$$
\begin{aligned}
&(l+1)^{1-p}\left(l+\frac{p}{2}\right) - l^{1-p}\left(l+1-\frac{p}{2}\right) \\
=&(l+1)^{1-p}\left(l+\frac{p}{2}\right) - \left(l+1-\frac{p}{2}\right)\sum_{n=0}^{\infty}\binom{1-p}{n}(l+1)^{1-p-n}(-1)^n \\
=&(l+1)^{1-p}\left[\left(l+\frac{p}{2}\right) - \left(l+1-\frac{p}{2}\right)\right] - \left(l+1-\frac{p}{2}\right)\sum_{n=1}^{\infty}\binom{1-p}{n}(l+1)^{1-p-n}(-1)^n \\
=&(p-1)(l+1)^{1-p} - \left(l+1-\frac{p}{2}\right)\sum_{n=1}^{\infty}\binom{1-p}{n}(l+1)^{1-p-n}(-1)^n \\
=&(p-1)(l+1)^{1-p} - \sum_{n=1}^{\infty}\binom{1-p}{n}(l+1)^{2-p-n}(-1)^n + \frac{p}{2}\sum_{n=1}^{\infty}\binom{1-p}{n}(l+1)^{1-p-n}(-1)^n \\
=&-\sum_{n=2}^{\infty}\binom{1-p}{n}(l+1)^{2-p-n}(-1)^n + \frac{p}{2}\sum_{n=1}^{\infty}\binom{1-p}{n}(l+1)^{1-p-n}(-1)^n \ . \qquad \text{(B.85)}
\end{aligned}
$$

Combining the summations we obtain

$$
(l+1)^{1-p}\left(l+\frac{p}{2}\right) - l^{1-p}\left(l+1-\frac{p}{2}\right) = \sum_{n=1}^{\infty}(l+1)^{1-p-n}(-1)^n\left[\binom{1-p}{n+1} + \frac{p}{2}\binom{1-p}{n}\right] ,
$$

where we have rewritten the first summation as

$$
-\sum_{n=2}^{\infty}\binom{1-p}{n}(l+1)^{2-p-n}(-1)^n = \sum_{n=1}^{\infty}\binom{1-p}{n+1}(l+1)^{1-p-n}(-1)^n.
$$

Note if $n=1$

$$
\left[\binom{1-p}{2} + \frac{p}{2}\binom{1-p}{1}\right] = \frac{(1-p)(-p)}{2} + \frac{p(1-p)}{2} = 0, \qquad \text{(B.86)}
$$

hence for $n=1$ the term is zero and so we have if $l \geq 1$

$$
(l+1)^{1-p}\left(l+\frac{p}{2}\right) - l^{1-p}\left(l+1-\frac{p}{2}\right) = \sum_{n=2}^{\infty}(l+1)^{1-p-n}\left((-1)^n\left[\binom{1-p}{n+1} + \frac{p}{2}\binom{1-p}{n}\right]\right). \qquad \text{(B.87)}
$$

Since the term $(-1)^n\left[\binom{1-p}{n+1} + \frac{p}{2}\binom{1-p}{n}\right] > 0$, (for $n \geq 2$ and $0 < p < 1$) as shown in Section B.3 then the term in Equation (B.87) is positive.

So the sum $S$ in Equation (B.83) is, after using Equation (B.87), becomes

$$\begin{aligned} S &= \sum_{l=0}^{j-1} \left[ (l+1)^{1-p} \left( l + \frac{p}{2} \right) - l^{1-p} \left( l + 1 - \frac{p}{2} \right) \right] \\ &= \sum_{l=0}^{j-1} \sum_{n=2}^{\infty} (l+1)^{1-p-n} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \\ &= \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \sum_{l=0}^{j-1} (l+1)^{1-p-n}. \end{aligned} \tag{B.88}$$

Now

$$\begin{aligned} \sum_{l=0}^{j-1} (l+1)^{1-p-n} &= \sum_{l=0}^{\infty} (l+1)^{1-p-n} - \sum_{l=j}^{\infty} (l+1)^{1-p-n} \\ &= \sum_{l=0}^{\infty} (l+1)^{1-p-n} - \sum_{l=0}^{\infty} (l+j)^{1-p-n} \\ &= \zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right), \end{aligned} \tag{B.89}$$

where $\zeta(s,a)$ is the Hurwitz Zeta function (Apostol et al. 1951). So we need to evaluate the bound

$$S = \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \left\{ \zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right) \right\} . \tag{B.90}$$

The coefficient is positive as shown earlier. In addition for $s > 1$ and $a > 1$, the Hurwitz Zeta function $\zeta(s,a)$ is a monotonically decaying function in both $s$ and $a$ so

$$\zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right) > 0$$

and so

$$\begin{aligned} S &= \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \left\{ \zeta\left(n-(1-p),1\right) - \zeta\left(n-(1-p),j\right) \right\} \\ &\le \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \zeta\left(n-(1-p),1\right) \\ &\le \sum_{n=2}^{\infty} (-1)^n \left[ \binom{1-p}{n+1} + \frac{p}{2} \binom{1-p}{n} \right] \zeta\left(1+p,1\right). \end{aligned}$$

Using Equation (B.71), we then obtain the equation

$$S \le \frac{p}{2} \zeta\left(1+p,1\right) \ , \tag{B.91}$$

which is finite for all $0 < p < 1$ and hence $S$ is bounded.

In the case of $p = 0$ and $p = 1$ the summation reduces to zero. In particular if $p = 0$ we find

$$S = \sum_{l=1}^{j} \left[ (l+1)^{1-p} \left( l + \frac{p}{2} \right) - l^{1-p} \left( l + 1 - \frac{p}{2} \right) \right] = 0, \tag{B.92}$$

and if $p = 1$ we obtain the result

$$S = \sum_{l=1}^{j} \left[ (l+1)^{1-p} \left( l + \frac{p}{2} \right) - l^{1-p} \left( l + 1 - \frac{p}{2} \right) \right] = 0. \tag{B.93}$$

So is $S$ is bounded for all $0 \leq p \leq 1$.

To show the second absolute term in Equation (2.172) is positive

$$\left[ \left( j + \frac{1}{2} \right)^{1-p} \left( j + \frac{1}{2} - \frac{2-p}{4} \right) - j^{1-p} \left( j + \frac{2-p}{4} \right) \right] > 0, \tag{B.94}$$

we let

$$A = \left( j + \frac{1}{2} \right)^{1-p} \left( j + \frac{p}{4} \right) - j^{1-p} \left( j + \frac{1}{2} - \frac{p}{4} \right). \tag{B.95}$$

Expanding $j^{1-p}$, if $j \geq 1$, as we find

$$j^{1-p} = \left( j + \frac{1}{2} - \frac{1}{2} \right)^{1-p} = \sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left( j + \frac{1}{2} \right)^{1-p-n} \left( -\frac{1}{2} \right)^{n}. \tag{B.96}$$

Then the term in Equation (B.94) becomes

$$\begin{aligned} A &= \left( j + \frac{1}{2} \right)^{1-p} \left( j + \frac{p}{4} \right) - j^{1-p} \left( j + \frac{1}{2} - \frac{p}{4} \right) \\ &= \left( j + \frac{1}{2} \right)^{1-p} \left( j + \frac{p}{4} \right) - \left( j + \frac{1}{2} - \frac{p}{4} \right) \sum_{n=0}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left( j + \frac{1}{2} \right)^{1-p-n} \left( -\frac{1}{2} \right)^{n} \\ &= \left( j + \frac{1}{2} \right)^{1-p} \left[ \left( j + \frac{p}{4} \right) - \left( j + \frac{1}{2} - \frac{p}{4} \right) \right] \\ &\qquad - \left( j + \frac{1}{2} - \frac{p}{4} \right) \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left( j + \frac{1}{2} \right)^{1-p-n} \left( -\frac{1}{2} \right)^{n} \\ &= \frac{1}{2}(p-1) \left( j + \frac{1}{2} \right)^{1-p} - \left( j + \frac{1}{2} - \frac{p}{4} \right) \sum_{n=1}^{\infty} \begin{pmatrix} 1-p \\ n \end{pmatrix} \left( j + \frac{1}{2} \right)^{1-p-n} \left( -\frac{1}{2} \right)^{n}. \end{aligned} \tag{B.97}$$

Simplifying further gives

$$
\begin{aligned}
A =& \frac{(p-1)}{2}\left(j+\frac{1}{2}\right)^{1-p} - \sum_{n=1}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{2-p-n}\left(-\frac{1}{2}\right)^{n} \\
&+ \frac{p}{4}\sum_{n=1}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{1-p-n}\left(-\frac{1}{2}\right)^{n} \\
=& \frac{(p-1)}{2}\left(j+\frac{1}{2}\right)^{1-p} + \frac{(1-p)}{2}\left(j+\frac{1}{2}\right)^{1-p} - \sum_{n=2}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{2-p-n}\left(-\frac{1}{2}\right)^{n} \\
&+ \frac{p}{4}\sum_{n=1}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{1-p-n}\left(-\frac{1}{2}\right)^{n} \\
=& -\sum_{n=2}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{2-p-n}\left(-\frac{1}{2}\right)^{n} \\
&+ \frac{p}{4}\sum_{n=1}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{1-p-n}\left(-\frac{1}{2}\right)^{n}.
\end{aligned}
\tag{B.98}
$$

Combining the summations we then obtain

$$
\begin{aligned}
A =& \sum_{n=1}^{\infty}\left(j+\frac{1}{2}\right)^{1-p-n}\left(-\frac{1}{2}\right)^{n}\left[\frac{1}{2}\left(\begin{array}{c}1-p\\ n+1\end{array}\right) + \frac{p}{4}\left(\begin{array}{c}1-p\\ n\end{array}\right)\right] \\
=& \sum_{n=1}^{\infty}\left(j+\frac{1}{2}\right)^{1-p-n}\left(\frac{1}{2}\right)^{n+1}(-1)^{n}\left[\left(\begin{array}{c}1-p\\ n+1\end{array}\right) + \frac{p}{2}\left(\begin{array}{c}1-p\\ n\end{array}\right)\right],
\end{aligned}
\tag{B.99}
$$

where the first summation in (B.98) was rewritten as

$$
-\frac{1}{2}\sum_{n=2}^{\infty}\left(\begin{array}{c}1-p\\ n\end{array}\right)\left(j+\frac{1}{2}\right)^{2-p-n}\left(-\frac{1}{2}\right)^{n} = \sum_{n=1}^{\infty}\left(\begin{array}{c}1-p\\ n+1\end{array}\right)\left(j+\frac{1}{2}\right)^{1-p-n}\left(-\frac{1}{2}\right)^{n+1}.
\tag{B.100}
$$

Note if $n = 1$

$$
\left[\left(\begin{array}{c}1-p\\ 2\end{array}\right) + \frac{p}{2}\left(\begin{array}{c}1-p\\ 1\end{array}\right)\right] = \frac{(1-p)(-p)}{2} + \frac{p(1-p)}{2} = 0,
\tag{B.101}
$$

and so we have if $l \geq 2$

$$
A = \sum_{n=2}^{\infty}\left(j+\frac{1}{2}\right)^{1-p-n}\left(\frac{1}{2}\right)^{n+1}(-1)^{n}\left[\left(\begin{array}{c}1-p\\ n+1\end{array}\right) + \frac{p}{2}\left(\begin{array}{c}1-p\\ n\end{array}\right)\right].
$$

Note the coefficient

$$(-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right] > 0 \tag{B.102}$$

for $n \geq 2$ and $0 < p < 1$ as shown in Section B.3 the term in Equation (B.102) is positive. Also the term $\left(j+\frac{1}{2}\right)^{1-p-n} \left(\frac{1}{2}\right)^{n+1}$ is positive, hence $A$ is positive.

To find a bound for $A$ we note, for $n \geq 2$ and $0 < p < 1$ the term $\left(j+\frac{1}{2}\right)^{1-p-n} < 1$, and we then have

$$A \leq \sum_{n=2}^{\infty} \left(\frac{1}{2}\right)^{n+1} (-1)^n \left[ \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} + \frac{p}{2} \begin{pmatrix} 1-p \\ n \end{pmatrix} \right]. \tag{B.103}$$

Evaluating the summations we find

$$\begin{aligned} \sum_{n=2}^{\infty} \left(\frac{1}{2}\right)^{n+1} (-1)^n \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} &= -\sum_{n=2}^{\infty} \left(\frac{1}{2}\right)^{n+1} (-1)^{n+1} \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} \\ &= -\sum_{n=2}^{\infty} \left(-\frac{1}{2}\right)^{n+1} \begin{pmatrix} 1-p \\ n+1 \end{pmatrix} \\ &= -\sum_{n=3}^{\infty} \left(-\frac{1}{2}\right)^{n} \begin{pmatrix} 1-p \\ n \end{pmatrix} \\ &= -\left[ \sum_{n=0}^{\infty} \left(-\frac{1}{2}\right)^{n} \begin{pmatrix} 1-p \\ n \end{pmatrix} - \begin{pmatrix} 1-p \\ 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1-p \\ 1 \end{pmatrix} - \frac{1}{4} \begin{pmatrix} 1-p \\ 2 \end{pmatrix} \right] \\ &= -\left[ \left(\frac{1}{2}\right)^{n} - 1 + \frac{1}{2}(1-p) - \frac{1}{4}\frac{(1-p)(-p)}{2} \right] \\ &= \frac{(4+p)(p-1)}{8} - \left(\frac{1}{2}\right)^{1-p}, \end{aligned} \tag{B.104}$$

and

$$\begin{aligned} \sum_{n=2}^{\infty} \left(-\frac{1}{2}\right)^{n} \begin{pmatrix} 1-p \\ n \end{pmatrix} &= \sum_{n=0}^{\infty} \left(-\frac{1}{2}\right)^{n} \begin{pmatrix} 1-p \\ n \end{pmatrix} - \begin{pmatrix} 1-p \\ 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1-p \\ 1 \end{pmatrix} \\ &= \left(\frac{1}{2}\right)^{1-p} - 1 + \frac{(1-p)}{2} . \end{aligned}$$

The bound in Equation (B.103) then becomes

$$A \leq \left[ \frac{(4+p)(p-1)}{8} - \left(\frac{1}{2}\right)^{1-p} + \frac{p}{4}\left( \left(\frac{1}{2}\right)^{1-p} - 1 + \frac{(1-p)}{2} \right) \right] = \frac{p-4}{4}\left(\frac{1}{2}\right)^{1-p} + \frac{p-2}{4}. \tag{B.105}$$

Hence $A$ is bounded by a constant.

## B.10 The weight $\beta_j(\gamma)$, given in Equation (4.9), is negative

**Lemma B.10.1.** The coefficients $\beta_j(\gamma)$ given in Equation (4.9) for $j \geq 1$ then $\beta_j(\gamma) < 0$.

*Proof.* First using binomial expansion on the coefficient in Equation (4.9), we then have

$$\begin{aligned}\beta_j(\gamma) &= \gamma j^{\gamma-1} - j^{\gamma} + \sum_{k=0}^{\infty} \binom{k}{\gamma} (-1)^k j^{\gamma-k} \\ &= \sum_{k=2}^{\infty} \binom{k}{\gamma} (-1)^k j^{\gamma-k} \ . \end{aligned} \tag{B.106}$$

Now using the result in Equation (B.7), we then find

$$\begin{aligned}\beta_j(\gamma) &= \sum_{k=2}^{\infty} \frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)} (-1)^{2k-1} j^{\gamma-k} \\ &= -\sum_{k=2}^{\infty} \frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)} j^{\gamma-k}, \end{aligned} \tag{B.107}$$

since $(-1)^{2k-1} = -1$. Now for $n \geq 2$ and $0 < \gamma \leq 1$ the term

$$\frac{\gamma\Gamma(k-\gamma)}{k!\Gamma(1-\gamma)} > 0,$$

is positive since the Gamma function is positive for positive arguments. The term $j^{\gamma-n} > 0$ is also positive, and hence the coefficient $\beta_j(\gamma)$ is negative. □

## B.11 Supporting information for Chapter 5

**Lemma B.11.1.** The parameter $z$ is given by Equation (5.437), satisfies

$$0 < \left| \frac{1}{1+z} \right| \leq 1, \tag{B.108}$$

if $\mathrm{Re}(z) > 0$.

*Proof.* From Equations (5.437) we have

$$z = \sin^2(q\Delta x/2) \left( \left(\frac{1}{2}\right)^{\gamma} d_1 - 1 \right) - \frac{d_2}{2} \left(\frac{1}{2}\right)^{\gamma} \sin(q\Delta x) i, \tag{B.109}$$

letting $a = \left(\left(\frac{1}{2}\right)^{\gamma} d_1 - 1\right)$, $b = d_2 \left(\frac{1}{2}\right)^{\gamma}$, and $x = \sin^2(q\Delta x/2)$, we note here $a \geq -1$ since $d_1 \geq 0$. Equation (B.109) becomes

$$z = ax^2 - b\sqrt{x(1-x)}i, \tag{B.110}$$

we then have

$$|1+z| = \sqrt{1 + x\left(2a + b^2\right) + x^2\left(a^2 - b^2\right)}. \tag{B.111}$$

Since $0 \leq \sin^2(q\Delta x/2) \leq 1$ then $0 \leq x \leq 1$. The sign of the terms $2a+b^2$ and $a^2-b^2$ may be positive or negative and so we need to consider four cases when checking the bound of the Equation (B.108).

These cases are where

1. $2a + b^2 \geq 0$ and $a^2 - b^2 \geq 0$,
2. $2a + b^2 \leq 0$ and $a^2 - b^2 \leq 0$,
3. $2a + b^2 \geq 0$ and $a^2 - b^2 \leq 0$, and
4. $2a + b^2 \leq 0$ and $a^2 - b^2 \geq 0$.

The range of values of $a$ and $b$ which satisfy each case is shown in Figure B.3 .

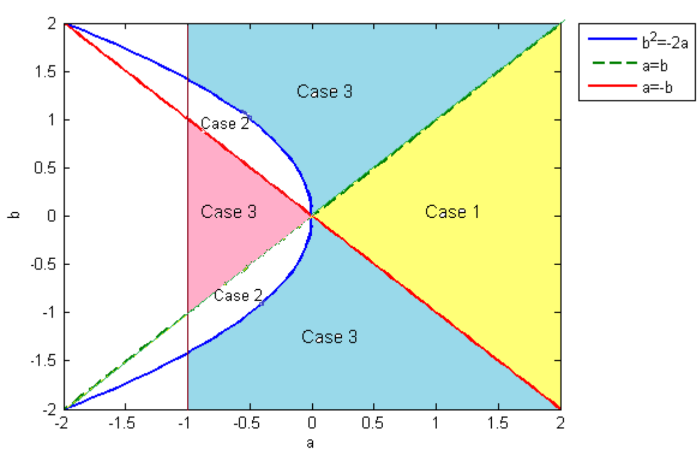



Figure B.3: The range of values of $a$ and $b$ for all cases to be considered when testing the bound of Equation (B.111)

**Case 1**:

If $2a + b^2 \geq 0$ from $2a \geq -b^2$, and $a^2 - b^2 \geq 0$ we then have $a^2 \geq b^2$. We then conclude that $|1+z| > 1$ from Equation (B.111). Hence

$$\left|\frac{1}{1+z}\right| \leq 1 \tag{B.112}$$

Equation (B.108) is satisfied. We note $\mathrm{Re}(z) = ax^2 \geq 0$ for this case.

**Case 2**: If $2a + b^2 \leq 0$ then $2a \leq -b^2$ and $a^2 - b^2 \leq 0$ then $a^2 \leq b^2$

$$|1+z| = \sqrt{1 + x\left(2a + b^2\right) + x^2\left(a^2 - b^2\right)} \leq 1, \tag{B.113}$$

and so (B.108) is not satisfied, for case 2 unless $a = b = 0$.

**Case 3**: If $2a + b^2 \geq 0$ then $2a \geq -b^2$ and $a^2 - b^2 \leq 0$ the $a^2 \leq b^2$, we then have

$$\begin{aligned} |1+z| &= \sqrt{1 + x\left(2a + b^2\right) + x^2\left(a^2 - b^2\right)} \\ &\geq \sqrt{1 + x^2\left(2a + b^2\right) + x^2\left(a^2 - b^2\right)} \\ &\geq \sqrt{1 + x^2\left(2a + a^2\right)}, \end{aligned} \tag{B.114}$$

since for $0 \leq x \leq 1$ then $0 \leq x^2 \leq x$ and if $a > 0$, (and so $\mathrm{Re}(z) \geq 0$), we then conclude that $|1+z| \geq 1$. Hence

$$\left|\frac{1}{1+z}\right| \leq 1 \tag{B.115}$$

is satisfied.

**Case 4**: If $2a + b^2 \leq 0$ then $2a \leq -b^2$ and $a^2 - b^2 \geq 0$ then $a^2 \geq b^2$, we then have

$$|1+z| = \sqrt{1 + x\left(2a + b^2\right) + x^2\left(a^2 - b^2\right)} \leq 1 \tag{B.116}$$

and so Equation (B.108) is not satisfied. □

**Lemma B.11.2.** Given $0 < \gamma \leq 1$, then the parameter $\widetilde{U_q}$ given in Equation (5.439) is bounded by $\left|\widetilde{U_q}\right| \leq 2^\gamma$ if $\mathrm{Re}(z) \geq 0$.

*Proof.* From Equation (5.439) we have

$$\widetilde{U_q} = 2^\gamma \left[\frac{x+z}{1+z}\right], \tag{B.117}$$

where $z = u - iv$, which $u$ and $v$ are defined as

$$u = \sin^2\left(q\Delta x/2\right)\left(\left(\frac{1}{2}\right)^\gamma d_1 - 1\right), \tag{B.118}$$

and

$$v = \frac{d_2}{2}\left(\frac{1}{2}\right)^{\gamma}\sin(q\Delta x), \tag{B.119}$$

and $x = \sin^2(q\Delta x/2)$ where $0 \le x \le 1$. Now taking the modulus, gives

$$\begin{aligned}\left|\widetilde{U_q}\right| &= 2^{\gamma}\left|\frac{x+z}{1+z}\right| \\ &= 2^{\gamma}\frac{\sqrt{(x+z)(x+\bar{z})}}{\sqrt{(1+z)(1+\bar{z})}} \\ &= 2^{\gamma}\frac{\sqrt{x^2+|z|^2+x(z+\bar{z})}}{\sqrt{1+|z|^2+(z+\bar{z})}} \\ &\le 2^{\gamma}\end{aligned} \tag{B.120}$$

since $0 \le x \le 1$ and $z+\bar{z} = 2\mathrm{Re}(z) = 2u \ge 0$. We then obtain the bound of $\left|\widetilde{U_q}\right| \le 2^{\gamma}$. $\square$

**Lemma B.11.3.** Given $0 < \gamma \le 1$, then the first term in the braces given in Equation (5.450) is bounded by $\left|1-\widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| \le 1$ if $\mathrm{Re}(z) \ge 0$, where $\widetilde{U_q}$ is defined in Equation (5.439).

*Proof.* From Equations (5.28) and (5.439) we have

$$\begin{aligned}\left|1-\widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| &= \left|1-2^{\gamma}\left[\frac{x+z}{1+z}\right]\left(\left(\frac{3}{2}\right)^{\gamma}-\left(\frac{1}{2}\right)^{\gamma}\right)\right| \\ &= \left|1-\left[\frac{x+z}{1+z}\right](3^{\gamma}-1)\right| \\ &= \left|\frac{(1+x-3^{\gamma}x)+(2-3^{\gamma})z}{1+z}\right| \\ &= \left|\frac{y_1+y_2z}{1+z}\right|,\end{aligned} \tag{B.121}$$

where $z = u-iv$, which $u$ and $v$ are defined in Equations (B.118) and (B.119) respectively, $x = \sin^2(q\Delta x/2)$, $y_1 = 1+x(1-3^{\gamma})$ and $y_2 = 2-3^{\gamma}$.

For $0 < \gamma \le 1$ and $0 < x \le 1$ we have $-1 \le a_1 \le 1$ and $-1 \le y_2 \le 1$ as shown in Figures B.4 and B.5. Equation (B.121) becomes

$$\begin{aligned}\left|1-\widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| &= \frac{\sqrt{(y_1+y_2z)(y_1+y_2\bar{z})}}{\sqrt{(1+z)(1+\bar{z})}} \\ &= \frac{\sqrt{y_1^2+y_2^2|z|^2+y_1y_2(z+\bar{z})}}{\sqrt{1+|z|^2+(z+\bar{z})}}.\end{aligned} \tag{B.122}$$

Since $y_1 \le 1$ and $y_2 \le 1$ then $y_1y_2 \le 1$. Also $z+\bar{z} = 2\mathrm{Re}(z) = 2u \ge 0$. We then conclude that $\left|1-\widetilde{U_q}\widetilde{\mu}_0(\gamma)\right| \le 1$.

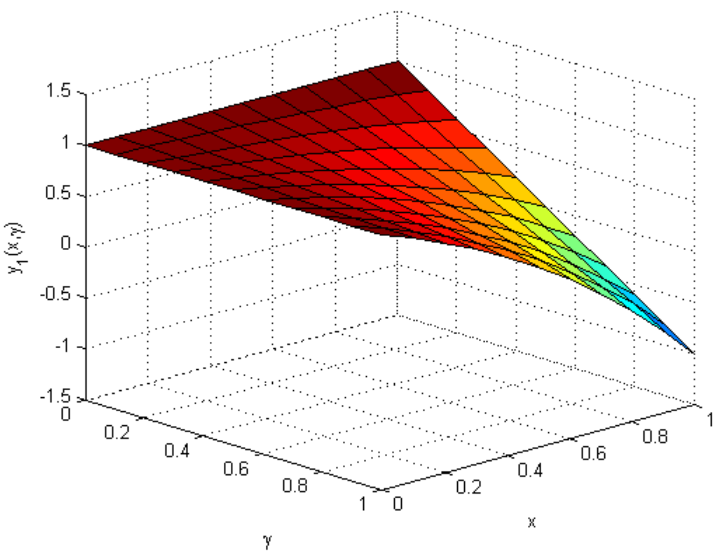



Figure B.4: Bound of $y_1$, where $y_1 = 1 + x(1 - 3^{\gamma})$ with $0 < \gamma \leq 1$ and $0 \leq x \leq 1$.

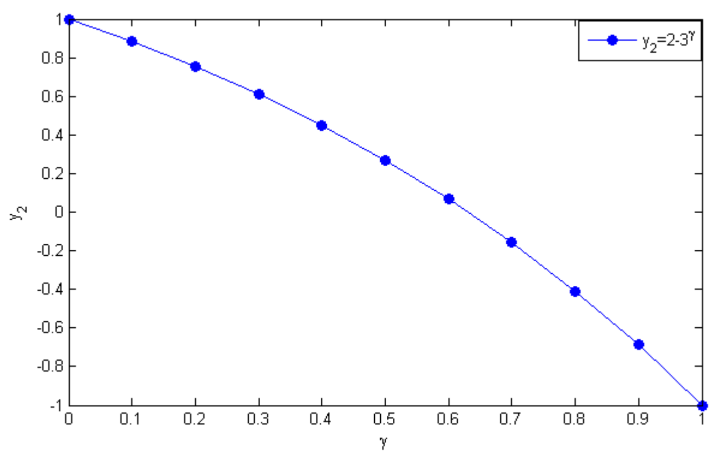



Figure B.5: Bound of $y_2$, where $y_2 = 2 - 3^{\gamma}$ with $0 < \gamma \leq 1$.

□

# Appendix C

# MATLAB Codes

In this appendix, we listed the programs that used to support this thesis. These are given on the CDROM.

## C.1 Programs used for Chapter 2

In this section we give the main programs that are used to determine the accuracy of the schemes in Chapter 2, as shown in the following table.

| The Main Programs used in Chapter 2 | | |
|---|---|---|
| Directory | File | Description |
| \Chapter 2\Accuracy-GL | \TestAccGL.m | The accuracy of the GL scheme |
| \Chapter 2\Accuracy_L1 | \Accuracy_L1.m | The accuracy of the L1 scheme |
| \Chapter 2\Accuracy_L1 | \RatDt_L1.m | Estimate of the convergence order for the L1 scheme |
| \Chapter 2\Accuracy_C1 | \AccuracyC1.m | The accuracy of the C1 scheme |
| \Chapter 2\Accuracy_C1 | \RatDt_C1.m | Estimate of the convergence order for the C1 scheme |
| \Chapter 2\Accuracy_C2 | \AccuracyC2.m | The accuracy of the C2 scheme |
| \Chapter 2\Accuracy_C2 | \RatDt_C2.m | Estimate of the convergence order for the C2 scheme |
| \Chapter 2\Accuracy_C3 | \AccuracyC3.m | The accuracy of the C2 scheme |
| \Chapter 2\Accuracy_C3 | \RatDt_C3.m | Estimate of the convergence order for the C3 scheme |
| \Chapter 2\Accuracy_RInt | \Accuracy_RI.m | The accuracy of the $RInt$ scheme |
| \Chapter 2\Accuracy_RInt | \RatDt_RI.m | Estimate of the convergence order for the $RInt$ scheme |
| \Chapter 2\L1star | \Accuracy.m | The accuracy of the $L1^*$ scheme |
| \Chapter 2\RL1 | \Accuracy.m | The accuracy of the RL1 scheme |
| \Chapter 2\LRA | \Accuracy.m | The accuracy of the LRA scheme |
| \Chapter 2\QRA | \Accuracy.m | The accuracy of the QRA scheme |
| \Chapter 2\NLRA | \Accuracy.m | The accuracy of the NLRA scheme |

## C.2 Programs used for Chapter 3

In this section, we give the main programs that are used in Chapter 3 to find the numerical solution using the IMC1 scheme as well as determine the stability and accuracy of this scheme. These are listed in the following table.

| The Main Programs used in Chapter 3 | | |
|---|---|---|
| Directory | File | Description |
| \Chapter 3\IMC1 | \IMC1.m | Numerical solution by using the IMC1 scheme |
| \Chapter 3\IMC1 | \St_C1.m | Stability for the IMC1 scheme |
| \Chapter 3\IMC1 | \RatDt.m | Estimate of the convergence order for the IMC1 scheme |

## C.3 Programs used for Chapter 4

In this section, we give the main programs that are used in Chapter 4 to find the numerical solution using the DFL1 scheme as well as its stability and accuracy of this scheme. These are listed in the following table.

| The Main Programs used in Chapter 4 | | |
|---|---|---|
| Directory | File | Description |
| \Chapter 4\DFL1 | \DuFort.m | The numerical solution by using the DFL1 scheme |
| \Chapter 4\DFL1 | \St_C1.m | Stability for the DFL1 scheme |
| \Chapter 4\DFL1 | \RatDt.m | Estimate of the convergence order for the DFL1 scheme |

## C.4 Programs used for Chapter 5

In this section, we give the main programs that obtain the numerical solution, stability and accuracy for the KBMC2, KBMC3, KBML1, and KBMC2–FADE schemes in Chapter 5, as shown in the following table.

| The Main Programs used in Chapter 5 | | |
|---|---|---|
| Directory | File | Description |
| \Chapter 5\KBMC2 | \SolutionKBMC2.m | The numerical solution by using the KBMC2 scheme |
| \Chapter 5\KBMC2 | \StKellerBox.m | The stability for the KBMC2 scheme |
| \Chapter 5\KBMC2 | \RatDt.m | Estimate of the convergence order for the KBMC2 scheme |
| \Chapter 5\KBMC3 | \SolnKBMC3.m | The numerical solution by using the KBMC3 scheme |
| \Chapter 5\KBMC3 | \ST.m | The stability for the KBMC3 scheme |
| \Chapter 5\KBMC3 | \RatDt.m | Estimate of the convergence order for the KBMC3 scheme |
| \Chapter 5\KBML1 | \SolnKeller1.m | The numerical solution by using the KBML1 scheme |
| \Chapter 5\KBML1 | \Test_Stability.m | The stability for the KBML1 scheme |
| \Chapter 5\KBML1 | \RatDt.m | Estimate of the convergence order for the KBML1 scheme |
| \Chapter 5\FADE_C2 | \Soln_FADE.m | The numerical solution by using the KBMC2–FADE scheme |
| \Chapter 5\FADE_C2 | \RatDt.m | Estimate of the convergence order for the KBMC2–FADE scheme |

## C.5 Programs used for Chapter 6

In this section, we give the main programs that are used in Chapter 6 to find the numerical solution of nonlinear fractional reaction diffusion equations by using the KBMC2 and IML1 schemes for Model Type 1 and Model Type 2. The main programs are listed in the following table.

| The Main Program used in Chapter 6 | | |
|---|---|---|
| Directory | File | Description |
| \Chapter 6\KBMC2 | \M1Soln_KBMC2.m | The numerical solution by using the KBMC2 scheme for Model Type 1 |
| \Chapter 6\KBMC2 | \RatDt.m | The convergence order of the KBMC2 scheme for Model Type 1 |
| \Chapter 6\KBMC2 | \M2Soln_KBMC2.m | The numerical solution by using the KBMC2 scheme for Model Type 2 |
| \Chapter 6\KBMC2 | \RatDt.m | The convergence order of the KBMC2 scheme for Model Type 2 |
| \Chapter 6\IML1 | \M1SolnIML1.m | The numerical solution by using the IML1 scheme for Model Type 1 |
| \Chapter 6\IML1 | \M2SolnIML1.m | The numerical solution by using the IML1 scheme for Model Type 2 |