From stochastic processes to numerical methods: A new scheme for solving reaction subdiffusion fractional partial differential equations.

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Abstract

We have introduced a new explicit numerical method, based on a discrete stochastic process, for solving a class of fractional partial differential equations that model reaction subdiffusion. The scheme is derived from the master equations for the evolution of the probability density of a sum of discrete time random walks. We show that the diffusion limit of the master equations recovers the fractional partial differential equation of interest. This limiting procedure guarantees the consistency of the numerical scheme. The positivity of the solution and stability results are simply obtained, provided that the underlying process is well posed. We also show that the method can be applied to standard reaction-diffusion equations. This work highlights the broader applicability of using discrete stochastic processes to provide numerical schemes for partial differential equations, including fractional partial differential equations.

1. Introduction

Reaction subdiffusion fractional partial differential equations have been widely used in recent years as mathematical models of systems of particles subject to, trapping, obstacles and reactions [1, 2, 3, 4, 5, 6, 7, 8]. Subdiffusion, characterised by a mean squared displacement of diffusing particles that grows slower

than linear with time, has been observed in hydrogeology [9, 8], physics [10], biology [11], finance [12] and chemistry [13].

Reaction subdiffusion fractional partial differential equations may be derived from generalised continuous time random walks (CTRWs) [14, 15] by incorporating reaction kinetics into the process [1, 2, 3, 5, 7]. In standard reaction-diffusion partial differential equations the reaction terms and the diffusion terms are additive [16, 17, 18, 19], whilst in reaction subdiffusion equations, derived from CTRWs, the reaction kinetics and the diffusion are entwined in the fractional partial differential equations [2, 3, 5]. In general it is not possible to obtain closed form algebraic solutions for non-linear reaction subdiffusion equations. This has stimulated a great deal of interest in the development of numerical methods for these equations. Some of the numerical methods developed for subdiffusion include, explicit and implicit finite difference methods [20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31], spectral methods [32, 33, 34, 35], and Galerkin methods [36, 37]. One of the simplest methods is to approximate the continuous fractional derivative using a Grünwald-Letnikov fractional derivative [38, 39].

There have been numerous articles published on numerical methods for time fractional reaction-diffusion equations. Most of the articles in this area consider fractional diffusion with the *ad-hoc* addition of standard reactions, or addition of reactions including the time fractional derivative on the reactions, or a combination of both [40, 41, 42, 43, 44]. The *ad-hoc* addition of subdiffusion and reactions may lead to unphysical negative solutions [2]. This can be avoided by taking a more physical approach, deriving the reaction subdiffusion equations from an underlying stochastic process, a continuous time random walk [2, 5, 6, 7]. The numerical method that we derive here is also based on an underlying stochastic process, a discrete time random walk (DTRW).

In [45], we introduced a novel numerical scheme for solving fractional Fokker-Planck equations that was based on a DTRW. Rather then discretising a continuum set of equations the numerical scheme is constructed by considering a discrete time and space stochastic process. The process was chosen such that, in the diffusion limit, the evolution equation of the probability density that described the system would become a fractional Fokker-Planck equation. As the process is discrete the probability density can be calculated recursively and used to approximate the diffusion limit density, and hence the solution of the fractional Fokker-Planck equation. A similar approach has also been used to solve sets of fractional ordinary differential equations arising from a modified SIR epidemic model [46].

In this article we have extended the DTRW formalism to provide a numerical scheme for solving reaction subdiffusion fractional partial differential equations of the form

$$\frac{\partial u}{\partial t} = D_\alpha \frac{\partial^2}{\partial x^2}\left[e^{-\int_0^t a(u,x,t')\,dt'}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{\int_0^t a(u,x,t')\,dt'}u\right)\right] + c(u,x,t) - a(u,x,t)u, \tag{1}$$

where $u = u(x,t)$, $a(u,x,t)$ and $c(u,x,t)$ are non-negative and ${}_0\mathcal{D}_t^{1-\alpha}$ is a

Riemann-Liouville fractional derivative of order $1-\alpha$. Equations of this form can be derived from a physically consistent theory of continuous time random walks [7], including extension to multiple species. The numerical scheme is obtained by first deriving a set of discrete time and space master equations for an ensemble of particles undergoing a DTRW with reactions. The evolution of these discrete equations provides the basis for a numerical solution of the fractional partial differential equations. The resulting numerical scheme is an explicit forward time-step method, Eq. (66) in this manuscript. Provided that the underlying process is well posed the solution is guaranteed to be positive, as is required for reaction diffusion processes, and stability results follow. The numerical scheme can be implemented without requiring a knowledge of stochastic processes, however additional symmetries, if known, can be incorporated into the scheme.

The remainder of the paper is organised as follows. In Section 2 we present the formalism for the DTRW with reactions, and derive the appropriate master equations. In Section 3 we consider specific forms for the jump and waiting time probability mass functions (pmfs) in the DTRWs. In Section 4, we show that in the continuous space and time limit, depending on the jump and waiting time pmfs, the master equations converge to standard reaction-diffusion PDEs or reaction subdiffusion fractional PDEs. In Section 5, we outline how to implement the discrete time master equations as a numerical scheme for the PDEs. In Section 6 we derive stability results from the underlying stochastic process. We show that the numerical scheme has positive solutions and is stable for physically consistent reaction kinetics. Detailed examples using the scheme are presented in Section 7.

2. The Master Equation for Discrete Time Random Walks With Reactions

In this section we derive the discrete time master equations of DTRWs with reactions an subdiffusion. These master requations underpin the numercial scheme. The derivation of the master equations follows the framework that we developed in [45] for the derivation of discrete time master equations of DTRWs subject to forcing. The additional complication of reactions in the discrete time master equations are treated in a manner similar to our treatment of reactions in continuous time master equations [47, 7] where the reactions are modelled as a birth (annihilation) and death (creation) process. The derivation of the master equations is broken into two main parts. Firstly we consider the evolution of a single particle subject to a space- and time-dependent probability of annihilation. Next, by considering an ensemble of such particles arising from a space- and time-dependent creation process, we construct the discrete master equations that govern the evolution of the reaction diffusion system.

2.1. A Discrete Time Random Walk with an Annihilation Rate

We begin by considering a particle traversing a one-dimensional lattice $V = \{L_1, ..., i-1, i, i+1, ..., L_2\}$, with $L_1, L_2 \in \mathbb{Z}$, in discrete time $n \in \mathbb{N}$. At each

time step the particle will randomly do one of three things; either remain at the current site, undergo a jump, or be annihilated and removed from further consideration. The probability of the actions are independent but may depend on the current site and time step, and the time step on which the particle arrived at the site.

For a particle that arrived at the site i on the m^{th} time step the probability of jumping to site j on the n^{th} time step is given by a transition probability mass function $\Psi(j, n|i, m)$. This function completely describes the evolution of the process. We make a further assumption that this probability mass function (pmf) can be decomposed into two independent pmfs,

$$\Psi(j, n|i, m) = \lambda(j|i)\psi(n - m), \tag{2}$$

where $\psi(n - m)$ is the pmf for waiting $n - m$ time steps before transitioning and $\lambda(j|i)$ is the pmf for jumping to site j conditional on being on site i. As usual, the pmfs are normalised,

$$\sum_{n=0}^{\infty} \psi(n) = 1, \tag{3}$$

and

$$\sum_{j=L_1}^{L_2} \lambda(j|i) = 1. \tag{4}$$

It is also important to note that we assume

$$\psi(0) = 0, \tag{5}$$

as we do not allow multiple jumps in the same time step. It is possible to incorporate a spatial dependence into the waiting time probabilities, and time dependence into the jump probabilities but this is not included here for simplicity.

The probability that a particle will be annihilated at site i on the n^{th} time step is denoted $A(i, n)$. This time- and space-dependence allows for the consideration of arbitrary functions provided that $0 \leq A(i, n) \leq 1$. The probability of not being annihilated over a number of time steps, between time m and n at site i, is then given by the survival function

$$\Theta(i, n, m) = \prod_{\ell=m}^{n-1} \left(1 - A(i, \ell)\right), \tag{6}$$

and we use the convention, $\Theta(i, n, n) = 1$. It is useful to note the semigroup property of Θ;

$$\Theta(i, n, m) = \Theta(i, n, k)\, \Theta(i, k, m) \;\; \forall\, m \leq k \leq n. \tag{7}$$

The probability of a particle arriving at site i on the n^{th} time step, given that it is created and begins walking at site i_0 on the n_0^{th} time step, is recursively defined by the probability flux;

$$Q(i,n|i_0,n_0) = \delta_{i,i_0}\delta_{n,n_0} + \sum_{j=L_1}^{L_2}\sum_{m=0}^{n-1} \Psi(i,n|j,m)\,\Theta(j,n,m)\,Q(j,m|i_0,n_0) \quad (8)$$

where $Q(i,m|i_0,n_0) = 0$ for all $m < n_0$. This equation expresses that the flux into site i at time step n is the sum of all the fluxes into site j at the earlier time step m that survived until time step n when they transition to site i. Note that the upper limit of the sum could be n, but $\Psi(i,n|j,n) = 0$ due to Eq. (5).

The probability of a particle at a site not jumping by time step n, given the particle arrived at the earlier time m is given by the survival probability

$$\Phi(n-m) = 1 - \sum_{k=0}^{n-m} \psi(k). \quad (9)$$

The probability of the particle being at site i on the n^{th} time step can then be written

$$X(i,n|i_0,n_0) = \sum_{m=0}^{n} \Phi(n-m)\,\Theta(i,n,m)\,Q(i,m|i_0,n_0). \quad (10)$$

The right hand side is the sum over all possibilities of the particle arriving at an earlier time step, m, and not being annihilated or jumping before the n^{th} time step.

The change in probability mass X between time steps n and $n-1$ is obtained directly from Eq. (10):

$$\begin{aligned} X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = &\sum_{m=0}^{n} \Phi(n-m)\,\Theta(i,n,m)\,Q(i,m|i_0,n_0) \\ &- \sum_{m=0}^{n-1} \Phi(n-1-m)\,\Theta(i,n-1,m)\,Q(i,m|i_0,n_0). \end{aligned} \quad (11)$$

This can be rewritten as

$$\begin{aligned} X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = &\,Q(i,n|i_0,n_0) \\ &+ \sum_{m=0}^{n-1} \Theta(i,n,m)\Phi(n-m)Q(i,m|i_0,n_0) \\ &- \sum_{m=0}^{n-1} \Theta(i,n-1,m)\Phi(n-1-m)Q(i,m|i_0,n_0)\,. \end{aligned} \quad (12)$$

From Eq. (9) we have that $\Phi(n-m) = \Phi(n-1-m) - \psi(n-m)$, and from Eq. (7) we see that $\Theta(i,n,m) = \Theta(i,n,n-1)\Theta(i,n-1,m)$, hence Eq. (12) can be rewritten as

$$X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = Q(i,n|i_0,n_0) - \sum_{m=0}^{n-1} \psi(n-m)\Theta(i,n,m)Q(i,m|i_0,n_0) - \sum_{m=0}^{n-1} \Phi(n-1-m)\Theta(i,n-1,m)\left(1-\Theta(i,n,n-1)\right)Q(i,m|i_0,n_0)\,. \tag{13}$$

Noting that from Eq. (6), $1-\Theta(i,n,n-1) = A(i,n-1)$ and we obtain

$$X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = Q(i,n|i_0,n_0) - \sum_{m=0}^{n-1} \psi(n-m)\Theta(i,n,m)Q(i,m|i_0,n_0) - A(i,n-1)\sum_{m=0}^{n-1} \Phi(n-1-m)\Theta(i,n-1,m)Q(i,m|i_0,n_0)\,. \tag{14}$$

Then by using the definition in Eq. (10), we substitute the last term with $X(i,n-1|i_0,n_0)$ to arrive at

$$\begin{aligned} X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = {} & Q(i,n|i_0,n_0) \\ & - \sum_{m=0}^{n-1} \psi(n-m)\Theta(i,n,m)Q(i,m|i_0,n_0) \\ & - A(i,n-1)X(i,n-1|i_0,n_0). \end{aligned} \tag{15}$$

We define the outgoing flux of site i at time step n to be

$$\zeta(i,n|i_0,n_0) \;=\; \sum_{m=0}^{n-1} \psi(n-m)\,\Theta(i,n,m)\,Q(i,m|i_0,n_0)\,. \tag{16}$$

Note from the definition of Q, Eq. (8), and recalling Eq. (2), that

$$Q(i,n|i_0,n_0) - \delta_{n,n_0}\delta_{i,i_0} \;=\; \sum_{j=L_1}^{L_2} \lambda(j|i)\,\zeta(j,n|i_0,n_0)\,. \tag{17}$$

Substituting this into Eq. (15) gives

$$\begin{aligned} X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = {} & \sum_{j=L_1}^{L_2} \lambda(j|i)\,\zeta(j,n|i_0,n_0) + \delta_{n,n_0}\delta_{i,i_0} \\ & - \zeta(i,n|i_0,n_0) - A(i,n-1)X(i,n-1|i_0,n_0)\,. \end{aligned} \tag{18}$$

To obtain the generalised master equation (GME) governing the evolution of the probability mass for the particle we use the semigroup property of Θ, given in Eq. (7), to write Eq. (10) as

$$\frac{X(i,n|i_0,n_0)}{\Theta(i,n,0)} = \sum_{m=0}^{n} \frac{Q(i,m|i_0,n_0)}{\Theta(i,m,0)}\,\Phi(n-m). \tag{19}$$

Similarly for Eq. (16) we get

$$\frac{\zeta(i,n|i_0,n_0)}{\Theta(i,n,0)} = \sum_{m=0}^{n} \frac{Q(i,m|i_0,n_0)}{\Theta(i,m,0)}\,\psi(n-m). \tag{20}$$

To proceed further, we make use of the single-sided $\mathcal{Z}$-transform [48] defined by

$$\mathcal{Z}_n\{Y(n)|z\} = \sum_{n=0}^{\infty} Y(n) z^{-n}. \tag{21}$$

Taking the $\mathcal{Z}$-transform of Eqs. (19) and (20) gives

$$\mathcal{Z}_n\left\{\frac{X(i,n|i_0,n_0)}{\Theta(i,n,0)}\middle|z\right\} = \mathcal{Z}_n\left\{\frac{Q(i,n|i_0,n_0)}{\Theta(i,n,0)}\middle|z\right\}\mathcal{Z}_n\{\Phi(n)|z\} \tag{22}$$

and

$$\mathcal{Z}_n\left\{\frac{\zeta(i,n|i_0,n_0)}{\Theta(i,n,0)}\middle|z\right\} = \mathcal{Z}_n\left\{\frac{Q(i,n|i_0,n_0)}{\Theta(i,n,0)}\middle|z\right\}\mathcal{Z}_n\{\psi(n)|z\}. \tag{23}$$

Similar to the analysis of CTRWs [7], it is convenient to define a discrete memory kernel $K(n)$ by the $\mathcal{Z}$-transform relation

$$\mathcal{Z}_n\{K(n)|z\} = \frac{\mathcal{Z}_n\{\psi(n)|z\}}{\mathcal{Z}_n\{\Phi(n)|z\}}. \tag{24}$$

Note that from Eq. (5) and Eq. (9), we have $K(0) = 0$. Dividing Eq. (23) by Eq. (22) and inverting the $\mathcal{Z}$-transform we can express ζ in terms of X,

$$\zeta(i,n|i_0,n_0) = \Theta(i,n,0)\sum_{m=0}^{n-1} K(n-m)\frac{X(i,m|i_0,n_0)}{\Theta(i,m,0)}. \tag{25}$$

We can substitute this expression for ζ in to Eq. (18) to obtain the following generalised master equation for the evolution of a single particle probability mass, X, subject to an annihilation process;

$$\begin{aligned} X(i,n|i_0,n_0) - X(i,n-1|i_0,n_0) = & \\ & \sum_{j=L_1}^{L_2} \lambda(j|i) \sum_{m=0}^{n-1} K(n-m)\,\Theta(j,n,m)\,X(j,m|i_0,n_0) \\ & - \sum_{m=0}^{n-1} K(n-m)\,\Theta(i,n,m) X(i,m|i_0,n_0) \\ & - A(i,n-1)\,X(i,n-1|i_0,n_0) + \delta_{n,n_0}\delta_{i,i_0}. \end{aligned} \tag{26}$$

2.2. An Ensemble of Discrete Time Random Walks With Creation and Annihilation

Under our model of reacting and diffusing particles the system comprises of an ensemble of particles that are created at some point, undergo a random walk and are annihilated at some other point. The evolution of this ensemble can be found by considering the evolution of the single particles in the ensemble. The GME for the single particle subject to an annihilation process, Eq. (26), can be thought of as propagating each single particle from some initial point onwards.

We assume that the creation process is Markovian and defined such that the expected number of particles created at lattice site i on time step n is given by the arbitrary function, $C(i,n) \geq 0$ for all i and n. The expected number of particles from the ensemble at position i at time n can then be found by propagating the creation of all the particles forward in time. The number of particles at site i on time step n is then given by,

$$U(i,n) \;=\; \sum_{i_0=L_1}^{L_2} \sum_{n_0=0}^{n} X(i,n|i_0,n_0) C(i_0,n_0). \tag{27}$$

As the creation process is Markovian, $C(i,n)$, can depend on the state of the system at the previous time step, $\{U(j,n-1)\}_j$. To find the evolution of U with time we multiply the single particle GME, Eq. (26), by $C(i_0,n_0)$ and then sum over all possible starting points; i_0 from L_1 to L_2 and n_0 from 0 to n. Using the definition in Eq. (27) we obtain

$$\begin{aligned} U(i,n) - U(i,n-1) \;=\; & \sum_{j=L_1}^{L_2} \lambda(j|i) \sum_{m=0}^{n-1} K(n-m)\, \Theta(j,n,m)\, U(j,m) \\ & - \sum_{m=0}^{n-1} K(n-m)\, \Theta(i,n,m) U(i,m) - A(i,n-1)\, U(i,n-1) + C(i,n). \end{aligned} \tag{28}$$

This is the generalised master equation for a single species discrete general reaction diffusion process. Note that $A(i,n-1)$ may also be dependent on $\{U(j,n-1)\}_j$. With the appropriate choice of the waiting time pmf, and hence the memory kernel K, Eq. (28) may model the cases of reaction-diffusion or reaction subdiffusion.

2.3. Interacting Ensembles of Discrete Time Random Walks With Annihilation and Creation

Similar to the approach in [7] we can generalise this master equation for the case of a multi-species ensemble of populations that have interactions between them. This can represent, for example, systems such as chemical reactions or microbiological population dynamics. To do so we allow the creation and annihilation rates to depend on all populations. As we have worked with creation and annihilation probabilities that are arbitrary in space and time we may

incorporate non-linear dependencies on populations into these probabilities. We calculate $\Theta_k(i,n,m)$ from the annihilation probabilities through

$$\Theta_k(i,n,m) = \prod_{\ell=m}^{n-1} (1 - A_k(i,\ell)), \tag{29}$$

where k is the species number. Note that $A_k(i,\ell)$ may also be dependent on the state of the system $\{U_p(j,\ell)\}_{j,p}$ at time ℓ.

Thus the multi-species DTRW master equation with non-linear reactions is given by

$$\begin{aligned} U_k(i,n) \; - \; U_k(i,n-1) \; = \; & \sum_{j=L_1}^{L_2} \lambda_k(i|j) \sum_{m=0}^{n-1} K_k(n-m)\, \Theta_k(j,n,m)\, U_k(j,m) \\ & - \sum_{m=0}^{n-1} K_k(n-m)\, \Theta_k(i,n,m)\, U_k(i,m) \\ & - A_k(i,n-1) U_k(i,n-1) + C_k(i,n). \end{aligned} \tag{30}$$

In these equations $C_k(i,n)$, can depend on the state of the system at the previous time step, $\{U_p(j,n-1)\}_{j,p}$.

3. Jump and Waiting Time Probability Mass Functions

The discrete generalised master equations can be used to formulate a numerical method for solving continuum reaction-diffusion type equations, including fractional reaction-diffusion equations. To obtain a numerical method for a given continuum reaction-diffusion equation from the discrete GME appropriate choices need to be made for the jump and waiting time distributions. Once these choices have been made, the discrete GMEs can be used as an explicit numerical scheme for approximating reaction-diffusion PDEs that are the continuum limit of the discrete GMEs. The corresponding continuum limit of the discrete GMEs will be obtained in section 4. This convergence in the continuum limit establishes the consistency of the numerical scheme.

3.1. Jump Probability Mass Functions

We considering a jump process composed of nearest neighbour and self jumps. The jump pmf is given by

$$\lambda(j|i) = \frac{r}{2}\delta_{i+1,j} + \frac{r}{2}\delta_{i-1,j} + (1-r)\delta_{i,j}. \tag{31}$$

Here $r \in [0,1]$ is the probability that a jump will not be a self jump. This jump pmf is symmetric. The incorporation of asymmetric space and time dependent jumps has previously been considered to model a space and time dependent force [45].

Substituting the jump pmf, Eq. (31), into the discrete GME, Eq. (28), gives,

$$\begin{aligned} U(i,n) - U(i,n-1) &= \frac{r}{2}\sum_{m=0}^{n-1} K(n-m)\,\Theta(i-1,n,m)\,U(i-1,m) \\ &+ \frac{r}{2}\sum_{m=0}^{n-1} K(n-m)\,\Theta(i+1,n,m)\,U(i+1,m) \\ &- r\sum_{m=0}^{n-1} K(n-m)\,\Theta(i,n,m)U(i,m) - A(i,n-1)\,U(i,n-1) + C(i,n). \end{aligned} \tag{32}$$

Using Eq. (7), we can express the sums in the above equation as discrete convolutions,

$$\begin{aligned} U(i,n) - U(i,n-1) &= \frac{r}{2}\Theta(i-1,n,0)\sum_{m=0}^{n-1} K(n-m)\frac{U(i-1,m)}{\Theta(i-1,m,0)} \\ &+ \frac{r}{2}\Theta(i+1,n,0)\sum_{m=0}^{n-1} K(n-m)\frac{U(i+1,m)}{\Theta(i+1,m,0)} \\ &- r\Theta(i,n,0)\sum_{m=0}^{n-1} K(n-m)\frac{U(i,m)}{\Theta(i,m,0)} - A(i,n-1)\,U(i,n-1) + C(i,n). \end{aligned} \tag{33}$$

3.2. Waiting Time Probability Mass Functions

3.2.1. Markovian

Assuming that the probability of the particle jumping to a new site on any given time step is ω and is independent of the time that the particle arrived at the current site, then it follows that waiting time pmf is given by,

$$\psi(n) = \omega(1-\omega)^n. \tag{34}$$

The corresponding survival function is,

$$\Phi(n) = (1-\omega)^n. \tag{35}$$

Equation (24) can now be used to obtain an explicit expression for the memory kernel,

$$K(n) = \omega\delta_{1,n}. \tag{36}$$

3.3. Sibuya

The waiting time pmf is non-Markovian when the probability of the particle jumping on any given time step depends on how many time steps the particle has waited for. A special case is when the probability of jumping on a given time step decreases the longer the particle waits without jumping. Sibuya waiting times arise by considering a particle that has a probability $\frac{\alpha}{n}$ of jumping after

waiting n time steps for some $0 < \alpha \leq 1$ [49]. The waiting time survival function is given by

$$\Phi(n) = \prod_{k=1}^{n} \left(1 - \frac{\alpha}{k}\right), \tag{37}$$

with $\Phi(0) = 1$. The corresponding waiting time pmf is,

$$\psi(n) = \frac{\alpha}{n} \prod_{k=1}^{n-1} \left(1 - \frac{\alpha}{k}\right), \tag{38}$$

with $\psi(0) = 0$ and $\psi(1) = \alpha$. As in [45], we can consider the $\mathcal{Z}$-transforms to obtain an analytic expression for the memory kernel, K, from Eq. (24),

$$\begin{aligned} \mathcal{Z}_n\{K(n)|z\} &= \frac{\mathcal{Z}_n\{\psi(n)|z\}}{\mathcal{Z}_n\{\Phi(n)|z\}} \\ &= \frac{1 - (1 - z^{-1})^{\alpha}}{(1 - z^{-1})^{\alpha - 1}} \\ &= (1 - z^{-1})^{1-\alpha} - (1 - z^{-1}), \end{aligned} \tag{39}$$

and hence it can be shown that the kernel, for $n \geq 1$ can be given by

$$K(n) = \prod_{k=1}^{n} \left(1 - \frac{2 - \alpha}{k}\right) + \delta_{1,n}, \tag{40}$$

with $K(0) = 0$. We may also write the Sibuya kernel in terms of binomial coefficients,

$$K(n) = \binom{1 - \alpha}{n} (-1)^n - \delta_{0,n} + \delta_{1,n}, \tag{41}$$

and the kernel can be obtained from a recursion relation [45]. It is interesting to note that the terms in the memory kernel can be related to the Grünwald-Letnikov fractional derivative via

$$\mathbb{D}^{1-\alpha}(f(x)) = \lim_{h \to 0} \sum_{k=0}^{n} \left(K(n) + \delta_{0,n} - \delta_{1,n}\right) \frac{f(x - kh)}{h^{1-\alpha}}. \tag{42}$$

4. Continuum Limit of the Discrete Generalised Master Equations

In this section we derive continuum limits of the GMEs, Eq. (33), corresponding to Markovian, and Sibuya waiting times. These continuum limits yield the standard reaction-diffusion PDEs and the fractional reaction-diffusion PDEs respectively. This shows that the discrete GMEs satisfy the consistency condition for an approximation to the PDEs, and can therefore be used as a consistent explicit numerical method.

4.1. Markovian Waiting Times

Using the Markovian memory kernel, Eq. (36), the discrete GME, Eq. (33), simplifies to,

$$\begin{aligned} U(i,n) - U(i,n-1) = \frac{r\omega}{2}\Big(&\Theta(i-1,n,n-1)U(i-1,n-1) \\ &- 2\Theta(i,n,n-1)U(i,n-1) + \Theta(i+1,n,n-1)U(i+1,n-1)\Big) \\ &- A(i,n-1)\,U(i,n-1) + C(i,n). \end{aligned} \tag{43}$$

Using Eq. (6) we have

$$\begin{aligned} U(i,n) - U(i,n-1) = \frac{r\omega}{2}\Big(&(1-A(i-1,n-1))U(i-1,n-1) \\ &- 2(1-A(i,n-1))U(i,n-1) + (1-A(i+1,n-1))U(i+1,n-1)\Big) \\ &- A(i,n-1)\,U(i,n-1) + C(i,n). \end{aligned} \tag{44}$$

We now relate our solution $U(i,n)$ of the discrete GME to a function in continuous space and time. We consider a uniform grid with spacings Δx and Δt, and associate the points $(i,n) \in \mathbb{Z}^2$ with points $(i\Delta x, n\Delta t) \in \mathbb{R}^2$. We associate the discrete function $U(i,n)$ with a continuous function $u_\Delta(x,t)$ that is dependent on the grid spacings Δx and Δt. The functions are related by requiring equality on the grid points, $u_\Delta(i\Delta x, n\Delta t) = U(i,n)$. At the grid points the function u_Δ is the solution of a two parameter family of discrete GMEs. The continuum limit is obtained when the separation between grid points, Δx and Δt, goes to zero, that is,

$$\lim_{\Delta x\to 0,\Delta t\to 0} u_\Delta(x,t) = u(x,t). \tag{45}$$

In order for this limit to exist we take a diffusion limit, which requires the ratio of Δx^2 and Δt to remain constant [50]. We also define a continuous version of the annihilation probability, $a_\Delta(x,t)$, where $a_\Delta(i\Delta x, n\Delta t) = A(i,n)$. The Δ dependence in the continuous function defines $a_\Delta(x,t)$ as the probability of an annihilation event between t and $t+\Delta t$. We can then define an annihilation rate as the limit,

$$a(x,t) = \lim_{\Delta t\to 0,\Delta x\to 0} \frac{a_\Delta(x,t)}{\Delta t}. \tag{46}$$

In a similar manner, we define a continuous creation rate,

$$c(x,t) = \lim_{\Delta t\to 0,\Delta x\to 0} \frac{c_\Delta(x,t)}{\Delta t}, \tag{47}$$

where $c_\Delta(i\Delta x, n\Delta t) = C(i,n)$.

With the above definitions of $u_\Delta, a_\Delta, c_\Delta$ the discrete GME, Eq. (44), then becomes,

$$\begin{aligned} u_\Delta(i\Delta x,n\Delta t) - u_\Delta(i\Delta x,(n-1)\Delta t) = \\ &\frac{r\omega}{2}\Big((1-a_\Delta((i-1)\Delta x,(n-1)\Delta t))u_\Delta((i-1)\Delta x,(n-1)\Delta t) \\ &-2(1-a_\Delta(i\Delta x,(n-1)\Delta t))u_\Delta(i\Delta x,(n-1)\Delta t) \\ &+(1-a_\Delta((i+1)\Delta x,(n-1)\Delta t))u_\Delta((i+1)\Delta x,(n-1)\Delta t)\Big) \\ &-a_\Delta(i\Delta x,(n-1)\Delta t)u_\Delta(i\Delta x,(n-1)\Delta t)+c_\Delta(i\Delta x,n\Delta t). \end{aligned} \tag{48}$$

We now introduce continuous variables x, t at the point $x = i\Delta x, t = n\Delta t$ and expand the continuous functions, $u_\Delta, a_\Delta, c_\Delta$, in Taylor series about x and t, with $a_\Delta(x,t) = o(\Delta t)$ and $c_\Delta(x,t) = o(\Delta t)$, to obtain

$$\begin{aligned} \Delta t\frac{\partial u_\Delta}{\partial t} + o(\Delta t^2) = &\frac{r\omega}{2}\Delta x^2\left(\frac{\partial^2}{\partial x^2}\Big(u_\Delta(x,t)+o(\Delta t)\Big)+o(\Delta x^2)\right) \\ &-a_\Delta(x,t)u_\Delta(x,t)+c_\Delta(x,t). \end{aligned} \tag{49}$$

Finally we divide by Δt and consider a sequence of processes corresponding to the above equation in the limit $\Delta x \to 0$ and $\Delta t \to 0$, such that

$$D = \lim_{\Delta x\to 0,\Delta t\to 0}\frac{r\Delta x^2}{2\Delta t}, \tag{50}$$

exists. Thus we obtain the diffusion limit of the GME arriving at a reaction-diffusion PDE,

$$\frac{\partial u(x,t)}{\partial t} = \omega D\frac{\partial^2 u(x,t)}{\partial x^2} - a(x,t)u(x,t)+c(x,t), \tag{51}$$

where $a(x,t)$ and $c(x,t)$ can be determined from the reaction kinetics for $u(x,t)$ and may depend explicitly on $u(x,t)$. The parameter ω, which is the probability of the particle jumping to a new site on any given time step in the discrete GMEs, can be interpreted as a time scale parameter in the continuum equation.

4.2. Sibuya Waiting Times

When using the Sibuya waiting time pmf a different approach needs to be taken when finding the continuum limit. The sum over the memory kernel is not amenable to direct calculation. However the sum can be written as a discrete convolution, which enables us to exploit properties of transform methods in finding the continuum limit.

The approach from the discrete to the continuum can be carried out in general by considering inverse Laplace transforms with limits to continuous time, and continuous space of star transforms from discrete time, and discrete space. To begin, we consider a general function of discrete space and time $Y(i,n)$ and

define the unilateral star transform with respect to the discrete time variable, n, as

$$\mathcal{Z}_n^* \{Y(i,n)|\, s, \Delta t\} = \sum_{n=0}^{\infty} Y(i,n)\, e^{-n\Delta t s}. \tag{52}$$

We define a bilateral star transform with respect to the discrete space variable, i, as

$$\hat{\mathcal{Z}}_i^* \{Y(i,n)|\, q, \Delta x\} = \sum_{i=-\infty}^{\infty} Y(i,n)\, e^{-i\Delta x q}. \tag{53}$$

These transforms are related to the unilateral $\mathcal{Z}$-transform with $z = e^{\Delta t s}$ and the bilateral $\mathcal{Z}$-transform with $z = e^{\Delta x q}$. Similar to the Markovian case, we consider a sequence of continuous functions, y_Δ, such that $y_\Delta(i\Delta x, n\Delta t) = Y(i,n)$. In this manner we associate an interval Δt between the time steps n and $n+1$ and an interval Δx between the space grid points i and $i+1$. The functions $y_\Delta(x,t)$ will be different for different interval sizes and the subscript Δ denotes this functional dependence. The continuum limit, $\Delta x \to 0, \Delta t \to 0$, can then be obtained from the inverse unilateral Laplace transform with limits to continuous time and the inverse bilateral Laplace transform with limits to continuous space of the unilateral star transform from discrete time and the bilateral star transform from discrete space. Explicitly, we have

$$y(x,t) = \lim_{\Delta x \to 0, \Delta t \to 0} \Delta t \Delta x \hat{\mathcal{L}}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \hat{\mathcal{Z}}_i^* \left\{ \mathcal{Z}_n^* \{Y(i,n)|\, s, \Delta t\} \,|\, q, \Delta x \right\} |\, t \right\} |\, x \right\}, \tag{54}$$

where $\mathcal{L}_s^{-1}\{F(s)|t\}$ denotes the inverse unilateral Laplace transform to continuous time t, and $\hat{\mathcal{L}}_q^{-1}\{G(q)|x\}$ denotes the inverse bilateral Laplace transform to continuous space x. To see the result in Eq. (54) we note that

$$\begin{aligned}
&\lim_{\Delta x \to 0, \Delta t \to 0} \Delta t \Delta x \hat{\mathcal{L}}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \hat{\mathcal{Z}}_i^* \left\{ \mathcal{Z}_n^* \{Y(i,n)|, s, \Delta t\} \,|\, q, \Delta x \right\} |\, t \right\} |\, x \right\} \\
&= \lim_{\Delta x \to 0, \Delta t \to 0} \Delta t \Delta x \hat{\mathcal{L}}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \sum_{i=-\infty}^{\infty} \sum_{n=0}^{\infty} y_\Delta(i\Delta x, n\Delta t)\, e^{-sn\Delta t} e^{-qi\Delta x}\, ds\, dq \,\middle|\, t \right\} \,\middle|\, x \right\}, \\
&= \lim_{\Delta x \to 0, \Delta t \to 0} \sum_{i=-\infty}^{\infty} \sum_{n=0}^{\infty} y_\Delta(i\Delta x, n\Delta t)\, \delta(t - n\Delta t)\delta(x - i\Delta x)\Delta t \Delta x, \\
&= \int_{-\infty}^{\infty} \int_{0}^{\infty} y(x', t')\, \delta(t - t')\delta(x - x')\, dt'\, dx' \\
&= y(x,t),
\end{aligned}$$

provided that $t > 0$. The continuum limit of the discrete generalized master equations with a Sibuya waiting time distribution can be found by first taking the unlilateral star transform with respect to the discrete time variable and the bilateral star transform with respect to the discrete space variable on each side of the GME, Eq. (33). The exponential functions arising in the star transforms

are expanded in Taylor series (see Appendix A) and then we take the inverse unilateral Laplace transform to continuous time, and the inverse bilateral Laplace transform to continuous space. The limit $\Delta x \to 0, \Delta t \to 0$, is then evaluated with the requirement that

$$D_\alpha = \lim_{\Delta x \to 0, \Delta t \to 0} \frac{r \Delta x^2}{2 \Delta t^\alpha} \tag{55}$$

exists.

The analysis, which is shown in Appendix A, results in the continuum diffusion limit of the discrete generalized master equation,

$$\frac{\partial u(x,t)}{\partial t} = D_\alpha \frac{\partial^2}{\partial x^2} \left[\theta(x,t,0)\, {}_0\mathcal{D}_t^{1-\alpha} \left(\frac{u(x,t)}{\theta(x,t,0)} \right) \right] - a(x,t) u(x,t) + c(x,t)\,. \tag{56}$$

This recovers the fractional reaction-diffusion equation derived from the diffusion limit of continuous time random walks in [7] where ${}_0\mathcal{D}_t^{1-\alpha}$ is the Riemann-Liouville fractional derivative, formally equivalent to the Grünwald-Letnikov fractional derivative in this setting. We note that Eq. (56) is potentially a non-linear equation, as the annihilation and creation rates, $a(x,t)$ and $c(x,t)$ respectively, are defined by the reaction kinetics, which may be dependent on the concentration $u(x,t)$.

5. Numerical Implementation

In this section we present a simplified method of matching parameters and implementing the explicit numerical scheme to solve the reaction-subdiffusion equation, Eq. (56). The standard reaction-diffusion equation can be recovered with $\alpha = 1$. First we set the step size Δt by inverting the relation for the diffusion coefficient given by

$$D_\alpha = \frac{r \Delta x^2}{2 \Delta t^\alpha}, \tag{57}$$

and treat Δx and r as free parameters, thus defining

$$\Delta t = \left(\frac{r \Delta x^2}{2 D_\alpha} \right)^{\frac{1}{\alpha}}. \tag{58}$$

We note that r may be a useful parameter for decoupling Δx, Δt and D_α. In the case of multiple species where each species has a different diffusion coefficient the lattice for each of the species needs to be the same. This can only be achieved by letting r be different for each species. If we have two species, A and B, with diffusion coefficients $D_{\alpha a} > D_{\alpha b}$, then we need to set,

$$r_b = \frac{r_a D_{\alpha b}}{D_{\alpha a}}. \tag{59}$$

This is done to ensure that $0 \leq r_b \leq 1$, given $0 \leq r_a \leq 1$. This choice will then give the same Δt, for a given Δx, for each species.

In modelling a physical system the annihilation and creation rates are prescribed by the reaction kinetics.

In a stochastic reaction-diffusion system the annihilation and creation processes may be modelled by inhomogeneous Poisson processes. In general, for an inhomogeneous Poisson process with $N(t)$ events up to time t, and rate function $\lambda(x,t)$, the expected number of events in the time interval $((n-1)\Delta t, n\Delta t)$ is given by

$$\mathbb{E}\left[N(n\Delta t) - N((n-1)\Delta t)\right] = \int_{(n-1)\Delta t}^{n\Delta t} \lambda(x,t')\,dt'. \tag{60}$$

For the same process, the probability that there is no event in the time interval $((n-1)\Delta t, n\Delta t)$ is given by

$$\mathbb{P}\left[N(n\Delta t) - N((n-1)\Delta t) = 0\right] = \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} \lambda(x,t')\,dt'\right). \tag{61}$$

If we assume that the annihilation process is modelled by an inhomogeneous Poisson process with rate parameter $a(x,t)$, then the probability of an annihilation event between $(n-1)\Delta t$ and $n\Delta t$ is one minus the probability that there is no annihilation event in this time. Thus

$$A(i,n-1) = 1 - \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} a(i\Delta x,t')\,\mathrm{d}t'\right). \tag{62}$$

The survival probability function for no annihilation event between time $m\Delta t$ and $n\Delta t$ is given by

$$\Theta(i,n,m) = \exp\left(-\int_{m\Delta t}^{n\Delta t} a(i\Delta x,t')\,\mathrm{d}t'\right). \tag{63}$$

If the creation process is independent of the annihilation process and may also be modelled as an inhomogeneous Poisson process with rate $c(x,t)$ then the expected number of particles created between $(n-1)\Delta t$ and $n\Delta t$ is given by

$$C(i,n) = \int_{(n-1)\Delta t}^{n\Delta t} c(i\Delta x,t')\,\mathrm{d}t'. \tag{64}$$

If the creation process is dependent on an annihilation process, such as in the case of multiple interacting chemical species, then a different approach may be used to find the expected number of particles created in the time step. The dependence of the processes may mean that a flux balance argument can be used to model the creation events. Considering a reaction such that the decay of a particle of species A, becomes a particle of species B. Then the number of particles of species B that are created would simply be the number of particles of species A lost. If we model the loss of species A by a Poisson process, i.e.

with $A(i,n)$ given by Eq. (62), then the expected number of species B particles created would be given by,

$$C_b(i,n) = \left(1 - \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} a_a(i\Delta x, t')\,\mathrm{d}t'\right)\right) u_a(i\Delta x, n\Delta t) \tag{65}$$

where the subscripts a and b denote species A and B respectively. Whilst the dependent and independent expected number of particles created in a time step look very different, they share the same limiting behaviour as $\Delta t \to 0$. Both the cases of dependent and independent creation processes are dealt with in the examples in Section 7.

In reaction dynamics obtained from the law of mass action the reaction terms are multinomials with positive coefficients identifying creation terms $c(x,t)$ and negative coefficients identifying annihilation terms $a(x,t)u(x,t)$. In general a numerical quadrature rule may be needed to evaluate the integrals in Eqs. (62), (63), (64), and (65). Taking the independent creation process, the explicit finite difference scheme for Eq. (56) can be written as,

$$\begin{aligned} U(i,n) = & \\ & \sum_{m=0}^{n-1} \left(\binom{1-\alpha}{n-m}(-1)^{n-m} - \delta_{0,n-m} + \delta_{1,n-m} \right) \left(\frac{r}{2} \exp\left(-\int_{m\Delta t}^{n\Delta t} a((i-1)\Delta x, t')\,\mathrm{d}t' \right) U(i-1,m) \right. \\ & \left. + \frac{r}{2} \exp\left(-\int_{m\Delta t}^{n\Delta t} a((i+1)\Delta x, t')\,\mathrm{d}t' \right) U(i+1,m) - r \exp\left(-\int_{m\Delta t}^{n\Delta t} a(i\Delta x, t')\,\mathrm{d}t' \right) U(i,m) \right) \\ & + \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} a(i\Delta x, t')\,\mathrm{d}t' \right) U(i,n-1) + \int_{(n-1)\Delta t}^{n\Delta t} c(i\Delta x, t')\,\mathrm{d}t', \end{aligned} \tag{66}$$

where Δt is given by Eq. (58).

5.1. Boundary Conditions

On the domain, $x \in [l_1, l_2]$, where $l_1 = L_1\Delta x$, and $l_2 = L_2\Delta x$ with $L_1, L_2 \in \mathbb{Z}$, boundary conditions can be set in the following manner:
Dirichlet: For

$$u(l_1,t) = b_1(t) \quad \text{and} \quad u(l_2,t) = b_2(t), \tag{67}$$

set

$$U(L_1,n) = b_1(n\Delta t) \quad \text{and} \quad U(L_2,n) = b_2(n\Delta t). \tag{68}$$

Zero-Flux: The conditions for a zero flux boundary can be found by integrating Eq. (56) over its domain. This gives,

$$\frac{\partial}{\partial t}\left[\int_{l_1}^{l_2} u(x,t)dx\right] = D_\alpha \frac{\partial}{\partial x}\left[\theta(x,t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{u(x,t)}{\theta(x,t,0)}\right)\right]\Bigg|_{x=l_1}^{x=l_2} + \int_{l_1}^{l_2} c(x,t) - a(x,t)u(x,t)dx. \tag{69}$$

Thus the zero flux boundary conditions are given by

$$D_\alpha \frac{\partial}{\partial x}\left[\theta(x,t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{u(x,t)}{\theta(x,t,0)}\right)\right]\Bigg|_{x=l_1}^{x=l_2} = 0. \tag{70}$$

These conditions is guaranteed to hold if we take

$$\left.\frac{\partial u(x,t)}{\partial x}\right|_{x=l_1} = \left.\frac{\partial u(x,t)}{\partial x}\right|_{x=l_2} = \left.\frac{\partial \theta(x,t,0)}{\partial x}\right|_{x=l_1} = \left.\frac{\partial \theta(x,t,0)}{\partial x}\right|_{x=l_2} = 0. \tag{71}$$

For the numerical scheme these boundary conditions are implemented by setting ghost points for all n as follows,

$$U(L_1-1,n) = U(L_1,n) \quad \text{and} \quad U(L_2+1,n) = U(L_2,n). \tag{72}$$

This is equivalent to redirecting outgoing flux that is destined to jump out of the domain back in to those end-points.

Alternatively the domain, $x \in [l_1, l_2]$, can be discretised such that, $l_1 = (L_1 - \frac{1}{2})\Delta x$, and $l_2 = (L_2 + \frac{1}{2})\Delta x$ with $L_1, L_2 \in \mathbb{Z}$. This results in the discrete points each being at the centre of an interval of width Δx. The Dirichlet and zero flux boundary conditions are implemented in the same manner as before.

5.2. Initial Conditions

For the initial condition

$$u(x,0) = u_0(x), \tag{73}$$

which we assume to be bounded, we simply sample $u_0(x)$ via

$$U(i,0) = u_0(i\Delta x). \tag{74}$$

However we may also treat unbounded initial conditions, provided that the integral of the initial condition over the domain is bounded. For example, if the initial condition is a Dirac delta function,

$$u(x,0) = \delta(x - x_0), \tag{75}$$

we take

$$U(i,0) = \frac{\delta_{i,i_0}}{\Delta x} \tag{76}$$

where δ_{i,i_0} is a Kronecker delta, $i_0 = \frac{x_0}{\Delta x}$. The justification for Eq. (76) follows from the identification

$$\begin{aligned}
\int_{l_1}^{l_2} u(x,0)\,dx &= \lim_{\Delta x\to 0,\Delta t\to 0} \int_{L_1\Delta x}^{L_2\Delta x} u_\Delta(x,0)\,dx \\
&= \lim_{\Delta x\to 0,\Delta t\to 0} \sum_{i=L_1}^{L_2} u_\Delta(i\Delta x,0)\Delta x \\
&= \lim_{\Delta x\to 0,\Delta t\to 0} \sum_{i=L_1}^{L_2} U(i,0)\Delta x.
\end{aligned}$$

with the left hand side and right hand side both equating to one.

6. Stability Analysis

For the numerical method to be stable we require the distance between the solution and its approximation from the numerical scheme to be bounded for all n, i.e.

$$\sum_i |U(i,n) - u(i\Delta x, n\Delta t)| \leq M \tag{77}$$

where $M \in \mathbb{R}^+$. To show this bound exists it is sufficient to show that both the solution is bound, and the approximation is bound, i.e.

$$\sum_i |U(i,n)| \leq M_1, \tag{78}$$

$$\sum_i |u(i\Delta x, n\Delta t)| \leq M_2, \tag{79}$$

with $M_1, M_2 \in \mathbb{R}^+$. If $u(x,t)$ is non-negative, and Riemann integrable then the condition in Eq. (79) is satisfied if,

$$\int_{l_1}^{l_2} u(x, n\Delta t)\mathrm{d}x \leq M_3, \tag{80}$$

with $M_3 \in \mathbb{R}^+$. The temporal evolution of the left hand side is given by Eq. (69). Taking zero-flux boundary conditions this further simplifies to,

$$\frac{\partial}{\partial t}\left[\int_{l_1}^{l_2} u(x,t)dx\right] = \int_{l_1}^{l_2} c(x,t) - a(x,t)u(x,t)dx. \tag{81}$$

Hence provided that the initial condition is bounded and

$$\int_{l_1}^{l_2} c(x,t) - a(x,t)u(x,t)dx \leq 0, \tag{82}$$

for all t then,

$$\int_{l_1}^{l_2} u(x,t)dx \leq \int_{l_1}^{l_2} u(x,0)dx, \tag{83}$$

and the condition in Eq. (80) will be satisfied. Equation (82) puts a sufficient condition on the reactions in order for the solution of the fractional PDE to remain bounded and simply states that in total at least as many particles are annihilated as created in the domain.

We also need to ensure that the condition in Eq. (78) is met. By construction, as a sum of pmfs in Eq. (27), $U(i,n)$ is non-negative, provided that the stochastic process is well posed. This is guaranteed if r, $A(i,n)$, $\psi(n)$ and $\lambda(i|j)$ are all probabilities, and thus restricted to $[0,1]$, for all i and n, and $C(i,n)$ and $U(i,0)$, are non-negative. This permits us to replace the condition in Eq. (78) with

$$\sum_i U(i,n) \leq M_1. \tag{84}$$

To obtain further conditions for the stability of the numerical scheme, we rearrange the GME, Eq. (28), and sum over i. Again taking zero-flux boundaries this gives,

$$\begin{aligned}\sum_i U(i,n) &= \sum_i U(i,n-1) + \\ &\sum_i \sum_j \left(\lambda(j|i) - \delta_{i,j}\right) \sum_{m=0}^{n} K(n-m)\,\Theta(j,n,m)\,U(j,m) \\ &- \sum_i \left(A(i,n-1)U(i,n-1) + C(i,n)\right) \\ &= \sum_i \left(U(i,n-1) - A(i,n-1)U(i,n-1) + C(i,n)\right). \end{aligned} \tag{85}$$

where we have used the fact that by Eq. (4),

$$\sum_i \left(\lambda(i|j) - \delta_{i,j}\right) = 0. \tag{86}$$

Provided that

$$\sum_i \left(C(i,n) - A(i,n-1)U(i,n-1)\right) \leq 0, \tag{87}$$

then

$$\sum_i U(i,n) \leq \sum_i U(i,n-1) \tag{88}$$

and hence if $\sum_i U(i,0)$ is bounded then the condition in Eq. (78) will be satisfied. Equation (87) is an analogous condition on the reactions to the continuous condition Eq. (82), and they are equivalent in the continuum limit.

The solution of the numerical scheme is therefore stable, as defined by Eq. (77), when the underlying stochastic process is well posed and Eqs. (82) and (87) hold. It should be emphasised that this stability result is valid for non-linear reactions. The simplicity of the provided stability analysis is due to deriving the numerical scheme from a stochastic process. An alternative derivation of the stability of the numerical scheme, in the absence of reactions, via a von Neumann type analysis is provided in Appendix B.

7. Numerical Examples

7.1. Example 1: Non-linear morphogen death rates on semi-infinite domain

In [51], the authors considered subdiffusion with self enhanced degradation as a model for morphogen concentrations in developmental biology. The fractional reaction subdiffusion equation in this case is

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left[D_\alpha e^{-\int_0^t ku(x,s)ds}\,{}_0\mathcal{D}_t^{1-\alpha}\left[e^{\int_0^t ku(x,s)ds}u(x,t)\right]\right] - ku(x,t)^2, \tag{89}$$

on the semi-infinite domain $x \in [0, \infty)$. The total mass is conserved over the domain by injecting a flux, which is equal to the integral of the reaction terms, at the origin. This corresponds to the boundary condition

$$D_\alpha \frac{\partial}{\partial x}\left[e^{-\int_0^t ku(x,s)ds}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{\int_0^t ku(x,s)ds}u(x,t)\right)\right]\Bigg|_{x=0} = \int_0^\infty ku(x,t)^2 dx. \tag{90}$$

7.1.1. Stationary Distribution

The stationary distribution is equivalent to the stationary distribution derived in [52]. In the long time limit we can replace the Riemann-Lioville fractional derivatives with Weyl fractional derivatives [46]. To find the stationary distributions, $u_{st}(x)$ we use the asymptotic relation

$$e^{-ku_{st}(x)t}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{ku_{st}(x)t}\right) \sim (ku_{st}(x))^{1-\alpha}. \tag{91}$$

Thus $u_{st}(x)$ satisfies the ordinary differential equation

$$D_\alpha k^{1-\alpha}\frac{d^2}{dx^2}\left(u_{st}(x)^{2-\alpha}\right) - ku_{st}(x)^2 = 0 \tag{92}$$

with boundary condition

$$D_\alpha k^{1-\alpha}\frac{d}{dx}\left(u_{st}(x)^{2-\alpha}\right)\Big|_0 = \int_0^\infty ku_{st}(x)dx. \tag{93}$$

The solution is given by [52, 51]

$$u_{st}(x) = u_{st}(0)\left(1+\frac{x}{\mu}\right)^{-\frac{2}{\alpha}} \tag{94}$$

where

$$u_{st}(0) = \left(\frac{g}{\sqrt{D_\alpha k^{2-\alpha}}}\sqrt{\frac{4-\alpha}{4-2\alpha}}\right)^{\frac{2}{4-\alpha}}, \tag{95}$$

$$g = \int_0^\infty ku_{st}(x)^2 dx, \tag{96}$$

and

$$\mu = \frac{4-2\alpha}{\alpha} g\left(\frac{4-\alpha}{4-2\alpha}\right)^{\frac{2-\alpha}{4-\alpha}}\sqrt{\frac{D_\alpha}{k^\alpha}}. \tag{97}$$

7.1.2. Numerical Solution

The numerical scheme for this problem is found by equating the process parameters in the fractional PDE, Eq.(89), with the discrete process parameters in the GME, Eq. (32), with the Sibuya waiting time kernel. The numerical scheme requires four parameters, Δx, Δt, r, and α, as well as two functions, $A(i,n)$, and $C(i,n)$. Comparing Eq. (89) with the general form given in Eq. (56) we see that we have a continuous annihilation process with a rate of $a(x,t) = ku(x,t)$, and no creation process, i.e. $c(x,t) = 0$. As there are no particles created in each time step we set $C(i,n) = 0$. Using Eq. (62), we set

$$\begin{aligned} A(i,n-1) &= 1 - \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} ku(i\Delta x, t')dt'\right) \\ &\approx 1 - \exp\left(-ku(i\Delta x,(n-1)\Delta t)\Delta t\right) \\ &= 1 - \exp\left(-kU(i,n-1)\Delta t\right). \end{aligned} \tag{98}$$

Here we have used a simple one point approximation for the integral, and the relation between the continuous and discrete solutions on the lattice points. We obtain $\Theta(i,n,m)$ from $A(i,n)$ through Eq. (6). The anomalous exponent in the fractional PDE, α, is equivalent to the fractional exponent parameter in the Sibuya memory kernel. The choice of the parameters Δx, Δt, and r, is dependent on the diffusion coefficient D_α and the fractional exponent from the fractional PDE. Treating Δx and r as free parameters we can set Δt using Eq. (58),

$$\Delta t = \left(\frac{r\Delta x^2}{2D_\alpha}\right)^{\frac{1}{\alpha}}. \tag{99}$$

Note that r is a probability and hence $0 \leq r \leq 1$ and, for a given Δx, the maximum Δt corresponds to $r = 1$.

The fractional PDE is defined over a semi-inifite domain, $x \in [0,\infty)$. This is approximated by taking an absorbing boundary a long distance from the origin, i.e. $u(l,t) = 0$, with $l \gg 0$. In the numerical scheme, we take $l = L\Delta x$ and this boundary condition corresponds to $U(L,n) = 0$. The conservation of mass boundary condition at the origin, Eq. (90), is implemented through a flux of particles inserted at the origin, equal to particles lost from the annihilation process and the flux at the $x = l$ boundary.

Substituting these functions and parameters in to the GME Eq. (32), we obtain

$$\begin{aligned} U(i,n) - U(i,n-1) \;=\; & \\ & \sum_{m=0}^{n-1} K(n-m)\frac{r}{2}\Bigg[\exp\left(-\sum_{p=m}^{n-1}\Delta t\, kU(i-1,p)\right)U(i-1,m) \\ & - 2\exp\left(-\sum_{p=m}^{n-1}\Delta t\, kU(i,p)\right)U(i,m) + \exp\left(-\sum_{p=m}^{n-1}\Delta t\, kU(i+1,p)\right)U(i+1,m)\Bigg] \\ & - \left[1-\exp(-\Delta t\, kU(i,n-1))\right]U(i,n-1), \end{aligned} \tag{100}$$

for $0 < i < L$, where $K(n-m)$ is the Sibuya kernel from Eq. (40). The boundary points are given by,

$$\begin{aligned} U(0,n) - U(0,n-1) = &\sum_{i=0}^{L} \left[1 - \exp(-k\Delta t\, U(i,n-1))\right] U(i,n-1) \\ &+ \sum_{m=0}^{n-1} K(n-m)\frac{r}{2}\Bigg[\exp\left(-\sum_{p=m}^{n-1} \Delta t\, kU(L-1,p)\right) U(L-1,m) \\ &- \exp\left(-\sum_{p=m}^{n-1} \Delta t\, kU(0,p)\right) U(0,m)\Bigg] \end{aligned} \tag{101}$$

and

$$U(L,n) = 0. \tag{102}$$

The discrete solution is related to the continuous solution at the lattice points, hence the numerical solution will be given using the relation,

$$u(i\Delta x, n\Delta t) = U(i,n). \tag{103}$$

To obtain a solution we take $k = 10$, $r = 1$, $D_\alpha = 1$, and $\alpha = 0.9$. We also choose an initial condition with $g = 1$ in Eq. (96), and start near the asymptotic steady state given by Eq.(94),

$$U(i,0) = u_{st}(i\Delta x). \tag{104}$$

As the steady state result is valid in the limit $l \to \infty$, we examine the convergence of the numerical method to this solution as we increase the length of the domain. We also examine a range of different Δx to demonstrate convergence to the steady state.

The numerical solutions were run to $t = 2$. At this time the numerical solution was found to have converged in the sense that

$$\sum_{i=0}^{L} (U(i,n) - U(i,n-1))^2 \Delta x \leq 10^{-3} ||U - u_{st}||_2 \tag{105}$$

where

$$||U - u_{st}||_2 = \sum_{i=0}^{L} (U(i,n) - u_{st}(i\Delta x))^2 \Delta x. \tag{106}$$

Figure 1 shows the analytic solution and the convergence of the numerical solutions. The method is shown to converge with decreasing Δx and increasing domain size $l = L\Delta x$.

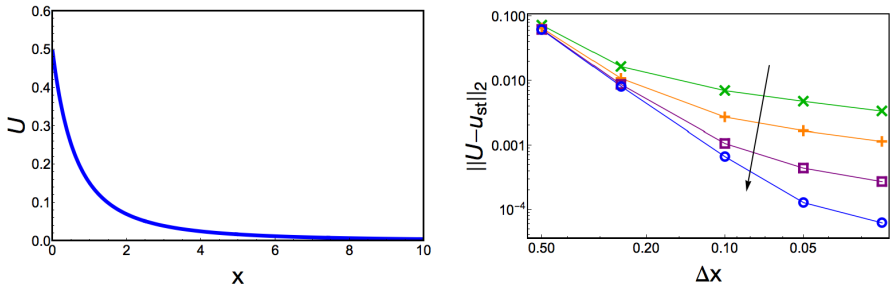

Figure 1: Left: Analytic steady state solution for example 1 at $t = 2$. Right: Convergence between the DTRW solution and the analytic steady state at $t = 2$ as a function of Δx for $l = 5$ (cross), $l = 10$ (plus), $l = 20$ (square) and $l = 50$ (circle).

7.2. Example 2: Multi-species chemical reaction model

In the second example, we consider a simple two-species chemical reaction-subdiffusion model with a simple transition from species A to species B and vice-versa with a constant rate k,

$$A \overset{k}{\rightleftharpoons} B\,.$$

We denote the population densities in time and space of A and B by u_a and u_b respectively. As a set of fractional partial differential equations, the model can then be expressed as [4],

$$\begin{aligned}\frac{\partial u_a(x,t)}{\partial t} &= D_\alpha \frac{\partial^2}{\partial x^2}\left[e^{-kt}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{kt}u_a(x,t)\right)\right] - ku_a(x,t) + ku_b(x,t)\\ \frac{\partial u_b(x,t)}{\partial t} &= D_\alpha \frac{\partial^2}{\partial x^2}\left[e^{-kt}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{kt}u_b(x,t)\right)\right] + ku_a(x,t) - ku_b(x,t)\,.\end{aligned} \tag{107}$$

We consider the case of zero flux boundaries located at $x = -l$, and $x = l$. This gives the conditions,

$$\begin{aligned}D_\alpha \frac{\partial}{\partial x}\left[e^{-kt}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{kt}u_a(x,t)\right)\right]\Big|_{x=-l} &= 0,\\ D_\alpha \frac{\partial}{\partial x}\left[e^{-kt}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{kt}u_a(x,t)\right)\right]\Big|_{x=l} &= 0,\end{aligned} \tag{108}$$

with equivalent conditions on $u_b(x,t)$. These conditions will be satisfied if,

$$\begin{aligned}\frac{\partial u_a(x,t)}{\partial x}\Big|_{x=-l} &= 0,\\ \frac{\partial u_a(x,t)}{\partial x}\Big|_{x=l} &= 0,\end{aligned} \tag{109}$$

and again equivalent conditions for $u_b(x,t)$. To facilitate a simple analytic solution we take the initial condition to be a Dirac delta function located at the origin for species A and zero every where for species B, i.e.

$$\begin{aligned} u_a(x,0) &= \delta(0-x) \\ u_b(x,0) &= 0 \end{aligned} \tag{110}$$

7.2.1. Analytic Solution

By summing both equations in Eq. (107) and substituting $u_z(x,t) = e^{kt}(u_a(x,t)+u_b(x,t))$, we obtain the equation,

$$\frac{\partial u_z(x,t)}{\partial t} = D_\alpha \, {}_0\mathcal{D}_t^{1-\alpha}\left[\frac{\partial^2 u_z(x,t)}{\partial x^2}\right] + k u_z(x,t). \tag{111}$$

This equation is of the same form as the fractional cable equation [53], where it was solved for the case $k < 0$. The boundary conditions are then,

$$\begin{aligned} \left.\frac{\partial u_z(x,t)}{\partial x}\right|_{x=-l} &= 0, \\ \left.\frac{\partial u_z(x,t)}{\partial x}\right|_{x=l} &= 0, \end{aligned} \tag{112}$$

and the initial condition is,

$$u_z(x,0) = \delta(0-x). \tag{113}$$

This equation can then be solved analytically via the method of images yielding

$$\begin{aligned} u_z(x,t) = \frac{1}{\sqrt{4\pi D_\alpha t^\alpha}} \sum_{j=0}^{\infty} \frac{(kt)^j}{j!} \sum_{n=-\infty}^{\infty} \Bigg(& H_{1,2}^{2,0}\left[\frac{(x+4nl)^2}{4D_\alpha t^\alpha}\middle| \begin{matrix}(1-\frac{\alpha}{2}+j,\alpha)\\(0,1)\ (\frac{1}{2}+j,1)\end{matrix}\right] \\ & + H_{1,2}^{2,0}\left[\frac{(2l-x+4nl)^2}{4D_\alpha t^\alpha}\middle| \begin{matrix}(1-\frac{\alpha}{2}+j,\alpha)\\(0,1)\ (\frac{1}{2}+j,1)\end{matrix}\right]\Bigg), \end{aligned} \tag{114}$$

where H are Fox H functions [54]. Alternatively the solution can be found by separation of variables [53] giving,

$$u_z(x,t) = \frac{\exp(kt)}{2L} + \sum_{m=1}^{\infty} \frac{1}{L}\cos\left(\frac{m\pi x}{L}\right) \sum_{j=0}^{\infty} \frac{(kt)^j}{j!} E_{\alpha,1+(1-\alpha)j}^{(j)}\left(-\frac{m^2\pi^2 D_\alpha t^\alpha}{L^2}\right), \tag{115}$$

where $E_{\alpha,\beta}^{(m)}(z)$ is the m^{th} derivative of a Mittag-Leffler function.

7.2.2. Numerical Solution

To construct the numerical solution to the set of fractional PDEs, Eq (107), we must parameterise an equivalent set of GMEs. The coupled GMEs will be of the same form as Eq. (32), using a Sibuya memory kernel and with the additional complication of a dependence in the annihilation and creation processes. The numerical scheme will require the identification of five parameters, Δx, Δt, r_a, r_b, and α, as well as four functions $A_a(i,n)$, $A_b(i,n)$, $C_a(i,n)$, and $C_b(i,n)$.

Similar to the first example we compare the fractional PDEs with the general form presented in Eq. (56). From this we see that that the continuous annihilation precess for both species A and B has a constant rate, i.e., $a_a(x,t) = a_b(x,t) = k$. The creation process arises out of a flux balance with the annihilation process, i.e. $c_a(x,t) = ku_b(x,t)$, and $c_b(x,t) = ku_a(x,t)$. The diffusion coefficients for species A and B are both equal to D_α.

The discrete annihilation probabilities are found from Eq. (62),

$$\begin{aligned} A_a(i,n-1) = A_b(i,n-1) &= 1 - \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} k dt'\right) \\ &= 1 - \exp\left(-k\Delta t\right). \end{aligned} \tag{116}$$

Again note that setting $A(i,n)$ also sets $\Theta(i,n,m)$ through Eq. (6). As we have a dependent creation process we will use the expected number of created particles of the form of Eq. (65), this will give,

$$\begin{aligned} C_a(i,n) &= \left(1 - \exp\left(-\int_{(n-1)\Delta t}^{n\Delta t} k dt'\right)\right) u_b(i\Delta x, n\Delta t) \\ &= \left(1 - \exp\left(-k\Delta t\right)\right)\right) U_b(i,n), \end{aligned} \tag{117}$$

where the correspondence between the discrete and continuous solutions has been used. Similarly we take,

$$C_b(i,n) = \left(1 - \exp\left(-k\Delta t\right)\right)\right) U_a(i,n) \tag{118}$$

The fractional exponent used in the Sibuya memory kernel must match the fractional exponent in Eq. (107). The choice of the parameters Δx, Δt, r_a, and r_b, is dependent on the diffusion coefficients, D_α, and the fractional exponent, α, of the fractional PDEs. As the diffusion coefficients of the two species are equal then the two r parameters must also be equal, i.e. $r_a = r_b = r$. Treating Δx and r as free parameters Δt will be given by Eq. (58).

The continuous boundary conditions are taken to be zero flux at $x = -l$ and $x = l$. We let $l = L\Delta x$, and define the discrete boundary conditions are found by creating ghost points at $-L-1$ and $L+1$ according to Eq. (72).

Putting these parameters and functions into the GMEs based on Eq.(32)

yields the numerical scheme,

$$
\begin{aligned}
&U_a(i,n) - U_a(i,n-1) \;= \\
&\sum_{m=0}^{n-1} K(n-m)\exp\left(-k\Delta t(n-m)\right)\frac{r}{2}\big(U_a(i-1,m) - 2U_a(i,m) + U_a(i+1,m)\big) \\
&- \left[1-\exp(-k\Delta t)\right]U_a(i,n-1) + \left[1-\exp(-k\Delta t)\right]U_b(i,n-1),
\end{aligned}
\tag{119}
$$

for $-L < i < L$, where the $K(n)$ is the Sibuya memory kernel given by Eq. (40). The boundary points evolve according to

$$
\begin{aligned}
&U_a(-L,n) - U_a(-L,n-1) \;= \\
&\sum_{m=0}^{n-1} K(n-m)\exp\left(-k\Delta t(n-m)\right)\frac{r}{2}\big(U_a(-L,m) + U_a(-L+1,m)\big) \\
&- \left[1-\exp(-k\Delta t)\right]U_a(-L,n-1) + \left[1-\exp(-k\Delta t)\right]U_b(-L,n-1),
\end{aligned}
\tag{120}
$$

and

$$
\begin{aligned}
&U_a(L,n) - U_a(L,n-1) \;= \\
&\sum_{m=0}^{n-1} K(n-m)\exp\left(-k\Delta t(n-m)\right)\frac{r}{2}\big(U_a(L-1,m) - U_a(i,m)\big) \\
&- \left[1-\exp(-k\Delta t)\right]U_a(L,n-1) + \left[1-\exp(-k\Delta t)\right]U_b(L,n-1).
\end{aligned}
\tag{121}
$$

Equivalent equations are also found for U_b.

As the continuum equations initial conditions involve a Dirac delta function we use Eq. (76) to obtain discrete initial conditions,

$$
\begin{aligned}
U_a(i,0) &= \frac{\delta_{i,0}}{\Delta x}, \\
U_b(i,0) &= 0.
\end{aligned}
\tag{122}
$$

The numerical solution is obtained by noting the correspondence between the discrete and continuous solutions, i.e.

$$
\begin{aligned}
u_a(i\Delta x, n\Delta t) &= U_a(i,n) \\
u_b(i\Delta x, n\Delta t) &= U_b(i,n)
\end{aligned}
\tag{123}
$$

To obtain a numerical solution we have taken $\alpha = 0.5$, $D_\alpha = 1$ and $k = 1$, with a spatial domain of $[-1,1]$. The solution was run up to time $t = 0.1$. A range of values for Δx were considered. Two separate discretisations of the domain were considered to examine the effect of the boundary points on the numerical solution. In the first the domain was discretised so that the discrete points aligned with the boundary points, i.e. $l = L\Delta x$. The second discretisation placed each point in the centre of an interval of width Δx, i.e. $l = (L + \frac{1}{2})\Delta x$.

For comparison with the analytical solution we consider the sum of the two species solutions, $U_Z(i,n) = (U_a(i,n) + U_b(i,n))\exp(kn\Delta t)$. This is compared with the solution obtained from Eq. (114) in Fig. 2 for the aligned boundary grid, and in Fig. 3 for the centred grid. We define the norm of the difference $\|U_Z - u_z\|_2$ in a similar fashion to Eq. (106). In each case the numerical solution converges to the analytical solution. For the case of the aligned boundary the numerical solution converges with order Δx^2, and for the case of the centred grid the convergence is of the order Δx^4. This suggests, for zero-flux boundary conditions, the centred grid discretisation of the domain is preferable to the aligned grid discretisation.

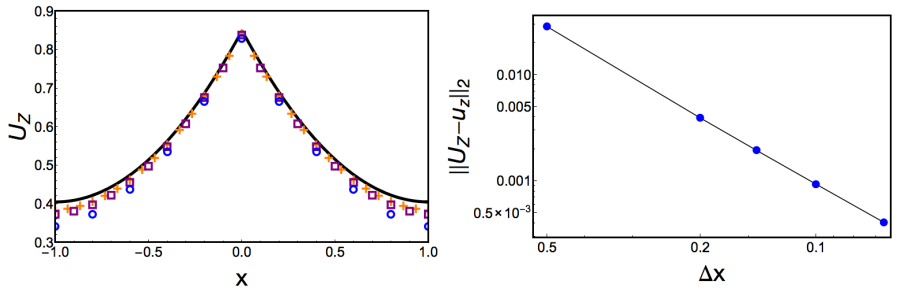

Figure 2: Solution of example 2 using aligned boundary grid discretisation. (Left): The solid line denotes the analytical solution $u_z(x,t)$, at $t = 0.1$. The points show the numerical solution, $U_Z(x,t)$, at $t = 0.1$ with $\Delta x = \frac{1}{5}$ (Blue Circle), $\Delta x = \frac{1}{10}$ (Purple Square), and $\Delta x = \frac{1}{15}$ (Orange Cross). (Right): Convergence of the numerical solution, $U_Z(x,t)$, to the analytic solution $u_z(x,t)$. For each Δx the solution is compared at the time $t = \lfloor \frac{0.1}{\Delta t} \rfloor \Delta t$.

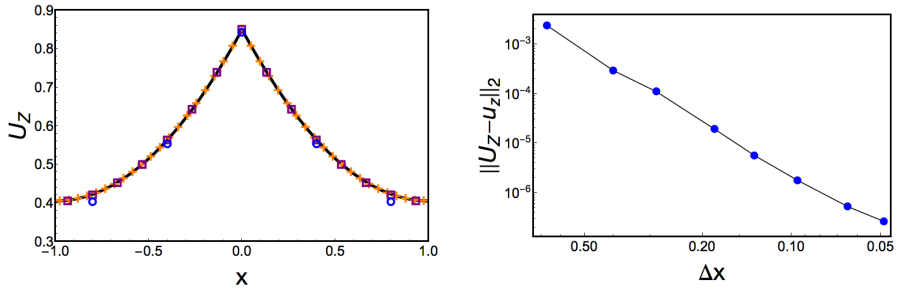

Figure 3: Solution of example 2 using centred grid discretisation. (Left): The solid line denotes the analytical solution $u_z(x,t)$ at $t = 0.1$. The points show the numerical solution, $U_Z(x,t)$, with $\Delta x = \frac{2}{5}$ (Blue Circle), $\Delta x = \frac{2}{15}$ (Purple Square), and $\Delta x = \frac{2}{41}$ (Orange Cross). Each numerical solution is evaluated at $t = \lfloor \frac{0.1}{\Delta t} \rfloor \Delta t$. (Right): Convergence of the numerical solution, $U_Z(x,t)$, to the analytic solution $u_z(x,t)$. For each Δx the solution is compared at the time $t = \lfloor \frac{0.1}{\Delta t} \rfloor \Delta t$.

8. Summary

Numerous numerical schemes have been proposed for solving nonlinear reaction diffusion processes. The simplest scheme to implement is an explicit finite difference scheme in which the time and space derivatives are replaced by local difference operators. However such schemes are known to be numerically unstable for general parameters and a formal stability analysis is required to investigate this. Here we have presented a new approach to obtaining numerical schemes for reaction diffusion equations and fractional reaction subdiffusion equations. The numerical schemes are implemented as explicit finite difference schemes but they are guaranteed to be stable, in the sense that the difference between the numerical solution and the exact solution remains bounded for all time, by construction, provided the stochastic process is well posed. The construction involves the derivation of discrete time master equations for a stochastic process with the consistency that the discrete time master equations converge to the reaction diffusion equation of interest in the continuum space and time limit. The utility of this construction as the basis of a stable numerical scheme is perhaps unsurprising. Reaction diffusion equations, including fractional reaction subdiffusion equations, are themselves formally derived from a continuous time stochastic process [7]. In implementing the numerical scheme, further information on the stochastic process, such as symmetries in the reaction kinetics, can be incorporated in a natural way. More generally it may be possible to formulate discrete time stochastic processes that converge to partial differential equations, and fractional partial differential equations, even in cases where the partial differential equations have not previously been obtained from a continuous time stochastic process. This opens up the possibility of new classes of explicit finite difference schemes that are inherently stable.

Appendix A

In this appendix we evaluate the continuum limit of the discrete generalized master equations, Eq. (33), based on transform methods with

$$y(x,t) = \lim_{\Delta x \to 0, \Delta t \to 0} \Delta t \Delta x \hat{\mathcal{L}}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \hat{\mathcal{Z}}_i^* \left\{ \mathcal{Z}_n^* \left\{ Y(i,n) | \, s, \Delta t \right\} | \, q, \Delta x \right\} | \, t \right\} | \, x \right\}, \tag{124}$$

where

$$\mathcal{Z}_n^* \left\{ Y(i,n) | \, s, \Delta t \right\} = \sum_{n=0}^{\infty} Y(i,n) \, e^{-n \Delta t s}, \tag{125}$$

is the unilateral star transform with respect to n,

$$\hat{\mathcal{Z}}_i^* \left\{ Y(i,n) | \, q, \Delta x \right\} = \sum_{i=-\infty}^{\infty} Y(i,n) \, e^{-i \Delta x q}, \tag{126}$$

is the bilateral star transform with respect to i, $\mathcal{L}_s^{-1} \left\{ F(s) | t \right\}$ is the inverse unilateral Laplace transform to continuous time and $\hat{\mathcal{L}}_q^{-1} \left\{ G(q) | x \right\}$ is the inverse bilateral Laplace transform to continuous space.

In taking the continuum limit we make use of a product rule

$$\begin{aligned}
&\lim_{\Delta x\to 0,\Delta t\to 0}\Delta t\Delta x\hat{\mathcal{L}}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{Y_1(i,n)Y_2(i,n)|\,s,\Delta t\right\}|\,q,\Delta x\right\}|\,t\right\}|\,x\right\}\\
&=\lim_{\Delta x\to 0,\Delta t\to 0}\Delta t\Delta x\hat{\mathcal{L}}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\sum_{i=-\infty}^{\infty}\sum_{n=0}^{\infty}y_{1,\Delta}(i\Delta x,n\Delta t)y_{2,\Delta}(i\Delta x,n\Delta t)e^{-n\Delta ts}e^{-i\Delta xq}|\,t\right\}|\,x\right\}\\
&=\lim_{\Delta x\to 0,\Delta t\to 0}\sum_{i=-\infty}^{\infty}\sum_{n=0}^{\infty}y_{1,\Delta}(i\Delta x,n\Delta t)y_{2,\Delta}(i\Delta x,n\Delta t)\delta(t-n\Delta t)\delta(x-i\Delta x)\Delta t\Delta x\\
&=y_1(x,t)y_2(x,t),\\
&=\left(\lim_{\Delta x\to 0,\Delta t\to 0}\sum_{n=0}^{\infty}y_{1,\Delta}(i\Delta x,n\Delta t)\delta(t-n\Delta t)\Delta t\right)\\
&\quad\times\left(\lim_{\Delta x\to 0,\Delta t\to 0}\sum_{n=0}^{\infty}y_{2,\Delta}(i\Delta x,n\Delta t)\delta(t-n\Delta t)\Delta t\right).
\end{aligned}\tag{127}$$

which is valid for $t>0$ and provided that both limits exist. We also make use of the shift properties

$$\mathcal{Z}_n^*\left\{Y(i,n-k)|\,s,\Delta t\right\} = e^{-k\Delta ts}\mathcal{Z}_n^*\left\{Y(i,n)|\,s,\Delta t\right\},\tag{128}$$

$$\hat{\mathcal{Z}}_i^*\left\{Y(i-k,n)|\,q,\Delta x\right\} = e^{-k\Delta xq}\hat{\mathcal{Z}}_i^*\left\{Y(i,n)|\,q,\Delta x\right\},\tag{129}$$

and, for notational convenience, we write

$$\hat{Y}_\Delta(s,q)=\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{Y(i,n)|\,s,\Delta t\right\}|\,q,\Delta x\right\}.\tag{130}$$

We now take the unilateral star transform with respect to the discrete time variable and the bilateral star transform with respect to the discrete space variable on each side of the GME, Eq. (33), to obtain

$$\hat{U}_\Delta(s,q)-e^{-\Delta ts}\hat{U}_\Delta(s,q)=\frac{r}{2}(e^{\Delta xq}+e^{-\Delta xq}-2)\hat{X}_\Delta(s,q)-e^{-\Delta ts}\hat{B}_\Delta(s,q)+\hat{C}_\Delta(s,q),\tag{131}$$

where

$$\hat{X}_\Delta(s,q)=\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{\Theta(i,n,0)\sum_{m=0}^{n}K(n-m)\frac{U(i,m)}{\Theta(i,m,0)}|\,s,\Delta t\right\}|\,q,\Delta x\right\},\tag{132}$$

and

$$\hat{B}_\Delta(s,q)=\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{A(i,n)U(i,n)|\,s,\Delta t\right\}|\,q,\Delta x\right\}.\tag{133}$$

We can expand the exponential functions in Eq. (131) to write

$$\begin{aligned}
\Delta ts\hat{U}_\Delta(s,q)-\frac{\Delta t^2s^2}{2}\hat{U}_\Delta(s,q)+O(\Delta t^3) &= \frac{r}{2}\Delta x^2q^2\hat{X}_\Delta(s,q)-\hat{B}_\Delta(s,q)\\
&+\Delta ts\hat{B}_\Delta(s,q)+\frac{\Delta t^2s^2}{2}\hat{B}_\Delta(s,q)+\hat{C}_\Delta(s,q)+O(\Delta x^4)+O(\Delta t^3).
\end{aligned}\tag{134}$$

We take the inverse unilateral Laplace transform with respect to s, with limits to continuous time, and we take the inverse bilateral Laplace transform with respect to q, with limits to continuous space. This yields

$$\begin{aligned}
&\Delta t \frac{\partial}{\partial t}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{U}_\Delta(s,q)|t\right\}|x\right\} - \frac{\Delta t^2}{2}\frac{\partial^2}{\partial t^2}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{U}_\Delta(s,q)|t\right\}|x\right\} \\
&= \frac{r}{2}\Delta x^2 \frac{\partial^2}{\partial x^2}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{X}_\Delta(s,q)|t\right\}|x\right\} - \mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{B}_\Delta(s,q)|t\right\}|x\right\} \\
&+ \Delta t \frac{\partial}{\partial t}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{B}_\Delta(s,q)|t\right\}|x\right\} - \frac{\Delta t^2}{2}\frac{\partial^2}{\partial t^2}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{B}_\Delta(s,q)|t\right\}|x\right\} \\
&+ \mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{C}_\Delta(s,q)|t\right\}|x\right\} + O(\Delta x^4) + O(\Delta t^3).
\end{aligned} \tag{135}$$

To take the continuum limit we first multiply by Δx and then take the limit $\Delta x \to 0, \Delta t \to 0$, thus arriving at

$$\frac{\partial}{\partial t}u(x,t) = f(x,t) - a(x,t)u(x,t) + c(x,t). \tag{136}$$

In taking the limits leading to Eq. (136) we identified

$$f(x,t) = \lim_{\Delta x\to 0,\Delta t\to 0} \frac{r}{2}\Delta x^3 \frac{\partial^2}{\partial x^2}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{X}_\Delta(s,q)|t\right\}|x\right\} \tag{137}$$

together with the continuous creation rate

$$c(x,t) = \lim_{\Delta x\to 0,\Delta t\to 0} \Delta t\Delta x \mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\frac{\hat{C}_\Delta(s,q)}{\Delta t}|t\right\}\Delta t|x\right\}, \tag{138}$$

and

$$a(x,t)u(x,t) = \lim_{\Delta x\to 0,\Delta t\to 0} \Delta t\Delta x \mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\frac{\hat{B}_\Delta(s,q)}{\Delta t}|t\right\}\Delta t|x\right\}, \tag{139}$$

where $a(x,t)$ is the annihilation rate. The result in Eq. (139) was obtained from the product rule, Eq. (127),together with the identification

$$a(x,t) = \lim_{\Delta x\to 0,\Delta t\to 0} \Delta t\Delta x \mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\frac{\hat{A}_\Delta(s,q)}{\Delta t}|t\right\}\Delta t|x\right\}. \tag{140}$$

It remains to evaluate the limit

$$\begin{aligned}
f(x,t) &= \lim_{\Delta x\to 0,\Delta t\to 0} \frac{r}{2}\Delta x^3 \frac{\partial^2}{\partial x^2}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{X}_\Delta(s,q)|t\right\}|x\right\} \\
&= \frac{\partial^2}{\partial x^2}\lim_{\Delta x\to 0,\Delta t\to 0} \frac{r\Delta x^3}{2}\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{\Theta(i,n,0)Y(i,n)|\, s,\Delta t\right\}|\, q,\Delta x\right\}|t\right\}|x\right\} \\
&= \frac{\partial^2}{\partial x^2}\theta(x,t,0)\lim_{\Delta x\to 0,\Delta t\to 0} \Delta x\Delta t \mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{\frac{r\Delta x^2}{2\Delta t}Y(i,n)|s,\Delta t\right\}|q,\Delta x\right\}|t\right\}|x\right\}.
\end{aligned} \tag{141}$$

In the last step we used the product rule, Eq. (127), with the identification

$$\theta(x,t,0) = \lim_{\Delta x\to 0,\Delta t\to 0} \Delta t\Delta x\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{\Theta}_\Delta(s,q)|t\right\}\Delta t|x\right\}, \tag{142}$$

and

$$Y(i,n) = \sum_{m=0}^{n} K(n-m)\frac{U(i,m)}{\Theta(i,m,0)}. \tag{143}$$

We can evaluate the unilateral star transform using the convolution theorem, thus

$$\mathcal{Z}_n^*\left\{Y(i,n)\right\} = \mathcal{Z}_n^*\left\{K(n)\right\}\mathcal{Z}_n^*\left\{V(i,n)\right\} \tag{144}$$

where

$$V(i,n) = \frac{U(i,n)}{\Theta(i,n,0)}. \tag{145}$$

The unilateral star transform of the Sibuya kernel is obtained by substituting $z = e^{-s\Delta t}$ into Eq. (39). Explicitly,

$$\mathcal{Z}_n^*\{K(n)\} = (1-e^{-s\Delta t})^{1-\alpha} - (1-e^{-s\Delta t}) \sim (s\Delta t)^{1-\alpha} + o(s\Delta t). \tag{146}$$

Substituting the results from Eqs. (144), (146) into Eq. (141) we have

$$f(x,t) = \frac{\partial^2}{\partial x^2}\theta(x,t,0)\lim_{\Delta x\to 0,\Delta t\to 0}\Delta x\Delta t\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\hat{\mathcal{Z}}_i^*\left\{\frac{r\Delta x^2}{2\Delta t^\alpha}s^{1-\alpha}\mathcal{Z}_n^*\left\{V(i,n)|s,\Delta t\right\}|q,\Delta x\right\}|t\right\}|x\right\}. \tag{147}$$

Provided that the limit

$$D_\alpha = \lim_{\Delta x\to 0,\Delta t\to 0}\frac{r\Delta x^2}{2\Delta t^\alpha} \tag{148}$$

exists, we can write this as

$$\begin{aligned}
f(x,t) &= D_\alpha\frac{\partial^2}{\partial x^2}\theta(x,t,0)\lim_{\Delta x\to 0,\Delta t\to 0}\Delta x\Delta t\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{s^{1-\alpha}\hat{\mathcal{Z}}_i^*\left\{\mathcal{Z}_n^*\left\{V(i,n)|s,\Delta t\right\}|q,\Delta x\right\}|t\right\}|x\right\}\\
&= D_\alpha\frac{\partial^2}{\partial x^2}\theta(x,t,0)\lim_{\Delta x\to 0,\Delta t\to 0}\Delta x\Delta t\\
&\quad\times\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{s^{1-\alpha}\sum_{i=-\infty}^{\infty}\sum_{n=0}^{\infty}v_\Delta(i\Delta x,n\Delta t)e^{-n\Delta ts}e^{-i\Delta xq}|t\right\}|x\right\}\\
&= D_\alpha\frac{\partial^2}{\partial x^2}\theta(x,t,0)\lim_{\Delta x\to 0,\Delta t\to 0}\Delta x\Delta t\\
&\quad\times\mathcal{L}_s^{-1}\left\{s^{1-\alpha}\sum_{i=-\infty}^{\infty}\sum_{n=0}^{\infty}v_\Delta(i\Delta x,n\Delta t)e^{-n\Delta ts}\delta(x-i\Delta x)|t\right\}\\
&= D_\alpha\frac{\partial^2}{\partial x^2}\theta(x,t,0)\lim_{\Delta x\to 0,\Delta t\to 0}\Delta x\Delta t\\
&\quad\times\mathcal{L}_s^{-1}\left\{s^{1-\alpha}\mathcal{L}_t\left\{\sum_{i=-\infty}^{\infty}\sum_{n=0}^{\infty}v_\Delta(i\Delta x,n\Delta t)\delta(t-n\Delta t)\delta(x-i\Delta x)|s\right\}|t\right\}.
\end{aligned} \tag{149}$$

In the last line of Eq. (149) we used the notation

$$\mathcal{L}_t \left\{ f(t) | s \right\} \tag{150}$$

to denote a unilateral Laplace transform with respect to time and with Laplace variable s.

This can be simplified further by noting that

$$\mathcal{L}_s^{-1} \left\{ s^{1-\alpha} \mathcal{L}_s \{ y(x,t) | s \} | t \right\} = {}_0\mathcal{D}_t^{1-\alpha} y(x,t) \tag{151}$$

where ${}_0D_t^{1-\alpha}$ denotes the Riemann-Liouville derivative of order $1-\alpha$. Using this result in Eq. (149) we can now write

$$f(x,t) = D_\alpha \frac{\partial^2}{\partial x^2} \theta(x,t,0) \, {}_0\mathcal{D}_t^{1-\alpha} v(x,t) \tag{152}$$

where

$$v(x,t) = \frac{u(x,t)}{\theta(x,t,0)}. \tag{153}$$

Finally we combine the results in Eq. (153) and Eq. (152) with Eq. (136) to obtain the continuum diffusion limit of the discrete generalized master equation,

$$\frac{\partial u(x,t)}{\partial t} = D_\alpha \frac{\partial^2}{\partial x^2} \left[\theta(x,t,0) \, {}_0\mathcal{D}_t^{1-\alpha} \left(\frac{u(x,t)}{\theta(x,t,0)} \right) \right] - a(x,t) u(x,t) + c(x,t) \,. \tag{154}$$

This recovers the fractional reaction-diffusion equation derived from the diffusion limit of continuous time random walks in [47]. We note that this is a potentially non-linear equation as $a(x,t)$ and $c(x,t)$ may be dependent on the concentration $u(x,t)$.

Appendix B: Stability Analysis

In this appendix we show the DTRW to be unconditionally stable in the reaction free case for the anomalous diffusion equation using a von Neumann type stability analysis introduced by Yuste and Acedo in [21]. We show that the stability bound obtained from the Sibuya waiting time pmf is superior to the bounds for the backward Euler formula of order 1 (BDF1), or the Grünwald-Letnikov in the anomalous case, as well as the backward Euler formula of order 2 (BDF2).

We begin by assuming the solution of our GME,

$$U(i,n) - U(i,n-1) = \sum_{m=0}^{n-1} K(n-m) \frac{r}{2} \left(U(i+1,m) - 2U(i,m) + U(i-1,m) \right) \tag{155}$$

is of the form

$$U(i,n) = \sigma_q(n) e^{Iiq\Delta x}, \tag{156}$$

where $I = \sqrt{-1}$ represents the complex number. This solution represents a single wave number, q, of a Fourier decomposed solution from the separation of variables approach. Substituting this solution form into our GME we obtain

$$\sigma_q(n)e^{Iiq\Delta x} - \sigma_q(n-1)e^{Iiq\Delta x} = \sum_{m=0}^{n-1} K(n-m)\frac{r}{2}\sigma_q(m)e^{Iiq\Delta x}\left(e^{Iq\Delta x} - 2 + e^{-Iq\Delta x}\right), \tag{157}$$

which gives

$$\frac{\sigma_q(n)}{\sigma_q(n-1)} = 1 - 2r\sin^2\left(\frac{q\Delta x}{2}\right)\sum_{m=0}^{n-1} K(n-m)\frac{\sigma_q(m)}{\sigma_q(n-1)}. \tag{158}$$

We now define

$$\rho(n) = \frac{\sigma_q(n)}{\sigma_q(n-1)}, \tag{159}$$

where $\rho(n)$ is an amplification factor which gives

$$\rho(n) = 1 - 2r\sin^2\left(\frac{q\Delta x}{2}\right)\sum_{m=0}^{n-1} K(n-m)\prod_{l=m}^{n-1}\rho(l)^{-1}. \tag{160}$$

If $|\rho(n)| > 1$ for all $n > N$ for some N, then $\rho(n)$ will grow temporally to infinity and the mode q is unstable. We therefore consider the extreme value $\rho = -1$ to establish a bound for stability,

$$r\sin^2\left(\frac{q\Delta x}{2}\right) \leq \frac{1}{\sum_{m=0}^{n-1} K(n-m)(-1)^{m-n+1}}. \tag{161}$$

Noting that

$$\sum_{m=0}^{n-1} K(n-m)(-1)^{m-n+1} = \sum_{m=1}^{n} K(m)(-1)^{-m+1}, \tag{162}$$

allows us to determine the behaviour of this bound as the number of iterations, n, tends to infinity. Using

$$\sum_{m=1}^{\infty} K(m)(-1)^{-m+1} = 2 - 2^{1-\alpha}, \tag{163}$$

we obtain the stability bound on r,

$$r = \frac{2D_\alpha \Delta t^\alpha}{\Delta x^2} \leq \frac{1}{2 - 2^{1-\alpha}}. \tag{164}$$

The derivation of the DTRW numerical scheme interprets r as a probability and hence $r \in [0, 1]$. The above stability bound is greater than or equal to 1 for all values of $\alpha \in [0, 1]$ resulting in an unconditionally stable numerical scheme for the reaction free case. The bounds obtained by Yuste and Acedo [21] for the BDF1 (Grünwald-Letinkov) and BDF2 schemes are $1/2^{2-\alpha}$ and $1/4^{3/2-\alpha}$ respectively. Figure 4 compares this stability bound for $\alpha \in [0, 1]$ for the BDF1, BDF2 and DTRW schemes.

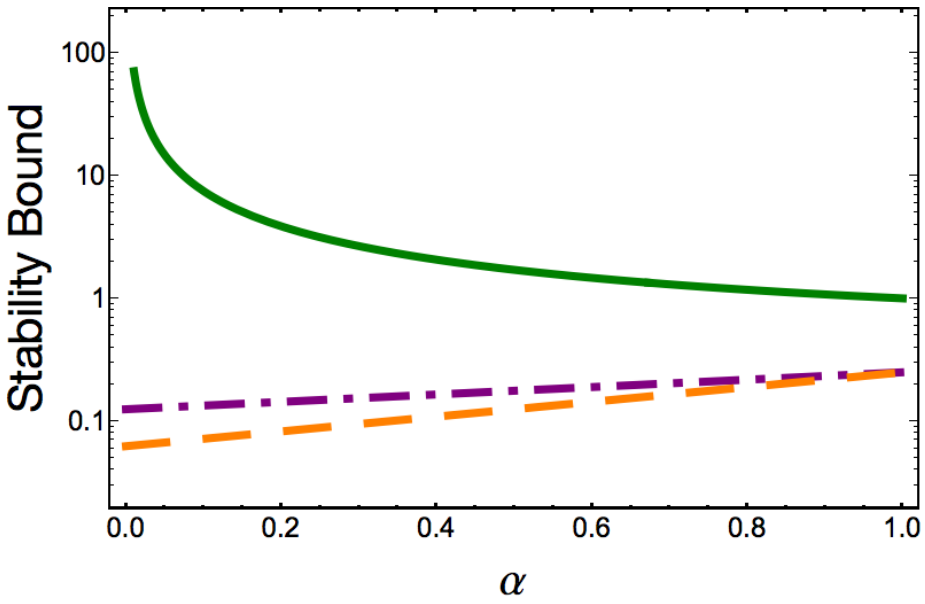

Figure 4: Stability bound on r for BDF1, BDF2 and DTRW over α.

Appendix C: Exact Solution of $\sigma_q(n)$

In this appendix we show that the function $\sigma_q(n)$, used in the stability analysis presented in appendix B, can be found in terms of Fox H functions. To begin we note that Eq. (170) can be rewritten as,

$$\sigma_q(n+1) = \sigma_q(n) - v\sum_{m=0}^{n} K(n-m+1)\sigma_q(m), \tag{165}$$

where

$$v = 2r\sin^2\left(\frac{q\Delta x}{2}\right). \tag{166}$$

Taking the $\mathcal{Z}$-transform gives

$$z\Sigma_q(z) - z\sigma_q(0) = \Sigma_q(z) - v(z\mathcal{K}(z) - zK(0))\Sigma(z) \tag{167}$$

where $\Sigma_q(z)$ and $\mathcal{K}(z)$ are the $\mathcal{Z}$-transforms of $\sigma_q(n)$ and $K(n)$ respectively. Solving for $\Sigma_q(z)$ and noting that $K(0) = 0$ we find,

$$\Sigma_q(z) = \frac{z\sigma_q(0)}{z - a + vz\mathcal{K}(z)}. \tag{168}$$

Now if the memory kernel is the Sibuya memory kernel we have,

$$\mathcal{K}(z) = (1-z^{-1})^{1-\alpha} - (1-z^{-1}), \tag{169}$$

which gives

$$\begin{aligned}\Sigma_q(z) &= \frac{z\sigma_q(0)}{z-1+vz((1-z^{-1})^{1-\alpha}-1(1-z^{-1}))} \\ &= \frac{z\sigma_q(0)}{z(1-z^{-1})-vz(1-z^{-1})+vz(1-z^{-1})^{1-\alpha}} \\ &= \frac{z\sigma_q(0)}{(1-z^{-1})(1-v)+v(1-z^{-1})^{1-\alpha}}\end{aligned} \tag{170}$$

If $0 \leq v < 1/2$ we can expand and find,

$$\begin{aligned}\Sigma_q(z) &= \frac{z\sigma_q(0)}{(1-z^{-1})(1-v)(1+\frac{v}{1-v}(1-z^{-1})^{-\alpha})} \\ &= \frac{z\sigma_q(0)}{(1-z^{-1})(1-v)}\sum_{j=0}^{\infty}\left(-\frac{v}{1-v}(1-z^{-1})^{-\alpha}\right) \\ &= \frac{z\sigma_q(0)}{(1-v)}\sum_{j=0}^{\infty}\left(-\frac{v}{1-v}\right)^j(1-z^{-1})^{-j\alpha-1}\end{aligned} \tag{171}$$

Inverting the $\mathcal{Z}$-transform then gives,

$$\sigma_q(n) = \frac{\sigma_q(0)}{(1-v)}\sum_{j=0}^{\infty}\left(-\frac{v}{1-v}\right)^j\binom{-j\alpha-1}{n}(-1)^n. \tag{172}$$

Note that,

$$\begin{aligned}\binom{-j\alpha-1}{n} &= \frac{\Gamma(-j\alpha)}{n!\Gamma(-j\alpha-n)} \\ &= \frac{(-1)^n}{n!}\frac{\Gamma(j\alpha+n+1)}{\Gamma(j\alpha+1)}\end{aligned} \tag{173}$$

so Eq. (172) can be written,

$$\sigma_q(n) = \frac{\sigma_q(0)}{(1-v)}\sum_{j=0}^{\infty}\left(-\frac{v}{1-v}\right)^j\frac{\Gamma(j\alpha+n+1)}{n!\Gamma(j\alpha+1)}. \tag{174}$$

Which may be expressed in terms of a Fox H function,

$$\sigma_q(n) = \frac{\sigma_q(0)}{(1-v)}H^{1,2}_{2,2}\left[\frac{v}{1-v}\middle|\begin{matrix}(0,1) & (-n,\alpha)\\ (0,1) & (0,\alpha)\end{matrix}\right] \tag{175}$$

Alternatively, expanding Eq. (170) in the case when $v \geq \frac{1}{2}$ we find,

$$\begin{aligned}\Sigma_q(z) &= \frac{z\sigma_q(0)}{v(1-z^{-1})(1+\frac{1-v}{v}(1-z^{-1})^{-\alpha})} \\ &= \frac{z\sigma_q(0)}{v(1-z^{-1})}\sum_{j=0}^{\infty}\left(-\frac{1-v}{v}(1-z^{-1})^{-\alpha}\right) \\ &= \frac{z\sigma_q(0)}{v}\sum_{j=0}^{\infty}\left(-\frac{1-v}{v}\right)^j(1-z^{-1})^{j\alpha+\alpha-1}\end{aligned} \tag{176}$$

Inverting the $\mathcal{Z}$-transform then gives,

$$\sigma_q(n) = \frac{\sigma_q(0)}{v}\sum_{j=0}^{\infty}\left(-\frac{1-v}{v}\right)^j\binom{j\alpha+\alpha-1}{n}(-1)^n. \tag{177}$$

Noting that,

$$\binom{-j\alpha-1}{n} = \frac{\Gamma(j\alpha+\alpha)}{n!\Gamma(j\alpha+\alpha-n)}, \tag{178}$$

this may be rewritten as,

$$\sigma_q(n) = \frac{(-1)^n\sigma_q(0)}{v}\sum_{j=0}^{\infty}\left(-\frac{1-v}{v}\right)^j\frac{\Gamma(j\alpha+\alpha)}{n!\Gamma(j\alpha+\alpha-n)}. \tag{179}$$

Which may be expressed in terms of a Fox H function,

$$\sigma_q(n) = \frac{(-1)^n\sigma_q(0)}{n!v}H^{1,2}_{2,2}\left[\frac{1-v}{v}\middle|\begin{matrix}(0,1) & (1-\alpha,\alpha)\\ (0,1) & (1-\alpha+n,\alpha)\end{matrix}\right]. \tag{180}$$

The expressions in terms of Fox functions may not be valid for all values of v. In both cases the absolute value of the argument needs to be less than $\alpha^{-2\alpha}$.

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