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Extrapolation techniques for first order hyperbolic partial differential equations.

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0. Abstract

A uniform grid of step size h is superimposed on the space variable x in the first order hyperbolic partial differential equation $\partial u/\partial t + a\,\partial u/\partial x = 0$ $(a > 0,\ x > 0,\ t > 0)$. The space derivative is approximated by its backward difference and central difference replacements and the resulting linear systems of first order ordinary differential equations are solved employing Padé approximants to the exponential function.

A number of difference schemes for solving the hyperbolic equation are thus developed and each is extrapolated to give higher order accuracy.

The schemes, and their extrapolated forms, are applied to two problems, one of which has a discontinuity in the solution across a characteristic.

1. The extrapolations

Given the firs t order hyperbolic partial differential equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \; ; \; a>0,\ x>0,\ t>0 \qquad (0)$$

with initial conditions u(x,0) = g(x) and boundary conditions u(0,t)= v(t), replacing the space derivative with the backward difference formula

$$\frac{\partial u}{\partial x} = \{u(x,t) - u(x-h,t)\}/h + 0(h)$$

leads to the system of first order ordinary differential equations

$$\frac{dU}{dt} = -\, aA\underline{U} + a\underline{v}_t \qquad (1)$$

where $\underline{U}(t) = [U_1(t),U_2(t),\ldots,U_N(t)]^T$, T denoting transpose, is the vector of computed solutions of (1) at time $t>0$ at N points whose x — coordinates are $x_i = ih$ ($i = 1,2,..,N$). Clearly that part of the x - axis for which the solution is sought is divided into N equal parts of width h . In equation (1) A is a square matrix of order N given by

$$hA = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ -1 & 1 & 0 & & \vdots \\ 0 & -1 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix}$$

and $\underline{v}_t$ is a vector with N components given by

$$h\underline{v}_t = [v_t,0,0,\ldots,0]^T$$

where v_t is the numerical (frozen) value of the boundary condition at time $t= n\ell$ ($n=0,1,\ldots$) and ℓ is a constant time step.

The solution of (1) is

$$\underline{U}(t) = A^{-1}\underline{v}_t + \exp(-atA)\{\underline{g} - A^{-1}\underline{v}_t\} \; , \qquad (2)$$

where $\underline{g}$ is the vector of initial values, and it is easy to show that $\underline{U}(t)$ satisfies

$$(3) \qquad \underline{U}(t+\ell) = A^{-1}\underline{v}_t + \exp(-a\ell A)\{\underline{U}(t) - A^{-1}\underline{v}_t\}\,.$$

Using the (0,1) Padé approximant to the exponential matrix function in (3) leads to

$$(4) \qquad \underline{U}(t+\ell) = A^{-1}\underline{v}_t + (I-a\ell A)\,\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^2).\,.$$

where I is the identity matrix of order N . Applying equation (4) to the point $(mh,n\ell)$ in the (x,t) plane, and using U_m^n to denote the computed value of $u(mh,n\ell)$, gives the three point explicit scheme

$$(5) \qquad U_m^{n+1} = (1-ap)U_m^n + apU_{m-1}^n$$

where $p=\ell/h$. This scheme appears in Mitchell[1;p.161] and is known to be first order accurate in time and to be stable for $0 \le ap \le 1$.

The scheme may be extrapolated to give second order accuracy as follows:

Writing (4) over a double interval 2ℓ gives

$$(6) \qquad \underline{U}^{(1)}(t+2\ell) = A^{-1}\underline{v}_t + (I - 2a\ell A)\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^2)$$

and writing (4) over two single time intervals gives

$$(7) \qquad \underline{U}^{(2)}(t+2\ell) = A^{-1}\underline{v}_t + (I - a\ell A)(I - a\ell A)\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^2)$$

Expanding the matrix products in (7) and comparing (6) and (7) with the Maclaurin expansion of the matrix exponential term in (3) written over a double time step, that is

$$(8) \qquad \underline{U}^{(m)}(t+2\ell) = A^{-1}v_t + \{I - 2a\ell A + 2a^2\ell^2A^2 - \frac{4}{3}a^3\ell^3A^3$$

$$+\frac{2}{3}a^4\ell^4A^4 - \frac{4}{15}a^5\ell^5A^5 + \ldots\}\{\underline{U}(t) - A^{-1}\underline{v}_t\}\,,$$

it is seen that, Whilst $\underline{U}^{(1)}$ and $U^{(2)}$ are each only first order accurate, the extrapolated solution $U^{(E)}$ defined by

$$(9) \qquad \underline{U}^{(E)} = 2\underline{U}^{(2)} - \underline{U}^{(1)} + O(\ell^3)$$

is seen to be second order accurate when compared with $\underline{U}^{(M)}(t+2\ell)$.

Using the (1,0) Padè approximant to the exponential matrix function in (3) gives

(10) $$\underline{U}(t+\ell) = A^{-1}v_t + (I+a\ell A)^{-1}\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^2)$$

Writing (10) in implicit form and replacing $\underline{v}_t$ with the N-component vector $\underline{v}_{t+\ell} = [v_{t+\ell}, 0,\ldots,0]^T$, where $\underline{v}_{t+\ell}$ is the numerical value of the boundary condition at time $t+\ell$, gives

(11) $$(I+a\ell A)\underline{U}(t+\ell) - a\ell\underline{v}_{t+\ell} + \underline{U}(t)$$

Applying (11) to the point $(mh,n\ell)$ gives the three point, implicit scheme

(12) $$(1+ap)\, U_m^{n+1} - apU_{m-1}^{n+1} = U_m^n$$

(see Mitchell [1;p.165]) which is also first order accurate.

The scheme is unconditionally stable and because of the form of the initial and boundary conditions may be used explicitly in the first quadrant of the (x,t) plane.

The scheme can be extrapolated to give second order accuracy: equations (6) and (7) become

(13) $$\underline{U}^{(1)}(t+2\ell) = A^{-1}\underline{v}_t + (I+2a\ell A)^{-1}\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^2)$$

and

(14) $$\underline{U}^{(1)}(t+2\ell) = A^{-1}\underline{v}_t + (I+a\ell A)^{-1}(I+a\ell A)^{-1}\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^2)$$

and it may be shown that the extrapolated solution $\underline{U}^{(E)}$ defined by (9) is second order accurate.

Using the (1,1) Padè approximant to the exponential matrix function in (3) gives

(15) $$\underline{U}(t+\ell) = A^{-1}\underline{v}_t + (I+\frac{1}{2}a\ell A)^{-1}(I-\frac{1}{2}a\ell A)\text{-}1\{\underline{U}(t) - A^{-1}v_t\} + O(\ell^3)$$

Written implicity, this leads to

(16) $$(I+\frac{1}{2}a\ell A)\underline{U}(t+\ell) - \frac{1}{2}a\ell A\underline{v}_{t+\ell} = (I-\frac{1}{2}a\ell A)\underline{U}(t) + \frac{1}{2}a\ell\underline{v}_t \quad ,$$

which, when applied to the mesh point $(mh,n\ell)$, gives the four point implicit scheme

(17) $$(1+\frac{1}{2}ap)U_m^{n+1} - \frac{1}{2}apU_{m-1}^{n+1} = (1-\frac{1}{2}ap)U_m^n + \frac{1}{2}apU_{m-1}^n .$$

A stability analysis shows that this new scheme is unconditionally stable. It, also, may be used explicitly in the first quadrant because of the form of the initial conditions and boundary conditions

Extrapolation of the scheme to give two more powers of accuracy may be achieved by writing

(18) $$\underline{U}^{(1)}(t+2\ell) = A^{-1}v_t + (I + a\ell A)^{-1}(I - a\ell A)\{\underline{U}(t) - A^{-1}v_t\} + O(\ell^3)$$

and

(19) $$U^{(2)}(t+2\ell) = A^{-1}v_t + (I+\frac{1}{2}a\ell A)^{-1}(I-\frac{1}{2}a\ell A)(I+\frac{1}{2}a\ell A)^{-1}(I-\frac{1}{2}a\ell A).$$
$$\{\underline{U}(t) - A^{-1}\underline{v}_t\} + O(\ell^3)$$

and defining

(20) $$\underline{U}(E) = \frac{4}{3}\underline{U}(2) - \frac{1}{3}\underline{U}(1) + O(\ell 5) .$$

which is seen to be fourth order accurate when compared with $\underline{U}^{(M)}$

Suppose now that instead of using the backward difference replacement of the space derivative, the central difference replacement

$$\frac{\partial u}{\partial x} = \{u(x+h, t) - u(x-h, t)\}/2h + O(h^2)$$

is used. Equation (1) is then replaced by the system

(21) $$\frac{d\underline{U}}{dt} = -\frac{1}{2}aB\underline{U} + \frac{1}{2}a\underline{w}_t$$

where B is the matrix given by

$$hB = \begin{bmatrix} 0 & 1 & 0 & \cdots & & & 0 \\ -1 & 0 & 1 & & & & \cdot \\ 0 & -1 & 0 & 1 & & & \cdot \\ \cdot & & \ddots & \ddots & \ddots & & \cdot \\ \cdot & & & \ddots & \ddots & \ddots & \cdot \\ \cdot & & & & -1 & 0 & 1 \\ 0 & \cdots & & & 0 & -1 & 0 \end{bmatrix}$$

and $\underline{w}_t = \frac{1}{h}[v_t, 0, \ldots. 0, -U_{N+1}^n]^T$ is an N-component vector whose first element is the numerical (frozen) value of the boundary condition at time $t = n\ell$ (n=0,1,...) and whose last element is minus the value of the solution at the point $((N+1)h,t)$. This means that knowledge of the solution is required on some "boundary" beyond that part of the x-axis under consideration. A brief account of how to deal with this difficulty is given by Mitchell [1;pp.167-1681, together with further references therein.

The solution of (21) is

(22) $$\underline{U}(t) = B^{-1}\underline{w}_t + \exp(-\frac{1}{2}atB)\{\underline{g} - B^{-1}\underline{w}_t\}$$

which satisfies the relation

(23) $$\underline{U}(t+\ell)=B^{-1}\underline{w}_t+\exp(-\frac{1}{2}a\ell B)\{\underline{U}(t)-B^{-1}\underline{W}_t\},$$

and replacing the exponential matrix function with its (0,1) Pade approximant gives

(24) $$\underline{U}(t+\ell)=B^{-1}\underline{w}_t+(I-\frac{1}{2}a\ell B)\{\underline{U}(t)-B^{-1}\underline{wt}\}+O(\ell^2).$$

Applying (24) to the point $(mh,n\ell)$ gives the scheme

(25) $$U_m^{n+1} = U_m^n - \frac{1}{2}ap(U_{m+1}^n - U_{m-1}^n).$$

A stability analysis shows that scheme (25) is unconditionally unstable and would not be used.

Using the (1,0) Fade approximant to the exponential matrix function in (23) gives

(26) $$\underline{U}(t+\ell) = B^{-1}\underline{w}_t + (I + \frac{1}{2}a\ell B)^{-1}\{\underline{U}(t) - B^{-1}\underline{w}_t\} + O(\ell^2).$$

Writing (26) in implicit form gives

(27) $$I + \frac{1}{2}a\ell B)\ \underline{U}(t+\ell) - \frac{1}{2}a\ell\underline{w}_{t+\ell} = \underline{U}(t),$$

Where $w_{t+\ell} = \frac{1}{h}[v_{t+\ell},0,.....,0,-U_{N+1}^{n+1}]^T$, and applying (27) to the point $(mh.n\ell)$ gives the new four point, two level, implicit scheme

(28) $$U_m^{n+1} + \frac{1}{2}ap(U_{m+1}^{n+1} - U_{m-1}^{n+1}) = {}_m^n$$

which may be shown to be unconditionally stable.

Considering (26), the scheme may be extrapolated by first writing (26) over a double time step 2ℓ to give

(29) $$\underline{U}^{(1)}(t+2\ell) = B^{-1}\underline{w}_t + (I + a\ell B)^{-1}\{\underline{U}(t) - B^{-1}\underline{w}_t\} + O(\ell^2).$$

and over two single time steps to give

(30) $$\underline{U}^{(2)}(t+2\ell) = B^{-1}\underline{w}_t + (I + \frac{1}{2}a\ell B)^{-1}(I + \frac{1}{2}a\ell B)^{-1}\{\underline{U}(t) - B^{-1}\underline{w}_t\} + O(\ell^2)$$

The Maclaurin expansion $\underline{U}^{(M)}(t+2\ell)$ of the exponential matrix function in (23) written over a double time step is given by

(31) $$\underline{U}^{(M)}(t+2\ell) = B^{-1}w_t + \{I - a\ell B + \frac{1}{2}a^2\ell^2B^2 - \frac{1}{6}a^3\ell^3B^2 - \frac{1}{24}a^4\ell^4B^4 - \frac{1}{120}a^5\ell^5B^5 + \dots\}\{\underline{U}(t) - B^{-1}w_t\}.$$

Expanding the matrix inverses in (29) and (30) and defining $\underline{U}^{(E)}(t+2\ell)$ as in equation (9), that is by

$$\underline{U}^{(E)} = 2\underline{U}^{(2)} - \underline{U}^{(1)} + O(\ell^3)$$

it is clear that the first order scheme given by (26) has been extrapolated to give second order accuracy.

Using the (1, 1) Padé approximant to the exponential matrix function in (23) gives

(32) $$U(t+\ell) = B^{-1}w_t + (I + \frac{1}{4}a\ell B)^{-1}(I - \frac{1}{4}a\ell B)\{\underline{U}(t) - B^{-1}w_t\} + O(\ell^3)$$

which, when written implicitly, gives

(33) $$(I + \frac{1}{4}a\ell B)\underline{U}(t+\ell) - \frac{1}{4}a\ell w_{t+\ell} = (I - \frac{1}{4}a\ell B)\underline{U}(t) + \frac{1}{4}a\ell w_t.$$

Applying (33) to the point $(mh, n\ell)$ gives the Crank-Nicolson type Implicit scheme

$$-\frac{1}{4}apU_{m-1}^{n+1} + U_m^{n+1} + \frac{1}{4}apU_{m+1}^{n+1} = \frac{1}{4}apU_{m-1}^{n} + U_m^{n} - \frac{1}{4}apU_{m+1}^{n}$$

(34)

which is known to be unconditionally stable (Mitchell [1;p.167]) but which also requires knowledge of the solution at the "boundary" $x = (N+1)h$ (Mitchell [1;pp. 167-168]).

To extrapolate the scheme, (32) is written over a double time step 2ℓ and over two single time steps giving, respectively,

(35) $$\underline{U}^{(1)}(t+2\ell) = B^{-1}\underline{w}_t + (I + \frac{1}{2}a\ell B)^{-1}(I - \frac{1}{2}a\ell B)\{\underline{U}(t) - B^{-1}\underline{w}_t\} + O(\ell^3).$$

(36) $$\underline{U}^{(2)}(t+2\ell) = B^{-1}\underline{w}_t + (I + \frac{1}{4}a\ell B)^{-1}(I - \frac{1}{4}a\ell B)(I + \frac{1}{4}a\ell B)^{-1}(I + \frac{1}{4}a\ell B). \{\underline{U}(t) - B^{-1}\underline{w}_t\} + O(\ell^3).$$

The extrapolated solution defined by (20) increases the accuracy to fourth order.

2. Numerical results

To examine the behaviour of the schemes developed and extrapolated in section 1, each was applied to equation (0) with $a = 1$, that is

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial t} = 0; \quad x > 0, \quad t > 0$$

with two different sets of initial conditions and boundary conditions:

Problem 1:

$$u(x,0) = 1 + x,$$
$$u(0,t) = t.$$

The theoretical solution of Problem 1 in the first quadrant of the (x,t) plane was taken to be

$$u(x,t) = 1 + x - t, \quad x \geq t$$
$$u(x,t) = t - x, \quad x < t$$

so that there exists a discontinuity in the solution across the line $t = x$ in the (x, t) plane.

Problem 2:

$$u(x,0) = e^{x},$$
$$u(0,t) - e^{t}.$$

The theoretical solution of Problem 2 in the first quadrant of the (x,t) plane was taken to be

$$u(x, t) = e^{x-t}, \quad x \geq t$$
$$u(x,t) = e^{t-x}, \quad x < t$$

Each problem was run with $h = \ell = 0.1$ and for formulas (28) and (34) the theoretical value of the solution along the line $x = 1.1$ was assumed. For $a = 1$ and $p - 1$ formula (5) reduces to

$$U_m^{n+1} = U_{m-1}^{n};$$

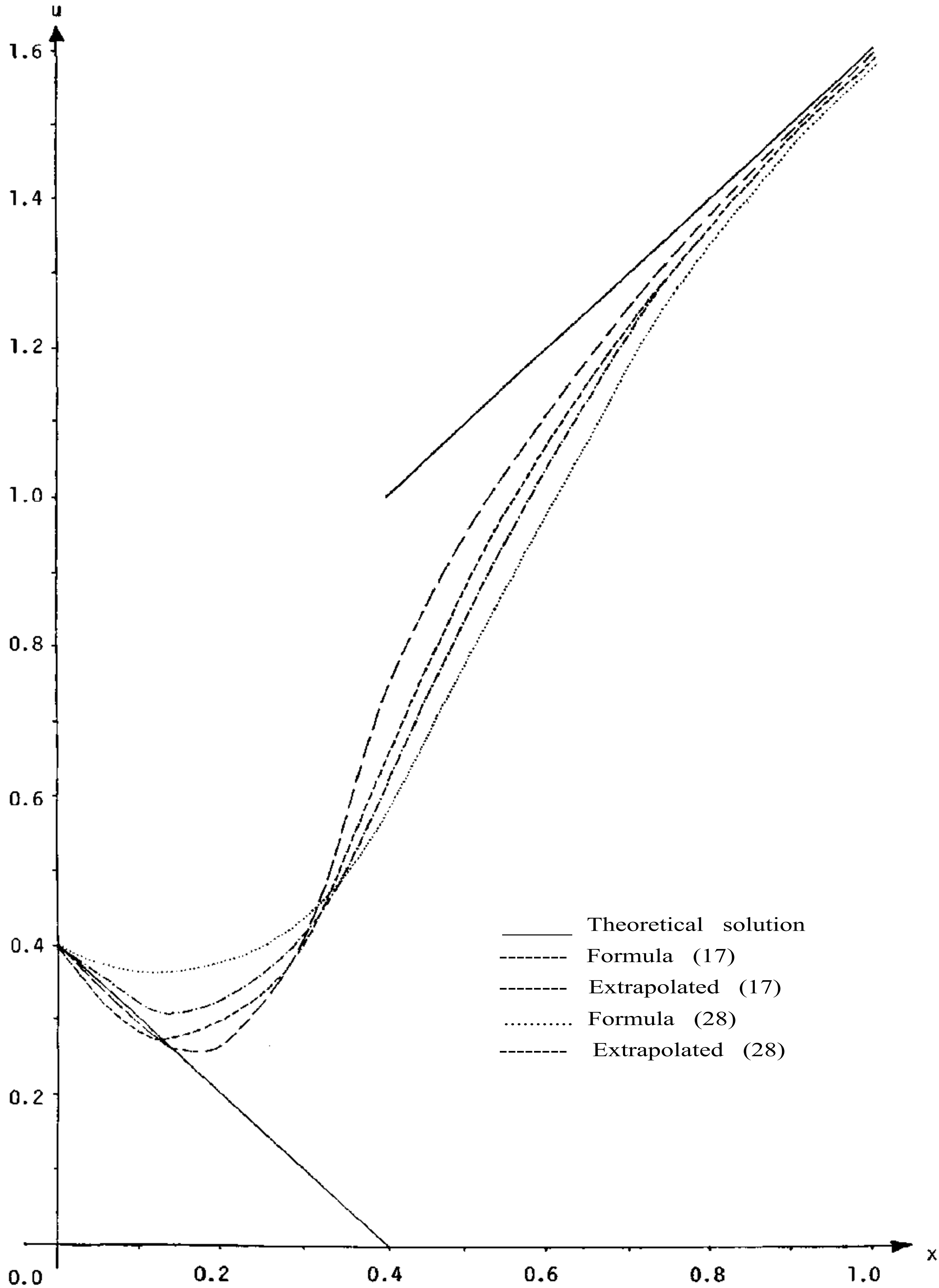
this scheme propagates the initial and boundary conditions along the characteristics and will not be discussed further.

Equations (12) and (34) have been discussed previously in the literature (see, for example, Mitchell [1;pp.165,167]) and the behaviour of schemes (17) and (28), together with their respective extrapolated forms, are depicted in Fig;1 for Problem I and in Fig:2

for Problem 2 for $0 \leq x \leq 1.0$ at time $t=0.4$. The two schemes are seen to behave in much the same manner when applied to both problems and the proximity of each to the theoretical solution is in agreement with the theory of section I.

The error moduli for $t = 0.2(0.2)\,1.0$ at the point $x=0.5$ using all four schemes given by formulas (12), (17),(28),(34), together with the error moduli of their respective extrapolated formulations, are given in Table 1 for Problem 1 and in Table 2 for Problem 2. In the case of Problem 1 it was found that all methods incurred their worst errors at points in the vicinity of the discontinuity of the solution across the line $t = x$; this phenomenon also occurred with Problem 2 which does not have a discontinuity in the solution but does have discontinuities in the first derivatives across this line.

It was generally found that all methods behaved as predicted in section 1. In particular, the novel formula (17) which is of the same order of accuracy as the Crank-Nicolson type method (34), was found to incur smaller errors with increasing time; this formula is also superior in that it is easier to use as it may be applied explicitly, and in that it does not require knowledge of the solution at a point outside the interval of x which is under discussion. For just the same reasons the well known formula (12) must be regarded as superior to formula (28). It is easily seen from the figures and tables that extrapolation of each scheme to improve accuracy is well justified.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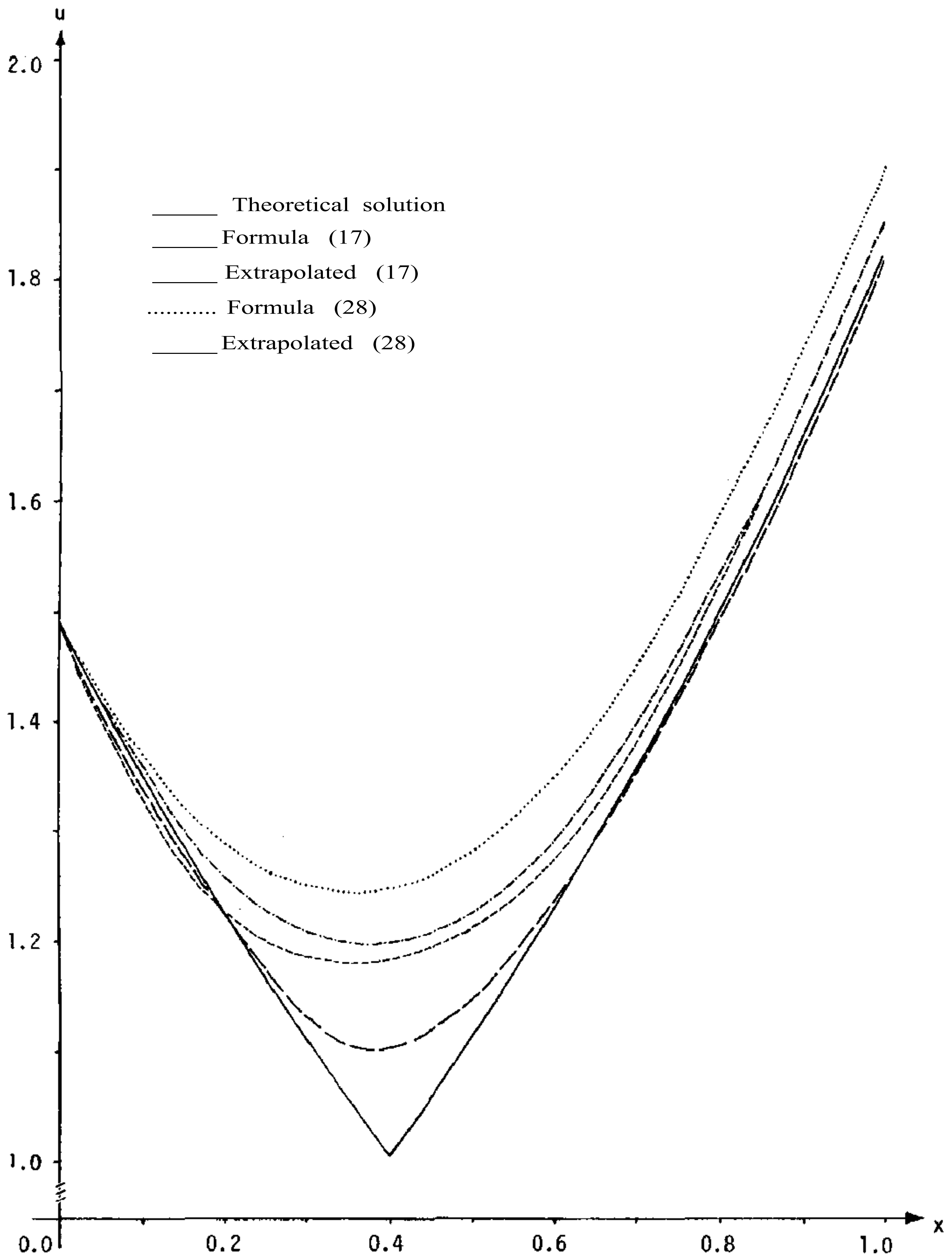
x
Theoretical solution
Formula (17)
Extrapolated (17)
Formula (28)
Extrapolated (28)

Figure 1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x
______ Theoretical solution
______ Formula (17)
______ Extrapolated (17)
.... Formula (28)
______ Extrapolated (28)

Figure 2

Table 1: Error moduli for Problem 1 at x=0.5 for t - 0,2(0.2) 1 .0 using the schemes given by formulas (12),(17),(28),(34) and their extrapolated formulations.

Method	Time				
	0.2	0.4	0.6	0.8	1.0
Formula (12) Extrapolation	8.1 (-2) 2.0(-2)	2.2(-1) 4.0(-2)	5.5(-1) 2.4(-1)	2.7(-l) 1.1(-1)	1.2(-1) 4.0(-2)
Formula (17) Extrapolation	2.0(-2) 2.7(-3)	2.7(-2) 1.2(-2)	2.4(-1) 3.2(-2)	1.2(-I) 1.3(-2)	3.1(-2) 1.1(-2)
Formula (28) Extrapolation	4.8(-2) 6.7(-3)	1.1(-1) 1.7(-2)	2.8(-1) 3.8(-2)	6.7(-l) 1.9(-1)	9.3(-1) 7.6(-2)
Formula (34) Extrapolation	3.3(-3) 1.7(-4)	5.6(-2) 5.3(-3)	2.7(-1) 2.8(-2)	9.4(-1) 2.4(-2)	1.2(-1) 2.5(-2)

Theoretical solution	1.3	1. 1	0.1	0.3	0.5

Table 2: Error moduli for Problem 2 at $x = 0.5$ for $t = 0.2(0.2)1.0$ using the schemes given by formulas (12), (17), (2-8), (34) and their extrapolated formulations.

Method	Time				
	0.2	0.4	0.6	0.8	1.0
Formula (12)	5.2(-2)	1.8(-1)	2.2(-1)	1.4(-1)	1.1(-1)
Extrapolation	1.0(-2)	4.0(-2)	4.0(-2)	5.0(-2)	4.6(-2)
Formula (17)	2.0(-2)	8.2(-2)	1.2(-1)	6.0(-2)	4.6(-2)
Extrapolation	1.0(-2)	1.6(-3)	1.3(-2)	2.0(-2)	1.1(-2)
Formula (28)	2.1(-1)	1.0(-1)	2.4(-1)	1.3(-1)	1.1(-1)
Extrapolation	1.8(-2)	1.0(-2)	1.0(-1)	1.8(-2)	4.7(-2)
Formula (34)	3.2(-3)	5.3(-2)	2.4(-1)	1.9(-1)	1.8(-1)
Extrapolation	1.0(-4)	3.7<-3)	1.0(-1)	1.0(-1)	9.0(-2)
Theoretical solution	1.34980	1.10517	1.10517	1.34986	1.64872

Reference

1. A.R. Mitchell, *Computational methods in partial differential equations*, Wiley, London, 1969.