

Second-order, L_0 -stable methods for the heat equation with time-dependent boundary conditions

E. H. Twizell, A. B. Gumel* and M. A. Arigu

Department of Mathematics and Statistics, Brunel University, Uxbridge, Middlesex UB8 3PH, UK

Dedicated to Professor J. Crank on the occasion of his 80th birthday

A family of second-order, L_0 -stable methods is developed and analysed for the numerical solution of the simple heat equation with time-dependent boundary conditions. Methods of the family need only real arithmetic in their implementation. In a series of numerical experiments no oscillations, which are a feature of some results obtained using A_0 -stable methods, are observed in the computed solutions. Splitting techniques for first- and second-order hyperbolic problems are also considered.

1. Introduction

It is well known that systems of parabolic partial differential equations (PDE's) of the second order, in one or more space dimensions, feature in the mathematical modelling of many phenomena. They arise, for example, in the study of removal of the organic vehicle from moulded ceramic bodies (Evans et al. [4]), in percutaneous drug absorption (Kubota and Ishizahi [9, 10]), and in models of travelling waves in simple isothermal chemical systems (Merkin et al. [14]).

One method of solution of the model initial/boundary-value problem, the so-called *method of lines*, discretizes the region in space over which the PDE's are to be integrated using some mesh or grid, following which the space derivatives in the PDE's, and in the boundary conditions, are replaced possibly by some finite-difference or finite-element approximants. Assuming that the space is one-dimensional, there results an initial-value problem consisting of MN first-order ordinary differential equations (ODE's), where M is the number of PDE's in the mathematical model and N is the number of points of the afore-mentioned mesh at which the solution will be computed.

* Present address: Faculty of Information Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia.

Models which feature one PDE and admit a time-dependent source term or time-dependent boundary conditions are transformed by the method of lines into an initial-value system of the form

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t) + \boldsymbol{\psi}(t), \quad t > 0; \quad \mathbf{U}(0) = \mathbf{g}, \quad (1.1)$$

in which all vectors have N elements and A is an N -square matrix which will be assumed to be constant with real, distinct, negative eigenvalues λ_i ($i = 1, 2, \dots, N$). In the case of the simple heat equation

$$\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2}; \quad 0 < x < X, \quad t > 0, \quad (1.2)$$

with Dirichlet boundary conditions, for instance, discretizing the interval $0 \leq x \leq X$ at the $N + 2$ points $x_m = mh$ ($m = 0, 1, \dots, N + 1$) with $(N + 1)h = X$, replacing the space derivative by the familiar second-order central-difference approximant

$$\frac{\partial^2 u(x, t)}{\partial x^2} = h^{-2} [u(x - h, t) - 2u(x, t) + u(x + h, t)] + O(h^2) \quad \text{as } h \rightarrow 0, \quad (1.3)$$

and applying (1.2) with (1.3) to each of the N interior points at which the solution is sought, leads to the familiar matrix A of the form

$$A = h^{-2} \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix} \quad (1.4)$$

for which $\lambda_i = -4h^{-2} \sin^2[i\pi/\{2(N + 1)\}] < 0$ with $i = 1, 2, \dots, N$.

The solution $\mathbf{U}(t)$ of the semi-discrete problem (1.1) satisfies the recurrence relation

$$\mathbf{U}(t + l) = \exp(lA)\mathbf{U}(t) + \int_t^{t+l} \exp[(t + l - k)A] \boldsymbol{\psi}(k) dk; \quad (1.5)$$

$$t = 0, l, 2l, \dots,$$

in which $l > 0$ is a constant time step in the discretization of the time variable $t \geq 0$ at the points $t_n = nl$ ($n = 0, 1, 2, \dots$).

It is convenient to denote by \mathbf{U}^n and $\tilde{\mathbf{U}}^n$ the solution of (1.5) at time $t = t_n$ and the solution actually obtained, respectively, and to define the vector \mathbf{Z}^n by $\mathbf{Z}^n = \mathbf{U}^n - \tilde{\mathbf{U}}^n$. A linearized stability analysis with $\boldsymbol{\psi} \equiv \mathbf{0}$, of von Neumann type, then

considers the growth of a perturbation in the initial vector $U^0 = g$ which satisfies the error equation

$$Z^{n+1} = R(lA)Z^n; \quad n = 0, 1, 2, \dots, \quad (1.6)$$

where $R(lA)$ is the approximation to $\exp(lA)$ on which the numerical method is based; $R(lA)$ is the amplification matrix. The numerical method based on $R(lA)$ is said to be A_0 -stable if $|R(-z)| \leq 1$, where $z = -l\lambda > 0$ and λ is an eigenvalue of A , and to be L_0 -stable if, in addition to being A_0 -stable, $R(-z) \rightarrow 0$ as $z \rightarrow \infty$. The quantity $R(-z)$ is called the symbol or amplification symbol of the numerical method: see Lawson and Morris [13] who emphasize the merits of L_0 -stable methods for use in solving initial/boundary-value problems for which there are discontinuities between initial conditions and boundary conditions.

One frequently-used family of methods is based on the approximant

$$R(lA) = (I - alA)^{-1} [I + (1 - a)lA], \quad (1.7)$$

in which $a \in [0, 1]$ is a parameter. In the context of (1.1) with $\psi \equiv 0$ (the semi-discretization of the simple heat equation with homogeneous boundary conditions in one space variable), replacement of the space derivative by second-order central-difference approximants leads to some familiar finite-difference methods for certain choices of a . These include

- (i) $a = 0$, leading to an explicit method which is conditionally stable, $O(h^2 + l)$ accurate as $h, l \rightarrow 0$, where $h > 0$ is the parameter of the space discretization.
- (ii) $a = 1/2$, leading to an A_0 -stable, $O(h^2 + l^2)$, implicit method due to Crank and Nicolson [3].
- (iii) $a = 1$, leading to an L_0 -stable, $O(h^2 + l)$, fully implicit method.

In the terminology of ODE's (Lambert [11]), the single initial-value problem of interest is given by

$$y'(t) = f(t, y(t)), \quad t > 0; \quad y(0) = y_0, \quad (1.8)$$

where $y'(t) \equiv Dy(t) = dy(t)/dt$, for which it will be assumed that $\text{Re}(\partial f / \partial y) < 0$. Implementing (1.7) in the form

$$R(lD) = (1 - alD)^{-1} [1 + (1 - a)lD] \quad (1.9)$$

for use in the Taylor expansion

$$y(t + l) = \exp(lD)y(t), \quad (1.10)$$

these three values of a lead, respectively, to

- (i) the Euler predictor formula $y_{n+1} = y_n + hf_n$,
- (ii) the Euler corrector formula $y_{n+1} = y_n + (1/2)h(f_n + f_{n+1})$,
- (iii) the backward Euler method $y_{n+1} = y_n + hf_{n+1}$,

where, in the notation of Lambert [11], y_n is an approximation to $y(t_n)$ and $f_n = f(t_n, y_n)$.

The values $a = 0, 1/2$ and 1 in (1.7) or (1.9) are also known as the $(0, 1)$, $(1, 1)$ and $(1, 0)$ Padé approximants (Padé [15]) to $\exp(lA)$ or $\exp(lD)$.

2. An alternative family of numerical methods

The family of numerical methods arising from (1.7) does not contain one method which is both L_0 -stable and $O(h^2 + l^2)$ accurate as $h, l \rightarrow 0$ when used to solve the simple heat equation. To this end, a new family of methods was used by Gumel [6] which is based on the approximation

$$R(lA) = (I - alA + bl^2A^2)^{-1}[I + (1 - a)lA], \quad (2.1)$$

in which a and b are parameters. This approximation, which was used simultaneously by Arigu [1] to solve hyperbolic PDEs, will be used in this section of the present paper to solve parabolic problems and in section 4 to solve hyperbolic problems. Voss and Khaliq [19] also report $O(h^2 + l^2)$ methods, which need only real arithmetic, to solve parabolic and hyperbolic problems and in [20] they extend their work to advection-diffusion problems for which they develop an $O(h^2 + l^4)$ technique. Taj [18] has developed $O(h^3 + l^3)$ and $O(h^4 + l^4)$, L_0 -stable methods, which also need only real arithmetic, to solve problems of the form (1.1) while Cheema [2] develops $O(h^3 + l^3)$ and $O(h^4 + l^4)$ methods for first-order and second-order hyperbolic equations.

Obviously, (2.1) reduces to (1.7) when $b = 0$. It is immediately clear that the family contains two approximations to $\exp(lA)$ which lead to existing L_0 -stable numerical methods for solving the simple heat equation. They are

- (i) the (2,0) Padé approximant obtained when $a = 1$ and $b = 1/2$; this is an $O(h^2 + l^2)$ method,
- (ii) the (2,1) Padé approximant obtained when $a = 2/3$ and $b = 1/6$; this is an $O(h^2 + l^3)$ method.

It is easy to see that, although the resulting numerical experiments give high accuracy (Khaliq [7]), they can be expensive to implement especially in multi-space dimension problems. Even in one space dimension, the user must employ a quin-diagonal solver or use a splitting technique with complex arithmetic. In what follows, it will be seen that by restricting a (and, consequently, b) to lie in certain ranges, numerical methods which are $O(h^2 + l^2)$ accurate as $h, l \rightarrow 0$, L_0 -stable and use only real arithmetic can be developed. The use of only real arithmetic especially in multi-space dimensions can yield large savings in CPU time used.

The $O(h^2)$ component of the local truncation error is not related to the choice of a or b . To establish the desired $O(l^2)$ component it is useful to consider (1.10). It is easy to see that the local truncation error (Lambert [11, p. 27]) of the multiderivative method arising from the use of the associated operator

$$R(lD) = (1 - alD + bl^2D^2)^{-1}[1 + (1 - a)lD] \quad (2.2)$$

in (1.10) is

$$\begin{aligned} \mathcal{L}[y(t); l] &= C_2 l^2 y''(t) + C_3 l^3 y'''(t) + O(l^4) \\ &= \left(\frac{1}{2} - a + b\right) l^2 y''(t) + \left(\frac{1}{6} - \frac{a}{2} + b\right) l^3 y'''(t) + O(l^4). \end{aligned} \quad (2.3)$$

Thus, $\mathcal{L}[y(t); l] = O(l^3)$ as $l \rightarrow 0$ provided

$$b = a - \frac{1}{2}, \quad (2.4)$$

which is the restriction to be placed on b to achieve $O(h^2 + l^2)$ accuracy as $h, l \rightarrow 0$ when solving the simple heat equation.

The amplification symbol associated with the family of numerical methods is seen to be

$$R(-z) = \frac{1 - (1 - a)z}{1 + az + (a - 1/2)z^2} \quad (2.5)$$

and it is an easy exercise to show that the methods are L_0 -stable provided

$$a > \frac{1}{2}. \quad (2.6)$$

To address the possibility of using only real arithmetic, it is convenient to note that (2.1) with (2.4) may be written in the form

$$R(lA) = (I - r_1 lA)^{-1} (I - r_2 lA)^{-1} [I + (1 - a)lA]; \quad a \neq \frac{1}{2}, \quad (2.7)$$

in which

$$r_1 = \frac{2a - 1}{a + (a^2 - 4a + 2)^{1/2}}, \quad r_2 = \frac{2a - 1}{a - (a^2 - 4a + 2)^{1/2}}, \quad (2.8)$$

and it follows that only real arithmetic is needed and $r_1 \neq r_2$ provided $a^2 - 4a + 2 > 0$, that is

$$a < 2 - \sqrt{2} \quad \text{or} \quad a > 2 + \sqrt{2}. \quad (2.9)$$

Combining (2.9) with (2.6) it may be concluded that (2.1) yields a family of numerical methods for solving the simple heat equation which are $O(h^2 + l^2)$ accurate as $h, l \rightarrow 0$ and L_0 -stable, and which need only real arithmetic in a splitting implementation, provided

$$\frac{1}{2} < a < 2 - \sqrt{2} \quad \text{or} \quad a > 2 + \sqrt{2}. \quad (2.10)$$

It is easy to see from (2.3) and (2.5) that $a = 2/3$, $b = 1/6$ (the aforementioned (2,1) Padé approximant) is the only $O(h^2 + l^3)$ method arising from (2.1). This method, however, needs complex arithmetic in a splitting implementation.

It may be seen from (2.3) and (2.4) that, subject to the restriction in (2.10), the local truncation error is minimized by taking $a = 2 - \sqrt{2} - \varepsilon$, where ε is the smallest positive (real) number available to the precision of the computer being used. The three aims of $O(h^2 + l^2)$ accuracy, L_0 -stability and the use of only real arithmetic are met by this choice of a .

It is easy to see that, in the case of the single test equation

$$y'(t) = \lambda y(t), \quad \lambda < 0, \quad t > 0, \quad y(0) = y_0, \quad (2.11)$$

oscillations in the numerical solution generated by (1.10), in which $\exp(lD)$ is replaced by $R(lD)$ given by (2.2), will not arise provided the amplification symbol $R(-z)$ given by (2.5) is positive. That is, for $a < 1$, whenever $z = -l\lambda < (1-a)^{-1}$.

Generalizing to the system (1.1) with $\psi(t) \equiv 0$, it follows that, interpreting λ to be an eigenvalue of the matrix A given in (1.4), the amplification symbol is positive provided h and l are chosen so that, for a given value of $a < 1$,

$$p < \frac{1}{[4S(1-a)]}, \quad (2.12)$$

where $p = l/h^2$ and S is the number of space dimensions in the partial differential equation with which A is associated. The amplification symbol is always positive (for $z > 0$) whenever $a \geq 1$ and there is no associated restriction on p . Thus, for the intervals in (2.10), it follows that if, in order to obtain a low local truncation error, a is chosen in the interval $1/2 < a < 2 - \sqrt{2}$, the discretization parameters h and l should be chosen to satisfy (2.12) in order to avoid contrived oscillations in the numerical solution. For $a > 2 + \sqrt{2}$, however, no such condition on p is needed.

The condition in (2.12) is restrictive and Lawson and Morris [13] note that oscillatory components in a numerical solution are permissible provided they decay to zero faster than the non-oscillatory components. To achieve this, Lawson and Morris impose the condition $|R(l\lambda_N)| < |R(l\lambda_1)|$ which leads in the present work to

$$\begin{aligned} -\frac{1 + (1-a)l\lambda_1}{1 - al\lambda_1 + (a-1/2)l^2\lambda_N^2} &< \frac{1 + (1-a)l\lambda_N}{1 - al\lambda_N + (a-1/2)l^2\lambda_N^2} \\ &< \frac{1 + (1-a)l\lambda_1}{1 - al\lambda_1 + (a-1/2)l^2\lambda_1^2}. \end{aligned} \quad (2.13)$$

The left-hand inequality leads, after some tedious manipulation, to the condition

$$\begin{aligned} \left(a - \frac{1}{2}\right)l[2(\lambda_1 + \lambda_N) - l(\lambda_1^2 + \lambda_N^2) - (1-a)l^2\lambda_1\lambda_N(\lambda_1 + \lambda_N)] \\ + 2a(1-a)l^2\lambda_1\lambda_N < 2, \end{aligned} \quad (2.14)$$

while the right-hand inequality leads to the condition

$$\left(a - \frac{1}{2}\right)l[\lambda_1 + \lambda_N + (1-a)l\lambda_1\lambda_N] < 1. \quad (2.15)$$

It may be noted that, when $a = 1/2$ (the Crank–Nicolson method), (2.14) reduces to $l^2\lambda_1\lambda_N < 4$ while (2.15) is trivially satisfied: these conclusions were also reached by Lawson and Morris [13].

Since, for the matrix A given in (1.4), $\lambda_1 < 0$ and $\lambda_N < 0$, (2.14) and (2.15) are both trivially satisfied for $a > 2 + \sqrt{2}$ (see (2.10)) confirming that no restriction on p is needed. To obtain the restrictions on p for a in the interval $1/2 < a < 2 - \sqrt{2}$, the values of λ_1 and λ_N must now be substituted in (2.14) and (2.15). Lawson and Morris [13] note that, for large N ,

$$\lambda_1 \simeq -\pi^2 / [(N+1)^2 h^2] \quad \text{and} \quad \lambda_N \simeq -4/h^2.$$

With these approximations (2.14) and (2.15) give the inequalities

$$\begin{aligned} & 4(1-a) \left(a - \frac{1}{2} \right) [4(N+1)^2 + \pi^2] \pi^2 S^3 p^3 \\ & + \left[8a(1-a)(N+1)^2 \pi^2 - \left(a - \frac{1}{2} \right) \{16(N+1)^4 + \pi^4\} \right] S^2 p^2 \\ & - 2 \left(a - \frac{1}{2} \right) (N+1)^2 [4(N+1)^2 + \pi^2] S p \\ & < 2(N+1)^4 \end{aligned} \quad (2.16)$$

and

$$4(1-a) \left(a - \frac{1}{2} \right) \pi^2 S^2 p^2 - \left(a - \frac{1}{2} \right) [4(N+1)^2 + \pi^2] S p < (N+1)^2, \quad (2.17)$$

both of which must be satisfied by the ratio p if oscillatory components are to decay faster than non-oscillatory components. In (2.16) and (2.17) $S = 1$ and it is noteworthy that, when $a = 1/2$ and $X = 2$, (2.16) reduces to the associated restriction given by Lawson and Morris [13, p. 1214] relating to the Crank–Nicolson method ($\tau < 2h/\pi$ in their terminology).

The integral in (1.5) may be approximated by a quadrature formula of the form

$$\int_t^{t+l} \exp[(t+l-k)A] \psi(k) dk \simeq W_1 \psi(k_1) + W_2 \psi(k_2), \quad k_1 \neq k_2, \quad (2.18)$$

in which $W_1 = W_1(lA)$ and $W_2 = W_2(lA)$. Putting $\psi(k) \equiv [1, 1, \dots, 1]^T$ and $\psi(k) \equiv [k, k, \dots, k]^T$, successively, in (2.18) it may be shown, following Lawson [12] and Swayne [16], that

$$W_1 + W_2 = M_1, \quad (2.19)$$

$$k_1 W_1 + k_2 W_2 = M_2, \quad (2.20)$$

in which

$$M_1 = M_1(lA) = A^{-1} \exp(lA) - A^{-1}$$

and

$$M_2 = M_2(lA) = A^{-1} [-(t+l)I + t \exp(lA) - A^{-1} + A^{-1} \exp(lA)].$$

Solving (2.19) and (2.20) gives

$$W_1 = (k_2 M_1 - M_2)/(k_2 - k_1) \quad \text{and} \quad W_2 = (k_1 M_1 - M_2)/(k_1 - k_2) \quad (2.21)$$

provided the abscissae k_1 and k_2 are distinct. Then, substituting (2.18), with W_1 and W_2 given by (2.21) and $k_1 = t$, $k_2 = t + l$, into (1.5) leads to

$$\begin{aligned} U(t+l) = & \exp(lA)U(t) + (lA)^{-1} [l \exp(lA) + A^{-1} - A^{-1} \exp(lA)] \psi(t) \\ & + (lA)^{-1} [A^{-1} \exp(lA) - lI - A^{-1}] \psi(t+l); \end{aligned} \quad (2.22)$$

$$t = 0, l, 2l, \dots$$

Substituting, next, the approximation $R(lA)$, given by (2.1) with $b = a - 1/2$, for $\exp(lA)$ in (2.22) leads to the numerical method

$$\begin{aligned} U(t+l) = & R(lA)U(t) + \frac{1}{2}l [S(lA)\psi(t) + T(lA)\psi(t+l)]; \\ t = & 0, l, 2l, \dots, \end{aligned} \quad (2.23)$$

in which

$$S(lA) = \left[I - alA + \left(a - \frac{1}{2} \right) l^2 A^2 \right]^{-1}, \quad (2.24)$$

$$T(lA) = \left[I - alA + \left(a - \frac{1}{2} \right) l^2 A^2 \right]^{-1} \left[I - 2 \left(a - \frac{1}{2} \right) lA \right]. \quad (2.25)$$

Implementation of the family using a parallel architecture with two processors is based on the partial-fraction decomposition of $R(lA)$ given in (2.7), $S(lA)$ given in (2.24) and $T(lA)$ given in (2.25). These have the forms

$$R(lA) = s_1(I - r_1 lA)^{-1} + s_2(I - r_2 lA)^{-1} \quad (2.26)$$

with

$$s_1 = \frac{1 - a + r_1}{r_1 - r_2}, \quad s_2 = \frac{1 - a + r_2}{r_2 - r_1}, \quad (2.27)$$

$$S(lA) = s_3(I - r_1 lA)^{-1} + s_4(I - r_2 lA)^{-1} \quad (2.28)$$

with

$$s_3 = \frac{r_1}{r_1 - r_2}, \quad s_4 = \frac{r_2}{r_2 - r_1} \quad (2.29)$$

and

$$T(lA) = s_5(I - r_1 lA)^{-1} + s_6(I - r_2 lA)^{-1} \quad (2.30)$$

with

$$s_5 = \frac{1 - 2a + r_1}{r_1 - r_2}, \quad s_6 = \frac{1 - 2a + r_2}{r_2 - r_1} \quad (2.31)$$

and r_1, r_2 given in (2.8). The algorithm, for $n = 0, 1, 2, \dots$, is thus:

$$\text{Processor 1:} \quad (I - r_1 lA)q_1 = s_1 U^n, \quad (2.32a)$$

$$(I - r_1 lA)q_3 = s_3 \psi^n, \quad (2.32b)$$

$$(I - r_1 lA)q_5 = s_5 \psi^{n+1}; \quad (2.32c)$$

$$\text{Processor 2:} \quad (I - r_2 lA)q_2 = s_2 U^n, \quad (2.32d)$$

$$(I - r_2 lA)q_4 = s_4 \psi^n, \quad (2.32e)$$

$$(I - r_2 lA)q_6 = s_6 \psi^{n+1}; \quad (2.32f)$$

$$\text{Then:} \quad U^{n+1} = q_1 + q_2 + \frac{1}{2}l(q_3 + q_4 + q_5 + q_6). \quad (2.32g)$$

In implementing (2.32a–g), processor 1 generates the once-only decomposition of $I - r_1 lA$ while processor 2 generates the once-only decomposition of $I - r_2 lA$. In the case of the simple heat equation, $\psi \equiv 0$ so that $q_3 = q_4 = q_5 = q_6 = 0$ and (2.32b,c,e,f) disappear from the algorithm.

Implementation of the family for use on a single-processor architecture is based on the multiplication of (2.23) by the matrix $I - alA + (a - 1/2)l^2 A^2$. This yields the algorithm

$$e = [I + (1 - a)lA]U^n + \frac{1}{2}l \left[\psi^n + \left\{ I - 2 \left(a - \frac{1}{2} \right) lA \right\} \psi^{n+1} \right],$$

$$(I - r_2 lA)v = e, \quad (2.33)$$

$$(I - r_1 lA)U^{n+1} = v,$$

in which e and v are intermediate vectors. In the case of the simple heat equation with homogeneous boundary conditions, $\psi \equiv 0$ so that $e = [I + (1 - a)lA]U^n$.

Splitting techniques using the approximation (2.7) to solve first- and second-order hyperbolic PDE's are outlined in section 4.

3. Numerical results

Lawson and Morris [13], Gourlay and Morris [5] and Khaliq and Twizell [8], for example, have illustrated the superior properties of L_0 -stable methods for solving one- and two-dimensional problems with homogeneous boundary conditions. However, the literature contains fewer numerical experiments reporting on the behaviour of L_0 -stable methods for problems with time-dependent boundary conditions, particularly in high-dimensional problems. Some examples are given in the papers by Swayne [16, 17].

To illustrate the behaviour of the L_0 -method arising from equation (2.1) the following one-dimensional problem with homogeneous boundary conditions was solved first of all.

Problem 1.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}; \quad 0 < x < 2, \quad t > 0, \quad (3.1a)$$

$$u(x, 0) = 1; \quad 0 \leq x \leq 2, \quad (3.1b)$$

$$u(0, t) = u(2, t) = 0; \quad t > 0, \quad (3.1c)$$

which has theoretical solution

$$u(x, t) = \sum_{k=1}^{\infty} [1 - (-1)^k] \frac{2}{k\pi} \sin\left(\frac{1}{2}k\pi x\right) \exp\left(-\frac{1}{4}k^2\pi^2 t\right). \quad (3.2)$$

This problem, which has discontinuities between initial and boundary conditions at $x = 0$ and $x = X = 2$, was used by Lawson and Morris [13] to compare their L_0 -stable, $O(h^2 + l^2)$ extrapolation method with the A_0 -stable method of the same order due to Crank and Nicolson [3].

Three of the numerical experiments reported by Lawson and Morris [13, table 1, p. 1217] were repeated: these well-chosen experiments illustrate clearly the respective behaviours of A_0 -stable and L_0 -stable methods in solving problems such as problem 1. The time-step, l , was given the value 0.1 and the space step, h , the values 0.1, 0.05 and 0.025, so that $N = 19, 39$ and 79 , respectively, and the problem was integrated to time $t = 1.0$.

The parameter a was given the value $1/2 + \varepsilon$, where $\varepsilon = 10^{-v}$ ($v = 1, 2, \dots$). It was found that, as $v \rightarrow 8$ so that ε approached the smallest, positive, real number available to the precision of the computer used, the L_0 -stable method based on (2.32a,d,g) began to behave in the same way as the Crank–Nicolson method (see Lawson and Morris [13, figure 2]).

Arbitrarily choosing $a = (1/2)(2.5 - \sqrt{2}) \simeq 0.54$, the mid-point of the first interval in (2.10), gives $C_3 \simeq -0.062$ compared to $C_3 = -1/12 \simeq -0.083$ for the Crank–Nicolson method and $C_3 = 1/6 \simeq 0.167$ for the $O(h^2 + l^2)$ extrapolation method of Lawson and Morris [13] when used over a single time step (the formulation of their method was over a double time step $2l$). The maximum (modulus) values of the errors $e_m^n = u_m^n - \tilde{u}_m^n$ at time $t = 1.0$ ($n = 10$) incurred by the three methods (retaining the sign in each case) are given in table 1.

It was found that, for the Crank–Nicolson method, the maximum modulus value of e_m^n always occurred at points adjacent to the boundaries ($m = 1$ and N) whereas

Table 1

Errors e_m^n and relative percentage errors E_m^n at time $t = 1$ and $l = 0.1$ using the method in (2.32a,d,g) with $a = (2.5 - \sqrt{2})/2$, the Lawson–Morris method and the Crank–Nicolson method.

	e_m^{10}			$E_m^{10}(\%)$		
	$h = 0.1$	$h = 0.05$	$h = 0.025$	$h = 0.1$	$h = 0.05$	$h = 0.025$
Method (2.32)	0.68E-03	0.93E-03	0.99E-03	0.62E+00	0.85E+00	0.90E+00
Lawson–Morris	-0.63E-02	-0.61E-02	-0.60E-02	-0.57E+01	-0.56E+01	-0.55E+01
Crank–Nicolson	-0.56E-01	-0.28E+00	-0.55E+00	-0.77E+02	-0.97E+02	-0.10E+03

for the two L_0 -stable methods the maximum modulus value of e_m^n always occurred at the mid point where $m = (N + 1)/2$ (note: $u(1, 1) \simeq 0.108$ from (3.2)). The relative percentage error at time $t = 1.0$ ($n = 10$) in each case, defined by $E_m^n = 100e_m^n/u_m^n\%$, is also given in table 1. The results in table 1 confirm that the L_0 -stable method (2.32a,d,g) is accurate when tested on this problem.

To illustrate the behaviour of the L_0 -stable method (2.32a–g) when used to solve problems with time-dependent boundary conditions, the following problems were solved.

Problem 2.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}; \quad 0 < x < 1, \quad t > 0, \quad (3.3a)$$

$$u(x, 0) = \sin \frac{1}{2}\pi x; \quad 0 \leq x \leq 1, \quad (3.3b)$$

$$u(0, t) = 1; \quad t > 0, \quad (3.3c)$$

$$u(1, t) = \exp\left(-\frac{1}{4}\pi^2 t\right); \quad t > 0, \quad (3.3d)$$

which has theoretical solution

$$u(x, t) = \exp\left(-\frac{1}{4}\pi^2 t\right) \sin \frac{1}{2}\pi x. \quad (3.4)$$

Clearly

$$\psi(t) = h^{-2} \left[0, \dots, 0, \exp\left(-\frac{1}{4}\pi^2 t\right) \right]^T$$

is of order N .

Taking $a = (1/2)(2.5 - \sqrt{2})$ once again the solution was computed to time $t = 1.0$ for $l = 0.1, 0.05, 0.025, 0.0125$ and $N = 9, 19, 39, 79$. The maximum errors (retaining the sign) and the corresponding relative errors, together with the points $x = x^*$ at which they occur, are reported in table 2 for all 16 experiments.

Problem 2 and its solution (3.4) have no axis of symmetry and it was noted that the maximum errors did not occur at the same point in each experiment. In some experiments the curves representing the theoretical and numerical solutions crossed (once) though, as can be seen from table 2, the maximum errors were always small. There were no oscillations in the computed solutions. Examination of the errors relating to the sequence of pairs $(l, N) = (0.1, 9), (0.05, 19), (0.025, 39), (0.0125, 79)$, in which l and h are successively halved, depicts that the method (2.32a–g) has observed order two. Errors relating to other, shorter sequences drawn from table 2 confirm this conclusion.

Table 2

Maximum errors and corresponding relative errors, and the point $x = x^*$ at which they occur, at time $t = 1.0$ using the method in (2.32a–g) with $a = (2.5 - \sqrt{2})/2$ for $l = 0.1, 0.05, 0.025, 0.0125$ and $N = 9, 19, 39, 79$.

l	N	x^*	Analytical solution	Error	Relative error (%)
0.1	9	0.8	0.81E-01	-0.69E-04	-0.85E-01
	19	0.9	0.84E-01	-0.54E-04	-0.64E-01
	39	0.9	0.84E-01	-0.51E-04	-0.61E-01
	79	0.9	0.84E-01	-0.51E-04	-0.61E-01
0.05	9	0.6	0.69E-01	-0.48E-04	-0.71E-01
	19	0.85	0.83E-01	-0.20E-04	-0.24E-01
	39	0.9	0.84E-01	-0.16E-04	-0.20E-01
	79	0.9125	0.84E-01	-0.16E-04	-0.19E-01
0.025	9	0.6	0.69E-01	-0.49E-04	-0.71E-01
	19	0.65	0.72E-01	-0.12E-04	-0.17E-01
	39	0.9	0.84E-01	-0.57E-05	-0.68E-02
	79	0.925	0.84E-01	-0.42E-05	-0.50E-02
0.0125	9	0.6	0.69E-01	-0.48E-04	-0.70E-01
	19	0.55	0.65E-01	-0.12E-04	-0.19E-01
	39	0.625	0.71E-01	-0.31E-05	-0.44E-02
	79	0.9375	0.84E-01	-0.13E-05	-0.15E-02

Problem 3.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}; \quad 0 < x, y < 1, \quad t > 0, \quad (3.5a)$$

$$u(x, y, 0) = \sin \frac{1}{2} \pi x \sin \frac{1}{2} \pi y; \quad 0 \leq x, y \leq 1, \quad (3.5b)$$

$$u(0, y, t) = u(x, 0, t); \quad 0 < x, y < 1, \quad t > 0, \quad (3.5c)$$

$$u(1, y, t) = \exp \left(-\frac{1}{2} \pi^2 t \right) \sin \frac{1}{2} \pi y; \quad 0 < y < 1, \quad t > 0, \quad (3.5d)$$

$$u(x, 1, t) = \exp \left(-\frac{1}{2} \pi^2 t \right) \sin \frac{1}{2} \pi x; \quad 0 < x < 1, \quad t > 0, \quad (3.5e)$$

in which $u = u(x, y, t)$, which has theoretical solution

$$u(x, y, t) = \exp \left(-\frac{1}{2} \pi^2 t \right) \sin \frac{1}{2} \pi x \sin \frac{1}{2} \pi y. \quad (3.6)$$

This problem is the two-dimensional analogue of problem 2 given by (3.3a–d).

Replacing the space derivatives in (3.5a) by their second-order central-difference replacements analogous to (1.3) and discretizing the square bounded by the lines

$x = 0, x = 1, y = 0, y = 1$ at the points $(x_k, y_m) = (kh, mh)$ with $k, m = 0, 1, \dots, N, N + 1$, leads to the matrix A in (1.5) having the form

$$A = h^{-2} \begin{bmatrix} A_1 & I & & & \\ I & A_1 & I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & I & A_1 & I \\ & & & I & A_1 \end{bmatrix} \quad (3.7)$$

with

$$A_1 = \begin{bmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 & -4 & 1 \\ & & & 1 & -4 \end{bmatrix}.$$

In (3.7) A is a block-tridiagonal matrix of order N^2 , I is the diagonal matrix of order N and A_1 is a tridiagonal matrix of order N . The vector $\psi(t)$ in (1.1) is now of order N^2 and may be written down from the boundary conditions (3.5c–e).

Taking $a = (1/2)(2.5 - \sqrt{2})$ once more, $N = 9$ and a time step $l = 0.001$, the problem was integrated to time $t = 0.1$. No oscillations were observed in the computed solution and the maximum error was observed at the point $x = 0.6, y = 0.5$ where $u \simeq 0.349$. The error was $-0.403\text{E}-03$ and the relative percentage error was $-0.115\text{E}+00$. The solution profile (produced using the *Mathematica* package, which is capable of showing only the solution at the interior points) is depicted in figure 1. To the scale used the graph of the analytical solution given by (3.6) is indistinguishable from that in figure 1.

Problem 4.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}; \quad 0 < x, y, z < 1, \quad t > 0, \quad (3.8a)$$

$$u(x, y, z, 0) = \sin \frac{1}{2}\pi x \sin \frac{1}{2}\pi y \sin \frac{1}{2}\pi z; \quad 0 \leq x, y, z \leq 1, \quad (3.8b)$$

$$u(0, y, z, t) = u(x, 0, z, t) = u(x, y, 0, t) = 0; \quad t > 0, \quad (3.8c)$$

$$u(1, y, z, t) = \exp\left(-\frac{3}{4}\pi^2 t\right) \sin \frac{1}{2}\pi y \sin \frac{1}{2}\pi z; \quad 0 < y, z < 1, \quad t > 0, \quad (3.8d)$$

$$u(x, 1, z, t) = \exp\left(-\frac{3}{4}\pi^2 t\right) \sin \frac{1}{2}\pi x \sin \frac{1}{2}\pi z; \quad 0 < x, z < 1, \quad t > 0, \quad (3.8e)$$

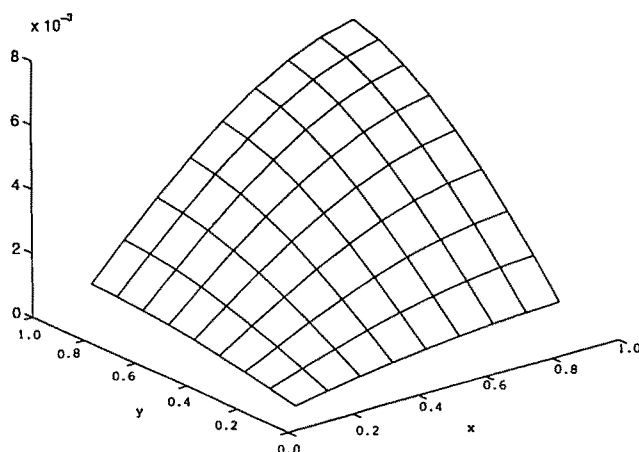


Figure 1. Solution profile for problem 3 at time $t = 0.1$ with $a = (1/2)(2.5 - \sqrt{2})$, $h = 0.1$ and $l = 0.001$.

$$u(x, y, 1, t) = \exp\left(-\frac{3}{4}\pi^2 t\right) \sin \frac{1}{2}\pi x \sin \frac{1}{2}\pi y; \quad 0 < x, y < 1, \quad t < 0, \quad (3.8f)$$

in which $u = u(x, y, z, t)$, which has theoretical solution

$$u(x, y, z, t) = \exp\left(-\frac{3}{4}\pi^2 t\right) \sin \frac{1}{2}\pi x \sin \frac{1}{2}\pi y \sin \frac{1}{2}\pi z. \quad (3.9)$$

This problem is the three-dimensional analogue of (3.1a-d).

The cube bounded by the planes $x = 0$, $x = 1$, $y = 0$, $y = 1$, $z = 0$, $z = 1$ is discretized at the points (x_k, y_m, z_j) with $k, m, j = 0, 1, \dots, N, N+1$. Replacing the space derivatives in (3.8a) by their second-order central-difference approximants analogous to (1.3) leads to the matrix A in (1.5) having the block-tridiagonal form

$$A = h^{-2} \begin{bmatrix} A_2 & I^* & & & \\ I^* & A_2 & I^* & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & I^* & A_2 & I^* \\ & & & I^* & A_2 \end{bmatrix}; \quad (3.10)$$

clearly the square matrix A is of order N^3 . In (3.10) I^* is the identity matrix of order N^2 and the square matrix A_2 is of order N^2 and is given by

$$A_2 = \begin{bmatrix} A_3 & I & & & \\ I & A_3 & I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & I & A_3 & I \\ & & & I & A_3 \end{bmatrix} \quad (3.11)$$

with

$$A_3 = \begin{bmatrix} -6 & 1 & & & & \\ 1 & -6 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -6 & 1 \\ & & & & 1 & -6 \end{bmatrix}$$

In (3.11), I is the identity matrix of order N and the tridiagonal matrix A_3 is of order N . The vector $\psi(t)$ in (1.1) is now of order N^3 and may be written down from the boundary conditions (3.8c-f).

Taking $a = (1/2)(2.5 - \sqrt{2})$, $N = 5$ and a time step $l = 0.001$, the solution was obtained at the 125 interior points of the cube at time $t = 0.1$ (after 100 time steps). No oscillations were observed in the numerical solution and the maximum error was observed at the point $x = y = z = 0.8$ where $u \simeq 0.308$ at time $t = 0.1$. The error at this point was $-0.646\text{E}-03$ (approximately) giving a relative percentage error of $-0.210\text{E}+00$.

4. Hyperbolic equations

4.1. First-order equations

Consider the first-order hyperbolic initial/boundary-value problem (IBVP)

$$\frac{\partial u}{\partial t} + \alpha \frac{\partial u}{\partial x} = 0; \quad \alpha > 0, \quad t > 0, \quad (4.1)$$

$$u(x, 0) = g(x); \quad x \geq 0, \quad (4.2)$$

$$u(0, t) = v(t); \quad t > 0, \quad (4.3)$$

and suppose that the solution $u(x, t)$ is sought in some region

$$R = [0 < x \leq X] \times [t > 0],$$

where $X < \infty$ is arbitrarily large. This IBVP may be transformed into an initial-value problem (IVP) of the form

$$\frac{dU(t)}{dt} = -\alpha CU(t) + \alpha \gamma(t); \quad t > 0, \quad U(0) = g, \quad (4.4)$$

by dividing the interval $0 \leq x \leq X$ into N subintervals each of width h so that, now, $Nh = X$ and by approximating the space derivative in (4.1) by the replacement

$$\frac{\partial u(x, t)}{\partial x} = \frac{u(x, t) - u(x - h, t)}{h} + O(h) \quad \text{as } h \rightarrow 0. \quad (4.5)$$

In (4.4), the N -square lower-bidiagonal matrix C and the N -vectors \mathbf{g} , $\gamma(t)$ and $\mathbf{U}(t)$ are given by

$$C = h^{-1} \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} g(x_1) \\ g(x_2) \\ \vdots \\ g(x_N) \end{bmatrix}, \quad \gamma(t) = h^{-1} \begin{bmatrix} v(t) \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

and

$$\mathbf{U}(t) = \begin{bmatrix} U_1(t) \\ U_2(t) \\ \vdots \\ U_N(t) \end{bmatrix}. \quad (4.6)$$

The solution can be generated at time $t_n = nl$ ($n = 1, 2, \dots$) using (2.32a–g) or (2.33) in which A is replaced by $-\alpha C$ and ψ is replaced by $\alpha \gamma$.

When $u(0, t) = v$, a constant, in (4.3), equation (4.4) becomes

$$\frac{d\mathbf{U}(t)}{dt} = -\alpha C \mathbf{U}(t) + \alpha \mathbf{c}; \quad t > 0, \quad \mathbf{U}(0) = \mathbf{g}, \quad (4.7)$$

where $\mathbf{c} = h^{-1}[v, 0, \dots, 0]^T$ is an N -vector. The solution of (4.7) satisfies the recurrence relation

$$\mathbf{U}(t+l) = C^{-1}\mathbf{c} + \exp(-\alpha l C)\{\mathbf{U}(t) - C^{-1}\mathbf{c}\}; \quad t = 0, l, 2l, \dots, \quad (4.8)$$

and approximating $\exp(-\alpha l C)$ by $R(-\alpha l C)$, see (2.1) and (2.10), gives

$$\left[I + a\alpha l C + \left(a - \frac{1}{2} \right) \alpha^2 l^2 C^2 \right] \mathbf{U}^{n+1} = [I - (1-a)\alpha l C] \mathbf{U}^n + \alpha l \mathbf{c};$$

$$n = 0, 1, 2, \dots \quad (4.9)$$

The solution may then be determined using the two-processor algorithm

$$\text{Processor 1:} \quad (I + r_1 \alpha l C) \mathbf{q}_1 = s_1 \mathbf{U}^n, \quad (4.10a)$$

$$(I + r_1 \alpha l C) \mathbf{q}_3 = s_3 \alpha l \mathbf{c}; \quad (4.10b)$$

$$\text{Processor 2:} \quad (I + r_2 \alpha l C) \mathbf{q}_2 = s_2 \mathbf{U}^n, \quad (4.10c)$$

$$(I + r_2 \alpha l C) \mathbf{q}_4 = s_4 \alpha l \mathbf{c}; \quad (4.10d)$$

$$\text{Then:} \quad \mathbf{U}^{n+1} = \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4, \quad (4.10e)$$

in which r_1 and r_2 are given in (2.8), s_1 and s_2 are given by (2.27) with (2.8) and s_3 and s_4 are given by (2.29) with (2.8). Alternatively, the solution may be computed sequentially using the algorithm

$$\mathbf{e} = [I - (1+a)\alpha l C] \mathbf{U}^n + \alpha l \mathbf{c}, \quad (4.11a)$$

$$(I + r_2 \alpha l C) \mathbf{w} = \mathbf{e}, \quad (4.11b)$$

$$(I + r_1 \alpha l C) \mathbf{U}^{n+1} = \mathbf{w}. \quad (4.11c)$$

Note that, in (4.10a–d) and (4.11b,c) the vectors \mathbf{q}_1 , \mathbf{q}_3 , \mathbf{q}_2 , \mathbf{q}_4 , \mathbf{w} and \mathbf{U}^{n+1} are obtained explicitly (by forward substitution) because the matrices $I + r_1 \alpha l C$ and $I + r_2 \alpha l C$ are lower bidiagonal.

4.2. Second-order equations

The method of lines transforms the second-order hyperbolic problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}; \quad 0 < x < X, \quad t > 0, \quad (4.12)$$

$$u(0, t) = u(X, t) = 0; \quad t > 0, \quad (4.13)$$

$$u(x, 0) = g(x), \quad \frac{\partial u(x, 0)}{\partial t} = f(x); \quad 0 \leq x \leq X, \quad (4.14)$$

into the second-order initial-value problem

$$\frac{d^2 \mathbf{U}(t)}{dt^2} = A\mathbf{U}(t); \quad t > 0, \quad \mathbf{U}(0) = \mathbf{g}, \quad \frac{d\mathbf{U}(t)}{dt} = \mathbf{f}, \quad (4.15)$$

the solution of which is known to satisfy the recurrence relation

$$\mathbf{U}(t + l) = \{ \exp(lB) + \exp(-lB) \} \mathbf{U}(t) - \mathbf{U}(t - l); \quad t = l, 2l, \dots \quad (4.16)$$

The solution at the first time step may be computed using the formula

$$\mathbf{U}(l) = \left(I + \frac{1}{2} l^2 A \right) \mathbf{g} + l \mathbf{f}. \quad (4.17)$$

In transforming the IBVP (4.12)–(4.14) into the IVP (4.15), the discretizations and notations introduced in section 1 have been retained, $\mathbf{g} = [g(x_1), g(x_2), \dots, g(x_N)]^T$, $\mathbf{f} = [f(x_1), f(x_2), \dots, f(x_N)]^T$ and the matrix A is given by (1.4). The matrix B in (4.16) is such that $B^2 = A$.

Using the approximation

$$\exp(lB) \simeq R(lB) = (I - r_1 lB)^{-1} (I - r_2 lB)^{-1} [I + (1 - a)lB]; \quad a \neq \frac{1}{2}, \quad (4.18)$$

it is easy to show that

$$\begin{aligned} R(lB) + R(-lB) &= 2 \left[I - \frac{1}{2} \{ (a - 1)^2 - a(a^2 - 4a + 2)^{1/2} \} l^2 A \right]^{-1} \\ &\quad \times \left[I - \frac{1}{2} \{ (a - 1)^2 + a(a^2 - 4a + 2)^{1/2} \} l^2 A \right]^{-1} \\ &\quad \times \left[I - \left(a^2 - 2a + \frac{1}{2} \right) l^2 A \right], \end{aligned} \quad (4.19)$$

so that, as in the parabolic case, real arithmetic is ensured provided

$$a < 2 - \sqrt{2} \quad \text{or} \quad a > 2 + \sqrt{2}. \quad (4.20)$$

Using (4.19) in (4.16) gives a numerical method which may be shown to have local truncation error with principal part

$$-\frac{1}{12}h^2\frac{\partial^4 u}{\partial x^4} + \left(a^2 - \frac{5}{12}\right)l^2\frac{\partial^4 u}{\partial t^4}, \quad (4.21)$$

verifying $O(h^2 + l^2)$ accuracy as $h, l \rightarrow 0$. A von Neumann stability analysis shows that the method is stable for any choice of h, l whenever $a > 1/2$ or $a < 3/2$. Overall, therefore, the numerical method is stable, $O(h^2 + l^2)$ accurate as $h, l \rightarrow 0$, requires only real arithmetic and does not require the square of the matrix A whenever

$$a < 1/2 \quad \text{or} \quad a > 2 + \sqrt{2}. \quad (4.22)$$

Following the partial-fraction decomposition of $R(lB) + R(-lB)$ in (4.19), the algorithm may be implemented using two processors in parallel as follows:

Processor 1: Solve for U^* from

$$\begin{aligned} & \left[I - \frac{1}{2} \{ (a-1)^2 - a(a^2 - 4a + 2)^{1/2} \} l^2 A \right] U^* \\ &= [I - (2-a)(a^2 - 4a + 2)^{-1}] U^n. \end{aligned} \quad (4.23)$$

Processor 2: Solve for U^+ from

$$\begin{aligned} & \left[I - \frac{1}{2} \{ (a-1)^2 + a(a^2 - 4a + 2)^{1/2} \} l^2 A \right] U^+ \\ &= [I + (2-a)(a^2 - 4a + 2)^{-1}] U^n. \end{aligned} \quad (4.24)$$

Then: $U^{n+1} = U^* + U^+ - U^{n-1}$.

On a serial computer, the algorithm arising from (4.16) and (4.19) may be implemented as follows: let

$$\begin{aligned} W &= 2 \left[I - \left(a^2 - 2a + \frac{1}{2} \right) l^2 A \right] U^n \\ &\quad - \left[I - \frac{1}{2} \{ (a-1)^2 - a(a^2 - 4a + 2)^{1/2} \} l^2 A \right] \\ &\quad \times \left[I - \frac{1}{2} \{ (a-1)^2 + a(a^2 - 4a + 2)^{1/2} \} l^2 A \right] U^{n-1}, \end{aligned}$$

then

$$\left[I - \frac{1}{2} \{ (a-1)^2 + a(a^2 - 4a + 2)^{1/2} \} l^2 A \right] V = W, \quad (4.25)$$

$$\left[I - \frac{1}{2} \{ (a-1)^2 - a(a^2 - 4a + 2)^{1/2} \} l^2 A \right] U^{n+1} = V, \quad (4.26)$$

in which V is an intermediate vector.

Arigu [1] reports numerical results using (4.25), (4.26) to solve the simple wave equation in one-, two- and three-space dimensions.

5. Summary

A family of L_0 -stable methods, suitable for use in solving the simple heat equation with time-dependent boundary conditions, has been developed and analysed in this paper. The methods are second order in space and time and use only real arithmetic.

In a series of numerical experiments, one member of the family was tested on a one-dimensional problem with homogeneous boundary conditions and on three problems with time-dependent boundary conditions (in one-, two- and three-space dimensions). All problems had discontinuities between initial conditions and boundary conditions but no oscillations were observed in the computed solution of any numerical experiment. Such oscillations are a feature of some numerical results obtained using A_0 -stable methods when the time step is too large in comparison to the space step (Lawson and Morris [13]). The work was also extended to first- and second-order hyperbolic problems.

References

- [1] M. A. Arigu, Parallel and sequential algorithms for hyperbolic partial differential equations, Ph.D. thesis, Brunel University (1993).
- [2] T. A. Cheema, Higher-order parallel splitting methods for hyperbolic partial differential equations, Ph.D. thesis, Brunel University, in preparation.
- [3] J. Crank and P. J. Nicolson, A practical method for numerical integration of solutions of partial differential equations of heat conduction type, *Proc. Camb. Phil. Soc.* 43 (1947) 50–67.
- [4] J. R. G. Evans, M. J. Edirisinghe, J. K. Wright and J. Crank, On the removal of organic vehicle from moulded ceramic bodies, *Proc. Roy. Soc. London Ser. A* 432 (1991) 321–340.
- [5] A. R. Gourlay and J. Ll. Morris, The extrapolation of first-order methods for parabolic partial differential equations II, *SIAM J. Numer. Anal.* 17 (1980) 641–655.
- [6] A. B. Gumel, Parallel and sequential algorithms for second-order parabolic equations with applications, Ph.D. thesis, Brunel University (1993).
- [7] A. Q. M. Khaliq, Numerical methods for ordinary differential equations with applications to partial differential equations, Ph.D. thesis, Brunel University (1983).
- [8] A. Q. M. Khaliq and E. H. Twizell, L_0 -stable splitting methods for the simple heat equation in two space dimensions with homogeneous boundary conditions, *SIAM J. Numer. Anal.* 23 (1986) 473–484.
- [9] K. Kubota and T. Ishizaki, A calculation of percutaneous drug absorption – I. Theoretical, *Comput. Biol. Med.* 16 (1986) 7–19.
- [10] K. Kubota and T. Ishizaki, A calculation of percutaneous drug absorption – II. Computation results, *Comput. Biol. Med.* 16 (1986) 21–37.
- [11] J. D. Lambert, *Numerical Methods for Ordinary Differential Systems: The Initial-Value Problem* (Wiley, Chichester, 1991).
- [12] J. D. Lawson, Some numerical methods for stiff ordinary and partial differential equations, in: *Proc. 2nd Manitoba Conf. on Numerical Mathematics*, Winnipeg, Canada (1972) pp. 27–34.
- [13] J. D. Lawson and J. Ll. Morris, The extrapolation of first-order methods for parabolic partial differential equations I, *SIAM J. Numer. Anal.* 15 (1978) 1212–1224.
- [14] J. H. Merkin, D. J. Needham and S. K. Scott, The development of travelling waves in a simple isothermal chemical system I. Quadratic autocatalysis with linear decay, *Proc. Roy. Soc. London Ser. A* 424 (1989) 187–209.
- [15] M. H. Padé, Sur la représentation approchée d'une fonction par des fractions rationnelles, *Ann. de l'École Normale Supérieure* 9 (1892).

- [16] D. A. Swayne, Time-dependent boundary and interior forcing in locally one-dimensional schemes, *SIAM J. Sci. Statist. Comput.* 8 (1987) 755–767.
- [17] D. A. Swayne, Time-dependent Dirichlet boundary conditions and fractional step methods, in: *Numerical Mathematics, Singapore 1988*, eds. R. P. Agarwal, Y. M. Chow and S. J. Wilson (Birkhäuser, Basel, 1988).
- [18] M. S. A. Taj, Higher-order parallel splitting methods for parabolic partial differential equations, Ph.D. thesis, Brunel University (1995).
- [19] D. A. Voss and A. Q. M. Khaliq, Parallel LOD methods for second-order time-dependent PDEs, *Comput. Math. Appl.* 30(10) (1995) 25–35.
- [20] D. A. Voss and A. Q. M. Khaliq, Time-stepping algorithms for semidiscretized linear parabolic PDEs based on rational approximants with distinct real poles, *Adv. Comput. Math.*, this issue.