Alternating direction methods for parabolic equations in two space dimensions with a mixed derivative

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An alternating direction implicit (A.D.I.) method, which requires the solution of two tridiagonal sets of equations at each time step, is derived for solving a parabolic equation with variable coefficients in two space dimensions with a mixed derivative. The method is shown to be unconditionally stable for two semi-infinite ranges of an auxiliary parameter. Other existing finite difference schemes are mentioned and numerical results are presented.

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1. Introduction

Consider the linear parabolic equation

$$\frac{\partial u}{\partial t} = Lu, \tag{1.1}$$

where

$$L \equiv a(x, y, t)\frac{\partial^2}{\partial x^2} + 2b(x, y, t)\frac{\partial^2}{\partial x \partial y} + c(x, y, t)\frac{\partial^2}{\partial y^2}$$

subject to $a > 0$, $c > 0$, $b^2 < ac$, in the region of (x, y, t) space given by $R \times (0 \leqslant t \leqslant T)$, where $R = (0 \leqslant x, y \leqslant 1)$, and x, y are the distance co-ordinates and t the time co-ordinate respectively. It is assumed that $u \epsilon C^4$ and $a, b, c \epsilon C^2$. Existence and uniqueness of the solution of the partial differential equation (1.1) with appropriate initial and boundary conditions have been studied by Dressel (1940), Protter and Weinberger (1967) and other authors.

The region is covered by a rectilinear grid with h the grid spacing in the x and y directions and k the grid spacing in the t direction. The point (x, y, t) is an internal grid point if

$$x = ih, y = jh, t = nk (1 \leqslant i, j \leqslant M - 1, 1 \leqslant n \leqslant N - 1)$$

where $Mh = 1$ and $Nk = T$. It is the purpose of this note to derive a two level alternating direction finite difference scheme which is an approximation to (1.1), and which, despite the presence of a mixed derivative, requires the solution of only two tridiagonal sets of equations at each time step. This is in contrast to the A.D.I. method of Douglas and Gunn (1964) which requires the solution of four tridiagonal sets of equations at each time step. We define notation consisting of $U^n_{i,j}$ the solution of the difference equation at the grid point $x = ih, y = jh, t = nk$; r the mesh ratio k/h^2; and

$$\begin{aligned}
\delta_x^2 U^n_{i,j} &= U^n_{i+1,j} - 2U^n_{i,j} + U^n_{i-1,j} \\
\delta_y^2 U^n_{i,j} &= U^n_{i,j+1} - 2U^n_{i,j} + U^n_{i,j-1} \\
H_x U^n_{i,j} &= U^n_{i+1,j} - U^n_{i-1,j} \\
H_y U^n_{i,j} &= U^n_{i,j+1} - U^n_{i,j-1} \\
\sigma^{(1)} U^n_{i,j} &= U^n_{i+1,j+1} - U^n_{i,j+1} - U^n_{i+1,j} + U^n_{i,j} \\
\sigma^{(2)} U^n_{i,j} &= U^n_{i,j+1} - U^n_{i-1,j+1} - U^n_{i,j} + U^n_{i-1,j} \\
\sigma^{(3)} U^n_{i,j} &= U^n_{i,j} - U^n_{i-1,j} - U^n_{i,j-1} + U^n_{i-1,j-1} \\
\sigma^{(4)} U^n_{i,j} &= U^n_{i+1,j} - U^n_{i,j} - U^n_{i+1,j-1} + U^n_{i,j-1}.
\end{aligned}$$

2. Existing two level difference methods for solving (1.1)

Several difference schemes have been proposed for the solution of (1.1) (and (1.1) with constant coefficients) subject to appropriate initial and boundary conditions. Lax and Richtmyer (1956) proposed the scheme

$$U^{n+1}_{i,j} - U^n_{i,j} = r[\theta L_h U^{n+1}_{i,j} + (1 - \theta) L_h U^n_{i,j}] \tag{2.1}$$

where $L_h \equiv a\delta_x^2 + \frac{1}{2}bH_xH_y + c\delta_y^2$, and $0 \leqslant \theta \leqslant 1$. The scheme is explicit when $\theta = 0$ and conditionally stable. For $0 < \theta \leqslant 1$, the scheme is implicit, and relaxation methods are suggested for solving the block tridiagonal set of equations at each time step. Even using modern relaxation methods like S.O.R. the method is exceedingly laborious. When $\theta = 1$ this scheme reduces to Saul'yev's scheme (1964).

Seidman (1963) constructed various types of schemes for the solution of (1.1). They consisted of explicit, completely implicit and sweep explicit schemes. The last named depended on splitting the difference operators which replaced the derivatives $\frac{\partial^2 u}{\partial x^2}$, $\frac{\partial^2 u}{\partial x \partial y}$, and $\frac{\partial^2 u}{\partial y^2}$ in such a way that in some problems, judicious use of the boundary conditions enabled the overall difference formulae to be solved explicitly.

Russian authors have suggested many split difference formulae for the solution of (1.1). The Russian name for these methods means literally 'fractional steps', and they include the schemes

$$(1 - ar\delta_x^2)U_{i,j}^{n+1/2} = (1 + \tfrac{1}{4}brH_xH_y)U_{i,j}^n$$
$$(1 - cr\delta_y^2)U_{i,j}^{n+1} = (1 + \tfrac{1}{4}brH_xH_y)U_{i,j}^{n+1/2} \quad (2.2)$$

of Yanenko, Suchkov and Pogodin (1959),

$$(1 - ar\delta_x^2)U_{i,j}^{n+1/2} = U_{i,j}^n$$
$$(1 - cr\delta_y^2)U_{i,j}^{n+1} = (1 + br(\sigma^{(2)} + \sigma^{(4)}))U_{i,j}^{n+1/2} \quad (2.3)$$

of Samarskii (1964) (see also Samarskii (1962)), and

$$(1 - ar\delta_x^2)U_{i,j}^{n+1/3} = U_{i,j}^n$$
$$(1 - cr\delta_y^2)U_{i,j}^{n+2/3} = U_{i,j}^{n+1/3}$$
$$U_{i,j}^{n+1} = (1 + \tfrac{1}{2}brH_xH_y)U_{i,j}^{n+2/3} \quad (2.4)$$

of Sofronov (1963). The schemes (2.2), (2.3), and (2.4) are classified as two level schemes, despite the presence of intermediate levels. The unsplit scheme

$$(1 - \lambda ar\delta_x^2)(1 - \lambda cr\delta_y^2)(U_{i,j}^{n+1} - U_{i,j}^n) = r(a\delta_x^2 + c\delta_y^2 + b(\sigma^{(2)} + \sigma^{(4)}))U_{i,j}^n \quad (2.5)$$

where λ is a parameter, has been proposed by Andreev (1967). These schemes were not derived in any systematic manner. They were considered because they looked feasible schemes and were shown to work under certain conditions.

Finally, Douglas and Gunn (1964) considered the scheme

$$U_{i,j}^{n+1} - U_{i,j}^n = r(a\delta_x^2 + c\delta_y^2 + 2b\delta_{xy}^*)U_{i,j}^{n+1} \quad (2.6)$$

where δ_{xy}^* is either $\tfrac{1}{2}(\sigma^{(1)} + \sigma^{(3)})$ or $\tfrac{1}{2}(\sigma^{(2)} + \sigma^{(4)})$, depending on whether $b > 0$ or $b < 0$. The alternating direction form of this scheme is extremely complicated and, in the case of b positive and negative in different parts of the region, four tridiagonal sets of equations have to be solved at each time step. The four basic directions are the x-direction, the y-direction, and directions inclined at an angle $\pi/4$ with the positive and negative x-axis respectively.

3. Derivation of A.D.I. scheme

In order to derive an A.D.I. scheme which meets our requirements, we assume *initially* that the coefficients a, b, c in (1.1) are constant. We then consider a general two level finite difference formula of the form

$$[A + BH_x + CH_y + D\delta_x^2 + E\delta_y^2 + FH_xH_y + G_1H_x\delta_y^2 + J_1H_y\delta_x^2 + K_1\delta_x^2\delta_y^2]U_{i,j}^{n+1}$$
$$= [A + BH_x + CH_y + (D + arA)\delta_x^2 + (E + crA)\delta_y^2 + (F + \tfrac{1}{2}brA)H_xH_y + G_2H_x\delta_y^2 + J_2H_y\delta_x^2 + K_2\delta_x^2\delta_y^2]U_{i,j}^n \quad (3.1)$$

where $A, B, C, D, E, F, G_1, J_1, K_1, G_2, J_2, K_2$ are arbitrary real parameters. Straight forward Taylor expansions of the operators in (3.1) show that the latter is a finite difference approximation of (1.1) of order of accuracy $0(h^2 + k)$. Moreover, despite the twelve arbitrary parameters in (3.1) which can be assigned any values we please, a two level scheme of local accuracy $0(h^2 + k^2)$ cannot be obtained from (3.1). When $a = c$, however, a scheme of accuracy $0(h^4 + k^2)$ can be obtained. It is

$$\left[1 - \frac{a}{2}\left(r - \frac{1}{6a}\right)\delta_x^2 - \frac{a}{2}\left(r - \frac{1}{6a}\right)\delta_y^2 - \frac{b}{4}\left(r - \frac{1}{6a}\right)H_xH_y + G_1H_x\delta_y^2 + J_1H_y\delta_x^2 + K_1\delta_x^2\delta_y^2\right]U_{i,j}^{n+1}$$
$$= \left[1 + \frac{a}{2}\left(r + \frac{1}{6a}\right)\delta_x^2 + \frac{a}{2}\left(r + \frac{1}{6a}\right)\delta_y^2 + \frac{b}{4}\left(r + \frac{1}{6a}\right)H_xH_y + G_1H_x\delta_y^2 + J_1H_y\delta_x^2 + \left\{K_1 + \frac{ar}{6}(1 + 4b^2/a^2)\right\}\delta_x^2\delta_y^2\right]U_{i,j}^n.$$

Since we have been unable to split this scheme and so ease the calculation of $U_{i,j}^{n+1}$, it is of little practical use, and its stability has not been considered.

A suitable condition in forming A.D.I. schemes is that the difference operator at the advanced time level is capable of factorisation. To facilitate this, the arbitrary parameters in (3.1) are chosen to satisfy the conditions

$$G_1 = J_1 = 0,$$
$$A = 1, B = C = F = 0, K_1 = DE.$$

The modified scheme, with $G_2 = J_2 = 0$ for convenience, becomes

$$(1 + D\delta_x^2)(1 + E\delta_y^2)U_{i,j}^{n+1} = [1 + (D + ar)\delta_x^2 + (E + cr)\delta_y^2 + \tfrac{1}{2}brH_xH_y + K_2\delta_x^2\delta_y^2]\,U_{i,j}^n \quad (3.2)$$

which can be written in the Douglas–Rachford alternating direction form

$$(1 + D\delta_x^2)U_{i,j}^{n+1*} = [1 + (D + ar)\delta_x^2 + cr\delta_y^2 + \tfrac{1}{2}brH_xH_y + (K_2 - DE)\delta_x^2\delta_y^2]U_{i,j}^n$$
$$(1 + E\delta_y^2)U_{i,j}^{n+1} = U_{i,j}^{n+1*} + E\delta_y^2U_{i,j}^n, \quad (3.3)$$

where $U_{i,j}^{n+1*}$ denotes an intermediate value of $U_{i,j}^{n+1}$. However, if we reduce the number of parameters further by setting

$$D = \frac{1}{f} - \frac{1}{2}ra,\ E = \frac{1}{f} - \frac{1}{2}rc,$$
$$K_2 = \left(\frac{1}{f} + \frac{1}{2}ra\right)\left(\frac{1}{f} + \frac{1}{2}rc\right),$$

the scheme

$$\left[1 + \left(\frac{1}{f} - \frac{1}{2}ra\right)\delta_x^2\right]\left[1 + \left(\frac{1}{f} - \frac{1}{2}rc\right)\delta_y^2\right]U_{i,j}^{n+1}$$
$$= \left\{\left[1 + \left(\frac{1}{f} + \frac{1}{2}ra\right)\delta_x^2\right]\left[1 + \left(\frac{1}{f} + \frac{1}{2}rc\right)\delta_y^2\right] + \frac{1}{2}rbH_xH_y\right\}U_{i,j}^n \quad (3.4)$$

is obtained, which involves the single parameter f. When split in Douglas–Rachford form, this scheme becomes

$$\left[1 + \left(\frac{1}{f} - \frac{1}{2}ra\right)\delta_x^2\right]U_{i,j}^{n+1*} = \left[1 + \left(\frac{1}{f} + \frac{1}{2}ra\right)\delta_x^2\right.$$

$$+ rc\delta_y^2 + \frac{1}{2} rbH_xH_y + \frac{r}{f}(a+c)\delta_x^2\delta_y^2\Big] U_{i,j}^n$$

$$\left[1 + \left(\frac{1}{f} - \frac{1}{2}rc\right)\delta_y^2\right] U_{i,j}^{n+1}$$

$$= U_{i,j}^{n+1*} + \left(\frac{1}{f} - \frac{1}{2}rc\right)\delta_y^2 U_{i,j}^n \qquad (3.5)$$

Special cases of (3.4) are already in existence when $a = c = 1$, and $b = 0$. These are the Peaceman–Rachford formula (1955) when $f = \infty$, and the high accuracy Mitchell–Fairweather scheme (1964) when $f = 12$. It should be noted that (3.3) (and (3.5)) involve the solution of two tridiagonal sets of equations at each time step.

The principal part of the truncation error of (3.4) can be shown to be

$$arh^4\left(\frac{1}{f} - \frac{1}{12}\right)\frac{\partial^4 u}{\partial x^4} + brh^4\left(ar + \frac{2}{f} + \frac{1}{3}\right)\frac{\partial^4 u}{\partial x^3 \partial y}$$

$$+ 2b^2r^2h^4\frac{\partial^4 u}{\partial x^2 \partial y^2} + brh^4\left(cr + \frac{2}{f} + \frac{1}{3}\right)\frac{\partial^4 u}{\partial x \partial y^3}$$

$$+ crh^4\left(\frac{1}{f} - \frac{1}{12}\right)\frac{\partial^4 u}{\partial y^4}. \qquad (3.6)$$

If we now return to the original equation (1.1) and allow a, b, and c to be functions of x, y, t, it can be verified by Taylor expansions that (3.4) (and (3.5)) still retain an order of accuracy $0(h^2 + k)$.

4. Stability

(i) Constant coefficients

For a two level scalar difference scheme such as (3.4), the von Neumann condition is sufficient as well as necessary for stability. The von Neumann method of examining stability will now be employed to demonstrate the stability of (3.4). It is assumed that the coefficients a, b, c are again constant, and that any initial and boundary conditions are periodic.

Fourier decomposition of the space variables in (3.4) leads to

$$\left[1 - 4\left(\frac{1}{f} - \frac{1}{2}ra\right)\sin^2\frac{\theta}{2}\right]\left[1 - 4\left(\frac{1}{f} - \frac{1}{2}rc\right)\sin^2\frac{\phi}{2}\right]\mu$$

$$= \left[1 - 4\left(\frac{1}{f} + \frac{1}{2}ra\right)\sin^2\frac{\theta}{2}\right]\left[1 - 4\left(\frac{1}{f} + \frac{1}{2}rc\right)\sin^2\frac{\phi}{2}\right]$$

$$- 2rb\sin\theta\sin\phi, \qquad (4.1)$$

where $\theta = \beta h$, $\phi = \gamma h$, with β and γ arbitrary real numbers, and where μ is the amplification factor of a Fourier component. The von Neumann condition for stability is $|\mu| \leqslant 1$. Provided

$$1 + 4\left(\frac{1}{2}ra - \frac{1}{f}\right)\sin^2\frac{\theta}{2} > 0 \text{ and } 1 + 4\left(\frac{1}{2}rc - \frac{1}{f}\right)\sin^2\frac{\phi}{2} > 0, \qquad (4.1a)$$

the two inequalities resulting from applying this condition to (4.1) are

$$1 - \frac{4}{f}\sin^2\frac{\theta}{2} - \frac{4}{f}\sin^2\frac{\phi}{2} + \left(\frac{16}{f^2} + 4r^2ac\right)\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2}$$

$$- rb\sin\theta\sin\phi \geqslant 0, \qquad (4.2)$$

and

$$a\sin^2\frac{\theta}{2} + c\sin^2\frac{\phi}{2} - \frac{4}{f}(a+c)\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2}$$

$$+ \tfrac{1}{2}b\sin\theta\sin\phi \geqslant 0. \qquad (4.3)$$

If $\phi = 0$ or 2π, (4.2) reduces to

$$1 - \frac{4}{f}\sin^2\frac{\theta}{2} \geqslant 0. \qquad (4.4)$$

This will (only) be true if $f < 0$ or $f \geqslant 4$, and so a necessary condition for (4.2) to hold is

$$f < 0 \quad \text{or} \quad f \geqslant 4.$$

This condition implies that (4.1a) is true.

Consider (4.2) again and let $\frac{4}{f} = 1 - \epsilon$ (ϵ not necessarily small). This time (4.2) becomes

$$1 - \left(\sin^2\frac{\theta}{2} + \sin^2\frac{\phi}{2}\right) + \epsilon\left(\sin^2\frac{\theta}{2} + \sin^2\frac{\phi}{2}\right)$$

$$+ [(1-\epsilon)^2 + 4r^2ac]\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2} - rb\sin\theta\sin\phi \geqslant 0,$$

which leads to

$$\cos^2\frac{\theta}{2}\cos^2\frac{\phi}{2} + \epsilon\left(\sin^2\frac{\theta}{2} + \sin^2\frac{\phi}{2}\right)$$

$$+ [\epsilon^2 - 2\epsilon + 4r^2ac]\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2}$$

$$- 4rb\sin\frac{\theta}{2}\cos\frac{\theta}{2}\sin\frac{\phi}{2}\cos\frac{\phi}{2} \geqslant 0,$$

and then

$$\left[2r\sqrt{ac}\sin\frac{\theta}{2}\sin\frac{\phi}{2} - \frac{b}{\sqrt{ac}}\cos\frac{\theta}{2}\cos\frac{\phi}{2}\right]^2$$

$$+ \frac{(ac - b^2)}{ac}\cos^2\frac{\theta}{2}\cos^2\frac{\phi}{2}$$

$$+ \epsilon\left(\sin^2\frac{\theta}{2} + \sin^2\frac{\phi}{2}\right) - 2\epsilon\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2}$$

$$+ \epsilon^2\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2} \geqslant 0,$$

and finally

$$\left[2r\sqrt{ac}\sin\frac{\theta}{2}\sin\frac{\phi}{2} - \frac{b}{\sqrt{ac}}\cos\frac{\theta}{2}\cos\frac{\phi}{2}\right]^2$$

$$+ \frac{(ac - b^2)}{ac}\cos^2\frac{\theta}{2}\cos^2\frac{\phi}{2} + \epsilon\sin^2\frac{\theta}{2}\cos^2\frac{\phi}{2}$$

$$+ \epsilon\sin^2\frac{\phi}{2}\cos^2\frac{\theta}{2} + \epsilon^2\sin^2\frac{\theta}{2}\sin^2\frac{\phi}{2} \geqslant 0.$$

This result is true if $\epsilon \geqslant 0$. But $\epsilon \geqslant 0$ implies either $f \leqslant 0$ or $f \geqslant 4$ according as ϵ is greater or less than 1. Note $f = 0$ is meaningless in practice and can be disregarded. Since the sufficient condition for (4.2) to hold coincides with the necessary condition, it is clear that the unique necessary and sufficient condition for (4.2) to be true is

$$f < 0 \quad \text{or} \quad f \geqslant 4.$$

Now consider (4.3) and let $\frac{4}{f} = 1 - \epsilon$ (ϵ not necessarily small). Condition (4.3) becomes

$$a \sin^2 \frac{\theta}{2} + c \sin^2 \frac{\phi}{2} - (a + c) \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2}$$
$$+ \epsilon(a + c) \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2}$$
$$+ 2b \sin \frac{\theta}{2} \sin \frac{\phi}{2} \cos \frac{\theta}{2} \cos \frac{\phi}{2} \geqslant 0,$$

which gives

$$a \sin^2 \frac{\theta}{2} \cos^2 \frac{\phi}{2} + c \sin^2 \frac{\phi}{2} \cos^2 \frac{\theta}{2}$$
$$+ 2b \sin \frac{\theta}{2} \sin \frac{\phi}{2} \cos \frac{\theta}{2} \cos \frac{\phi}{2}$$
$$+ \epsilon(a + c) \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2} \geqslant 0,$$

and finally

$$\left[\sqrt{a} \sin \frac{\theta}{2} \cos \frac{\phi}{2} + \frac{b}{\sqrt{a}} \sin \frac{\phi}{2} \cos \frac{\theta}{2}\right]^2$$
$$+ \frac{(ac - b^2)}{a} \sin^2 \frac{\phi}{2} \cos^2 \frac{\theta}{2}$$
$$+ \epsilon(a + c) \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2} \geqslant 0$$

which is true if $\epsilon \geqslant 0$. Thus the necessary and sufficient condition for the stability of (3.4) is $f < 0$ or $f \geqslant 4$.

(ii) *Variable coefficients*

To establish the stability of (3.4) for the case of variable coefficients, reference is made to an important paper by Widlund (1965). For convenience in this paper, it is assumed that the coefficients are independent of t. The extension to the general case presents no new difficulties. In Widlund's notation, (3.4) is re-written in the form

$$U_{i,j}^{n+1} = U_{i,j}^n + Q_{-1} U_{i,j}^{n+1} + Q_0 U_{i,j}^n$$

where

$$Q_{-1} = 1 - \left[1 + \left(\frac{1}{f} - \frac{1}{2} ra\right) \delta_x^2\right]\left[1 + \left(\frac{1}{f} - \frac{1}{2} rc\right) \delta_y^2\right]$$

and

$$Q_0 = \left\{\left[1 + \left(\frac{1}{f} + \frac{1}{2} ra\right) \delta_x^2\right]\right.$$
$$\left.\left[1 + \left(\frac{1}{f} + \frac{1}{2} rc\right) \delta_y^2\right] + \frac{1}{2} rbH_x H_y\right\} - 1.$$

The principal parts of these as defined by Widlund are

$$Q_{-1}^{(1)} = -\left(\frac{1}{f} - \frac{1}{2} ra\right) (hD_{+x})(hD_{-x})$$
$$- \left(\frac{1}{f} - \frac{1}{2} rc\right) (hD_{+y})(hD_{-y})$$
$$- \left(\frac{1}{f} - \frac{1}{2} ra\right)\left(\frac{1}{f} - \frac{1}{2} rc\right)(hD_{+x})(hD_{-x})(hD_{+y})(hD_{-y}),$$

and

$$Q_0^{(1)} = \left(\frac{1}{f} + \frac{1}{2} ra\right) (hD_{+x})(hD_{-x})$$
$$+ \left(\frac{1}{f} + \frac{1}{2} rc\right) (hD_{+y})(hD_{-y})$$
$$+ \left(\frac{1}{f} + \frac{1}{2} ra\right)\left(\frac{1}{f} + \frac{1}{2} rc\right)(hD_{+x})(hD_{-x})(hD_{+y})(hD_{-y})$$
$$+ 2rb(hD_{0x})(hD_{0y}),$$

where

$$hD_{\pm x} U(x, y) = \pm(U(x \pm h, y) - U(x, y)),$$
$$hD_{\pm y} U(x, y) = \pm(U(x, y \pm h) - U(x, y)),$$
$$2hD_{0x} U(x, y) = U(x + h, y) - U(x - h, y),$$
$$2hD_{0y} U(x, y) = U(x, y + h) - U(x, y - h).$$

If $hD_{\pm x}$ is replaced by $2i \sin \frac{\theta}{2} e^{\pm i\theta/2}$, $hD_{\pm y}$ by $2i \sin \frac{\phi}{2} e^{\pm i\phi/2}$, hD_{0x} by $i \sin \theta$, and hD_{0y} by $i \sin \phi$, the functions of period 2π

$$\hat{Q}_{-1}^{(1)} = 4\left(\frac{1}{f} - \frac{1}{2} ra\right) \sin^2 \frac{\theta}{2} + 4\left(\frac{1}{f} - \frac{1}{2} rc\right) \sin^2 \frac{\phi}{2}$$
$$- 16\left(\frac{1}{f} - \frac{1}{2} ra\right)\left(\frac{1}{f} - \frac{1}{2} rc\right) \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2},$$

$$\hat{Q}_0^{(1)} = -4\left(\frac{1}{f} + \frac{1}{2} ra\right) \sin^2 \frac{\theta}{2} - 4\left(\frac{1}{f} + \frac{1}{2} rc\right) \sin^2 \frac{\phi}{2}$$
$$+ 16\left(\frac{1}{f} + \frac{1}{2} ra\right)\left(\frac{1}{f} + \frac{1}{2} rc\right) \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2} - 2rb \sin \theta \sin \phi$$

are obtained and so

$$(1 - \hat{Q}_{-1}^{(1)})^{-1}(1 + \hat{Q}_0^{(1)}) =$$
$$\left[1 - 4\left(\frac{1}{f} - \frac{1}{2} ra\right) \sin^2 \frac{\theta}{2}\right]^{-1} \left[1 - 4\left(\frac{1}{f} - \frac{1}{2} rc\right) \sin^2 \frac{\phi}{2}\right]^{-1}$$
$$\times \left\{\left[1 - 4\left(\frac{1}{f} + \frac{1}{2} ra\right) \sin^2 \frac{\theta}{2}\right]\left[1 - 4\left(\frac{1}{f} + \frac{1}{2} rc\right) \sin^2 \frac{\phi}{2}\right]\right.$$
$$\left. - 2rb \sin \theta \sin \phi\right\}$$

It is only necessary to show that

$$\left|\left[1 - 4\left(\frac{1}{f} - \frac{1}{2} ra\right) \sin^2 \frac{\theta}{2}\right]^{-1}\right.$$
$$\left[1 - 4\left(\frac{1}{f} - \frac{1}{2} rc\right) \sin^2 \frac{\phi}{2}\right]^{-1}$$
$$\times \left\{\left[1 - 4\left(\frac{1}{f} + \frac{1}{2} ra\right) \sin^2 \frac{\theta}{2}\right]\right.$$
$$\left.\left.\left[1 - 4\left(\frac{1}{f} + \frac{1}{2} rc\right) \sin^2 \frac{\phi}{2}\right] - 2rb \sin \theta \sin \phi\right\}\right| \leqslant 1.$$

Thus Widlund's analysis in this case is equivalent to von Neumann's analysis and so (3.4) is a stable approximation to the original equation (1.1) with variable coefficients when $f < 0$ or $f \geqslant 4$.

The question of obtaining an optimum value of f in these ranges is difficult to answer. Such a value would probably minimise (3.6), but it is unlikely that this optimum value can be obtained.

5. Numerical results

The A.D.I. method (3.5) is now used to solve examples involving the partial differential equation (1.1) with constant and variable coefficients.

Example 1. Constant coefficients

Here the problem consists of (1.1) with $a = 1$, $b = \frac{1}{2}$, $c = 2$, together with the initial condition

$$u(x, y, 0) = \sin \pi(x + y) \qquad 0 \leqslant x, y \leqslant 1$$

and the boundary conditions

$$\begin{aligned} u(0, y, t) &= e^{-\pi^2(a+2b+c)t} \sin \pi y \\ u(1, y, t) &= -e^{-\pi^2(a+2b+c)t} \sin \pi y \\ u(x, 0, t) &= e^{-\pi^2(a+2b+c)t} \sin \pi x \\ u(x, 1, t) &= -e^{-\pi^2(a+2b+c)t} \sin \pi x. \end{aligned}$$

The theoretical solution is

$$u(x, y, t) = e^{-\pi^2(a+2b+c)t} \sin \pi(x + y).$$

Numerical calculations using (3.5) with $f = -4$, 12 and $h = 0{\cdot}1$ were carried out for four values of the mesh ratio r. The maximum differences between the computed and the theoretical solutions are shown in **Table 1.** A comparison is given with numerical solutions obtained using Samarskii's scheme (2.3), which is probably the best of existing split operator schemes.

Partial verification of the stability analysis presented in this paper for A.D.I. method (3.4) is given in **Table 2.** Here it is shown that instability occurs for $f = 2$, whereas the calculations for $f = -4$, 4, 12 are stable. The errors quoted in Table 2 are at $t = \frac{1}{10}$.

Example 2. Variable coefficients

This time the problem consists of (1.1) with $a = \frac{1}{2}x^2 + y^2$, $b = -\frac{1}{2}(x^2 + y^2)$, $c = x^2 + \frac{1}{2}y^2$ together with the initial conditions

$$u(x, y, 0) = x^2y + xy^2, \qquad 0 \leqslant x, y \leqslant 1$$

and the boundary conditions

$$\begin{aligned} u(0, y, t) &= 0 \\ u(1, y, t) &= y(1 + y)e^{-t} \\ u(x, 0, t) &= 0 \\ u(x, 1, t) &= x(1 + x)e^{-t}. \end{aligned}$$

The theoretical solution is

$$u(x, y, t) = e^{-t}(x^2y + xy^2).$$

The same numerical calculations were carried out as in the constant coefficient case and comparative results between the present scheme and Samarskii's scheme are given in **Table 3.** This time the mean deviation of the difference between the computed and theoretical solution is quoted.

6. Concluding remarks

Although the A.D.I. method (3.5) and most other two level methods referred to in this paper have the same order of local accuracy, namely $0(h^2 + k)$, it appears from Tables 1 and 3 that (3.5), at least for certain values of f, has superior overall accuracy. A contributory factor towards this increased accuracy is almost certainly the fact that intermediate boundary corrections (see Fairweather and Mitchell (1967)) can be applied to (3.5) but not to any of the other methods mentioned in this paper. From (3.5), the intermediate boundary values are given by

$$U_{i,j}^{n+1*} = \left[1 + \left(\frac{1}{f} - \frac{1}{2}rc\right)\delta_y^2\right] g_{i,j}^{n+1} - \left(\frac{1}{f} - \frac{1}{2}rc\right)\delta_y^2 g_{i,j}^n,$$

whereas Samarskii, for example, has to be content with

$$U_{i,j}^{n+1*} = g_{i,j}^{n+1}.$$

Here g is written for U when the grid point is on the boundary of the region. The values of g are of course known and so the intermediate boundary values $U_{i,j}^{n+1*}$ can be calculated from the boundary data, in advance of the main calculation.

Table 1

VALUE OF r	TIME	NUMBER OF TIME STEPS	MAXIMUM DIFFERENCE BETWEEN COMPUTED AND THEORETICAL SOLUTIONS			MAXIMUM THEORETICAL SOLUTION
			McKEE–MITCHELL		SAMARSKII	
			$f = -4$	$f = 12$		
0·1	1/20	50	0·0062	0·0001	0·0025	0·1389
	1/10	100	0·0012	0·0000	0·0005	0·0193
0·5	1/20	10	0·0030	0·0035	0·0130	0·1389
	1/10	20	0·0006	0·0006	0·0022	0·0193
1	1/20	5	0·0016	0·0083	0·0263	0·1389
	1/10	10	0·0003	0·0015	0·0046	0·0193
5	1/20	1	0·1095	0·1287	0·1451	0·1389
	1/10	2	0·0159	0·0218	0·0354	0·0193

There is also little doubt that (3.5) is a much simpler A.D.I. method than that based on (2.7) which is the only other genuine A.D.I. method known to the authors for solving (1.1).

Finally, the method of the present paper can be extended to three level difference formulae, which will certainly enable split schemes of an order of local accuracy of at least $0(h^2 + k^2)$ to be obtained. Of course, this increased accuracy of three level schemes will have to be balanced against their additional complexity.

All calculations were carried out to ten places of decimals on the Elliot 4130 computer of the University of Dundee.

Table 2

Errors at $t = 1/10$

$f \backslash r$	0·1	0·5	1	5
−4	0·0012	0·0006	0·0003	0·0159
2	$0(10^{80})$	$0(10^{38})$	7·2300	0·0317*
4	0·0006	0·0012	0·0021	0·0254
12	0·0000	0·0006	0·0015	0·0218

* Although this value does not demonstrate instability, it can be shown that scheme (3·5) is unstable for $f = 2$ and $r = 5$ by running the scheme for a greater length of time.

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Table 3

VALUE OF r	TIME	NUMBER OF TIME STEPS	MEAN DEVIATION OF THE DIFFERENCE BETWEEN COMPUTED AND THEORETICAL SOLUTIONS			THEORETICAL SOLUTION AT CENTRAL NODAL POINT
			McKEE–MITCHELL		SAMARSKII	
			$f = -4$	$f = 12$		
0·1	1/20	50	0·0122	0·0129	0·0255	0·2378
	1/10	100	0·0152	0·0159	0·0316	0·2262
0·5	1/20	10	0·0123	0·0129	0·0248	0·2378
	1/10	20	0·0152	0·0159	0·0307	0·2262
1	1/20	5	0·0124	0·0130	0·0240	0·2378
	1/10	10	0·0152	0·0158	0·0298	0·2262
5	1/20	1	0·0144	0·0155	0·0189	0·2378
	1/10	2	0·0158	0·0164	0·0252	0·2262

References

Andreev, V. B. (1967). On difference schemes with a splitting operator for general p-dimensional parabolic equations of second order with mixed derivatives. *Zh. Vych. Mat. i mat. fiz.*, Vol. 7, pp. 312–321.

Douglas, J. (Jr.), and Gunn, J. E. (1964). A general formulation of alternating direction methods. Part 1. Parabolic and hyperbolic problems. *Num. Math.*, Vol. 6, pp. 428–453.

Dressel, F. G. (1940). The fundamental solution of the parabolic equation. *Duke Math. J.*, Vol. 7, pp. 186–203.

Fairweather, G., and Mitchell, A. R. (1967). A new computational procedure for A.D.I. methods. *SIAM J.*, Vol. 4, No. 2, pp. 163–170.

Lax, P. D., and Richtmyer, R. D. (1956). Survey of the stability of linear finite difference equations. *Comm. Pure Appl. Math.*, Vol. 9, pp. 267–293.

Mitchell, A. R., and Fairweather, G. (1964). Improved forms of the alternating direction methods of Douglas, Peaceman and Rachford for solving parabolic and elliptic equations. *Num. Math.*, Vol. 6, pp. 285–292.

Peaceman, D. W., and Rachford, H. H. (1955). The numerical solution of parabolic and elliptic differential equations. *J. Soc. Indust. Appl. Math.*, Vol. 3, pp. 28–41.

Protter, M. H., and Weinberger, Hans F. (1967). *Maximum Principles in Differential Equations.* New Jersey: Prentice Hall.

Samarskii, A. A. (1962). On an economical difference method for the solution of a multidimensional parabolic equation in an arbitrary region. *Zh. Vych. Mat. i mat. fiz.*,Vol. 2, No. 5, pp. 787–811.

Samarskii, A. A. (1964). Economical difference schemes for parabolic equations with mixed derivatives. *Zh. Vych. Mat. i mat. fiz.*, Vol. 4, No. 4, pp. 753–759.

Saul'yev, V. K. (1964). *Integration of Equations of Parabolic Type by the Method of Nets*, London, Pergamon Press.

Seidman, T. I. (1963). On stability of certain difference schemes. *Num. Math.*, Vol. 5, pp. 201–210.

Sofronov, I. D. (1963). A contribution to the difference solution of the heat conduction equation in curvilinear co-ordinates. *Zh. Vych. Mat. i mat. fiz.*, Vol. 3, No. 4, pp. 786–788.

Widlund, O. B. (1965). On stability of parabolic difference schemes. *Maths. Comp.*, Vol. 19, No. 89, pp. 1–13.

Yanenko, N. N., Suchkov, V. A., and Podogin, Yu. Ya. (1959) О РАЗНОСТНОМ РЕШЕНИИ УРАВНЕНИЯ ТЕПЛОПРОВОДНОСТИ В КРИВОЛИНЕЙНЫХ КООРДИНАТАХ. *Dokl. Akad. Nauk. SSSR*, Vol. 128, No. 5, pp. 903–905.