Alternating direction methods for parabolic equations in three space dimensions with mixed derivatives

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An alternating direction implicit (ADI) method which requires the solution of three tridiagonal sets of equations at each time step is suggested for solving the general parabolic equation with variable coefficients in three space dimensions. A sufficient condition for stability is proved in the pure initial value case. Other existing finite difference schemes are mentioned and numerical results are presented.

(Received February 1970)

1. Introduction

In the region of (x, t) space given by $R \times (0 \leqslant t \leqslant T)$ where $R = \{0 \leqslant x_i \leqslant 1,\ i = 1, 2, 3\}$ consider the linear parabolic equation

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

where

$$L \equiv \sum_{i=1}^{3} \sum_{j=1}^{3} a_{ij}(x, t) \frac{\partial^2}{\partial x_i \partial x_j} \ ;$$

$$u\,|_{x_i=0} = u_i^-(x, t)\ ,\ u\,|_{x_i=1} = u_i^+(x, t)\ ,\ i = 1, 2, 3\ ;$$

$$u(x, 0) = u_0(x)\ ,\ x = (x_1, x_2, x_3)\ .$$

The matrix of the coefficients $(a_{ij})_{3\times 3}$ is positive definite, that is there exists a $\delta > 0$ such that

$$\sum_{i=1}^{3} \sum_{j=1}^{3} a_{ij}\zeta_i\zeta_j > \delta \sum_{i=1}^{3} \zeta_i^2\ ,\ \zeta = (\zeta_1, \zeta_2, \zeta_3)$$

is any real vector, $\zeta \neq 0$.

A consequence of this definition is that $a_{11} > 0$, $a_{22} > 0$, and $a_{33} > 0$. We assume that the matrix of coefficients is symmetric, $a_{ij} = a_{ji}$.

It is assumed that $u \in C^4$ and $a_{ij} \in C^2$. Existence and uniqueness of the solution of the partial differential equation (1.1) with the appropriate initial and boundary conditions has been studied by Dressel (1940), Protter and Weinberger (1967) and other authors.

The region is covered by a rectilinear grid with $h_i = h$ the grid spacing in the x_i-direction $(i = 1, 2, 3)$ and k the grid spacing in the t-direction. The point (x, t) is a grid point if $x = (\alpha_1 h, \alpha_2 h, \alpha_3 h)$ $(0 \leqslant \alpha_i \leqslant M)$, $t = nk$ $(0 \leqslant n \leqslant L)$ where $Mh = 1$ and $Lk = T$.

It is the purpose of this paper to present an alternating direction finite difference scheme for the numerical solution of (1.1) despite the presence of mixed derivatives; and which requires the solution of only three tridiagonal sets of equations at each time step. We shall define notation consisting of U_n the solution of the difference equation at the grid point $x = (\alpha_1 h, \alpha_2 h, \alpha_3 h)$, $t = nk$, r the mesh ratio k/h^2 and

$$\delta_{x_i}^2 U_n = U(x+he_i, t) - 2U(x, t) + U(x-he_i, t) \quad (i = 1, 2, 3)\ ,$$

$$Hx_iHx_jUn = U(x+he_i+he_j, t) - U(x+he_i-he_j, t) - U(x-he_i+he_j, t) + U(x-he_i-he_j, t)\ (i, j = 1, 2, 3, i \neq j)\ ,$$

$$\sigma_{x_i x_j}^2 U_n = U(x+he_j, t) - U(x-he_i+he_j, t) - U(x, t) + U(x-he_i, t) \quad (i, j = 1, 2, 3, i \neq j)\ ,$$

$$\sigma_{x_i x_j}^4 U_n = U(x+he_i, t) - U(x, t) - U(x+he_i-he_j, t) - U(x-he_j, t) \quad (i, j = 1, 2, 3, i \neq j)\ ,$$

where e_1, e_2, e_3 are the unit vectors in the directions of the x_1-, x_2-, x_3- co-ordinate axes respectively.

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

Several difference schemes have been proposed for the solution of (1.1) subject to appropriate initial and boundary conditions.

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 $\partial^2 u/\partial x_i \partial x_j$, $i, j = 1, 2, 3$ $(i \neq j)$ 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 several difference formulae for the solution of (1.1). These include the schemes

$$\begin{aligned}
\left(1 - \frac{r}{2} a_{11}\delta x_1^2\right) U_{n+1/6} &= \left(1 + \frac{r}{4} a_{12} Hx_1 Hx_2\right) U_n \\
\left(1 - \frac{r}{2} a_{22}\delta x_2^2\right) U_{n+2/6} &= \left(1 + \frac{r}{4} a_{21} Hx_1 Hx_2\right) U_{n+1/6} \\
\left(1 - \frac{r}{2} a_{11}\delta x_1^2\right) U_{n+3/6} &= \left(1 + \frac{r}{4} a_{13} Hx_1 Hx_3\right) U_{n+2/6} \\
\left(1 - \frac{r}{2} a_{33}\delta x_3^2\right) U_{n+4/6} &= \left(1 + \frac{r}{4} a_{31} Hx_1 Hx_3\right) U_{n+3/6} \\
\left(1 - \frac{r}{2} a_{22}\delta x_2^2\right) U_{n+5/6} &= \left(1 + \frac{r}{4} a_{23} Hx_2 Hx_3\right) U_{n+4/6} \\
\left(1 - \frac{r}{2} a_{33}\delta x_3^2\right) U_{n+1} &= \left(1 + \frac{r}{4} a_{32} Hx_3 Hx_2\right) U_{n+5/6}
\end{aligned} \tag{2.1}$$

of Yanenko (1961) (for constant coefficients only),

$$(1 - ra_{ii}\delta x_i^2)\ U_{n+i/3} = \left[1 + r\sum_{j=1}^{i-1} a_{ij}(\sigma_{x_i x_j}^2 + \sigma_{x_i x_j}^4)\right] U_{n+(i-1/3)}$$

$$(i = 1, 2, 3,\ \sum_{j=1}^{0} \equiv 0) \tag{2.2}$$

of Samarskii (1964)

$$\prod_{i=1}^{3}(1 - r\bar{a}_{ii}\delta x_i^2)\ U_{n+1} = \left[1 + r\sum_{i=1}^{3} \overset{+}{a}_{ii}\delta x_i^2 + \tfrac{1}{2} r \sum_{i=1}^{2} \sum_{j>i} a_{ij} Hx_i Hx_j\right] U_n \tag{2.3}$$

of D'Yakonov (1964) where

$$a_{ii} = \bar{a}_{ii} + \overset{+}{a}_{ii}\ ,$$

and finally

$$\prod_{i=1}^{3}(1-\lambda r a_{ii}\delta x_i^2)(U_{n+1}-U_n) = r\left[\sum_{i=1}^{3} a_{ii}\delta x_i^2+\sum_{i=1}^{2}\sum_{j>i} a_{ij}(\sigma^2_{x_i x_j}+\sigma^4_{x_i x_j})\right]U_n \quad (2.4)$$

of Andreev (1967) where λ is a parameter.

3. ADI schemes

The authors (1970) have already proposed the finite difference scheme

$$\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{11}\right)\delta x_1^2\right]\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{22}\right)\delta x_2^2\right]U_{n+1} = \left\{\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{11}\right)\delta x_1^2\right]\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{22}\right)\delta x_2^2\right] + \tfrac{1}{2}ra_{12}Hx_1Hx_2\right\}U_n \quad (3.1)$$

for the parabolic equation in two space dimensions

$$\frac{\partial u}{\partial t} = a_{11}(x,t)\frac{\partial^2 u}{\partial x_1^2}+2a_{12}(x,t)\frac{\partial^2 u}{\partial x_1\partial x_2}+a_{22}(x,t)\frac{\partial^2 u}{\partial x_2^2}$$

subject to

$$a_{11}a_{22}-a_{12}^2>0\,,\ a_{11}>0\,,\ a_{22}>0\,,$$

with $a_{12} = a_{21}$, $x = (x_1x_2)$.

The obvious extension of this scheme to three space dimensions is

$$\prod_{i=1}^{3}\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)\delta x_i^2\right]U_{n+1} = \prod_{i=1}^{3}\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\delta x_i^2\right]U_n + \tfrac{1}{2}r\sum_{i=1}^{2}\sum_{j>i}a_{ij}Hx_iHx_jU_n \quad (3.2)$$

where f is an arbitrary real parameter.

Straightforward Taylor expansions of the operators in (3.2) shows that the latter is a finite difference approximation to (1.1) with local accuracy of order $O(h^2 + k)$.

The Douglas Rachford type splitting of (3.2) is

$$\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{11}\right)\delta x_1^2\right]U^*_{n+1} = \prod_{i=1}^{3}\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\delta x_i^2\right]U_n - \prod_{i=1}^{3}\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)\delta x_i^2\right]U_n + \left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{11}\right)\delta x_1^2\right]U_n + \tfrac{1}{2}r\sum_{i=1}^{2}\sum_{j>i}a_{ij}Hx_iHx_jU_n \quad (3.3)$$

$$\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{22}\right)\delta x_2^2\right]U^{**}_{n+1} = U^*_{n+1}+\left(\frac{1}{f}-\frac{1}{2}ra_{22}\right)\delta x_2^2U_n$$

$$\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{33}\right)\delta x_3^2\right]U_{n+1} = U^{**}_{n+1}+\left(\frac{1}{f}-\frac{1}{2}ra_{33}\right)\delta x_3^2U_n$$

Special cases of (3.2) are already in existence when $a_{11} = a_{22} = a_{33} = 1$, and the mixed derivative terms are zero. These are the three space dimensional analogue of the Peaceman-Rachford formula (see Gourlay and Mitchell, 1967) when $f = \infty$ and the high accuracy extended Mitchell-Fairweather scheme (EMF) (see Fairweather *et al.*, 1966) when $f = 12$.

4. Stability

We shall first establish the following lemmas.

Lemma 1:

The positive definiteness of the matrix of coefficients implies that the following inequalities hold:

$$\text{I1}: a_{11}\sin^2\theta_1+a_{22}\sin^2\theta_2+a_{33}\sin^2\theta_3+2a_{12}\sin\theta_1\sin\theta_2 +2a_{13}\sin\theta_1\sin\theta_3+2a_{23}\sin\theta_2\sin\theta_3>0\,,$$

$$\text{I2}: a_{11}\sin^2\theta_1+a_{22}\sin^2\theta_2+a_{33}\sin^2\theta_3+2a_{12}\sin\theta_1\sin\theta_2 -2a_{13}\sin\theta_1\sin\theta_3-2a_{23}\sin\theta_2\sin\theta_3>0\,.$$

Proof of I1:

Positive definiteness of $(a_{ij})_{3\times 3}$ implies that

$$\sum_{i=1}^{3}\sum_{j=1}^{3}a_{ij}\zeta_i\zeta_j>0\,,$$

for all real vectors, $\zeta \neq 0$, that is

$$a_{11}\zeta_1^2+a_{22}\zeta_2^2+a_{33}\zeta_3^2+2a_{12}\zeta_1\zeta_2+2a_{13}\zeta_1\zeta_3+2a_{23}\zeta_2\zeta_3>0 \quad (4{\cdot}1)$$

But since this is true for all ζ_1, ζ_2, ζ_3 it is true in particular for $\zeta_i = \sin\theta_i (i = 1, 2, 3)$. This gives the required result.

Proof of I2:

Since (4.1) holds for all real ζ_1, ζ_2, ζ_3 it is true in particular for $\zeta_1 = \sin\theta_1$, $\zeta_2 = \sin\theta_2$, $\zeta_3 = -\sin\theta_3$.

The inequality

$$a_{11}\sin^2\theta_1+a_{22}\sin^2\theta_2+a_{33}\sin^2\theta_3+2a_{12}\sin\theta_1\sin\theta_2 -2a_{13}\sin\theta_1\sin\theta_3-2a_{23}\sin\theta_2\sin\theta_3>0$$

is obtained and the second part of the lemma is proved.

Lemma 2:

Necessary and sufficient conditions for the matrix of coefficients $(a_{ij})_{3\times 3}$ to be positive definite are:

1. $a_{11}a_{22}-a_{12}^2>0\,,\ a_{11}a_{22}a_{33}-a_{11}a_{23}^2-a_{22}a_{13}^2-a_{33}a_{12}^2+2a_{12}a_{13}a_{23}>0$
2. $a_{11}a_{33}-a_{13}^2>0\,,\ a_{11}a_{22}a_{33}-a_{11}a_{23}^2-a_{22}a_{13}^2-a_{33}a_{12}^2+2a_{12}a_{13}a_{23}>0$
3. $a_{22}a_{33}-a_{23}^2>0\,,\ a_{11}a_{22}a_{33}-a_{11}a_{23}^2-a_{22}a_{13}^2-a_{33}a_{12}^2+2a_{12}a_{13}a_{23}>0$

These results are well known and follow from completion of squares. The proof is given in Fraser, Duncan, and Collar (1963).

To establish the stability of (3.2) for the case of variable coefficients, reference is made to an important paper by Widlund (1965). For convenience, it is assumed that the coefficients are independent of t. The extension to the general case presents no new difficulties.

Theorem 1:

A sufficient condition for the stability of (3.2) is

$$-\frac{2}{r\max_i\{\max_{0\leqslant x\leqslant 1} a_{ii}(x)\}}<f<0$$

Proof:

In Widlund's notation (3.2) is re-written in the form

$$U_{n+1} = U_n+Q_{-1}U_{n+1}+Q_0U_n$$

where

$$Q_{-1} = 1-\prod_{i=1}^{3}\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\delta x_i^2\right]$$

and

$$Q_0 = \prod_{i=1}^{3}\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\delta_{x_i}^2\right]-1+\tfrac{1}{2}r\sum_{i=1}^{2}\sum_{j>i}a_{ij}Hx_iHx_j\ .$$

The principal parts of these are

$$Q_{-1}^{(1)} = 1-\prod_{i=1}^{3}\left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)(hD_{+i}(h))\,(hD_{-i}(h))\right],$$

and

$$Q_0^{(1)} = \prod_{i=1}^{3}\left[1+\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)(hD_{+i}(h))\,(hD_{-i}(h))\right]$$

$$-1+2r\sum_{i=1}^{2}\sum_{j>i}a_{ij}(hD_{0i}(h))\,(hD_{0j}(h))\ ,$$

where

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

If $hD_{\pm i}(h)$ is replaced by

$$2\sqrt{-1}\,\sin\frac{\theta_i}{2}\,e^{\pm\sqrt{-1}\,\frac{\theta_i}{2}}\ ,\ hD_{0i}(h)\text{ by }\sqrt{-1}\,\sin\theta_i$$

the functions of period 2π

$$\hat{Q}_{-1}^{(1)} = 1-\prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right],$$

and

$$\hat{Q}_0^{(1)} = \prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]-1$$

$$-2r\sum_{i=1}^{2}\sum_{j>i}a_{ij}\sin\theta_i\sin\theta_j$$

are obtained and so

$$(I-\hat{Q}_{-1}^{(1)})^{-1}(I+\hat{Q}_0^{(1)})$$

$$=\left[\prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]\right]^{-1}$$

$$\times\left\{\prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]-2r\sum_{i=1}^{2}\sum_{j>i}a_{ij}\sin\theta_i\sin\theta_j\right\}$$

Since $(I-\hat{Q}_{-1}^{(1)})^{-1}(I+\hat{Q}_0^{(1)})$ is scalar, Widlund requires for stability in the L_2 norm that

$$\left|\left\{\prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]\right\}^{-1}\times\left\{\prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}+\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]-2r\sum_{i=1}^{2}\sum_{j>i}a_{ij}\sin\theta_i\sin\theta_j\right\}\right|<1\ , \quad (4.2)$$

allowing equality only when $\sin\theta_i = 0$ ($i = 1, 2, 3$). The result (4.2) leads to

$$4a_{11}\sin^2\frac{\theta_1}{2}+4a_{22}\sin^2\frac{\theta_2}{2}+4a_{33}\sin^2\frac{\theta_3}{2}$$
$$-\frac{16}{f}(a_{11}+a_{22})\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}$$
$$-\frac{16}{f}(a_{11}+a_{33})\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_3}{2}$$
$$-\frac{16}{f}(a_{22}+a_{33})\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2}$$
$$+64\left[\frac{a_{11}}{f^2}+\frac{a_{22}}{f^2}+\frac{a_{33}}{f^2}+\frac{1}{4}r^2a_{11}a_{22}a_{33}\right]$$
$$\times\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2}$$
$$+2a_{12}\sin\theta_1\sin\theta_2+2a_{13}\sin\theta_1\sin\theta_3$$
$$+2a_{23}\sin\theta_2\sin\theta_3>0\ , \quad (4.3)$$

$$1-\frac{4}{f}\left(\sin^2\frac{\theta_1}{2}+\sin^2\frac{\theta_2}{2}+\sin^2\frac{\theta_3}{2}\right)$$
$$+16\left(\frac{1}{f^2}+\frac{1}{4}r^2a_{11}a_{22}\right)\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}$$
$$+16\left(\frac{1}{f^2}+\frac{1}{4}r^2a_{11}a_{33}\right)\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_3}{2}$$
$$+16\left(\frac{1}{f^2}+\frac{1}{4}r^2a_{22}a_{33}\right)\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2}$$
$$-64\left[\frac{1}{f^3}+r^2\frac{a_{11}}{4f}a_{22}+r^2\frac{a_{11}}{4f}a_{33}+r^2\frac{a_{22}}{4f}a_{33}\right]$$
$$\times\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2}$$
$$-ra_{12}\sin\theta_1\sin\theta_2-ra_{13}\sin\theta_1\sin\theta_3$$
$$-ra_{23}\sin\theta_2\sin\theta_3>0\ , \quad (4.4)$$

together with

$$\prod_{i=1}^{3}\left[1-4\left(\frac{1}{f}-\frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]>0\ . \quad (4.5)$$

Using the result that $\sin^2\theta_i \leqslant 4\sin^2(\theta_i/2)$ and with the aid of inequality I1 of lemma 1, it can be seen that a sufficient condition for (4.3) to hold is that $f < 0$. This condition ensures that (4.5) holds.

By means of inequality I2 of the lemma 1 re-written in the form

$$-a_{13}\sin\theta_1\sin\theta_3-a_{23}\sin\theta_2\sin\theta_3>-\tfrac{1}{2}(a_{11}\sin^2\theta_1+a_{22}\sin^2\theta_2+a_{33}\sin^2\theta_3)-a_{12}\sin\theta_1\sin\theta_2\ ,$$

the left hand side of (4.4) is greater than

$$1-\frac{4}{f}\left(\sin^2\frac{\theta_1}{2}+\sin^2\frac{\theta_2}{2}+\sin^2\frac{\theta_3}{2}\right)-\frac{ra_{11}}{2}\sin^2\theta_1$$
$$-\frac{ra_{22}}{2}\sin^2\theta_2-\frac{ra_{33}}{2}\sin^2\theta_3-ra_{12}\sin\theta_1\sin\theta_2$$
$$+16\left(\frac{1}{f^2}+\frac{1}{4}r^2a_{11}a_{22}\right)\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}$$
$$+16\left(\frac{1}{f^2}+\frac{1}{4}r^2a_{11}a_{33}\right)\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_3}{2}$$
$$+16\left(\frac{1}{f^2}+\frac{1}{4}r^2a_{22}a_{33}\right)\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2}$$
$$-64\left[\frac{1}{f^3}+r^2\frac{a_{11}}{4f}a_{22}+r^2\frac{a_{11}}{4f}a_{33}+r^2\frac{a_{22}}{4f}a_{33}\right]$$
$$\times\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2} \quad (4.6)$$

Let

$$\frac{4}{f} = -2r \max_{i}\left\{\max_{0\leqslant x\leqslant 1} a_{ii}(x)\right\} - \varepsilon$$

and for convenience denote $\max_{i}\{\max_{0\leqslant x\leqslant 1} a_{ii}(x)\}$ by $a_{\max}$. The left hand side of (4.6) then becomes

$$\begin{aligned}
1 &+ 2r\sin^2\frac{\theta_1}{2}\left[a_{\max} - a_{11}\cos^2\frac{\theta_1}{2}\right] \\
&+ 2r\sin^2\frac{\theta_2}{2}\left[a_{\max} - a_{22}\cos^2\frac{\theta_2}{2}\right] \\
&+ 2r\sin^2\frac{\theta_3}{2}\left[a_{\max} - a_{33}\cos^2\frac{\theta_3}{2}\right] \\
&+ \varepsilon\left(\sin^2\frac{\theta_1}{2} + \sin^2\frac{\theta_2}{2} + \sin^2\frac{\theta_3}{2}\right) \\
&- ra_{12}\sin\theta_1\sin\theta_2 \\
&+ [(2ra_{\max}+\varepsilon)^2 + 4r^2 a_{11}a_{22}]\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2} \\
&+ [(2ra_{\max}+\varepsilon)^2 + 4r^2 a_{11}a_{33}]\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_3}{2} \\
&+ [(2ra_{\max}+\varepsilon)^2 + 4r^2 a_{22}a_{33}] \\
&\times \sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_3}{2} + [(2ra_{\max}+\varepsilon)^2 \\
&+ 4r^2 a_{11}a_{22}(2ra_{\max}+\varepsilon) \\
&+ 4r^2 a_{11}a_{33}(2ra_{\max}+\varepsilon) \\
&+ 4r^2 a_{22}a_{33}(2ra_{\max}+\varepsilon)]\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2},
\end{aligned}$$

which can be re-written in the form

$$\begin{aligned}
&\left[\frac{a_{12}}{\sqrt{a_{11}a_{22}}}\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2} - 2r\sqrt{a_{11}a_{22}}\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\right]^2 \\
&+ \frac{\left(a_{11}a_{22} - a_{12}^2\cos^2\frac{\theta_1}{2}\cos^2\frac{\theta_2}{2}\right)}{a_{11}a_{22}} \\
&+ 2r\sin^2\frac{\theta_1}{2}\left[a_{\max} - a_{11}\cos^2\frac{\theta_1}{2}\right] \\
&+ 2r\sin^2\frac{\theta_2}{2}\left[a_{\max} - a_{22}\cos^2\frac{\theta_2}{2}\right] \\
&+ 2r\sin^2\frac{\theta_3}{2}\left[a_{\max} - a_{33}\cos^2\frac{\theta_3}{2}\right] \\
&+ (2ra_{\max}+\varepsilon)^2\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2} \\
&+ [(2ra_{\max}+\varepsilon)^2 + 4r^2 a_{11}a_{33}]\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_3}{2} \\
&+ [(2ra_{\max}+\varepsilon)^2 + 4r^2 a_{22}a_{33}]\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2} \\
&+ [(2ra_{\max}+\varepsilon)^3 + 4r^2 a_{11}a_{22}(2ra_{\max}+\varepsilon) \\
&+ 4r^2 a_{11}a_{33}(2ra_{\max}+\varepsilon) \\
&+ 4r^2 a_{22}a_{33}(2ra_{\max}+\varepsilon)]\sin^2\frac{\theta_1}{2}\sin^2\frac{\theta_2}{2}\sin^2\frac{\theta_3}{2} \\
&+ \varepsilon\left(\sin^2\frac{\theta_1}{2} + \sin^2\frac{\theta_2}{2} + \sin^2\frac{\theta_3}{2}\right),
\end{aligned}$$

which by lemma 2 is greater than zero for all $r > 0$ and $\sin\theta_i \neq 0$ $(i = 1, 2, 3)$ if $\varepsilon > 0$. But $\varepsilon > 0$ implies that

$$f > -\frac{2}{ra_{\max}}$$

Therefore a sufficient condition for stability of (3.2) is

$$-\frac{2}{r\max_{i}\{\max_{0\leqslant x\leqslant 1} a_{ii}(x)\}} < f < 0 \ . \qquad (4.7)$$

In an earlier paper (McKee and Mitchell, 1970) we proved that a necessary and sufficient condition for the stability of (3.1) is that f lies in either of the two semi-infinite ranges $f < 0$ or $f \geqslant 4$. This result is very satisfactory and it includes two well-known stable schemes when $a_{12} = 0$ namely, the Peaceman-Rachford scheme (1955) when $f = \infty$, and the high accuracy Fairweather-Mitchell scheme (1964) when $f = 12$. However, in the three space dimensional case this condition for stability does not hold in general (as counter examples show), although in the particular case when the coefficients of the mixed derivative terms are zero, this condition remains as a necessary and sufficient condition for stability (see Theorem 2).

Theorem 2:

A necessary and sufficient condition for stability of (3.2) when the coefficients of the mixed derivatives of (1.1) are zero is that f lies in either of the two semi-infinite ranges

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

Proof:

In this particular case application of Widlund's analysis leads to the inequality

$$\left|\left\{\prod_{i=1}^{3}\left[1 - 4\left(\frac{1}{f} - \frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]\right\}^{-1}\left\{\prod_{i=1}^{3}\left[1 - 4\left(\frac{1}{f} + \frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]\right\}\right| < 1 \qquad (4.8)$$

where equality is only allowed when $\sin\theta_i = 0$ $(i = 1, 2, 3.)$. This can be re-written as

$$\left|\prod_{i=1}^{3} F(a_{ii}, \theta_i)\right| < 1$$

where

$$F(a_{ii}, \theta_i) = \frac{\left[1 - 4\left(\frac{1}{f} + \frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]}{\left[1 - 4\left(\frac{1}{f} - \frac{1}{2}ra_{ii}\right)\sin^2\frac{\theta_i}{2}\right]} \qquad (4.9)$$

Clearly $|F(a_{ii}, \theta_i)| < 1$ for arbitrary i is a necessary and sufficient condition for (4.8) to hold.

Let $(4/f) = 1 - \varepsilon$ in (4.9) to obtain

$$|F(a_{ii}, \theta_i)| = \left|\frac{\left(1 - \sin^2\frac{\theta_i}{2}\right) + (\varepsilon - 2ra_{ii})\sin^2\frac{\theta_i}{2}}{\left(1 - \sin^2\frac{\theta_i}{2}\right) + (\varepsilon + 2ra_{ii})\sin^2\frac{\theta_i}{2}}\right|,$$

and it is now evident that $\varepsilon > 0$ is a necessary and sufficient condition for the inequality

$$|F(a_{ii}, \theta_i)| < 1$$

to hold for all $r > 0$. Since $\varepsilon > 0$ implies $f < 0$ or $f \geqslant 4$ we have proved the theorem.

We now give two counter examples to demonstrate that the stability conditions for the two space dimensional problem with a mixed derivative (i.e. $f < 0$ or $f \geqslant 4$) do not hold for the three space dimensional problem when mixed derivatives are present.

Counter Example 1:

By choosing the variables in the following manner:

$$r = 1\,,\ a_{11} = a_{22} = a_{33} = 196$$
$$a_{12} = a_{13} = a_{23} = 195$$
$$\theta_1 = \theta_2 = \theta_3 = \pi/30$$

and by choosing f to be negative and sufficiently small (i.e. close to $-\infty$) it can be shown that inequality (4.4) is violated.

Counter Example 2:

By choosing the variables in the following manner:

$$r = 0{\cdot}1\,,\ a_{11} = a_{22} = 10\,,\ a_{33} = 1\,,$$
$$a_{13} = a_{23} = 1\,,\ a_{12} = 9\,,$$
$$\theta_1 = -\pi/2\,,\ \theta_2 = \pi/2\,,\ \theta_3 = \pi\,,$$

and by choosing f to be sufficiently close to $+4$ it can be shown that inequality (4.3) is violated.

It is important to remember that Widlund's analysis is applicable to pure initial value problems only and so the above theorems are similarly restricted. However, numerical experimentation, the results of which are shown in the next section, leads to the belief that the stability condition (4.7) obtained using Widlund's analysis, applies to a large class of initial boundary value problems.

5. Numerical results

The ADI method (3.3) is now used to solve examples involving the equation (1.1) with constant and variable coefficients.

Example 1, *constant coefficients*:

Here the problem consists of (1.1) with $a_{11} = a_{22} = a_{33} = 0{\cdot}1$, $a_{12} = a_{13} = -0{\cdot}05$, $a_{23} = 0{\cdot}05$ together with the initial condition

$$u(x_1, x_2, x_3, 0) = \sin(x_1+x_2+x_3) \quad 0 \leqslant x_1, x_2, x_3 \leqslant 1$$

and the boundary conditions

$$u(0, x_2, x_3, t) = e^{-\alpha t}\sin(x_2+x_3)$$
$$u(1, x_2, x_3, t) = e^{-\alpha t}\sin(1+x_2+x_3)$$
$$u(x_1, 0, x_3, t) = e^{-\alpha t}\sin(x_1+x_3)$$
$$u(x_1, 1, x_3, t) = e^{-\alpha t}\sin(x_1+1+x_3)$$
$$u(x_1, x_2, 0, t) = e^{-\alpha t}\sin(x_1+x_2)$$
$$u(x_1, x_2, 1, t) = e^{-\alpha t}\sin(x_1+x_2+1)$$

where $\alpha = \sum_{i=1}^{3}\sum_{j=1}^{3} a_{ij}$. The theoretical solution is

$$u(x_1, x_2, x_3, t) = e^{-\alpha t}\sin(x_1+x_2+x_3).$$

Numerical calculations using (3.3) with $f = -4$ were carried out for four values of the mesh ratio r. The absolute value of the central node with the corresponding theoretical solution is shown in **Table 1.** In this example, the sufficient condition for stability (4.7) reduces to $r < 5$.

Example 2, *variable coefficients*:

This time the problem consists of (1.1) with $a_{11} = a_{22} = 0{\cdot}5$, $a_{33} = 1 - x_3^2/2$, $a_{12} = -x_1x_2/8$, $a_{13} = a_{23} = 0$, together with the initial condition

$$u(x_1, x_2, x_3, 0) = x_1^2+x_2^2-x_3^2-x_1^2x_2^2\,,\ 0 \leqslant x_1, x_2, x_3 \leqslant 1\,,$$

and the boundary conditions

$$u(0, x_2, x_3, t) = (x_2^2-x_3^2)\,e^{-t}$$
$$u(1, x_2, x_3, t) = (1-x_3^2)\,e^{-t}$$
$$u(x_1, 0, x_3, t) = (x_1^2-x_3^2)\,e^{-t}$$
$$u(x_1, 1, x_3, t) = (1-x_3^2)\,e^{-t}$$
$$u(x_1, x_2, 0, t) = (x_1^2+x_2^2-x_1^2x_2^2)\,e^{-t}$$
$$u(x_1, x_2, 1, t) = (x_1^2+x_2^2-1-x_1^2x_2^2)\,e^{-t}\,.$$

The theoretical solution is

$$u(x_1, x_2, x_3, t) = (x_1^2+x_2^2-x_3^2-x_1^2x_2^2)\,e^{-t}\,.$$

The same numerical calculations were carried out and are presented in **Table 2.**

Note that in this example the sufficient condition for stability given by (4.7) in Theorem 1 gives $r < \frac{1}{2}$. This condition is violated by three of the calculations recorded in Table 2. However, since in this example we can omit the use of inequality *I*2 and as before by completion of the square we can show that a sufficient condition for stability in this case is $f < 0$. This is, of course, only true when two of the coefficients of the mixed derivative terms are zero.

It is also worth pointing out that although the errors in the constant coefficient case are decidedly smaller than in the variable coefficient case, this does not mean that (3.3) gives better results in the constant coefficient case; the greater accuracy is purely a function of the particular problem chosen as an examination of the principal part of the truncation error will demonstrate.

6. Concluding remarks

The accuracy of this method is almost certainly enhanced by means of boundary correction (see Gourlay and Mitchell, 1967). The intermediate boundary values are given by

$$U^*_{n+1} = \left[1+\left(\frac{1}{f}-\frac{1}{2}ra_{22}\right)\delta x_2^2\right] \times\left\{g_{n+1}+\left(\frac{1}{f}-\frac{1}{2}ra_{33}\right)\delta x_3^2(g_{n+1}-g_n)\right\} - \left(\frac{1}{f}-\frac{1}{2}ra_{22}\right)\delta x_2^2 g_n$$

Table 1

VALUE OF r	TIME	NUMBER OF TIME STEPS	ABSOLUTE VALUE OF THE ERROR AT THE CENTRAL NODE $f = -4$	CORRESPONDING THEORETICAL SOLUTION
0·1	1/10	100	$0(10^{-5})$	0(1)
0·5	1/10	20	$0(10^{-6})$	0(1)
1	1/10	10	$0(10^{-6})$	0(1)
5	1/10	2	$0(10^{-5})$	0(1)

Table 2

VALUE OF r	TIME	NUMBER OF TIME STEPS	ABSOLUTE VALUE OF THE ERROR AT THE CENTRAL NODE $f = -4$	CORRESPONDING THEORETICAL SOLUTION
0·1	1/10	100	$0(10^{-3})$	0(·1)
0·5	1/10	20	$0(10^{-3})$	0(·1)
1	1/10	10	$0(10^{-3})$	0(·1)
5	1/10	2	$0(10^{-3})$	0(·1)

and

$$U_{n+1}^{**} = g_{n+1} + \left(\frac{1}{f} - \frac{1}{2}ra_{33}\right)\delta x_3^2(g_{n+1} - g_n)$$

as opposed to, say $U_{n+1}^{**} = U_{n+1}^{*} = g_{n+1}$. 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 can be calculated from the boundary data in advance of the main calculation.

Finally, three level difference schemes have been considered for the solution of (1.1). These enable split difference schemes of an order of local accuracy of at least $O(h^2 + k^2)$ to be obtained but, of course, this increased accuracy has to be balanced against their additional complexity.

All calculations were carried out to eight places of decimals on the Elliott 4130 computer at the University of Dundee.

Acknowledgement

Dr. McKee's share of the work was carried out whilst he was in receipt of a Science Research Council grant.

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