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AN ALTERNATING-DIRECTION IMPLICIT SCHEME FOR PARABOLIC EQUATIONS WITH MIXED DERIVATIVES

I. J. D. CRAIG and A. D. SNEYD

Department of Mathematics, University of Waikato, Hamilton, New Zealand

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Abstract—An alternating-direction implicit method for N -dimensional parabolic equations with mixed derivatives is considered. The method requires the solution of N tridiagonal matrix equations per time-step and combines computational simplicity with the possibility of unconditional stability for any N . The regimes of conditional stability for $N \leq 6$ show that the scheme is less effective for higher dimensional problems, owing to the proliferation of mixed derivatives. An alternative scheme (requiring $2N$ tridiagonal operations) which involves a single iteration to time-centre the mixed derivatives is shown to improve accuracy and stability. In particular the iterative scheme allows second-order accuracy and unconditional stability in the important special cases of two and three space dimensions.

1. INTRODUCTION

We consider initial value problems of the form

$$\frac{\partial u}{\partial t} = Lu, \quad (1)$$

where L is an elliptic partial differential operator

$$L = \sum_{i=1}^N \sum_{j=1}^N q_{ij} \partial_i \partial_j \quad \left(\partial_i = \frac{\partial}{\partial x_i} \right), \quad (2)$$

defined in some rectangular region R , $0 \leq x_i \leq 1$, and whose coefficients are functions of the x_i and t having continuous second partial derivatives. The parabolicity of problem (1) implies that the symmetric matrix $Q = (q_{ij})$ is positive definite so that problem (1) is well-posed [cf. 1].

Our present purpose is to construct an unconditionally stable finite difference approximation to problem (1) that can be resolved in terms of alternating-direction implicit (ADI) methods in three or more space dimensions. Although a variety of stable ADI schemes are available for multi-dimensional parabolic equations *in the absence of mixed derivatives*, it is well-known that “cross terms” can be difficult to handle implicitly using the ADI technique [2]. Lax and Richtmyer [3], for example, resorted to relaxation methods to resolve the implicit system of equations that derive from problem (1) in the case of two space dimensions. Russian authors however, invoking “fractional step” methods, have shown that 2-D problems can be reduced to the solution of just two tridiagonal matrix equations per time-step [e.g. 4], while McKee and Mitchell [5] have developed an equally effective ADI scheme. Russian workers [6–9] have also considered extensions to N dimensions but the stability criteria they employ are too crude to be of practical use (as discussed in Sections 2 and 3). More recent work has established convergence results for N -dimensional fractional step methods [10] and semi-discrete projection methods [11–13]. In this paper we consider an ADI method applicable to any number N of space dimensions, and determine detailed stability criteria up to $N = 6$ —the dimensionality of the Fokker–Planck equation, for example.

The main motivation for this study is that complicated problems involving the solution of *parabolic systems of partial differential equations* can often be tackled effectively with a sequence of ADI operations [14]. In such applications it is vital to use robust numerical schemes that permit a generous trade-off between computational accuracy and stability [15]. A specific application of the present ADI method to an astrophysical problem involving the structure and stability of 3-D fields *over a non-rectangular region* is described in Ref. [14].

The numerical scheme is outlined in Section 2. We begin by discussing a simple scheme in which the mixed derivatives are treated explicitly. It turns out that some advantage may be obtained in terms of increased accuracy and stability by employing an iterative version of the scheme to "time-centre" the mixed derivatives. In Section 3 the stability of the simple method is examined in detail, and it appears that unconditional stability is always possible but entails some loss of accuracy for $N \geq 5$. Domains of conditional stability are examined in all cases. Section 4 discusses the stability of the iterated scheme, and we find that one iteration will lead to significant improvements in stability and accuracy. In the important case of three space dimensions, second-order accuracy and unconditional stability can be attained. In Section 5 some extensions of the method to operators with lower-order space derivatives or non-constant coefficients, are outlined.

In what follows we shall use the symbol u_{j_1, \dots, j_N}^n to denote the finite difference solution at the node point $(j_1 \Delta x_1, \dots, j_N \Delta x_N, n \Delta t)$ under the assumption that $\Delta x_i = \Delta$ defines a uniform space mesh. Operations such as (for example, in two space dimensions)

$$\delta_x^2 u_{ij} = u_{i+1,j} - 2u_{ij} + u_{i-1,j},$$

and

$$\delta_{xy} u_{ij} = u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}$$

define conventional central difference operators.

2. THE NUMERICAL SCHEME

The basic scheme we consider can be written in the "unsplit" form

$$Au^{n+1} = (A + B)u^n, \quad (3)$$

where

$$A = \prod_{i=1}^N (1 - \theta r q_{ii} \delta_{x_i}^2) \quad (4)$$

and

$$B = r \sum_{i=1}^N q_{ii} \delta_{x_i}^2 + \frac{1}{2} r \sum_{i=2}^N \sum_{j=1}^{i-1} q_{ij} \delta_{x_i x_j}; \quad (5)$$

$r = \Delta t / \Delta^2$ and θ is a real parameter that determines the implicitness of the method. In practice the scheme is split into ADI form and resolved as a sequence of N tridiagonal matrix operations, namely

$$\begin{aligned} (1 - \theta q_{11} r \delta_{x_1}^2) u^{n+1(1)} &= \left[1 + r(1 - \theta) q_{11} \delta_{x_1}^2 + r \sum_{i=2}^N q_{ii} \delta_{x_i}^2 + \frac{1}{2} r \sum_{i=2}^N \sum_{j=1}^{i-1} q_{ij} \delta_{x_i x_j} \right] u^n, \\ (1 - \theta q_{22} r \delta_{x_2}^2) u^{n+1(2)} &= u^{n+1(1)} - \theta q_{22} r \delta_{x_2}^2 u^n, \\ &\vdots \\ (1 - \theta q_{NN} r \delta_{x_N}^2) u^{n+1} &= u^{n+1(N-1)} - \theta q_{NN} r \delta_{x_N}^2 u^n, \end{aligned} \quad (6)$$

where $u^{n+1(i)}$ denotes the approximation to u^{n+1} at split level (i) .

We note, first of all that this scheme can be regarded as a natural extension of previous ADI methods for parabolic equations. For example when $N = 3$ and the cross terms are absent (i.e. $q_{ij} = 0$, $i \neq j$), the choice $\theta = 1$ defines an unconditionally stable Douglas-Rachford method [16] of $O(\Delta t) + O(\Delta^2)$, whereas the choice $\theta = \frac{1}{2}$ yields a higher-order scheme [$O(\Delta t^2) + O(\Delta^2)$] which is again unconditionally stable [17]. When mixed derivatives are present however, the accuracy remains [$O(\Delta t) + O(\Delta^2)$] independent of θ , owing to the one-sided time differencing of the cross terms.

In the case of two space dimensions with mixed derivatives, scheme (6) has the same structure as the stable ($\theta \geq \frac{1}{2}$) ADI scheme advocated by McKee and Mitchell [5 cf. 18]. Russian authors [6, 8] have also considered schemes very similar to scheme (6) but have assumed very crude stability bounds [cf. condition (16)].

In applying the method it is essential that the boundary conditions be handled in a way which involves no loss of accuracy. This can sometimes be difficult in split-level schemes since intermediate values such as $u^{n+1(i)}$ often emerge as mathematical artifacts of the numerical method, bearing no simple relation to the analytic solution at the advanced time level $(n + 1)$. In the present case we note that formal accuracy can always be maintained by expressing the intermediate boundary values $u_b^{n+1(i)}$ in terms of u_b^{n+1} and u_b^n , via

$$u_b^{n+1(i)} = u_b^n + \prod_{j=i+1}^N (1 - \theta q_{jj} r \delta_{x_j}^2) (u_b^{n+1} - u_b^n)$$

as discussed more generally in Ref. [19].

We also consider an iterative application of the basic scheme which includes a second step to time-centre the mixed derivatives, namely

$$Au_{(1)}^{n+1} = (A + B)u^n \tag{7a}$$

and

$$Au^{n+1} = (A + B)u^n + \lambda M(u_{(1)}^{n+1} - u^n), \tag{7b}$$

where the operator

$$M = \frac{1}{2}r \sum_{i=2}^N \sum_{j=1}^{i-1} q_{ij} \delta_{x_i x_j} = B - D \quad \text{say.} \tag{8}$$

Thus, D and M denote the diagonal and off-diagonal (or mixed derivative) components of the operator B . The variable λ is a positive weighting parameter, and the obvious choice of $\lambda = \theta = \frac{1}{2}$ yields a time-centred scheme of increased accuracy [$O(\Delta t)^2 + O(\Delta^2)$, see Section 4] but this selection cannot be guaranteed to yield unconditional stability for arbitrary N . In Section 4 we show however that this scheme yields an unconditionally stable, second-order method in the important special case of three space dimensions. Some advantage in terms of accuracy and stability is also gained for higher dimensional problems. The effect of repeated iterations is also considered.

3. STABILITY OF THE SIMPLE SCHEME (3)

In this section we derive the von Neumann condition for the simple scheme (3), which is necessary and sufficient for stability in the case of constant coefficients q_{ij} . This condition is used to find estimates of the smallest value of θ necessary for unconditional stability for $N = 2 - 6$. We then find the (r, θ) regions of conditional stability in the “worst” possible case when all the q_{ij} are equal and the diagonal terms least dominant.

3.1. Stability conditions for constant coefficients

In the case of constant coefficients, stability can be established using the traditional von Neumann method [e.g. 1]. Accordingly, we consider a single Fourier component,

$$u_F^n(x_1, x_2, \dots, x_n) = \zeta^n \exp[i(\omega_1 x_1 + \omega_2 x_2 + \dots + \omega_n x_n)],$$

where the ω_i are constant wavenumbers and ζ an amplification factor. Substituting into scheme (3) and using the identities

$$Au_F^n = \hat{A}u_F^n \quad \text{and} \quad Bu_F^n = -\hat{B}u_F^n, \tag{9a,b}$$

where

$$\hat{A} = \prod_{i=1}^N (1 + 4\theta r q_{ii} s_i^2), \quad s_i = \sin(\frac{1}{2}\omega_i \Delta). \tag{10}$$

and

$$\hat{B} = 4r \left(\sum_{i=1}^N q_{ii} s_i^2 + 2 \sum_{i=2}^N \sum_{j=1}^{i-1} q_{ij} s_i c_i s_j c_j \right), \quad c_i = \cos(\frac{1}{2}\omega_i \Delta), \tag{11}$$

we find that the amplification factor is given by

$$\xi = \frac{\hat{A} - \hat{B}}{\hat{A}}.$$

Stability requires that $|\xi| \leq 1$ for all ω_i , or equivalently

$$\hat{B} \geq 0 \quad \text{and} \quad 2\hat{A} - \hat{B} \geq 0. \tag{12a,b}$$

Requirement (12a) is always satisfied since Q is positive definite, and we can write

$$\hat{B} = 4r \left(\mathbf{x}^T Q \mathbf{x} + \sum_{i=1}^N q_{ii} s_i^4 \right),$$

where $\mathbf{x}^T = (s_1 c_1, \dots, s_N c_N)$. Condition (12b) is more difficult since it depends on the parameters r and θ , and will determine the regime of unconditional stability.

3.2. Sufficient conditions

Before the detailed stability discussion of subsection 3.3, we determine a simple analytic condition that guarantees stability. We can write

$$2\hat{A} - \hat{B} = \sum_{i=2}^N \sum_{j=1}^{i-1} T_{ij} + \text{positive terms}, \tag{13}$$

where

$$T_{ij} = \frac{4}{N(N-1)} + \frac{4r}{N-1} (2\theta - 1)(q_{ii}s_i^2 + q_{jj}s_j^2) + 32\theta^2 r^2 q_{ii}q_{jj}s_i^2s_j^2 - 8rq_{ij}s_i c_i s_j c_j. \tag{14}$$

It is clear that for $\theta \geq \frac{1}{2}$ only the last term in T_{ij} can be negative, and

$$T_{ij} > \frac{4}{N(N-1)} + \frac{8}{N-1} (2\theta - N)x + 32\theta^2 x^2, \tag{15}$$

where $x = r\sqrt{q_{ii}q_{jj}}|s_i s_j|$ and we have used the inequality $q_{ii}q_{jj} > q_{ij}^2$ which follows from the fact that Q is positive definite. By retaining only the linear term we obtain the stability bound $\theta \geq \frac{1}{2}N$ adopted in Refs [6, 8]. The r.h.s. of inequality (15) is however a quadratic in x which will always be positive if its discriminant is negative, i.e. if

$$\theta \geq \hat{\theta} = \begin{cases} \frac{1}{2} & \text{if } N = 2, \\ \frac{N^2}{2(N-2)} [(1 + (N-2)/N)^{1/2} - 1] & \text{if } N \geq 3. \end{cases} \tag{16}$$

Values of $\hat{\theta}$ for $N = 2$ to 6 are given in Table 1. These results show that the scheme can always be made unconditionally stable but that for $N \geq 5$ it is necessary to choose $\theta > 1$. As N increases, $\hat{\theta}$ increases almost linearly and accuracy will be lost progressively. Note that $\theta = \frac{1}{2}$ will guarantee stability for all N in the absence of mixed derivatives (i.e. when $M = 0$).

3.3. Necessary and sufficient conditions in the worst case

It is desirable to formulate a stability condition which depends on as little as possible detailed knowledge of the q_{ij} , and we can achieve this by considering the worst possible case.

Table 1. Stability limits for $N = 2 - 6$. The symbol θ_c denotes the smallest value of θ necessary for unconditional stability (see condition (24)). The symbols R_0 and R_1 denotes the largest possible values of $R = r \times$ the maximum of the q_{ij} , which will give a stable scheme for $\theta = 0$ and $\theta = 1$ respectively

N	$\hat{\theta}$	θ_c	$R_0(\theta = 0)$	$R_1(\theta = 1)$
2	0.500	$\frac{1}{2} = 0.500$	$\frac{1}{4} = 0.250$	∞
3	0.696	$\frac{2}{3} = 0.666$	$\frac{4}{27} = 0.148$	∞
4	0.899	$\frac{27}{32} = 0.844$	$\frac{3}{32} = 0.093$	∞
5	1.104	$\frac{128}{125} = 1.024$	$\frac{8}{125} = 0.064$	2.1016
6	1.309	$\frac{3125}{2592} = 1.206$	$\frac{5}{108} = 0.046$	0.2163

The stability condition (12b) can be written as

$$\min(2\hat{A} - \hat{B}) \geq 0, \tag{17}$$

where the minimum is taken over all possible s_i . The matrix q_{ij} is positive definite so all $q_{ii} > 0$, $q_{ii}q_{jj} > q_{ij}^2$, and

$$\begin{aligned} \min(2\hat{A} - \hat{B}) \geq \min \left[2 \prod_{i=1}^N (1 + 4\theta r a_i^2 s_i^2) - 4r \left(\sum_{i=1}^N a_i^2 s_i^2 + 2 \sum_{i=2}^N \sum_{j=1}^{i-1} a_i a_j s_i s_j c_i c_j \right) \right] \\ = \min f(a_1, \dots, a_N, s_1, \dots, s_N) \text{ say,} \end{aligned} \tag{18}$$

where $a_i = \sqrt{q_{ii}}$. Clearly the minimum of f will occur when all s_i and c_i are positive, so only such values need be considered. We can further show that the worst possible case occurs when all the a_i are equal. Let

$$g(a, s_1, \dots, s_N) = f(a, a, \dots, a, s_1, \dots, s_N),$$

where a is the maximum of the a_i , and suppose we know that

$$g(a, s_1, \dots, s_N) \geq 0$$

$\forall s_1, \dots, s_N$. Then writing $a_i = \eta_i a$, where $0 < \eta_i \leq 1$, $s'_i = \eta_i s_i$, we find

$$f(a_1, \dots, a_N, s_1, \dots, s_N) = g(a, s'_1, \dots, s'_N) + 8r \sum_{i=2}^N \sum_{j=1}^{i-1} a^2 s'_i s'_j (c'_i c'_j - c_i c_j),$$

where $c'_i = (1 - \eta_i^2 s_i^2)^{1/2}$. Since $c'_i \geq c_i$ it follows that

$$f(a_1, \dots, a_N, s_1, \dots, s_N) \geq 0$$

$\forall s_i$. Thus, stability is ensured if

$$\frac{1}{2}g(a, s_1, \dots, s_N) = \prod_{i=1}^N (1 + 4\theta R s_i^2) - 2R \left(\sum_{i=1}^N s_i^2 + 2 \sum_{i=2}^N \sum_{j=1}^{i-1} s_i s_j c_i c_j \right) \geq 0 \tag{19}$$

$\forall s_i$, where $R = r \times$ the maximum of the q_{ii} .

It is not generally possible to locate the minimum of g analytically but by symmetry there will always be a local minimum on the "diagonal" $s_1 = s_2 = \dots = s_N$. Although other non-diagonal minima can occur, we have verified numerically for $N \leq 6$ that condition (19) holds $\forall s_i$, iff the *diagonal minimum* is non-negative.

Assuming then that we need consider only the diagonal minimum of g and writing $s_1^2 = s_2^2 = \dots = s_N^2 = x$ say, the stability criterion (19) becomes

$$\min(0 \leq x \leq 1) h(R, \theta, x) \geq 0, \tag{20}$$

where

$$h(R, \theta, x) = (1 + 4R\theta x)^N - 2R[N^2 x - N(N - 1)x^2]. \tag{21}$$

Note that for $\theta < 2$ and $N \geq 2$,

$$h_x(R, \theta, 0) = 2R(2\theta - N^2) < 0$$

and

$$h_x(R, \theta, 1) = 4RN\theta(1 + 4R\theta)^{N-1} + 2RN(N - 2) > 0,$$

so there must be at least one local minimum of h in the interval $0 \leq x \leq 1$.

For $N = 2$ it is possible to find analytically the region of conditional stability in the (R, θ) -plane, given by condition (20). In this case,

$$h = (1 + 4R\theta x)^2 + 4R(x^2 - 2x)$$

and the minimum value, which occurs at $x = (1 - \theta)/(1 + 4R\theta^2)$ is

$$h_{\min} = \frac{1 - 4R(1 - 2\theta)}{1 + 4\theta^2 R}.$$

It follows that the region of conditional stability is

$$R \leq \frac{1}{4(1-2\theta)} \quad (\theta \leq \frac{1}{2}). \tag{22}$$

Note that this stability regime coincides with that of Richtmyer and Morton [1, Section 8.7] who handle the mixed derivative implicitly via relaxation methods.

For $N \geq 3$ the stability region is found by locating numerically, for a given θ , the value of R which makes the minimum value of $h(R, \theta, x)$ equal to zero. Results up to $N = 6$ are shown in Fig. 1. In each case there is a critical value of θ , say θ_c , beyond which the stability is unconditional (for $N = 2$, $\theta_c = \frac{1}{2}$). For $N \geq 3$, θ_c can also be determined as follows. Substituting $y = 1 + 4R\theta x$ in criterion (20) gives

$$h = y^N - \frac{N^2}{2\theta}(y-1) + \frac{N(N-1)}{8R\theta^2}(y-1)^2. \tag{23}$$

For large R we ignore the last term in equation (23); the minimum then occurs at $y = y_0$, say $=(N/2\theta)^{1/(N-1)}$, and its value is $N[N - y_0(N-1)]/2\theta$. Thus h is non-negative provided $y_0 \leq N/(N-1)$, or

$$\theta \geq \frac{1}{2}N \left(\frac{N-1}{N} \right)^{N-1} = \theta_c. \tag{24}$$

Values of θ_c for $N = 2$ to 6 are given in Table 1. For $N \geq 5$, $\theta_c > 1$, which means that unconditional stability is achieved at the expense of accuracy. The reason is that as N increases, the number of cross terms increases faster than the number of diagonal terms— $N(N-1)$ compared with N —which makes stability more difficult to achieve. (Note that $\theta_c \rightarrow N/2e$ as $N \rightarrow \infty$.)

The stability condition on R when $\theta = 0$ can be determined analytically. In this case

$$h = 1 - 2RN^2x + 2RN(N-1)x^2$$

and the minimum is $1 - RN^3/2(N-1)$. The scheme will be stable if

$$R \leq \frac{2(N-1)}{N^3} = R_0 \quad \text{say.} \tag{25}$$

Values of R_0 are given in Table 1. Note that $R_0 = O(N^{-2})$ as $N \rightarrow \infty$.

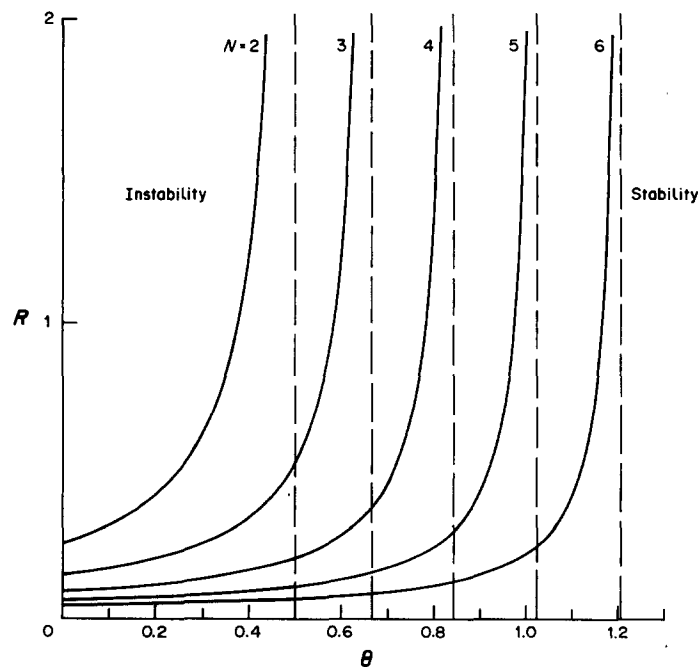


Fig. 1. Regions of conditional stability for the simple scheme (3). The solid curve for each N represents the boundary between stability and instability. The dashed lines are the asymptotes to each curve at $\theta = \theta_c$, beyond which value stability is unconditional.

4. STABILITY OF THE ITERATED SCHEME (7a, b)

We now explore the extent to which the iterated scheme (7a, b) is capable of relaxing the stability restrictions established in Section 3. From equations (7a, b) it follows that

$$A^2 u^{n+1} = A^2 u^n + B(A + \lambda M)u^n. \quad (26)$$

The second iteration leads to the possibility of time-centring the scheme. For example, in the case $N = 2$, $\theta = \frac{1}{2}$, expansion of the operators in scheme (3) shows that the leading error of $O(\Delta t)$ is

$$q_{xy} u_{xy} r \Delta^2,$$

whereas with a second iteration and $\theta = \lambda = \frac{1}{2}$ we can show from equation (26) that the leading error is

$$\frac{-\Delta^2}{12} (q_{xx} u_{xxx} + 4q_{xy} (u_{xyyy} + u_{yxxx}) + q_{yy} u_{yyyy}).$$

(Note that in the above equations we have reverted to the use of x and y as independent variables.)

Using equations (9a, b) we find that the von Neumann amplification factor of scheme (26) is given by

$$\xi = 1 - \frac{\hat{B}}{\hat{A}} \left(1 - \frac{\lambda \hat{M}}{\hat{A}} \right), \quad (27)$$

\hat{M} being the mixed derivative component of \hat{B} —i.e.

$$\hat{M} = \hat{B} - \hat{D} = 8r \sum_{i=2}^N \sum_{j=1}^{i-1} q_{ij} s_i c_i s_j c_j.$$

Since \hat{B} is non-negative the stability conditions $\xi \leq 1$ and $\xi \geq -1$ yield, respectively,

$$\lambda \hat{M} \leq \hat{A} \quad \text{and} \quad 2\hat{A}^2 - \hat{B}(\hat{A} - \lambda \hat{M}) \geq 0. \quad (28a, b)$$

4.1. Analysis of condition (28a)

To analyse the implications of condition (28a) we use equation (10) and (11), making the substitutions

$$\lambda = \bar{\lambda} \theta \quad \text{and} \quad x_i = 2\sqrt{r\theta q_{ii}} |s_i| |c_i|.$$

Then,

$$\hat{A} - \lambda \hat{M} \geq \prod_{i=1}^N (1 + x_i^2 + 4r\theta q_{ii} s_i^4) - 2\bar{\lambda} \sum_{i=2}^N \sum_{j=1}^{i-1} x_i x_j, \quad (29)$$

where we have again made use of the inequality $q_{ii} q_{jj} \geq q_{ij}^2$ which follows from the fact that (q_{ij}) is a positive definite matrix. For unconditional stability condition (28) must be valid for all possible values of s_i , c_i and r , so in view of inequality (29) a necessary and sufficient condition will be

$$p(x_1, x_2, \dots, x_n) = \prod_{i=1}^N (1 + x_i^2) - 2\bar{\lambda} \sum_{i=2}^N \sum_{j=1}^{i-1} x_i x_j \geq 0, \quad (30)$$

\forall positive x_i .

We have verified numerically for $N = 3$ to 6 that the minimum of the polynomial p always lies on the "diagonal", $x_1 = x_2 = \dots = x_n$, so to decide if p is always positive we consider just

$$p(x, x, \dots, x) = (1 + y)^n - \bar{\lambda} N(N-1)y = p_1(y)$$

say, where $y = x^2$. Since p_1 is a function of a single variable it can be minimized easily, and one finds that the condition for p to remain positive is

$$\lambda \leq \frac{N^{N-1}}{(N-1)^N} \theta. \quad (31)$$

Values of the coefficient of θ in condition (31) are given in Table 2 for $N = 2$ to 6.

Table 2. Maximum permissible values of λ/θ for unconditional stability. The last row of the table gives values of θ_{\min} —the minimum value of θ for unconditional stability ($\lambda = \frac{1}{2}$)

N	2	3	4	5	6
	$\frac{2}{1}$	$\frac{9}{8}$	$\frac{64}{81}$	$\frac{625}{1024}$	$\frac{7776}{15625}$
$\frac{N^{N-1}}{(N-1)^N}$	2.00	1.125	0.790	0.610	0.498
θ_{\min}	0.5	0.5	0.633	0.820	1.004

4.2. Analysis of condition (28b)

On making the substitution $\hat{B} = \hat{D} + \hat{M}$ into condition (28b) we find that this condition is equivalent to

$$\hat{A}(2\hat{A} - \hat{D}) - \hat{M}(\hat{A} - \lambda\hat{D}) + \lambda\hat{M}^2 \geq 0. \tag{32}$$

Now on setting $q_{ij} = 0, i \neq j$, in equations (13) and (14) it follows that $2\hat{A} - \hat{D} \geq 0$ when $\theta \geq \frac{1}{2}$. Also it is easily verified that $\hat{A} - \lambda\hat{D} \geq 0$ provided $\lambda \leq \theta$, so then condition (32) can be violated only if $\hat{M} > 0$. In this case we can use condition (28a) to show that condition (32) will be satisfied provided

$$\hat{A}^2(2\lambda - 1) + \lambda^2\hat{M}^2 \geq 0.$$

i.e. if $\lambda \geq \frac{1}{2}$. To summarize, condition (28b) will hold, provided

$$\theta \geq \frac{1}{2}, \quad \frac{1}{2} \leq \lambda \leq \theta. \tag{33}$$

4.3. Sufficient conditions for unconditional stability

It can be seen from Table 2 that for $N = 2$ and 3 , condition (31) is redundant, so condition (33) gives sufficient condition for unconditional stability. In particular, the choice $\lambda = \theta = \frac{1}{2}$ will yield unconditional stability and second-order accuracy in two or three space dimensions. In four or more dimensions, the condition will be

$$\theta \geq \frac{1}{2}, \quad \frac{1}{2} \leq \lambda \leq \frac{N^{N-1}}{(N-1)^N} \theta, \tag{34}$$

which becomes increasingly restrictive as N becomes large. In particular, for $N > 6$ we must choose $\theta > 1$, which entails loss of accuracy. Nonetheless the iterated scheme represents a considerable improvement over the simple scheme (3) in that smaller values of θ are necessary for unconditional stability. The minimum necessary value θ_{\min} is given by

$$\theta_{\min} = \frac{1}{2}, \quad N = 2, 3; \quad \theta_{\min} = \frac{(N-1)^N}{2N^{N-1}}, \quad N > 3.$$

These values of θ_{\min} are shown in Table 2.

4.4. Further iterations

In view of the improved characteristics of the iterated version of the ADI scheme, it is interesting to see if further iterations will permit more generous stability margins. Suppose that equation (7b) is replaced by a k -stage iteration,

$$Au_{(k)}^{n+1} = (A + B)u^n + \lambda M(u_{(k-1)}^{n+1} - u^n), \quad k = 1, 2, \dots$$

It is readily shown that the stability conditions $\zeta \leq 1$ and $\zeta \geq -1$ are equivalent to

$$p_k \hat{B} \geq 0 \quad \text{and} \quad 2\hat{A} - p_k \hat{B} \geq 0,$$

where

$$p_k = \sum_{n=0}^k (-1)^n \left(\frac{\lambda \hat{M}}{\hat{A}} \right)^n = \frac{1 + (-1)^k (\lambda \hat{M} / \hat{A})^{k+1}}{1 + (\lambda \hat{M} / \hat{A})}. \tag{35a, b}$$

These conditions clearly incorporate the simple and single-iterated schemes ($k = 0, 1$) discussed previously.

Consider, the example, the case $k = 2$. Condition (35a) is satisfied automatically, since $\hat{B} \geq 0$ and p_k is a positive definite quadratic in $\lambda\hat{M}/\hat{A}$. Condition (35b) can be expressed in the form

$$\hat{A}^2(2\hat{A} - \hat{B}) + \lambda\hat{M}\hat{B}(\hat{A} - \lambda\hat{M}) \geq 0.$$

The first term will be non-negative if $\theta \geq \theta_c$ (see Section 3), and indeed it can be zero for this value of θ in the worst possible case. The second term will be non-negative iff

$$0 \leq \lambda\hat{M} \leq \hat{A},$$

so the stability conditions are more stringent than for $k = 1$, when $N > 2$ and $\theta_c > \frac{1}{2}$. Thus, it seems there is no advantage to be gained by carrying out further iterations.

5. EXTENSIONS OF THE METHOD

5.1. Effect of lower-order derivatives

An equation of the form

$$\frac{\partial u}{\partial t} = \left(L + \sum_{i=1}^N p_i \partial_i + b \right) u$$

is easily accommodated in the general scheme by modifying the operator B in scheme (7a, b). If we impose the von Neumann condition $|\xi| \leq 1 + O(\Delta t)$, as required for solutions that possess a legitimate exponential growth, then the previous stability conditions are unchanged for sufficiently small Δt [cf. 1, p. 270; 18].

5.2. Extension to non-constant coefficients

To extend the stability analysis to the case of non-constant coefficients ($q_{ij} = q_{ij}(\mathbf{x}, t)$) we may invoke the analysis of Widlund [20; cf. 1, Chap. 5]. Following the steps of McKee and Mitchell [5] we find that Widlund's criterion reduces to the von Neumann conditions discussed previously.

6. CONCLUSIONS

We have presented an ADI method that combines computational simplicity with the possibility of unrestricted stability for multi-dimensional parabolic equations in the presence of mixed derivatives. In the simplest version of the scheme the mixed derivatives are treated entirely explicitly so the accuracy is $O(\Delta t) + O(\Delta^2)$. The stability conditions for this scheme are summarized in Table 1. In five or more space dimensions unconditional stability requires $\theta > 1$, which entails some loss of accuracy. However, the scheme remains feasible provided the dominant matrix coefficients are not too large—for example, in five space dimensions the fully backward method ($\theta = 1$) increases the stability boundary of the explicit scheme ($\theta = 0$) by a factor of approx. 30.

In general however it seems worthwhile to perform a second iteration to time-centre the mixed derivatives. This allows the possibility of second-order accuracy [$O(\Delta t^2) + O(\Delta^2)$] and permits a relaxation of the stability conditions in Table 1 for $N \geq 3$ (see Table 2). The choice $\theta = 1$ will guarantee unconditional stability for $N \leq 5$, and for $N = 6$ we need increase this value by only 0.004! Little advantage seems to be gained however by performing more than one iteration.

It should be emphasized that our stability arguments involve no assumptions about the coefficient matrix (q_{ij}), other than that it is positive definite. This property can often be guaranteed [e.g. 14] even when the coefficients are non-linear functions of the dependent variable u and its first derivatives, so one would expect the scheme to be feasible in such non-linear applications.

Finally, we note one apparent disadvantage of ADI schemes—that their application is restricted to domains which are unions of rectangles with sides parallel to the co-ordinate axes. It is often possible to transform an arbitrary domain to a rectangular one by a change of variable [e.g. 14], which will not affect the parabolicity of the operator and hence the viability of the scheme.

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