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AN EXTENSION OF A-STABILITY TO ALTERNATING DIRECTION IMPLICIT METHODS*

R.F. WARMING AND RICHARD M. BEAM

Abstract.

Completely implicit, noniterative, finite-difference schemes have recently been developed by several authors for nonlinear, multidimensional systems of hyperbolic and mixed hyperbolic-parabolic partial differential equations. The method of Douglas and Gunn or the method of approximate factorization can be used to reduce the computational problem to a sequence of one-dimensional or alternating direction implicit (ADI) steps. Since the eigenvalues of partial differential equations (for example, the equations of compressible fluid dynamics) are often widely distributed with large imaginary parts, A-stable integration formulas provide ideal time-differencing approximations. In this paper it is shown that if an A-stable linear multistep method is used to integrate a model two-dimensional hyperbolic-parabolic partial differential equation, then one can always construct an ADI scheme by the method of approximate factorization which is also A-stable, i.e., unconditionally stable. A more restrictive result is given for three spatial dimensions. Since necessary

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and sufficient conditions for A-stability can easily be determined by using the theory of positive real functions, the stability analysis of the factored partial difference equations is reduced to a simple algebraic test.

1. Introduction.

Alternating direction implicit (ADI) methods for parabolic equations were originated by Douglas [10] and Peaceman and Rachford [24]. A general procedure for constructing ADI schemes for multidimensional parabolic equations and the second-order wave equation was devised by Douglas and Gunn [12]. An ADI method for first-order linear hyperbolic systems in two space dimensions was constructed by Gourley and Mitchell [15].

Recently, completely implicit, noniterative, finite-difference schemes have been developed by several authors for nonlinear, multidimensional systems of hyperbolic [1,25] and mixed hyperbolic-parabolic [2,5,6,19,25] partial differential equations. Lindemuth and Killeen formulated their ADI scheme by following the Douglas, Peaceman-Rachford procedure, Briley and MacDonald devised their ADI algorithm by a formal application of the Douglas-Gunn procedure, while Beam and Warming constructed an ADI method by using approximate factorization.

The linear stability analysis for the algorithms applied to systems of hyperbolic-parabolic equations is in a very rudimentary state. The primary reason is that the operators involved do not commute. In addition, the stability analysis of schemes for mixed hyperbolic-parabolic equations is generally more difficult than the analysis for either type treated separately. This is particularly true for schemes using more than two time levels. In fact, we are aware of only one stability proof for a multistep ADI scheme applied to a model equation with both convection (hyperbolic) and diffusion (parabolic) terms [7].

The eigenvalues associated with a mixed hyperbolic-parabolic system (for example, the equations of compressible fluid dynamics) are often widely distributed with large imaginary parts. Since the eigenvalue spectrum cannot be bounded away from the imaginary axis, A-stable linear multistep integration formulas provide ideal time-differencing approximations (For the definition of A-stable methods, see, e.g., [8,14] or section 2.) Although the temporal accuracy of an A-stable linear multistep method (LMM) cannot exceed two [8], this is compatible with the accuracy achievable with typical ADI schemes.

The purpose of this paper is to show that if one uses an A-stable LMM to integrate an evolutionary partial differential equation (PDE) of the form

$$\frac{\partial u}{\partial t} = (L_x + L_y)u \quad , \tag{1.1}$$

where L_x and L_y are linear scalar differential operators, then one can always construct an ADI scheme by the method of approximate factorization which is also A-stable, i.e., unconditionally stable. Since necessary and sufficient conditions for the A-stability of an LMM can easily be determined by applying the theory of positive real functions [9], the stability analysis of the factored partial difference equations is reduced to a simple algebraic test. Our most general result is for two spatial dimensions with a more restrictive result for three spatial dimensions. We should add that the stability analysis is for simple linear test equations and we have not dealt with noncommuting operators.

In section 2 we briefly review the theory of linear multistep methods. In section 3 we describe a method of constructing an ADI method by starting with a linear multistep method and then using the method of approximate factorization. A linear (model) test equation for partial differential equations is defined (section 4) and then used to analyze the stability of approximate factorization schemes (section 5). The natural extension of approximate factorization methods to three spatial dimensions is discussed in section 6. In section 7 we examine in detail the family of A-stable linear two-step methods. To illustrate the notions of this paper, we write out an ADI method for the three-dimensional heat equation (section 8). Section 9 contains an illustration of a reduced stability range for an approximate factorization formulation which does not follow the formulation of section 3. The connection between this paper and the classic paper on ADI methods by Douglas and Gunn [12] is discussed in section 10. The final section includes a summary of the approximate factorization approach described in this paper.

2. Preliminaries: A review of linear multistep methods (LMM) and A-stability.

A linear k-step method for integrating the first-order ordinary differential equation

$$\frac{du}{dt} = f(u) \quad , \quad t > 0 \quad , \quad u(0) = u_o \quad , \tag{2.1}$$

is defined by

$$\sum_{j=0}^{k} \alpha_j u^{n+j} = \Delta t \sum_{j=0}^{k} \beta_j \frac{du^{n+j}}{dt} \quad , \tag{2.2}$$

where Δt is the step size ($t = n\Delta t$), the coefficients α_j and β_j are real constants with $\alpha_k \neq 0$ and not both α_0 and β_0 are zero.

The method is said to be explicit if $\beta_k = 0$ and implicit otherwise. Consistency and normalization are expressed by the relations

$$(2.3a,b,c) \qquad \sum_{j=0}^{k} \alpha_j = 0 \;, \quad \sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j = 1 \;.$$

It is convenient to associate with (2.2) the polynomials

$$(2.4a) \qquad \rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j \;,$$

$$(2.4b) \qquad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j \;.$$

Consequently the LMM (2.2) can be rewritten as

$$(2.5) \qquad \rho(E)u^n = \Delta t \; \sigma(E)\frac{du^n}{dt} \;,$$

where the shift operator E is defined by

$$(2.6) \qquad Eu^n = u^{n+1} \;.$$

Linear stability of an LMM is analyzed by applying (2.2) to the linear test equation

$$(2.7) \qquad \frac{du}{dt} = \lambda u$$

where in general

$$\lambda = \lambda_R + i\lambda_I$$

is a complex constant. If one assumes a solution of the form $u^n = \zeta^n$ (ζ to the nth power), there follows the characteristic equation

$$\rho(\zeta) - \lambda\,\Delta t\,\sigma(\zeta) = 0 \quad , \tag{2.8}$$

where the polynomials ρ and σ are defined by (2.4). The stability region of an LMM consists of those values of $\lambda\,\Delta t$ for which the characteristic equation (2.8) satisfies the root condition, i.e., its roots ζ_ℓ satisfy $|\zeta_\ell| \le 1$ and the roots of unit modulus are simple.

An LMM is said to be A-stable if its stability region contains all of the left half of the complex $\lambda\,\Delta t$ plane including the imaginary axis (Dahlquist [8]). Since the linear test equation (2.7) has a bounded solution if and only if $\mathrm{Re}\,\lambda \le 0$, the notion of A-stability is equivalent to

$$\text{stability of ODE} \Longrightarrow \text{stability of LMM} \tag{2.9}$$

where ODE denotes ordinary differential equation. Dahlquist [8] proved that the order of accuracy of an A-stable LMM cannot exceed two and that an A-stable method must be implicit. In addition, he showed that the trapezoidal formula

$$u^{n+1} - u^n = \frac{\Delta t}{2}\left(\frac{du}{dt}^{n+1} + \frac{du}{dt}^{n}\right) \tag{2.10}$$

has the smallest truncation error of all the A-stable LMMs.

The advantage of an A-stable LMM is that the stability of the ODE is a sufficient condition for the unconditional stability (i.e., stability for an arbitrary value of Δt) of the LMM. In this paper we extend the notion of A-stability to LMM methods applied to partial differential equations (PDEs). The numerical scheme is constructed so that approximate spatial factoring into a product of one-dimensional operators retains the A-stable property:

(2.11) stability of PDE $\Longrightarrow$ stability of factored LMM .

The precise meaning of a factored method will be clarified in the following section.

3. Construction of an ADI scheme using an LMM and approximate factorization.

For the development that follows, a convenient form of the LMM (2.5) is

$$\rho(E)u^n - \omega\Delta t\rho(E)\frac{du^n}{dt} = \Delta t[\sigma(E) - \omega\rho(E)]\frac{du^n}{dt} + O(\Delta t^3) \tag{3.1}$$

where

$$\omega = \frac{\beta_k}{\alpha_k} .$$

Henceforth we consider only A-stable LMMs and assume that (3.1) is A-stable. Since the order of accuracy of an A-stable LMM cannot exceed two, we concentrate in this paper on the second-order schemes as indicated by the symbol $O(\Delta t^3)$ on the right-hand side of (3.1). The parameter ω is defined so that the operator $\sigma(E) - \omega\rho(E)$ on the right-hand side of (3.1) is at least one degree lower than the operator $\rho(E)$ on the left-hand side. This is obvious by noting that

$$\sigma(E) = \beta_k E^k + \beta_{k-1} E^{k-1} + \ldots$$

$$\omega\rho(E) = \frac{\beta_k}{\alpha_k}\left(\alpha_k E^k + \alpha_{k-1} E^{k-1} + \ldots\right) ,$$

and hence

$$\sigma(E) - \omega\rho(E) = \left(\beta_{k-1} - \frac{\beta_k}{\alpha_k}\alpha_{k-1}\right) E^{k-1} + \ldots \quad .$$

Consequently, the right-hand side of (3.1) can be computed explicitly from known data when advancing the numerical solution from $n + k - 1$ to $n + k$.

Insertion of the linear PDE (1.1) into (3.1) yields

$$(3.2) \qquad [I - \omega\Delta t(L_x + L_y)]\rho(E)u^n = \Delta t[\sigma(E) - \omega\rho(E)](L_x + L_y)u^n + O(\Delta t^3) \quad .$$

Here, for simplicity, we have assumed that the linear operators L_x and L_y are independent of time although the case of time-dependent and/or nonlinear coefficients can be handled without difficulty [3]. It is important to note that the unknown variable to be computed is $\rho(E)u^n$ and not u^{n+k}. This choice ensures that the approximate factorization does not upset either the temporal accuracy of the scheme (see below) or the unconditional stability (section 5).

If the spatial operators L_x and L_y are approximated by appropriate difference quotients, one obtains, in general, an enormous linear system to solve for $\rho(E)u^n$. The computational problem can be reduced to a sequence of one-dimensional (inversion) problems by an approximate factorization of the left-hand side of (3.2):

$$(3.3) \qquad (I - \omega\Delta t\, L_x)(I - \omega\Delta t\, L_y)\rho(E)u^n = \Delta t[\sigma(E) - \omega\rho(E)](L_x + L_y)u^n + O(\Delta t^3) \quad .$$

On comparing the left-hand sides of (3.2) and (3.3), we see that they differ by the cross product term

$$\omega^2\, \Delta t^2\, L_x L_y \rho(E)u^n \quad .$$

But by expanding $\rho(E)u^n$ in a Taylor series about u^n and using the consistency and normalization conditions (2.3a,b), there follows

$$\rho(E)u^n = \Delta t\, \frac{\partial u^n}{\partial t} + O(\Delta t^{\alpha+1}) \quad , \quad \alpha \geq 1 \quad .$$

Consequently, the cross product term

$$\omega^2 \Delta t^2\, L_x L_y \rho(E)u^n = \omega^2\, \Delta t^3\, L_x L_y\, \frac{\partial u^n}{\partial t} + O(\Delta t^{\alpha+3})$$

$$= O(\Delta t^3)$$

is a third-order term and formal accuracy of the scheme (3.2) is not upset by the approximate factorization (3.3). The computational sequence to implement the factored scheme (3.3) as an alternating direction sequence is not unique. Perhaps the most obvious choice is

$$(3.4a) \qquad (I - \omega\Delta t\, L_x)\rho(E)u^* = \Delta t[\sigma(E) - \omega\rho(E)](L_x + L_y)u^n \quad ,$$

(3.4b) $$(I - \omega \Delta t\, L_y)\rho(E)u^n = \rho(E)u^* ,$$

(3.4c) $$u^{n+k} = \frac{1}{\alpha_k}\left[\rho(E)u^n - \sum_{j=0}^{k-1} \alpha_j E^j u^n\right] ,$$

where $\rho(E)u^*$ is a dummy temporal difference. Here we have used notation from the theory of LMM for ordinary differential equations and consequently the algorithm (3.4) looks rather unfamiliar. In section 8 we write out an example following notation more conventional for partial differential equations.

An important aspect of implementing an ADI scheme is determining the proper boundary values for the intermediate dummy variables such as $\rho(E)u^*$. Although such considerations are outside the scope of the present paper, they have been discussed elsewhere (see, e.g., [13,2]).

4. A linear test equation for partial differential equations.

For first-order ordinary differential equations, Eq. (2.7) is known as the linear test equation. For a first-order evolutionary PDE, we define a linear test equation for two spatial dimensions as

(4.1) $$\frac{\partial u}{\partial t} + c_1 \frac{\partial u}{\partial x} + c_2 \frac{\partial u}{\partial y} = a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2} ,$$

where c_1, c_2, a, b and c are real constants. In order to determine the conditions to be imposed on these constants for which the PDE (4.1) has a bounded solution, we seek a solution of the form

(4.2) $$u(x,y,t) = v(t)e^{i(\kappa_1 x+\kappa_2 y)} ,$$

where $v(t)$ is the Fourier coefficient, and κ_1, κ_2 are the Fourier variables (wave numbers). The Fourier coefficient $v(t)$ satisfies

(4.3a) $$\frac{dv}{dt} = \lambda v \quad ,$$

where

(4.3b) $$\lambda = -i(c_1\kappa_1 + c_2\kappa_2) - (a\kappa_1^2 + b\kappa_1\kappa_2 + c\kappa_2^2) \quad .$$

For the PDE (4.1) to have bounded solutions, Re $\lambda \le 0$. Consequently, the quadratic form

$$a\kappa_1^2 + b\kappa_1\kappa_2 + c\kappa_2^2$$

must be nonnegative for arbitrary values of κ_1 and κ_2, which implies that $a, c \ge 0$, $b^2 \le 4ac$. In the absence of the convective terms, i.e., $c_1 = c_2 = 0$, the inequalities $a > 0$, $b^2 < 4ac$ are the conditions under which (4.1) is parabolic. The convection coefficients c_1 and c_2 are arbitrary real numbers, and in the absence of diffusion, i.e., $a = b = c = 0$, the eigenvalue λ is pure imaginary.

5. Linear stability analysis for two-dimensional unfactored and factored schemes.

In this section we examine the stability of the unfactored scheme (3.2) and its factored counterpart (3.3) when applied to the linear test equation (4.1) with the mixed derivative bu_{xy} set to zero. The linear operators L_x and L_y are

(5.1)

$$L_x = -c_1 \frac{\partial}{\partial x} + a \frac{\partial^2}{\partial x^2} ,$$

$$L_y = -c_2 \frac{\partial}{\partial y} + c \frac{\partial^2}{\partial y^2} .$$

A stability analysis including the mixed spatial derivative is considered in appendix A.

We assume for simplicity that u^n is spatially continuous and assume a solution of the form

(5.2) $$u^n = v^n e^{i(\kappa_1 x + \kappa_2 y)} ,$$

where v^n is the Fourier coefficient and κ_1, κ_2 are the Fourier variables. In practice, the spatial derivatives are replaced by discrete difference quotients; however, as indicated at the end of this section, the stability proof for the spatially discrete case requires only a minor modification of the following stability proof. We first consider the stability of the unfactored scheme (3.2). Equation (3.2) was written in the particular form shown as a precursor to factoring the scheme into a product of one-dimensional operators. However, as it stands, (3.2) is simply

$$\rho(E)u^n = \Delta t\ \sigma(E)(L_x + L_y)u^n ,$$

where, for the present analysis, L_x and L_y are defined by (5.1). Assuming a solution of the form (5.2), we obtain the characteristic equation

(5.3a) $$\rho(\zeta) - \lambda\,\Delta t\,\sigma(\zeta) = 0 \quad ,$$

where

(5.3b) $$\lambda = -i(c_1\kappa_1 + c_2\kappa_2) - (a\kappa_1^2 + c\kappa_2^2)$$

and ζ is the amplification factor defined by

(5.4) $$v^{n+1} = \zeta v^n \quad .$$

But (5.3a) has the same form as the characteristic equation (2.8) obtained when an LMM method is applied to the linear test equation (2.7) for ordinary differential equations. Since $\mathrm{Re}\,\lambda \leq 0$, the resulting scheme is unconditionally stable since we have assumed that the original LMM is A-stable. We note that for an unfactored scheme with u^n assumed to be spatially continuous, an equivalent way of obtaining the characteristic equation (5.3a) would be to apply an LMM directly to the ODE (4.3) satisfied by the Fourier coefficient.

For the factored scheme (3.3) where L_x and L_y are defined by (5.1), we again assume a solution of the form (5.2) and obtain the following characteristic equation for the amplification factor:

(5.5a) $$\rho(\zeta) - \frac{(\lambda_1 + \lambda_2)\Delta t}{1 + \omega^2\,\Delta t^2\,\lambda_1\lambda_2}\,\sigma(\zeta) = 0 \quad ,$$

where

(5.5b) $$\lambda_1 = -ic_1\kappa_1 - a\kappa_1^2 \quad , \quad \lambda_2 = -ic_2\kappa_2 - c\kappa_2^2$$

with

$$\mathrm{Re}\ \lambda_1\ ,\ \mathrm{Re}\ \lambda_2 \le 0\ .$$

On comparing (5.3) and (5.5) we see that $\lambda = \lambda_1 + \lambda_2$ has been replaced by

$$\lambda_{AF} = \frac{\lambda_1 + \lambda_2}{1 + \omega^2\ \Delta t^2\ \lambda_1\lambda_2}\ . \tag{5.6}$$

The product term in the denominator is a direct result of the approximate factorization (AF) and hence we call this "eigenvalue" λ_{AF}. A sufficient condition for the factored scheme to be unconditionally stable is $\mathrm{Re}\ \lambda_{AF} \le 0$ which follows directly from the following lemma:

$$\mathrm{Re}\ \lambda_1,\ \mathrm{Re}\ \lambda_2 \le 0 \Longrightarrow \mathrm{Re}\ \frac{\lambda_1 + \lambda_2}{1 + \alpha^2\lambda_1\lambda_2} \le 0 \tag{5.7}$$

for arbitrary real α.

PROOF. Recall for an arbitrary complex number z that if $\mathrm{Re}\ z \le 0$, then $\mathrm{Re}\ z^{-1} \le 0$. Then, by noting that

$$\frac{1 + \alpha^2\lambda_1\lambda_2}{\lambda_1 + \lambda_2} = \frac{1}{\lambda_1 + \lambda_2} + \frac{\alpha^2\lambda_1\lambda_2}{\lambda_1 + \lambda_2}$$

$$= \frac{1}{\lambda_1 + \lambda_2} + \frac{\alpha^2}{1/\lambda_1 + 1/\lambda_2}$$

the lemma obviously follows.□

In the above analysis we assumed that spatial derivatives were continuous. It remains to consider the spatially discrete case. We consider the case where the spatial derivatives in (5.1) are replaced by three-point central difference quotients:

$$\left.\frac{\partial u}{\partial x}\right|_j = \frac{u_{j+1} - u_{j-1}}{2\Delta x} + O(\Delta x^2) \quad , \quad x = j\,\Delta x \quad ,$$

(5.8)

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} + O(\Delta x^2)$$

with analogous expressions for the y-derivatives. The stability analysis proceeds as in the spatially continuous case with the exception that the exponential in (5.2) is replaced by

(5.9)
$$u^{n} = v^n\, e^{i(\kappa_1 j\Delta x + \kappa_2 k\Delta y)} \quad ,$$

where $x = j\,\Delta x$, $y = k\,\Delta y$. If we make the following correspondence

(5.10)
$$\kappa_1 \longleftarrow \frac{2\sin(\theta_1/2)}{\Delta x} \quad , \quad \kappa_2 \longleftarrow \frac{2\sin(\theta_2/2)}{\Delta y} \quad ,$$

$$c_1 \longleftarrow c_1\cos(\theta_1/2) \quad , \quad c_2 \longleftarrow c_2\cos(\theta_2/2) \quad ,$$

where

$$\theta_1 = \kappa_1\,\Delta x \quad , \quad \theta_2 = \kappa_2\,\Delta y \quad ,$$

between the parameters for the discrete and continuous case, then the eigenvalue (5.[illegible]) has the same form for both the continuous and the discrete case. Recall for the spatially continuous case that $\text{Re}\,\lambda \leq 0$ for arbitrary real values of $c_1, c_2, \kappa_1, \kappa_2$ and hence the discretization does not change the essential property for A-stability that $\text{Re}\,\lambda \leq 0$. Likewise, for the factored algorithm (3.3) with discrete spatial derivative approximations, one obtains by using the correspondence (5.10) the same characteristic equation (5.5) as for the spatially continuous case and again the algorithm is unconditionally stable.

In this section we considered the stability of the factored scheme (3.3) when applied to the linear test equation (4.1) with the mixed derivative bu_{xy} set to zero. In appendix A we prove that if the mixed derivative is treated explicitly, then the resulting factored scheme is unconditionally stable. The particular explicit method considered in appendix A has the defect that the resulting scheme is first-order accurate in time for the mixed derivative. Beam and Warming [2] showed that it was possible to construct an unconditionally stable two-step scheme where the mixed derivative is second-order time accurate by using linear extrapolation. However, the characteristic equation for the amplification factor did not have the form (5.5a); and the stability analysis did not include the convective terms $c_1 u_x$ and $c_2 u_y$.

6. Extension to three spatial dimensions.

In three spatial dimensions, an obvious generalization of the two-dimensional approximate factorization scheme (3.3) is

$$(I - \omega\Delta t\, L_x)(I - \omega\Delta t\, L_y)(I - \omega\Delta t\, L_z)\rho(E)u^n =$$

$$\Delta t[\sigma(E) - \omega\rho(E)](L_x + L_y + L_z)u^n \quad . \tag{6.1}$$

For three spatial dimensions a linear test equation (without mixed derivatives) is

(6.2) $$\frac{\partial u}{\partial t} + c_1 \frac{\partial u}{\partial x} + c_2 \frac{\partial u}{\partial y} + c_3 \frac{\partial u}{\partial z} = a_1 \frac{\partial^2 u}{\partial x^2} + a_2 \frac{\partial^2 u}{\partial y^2} + a_3 \frac{\partial^2 u}{\partial z^2} ,$$

where the coefficients c_ℓ are arbitrary real numbers and $a_\ell \geq 0$. If the approximate factorization scheme (6.1) is applied to the test equation (6.2), one obtains the following characteristic equation for the amplification factor:

(6.3a) $$\rho(\zeta) - \lambda_{AF} \Delta t \, \sigma(\zeta) = 0 ,$$

where

(6.3b) $$\lambda_{AF} = \frac{\lambda_1 + \lambda_2 + \lambda_3}{1 + \omega^2 \Delta t^2 (\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1) - \omega^3 \Delta t^3 \lambda_1\lambda_2\lambda_3}$$

and

$$\lambda_\ell = -ic_\ell\kappa_\ell - a_\ell\kappa_\ell^2 , \quad \text{Re } \lambda_\ell \leq 0 .$$

The lemma (5.6) of the previous section does not extend to three dimensions for arbitrary values of λ_ℓ with Re $\lambda_\ell \leq 0$. We consider two special cases. If λ_ℓ is pure real, i.e., $\lambda_\ell = -a_\ell\kappa_\ell^2$, then the denominator of (6.3b) is positive and, consequently, Re $\lambda_{AF} = \lambda_{AF} \leq 0$ and the scheme is unconditionally stable. If λ_ℓ is pure imaginary, i.e., $\lambda_\ell = -ic_\ell\kappa_\ell$, then λ_{AF} has the form

(6.4) $$\lambda_{AF} = \frac{i\beta_1}{\alpha_2 + i\beta_2} ,$$

where

$$\beta_1 = -(c_1\kappa_1 + c_2\kappa_2 + c_3\kappa_3) ,$$

$$\beta_2 = -\omega^3 \Delta t^3 c_1c_2c_3\kappa_1\kappa_2\kappa_3 ,$$

$$\alpha_2 = 1 - \omega^2 \Delta t^2(c_1c_2\kappa_1\kappa_2 + c_2c_3\kappa_2\kappa_3 + c_3c_1\kappa_3\kappa_1) .$$

The region of stability for a typical A-stable LMM is illustrated in figure 1. For given values of c_1,c_2,c_3, one can always pick wave numbers $\kappa_1,\kappa_2,\kappa_3$ such that $\lambda_{AF}\,\Delta t$ as defined by (6.4) has a positive real part and falls in the unstable "hole" of figure 1. Consequently, for pure imaginary eigenvalues ($a_\ell = 0$), the unconditional stability of the three-dimensional factored algorithm for the model equation (6.2) is not retained.

7. A-stable linear two-step methods.

Since the order of an A-stable LMM cannot exceed two, one- and two-step schemes are of primary interest. The addition of more steps or time levels complicates the numerical scheme and generally increases computer storage requirements with no attendant increase in accuracy. The most general consistent two-step method [i.e., k = 2 in (2.2)] can be written as

$$(7.1) \qquad (1+\xi)u^{n+2} - (1+2\xi)u^{n+1} + \xi u^n =$$

$$\Delta t\left[\theta \frac{du}{dt}^{n+2} + (1-\theta+\phi)\frac{du}{dt}^{n+1} - \phi\frac{du}{dt}^{n}\right] - e^n ,$$

where the parameters θ,ξ,ϕ are arbitrary real numbers and e^n is the local truncation error

$$(7.2) \qquad e^n = (\phi - \xi + \theta - \tfrac{1}{2})\Delta t^2 \frac{d^2u^n}{dt^2} + O(\Delta t^3)$$

determined by a Taylor series expansion about $t = n\,\Delta t$. The class of all two-step methods that are at least second-order accurate is obtained by setting the coefficient of d^2u/dt^2 in (7.2) to zero,

$$(7.3) \qquad \phi = \xi - \theta + \frac{1}{2}$$

in which case the local truncation error is

$$(7.4) \qquad e^n = (2\theta - \xi - \frac{5}{6})\frac{\Delta t^3}{2}\frac{d^3u^n}{dt^3} + O(\Delta t^4) \quad .$$

If $\xi = \phi = 0$ in (7.1), we obtain the linear one-step method (which is a subclass of the two-step method),

$$(7.5) \qquad u^{n+1} - u^n = \Delta t\left[\theta\frac{du}{dt}^{n+1} + (1-\theta)\frac{du}{dt}^{n}\right] - e^n \quad ,$$

where we have shifted the time index down by one. This scheme is sometimes called the θ-method. If $\theta = 1/2$, we obtain the trapezoidal formula (2.10), which is the only second-order-accurate one-step method.

Because the trapezoidal formula has the smallest truncation error of all A-stable LMMs [8], one might ask why we bother to consider the class of A-stable linear two-step schemes. Unfortunately, the trapezoidal formula has the property that the characteristic root $\zeta \to -1$ as $\lambda \Delta t \to \infty$. Consequently, when applied to stiff ordinary differential equations, the trapezoidal formula can produce slowly decaying numerical oscillations. When the trapezoidal formula is applied to hyperbolic partial differential equations where central spatial difference approximations are used, the resulting algorithm is neutrally stable, i.e., the eigenvalues of the amplification matrix have unit modulus. If the solution is nonsmooth by virtue of the presence of shock waves, shear layers, etc., the resulting solution can exhibit highly oscillatory errors. In both of these applications, the oscillatory errors can be damped by a filtering procedure [18] or by the addition of dissipative terms in the case of hyperbolic equations [1,2]. An alternative to using the trapezoidal rule with smoothing is to use a "nonsymmetric" A-stable scheme such as the second-order backward differentiation formula [(7.1) with $\theta = 1$, $\xi = 1/2$, $\phi = 0$]. Nevanlinna and Liniger [23] have recently suggested contractive methods for problems with nonsmooth solutions or where the lack of smoothness is introduced by rapidly varying integration step sizes. A particular example is a method called the contractive Adams method [23] [(7.1) with $\theta = 3/4$, $\xi = 0$, $\phi = -1/4$].

An elegant and simple test for A-stability can be formulated in terms of positive real functions. This terminology is borrowed from the literature of electrical engineering (see, e.g., [16], page 409). Dahlquist [9] has recently extended the theory of positive real functions and considered applications to stability problems arising in numerical analysis. By applying this theory, it is easy to show that the linear two-step method (7.1) is A-stable if and only if the parameters (θ,ξ,ϕ) satisfy the following inequalities:

$$\theta \geq \phi + 1/2 \ ,$$
$$(7.6) \qquad \xi \geq -1/2 \ ,$$
$$\xi \leq \theta + \phi - 1/2 \ .$$

The details of the analysis for obtaining these inequalities are described in [3].

In particular we are interested in the class of all A-stable methods that are second-order accurate as determined by the condition (7.3). In this case two parameters (θ,ξ) remain and the inequalities (7.6) defining the A-stable schemes become

$$(7.7) \qquad \xi \leq 2\theta - 1 \ , \quad \xi \geq -1/2 \ .$$

The shaded region of figure 2 shows the range of the parameters (θ,ξ) for which this class of methods is A-stable. Liniger [20] devised a sufficient and "almost necessary" condition for A-stability of LMMs. As an application of the criterion he developed, Liniger determined the constraints for A-stability on the parameters that define the family of all linear two-step schemes that are at least second-order accurate. The shaded domain of figure 2 reproduces the result determined by Liniger. (Our parameterization of the two-step methods differs from Liniger but it is easy to make the proper correspondence.)

In numerical algorithms for partial differential equations it is conventional to use $n + 1$ as the most advanced time level. Hence we multiply the linear two-step scheme (7.1) by the shift operator E^{-1} to obtain

$$E^{-1}\rho(E)u^n = \Delta t \, E^{-1}\sigma(E) \frac{du^n}{dt} \quad , \tag{7.8}$$

where

$$E^{-1}\rho(E) = (1 + \xi)\Delta - \xi\nabla \quad , \tag{7.9}$$

$$E^{-1}\sigma(E) = 1 + \theta\Delta + \phi\nabla \quad , \tag{7.10}$$

where Δ and ∇ are classical forward and backward difference operators defined by

$$\Delta u^n = u^{n+1} - u^n \quad , \quad \nabla u^n = u^n - u^{n-1} \quad . \tag{7.11}$$

As a notational simplification we denote $E^{-1}\rho(E)$ by the operator Λ:

$$\begin{aligned} \Lambda u^n = E^{-1}\rho(E)u^n &= [(1 + \xi)\Delta - \xi\nabla]u^n \\ &= (1 + \xi)u^{n+1} - (1 + 2\xi)u^n + \xi u^{n-1} \\ &= \Delta u^n + \xi\delta^2 u^n \quad , \end{aligned} \tag{7.12}$$

where δ^2 is the second-central difference operator

$$\delta^2 u^n = u^{n+1} - 2u^n + u^{n-1} \quad .$$

The class of A-stable, two-step, second-order methods (see figure 2) is quite large. Certain subclasses offer particular advantages in regard to computer storage, numerical dissipation, etc. As an example we consider one special subclass that has a particularly simple computational form. Let (6.1) be an ADI scheme where the time differencing is the two-step method (7.1). In this particular case $\omega = \beta_2/\alpha_2 = \theta/(1 + \xi)$. Multiply (6.1) by E^{-1} to conform to the convention that the most advanced time level is $n + 1$. The computational algorithm is simplified when the difference operator in the brackets on the right-hand side of (6.1) is the identity operator. Since from (7.9) and (7.10)

$$E^{-1}[\sigma(E) - \omega\rho(E)] = 1 + \left(\phi + \frac{\theta\xi}{1 + \xi}\right)\nabla \tag{7.13}$$

this becomes the identity operator if

$$\phi + \frac{\theta\xi}{1 + \xi} = 0 \quad . \tag{7.14}$$

For the class of second-order methods, (θ,ξ,ϕ) are related by (7.3) and hence (7.14) can be written in terms of (θ,ξ) as

$$\theta = (\xi + 1)(\xi + 1/2) \quad . \tag{7.15}$$

This curve is shown in figure 2 as a dashed line. With the notation (7.12) and the condition (7.14), which reduces (7.13) to the identity operator, the factored scheme (6.1) becomes

$$(I - \omega\Delta t\, L_x)(I - \omega\Delta t\, L_y)(I - \omega\Delta t\, L_z)\Delta u^n = \Delta t(L_x + L_y + L_z)u^n \quad , \tag{7.16}$$

where $\omega = \theta/(1 + \xi)$.

8. An ADI scheme for the heat equation in three dimensions.

To illustrate the results of the preceding sections we write out an ADI scheme for the linear heat equation

$$(8.1) \qquad \frac{\partial u}{\partial t} = a_1 \frac{\partial^2 u}{\partial x^2} + a_2 \frac{\partial^2 u}{\partial y^2} + a_3 \frac{\partial^2 u}{\partial z^2} \quad ,$$

where $a_\ell \geq 0$. The scheme considered will be for the class of second-order A-stable schemes represented by the portion of the curve $\theta = (\xi + 1)(\xi + 1/2)$ of figure 2 in the shaded region. When applied to the heat equation (8.1), the factored algorithm (7.16) is

$$(8.2) \qquad \left(1 - \omega\Delta t \; a_1 \frac{\partial^2}{\partial x^2}\right)\left(1 - \omega\Delta t \; a_2 \frac{\partial^2}{\partial y^2}\right)\left(1 - \omega\Delta t \; a_3 \frac{\partial^2}{\partial z^2}\right)\Delta u^n = \Delta t\left(a_1 \frac{\partial^2}{\partial x^2} + a_2 \frac{\partial^2}{\partial y^2} + a_3 \frac{\partial^2}{\partial z^2}\right)u^n \quad .$$

An obvious implementation of (8.2) is

$$(8.3a) \qquad \left(1 - \omega\Delta t \; a_1 \frac{\partial^2}{\partial x^2}\right)\Delta u^* = \Delta t\left(a_1 \frac{\partial^2}{\partial x^2} + a_2 \frac{\partial^2}{\partial y^2} + a_3 \frac{\partial^2}{\partial z^2}\right)u^n \quad ,$$

$$(8.3b) \qquad \left(1 - \omega\Delta t \; a_2 \frac{\partial^2}{\partial y^2}\right)\Delta u^{**} = \Delta u^* \quad ,$$

$$(8.3c) \qquad \left(1 - \omega\Delta t \; a_3 \frac{\partial^2}{\partial z^2}\right)\Delta u^n = \Delta u^{**} \quad ,$$

$$(8.3d) \qquad (1 + \xi)u^{n+1} = \Delta u^n + (1 + 2\xi)u^n - \xi u^{n-1} \quad .$$

where $\omega = \theta/(1 + \xi) = \xi + 1/2$ and Λu^{*} and Λu^{**} are dummy variables. If the space derivatives $\partial^2/\partial x^2$, etc., are approximated by central difference quotients, then the x-, y-, z-operators on the left side of (9.3a,b,c) each require the solution of a tridiagonal system. There is a well-known and highly efficient algorithm for the solution of tridiagonal systems (see, e.g. [17, page 55]). The final step (8.3d) is to compute the solution u^{n+1} from known values of Λu^{n}, u^{n} and u^{n-1}.

9. Reduced stability boundary for an alternative formulation.

It has been demonstrated that an approximate factorization scheme for the model equation (4.1) can be constructed that is unconditionally stable if the time differencing is based on an A-stable LMM. In this section we show that an alternative formulation leads to a reduced stability range.

Here we consider only the hyperbolic model equation

$$\frac{\partial u}{\partial t} + c_1 \frac{\partial u}{\partial x} + c_2 \frac{\partial u}{\partial y} = 0 \tag{9.1}$$

and the linear two-step scheme (7.1). After multiplying (7.1) by E^{-1}, one can rewrite the two-step scheme (7.1) as (7.8):

$$[(1 + \xi)\Delta - \xi\nabla]u^{n} = \Delta t[1 + \theta\Delta + \phi\nabla]\frac{du^{n}}{dt} \quad , \tag{9.2}$$

where Δ and ∇ are forward and backward difference operators defined by (7.11). The operator on the left-hand side of (9.2) is $\Lambda = E^{-1}\rho(E)$ as defined by (7.12). As formulated in section 3, the unknown variable to be computed is Λu^n. In this section we alter the procedure and take Δu^n as the unknown variable.

If the time derivative on the right-hand side of (9.2) is replaced by spatial derivatives from (9.1) there follows

$$(9.3)\quad \left[1 + \frac{\theta\,\Delta t}{1+\xi}\left(c_1 \frac{\partial}{\partial x} + c_2 \frac{\partial}{\partial y}\right)\right]\Delta u^n = - \frac{\Delta t}{1+\xi}\left(c_1 \frac{\partial}{\partial x} + c_2 \frac{\partial}{\partial y}\right)u^n - \frac{\phi\,\Delta t}{1+\xi}\left(c_1 \frac{\partial}{\partial x} + c_2 \frac{\partial}{\partial y}\right)\nabla u^n + \frac{\xi}{1+\xi}\nabla u^n \ .$$

An approximate factorization of the left-hand side of (9.3) yields

$$(9.4)\quad \left(1 + \frac{\theta\,\Delta t}{1+\xi}\, c_1 \frac{\partial}{\partial x}\right)\left(1 + \frac{\theta\,\Delta t}{1+\xi}\, c_2 \frac{\partial}{\partial y}\right)\Delta u^n = \mathrm{RHS}(9.3) \ ,$$

where RHS (9.3) denotes the right-hand side of (9.3). In appendix B we analyze the stability of the factored scheme (9.4). For the class of all two-step methods (9.2) that are at least second-order accurate, the parameters (θ,ξ,ϕ) are related by (7.3). For this class of methods, the parameter space (θ,ξ) for which the factored scheme (9.4) is unconditionally stable is shown by the shaded region of figure 3. The wedge shaped region to the "right" of the dotted lines shows the parameter space for which the LMM scheme (7.1) with condition (7.3) is A-stable (this region coincides with the shaded region of figure 2). Consequently, a fairly large class of factored schemes that are unconditionally stable according to the formulation of section 3 are not unconditionally stable if the unknown variable is taken to be Δu^n rather than $E^{-1}\rho(E)u^n = \Lambda u^n$. We should note that the Δu^n and the Λu^n formulations are identical for the subclass of two-step schemes where $\xi = 0$, since in this special case $\Delta u^n = \Delta u^n$, as is obvious from (7.12).

The simplest computational version of (9.4) is the variant where $\phi = 0$. In this case (7.3) becomes $\xi = \theta - 1/2$ and this subclass of schemes was considered in [2] and [25]. The line $\xi = \theta - 1/2$ is shown in figure 3 and falls in the region of unconditionally stable schemes for $\theta \geq 1/2$.

The reduced stability range illustrated in figure 3 results from applying the linear two-step method (9.2) to the model hyperbolic equation (9.1) and taking Δu^n to be the unknown variable. If we had followed exactly the same procedure for the parabolic model equation

$$\frac{\partial u}{\partial t} = a \frac{\partial^2 u}{\partial x^2} + c \frac{\partial^2 u}{\partial y^2} ,$$

the resulting approximate factorization scheme in the Δu^n variable would not have resulted in a reduced stability range in the parameter space (θ, ξ). The example of this section and the result of section 6 for three spatial dimensions show that maintaining unconditional stability of approximate factorization schemes is more difficult for hyperbolic equations than for parabolic equations.

10. The relation between the Douglas-Gunn method and the method of approximate factorization

A general procedure for devising ADI schemes from fully implicit schemes for parabolic equations and the second-order wave equation was developed by Douglas and Gunn [12]. In this section we briefly discuss the relation between the method of Douglas and Gunn and the method of approximate factorization as formulated in section 3.

Linear one-step methods [defined by (7.5)] are called two-level difference schemes by Douglas and Gunn. For linear one-step methods, the operator $\rho(E)u^n$ is simply the forward difference operator

$$\rho(E)u^n = \Delta u^n = u^{n+1} - u^n \quad . \tag{10.1}$$

A method where the increment $\rho(E)u^n = \Delta u^n$ is taken to be the unknown variable (rather than u^{n+1}) is sometimes said to be in the "delta" form. For a linear one-step method, the time-differencing method for the ADI scheme (8.3) with $\xi = 0$ corresponds to the trapezoidal formula (2.10). In this special case, the scheme (8.3) for the heat equation is equivalent to the Douglas-Gunn scheme and to a scheme given earlier and independently by Brian [4] and Douglas [11]. The form that Douglas and Gunn recommend for machine computation (see (2.7) of [12]) is not in the delta form, but it can easily be rewritten in delta form. The delta form generally leads to the most efficient computational algorithm.

To simplify the comparison of the Douglas-Gunn scheme and the formulation of this paper for linear multistep methods, we consider two-step methods. The role of the operator Λu^n defined by (7.12) is taken in the Douglas-Gunn formulation ([12], page 441) by

$$\left(u^{n+1} - u_*^{n+1}\right) , \tag{10.2a}$$

where

$$u_*^{n+1} = \phi_0 u^n + \phi_1 u^{n-1} \tag{10.2b}$$

and

$$\phi_0 + \phi_1 = 1 \quad . \tag{10.2c}$$

Here u_*^{n+1} is a prediction of u^{n+1} based on u^n and u^{n-1}. The choice of (ϕ_0, ϕ_1) is ambiguous unless some condition in addition to (10.2c) is imposed. The interested reader should refer to the discussion by Douglas and Gunn.

In the formulation of this paper, the variable to be determined from the scheme is $E^{-1}\rho(E)u^n$ rather than u^{n+1}. It is obvious from (2.5) that $\rho(E)u^n$ must be an approximation to $\Delta t\ \partial u/\partial t$ for any consistent scheme. Choosing $E^{-1}\rho(E)u^n$ as the unknown variable is equivalent to imposing the condition

$$u^{n+1} - u_*^{n+1} = \frac{\Delta t}{1 + \xi} \frac{\partial u^n}{\partial t} + O(\Delta t^2) \tag{10.3}$$

in the Douglas-Gunn method. The normalization factor $(1 + \xi)^{-1}$ results from the parameterization chosen for the two-step method, as can be seen by comparing (7.12) and (10.2). By imposing (10.3) and using (10.2b), we obtain (10.2c) and, in addition,

$$\phi_0 + 2\phi_1 = \frac{1}{1 + \xi} \quad . \tag{10.4}$$

Hence

$$\phi_0 = \frac{1 + 2\xi}{1 + \xi} \quad , \quad \phi_1 = -\frac{\xi}{1 + \xi} \quad . \tag{10.5}$$

Consequently, if one applies a linear two-step scheme [with the parameterization (7.1)] to the heat equation (9.1) and uses the Douglas-Gunn method with (ϕ_0, ϕ_1) determined by (10.5), then the resulting algorithm will be equivalent to (8.3). Since condition (10.3) is not part of the Douglas-Gunn formulation, the scheme (8.3) will not, in general, coincide with the Douglas-Gunn method. It is obvious that if the constants (ϕ_0, ϕ_1) are determined by (10.5), then u_*^{n+1} will depend on the particular time differencing method chosen.

We should mention that since Douglas and Gunn did not include first-order hyperbolic equations in their formulation, we are demanding a more stringent stability condition (namely A-stability) than one would require if the eigenvalue [see (4.3b)] were pure real. In the latter case, $\lambda = \lambda_R \leq 0$ and A_0-stability is sufficient for unconditional stability. A_0-stability means that the region of stability (see section 2) contains only the interval $(-\infty, 0]$ rather than the entire left-half plane as required for A-stability. (See also last paragraph of section 9.)

11. Concluding remarks and summary.

In this paper we have combined A-stable LMMs and approximate factorization to construct unconditionally stable ADI schemes for partial differential equations with both convection (hyperbolic) and diffusion (parabolic) terms. Linear stability analysis for multilevel partial difference equations is usually very difficult. The stability of a particular scheme is determined by the location of the roots of the characteristic polynomial relative to the unit circle in the complex plane. There are tests such as the Schur-Cohn criterion to determine when the roots of the characteristic polynomial have modulus less than or equal to unity (see, e.g., [21,22]). However, it is often difficult in practice to apply these tests because of the complicated nature of the coefficients (generally complex) of the characteristic polynomial. (See appendix B for the complexity involved for a simple model problem.) We have circumvented this difficulty by constructing a class of ADI schemes such that a sufficient condition for unconditional stability (A-stability) is maintained in the step by step development of the scheme.

The approach is summarized as follows. An A-stable LMM is chosen as the basic time differencing scheme. Next, one discretizes in time but not in space and applies the LMM method to a (model) linear PDE (4.1). The resulting (space continuous) scheme retains the A-stable property since the requirement that the real part of the eigenvalue (4.3b) be nonpositive is the parabolicity condition for the PDE. The ensuing approximations in the construction of an ADI scheme are such that the real part of the "eigenvalue" remains nonpositive. The implicit operator to be inverted is constructed so that the unknown variable to be determined is $\rho(E)u^n$. This ensures that the approximate factorization does not upset either the temporal accuracy (second-order) or the stability of the scheme [by lemma (5.7)]. Finally, one notes that (central) spatial discretizations do not alter the essential property for A-stability, i.e., the real part of the eigenvalue is nonpositive.

Since our main emphasis in this paper is linear stability theory, we have considered only model equations. In a companion paper [3], we apply the method outlined in section 3 to derive an ADI algorithm for a mixed hyperbolic-parabolic system of nonlinear equations where the time differencing is the class of A-stable linear two-step methods. Earlier references on the development of noniterative ADI schemes for nonlinear systems of partial differential equations are listed in the introduction.

Appendix A. Stability analysis when model equation includes a mixed spatial derivative.

In the stability analysis of section 5 we assumed that the mixed derivative term bu_{xy} of the model equation (4.1) was zero. In this appendix we show that if the mixed derivative is treated explicitly by a first-order method, then the resulting ADI scheme remains unconditionally stable. An explicit treatment of the mixed derivative means that bu_{xy} does not appear on the left-hand side of the factored scheme (3.3) but does appear on the right-hand side. Let the mixed derivative be appended to (3.3) as follows:

$$(1 - \omega\Delta t\, L_x)(1 - \omega\Delta t\, L_y)\rho(E)u^n = \Delta t[\sigma(E) - \omega\rho(E)]\left(L_x + L_y + b\frac{\partial^2}{\partial x\partial y}\right)u^n \quad , \tag{A1}$$

where L_x and L_y are defined by (5.1).

By following the same stability analysis that led to characteristic equation (5.5a), we obtain

$$\rho(\zeta) - \lambda_{AF}\,\Delta t\,\sigma(\zeta) = 0 \quad , \tag{A2a}$$

where λ_{AF} is now defined by

$$\lambda_{AF} = \frac{\lambda_1 + \lambda_2 - b\kappa_1\kappa_2}{1 + \omega^2\Delta t^2\,\lambda_1\lambda_2 - \omega\Delta t\; b\kappa_1\kappa_2} \tag{A2b}$$

and λ_1 and λ_2 are defined by (5.5b) and b is the coefficient of u_{xy} in the partial differential equation. A sufficient condition for unconditional stability is that the Re $\lambda_{AF} \le 0$. Since λ_{AF} has the form

(A3) $$\lambda_{AF} = \frac{\alpha_1 + i\beta_1}{\alpha_2 + i\beta_2} ,$$

Re $\lambda_{AF} \le 0$ if and only if

(A4) $$\alpha_1\alpha_2 + \beta_1\beta_2 \le 0 .$$

By a direct calculation we find

$$\alpha_1\alpha_2 + \beta_1\beta_2 = -\left(a\kappa_1^{\,2} + b\kappa_1\kappa_2 + c\kappa_2^{\,2}\right)\left(ac\psi^2 - b\psi + 1\right)$$
$$- \omega^2\kappa_1^{\,2}\kappa_2^{\,2}\left(cc_1^{\,2} - bc_1c_2 + ac_2^{\,2}\right) ,$$

where $\psi = \omega\,\Delta t\,\kappa_1\kappa_2$. The quadratic forms

$$a\kappa_1^{\,2} + b\kappa_1\kappa_2 + c\kappa_2^{\,2}$$

and

$$cc_1^{\,2} - bc_1c_2 + ac_2^{\,2}$$

are nonnegative if and only if $a,c \ge 0$ and $b^2 \le 4ac$, which is the parabolicity condition for the PDE. (If equality holds the equation is hyperbolic.) Likewise, the quadratic

$$ac\psi^2 - b\psi + 1$$

is nonnegative if and only if $b^2 \leq 4ac$. Consequently, Re $\lambda_{AF} \leq 0$ and the ADI scheme with the mixed derivative term treated explicitly is unconditionally stable. The above analysis is for the spatially continuous case. However, in the spatially discrete case, λ_{AF} will also have the same form as (A2) and thus the spatially discrete ADI scheme will be unconditionally stable.

It is very interesting to observe that if one treats the mixed derivative term explicitly but does not use a factored scheme, the product term $\omega^2 \Delta t^2 \lambda_1 \lambda_2$ would be missing from the denominator of (A2b). In this case one can always pick wave numbers κ_1, κ_2 so that the denominator is negative, and then Re $\lambda_{AF} > 0$. Consequently, the unfactored scheme is not unconditionally stable.

Finally, we should point out that if the cross derivative term is treated explicitly as above, then the resulting scheme is first-order accurate in time for the mixed derivative. (See last paragraph of section 5.)

Appendix B. Stability analysis for an alternative formulation.

In this appendix we carry out a linear stability analysis for the factored scheme (9.4). We assume a solution of the form (5.2) and find that the Fourier coefficient satisfies

$$(B1)\qquad (1 + i\bar{c}_1)(1 + i\bar{c}_2)\Delta v^n = -\frac{1}{\theta}(i\bar{c}_1 + i\bar{c}_2)v^n - \frac{\phi}{\theta}[i\bar{c}_1 + i\bar{c}_2]\Delta v^{n-1} + \frac{\xi}{1+\xi}\Delta v^{n-1} ,$$

where we have defined

$$(B2)\qquad \bar{c}_1 = \frac{\theta\,\Delta t}{1+\xi}\kappa_1 c_1 , \quad \bar{c}_2 = \frac{\theta\,\Delta t}{1+\xi}\kappa_2 c_2 .$$

and used the identity

$$(B3)\qquad \nabla v^n = \Delta v^{n-1} .$$

From (B1) it follows that the amplification factor defined by (5.4) satisfies the quadratic equation

$$(B4)\qquad a_2\zeta^2 + a_1\zeta + a_0 = 0 ,$$

where

$$(B5)\qquad \begin{aligned} a_2 &= (1 + i\bar{c}_1)(1 + i\bar{c}_2) , \\ a_1 &= -(1 + i\bar{c}_1)(1 + i\bar{c}_2) + \left(\frac{1}{\theta} + \frac{\phi}{\theta}\right)(i\bar{c}_1 + i\bar{c}_2) - \frac{\xi}{1+\xi} , \\ a_0 &= -\frac{\phi}{\theta}(i\bar{c}_1 + i\bar{c}_2) + \frac{\xi}{1+\xi} . \end{aligned}$$

The characteristic equation (B4) with coefficients (B5) cannot be put in the form (5.3a) and, consequently, we must use some other method of determining when the modulus of the roots of (B4) are bounded by unity. Here we use the Schur-Cohn criterion [21] as formulated by Miller [22].

The polynomial (B4) is a von Neumann polynomial [22], that is, $|\zeta| \leq 1$, if and only if either

$$\text{(B6a)} \qquad \Delta_1 = a_0\bar{a}_0 - a_2\bar{a}_2 < 0$$

and

$$\text{(B6b)}. \qquad \Delta_2 = (a_0\bar{a}_0 - a_2\bar{a}_2)^2 - (\bar{a}_2a_1 - a_0\bar{a}_1)(a_2\bar{a}_1 - \bar{a}_0a_1) \geq 0$$

or

$$\text{(B6c)} \qquad \Delta_1 = \Delta_2 = 0 \quad , \quad 4a_2\bar{a}_2 - a_1\bar{a}_1 \geq 0 \quad .$$

Substitution of the coefficients (B5) into (B6a,b) yields, after some algebraic manipulations,

$$\text{(B7)} \quad \Delta_1 = \bar{\xi}^2 - 1 - \left[\left(1 - \frac{\phi^2}{\theta^2}\right)\bar{c}_1^{\,2} - 2\,\frac{\phi^2}{\theta^2}\,\bar{c}_1\bar{c}_2 + \left(1 - \frac{\phi^2}{\theta^2}\right)\bar{c}_2^{\,2} + \bar{c}_1^{\,2}\bar{c}_2^{\,2}\right] ,$$

(B8)
$$\Delta_2 = \left(\frac{\bar{c}_1 + \bar{c}_2}{\theta}\right)^2 \Bigg\{(1 + \bar{\xi})[(2\theta + 2\phi - 1) - \bar{\xi}(2\theta + 2\phi + 1)]$$
$$+ (2\theta + 2\phi - 1)\bar{c}_1^{\,2}\bar{c}_2^{\,2} + \left(\frac{\theta + \phi}{\theta}\right)^2 (2\theta - 2\phi - 1)\bar{c}_1^{\,2}$$
$$+ 2\left[\bar{\xi} - (2\theta + 2\phi - 1) + \left(\frac{\theta + \phi}{\theta}\right)^2 (2\theta - 2\phi - 1)\right]\bar{c}_1\bar{c}_2$$
$$+ \left(\frac{\theta + \phi}{\theta}\right)^2 (2\theta - 2\phi - 1)\bar{c}_2^{\,2}\Bigg\} \ ,$$

where $\bar{\xi} = \xi/(1 + \xi)$. For the class of all two-step methods (9.2) that are at least second-order accurate, the parameters (θ,ξ,ϕ) are related by (7.3). For this class of methods we want to determine the parameter space (θ,ξ) for which the factored scheme (9.4) is unconditionally stable.

First, we consider the conditions under which Δ_2 as given by (B8) is nonnegative. Using (7.3) we find that the expression enclosed in the first pair of brackets within the braces of (B8) is zero. The coefficient of $\bar{c}_1^{\,2}\bar{c}_2^{\,2}$ is nonnegative if and only if

(B9)
$$\xi \geq 0 \ .$$

The remaining terms within the braces constitute a quadratic form

(B10)
$$A\bar{c}_1^{\,2} + B\bar{c}_1\bar{c}_2 + C\bar{c}_2^{\,2} \ ,$$

which is nonnegative if and only if

(B11a,b,c)
$$A \geq 0 \ , \quad C \geq 0 \ , \quad B^2 \leq 4AC \ .$$

The first two inequalities (B11a,b) require

(B12a) $$\xi \le 2\theta - 1 \ .$$

Necessary and sufficient conditions for the third inequality (B11c) are

(B13a) $$\theta \ge (1 + \xi)\left[(1 + 2\xi) - \sqrt{(1 + 2\xi)(1 + \xi)}\right]/\xi \ ,$$

(B13b) $$\theta \le (1 + \xi)\left[(1 + 2\xi) + \sqrt{(1 + 2\xi)(1 + \xi)}\right]/\xi$$

for $\xi \ge 0$.

Formula (B7) for Δ_1 can be rewritten as the sum of two quadratic forms:

$$\Delta_1 = -\left[d_1 + d_2\bar{c}_1\bar{c}_2 + \left(\bar{c}_1\bar{c}_2\right)^2 + d_3\bar{c}_1{}^2 + d_4\bar{c}_1\bar{c}_2 + d_3\bar{c}_2{}^2\right] \ ,$$

where

$$d_1 = 1 - \bar{\xi}^2 \ , \quad d_2 + d_4 = -2\left(\frac{\phi}{\theta}\right)^2 \ , \quad d_3 = 1 - \left(\frac{\phi}{\theta}\right)^2 \ .$$

Necessary and sufficient conditions to satisfy $\Delta_1 < 0$ are less restrictive than conditions (B9) and (B13a,b), as the interested reader can verify. Hence, the region of unconditional stability is defined by the inequalities (B9) and (B13) and is indicated by the shaded region of figure 3 of the text.

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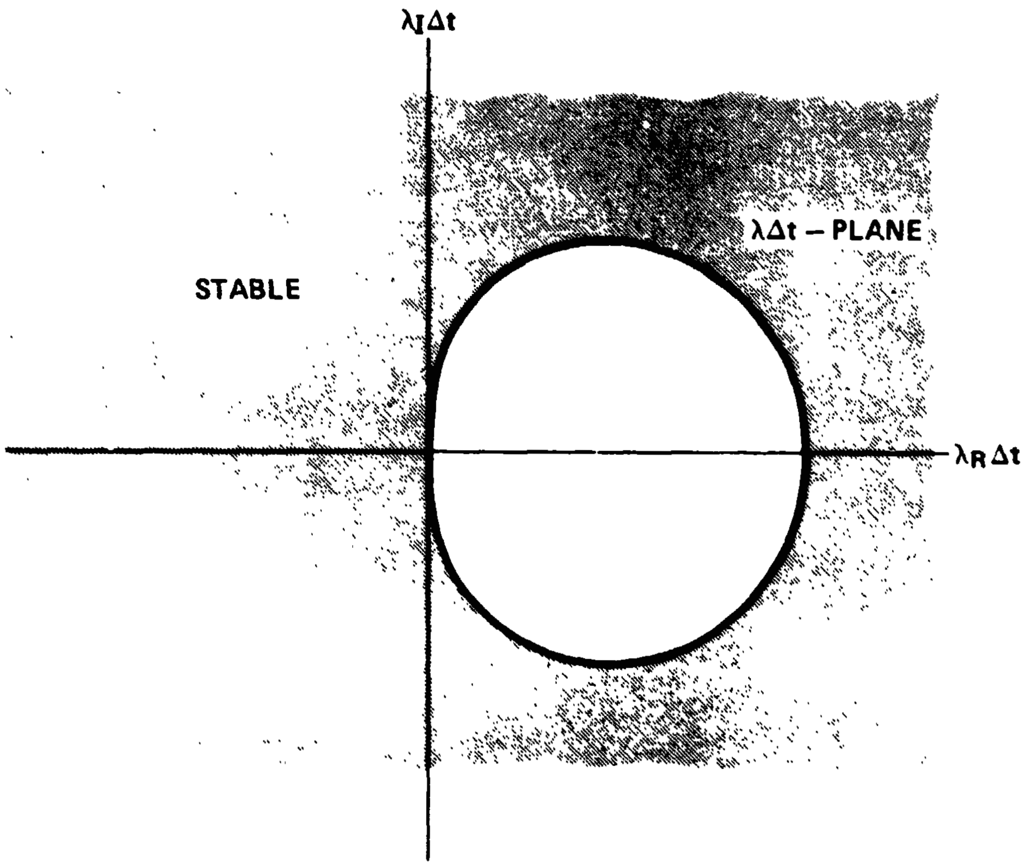

Fig. 1. Region of stability for a typical A-stable scheme.

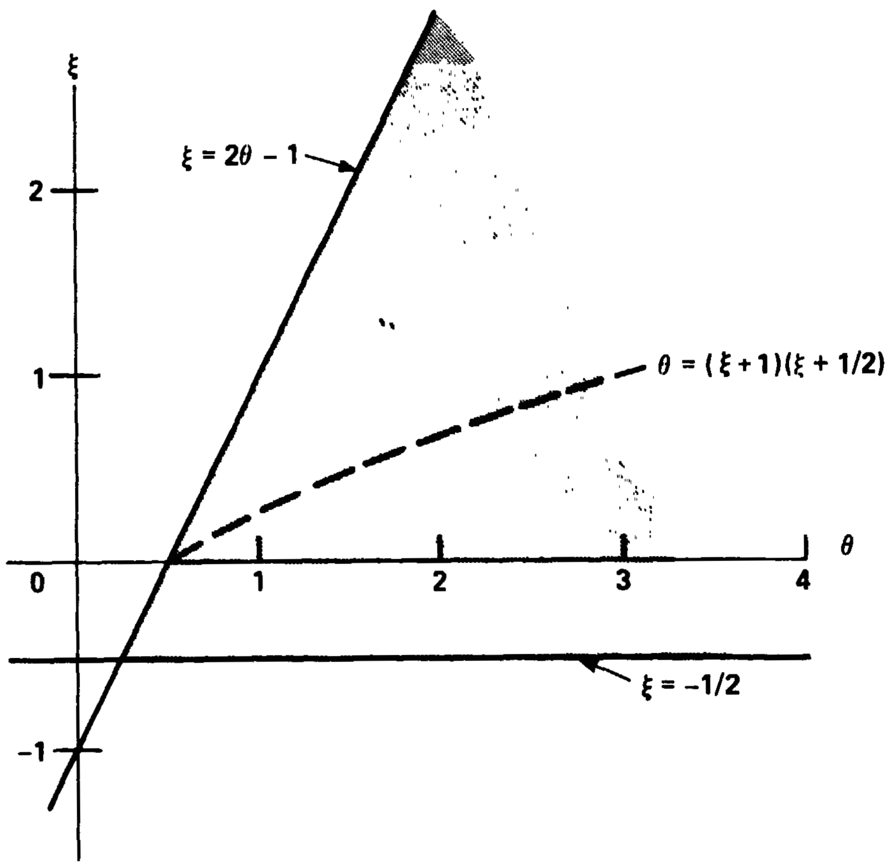

Fig. 2. A-stable range of the parameters (θ,ξ) for the class of all second-order linear two-step methods.

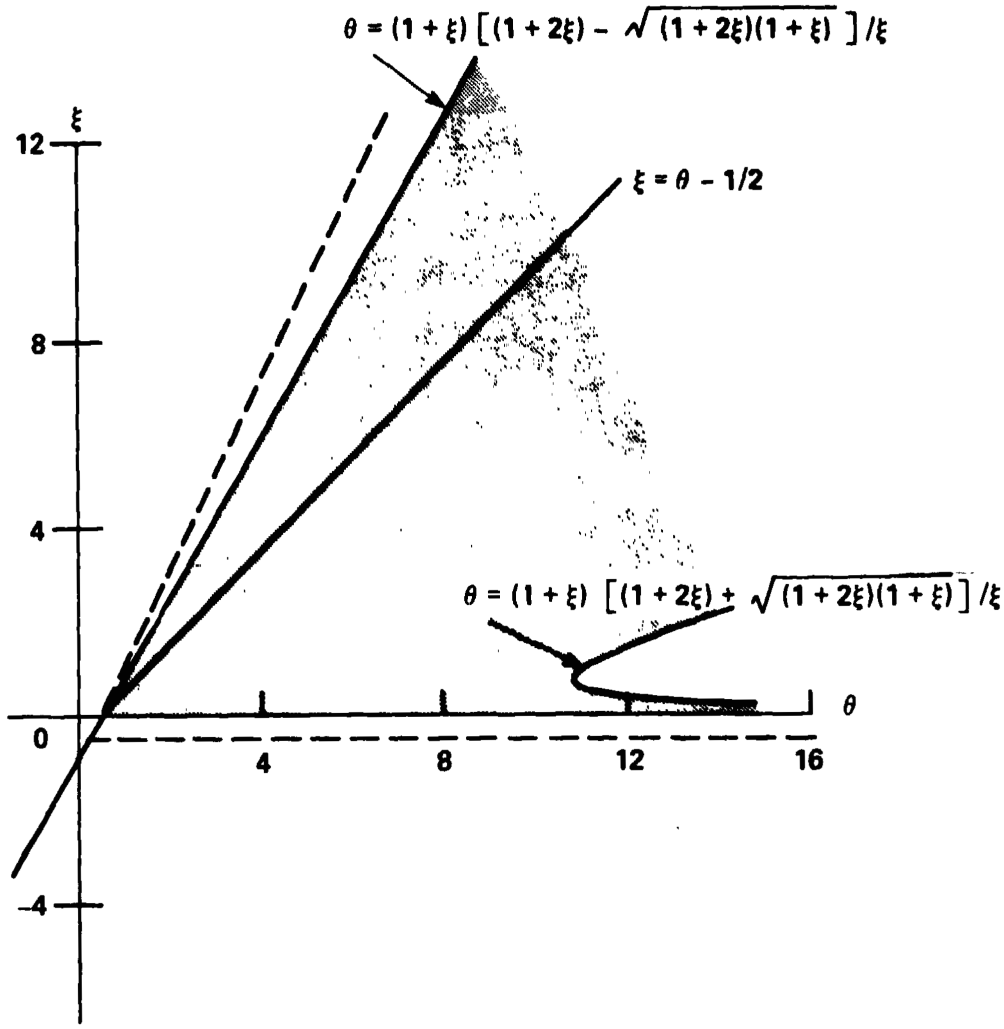

Fig. 3. Unconditionally stable range of the parameters (θ,ξ) for the factored scheme (9.4).