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The Modified Equation Approach to the Stability and Accuracy Analysis of Finite-Difference Methods

R. F. WARMING AND B. J. HYETT

Computational Fluid Dynamics Branch, Ames Research Center, NASA, Moffett Field, California 94035

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The stability and accuracy of finite-difference approximations to simple linear partial differential equations are analyzed by studying the modified partial differential equation. Aside from round-off error, the modified equation represents the actual partial differential equation solved when a numerical solution is computed using a finite-difference equation. The modified equation is derived by first expanding each term of a difference scheme in a Taylor series and then eliminating time derivatives higher than first order by the algebraic manipulations described herein. The connection between "heuristic" stability theory based on the modified equation approach and the von Neumann (Fourier) method is established. In addition to the determination of necessary and sufficient conditions for computational stability, a truncated version of the modified equation can be used to gain insight into the nature of both dissipative and dispersive errors.

INTRODUCTION

This paper describes a technique for evaluating various qualities or properties of a finite-difference analogue of a given partial differential equation. These qualities include order of accuracy, consistency, stability, dissipation, and dispersion. The technique involves determining the actual partial differential equation which is solved numerically, aside from round-off error, by the application of a given difference method to solve an initial-value problem. This actual partial differential equation is called the modified equation. It is derived by expanding each term of a finite-difference equation into a Taylor series and then eliminating time derivatives higher than first order and mixed time and space derivatives by a method described in Section 1. It is emphasized that, contrary to common practice, the original partial differential equation should not be used to eliminate these derivatives.

Although the modified equation has infinitely many terms, in practice only the first several lowest-order terms need to be computed. Terms appearing in the modified equation which are not in the original partial differential equation represent a type of truncation error. These error terms allow one to determine by inspection the order of accuracy and consistency (Section 2) of a finite-difference approximation.

Stability analysis based on an examination of the error terms of a truncated version of the modified equation has heretofore been called "heuristic" and is outlined in Section 3. One of the primary results of this paper is to establish the connection between this approach and the von Neumann method for simple linear equations. To this end we review the von Neumann method in Section 4 and express the square of the modulus of the amplification factor for two-level schemes in a succinct rational function form. This expression provides an important link in understanding the relation between the number of spatial points used in an algorithm, the order of the dissipative error, and the stability bound. With the aid of the rational function formula, the relation and, in fact, equivalence between the von Neumann method and the heuristic approach is established in Section 5. This connection allows us to develop both necessary and sufficient conditions for stability based on the error terms of the modified equation. Finally, in Section 6, dispersive errors for convective equations are discussed.

This article evolved from our interest in the work of several authors. In particular, our prescription for the derivation of the modified equation followed from a discussion by Richtmyer and Morton [1, p. 331] of the Lax–Wendroff scheme for the hyperbolic system $\mathbf{u}_t + A\mathbf{u}_x = 0$. It is well-known that the Lax–Wendroff algorithm attenuates large-wave-number Fourier components. Richtmyer and Morton derived "corrective" dispersive and dissipative operators which, when appended to the right side of the above equation, allowed them to properly interpret the implicit damping of the Lax–Wendroff scheme. The term "modified equation" was suggested to us by our colleague H. Lomax [2], who used the modified equation concept in an analysis of time-continuous methods. Finally, the work of Hirt [3] was instructive in showing that one can deduce stability conditions by examining a truncated version of the modified equation.

1. Concept of the Modified Equation

The linear partial differential equations considered in this paper for initial-value problems will be indicated symbolically as

$$(\partial \tilde{u}/\partial t) + \mathscr{L}_x(\tilde{u}) = 0, \tag{1.1}$$

where $\mathscr{L}_x(\tilde{u})$ represents a linear spatial differential operator and $\tilde{u}$ is dependent variable which is a function of a spatial variable x and a temporal variable t. A specific example is the scalar convective equation:

$$(\partial \tilde{u}/\partial t) + c(\partial \tilde{u}/\partial x) = 0, \tag{1.2}$$

where c is a real constant.

To calculate a solution of a differential equation (1.1) by the method of finite differences, a grid of mesh points is introduced in $x - t$ space with increments Δx and Δt and with indexing defined, e.g., by

$$t = t^n = n\,\Delta t, \qquad x = x_j = j\,\Delta x.$$

The partial differential equation (1.1) is replaced by a finite-difference analogue whose solution on the discrete mesh will be denoted by $u(j\,\Delta x, n\,\Delta t) = u_j^n$. As an example, the second-order Lax–Wendroff scheme [1] applied to the linear convective equation (1.2) is

$$u_j^{n+1} - u_j^n + \frac{c\,\Delta t}{\Delta x}(\mu\delta)\,u_j^n - \frac{1}{2}\left(\frac{c\,\Delta t}{\Delta x}\right)^2 (\delta^2)\,u_j^n = 0, \tag{1.3}$$

where the conventional difference operators

$$(\mu\delta)\,u_j^n = (u_{j+1}^n - u_{j-1}^n)/2, \qquad (\delta^2)\,u_j = u_{j+1}^n - 2u_j^n + u_{j-1}^n \tag{1.4}$$

are employed as a notational convenience. The operators μ and δ are defined individually by

$$\mu u_j = (u_{j+1/2}^n + u_{j-1/2}^n)/2, \qquad \delta u_j = u_{j+1/2}^n - u_{j-1/2}^n\,.$$

In our analysis, it will be important to maintain a distinction between an exact solution of a differential equation, represented by $\tilde{u}$, and a solution of the difference analogue, represented by u, and so a tilde will be retained on a solution of the former.

Since the goal of a finite-difference approximation is to provide a numerical solution to a given partial differential equation, it would seem expedient to know what differential equation is, in fact, being solved by a finite-difference algorithm. The differential equation actually solved by a difference scheme will be called the modified equation.

The modified equation is derived by a two-step procedure outlined as follows. The first step is to expand each term of a given difference algorithm in a Taylor series about u_j^n or, more precisely, the point $(x = j\,\Delta x,\ t = n\,\Delta t)$. Since the solution of a difference equation is defined only at the mesh points, one might question the validity of this expansion. However, for the purpose of analysis, we assume the existence of a continuously differentiable function $u(x, t)$ which coincides at the mesh points—at least in some local sense—with the exact solution of the difference equation, i.e.,

$$u(x, t) = u_j^n \quad \text{for} \quad x = j\,\Delta x, \quad t = n\,\Delta t.$$

TABLE I

Partial Derivatives	$\frac{\partial u}{\partial t}$	$\frac{\partial u}{\partial x}$	$\frac{\partial^2 u}{\partial t^2}$	$\frac{\partial^2 u}{\partial t\,\partial x}$	$\frac{\partial^2 u}{\partial x^2}$	$\frac{\partial^3 u}{\partial t^3}$	$\frac{\partial^3 u}{\partial t^2\,\partial x}$
Coefficients of Eq. (1.5)	1	c	$\frac{\Delta t}{2}$	0	$-\frac{c^2}{2}\Delta t$	$\frac{\Delta t^2}{6}$	0
$-\frac{\Delta t}{2}\frac{\partial}{\partial t}$[Eq. (1.5)]			$-\frac{\Delta t}{2}$	$-\frac{c}{2}\Delta t$	0	$-\frac{\Delta t^2}{4}$	0
$\frac{c}{2}\Delta t\frac{\partial}{\partial x}$ [Eq. (1.5)]				$\frac{c}{2}\Delta t$	$\frac{c^2}{2}\Delta t$	0	$\frac{c}{4}\Delta t^2$
$\frac{\Delta t^2}{12}\frac{\partial^2}{\partial t^2}$ [Eq. (1.5)]						$\frac{\Delta t^2}{12}$	$\frac{c}{12}\Delta t^2$
$-\frac{c}{3}\Delta t^2\frac{\partial^2}{\partial t\,\partial x}$ [Eq. (1.5)]							$-\frac{c}{3}\Delta t^2$
$\frac{c^2}{12}\Delta t^2\frac{\partial^2}{\partial x^2}$ [Eq. (1.5)]							
$\frac{c}{12}\Delta t^3\frac{\partial^3}{\partial t^2\,\partial x}$ [Eq. (1.5)]							
$-\frac{c^2}{12}\Delta t^3\frac{\partial^3}{\partial t\,\partial x^2}$ [Eq. (1.5)]							
$\frac{c\,\Delta t}{12}(\Delta x^2 - c^2\Delta t^2)\frac{\partial^3}{\partial x^3}$ [Eq. (1.5)]							
. . .							
Sum of coefficients in each column	1	c	0	0	0	0	0

Procedure for the Calculation of the Modified Equation.

$\frac{\partial^3 u}{\partial t\,\partial x^2}$	$\frac{\partial^3 u}{\partial x^3}$	$\frac{\partial^4 u}{\partial t^4}$	$\frac{\partial^4 u}{\partial t^3\,\partial x}$	$\frac{\partial^4 u}{\partial t^2\,\partial x^2}$	$\frac{\partial^4 u}{\partial t\,\partial x^3}$	$\frac{\partial^4 u}{\partial x^4}$
0	$\frac{c}{6}\,\Delta x^2$	$\frac{\Delta t^3}{24}$	0	0	0	$-\frac{c^2}{24}\,\Delta t\,\Delta x^2$
$\frac{c^2}{4}\,\Delta t^2$	0	$-\frac{\Delta t^3}{12}$	0	0	$-\frac{c}{12}\,\Delta t\,\Delta x^2$	0
0	$-\frac{c^3}{4}\,\Delta t^2$	0	$\frac{c}{12}\,\Delta t^3$	0	0	$\frac{c^2}{12}\,\Delta t\,\Delta x^2$
0	0	$\frac{\Delta t^3}{24}$	0	$-\frac{c^2}{24}\,\Delta t^3$	0	0
$-\frac{c^2}{3}\,\Delta t^2$	0	0	$-\frac{c}{6}\,\Delta t^3$	0	$\frac{c^3}{6}\,\Delta t^3$	0
$\frac{c^2}{12}\,\Delta t^2$	$\frac{c^3}{12}\,\Delta t^2$	0	0	$\frac{c^2}{24}\,\Delta t^3$	0	$-\frac{c^4}{24}\,\Delta t^3$
			$\frac{c}{12}\,\Delta t^3$	$\frac{c^2}{12}\,\Delta t^3$	0	0
				$-\frac{c^2}{12}\,\Delta t^3$	$-\frac{c^3}{12}\,\Delta t^3$	0
					$\frac{c\,\Delta t}{12}(\Delta x^2 - c^2\,\Delta t^2)$	$\frac{c^2\,\Delta t}{12}\,(\Delta x^2 - c^2 \Delta t^2)$
0	$\frac{c}{6}\,(\Delta x^2 - c^2\,\Delta t^2)$	0	0	0	0	$\frac{c^2\,\Delta t}{8}(\Delta x^2 - c^2\,\Delta t^2)$

Additional comments on the generalization of point functions to continuous functions can be found in the book by Richtmyer and Morton [1, p. 30]. Once the Taylor series expansions have been made, there follows a partial differential equation which includes an infinite number of both space and time derivatives. For example, one obtains, for the Lax–Wendroff scheme (1.3), the expansion

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} - \frac{c^2\,\Delta t}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\Delta t^2}{6}\frac{\partial^3 u}{\partial t^3} + \frac{c\,\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + \frac{\Delta t^3}{24}\frac{\partial^4 u}{\partial t^4} - \frac{c^2\,\Delta t\,\Delta x^2}{24}\frac{\partial^4 u}{\partial x^4} + \cdots = 0. \tag{1.5}$$

In order to obtain an equation amenable to physical interpretation (Section 3), we eliminate in the second step all the time derivatives appearing in the above equation with the exception of u_t by a method to be described below. It is important to emphasize that the original partial differential equation (1.1) should not be used to eliminate the unwanted time derivatives. In general, a solution of the partial differential equation will not satisfy the difference equation, and since the modified equation is to represent the difference equation, it is clear that the original partial differential equation should play no role in the elimination of the higher-order time derivatives. Among recent articles containing modified-equation analyses differing from the following prescription for obtaining the modified equation are those by Tyler [4] and Roache [5].

The proper method for removing the time derivatives can most easily be demonstrated by example for the differential equation (1.5). The procedure requires repeated use of Eq. (1.5) itself. To eliminate the $\partial^2 u/\partial t^2$ term, we multiply Eq. (1.5) by the operator $-(\Delta t/2)\,\partial/\partial t$ and then add the result to (1.5). The resulting new equation has a term $-(c\,\Delta t/2)\,\partial^2 u/\partial t\,\partial x$ which, in turn, can be removed by applying the operator $(c\,\Delta t/2)\,\partial/\partial x$ to Eq. (1.5) and adding the result to the new equation. This calculation can be conveniently organized into a table as illustrated in Table I. The first two rows list the derivatives through fourth order and their coefficients appearing in Eq. (1.5). The subsequent rows show the coefficients of the derivative terms obtained after operation on (1.5) with the differential operator shown on the left-most column. The table is continued until the desired number of time derivatives are deleted. The final equation is obtained by adding the coefficients in each column and multiplying by the derivative at the top of the column. Hence, for the Lax–Wendroff algorithm (1.3), we obtain the modified equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = -\frac{c}{6}(\Delta x^2 - c^2\,\Delta t^2)\frac{\partial^3 u}{\partial x^3} - \frac{c^2\,\Delta t}{8}(\Delta x^2 - c^2\,\Delta t^2)\frac{\partial^4 u}{\partial x^4} + \cdots. \tag{1.6}$$

Although the algebra required in the derivation of the modified equation is tedious, it is completely routine and thus lends itself to automated machine computation by use of a system such as FORMAC [6] capable of performing algebraic operations. All the examples discussed in this paper were computed using a FORMAC language code on an IBM 360/67 computer.

In general, for a given finite-difference analogue of the partial differential equation (1.1), the procedure described above provides the modified equation:

$$\frac{\partial u}{\partial t} + \mathscr{L}_x(u) = \sum_p \mu(p) \frac{\partial^p u}{\partial x^p}. \tag{1.7}$$

The coefficient $\mu(p)$ appearing in the sum denotes the coefficient of the pth spatial derivative. These derivative terms are not in the original partial differential equation and constitute a form of truncation error introduced by the finite-difference analogue. Aside from round-off error, the modified equation represents the exact partial differential equation solved by the finite-difference algorithm. This assertion of the equivalence of the modified equation and the difference algorithm should be qualified since the modified equation contains spatial derivatives of arbitrarily high order. Thus, strictly speaking, an infinite number of boundary conditions are required to define a solution. In our analysis (Sections 3 and 5), we assume spatial periodicity to replace the required boundary conditions.

The essence of the modified-equation approach is that various properties of a finite-difference scheme can be deduced quite simply by examining a truncated version of the modified equation. The first two properties we consider, i.e., order of accuracy and consistency, are discussed in the following section.

2. Order of Accuracy and Consistency

The order of accuracy of a finite-difference scheme is defined by the lowest-order powers of the increments Δt and Δx appearing in the error terms of the modified equation (the right side of Eq. (1.7)). Thus, according to Eq. (1.6), the Lax–Wendroff scheme is uniformly second-order accurate in the increments Δx and Δt. The formal order of accuracy based on the error terms of the modified equation is consistent with that obtained from an examination of truncation error as conventionally defined (see, e.g., Richtmyer and Morton [1, p. 19]). Roughly speaking, the truncation error is a measure of how well a solution of the differential equation satisfies the difference equation, while the modified equation provides a measure of how closely the difference equation models the differential equation.

From the modified-equation viewpoint, a finite-difference scheme is said to be consistent with a given partial differential equation if the right side of Eq. (1.7) tends to zero as Δt and Δx approach zero in an arbitrary manner. Thus, for example, it is obvious from the modified equation (1.6) that the Lax–Wendroff scheme is consistent with the convective equation (1.2). If, by some special relationship between Δt and Δx, the right side of Eq. (1.7) does not tend to zero as the increments vanish, then a finite-difference scheme is said to be inconsistent with the original partial differential equation. In this situation, the modified equation yields directly the differential equation with which the difference scheme is consistent.

3. Heuristic Stability Theory

In this section, we briefly describe a heuristic stability theory based on the modified equation (1.7). The connection between this heuristic description and the von Neumann method will be established in Section 5.

The modified equation (1.7) can be rewritten as

$$\frac{\partial u}{\partial t} = \sum_{p=0}^{\infty} \mu(2p+1) \frac{\partial^{2p+1} u}{\partial x^{2p+1}} + \sum_{p=1}^{\infty} \mu(2p) \frac{\partial^{2p} u}{\partial x^{2p}} \tag{3.1}$$

where the linear spatial operator $\mathscr{L}_x(u)$ has been moved to the right side and included in the sums on the right by appropriate redefinition of the coefficients $\mu(p)$. If we assume an elementary solution for Eq. (3.1) of the form

$$u(x, t) = e^{\alpha t} e^{ikx} \tag{3.2}$$

where the wave number k is real and $\alpha = a + ib$ is complex, then a and b must satisfy

$$a = \sum_{p=1}^{\infty} (-1)^p \, k^{2p} \mu(2p), \tag{3.3}$$

$$b = \sum_{p=0}^{\infty} (-1)^p \, k^{2p+1} \mu(2p+1). \tag{3.4}$$

The elementary solution (3.2) damps or decays as a function of time if $a < 0$, or grows exponentially if $a > 0$. There are difference methods for the convective equation (1.2) without inherent damping in which case $a = 0$ (see, e.g., Roberts and Weiss [7]). Subsequently, we will limit our attention to difference schemes with inherent damping, and, as a consequence, there exist nonvanishing even-order coefficients $\mu(2p)$ in the modified equation.

If the modified equation is to be of practical value, then one should be able to deduce useful stability information by examining a truncated version containing only the first few error terms. Equation (3.3) shows that in the small-wave-number limit, $k \to 0$, we should be able to neglect all the terms except the lowest-order nonzero coefficient, say, $\mu(2r)$. Thus, in order that $a < 0$ for small k, it follows that a necessary (heuristic) condition for the stability of a finite difference scheme is that

$$(-1)^{r-1}\mu(2r) > 0. \tag{3.5}$$

As an application of the above stability condition, consider the modified equation (1.6) associated with the Lax–Wendroff scheme. The lowest even-order derivative is of fourth order, and thus by Eq. (3.5) its coefficient $\mu(4)$ should be negative for stability. Thus we obtain the well-known stability condition $|\nu| < 1$ for the Lax–Wendroff scheme where

$$\nu = c\,\Delta t/\Delta x \tag{3.6}$$

is defined to be the Courant number. Actually, this example was a fortuitous choice as will become apparent in Section 5.

As an example of a higher-order algorithm for the solution of the convective equation (1.2), we examine the linear version of an algorithm due to Rusanov [8] and Burstein and Mirin [9] which is uniformly third order in both the time and spatial increments. In terms of the difference operators defined by Eq. (1.4), this scheme can be written as

$$u_j^{n+1} = u_j^n - \nu(\mu\delta)\left[1 - \frac{1}{6}\delta^2\right]u_j^n + \nu^2(\delta^2)\left[\frac{1}{2} + \frac{1}{8}\delta^2\right]u_j^n$$
$$- \frac{\nu^3}{6}(\mu\delta^3)\,u_j^n - \frac{\omega}{24}(\delta^4)\,u_j^n. \tag{3.7}$$

The last term on the right side is a fourth-order spatial difference operator with a multiplicative parameter ω, which was appended to the scheme to achieve numerical stability. According to the von Neumann analysis [9], the algorithm is stable if

$$4\nu^2 - \nu^4 < \omega \leqslant 3 \quad \text{and} \quad |\nu| < 1. \tag{3.8}$$

The modified equation corresponding to this difference algorithm is

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \frac{-\Delta x^4}{24\Delta t}(\omega - 4\nu^2 + \nu^4)\frac{\partial^4 u}{\partial x^4}$$
$$+ \frac{c\,\Delta x^4}{120}[-5\omega + (4\nu^2 + 1)(4 - \nu^2)]\frac{\partial^5 u}{\partial x^5} + \cdots. \tag{3.9}$$

If the stability criterion (3.5) is applied to the above modified equation, we obtain only the left-most inequality of Eq. (3.8), and so we have obtained only partial information about the complete stability bound. In other situations, in particular when applied to heat-equation algorithms, the heuristic stability condition yields no obvious information about stability. Since condition (3.5) was obtained from a plausibility argument in the small-wave-number limit, the insufficiency of the condition is certainly no surprise.

The largest wave number that can be resolved by a finite-difference scheme is $k = \pi/\Delta x$. The determination of the stability bound in this limit is of critical importance since Fourier components corresponding to the largest wave numbers tend to be the least stable. It does not appear feasible to use the modified equation to predict a stability bound when $k \sim O(1/\Delta x)$ for the following reason. For a finite-difference analogue of either the simple convective equation where $\mu(2p) \sim O(\Delta x^{2p-1})$ if $\Delta t \sim O(\Delta x)$, or the heat equation where $\mu(2p) \sim O(\Delta x^{2p-2})$, if $\Delta t \sim O(\Delta x^2)$, each term of the series (3.3) is of the same order if $k \sim O(1/\Delta x)$. Hence, one should hardly expect to obtain a sensible bound from a truncated version of the modified equation. However, we will describe in Section 5 a stratagem to circumvent this apparent difficulty.

4. Square of the Amplification Factor Modulus as a Rational Function

In this section, we briefly review the von Neumann method for two-level schemes and give a formula for the square of the amplification factor modulus in the form of a rational function. The particular structure of this formula provides the key to understanding the relation between the number of spatial points used in an algorithm, the order of the dissipative error (to be defined), the stability bound for the method, and the connection between the heuristic condition (3.5) and that found by the von Neumann method.

A two-level difference analogue of the differential equation (1.1) can be written in the form

$$\sum_{q=-m_\ell}^{m_r} B_q u_{j+q}^{n+1} = \sum_{q=-n_\ell}^{n_r} A_q u_{j+q}^{n}, \tag{4.1}$$

where m_ℓ, m_r, n_ℓ, and n_r are nonnegative integers. The condition

$$\sum_{q=-m_\ell}^{m_r} B_q = \sum_{q=-n_\ell}^{n_r} A_q \tag{4.2}$$

is necessary for consistency. The von Neumann stability procedure [1] consists of replacing each term u_j^n of the difference equation (4.1) by the kth Fourier component of a harmonic decomposition of u_j^n, i.e., by $v^n(k)\exp(ikj\,\Delta x)$, where $v^n(k)$ denotes the kth Fourier coefficient. The Fourier coefficients at $n+1$ and n are related by

$$v^{n+1}(k) = g(k)\, v^n(k), \tag{4.3}$$

where $g(k)$ is the amplification factor of the finite-difference method. In general, this factor is complex and can be expressed as

$$g(k) = |g(k)| e^{i\phi}. \tag{4.4}$$

Since the two-level algorithm (4.1) has only one dependent variable, a necessary and sufficient condition for stability is [1, p. 72]

$$|g(k)| \leqslant 1 \tag{4.5}$$

for all values of k. If $|g(k)| = 1$ for all k, then the difference scheme is said to be nondissipative or marginally stable, and if $|g(k)| > 1$ for some k, the scheme is unstable. Henceforth, we restrict our attention to algorithms where $|g(k)|$ is not identically one.

For two-level schemes, it can be shown (see Appendix) that $|g(k)|^2$ can always be expressed as the following rational function:

$$|g(k)|^2 - 1 = -4z^r S(z)/P(z), \tag{4.6a}$$

where

$$z = \sin^2(\theta/2), \qquad \theta = k\,\Delta x, \tag{4.6b}$$

$$S(z) = \sum_{i=0}^{s} \alpha_i z^i, \qquad \alpha_0 = S(0) \neq 0, \tag{4.6c}$$

$$P(z) = \sum_{i=0}^{d} \beta_i z^i > 0, \qquad \beta_0 = 1. \tag{4.6d}$$

Here, r is a positive integer and s is a nonnegative integer, and they are related by the formula

$$r + s = m, \tag{4.7a}$$

where

$$m = \max(m_\ell + m_r, n_\ell + n_r) \tag{4.7b}$$

is determined by the number of spatial grid points to the left and right of x_j used in the algorithm (4.1). The integer d of Eq. (4.6d) is nonnegative and $d = m_r + m_\ell$.

[redacted]

the order of the polynomial $S(z)$ as predicted by Eq. (4.7a) is decreased by at least one (see Appendix Eqs. (A.2)–(A.4)). An example of this situation is algorithm (5.7) of Section 5. If a scheme is explicit, then all the coefficients B_q of Eq. (4.1) are zero with the exception of B_0 and $P(z) = 1$.

The polynomial $S(z)$ determines the stability of a given difference scheme since by comparing Eq. (4.6a) with (4.5) and using the fact $P(z) > 0$, it follows that a necessary and sufficient condition for stability is

$$S(0) > 0, \qquad S(z) \geqslant 0 \qquad \text{for} \quad 0 < z \leqslant 1. \tag{4.9}$$

As an example of the polynomial form (4.6) for an explicit scheme, consider the explicit third-order scheme (3.7). This method uses the five points x_j, $x_{j\pm1}$, and $x_{j\pm2}$ to advance the solution one time step and hence $m = 4$. From a direct but tedious calculation of $|g(k)|^2$, one finds that $r = 2$ and $S(z)$ is the following quadratic polynomial [8]:

$$S(z) = \tfrac{1}{3}(\omega - 4\nu^2 + \nu^4) - \tfrac{2}{9}[2\nu^2(1-\nu^2)^2 + 3\nu^2(\omega - \nu^2 - 2)]\, z \\ + \tfrac{1}{9}[4\nu^2(1-\nu^2)^2 - (\omega - 3\nu^2)^2]\, z^2. \tag{4.10}$$

The stability constraint (3.8) on the parameter ω follows directly by evaluating $S(z)$ in the small- and large-wave-number limits, i.e., $S(0)$ and $S(1)$. The corresponding bound on ν is $0 < |\nu| < 1$ and $\sqrt{3} < |\nu|$. Strictly speaking, this latter possible stable range for ν cannot be excluded solely by an examination of the small- and large-wave-number limits.

Schemes for hyperbolic equations with inherent damping may be divided into two main categories as follows. If $S(z) > 0$ for $0 \leqslant z \leqslant 1$, then the difference scheme is said to be strongly dissipative of order $2r$ where r is the positive integer appearing on the right of Eq. (4.6a). If $S(0) > 0$, $S(z) \geqslant 0$ for $0 < z < 1$, and $S(1) = 0$, the scheme is said to be weakly dissipative of order $2r$. A strongly dissipative scheme is characterized by damping of all Fourier components corresponding to nonzero wave numbers and, in particular, the ones with the largest wave numbers. But a weakly dissipative scheme need not damp all components and also the damping tends to zero in the large-wave-number limit since $S(1) = 0$. Our motivation for defining the order of the dissipation to be $2r$ is that in the small-wave-number limit

$$|g(k)| = 1 - 2S(0)(k\,\Delta x)^{2r}/4^r + O[(k\,\Delta x)^{2(r+1)}], \qquad k\,\Delta x \to 0, \tag{4.11}$$

which follows by expanding Eq. (4.6a) for small z. Furthermore, for a strongly disspative scheme, one can show directly from Eq. (4.6) without a small-wave-number assumption that

$$|g(k)| \leqslant 1 - C\theta^{2r}, \tag{4.12}$$

where C is a positive constant independent of θ. The notion of a strongly dissipative scheme as defined above agrees with Kreiss' definition [1] of a dissipative scheme.

5. Relation Between the von Neumann Method and Heuristic Stability Theory

The precise relation between the (heuristic) stability condition (3.5) of Section 3 and the von Neumann theory of the last section can be clarified by the following discussion.

The elementary solution (3.2) of the modified equation (3.1) has the amplification factor

$$g_m(k) = e^{\alpha \Delta t} = e^{a \Delta t} e^{i b \Delta t} \tag{5.1}$$

for one time increment. But since the modified equation represents the exact partial differential equation solved by a finite-difference scheme, the amplification factor (5.1) must equal the amplification factor (4.4) of the difference scheme. Thus,

$$g(k) = g_m(k), \tag{5.2}$$

and by comparison

$$| g(k)| = e^{a \Delta t}, \tag{5.3a}$$

$$e^{i\phi} = e^{i b \Delta t}. \tag{5.3b}$$

Thus from Eqs. (3.3) and (3.4), it is clear that the modulus of $g(k)$ is related to the even-order coefficients $\mu(2p)$ of the modified equation, and the phase shift ϕ is related to the odd-order coefficients. Phase-shift relations will be considered in Section 6; in the present section we concentrate on stability.

We first consider the small-wave-number limit. Let $\mu(2p = 2r)$ be the lowest-order nonzero coefficient appearing on the right side of Eq. (3.3). If one expands $\exp(a\, \Delta t)$ and retains only the lowest-order term in k and then compares with the limiting form (4.11), there follows the relation

$$\mu(2r) = ((-1)^{r-1}/2^{(2r-1)})(\Delta x^{2r}/\Delta t)\, S(0). \tag{5.4}$$

Since a necessary condition for stability is $S(0) > 0$, the lowest even-order nonvanishing coefficient $\mu(2r)$ must satisfy

$$(-1)^{r-1} \mu(2r) > 0. \tag{5.5}$$

But this inequality is precisely the stability condition (3.5) obtained by a heuristic argument.

It is now obvious that the simplest algorithms to analyze using the modified equation are ones for which $S(z) = \text{constant} = S(0)$. In this case, inequality (5.5) is both necessary and sufficient for stability. An example of this situation is the Lax–Wendroff algorithm (1.3) whose amplification factor modulus is

$$| g(k)|^2 - 1 = -4z^2 S(z); \qquad S(z) = \nu^2(1 - \nu^2), \tag{5.6}$$

where $S(z)$ is a constant independent of z. As a second example, consider the Crank–Nicholson algorithm [1]

$$u_j^{n+1} = u_j^n + (\sigma\, \Delta t/2\Delta x^2)[(\delta^2)\, u_j^{n+1} + (\delta^2)\, u_j^n] \tag{5.7}$$

for the heat equation $\tilde{u}_t = \sigma \tilde{u}_{xx}$, $\sigma > 0$. The modified equation is

$$\partial u/\partial t = \sigma(\partial^2 u/\partial x^2) + (\sigma\, \Delta x^2/12)\, \partial^4 u/\partial x^4 + \cdots. \tag{5.8}$$

The coefficient of the lowest even-order derivative of the modified equation is $\mu(2r = 2) = \sigma$ so $r = 1$. By comparing this algorithm (5.7) with the general two-level formula (4.1), one can easily verify that this scheme is a special case covered by Eq. (4.8) where $m_\ell + m_r = m = 2$. Thus, the order of the polynomial $S(z)$ must be at least one order lower than given by formula (4.7a) and consequently $s = 0$ and $S(z)$ is a constant. But by Eq. (5.4), $S(0)$ is given by

$$\mu(2) = \sigma = (1/2)(\Delta x^2/\Delta t)\, S(0) > 0.$$

Here we have the curious result that the unconditionally stable nature of the algorithm is predicted by the coefficient of u_{xx} which is not an error term of the modified equation.

If one calculates the modified equation for a given algorithm, then the order s of the polynomial $S(z)$ can be determined directly from Eq. (4.7a) since m is known and r is determined by the lowest-order nonvanishing coefficient $\mu(2r)$. For example, in the case of third-order algorithm (3.7), $r = 2$ since in the modified equation (3.9) $\mu(4)$ is the lowest even-order nonzero coefficient and $m = 4$ by Eq. (4.7b). Hence, $s = 2$, and thus we know that $S(z)$ is a quadratic and we cannot expect more than a necessary condition by applying condition (5.5).

At the end of Section 3, we argued that it did not appear feasible to determine from the modified equation the stability bound in the large-wave-number limit, i.e., the stability bound imposed by $S(1)$. However, if we can establish a relation between the even-order coefficients $\mu(2p)$ of the modified equation and the coefficients α_i of the polynomial $S(z)$, then we could use the modified equation to obtain a complete stability analysis. This can in fact be done as follows. Rewrite Eq. (5.3a) as

$$|\, g(k)|^2 = e^{2a\Delta t}, \tag{5.9}$$

and replace the left side of this equation by (4.6a) and the parameter a in the exponential by Eq. (3.3). Then expand both sides in powers of $\theta = k\, \Delta x$ and compare coefficients.

In order to demonstrate this approach, we examine explicit schemes where

$$S(z) = \alpha_0 + \alpha_1 z, \qquad \alpha_0 \neq 0. \tag{5.10}$$

This linear case actually encompasses a large number of algorithms because if the order s of the polynomial $S(z)$ is greater than unity, this generally indicates that more spatial points are used in the algorithm than necessary for the order of accuracy achieved. If both sides of Eq. (5.9) are expanded as described above, we find for $r = 1$

$$S(1) = (8\,\Delta t/\Delta x^4)[(\Delta x^2/3)\,\mu(2) - \Delta t\mu^2(2) - \mu(4)], \qquad r = 1, \tag{5.11}$$

and for $r \geqslant 2$

$$S(1) = ((-4)^{r+1}\,\Delta t/(2\,\Delta x^{(2r+2)}))[(1/12)(3 + r)\,\Delta x^2\,\mu(2r) - \mu(2r + 2)], \qquad r \geqslant 2. \tag{5.12}$$

In either case, $S(0)$ is given by Eq. (5.4.) For linear $S(z)$, it is obvious that $S(0) > 0$ and $S(1) \geqslant 0$ are both necessary and sufficient for stability since $S(z) \geqslant \min(S(0), S(1))$.

In a recent paper, Morton [10] considered the effect on numerical stability when the viscous term $\sigma\tilde{u}_{xx}$ is added to the right side of convective equation (1.2) yielding

$$(\partial\tilde{u}/\partial t) + c(\partial\tilde{u}/\partial x) = \sigma(\partial^2\tilde{u}/\partial x^2), \qquad \sigma > 0. \tag{5.13}$$

The explicit finite-difference algorithm he analyzed was

$$u_j^{n+1} = u_j^{\,n} - \nu(\mu\delta - (\nu/2)\,\delta^2)\,u_j^{\,n} + \gamma(\delta^2)\,u_j^{\,n}, \tag{5.14}$$

where $\nu = c\,\Delta t/\Delta x$ and $\gamma = \sigma\,\Delta t/\Delta x^2$. The modified equation is

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \sigma\frac{\partial^2 u}{\partial x^2} - \frac{c\,\Delta x^2}{6}(1 - \nu^2 - 6\gamma)\frac{\partial^3 u}{\partial x^3} + \frac{\Delta x^4}{24\Delta t}[2\gamma(1 - 6\gamma) + 3\nu^2(\nu^2 + 4\gamma - 1)]\frac{\partial^4 u}{\partial x^4} + \cdots. \tag{5.15}$$

The lowest nonzero even-order coefficient $\mu(2) = \sigma$ is positive for arbitrary Δx and Δt and consequently we learn nothing about the stability of the algorithm from the stability condition (5.5). But we can still use the modified equation to determine the stability bound. Since the algorithm uses the points x_j, $x_{j\pm 1}$, the integer m equals 2 and from Eq. (4.7a) s equals 1; thus $S(z)$ is linear. By applying formula (5.11) and using values of $\mu(2)$ and $\mu(4)$ determined from the modified equation (5.15), we find

$$S(1) = (\nu^2 + 2\gamma)(1 - \nu^2 - 2\gamma), \tag{5.16}$$

and consequently a necessary and sufficient condition for stability is

$$\nu^2 + 2\gamma \leqslant 1. \tag{5.17}$$

If ν is set to zero in the difference algorithm (5.14), one gets the explicit scheme for the heat equation, and from inequality (5.17), there follows the well-known stability bound $\gamma \leqslant 1/2$.

6. Phase Error Analysis for Convective Schemes

A stable numerical solution of the scalar convective equation (1.2) computed from a finite-difference scheme will generally exhibit errors in both amplitude (dissipation) and phase (dispersion). The modified equation provides a natural resolution of these errors since even-order spatial derivatives correspond to dissipative effects and odd-order spatial derivatives are related to dispersive effects.

Phase shift errors resulting from a finite-difference solution can be analyzed by the von Neumann method as follows. A Fourier expansion of an exact solution of Eq. (1.2) has elementary modes $\exp[ik(x - ct)]$, and thus for one time-increment Δt, the amplification factor is

$$g_e(k) = e^{-ick\Delta t}. \tag{6.1}$$

The phase shift per time step is

$$\phi_e = -ck\,\Delta t = -\nu\theta, \tag{6.2}$$

where $\theta = k\,\Delta x$ and ν is the Courant number $c\,\Delta t/\Delta x$. Consequently, the relative phase shift error or velocity dispersion per time increment is given by the ratio ϕ/ϕ_e, where ϕ is computed from the amplification factor (4.4) of the finite-difference scheme. Figure 1 is a plot of the phase error ϕ/ϕ_e as a function of θ for the second-order Lax–Wendroff scheme (1.3) and the third-order method (3.7) for $\nu = 0.3$ and 0.8 and several values of the parameter ω. If the phase error exceeds 1 for a given value of θ, the corresponding Fourier mode will have a wave speed exceeding the exact solution with the converse being the case for a phase error less than 1.

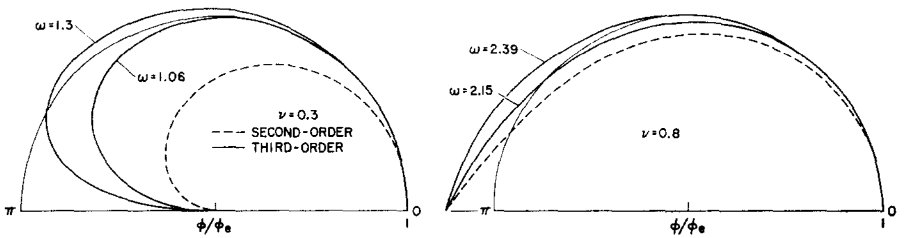

Fig. 1. Comparison of phase error ϕ/ϕ_e for second- and third-order methods for $\nu = 0.3$ and $\nu = 0.8$.

The phase shift ϕ for a difference algorithm in terms of the odd-order coefficients of the modified equation is given by

$$\phi = \Delta t \sum_{p=0}^{\infty} (-1)^p k^{2p+1} \mu(2p+1) \tag{6.3}$$

which follows from Eq. (5.3b) with b given by the sum (3.4). Since any sensible difference analogue of the convective equation (1.2) will have a modified equation with $\mu(1) = -c$, the above equation can be rewritten as

$$\frac{\phi}{\phi_e} = 1 - \frac{1}{c} \sum_{p=1}^{\infty} (-1)^p k^{2p} \mu(2p+1). \tag{6.4}$$

Let $\mu(2q+1)$ be the lowest-order nonvanishing coefficient in the summation of Eq. (6.4). For small wave numbers, one can neglect all but the lowest-order term and, consequently,

$$\frac{\phi}{\phi_e} = 1 - \frac{(-1)^q k^{2q}}{c} \mu(2q+1) + O[(k \, \Delta x)^{2(q+1)}], \qquad k \, \Delta x \to 0. \tag{6.5}$$

On the basis of this limiting form, a convective difference scheme is said to be dispersive or order $2q$, where q is the positive integer appearing in the above equation.

According to the limiting form (6.5), a Fourier mode for small k will lag or have a lower wave speed than the exact mode if

$$((-1)^q/c) \, \mu(2q+1) > 0 \qquad \text{(phase lag).} \tag{6.6}$$

Although this inequality is strictly true only for small wave numbers, it provides a practical criterion for judging whether a particular algorithm has a dominant leading or lagging phase error. From the modified equation (1.6) for the Lax–Wendroff scheme, $-\mu(3)/c$ is positive in the stable range, indicating a predominant lagging phase error even though ϕ/ϕ_e can exceed 1 for large wave numbers as illustrated in Fig. 1 for $\nu = 0.8$.

As an example of a second-order scheme with a leading phase error, consider the "upwind" scheme for $c > 0$

$$u_j^{n+1} = u_j^n - \nu(1 + \tfrac{1}{2}\nabla) \nabla u_j^n + \tfrac{1}{2}\nu^2 \nabla^2 u_j^n, \qquad c > 0, \tag{6.7}$$

where ∇ is the backward difference operator defined by

$$\nabla u_j^n = u_j^n - u_{j-1}^n .$$

The modified equation is

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \frac{c\,\Delta x^2}{6}(1-\nu)(2-\nu)\frac{\partial^3 u}{\partial x^3} - \frac{\Delta x^4}{8\Delta t}\nu(1-\nu)^2(2-\nu)\frac{\partial^4 u}{\partial x^4} + \cdots. \quad (6.8)$$

By virtue of Eq. (6.6), this upwind scheme has a leading phase error for $0 < \nu < 1$.

Fromm [11] based his method of zero-average phase error on the observation that a reduction of dispersion should occur by using a linear combination of methods of opposite phase error. If we represent the Lax–Wendroff scheme (1.3) as $u_j^{n+1} = L_w(u_j^n)$ and the upwind scheme (6.7) by $u_j^{n+1} = L_u(u_j^n)$ and form the average

$$u_j^{n+1} = 1/2(L_w + L_u)\,u_j^n,$$

we obtain the one-dimensional version of Fromm's scheme. The modified equation for Fromm's scheme is a simple average of Eqs. (1.6) and (6.8) corresponding to the Lax–Wendroff and upwind schemes. The reduction in phase error is apparent by comparing the coefficient $\mu(3)$ of the three methods for $0 < \nu < 1$.

The third-order method (3.7) can have either a predominantly leading or lagging phase error, depending on the choice of the parameter ω as illustrated in Fig. 1. A difficulty with the third-order method is finding a practical criterion for choosing the free parameter in the stable range (3.8). We have shown, in a recent paper [12], that the modified equation (3.9) can be used to advantage to provide such a criterion. If it is desirable to minimize dispersive error, then ω is selected so that the coefficient of the lowest-order odd derivative on the right side of Eq. (3.9) is zero, i.e.,

$$\omega = (4\nu^2 + 1)(4 - \nu^2)/5. \quad (6.9)$$

A more detailed analysis including phase error plots and numerical examples for both linear and nonlinear problems is presented in Refs. 12 and 13.

In a recent paper, Taylor *et al.* [14] evaluated several methods for integrating the one-dimensional inviscid gasdynamic equations. By numerical experiment, they found for Rusanov's [8] third-order method that the best results were obtained for $\nu = 0.7$ and $\omega = 2.0$. For a Courant number of 0.7, the minimum dispersion formula (6.9) yields $\omega = 2.08$. This predicted value certainly adds credence to the practical utility of the modified equation analysis.

7. Summary of the Modified-Equation Approach

To summarize the modified-equation method of evaluating a finite-difference approximation to a simple partial differential equation, we analyze the following second-order explicit algorithm proposed by Crowley [15] for the convective equation (1.2):

$$u_j^{n+1} = u_j^n - \nu(\mu\delta)\, u_j^n + (\nu^2/2)(\mu^2\delta^2)\, u_j^n - (1/8)\, \nu^3(\mu\delta^3)\, u_j^n,$$

where $\nu = c\,\Delta t/\Delta x$. The corresponding modified equation is

$$\begin{aligned}\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = &-\frac{c\,\Delta x^2}{24}(4 - \nu^2)\frac{\partial^3 u}{\partial x^3} - \frac{c\,\Delta x^4}{480}(4 - \nu^2)(1 - 6\nu^2)\frac{\partial^5 u}{\partial x^5} \\ &+ \frac{c^4\,\Delta x^2\,\Delta t^3}{128}(4 - \nu^2)\frac{\partial^6 u}{\partial x^6} + \mu(7)\frac{\partial^7 u}{\partial x^7} \\ &+ \frac{c^4\,\Delta x^4\,\Delta t^3}{256}(4 - \nu^2)\frac{\partial^8 u}{\partial x^8} + \cdots . \end{aligned} \tag{7.1}$$

The lowest-order error term is

$$\mu(3) = -(c/24)(4\,\Delta x^2 - c^2\,\Delta t^2),$$

so the scheme is uniformly second-order accurate in Δx and Δt. The error terms on the right side of the modified equation (7.1) tend to zero as Δt and Δx approach zero, so clearly the scheme is consistent with the convective equation (1.2). The lowest-order even-derivative coefficient of the modified equation is $\mu(6 = 2r)$, so $r = 3$. From inequality (5.5), a necessary condition for stability is $\mu(6) > 0$, and hence a bound on the Courant number is

$$0 < |\nu| < 2. \tag{7.2}$$

The Crowley algorithm uses data at the five spatial points x_j, $x_{j\pm 1}$, and $x_{j\pm 2}$ to advance the solution one time step, and thus the integer m defined by Eq. (4.7b) is 4. Then by Eq. (4.7a), $s = 1$ and the polynomial $S(z)$ is linear, and, consequently, $S(1)$ can be determined by formula (5.12). We find that $S(1) = 0$, so inequality (7.2) is both necessary and sufficient for stability. By the definition in Section 4, the scheme is weakly dissipative of order 6 for ν in the range (7.2). Utilizing inequality (6.6), it follows that the phase error will be predominantly lagging. Finally, since the scheme is consistent and stable for $|\nu| < 2$, u will converge uniformly to $\tilde{u}$ as Δt tends to zero for a fixed constant $|\nu| = |c|\,\Delta t/\Delta x < 2$ (Lax equivalence theorem [1]).

Concluding Remarks

The modified-equation approach has been shown to be a viable technique for analyzing linear finite-difference approximations to partial differential equations.

Since the algebraic operations involved in the analysis are readily amenable to automated machine calculation by a language such as FORMAC [6], the technique can be applied with little effort on the part of the user. We have found it to be particularly valuable in analyzing the relative merits of proposed schemes or in constructing new ones.

We believe the modified equation concept can be used as an effective didactic device since one quite often has, from experience, more physical intuition about the properties of simple partial differential equations than for those of difference equations. Thus it can be applied effectively to give insight into the nature and control of dispersive and dissipative errors.

Finally, we should emphasize that although the stability analysis of this paper has been confined to linear problems, Hirt [3] has argued that a criterion similar to the heuristic necessary condition (3.5) is applicable to nonlinear equations with variable coefficients. In a recent paper, Lerat and Peyret [16] have used a nonlinear modified equation analysis to demonstrate that the oscillations observed behind a shock front are not always due to dispersive error but are also attributable to a small local nonlinear instability.

APPENDIX: Derivation of Equation (4.6)

Our original derivation of formula (4.6) was somewhat cumbersome. The following simplified proof was suggested to us by Marcel Vinokur. The amplification factor for the two-level algorithm (4.1) is

$$g(k) = \sum_{q=-n_\ell}^{n_r} A_q e^{iq\theta} \Big/ \sum_{q=-m_\ell}^{m_r} B_q e^{iq\theta}, \tag{A.1}$$

where $\theta = k\,\Delta x$. The square of the modulus of the sum in the numerator can be expressed as

$$\left| \sum_{q=-n_\ell}^{n_r} A_q e^{iq\theta} \right|^2 = \sum_{q=-n_\ell}^{n_r} \sum_{p=-n_\ell}^{n_r} A_p A_q \cos(q-p)\theta.$$

But since $\cos\theta = 1 - 2z$, where $z = \sin^2(\theta/2)$, one finds by using a trigonometric multiple angle formula that

$$\cos n\theta = \sum_{i=0}^{n} D_i z^i, \qquad D_0 = 1, \qquad D_n = (-1)^n\, 2^{2n-1}.$$

If we define $w = n_\ell + n_r$, then

$$\left| \sum_{q=-n_\ell}^{n_r} A_q e^{iq\theta} \right|^2 = \sum_{i=0}^{w} \gamma_i z^i, \qquad \gamma_0 = 1, \qquad \gamma_w = (-1)^w \, 2^{2w} A_{-n_\ell} A_{n_r}, \tag{A.2}$$

where without loss of generality we have normalized the coefficients A_q such that the consistency condition (4.2) is $\sum A_q = 1$. Hence, one obtains for $|g(k)|^2$ the formula

$$|g(k)|^2 = \sum_{i=0}^{w} \gamma_i z^i \Big/ \sum_{i=0}^{d} \beta_i z^i = 1 + \sum_{i=0}^{m} (\gamma_i - \beta_i) \, z^i \Big/ \sum_{i=0}^{d} \beta_i z^i, \tag{A.3}$$

where

$$d = m_\ell + m_r, \qquad m = \max(d, w), \qquad \beta_0 = 1, \qquad \beta_d = (-1)^d \, 2^{2d} B_{-m_\ell} B_{m_r}. \tag{A.4}$$

Finally, if r is a positive integer defined by

$$\gamma_i = \beta_i \qquad \text{for} \quad i < r, \qquad \gamma_i \neq \beta_i \qquad \text{for} \quad i = r,$$

and if a coefficient α_i is defined as $-4\alpha_i = \gamma_{i+r} - \beta_{i+r}$, then Eq. (A.3) can be

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