JOURNAL OF COMPUTATIONAL PHYSICS 70, 262–268 (1987)

Note

Stability of Finite Difference Representations of Partial Differential Equations—A Two-Step Process

Two classical methods are currently available for the determination of the numerical stability of finite difference representations of partial differential equations. These are the Fourier and the Matrix methods [1]. These methods require one to represent all of the partial derivatives as finite differences before they can be applied. Furthermore, if the result is negative (an unstable case), little information is obtained as to the cause of the instability.

The method proposed in this paper is identical to the matrix method, except that the procedure is divided into two sequential steps. The additional information obtained after the first step can help identify the cause of any instability found.

The first step requires that finite difference representations of the partial derivatives, with respect to all but one of the independent variables, be constructed. This results in a set of ordinary differential equations. The stability of this set of ordinary differential equations can then be determined via several methods, typically by linearization about equilibrium points.

The second step consists of representing the remaining derivatives as finite differences to obtain a set of algebraic equations. The stability of this finite difference approximation can be easily evaluated via well-known methods for ordinary differential equations [2].

Since the method involves two independent steps, accuracy and stability of the many possible approximations for the derivatives with respect to the remaining independent variable can be quickly evaluated. The first step need not be repeated. Furthermore, if there are more than two independent variables, the method can be repeated so as to isolate the finite difference approximations with respect to each variable. This may help determine which finite difference approximations contributed to any numerical instability.

The proposed method is best applied to mathematical models of physical systems that exhibit a physical instability, for it allows one to more easily distinguish between physical and numerical instabilities. This is done via the additional information that is obtained from the first step and is discussed later in this paper.

It is easy to demonstrate the equivalence of the two-step process to the classical one-step procedure of the matrix method. First, consider a general partial differential equation. If one chooses finite difference approximations for the partial derivatives with respect to all the independent variables, save one, an ordinary differential equation set results,

$$\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}). \tag{1}$$

0021-9991/87 $3.00

The time variable has been assumed to be the remaining independent variable here for case of physical interpretation. The other independent variables will be assumed to represent spatial locations. If the time derivatives are not all of first order, this form can still be obtained by introducing additional state variables.

In general, Eq. (1) can be linearized to test the stability of the ordinary differential equation set about equilibrium points,

$$\dot{\mathbf{u}} = \mathbf{A}\mathbf{u}. \tag{2}$$

The stability of the above equation set can be determined by examining the eigenvalues, λ, of $\mathbf{A}$, obtained from

$$|\mathbf{A} - \lambda \mathbf{I}| = 0. \tag{3}$$

If all the eigenvalues have negative real parts, the ordinary differential equation set is stable (at least in the region of the equilibrium point, or globally if Eq. (1) is linear). This completes step one of the proposed method.

The second, and final, step involves choosing a finite difference method for the derivatives with respect to time. Several implicit and explicit methods are available, and their stability characteristics can all be expressed based on the eigenvalues obtained from Eq. (3).

A general ordinary differential equation multistep method will be considered here for the finite difference approximations of the time derivatives,

$$\mathbf{u}_{n+1} = \sum_{j=0}^{p} a_j \mathbf{u}_{n-j} + h \sum_{j=-1}^{p} \beta_j \mathbf{A}\mathbf{u}_{n-j}. \tag{4}$$

In Eq. (4) the subscripts represent the step (or time plane) in the multistep integration, $\mathbf{A}$ is defined in Eq. (2), and h is the time-step size. The terms a_j and β_j are coefficients obtained from a particular multistep method, and the value of p represents the number of steps in the multistep method.

It has been shown [2] that for absolute stability of the multistep method, the roots of the following polynomial should be less than unity in magnitude for all eigenvalues, λ_i, of the matrix $\mathbf{A}$,

$$(1 - h\lambda_i \beta_{-1})\, r^{p+1} = \sum_{j=0}^{p} (a_j + h\lambda_i \beta_j)\, r^{p-j}, \tag{5}$$

where the superscripts represent integer powers.

Next, the standard stability calculation for the classical matrix method is briefly presented for a comparison of the results. This requires finite difference

approximations of all partials, including those with respect to time, be constructed in the beginning. Then if the eigenvalues of the matrix **S** in the following equation are less than unity in magnitude, the numerical representation is stable;

$$\mathbf{U}_{n+1} = \mathbf{S}\mathbf{U}_n,$$

where

$$\mathbf{U}_{n+1} = \begin{bmatrix} \mathbf{u}_{n+1} \\ \mathbf{u}_n \\ \vdots \\ \mathbf{u}_{n-p+1} \end{bmatrix} \quad \text{and} \quad \mathbf{U}_n = \begin{bmatrix} \mathbf{u}_n \\ \mathbf{u}_{n-1} \\ \vdots \\ \mathbf{u}_{n-p} \end{bmatrix}. \tag{6}$$

From Eqs. (2), (4), and (6), the matrix **S** can be represented in partitioned form

$$\mathbf{S} = \begin{bmatrix} \mathbf{B}(a_0\mathbf{I} + \beta_0 h\mathbf{A}) & \mathbf{B}(a_1\mathbf{I} + \beta_1 h\mathbf{A}) & \cdots & \mathbf{B}(a_p\mathbf{I} + \beta_p h\mathbf{A}) \\ \mathbf{I} & \mathbf{O} & & \cdot \\ \mathbf{O} & \mathbf{I} & & \cdot \\ \mathbf{O} & \mathbf{O} & \ddots & \cdot \\ \cdot & \cdot & & \\ \cdot & \cdot & \mathbf{I}\ \mathbf{O} & \mathbf{O} \\ \cdot & & \mathbf{O}\ \mathbf{I} & \mathbf{O} \end{bmatrix},$$

where $\mathbf{B} = (\mathbf{I} - \beta_{-1} h\mathbf{A})^{-1}$.

The eigenvalues of **S** can be determined from consideration of the form that the eigenvectors must take,

$$\begin{bmatrix} c_0 & \mathbf{v} \\ c_1 & \mathbf{v} \\ c_2 & \mathbf{v} \\ \vdots & \\ c_p & \mathbf{v} \end{bmatrix},$$

where $c_{k-1} = \mu c_k$ and μ is an eigenvalue of the matrix **S** and **v** is a yet to be determined vector.

Setting $c_p = 1$ for scaling results in

$$c_k = \mu^{p-k}. \tag{7}$$

The final partitioned matrix equation (top row of Eq. (6)) can now be written as

$$\sum_{j=0}^{p} (a_j\mathbf{I} + h\beta_j\mathbf{A})\,\mu^{p-j}\mathbf{v} = \mu^{p+1}(\mathbf{I} - \beta_{-1} h\mathbf{A})\,\mathbf{v}. \tag{8}$$

Examination of Eq. (8) reveals that the vector $\mathbf{v}$ must be an eigenvector of the matrix $\mathbf{A}$, so we can replace $\mathbf{Av}$ by $\lambda_i \mathbf{v}$, which yields

$$(1 - h\lambda_i \beta_{-1})\, \mu^{p+1} = \sum_{j=0}^{p} (a_j + h\lambda_i \beta_j)\, \mu^{p-j}. \tag{9}$$

This is identical to Eq. (5), which demonstrates the equivalence of the proposed two-step method to the classical one-step method. Recall that the derivations of both Eq. (5) and Eq. (9) require that the roots be less than unity in magnitude. Also note that one obtains $(p+1)$ eigenvalues of the matrix $\mathbf{S}$ for every eigenvalue of the matrix $\mathbf{A}$. This demonstrates another advantage of the two-step application of the matrix method. The largest matrix that needs to be analyzed is $\mathbf{A}$, which is smaller than the matrix $\mathbf{S}$.

The advantages of the two-step application of the matrix method are many. The additional information obtained from the first step can be quite helpful in choosing a proper numerical method for a particular problem. First, consider a case when the eigenvalues from Eq. (3) all have negative real parts. This would indicate that the ordinary differential equation set is stable and would be the proper result if it is known that the physical system is also stable. Each choice of a finite difference approximation for the partial derivatives with respect to the time variable can now be easily evaluated for its effect on numerical stability.

The second, and more interesting, case is when some of the eigenvalues from Eq. (3) have positive real parts. Growth rates and frequencies of the instabilities can be determined by examining the real and imaginary parts of the associated eigenvalues. If the physical system is subject to an instability, the growth rates and frequencies can be compared to experimental results to determine if the model is sufficient. Even if no experimental stability results are available, it is often possible to distinguish between real and numerical instabilities upon examination of the eigenvalues and their response to simple modeling changes. Numerical instabilities usually can be identified by the following properties:

- typically very large growth rates and frequencies,
- sensitivity of eigenvalues to node sizes,
- insensitivity of eigenvalues to physical damping in the model.

Examination of the corresponding system eigenvectors may also yield some insight into the cause of the instabilities. Of course, it is desired to eliminate the numerical instabilities while retaining the physical ones. The proposed two-step method allows one to easily evaluate the relative stabilities of the different modes. If the indication is that the physical instability will grow much faster than the numerical one, it is not strictly required to eliminate the numerical instability.

All of these insights into instability are obtained from examination of the first step of the proposed two-step method. The eigenvalues obtained from the classical one-step matrix method do not permit a similar ease of physical interpretation and,

therefore, are much less useful in determining relative stabilities, frequencies, growth rates, and causes of instabilities.

The two-step method was succesfully applied by the author and colleagues in analyzing the numerical and physical instabilities of boiling flow systems. The physical instability results have been reported elsewhere [3]. In this problem, it was essential to be able to distinguish between physical instabilities and numerical ones to allow elimination of the latter. The eigenvalues obtained from Eq. (3), step one, allowed this. The Appendix shows a very simple application of the proposed method.

Concluding Remarks

A two-step method for determination of the stability of finite difference approximations to partial differential equations is introduced. The method yields a necessary and sufficient condition for absolute stability. It offers an advantage over the classical matrix method in that it can isolate partial derivatives with respect to one independent variable at a time. Intermediate answers can then help pinpoint the cause of any numerical instability. However, its greatest advantage is that it allows easier distinction between numerical and physical instabilities. Furthermore, comparison of their relative stabilities is made possible.

These advantages are all derived from the fact that the eigenvalues obtained from the first step can be used not only as a test for stability but as an indication of the actual time response of the model.

APPENDIX: Simple Example Application

Consider the following partial differential equations which describe the flow of a compressible fluid in one dimension,

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial z} \tag{A1}$$

$$\frac{\partial(\rho u)}{\partial t} = -\frac{\partial P}{\partial z} - \frac{\partial(\rho u^2)}{\partial z} - f\rho u^2. \tag{A2}$$

A constitutive equation is also required to describe the density (ρ) in terms of the pressure (P),

$$\rho = \rho_0 + b(P - P_0). \tag{A3}$$

The equations will be represented in finite difference form using a grid with the pressure defined on the cell boundaries and the velocity (u) defined as cell averages.

The donor cell method will be used to define the convected quantities. This yields the finite difference equations (assuming u positive velocity),

$$\frac{\partial \rho_k}{\partial t} = \frac{\rho_{k-1} u_{k-1} - \rho_k u_k}{\Delta z} \tag{A4}$$

$$\frac{\partial (\rho_k u_k)}{\partial t} = \frac{P_i - P_e}{\Delta z} + \frac{\rho_{k-1} u_{k-1}^2 - \rho_k u_k^2}{\Delta z} - f p_k u_k^2 \tag{A5}$$

and the following constitutive relation

$$\rho_k = \rho_0 + b(P_k - P_0). \tag{A6}$$

One still needs to specify the cell pressure (P_k) in terms of the cell inlet and cell exit pressures. Two simple schemes are immediately evident,

$$\text{Case I} \qquad P_k = P_e \tag{A7}$$

$$\text{Case II} \qquad P_k = P_i. \tag{A8}$$

A single cell problem will be considered here, since it has been found in the course of this work that most numerical instabilities (that occur due to improper spacial finite differences) are evident no matter the number of cells in the grid. All variables in Eqs. (A4), (A5), other than ρ_k, u_k, and P_k, will be treated as boundary conditions, and not state variables.

First, the equations are linearized and put into the form (the 'o' that is included in some of the subscripts indicates the state about which the linearization was performed),

$$\mathbf{M} \frac{d}{dt} \begin{bmatrix} P_k \\ u_k \end{bmatrix} = \mathbf{N} \begin{bmatrix} P_k \\ u_k \end{bmatrix} + \mathbf{C}, \tag{A9}$$

where

$$\mathbf{M} = \begin{bmatrix} b & 0 \\ u_{ko} b & \rho_{ko} \end{bmatrix}$$

$$\mathbf{N} = \frac{1}{\Delta z} \begin{bmatrix} -u_{ko} b & -\rho_{ko} \\ \mp 1 - b u_{ko}^2 (1 + f \Delta z) & -2 u_{ko} \rho_{ko} (1 + f \Delta z) \end{bmatrix}.$$

In the above description of the matrix $\mathbf{N}$, one term offers a choice in the sign. The top sign applies to Case I, and the bottom sign applies to Case II. In more complicated problems, the linearization should be done numerically.

The eigenvalues of interest are those of $\mathbf{M}^{-1}\mathbf{N}$ (which is the same as matrix $\mathbf{A}$ in the main body of this paper). These eigenvalues determine the stability of the

spacial finite differences and constitute the output of step one. The eigenvalues were found analytically to be

$$\lambda = -u(1+f\Delta z) \pm \sqrt{u^2(1+f\Delta z)^2 - u^2 f\Delta z \pm 1/b}.$$

Note that if the term $-u^2 f\Delta z \pm 1/b$ is greater than zero, then one of the eigenvalues will be positive. This is not only possible but likely for Case I where the top sign applies.

This means that in the limit of very small time steps, any proper finite difference scheme of the time variable will likely yield an unstable result for Case I. This goes against physical understanding of the process that is being modeled, so the analysis would normally stop here after the first step to try to correct the problem.

The spacial finite differences for Case II are shown to be always stable. This is what is expected for a one-dimensional flow with a friction term in the momentum equation. From these eigenvalues, one can select a finite difference method for the time variable and a maximum allowable time step to guarantee stability of the numerical model.

It should be noted here that Case I is not causal [4]. A cell should not output both the pressure and velocity at the same location. (Note that in the donor cell scheme, the exit velocity is the same as the cell average velocity.) Liles and Reed [5] also found that the density of a cell should be based on the upstream pressure for stability; however, they did not identify any reason for this fact. An interesting topic for investigation might be the relationship between causality and numerical instability.

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RECEIVED: August 6, 1985; REVISED: July 16, 1986

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