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AN ELEMENTARY INTRODUCTION TO FINITE DIFFERENCE EQUATIONS

John W. White

May 3, 1976

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AN ELEMENTARY INTRODUCTION TO FINITE DIFFERENCE EQUATIONS

Abstract

This paper is an elementary description of the basic vocabulary and concepts associated with finite difference modeling. The material discussed is biased toward the types of large computer programs used at the Lawrence Livermore Laboratory. Particular attention is focused on truncation error and how it can be affected by zoning patterns. The principle of convergence is discussed, and convergence as a tool for improving calculational accuracy and efficiency is emphasized.

Introduction

Since this description of finite difference methods is intended to accompany a brief, introductory course, it is very elementary. The survey is oriented toward the user of large computer programs who has no previous experience with numerical methods rather than the writer of such programs. It introduces basic vocabulary and provides references for further reading.

This paper is biased toward computer programs at Lawrence Livermore Laboratory (LLL) where codes are dominated by computations for hydrodynamic effects and other transport processes (e.g., the diffusion equation). The equations of hydrodynamics are singled out for special emphasis because I believe that more often than not they limit the accuracy of the computer code calculations performed at LLL.

In general, a rigorous treatment of finite difference methods is severely limited, partly because of the newness of the field but more fundamentally because many interesting physical systems involve coupled sets of nonlinear differential equations. This area of mathematics has had analytical difficulties for a long time, and in fact that is the reason we resort to finite differences methods. After we establish a foundation of fundamental principles, we can apply finite difference methods with a fair amount of confidence; however, a significant amount of subjective judgment will still be involved, and it is usually wise to view the results of any calculation with caution.

THE FINITE DIFFERENCE APPROXIMATION

The standard analytic calculus definition of a derivative is given by the following equation:

$$\frac{df}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}, \quad (1)$$

where f is a "well behaved" function of x in the vicinity of the value for x at which the derivative is evaluated. Typically, the values of x constitute an unbounded ($-\infty < x < +\infty$) continuum. One concern of classical mathematical analysis is to find solutions for differential equations (or partial differential equations). However, not all equations of interest are readily solvable. This is particularly true for the nonlinear differential equations frequently encountered when modeling physical systems. To obtain solutions, we resort to finite difference approximations of derivatives or partial derivatives as follows:

$$\frac{df}{dx} \approx \frac{\Delta f}{\Delta x} = \frac{f(x+\Delta x) - f(x)}{\Delta x}, \quad (2)$$

i.e., we omit the limiting process.

Values of f exist only at discrete points on a mesh for which x is bounded. If time is an independent variable, the same argument applies, except that the initial conditions form a single theoretical boundary. Such a mesh is shown in Fig. 1. We need boundary conditions at x_0 and $x_{\max}$ for all possible mesh values of t , and we need the initial values ($t = t_0$) for all possible mesh values of x . When such a solution is found, it is a particular solution, not a general solution.

CLASSIFICATION OF PARTIAL DIFFERENTIAL EQUATIONS (PDE's)

First, we examine the general second order linear partial differential equation (PDE).

$$A U_{xx} + 2 B U_{xy} + C U_{yy} + D U_x + E U_y + F U = G \quad (3)$$

$$A = A(x, y), \text{ etc.}$$

Fig. 1 General time-space mesh.

If $B^2 - AC > 0$, the equation is hyperbolic. But, consider a change of variables:

$$\zeta = \zeta(xy) \quad \text{and} \quad \eta = \eta(xy). \quad (4)$$

If Eq.(3) is hyperbolic, a change of variables can be found such that either of the following canonical forms will result:

$$U_{\zeta\eta} + \text{l.o.t.} = 0 \quad \text{or} \quad U_{\zeta\zeta} - U_{\eta\eta} + \text{l.o.t.} = 0 \quad (\text{l.o.t.} = \text{lower order terms}) \quad (5)$$

If $B^2 - AC = 0$, the equation is parabolic. With the canonical form:

$$U_{\zeta\zeta} + \text{l.o.t.} = 0. \quad (6)$$

If $B^2 - AC < 0$, the equation is elliptic. With the canonical form:

$$U_{\zeta\zeta} + U_{\eta\eta} + \text{l.o.t.} = 0.$$

The fact that A, B, and C are functions of the independent variables means that the classification of the PDE may change in different regions of the variable space.

The significance of the PDE classifications can be emphasized by the set of equations for hydrodynamics. This set of equations is hyperbolic for inviscid fluid flow. Allowed solutions then can include discontinuities such as those found at shock fronts, but discontinuities are not compatible with discretized functions. The inclusion of viscous effects, however, changes the set of equations from hyperbolic to parabolic, and parabolic equations do not permit discontinuities in their solutions. These can be readily handled by the finite difference method.

EXAMPLES OF PARTIAL DIFFERENCE EQUATIONS

The following equations are examples of PDE's:

- Hyperbolic Equation:

$$\frac{\partial^2 \phi}{\partial t^2} - c^2 \frac{\partial^2 \phi}{\partial x^2} = 0 \quad (7)$$

(the wave equation).

Conditions for a vibrating string with clamped ends are:

$$0 \leq x \leq l \quad ; \quad \phi(t_0) = \phi(2t) = 0,$$

$$\phi(t=0) = f(x) \quad \text{and} \quad \left. \frac{\partial \phi}{\partial t} \right|_{t=0} = g(x).$$

- Parabolic Equation:

$$\frac{\partial \phi}{\partial t} = \sigma \frac{\partial^2 \phi}{\partial x^2} \quad (8)$$

(diffusion equation).

Conditions for slab heat flow with ends clamped at $t = 0$ are similar to the above but with no need for derivative boundary conditions.

- Elliptic Equation:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \quad (9)$$

(Laplace's equation). The value of ϕ must be specified along the boundaries of the problem.

Major Accuracy Considerations

TRUNCATION ERROR

We can approximate the derivative $\frac{dy}{dt}$ by several different algorithms:

Forward difference:

$$\left. \frac{dy}{dt} \right|_{t_0} \approx \frac{y(t_0 + \Delta t) - y(t_0)}{\Delta t} . \quad (10)$$

Backward difference:

$$\left. \frac{dy}{dt} \right|_{t_0} \approx \frac{y(t_0) - y(t_0 - \Delta t)}{\Delta t} . \quad (11)$$

Central difference:

$$\left. \frac{dy}{dt} \right|_{t_0} \approx \frac{y(t_0 + \frac{\Delta t}{2}) - y(t_0 - \frac{\Delta t}{2})}{\Delta t} \quad \text{or} \quad \approx \frac{y(t_0 + \Delta t) - y(t_0 - \Delta t)}{2\Delta t} . \quad (12)$$

Let us use a series expansion of y in a form compatible with the forward difference algorithm, i.e.,

$$y(t_0 + \Delta t) = y(t_0) + \Delta t y'(t_0) + \frac{(\Delta t)^2}{2!} y''(t_0) + \dots$$

By rearranging terms and dividing by t , we obtain the following:

$$y'(t_0) = \frac{y(t_0 + \Delta t) - y(t_0)}{\Delta t} + \alpha \Delta t + \beta (\Delta t)^2 + \dots \quad (13)$$

where $\alpha, \beta \dots$ are functions of t and derivatives (second order and higher) of y evaluated at t_0 .

In other words, the error in Eq. (10) is proportional to Δt and higher powers of Δt . If Δt is small, the error will be dominated by the lowest power of Δt in the error term, and for this case it is the first power. This approximation is said to be first order accurate.

Problem: Determine the order of the error terms for both
Eqs. (11) and (12).

In summary, the truncation error refers to the truncation of a series expansion for a given derivative. To reduce the truncation error order at a given mesh point, we must use a finer mesh or use a higher-order algorithm and include information from many more neighboring mesh points in the calculation of the derivative; either of these choices can be very expensive. In most computer calculations the truncation error is the dominant error. Note that truncation error does not give the size of the error. Rather, it indicates how rapidly the error vanishes as the mesh is refined. Most practical calculations are done with a mesh size such that a higher-order truncation error scheme produces a smaller error than a lower-order scheme.

ROUND OFF ERROR

Von Neumann and Goldstein have listed four major sources of errors which are nearly unavoidable when describing physical systems.¹

1. The mathematical models of nature are approximations.
2. Most descriptions require measured data (equations of state, electric charge, etc.).
3. Most descriptions involve an infinite continuum, and limiting processes cannot be completed. The result is a truncation error.
4. However, the numbers manipulated in any calculations must be finite. The dropping of digits is roundoff error.

In computer calculations this last item reflects the fact that only a finite number of bits are available to calculate the differences used to approximate derivatives. The expectation is that numbers will round down as often as up, with no accumulating error. However, it is possible that all numbers would be rounded up, although the probability of such an occurrence is small. The expected error is proportional to the standard deviation expected for such random events. But we know

$$\sigma \propto \sqrt{N}$$

where σ is the standard deviation and N is the number of such calculational roundoffs.

As calculations use a finer mesh, the truncation error decreases but the roundoff error increases due to the increased number of computations performed. The economies of computers, however, indicates that the truncation error is the limiting factor for most problems. That is, most calculations in large electronic computers have considerably larger truncation errors than roundoff errors. This can be understood by the following example. Let the truncation error be proportional to grid size and time step for a time-dependent problem with one spatial dimension. Reduce the truncation error a factor of two by halving Δx and Δt . The problem then requires twice as much memory and four times as many calculations. Four times as many calculations means an increase in roundoff error of a factor of two. Reducing the truncation error by a factor of two relative to its original value requires an overall improvement in roundoff of a factor of four. Thus, if we want to maintain the same relative value of roundoff error and truncation error, only two more binary bits per number are required. For a factor of two improvement in truncation error and roundoff error, the increase in memory for improving truncation error is much larger than that required for improving roundoff error.

When roundoff error is large enough to seriously affect the solution, it can usually be detected readily. If insignificant changes in the physical system result in large changes in the solution, roundoff error is the likely culprit.

STABILITY AND CONVERGENCE

Let $U(x_j, t_n)$ be the exact solution of the PDE and $\bar{U}_j^n$ be the solution obtained by the Finite Difference Approximation (FDA) of the PDE. Then define A as follows:

$$A = |\bar{U}_j^n - U(x_j, t_n)| \quad (14)$$

Stability is concerned with the following question. What is the behavior of A as n approaches infinity? If A grows in an unbounded manner, then the FDA is unstable. This usually means that the calculation crashes which frequently results when the time step (Δt) has exceeded a prescribed limit (the stability condition).

Convergence is concerned with the following question. What is the behavior of A for a fixed value of t as Δx and Δt approaches zero? If A

approaches zero, then the difference equation and the differential equation converge. We will find that under most conditions, the criteria for stability will be necessary and sufficient to insure convergence.

Linear Partial Differential Equations

EXPLICIT ALGORITHM EXAMPLE

Consider the diffusion equation

$$\frac{\partial U}{\partial t} = \sigma \frac{\partial^2 U}{\partial x^2} \quad \text{where} \quad \begin{array}{l} \sigma > 0 \\ 0 \leq x \leq \pi, \\ t \geq 0 \end{array}$$

where $U(x, 0) = f(x)$ and $U(0, t) = U(\pi, t) = 0$ (for $t > 0$).

Also consider the explicit difference equation

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2} \quad (15)$$

where $U_j^0 = f(x_j)$ and $U_0^n = U_{j_{\max}}^n = 0$.

Thus as shown in Fig. 2, the values of U at three spatial points for $t = t_n$ are used to obtain the value of U at $t = t_{n+1}$ at one spatial point.

Fig. 2 Local time-space mesh.

We know the general solution of the differential solution is as follows:

$$U(x,t) = \sum_{m=-\infty}^{+\infty} A_m e^{imx - m^2 \sigma t}$$

where

$$A_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-imx} dx.$$

We have been able to use separation of variables to solve the differential equation because the system is linear. Note that σ is assumed constant. Now try a separation of variables for the FDE for each mode of the Fourier series with the following arbitrary form:

$$U_j^n = \sum_{m=-\infty}^{\infty} A_m e^{imj\Delta x} \left(\zeta_m^n(t) \right). \quad (16)$$

If we rewrite Eq. (15) by substituting the relationships in Eq. (16), we then obtain an equation for the required form of ζ_m (called the amplification factor).

$$\zeta_m = 1 - \frac{2\sigma \Delta t}{(\Delta x)^2} (1 - \cos m\Delta x) \quad (17)$$

or by series expansion

$$\zeta_m = 1 - m^2 \sigma \Delta t + \frac{1}{12} m^4 \sigma \Delta t (\Delta x)^2 + \dots \quad (18)$$

Likewise, the PDE time component can be expanded

$$e^{-m^2 \sigma \Delta t} = 1 - m^2 \sigma \Delta t + \frac{1}{2} m^4 \sigma^2 (\Delta t)^2 + \dots \quad (19)$$

Hence $\zeta_m \rightarrow e^{-m^2 \sigma \Delta t}$ as $\Delta x, \Delta t \rightarrow 0$.

Thus we have demonstrated convergence. For stability we want ζ_m to be bounded, and this requires that

$$|\zeta_m| < 1$$

Which results in a requirement that

$$\frac{2\sigma \Delta t}{(\Delta x)^2} < 1 .$$

This relates the maximum permissible time step to the grid size and is the condition necessary for stability. Comparing Eqs. (18) and (19) we noted that the error is of order $\Delta t (\Delta x)^2$ or $(\Delta t)^2$ by comparing terms in the series expansion. However, by enforcing the following constraint the truncation error can be made higher order. Let

$$\frac{6\sigma \Delta t}{(\Delta x)^2} = 1 .$$

That is, the two series expansions can be made identical by one more term with the above relationship for Δt and Δx . Note that it does satisfy the stability condition.

In the previous problem on page 6 we encountered a similar situation. The forward difference operator and the backward difference operators were combined (added) to obtain the central difference algorithm. The result was that the lowest order error terms in each of the forward and backward algorithms cancelled when combined to form the central difference. However, a constraint is implied for the central difference operator to be higher-order accurate. That is, the positive Δt must be equal to the negative Δt . Or equivalently, Δt must be a constant throughout the calculation. Later we will examine the equations of hydrodynamics and see that they need constant Δt and Δx to achieve highest order accuracy.

Remember that we used a linear equation whose solution is known in order to examine stability conditions. Any analysis of other equations will also be linear. By implication, the assumption is that the basic principles uncovered by such linear analysis can be applied to nonlinear equations.

Truncation error has meaning only relative to the convergence process. It tells how rapidly the error vanishes as the mesh is refined. Determination of the absolute error is more complicated.

IMPLICIT ALGORITHM EXAMPLE

The implicit difference equation

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} \quad (20)$$

is unconditionally stable. When we solve for the new values implicitly by using these new values in the equations, a form of self-consistency in the equations is assured. In general, it turns out that most implicit algorithms are unconditionally stable. However, the solution is more difficult to obtain, since unknowns are found on both sides of the equality. Thus one is in effect inverting a large matrix obtained from simultaneous equations. Intuitively, it seems plausible that such solutions might be inherently stable, since obtaining simultaneous equations in this manner implies a form of self-consistency, which is probably desirable. However, though any size time step may be stable, if it is very large it can produce a large error. Most computer code writers do not find it worthwhile to try for third-, fourth-, or higher-order accuracy in their algorithms. They will usually accept first- or second-order accuracy, but they will also usually require that for very large time steps, the physical solution must reduce to an equilibrium description. Let

$$u_{j+1} - 2u_j + u_{j-1} = \delta^2 u_j.$$

Then one can write a more general equation as follows:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \frac{\theta(\delta^2 u)_j^{n+1} + (1-\theta)(\delta^2 u)_j^n}{(\Delta x)^2}, \quad (21)$$

if

$$0 \leq \theta < \frac{1}{2}, \quad \frac{2\sigma \Delta t}{(\Delta x)^2} \leq \frac{1}{1-2\theta}$$

is the stability condition.

For $\theta \geq \frac{1}{2}$ the equations are unconditionally stable. If $\theta = \frac{1}{2}$, second-order accuracy is obtained in addition to unconditional stability.

PARTIAL DIFFERENTIAL EQUATION EXAMPLES

Laplace's equation ($\nabla^2 U = 0$) can be solved explicitly

$$U_{i,j}^{n+1} = \frac{1}{4} (U_{i+1,j}^n + U_{i-1,j}^n + U_{i,j+1}^n + U_{i,j-1}^n), \quad (22)$$

where n is the number of iterations performed, or implicitly just like Eq. (22) with n replaced by $n+1$ on the right-hand side. Both equations are unconditionally stable, but the implicit scheme converges faster.

The wave equation can likewise be solved either implicitly or explicitly. The explicit example is

$$\frac{U_{i,j}^{n+1} - 2U_{i,j}^n + U_{i,j}^{n-1}}{(\Delta t)^2} = C^2 \frac{U_{i+1,j}^n - 2U_{i,j}^n + U_{i-1,j}^n}{(\Delta x)^2}.$$

The stability condition is

$$\frac{C \Delta t}{\Delta x} \leq 1.$$

This condition can be interpreted as limiting a sound signal so that it can cross no more than one zone in one time step. This also has implications regarding accuracy. If a larger time step is desired, it might be obtained by a larger Δx , rather than by employing an implicit scheme. However, if material velocities are comparable to the value of C (the sound speed), accuracy considerations will not permit a larger Δx , and it may be hard to justify a larger Δt , and not worthwhile to develop an implicit scheme. However, if material speeds are slow compared to the sound speed (as is the case for weather models), then such a correlation between a stability condition like the above and accuracy considerations would be inappropriate. Then an unconditionally stable implicit scheme would be desirable. Similar arguments can be made for astrophysics problems concerning energy flow by radiation and stability conditions dependent on the speed of light.

Nonlinear Partial Difference Equations

EQUATIONS OF HYDRODYNAMICS

When fluid flow is described, two distinctly different formulations are popular. In the Eulerian formulation, the coordinate system remains fixed and the fluid moves relative to it. The FDE for such a formulation requires an equation accounting for material flow into and out of each zone. In a Lagrangian formulation, the coordinate system moves with the mass particles; thus, the mass in each zone remains constant, and we then describe the movement of the Lagrangian coordinate system. The Lagrangian approach has the advantage of providing higher-order accuracy at the least cost in computer time. However, since the finite difference mesh follows the flow of the material, the mesh can become hopelessly distorted for turbulent flow. The calculation can yield meaningless results under such circumstances, or it can even crash. The Eulerian approach can handle turbulent flow more readily, since the finite difference mesh remains fixed, and material is transported through it. However, it is a more expensive approach. This paper will deal with the Lagrangian system only. A standard sequence of FDE's in the Lagrangian formulation is given by Eqs. (23) through (27).

Some quantities are zone-centered and some quantities are on the zone boundaries to improve the accuracy of the scheme in a manner analogous to the central differencing method examined earlier. The set of equations is analogous to a spring-mass system. The volume, pressure, and energy act like the spring; the others act like the mass points.

$$\begin{array}{ccccc}
 & & V & & V \\
 & & | & & | \\
 & & P & & P \\
 & & | & & | \\
 & & E & & E \\
 & & | & & | \\
 & & (j\frac{1}{2}) & & (j+\frac{1}{2}) \\
 (j-1) & & & (j) & & (j+1)
 \end{array}$$

$$\frac{y_{j+1/2}^{n+1/2} - y_j^{n+1/2}}{\Delta t} = -v_0 \left(\frac{R_j^n}{r_j} \right)^{\alpha-1} \left(\frac{p_{j+1/2}^n - p_{j-1/2}^n}{\Delta r} \right)$$

for $j = 2, 3, \dots, J-1$ and where $V_0 = \frac{1}{\rho_0}$. In other words acceleration is pressure gradient divided by mass. This is the equation of motion, or a restatement of the conservation of momentum.

We can use boundary conditions to get $U_1^{n+1/2}$, $U_J^{n+1/2}$;

$$R_j^{n+1} = R_j^n + \Delta t U_j^{n+1/2}, \text{ calculate new radius;} \quad (24)$$

$$V_{j+1/2}^{n+1} = V_0 \frac{(R_{j+1}^{n+1})^\alpha - (R_j^{n+1})^\alpha}{(r_{j+1})^\alpha - (r_j)^\alpha}, \text{ calculate new volume;} \quad (25)$$

$$\epsilon_{j+1/2}^{n+1} = \epsilon_j^n - p_{j+1/2}^{n+1/2} \left(V_{j+1/2}^{n+1} - V_{j+1/2}^n \right), \text{ conservation of energy} \quad (26)$$

($d\epsilon = P dV$);

$$p_{j+1/2}^{n+1} = f \left(\epsilon_{j+1/2}^{n+1}, V_{j+1/2}^{n+1} \right), \text{ equation of state (EOS)} \quad (27)$$

$\alpha = 1$ for a slab, 2 for a cylinder, 3 for a sphere.

R is the Eulerian coordinate and r is the Lagrangian coordinate. That is, R gives the position of a mass point at time t which was initially at position r .

Note that these form a set of nonlinear equations. The last two equations may involve an iteration or two. However, the scheme is completely explicit and second order for constant Δt and Δx . The stability condition is:

$$\frac{C_s \Delta t}{\Delta x} \leq 1$$

where C_s is the sound speed. (Again the signal cannot go across more than 1 zone in Δt .) For an ideal gas

$$C_s = \sqrt{\frac{dP}{d\rho}} = \sqrt{\frac{\gamma P}{\rho}}.$$

INTERFACES

In the absence of interfaces, and assuming density is constant, the greatest accuracy is achieved by keeping the zone size constant. This also means that the zone mass is approximately constant. This is desirable because velocities and accelerations are calculated at zone boundaries, and constant zone size means that the pressure gradient is also located at the

zone boundary as is the center of mass which is being accelerated. Thus the mass and its acceleration are located at the same point, which is obviously desirable for best accuracy. However, when there is an interface involving a density discontinuity, then either the pressure gradient can be evaluated at the zone boundary or the mass undergoing acceleration can be located at the zone boundary. But both cannot be located at the zone boundary simultaneously. Keeping Δx constant across the interface locates the pressure gradient at the boundary; matching zone mass across the interface locates the center of mass at the zone boundary.

Assume a zoning pattern at the interface with equal Δx , but with the density in the right-hand zone (rhz) being a multiple (m) of that in the left-hand side. The mass associated with the acceleration of the interface is half the mass of the left hand zone (lhz) and half the mass of the rhz. Each half mass is centered halfway between the zone boundary and the zone center. (See Fig. 3). Then m is not located exactly at the interface as is dp/dR but is located at

$$\frac{-(m-1) \ell}{(m+1) 2}$$

with respect to the interface. Since ℓ is negative, this means that the center of mass is located in the high density side, as expected.

A similar argument can be made when the zones are mass-matched and the center of mass is at the boundary. Then we calculate the displacement of the center of the pressure gradient. See Fig. 4; again the rhz density is a factor m greater than the lhz.

Fig. 3 Location of zonal quantities: equal Δx case.

where Δ_r and Δ_{+r} are the zone sizes on the minus and plus sides of the interface. This formula ensures that the pressure gradient is calculated at the interface and applies even if the interface is not real (only a zoning discontinuity or a material density gradient). This more accurate algorithm is required because our original algorithm assumed constant values for Δx and for density. That is, we assumed that the zone interface position and velocity, the mass associated with the interface, and the pressure gradient accelerating that mass were all co-located. To get complete second order accuracy, an improvement similar to Eq. (28) for Δt is required, and zone masses must be matched across the interface.

Generalizing to two dimensions is not easy. We may need slip surfaces, or zones may have irregular shapes. The most serious difficulty with two-dimension calculations may be that their algorithms are usually very inaccurate when the mesh is not orthogonal (i.e., when the corners of the zones are not at right angles). Equation (28) represents a correction for the simple Eq. (23) because of a lack of equal-sized zones in Eq. (23), and it locates the pressure gradient at the zone interface. Likewise the simplest two-dimension calculations require corrections when the grid is nonorthogonal, and similar accuracy considerations with respect to the mesh are encountered with other equations such as the diffusion equation. Unfortunately, these corrections are quite complicated and usually omitted. We should keep in mind that zoning patterns can significantly affect the accuracy of the numerical calculation.

SHOCKS

The simulation of shocks by FDE's presents a fundamental difficulty. A shock in the physical world has no discontinuities in the mathematical sense. However, its dissipative mechanisms operate over distances comparable to atomic lengths with the result that variables (e.g., ρ , θ , P , U) rise very abruptly. To model such real physics would require zone sizes smaller than the width of the shock, and this would be prohibitively expensive. However, if the zones are larger, the finite difference scheme will "ring" since its discrete nature cannot cope with such a discontinuity. The discontinuous character of the process we are trying to model is shown in Fig. 5.

A shock is an irreversible thermodynamic process with an accompanying change in entropy in which some kinetic energy is converted to potential energy. One standard way of obtaining the proper entropy change and avoiding

the "ringing" is given by Ref. 1 which introduces an artificial viscosity. The adjective "artificial" is used because the viscosity is dependent on zone size. The addition of this artificial viscosity results in an artificial pressure (q) which changes the set of equations from hyperbolic to parabolic and eliminates discontinuities in the solutions. The standard form follows:

$$q = \rho(c \Delta x)^2 \left(\frac{\Delta u}{\Delta x} \right)^2 \quad (29)$$

$q = 0$ for an expanding zone,

c is a dimensionless constant, $q \rightarrow 0$ as $\Delta x \rightarrow 0$ as an artifice should.

Wherever the FDE's included a term for the pressure, $q + P$ is substituted, and the result is that the shock is spread over a number of zones. This technique was introduced by Von Neumann and is sometimes simply called the "q" method. The method is widely used, partly because it is convenient. Alternative shock handling methods are described in Ref. 1. A common test applied to any such method is to see if the Rankine-Hugoniot (R-H) equations which are restatements of conservation laws, are satisfied when the method is employed.

The R-H equations relate the thermodynamic variables in the shocked region to those in the undisturbed region. See Fig. 5.

Fig. 5 Schematic of shock front.

$$\rho_2 \frac{d\zeta}{dt} = \sqrt{\frac{p_1 - p_2}{v_2 - v_1}} \quad (30)$$

$$|u_1 - u_2|^2 = (p_1 - p_2) (v_2 - v_1) \quad (31)$$

$$\epsilon_1 - \epsilon_2 = \frac{p_1 + p_2}{2} (v_2 - v_1) \quad (32)$$

where ζ is the shock position. In the limit of weak or reversible shocks Eq. (31) modifies to

$$\frac{du}{dx} = \frac{1}{\rho C_s} \frac{dp}{dx},$$

where C_s is again the sound speed.

STABILITY ANALYSIS

Stability analysis will be performed on the partial differential equations rather than the FDE's so that we can use the methods of variational calculus.

The differential equations for an ideal gas in Lagrangian form are:

$$V(xt) = \frac{1}{\rho_0(x)} \frac{\partial X}{\partial x} \quad (34)$$

$$U(xt) = \frac{\partial X}{\partial t} \quad (35)$$

$$\rho_0 \frac{\partial U}{\partial t} = \frac{\partial}{\partial x} (P + q) \quad (36)$$

$$\frac{\partial \epsilon}{\partial t} + (P + q) \frac{\partial V}{\partial t} = 0 \quad (37)$$

$$\rho_0 \frac{\partial V}{\partial t} = \frac{\partial U}{\partial x} \quad (38)$$

$$\epsilon = P \frac{V}{(\gamma-1)} \quad (\gamma \text{ is the ideal gas constant}) \quad (39)$$

$$\text{where } q = - \frac{(C \Delta n)^2}{V} \frac{\partial U}{\partial x} \bigg| \frac{\partial U}{\partial x} \bigg| \quad (40)$$

The equations using a q should have the following properties:

1. Equations (36), (37), and (38) should have continuous solutions.
2. The shock thickness should be zone-size dependent.

3. The effect of q should be negligible outside the shock.
4. The Hugoniot conditions must hold when all other dimensions describing the flow are large compared to the shock thickness. The q method meets all of the above requirements. We will examine only some of these.

The solution for a steady state plane shock is^{1,2}:

$$V = \frac{V_i - V_f}{2} \sin \frac{\omega}{\omega_0} \quad \text{for } -\frac{\pi\omega_0}{2} \leq \omega \leq \frac{\pi\omega_0}{2}$$

where i and f refer to initial and final values (undisturbed and shocked),
 $\omega = x - \dot{S}t$, $\dot{S}$ is the speed of the shock relative to the Lagrangian frame, and
 where

$$\omega_0 = \left[\frac{2}{\gamma+1} \right]^{1/2} C \Delta x \quad \text{and} \quad V = V_i \quad \text{for } \omega \geq \frac{\pi\omega_0}{2},$$

$$V = V_f \quad \text{for } \omega \leq -\frac{\pi\omega_0}{2}.$$

Let us look at the stability of the differential equations for the above system. Let us impose a small perturbation* on the desired solution ($U + \delta U$, $V + \delta V$, etc.) and Eq. (39) in Eq. (37) to get (before taking variation)

$$\left[\gamma p + (\gamma-1) q \right] \frac{\partial V}{\partial t} + V \frac{\partial p}{\partial t} = 0.$$

The equations of first variation are:

$$\rho_0 \frac{\partial}{\partial t} \delta U = - \frac{\partial}{\partial x} (\delta p + \delta \epsilon), \quad (41)$$

$$0 = \frac{\partial V}{\partial t} (\gamma \delta p + (\gamma-1) \delta q) + \left[\gamma p + (\gamma-1) q \right] \frac{\partial \delta V}{\partial t} \quad (42)$$

$$+ V \frac{\partial}{\partial t} \delta p + \frac{\partial p}{\partial t} \delta V,$$

$$\delta q = \frac{(C \Delta x)^2}{V} \frac{\partial U}{\partial x} \left[\frac{\partial U}{\partial x} \delta V - 2 \frac{(C \Delta x)^2}{V} \frac{\partial U}{\partial x} \frac{\partial}{\partial x} \delta U \right], \quad (43)$$

and, assuming that $\frac{\partial U}{\partial x}$ does not change its sign when the variation is taken

$$\rho_0 \frac{\partial}{\partial t} \delta V = \frac{\partial}{\partial x} \delta U. \quad (44)$$

*Perturbations are guaranteed because of roundoff error.

The above equations form a set of simultaneous differential equations for δU , δV , δP , and δq . If we are not concerned with rapidly varying perturbations, then their coefficients can be considered as approximately constant and the equations as linear. Let us look for solutions of the form $\delta U = \delta U_0 \exp(ikx + \alpha t)$, $\delta V = \delta V_0 \exp(ikx + \alpha t)$, etc., where k and α are constants and k is real. We choose this form because all the derivatives are first order with respect to either t or x . Then the four equations become simple linear homogeneous algebraic equations. This system of equations will be satisfied if the determinant of the coefficients vanishes. By solving this determinant and examining the results for large values of k and α , we can obtain expressions for α in terms of k in the shocked and unshocked regions. This will reveal the nature of the solutions.

$$[\rho_0 \alpha] \delta U_0 + [ik] \delta P_0 + [ik] \delta q_0 = 0$$

$$\left[v\alpha + \frac{\partial v}{\partial t} \gamma \right] \delta P_0 + \left[(\gamma-1) \frac{\partial v}{\partial t} \right] \delta q_0 + \left[\frac{\partial p}{\partial t} + \alpha [\gamma p + (\gamma-1) q] \right] \delta V_0 = 0$$

$$\left[-2 \frac{(c \Delta x)^2}{v} \frac{\partial U}{\partial x} ik \right] \delta U_0 + [-1] \delta q_0 + \left[\frac{(c \Delta x)^2}{v^2} \frac{\partial U}{\partial x} \left| \frac{\partial U}{\partial x} \right| \right] \delta V_0 = 0$$

$$[ik] \delta U_0 + [-\rho_0 \alpha] \delta V_0 = 0.$$

We will restrict our attention to the large values of k and α as mentioned before for both the solution in the shock region and in the regions outside of the shock. Outside the shock region, we can neglect the terms with $(\Delta x)^2$ in them, but in the shock region all terms are considered. Then the dominant terms are obtained by keeping highest powers in both k and α .

In the shock regions:

$$2 (c \Delta x)^2 \frac{\partial U}{\partial x} k^2 P_0 \alpha^2 + \rho_0^2 \alpha^3 v = 0$$

$$\alpha = -2 \frac{(ck \Delta x)^2}{v \rho_0} \left| \frac{\partial U}{\partial x} \right|$$

(hence α is real and negative).

In the normal regions:

$$k^2 \propto (\gamma_p + [\gamma-1] \frac{0}{q}) + \rho_0^2 \alpha^3 v \approx 0$$

$$\alpha^2 = - \frac{k^2 \gamma_p}{\rho_0^2 v} \approx - \frac{k^2}{\rho_0^2 v} \frac{\gamma_p}{\rho_0}$$

(i.e., α is purely imaginary).

Thus we see that small perturbations are damped out in the shock layer but that they propagate without change in normal regions. The first solution is the diffusion equation solution for the following equation:

$$\frac{\partial}{\partial t} \delta U \approx - \frac{\partial^2}{\partial x^2} \delta U$$

where

$$\sigma = \frac{2}{v} \frac{(c \Delta x)^2}{\rho_0} \left| \frac{\partial U}{\partial x} \right|_0$$

and $\frac{2\sigma \Delta t}{(\Delta x)^2} \leq 1$ is the stability condition.

Likewise the second solution is for the wave equation.

$$\frac{\partial^2}{\partial t^2} \delta U = S_0^2 \frac{\partial^2}{\partial x^2} \delta U$$

where

$$S_0^2 = \frac{\gamma_p}{\rho_0^2 v} \quad [S_0 \text{ is approximately the sound speed}]$$

and $\frac{S_0 \Delta t}{\Delta x} \leq 1$ is the stability condition. Unfortunately, the above analysis is only approximately correct, and slightly different conditions are required in practice.³

GENERAL COMMENTS

We noted earlier that q should only be significant in shocked regions. To determine if this is so one must compare q to P .

For an ideal gas, in the limit of weak shocks

$$\frac{q}{P} = \frac{C^2}{P} \frac{(\Delta P)^2}{\rho C_s^2} \text{ using } \Delta U = \frac{\Delta P}{\rho C_s}$$

$$\text{but } C_s^2 = \frac{\gamma P}{\rho} \therefore \frac{q}{P} = \frac{C^2}{\gamma(P)^2} \frac{(\Delta P)^2}{\rho} . \quad (45)$$

Thus q/P vanishes rapidly as shocks become weak. A linear q of the following type is frequently employed.

$$q_L = \rho(c \Delta x) C_s \left| \frac{\Delta U}{\Delta x} \right|$$

Then regardless of equation of state

$$\frac{q}{P} \propto \frac{\Delta P}{P} .$$

The linear q is apparently not attractive for accuracy considerations. However, it is very useful in practical applications. Elastic solids present special difficulties for q 's and are discussed in Ref. 4.

Another problem occurs when $|\Delta U|$ is large even though no large signal is present. This can happen due to geometry considerations such as the adiabatic compression of a sphere. The form for q can be rewritten to make it more sensitive to physical behavior characteristic of shocks by sampling other variables. The most obvious variable substitution is to replace ΔU by a variable equal to ΔU through the Rankine-Hugoniot equations,

$$q = \rho(c \Delta x)^2 \left| \frac{\Delta U}{\Delta x} \right| \left| \frac{\Delta P}{\Delta x} \right| \left| \frac{\Delta \rho}{\Delta x} \right|^{1/2} \quad (\text{again } q = 0 \text{ for expanding zones})$$

or

$$q = \rho(c \Delta x)^2 \left| \frac{\Delta U}{\Delta x} \right|^{3/2} \left| \frac{\Delta P}{\Delta x} \right| \left| \frac{1}{\rho C_s} \right|^{1/2} .$$

The Von Neumann q can be made to give more accurate thermodynamics by either of these substitutions. However, shocks are not the only causes of undesirable numerical noise. When we solve two-dimensional problems, the mesh can also require a so-called "tensor q " to damp ringing of a shearing type. When a " q " is added to the equations of hydrodynamics, an additional truncation error is introduced. However, the mesh is made to behave more regularly, with the seemingly contradictory result that the final solution may be more accurate. Unfortunately, our previous analysis regarding interfaces is nullified by the presence of a q in the equations because the q spreads a shock over a given number of zones rather than a physical distance. Every time the zoning changes, such as can happen at an interface, the shape of the shock changes, and transient noise and errors are introduced. These errors will disappear from interfaces or boundaries only if the shock propagates through a uniform material (constant density and sound speed) with constant zone size ahead of the shock.

Understanding the computer simulation of physically dynamic systems requires a good knowledge of numerical hydrodynamics. This means understanding artificial viscosity. Hydrodynamic equations are concerned with material transport, and the diffusion equation can be concerned with energy (e.g., heat) and particle (e.g., neutron) transport. These two examples have been used to illustrate the fundamental considerations of finite difference methods (e.g., truncation error, roundoff error, stability, and convergence). We have shown that zoning patterns and time-step constraints can influence these items in a significant way

The examples were chosen for their simplicity, but the reader should be warned that the schemes used to solve some real two-dimensional calculations can become very complicated. This frequently happens when attempts are made to run problems faster and with greater accuracy. To delve into such algorithms or the theory in depth requires a much more detailed and time-consuming exposition.

Zoning Considerations

ZONING DENSITY

We have observed that computational error is dominated by truncation error, which in turn is significantly determined by zone size. Thus we want small zones. The question naturally arises, how small? What do we use as a yardstick when measuring zone size? The answer is that we want zones fine enough to resolve those physical distances in which we are interested.

For example, if we are to simulate a vibrating string, then we want a significant number of zones in the smallest wavelength of interest. We can observe a second example by simulating laser fusion phenomena. When laser light shines on a fusion target, it penetrates a finite distance (determined by plasma conditions) and the material which has been penetrated ablates. Thus a density gradient is created in the ablated material. A significant number of zones are required to define such a density gradient accurately. Such a density gradient might be analogous to a half-wavelength since it goes from a maximum to a minimum but not back again to a maximum. However, some portions of the problem are physically more important than others, and the resolution must be treated more accurately in those portions. Thus it is very important to have a general physical understanding of the system being simulated and to exercise judgment about the resolution required in different regions of the problem based on this understanding. A fairly common guideline is 20 zones per wavelength for good accuracy and 10 zones per wavelength for fair accuracy.

Consider a spherical nuclear reactor made of concentric shells of enriched uranium and heavy water as in Fig. 6. Assume that the overall neutron gradient does not change much when crossing one of the metal shells. Thus we have a neutron density half-wave of length R on which are imposed some slightly shorter wavelength perturbations crossing the metal shells. Then 5 zones per metal shell might suffice, and the heavy water might require one zone per $.05 R$. Thus there might be 15 zones in the metal and 17 zones in the heavy water for a total of 32 zones. That description might be satisfactory for a purely neutronic simulation. However, let us assume that the above physical system is supercritical and explodes. In that case each metal shell will undergo hydrodynamic motion characteristic of one wavelength. Thus for hydrodynamic purposes, the zoning would need to be quite a bit finer. This illustrates an

Fig. 6 Simplified reactor schematic.

important consideration. Most computer simulations involve many physical processes, and the one requiring the finest zoning determines the zoning.

TWO-DIMENSIONAL MESHES

In previous sections we observed that the truncation error could be affected by algorithm type (e.g., forward difference vs central difference) and/or by special conditions (e.g., constant time step or uniform spatial mesh). In two-dimensional calculations, the mesh orthogonality (or lack thereof) is an important factor in determining the accuracy of the calculations. Figure 7 shows a regular but nonorthogonal 2-D mesh. If neutrons are introduced at zone A and allowed to diffuse out, physically they should arrive on the other side first at zone 1. However, a standard implicit algorithm will show them arriving first at zone 3 because of a failure to include the nonorthogonality of the mesh in the calculation. The lines of the mesh are given indices ($k = 1, 2, \dots, 16$ and $l = 1, 2, \dots, 8$). In the example given, the neutrons seem to be flowing along the k -lines. Other algorithms may attempt to include such considerations inadequately and end up predicting that neutrons arrive first at an intermediate zone such as 2. Note that the zone dimensions in the x and y directions are nearly equal for the example given, or their aspect ratios are nearly 1. When aspect ratios are far from 1,

Fig. 7 half-life vs zone size: convergence example.

the problems associated with mesh nonorthogonality become exaggerated. The same holds true when the mesh becomes highly irregular as in Fig. 8, where it becomes very difficult to describe the neutron flux flowing across the interface that separates zone A from zone B.

Our discussion to this point has been directed toward Lagrangian grids. However, Eulerian codes have the same troubles describing interfaces as they pass through the mesh. An interface may then split a zone into two pieces, and such partial zones may have large aspect ratios, or their corners may have angles which are far from right angles. Additionally, Eulerian codes find it difficult to place fine zoning in certain sections of the problem and coarse zoning in others.

It is desirable to have a balance between the zoning density in the k direction and that in the l direction. Put another way, it is foolish to have fine zoning (in the sense of wavelengths) in the mesh in the k direction and coarse zoning in the l direction. One would like the physical resolution in the two directions to be comparable. Note, this does not mean that the number of k lines should equal the number of l lines!

ZONE SIZE STUDIES AND CONVERGENCE

Assume that one has achieved an appropriate zoning pattern with respect to zoning density, mesh orthogonality, and aspect ratios. Most likely, we will find it efficient to examine solution convergence as a function of zone size. This can be achieved by starting with a coarsely zoned calculation and proceeding to a more finely zoned calculation. For a 2-D problem the zone

Fig. 8 Highly distorted mesh example.

might be halved in each direction, thereby resulting in a quadrupling of zones and an increase of a factor of eight in computer time (Δt cut in half also). Some planning is required to ensure that such a finely zoned problem will not exceed the memory capabilities of the computer. It may be possible to halve the zone size once or even more in a zone size study.

The advantages of this process are obvious. Coarsely zoned calculations may provide sufficient accuracy at a large factor of savings in machine time. This would allow the applied scientist to examine more design options and to test the sensitivity of his calculations to more input variations. We may also be able to obtain more accurate solutions by extrapolating the results to zero zone size.

Of course, the coarsely zoned problems must not disrupt the ability of the mesh to resolve physical phenomena. Even when we are using all of the computer memory, the accuracy of the calculations may be only minimally acceptable or even unacceptable. Each problem must be examined individually.

A certain amount of subjective judgement is required to determine the usefulness of the convergence process for any given problem. Let us return to the example of the reactor composed of concentric spherical shells of fissile material in heavy water. Assume that the system is subcritical, that only neutronic behavior is of interest, and that the system radius (R_0) is many mean free paths. If a burst of neutrons is introduced, the neutron population will be redistributed in a short time and will "settle" into a fundamental spatial mode (eigenvalue) which will decay exponentially in time with a half-life characteristic of the system. We want to determine this half-life using a computer code. Assume that the results of a zone size study are given

by the plot in Fig. 9. By drawing a smooth curve through the three points from different calculations, we can extrapolate to the value (x) at infinitely small zone size. If the value B is 1% greater than the value A, then the extrapolation involves an error of considerably less than 1%. Also solution B is off by less than 2% and solution C is off by about 5%. Thus we might conclude that the coarse zoning is adequate for most calculations. However, if the value B is 20% greater than value A, even the accuracy of the finely zoned calculation may not be adequate. But it may be that the convergence/extrapolation process will produce an accurate answer. Of course, we might obtain intermediate results, such as finding that medium zoning produces satisfactory accuracy for most calculations but that coarsely zoned results are useless.

Fig. 9 2-D non-orthogonal mesh example.

CONCLUSIONS AND RECOMMENDATIONS

We have very briefly reviewed the basic ideas of finite difference methods. These include truncation error, roundoff error, stability, convergence, explicit algorithms, and implicit algorithms. We have observed that truncation error is usually the dominant factor affecting calculational accuracy. Fortunately, this variable is the one over which a moderate

amount of control can be exercised by the code user by controlling zone size and zoning pattern. There can be no single computational procedure guaranteed most efficient for all simulations. However, for those who would like a starting point guideline, the next paragraph provides a reasonably good procedure for considering 2-D calculations.

First, examine the physical system wanted to simulate and determine the spatial resolution required to define all important variables. These include material boundary shapes, density gradients, particle density gradients, energy, temperature gradients, etc. Characterize all such spatial definition with a common unit of measure (e.g., wavelength). Then determine the number of such physical wavelengths in the k direction and l direction, and proportion the number of zones accordingly with a weighting factor to account for the relative physical importance of different regions. Next, select a mesh as regular and orthogonal as possible, striving for equal zone spacing in any direction within any region. Do not be overly concerned about mass matching or Δx matching at interfaces, and try to avoid using zones with large aspect ratios. Whenever possible, start with a fairly coarse zoning density (perhaps 10 zones per wavelength). Then double the zoning in each direction and examine the solution convergence. We can then redistribute the same number of zones (more zones in some regions and fewer in others, different patterns, etc.) and examine solution convergence to find the zoning pattern which converges most rapidly.

A number of iterations may be necessary to optimize the zoning density and pattern for an adequate coarsely zoned calculation, if such a calculation can be obtained. This process is somewhat time consuming and is all aimed at minimizing the truncation error. However, if successful, it will allow us to quickly examine other error sources such as roundoff, data uncertainties, and modeling choices. For example, cross sections could be multiplied by arbitrary values to test the importance of the data's accuracy. Or neutronics calculations could be run, using several different models (e.g., diffusion theory, transport theory, or a Monte Carlo model). All of these can be examined with cheap, coarsely zoned problems. Naturally, the major effort of design variations can also be handled in the same manner, with an occasional double-zoned calculation to check on convergence. If convergence works, efficiency is not the only beneficial result; an accurate answer is also assured. In fact, we may want to select a design approach because of our confidence that it can be calculated accurately.

In closing, a cautionary note seems appropriate. There are many approximations involved in the modeling process, and the results of computer code calculations are not to be trusted without question. Whenever possible, it is good practice to try to calculate the same problem on different computer codes, and also to check a code's performance against known analytic solutions.

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References

1. J. Von Neuman and R. Richtmyer, J. Appl. Phys. **21**, 232 (1950).
2. R. Richtmyer and K. Morton, Difference Methods for Initial Value Problems, (Interscience, New York, 1967).
3. See Ref. 2, p. 230.
4. J. White, J. Comp. Phys. **16** (2), 119 (1974).

Recommended References

- Crowley, W. P., Lectures: Introduction to Finite Differences Methods, Lawrence Livermore Laboratory, Instructional TV Course, 1974.
- Handbook of Numerical Methods and Applications, Louis G. Kelly, Ed. (Addison-Wesley, Reading, Massachusetts, 1967).
- Harlow, F. H. and A. A. Amsden, Fluid Dynamics, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, Rept. LA-4700 (1971).
- Roche, P. J., Computational Fluid Dynamics (Hermosa Publishers, Albuquerque, New Mexico 1972).
- Wilkins, M. L., Introduction to Hydrodynamics, Lawrence Livermore Laboratory, Rept. UCRL-51178 (1972).