THE METHOD OF INDEPENDENT TIMESTEPS IN THE NUMERICAL SOLUTION OF INITIAL VALUE PROBLEMS

Andrew Peabody Porter

(Ph. D. Thesis)

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ABSTRACT

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Andrew P. Porter

In the numerical solution of initial value problems in several independent variables the timestep is controlled, especially in the presence of shocks, by a small portion of the logical mesh, what one may call the crisis zone. One is frustrated by the necessity of doing in the whole mesh frequent calculations required by only a small part of the mesh. It is shown that it is possible to choose different timesteps natural to different parts of the mesh and to advance each zone in time only as often as is appropriate to that zone's own natural timestep, in what may be called the Method of Independent Timesteps. The prior work is reviewed and for the first time an investigation of the conditions for well posedness, consistency and stability in independent timesteps is presented, resulting in a new method. The prochronic and parachronic Cauchy surfaces are identified and the reasons (well posedness) for constraining the Cauchy surfaces to be prochronic, (in distinction from the method of Grandey) that is, to lie prior to the time of the crisis zone, (the zone of least timestep) are indicated. Stability (in the *maximum norm*) of parabolic equations and (in the L_2 norm) of hyperbolic equations is reviewed, without restricting the treatment to linear equations or constant coefficients, and stability of the new method is proven in this framework. The details of the method of independent timesteps, the rules for choosing timesteps and for deciding when to update and when to skip zones, and the method of joining adjacent regions of differing timestep are described. The stability of independent timestep difference schemes is analysed and exhibited. A summary of experience with the method is appended. The economic advantages of the method, which often amount to an order of magnitude decrease in running time relative to conventional or implicit difference methods, are noted.

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SYMBOL TABLE

Indices

- j As a subscript, the zone index in one dimensional calculations.
- J Greatest zone index in one dimensional calculations.
- k Zone index in two dimensional problems.
- n Indexes quantities at time t^n .

Operators

$$\Delta_+ x_j = x_{j+1} - x_j$$

$$\Delta_- x_j = x_j - x_{j-1}$$

$$\delta_+ x^n = x^{n+1} - x^n$$

$$\delta_- x^n = x^n - x^{n-1}$$

$$\sigma_+ x^n = x^n + x^{n+1}$$

$$\sigma_- x^n = x^n + x^{n-1}$$

$$\Sigma_+ \quad \Sigma_+ x_j = x_j + x_{j+1}$$

$$\Sigma_- \quad \Sigma_- x_j = x_{j-1} + x_j$$

Physical Quantities

- A** A product of constants, finite differences, properties of matter, as is convenient. See for example Eqs. (3.22,3.23), (4.30), (5.13)
- a** Coefficient in Eqn. (7.1)
- a_j** General averaging function of temperatures adjacent to zone *j*
- B_j** Auxiliary quantity, Eqn. (4.29)
- B_j** Collection of constants and coefficients, Eqs. (5.13), (4.29)
- BT, BTⁿ** Boundary terms in Eqn. (5.17)
- C_j** Auxiliary quantity in a tri-diagonal matrix inversion routine.
- C** A general finite difference operator, Eqn. (4.21)
- c** Wave propagation speed in hyperbolic equations.
- D_j** Auxiliary quantity in tri-diagonal matrix inversion routine.
- E_j** Internal energy per unit mass in hydrodynamics
- E** Number of times a code does major output, Eqn. (7.1)

- F General function, see context.
- f General function, see context.
- G_j Divergence of flux.
- G_j Product of conductivity and geometry factors, as in Eqn. (4.27)
- g Variable parameter, $0 \leq g \leq 1$, $g = 0$ for backward differencing, $g = 1$ for forward differencing; see Eqn. (4.35)
- $G_{k,j}$ Product of conductivity and geometry factors, as in Eqn. (3.25)
- $G(\Delta t)$ One of a family of operators, ch. VI.
- K Constant, Eqn. (4.19)
- $K_{k,j}$ Product of conductivity and geometry factors, as in Eqn. (3.25)
- K_j Product of conductivity and geometry factors, as in Eqn. (4.27)
- m_j Zonal mass.
- $\mathcal{M}$ A mesh
- N Number of cycles a problem has run, as in Eqn. (7.1)
- τ Geometry sentinel, as in Eqn. (3.8)
- JXN Number of zones times number of cycles run.
- P_j Pressure from equation of state
- P_j $p_j + Q_j$

P_t	Time derivative of P .
p^*	Extrapolated value of P .
Q_i^n	A term in the sum R^n , Eqs. (5.25), (5.6)
Q_j	Artificial viscosity.
R^n	Square of the wave norm, as in Eqn. (5.18)
R	Ratio of successive timesteps in one cone.
r	Radial coordinate
s_j	Computation sentinel
SS/N	Number of zone cycles actually computed
$SRAT$	J/N SS/N .
S	General operator, Eqn. (4.17)
s	Bound of operator S , as in Eqn. (4.17)
t	Time
t^n	Time at cycle n .
t_0	Time at which initial conditions are specified.
t_j	Proper time of the j^{th} zone.
T, x'	Cauchy surface on which initial conditions are specified.
T_j^n	Temperature

u	Dependent variable, typically a temperature.
u_j	Scalar wave function, Eqns. (5.9),(5.35)
u_j	Lagrangian velocity in hydrodynamics.
u_t	Time derivative of u .
u_x	space derivative of u
u^*	Extrapolated temperature in a neighboring zone.
u	Shock speed, in Chapter 11.
u_{ttt}	$\partial^3 u / \partial t^3$.
v	Component of a vector wave function.
v_j	Specific volume, or reciprocal of the density in hydrodynamics.
v_j^n	Auxiliary quantity defined in Eqn. (4.24)
v	Approximate solution to an equation whose exact solution is u .
w	Component of a vector wave function.
t_j^n	For times with both superscripts and subscripts, see the first section of chapter III.
x	Cartesian coordinate
x_j	Lagrangian position coordinate in hydrodynamics.
y	Cartesian coordinate.

y_j	A component of a vector wave function.
y	$k\Delta x$, in Eqn. (4.5)
z	Coefficient in Eqn. (7.1)
z	Cartesian coordinate
Z	A general vector wave function.
γ	Constant in perfect gas Equation of state.
Δt	Timestep
Δx	Spacing between adjacent mesh points: x_j, x_{j+1} .
Δt_c	Courant timestep, defined in Eqn. (2.2).
Δt_p	Physical timestep, defined in Eqn. (2.3).
Δu	Change in u in one cycle.
ϵ	A small number, $0 < \epsilon \ll 1$.
ζ	Amplification factor, Eqns. (4.1-4.5)
η	Shock density ratio: (density behind)/(density in front).
ξ	Shock strength: (pressure behind)/(pressure in front).
Δr	Mesh spacing in cylindrical coordinates.
ν	Density
σ	Diffusion coefficient.

Φ_1

Flux of heat

CHAPTER I

INTRODUCTION: MOTIVATION AND STRATEGY

Shock Hydrodynamics, the Context of the Present Work

This dissertation develops and describes a method of speeding up shock hydrodynamics and related calculations by an order of magnitude, a gain in effective computing power usually realised only over several generations of digital computers. The methodology developed treats its calculations with elements of the perspective and discrimination until now seen only in the human approach to such problems. The present work grew out of the frustrating experience that numerical simulation of shock hydrodynamics problems can be very slow, even with the fastest modern digital computers. Such a hydrodynamic simulation requires many computations, with varying degrees of accuracy appropriate to each. The usual practise (in finite approximation of partial differential equations as well as in their analytic treatment) is to provide a single approximation which is uniformly adequate to all parts of the calculation. A human calculator, by contrast, has a sure feeling for where he must be careful and where he can tolerate

imprecision and still obtain stable and acceptably accurate answers in a reasonable amount of time. The same motivation governs the present numerical strategy. Before making concrete its outline and details of its implementation, it is perhaps better to wait until the terms and usage of this field have been defined in the next section. It is appropriate to point out now, however, the place of shock hydrodynamics in the history of numerical analysis, and to indicate that, because of its sophistication of physical effects and conceptual simplicity of numerical techniques, it presents a singularly fortuitous opportunity for a computational programme such as the present one.

There are many genera of problems which lend themselves readily to numerical solution, among which one may single out initial value or time evolution problems, problems in time and one or more space variables. Shock hydrodynamics forms a somewhat more limited genus of differential equations than this broad class, but it is not too much to claim that it has motivated much of modern numerical analysis. By contrast, the early numerical work, which paralleled the conceptual development of the differential calculus, was in ordinary differential equations; this work was motivated largely by celestial mechanics. Its strategy was inspired by the Taylor series, and it has sufficed rather well for ordinary differential equations. Partial differential equations had to wait for large digital computers, not available until after 1945. George Boole¹ in 1872 laid the foundations for a formal treatment of finite difference equations, and Courant, Friedrichs, and Lewy in 1928 published the classic work on stability of difference approximations to equations in

¹ Boole, (1872).

several independent variables². The name of John von Neumann is most widely associated with the next significant work, both in construction of computers themselves, necessary for any practical work in partial difference equations, and in the theoretical and programming techniques of approximation in such equations. His interests were in shock hydrodynamics, beginning with theoretical³ applications. Since then engineering⁴ and astrophysical⁵ concerns have flourished. These practical motives have provided the impetus for a major theoretical body of art and science in numerical methods⁶.

Like so much that has gone before it, the present work is situated in shock hydrodynamics, and for two reasons. Shock hydrodynamics, broadly construed, encompasses great subtlety and richness of physical effect, and numerically it is essentially simple. Detailed calculations of real rather than idealised physical effects can lead to frustratingly slow hydrodynamic calculations. One would like to see the computer structure its calculations with a little more care, as does the human calculator, rather than indiscriminately recalculating many times physical quantities it already had available if only it could recognise them. This constitutes a major departure from nearly universal philosophy, for all previous practise has been to find an approximation

² Courant, Friedrichs, Lewy, (1928).

³ von Neumann & Richtmyer, (1950).

⁴ For a recent example of engineering applications of shock hydrodynamics, see the references by Zimmermann, Wood, Nuckolls, Thiessen.

⁵ For recent astrophysical applications, see Weaver (1976) Wilson, LePiane (1970) May, White (1966) Colgate, White (1966) Chevalier, R. A. (1976)

⁶ For a handbook of numerical methods in the solution of time dependent partial differential equations, see Richtmyer & Morton (1967).

which is adequate (uniformly) even in the worst parts of one's calculational problem, regardless of how over-fine it may be in other parts of the problem. The work here described is a method of locally suiting the fineness of the approximation to the conditions at hand, and it will be introduced a little more fully in the next section.

Hydrodynamics is numerically simple and tractable enough so that this program may be carried out practically, and the physics is sophisticated enough that the faculties gained are of great significance. This is an unusual combination of circumstances, and a brief survey of other kinds of initial value problems will indicate how fertile a setting is hydrodynamics for the numerical programme to be outlined shortly.

It is sufficient simply to catalogue different regimes of physics and to note which aspects of each require or lend themselves to special treatment, and it will be apparent why the present programme is situated in shock hydrodynamics. In the case of weather prediction, one is confronted with a fluid medium which is homogeneous and subsonic, suggesting Eulerian hydrodynamics. The time scales of processes are similar throughout the spatial extent of the problem, obviating the need for special handling of shocks by means such as artificial viscosity, and rendering a method such as independent timesteps unnecessary. There is spatial structure at all scales, from one meter turbulence to kilometer topographic effects to 100 kilometer storms to global weather patterns. Weather is intrinsically three-dimensional, implying that (now, in 1976 and for at least a few more years) computer memory must be husbanded with care. Appropriate numerical strategies have evolved to suit the simulation of the atmosphere⁷. Turbulent hydrodynamics by

⁷ Leith, C. E. (1964,1965).

virtue of its very fine spatial structure has difficulties of its own, taxing all the resources of a digital computer and its programmer.

The numerical modelling of plasmas can confront one with equations that defy stable integration by ordinary means. The Boltzmann equation in all its variations presents one with physics in as many as six dimensions (three of position and three of velocity). In the velocity dimensions, the interactions are quite non-local, and the implications for computational simulation do not promise an easy or early solution.

Shock hydrodynamics is in many ways the simplest, and certainly the earliest explored genus of initial value problems. The physics is confined to one scale, always macroscopic; shocks can be treated easily by an artificial viscosity⁸; one needs only fairly conventional finite difference integrations motivated by the Taylor series expansion of the physical quantities at hand. Shock hydrodynamics may seem a limited area of numerical work, but there is room even here for a surprising richness of method and experience, as the written and oral tradition amply show⁹. In practical shock hydrodynamics problems¹⁰ one is usually obliged to treat also physics of one or more diffusion processes, such as neutron flow, heat conduction, conduction of heat by free electrons and even by positrons¹¹. Such an effort can quickly come to resemble a symphony more than a sonata, and as the computation progresses, many physical and computational effects will contribute to the time evolution

⁸ von Neumann & Richtmyer (1950).

⁹ See for example the literature cited in Richtmyer & Morton (1967)

¹⁰ See the references by Zimmermann, Nuckolls, Wood, and Thiessen.

¹¹ Weaver (in press)

of the problem, but despite all the physical complications, the numerical work remains essentially simple.

Posing the Problem

Initial value problems of shock hydrodynamics may be described by coupled partial differential equations in the physical quantities of interest. There are at least two independent variables, one or more having the character of cartesian coordinates in space, and one and only one independent variable having the character of time; denoted by t , rarely by T . The equations are of such a nature that if the state of the physical system is specified at some time $t = t_0$, a solution of those equations exists for times $t \geq t_0$. The physical extent of the problem is defined by some region R with boundary ∂R , and it is usually necessary not only to specify some conditions throughout R at time t_0 but also on ∂R at all times $t \geq t_0$. These are the *initial conditions* and the *boundary conditions*.

By way of a specific example, the heat conduction equation may be considered:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\sigma \frac{\partial u}{\partial x} \right), \quad (1.1)$$

its domain R may be taken as $x = [0, X]$, and its initial and boundary conditions specified by functions $f(x)$, $g(t)$, and $h(t)$:

$$\begin{aligned}
 u(x, 0) &= f(x) & \text{for } 0 \leq x \leq X \\
 u(0, t) &= g(t) & \text{for } t \geq t_0 \\
 u(X, t) &= h(t) & \text{for } t \geq t_0
 \end{aligned}
 \tag{1.2}$$

It may be proven that a solution $u(x, t)$ of Eqns. (1.1-1.2) exists and is unique¹².

The system Eqns. (1.1-1.2) may be approximated, not at all points (x, t) in R , but on a finite grid or mesh of points x_j at times t^n . The subscripts (usually j and k) will index the space coordinates of all quantities defined on this mesh, and superscripts (usually n , occasionally m or some other letter) will index the time. Thus u_j^n is the temperature u at point x_j and time t^n . The mesh may be defined by the sequence of points x_j , for $1 \leq j \leq J$, with $x_1 = 0$ and $x_J = X$; and by the sequence of times t^n , with $t^0 = t_0$ and $t = T$, the "stop time" for the problem. The portion of the problem delineated by points x_j and x_{j+1} may be called a zone, zone j . The symbol u^n with no subscript may denote the whole array $(u_1, u_2, \dots, u_{j-1}, u_j)$, and $u_j(t^m)$ may denote u at x_j and some for the moment variable time t^m . One finite approximation to Eqns. (1.1-1.2) may be exhibited:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\sigma}{\Delta x^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n), \tag{1.3}$$

together with its initial and boundary conditions:

¹² Garabedian (1966).

$$\begin{aligned}
 u_j^0 &= f(x_j) & \text{for } j=1,2,\dots,J \\
 u_j^n &= g_j(t^n) & \text{for } n=1,2,\dots \\
 u_j^n &= h_j(t^n) & \text{for } n=1,2,\dots
 \end{aligned}
 \tag{1.4}$$

The equation (1.3) may be used to advance the array u^n from time t^n to time t^{n+1} ; the quantity $\Delta t = t^{n+1} - t^n$ is known as the *timestep*. Note that every zone is defined at time t^n and that all are moved in lockstep to time t^{n+1} . This may be called a *synchronous calculation*, since all the zones are advanced synchronously. The timestep Δt does not depend on j , the zone index. Shortly Eqns. (1.1-1.2) will be examined a little more closely and *asynchronous calculations* will be defined, with timesteps Δt_j that may vary from one zone to the next. *Asynchronous* is used interchangeably with *independent timesteps*. When a particular zone is advanced from time t^n to t^{n+1} , it is said to be *updated* or *calculated*. The total number of times that zones have been updated is the number of *zone-cycles* (represented by $SSJN$) that the problem has done. In a synchronous calculation, $SSJN$ is equal to the product of the number of zones times the number of cycles run (this product is denoted by JXN). For an asynchronous calculation, $SSJN$ may be less than JXN . The ratio $(JXN/SSJN)$ may be called the *computation ratio*, denoted by $SRAT$.

Eqn. (1.1) may be generalised in several ways. First, one may note that it is a single equation in a scalar quantity u . By contrast, there may be posed the wave equation

$$\frac{\partial v}{\partial t} = \frac{\partial v}{\partial x} \quad (1.5)$$

$$\frac{\partial v}{\partial t} = \frac{\partial v}{\partial x}$$

It may be provided with initial and boundary conditions analogous to Eqns. (1.2) and (1.4); quantities v_j^n and u_j^n may be defined on a mesh as before, and a pair of coupled finite difference equations play the role of Eqn. (1.3). In hydrodynamics, there will be not two but six or more such coupled equations.

Secondly, it may be noted that in Eqn. (1.1) there is only one space variable x ; there are commonly as many as three, x, y, z ; and the temperature will accordingly carry three subscripts: u_{jkl}^n . It may also be noted that the symbol x in Eqn. (1.1) defines a coordinate in a problem with plane symmetry; implicitly, u is defined for cartesian coordinates y and z also, but does not depend on them. The problem might have been posed in spherical geometry, with $u = u(r) = u(r, \theta, \phi)$ and u independent of θ and ϕ ; or in cylindrical geometry, with $u = u(r) = u(r, z, \phi)$ and u independent of ϕ and z ¹³.

¹³ For a two dimensional problem in cylindrical coordinates r, z , see LeBlanc & Wilson (1970); for a one dimensional problem in spherical geometry, see May & White (1966). For three dimensional work, see e.g. Leith (1964, 1965). For two dimensional Lagrangian hydrodynamics in plane and cylindrical geometry, see Schulz, (1964).

Two terms from hydrodynamic usage may be defined at this point: *Eulerian* and *Lagrangian* hydrodynamics. Among the physical quantities appearing in the hydrodynamic equations as dependent variables are the velocity, pressure, density, and internal energy density. The position x_j may be taken as dependent or independent, according as the points x_j are fixed in the moving fluid or fixed in the laboratory. In the former case, the Lagrangian formalism, the position x is a dependent variable and the mass m_j of the fluid zone j is a fixed parameter. Here the quantity x_j is the position of the point j , which moves with the fluid. In Eulerian hydrodynamics by contrast, the positions x_j are fixed parameters, and the masses m_j are dependent variables. Matter flows into and out of zones, and this flow must be calculated. In textbooks of hydrodynamics, the usual formalism is Eulerian¹⁴, and the Lagrangian equations are less common¹⁵.

To return to the system, Eqs. (1.1-1.2), and to indicate one more way in which it is not general, the initial conditions in Eqn. (1.2) were specified on a line $T(x) = t_0$. This curve $T(x)$, called a *Cauchy surface*, might have been more general, a function not independent of x . The terms *Cauchy Problem* and *initial Value Problem* are synonymous. With initial and boundary conditions specified by Eqn. (1.2) on $T(x) = t_0$ or on some curve $T(x)$ not a constant, the pertinent generalisations of Eqn. (1.1) are always in some sense hyperbolic¹⁶. It is known from the theory of partial differential equations¹⁷ that if the Cauchy surface $T(x)$ is not a constant, neither $T(x)$ nor the function $f(x)$ defining the initial conditions are completely free of restrictions. The nature and

¹⁴ Landau, Lifshitz, (1959), p. 1, ff.

¹⁵ Zel'dovich, Raizer (1966), section 2, p. 4, ff.

¹⁶ Garabedian (1964), chapter 3.

¹⁷ Garabedian (1964), chapter 4.

causes of these restrictions will be made clear below, when the plan of the present work is outlined.

Allocation of Computational Effort

At each particular stage of the computation, one must decide how far in time to advance it on the next round of computations. For example, one must select in Eqn. (1.3) a value for the parameter Δt if one is to advance the problem from t^n to $t^{n+1} = t^n + \Delta t$. In only the simplest of problems may the timestep be set once and for all time at the start of the calculation. Usually as events transpire, longer or shorter timesteps are appropriate to different epochs in the history of the problem, brief in times of rapid change, and of longer duration when little is happening.

Different zones of the problem may for reasons of stability and accuracy discussed below require quite incommensurate timesteps -- differing even by orders of magnitude. One is then apparently obliged to step the problem not further than the briefest of these timesteps, in order to escape instability or avoid unacceptable inaccuracy in the most stringently limited zone. It does not matter that most of the zones in the fluid body being simulated will be computed far more frequently than they require -- even recomputed when they are barely changing at all. One may in a one dimensional context plot the timestep as a function of position, as in Fig. (2.2). This situation (and it is a common one) cries for improvement. To the extent that the briefest timestep is unacceptably small because of stability considerations, one can resort

to implicit difference methods, which usually are unconditionally stable¹⁸. However, in problems of any complexity at all experience with implicit equations indicates that the timestep is still controlled severely by one or two zones for reasons not of stability but of accuracy. One can use five or seven point integration formulas, in which a zone is allowed to interact not just with its nearest neighbors but with matter several zones distant¹⁹. Here, one can expect the Courant condition²⁰ on the timestep to be relaxed by a factor of two or three. There are even explicit difference methods which are unconditionally stable, such as that of du Fort and Frankel, for the diffusion equation²¹, a matter to be discussed below in Chapter IV.

What one would like to do if only one could is simply to skip calculations in those zones where the timestep can be long until enough time has elapsed since their last updating to fill out their own natural timesteps. Inspecting Fig. (2.2), zone number 10 has a timestep smaller by an order of magnitude than any other. This problem of 80 zones must allocate ten times as much effort to the body of the problem (zones 1-9 and 11-80, at the present) as it would require from stability and accuracy conditions prevailing in the majority of the zones. Because the region of brief timestep is so small, there is a potential savings of about a factor of ten in effort -- in problem running time.

In fact, much of this potential savings can be realised. It is possible to step zone 10 ten times for every one time zones 1-9 and 11-80 are stepped forward in time, and it is possible to do so in a way

¹⁸ Richtmyer & Morton (1967), p. 16; Yanenko (1971), p.

¹⁹ Joubert (1971, 1972).

²⁰ Courant, Friedrichs, Lewy (1928); J. R. Joubert

²¹ du Fort, Frankel (1953).

such that the zone frequently calculated is not always some fixed zone (zone 10, e.g.) but is whatever zone momentarily needs the frequent attention. For as the shock progresses across the problem, each zone in turn requires a timestep briefer than all the others. With an algorithm of no great complexity, each zone can enjoy the treatment it deserves without unduly delaying the rest of the problem. Or, if several zones at once require brief timesteps, that can be handled easily. The method requires none of the global perspective of the human calculator, but handles its calculations and decisions on purely local considerations. What follows will indicate the approach and the modest precautions necessary to maintain stability and accuracy.

The Experience of Celestial Mechanics

A remedy for the difficulties of hydrodynamics may be had by following the example of recent practise in some problems of celestial mechanics. This problem is treated in comprehensive generality for ordinary differential equations by Gear²² and others, but my own acquaintance with it is via the particular case of celestial mechanics, and that example will provide a nicely concrete motivation for the contemplated programme in partial differential equations. Integration of the equations of motion of the ten major bodies of the solar system presents problems similar in some respects to shock hydrodynamics. There is a great disparity in celestial time scales, from the 28 day orbit of the moon to the 90,465 day orbit of Pluto, a factor of 3000. Methods of integration in celestial mechanics take advantage of the

²² Gear (1971), Hindmarsh (1972).

positions of the planets at many previous points in their orbits, and consequently can move a planet around its orbit in a dozen or so timesteps. But if the moon sets the timestep at approximately 2 days, one is called to step Pluto 40,000 times in its orbit, and that hardly seems called for.

The experience of S. J. Aarseth and others²³ indicates that indeed each planet can enjoy its own natural timestep of about a tenth of its year. In estimating the gravitational forces on one of the ten bodies one needs the positions of the other nine. These may be had by interpolation or extrapolation as is convenient. The same strategy works for the solution of partial differential equations as for coupled ordinaries. There are some critical differences, however. Stability is always an uncertain matter until it is investigated and proven. There is at least one example of an unconditionally stable integration scheme for the heat equation being rendered at best conditionally stable by independent timesteps.

Hydrodynamics presents a new situation in as much as no one zone always has the briefest timestep, leaving others to be updated less often. In the motion of the planets, Mercury will always have an 88 day period, and the Earth will always have one of 365 days. But no zone in hydrodynamics always plays the role of Mercury while some other zone plays the role of Pluto. One cannot permanently and ahead of time

²³ The Work of S. J. Aarseth referenced is an extension of the described work from the solar system to the N-Body problem, specifically the simulation of globular clusters. The need for independent timesteps there is critical, and arises from a few close encounters of stars. Close encounters require timesteps far briefer than those sufficient for the integration of the other bodies of the cluster.

assign timesteps to different zones. Somewhat more sophisticated logical machinery is required to assign timesteps and to select zones due for calculation. Nevertheless, to be useful and general as a method, this logical apparatus must operate without help from the human user of the method, and it must not consume too much time in comparison to the effort spent on actually doing the physics.

The Strategy of Approach

As a general, if somewhat simple instance of the equations to be integrated, one may take, with a, b, c, e all positive:

$$a \frac{\partial u}{\partial t} + b \frac{\partial^2 u}{\partial t^2} = c - e \frac{\partial u}{\partial x} \quad (1.6)$$

The coefficients a, b, c, e may all be variable functions of x and t and more significantly, of u . If b is zero, the equation is parabolic, otherwise it is hyperbolic²⁴. This is a scalar equation in one variable, u , and almost invariably practical situations call for integrating several coupled equations. But this equation is for the moment quite sufficient to illustrate the pertinent considerations. Together with this equation, one must specify initial and boundary conditions on some Cauchy surface $T(x)$, as in Fig. (1.1)²⁵. For present purposes, all problems may be considered hyperbolic, and so initial conditions at point P influence subsequent events in the region D bounded by the two characteristics $q(x)$ and $s(x)$; and in Fig. (1.2), the events at point Q are determined by the conditions on the Cauchy surface

²⁴ Garabedian (1964), Ch. 3.

²⁵ Garabedian (1964), p. 104

T between points R and S and possibly (usually) by the conditions in the region E bounded by T and the characteristics q and s through the point Q.

In order for the problem to be well posed, it is necessary that figures such as Figs. (1.1) and (1.2) exist. This is in fact a condition on the slopes of the curves $T(x)$, $q(x)$, and $s(x)$: $q(x)$ and $s(x)$ must both be steeper than $T(x)$. In usual circumstances this could be passed over without mention, since Cauchy conditions are commonly prescribed on a line $t = 0$. But as the computation proceeds, if different zones have different timesteps, they will also be referred to different times. Thus, at any stage of the calculation the aggregate of data stored for the set of all zones represents Cauchy conditions specifying the further development of the problem, so that a problem which was initially well posed could evolve into one which is not well posed. Such a pathological situation is illustrated in Fig. (1.3). Suppose that in Eqn. (1.6), u represents a temperature, and that at point P in Fig. (1.3) due to non-linear effects, the characteristics are significantly flattened. Now the slope ($\partial q/\partial x$) of the characteristic q is just the reciprocal of the sound speed, so we may expect the curve $q(x)$ to bend over, and in fact it can intersect $T(x)$. Here there is trouble, for the point Q is specified already, since it is on $T(x)$, which is to say it is the result of prior essentially local evolution of the problem. But Q is now alleged to depend on conditions in the neighborhood of P, and this is impossible. For computational purposes, Q lies in the past of P, and P has succeeded in propagating information into Q's past. There is no proper way to handle this trouble; the problem is no longer well posed. Because real equations are not

Fig. (1.1) Initial Conditions

Fig. (1.2) Domain of Dependence

commonly linear, it is not in general possible, given the information on the Cauchy surface $T(x)$, to predict the shape of the characteristics, except by actually solving the problem incrementally in time. And so, with Cauchy surfaces concave forward in time, one is always vulnerable to this kind of misfortune. It is apparently possible to protect oneself from it, as is reported by Grandey, although his published work does not indicate how²⁶; he indicates that stringent timestep controls will suffice²⁷.

This may be made clearer by indicating the possible methods of selecting the next zones to be updated, since this choice determines the character of the Cauchy surfaces $T(x)$. As each zone is updated, to it is assigned a time T , specifying some point on the curve $T(x)$. In the approach of Grandey, the next zone to be computed is always the zone most out of date, the zone of earliest or least time T . To the problem as a whole, at this particular stage of the computation, can be assigned the time t of this zone. Thus, all the T 's are larger than t , that is, *parachronic* with respect to t . Most of the time the next zone to be computed is the zone of least timestep, and this is the zone where events are developing at the greatest rate. It might be called the *crisis zone*. It is also the place most likely to originate trouble of the kind illustrated in Fig. (1.3). Whenever a zone of longer timestep is momentarily the zone most out of date, it is updated far into the future of its neighbors of briefer timestep. Thus, one may plot the Cauchy surface $T(x)$ and the timestep $\Delta t(x)$ on the same graph, as in Fig. (1.4) For the price of potential trouble, and the stringent timesteps

²⁶ The work known as *Variable Timesteps* is reported in the references of R. A. Grandey and C. W. Davis.

²⁷ R. A. Grandey, private communication, (1975)

Fig. (1.3) Pathological Initial Conditions

Fig. (1.4) Cauchy Surfaces in the Method of Grandey

needed to avoid this trouble, one enjoys the opportunity of time interpolating instead of extrapolating quantities in neighboring zones as one needs them when they are not isochronic with the zone of interest.

In the work here detailed below, the zones of long characteristic timestep are simply neglected until their time falls due. One assigns to the whole problem a time t^n and to each zone a time $T(x)$ and a timestep $\Delta t(x)$. In advancing the problem from t^n to an intended next time t^{n+1} , one asks at each point x , is $T(x) + \Delta t(x)$ less than t^{n+1} ? If so, then the zone at point x is due to be updated, otherwise not. The zone of least timestep will be the zone of latest proper time $T(x)$; for that zone $T(x) = t^{n+1}$. Thus, all times $T(x)$ are earlier than t^{n+1} , or prochronic to the problem time. If in calculating some zone one needs quantities from a neighboring zone it may be necessary to extrapolate them forward in time. This can safely be done, subject to simple precautions, the chief of which is that adjacent zones have timesteps differing by no more than a factor of two (this restriction will be motivated in detail at Eqn. (3.6)). It is this precaution which is responsible for the constant slope of $\Delta t(x)$ in Figs. (2.2) to (2.4) adjacent to the zone of least timestep. The strategy of the present work may be illustrated in Fig. (1.5) Four successive stages in the computation are presented as surfaces T^1 to T^4 . On the surface T^n are indicated points P and Q of long and short timesteps, respectively. It is possible, but in practise quite unlikely, that point P could originate a disturbance propagating into the past of point Q. The reason is that points which are potential sources of trouble tend to be the points of briefest timestep, such as point Q, and other points are

safely in the past of these crisis zones. In Fig. (1.6) is illustrated the relative shape of the curves $T(x)$ and $\Delta t(x)$ in the present work. Note that the maximum proper time occurs in the zone of minimum timestep. This is sufficient to keep the problem well posed.

It is fair to ask what precisely is new, what has been done before, and what is drawn from the common practise of the field. R. A. Grandey first attempted what is known as *variable timesteps*, with mixed success, and no investigation of that method's stability, convergence or well posedness. For reasons of well posedness a different approach is taken here, with different methods of approximation (those reasons were just indicated; the details of implementation are illustrated in Chapter II and generalised in Chapter III) and a different sequence of logical control (for reasons of computational economy, discussed in Chapter VII). The methods of stability argument presented below are well enough known (though not widely used) but new in their application to independent timesteps.

In what follows, the method of independent timesteps will be illustrated in chapter II by a simple example, one-dimensional von Neumann hydrodynamics. In chapter III will be presented rules specifying a general approach to implementing independent timesteps in any difference scheme, together with comments on specific instances of particular difference schemes. Chapters IV and V will detail stability analyses of synchronous (conventional) parabolic and hyperbolic difference equations. Chapter VI will present these arguments modified by the presence of asynchronous (independent timesteps) calculations, together with an error analysis of difference equations with independent timesteps. Chapter VII will present the experience of comparative

Fig. (1.5) Prochronic Cauchy Surfaces

Fig. (1.6) Timesteps and Prochronic Cauchy Surfaces

timing trials, in which independent timesteps are seen to afford a ready gain in speed by a factor by three to ten.

CHAPTER 11

AN ILLUSTRATIVE EXAMPLE OF INDEPENDENT TIMESTEPS

General Considerations

It is typical in a one-dimensional program doing Lagrangian hydrodynamics with the method of von Neumann¹ & Richtmyer to use roughly 100 to 200 spatial zones and take from 100 to 10,000 timesteps. This is adequate to describe, say, a dozen material regions and several shock transits. With half a dozen numbers describing each zone, for a problem of 100 zones run for 1000 cycles, there will be generated 6×10^5 numbers -- these form the "answer" to the Cauchy problem.

Fig. (2.1) is a graphic summary of the kinematic portion of such an "answer" (in the Lagrangian formulation) -- it plots the zonal coordinate vs. time for selected zones. It may be seen that various regions expand and are compressed in their turn as the problem evolves. Taking the number of inflection points as a very rough index of the degree of a polynomial required to fit these curves, it appears that a dozen sixth or seventh degree curves are involved. Twelve seventh

¹ von neumann & Richtmyer, (1950).

R vs. t Problem History Output of a
Hydrodynamics Program

Fig. (2.1) A Problem History

degree polynomials can be defined in $12 \times 8 = 96$ numbers, whereas code output is 100,000 position coordinates alone, not to mention pressures, energies, etc. This is a factor of 1,000 more "information" than one naively suspected would be required. One thousand numbers might provide 100 curves -- a history for each zone.

Since the code takes so many more timesteps than one thought necessary, one may ask how the timesteps were set. A finite difference program in hydrodynamics is limited in its timestep by a stability condition, the Courant condition, and by some "reasonability" condition -- that no zone volume change by more than 10% or 20% in a single timestep. This second condition sets what may be called a physical timestep; it ensures the accuracy of the calculation. Each zone has its own individual Courant timestep and its own physical timestep; the whole problem takes the least of all these timesteps. In other words, the zone with the smallest timestep of either kind sets the timestep for the whole problem.

Conversations with L. D. Howard suggested one way to speed up a calculation, namely, to let each zone calculate at its own timestep. It is possible to implement such a scheme, and the initial results were encouraging in that the method worked at all, and discouraging in that the experimental code -- the "hare" -- computed only a little (0-50%) faster than the standard von Neumann algorithm -- the "tortoise". Subsequent work was much more encouraging, as will be detailed in chapter VII. As the code was rewritten to do more physics, the logic required for independent timesteps occupied proportionately far less of its time, and was able to effect the savings of a significantly greater effort.

The Method of Individual Timesteps

DENEB, a shock hydrodynamics code in which each zone steps forward in time at its own natural rate, was created to study the individual timesteps scheme. Fig. (2.2) plots the Courant timesteps and the physical timesteps for a sample problem. Here one can see the disparity in timestep from the briefest to the longest. This test problem consists of two regions, zones 2 through 42 and 43 through 82, of different densities. The position at zone 2 is fixed, and a shock is moving from zone 82 towards zone 2. At zone 42, one can see the jump in Courant time due to the density discontinuity; at zone 75 is the reflected shock, and the transmitted shock is at zone 10. The zone presently in the shock (zone 10) is being compressed rapidly, and it will set the timestep for the problem, a factor of ten smaller than the natural timesteps for most of the other zones.

In fact, however, since (in DENEB) zone 10 holds down the timesteps only of its neighbors, most of the problem does proceed at its own rate. The difference equations are set up to compute the zone with the currently smallest timestep every cycle and (most of the time) skip zones of longer timesteps. The problem proceeds for 5,000 cycles as it normally would, but where one would have expected 400,000 zone-cycles of computation, only 33,000 have been done, so that on the average each zone is computed less often than once every 10 cycles. There is no noticeable difference in accuracy relative to the calculation done without individual timesteps, as is seen in the last section of this chapter.

Fig. (2.2) Courant and Physical Timesteps

There is no great strain on memory requirements by the difference scheme in DENEb. Hydrodynamics commonly stores at least nine numbers per zone (e.g., mass, position, velocity, specific volume, artificial viscosity, material pressure, effective pressure, internal energy, and gas law γ), and for this scheme four more numbers per zone are needed: the time when that zone was last updated, that zone's individual timestep, a sentinel which says "compute me next cycle" or "skip me", and the rate of change of that zone's pressure. The *computation sentinel* is the code's note to itself indicating whether that zone is due to be updated or not. The timestep stored for each zone is the maximum permissible; the actual step taken may be briefer. The time rate of change of pressure may be needed by neighboring zones in order to estimate that zone's pressure at times other than when it was last updated.

Two programs were written -- an asynchronous code with individual timesteps for each zone, and a synchronous code with a common timestep for all zones; both programs used the same difference equations taken from Richtmyer and Morton². DENEb, with individual timesteps for each zone, generally requires less computing time than does RIGEL, which employs a single timestep. DENEb indeed spent much less time doing calculations of physics, as its computation ratio ($400,000/33,000 = 12.1$) indicates. With physics as simple as this (no non-hydrodynamic energy transport, perfect gas equation of state), the physics time saved by using individual timesteps was comparable to the time used in doing the extra logical work required to manage the

² Richtmyer & Morton (1967) See for example, p. 295.

Fig. (2.3) Timesteps for Various Zones

Fig. (2.4) Timesteps for Various Zones

Fig. (2.5) Timesteps for Various Zones

Fig. (2.6) Timesteps for Various Zones

computation. Since these initial trials, this logical apparatus has been streamlined (it was very clumsy in DENEb), and with only a little more physics added, the timing comparisons between the two methods can be quite striking.

As a graphic indication of what occurs in DENEb and RIGEL, Figs. (2.3-2.6) plot Δt_j vs. j for various times in the test problem of Fig. (2.7), showing the shock progressing across the problem. (This test problem is described in detail below.) In Fig. (2.3), the shock is at zone 56, and the logarithmically regular interval in timestep between neighboring zones may be noted on both sides of the shock. (Neighboring zones are allowed to have timesteps different by no more than a factor of two, resulting in the timestep spacing around zone 56, as in Fig. (2.3). This restriction lowers the timesteps ahead of the shock, insuring that zones 50 through 55 are not "surprised" by the shock, an event which could leave those zones with negative volumes.) The zones ahead of and behind the shock have timesteps set by the Courant condition, but the region behind the shock is much hotter and denser and develops a timestep accordingly briefer. In the shock itself, the limiting consideration is the volume timestep. In Fig. (2.4), the shock has crossed the region boundary, and the timestep discontinuities mark the boundary and the two shocks now present in the problem. Fig. (2.5) is at the same time as Fig. (2.2), but plots the maximum permissible timestep for each zone (as do Figs. (2.3-2.4)), not the Courant or physical timesteps (as in Fig. (2.2)). The actual maximum Δt_j is sometimes less than either the Courant or the physical timestep, in order not to exceed $\Delta t_{j,f}$ or $\Delta t_{j,-f}$ by more than a factor of two. Fig.

(2.6) is plotted after the shock has reflected from the fixed wall and the entire problem is in more or less uniform expansion.

A method such as this one appears to be well suited to a problem in which a few zones require very frequent advancements in time over very brief intervals, while the vast majority of the zones can proceed forward in time with much more infrequent computations. The usually striking overall savings in computation achieved by this method in one spatial dimension made it seem natural to try it in problems of two spatial dimension: where the ratio of high frequency zones to low frequency zones ought to be much smaller than the one dimensional cases. It also seemed opportune to do more complex physics in one dimensional problems, e.g., to add heat conduction and other kinetic processes. The computation labor for timestep logic did not increase, while such programs did indeed save much more computation time in doing calculations of physics.

One point may be noted, that the independent timesteps code is everywhere at least Courant limited. This limitation requires the program to include in its "answer" calculational results at many more points than seem intuitively necessary to define the solution to the Cauchy problem. Nevertheless, independent timesteps codes with explicit transport run faster than synchronous codes with implicit transport (the fastest codes heretofore available). These results will be detailed in Chapter VII.

The Difference Schemes

By exhibiting the difference schemes in detail, it is possible to show exactly what modifications are necessary to implement independent timesteps in one dimensional hydrodynamics. Both the synchronous von Neumann - Richtmyer method and the modified asynchronous method are very similar in most respects. Nine variables per zone are kept for physics:

m_j	mass
x_j	position of the j th zone interface in the lab system
u_j	$\partial x / \partial t$
V_j	specific volume; $= (x_{j+1/2} - x_j) / m_j$
Q_j	von Neumann artificial viscosity
p_j	pressure from equation of state
P_j	$p_j + Q_j$
E_j	internal energy per unit mass
γ_j	the constant γ in the equation of state.
	$pV = (\gamma - 1)E$

The mass, density, pressure, artificial viscosity, energy and gamma are kept at the center of the zone. Position and velocity are kept for the j^{th} zone at its boundary; $x_{j+1/2} \approx x_j$. Zone 1 is a logically convenient dummy, as is one zone outside of the other boundary. Thus, x_2 is the position of one boundary and x_{jM0} is the position of the other boundary, as in Fig. (2.7).

In addition, the timestep logic requires four variables per zone:

t_j	the time when the j^{th} zone was last updated
Δt_j	the longest timestep permitted to the j^{th} zone

The Test Problem of Figures 2-6

Fig. (2.7) The Test Problem of Figs. (2.2-2.6)

$x_1 = u_1 = 0$ always

x_{jmo}, u_{jmo} are free

P_{jmo} is set once for all time, $= 10^6 \text{ erg/cm}^3$; $P_j, j = 2, jmo-1 = 10 \text{ erg/cm}^3$ initially.

s_j a sentinel to update or not on the next cycle
 $(P_t)_j$ $\partial P / \partial t$, the time rate of change of
 the j^{th} total pressure P_j .

For simplicity and clarity of exposition, the calculation is in plane geometry. For the case of a common timestep for the whole problem, the difference equations are³:

$$\begin{aligned}
 u_j^{n+1} &= u_j^n + 2\Delta t^n (P_{j-1}^n - P_j^n) / (m_{j-1} + m_j) \\
 x_j^{n+1} &= x_j^n + \Delta t^n u_j^{n+1} \\
 v_j^{n+1} &= (x_{j+1}^{n+1} - x_j^{n+1}) / m_j \\
 \text{if } u_{j+1}^{n+1} - u_j^{n+1} < 0, \text{ then} \\
 Q_j^{n+1} &= 2(u_{j+1}^{n+1} - u_j^{n+1})^2 / v_j^{n+1} \\
 \text{else,} & \\
 Q_j^{n+1} &= 0. \\
 P_j &= P_j + Q_j^{n+1} \\
 E_j^{n+1} &= E_j^n - P_j (v_j^{n+1} - v_j^n) \\
 p_j^{n+1} &= (\gamma_j - 1) E_j^{n+1} / v_j^{n+1} \\
 p_j^{n+1} &= Q_j^{n+1} + p_j^{n+1}
 \end{aligned} \tag{2.1}$$

The equations are presented in the order in which they are solved, with the right hand side being evaluated and becoming the new value of the quantity on the left hand side. For convenience, the pressure (P) includes both the material pressure and artificial viscosity, and the latter is updated before the energy equation computation, while the material pressure (p) is updated afterwards.

³ Richtmyer & Morton (1967)

The units employed are cgs metric. The equation of state is that of a perfect gas,

$$p = (\gamma - 1)E/V,$$

though each zone may have its own γ , set once for all time.

The timestep is limited by two considerations, stability and accuracy, which, as Fig. (2.2) illustrates, are generally not too radically different. If c_j is the local sound speed, we assign to each zone two timesteps:

$$\Delta t_{c_j} = (x_{j+1} - x_j) / 2c_j \quad (2.2)$$

or one half the Courant time, and

$$\Delta t_{v_j} = 0.1 \left| \frac{x_{j+1} - x_j}{u_{j+1} - u_j} \right| \quad (2.3)$$

the time for a ten percent volume change. The timestep for the whole problem, Δt^n , is the least of the $[\Delta t_{c_j}^n, \Delta t_{v_j}^n]$. In RIGEL every zone is calculated at every timestep. In DENEb, a zone may be passed over for a thousand cycles if its timesteps Δt_{c_j} and Δt_{v_j} are both a thousand times longer than Δt^n , the smallest timestep of the problem.

One must be slightly more careful than merely to set Δt_j to the lesser of Δt_{c_j} and Δt_{v_j} . If Δt_j and Δt_{j+1} are grossly different, one zone may be computed many times while its neighbor does nothing. When its neighbor finally "wakes up", it is likely to be too late. It has been observed in this situation that the neighbor zone may "wake up" to

find itself with a negative volume. To eliminate such possibilities, we insist that adjacent timesteps differ by at most a factor of two. The number two may seem arbitrary; it is. But it sufficed to allow the computation to proceed without untoward event; a value of four for this ratio proved too large. As a second requirement on the timestep, we let no Δt_j increase more than twofold from one timestep to the next. Each timestep Δt_j is thus constrained by five conditions:

$$\begin{aligned}
 \Delta t_j^n &\leq \Delta t_{c,j} \\
 \Delta t_j^n &\leq \Delta t_{v,j} \\
 \Delta t_j^n &\leq 2\Delta t_{j+1}^{n-1} \\
 \Delta t_j^n &\leq 2\Delta t_{j-1}^{n-1} \\
 \Delta t_j^n &\leq 2\Delta t_j^{n-1}
 \end{aligned}
 \tag{2.4}$$

The first and second conditions of Eqn. (2.4) were enforced only as often as zone j is computed; The remaining conditions were imposed on every zone every cycle.

Consider now a point in the computation at the end of the n^{th} cycle, as the code is about to set the timesteps Δt_j^{n+1} and choose a next time t^{n+1} and choose zones to be advanced to that time. DENEb already has the timesteps Δt_j for zones which were not calculated at time t^n , and it has $\Delta t_{v,j}$ and $\Delta t_{c,j}$ for zones which were computed at time t^n . For these last zones, set $\Delta t_j = \min(\Delta t_{v,j}, \Delta t_{c,j})$, insuring the first and second conditions of Eqn. (2.4). Now the third, fourth, and fifth conditions of Eqn. (2.4) may be imposed at all zones. This requires passing through the mesh once in each direction. Having done this much, it is time to choose a next time, t^{n+1} . For each zone there is a time t_j when that zone was last calculated; t_j can be as recent as t^n . The

least (which is to say, the earliest) of the times $t_j + \Delta t_j$, will be the new time t^{n+1} , and the problem timestep (as distinguished from any one zonal timestep) may be found from $\Delta t = t^{n+1} - t^n$. Clearly only one zone absolutely must be calculated as early as time t^{n+1} . But if several zones fall due at nearly the same time, it would be unreasonable to update only one of them, because then the following timestep would have to be much smaller than the present one. The code therefore calculates at cycle $n+1$ all the zones for which

$$t_j + \Delta t_j \leq t^n + 2\Delta t^n. \quad (2.5)$$

Fig. (2.8) illustrates this situation.

Frequently, the neighboring zones $j-1, j, j+1$ were all last calculated at the same time, t^m , for some $m < n$, and they all fall due at time t^{n+1} . In this case the straightforward difference equations, Eqns. (2.1), may be used, but with the timestep here given by $\Delta t = t^{n+1} - t^m$.

Less often, zones j and $j-1$, say, were last calculated at different times, $t_j \neq t_{j-1}$, and the situation of Fig. (2.9) occurs. Here the numbers x_{j-1}, p_{j-1} are all referenced to time t_{j-1} ; the quantities x_j, p_j are at time t_j . The code must step the j^{th} zone interface, (the quantities x_j, u_j) from time t_j to time t^{n+1} . But in order to do this, the first of Eqns. (2.1) requires a pressure gradient constructed from two pressures both referenced to time t_j . This is not immediately possible, since the pressure p_{j-1} is at time t_{j-1} . It is necessary to extrapolate the pressure in zone $j-1$ forward to time t_j , before the difference Eqns. (2.1) may be solved at zone j to move x_j and u_j from time t_j to time t^{n+1} .

Fig. (2.8) Setting Computational Sentinels

Figs. (2.9-2.10) illustrate the typical situation in the computation. The arrays x_j and u_j are zone-edged quantities and are not isochronous. For instance, in Fig. (2.10), the numbers x_2 and x_3 are at different times, as are the pressures P_1 and P_2 . The zone centered quantities, including the zone times t_j , are typified by the pressures in Fig. (2.10).

In this situation, positions x_7 , x_8 and pressures P_6 , P_7 , P_8 can be advanced to time t^{n+1} in the normal way. Zone 2, however, is more complex. Nonetheless, only a pressure P_2^n is required at time t_j to advance x_2 and u_2 to time t^{n+1} . The position and velocity x_3 and u_3 may be advanced directly from time t^{n-1} .

The new x_2^{n+1} , x_3^{n+1} and the mass m_2 yield a new specific volume V_2^{n+1} , and the change $V_2^{n+1} - V_2^{n-2}$, together with the pressure P_2^{n+1} , yield a new energy E_2^{n+1} . The new artificial viscosity, Q_2^{n+1} , is obtained from u_2^{n+1} and u_3^{n+1} . Thus, only the total pressure (which includes the artificial viscosity) need be extrapolated at time $t_j = t^{n-3}$. This extrapolation can be accomplished as follows: if one keeps at each zone center a quantity

$$P_t = \frac{\partial}{\partial t} (p_j + Q_j) = \frac{p_j^n + Q_j^n - p_j^k - Q_j^k}{t_j^n - t_j^k} \quad (2.6)$$

where t^n, t^k are the last two times zone j was updated, then the extrapolated total pressure P_2^* may be obtained in the example of Fig. (2.10) from the equation

$$P_2^* = P_2 + P_t (t_j - t_2) \quad (2.7)$$

Fig. (2.9) Adjacent Zones with Different Timesteps

Fig. (2.10) A Mesh with Independent Timesteps

Figure 10

Zone 1 through 9 are to be updated to time t^{n+1} . Figure 10 shows how the arrays p_j , x_j and t_j are arranged in the problem history and in the computer memory just before the update to t^{n+1} .

In this manner the calculation may proceed and obtain results differing not noticeably from those of a synchronous von Neumann - Richtmyer calculation, as the remarks of the next section will show.

Test Problems

Several early test problems were run, comparing DENEB (with individual timesteps for each zone), with RIGEL (taking a common timestep for the whole problem). In the case of a rarefaction of a perfect gas into a vacuum, the timesteps do not differ enough from one zone to the next for DENEB ever to gain any advantage, and DENEB runs more slowly. Both DENEB and RIGEL obtain the same results at all times to within about one percent.

Shock compression of a perfect gas engenders widely different timesteps, as noted earlier in this chapter, and here the difference in computation time is often considerable. Figs. (2.2) through (2.6) illustrate the zonal timesteps at various stages in a typical problem history. Fig. (2.11) diagrams the shock test problem. Two regions at an initial pressure of 10 ergs/cm^3 comprise the initial conditions. Region I has a density of 4 g/cm^3 , region II has a density of 1 g/cm^3 . Regions I and II have gas law gammas of $5/3$ and $7/5$, respectively. Each region is of mass 50 g and comprises 40 zones. One outer boundary, that of region I, is fixed in position for all time. The other is free, but has a pressure of 10^6 ergs/cm^3 placed on it, driving a shock into the problem.

A Test Problem

Fig. (2.11) A Test Problem

The shock is partially reflected and partially transmitted at the material interface, the reflected shock being amplified by a factor of 2.1. The problem has an analytic solution⁴. The analytic solution, DENEb, and RIGEL all agree to within about one percent. Tables (2.1-2.2) present the comparative results for two problems. One is the problem just described, the other is identical except that the boundary pressure is 10^4 ergs/cm³ instead of 10^6 ergs/cm³. The row headings are:

ξ	initial shock strength in region 2
ξ_1	transmitted shock strength in region 1
ξ_2	reflected shock strength in region 2
η	initial compression in region 2
η_1	transmitted compression
η_2	reflected compression
u	initial shock speed
u_1	transmitted shock speed.

The quantities from the codes DENEb and RIGEL have an error associated with them, since there is some variation in the pressure and density behind a shock; where this error is known, it is quoted with the results from these codes. The analytic results are usually presented to greater precision than that of the computational results of DENEb and RIGEL.

⁴ R. LeLevier (1954) See pp. 25-27; LeLevier treats the case of strong shocks in a problem with zero initial pressure. Actually it is possible to treat shocks of any strength in a problem with finite initial pressure. For given initial conditions and incident shock strength an implicit equation in the reflected shock strength may be solved numerically. From the reflected shock strength all other quantities may be obtained explicitly.

Table (2.1)
Shock strength = 10^5

ξ	DENEB	Analytic	RIGEL
ξ_2	$2.14 \pm .03$	2.139	$2.14 \pm .02$
ξ_1	$2.14 \pm .03 \times 10^5$	2.139×10^5	$2.13 \pm .04 \times 10^5$
η	$6.0 \pm .05$	5.999	$6. \pm .1$
η_2	$1.69 \pm .01$	1.6997	1.71
η_1	4.02	4.00	4.02
u	1125.	1095.	1110.
u_1	810.	844.	850.

Table (2.2)
Shock Strength = 10^3

ξ	Analytic	DENEB
ξ_2	2.1345	$2.14 \pm .03$
ξ_1	2.1345×10^3	$2.14 \pm .04 \times 10^3$
η	5.96	$6.0 \pm .1$
η_2	1.697	1.705
η_1	4.	4.04
u	109.5	110.
u_1	84.3	84.

CHAPTER III

THE GENERAL METHOD OF INDEPENDENT TIMESTEPS

On Notation

In a problem with a common timestep, notation regarding time and timestep is relatively simple; t and Δt will suffice -- more specifically, $\Delta t^n = t^{n+1} - t^n$. For the present work each zone has its own timestep Δt_j ; the actual time stepped by that zone may be briefer than Δt_j . Let t^n , t^{n+1} , etc., written without a subscript j refer to whole problem times. When the computation has reached $t = t^n$ at some cycle number n , some zone has been advanced to time t^n , and no zone has yet been advanced beyond time t^n . Contemplating the advance of some zones to time t^{n+1} we find that at this cycle (number n) these zones are referred to times t_j , not all equal to t^n , but to various times t_j^n with $0 < m \leq n$. Nevertheless, it is convenient to label these several times t_j^n . The set of times t_j^n specifies the Cauchy surface at computation cycle n . All this may be illustrated in Fig. (3.1). It may be noted that $t_j^n \neq t_{j-1}^n$. Although the set of times t_j^n define the Cauchy surface at cycle n , the set of times t_j^{n-1} do not define the prior Cauchy surface

at cycle $n-1$. The time t_j^{n-1} is meant to refer simply to that time t_j at which zone j was last updated prior to cycle $n+1$, regardless of what cycle that update occurred at. The time t_j^{n-1} may have fallen one or several or hundreds of cycles before cycle n . In the same way time t_j^{n-2} is defined simply as two updates before time t_j^n . In somewhat different words, the times t_j^n are labeled at computation cycle n , and the times t_j^{n-1} , t_j^{n-2} , etc., are labeled in sequence backwards by updates at zone $j-1$, not by cycles $n-1$, $n-2$, etc.

With this in mind, the timesteps may be labeled. Δt_j^n is the time $t_j^{n+1} - t_j^n$, and so is different for different zones. In some places Δt_j^n will refer to the step actually taken; in others, notably in parts of the following section, to the maximum time allowed for that step. Where Δt_j^n (or $\Delta t_j^{n-1} = t_j^n - t_j^{n-1}$) appears in a difference equation, it denotes the step actually taken. In considerations of what the timestep should actually be, it denotes merely the bound at zone j on that timestep.

The Method

Having provided in Chapter II an example of independent timesteps in the context of von Neumann hydrodynamics, it is time to indicate in a somewhat more general way how to implement independent timesteps in any difference scheme. For, if the method is applicable to just one or two difference schemes, it is only of theoretical curiosity value no matter how great its practical significance for its few applications. Its theoretical significance lies in its motivation (to instruct the machine how to approach its work along the lines of the human calculator, i.e.,

Fig. (3.1) Nomenclature of Times and Timesteps

to allocate computational effort where it is needed instead of indiscriminately) and in its broad applicability.

One is interested in predicting the time evolution of some physical quantity which we may designate as u . This is usually a vector quantity -- not just temperature, but an ensemble of quantities: temperature, pressure, velocity, density, composition, energy, etc. The finite difference equation can be conceived in the form

$$u_j^{n+1} = F(u_j(t^n), u_{j+1}(t^n), u_{j-1}(t^n), t^{n+1}, t^n \dots etc.) \quad (3.1)$$

Here we have indicated the neighbors only in one dimension, u_{j+1} and u_{j-1} . But for our purposes, two and three dimensions are not qualitatively different. The function F may be any procedure for generating u_j^{n+1} from the given arguments, but note that it is an explicit operation: u_j^{n+1} does not depend on u_{j+1}^{n+1} or u_{j-1}^{n+1} , the values of u in the neighboring zones at the end of the timestep.

The arguments are all contemporaneous: all are evaluated at time t^n . To implement independent timesteps, the quantities u_j may have been evaluated at various times t_j^n . But the function F still requires contemporaneous arguments, so we can rewrite Eqn. (3.1) for independent timesteps as follows:

$$u_j^{n+1} = F(u_j(t_j^n), u_{j+1}(t_j^n), u_{j-1}(t_j^n), t^{n+1}, t_j^n \dots etc.) \quad (3.2)$$

Note that now the neighboring quantities u_{j+1} and u_{j-1} must be treated differently from u_j . They may not have been evaluated at time t_j^n when zone j was last updated, but for the present update of zone j ,

the neighboring quantities are required at time t_j^n : $u_{j+1}(t_j^n)$, $u_{j-1}(t_j^n)$. These quantities are generated from the old values at the zones $j+1$ and $j-1$ and their time derivatives:

$$u_{j+1}(t_j^n) = u_{j+1}(t_{j+1}^n) + (u_t)_{j+1}^n(t_j^n - t_{j+1}^n) \quad (3.3)$$

The time derivatives u_t , may be approximated in whatever manner is convenient, and, as noted above, memory space must be reserved for these quantities.

Having indicated the form of the finite differencing, it remains to comment on the selection of timesteps Δt_j and the decision when to update a zone in order that the calculation may proceed stably and expeditiously. As in any complicated physical situation, there are various processes occurring at different rates, and characteristic times associated with each. There are often (usually) stability condition(s) on the timestep arising from the difference equations. So, just as in a conventional situation, one is faced with the choice of the briefest of several candidate timesteps:

$$\Delta t = \min(\Delta t_{1j}, \Delta t_{2j}, \Delta t_{3j}, \dots) \quad (3.4)$$

The quantities Δt_{1j} , Δt_{2j} , etc., arise from different processes, accuracy considerations, stability conditions, exactly as one would determine them without using independent timesteps. The timestep Δt_j need be evaluated only as often as its arguments change, and this means in practise only as often as zone j is updated. It happens that for explicit difference equations, stability is usually not affected by the presence of independent timesteps. (To my knowledge, there is no

contrary example, but as much cannot be said for independent timesteps in implicit equations, a matter to be mentioned at greater length below.) Stability will be proven quite rigorously in Chapter VI for the common diffusion and hydrodynamic difference equations with independent timesteps. It is a matter of some significance that independent timesteps should not affect the stability conditions for the common explicit difference equations so far encountered. However, there is not any readily evident simple proof that this is true in general; so each difference equation, or class of equations, must be considered on its own merits.

There is an additional condition on timesteps which are independent. It arises not so much to assure stability as to insure that the problem remain well posed. Successive timesteps in one zone are constrained to increase if at all by no more than a factor of two, and neighboring timesteps to differ by no more than a factor of two. The number "2" was chosen arbitrarily at first, as a guess at the limits beyond which one might not reasonably stray. These conditions may occasionally be relaxed, but for the moment they may be stated thus:

$$\Delta t = \min(\Delta t_j^n, 2\Delta t_{j-1}^{n-1}) \quad (3.5)$$

$$\Delta t = \min(\Delta t_j^n, 2\Delta t_{j+1}^n, 2\Delta t_{j-1}^n) \quad (3.6)$$

The reason for the restriction of Eqn. (3.5) on successive timesteps is that extrapolated values of u_j will be required, and it is risky to extrapolate for a time much greater than the interval over which $(u_t)_j^n$ was itself approximated. Relaxing the restraint of Eqn.

(3.5) in fact led to trouble of precisely the nature indicated. This restriction will be used as a premise in the stability arguments in Chapter VI, so it may not be relaxed casually.

The motivation for Eqn. (3.6), the restriction on neighboring timesteps, is a little different and less quantitative. If, for instance, some zone j is updated many times while zone $j+1$ is updated not at all, then the two zones may lose contact with each other. A natural apprehension suggests itself that the original long estimate for Δt_{j+1} was not realistic; subsequent events in zone j have rendered it quite dated and even quite dangerous. The imagined situation may be diagrammed as in Fig. (3.2). Both zones, suppose, were computed at time t^0 and both timesteps were set then also. Zone $j+1$ will not fall due until t^6 , but zone j will need to be updated at time t^2 . As events transpire, let us say zone j requires updating five times before zone $j+1$ receives any attention. One cannot really believe that all that activity in zone j can leave zone $j+1$ unaffected. So it is reasonable to require that zone $j+1$ fall due at least at times t^4 and t^6 , or, equivalently, to put the restriction as in Eqn. (3.6). Once again, this restriction grew out of experience; for relaxing Eqn. (3.6) completely soon leads to grief. The value of "2" for the ratio of adjacent timesteps is not critical, but a ratio of approximately this value must be used. The experience leading to Eqn. (3.6) and its safe relaxation will be discussed at the end of this chapter. In fact however, the restriction as stated here (Eqn. (3.6)) is economically the most useful and (for programming purposes) the simplest form.

Fig. (3.2) Disparate Neighboring Timesleps

All that now remains to complete the general specification of calculations with independent timesteps is the rule for selecting zones due for updating. The remarks in Chapter 11 are quite general and not at all restricted to hydrodynamics. As was illustrated in Fig. (2.8), we require the updating of those zones for which

$$t_j^n + \Delta t_j^n > t^{n+1} + 2\Delta t^n \quad (3.7)$$

The reasons for the stringent condition of Eqn. (3.7) instead of say, $t_j^n + \Delta t_j^n > t^{n+1}$, were discussed in Chapter 11 at Eqn. (2.5) and illustrated in Fig. (2.8)

Examples in One Dimension

The principal example in one dimension, and the only one to be examined in great detail, is that of Chapter 11, one dimensional von Neumann hydrodynamics. The experience here summarized is included for several reasons. It is pertinent to indicate the range over which independent timesteps have been tested, and also to note places where special considerations were (or were not) necessary.

The bulk of the experience to date has been in one dimensional calculations, coupled hydrodynamics and one or several diffusion processes. The method of duFort and Frankel was examined and deserves some comment simply because the standard manuals all note it in passing with only only the briefest indication of its special character. A considerable effort was expended attempting to implement independent

timesteps in an implicit difference scheme for the diffusion equation, and not without some success; but the results were such as to render it impractical except as a curiosity. And lastly is mentioned two dimensional explicit heat diffusion, explored both to prove that, as expected, nothing essentially new is encountered here, and to get some idea of the computational economics of independent timesteps in two dimensions.

To deal first with one dimensional problems, the hydrodynamics of Chapter II is simpler than common practical problems in several respects. It assumes plane geometry, and calculations are often carried out in cylindrical (and, for astrophysical problems in spherical) geometry. Usually all three geometries are coded together, and setting an index to a value of 1, 2, or 3 is all that is needed to select the desired geometry. The implications for independent timesteps are marginal. The first equation of Eqn:(2.1) is changed, as is the third: the force equation becomes

$$\frac{u_j^{n+1} - u_j^n}{\Delta t^n} = 2 \frac{p_{j-1}^n - p_j^n}{m_j + m_{j-1}} (x_j)^{i-1} \quad (3.8)$$

and the specific volume

$$v_j^{n+1} = \frac{(x_{j+1}^{n+1})^i - (x_j^{n+1})^i}{(m_j)^i} \quad (3.9)$$

where $i = 1, 2$, or 3 , depending on the geometry. Neither of these changes affects the use of independent timesteps. The situation here is typical of difference equations for diffusion as well, which can be

constructed straightforwardly in any geometry in the presence of independent timesteps.

When hydrodynamics is coupled to diffusion, the difference equations may be written as a modification of Eqn. (2.1), here in plane geometry. Where in Eqn. (2.1) pressure was considered a function of energy and specific volume, here temperature also will be treated this way. Energy is differenced by analogy to the energy equation of Eqn. (2.1) and temperature is looked up in equation of state tables. One could easily do it the other way, differencing the temperature and treating the energy by means of an equation of state as a function of temperature and specific volume. A new quantity, the energy flux, is defined by an equation of the form of Eqn. (3.17); its gradient appears in the energy equation eqn. (3.20). When a zone falls due for computations, some of the equations (3.10-3.21) are done at zone j , and some both at zones j and $j+1$. The zone centered quantities, volume, pressure, energy, temperature, are updated only at zone j . The zone edged quantities, position, velocity, flux, are updated at zone edges j and $j+1$: at both edges of zone j . So it should be noted that a zone edged quantity (e.g. x_j^n) is not necessarily contemporaneous with its companion zone centered quantities (e.g., E_j^n). The zone edged quantities are contemporaneous with the more recently updated of the zone centered quantities at zones j and $j-1$. One may list the difference equations:

$$\Delta t_j^n = t^{n+1/2} - t_j^n \quad (3.10)$$

$$u_j^{n+1} = u_j^n + 2\Delta t_j^n \left(\frac{P_{j-1}(t_j^n) - P_j^n}{m_j + m_{j-1}} \right) \quad (3.11)$$

$$x_j^{n+1} = x_j^n + u_j^{n+1} \Delta t_j^n \quad (3.12)$$

$$V_j^{n+1} = \frac{x_{j+1}^{n+1} - x_j^{n+1}}{m_j} \quad (3.13)$$

$$\text{if } u_{j+1}^{n+1} - u_j^{n+1} < 0, \text{ then} \quad (3.14)$$

$$Q_j^{n+1} = 2(u_{j+1}^{n+1} - u_j^{n+1})^2 / V_j^{n+1}$$

$$\text{else,} \quad (3.15)$$

$$Q_j^{n+1} = 0.$$

$$P_j = p_j + Q_j^{n+1} \quad (3.16)$$

$$E_j^{n+1} = E_j^n - P_j(V_j^{n+1} - V_j^n) + \Delta t_j^n C_j^n \quad (3.17)$$

$$p_j^{n+1} = p(V_j^{n+1}, E_j^{n+1}) \quad (3.18)$$

$$T_j^{n+1} = T(V_j^{n+1}, E_j^{n+1}) \quad (3.19)$$

$$\Phi_j^{n+1} = \Phi \left((T_j^{n+1} - T_{j-1}^{n+1}) / (x_{j+1}^{n+1} - x_{j-1}^{n+1}) \right) \quad (3.20)$$

$$C_j^{n+1} = (\Phi_{j+1}^{n+1} - \Phi_j^{n+1}) / m_j \quad (3.21)$$

So, when zone j falls due, Eqns. (3.10,13-19,21) are solved at the center of zone j , and Eqns. (3.11,12,20) are solved at zone edges j and $j-1$. In Eqn. (3.21) the difference of energy fluxes across zone j is saved as the quantity C_j^{n+1} . Eqns. (3.11,20) require zone centered quantities from neighboring zones, pressures P_{j-1} , P_{j+1} and temperatures T_{j-1} and T_{j+1} . These are required at time t_j^n although they may have been computed at some other time. Therefore, they are extrapolated to

that time t_j^n , and for this purpose one must save both of their time derivatives. This fairly conventional set of coupled equations can be differenced quite straightforwardly with independent timesteps.

It is sometimes convenient to require one's difference equations explicitly to observe some conservation law, for example, conservation of energy. It is fair to note that this, too, can be done in the presence of independent timesteps. The approach is to construct the difference equations in a way that takes exactly as much energy out of one zone as is passed to the neighboring zone. If all zones are updated synchronously in lockstep, this is of course very easy. If they are updated asynchronously, it is not too much more intricate. For, suppose that zones j and $j+1$ are contemporaneous at some time and that a little later zone j falls due before zone $j+1$, and is updated accordingly. Then there is some energy transferred into zone j but not yet taken out of zone $j+1$. This floating energy balance may be simply saved zone by zone, together with a sentinel which indicates at each zone edge for which of the two zones there bounded the float is being saved.

The work of duFort and Frankel¹ deserves some discussion where economies of computation are sought. They constructed and published in 1953 (early in the modern history of finite differences) a difference approximation for the diffusion equation which is quite remarkable. It is explicit and unconditionally stable and can even be generalized to two or three dimensions without displaying any essentially new behavior. It is mentioned in all the standard difference manuals² for its peculiar stability and convergence properties. This kind of equation may be

¹ duFort & Frankel (1953).

² Richtmyer & Morton (1967), p. 176; or Yanenko (1971), p. 11.

quoted in several forms having slightly different accuracy, but essentially the same character:

$$\frac{u_j^{n+1} - u_j^n}{2\Delta t} = A(u_{j+1}^n - u_j^{n+1} - u_j^{n-1} + u_{j-1}^n) \quad (3.22)$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = A(u_{j+1}^n - u_j^{n+1} - u_j^{n-1} + u_{j-1}^n) \quad (3.23)$$

For present purposes it is enough to observe that neither presents anything new to independent timesteps. The temperatures u_{j+1} and u_{j-1} must be supplied at time t_j^n by the usual independent timesteps formula, Eqn. (3.3); then the calculation may proceed normally.

Diffusion in Two Dimensions

Diffusion in two dimensions is worth some attention both because it is essentially similar to the one dimensional case and because it pays greatly to code carefully Eqn. (3.6), which restricts neighboring zones to have timesteps differing by no more than a factor of two. This aspect of the coding will serve to illustrate the sort of considerations one encounters in managing the logic of asynchronous calculations.

The equation to be solved is:

$$\frac{\partial u}{\partial t} = -\sigma \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial y^2} \quad (3.24)$$

and its common explicit backward differenced finite representation is

$$\frac{u_{k,j}^{n+1} - u_{k,j}^n}{\Delta t} = \left\{ G_{k,j} \left(u_{k,j+1}^n - u_{k,j}^n \right) + G_{k,j-1} \left(u_{k,j-1}^n - u_{k,j}^n \right) \right. \\ \left. + K_{k,j} \left(u_{k+1,j}^n - u_{k,j}^n \right) + K_{k-1,j} \left(u_{k-1,j}^n - u_{k,j}^n \right) \right\} \quad (3.25)$$

A word of explanation is in order, for the similarity of Eqn. (2.25) to (3.24) may appear strained. The σ in Eqn. (3.24), the heat conductivity, may be a function of temperature. It appears in Eqn. (3.25) as a factor in the coefficients $G_{k,j}$ and $K_{k,j}$, which also include the difference approximations Δx to the denominators of the space derivatives in Eqn. (3.24). The first two terms on the right of Eqn. (3.25) approximate the x derivatives, and the last two terms approximate the y derivatives. Out of those derivatives have been factored the numerators, the temperature differences. All other factors have been collected in the coefficients G and K . It is the temperatures at the neighboring zone centers that may be asynchronous to the temperature $u_{k,j}^n$ in the zone being updated currently. The indexing conventions may be seen in Fig. (3.3). The zone centered quantities are referred to the point Q in this figure; the point quantities to the zone's upper right corner. The conductivities are zone edged quantities and stand between zones as shown in Fig. (3.4).

For reasons of economy, the common method of approximating Eqn. (3.24) is not with Eqn. (3.25) but with an alternating-directions-implicit technique (ADI), and as this is well known³, it need not be described again here. Thus, the explicit

³ Yanenko (1971), chapter 2.

at P: $x_{k,j}$, $y_{k,j}$

at Q: $u_{k,j}$, $t_{k,j}^n$, $m_{k,j}$

Fig. (3.3) Indexing Conventions

$G_{k,j}$ stands between zones k,j and $k,j+1$

$K_{k,j}$ stands between zero k,j and $k+1,j$

Fig. (3.4) Conductivity Coefficients

difference equation with independent timesteps must compete not with conventional explicit but with ADI equations. To indicate what must be done to implement independent timesteps in Eqn. (3.25), the neighboring temperatures must, of course, be brought by extrapolation to a time contemporaneous with $u_{k,j}^n$, and the timestep Δt must be replaced by the quantity $(t^{n+1} - t_{k,j}^n)$. This much corresponds quite closely to Eqns. (3.2-3.3).

Eqns. (3.4-3.7) are the same in any asynchronous calculation, but their coding can yield great dividends if it is done with care. Eqn. (3.7) must be inspected for every zone every cycle, as it selects those zones due for computation on the next cycle. Eqns. (3.4-3.5) need only be solved as often as the zone at k,j is itself updated, not very often on the average. The condition in Eqn. (3.6), which requires neighboring timesteps not to be too disparate, can be handled several ways. One could at every cycle readjust all the timesteps $\Delta t_{k,j}$. Or, one could let matters in zone k,j ride unattended until one of its four neighbors' timesteps is reset, and then enforce condition (3.6) at zone k,j . Now if on some cycle the new minimum timestep appears at zone k',j' , it is necessary to apply Eqn. (3.6) at its four neighbors. And for each of these, only if their timestep is reduced by Eqn. (3.6) does one continue the enforcement of Eqn. (3.6). This specification is recursive if it is extended to cover the whole mesh starting from each zone, but experience shows that it may be terminated after dealing with the adjacent neighbors. The reason for indicating the method of coding Eqn. (3.6) is that if done this way, it is encountered only a little more often than zones are updated, whereas naively coded it can be executed for every

every zone at every cycle, and this can have a significant effect on running times.

The conventional explicit, explicit with independent timesteps, and ADI methods may be compared (here for their accuracy; in Chapter VII for their running times) in their solution of similar problems. A useful test problem for any scheme is an initial temperature distribution of the form $u = \cos(x)\cos(y)$, with the temperature held at $u=0$ on the (square) boundaries. It has a known solution, but suffers from the disadvantage that the characteristic timesteps are identical always and everywhere, so the independent timesteps coding solves the problem in exactly the same way as the conventional explicit version, without, in fact, ever doing any asynchronous calculations at all. Another problem, in which a corner zone is held at a fixed high temperature of $10^{6^{\circ}}$ and all other zones start out at a uniform temperature of 1° , provides a good comparison of methods. These initial conditions are illustrated in Fig. (3.5). The problem is defined on a mesh 30 zones by 30 zones, each one centimeter square.

For numerical purposes all monotonic temperature dependent conductivities are alike. As the heat propagates out from the source, there are great disparities of timesteps, and the more so if the heat conductivity is taken as proportional to some power of the temperature. If σ goes as the first power of u or higher, one zone must warm up almost completely before its conductivity is great enough to begin warming the next zone. The time scale may be different for different conductivities, but the numerical sequence of events is pretty much the same for all. Zones warm up one at a time, and the zone currently

warming up will set the timestep. Electron thermal conductivity⁴ is a typical physical process displaying this numerical behavior

Figs. (3.6) and (3.7) are output from ADI and independent timesteps calculations with the same initial and boundary conditions. The number of cycles required to calculate the time evolution of the problem is about the same (contrary to what one would expect), and is determined not by stability conditions but by accuracy constraints. What is plotted in these figures is the temperature distribution, and these pictures are fairly early in the problem. At the stop time, 5.28×10^{-5} sec., the calculations have reached in zone (6,6) a temperature of 7.143, 7.105, and 7.125×10^3 °K by the explicit, independent timestep, and ADI methods respectively, a spread of 0.5%.

Figs. (3.5-3.12) are all output from two codes, ADI and TDH. ADI is an alternating-directions-implicit two dimensional heat diffusion code, forward differenced. TDH is an explicit backward differenced two dimensional heat diffusion code using the method of independent timesteps. Various functions of (x,y) are plotted as surfaces using the system plotting routine PICTURE. A function of two variables (x,y) defined by the FORTRAN array, $f(x,y) = F(J,K)$, is plotted by PICTURE as a surface, with x and y coordinates equal to the integer indices J and K , and the ordinate z (scaled) equal to $F(J,K)$. The point of view is chosen to show as much of the surface as possible, such that the temperature source appears variously at the far right or near left corner. The first line of labelling at the bottom names the code (ADI or TDH), the problem name (POINT SORS), the variable plotted ($U (=u)$; $UD (=u_t)$; $D (= \Delta t_{k_j})$, $TJ (=t_{k_j}^n)$), and operating system statistics. On the

⁴ Spitzer (1962), p. 133.

third line appear the cycle number, time, and timestep. On the third line under SSJN and JXN are the number of zone-cycles of computation actually done, and the product of the mesh size (900) and the number of cycles. For ADI, SSJN is always equal to JXN. For TDH, SSJN is usually much less than JXN. SRAT is the computation ratio, $JXN/SSJN$. The last two integers, under K,LWST, are the indices of the zone with the briefest timestep. On the fourth line, after "SCALE", is "LOG" or "LIN", according as the vertical scale in the picture is logarithmic or linear. After "PI" is printed the angle in radians from the line $J = 1$ to to the point of view of the picture. On the fourth line, as MAX and MIN, are the maximum and minimum values of the plotted function at the top and bottom of the picture box.

In Figs. (3.8) and (3.9) are plotted logarithmically the time derivative ($\Delta T/\Delta t$) of the temperature as calculated by ADI and by TDH. In Figs. (3.10) and (3.11) are plotted the timesteps $\Delta t_{k,j}$. The comparison is instructive, for the minimum timesteps are found in a "trench" in the plotted surface, at the edge of the growing heated region, and are not set by the stability condition. Behind this region, the timesteps are set by the Courant condition for this difference equation in the explicit calculation, and in the implicit one by the equation $\Delta t = 0.05u/(\partial u/\partial t)$. This adjusts the timestep so that no temperature is expected to change by more than 5% per cycle. Ahead of the heated region, the timesteps are uniformly quite large. The implicit code is constrained to step all zones at roughly the same brief timestep as the explicit code; they both advanced the problem 5.26×10^{-5} sec in about 3500 cycles.

Fig. (3.12) shows the Cauchy surface at this stage in the explicit calculation. Zones ahead of the heated region have not been computed at all, and those near it and behind it are more or less up to date. This graph is in linear scale. Comparison of Fig. (3.12) and Fig. (3.7) will show how far ahead of the heated region the calculations have been brought up to date by the enforcement of the condition of Eqn. (3.6)

Implicit Equations

It was reasoned at one point that in an attempt to speed up calculations one should start with the fastest difference equations available, namely, implicit ones. And proceeding along the lines indicated at the beginning of this chapter yielded some successes with implicit equations. In a one dimensional problem describing a bar heated at one end, no difficulties arose until the temperatures everywhere approached equilibrium. Then an instability of unknown cause manifested itself, and the temperature distribution would blow up in isolated areas, but not everywhere. The mystery was compounded by the fact that not just a simple test code behaved this way, but also a complicated problem including hydrodynamics and multi-temperature diffusion.

The implicit equations require solving a series of recursion relations for the temperatures at the future time t^{n+1} :

$$u_j^{n+1} = C_j u_{j-1}^n + D_j \quad j = J, J-1, \dots, 1 \quad (3.26)$$

The coefficients C_j and D_j are given at zone j as functions of


```

IHEADR = 1 ONPOINT SORS      DTMAX = 0.2
UCHANGE = 0.05              DTSTRT = 1.E=009
LOOSE = 0                   YSTRT = 1.E-006
NGANG = 0                   TKA = 1
NONEI = 2                   TKB = 6
YED = 5.E+007               TLA = 1
YSTOP = 1.561E+18           TLB = 6
TED = 5.E-006               ICK = 1
ND = 3                      CRITFCTR = 1.E-008
NED = 3000                  NOEDIT = 0
TSTOP = 5.264E-05           ICOS = 0
NSTOP = 40000               AKEXP = 4.
AKCOEF = 8.E-018           END

```

```

ADI      POINT SORS  U      PCTS,XTIME
  KC      T      DT
  0  0.      1.000000E-09
SCALE: LOG FI 1.00 MAX 1.00E+06 MIN

    035:51:12    0.22
SSJN      JXN      SRAT    UTOT K,LWST
  0      0  0.      1.0E+06 29 29
1.00E-01

```

Fig. (3.5) Initial Conditions of a Two Dimensional Problem

Fig. (3.6) Temperature from an ADI Calculation

TOW	POINT SORS	U	PCTS,XTIME	099:00:00	35.15		
NC	T		DT	SSJN	JXN	SRAT	UTOT K,LWST
3357	5.263426E-05	2.630535E-08	96078	2631888	2.7E+01	5.8E+07	11 8
SCALE:	LOG FJ 1.00 MAX	1.00E+06 MIN	1.00E-01				

Fig. (3.7) Temperature from a MITS Calculation

ADI POINT SORS UD PCTS.XTIME 099:00:00 268.72
 NC T DT 55JN JKN SRAT UTOT K,LWST
 3596 5.263782E-05 3.183143E-08 281926 2819264 1.0E+00 6.0E+07 8 11
 SCALE: LOG Ff 1.00 MAX 1.00E+12 MIN 1.00E-01

Fig. (3.8) Rate of Change of Temperature: ADI

Fig. (3.9) Rate of Change of Temperature: MITS

ADI	POINT SORS	D	PCTS.XTIME	099:00:00	268.72			
NC	T		QT	SSJN	JXN	SRAT	UTOT K.LWST	
3596	5.263782E-05	3.183143E-08	2819264	2819264	1.0E+00	6.0E+07	8 11	
SCALE:	LOG F1 5.00	MAX	2.50E-01	MIN	1.00E-10			

Fig. (3.10) Timesteps in an ADI Calculation

TDH	POINT	SQRS	D	PCTS, XTIME	099:00:00	35.15		
NC	T			DT	SSJN	JKN	SRAT	U*OT K,LWST
3357	5.263426E-05	2.630335E-08		96078	2631888	2.7E+01	5.8E+07	11 8
SCALE:	LOG F1 5.00 MAX	2.50E-01 MIN		1.00E-10				

Fig. (3.11) Timesteps in a MITS Calculation

TDM	POINT SORS	TJ	PCTS.XTIME	099:00:00	35.15		
NC	T	DT	SSUN	JXN	SRAT	UTOT K,LWST	
3357	5.263426E-05	2.630535E-08	96078	2631888	2.7E+01	5.6E+07 11 8	
SCALE:	LIN FI 1.00 MAX	5.26E-05 MIN	D.				

Fig. (3.12) Cauchy Surface in a MITS Calculation

quantities known at zone j and quantities required from the neighboring zones:

$$\begin{aligned} C_j^n &= f(u_j^n, u_{j+1}^n, u_{j-1}^n, C_{j-1}^n) \\ D_j^n &= f(u_j^n, u_{j+1}^n, u_{j-1}^n, C_{j-1}^n, D_{j-1}^n) \end{aligned} \quad (3.27)$$

And so, when a neighboring zone was not computed, its C_j and D_j were extrapolated from old values and their time derivatives. It is remarkable that this procedure worked at all, because independent timesteps do violence to the motivating philosophy of implicit equations. The implicit solution is of the form

$$u_j^{n+1} = f(u_j^n, u_2^n, \dots, u_{j-1}^n, u_j^n) \quad (3.28)$$

and each temperature u_j^{n+1} at the future time depends on all the temperatures u_j^n at the old time t^n . It is from this that the implicit method derives its stability, as will be made clearer in Chapter IV. Interrupting the recursion Eqn. (3.26) at any point completely destroys the dependence of the form of Eqn. (3.28). Thus, implicit diffusion with independent timesteps is not nearly the simple matter that explicit equations are.

Considerations in Implementing Independent Timesteps

It is pertinent to speak more of the details of managing asynchronous calculations. For once the simultaneous quantities have been generated at some zone, its calculations proceed pretty much as usual. But the solution of Eqns. (3.2) may be interleaved with the

solutions of Eqns. (3.3-3.7), instead of proceeding in the order given. For example, it may be convenient to find the time derivatives du/dt on physical grounds and then get the timesteps, and only then proceed to update the u 's at time t . It is a matter again of convenience where in this cycle one enforces the neighbor restrictions on the timesteps and selects those zones to be updated next. The present experience is that it can be done in various ways without peculiar difficulties in any approach.

The neighbor constraint on the timesteps, Eqn. (3.6), can often be relaxed, as was mentioned above. Specifically, where there is not much activity (which is to say where all the time derivatives are small), it can be relaxed, but it must be enforced in the vicinity of those zones of briefest timestep (where the time derivatives are not small). This involves more coding than one would usually care for, and greatest savings in computation time come not from eliminating physics in just a few more zones, but from reducing the logical "overhead" one must pay to manage independent timesteps at all. For example, suppose zone j has the least timestep and, in accordance with Eqn. (3.6), zones $j+1$, $j+2$, etc., have timesteps each increasing by a factor of two, as far as zone $j+n$. In the time that zone $j+n$ is updated once, zone j is updated 2^n times, zone $j+1$ 2^{n-1} times, and so on. The total number of zone cycles of computation is $2^n + 2^{n-1} + \dots + 2 + 1 = 2^{n+1}$. An equivalent number of zone cycles of physics would have been done if zone $j+1$ was held at the timestep of zone j and zones $j+2$, $j+3$, ..., $j+n$ were all held at the much longer timestep of zone $j+n$. Although the enforcement of Eqn. (3.6) has greatly lowered the timesteps of some zones, it has, in effect, only cost the computational effort of lowering the timestep in

one zone. In Fig. (2.4) the regular (and steep) slope of the $\Delta t(j)$ curve is caused by Eqn. (3.6) restraining the timesteps in the vicinity of the shock zone of that problem.

CHAPTER IV

STABILITY OF PARABOLIC EQUATIONS IN THE MAXIMUM NORM

The Classical Stability Analysis

The method of stability analysis by Fourier components which was developed by von Neumann and Richtmyer¹ is quite sufficient to deal with most problems. As it happens, the method of independent timesteps is quite refractory to this approach, and it was necessary to resort to other means. A few remarks may illustrate the difficulties encountered. The solution $u(x)$ of any problem in one dimension can be represented as a Fourier series $u = \sum_k u_k \cos(kx)$. The difference equations can be linearized so that each of the components $u_k \cos(kx)$ is propagated forward in time independently of the others. Stability requires proof that the solution remains bounded as the mesh is refined. If each component $u_k \cos(kx)$ is damped in time, then the solution is clearly stable. If any component is amplified, then there are grounds for suspecting instability (but not, it may be noted, proof of instability in fact).

¹ von Neumann & Richtmyer (1950).

One substitutes in the linearized difference equations a solution of the form

$$u_j^n = \zeta^n e^{i j \Delta x} \quad (4.1)$$

and solves for ζ , the amplification factor. The difficulty is that this method assumes in the approximations of its premises precisely all the properties which independent timesteps never possess, namely constant coefficients in the difference equations and a mesh that is always and everywhere uniform in Δx and more importantly in Δt . For suppose in the difference equation

$$u_j^{n+1} - u_j^n = A(u_{j-1}^n, 2u_j^n, u_{j+1}^n) \quad (4.2)$$

with $A = \sigma \Delta t / (\Delta x)^2$, that u_{j+1}^n is available at time t_j^n but u_{j-1}^n is not. The temperature at zone $j-1$ may be approximated by

$$u_{j-1}(t_j^n) = u_{j-1}^n + \frac{u_{j-1}^n - u_{j-2}^n}{t_j^n - t_{j-1}^n} (t_j^n - t_{j-1}^n) \quad (4.3)$$

This is the linear extrapolation forward from the two previous values at $j-1$. In $R = (t_j^n - t_{j-1}^n) / (t_{j-1}^n - t_{j-2}^n)$, one may substitute in Eqn. (4.2), giving

$$u_j^{n+1} - u_j^n = A \left(u_{j-1}^n - 2u_j^n + u_{j+1}^n + R(u_{j-1}^n - u_{j-2}^n) \right) \quad (4.4)$$

Into this may be substituted Eqn. (4.1), and simplifying, there results an equation in ζ :

$$\zeta - 1 = A \left(e^{i\psi} - 2 + e^{-i\psi} \left(\frac{1+R}{\zeta} - \frac{R}{\zeta^2} \right) \right) \quad (4.5)$$

with $y = k\Delta x$. This may be rearranged to exhibit a cubic in ζ , the amplification factor:

$$\zeta^3 + \zeta^2 \left(2A - Ae^{i\psi} - 1 \right) - \zeta Ae^{i\psi}(1+R) + Ae^{i\psi} = 0 \quad (4.6)$$

Now the roots of this equation are not inaccessible, but before considering them it is sobering to note that R was tacitly assumed equal to unity. For, if Eqn. (4.1) is to be tested as a solution to any form of Eqn. (4.2), it must be that u is amplified by the same factor ζ at every zone and over every timestep, and this requires timesteps of equal size, not only in adjacent zones, but also in succession in the same zone. So, any results based on Eqn. (4.6) are suspect for values of R not equal to one.

While this is one of the more tractable equations in an amplification factor, it still requires a numerical solution. Even the method of Routh and Hurwitz will not easily confine its roots to within the unit circle. Its roots are plotted in Fig. (4.1) in the complex plane. The unit circle and the positive real axis are shown for scale. As the parameter $y = k\Delta x$ is varied from 0 to 2π , the roots fall on two loci, one a balloon near unity, and the other, a deformed circular locus with approximate radius proportional to A . When A is roughly equal to 0.25, this locus first strays outside of the unit circle, thus indicating the limits of stability. As encouraging as this was, it was

Fig. (4.1) Amplification Factors

felt to be no more than suggestive, and other assurances for stability were sought.

The Equation of DuFort and Frankel

In 1953 was published a rather remarkable finite difference approximation to the heat equation². It is quite explicit and unconditionally stable. The fact that its convergence is conditional on the way in which the mesh is refined does not make clear its true character, and little more is said about it in the various finite difference handbooks. The equation published in 1953 is actually one of a broad class of difference equations which are explicit and unconditionally stable, two of which were quoted at Eqns. (3.22) and (3.23). Because of its stability, it was felt that such an equation,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\sigma}{\Delta x^2} \left(u_{j-1}^n - u_j^{n+1} - u_j^{n-1} + u_{j+1}^n \right) \quad (4.7)$$

might provide the best starting point for independent timesteps. Such an expectation was not confirmed, but this equation turned out to be very instructive and to provide good illustrations of precisely what stability is. The common rationalization notes that since in these equations the temperature u_j^{n+1} at the future time t^{n+1} depends only on present and past temperatures at the three zones $j-1, j, j+1$, the timestep cannot be extended too far without asking for trouble. This is indeed true, and the reasons why will indicate that the concept of stability is not as difficult as commonly supposed. In actual fact, Eqn. (4.7)

² duFort & Frankel (1953)

yields very bad approximations to the heat equation for timesteps large compared to those permitted by stability considerations to simple backward differenced explicit equations. Moreover, the solutions, while bounded and therefore formally quite stable, exhibit thoroughly unacceptable pathologies.

Eqn. (4.7) may be solved explicitly for u_j^{n+1} , with $A = \sigma \Delta x^2$:

$$u_j^{n+1} = u_j^n + \frac{A\Delta t}{1+A\Delta t} (u_{j+1}^n - u_j^n) + \frac{A\Delta t}{1+A\Delta t} (u_j^n - u_{j-1}^n) \quad (4.8)$$

In the limit of large timesteps,

$$u_j^{n+1} = u_{j+1}^n, u_j^n + u_{j-1}^n \quad (4.9)$$

A little graphic work suffices to explain what was happening. In Fig. (4.2), if u_j^n , u_{j+1}^n , and u_{j-1}^n are as shown, u_j^{n+1} approaches point Q asymptotically as Δt increases without limit. Point R is the average of u_j^n and u_{j+1}^n , and point Q is as far above R as u_j^n is below R . The calculated solution of a DuFort and Frankel type equation exhibits ripples of a quite unphysical nature, which, however, do not grow without bound in time, and thus are formally stable. It should also be clear that at late times the true solution $u(x,t)$ can be arbitrary, but the calculated value of u_j^{n+1} will bear no relation to it at all, if the calculation consists of one long timestep.

Thus, armed with an example of an equation which is stable but nevertheless not satisfactory, a similar inspection of the common backward differenced explicit equation

Fig. (4.2) The Solution to the Du Fort-Frankel Equation.

$$u_j^{n+1} - u_j^n = A(u_{j-1}^n, 2u_j^n, u_{j+1}^n) \Delta t, \quad (4.10)$$

sufficed to reveal the reasons for its stability condition. If one supposes u_{j-1}^n , u_j^n , and u_{j+1}^n to have arbitrary values, the diagram in Fig. (4.3) may be constructed. Here there is no point Q for u_j^{n+1} increases without limit as Δt increases without limit:

$$u_j^{n+1} - u_j^n = 2A\Delta t \left(\frac{u_{j-1}^n + u_{j+1}^n}{2} - u_j^n \right) \quad (4.11)$$

If u_j^n is greater than $(u_{j-1}^n + u_{j+1}^n)/2$, then u_j^{n+1} decreases without limit. The stability condition is known to require that $A\Delta t \leq 0.5$, which is to say that instability occurs as soon as u_j^{n+1} crosses point R in Fig. (4.3), but the difference equations are stable as long as u_j^{n+1} lies between u_j^n and the average of u_{j-1}^n and u_{j+1}^n .

Stability in General

Faced with the phenomena described above, one naturally returns to the definitions of stability to inquire just what one is dealing with. Following Richtmyer & Morton³ (the Russian nomenclature⁴ is generally at odds with this), one constructs an approximation to $u(x, t)$, and as the difference mesh is refined, if the approximation to $u(x, t)$ remains finite, then the method is said to be stable, otherwise not. Note that

³ Richtmyer & Morton (1967), p. 45.

⁴ Yanenko (1971), pp. 4-8.

Fig. (4.3) Solutions of Eqn. (4.10)

the approximate $u(x, t)$ is not required to decrease as the mesh is refined, only not to increase *without limit*.

In speaking of refining the mesh, one has in mind a series of ever finer meshes, $\mathfrak{M}_\alpha$, $\alpha=1, 2, \dots$, with each mesh $\mathfrak{M}_\alpha = \{(x_j, t^n)\}$. Mesh $\mathfrak{M}_\alpha$ is characterised by its mesh spacings, $\Delta x = x_{j+1} - x_j$, and $\Delta t = t^{n+1} - t^n$. Mesh $\mathfrak{M}_{\alpha+1}$ is finer than $\mathfrak{M}_\alpha$ if $\Delta x_{j+1} \leq \Delta x_j$ and $\Delta t_{n+1} \leq \Delta t_n$. For a given mesh $\mathfrak{M}_\alpha$, there is an approximation (calculated by means of the finite difference equation on that mesh) to the quantity $u(x, t)$: $(u_j^n)_\alpha$. For mesh $\mathfrak{M}_{\alpha+1}$, and its approximation $(u_j^n)_{\alpha+1}$, $j_{\alpha+1} \geq j_\alpha$ and $n_{\alpha+1} \geq n_\alpha$. The point $u(x, t)$ and its dependent variables $u(x, t)$ are reached in ever more and ever finer increments. The definition of stability speaks of the series $\{u(x, t)_\alpha, \alpha=1, 2, \dots\}$, and requires that this series converge (uniformly on all x and t) to some finite value. It does not have to be a monotonic decreasing series. Conditional stability generally asserts convergence of the series $\{u_\alpha\}$ given only the stronger additional premise that for each mesh $\mathfrak{M}_\alpha$, Δx_α and Δt_α are connected by some stability condition, as for example for some constant K , $\Delta t / \Delta x \leq K$ or $\Delta t / (\Delta x^2) \leq K$. These conditions were first stated by Courant, Friedrichs, and Lewy⁵ and are often called *Courant conditions*.

The problem may be specified precisely by naming the equation to be solved,

$$\partial u / \partial t = F(u, \partial u / \partial x, \text{etc.}) \quad (4.12)$$

its initial and boundary conditions,

⁵ Courant, Friedrichs, & Lewy (1928)

$$\begin{aligned}
 u(x, 0) &= f(x) \\
 u(0, t) &= g(t) \\
 u(X, t) &= h(t)
 \end{aligned}
 \tag{4.13}$$

and an approximate solution $v(x, t)$ together with its finite difference equation:

$$v(x, t + \Delta t) = S(x, t, \Delta x, \Delta t)v(x, t) \tag{4.14}$$

S is some for the moment unspecified finite difference operator. The approximation v is subject to the initial and boundary conditions of Eqn. (4.13). To define stability it is necessary to consider $v(x, t)$ as an element of a complete vector space in which there is a norm⁶ $\|v\|$. There are two common norms useful for our purposes, the maximum norm and the L_2 norm. The maximum norm is defined by

$$\|v\|_{MAX} = \max_x \{|v(x)|\} \tag{4.15}$$

and the L_2 norm by

$$\|v\|_{L_2}^2 = \int |v(x)|^2 dx \tag{4.16}$$

The operator S is said to have a bound s , if for any permissible function $v(x)$,

$$\|Sv(x)\| \leq s \|v(x)\| \tag{4.17}$$

This bound s may be written as $\|S\|$. A difference equation is really a

⁶ A Banach space; see Richtmyer & Morton (1967), p. 30.

schema of operators $S(x, t, \Delta x, \Delta t)$. Δx may be taken as a function of Δt , since we are interested in the behavior of approximations as one varies Δt , and in practise, Δx and Δt are connected by some fixed relationship. Thus the operators S may be considered as functions of Δt ; for, having specified Δt , one has a rule at every point (x, t) for specifying Δx , and so S . As Δt is lowered, with $n\Delta t = t$ held constant, one expects $S^n(\Delta t)$, the operator which brings $v(x, 0)$ to $v(x, t)$, to give an ever better approximation to $u(x, t)$. The approximation by means of $S^n(\Delta t)$ is called stable if there is some number K such that for any Δt in the finite range specified by

$$\begin{aligned} 0 < \Delta t < T_{\max} \\ 0 < n\Delta t < T \end{aligned} \tag{4.18}$$

it is the case that for all permitted $f(x)$,

$$\|S^n f(x)\| = \|v(x, t)\| \leq K \|f(x)\| \tag{4.19}$$

Stability in the Maximum Norm

The insight gained from the equation of DuFort and Frankel can be formalized in a method mentioned in passing by Richtmyer & Morton⁷. The Fourier analysis may be taken as proof of stability in either the L_2 norm or the maximum norm, but it is much easier for present purposes to prove stability for parabolic equations in the maximum norm. Moreover,

⁷ Richtmyer & Morton (1967), p. 12. It is surprising that these authors did not acknowledge the power and generality of the method they mention so briefly and decline to develop fully.

the proof supplied here is rigorously true for equations that are nonlinear and which have variable coefficients, and for neither of these cases will the Fourier analysis guarantee stability. Hyperbolic equations are best analysed in the L_2 norm, but again, by methods other than Fourier analysis.

It will be convenient to define an averaging function: $g(a,b)$ is an averaging function of its two arguments a and b if

$$|g| \leq \max(|a|, |b|) . \quad (4.20)$$

This definition is a little more broad than the intuitive idea of an average, but it captures precisely that property of averages which is used as a premise in the following arguments. The discussions of Figs. (4.2-4.3) hinged on the point at which u_j^{n+1} overtakes the average of its neighbors, u_{j-1}^n , and u_{j+1}^n , and this is the place where instability sets in. Averaging functions will figure prominently in all the stability arguments in the maximum norm.

It is useful to think of difference schemes as operators: the operator C applied to the function $u^n = u(x, t^n)$, gives the new function u^{n+1} at the time t^{n+1} :

$$u^{n+1} = Cu^n \quad (4.21)$$

The form of all stability arguments in the maximum norm is quite simple; an example may be stated in the following theorem:

Theorem 4.1 For a difference scheme $u^{n+1} = Cu^n$, and a function

u_j^n , if a_j^n is an averaging function $a_j^n(u_{j-1}, u_{j+1})$ of its arguments, and if

$$|u_j^{n+1}| \leq \max(|u_j^n|, |a_j^n|), \quad (4.22)$$

then the scheme is stable in the maximum norm.

For the proof, one may note first that from Eqn. (4.20),

$$|a_j^n| \leq \max(|u_{j-1}^n|, |u_{j+1}^n|). \quad (4.23)$$

It follows from Eqns. (4.22) and (4.23) that

$$|u_j^{n+1}| \leq \max(|u_j^n|, |u_{j-1}^n|, |u_{j+1}^n|) \quad (4.24)$$

and so that

$$\|u^{n+1}\| \leq \|u^n\| \quad (4.25)$$

whence the bound on $\|u^n\|$ ($\|u^n\| \leq \|u^0\|$), proving stability as expressed in Eqn. (4.19).

We note without proof that $g(x, y) = \alpha x + (1 - \alpha)y$ is an averaging function if $0 < \alpha < 1$.

There follows readily from Theorem (4.1):

Theorem (4.2) The difference scheme

$$u_j^{n+1} = u_j^n + A(a_j^n) u_j^n, \quad (4.26)$$

with a_j^n an averaging function of u_{j-1}^n and u_{j+1}^n , and $0 < A < 1$, is stable in

the maximum norm. The quantity A_j is generally $2\sigma\Delta t \Delta x^2$, where σ is the diffusion constant and Δt and Δx specify the mesh size. This is just the common stability condition. Note that it is a local argument; the mesh size may be variable, and the averaging function α and the diffusion coefficient σ may both be very nonlinearly dependent on u , but Theorem (4.2) still quite rigorously proves stability. One may see this in the common explicit backward differenced equation:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = - \frac{G_j}{x_{j+1} - x_{j-1}} \left(\frac{K_j(u_{j+1}^n - u_j^n)}{x_{j+1} - x_j} - \frac{K_{j-1}(u_j^n - u_{j-1}^n)}{x_j - x_{j-2}} \right). \quad (4.27)$$

Here σ_j is the diffusion coefficient, specified at the zone edge, and is a function of the temperatures u_j^n . The quantities G_j contain information about the geometry, (plane, cylindrical, or spherical) and the mesh size. Eqn. (4.27) may be rearranged:

$$u_j^{n+1} = u_j^n + \frac{2G_j\Delta t}{x_{j+1} - x_{j-1}} \left\{ \frac{K_j/2}{x_{j+1} - x_{j-1}} u_{j+1}^n + \frac{K_{j-1}/2}{x_j - x_{j-2}} u_{j-1}^n - \left(\frac{K_j/2}{x_{j+1} - x_{j-1}} + \frac{K_{j-1}/2}{x_j - x_{j-2}} \right) u_j^n \right\} \quad (4.28)$$

Here the auxiliary quantities B_j and C_j may be defined:

$$B_j = \frac{K_j/2}{x_{j+1} - x_{j-1}}, \quad \text{and} \quad C_j = \frac{K_{j-1}/2}{x_j - x_{j-2}},$$

and the averaging function α_j^n of Eqn. (4.26) here is given by

$$a_j^n = \frac{B_j u_{j+1}^n + C_j u_{j-1}^n}{B_j + C_j} \quad (4.29)$$

and A_j is given by

$$A_j^n = C_j \Delta t \frac{B_j + C_j}{x_j - x_{j-1}} \quad (4.30)$$

Thus, the difference Eqn. (4.27) is indeed of the same form as Eqn. (4.26).

Implicit Differences Equations

It is not difficult to extend this method to the forward differenced implicit equations. In order to demonstrate the quite broad general application of stability analysis by means of a bound in the maximum norm using simple arithmetic inequalities, the treatment of implicit equations is included here. This will provide the means of justifying the assertion of Chapter III from another point of view why independent timesteps are not suitable for implicit equations. It may be proven that

Theorem (4.3) A difference scheme $u^{n+1} = Cu^n$ is stable in the maximum norm if there exists an averaging function $a_j^n(u_{j+1}^n, u_{j-1}^n)$ such that

$$|u_j^{n+1}| \leq \max(|u_j^n|, |a_j^n|) \quad (4.31)$$

For the proof, note that in the premise the average is not taken at time t^n but at time t^{n+1} . Eqn. (4.31) states in effect that u_j^{n+1} is smaller in absolute value than one of u_j^n , u_{j+1}^{n+1} , and u_{j-1}^{n+1} . But one may proceed recursively from zone j to the boundaries and bound u_j^n by either some u_k^n or by a value of u at the boundary, and this is precisely to say that

$$\|u^{n+1}\| \leq \|u^n\|, \quad (4.32)$$

proving stability.

As a corollary, one may note:

Theorem (4.4) Difference schemes of the form

$$u_j^{n+1} = u_j^n + A(a_j^{n+1} - u_j^{n+1}) \quad (4.33)$$

are stable in the maximum norm for $0 < A < \infty$, if a_j^{n+1} is an averaging function of u_{j+1}^{n+1} and u_{j-1}^{n+1} .

For proof, one may note that u_j^{n+1} is given in Eqn. (4.33) by an averaging function of u_j^n and a_j^{n+1} , thus fulfilling the premise, Eqn. (4.31) of Theorem (4.3). One may also note that,

$$u_j^{n+1} = \frac{u_j^n + A a_j^{n+1}}{1+A}, \quad (4.34)$$

and that for the entire range $0 < A < \infty$, u_j^{n+1} lies between u_j^n and a_j^{n+1} . As before, A is taken as $2\sigma\Delta t \cdot \Delta x^2$, and the scheme, Eqn. (4.33) is stable for all timesteps. This is just the fully forward differenced implicit equation. Note that in this scheme each u_j^{n+1} is bounded not by one of

$u_j^n, u_{j-1}^n, u_{j+1}^n$, but by some element of the much larger set $\{u_1^n, u_2^n, u_3^n, \dots, u_j^n\}$.

The Crank-Nicholson scheme may be written as follows:

$$u_j^{n+1} = u_j^n + A \left\{ \left(ga_j^n + (1-g)a_j^{n+1} \right) - \left(gu_j^n + (1-g)u_j^{n+1} \right) \right\} \quad (4.35)$$

Here $0 < g < 1$, and a_j^n is an average of u_{j+1}^n and u_{j-1}^n , as before. Eqn.

(4.35) may be rewritten as

$$u_j^{n+1} = u_j^n \frac{1-Ag}{1+A(1-g)} + \frac{A}{1+A(1-g)} (ga_j^n + (1-g)a_j^{n+1}) \quad (4.36)$$

The right hand side averages u_j^n and $(ga_j^n + (1-g)a_j^{n+1})$ if and only if

$0.5 \leq g$. In this case, u_j^{n+1} may be bounded by one of u_j^n and

$(ga_j^n + (1-g)a_j^{n+1})$; or equivalently by one of $u_j^n, u_{j+1}^n, u_{j-1}^n, u_{j+1}^{n+1},$

u_{j-1}^{n+1} ; and one may proceed recursively as before until one bounds u_j^n by

some u_k^n or a value of u on the problem boundary. The number g specifies

how far "forward" the difference equation is: when $g=0$, the equation is

backward differenced, and when $g=1$, it is fully forward differenced.

For the Crank-Nicholson scheme, $g=0.5$.

CHAPTER V

STABILITY OF HYPERBOLIC EQUATIONS IN THE L_2 NORM

An example with Variable Coefficients

The usually superb convenience of Fourier analysis of stability is not universal. There are problems resistant to it, and one here described leads to a stability analysis later suitable for independent timesteps. The strategy is known as the *energy method*, and has been known for some time¹. This chapter will deal with stability of hyperbolic equations without independent timesteps, and the next will detail how the arguments in this chapter are modified by independent timesteps.

The example following was related to me by K. Marx². One difference is the cylindrical wave equation in the straightforward manner explicitly. This equation has coefficients variable in r , and its behavior is known from experience to be stable with the usual Courant condition for such equations. However, the Fourier method fails to prove stability. This

¹ Richtmyer & Morton (1967), chapter 6.

² Private communication.

is generally (and here erroneously) taken to be diagnostic of instability. It may be remembered from the discussion above in Chapter IV that a stable solution of the difference equation is merely forbidden to grow without bound; it is not required to decay.

The cylindrical wave equation,

$$\frac{\partial^2 u}{\partial t^2} = \frac{c^2}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) = c^2 \frac{\partial^2 u}{\partial r^2} + \frac{c^2}{r} \frac{\partial u}{\partial r} \quad (5.1)$$

may be differenced,

$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{(\Delta t)^2} = c^2 \left\{ \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta r)^2} + \frac{u_{j+1}^n - u_{j-1}^n}{2r_j \Delta r} \right\} \quad (5.2)$$

where Δt and Δr specify the mesh size. The Eqn. (5.1) is to be approximated by Eqn. (5.2) on some domain $0 < a \leq r \leq b$, not including the axis of coordinates. One may substitute

$$u_j^n = \zeta^n e^{ik\Delta r} \quad (5.3)$$

and with a little algebra obtain

$$\frac{\zeta^2 - 2\zeta + 1}{\Delta t^2} = 2c^2 \frac{\cos(k\Delta r) - 1}{(\Delta r)^2} + 2i \frac{\sin(k\Delta r)}{r\Delta r}$$

from which

$$\zeta^2 - 2G\zeta + 1 = 0 \quad (5.4)$$

with

$$G = f + (A \cos(k\Delta r) - f) - 2iA\Delta r \sin(k\Delta r)/r, \quad (5.5)$$

and with

$$A = c^2 \Delta t^2 / \Delta r^2 \quad (5.6)$$

Now the two roots ζ_1 and ζ_2 must satisfy

$$\zeta_1 \zeta_2 = 1, \quad \zeta_1 + \zeta_2 = -2G \quad (5.7)$$

If $\zeta_1 \zeta_2 = 1$ and $|\zeta_1| = |\zeta_2| = 1$, then $\zeta_1 = \zeta_2^*$. But if $\zeta_1 = \zeta_2^*$, then $\zeta_1 + \zeta_2$ is real. This cannot be the case, since G is not real. Therefore, one of $|\zeta_1|$, $|\zeta_2|$ must be greater than unity, and some Fourier component of the solution grows with time, leaving the stability of Eqn. (5.2) unproven.

Plane Waves

Before tackling cylindrical waves with the energy method, it is instructive to exhibit this strategy in its application to plane waves, because here it may be seen in the greatest clarity. Cylindrical waves and hydrodynamic difference equations may later be reduced to this case. In one dimension, in plane geometry, the wave equation is

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial r^2} \quad (5.8)$$

and its common finite form is,

$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{(\Delta t)^2} = \frac{2c^2}{r_{j+1} - r_{j-1}} \left\{ \frac{u_{j+1}^n - u_j^n}{r_{j+1} - r_j} - \frac{u_j^n - u_{j-1}^n}{r_j - r_{j-1}} \right\} \quad (5.9)$$

It is convenient to rewrite this as a pair of first order equations. To this end one defines quantities v and w by

$$v_j^n = \frac{u_j^n - u_{j-1}^{n-1}}{c\Delta t}, \quad \text{and} \quad u_j^n = \frac{u_j^n - u_{j-1}^n}{r_j - r_{j-1}} \quad (5.10)$$

Eqn. (5.9) may be written as

$$\frac{v_j^{n+1} - v_j^n}{c\Delta t} = \frac{2(u_{j+1}^n - w_j^n)}{r_{j+1} - r_{j-1}} \quad (5.11)$$

One may construct from Eqn. (5.10) an equation in w :

$$\frac{w_j^{n+1} - w_j^n}{c\Delta t} = \frac{v_j^{n+1} - v_{j-1}^{n+1}}{r_j - r_{j-1}} \quad (5.12)$$

It is convenient to define

$$A_j = \frac{r_{j+1} - r_{j-1}}{2c\Delta t}, \quad B_j = \frac{r_j - r_{j-1}}{c\Delta t} \quad (5.13)$$

Eqns. (5.11) and (5.12) may be rewritten

$$\begin{aligned} A_j(v_j^{n+1} - v_j^n) &= u_{j+1}^n - w_j^n \\ B_j(w_j^{n+1} - w_j^n) &= v_j^{n+1} - v_{j-1}^{n+1} \end{aligned} \quad (5.14)$$

The first of these may be multiplied by $(v_j^{n+1} - v_j^n)$ and the second by

$(w_j^{n+1} + w_j^n)$ to obtain a pair of equations:

$$\begin{aligned} A_j \left((v_j^{n+1})^2 - (v_j^n)^2 \right) &= (w_{j+1}^n - w_j^n) (v_j^{n+1} + v_j^n) \\ B_j \left((w_j^{n+1})^2 - (w_j^n)^2 \right) &= (v_j^{n+1} - v_{j-1}^n) (w_j^{n+1} + w_j^n) \end{aligned} \quad (5.15)$$

If Eqns. (5.15) are summed from $j = 1$ to $j = J$, one has

$$\begin{aligned} \sum_{j=1}^J \left\{ A_j \left((v_j^{n+1})^2 - (v_j^n)^2 \right) + B_j \left((w_j^{n+1})^2 - (w_j^n)^2 \right) \right\} \\ = \sum_{j=1}^J \left\{ (v_j^{n+1} + v_j^n) (w_{j+1}^n - w_j^n) + (w_j^{n+1} + w_j^n) (v_j^{n+1} - v_{j-1}^n) \right\} \end{aligned} \quad (5.16)$$

The right hand side of Eqn. (5.16) may be summed by parts:

$$\begin{aligned} R.H.S. &= \sum_{j=1}^J \left\{ (v_j^{n+1} + v_j^n) (w_{j+1}^n - w_j^n) + v_j^{n+1} (w_j^{n+1} - w_{j-1}^n + w_{j-1}^n - w_j^n) \right\} \\ &\quad - v_1^{n+1} (w_2^{n+1} + w_2^n) + v_J^{n+1} (w_{J+1}^n + w_{J+1}^n) \end{aligned} \quad (5.17)$$

The last, unsummed terms, may be termed BT^n , the boundary terms. One may define

$$R^n = \sum \left(A_j (v_j^n)^2 + B_j (w_j^n)^2 + v_j^n (w_{j+1}^n - w_j^n) \right). \quad (5.18)$$

and rearranging Eqn. (5.17) and substituting into Eqn. (5.18), one has

$$R^{n+1} = R^n + BT^n.$$

As stability problems at the boundary are usually of a different and altogether more tractable character than stability in the interior of

the mesh, it will simply be assumed that BT^n has no effect on stability. The boundary term may be set to zero for present purposes, and so

$$R^{n+1} = R^n \quad (5.19)$$

The quantity R^n has a form appearing very much like that of the square of a finite L_2 norm, and in fact, it may be shown to define a norm equivalent to the L_2 norm, which may be called the wave norm. Eqn. (5.19) proves stability in the wave norm under conditions which will be explored forthwith. It should be noted that nowhere were constant or linear coefficients assumed for the difference equations.

The Wave Norm

Let Z represent a vector function with two components x_j and y_j at each index j for $j = 1, \dots, J$; similarly, let U be a function with components v_j, w_j . One may define an inner product in the space of these functions:

$$(Z, U) = \sum \left(A_j x_j y_j + B_j y_j w_j + \frac{1}{2} (x_j \Delta_+ w_j + v_j \Delta_+ y_j) \right) \quad (5.20)$$

Here Δ_+ is the forward difference operator: $\Delta_+ w_j = w_{j+1} - w_j$. The A_j and B_j are positive coefficients, and conditions will be imposed on them in order that Eqn. (5.20) in fact define an inner product. For Eqn. (5.20) to qualify as an inner product, it is necessary that³

$$(Z, U) = (U, Z) \quad (5.21)$$

³ Herstein (1964), p. 152.

$$(Z, Z) \geq 0; \text{ and } (Z, Z) = 0 \text{ iff } Z = 0 \quad (5.22)$$

$$(aZ + bU, T) = a(Z, T) + b(U, T) \quad (5.23)$$

Eqn. (5.21) is easily verified, and Eqn. (5.23) is dealt with momentarily. Eqn. (5.22) yields the familiar Courant condition. For Eqn. (5.22) to hold, it is necessary that

$$A_j > 1, \quad B_j > 1. \quad (5.24)$$

Recalling the definition of B_j , one has

$$B_j = \frac{r_j - r_{j-1}}{c \Delta t} > 1,$$

and a similar condition results from $A_j > 1$. In order to prove the necessity of Eqn. (5.24) one may rewrite Eqn. (5.19), with $\|U\|_{NN}^2 = (U, U)$, as

$$\begin{aligned} R^n &= \|U\|_{NN}^2 = \sum Q_j^n \\ &= \frac{1}{2} \sum \left\{ \left(A_j (v_j^n)^2 + B_j (w_j^n)^2 - 2v_j^n w_j^n \right) \right. \\ &\quad \left. + \left(A_j (v_j^n)^2 + B_{j+1} (w_{j+1}^n)^2 + 2v_j^n w_{j+1}^n \right) \right\} \end{aligned} \quad (5.25)$$

The boundary term is different than in Eqn. (5.17) if one is to construct from Eqn. (5.25) the quantity $R^{n+1} - R^n = B T^n$. The squared norm Eqn. (5.25) was constructed from Eqn. (5.18) by apportioning the terms $B_j (w_j^n)^2$ not all at zone j in the summation, but half and half at zones j and $j+1$. The two terms in Eqn. (5.25) under the summation sign are each positive definite, if the A 's and B 's are all greater than unity. Together, as indicated in Eqn. (5.25), they are denoted by Q_j^n . Eqn.

(5.19) bounds $R^n = \|U\|_{\#N}^2$, and this gives a bound on the individual quantities under the sum of Eqn. (5.25) if those quantities are themselves all positive. Relaxing Eqn. (5.24) not only means that $R^n = \|U\|_{\#N}^2$ no longer defines a norm, but that the quantities r and w may increase without bound, which is precisely instability.

To complete the proof that Eqn. (5.20) defines an inner product, if in Eqn. (5.23), T is the set of quantities (r_j, s_j) , one has on writing out in full, and omitting the subscript j ,

$$\begin{aligned} (aZ+bU, T) = & \sum \left(A(ax+bv)r + B(ay+bw)s \right) \\ & + \frac{1}{2} \sum \left((ax+bv)\Delta_x s + r\Delta_x(ay+bw) \right) \end{aligned} \quad (5.26)$$

The first term is given by

$$\sum aAxr + bAur + aBys + bBws$$

and the second by

$$\frac{1}{2} \sum ax\Delta_x s + bv\Delta_x s + ar\Delta_x y + br\Delta_x w$$

Together, they are

$$\begin{aligned} a \sum Axr + Bys + \frac{1}{2} (x\Delta_x s + r\Delta_x y) \\ + b \sum Aur + Bws + \frac{1}{2} (v\Delta_x s + r\Delta_x w). \end{aligned}$$

or just

$$a(Z, T) + b(U, T),$$

proving Eqn. (5.239). One may now define the wave norm:

$$\|Z\|^2 = (Z, Z) \quad (5.27)$$

To qualify as a norm, it must satisfy⁴

$$\|aZ\| \leq |a| \|Z\| \quad (5.28)$$

$$\|Z\| \geq 0; \|Z\| = 0 \text{ iff } Z = 0 \quad (5.29)$$

$$\|Z+U\| \leq \|Z\| + \|U\| \quad (5.30)$$

Equation (5.28) follows immediately from Eqn. (5.23). Eqn. (5.29) is the same as (5.22), and Eqn. (5.30), the triangle inequality, follows from the properties of inner products⁵. The L2 norm may be defined by

$$\|Z\|_{L2}^2 = \sum (A_j x_j^2 + B_j y_j^2) \quad (5.31)$$

It remains to show under what circumstances an argument in the wave norm implies the same conclusion in the L2 norm, for we have already proven stability in the wave norm, at Eqn. (5.19). Equivalence of these two norms requires the existence of positive constants⁶ K_1 and K_2 such that

$$K_1 \|Z\|_{L2} \leq \|Z\|_{WN} \leq K_2 \|Z\|_{L2} \quad (5.32)$$

That such constants must exist may be seen from the positive definiteness condition, for, one may write,

$$\|Z\|_{WN}^2 = \sum (A_j x_j^2 + B_j y_j^2 + x_j \Delta_j y_j) \quad (5.33)$$

or

⁴ Richtmyer & Morton (1967), p. 31.

⁵ MacLane & Birkhoff (1967) p. 392, ff.

⁶ Richtmyer & Morton (1967), p. 57.

$$Z_{L2}^2 = (Z_{L2}^2 + \sum_j \Delta_j v_j) \quad (5.34)$$

For the right hand sides of Eqns. (5.31-34) to be positive it is necessary that

$$Z_{L2}^2 = \sum_j \Delta_j v_j$$

A_2 in Eqn. (5.32) may be taken as 2, and A_1 is greater than zero if $A_j = 1$, and $B_j = 1$ in Eqn. (5.31). This completes the proof of stability of the plane wave difference equations in the wave norm and therefore also in the L2 norm.

Cylindrical Waves

The case of cylindrical waves may be reduced to that of plane waves. Eqn. (5.2) may be written in full

$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{c^2 \Delta t^2} = \frac{1}{r_{j+1/2} r_{j-1/2}} \left\{ \frac{u_{j+1}^n - u_j^n}{r_{j+1/2} - r_j} - \frac{u_j^n - u_{j-1}^n}{r_j - r_{j-1/2}} \right\} \quad (5.35)$$

To deal with the left hand side first, one may define

$$v_j^n = \frac{r_j (u_j^n - u_{j-1}^{n-1})}{c \Delta t} \quad (5.36)$$

and write

$$A_j(v_j^{n+1} - v_j^n) = r_j \left(\frac{u_{j+1} - u_j}{r_{j+1} - r_j} - \frac{u_j - u_{j-1}}{r_j - r_{j-1}} \right) + u_{j+1} - u_{j-1} \quad (5.37)$$

with $A_j = (r_{j+1} - r_{j-1})/2c\Delta t$, as before. The right hand side may be rearranged as

$$\frac{u_{j+1}(r_{j+1} + r_{j-1} - r_j) - r_j u_j}{r_{j+1} - r_j} - \frac{u_j r_j - u_{j-1}(r_j - r_{j-1} + r_{j-1})}{r_j - r_{j-1}}$$

or,

$$\frac{r_{j+1} u_{j+1} - r_j u_j}{r_{j+1} - r_j} - \frac{r_j u_j - r_{j-1} u_{j-1}}{r_j - r_{j-1}}$$

Defining

$$w_j^n = \frac{r_j u_j^n - r_{j-1} u_{j-1}^n}{r_j - r_{j-1}} \quad (5.38)$$

the difference equation (5.35) may be written as

$$A_j(v_j^{n+1} - v_j^n) = w_{j+1}^n - w_j^n \quad (5.39)$$

A first order difference equation in w may be constructed,

$$B_j(w_j^{n+1} - w_j^n) = v_j^{n+1} - v_{j-1}^n \quad (5.40)$$

with $B_j = (r_j - r_{j-1})/c\Delta t$, as before. Eqns. (5.39) and (5.40) are identical to Eqn. (5.19), although v_j and w_j have been defined a little differently for the cylindrical case. The definition of the wave norm,

of course, proceeds as before, and the Courant condition on the timestep is obtained in the same way.

Hydrodynamics

Hydrodynamics may also be reduced to the plane wave treatment. One obtains a wave norm based only on the pressures, and we tacitly assume that instability will always include instability of the pressures⁷. Thus, stability of the pressure equation is taken to imply stability of the entire system of equations. Only the plane case is considered here, as the other geometries introduce nothing qualitatively new.

The difference equations may be exhibited:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{P_{j+1} - P_j}{m_j + m_{j+1}} \quad (5.41)$$

$$x_j^{n+1} - x_j^n = u_j^{n+1} \Delta t \quad (5.42)$$

$$V_j^n = (x_{j+1}^n - x_j^n) \cdot m_j \quad (5.43)$$

The rest of the equations will only bear indirectly on what follows.

The quantities x_j , u_j , V_j , are the (Lagrangian) position, velocity, and specific volume. P_j is the pressure, including the artificial

⁷ It must include instability of pressures; for the Lagrangian coordinates to diverge requires that the pressures vanish, by the equation of state, but this is forbidden by the boundary conditions. For any other quantity to diverge requires (again through the equation of state) that the pressures also diverge.

viscosity. Eqn. (5.41) written at zone j and again at zone $j+1$ may be combined to give

$$2\Delta t \left\{ \frac{P_{j+1}-P_j}{m_{j+1}+m_j} - \frac{P_j-P_{j-1}}{m_j+m_{j-1}} \right\} = u_j^{n+1} - u_j^n - u_{j+1}^n + u_{j+1}^{n+1} \quad (5.44)$$

The sound speed c may be defined by

$$V^2 dP = -c^2 dV \quad (5.45)$$

Here in the definition of the sound speed is where the effect of difference equations in energy and the equation of state for the pressure are felt. The volume change dV in Eqn. (5.43) is envisioned as

$$V_j^{n+1} - V_j^n = (u_{j+1}^n - u_j^n) \Delta t / m_j \quad (5.46)$$

Eqns. (5.43) and (5.44) may be combined to give

$$\begin{aligned} u_{j+1}^{n+1} - u_j^{n+1} &= \frac{m_j V_j^2}{c^2 \Delta t} (p_j^{n+1} - p_j^n) \\ u_{j+1}^n - u_j^n &= - \frac{m_j V_j^2}{c^2 \Delta t} (p_j^n - p_j^{n-1}) \end{aligned} \quad (5.47)$$

These may be combined with Eqn. (5.44) to give

$$2 \left(\frac{P_{j+1}-P_j}{m_{j+1}+m_j} - \frac{P_j-P_{j-1}}{m_j+m_{j-1}} \right) = \frac{m_j V_j^2}{c^2 \Delta t^2} (p_j^{n+1} - 2p_j^n + p_j^{n-1}) \quad (5.48)$$

One may now define two quantities y_j and w_j by

$$y_j^{n+1} = \frac{p_j^{n+1} - p_j^n}{c\Delta t}$$

$$w_j^n = 2 \frac{p_j^n - p_{j-1}^n}{m_{j-1} + m_j} \quad (5.49)$$

and reduce Eqn. (5.46) to a pair of first order equations:

$$y_j^{n+1} - y_j^n = \frac{c\Delta t}{m_j v_j^2} (w_{j+1}^n - w_j^n)$$

$$w_j^{n+1} - w_j^n = \frac{2c\Delta t}{m_j + m_{j+1}} (y_j^{n+1} - y_{j+1}^{n+1}) \quad (5.50)$$

And with

$$A_j^{-1} = \frac{c\Delta t}{m_j v_j^2} \quad \text{and} \quad B_j^{-1} = \frac{2c\Delta t}{m_j + m_{j+1}} \quad (5.51)$$

one has again exactly Eqn. (5.14), the plane wave equations proven stable above.

CHAPTER VI
STABILITY AND CONVERGENCE
IN THE PRESENCE OF
THE METHOD OF INDEPENDENT TIMESTEPS

Parabolic Equations: Stability

The last two chapters provided stability analyses of parabolic and hyperbolic difference equations. While there are more common and intuitively simple techniques for stability analysis, independent timesteps render these approaches a bit difficult and unconvincing. It was felt clearer to present the analyses of Chapters IV and V for equations with a common timestep and to wait until now to show how the argument needs to be modified to accomodate individual timesteps. Parabolic equations will have stability properties hardly different in the presence of independent timesteps. Hyperbolic equations will be a little more intricate. It is also necessary, if one would warrant a difference technique for general use, to say something about its truncation error, which is to indicate its consistency with its

differential equation. Having established consistency and stability, there are various theorems which ensure convergence; i.e., that with refinement of the mesh the calculation gives a solution which is not only finite (stability is no more than this) but which approximates the true answer.

In the common explicit difference scheme (Eqn. (4.10) or (4.27)), the temperature at the forward time, u_j^{n+1} must be bounded by one of the values of u at the time t^n , u_j^n , u_{j+1}^n , or u_{j-1}^n . This was easy enough to do, but suppose, as in Fig. (6.1), one of u_{j+1}^n or u_{j-1}^n was not available at time t^n and an estimate was supplied from earlier values:

$$\frac{u_j^{n+1} - u_j^n}{t_j^{n+1} - t_j^n} = \frac{u_j^{n+1} - u_j^n}{\Delta t_j^n} = A(u_j^{n+1} - 2u_j^n + u_{j-1}^n) \quad (6.1)$$

with

$$u_{j-1}^n = u_{j-1}^{n-1} + (t_j^n - t_{j-1}^{n-1}) \frac{u_{j-1}^{n-1} - u_{j-1}^{n-2}}{t_{j-1}^{n-1} - t_{j-1}^{n-2}} \quad (6.2)$$

It is, of course, easy to bound u_j^{n+1} by one of u_j^n , u_{j+1}^n , or u_{j-1}^n , but how is one to bound u_{j-1}^n , the estimate of u_{j-1}^n ?

The answer lies in looking at how u_{j-1}^{n-1} was itself calculated, and how the time t_{j-1}^{n-1} was selected for that calculation. It was then decided that zone $j-1$ could go unattended for some length of time Δt_{j-1}^{n-2} after which u_{j-1}^{n-1} would no longer be bounded. Since we are interested in using the same process to get u_{j-1}^n at time t_j^n , the original constraint on Δt_{j-1}^{n-2} must be tightened. For the estimate of $(\partial u / \partial t)$ at x_{j-1} and t_{j-1}^{n-2} must now be safely usable as late as t_j^n . Now the timesteps in

zones j and $j-1$ can differ by no more than a factor of two; this was demanded at Eqn. (3.56). If Δt_j is longer than Δt_{j-1} , zone $j-1$ will fall due before zone j , and there will be no need for an estimate u_{j-1}^n . So, assuming that $\Delta t_j < \Delta t_{j-1}$, it must then be that t_j^n falls no later than $t_{j-1}^{n-2} + 2\Delta t_{j-1}^{n-2}$. And, in order to warrant u_{j-1}^n at a time as late as t_j^n , it is sufficient that the difference equation be stable for a time of duration $\Delta t_{j-1}^{n-2} + \Delta t_j^{n-1} \leq 3\Delta t_{j-1}^{n-2}$ (by Eqn. (3.1)). In most situations, however, the timestep need not be cut. If both the first and second time derivative of the temperature are positive, the temperature estimate for a neighboring zone will be low, by using an old value of the first derivative, and therefore it will be safely bounded. If the second derivative is negative and the first positive, more caution is indicated, according to the rule just indicated. If the first derivative is negative, the timestep need not be cut, since the temperatures will always be safely bounded.

Having thus prepared the calculations at zone $j-1$, it is now safe to use u_{j-1}^n and the calculation at zone j may proceed in complete assurance of stability, and, therefore, the entire calculation is stable.

Hydrodynamics: Stability

There are many hyperbolic equations, but the argument for stability here is intended specifically for those of hydrodynamics. The work in independent timesteps was all done with hydrodynamics and the situation there should be typical.

Fig. (6.1) An Estimate of a Neighboring Temperature

The reduction to a pair of first order equations is straightforward, along the lines of the argument of the last chapter. In the requisite definitions the timesteps have been changed in order to yield the altered difference equations. The norm may be defined as before. Proving that it is bounded is no longer so simple, however. There is a theorem which states that a stable system of difference equations can tolerate small perturbations and still remain stable; and it may be seen that independent timesteps introduce just such a small perturbation.

The reduction to a pair of first order equations (eqn. (5.14)) may proceed as before if one now defines the quantities y and w by

$$y_j^n = \frac{p_j^n - p_j^{n-1}}{c \Delta t_j^n}, \quad w_j^n = 2 \frac{p_j^n - p_j^{n-1}}{m_j + m_{j-1}} \quad (6.3)$$

and the coefficients a and b by

$$A_j^n = \frac{2m_j V_j^2}{c(t_j^{n+1} - t_j^{n-1})}, \quad B_j^n = \frac{m_j + m_{j-1}}{2c \Delta t_j^n} \quad (6.4)$$

The difference equations then become

$$\begin{aligned} A_j^n (y_j^{n+1} - y_j^n) &= w_{j+1}^n - w_j^n \\ B_j^n (w_j^{n+1} - w_j^n) &= y_j^{n+1} - y_{j-1}^n \end{aligned} \quad (6.5)$$

The timestep in the denominator of A_j^n is chosen to cover the time spanned by the two quantities y_j^{n+1} and y_j^n .

Fig. (6.2) A Mesh with Independent Timesteps

The squared norm of the function (y, w) may be defined exactly as in Eqn. (5.25),

$$\|Z\|^2 = \Sigma Q_j^n, \text{ with} \quad (6.6)$$

$$Q_j^n = \frac{1}{2} \left(A_j y_j^2 + B_j w_j^2 - 2y_j w_j \right) + \frac{1}{2} \left(A_j y_{j+1}^2 + B_j w_{j+1}^2 + 2y_{j+1} w_{j+1} \right)$$

with the terms a, b, y, w here defined for independent timesteps by Eqns. (6.3-4). In regions of a computation mesh which have a common timestep, advancing the computation will not change ΣQ_j , and this is so in different regions regardless of the fact that they proceed with different timesteps. But where adjacent zones do not share a common timestep, it is not clear that what is taken from one Q_j is what is given to its neighbor, Q_{j+1} . The mesh contemplated is illustrated in Fig. (6.2). At time t^{n+1} , the pressure P_j^{n+1} is unavailable and is approximated by P_j^n . So, following Eqns. (2.1-2.6), as x_{j+1} is advanced from t^{n+1} to t^{n+2} , the effect shows up in the volumes V_{j+1}^{n+2} and V_j^{n+2} , and from there by the energy equation and the pressure equation of state the change shows up in the pressures P_{j+1}^{n+2} and P_j^{n+2} . The two pressures P_{j+1}^{n+2} and P_j^{n+2} contribute to the terms Q_{j+1}^{n+2} , Q_j^{n+2} , Q_{j+1}^{n+2} , Q_j^{n+2} in the sum ΣQ_k^{n+2} , for each term Q_k^n in that sum depends on the four pressures P_k^{n-1} , P_k^n , P_{k+1}^n , P_{k-1}^n , through its dependence on y_k^n , w_k^n , and w_{k+1}^n . In the mesh illustrated in Fig. (6.2), there is no effect on Q_k for $k < j-1$ or $k > j+2$. It is now necessary to estimate how serious is the effect on the terms $Q_{j-1}, \dots, Q_{j+2}$.

There is a theorem of Kreiss and Strang summarized by Richtmyer¹ which

¹ Richtmyer & Morton (1967), pp. 58-59.

says in effect that a sufficiently small perturbation will not affect the stability of an already stable difference scheme. If the difference system $u^{n+1} = C(\Delta t)u^n$ is stable, and if $C(\Delta t)$ is a bounded family of operators, then the system $u^{n+1} = (C + \Delta t G)u^n$ is also stable. The operator $C + \Delta t G$ depends through C and G on Δt . What is in effect said is that the perturbation operator $\Delta t G$ must vanish as Δt is refined. Then the operator

$$\left(C(\Delta t/m) + (\Delta t/m)G(\Delta t/m) \right)$$

remains finite as m tends to infinity, and it is this operator which carries the function u^n forward to some fixed time $t = m(\Delta t/m)$. (It is by the same principle that interest at a constant rate compounded ever more finely still only yields a finite return on investment.)

So, if the perturbation on the terms $Q_{j-1}^{n+2}, \dots, Q_{j+2}^{n+2}$ can be shown to be of first or higher order in Δt , then the sum $\Sigma Q(t^{n+2})$ will remain finite as the mesh is refined and time t^{n+2} is reached in ever more and ever briefer timesteps.

The argument is pretty much the same for each of the four Q 's mentioned, and so only Q_j^{n+2} will be examined in any detail. The perturbation on Q_j^{n+2} will be found by repeated use of the chain rule for derivatives. Suppose, in Fig. (6.2), the pressure P_j^{n+1} were available. The perturbation first appears as $dP = P_j^* - P_j^{n+1}$. Let this be denoted as dP_j^{n+1} , or simply dP if no indices are specified. It is required to find dP_j^{n+2} and dP_{j+2}^{n+2} , and from these, the dQ_j^{n+2} . Following Eqns. (2.1-3), one has

$$u_{j+1}^{n+2} - u_{j+1}^{n+1} = -2(t^{n+2} - t_{j+1}^{n+1})(p_{j+1}^{n+1} - p_j^n) / (m_j + m_{j+1}) \quad (6.7)$$

$$du_{j+1}^{n+2} = 2\Delta t_{j+1}^{n+1} dp / (m_j + m_{j+1}) \quad (6.8)$$

$$dx_{j+1}^{n+2} = 2(\Delta t_{j+1}^{n+1})^2 dp / (m_j + m_{j+1}) \quad (6.9)$$

$$dv_{j+1}^{n+2} = 2 \frac{-(\Delta t_{j+1}^{n+1})^2 dp}{m_{j+1}(m_j + m_{j+1})} \quad (6.10)$$

$$dv_j^{n+2} = 2 \frac{(\Delta t_{j+1}^{n+1})^2 dp}{m_j(m_j + m_{j+1})}$$

From the definition $-V^2 dp = c^2 dV$ of the sound speed c , one may obtain the pressure perturbations at time t^{n+2} :

$$\begin{aligned} dp_{j+1}^{n+2} &= \frac{c^2 (\Delta t_{j+1}^{n+1})^2 dp}{V_{j+1}^2 m_{j+1} (m_j + m_{j+1})} \\ dp_j^{n+2} &= -2 \frac{c^2 (\Delta t_{j+1}^{n+1})^2 dp}{V_j^2 m_j (m_j + m_{j+1})} \end{aligned} \quad (6.11)$$

These, together with Eqn. (6.3) yield

$$dy_j^{n+2} = \frac{-2c(\Delta t_{j+1}^{n+1})^2 dp}{V_j^2 m_j (m_j + m_{j+1}) (t^{n+2} - t_j^n)} \quad (6.12)$$

$$du_j^{n+2} = \frac{-4c^2(\Delta t_{j+1}^{n+1})^2 dP}{V_{j+1}^2 m_j (m_j + m_{j+1}) (m_j + m_{j+1})} \quad (6.13)$$

$$du_{j+1}^{n+2} = 4 \frac{c^2(\Delta t_{j+1}^{n+1})^2 dP}{V_{j+1}^2 m_j (m_j + m_{j+1})^2} \quad (6.14)$$

The expansion of dQ_j^{n+2} may be written:

$$\begin{aligned} Q_j &= A_j y_j^2 + \frac{1}{2} B_j u_j^2 + \frac{1}{2} B_{j+1} u_{j+1}^2 - 2y_j w_j + 2y_j w_{j+1} \\ dQ_j^{n+2} &= \left(2A_j y_j dy_j + B_j w_j du_j + B_{j+1} w_{j+1} du_{j+1} \right. \\ &\quad \left. + 2y_j dw_j - 2w_j dy_j + 2y_j dw_{j+1} + 2w_{j+1} dy_j \right) \end{aligned} \quad (6.15)$$

The expansions of dQ_{j-1} , dQ_{j+1} , and dQ_{j+2} are similar. To deal with the first of the seven terms of Eqn. (6.15):

$$2A_j y_j dy_j = \frac{-B(P_j^{n+2} - P_j^n)(\Delta t_{j+1}^{n+1})^2 dP}{(m_j + m_{j+1})(\Delta t_j^n)^2 (t^{n+2} - t_j^{n-1})} \quad (6.16)$$

This is of the same order as dP , for, $(\Delta t_{j+1}^{n+1})^2 / (\Delta t_j^n)^2 = 1/4$; and $(P_j^{n+2} - P_j^n) / (t^{n+2} - t_j^{n-1})$ is roughly constant as Δt is reduced. This leaves dP , which may be shown of order Δt .

The timestep is set by a condition on the permissible change in pressure:

$$P_j^{n+2} - P_j^n \leq \epsilon P_j^n \quad (6.17)$$

where ϵ is some small number, typically 0.05 or less. Now P_j^n and P_j^{n+1}

both will fall in the range of (P_j^n, P_j^{n+2}) , so their difference, dP , will be limited by

$$|dP| \leq |P_j^{n+2} - P_j^n| = (\partial P / \partial t) \Delta t_j^n. \quad (6.18)$$

proving that as Δt is reduced, dP must vanish also. Thus, the first term of Eqn. (6.15) is of first order in Δt , and by similar arguments it may be verified that the other terms are all second or third order in the timesteps. This completes the proof that the equations of hydrodynamics are stable in the presence of independent timesteps.

Parabolic Equations: Truncation Error

Having shown stability of asynchronous calculations, it is necessary that the finite equations do in fact approximate the differential equation over a period of one timestep. This is the property of consistency. Given these two properties, it is assured that the system of interest will yield answers converging to the true solution². Analysis of consistency will indicate how the error at each timestep depends on the mesh size. This analysis is obtained by comparing the exact solution with the finite difference solution by means of the Taylor expansion of the exact solution.

In the case of the diffusion equation, one needs Taylor series for u_j^{n+1} , u_{j+1}^n , u_{j-1}^n :

² Richtmyer & Morton (1967), see for example p. 45.

$$u_j^{n+1} = u_j^n + \Delta t u_t + \frac{1}{2} \Delta t^2 u_{tt} + \frac{1}{6} \Delta t^3 u_{ttt} + \dots \quad (6.19)$$

$$u_{j+1}^n = u_j^n + \Delta x u_x + \frac{1}{2} \Delta x^2 u_{xx} + \frac{1}{6} \Delta x^3 u_{xxx} + (1/24) \Delta x^4 u_{xxxx} + \dots \quad (6.20)$$

$$u_{j-1}^n = u_j^n - \Delta x u_x + \frac{1}{2} \Delta x^2 u_{xx} - \frac{1}{6} \Delta x^3 u_{xxx} + (1/24) \Delta x^4 u_{xxxx} + \dots \quad (6.21)$$

The error may be constructed:

$$E = \frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\sigma}{\Delta x^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) - (u_t - \sigma u_{xx})_j^n \quad (6.22)$$

And substituting Eqns (6.19-6.21) into Eqn. (6.22) gives

$$E = \frac{1}{2} \Delta t u_t - (1/12) \Delta x^2 \sigma u_{xxxx} + \dots \quad (6.23)$$

This will be modified somewhat in the presence of individual timesteps.

For u_{j-1}^n in Eqn. (6.22) substitute

$$u_{j-1}^n = u_{j-1}^{n-1} + (t_j^n - t_{j-1}^{n-1}) \frac{u_{j-1}^{n-1} - u_{j-1}^{n-2}}{t_{j-1}^{n-1} - t_{j-1}^{n-2}} \quad (6.24)$$

Defining

$$R = \frac{t_j^n - t_{j-1}^{n-1}}{t_{j-1}^{n-1} - t_{j-1}^{n-2}}$$

one has

$$\begin{aligned}
u_{j-1}^n = & (1+R) \left(u_j^n - \Delta x u_x - \Delta t u_t + \frac{1}{2} \Delta x^2 u_{xx} \right. \\
& + \frac{1}{2} \Delta t^2 u_{tt} - \frac{1}{3} \Delta t^3 u_{3t} - \frac{1}{6} \Delta x^3 u_{3x} + (1/24) \Delta x^2 u_{4x} \Big) \\
& - R \left(u_j^n - \Delta x u_x - 2 \Delta t u_t + \frac{1}{2} \Delta x^2 u_{xx} + 2 \Delta t^2 u_{tt} \right. \\
& \left. - \frac{1}{6} \Delta t^3 u_{3t} - \frac{1}{6} \Delta x^3 u_{3x} + (1/24) \Delta x^4 u_{4x} \right)
\end{aligned} \tag{6.25}$$

By comparison with Eqn. (6.21) this may be reduced to

$$u_{j-1}^n = u_j^n + (R-1) \Delta t u_t + \left(\frac{1}{2} - \frac{3}{2} R \right) \Delta t^2 u_{tt} + \tag{6.26}$$

Substituting Eqn. (6.26) into Eqn. (6.22) in place of u_{j-1}^n , the new error E' is given by

$$E' = E + \frac{\sigma \Delta t}{\Delta x^2} (R-1) u_t + \Delta t \left(\frac{1}{2} - \frac{3}{2} R \right) \frac{\sigma \Delta t}{\Delta x^2} u_{tt} \tag{6.27}$$

This equation indicates the additional error introduced where the timestep changes from one zone to the next. Where adjacent timesteps are the same, the error is given by Eqn. (6.23) as before. The quantity $u_t \Delta t$ is generally used to set the timestep (in the absence of stronger stability constraints) in order to control the error. With independent timesteps the contributions to the error are commensurate throughout the mesh. In Eqn. (6.27) the quantity $\sigma \Delta t / \Delta x^2$ is zero order in time, and so the most serious contribution to the error is the term $(\sigma \Delta t / \Delta x^2) (R-1) u_t$.

It should be noted that the error of Eqn. (6.23) or Eqn. (6.27) is the error not in u_j^{n+1} itself but the difference between the differential equation and its finite approximation: the error quoted is the error in the first derivative of u . And where adjacent timesteps differ, this

error appears as an inconsistency with the differential equation. Although only conditionally consistent, calculation with independent timesteps yields answers within 1 to 3 percent of the same calculations with a common timestep. So, the error of Eqn. (6.27) (and it is an occasional error, not a chronic one) evidently does not adversely affect the results. The error in approximating the differential equation is (occasionally) of zero order in Δt , amounting to altering the value of σ . The resultant error in u_j^{n+1} is roughly given by factors of order unity times $u_j \Delta t$.

Hydrodynamics: Truncation Error

The equations of hydrodynamics present consistency behavior essentially like that of parabolic equations. It is sufficient to examine the acceleration equation. As written, the pressures were referred to zones j and $j-1$, since in FORTRAN, one has only integral indices of variables. But to be more precise, the pressure P_j at the zone center should be called $P_{j+1/2}$, and P_{j-1} should be called $P_{j-1/2}$, and their Taylor series constructed accordingly. The error in the equation is

$$E = \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{P_{j+1/2} - P_{j-1/2}}{\rho \Delta x} - (u_t + P_{x/x}) \quad (6.28)$$

The Taylor expansions required are

$$u_j^{n+1} = u_j^n + \Delta t u_{jt} + \frac{1}{2} \Delta t^2 u_{jtt} + \frac{1}{6} \Delta t^3 u_{jt t t} + \dots \quad (6.29)$$

$$P_{j+1/2} = P_j^n + \frac{1}{2}\Delta x P_x + \frac{1}{6}\Delta x^2 P_{xx} + (1/48)\Delta x^3 P_{3x} + \dots \quad (6.30)$$

$$P_{j-1/2} = P_j^n - \frac{1}{2}\Delta x P_x + \frac{1}{6}\Delta x^2 P_{xx} - (1/48)\Delta x^3 P_{3x} + \dots \quad (6.31)$$

The error may be exhibited:

$$E = \frac{1}{2}\Delta t u_{tt} + \frac{1}{6}\Delta t^2 u_{3t} + (1/48)\Delta x^2 P_{3x} + \dots \quad (6.32)$$

As before, the quantity $P_{j-1/2}^*$ used in the absence of $P_{j-1/2}^n$ is given by

$$P_{j-1/2}^* = P_{j-1/2}^{n-1} + (t_j^n - t_{j-1}^{n-1}) \frac{P_{j-1/2}^{n-1} - P_{j-1/2}^{n-2}}{t_j^{n-1} - t_{j-1}^{n-2}} \quad (6.33)$$

Its Taylor series is

$$P_{j-1/2}^* = P_{j-1/2}^n + \left(\frac{1}{2} - \frac{3}{2}R\right)\Delta t^2 P_{tt} + \dots \quad (6.34)$$

The resulting altered error is

$$E' = E - \frac{(R-1)\Delta t}{\Delta x} P_t - \left(\frac{1}{2} - \frac{3}{2}R\right) \frac{\Delta t^2}{\mu \Delta x} P_{tt} \quad (6.35)$$

The same observations might be made here as applied to the case of parabolic equations. The error is of zero order, occasionally, and usually of first order in Δt . The remarks of Chapter II on the accuracy of hydrodynamics with independent timesteps should provide an index of their effect on the answers obtained.

CHAPTER VII

COMPARATIVE ECONOMICS: TIMING TRIALS

Time Trials in One Dimension: Hydrodynamics

As this work has progressed there has been a continuing interest in timing comparisons between asynchronous and synchronous methods, whatever the synchronous difference techniques appropriate to that problem were. The early results were encouraging, albeit barely so. All of the time trials used very simple test problems; this is the conservative way to test the method, inasmuch as more complex problems may be expected to show the method of independent timesteps in a much better light. Such problems are common in real applications, and there it should not be out of the ordinary for a very few zones to want timesteps much briefer than the rest of the mesh. The present timing trials are unrealistically conservative in two other respects as well. Nowhere have real world properties of matter been approximated, and as physical equations of state are computationally expensive to handle, independent timesteps should yield proportionately larger savings. Instead, a perfect gas equation of state and simple analytic heat

conductivities have been assumed. Also nowhere have advantages been taken of hand coding the management of independent timestep logic; in particular, there are fast search routines which could search a mesh for zones due for updating (Eqn. (3.7)). Eqn. (3.7) was everywhere coded in FORTRAN, and in the hydrodynamic work, very inefficiently.

In fact the hydrodynamic time trials in one dimension yielded results consistently but barely faster than conventional explicit von Neumann difference equations. A factor of two or better was occasionally seen, but 50% speed increases were often only to be hoped for. And looking at the FORTRAN in question, one may be amazed that independent timesteps ever did as well as conventional methods. For seemingly at every opportunity, the entire mesh was searched (after a subroutine jump!), and operations which could have been combined in one loop were apportioned among several, for ease in debugging.

Still, it is fair to describe the experience with one dimensional hydrodynamics. A shock problem of 81 zones and three regions was computed. The shock is created by a constant over-pressure at one boundary, while the other boundary is held fixed in position. The dimensionless shock strength varied from 10 to 10^5 , and the shock impinges first on a region of density 2 g/cc, then a thin region of density 20 g/cc, and then into a region of density 0.001 g/cc, affording a situation with several shock reflections. The timing results were pretty much the same regardless of shock strength. In one such problem, independent timesteps completed the task in 0.307 minutes, and the conventional method in 0.313; in another the comparison was 0.386 minutes (independent timesteps) and 0.428 (conventional), a difference

of about 10%. Times of 8.53 and 10.36 minutes were observed in a simpler problem (two regions, comparable densities), a time difference of 15%. The chief reason why independent timesteps took so long is that the FORTRAN coding of the control logic was so fearsomely inefficient. These comparisons were made on a CDC 6600. That the method of independent timesteps did so well under such burdensome circumstances motivated more study and development of the technique.

Time Trials in One Dimension: Diffusion

In preparation for two dimensional diffusion trials, the one dimensional diffusion equations were differenced and tested with independent timesteps. The timing results were quite favorable, yielding comparisons of a factor of 3 to 6 quite routinely on very conservative test problems. The equation to be integrated was discussed at Eqns. (4.2-4.3). The boundary conditions represented a bar heated at one end, and the problems were terminated only when nearly in temperature equilibrium. Forty zones were used and the diffusion coefficient was taken as having the form $\sigma = Au^m$. This represents the minimum of realism necessary to use independent timesteps at all. If a constant diffusion coefficient is used, the timesteps will be commensurate in all zones, and an implicit code will always run faster, but if the exponent in the diffusion coefficient is taken as low as 1, the situation is altogether reversed. In all calculations, the timestep was governed by the requirement that $\Delta u/u$ be less than ϵ , with $\epsilon = 0.01$ to $\epsilon = 0.05$. In the independent timestep code, which is explicit, the timestep is limited also by the Courant condition. With a

conductivity proportional to the temperature, the temperature profile resembles that of a shock, as in Fig. (7.1). Ahead of the thermal wave the conductivity is small and behind it very large, resulting in near equilibrium behind the front. In these calculations, eqn. (3.6), the restriction on disparity of neighboring timesteps, was enforced at every cycle over the whole mesh. The briefest timestep is in the growing edge of the warmed region, at about zone 22 in Fig. (7.1), and the timesteps on either side of this zone may be seen to increase by a factor of two per zone. The temperatures and timesteps plotted in Fig. (7.1) are taken from data at cycle 3731 of a computation with diffusion coefficient given by $\sigma = 10^{-12}u^3$, and $\Delta u/u \leq 0.05$.

The calculations were terminated when a fixed amount of heat has diffused into the problem across the hot boundary. The stop time is therefore somewhat variable, depending on the accuracy demanded, and its convergence may taken as a measure of that accuracy. The results of the time trials are summarised in Table (7.1). The first column identifies the code; MITS, the Method of Independent TimeSteps, IMPD, IMplicit Forward Differences, or EXBD, EXplicit Backward Differences. The second column is the time in seconds required for the calculation as monitored by the system timing routine TICHECK. The third and fourth columns are the cycle number and physical time at the end of computation, when the heat source has warmed almost all of the problem. The column labelled $\Delta u/u$ identifies the maximum permissible change per cycle in any temperature. It will be seen that $\Delta u/u$ and the ending cycle number vary more or less inversely as one another. The last column indicates for the MITS code the ratio of the number of zone-cycles it would have computed if it never skipped calculations, to the number of zone-cycles

actually calculated. It may be seen that a more stringent $\Delta u/u$ control requires that MITS calculate some zones more often, but not all. It may also be seen that the implicit code required a tighter $\Delta u/u$ control and briefer timesteps to approach its limiting value of the stop time. The trials are presented in three groups, for the diffusion coefficients of $10^{-12}u^3$, u , and 10^{12} respectively. In the first group, with $\sigma = 10^{-12}u^3$, it may be seen that all three codes eventually converged to a stop time of 8.084 to 8.101×10^{-4} sec, a range of 0.2%. At 7.82×10^{-4} sec, the initial guess by IMFD (with $\Delta u/u = .05$) is bad by about 3%. This raises the question of which run time, 65.7 sec (with $\Delta u/u = .05$) or 155.6 sec (with $\Delta u/u = .01$) should be used for IMFD. The ratio of run times, IMFD/MITS, is 7.13 or 3.01 depending on which value one prefers. In the second group of trials, as in the first, the timestep must be briefer for the implicit code to yield accuracy comparable to the explicit results. The run time ratio may be estimated at 4.0 to 9.5. In the last group, with the diffusion coefficient a constant independent of u , IMFD runs about twice as fast as the MITS or EXBD codes, as expected. Two conclusions may be drawn from this experience. First, as hoped, even on very conservative test problems, independent timesteps run significantly faster than implicit methods. Secondly, it is possible to demand fine accuracy of MITS in a few crucial zones without bogging down the whole problem in needlessly precise calculations.

Table (7.1) Time Trials in One Dimension: Diffusion

Diffusion Coefficient = $10^{-12}u^3$					
code	compu- tation time,	cycle number	stop time, 10^{-4} sec sec	$\Delta u/u$	compu- tation ratio
MITS	21.8	10829	8.091	.05	1.72
IMFD	65.7	8086	7.820	.05	
EXBD	23.1	10549	8.101	.05	
MITS	64.1	41983	8.098	.01	2.54
IMFD	155.6	40316	8.084	.01	
EXBD	99.4	41351	8.101	.01	
Diffusion Coefficient = u					
code	compu- tation time,	cycle number	stop time, 10^{-4} sec sec	$\Delta u/u$	compu- tation ratio
MITS	16.0	8315	2.111	.05	1.69
EXBD	19.9	8176	2.113	.05	
MITS	35.2	28988	2.112	.01	2.44
IMFD	58.7	25739	2.083	.01	
IMFD	155.9	85739	2.112	.003	
EXBD	55.1	28498	2.113	.01	
Diffusion Coefficient = 10^{12}					
code	compu- tation time,	cycle number	stop time, 10^{-4} sec sec	$\Delta u/u$	compu- tation ratio
MITS	10.5	4334	3.300	.05	1.00
EXBD	10.6	4332	3.300	.05	
IMFD	5.3	1280	3.139	.05	
MITS	19.3	9095	3.300	.01	1.01
EXBD	19.4	9095	3.300	.01	
IMFD	14.4	6370	3.321	.01

Fig. (7.1) A One Dimensional Heat Diffusion Problem

Time Trials in Two Dimensions

The experience in two dimensional calculations of heat diffusion problems confirms and extends the conclusions drawn from one dimensional work. There were very few peculiarities of two dimensions which required different handling than in one dimension, and these were treated in chapter III. It was remarked there that careful coding of Eqn. (3.6), the restriction on neighboring timesteps, affords a savings of up to 50% in running time, clearly well worth while.

As in the one dimensional calculations, the two dimensional time trials were made with conservative test problems, some of which do not have much two dimensional structure. The results are a factor of three to ten observed in running speed between the 2D MITS and the ADI codes. The equations integrated were discussed at Eqns. (3.24-3.25), and independent timesteps were implemented as discussed in the beginning of chapter III, Eqns. (3.1-3.7), and at Eqns. (4.2-4.3). The diffusion coefficient is taken as variable, again of the form $\sigma = Au^m$.

The problem of chapter III may be summarized. The diffusion coefficient was $\sigma = 8 \times 10^{-16} u^4$, the mesh was 30x30 zones square, and $\Delta u/u \leq .05$. The problems were all stopped at $t = 5.263 \times 10^{-5}$ sec, and the running times are as follows:

Table (7.2) Timing in the Problem of Chapter III

	cycle	time
MITS	3357	34.85
ADI	3596	268.62
EXBD	3454	107.45

The computation ratio for MITS was 27; and the ratio of running times is 7.7. This problem was not run very far towards equilibrium, as Figs. (3.5-3.6) show.

Two problems were run which are very similar to the one dimensional tests, one with $\sigma = 10^{-12}u^3$ and one with $\sigma = u$. The heat is supplied at the corner of the mesh, which is 16x16 zones. The initial temperatures are 1° and the source is at 10^{60} . The first problem, with $\sigma = u$, may be summarized at two times, roughly 1.5×10^{-4} sec and 6.6×10^{-4} sec:

Table (7.3) Two Dimensional Timing Comparisons

code	time 10^{-4} sec	cycle	run time sec
MITS	1.68	3003	10.96
ADI	1.51	2905	62.88
MITS	8.68	5661	26.60
ADI	8.52	3723	80.51

The ratios of run times are about 6 and 3. These latter numbers are taken as the problem reaches equilibrium. The temperature distributions plotted by MITS at cycle 3003 is shown in Fig. (7.2).

TDH	AS ID PROB	U	PCTS,XTIME	059:00:00	10.96		
NC	T	DT	SSJN	JKN	SRAT	UTOT K,LWST	
3003	1.684823E-04	1.589246E-07	106704	5.0588	5.5E+00	5.5E+07 12 15	
SCALE:	LOG F: 1.00 MAX	1.00E+06 MIN	1.00E-01				

Fig. (7.2) A Two Dimensional Heat Diffusion Problem.

TDH	AS ID PROB	U	PCTS,XTIME	099:00:00	9.65		
NC	T	DT	SSJN	JXN	SRAT	UTOT K,LWST	
3003	2.638571E-04	2.117963E-07	77128	588588	7.6E+00	4.8E+07	7 11
SCALE:	LOG F? 1.00 MAX	1.00E+06 MIN	1.00E-01				

Fig. (7.3) A Two Dimensional Heat Diffusion Problem.

The problem with $K = 10^{-12}u^3$ and $\Delta u/u \approx .05$ produced results which may be quoted at three successive times close to equilibrium:

Table (7.4) Two Dimensional Timing Comparisons

code	time, 10^{-4} sec	compu- tation time sec	cycle	compu- lation ratio
MITs	2.6	9.61	3003	7.6
ADI	2.5	64.87	3003	
MITs	7.6	21.06	5171	4.5
ADI	6.4	101.8	4716	
MITs	12.6	32.38	7168	3.7
ADI	11.0	124.2	5749	

The ratio of run times starts at about 8 and degrades to about 4 as equilibrium is approached more closely. This latter situation corresponds to a substantially isothermal problem, in which the effective thermal conductivity is everywhere about the same. We have seen previously that implicit equations are strongly preferred over explicit methods in such circumstances, but that such circumstances are generally of very little interest. The first comparison, at about 2.5×10^{-4} sec, is about half way to equilibrium; the last two temperature distributions are essentially similar to Fig. (7.3). The agreement between MITs and ADI at cycle 3003, corrected for being at slightly different times, is about 1%. These trials seem to be typical of the experience to date in two dimensions.

General Considerations in Attaining Speed

For each difference technique there are particular aspects of the programming which require special care. As in forward differenced work, the solution of the implicit equations requires its own handling. So also in explicit equations with independent timesteps, the machinery of independent timesteps requires special attention. It is of course not for this that a code earns its pay; that comes from doing physics. And the explicit physics is pretty much the same with or without independent timesteps. The time spent by the code may roughly be apportioned between logic and physics: the logic manages the difference equations which do the physics. In conventional explicit codes that logic is fairly simple and it is directly proportional to the amount of physics done. With independent timesteps, the logic required is a little more intricate, comprising the coding of Eqns. (3.3-3.7). Here the logic is somewhat more than proportional to the physics. The success of independent timesteps depends wholly on discharging its logical duties with a minimum of effort. Comparisons of conventional explicit and explicit-with-independent timesteps codes always indicate that a significant portion of the time gained by not doing physics is lost to the extra logic required. Grievous as that loss may be, the results of the timing trials indicate that independent timesteps still run three to eight times as fast as the best conventional codes on conservative test problems. Much greater gains are to be expected from codes embodying the method of independent timesteps which are tightly coded for production, rather than research purposes, and which treat correspondingly more complex physics.

A computation may be described for economic purposes by four numbers. How many cycles (N) did it run? How many times (E) did it do major printout? How many zones (J) does it have? And how many zone-cycles ($SSJN$) of physics did it do? Normally in a synchronous explicit code, $SSJN = JXN$. Here $SSJN \sim JXN$, by a factor commonly of 5 to 20. The time spent in computations is proportional in part to all of these parameters:

$$t = a + zSSJN + kJXN + eE + nN \quad (7.1)$$

For different codes, the coefficients a , z , k , e , n may vary. For a conventional synchronous code, k may be taken as zero and the $SSJN$ and JN terms combined. Independent timesteps seek to minimize $SSJN$ with respect to JXN . And so to take full advantage of this, one must minimize k with respect to z . Still, there is a minimum of work that must be done at every zone for every cycle. Equation (3.7) is in this category, and its coding significantly affects the size of the coefficient k . Equations (3.4-3.5), the normal timestep control, need be done only with the physics, and so contribute to the coefficient z . Equation (3.6), as remarked in chapter III, may be coded in a variety of ways. In all the one dimensional work, it was enforced over the whole mesh at every cycle, and so contributes to the coefficient k . In the two dimensional codes, it was done more carefully and it contributes roughly to z ; it was enforced only as often as a timestep was actually used, which is to say only as often as the zone was updated. Equation (3.3), the interpolations necessary to supply wanting adjacent quantities, are done somewhat less often than every zone-cycle, but may be taken as nevertheless contributing to z . The coefficient a

represents that overhead which one must pay to run a problem at all: initialization, and so forth. It was generally considered to be negligible. The time spent in I/O also was neglected, as suppressing all output affects the run times imperceptibly.

There are many coding effects which contribute to k , namely, all those things which must be done for every zone every cycle. The simple mechanics of cycling a FORTRAN DO loop through the mesh contributes noticeably to k . It paid 20% or so to combine loops in the two dimensional work in order to minimize this effect. It may be noted that in the method of Grandey, the entire mesh must be searched every zone cycle in order to find the next zone to be updated, and one suspects that this requirement may contribute seriously to k . In the present work, as long as several zones fall due at once this problem should not be too severe. It is for this reason in addition to those of Chapter 1 that the present work sought a method different from that of Grandey.

The timing experience of the previous sections may be analysed in the light of Eqn. (7.1). The limiting value of speed advantage over conventional explicit codes is $JXN/SSJN$, the computation ratio. The advantage is somewhat less over implicit calculations, since these are permitted longer timesteps. In the work reported the speed advantage is generally a factor of two or so down from the maximum, $JXN/SSJN$. There are several reasons for this. First, as noted, the logic peculiar to MITS was never hand coded in machine language; and secondly, there were often unnecessary loops over the whole mesh.

The FORTRAN in the two dimensional work was done fairly carefully, and it may be seen from Table (7.4) that at cycle 3003 the ratio of run times is about 7.1, almost equal to *SRA7*, 7.6. But the real difference between these test problems and practical problems is in the complexity of the physics. For the z coefficient in Eqn. (7.1) will always be greater for a MITS than for a synchronous code, and greater by the amount of logic done. But if the contribution of the physics to z is itself very great, this will be a negligible affect. One hears¹ that shock hydrodynamic calculations can spend 30% to 40% of their time in equation of state routines alone, in spite of great care lavished on efficient coding of those routines, to name only one aspect of calculations with real properties of matter. Applied to real world problems instead of research tests, the method of independent timesteps should be expected to yield substantially greater computation savings than have been seen above.

¹ Zimmerman, private communication.

CHAPTER VIII

CONCLUSIONS

In summary

The method of independent timesteps has been presented in its conception and motivation, in the context of related work, and in the details of implementation in several finite difference schemes. In order to maintain a well posed problem as the computation proceeds, a different approach was taken from the work of Grandey. The present work maintains a Cauchy surface everywhere prochronic to the crisis zones of the problem. General specifications for independent timesteps were presented together with details of specific instances in particular finite difference schemes.

In order to prove stability, asynchronous techniques require resources somewhat different from those adequate for conventional synchronous difference methods, and those arguments were exhibited as applied to both synchronous and asynchronous computations. The expected speed advantage was indeed observed, and even on very conservative test

problems. The accuracy was not degraded materially by independent timesteps. The considerations pertinent to the timing economies were indicated. The method of independent timesteps was tested on a sample of equations of a vast class, but it is believed that with the examples tested, from both parabolic and hyperbolic problems, this sampling is representative. And the sample of equations tested with independent timesteps may be small compared to the whole field of initial value problems, but it is nevertheless large enough so that it may be said with confidence that the successes observed were not accidental or peculiar but typical of all shock hydrodynamics problems with stiffly nonlinear equations.

Implications

In chapter I, an interest was announced in a very limited portion of the even broader class of all initial value problems. This limited subset is shock hydrodynamics, broadly construed. It is fair to note that even this is a broad area, and in the years since the first modern digital computers, a tremendous oral and written tradition has grown up in this work. There are many computational techniques, and many physical affects must be treated meticulously if one is to model high temperature shocks, for example.

Indeed, the development of large and fast digital computers may be credited to the need for practical solutions to problems in shock hydrodynamics. As much can also be said for the theoretical foundation work in numerical solution of partial differential equations with time

as one independent variable. The effort expended on this kind of problem is still great, and large new machines are still built with the prime design consideration being fast simulation of shock hydrodynamics problems. So a numerical technique which affords proven speed advantages of a factor of three to eight and substantially greater promised advantages is of no mean significance. It is also philosophically significant, in that it constitutes the commencement of doing for the logic of computation what digital computers have done for computation itself: greatly speeding up what humans do, but without loss of quality in how humans do it.

The history of numerical computation in differential equations since 1945 has been a steady progression of ever more complex problems treated in ever more detail. If a problem of one hundred zones could be treated before, ten thousand can be handled now. If some property of matter had to be idealised before, and evaluated with no more than a handful of arithmetic operations, now one can afford painstaking care in estimating properties of matter. And as it was pointed out in chapter VII, the more complex the physics of interest, the more suitable the problem is to independent timesteps. The logic required for this method should not in principle become more onerous as the physics is treated more accurately.

As in all endeavors, to get something, one must pay something. Here the price of speed is paid in memory requirements, as illustrated in chapter II. But at the present state of the art of digital hardware design, memory is becoming more plentiful much faster than is computing speed. There is a price paid in accuracy also, but as remarked in chapters II, VI, and VII, accuracy is not greatly affected by

independent timesteps. The cost in memory requirements is not too great: in hydrodynamics it was of the order of 50% additional, and will be relatively less in more complex problems.

The present work is only a beginning in a new area of computational hydrodynamics, and some idea may be sketched of the immediate work yet to be done. It is with some regret that the case of spherical waves could not be included in the stability arguments of Chapter V, for the sake of the current research in supernova dynamics. No wave norm is known to me and the problem has resisted efforts to devise one. The method of independent timesteps has so far been tested only on small problems for research purposes, not yet on real problems for practical motives. Two dimensional Lagrangian hydrodynamics is yet to be tested, as is Eulerian hydrodynamics. The method seems suitable for generalization in parabolic problems to any number of dependent or independent variables, with no qualitatively new behavior anticipated.

The initial motivation for this work was simply to instruct the modern digital computer how to operate more like a human, who does not add or multiply very quickly but does his arithmetic selectively and to great advantage. Now, it may be said that the machine's strength is arithmetic, and it should be used as a dumb adding machine, taking maximum advantage of its strengths. The logical capacities of modern digital computers are also great, however, and very little used by computational physicists. It has been noted above that at present, computer speed is not increasing nearly as quickly as people would like it to, and so at 50 multiplies per microsecond, even computers can be frustratingly slow in their arithmetic. The philosophy of independent timesteps will someday prove crudely simple, but now it is quite

unusual. That philosophy may fairly be stated as "skip calculations where you can", and the work here outlined merely indicates how to do so, which is to say, how to tell "when and where you can". It is still a very local approach to problems, employing none of the global perspective that affords the human calculator (one might more appropriately call him an estimator!) his advantages of speed for the amount of arithmetic he does. The human will first crudely solve the whole problem and then refine his estimate; there has as yet been no way to model independent timesteps on this virtue of human calculation. When confronted with a new problem and a computer to solve it with, there is always the temptation to treat it with as little thought and as much computation as possible. If a problem is to be solved only once, this may be cheaper in human effort, yielding an acceptable answer quickly. But if one is faced with a whole class of problems, then it behoves one to spend a little more time thinking, since even computers still only run at finite speeds. One is always faced with the choice between thinking or computing, and there are usually ample rewards for choosing the former. The method of independent timesteps is a first effort in teaching the computer also to take this attitude.

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