FINITE DIFFERENCE SOLUTION OF THE DIFFUSION EQUATION ON COUPLED EULERIAN AND LAGRANGIAN GRIDS

Richard Bruce Hickman
(Ph.D. Thesis)

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Richard B. Hickman

Abstract

A diffusion equation modeling the flow of radiation has been added to the hydrodynamic equations of two coupled Eulerian and Lagrangian finite difference computer codes. This permits the extension of the range of problems to which these codes may be applied to include those in which temperatures on the order of a thousand electron volts are attained.

The coupled codes are first order accurate shock hydrodynamics programs designed to calculate transient effects resulting from concentrations of high energy density. Such phenomena occur when a projectile impacts a target or when a high explosive is detonated. When the energy density is very high, as when a nuclear explosive is fired or a laser fusion pellet is imploded, radiation energy becomes a significant portion of the total energy and must be accounted for. The diffusion approximation has proven to be a useful means of incorporating radiation physics in codes of this type.

The three principal problems associated with the finite difference solution of the diffusion equation are the conservation of energy, the spatial differencing on grids that are becoming distorted with the passage of time, and the coupling of calculations done on the separate regional grids that together constitute the geometry of the problem.

The approximate conservation of energy in the diffusion calculation is achieved by an extrapolation in time that allows an accurate estimate of the heat capacity of each zone. In order that the approach of a nonlinear thermal wave be properly anticipated, the extrapolation uses information from surrounding zones and employs a functional iteration technique which has been modified to assure convergence.

The space differencing of the diffusion operator requires a nine point difference star. An implicit time difference scheme is required to achieve reasonable time steps. A method of implicit sweeps based on operator splitting was selected. To use one dimensional sweeps it is necessary to treat the diagonal terms in such a manner that the effective diffusion coefficient is not negative under severe zone distortion. This is accomplished by multiplying each of the diagonal terms, which are evaluated explicitly, by a ratio of temperature values that causes the magnitude of the product to decrease along with the zone temperature. It is shown that these modified terms lead to a solvable system of equations which are stable if energy is conserved.

The radiation diffusion equation is solved separately on each of the regional grids and communication between the grids is by means of boundary information passed from one grid to another. A combination of temperature and temperature gradient information is used in a manner that is shown to be stable in the limit of large time steps for an idealized case. This permits a fully implicit scheme with no restriction on the time step to be employed in each region and all the regions to be coupled in a manner that also requires no conditions other than those required for accuracy.

The difference techniques described in the thesis are applied to the calculation of the prompt effects of an explosive detonated at the earth's surface. This problem required five separate regions. The explosive, as well as the region of the earth more than three meters from the explosive, were zoned with Lagrangian coordinates. The air, the earth directly under the explosive, and a distant sink region were zoned in Eulerian coordinates. The calculation was carried out until most of the energy of the explosive, initially in the form of internal and radiation energy, was converted into kinetic energy and thermal energy in the air and earth. The results show that a smooth thermal front expands into the earth and no sign of instability was detected.

I. INTRODUCTION

The last thirty years has seen an unprecedented expansion in the capability of calculating continuum mechanics problems which possess complexities which place their analytic solution beyond reach. This has been the result of increased speed and storage capacity of electronic computers as well as the creation and refinement of numerical techniques which can be applied to these problems in an efficient manner to yield accurate approximations to the correct solution.¹ In particular, a variety of coordinate or indexing systems has arisen to associate material properties with location in space. The two most common such systems are the Lagrangian and Eulerian coordinate systems.

In a Lagrangian coordinate system each discrete coordinate is associated with a particular mass point and the position of that point is calculated from the equations of motion. In one space dimension, including cases where variation is permitted only along the radius of a cylindrical or spherical coordinate system, the advantages of Lagrangian coordinates, which permit a spatial resolution which adjusts to the state of the matter as well as an unambiguous identification of each material present, are especially evident.² When variation in more than one space dimension is permitted and indexed points are expected to traverse distances which are large compared to their original spacing during the time of interest, the possibility of gross distortions of the zones exists.³ Some distortions are physically reasonable but computationally unacceptable. Thus if an initially square zone were to distort to a rectangle of large aspect ratio while maintaining the same area, the increment of time used to advance the solution might decrease. This occurs in calculations where the Courant condition⁴ restricting the time

step to be no more than the sound transit time across the smallest dimension of the zone is used to assure stability. Nonphysical distortions such as zone inversion, which causes the orientation of the coordinate lines to change, are equally serious as they typically result in a negative volume and abort the solution process.⁵

An Eulerian coordinate system is fixed in space and hence matter may flow through coordinate lines. As the zone shapes do not change, time step decreases due to distortion do not occur. Flows with eddies or jets which would be prohibitively expensive for a Lagrangian calculation may be attempted in an Eulerian framework. The price to be paid for this capability includes the numerical diffusion caused by advection of mass, momentum, and energy across the zone boundaries.⁶ At each cycle densities of these quantities are averaged among those of the material remaining in a zone and those of the material entering the zone. Thus any sharp gradients, such as may be associated with a contact discontinuity, disappear. If there are to be more than one material in an Eulerian region some means of determining an equation of state appropriate to a mixture must be determined or an algorithm introduced to maintain and transport the components separately.

Because both the Lagrangian and Eulerian coordinate systems have flaws as well as virtues, efforts have been made to devise indexing schemes which minimize the deficiencies of either for some class of problems. These schemes include the free Lagrange method⁷, in which the indices of the points which are neighbors to a given point may change in time, as well as the arbitrary Lagrange Eulerian or ALE⁸ scheme which permits coordinate points to move but not necessarily with the velocity of the

matter. In the framework of a Lagrangian system the HEMP⁹ code permits slide lines which allow a shearing motion without causing zone distortion.

The particular variant of the coordinate schemes to be considered here is known as the Coupled Euler Lagrange or CEL method.¹⁰ In this case the region of space to be considered is indexed by both Lagrangian and Eulerian coordinates. An Eulerian grid underlays the entire problem area and several simply connected Lagrangian grids may exist within that area. The portion of Eulerian region not covered by Lagrangian grids may or may not be simply connected. No Eulerian calculation is performed in those zones which are covered. The finite difference form of the equations of motion in any Lagrangian region are solved with normal stresses as boundary conditions. The normal stresses are computed as functions of the local Eulerian and Lagrangian variables. In this way the calculations in the various regions are coupled.

In a large class of problems there exist regions in which displacements are to be small. These are zoned in the Lagrangian description. Where displacements are expected to be large the Eulerian description is used. For example, in studying the effects of an accident involving a nuclear reactor, the containment vessel as well as some internal structures would be expected to remain very near their original position and might be represented by Lagrangian grids. This representation would not be appropriate for the coolant fluid which would traverse over distances comparable to the entire underlying Eulerian grid. It is possible to use different equations of state in Eulerian regions that are separated by a Lagrange region but in any connected Eulerian region only one material may be present. This restriction is modified in the CHAMP code¹¹ which permits independent Eulerian regions

to be separated by a piecewise linear boundary. The grid spacing may vary from one Eulerian region to another and Lagrange regions may cover portions of several Eulerian grids.

The hydrodynamic equations upon which the CEL and CHAMP codes are based are Euler's equations. These are discussed in Chapter II. For physical situations in which temperatures are on the order of a thousand electron volts (or 1 keV) it is necessary for a proper description of the phenomena to include the transport of radiation. Near regions of high energy density such as nuclear explosives or laser fusion targets such temperatures exist and a code capable of simulating both radiative and hydrodynamic processes is needed. Although radiation transport is a complicated phenomenon, in many cases it is possible to use a simpler description, the diffusion approximation,¹² also described in Chapter II.

The hydrodynamic equations of CEL and CHAMP are differenced explicitly in time, that is the values of the variables at the new time are computed directly from the value of the local variables at the previous time. Thus no signal can propagate past the local region in one time step. This is consistent with the hyperbolic nature of the hydrodynamic equations.

The diffusion equation, however, is parabolic and admits an infinite signal velocity. Although the diffusion equation can be differenced explicitly, the stability constraint on the time step is likely to be much more severe than the Courant condition on the hydrodynamic time step unless there are hydrodynamic signal speeds approaching the speed of light, the radiative contribution to the heat capacity is small, the radiation mean free path is small compared to the zone size or some combination of these obtains. It should be noted that the stability condition is less restrictive than a reasonable accuracy condition for the

shortest wavelengths which the grid can sustain and there is no penalty while these components have non-trivial amplitudes. However as the diffusion process damps these waves the stability condition remains unchanged as the accuracy condition becomes less restrictive. It may become prohibitively expensive to proceed with an explicit difference method for the diffusion equation.

Implicit schemes, those requiring simultaneous solution for variables at the advanced time, may be devised such that there is no stability restriction on the time increment. In one space dimension implicit schemes require the solution of linear systems with small bandwidth and are thus nearly as economical as explicit methods.¹³

In spaces of higher dimension storage and time problems often indicate that the solution of the linear system be approximated by the solution of a collection of one dimensional problems. This can be done with any of a number of procedures¹⁴ for an orthogonal grid.

As Lagrangian grids nearly always become non-orthogonal during the course of calculation some means must be devised to accommodate this within the framework of the one dimensional sweep algorithms. When several grids are to be coupled hydrodynamically and by radiation diffusion there may be no straightforward way of extending one dimensional sweeps throughout the problem. A coupling algorithm must be devised which permits the diffusion process to proceed separately on each grid with grid-to-grid communication achieved by means of boundary conditions. As the advanced time values in zones near the boundary cannot be available for both grids, the coupling will be explicit to some extent. The question arises as to whether the time step need be restricted as a result

of this. Algorithms which may not impose a stability restriction are discussed in Chapter IV.

An illustration of the performance of these algorithms in computing the energy transfer of an explosive to the ground on which it rests is presented in Chapter V. This type of nuclear weapons effects problem requires the zoning flexibility permitted by a coupled grid code. The air surrounding the explosive undergoes rapid expansion and discontinuity of tangential velocity components at interfaces must be provided for. This capability of maintaining well defined interfaces while allowing a variety of zoning decisions has previously been used in modelling subsurface explosions with the CEL code.¹⁵ In Chapter V of this dissertation the CHAMP code was employed to model the early time coupling of energy from the explosive to the ground beneath it. The calculation proceeded until 90% of the initial energy of the problem, which had the form of internal energy in the explosive, had been transferred. Although most of the energy has been released to the air, a significant fraction was delivered to the ground and it is this transfer that is potentially important for studying the effects of explosives on buried structures. The radiative transfer process appeared to be well modeled and no instabilities, developed or incipient, appeared due to the diffusion differencing.

II. PHYSICS OF THE CEL AND CHAMP CODES

A. The Diffusion Approximation

Radiation transport must be one of the modeled phenomena if a hydrodynamics code is to be applied to problems in which temperatures of the order of hundreds of electron volts or more are to be expected. Radiative energy may vary with position, time, frequency and direction.¹⁶ It may be subject to a variety of scattering, absorption and emission processes. Useful results may be gained without considering all possible complexities. In the CEL and CHAMP codes the equilibrium diffusion approximation is employed to model radiation physics. We derive here the diffusion approximation and note in what regime it may be expected to be of value.

As a starting point we select the equation of radiative transfer without scattering.¹⁶

$$\frac{1}{c} \frac{\partial I_{\mathbf{n}}^{\nu}}{\partial t} + \vec{\mathbf{n}} \cdot \vec{\nabla} I_{\mathbf{n}}^{\nu} = S_{\mathbf{n}}^{\nu} - \sigma^{\nu} I_{\mathbf{n}}^{\nu} \quad (2.1)$$

where $I_{\mathbf{n}}^{\nu}(\vec{r}, t)$ is the energy of radiation with frequency ν and direction $\vec{\mathbf{n}}$ per unit area per unit time per steradian per unit frequency,

$S_{\mathbf{n}}^{\nu}(\vec{r}, t)$ is the emitted energy with frequency ν and direction $\vec{\mathbf{n}}$ per unit volume per unit time per steradian per unit frequency, and $\sigma^{\nu}(\vec{r}, t)$ is the absorption coefficient for radiation of frequency ν in units of inverse length.

In a region which is optically thick, that is one in which $(\sigma^{\nu})^{-1}$ is much smaller than any dimension of macroscopic interest throughout the range of frequency in which $I_{\mathbf{n}}^{\nu}$ has significant magnitude, and in which the matter is in local thermodynamic equilibrium at a temperature not

exceeding a few keV the right side of equation (2.1) may be replaced by the expression

$$\sigma^j (B^j / (4\pi) - I_n^j)$$

where B^j is a function of the local matter temperature. Two new equations can be obtained by integrating the equation of transfer over all angles and by performing such an integration after first multiplying by $\vec{n}$.

$$\frac{1}{c} \frac{\partial I^j}{\partial t} + \vec{\nabla} \cdot \vec{F}^j = \sigma^j (B^j - I^j) \quad (2.2)$$

$$\frac{1}{c} \frac{\partial \vec{F}}{\partial t} + \vec{\nabla} \cdot \vec{P}^j + \sigma^j \vec{F}^j = 0 \quad (2.3)$$

In these equations

$$I^j \equiv \int_{4\pi} I_n^j d\Omega$$

$$\vec{F}^j \equiv \int_{4\pi} \vec{n} I_n^j d\Omega$$

$$\text{and} \quad \vec{P}^j \equiv \int_{4\pi} \vec{n} \vec{n} I_n^j d\Omega.$$

As these equations are not a closed set we replace $\vec{\nabla} \cdot \vec{P}^j$ by a linear combination of $\vec{\nabla} I^j$ and $1/c \frac{\partial \vec{F}^j}{\partial t}$ as suggested by DeBar.¹⁷ The constant coefficients in the linear combination are determined by imposing two requirements dealing with limiting cases. First, in the limit of

vanishing interaction between radiation and matter ($\sigma^0 \rightarrow 0$) the equations are to reduce to a wave equation with c , the velocity of light in vacuum, as the characteristic velocity. The second requirement is that in the limit of large interaction with matter the radiation be isotropic and hence

$$(\vec{P}^0)_i^i = \delta_i^i I^0 / 3.$$

With these assumptions equation (2.3) is replaced by

$$\frac{1}{c} \frac{\partial \vec{F}^0}{\partial t} + \vec{\nabla} I^0 + 3\sigma^0 \vec{F}^0 = 0. \quad (2.4)$$

Embodied in this equation are assumptions about the angular distribution of the radiation in two important limiting cases. For optically thick regions a further approximation may be made. It is assumed that

$$\left| \frac{\partial \vec{F}^0}{\partial t} \right| \ll c \sigma^0 \left| \vec{F}^0 \right|. \quad (2.5)$$

This assumption is valid if the flux vector, $\vec{F}^0$, does not undergo significant change in times less than one collision time ($\approx 1/(c\sigma^0)$). In this case equation (2.4) serves as a definition of $\vec{F}^0$ in terms of I^0 ,

$$\vec{F}^0 = -1/(3\sigma^0) \vec{\nabla} I^0. \quad (2.6)$$

Equation (2.2) then becomes

$$\frac{1}{c} \frac{\partial I^0}{\partial t} - \vec{\nabla} \cdot [1/(3\sigma^0) \vec{\nabla} I^0] = \sigma^0 (B^0 - I^0). \quad (2.7)$$

This is the equation for nonequilibrium diffusion. If it is further assumed that relaxation times are less than times of interest at a single temperature, T , may be used for the matter and radiation. Defining $E_m(T)$ to be the material energy density and

$$E_r \equiv \frac{1}{c} \int I^{\nu} d\nu$$

the radiation energy density, we have

$$E(T) \equiv E_m(T) + E_r(T)$$

the total energy density. In the case of local thermal equilibrium I^{ν} becomes identical with B^{ν} . The term on the right hand side of equation (2.7) represents the net loss of radiation energy of frequency ν to the matter and combines with the first term of that equation upon integrating over all frequencies to yield

$$\frac{\partial E}{\partial t} - \frac{1}{3} \vec{\nabla} \cdot \int \vec{\nabla} B^{\nu}(T) / \sigma^{\nu} d\nu = 0. \quad (2.8)$$

As B^{ν} is a function of temperature only we see that

$$\int \vec{\nabla} B^{\nu}(T) / \sigma^{\nu} d\nu = \vec{\nabla} T \int \frac{\partial B^{\nu}}{\partial T} / \sigma^{\nu} d\nu \quad (2.9)$$

and

$$c \vec{\nabla} E_r = \vec{\nabla} \int B^{\nu} d\nu = \vec{\nabla} T \int \frac{\partial B^{\nu}}{\partial T} d\nu. \quad (2.10)$$

Thus

$$\int \vec{\nabla} B^{\nu} / \sigma^{\nu} d\nu = c \lambda_R \vec{\nabla} E_r \quad (2.11)$$

where λ_R , the Rosseland mean free path,¹⁶ is given by

$$\lambda_R \equiv \int \frac{\partial B^0}{\partial T} / \sigma^0 d\nu \bigg/ \int \frac{\partial B^0}{\partial T} d\nu. \quad (2.12)$$

For thermal equilibrium

$$E_r = a T^4 \equiv a \phi. \quad (2.13)$$

The constant, a , is related to the Stefan-Boltzman constant, σ , by

$$\sigma = ac/4 \quad (2.14)$$

and has a value of 137.2 megabars per (keV)⁴. Megabar units are those of energy per unit volume appropriate to a selection of fundamental units to be grams, centimeters, and microseconds. With these definitions plus

$$\lambda \equiv ac \lambda_R / 3 \quad (2.15)$$

we may rewrite equation (2.8) as the diffusion equation

$$\frac{\partial E}{\partial t} = \vec{\nabla} \cdot \lambda \vec{\nabla} \phi. \quad (2.16)$$

B. Hydrodynamics of CEL and CHAMP

Both the CEL and CHAMP codes are based on Euler's equations for a compressible inviscid fluid. These equations are

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0 \quad (2.17)$$

$$\frac{\partial \rho \vec{v}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v} \vec{v}) = -\vec{\nabla} p \quad (2.18)$$

$$\frac{\partial \epsilon}{\partial t} + \vec{\nabla} \cdot (\epsilon \vec{v}) = -p \vec{\nabla} \cdot \vec{v} \quad (2.19)$$

where ρ is the mass density

ϵ is the internal energy per unit volume

$\vec{v}$ is the fluid velocity relative to fixed coordinates and

p is pressure.

In addition to these an equation of state relating ρ , ϵ , and p is required to complete the set. The equations in this form are differenced in the Eulerian regions. In the Lagrangian regions an equivalent set is used. This set is:

$$\frac{D \vec{r}}{Dt} = \vec{v} \quad (2.20)$$

$$\frac{D \rho}{Dt} = -\rho \vec{\nabla} \cdot \vec{v} \quad (2.21)$$

$$\frac{D \vec{v}}{Dt} = -1/\rho \vec{\nabla} p \quad (2.22)$$

$$\frac{D \epsilon}{Dt} = -p/\rho \vec{\nabla} \cdot \vec{v} \quad (2.23)$$

where $e = \epsilon/\rho$ and

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \vec{v} \cdot \vec{\nabla}$$

is the total or Lagrange derivative. There may be zones in an Eulerian region which are partially covered by a Lagrange region or some other Eulerian region. In Figure 2.1 the central zone is partially obscured (denoted by dashed boundaries). In such a zone equations (2.17)-(2.19) are not appropriate. For these zones a set of equations in terms of a coordinate set $\vec{R}$ moving arbitrarily with respect to the fluid was derived by Noh.¹⁰ If $\vec{A}$ represents the Lagrange index vector and J the Jacobian of the components of $\vec{R}$ with respect to those of $\vec{A}$ then Noh's equations are

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial J}{\partial t} / J + \vec{\nabla} \cdot (\rho \vec{\Omega}) = 0 \quad (2.24)$$

$$\frac{\partial \rho \vec{v}}{\partial t} + \rho \vec{v} \frac{\partial J}{\partial t} / J + \vec{\nabla} \cdot (\rho \vec{v} \vec{\Omega}) = -\vec{\nabla} p \quad (2.25)$$

$$\frac{\partial \epsilon}{\partial t} + \epsilon \frac{\partial J}{\partial t} / J + \vec{\nabla} \cdot (\epsilon \vec{\Omega}) = -p \vec{\nabla} \cdot \vec{v} \quad (2.26)$$

where $\vec{\Omega} \equiv \vec{v} - \frac{\partial \vec{R}}{\partial t}$.

For interior Eulerian zones we take $\vec{R}$ fixed and $\vec{\Omega} = \vec{v}$ and $\frac{\partial J}{\partial t} = 0$.

Thus the Eulerian equations are recovered. For a purely Lagrange calculation

$\frac{\partial \vec{R}}{\partial t} = \vec{v}$ and so $\vec{\Omega} = 0$. As $\frac{\partial J p}{\partial t} = 0$ in this case the equations (2.20)-(2.23) result. The Eulerian equations are in conservation form and are differenced in such a manner as to preserve this feature. The

2.1 A partially covered Eulerian zone

2.2 Lagrange zoning. Density and specific internal energy are evaluated at zone centers while position and velocity vectors are centered at grid vertices.

2.3 Cell Eulerian grid. Density and internal energy density are evaluated at zone centers while velocities or momenta are centered at grid vertices

2.4 Champ Eulerian zoning. Density, internal energy density, and velocity are all evaluated at zone centers

advection terms are differenced using Lelevier's method,^{2,18} which is first order accurate in time.

The fact that some of the energy and momentum resides in the radiation field is accounted for in the hydrodynamic phase by adding α^4 to the material internal energy and one third of that to the pressure in all references to the equation of state.

Some of the indexing conventions used in the codes are indicated in Figures 2.2-2.4. Both codes allow plane or cylindrical symmetry. We shall discuss the case of planar coordinates x and y although an effort will be made to define operators invariant with respect to coordinate system; x and y are to form a right hand system and there is no variation of any variable in a direction perpendicular to the x - y plane. Grid vertices in the Eulerian regions are indexed by l and k which also form a right handed system. The Eulerian grids are rectangular and fixed in time. The Lagrange grids are not fixed in time and are indexed by separate l - k coordinate sets. These are oriented so that as the $k=0$ boundary is traversed in the direction of increasing l , the Eulerian region is to the right and the Lagrangian region is to the left.

In the Eulerian regions the density, internal energy and pressure are defined at zone centers, i.e., at the intersections of lines for which l and k have values differing by $1/2$ from integers. Momenta are defined at the same location in CHAMP but at grid vertices in CEL. As the quantities of interest in the radiation diffusion calculation are evaluated at zone centers, CEL and CHAMP do not differ in spatial differencing. In the Lagrange regions density, internal energy and pressure are zone centered quantities while velocities and grid coordinates are defined at vertices.

The following order of calculation is observed in a single cycle for which time is advanced from t^n to t^{n+1} :

1. Lagrange velocities $\vec{v}^{n+1}$ are calculated.
2. The coordinates $\vec{r}^{n+1}$ of the Lagrange grid vertices are computed.
3. The Lagrange zone centered quantities ρ^{n+1} , e^{n+1} , $\vec{p}^{n+1}$ are determined.

At this point CEL and CHAMP differ. The CHAMP procedure for the Eulerian region is described.

4. New positions of the interface points, those lying on the boundaries between Eulerian regions are calculated.
5. Eulerian densities, internal energies and momentum densities are updated for advection.
6. One half the work term of the form $\rho^{n+1}(\Delta V/V)^{n+1/2}$ is subtracted from the internal energy.
7. The momentum densities are advanced by the pressure terms, $\vec{v} \cdot \vec{p}^{n+1}$.
8. The other half of the work term is added to the internal energy.

One further concept must be defined at this point. Referring to Figure 2.5, the Eulerian zone centered at $j + 1/2$, $k+3/2$ is so nearly covered by the Lagrange region that its dimensions are no longer typical of the resolution specified by the grid spacing. In this case it is adjoined or blended to a neighboring zone (in this case the zone centered at $j+1/2$, $k+1/2$) and all zone centered quantities are recalculated for the new larger zone or blended complex in a fashion which conserves mass,

momentum, and energy. Subject to some restrictions on indices, as many as nine zones may be blended together. The blending occurs when the volume of the portion of the zone not covered is reduced to some specified fraction of the volume the zone would have if no portion of it were covered. For purposes of the hydrodynamic calculation this blended complex is a single zone and all densities have the same values in each member zone. Quantities advected through any zone side are added or subtracted from the entire complex. Likewise pressure exerted on a zone side accelerates the entire complex.

2.5 The zone at $L + 1/2, K + 3/2$ is blended to the zone centered at $L + 1/2, K + 1/2$

III. SPATIAL DIFFERENCING OF THE DIFFUSION OPERATOR

The diffusion equation (2.16) models the flow of radiation in the problem environment while the equations of hydrodynamics in Section II.B are used to represent the flow of matter. The way in which these physical processes interact is discussed in the next chapter. In this chapter we deal with the problem of estimating $\frac{\partial \mathcal{E}}{\partial t}$ at some point in time from values of the state variables specified only at zone centers. Some time average of derivatives thus obtained will be used to advance the solution from one time to the next. Rewriting equation (2.16)

$$\frac{\partial \mathcal{E}}{\partial t} = D\phi \quad (3.1)$$

where $D\phi \equiv \vec{\nabla} \cdot \lambda \vec{\nabla} \phi \quad (3.2)$

we seek an operator $\bar{D}$ defined on the collection of real functions such that $\lambda \vec{\nabla} \phi$ exists and $\lambda \vec{\nabla} \phi$ is differentiable where λ is a piecewise continuous function. $\bar{D}$ is to depend only on values of ϕ at zone centers and is defined at zone centers. It must further have the property that in the limit of vanishing grid mesh spacing, $\bar{D}\phi$ tends to $D\phi$ at each zone center. Furthermore it must yield values which do not defy physical intuition for any grid no matter how distorted.

A. Derivation of the Difference Operator

In this section an operator, $\bar{D}$, which approximates D , is defined in equation (3.25). The derivation proceeds by using the mean value theorem and the divergence theorem to replace the differential operator, D , by an integral operator, and Green's theorem to replace the resulting area integrals by line integrals, which are approximated in a simple

manner. The result is an expression for D which requires values of ϕ at grid points as well as zone centers. In the remainder of this section the rationale for expressing grid values in terms of zone centered values is presented.

Consider the zone indicated in Figure 3.1 which indicates the intersection of the zone with the x-y plane. We shall discuss the case of plane symmetry and indicate the manner in which algorithms must be altered to accommodate cylindrical symmetry. The extent of the zone in the direction perpendicular to the x-y plane is taken to be unity. We begin by applying an integral mean value theorem which states that

$$D\phi(\xi) = |V|^{-1} \int_V D\phi \, d\tau \quad (3.3)$$

where V denotes the region occupied by the zone

$|V|$ is its volume

and ξ is some point within the zone.

Although the location of ξ is unknown we shall assume that it is the zone center. Applying the divergence theorem to the right hand side of equation (3.3) we obtain

$$D\phi(\xi) = |V|^{-1} \int_{\partial V} \lambda \vec{\nabla} \phi \cdot d\vec{s} \quad (3.4)$$

The integrand has components

$$\left(\lambda \frac{\partial \phi}{\partial x}, \lambda \frac{\partial \phi}{\partial y}, 0 \right)$$

3.1 General zoning used for spatial differencing

where the third component vanishes because of the symmetry of the problem. Thus although the integration in equation (3.4) is over a six faceted surface, there is not a contribution over two of them. The integral is then a sum of four integrals, each of which will be denoted by the letter F so that

$$D\phi(\xi) = |V|^{-1} [F_{\ell+1, \kappa+1/2} - F_{\ell, \kappa+1/2} + F_{\ell+1/2, \kappa+1} - F_{\ell+1/2, \kappa}]. \quad (3.5)$$

We examine in some detail $F_{\ell+1, \kappa+1/2}$.

$$F_{\ell+1, \kappa+1/2} = \int_{S_{\ell+1, \kappa+1/2}} \lambda \vec{\nabla} \phi \cdot d\vec{S} \quad (3.6)$$

where $S_{\ell+1, \kappa+1/2}$ is one of the facets of the zone. In the x-y plane the zones appear as quadrilaterals. We define for each zone side the difference operators Δ and δ which represent differences along the side of the zone and transverse to it respectively. Thus as we are discussing the zone side centered at $\ell+1$ and $\kappa+1/2$ we have for any variable f:

$$\Delta f \equiv f_{\ell+1, \kappa+1} - f_{\ell+1, \kappa} \quad (3.7)$$

and

$$\delta f \equiv f_{\ell+1/2, \kappa+1/2} - f_{\ell+1/2, \kappa+1/2}. \quad (3.8)$$

The zone is traversed in a counter clockwise direction in defining Δ and $\delta^2 \times \Delta^2$ is always positive. With these definitions the length of the zone side is

$$\Delta \equiv \left((\Delta x)^2 + (\Delta y)^2 \right)^{1/2} \quad (3.9)$$

and the outward normal vector is

$$\vec{n} = (\Delta y / \Delta, -\Delta x / \Delta, 0). \quad (3.10)$$

Then applying the mean value theorem again

$$F_{\ell+1/2, K+1/2} = \lambda \nabla \phi \cdot \vec{n} |S| \quad (3.11)$$

where $\lambda \nabla \phi$ is evaluated at some point on the facet and $|S|$ is the area of the facet.

The vector $\lambda \nabla \phi$ will be estimated by an application of Green's theorem which states that

$$\int_A \frac{\partial \phi}{\partial \tau_x} d\tau_x dy = \int_{\partial A} \phi dy \quad (3.12)$$

$$\text{and} \quad \int_A \frac{\partial \phi}{\partial \tau_y} dx d\tau_y = - \int_{\partial A} \phi dx \quad (3.13)$$

where $d\tau_x = dx / \lambda$

and $d\tau_y = dy / \lambda$.

The region A is shaded in Figure 3.2.

3.2 Regions over which line integrals in flux approximation are taken

If φ is assumed to be linear between adjacent vertices of the region A, then

$$\int_{\partial A} \varphi dy \approx [\varphi, y] \quad (3.14)$$

$$\text{where } [\varphi, y] \equiv \frac{1}{2} (\delta \varphi \Delta y - \Delta \varphi \delta y) \quad (3.15)$$

$$\text{Similarly } \int_{\partial A} \varphi dx \approx [\varphi, x] \quad (3.16)$$

$$\text{and } [\varphi, x] \equiv \frac{1}{2} (\delta \varphi \Delta x - \Delta \varphi \delta x). \quad (3.17)$$

Applying the mean value theorem once again

$$\int_A \frac{\partial \varphi}{\partial x} dx dy = \lambda \frac{\partial \varphi}{\partial x}(\eta_1) \int_A dx dy \quad (3.18)$$

$$\int_A \frac{\partial \varphi}{\partial y} dx dy = \lambda \frac{\partial \varphi}{\partial y}(\eta_2) \int_A dx dy \quad (3.19)$$

where η_1 and η_2 are points in the region A. The integrals on the right hand side of equations (3.18) and (3.19) are equal and have the common value given by

$$\int_A \frac{dx dy}{\lambda} = \int_{A_1} \frac{dx dy}{\lambda} + \int_{A_2} \frac{dx dy}{\lambda} \quad (3.20)$$

where A_1 and A_2 are the triangular regions indicated in Fig. 3.2.

Each integral on the right hand side of equation (3.20) is evaluated by the mean value theorem to be the area of the region divided by λ evaluated somewhere within the region. The mean free path, λ , is a function of

density, temperature, and the chemical nature of the material. The density and chemical composition can be evaluated at the zone center but the temperature should not be. If this were done a very small value of λ due to a low temperature could effectively block diffusion into a zone and the temperature would rise much too slowly. Hence for each of the triangles, A_1 and A_2 , the temperature selected is that obtained by averaging the values of ϕ at the zone centers. This value is

$$\bar{\phi}_{\ell+1/2, k+1/2} \equiv 1/2 (\phi_{\ell+3/2, k+1/2} + \phi_{\ell+1/2, k+1/2}). \quad (3.21)$$

We have then that

$$\int \frac{dx dy}{\lambda} \approx \left| \frac{A}{\lambda} \right| = \frac{|A_1|}{\lambda_1} + \frac{|A_2|}{\lambda_2}. \quad (3.22)$$

Summarizing the equations (3.6) through (3.21), if

$$\bar{F}_{\ell+1/2, k+1/2} \equiv \left\{ \frac{[\phi, y] \Delta y + [\phi, x] \Delta x}{|A/\lambda|} \frac{|S|}{\Delta} \right\} \quad (3.23)$$

$$\text{then } \bar{F}_{\ell+1/2, k+1/2} \approx \bar{F}_{\ell+1/2, k+1/2} \quad (3.24)$$

$$\text{and } \bar{D}\phi_{\ell+1/2, k+1/2} \equiv |V|^{-1}_{\ell+1/2, k+1/2} \left\{ \bar{F}_{\ell+1/2, k+1/2} - \bar{F}_{\ell, k+1/2} + \bar{F}_{\ell+1/2, k+1} - \bar{F}_{\ell+1/2, k} \right\}. \quad (3.25)$$

We have thus derived an expression, $\bar{D}$, which we shall assume to be a satisfactory discrete approximation to the differential operator, D , defined in equation (3.2). This approximation, defined by equation (3.23)

and (3.25) will be referred to in Chapter IV where the second part of the discretization procedure, differencing in time, will be discussed.

If cylindrical symmetry were observed instead of plane symmetry and a z - r coordinate system replaced the x - y system the only changes would be in the calculation of the volume, $|V|$, and areas, $|S|$, in equation (3.23).

The integral approximation $\{\phi, x\}$ and $\{\phi, y\}$ require knowledge of ϕ at grid points as well as zone centers. Although an arithmetic average of the values of ϕ at the surrounding four zone centers would have satisfactory formal error properties, it would not be appropriate for situations in which there were sharp changes in λ or grid spacing. Referring to Figure 3.3, consider a grid with constant mesh angle, θ but varying λ and grid spacing, h_k and h_λ . This may be a local approximation to a more general situation. We seek a representation of ϕ_0 which is consistent in the limit of constant flux, $\vec{F}$. In this case

$$\phi_i = \phi_0 + \vec{S}_i \cdot (\vec{\nabla} \phi) = \phi_0 + \frac{1}{\lambda_i} \vec{S}_i \cdot \vec{F} \quad (3.26)$$

where $\vec{S}_i$ is the vector from the vertex to the center of the i th zone and λ_i is the value of λ at the center of the i th zone. The desired average will be written as

$$\phi_0 = \sum_i \sigma_i \phi_i. \quad (3.27)$$

Substituting (3.27) in (3.26) we have

3.3 Notation for averaging algorithm to assign temperatures at grid vertices

$$\phi_o = \sum_i \gamma_i \phi_o + \sum_i \gamma_i / \lambda_i \vec{S}_i \cdot \vec{F} \quad (3.28)$$

As $\vec{F}$ is arbitrary we see that

$$\sum_i \gamma_i = 1 \quad (3.29)$$

and

$$\sum_i (\gamma_i / \lambda_i) \vec{S}_i = 0 \quad (3.30)$$

As

$$h_k^+ (\vec{S}_2 + \vec{S}_3) = h_k^- (\vec{S}_1 + \vec{S}_4) \quad (3.31)$$

and

$$h_\ell^+ (\vec{S}_3 + \vec{S}_4) = h_\ell^- (\vec{S}_1 + \vec{S}_2) \quad (3.32)$$

where the h's are the mesh constants indicated in Figure 3.3, we select

$$\begin{aligned} \gamma_1 &= c \lambda_1 / (h_\ell^+ h_k^+) \\ \gamma_2 &= c \lambda_2 / (h_\ell^+ h_k^-) \\ \gamma_3 &= c \lambda_3 / (h_\ell^- h_k^-) \\ \gamma_4 &= c \lambda_4 / (h_\ell^- h_k^+) \end{aligned} \quad (3.33)$$

where c is a constant of proportionality. In order to generalize to the case of a more general grid and also satisfy equation (3.29) we set

$$\gamma_i = \lambda_i / (|A_i| \sum_i (\lambda_i / |A_i|)) \quad (3.34)$$

where $|A_i|$ is the area of the i th zone projected onto the x - y plane.

We might determine at this point the form the difference operator, $\bar{D}$, assumes for a one-dimensional problem. If variation is permitted only in the x direction the $\bar{F}/|S|$ of equation (3.23) becomes

$$(\phi_2 - \phi_1) / ((\Delta x/\lambda)_1 + (\Delta x/\lambda)_2).$$

This expression is the result also of equating the fluxes in each zone based on a value $\bar{\phi}$ at the boundary between the zones. Then

$$\bar{F}/|S| = (\phi_2 - \bar{\phi}) / (\Delta x/\lambda)_1 = (\bar{\phi} - \phi_1) / (\Delta x/\lambda)_2 \quad (3.35)$$

and

$$\bar{\phi} = [(\Delta x/\lambda)_1 \phi_2 + (\Delta x/\lambda)_2 \phi_1] / [(\Delta x/\lambda)_1 + (\Delta x/\lambda)_2]. \quad (3.36)$$

This procedure can also be followed in two dimensions by calculating an energy flux through a zone boundary on each side of the boundary and equating them. This is done exactly as in equation (3.23) with the exception that one of the triangles in Figure 3.2 shrinks to zero, and the value of $\phi_{\ell+1/2, k+1/2}$ is to be determined. The result is that

$$\phi_{\ell+1/2, k+1/2} = \bar{\phi}_{\ell+1/2, k+1/2} + \phi_{\ell+1/2, k+1/2}^D \quad (3.37)$$

where

$$\bar{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} = \left[(A/\lambda)_1 \phi_{l+\frac{1}{2}, k+\frac{1}{2}} + (A/\lambda)_2 \phi_{l+\frac{1}{2}, k+\frac{1}{2}} \right] / \left[(A/\lambda)_1 + (A/\lambda)_2 \right] \quad (3.38)$$

and

$$\phi^D_{l+\frac{1}{2}, k+\frac{1}{2}} = \frac{\Delta \phi \left[(\vec{r}_{l+\frac{1}{2}, k+\frac{1}{2}} - \vec{r}_{l+\frac{1}{2}, k+\frac{1}{2}})(A/\lambda)_1 - (\vec{r}_{l+\frac{1}{2}, k+\frac{1}{2}} - \vec{r}_{l+\frac{1}{2}, k+\frac{1}{2}})(A/\lambda)_2 \right] \cdot (\vec{r}_{l+\frac{1}{2}, k+\frac{1}{2}} - \vec{r}_{l+\frac{1}{2}, k+\frac{1}{2}})}{\Delta^2 [(A/\lambda)_1 + (A/\lambda)_2]} \quad (3.39)$$

The first term $\bar{\phi}$ is analogous to the $\bar{\phi}$ of equation (3.36) while the second term vanishes for an orthogonal grid but for skewed grids may become important.

B. Accuracy of the Difference Operator

It is now appropriate to determine what errors are introduced by replacing the operator D by $\bar{D}$. For a first estimate we assume a regular grid of orthogonal coordinates with grid spacing h_x and h_y . In this case

$$\begin{aligned} (\bar{D}\phi)_{l+\frac{1}{2}, k+\frac{1}{2}} &= \bar{\lambda}_{l+\frac{1}{2}, k+\frac{1}{2}} (\phi_{l+\frac{1}{2}, k+\frac{1}{2}} - \phi_{l+\frac{1}{2}, k+\frac{1}{2}}) / h_x^2 \\ &+ \bar{\lambda}_{l, k+\frac{1}{2}} (\phi_{l-\frac{1}{2}, k+\frac{1}{2}} - \phi_{l+\frac{1}{2}, k+\frac{1}{2}}) / h_x^2 \\ &+ \bar{\lambda}_{l+\frac{1}{2}, k+1} (\phi_{l+\frac{1}{2}, k+\frac{1}{2}} - \phi_{l+\frac{1}{2}, k+\frac{3}{2}}) / h_y^2 \\ &+ \bar{\lambda}_{l+\frac{1}{2}, k} (\phi_{l+\frac{1}{2}, k-\frac{1}{2}} - \phi_{l+\frac{1}{2}, k+\frac{1}{2}}) / h_y^2 \end{aligned} \quad (3.40)$$

where, for instance

$$2/\bar{\lambda}_{l+1/2, k+1/2} = 1/\lambda(\rho_{l+1/2, k+1/2}, \bar{\varphi}_{l+1/2, k+1/2}) + 1/\lambda(\rho_{l+1/2, k+1/2}, \bar{\varphi}_{l+1/2, k+1/2}). \quad (3.41)$$

Upon expanding the above expression about values at the zone center ($l + 1/2, k + 1/2$) it is seen that

$$(\bar{D}\varphi)_{l+1/2, k+1/2} = (D\varphi)_{l+1/2, k+1/2} + (\text{terms of order } h_x^2, h_y^2 \text{ and higher order}) \quad (3.42)$$

indicating that

$$\lim_{\substack{h_x \rightarrow 0 \\ h_y \rightarrow 0}} \bar{D}\varphi = D\varphi \quad (3.43)$$

for functions φ, λ which are sufficiently well behaved. Unfortunately restrictions on computer storage and time do not permit proceeding far toward this limit so it is necessary to estimate the divergence of $\bar{D}$ from D in the case that h_x and h_y cannot be considered infinitesimal. To perceive the nature of the approximations made in the derivation of $\bar{D}$ we list them and apply them to the simplest meaningful case, i.e., a regular orthogonal grid with constant λ . Summarizing these approximations, we

1. replaced $D\varphi$ by $\int D\varphi \, d\tau / (V)$
2. approximated the components of $\lambda \nabla \varphi$ in $\int \lambda \nabla \varphi \cdot d\vec{s}$ by

$$\int \frac{\partial \varphi}{\partial \tau_i} d\tau_i \, dy / \int \frac{dx \, dy}{\lambda} \quad \text{and} \quad \int \frac{\partial \varphi}{\partial \tau_i} dx \, d\tau_i / \int \frac{dx \, dy}{\lambda}$$

3. replaced $\int \phi \, dx$ and $\int \phi \, dy$ by $[\phi, x]$ and $[\phi, y]$ and
4. approximated $\int \frac{dx \, dy}{\lambda}$ by A/λ .

In the case of constant λ , which we consider here, 4, is exact so we treat only the first three.

We first note that on an unbounded mesh, or one with periodic boundary conditions both $\bar{D}$ and D have as eigenfunctions

$$\phi_{\nu_x \nu_y} = e^{i(\nu_x x + \nu_y y)} \quad (3.44)$$

In particular

$$D \phi_{\nu_x \nu_y} = -\lambda (\nu_x^2 + \nu_y^2) \phi_{\nu_x \nu_y} \quad (3.45)$$

while

$$\bar{D} \phi_{\nu_x \nu_y} = -2\lambda \left[(1 - \cos \nu_x h_x) / h_x^2 + (1 - \cos \nu_y h_y) / h_y^2 \right] \phi_{\nu_x \nu_y}. \quad (3.46)$$

As the mesh increments h_x and h_y approach zero the eigenvalue of $\bar{D}$ is

$$-\lambda (\nu_x^2 + \nu_y^2 - (\nu_x^4 h_x^2 + \nu_y^4 h_y^2) / 12 + O(h_x^4, h_y^4)). \quad (3.47)$$

If one could afford zoning so fine that for any component of ϕ which had a nonzero coefficient the values of $\nu_x h_x$ and $\nu_y h_y$ were very small the eigenvalues of $\bar{D}$ and D for these components would be nearly equal. However, if there were major changes in ϕ from zone to zone then the shortest wavelength in the x direction which the mesh can support, $\nu_x h_x = \pi$ would contribute in an important fashion to the expansion

of ϕ and in this case the x contribution to the eigenvalue of D is $-\gamma\lambda/h_x^2$ compared to $-\pi^2\lambda/h_x^2$ for D. This represents considerable divergence, indicating that short wavelengths are not sufficiently damped by the difference operator. In noting the effects of each of the three major approximations we assume ψ_y constant and consider three values of ψ_x :

1. $\psi_x h_x = \epsilon$, a small value characteristic of long waves,
2. $\psi_x h_x = \pi/4$, an intermediate, perhaps typical, wavelength, and
3. $\psi_x h_x = \pi$, the shortest wavelength.

Replacing $D\phi$ by

$$\int_V D\phi d\tau / |V|$$

means that the $-\lambda(\psi_x^2 + \psi_y^2)$ is replaced by

$$-\lambda(\psi_x^2 + \psi_y^2) \frac{\sin(\psi_x h_x/2)}{(\psi_x h_x/2)} \frac{\sin(\psi_y h_y/2)}{(\psi_y h_y/2)}.$$

The factor

$$\frac{\sin(\psi_x h_x/2)}{(\psi_x h_x/2)}$$

takes on the values

$$1 - \epsilon^2/6,$$

$$(4\sqrt{2 - \sqrt{2}})/\pi \text{ or } \approx 0.974,$$

$$\text{and } 2/\pi, \approx 0.637,$$

for the three test values.

The second and third approximations combine to replace, for instance,

$$\int_{S_{\ell+1/2, K+1/2}} \frac{\partial \phi}{\partial x} ds \text{ by } \frac{|S|}{|A|} [\phi, y]_{\ell+1/2, K+1/2}.$$

As we are considering orthogonal coordinates the values of ϕ at grid points are irrelevant and

$$[\phi, y]_{\ell+1/2, K+1/2} = \frac{1}{2} h_y (\phi_{\ell+1/2, K+1/2} - \phi_{\ell+1/2, K+1/2}) \quad (3.48)$$

The result here is that a factor of

$$\frac{\partial_x}{\partial_y} \sin(\partial_y h_y / 2)$$

is replaced in the approximation by

$$\frac{h_y}{h_x} \sin(\partial_x h_x / 2).$$

These quantities may differ greatly, yet the effect of all three approximations is indicated by equation (3.46) which shows that for long wavelengths ($\partial h < \pi/4$) the approximate eigenvalues are within 5% of the true values. Although this description is straightforward for the simple geometry considered it lends insight into the nature of the approximation for more complex cases.

C. Problem Boundaries

When a zone for which we are seeking a difference equation has one or more sides coincident with a problem boundary we must determine what modifications to the scheme which we have accepted for interior zones are indicated. There are several external boundary conditions permitted for the diffusion physics in the CEL and CHAMP codes. These are insulated or symmetry boundaries, prescribed temperature boundaries, and vacuum boundaries.

In the case of an insulated or symmetry boundary there is no flow of energy through the boundary. This may be due to the fact that in the physical situation considered the boundary adjoins a region in which conduction of radiation is very small due to a small mean free path. In this case the appropriate $\bar{F}$ in equation (3.25) is set to zero. In order to calculate flow parallel to the boundary, values of ϕ at grid points on the boundary are needed. The procedure here is to reflect each boundary zone across the boundary to create a virtual zone of identical area and λ on the outside. Then the averaging algorithm of equation (3.27) and (3.34) may be applied.

When a problem is driven from the outside or is bounded by a region, which because of its large heat capacity is assumed to maintain a certain temperature throughout the time of interest, a prescribed temperature boundary is needed. In this case an imaginary zone of infinitesimal thickness is adjoined to each boundary segment. The center of this zone is at the center of the boundary segment and the value of A in equation (3.22) is zero, making the corresponding value of λ immaterial. The calculation of ϕ at the boundary points degenerates in equation (3.29) to a sum over only two terms as two of the areas are zero.

In the case that a boundary is adjoined by a region in which λ is so large that all energy leaving the boundary is lost and there is no energy incident from the outside we apply a vacuum boundary condition. It is not proper in this case to treat the boundary as a zero temperature Dirichlet condition nor is it appropriate to treat the boundary as a black body emitter at the temperature of the boundary zone. The boundary may however be considered to be a black body emitter at some reduced effective temperature. Returning to the definition of $\vec{F}$ given after equation (2.3) and considering variation only in the direction normal to the boundary we have

$$F = |\vec{F}| = \left| \int_{4\pi} I \vec{n} d\Omega \right| = 2\pi \int_{-1}^1 I \cos\theta d(\cos\theta) \quad (3.49)$$

If θ is measured from the outward normal and a mean value theorem applied to the integral on the right hand side we have

$$\begin{aligned} F &= 2\pi \int_{-1}^0 I \cos\theta d(\cos\theta) + 2\pi \int_0^1 I \cos\theta d(\cos\theta) \\ &= -\pi I^i + \pi I^o \end{aligned} \quad (3.50)$$

where I^i and I^o are the inward and outward directed average intensities. A similar approximation yields

$$\vec{E} = \frac{1}{c} \int_{4\pi} I d\Omega = 2\pi/c (I^i + I^o). \quad (3.51)$$

As there is no inward directed radiation at the boundary $I^i = 0$ so

$$F = c E / 2 \quad (3.52)$$

As $E = a\phi$ we have

$$F = ac\phi/2 \quad (3.53)$$

which means the effective value of T^4 is twice the value of T^4 for a black body. We equate this flux to the diffusion flux to find a boundary value ϕ_b .

$$\frac{ac}{3\tau} (\phi - \phi_b) = ac\phi_b/2 \quad (3.54)$$

so

$$\phi_b = \phi / (1 + \frac{3}{2}\tau) \quad (3.55)$$

where ϕ is the value at the center of the boundary zone and τ is the normal distance from zone center to boundary divided by the Rosseland mean free path evaluated at the zone center. Thereafter the boundary is treated as a prescribed temperature boundary.

D. Coupled Boundaries

At the boundary between two regions, whether they both are Eulerian regions or one is a Lagrange region, some modification of the differencing scheme must be employed. The nature of the modification will depend on whether we are examining the effect on an Eulerian or Lagrange

region, and also whether the boundary condition is to be of the Dirichlet or Neumann type.

We consider first the Lagrange region as it is more straightforward. We must find an expression for the $\bar{F}$ of equation (3.23). As this term has the dimensions of energy per unit time, a Neumann, or flux, boundary condition is satisfied by setting $\bar{F}$ to the prescribed value of the energy flux. In the case of a prescribed value of ϕ at the boundary we assume that a pseudo-zone abuts the Lagrange zone and shares one of its sides. If we further assume that the line joining the centers of the Lagrange zone and the pseudo-zone is normal to the shared side, equation (3.23) can be rewritten as

$$\bar{F}_b = (\phi_b - \phi_L) / (\tau_b + \tau_L) \cdot |S| \quad (3.56)$$

where ϕ_b is the boundary value

ϕ_L is the value at the center of the Lagrange zone and

$$\tau_L = 2 A_L / (\lambda_L \Delta).$$

The values of ϕ_b and τ_b must be computed as averages over the Eulerian zones which share a boundary with the Lagrange zone. Referring to Figure 3.4 we see a number of Eulerian zones along the segment labeled J. If the value τ_L was known to be associated with the other side of that segment then one could require that

$$\sum_i \frac{|S_i| (\phi_i - \phi_L)}{\tau_i + \tau_L} = \frac{|S| (\phi_b - \phi_L)}{\tau_b + \tau_L} \quad (3.57)$$

3.4 Jth segment of Eulerian-Lagrangian interface. Boundary conditions are transmitted for each such segment

be satisfied identically in ϕ_L . In this equation the $|S_i|$ are the areas which each Eulerian zone shares with the boundary and the ϕ_i and τ_i are values for each Eulerian zone. Thus equation (3.57) means that the sum of energy flows across subsegments of the boundary be represented by the single term on the right. If (3.57) is to be an identity in ϕ_L we must have

$$\sum_i \frac{|S_i|}{\tau_i + \tau_L} = \frac{|S|}{\tau_b + \tau_L} \quad (3.58)$$

and

$$\sum_i \frac{|S_i| \phi_i}{\tau_i + \tau_L} = \frac{|S| \phi_b}{\tau_b + \tau_L} \quad (3.59)$$

leading to

$$\tau_b = \left(\sum_i (|S_i|/|S|) / (\tau_i + \tau_L) \right)^{-1} - \tau_L \quad (3.60)$$

and

$$\phi_b = \left(\sum_i (|S_i|/|S|) \phi_i / (\tau_i + \tau_L) \right) / \left(\sum_i (|S_i|/|S|) / (\tau_i + \tau_L) \right). \quad (3.61)$$

Summarizing, the knowledge of τ_L and the τ_i and ϕ_i from the Eulerian side permit the calculation of ϕ_b and τ_b which are used in equation (3.56) to calculate the energy flow across a portion of the boundary.

When viewing the situation in an Eulerian boundary zone a somewhat more complex situation develops. Now the sum in equation (3.25) is over only those sides of the Eulerian zone which are not covered by another region. Each term, $\bar{F}$, of the sum is of the form

$$\bar{F} = (\phi_2 - \phi_1) / (\tau_1 + \tau_2) \cdot |S| \quad (3.62)$$

where the zone indexed by 1 is the one for which the sum is being performed and the index 2 refers to an adjacent zone. The value of $|S|$ must be the portion of the area of the zone side which is not covered by another region. Some of the summands will be over areas which the Eulerian zone shares with another region. If a temperature boundary condition is to prevail then ϕ_L and τ_L are both prescribed and the $\bar{F}$ of equation (3.62) is computed directly. If, however, a flux condition is to be applied some means of apportioning the energy among the Eulerian zones that abut the boundary area must be devised. It is not satisfactory to adopt the natural convention that the energy flow per unit area is constant across the boundary. In the case of a steep temperature gradient tangent to the boundary some zones may be called upon to deliver up more energy than they possess. It is reasonable to treat the boundary condition as a temperature boundary condition first and calculate the partial energy flows, F_i , across each portion of the boundary area. Then if F is the prescribed boundary flux define

$$\tilde{F}_i = F_i + |F_i| \cdot (F - \sum_i F_i) / \sum_i |F_i|. \quad (3.63)$$

Note that $\tilde{F}_i = F_i$ if the sum of the individually calculated flows is in fact equal to the prescribed flux and also that

$$\sum_i \tilde{F}_i = F \quad (3.64)$$

so that energy is conserved. If this procedure is followed, zones which should be contributing little to the total flux are not greatly affected by a large tangential temperature gradient.

The blending procedure, described at the end of Section II B, was conceived to allow each Eulerian zone to maintain dimensions comparable to that of the underlying grid in order that the Courant stability condition for the hydrodynamics calculation not be too restrictive. In the sequel it will be seen that it is not efficient to use a similar construct for the diffusion equation differencing. Yet neither is it appropriate to permit blended zones, which may have volumes many times smaller than the nearby interior zones, to deal exclusively with the transport across the region boundaries which they share. Because for high temperatures heat capacity is proportional to volume, the interregion coupling terms are apportioned between the blended zone in which the boundary lies and the zone into which it has blended according to the ratio of their volumes.

IV. Differencing in Time

We are now prepared to discuss the means of solving the model problem which we pose for ourselves, i.e., given a physical situation which we believe to be adequately described by Euler's equations of hydrodynamics and the diffusion equation of radiation transfer together with initial and boundary conditions, to find an algorithm which provides a useful approximation to the physical state of the system at some later time. We may be somewhat more specific in that the class of problems for which the CEL¹⁰ and CHAMP¹¹ codes are intended are those in which transient phenomena are those of greatest interest. Thus the time of interest will be that in which the initial conditions and local sources dominate the solution. More stringent demands are made upon a code which must calculate until some steady state or equilibrium condition is achieved.

This chapter deals primarily with the manner in which the diffusion equation is differenced. A discussion of the means by which the hydrodynamics is accommodated is reserved until section IV.E.

A. Selecting a differencing scheme

The diffusion equation, (2.16), is now replaced by a system of ordinary differential equations

$$\frac{d\bar{\phi}}{dt} = \frac{1}{c_v} \bar{D} \bar{\phi} \quad (4.1)$$

where $c_v = \left. \frac{\partial \epsilon}{\partial \phi} \right|_p$,

is the sum of internal and radiation energy per unit volume,

$\bar{D}$ is the operator defined in equation (3.25) and

$\bar{\phi}$ is the vector whose components are the values of ϕ at zone centers.

We shall drop the overbars on $\bar{D}$ and $\bar{\phi}$ in what follows.

Many considerations present themselves in the process of determining an appropriate differencing scheme for the approximate solution of equation (4.1). The first of these is the feasibility of simultaneously considering all the regions, Lagrange and Eulerian, that make up the problem. Because each region may have tens of thousands of zones and the pattern of incidence of one region upon another may be very complex geometrically, it is more efficient to process each region separately, if a suitable interregion coupling can be achieved. This coupling is the subject of section IV.D.

Within a given region it is necessary to decide how many levels in time are to influence the calculation of the solution at the next time. In absence of any compelling superiority of multi-level schemes and the extra storage requirement which they impose a two level scheme was deemed adequate. Thus the time discretization of equation (4.1) is to involve only values at t^n and t^{n+1} and superscripts will henceforth denote which of these applies. The discrete form of equation (4.1) will then be

$$\phi^{n+1} - \phi^n = \frac{\Delta t}{c_v} (D_1 \phi^n + D_2 \phi^{n+1}) \quad (4.2)$$

where D_1 and D_2 are chosen to be consistent with equation (4.1) and also the definition of $D(D)$ in equation (3.24).

If D_2 is the null operator and $D_1 = D$ then the solution procedure is explicit, fast, and unacceptable due to the stability imposed limit on Δt .² If the time of interest exceeds by a significant amount the time during which the shortest wavelengths are damped then the explicit procedure requires many more time steps than the relaxation time of the

physical problem would indicate. Alternatively if $D_1 = 0$ and $D_2 = D$ then a large set of simultaneous equations must be solved. Although recent advances¹⁹ in solving systems which arise from partial differential equations indicate that the cost in storage and computational time per cycle is no longer prohibitive, experience since the 1955 publication of the Peaceman-Rachford method¹³ for solution of parabolic equations has shown that methods relying on one dimensional sweeps²⁰ are efficient and accurate for a wide class of problems. To apply such a method in the case of orthogonal zoning it is necessary to separate the operator D of equation (3.25) into two components, D_ℓ and D_K

$$\text{where } D_\ell \phi_{\ell+1/2, k+1/2} = \frac{\Delta t}{C_v} |V|_{\ell+1/2, k+1/2}^{-1} \left(\bar{F}_{\ell+1, k+1/2} - \bar{F}_{\ell, k+1/2} \right) \quad (4.3a)$$

$$\text{and } D_K \phi_{\ell+1/2, k+1/2} = \frac{\Delta t}{C_v} |V|_{\ell+1/2, k+1/2}^{-1} \left(\bar{F}_{\ell+1/2, k+1} - \bar{F}_{\ell+1/2, k} \right). \quad (4.3b)$$

The case where the zones are not rectangular is deferred to section IV.C.

The primary appeal of the fractional step methods is that the equations to be solved have a banded matrix with small bandwidth. Most often the matrices are tridiagonal and very efficient means have been devised for the solution of such systems.² Of all such schemes the one selected was the simplest splitting scheme:

$$(I - D_K)(I - D_\ell)\phi^{n+1} = \phi^n \quad (4.4)$$

The chief disadvantage of such a scheme is that it is only correct to terms of first order in Δt while almost every other scheme is correct to at least second order in Δt .¹⁴ However the hydrodynamics portion of the code is also correct to only first order in its advection phase¹¹ and so there is no possibility of improving the formal accuracy of the program by selecting a second order method for the diffusion portion.

More important, however, the scheme of equation (4.4) possesses a stability based on a maximum principle rather than one based on a linear analysis of spectral components as is the case for second order schemes. In that linear analysis two disturbing features of the second order schemes are revealed.²⁰ One feature is that as short wavelengths are damped and the time step rises to exceed the relaxation time for those wavelengths, the solution process ceases to damp them further but in the limit of large time step merely inverts their amplitude each cycle. Thus, as the solution evolves they represent components on the threshold of instability. As the algorithm is to be applied to a nonlinear problem with possibly distorted geometry the possibility of an instability occurring must be considered. As will be noted in section IV.D. the interregion coupling is also stable only by the same margin, thus the comfort of an internal differencing method the stability of which required no strong assumptions was sought.

The second feature of the second order schemes which was found to be disturbing was that the final value of ϕ was the result of several steps and intermediate values could be the result of unstable one dimensional sweeps followed by stabilizing successive sweeps. As will be noted in section IV.B. the values of C_v which are to be calculated for each

sweep are of essential importance to the accuracy of the solution. Their calculation on the basis of unphysical intermediate values would be an invitation to invalidate the solution process.

Thus although the algorithm suggested in equation (4.4) falls short of the best available in terms of formal accuracy, for the calculation of transients in a nonlinear system described on a collection of space grids, this fully implicit splitting is appropriate.

B. Calculation of Coefficients

Considering a single step of the splitting procedure, e.g.

$$(I - D) \phi_{\ell, n_2}^* = \phi_{\ell, n_2}^n \quad (4.5)$$

we examine the time dependence of the coefficients in D_ℓ . Many of these,

$|V|_{\ell, n_2}$ for example, are geometric in nature and are evaluated using the latest position of Lagrange and interface vertices. Two coefficients depend on the state of the material through which the radiation is diffusing. The first of these is the radiation mean free path, λ , which is a function of the chemical identity of the material as well as its thermodynamic state as specified by its density and temperature. As we have already decided to admit errors of second order in Δt it is not inappropriate to evaluate the mean free path at a time other than a centered time. Hence we do not extrapolate in time to achieve a formally superior coefficient but rather accept the thermodynamic state of the material at the beginning of each diffusion time step as representative of the state throughout that time step.

Such a procedure is not appropriate for the calculation of the specific heat, $\frac{\partial \epsilon}{\partial \varphi}$, however. Although energy is not formally conserved when differencing φ , the effectiveness of the diffusion approximation in solving highly nonlinear radiation transport problems rests heavily on the approximate conservation of energy. If we rewrite equation (4.5) locally for the ℓ th zone we have

$$\varphi_{\ell+1/2}^* = \varphi_{\ell+1/2}^n + \Delta t (F_{\ell+1} - F_{\ell}) / (|V|_{\ell+1/2} \frac{\partial \epsilon}{\partial \varphi}_{\ell+1/2}). \quad (4.6)$$

Summing to find the total energy, E^* , for this row or column of zones we have

$$\begin{aligned} E^* &= \sum_{\ell} |V|_{\ell+1/2} \epsilon_{\ell+1/2}^* \\ &= \sum_{\ell} |V|_{\ell+1/2} \left(\epsilon_{\ell+1/2}^n + \frac{\epsilon_{\ell+1/2}^* - \epsilon_{\ell+1/2}^n}{\varphi_{\ell+1/2}^* - \varphi_{\ell+1/2}^n} (\varphi_{\ell+1/2}^* - \varphi_{\ell+1/2}^n) \right) \\ &= E^n + \Delta t \sum_{\ell} |V|_{\ell+1/2} \frac{\epsilon_{\ell+1/2}^* - \epsilon_{\ell+1/2}^n}{\varphi_{\ell+1/2}^* - \varphi_{\ell+1/2}^n} (F_{\ell+1} - F_{\ell}) / (|V|_{\ell+1/2} \frac{\partial \epsilon}{\partial \varphi}_{\ell+1/2}) \\ &= E^n + \Delta t \sum_{\ell} (F_{\ell+1} - F_{\ell}) \frac{\epsilon_{\ell+1/2}^* - \epsilon_{\ell+1/2}^n}{\varphi_{\ell+1/2}^* - \varphi_{\ell+1/2}^n} / \frac{\partial \epsilon}{\partial \varphi}_{\ell+1/2}. \end{aligned} \quad (4.7)$$

Now if in each instance the secant to the $\epsilon - \varphi$ plot,

$$\frac{\epsilon_{\varphi^{n+1/2}}^* - \epsilon_{\varphi^{n+1/2}}^n}{\varphi_{\varphi^{n+1/2}}^n - \varphi_{\varphi^{n+1/2}}^n}$$

were equal to the value of $\frac{\partial \epsilon}{\partial \varphi_{\varphi^{n+1/2}}}$ which is used in equation (4.6), the sum in equation (4.7) would vanish except for boundary terms as each transfer term, F_x , would appear twice, but with opposite signs. Hence the degree to which energy conservation is achieved will depend on how closely $\frac{\partial \epsilon}{\partial \varphi}$ approximates the secant.

It is possible to extrapolate in time to estimate $\varphi^{n+1/2}$ for each zone but there are three disadvantages to this approach. First there is the problem of storage as at least one value of φ before time t^n would be carried and for a problem with tens of thousands of zones this is a significant consideration. Secondly, even if we could estimate

$\varphi^{n+1/2}$ exactly it is not $\frac{\partial \epsilon}{\partial \varphi}(\varphi^{n+1/2})$ that is demanded for

conservation but rather the secant. Finally, a very sensitive extrapolation is necessary to propagate a nonlinear wave. Because $\frac{\partial \epsilon}{\partial \varphi}$ is proportional to $\varphi^{-3/4}$ at low temperatures it attains very large values in that case. As $\frac{\partial \epsilon}{\partial \varphi}$ appears in the denominator of equation (4.6), if the approach of a thermal wave is not properly anticipated by the extrapolation procedure an initially cold zone will not be able to accept energy. This will lead the time extrapolation to continue to predict low temperatures and hence high specific heats.

To obviate these difficulties an extrapolation is made on the basis of space differencing. In each zone equation (4.6) is rewritten

$$\frac{\partial \epsilon}{\partial \varphi_{\ell+1/2}} (\varphi_{\ell+1/2}^* - \varphi_{\ell+1/2}^n) = a_1 \varphi_{\ell+1/2}^* + a_2 \varphi_{\ell+1/2}^* + a_3 \varphi_{\ell+1/2}^* + a_4. \quad (4.8)$$

We define an extrapolated φ^{ext} by

$$\frac{\partial \epsilon}{\partial \varphi_{\ell+1/2}} (\varphi_{\ell+1/2}^{\text{ext}} - \varphi_{\ell+1/2}^n) = a_1 \varphi_{\ell+1/2}^{\text{ext}} + a_2 \varphi_{\ell+1/2}^n + a_3 \varphi_{\ell+1/2}^n + a_4. \quad (4.9)$$

This can be solved for $\varphi_{\ell+1/2}^{\text{ext}}$ to yield

$$\varphi_{\ell+1/2}^{\text{ext}} = (\varphi_{\ell+1/2}^n + x \varphi_{\ell+1/2}^{\text{eq}}) / (1 + x) \quad (4.10)$$

where

$$\varphi_{\ell+1/2}^{\text{eq}} = -(a_2 \varphi_{\ell+1/2}^n + a_3 \varphi_{\ell+1/2}^n + a_4) / a_1,$$

and

$$x = -a_1 / \frac{\partial \epsilon}{\partial \varphi_{\ell+1/2}}.$$

As $\varphi_{\ell+1/2}^{\text{eq}}$ is independent of $\frac{\partial \epsilon}{\partial \varphi}$ we may iterate to find new values of x with

$$x^{(m)} = -a_1 / \frac{\partial \epsilon}{\partial \varphi_{\ell+1/2}}^{(m)}. \quad (4.11)$$

$$\varphi_{\ell+1/2}^{\text{ext}^{(m)}} = (\varphi_{\ell+1/2}^n + x^{(m)} \varphi_{\ell+1/2}^{\text{eq}}) / (1 + x^{(m)}) \quad (4.12)$$

$$\frac{\partial \epsilon}{\partial \varphi}^{(m+1)} = \left(\epsilon(\varphi_{\ell, \nu_2}^{\text{ext}(m+1)}) - \epsilon_{\ell, \nu_2}^{\eta} \right) / \left(\varphi_{\ell, \nu_2}^{\text{ext}(m+1)} - \varphi_{\ell, \nu_2}^{\eta} \right) \quad (4.13)$$

starting with

$$\frac{\partial \epsilon}{\partial \varphi}^{(0)} = \left(\epsilon(\varphi_{\ell, \nu_2}^{\text{eq}}) - \epsilon_{\ell, \nu_2}^{\eta} \right) / \left(\varphi_{\ell, \nu_2}^{\text{eq}} - \varphi_{\ell, \nu_2}^{\eta} \right). \quad (4.14)$$

We proceed until successive values of $\frac{\partial \epsilon}{\partial \varphi}^{(m)}$ are nearly equal.

Unfortunately there are cases for which this iteration does not converge and the remedy is discussed in Appendix IV.A.

It is possible to appraise the value of this extrapolation for the case of constant coefficients, i.e.

$$-a_1 = 2a_2 = 2a_3 = 2\alpha > 0$$

and

$$a_4 = 0.$$

In this case $\varphi_{\ell, \nu_2}^{\text{eq}}$ lies between $\varphi_{\ell, \nu_2}^{\eta}$ and $\varphi_{\ell, \nu_2}^{\eta}$ and $\varphi_{\ell, \nu_2}^{\text{ext}}$ is a convex combination of the values of φ^{η} at three successive locations. If one spectral component is considered, for example space dependence proportional to e^{ikx} , then

$$\varphi_{\ell, \nu_2}^{\text{ext}} / \varphi_{\ell, \nu_2}^{\eta} = (1 + \alpha \cos K\Delta x) / (1 + \alpha) \quad (4.15)$$

while

$$\phi_{\ell, \nu_2}^* / \phi_{\ell, \nu_1}^* = 1 / (1 + \alpha (1 - \cos K \Delta x)) \quad (4.16)$$

and both are of the form

$$1 + \alpha (\cos K \Delta x - 1) + O(\alpha^2)$$

Thus in the regime where there are large amplitudes for short wavelengths and hence α is small, ϕ^{ext} will be a good approximation to ϕ^* and hence the secants will be in good agreement. Certainly a cold zone abutting a hot zone will have a value of $\frac{\partial \epsilon}{\partial \phi}$ that reflects the fact that it is being directly heated. When the short wavelengths have been damped ϕ^{ext} may diverge from ϕ^* but $\alpha(1 - \cos K \Delta x)$ will always be small as it is the consequence of an accuracy time step limitation. If the long wavelengths dominate in a region where the radiation energy density exceeds the material internal energy then total internal energy, ϵ , is nearly linear in ϕ so the error in estimating $\frac{\partial \epsilon}{\partial \phi}$ is small. If long wavelengths dominate in a cold region the value of α will be very small and again $\frac{\partial \epsilon}{\partial \phi}$ will be well approximated.

C. Treatment of Skewed Grids

1. Description of a method for treating skewed grids

As we have mentioned in the first section of this chapter, the method of one dimensional sweeps is particularly appealing because in its simplest form it leads to the solution of tridiagonal systems of

equations. A typical equation of such a system might be written in the form

$$-A_j \phi_{j+1} + B_j \phi_j - C_j \phi_{j-1} = D_j \quad (4.17)$$

The simple algorithm for the solution of the system³ proceeds by assuming that

$$\phi_j = E_j \phi_{j+1} + F_j \quad (4.18)$$

and substituting into equation (4.17) to obtain

$$E_j = A_j / (B_j - C_j E_{j-1}) \quad (4.19)$$

$$F_j = (D_j + C_j F_{j-1}) / (B_j - C_j E_{j-1}) \quad (4.20)$$

The first and last values of the E's and F's depend upon the boundary conditions but generally if all A's, B's, and C's are greater than zero and each B exceeds the sum of the corresponding A and C then the E's and F's can be found recursively from equations (4.19) and (4.20) and the equation (4.18) can be used to find the ϕ 's starting at the highest value of j. Although the splitting into these one dimensional sweeps indicated in equations (4.1)-(4.4) is straightforward when the mesh is orthogonal, if the grid is skewed each zone is coupled to its eight nearest neighbors and the simple splitting into two sweeps is not possible. Very likely this situation will arise in the Lagrange regions

and a discussion of some means of dealing with it will be found in Appendix IV.B. We describe here the particular scheme used in the CEL and CHAMP codes.

Recall from equation (3.23) that the flux across a zone face has the form

$$\bar{F}_{\ell+1/2, K+1/2} = \left\{ \frac{[\phi_y] \Delta y + [\phi_x] \Delta x}{|A/\lambda|} \frac{|S|}{\Delta} \right\}$$

We rewrite this for use in an ℓ sweep

$$\bar{F}_{\ell+1} = \chi_{\ell+1}^0 \left(\chi'_{\ell+1} (\phi_{\ell+1/2, K+1/2} - \phi_{\ell+1/2, K+1/2}) + \chi_{\ell+1}^2 (\phi_{\ell+1/2, K+1} - \phi_{\ell+1/2, K}) \right) \quad (4.21)$$

where

$$\chi^0 \equiv |S| / (|A/\lambda| \Delta)$$

$$\chi' \equiv \Delta^2$$

$$\chi^2 \equiv -\vec{\Delta} \mathbf{r} \cdot \delta \vec{r}$$

If χ^2 is zero then the values of ϕ at the grid vertices are not germane. If this is not the case the tridiagonal form can be maintained by evaluating the term multiplied by χ^2 explicitly, i.e., at time t^n , or to introduce splitting in more than two directions. If separate sweeps are employed to deal with these diagonal terms the conditions on

the A's, B's, and C's mentioned after equation (4.20) may not be satisfied and the solution may not exist or may lead to an instability even if it does.

In view of this we employ here a strategem of treating the term

$$\chi_{\ell+1}^0 \chi_{\ell+1}^2 (\phi_{\ell+1/2, \kappa+1} - \phi_{\ell+1, \kappa})$$

in a manner depending upon its sign. The ϕ 's are the most recent values which we denote by ϕ^n . If the term is positive it is multiplied by

$$\phi_{\ell+1/2, \kappa+1/2}^{n+1} / \phi_{\ell+1/2, \kappa+1/2}^n$$

where the superscript (n+1) refers to the value after solution of the tridiagonal system. If the term is negative it is multiplied by

$$\phi_{\ell+1/2, \kappa+1/2}^{n+1} / \phi_{\ell+1/2, \kappa+1/2}^n$$

Each of the diagonal flux contributions is treated in this manner so that a zone which would lose energy due to such a term finds the term decreases with its own value of ϕ . These diagonal flux terms can never drive ϕ negative in a zone where it was positive at the start of the sweep.

On a typical ℓ sweep each equation is then of the form (with k indices deleted)

$$\alpha_{l+1/2} (\varphi_{l+1/2}^{n+1} - \varphi_{l+1/2}^n) = \beta_{l+1} (\varphi_{l+1/2}^{n+1} - \varphi_{l+1/2}^{n+1/2}) + \beta_l (\varphi_{l+1/2}^{n+1} - \varphi_{l+1/2}^{n+1/2}) \quad (4.22)$$

$$+ \delta_{l+1/2} \varphi_{l+1/2}^{n+1} + \eta_{l+1/2} \varphi_{l+1/2}^{n+1} - (\delta_{l+1/2} + \eta_{l+1/2}) \varphi_{l+1/2}^{n+1/2}.$$

The α terms are composed of specific heat and volume, while the β 's are positive terms derived from geometric and opacity calculations. The terms in δ and η are selected as mentioned above to appear positively, i.e. if the explicit diagonal flux across the boundary at $l+1$ carried energy from the zone at $l+3/2$ to the zone labeled $l+1/2$ then $\delta_{l+1/2}$ is nonzero and $\eta_{l+1/2}$ will be zero. In this case

$$\delta_{l+1/2} = (\chi^0 \chi^1)_{l+1/2, l+1/2} (\varphi_{l+1/2, l+1}^n - \varphi_{l+1/2, l+1}^n) / \varphi_{l+1/2, l+1/2}^n \quad (4.23)$$

and $\eta_{l+1/2} = 0.$

If the flow had gone from zone $l+1/2$ to zone $l+3/2$, then

$$\delta_{l+1/2} = 0$$

and $\eta_{l+1/2} = (\chi^0 \chi^1)_{l+1/2, l+1/2} (\varphi_{l+1/2, l+1}^n - \varphi_{l+1/2, l+1}^n) / \varphi_{l+1/2, l+1/2}^n. \quad (4.24)$

Thus the δ 's and η 's are positive if the φ 's in the denominators are positive. In the case that the φ in the zone from which the energy is to flow is zero, both δ and η are set to zero.

We now examine the coefficients, $E_{\ell+\nu_2}$ and $F_{\ell+\nu_2}$ of the tridiagonal algorithm to determine if the system can be solved and also whether the ϕ 's remain non-negative. Proceeding as before we find

$$E_{\ell+\nu_2} = (\beta_{\ell+1} + \delta_{\ell+\nu_2}) / G_{\ell+\nu_2} \quad (4.25)$$

$$F_{\ell+\nu_2} = (\alpha_{\ell+\nu_2} \phi_{\ell+\nu_2}^n + (\beta_{\ell} + \eta_{\ell+\nu_2}) F_{\ell+\nu_1}) / G_{\ell+\nu_2} \quad (4.26)$$

$$G_{\ell+\nu_2} = \alpha_{\ell+\nu_2} + \beta_{\ell+1} + \eta_{\ell+\nu_2} + \mu_{\ell+\nu_2} \quad (4.27)$$

$$\mu_{\ell+\nu_2} = \beta_{\ell} + \delta_{\ell+\nu_2} - E_{\ell+\nu_2} (\beta_{\ell} + \eta_{\ell+\nu_2}). \quad (4.28)$$

The set of equations for the $\phi^{(n)}$ will be soluble if all the G 's are greater than zero. This is so if the μ 's are non-negative. We show this by induction. We see that $\mu_{\nu_1} > 0$ as it involves only a positive coupling term to a region on the other side of the boundary.

If $\mu_{i+\nu_i} \geq 0$ for all $i < \ell$ then as

$$\mu_{\ell+\nu_2} = \beta_{\ell} + \delta_{\ell+\nu_2} - (\beta_{\ell} + \delta_{\ell+\nu_2})(\beta_{\ell} + \eta_{\ell+\nu_2}) / (\alpha_{\ell+\nu_2} + \beta_{\ell} + \eta_{\ell+\nu_2} + \mu_{\ell+\nu_2})$$

we see that

$$\mu_{\ell, \nu_2} = (\beta_\ell + \delta_{\ell, \nu_2})(\alpha_{\ell, \nu_2} + \mu_{\ell, \nu_2}) / (\alpha_{\ell, \nu_2} + \beta_\ell + \eta_{\ell, \nu_2} + \mu_{\ell, \nu_2}). \quad (4.29)$$

As all terms involving $\alpha, \beta, \delta, \eta$ are non-negative by selection and μ_{ℓ, ν_2} is non-negative by hypothesis we see that μ_{ℓ, ν_2} is also non-negative. We now ask whether any of the $\varphi^{(n)}$ are negative. Again induction shows that the F's are positive if the interregion coupling term does not drive $F_{1/2}$ negative. Then as all the E's and F's are positive only a boundary term at the last zone can cause a negative $\varphi^{(n)}$. To summarize then the linear system can be solved and yields a non-negative solution if the initial values are also non-negative and the boundary conditions are properly bounded. This together with the fact that energy is conserved if the specific heats are accurately estimated means that the range of values for φ is bounded above and below and stability is then indicated.

2. Analysis of the method

The stability analysis outlined in Appendix IV.B. is not appropriate for this scheme as the coefficients δ and η depend on in a way that would make them different for different wavelengths so a linear constant coefficient situation does not obtain. To further study the properties of this differencing scheme in skewed coordinates it will be helpful to display the quantity $\vec{\nabla} \cdot \lambda \vec{\nabla} \varphi$ in the ℓ - k coordinate system. The metric tensor g_{ij} in this system is

$$g_{ij} = \begin{bmatrix} \delta l^2 & \delta l \delta \kappa \cos \ell \kappa & 0 \\ \delta l \delta \kappa \cos \ell \kappa & \delta \kappa^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (4.30)$$

so that the volume element is $\sqrt{g} = \delta l \delta \kappa \sin \ell \kappa$. Here

$$\delta l = \left| \frac{\partial \vec{r}}{\partial l} \right|$$

$$\delta \kappa = \left| \frac{\partial \vec{r}}{\partial \kappa} \right|$$

and $\cos \ell \kappa$ and $\sin \ell \kappa$ are the cosine and sine of the angle between the coordinate lines. Then the contravariant form of the metric tensor is given by

$$g^{ij} = \begin{bmatrix} \delta \kappa^2 & -\delta l \delta \kappa \cos \ell \kappa & 0 \\ -\delta l \delta \kappa \cos \ell \kappa & \delta l^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (4.31)$$

Finally

$$\begin{aligned}
 \vec{\nabla} \cdot \lambda \vec{\nabla} \phi &= \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left(\sqrt{g} \lambda g^{ij} \frac{\partial \phi}{\partial x^j} \right) \\
 &= \frac{1}{\delta l \delta k \sin \theta k} \left\{ \frac{\partial}{\partial l} \left(\frac{\lambda \delta k}{\delta l \sin \theta k} \frac{\partial \phi}{\partial l} - \lambda \cos \theta k \frac{\partial \phi}{\partial k} \right) \right. \\
 &\quad \left. + \frac{\partial}{\partial k} \left(\frac{\lambda \delta l}{\delta k \sin \theta k} \frac{\partial \phi}{\partial k} - \lambda \cos \theta l \frac{\partial \phi}{\partial l} \right) \right\}
 \end{aligned} \tag{4.32}$$

Note that the ratio of coefficients of the cross derivative terms to the term which will remain in orthogonal coordinates is

$$\frac{-\delta l \cos \theta k}{\delta k} \quad \text{for the } l \text{ sweep,}$$

$$\text{and} \quad \frac{-\delta k \cos \theta l}{\delta l} \quad \text{for the } k \text{ sweep.}$$

This shows that the ratio is small if the grid is nearly orthogonal but that if such is not the case and δl and δk differ greatly in magnitude then one ratio will be small and the other large. This points up the need for updating the values of ϕ used in evaluating the cross derivatives after each sweep. Even though the formal error introduced by evaluating these terms at t^n for both sweeps may be of the same order as errors already accepted, it is important that whichever sweep has dominant cross derivative terms be preceded by a sweep which is able to smooth the distribution of ϕ 's.

Finally a word should be said about the truncation error of this scheme. If the cross derivative or diagonal coupling terms were taken

explicitly or fully implicitly in time the difference equations would have errors of order $\Delta t (\Delta t + \delta l^2 + \delta \kappa^2 + \delta l \delta \kappa)$. Multiplying these terms by a factor of the form ϕ_i^{n+1}/ϕ_i^n where the subscript i depends on the sign of the term in fact multiplies by a coefficient which can be written $1 + O(\Delta t)$ so the error introduced is of the same order as those already accepted. It is however important to note that if the problem has a symmetry in Z the difference scheme will also have that symmetry.

An appreciation for the problem discussed here may be gained by considering a specific example. Fig. 4.1 illustrates a pair of long slender zones in a mesh which is not orthogonal. We consider the flow of energy across the zone boundary centered at $l+1$ and $k+1/2$. This flow is dealt with in the course of an l sweep. In particular we assume that the flux intensity vector, $\vec{F}$, has the direction indicated in the figure. Then $\Delta \phi$ may be as large as or larger than $\delta \phi$ while χ^2 is much larger than χ^1 . That this situation may exist in the course of a calculation is verified by Fig. 5.14. The result is that the second term in equation (4.21) dominates the first. If this term is treated explicitly it serves as a strong source or sink. If the zoning is reasonably uniform each zone will have both source and sink terms of comparable magnitude from the low l and high l boundaries. If the grid is sufficiently distorted however some zone may be driven to a negative temperature by some explicit term, leading to a physically unrealistic state.

4.1 High aspect ratio skewed zones. Although the direction of the flux vector, $\vec{F}$, indicates that the left zone is hotter than the right zone, energy flows from the right zone to the left zone

D. Interregion Coupling

1. Coupling in the CEL Code

The possibility of solving only tri-diagonal sets of equations is seriously threatened by the coexistence of several Eulerian and/or Lagrange regions. For a two dimensional problem it may be impossible to devise a splitting of the diffusion operator that will result in a banded set of equations to solve. Hence it was decided to consider the regions as separate problems communicating only through the boundary conditions which one imposed upon the other.

Several methods for constructing such boundary conditions suggested themselves and we consider first a few which were discarded and the reasons for so doing. It will simplify the presentation to consider a one dimensional problem with zones with index $j=1, J$ representing one region and indices $j = J+1, N$ a second region. The existence of the separate Eulerian regions and Lagrange regions is reflected in this simpler problem by the requirement that the diffusion equation be solved separately in each region. The problem then is evaluating the boundary term

$$\alpha (\phi_{J+1} - \phi_J)$$

where α is the nondimensional coupling coefficient at the boundary between the J and $J+1$ zones. Evaluating this term explicitly, i.e., as

$$\alpha (\phi_{J+1}^n - \phi_J^n)$$

is surely unstable for large values of α . Evaluating the term with the latest state information

$$\alpha (\phi_{J+1}^n - \phi_J^{n+1}) \quad \text{for the first region}$$

$$\alpha (\phi_{J+1}^{n+1} - \phi_J^{n+1}) \quad \text{for the second region}$$

is just as surely stable but is not in a form which formally conserves energy.

Another possibility would be to estimate a response parameter for each boundary segment. That is, from past history, the change in ϕ of the J+1 zone due to a flux across the lower zone boundary, can be estimated as a parameter, b. Then the temperature of the J+1 zone can be predicted by an extrapolation,

$$\tilde{\phi}_{J+1} = \phi_{J+1}^n + \alpha b (\phi_J^{n+1} - \tilde{\phi}_{J+1}) \quad (4.33)$$

This leads to a coupling coefficient of the form

$$\alpha / (1 + \alpha b)$$

which is bounded by b^{-1} for large α , an eventuality which may prevent an asymptotic approach to the proper steady state solution.

Finally we consider replacing the term by

$$\alpha(\varphi_{j+1}^n - \varphi_j^{n+1}).$$

This permits the first region to be handled with the boundary condition φ_{j+1}^n known and then solve the equations in the second region with the boundary flux,

$$\alpha(\varphi_{j+1}^n - \varphi_j^{n+1}) \quad , \text{ known.}$$

To examine the stability of this scheme we again consider the case of constant coefficients with no energy flow through exterior boundaries for which the equations are

$$\varphi_1^{n+1} - \varphi_1^n = \alpha(\varphi_2^{n+1} - \varphi_1^{n+1}) \quad (4.34)$$

$$\varphi_2^{n+1} - \varphi_2^n = \alpha(\varphi_3^{n+1} - 2\varphi_2^{n+1} + \varphi_1^{n+1})$$

⋮

$$\varphi_j^{n+1} - \varphi_j^n = \alpha(\varphi_{j+1}^n - 2\varphi_j^{n+1} + \varphi_{j-1}^{n+1})$$

$$\varphi_{j+1}^{n+1} - \varphi_{j+1}^n = \alpha(\varphi_{j+2}^{n+1} - \varphi_{j+1}^{n+1} - \varphi_{j+1}^n + \varphi_j^{n+1})$$

⋮

$$\varphi_N^{n+1} - \varphi_N^n = \alpha(\varphi_{N-1}^{n+1} - \varphi_N^{n+1}).$$

In the sequel matrices defined by equation will be more explicitly represented in Appendix IV.C. Equations (4.34) then appear in matrix form as

$$P\varphi^{n+1} = Q\varphi^n \quad (4.35)$$

The matrix Q is easily inverted for α not equal to unity and premultiplication by this inverse results in

$$G\varphi^{n+1} \equiv Q^{-1}P\varphi^{n+1} = \varphi^n. \quad (4.36)$$

We require that the matrix G have no eigenvalues smaller than one in magnitude, for if such were the case and φ^0 had a nonvanishing projection along the corresponding eigenvector, then the scheme would be unstable. Because it is not known that G has a complete set of eigenvectors it cannot be claimed that the coupling is stable even in this idealized case if G is found to have only eigenvalues whose magnitudes are greater than or equal to unity. Nonetheless we proceed in order to determine whether the coupling is demonstrably unstable. Thus we seek a necessary rather than a sufficient condition for stability. We do this specifically for large α , which corresponds to large values of Δt , as many instabilities become manifest in this regime. For large α the matrix G can be written, to first order in $\epsilon \equiv 1/\alpha$, as

$$G = \bar{\alpha} (A + \epsilon B) + O(\epsilon^2). \quad (4.37)$$

Here $\tilde{\alpha}$ and $\tilde{\epsilon}$ denote scalar matrices with diagonal elements equal to α and ϵ respectively. Equation (4.37) serves to define A and B, which are displayed in Appendix IV.C. We are particularly interested in vanishing eigenvalues of A as any non-vanishing eigenvalues are to be multiplied by α and have magnitude greater than one in the limit of large α . As A^T has the same eigenvalues as A we look at the columns of A and conclude that for any eigen- vector of A^T which corresponds to an eigenvalue of zero,

$$\phi_1 = \phi_2 = \dots = \phi_j = \phi_{j+2} = \dots = \phi_N.$$

Hence the eigenvalue zero has multiplicity two and we take as corresponding eigenvectors of A^T ,

$$Y_1 = (1, 1, 1, \dots, 1, 0, 1, 1, \dots, 1, 1)$$

$\quad \quad \quad j$

and

$$Y_2 = (0, 0, \dots, 0, 1, 0, 0, \dots, 0, 0) \quad (4.38)$$

$\quad \quad \quad j$

which are independent. It can also be seen that

$$X_1 = (1, 1, 1, \dots, 1, 0, 0, \dots, 0, 0) \quad (4.39)$$

$\quad \quad \quad j$

and

$$X_2 = (0, 0, 0, \dots, 0, 1, 1, \dots, 1, 1)$$

$\quad \quad \quad j$

are eigenvectors of A corresponding to the null eigenvalue and again are independent.

We now seek the eigenvalues of the perturbed matrix $A + \epsilon B$. We let

$$c_{i1} X_1 + c_{i2} X_2 \quad \text{and} \quad c_{i1} X_1 + c_{i2} X_2$$

be the unperturbed eigenvectors and $\epsilon \lambda_i$ and $\epsilon \lambda_i$ the perturbed eigenvalues while ϵX_{31} and ϵX_{32} will be the perturbation to the eigenvectors. Then

$$(A + \epsilon B)(c_{i1} X_1 + c_{i2} X_2 + \epsilon X_{3i}) = \epsilon \lambda_i (c_{i1} X_1 + c_{i2} X_2 + \epsilon X_{3i}) \quad (4.40)$$

or to first order in ϵ

$$A X_{3i} = (\lambda_i - B)(c_{i1} X_1 + c_{i2} X_2) \quad \text{for } i = 1, 2. \quad (4.41)$$

In order that there be a solution for X_{31} the right hand side must be orthogonal to all solutions of the homogeneous adjoint equation, i.e., orthogonal to Y_1 and Y_2 . Thus

$$Y_k^T (\lambda_i - B)(c_{i1} X_1 + c_{i2} X_2) = 0 \quad \begin{matrix} \text{for } k = 1, 2 \\ i = 1, 2. \end{matrix} \quad (4.42)$$

This set of requirements can be written as

$$\begin{bmatrix} \lambda_i Y_i X_i - Y_i (BX_1) & \lambda_i Y_i X_i - Y_i (BX_2) \\ \lambda_i Y_i X_i - Y_i (BX_1) & \lambda_i Y_i X_i - Y_i (BX_2) \end{bmatrix} \begin{bmatrix} c_{i1} \\ c_{i2} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (4.43)$$

But

$$Y_i X_i = J$$

$$Y_i X_i = 0$$

$$Y_i X_i = N - J - 1$$

$$Y_i X_i = 1$$

(4.44)

while,

$$BX_1 = (1, 1, \dots, 1, 0, 0, \dots, 0, 0)$$

$$BX_2 = (0, 0, \dots, 0, 1, 0, 1, \dots, 1, 1)$$

(4.45)

so that

$$Y_1 \cdot (BX_1) = J-1$$

$$Y_2 \cdot (BX_1) = 1$$

$$Y_1 \cdot (BX_2) = N-J$$

$$Y_2 \cdot (BX_2) = 0$$

(4.46)

so the condition that there exist non-null (c_{11}, c_{12}) is that

$$\begin{vmatrix} J\lambda_i - J + 1 & (N - J - 1)\lambda_i + J - N \\ -1 & \lambda_i \end{vmatrix} = 0 \quad (4.47)$$

or

$$\lambda_i = 1, (1 - N/J) \quad (4.48)$$

The necessary condition for stability is that these eigenvalues have magnitude greater than or equal to one. Clearly this cannot be the case if $N < 2J$. In physical terms this means that instability will result if the heat capacity of the second region is less than that of the first.

Consider an example where J is ten and N is fifteen. The initial conditions are that ϕ is one in the first region and zero in the second.

Then for large α the value of ϕ at each zone in the first region will go to zero in the first cycle. The value of ϕ at each zone of the second region will be two in order for energy, here proportional to ϕ , to be conserved. In the second cycle the first region will have ϕ 's of two and the second region negative two. After ten cycles ϕ will be 342 in the first region and -682 in the second region and the change in ϕ for either region doubles in magnitude for each cycle.

In fact in the nonlinear case where the diffusion coefficient varies sharply with ϕ there may result a pseudo-instability where the heat capacity of that portion of the second region which has been heated sufficiently to have a large diffusion coefficient is less than that of the first region even if the entire second region has large heat capacity. This is because a flow of energy into the second region cannot be distributed throughout that region due to high opacities and specific heats.

Fortunately the above investigation suggests a way to stabilize the calculation. If the term connecting the two regions were written as

$$\propto (\phi_{J+1}^{n+1} - \phi_J^n)$$

and the second region were done first, the unperturbed eigenvectors would remain the same and the perturbed eigenvalues would be

$$\lambda_i = 1, J/(J-N) \quad (4.49)$$

and the product of eigenvalues for the pair of calculations will be

$$\lambda_i^1 \lambda_i^2 = 1. \quad (4.50)$$

Hence stability can be achieved by alternating the time indices in the term connecting the two regions.

This product of possibly unstable operators leads to an inaccuracy in the case of nonlinear coefficients. In particular, as consecutive time values of ϕ at some point might oscillate even though the values spaced $2\Delta t$ apart presented very smooth behavior, the heat capacity must be estimated for each time step and errors in that estimation lead to the presence of local energy discrepancies. A partial solution employed in the CEL code was to combine two successive steps in the Eulerian region. That is, while advancing the internal diffusion by $2\Delta t$ the Eulerian had a boundary condition of the third kind imposed upon it. Each Eulerian zone adjacent to the Lagrange region was associated with an equation of the form

$$\begin{aligned} \phi_j^{n+2} = & \phi_j^n + \frac{\delta \phi}{\delta t_{\text{internal}}} (2\Delta t) + a_1 \Delta (\phi_{\text{Lagrange}}^{n+1} - \phi_j^{n+2}) \\ & + a_2 \Delta t (\phi_{\text{Lagrange}}^{n+1} - \phi_j^n) \end{aligned} \quad (4.51)$$

where a_1 and a_2 involve geometry, opacity and heat capacity.

2. Coupling in the CHAMP Code

In considering a means of differencing the diffusion equation in the CHAMP code, which enjoys a multifluid Eulerian capability, it was decided to employ equations of the above type for boundary zones in both the Eulerian and Lagrange boundary zones including zones abutting the interface between Eulerian regions representing different materials. In order to investigate stability we proceed as before with a one-dimensional constant coefficient analysis with a single interface.

Thus the difference equations replacing

$$\frac{\partial \phi}{\partial t} = \alpha' \frac{\partial^2 \phi}{\partial x^2} \quad (4.52)$$

with insulated boundaries are:

$$\phi_1^{n+1} - \phi_1^n = \alpha (\phi_2^{n+1} - \phi_1^{n+1})$$

$$\phi_2^{n+1} - \phi_2^n = \alpha (\phi_3^{n+1} - \alpha \phi_2^{n+1} + \phi_1^{n+1})$$

$$\phi_J^{n+1} - \phi_J^n = \alpha (\phi_{J+1}^n - \frac{1}{2} \phi_J^n - \frac{3}{2} \phi_J^{n+1} + \phi_{J+1}^{n+1})$$

$$\phi_{J+1}^{n+1} - \phi_{J+1}^n = \alpha (\phi_{J+2}^{n+1} - \frac{1}{2} \phi_{J+1}^n - \frac{3}{2} \phi_{J+1}^{n+1} + \phi_J^{n+1}) \quad (4.53)$$

$$\begin{aligned} & \vdots \\ & \vdots \\ & \vdots \\ \varphi_{N-1}^{n+1} - \varphi_{N-1}^n &= \alpha (\varphi_{N-2}^{n+1} - 2\varphi_{N-1}^{n+1} + \varphi_N^{n+1}) \\ \varphi_N^{n+1} - \varphi_N^n &= \alpha (\varphi_{N-1}^{n+1} - \varphi_N^{n+1}). \end{aligned}$$

Here $\alpha = \frac{\alpha' \Delta t}{\Delta x^2}$ and the interregion boundary lies between points labeled J and $J+1$. Proceeding as before we write the equations in matrix form:

$$P\varphi^{n+1} = Q\varphi^n \quad (4.54)$$

where, again, the matrices in this section are displayed in Appendix IV.C. For $\alpha > 2$ the matrix on the right is invertible and we have

$$G\varphi^{n+1} \equiv Q^{-1}P\varphi^{n+1} = \varphi^n \quad (4.55)$$

The matrix G takes the form upon expanding in powers of $1/\alpha$,

$$\bar{\alpha} (A + \bar{\epsilon} B + \bar{\epsilon}^2 C + \bar{\epsilon}^3 D + O(\bar{\epsilon}^4)) \varphi^{n+1} = \varphi^n \quad (4.56)$$

Here $\bar{\alpha}$ and $\bar{\epsilon}$ are as defined after equation (4.37). Again we investigate the limit of large Δt , hence large α , using perturbation theory. As before our interest is directed to the eigenvectors of A corresponding to eigenvalue zero.

$A \phi_0 = 0$ implies that ϕ_0 is a linear combination of

$$\phi_0^0 = (1, 1, 1, \dots, 1, 0, 0, \dots, 0)$$

and

(4.57)

$$\phi_0^1 = (0, 0, 0, \dots, 0, 1, 1, \dots, 1).$$

In this case however $A^T \psi_0 = 0$ means ψ_0 is in the space spanned by

$$\psi_0^0 = (0, 0, 0, \dots, 1, 0, 0, \dots, 0)$$

and

(4.58)

$$\psi_0^1 = (0, 0, 0, \dots, 0, 1, 0, 0, \dots, 0).$$

Consider an eigenfunction of the original matrix to be

$$\phi = a_0 \phi_0^0 + a_1 \phi_0^1 + \epsilon \phi_1 + \epsilon^2 \phi_2 + \epsilon^3 \phi_3 + \dots$$

corresponding to an eigenvalue of $0 + \epsilon \lambda_1 + \epsilon^2 \lambda_2 + \epsilon^3 \lambda_3 + \dots$

Then matching powers of ϵ yields

$$A(a_0 \phi_0^0 + a_1 \phi_0^1) = 0$$

(4.59)

$$A\phi_1 + B(a_0 \phi_0^0 + a_1 \phi_0^1) = \lambda_1 (a_0 \phi_0^0 + a_1 \phi_0^1)$$

$$A\phi_2 + B\phi_1 + C(a_0 \phi_0^0 + a_1 \phi_0^1) = \lambda_1 \phi_1 + \lambda_2 (a_0 \phi_0^0 + a_1 \phi_0^1)$$

$$A\phi_3 + B\phi_2 + C\phi_1 + D(a_0 \phi_0^0 + a_1 \phi_0^1) = \lambda_1 \phi_2 + \lambda_2 \phi_1 + \lambda_3 (a_0 \phi_0^0 + a_1 \phi_0^1) .$$

$\vdots$

The first of these is of course satisfied for any choice of a_0 and a_1 . The condition that the second of these perturbation equations be solvable for ϕ_1 is

$$\psi_0^i \cdot (\lambda_i - B)(a_0 \phi_0^i + a_1 \phi_1^i) = 0 \quad \text{for } i = 0, 1. \quad (4.60)$$

This means that

$$(\lambda_1 - 3)a_0 + (-2)a_1 = 0 \quad (4.61)$$

$$2a_0 + (\lambda_1 - 1)a_1 = 0. \quad (4.62)$$

If this pair of homogeneous equations for a_0 and a_1 is to have a solution the determinant, $\lambda_1^2 - 2\lambda_1 + 1$, will be zero so $\lambda_1 = 1$ and $a_0 = a_1$. Note that in contrast to the previous case the degeneracy is not removed by the first order perturbation so we must proceed to higher orders. We first normalize the eigenvector by setting $a_0 = a_1 = 1$ and define

$$\phi_0 \equiv \phi_0^0 + \phi_0^1$$

The second perturbation equation then becomes

$$A\phi_1 = (I - B)\phi_0 = 0, \quad (4.63)$$

so ϕ_1 is again a member of the space spanned by ϕ_0 and ϕ_0' .

Consistency with our normalization suggests we select ϕ_1 normal to ϕ_0 so we define

$$\phi_1 = b (J_1, J_1, J_1, \dots, J_1, -J, -J, \dots, -J) \quad \text{where } J_1 = N-J \quad (4.64)$$

Considering now the third perturbation equation we find

$$A \phi_2 = (\lambda_1 - B) \phi_1 + (\lambda_2 - C) \phi_0 \quad (4.65)$$

and again require the orthogonality of the right hand side with ψ_0 and ψ_0' , which leads to

$$-2J_1 b - 2Jb + \lambda_2 = 0$$

$$\text{or} \quad (4.66)$$

$$\lambda_2 = 2Nb.$$

Solving then for ϕ_2 we have

$$A \phi_2 = 2Nb (J_1, J_1, J_1, \dots, J_1, 0, 0, J_1, \dots, J_1) \quad (4.67)$$

so

$$\phi_2 = 2Nb \left(\frac{J_1-1}{6}, \frac{J_1-1}{6}, \frac{J_1-1}{6}, \dots, \frac{-J(J-1)(J-2)}{6}, \frac{-(J-1)(2J-1)}{6}, \dots, \frac{J_1-1}{6} \right) \quad (4.68)$$

which is orthogonal to ϕ_0 and ϕ_1 .

Looking at the last of the perturbation equations which we have written, the condition for solvability requires that $b = 0$ or 2 . The condition that $b = 0$ leads to $\lambda_3 = 0$ and represents the fact that the constant vector ϕ_0 is unchanged by the diffusion process. The value $b = 2$ leads to

$$\lambda_3 = 8/3N^2 (J_1 - J + 3). \quad (4.69)$$

Although λ_3 may be positive or negative, in the limit of large Δt the eigenvalue has the form

$$\lambda = 1 + 4N/\alpha + O(\epsilon^2) \quad (4.70)$$

which exceeds one in magnitude. Once again although unconditional stability has not been shown we do see that this scheme does not lead to large Δt instability for our model equation. This scheme has the advantage that solutions are smooth in time near the boundary as the equations are the same at each time step. However there is a caution to be noted. At no step is the sum of the energies for the two regions equal to the total energy as there is always some energy in transit across the interface, namely

$$\alpha/2 (\phi_{J+1}^{n+1} - \phi_J^{n+1}).$$

If this is a significant portion of the energy being transported in the problem then the time step must be abbreviated to an extent necessary to insure that this residual interface transfer does not lead to a serious misrepresentation of the energy distribution.

It is proper here to reflect upon the significance of these perturbation analyses and that is two fold. First, they give some insight into the mechanism of the interface transfer and thereby suggest extensions and modifications. Taken together with computational experience they provide the basis for treating any new problem of interface coupling that might arise. In addition, although it is realized that the actual problem is nonlinear, two dimensional, and requiring a range of time steps, none of which conditions is dealt with in the analysis, it is of importance that a negative result was not obtained. At worst the results give license to proceed with the coupling scheme until numerical experiment or further theoretical study indicate otherwise.

E. Interrelation of Hydrodynamics and Radiation Diffusion

The radiation diffusion equation, equation (2.16) is differenced as outlined in this chapter. The sequence of operations used to advance the hydrodynamics is indicated in Chapter II. It is necessary now to integrate these processes and for this purpose we again choose a splitting method. Schematically this is modelled by replacing

$$\phi^{n+1} = (I + H + R)\phi^n \quad (4.71)$$

by

$$\phi^* = (I + H)\phi^n \quad (4.72)$$

and

$$\phi^{n+1} = (I + R)\phi^* \quad (4.73)$$

where ϕ is the state vector,

ϕ^* is an intermediate state vector,

H is a hydrodynamics operator,

and R is a radiation diffusion operator.

Again this simple splitting is only correct to first order but some of the methods of obtaining greater accuracy have pitfalls also. One might extrapolate in time for both processes and obtain a centered specific heat and advance temperature in both phases rather than energy in the hydrodynamic phase and the fourth power of temperature in the diffusion phase. But as energy conservation is so important in the class of problems under consideration the centered specific heat may not be appropriate for the diffusion calculation. Hence in this code the two processes are treated separately and sequentially in the following manner.

After the hydrodynamics has been completed in the Lagrange regions the radiation calculation proceeds with the most recent geometry and energy values providing the initial conditions. The energy fluxes and boundary temperatures calculated in the Eulerian regions during the last cycle provide the boundary conditions. Each Eulerian region is then advanced in terms of advection as well as the first half of the hydrodynamic kinetic to internal energy conversion. At this point the diffusion is done in each of the Eulerian regions. The initial conditions are provided through an inverse equation of state table look up which provides temperature as a function of mass density and internal

energy density. The boundary conditions relating to other computational regions are provided by the most recently calculated energy fluxes and temperatures from the adjoining regions. This means that not all fluxes are associated with the same computational cycle.

At the end of the radiation diffusion the energy density is calculated from the new temperature but the pressure is not advanced in time. Conservation of energy in the hydrodynamic phase relies upon using the same pressures in the equations of motion as are used in the work terms in the energy equation. When the pressure is updated it is augmented by the equilibrium radiation pressure, which is one third of the radiation energy density.

Appendix IV.A. Iteration for $\partial \epsilon / \partial \varphi$ Calculation

As noted in section IV.B. the functional iteration used to calculate the estimate of the secant $\partial \epsilon / \partial \varphi$ may not converge unless precautions are taken. In particular the provision that $|(\partial F / \partial x)_{x=x_0}| \leq 1$ in some neighborhood of the solution, x_0 , of the equation

$$x = F(x) \quad (4.74)$$

may not be satisfied. Here x represents the secant, $\partial \epsilon / \partial \varphi$. For large values of $\frac{\partial \epsilon}{\partial \varphi}$ the extrapolated value of φ will be very near the initial value, φ^n , and hence F will take on the value of the slope of the $\epsilon(\varphi)$ curve at φ^n . For $\frac{\partial \epsilon}{\partial \varphi}$ small the extrapolated φ approaches φ^{n+1} and F approaches the secant,

$$\frac{\epsilon(\varphi^{n+1}) - \epsilon^n}{\varphi^{n+1} - \varphi^n}$$

It is not expected that negative values of $\frac{\partial \epsilon}{\partial \varphi}$ need be explored as ϵ is assumed to be a monotonically increasing function of φ . Hence we are to consider the iteration

$$x^{m+1} = F(x^m) \quad (4.75)$$

where $F(0)$ is some positive number and $\lim_{x \rightarrow 0} F(x)$ exists and is also positive. Thus as F is continuous, a solution to (4.74) exists and $\lim_{x \rightarrow 0} F(x)/x = 0$. These conditions permit the development of an algorithm modifying equation (4.75) which permits the calculation of a sequence $\{x^m\}$ which converges to x_0 .

The failure of the algorithm (4.75) is made manifest in a sequence $\{x^m\}$ of approximants which alternately are less than and greater than the solution. The modified algorithm does not accept such values and eventually creates a monotone sequence.

In the case where $x^1 > x^0$ successive iterates are accepted for as long as $x^{m+1} > x^m$. When this inequality fails to be satisfied neither x^{m+1} nor x^m is accepted and a new sequence x_i^m is calculated by the algorithm:

$$x_0^m = F(x^m) \quad (4.76)$$

$$x_{i+1}^m = (x_i^m \cdot x^m - F(x_i^m) \cdot x^{m-1}) / ((x^m - x^{m-1}) + (x_i^m - F(x_i^m)))$$

This procedure is continued until $x_1^m < F(x_1^m)$ in which case x_1^m becomes the new x^m . The x^m then form a monotone sequence bounded above by the largest root of (4.74). It may happen that for given m an infinite sequence of x_i^m is generated. This sequence is also monotone and bounded below by some root of (4.74). In either case a convergent sequence is generated. It need not be feared that the denominator in eq. (4.76) may vanish as in either of the cases $x_0 > x_1$ or $x_1 > x_0$ it is so that $(x^m - x^{m-1})$ and $x_1^m - F(x_1^m)$ have the same sign if the iteration is to proceed.

Geometrically this algorithm may be seen to reflect the replacement of the function F by a line segment joining (x^{m-1}, x^m) and $(x_i^m, F(x_i^m))$ when it is known that a root lies in the interval (x^{m-1}, x^m) . If there are multiple roots in $[0, \infty]$ there is no guarantee other than that

the procedure will yield a sequence converging to one of the roots. This applies also for the case where $x^1 < x^0$ using the same algorithm.

Appendix IV.B. Non-Orthogonal Meshes

As mentioned in Section IV.C., a skewed grid requires the use of functional values at the eight nearest neighbors of the zone for which the diffusion operator is to be evaluated. This makes splitting into stable sweeps difficult and although a resolution of this problem was presented in the above mentioned section, it is instructive to examine other possibilities. Immediately we must insist that we deal with a uniform plane grid with l and k lines meeting at a constant angle, θ , and that all other properties ($\lambda, \partial \epsilon / \partial \rho$) are constants in order that we may apply the Fourier stability analysis. In this case the diffusion operator in difference form becomes

$$\begin{aligned}
 D\phi_{l+\frac{1}{2}, k+\frac{1}{2}} = & \frac{\lambda \Delta t}{\partial \epsilon / \partial \rho} \frac{1}{\Delta^2 \delta^2 \sin^2 \theta} \left\{ \Delta^2 \left(\phi_{l+\frac{3}{2}, k+\frac{1}{2}} - 2\phi_{l+\frac{1}{2}, k+\frac{1}{2}} + \phi_{l-\frac{1}{2}, k+\frac{1}{2}} \right) \right. \\
 & + \delta^2 \left(\phi_{l+\frac{1}{2}, k+\frac{3}{2}} - 2\phi_{l+\frac{1}{2}, k+\frac{1}{2}} + \phi_{l+\frac{1}{2}, k-\frac{1}{2}} \right) \\
 & \left. + 2\Delta\delta\cos\theta \left(\phi_{l+1, k} + \phi_{l, k+1} - \phi_{l+1, k+1} - \phi_{l, k} \right) \right\} \quad (4.77)
 \end{aligned}$$

In this constant coefficient analysis each value at a grid point in the last term is just the uniform average of the values at the four surrounding zone centers, and the pattern of signs will cause some cancelling that would not occur in a problem with space dependent coefficients. It has been shown that grouping the terms in the l and k directions with like terms earlier in the expression leaves just four "diagonal" terms which may serve as explicit source terms for two implicit sweeps in the l and k directions the product of which is

stable. Here however we shall leave each grid value of ϕ explicit in the hope that the resultant calculation will be less dependent on the restrictions which have been placed on the problem. Hence we set

$$\begin{aligned} \tilde{\phi}_{l+1/2, k+1/2}^n = & \phi_{l+1/2, k+1/2}^n + \alpha \left\{ \Delta^2 (\tilde{\phi}_{l+1/2, k+1/2}^n - 2\tilde{\phi}_{l+1/2, k+1/2}^n + \tilde{\phi}_{l+1/2, k+1/2}^n) \right. \\ & \left. + \Delta \delta \cos \theta (\phi_{l+1, k}^n + \phi_{l, k+1}^n - \phi_{l+1, k+1}^n - \phi_{l, k}^n) \right\} \end{aligned} \quad (4.78)$$

$$\begin{aligned} \phi_{l+1/2, k+1/2}^{n+1} = & \tilde{\phi}_{l+1/2, k+1/2}^n + \alpha \left\{ \delta^2 (\phi_{l+1/2, k+1/2}^{n+1} - 2\phi_{l+1/2, k+1/2}^{n+1} + \phi_{l+1/2, k+1/2}^{n+1}) \right. \\ & \left. + \Delta \delta \cos \theta (\tilde{\phi}_{l+1, k}^n + \tilde{\phi}_{l, k+1}^n - \tilde{\phi}_{l+1, k+1}^n - \tilde{\phi}_{l, k}^n) \right\} \end{aligned}$$

where

$$\alpha = \frac{\lambda \Delta t}{\partial \epsilon / \partial \phi} \frac{1}{\Delta^2 \delta^2 \sin^2 \theta}$$

This is the splitting derived from taking $(F_{l+1, k+1/2} - F_{l, k+1/2})$ on the first sweep and $(F_{l+1/2, k+1} - F_{l+1/2, k})$ on the second. Letting

$$\varphi^n = e^{i(\ell m_\ell + K m_K)}$$

$$\tilde{\varphi} = \xi_1 \varphi^n$$

$$\varphi^{n''} = \xi_2 \tilde{\varphi}$$

we see that

$$\xi_1 = \frac{1 + \alpha \Delta \delta \cos \theta \sin m_\ell \sin m_K}{1 + 2\alpha \Delta^2 (1 - \cos m_\ell)} \quad (4.79)$$

and

$$\xi_2 = \frac{1 + \alpha \Delta \delta \cos \theta \sin m_\ell \sin m_K}{1 + 2\alpha \delta^2 (1 - \cos m_K)} \quad (4.80)$$

Hence $\varphi^{n''} = \xi_1 \xi_2 \varphi^n$ where

$$\xi_1 \xi_2 = \frac{(1 + \alpha \Delta \delta \cos \theta \sin m_\ell \sin m_K)^2}{(1 + 2\alpha \Delta^2 (1 - \cos m_\ell))(1 + 2\alpha \delta^2 (1 - \cos m_K))} \quad (4.81)$$

and for stability we must show $|\xi_1 \xi_2| \leq 1$. It is easy to see that the product is positive so we need only that $\xi_1 \xi_2 \leq 1$.

As $1 - \cos m_\theta = \frac{\sin^2 m_\theta}{1 + \cos m_\theta} \geq \frac{\sin^2 m_\theta}{2}$ we have

$$\xi_1 \xi_2 \leq \frac{(1 + \alpha \Delta \delta \cos \theta \sin m_\theta \sin m_\kappa)^2}{(1 + \alpha \Delta^2 \sin^2 m_\theta)(1 + \alpha \delta^2 \sin^2 m_\kappa)} \quad (4.82)$$

$$= \frac{1 + 2\alpha\Delta\delta\cos\theta\sin m_\theta\sin m_\kappa + \alpha^2\Delta^2\delta^2\cos^2\theta\sin^2 m_\theta\sin^2 m_\kappa}{1 + \alpha(\Delta^2\sin^2 m_\theta + \delta^2\sin^2 m_\kappa) + \alpha^2\Delta^2\delta^2\sin^2 m_\theta\sin^2 m_\kappa}$$

$$\leq \frac{1 + 2\alpha\Delta\delta\cos\theta\sin m_\theta\sin m_\kappa + \alpha^2\Delta^2\delta^2\sin^2 m_\theta\sin^2 m_\kappa}{1 + \alpha(\Delta^2\sin^2 m_\theta + \delta^2\sin^2 m_\kappa) + \alpha^2\Delta^2\delta^2\sin^2 m_\theta\sin^2 m_\kappa}$$

The numerator and denominator of this bound differ only in the terms

$$2\alpha\Delta\delta\cos\theta\sin m_\theta\sin m_\kappa$$

and

$$\alpha(\Delta^2\sin^2 m_\theta + \delta^2\sin^2 m_\kappa)$$

so we must show that the latter exceeds the former. But

$$\begin{aligned} \Delta^2\sin^2 m_\theta + \delta^2\sin^2 m_\kappa &= (\Delta\sin m_\theta - \delta\sin m_\kappa)^2 + 2\Delta\delta\sin m_\theta\sin m_\kappa \\ &\geq 2\Delta\delta\sin m_\theta\sin m_\kappa \\ &\geq 2\Delta\delta\cos\theta\sin m_\theta\sin m_\kappa \end{aligned} \quad (4.83)$$

Thus we are assured of stability in this case for the product of sweeps although the magnitude of either f_1 or f_2 may exceed one.

There is a way of splitting the operator into two stable sweeps where each sweep changes direction from l to k and back again for successive zones. This algorithm is obtained by replacing $\phi_{l+1, k+1}$ by $\frac{1}{2}(\phi_{l+\frac{1}{2}, k+\frac{1}{2}} + \phi_{l+\frac{1}{2}, k+\frac{3}{2}})$ and similarly for other grid values. The centering is thus correct and the equations become

$$\begin{aligned}\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} &= \phi_{l+\frac{1}{2}, k+\frac{1}{2}}^n + \alpha \left\{ \Delta^2 (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} - \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}}) + \delta^2 (\phi_{l+\frac{1}{2}, k-\frac{1}{2}} - \phi_{l+\frac{1}{2}, k+\frac{1}{2}}) \right. \\ &\quad \left. + \Delta \delta \omega \theta (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} + \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}} - \tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} - \frac{1}{2} (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} + \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}})) \right\} \\ &\equiv \phi_{l+\frac{1}{2}, k+\frac{1}{2}}^n + \alpha D_1 \tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}}\end{aligned}$$

if $l+k$ is even (4.84)

$$\begin{aligned}\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} &= \phi_{l+\frac{1}{2}, k+\frac{1}{2}}^n + \alpha \left\{ \delta^2 (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} - \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}}) + \Delta^2 (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} - \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}}) \right. \\ &\quad \left. + \Delta \delta \omega \theta (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} + \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}} - \tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} - \frac{1}{2} (\tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} + \tilde{\phi}_{l+\frac{1}{2}, k+\frac{3}{2}})) \right\}\end{aligned}$$

if $l+k$ is odd. (4.85)

For the second sweep

$$\phi_{l+\frac{1}{2}, k+\frac{1}{2}}^{n+1} = \tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} + \alpha D_z \phi_{l+\frac{1}{2}, k+\frac{1}{2}}^{n+1} \quad (4.86)$$

if $l+k$ is even, and

$$\phi_{l+\frac{1}{2}, k+\frac{1}{2}}^{n+1} = \tilde{\phi}_{l+\frac{1}{2}, k+\frac{1}{2}} + \alpha D_z \phi_{l+\frac{1}{2}, k+\frac{1}{2}}^{n+1} \quad (4.87)$$

if $l+k$ is odd.

Now if $\phi^n = e^{i(lm_k + km_k)}$ again and

$$\tilde{\phi} = \xi \phi^n \quad \text{if } l+k \text{ is even}$$

$$\tilde{\phi} = \eta \phi^n \quad \text{if } l+k \text{ is odd}$$

then

$$\begin{aligned} \xi = 1 + \alpha \{ & \Delta^2 (\eta e^{im_k} - \xi) + \delta^2 (\eta e^{-im_k} - \xi) \\ & + \Delta \delta \cos \theta (\eta e^{im_k} + \eta e^{-im_k} - \xi (1 + \cos \psi)) \} \end{aligned} \quad (4.88)$$

$$\begin{aligned} \eta = 1 + \alpha \{ & \delta^2 (\xi e^{im_k} - \eta) + \Delta^2 (\xi e^{-im_k} - \eta) \\ & + \Delta \delta \cos \theta (\xi e^{im_k} + \xi e^{-im_k} - \eta (1 + \cos \psi)) \} \end{aligned} \quad (4.89)$$

where $\Psi = m_l + m_k$. In matrix form

$$\begin{bmatrix} 1 + \alpha(\Delta^2 + \delta^2 + \alpha\delta\cos\theta(1 + \cos\Psi)) & -\alpha(\Delta^2 e^{im_l} + \delta^2 e^{-im_k} + \alpha\delta\cos\theta(e^{-im_k} - e^{im_l})) \\ -\alpha(\delta^2 e^{im_k} + \Delta^2 e^{-im_l} + \alpha\delta\cos\theta(e^{im_k} - e^{-im_l})) & 1 + \alpha(\Delta^2 + \delta^2 + \alpha\delta\cos\theta(1 + \cos\Psi)) \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (4.90)$$

and we must have eigenvalues of magnitude at least one for stability.

The matrix above has the form

$$\begin{bmatrix} 1+x & -y \\ -y^* & 1+x \end{bmatrix}$$

and Gershgorin's theorem will guarantee that the desired condition is satisfied if $|y| \leq |x|$. But

$$x^2 = \alpha^2(\Delta^4 + \delta^4 + 2\alpha\delta\cos\theta(\Delta^2 + \delta^2)(1 + \cos\Psi) + 2\Delta^2\delta^2 + (\alpha\delta\cos\theta)^2(1 + \cos\Psi)^2) \quad (4.91)$$

while

$$y^2 = \alpha^2(\Delta^4 + \delta^4 + 2\alpha\delta\cos\theta(\Delta^2 + \delta^2)(1 + \cos\Psi) + 2\Delta^2\delta^2\cos^2\Psi + 2(\alpha\delta\cos\theta)^2(1 + \cos\Psi)) \quad (4.92)$$

which agree but for the last two terms which, if a common factor of $2\Delta^2\delta^2$ is removed, are

$1 + \cos^2 \theta (1 + \cos \psi)^2 / 2$ in the expression for x^2
and $\cos \psi + \cos^2 \theta (1 + \cos \psi)$ in the expression for y^2 .

Hence

$$\begin{aligned} X^2 - Y^2 &= 2\delta^2 \left\{ (1 - \cos \psi) + \frac{1}{2} (\cos^2 \psi - 1) \cos^2 \theta \right\} \\ &= 2\delta^2 \cos^2 \theta (1 - \cos \psi) \left\{ 1 - \frac{1}{2} (1 + \cos \psi) \cos^2 \theta \right\} \\ &\geq 0 \end{aligned} \tag{4.93}$$

and we find that there is no magnification going from ϕ^n to $\tilde{\phi}$. As the matrix for the transition from $\tilde{\phi}$ to ϕ^{n+1} merely has the rows interchanged it too represents a stable change. In this case then each sweep is stable separately but there are two possible disadvantages. First, this algorithm links each zone with four neighbors on each sweep and the resulting set of equations is pentadiagonal rather than tridiagonal so slightly more time and 50% more storage is necessary to solve it. Secondly each sweep is from lower left to upper right in $l-k$ space which may lead to problems if the entire grid is not easily accessible in the computer and is unlikely to be a natural direction for many problems. It would of course be appropriate to alter applications of the above scheme with a similar scheme sweeping from upper left to lower right in $l-k$ space.

Appendix IV.C. Display of Matrices

The matrices introduced in section IV.D. will be displayed in a more explicit fashion in this appendix. Each matrix will be divided by rows into three submatrices, the first containing the first $J-1$ rows, the second containing rows J and $J+1$, and the third rows $J+2$ through N . The first submatrix will be represented by only its first two rows as it is at most tridiagonal and the nature of successive rows is apparent. The lowest submatrix will be represented by the last two rows, whose nonzero elements will be in the last three columns only. The central submatrix will be further divided into three submatrices; the leftmost for the first $J-2$ columns, then another for columns $J-1$ through $J+2$ and finally the rightmost for columns $J+3$ through N . All elements not explicitly displayed should be taken to be zero. There follows a list of matrices identified by letter and equation number of first appearance. The matrix itself is displayed in the manner indicated here after each member of the list.

P of equation (4.35)

$$\begin{bmatrix} 1+\alpha & -\alpha & & & & & \\ -\alpha & 1+2\alpha & -\alpha & & & & \\ & \vdots & & & & & \\ & & -\alpha & 1+2\alpha & & & \\ & & & -\alpha & 1+\alpha & -\alpha & \\ & & & & \vdots & & \\ & & & & -\alpha & 1+2\alpha & -\alpha \\ & & & & & -\alpha & 1+\alpha \end{bmatrix}$$

P of equation (4.54)

$$P = \begin{bmatrix} 1+\alpha & -\alpha & & & & \\ -\alpha & 1+2\alpha & -\alpha & & & \\ & \vdots & & & & \\ & & -\alpha & 1+\frac{3}{2}\alpha & & \\ & & & -\alpha & 1+\frac{3}{2}\alpha & -\alpha \\ & & & & \vdots & \\ & & & & & -\alpha & 1+2\alpha & -\alpha \\ & & & & & & -\alpha & 1+\alpha \end{bmatrix}$$

Q of equation (4.54)

$$Q = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & \vdots & & & \\ & & & 0 & 1-\alpha/2 & \alpha & 0 \\ & & & 0 & 0 & 1-\alpha/2 & 0 \\ & & & & & & \vdots \\ & & & & & & & 1 \end{bmatrix}$$

B of equation (4.56)

$$\begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 2 & 1 & -6 & 4 \\ & & 0 & 2 & -3 & 2 \\ & & & & & 1 \\ & & & & & & 1 \end{bmatrix}$$

C of equation (4.56)

$$\begin{bmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 4 & 8 & -28 & 16 \\ & & 0 & 4 & -8 & 4 \\ & & & & & 0 \end{bmatrix}$$

D of equation (4.56)

$$\begin{bmatrix}
 0 & & & & \\
 & \cdot & & & \\
 & & \cdot & & \\
 & & & \cdot & \\
 & 8 & 32 & -88 & 48 \\
 & 0 & 8 & -16 & 8 \\
 & & & & \cdot \\
 & & & & \cdot \\
 & & & & 0
 \end{bmatrix}$$

V. MODELLING A SURFACE BURST

The phenomena associated with the release of a large quantity of energy in a transparent halfspace immediately adjacent to an opaque halfspace are worth investigation for practical reasons as well as for the evaluation of the computational procedure outlined in the preceding chapters. For this reason the problem selected as an application of the coupled radiation hydrodynamics code is an idealization of a nuclear weapons effects calculation.

A. Description of the Model

Although the CHAMP¹¹ code, which was used for this problem, has access to a large library of equation of state tables, each of the three materials in this configuration was assumed to have material pressure directly varying with material energy density which in turn was proportional to mass density and temperature. The geometric disposition of the various regions is indicated in Figure 5.1, which shows the region immediately around the sphere, referred to hereafter as the source. The upper halfspace, in which the source initially resides, is a low density gas and is referred to as the air. The lower halfspace simulates the earth. The early behavior is dominated by the radiative release of energy, primarily to the air. The principal focus here will be on the coupling of energy to the earth as the effect of ground shocks on structures is an important area for study.

It is apparent that a coupled Eulerian and Lagrangian code is well suited for a problem of this type. The source is represented by a

5.1 Initial geometry for surface burst calculation

Lagrange region so that its integrity and spherical expansion are well represented. It is possible at some later time to map the source into an additional and distinct Eulerian region.

The CHAMP code allows for the possibility of two kinds of Lagrange region. A separate controllee may be initiated to run a HEMP⁹ calculation for each time step with CHAMP as the controller. The HEMP simulates both hydrodynamic and radiative processes and may be subcycled if a time step smaller than the CHAMP time step is necessary for stability or accuracy. The HEMP calculation allows for a full stress tensor rather than a scalar pressure and also has the capability of decoupling along slide lines. The radiation flow between the HEMP Lagrange regions and the other region is as described in Chapter IV.

Although HEMP calculations would be appropriate if wave propagation in the earth were to be studied, for the initial phase considered here the Lagrange routines internal to the CHAMP code were deemed satisfactory. The air experiences large shear strains in the region where it meets the source and the earth and is thus not well suited to a Lagrange representation. Consequently, it is in an Eulerian region.

The earth was divided into two regions, one Eulerian and one Lagrangian. The Eulerian region was directly beneath the source and experiences motion comparable to grid size. Farther from the source, where displacements are smaller, the earth was represented by a Lagrangian region, which was zoned to accommodate the spherically diverging shock emanating from the origin of coordinates.

The calculation was run with the cylindrical symmetry option with axes labelled R and Z. Although positive Z may be thought of as the

"up" direction and the code permits introduction of a gravity body force, the short duration of the calculation does not warrant the inclusion of that effect.

Rather than apply radiative escape boundary conditions, each region was extended past the anticipated area of activity with coarse zoning so that zero flux boundary conditions at the extremes of each Eulerian region would be satisfactory. A third Eulerian region, surrounding the Lagrangian earth is demanded by the code logic and is displayed in Figure 5.2.

Initially there was no motion and the entire energy content of the problem, four thousand terajoules (approximately one megaton equivalent of TNT), was uniformly distributed in the spherical source. The mass density of the source was two grams per cubic centimeter. This led to a temperature of 4.7 keV throughout the source. For all materials in the problem a constant specific heat for the matter of one hundred megajoules per keV per gram was used. Hence nearly ninety percent of the initial energy was in the radiation field. The material contribution to the pressure in the source was .15 times the material energy per cubic centimeter.

The source was zoned as shown in Figure 5.3. The finer zoning toward the surface of the sphere is to reduce the optical depth to the center of the first zone. The Rosseland mean free path in the source was modeled as

$$\lambda_{\text{source}} = T^2 / (20\rho) \quad (5.1)$$

5.2 Location of Eulerian sink

5.3 Zoning in the Lagrangian source region

where T and ρ are the temperature and density respectively. For these initial conditions the mean free path was slightly more than half a centimeter so the optical depth, $\Delta x/\lambda$, to the center of the outermost zone was near unity. There were more zones azimuthally near the bottom of the sphere to ameliorate the problem of a large ratio of zone length to zone width as that region became compressed.

The air region had an initial mass density of .001 grams per cubic centimeter and no energy. The equation of state was that of a gamma law gas with gamma of 1.36. The mean free path was given by

$$\lambda_{\text{air}} = T^2 / (50\rho). \quad (5.2)$$

With its low density, air is very transparent at the temperatures encountered in this problem near the source. For this reason a flux limiter was employed to preclude physically unreasonable results in the Eulerian regions.

The flux limiter is a device to prevent energy from being transported faster than the speed of light. The diffusion approximation leads to a parabolic partial differential equation, which admits an infinite signal velocity. For opaque materials the energy transported more than a few mean free paths in the time it takes light to cover the same distance is negligible. As the medium becomes more and more transparent as evidenced by the mean free path growing larger than the local mesh width it becomes possible for substantial energy transport to occur at velocities which exceed that of light. To prevent this a common technique²¹ is to modify the diffusion coefficient. This was done in the Eulerian region by adding a term to the optical depth which restricts

the energy flux between two zones in a transparent region to some fraction of the flux that would occur if the angular distribution of the radiation intensity were a delta function with respect to the outward direction from the hotter zone. Thus if the zonal energy densities are represented by ϕ_i , the optical thickness of each zone by τ_i and α is the required fraction of the maximum possible flux then the equivalent optical depth for the diffusion flux, τ_{FL} , is found by equating the diffusion flux to the permitted flux.

$$\frac{ac}{3\tau_{FL}} (\phi_1 - \phi_2) = \alpha ac \phi_1 \quad (5.3)$$

Here ϕ_1 is the fourth power of the temperature of the hotter zone.

Solving for τ_{FL} ,

$$\tau_{FL} = \frac{1}{3\alpha} \frac{\phi_1 - \phi_2}{\phi_1} \quad (5.4)$$

This particular problem was run with α set to one half so that the optical thickness between zone centers was computed as

$$\tau = \tau_1 + \tau_2 + \frac{2}{3} \frac{\phi_1 - \phi_2}{\phi_1} \quad (5.5)$$

Only if the τ_i are both of the order of unity or less is this additional term significant.

For this problem, which was run to a third of a microsecond, the maximum distance that the radiation could travel would be about one hundred meters and the code deposited energy out to about half that distance.

The zoning in the air is shown in Figures 5.4 and 5.5. Additional zoning extends to a few thousand meters but is very coarse and serves only as a sink.

The zoning in the earth is shown in Figure 5.6 and 5.7. The equation of state for earth had the pressure equal to three tenths of the internal energy density and the radiation mean free path given by

$$\lambda_{\text{earth}} = T^2 / \rho \quad . \quad (5.6)$$

The initial density of the earth was two grams per cubic centimeter. At this density the mean free path would be half a centimeter at a temperature of one keV and two centimeters at two keV.

B. Results

The phenomena associated with this surface burst are indicated by figures 5.8 and 5.9. During the course of the calculation the internal energy of the source decreased to less than one tenth its original value. The principal recipient of this energy was the radiation field in the air. The energy in the earth had been transported primarily by radiation, both from the source and the air. It might be thought that the air would be far out of equilibrium between the source and the earth, especially in close to the source. This is because the air is so transparent that it might not become as hot as the radiation field. That this need not be significant is demonstrated by considering that the material heat capacity of the air is less than ten per cent of the radiation heat capacity during most of the calculation and is often less than one percent.

5.4 Zoning in the Eulerian air region near the source

6.5 Zoning in the Eulerian region at intermediate distance from the source

5.6 Near field zoning in the earth for Eulerian and Lagrangian regions

5.7 Far field zoning in the Lagrangian earth region

5.8 Relative disposition of energy as a function of time

5.9 Relative disposition of energy in each material as a function of time

It is seen by comparing the energy curves for the earth in the Eulerian region with that in the Lagrangian region that after a few tenths of a microsecond the heating of the earth is caused in large measure by radiative transfer from the expanding thermal wave in the air.

It may be recalled that the Eulerian earth region extends only three meters from the center line. At a time of .2 microseconds the air has been heated to a temperature of several hundred electron volts out to fifteen meters. The temperature gradient between the source and the earth at ground zero has nearly vanished and so the rate of increase of the energy in the earth immediately beneath the source is not as great as that of the ever increasing earth exposed to the thermal wave in the air. This is shown by the rapid increase in internal energy of the Lagrange earth region which can be due only to the absorption of radiant energy from the fireball. Although the kinetic energy of the earth remains comparatively small the momentum coupled to the earth is important and is shown in Figure 5.10.

Figures 5.11, 5.12 and 5.13 show the expansion of the source at three representative times. Note that the Lagrangian grid has modeled the spherical expansion of the source well. The motion of the surface has averaged 1.5 meters per microsecond and has resulted in a doubling of the radius in the third picture of this series. The isotherms in the earth show that the earth directly beneath the source is cooling as the earth at greater depths grows hotter. The thermal wave in the earth has penetrated to a depth of .6 meters at the final time of .34 microseconds.

Three features of the code warrant examination as their unsatisfactory performance would be egregious. The first such feature would be the energy conservation properties of the extrapolation which is

5.10 Magnitude of the axial momentum in the earth as a function of time

5.11 Isotherms in the earth and zoning in the source at 0.11 microseconds. The isotherms represent temperature values of 0.5, 1, 1.5, and 2 keV

5.12 As the source expands away from the earth the zones near the earth collapse. Note that the 2 keV isotherm has disappeared. The time here is 0.24 microseconds

5.13 Lagrange zoning and isotherms in the earth at time 0.34 microseconds

used to compute the heat capacity of each zone. To test this the total energy of a region was calculated before and after the radiation calculation for each cycle. The difference of these quantities was summed to yield a total energy change due to radiation. The total radiative energy passed through each region boundary was also summed. These two accumulated radiative energy changes were compared at the end of the problem run for two Eulerian regions, earth and air, and were found to disagree by two tenths of one percent and six tenths of one percent respectively. The high quality of energy conservation is important because of the nonlinear nature of the radiative transport. If the transport is slow for some reason but energy is conserved the temperature gradients remain high and there is a tendency to self correct. If energy were not conserved, this self regulating mechanism might not be evidenced.

Another code feature is the treatment of highly skewed zones. Figure 5.14 shows several zones in the source near the earth which have become distorted. When sweeping in the azimuthal direction the flux across the direction of the sweep is twenty times that of the flux in the direction of the sweep at the indicated zone face. This is a situation which is often treated by artificially limiting this cross flux due to non-orthogonal grid lines. Here however inspection shows that taking full account of the cross flow has not disturbed the smooth behavior of the temperature field, which exhibits no local extrema.

C. Stability

Finally we consider the stability of the coupling and see that the time step exceeded that required by the explicit stability criterion

5.14 Local zoning in the Lagrange source region at 0.24 microseconds. Note that there are high aspect ratio zones in a region where the grid lines are far from orthogonal

in the air near the juncture of the source and the earth for many cycles. There was no evidence of an increasing oscillation that one might expect if the coupling were in fact unstable. In fact in one dimensional test problems a time step of many times that required for stability of explicit differencing has been used and compared to an implicit code with good agreement.

Although the explicit stability condition for one dimensional linear problems has no direct application here, it is instructive to look at the magnitude of the local diffusion coefficients to see if the coupling mechanism has been tested at all. We investigate the situation near the junction of the air, earth and source after twenty-five nanoseconds. There were large heat flows at this time so the accuracy condition was restrictive. The time step was slightly larger than one nanosecond. The dimensionless diffusion coefficient may be thought of as the product of three dimensionless factors:

$$a/\frac{\partial \epsilon}{\partial \phi} \quad ,$$

$$c\Delta t/3\Delta x, \text{ and}$$

$$1/\tau.$$

The first of these is the ratio of the radiative specific heat to the total specific heat and ranges at this time and place from slightly greater than .8 in the earth to nearly one in the air. It is a factor of order unity. The second term, resembling a Courant number for light is about two in the Eulerian regions to twelve in the source. The last

term, the reciprocal of the zonal optical depth, is .25 in the source where the temperature is 3 keV and the specific gravity is 2.5. In the Eulerian regions the effect of the flux limiter is significant where there are substantial temperature gradients. The only large temperature difference is between the source and the air but the optical depth in the source still dominates. In summary the diffusion coefficient is five times the explicit stability criterion of one half in the air and source. The coupling coefficient, taking account of the partially covered Eulerian zones is of the same magnitude for coupling of each of the three pairs of regions. If an instability of the type associated with explicit differencing were to occur with a coefficient of this magnitude it would destroy the calculation in a few cycles starting from the conditions extant at .024 microseconds. It would require less than forty cycles for an instability driven by a coefficient of this magnitude to dominate the solution starting from round off error. The fact that there is no sign of any such ill effect caused by an instability lends credibility to the proposition that this coupling algorithm is indeed stable.

VI. CONCLUSION

A. Summary

There has been presented in this dissertation a means of adding a radiation diffusion calculation to a particular sort of hydrodynamics code. The requirement of consistency with the hydrodynamics code, whether CHAMP or CEL, led to certain decisions in deciding how the diffusion equation was to be differenced.

These codes are designed to simulate transient phenomena associated with the release of large amounts of energy and the concomitant large displacements of nearby matter. Because transients are of prime interest the code is only accurate to first order in time. This is not to say however that accuracy is given cavalier treatment. The philosophy of these codes has been that conservation of mass, momentum, and energy is of paramount importance and that in the short term propagation and conversion rates for these conserved quantities can be adequately calculated with low order approximations. The need for energy conservation led to the temperature extrapolation scheme which recognized the approach of a steep thermal front and made a prediction of temperature change in a stable fashion.

The expectation of large zone distortion in the Lagrange regions led to an algorithm capable of dealing with zones whose sides are of dissimilar magnitude as well as being far from rectangular. The algorithm provides bounded temperature distributions on a distorted grid regardless of the direction of the energy flux vector.

The coupling of distinct grids places the principal constraint upon the differencing technique. To be sure, the entire collection of

grids could be coupled in an implicit manner but the great range of geometric possibilities means that a great price in computing time would have to be paid. The scheme presented here allows the grids to be coupled in a stable manner with accuracy the only criterion for time step selection.

The problem used to illustrate the features of the code in Chapter V was run on a CDC 7600 computer. The five computational grids, three Eulerian and two Lagrangian, used to describe the problem contained approximately eight thousand zones. The calculation proceeded at a rate of 5.6 seconds per cycle. This is about twice the time required for a hydrodynamics only calculation for a problem of comparable size but still less than one millisecond per zone per cycle. A typical cycle used a time step of about a nanosecond.

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References

1. Patrick J. Roache, Computational Fluid Dynamics (Hermosa, Albuquerque, 1972).
2. R. D. Richtmyer and K. W. Morton, Difference Methods for Initial Value Problems, (Interscience, New York, 1967), 2nd edition.
3. J. P. Boris and D. L. Book, "Solution of Continuity Equations by the Method of Flux-Corrected Transport", in Methods in Computational Physics, John Killeen, ed. (Academic Press, New York, 1976), V. 16, p. 85.
4. R. Courant, K. Friedrichs, and H. Lewy, Math. Annalen 100, 32 (1928).
5. William F. Noh, Numerical Methods in Hydrodynamic Calculations, Lawrence Livermore Laboratory Report UCRL-52112 (1976).
6. J. E. Fromm, Phys. Fluids Sup. II 12, II-3 (1969).
7. W. P. Crowley, "The Free-Lagrange Method", in Proc. Second International Conf. on Numerical Methods in Fluid Dynamics (Springer-Verlag, New York 1970), p. 37.
8. C. W. Hirt, A. A. Amsden and J. L. Cook, J. Comp. Phys. 14, 227 (1974).
9. Mark L. Wilkins, "Calculation of Elastic-Plastic Flow" in Methods in Computational Physics, B. Alder, S. Fernbach, and M. Rotenberg, eds. (Academic Press, New York 1964), V. 3, p. 211.
10. William F. Noh, "CEL: A Time-Dependent, Two-Space-Dimensional, Coupled Eulerian-Lagrange Code" in Methods in Computational Physics, B. Alder, S. Fernbach, and M. Rotenberg, eds. (Academic Press, New York 1964), V. 3, p. 117.

11. L. L. Edwards, R. B. Hicknan, J. K. Hobson and T. C. Michels, CHAMP: A Coupled HEMP and Multifluid Eulerian Program for Fluid Flow Simulations, Lawrence Livermore Laboratory Report, UCRL-52444 (1978).
12. Ya. B. Zeldovich and Yu. P. Raizer, Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena (Academic Press, New York, 1966).
13. D. W. Peaceman and H. H. Rachford, Jr., J. Soc. Indust. Appl. Math. 3, 28 (1955).
14. N. N. Yanenko, The Methods of Fractional Steps (Springer-Verlag, New York, 1971).
15. Minao Kamegai, Investigation of the Thermal Yield from the Subsurface Explosions, Lawrence Livermore Laboratory Internal Document, UCID 17221 (1976).
16. G. C. Pomraning, Radiation Hydrodynamics (Pergamon, New York, 1973).
17. Roger B. DeBar, Nuclear Science and Engineering 30, 159 (1967).
18. R. Lelevier, Lectures on Hydrodynamics and Shock Waves, Lawrence Radiation Laboratory Report UCRL-4333 (1954).
19. J. A. Meijerink and H. A. van der Vorst, Math. of Computation, 31, 148 (1977).
20. D. V. von Rosenberg, Methods for the Numerical Solution of Partial Differential Equations (American Elsevier, New York, 1969).
21. M. L. Alme and J. R. Wilson, Astrophysical Journal, 194, 147 (1974).