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**An Algorithm for the Computation of Nonlinear
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AN ALGORITHM FOR THE COMPUTATION OF NONLINEAR ELECTRON THERMAL CONDUCTION ON AN ARBITRARILY SHAPED, TWO-DIMENSIONAL DOMAIN

by

J. U. Brackbill and L. G. Margolin

ABSTRACT

A numerical algorithm is described for computing coupled heat and hydrodynamic flow on an arbitrarily shaped, time-varying domain. The algorithm extends the ICED-ALE method, for the computation of hydrodynamic motion using an arbitrary Eulerian-Lagrangian mesh, to include electron thermal conduction. Appropriate difference equations in conservation form are developed, and the Dufort-Frankel scheme is adapted to advance these equations in time. Results are presented which illustrate the application of the algorithm to the two-dimensional hydrodynamic motion induced by illuminating spherical and thin foil targets with a single laser beam.

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I. INTRODUCTION

Many problems of current interest in plasma physics are characterized by the competition between hydrodynamic flow and thermal conduction processes. Among these are the simultaneous fluid flow and thermal conduction induced in targets by laser illumination¹ and the energy and mass losses from open-ended, magnetic confinement devices.^{2,3} Solving these problems numerically requires the development of reasonably fast and accurate algorithms for the solution of nonlinear thermal conduction equations.

A two-dimensional algorithm for the computation of nonlinear electron thermal conduction on an arbitrarily shaped domain is reported here. The algorithm has been incorporated into a hydrodynamics code and used to compute

laser-induced flow and thermal conduction in spherical pellets and thin foils. The method of time advancement used in the algorithm is an adaptation to nonlinear equations of the Dufort Frankel method.⁴ The algorithm is, therefore, explicit and unconditionally stable. The spatial differencing used in the algorithm is appropriate for the irregularly shaped quadrilateral cells used in the arbitrary Lagrangian-Eulerian (ALE) mesh of the hydrodynamics code.^{5,6,7} Thus, the resulting code combines the advantages of the ALE method (among them the reduction of computational diffusion, the accumulation of mesh points in regions of strong flow gradients to provide increased resolution where it is needed, and the ability to cover arbitrarily shaped, time-dependent domains,) with a simple, explicit algorithm for the computation of nonlinear heat conduction.

In the following section, the heat conduction algorithm is presented. In the next section, an error estimate, based on a one-dimensional analysis, leads to a time-step restriction based on accuracy rather than stability. In the last section, the results of the application of the method to the computation of laser-induced flow and conduction in spherical pellets and thin foils are presented. Finally, in an Appendix, a Lagrange multiplier technique for forcing the global conservation of energy in the heat conduction process is derived. It is shown, both by analysis and by application to a one-dimensional test case, that the resulting conduction algorithm is computationally unstable. The discussion of this method is included on the theory that it is sometimes as useful to know what will not work as well as what will work.

II. ELECTRON THERMAL CONDUCTION

Electron thermal conduction in a fully ionized plasma is described by the equation

$$\frac{\partial I_e}{\partial t} = \frac{1}{M_e} \int_s ds (\hat{n} \cdot \nabla) \bar{\kappa} \nabla I_e^{7/2}, \quad (1)$$

where I_e is the specific electron energy, M_e is the total mass of electrons contained within a volume V whose surface is s with outward directed unit normal

$\hat{n}$, and $\bar{\kappa}$ is the conductivity.⁸ The conductivity is given by

$$\bar{\kappa} = \left(\frac{2}{7}\right) 20 \cdot \left(\frac{2}{\pi}\right)^{3/2} \frac{m_e^3 (\gamma-1)^{7/2}}{e^4 \ln \Lambda \underline{Z}}, \quad (2)$$

where γ is the ratio of specific heats, m_e is the electron mass, e the electronic charge, $\underline{Z}$ the average ionization state of the molecules in the material, and Λ the Coulomb integral.⁸

A complete numerical solution algorithm for this time-dependent equation is derived. First, a spatial difference equation appropriate for a nonrectilinear mesh is derived and then reduced to a compact, nine-point stencil. Second, an algorithm for the advancement in time of the resulting polynomial equation is given.

The spatial difference approximation to the electron thermal conduction equation, Eq. (1), is constructed by computing the energy flux across each face of a computation cell, and then integrating the fluxes over all faces of the cell. The energy flux is proportional to the gradient of $I_e^{7/2}$ and the conductivity at the center of a face. The gradient is computed from the values of $I_e^{7/2}$ at the vertices bounding a face and at the cell centers of the adjacent cells. The I_e 's at cell centers are stored quantities. The $I_e^{7/2}$'s at cell vertices are defined to be the linear average of the $I_e^{7/2}$'s at the four cell centers neighboring a vertex. Where the local indexing is defined as shown in Fig. 1, the value of $\bar{I}$ at vertex of 2, for example, is given by,

$$\bar{I}_2 \equiv \frac{1}{4} (\bar{I}_a + \bar{I}_b + \bar{I}_c + \bar{I}_o), \quad (3)$$

where $\bar{I}$ is defined by,

$$\bar{I} \equiv I^{7/2}. \quad (4)$$

The difference equations used to define the gradient are similar to those given in Ref. 7. The component equations for the gradient on side 1-2 are given here to illustrate their form, and are written

$$\left\langle \frac{\partial \bar{I}}{\partial x} \right\rangle_{12} = \left\{ (\bar{I}_a - \bar{I}_o) (y_2 - y_1) - (\bar{I}_2 - \bar{I}_1) (y_a - y_o) \right\} / A_{12} , \quad (5)$$

and

$$\left\langle \frac{\partial \bar{I}}{\partial y} \right\rangle_{12} = \left\{ (\bar{I}_2 - \bar{I}_1) (x_a - x_o) - (\bar{I}_a - \bar{I}_o) (x_2 - x_1) \right\} / A_{12} , \quad (6)$$

and where A_{12} is given by

$$A_{12} = \left\{ (x_a - x_o) (y_2 - y_1) - (y_a - y_o) (x_2 - x_1) \right\} . \quad (7)$$

The cell-centered coordinates, x_o and y_o , for example, are given by

$$x_o = (x_1 + x_2 + x_3 + x_4) / 4 , \text{ and}$$

$$y_o = (y_1 + y_2 + y_3 + y_4) / 4 . \quad (8)$$

The integral, Q , of the flux over all surfaces of the cell is given by

$$\begin{aligned}
Q = \frac{1}{2} \left[\kappa_{12} (r_1 + r_2) \left\{ \left\langle \frac{\partial \bar{I}}{\partial x} \right\rangle_{12} (y_2 - y_1) - \left\langle \frac{\partial \bar{I}}{\partial y} \right\rangle_{12} (x_2 - x_1) \right\} \right. \\
+ \kappa_{23} (r_2 + r_3) \left\{ \left\langle \frac{\partial \bar{I}}{\partial x} \right\rangle_{23} (y_3 - y_2) - \left\langle \frac{\partial \bar{I}}{\partial y} \right\rangle_{23} (x_3 - x_2) \right\} \\
+ \kappa_{34} (r_3 + r_4) \left\{ \left\langle \frac{\partial \bar{I}}{\partial x} \right\rangle_{34} (y_4 - y_3) - \left\langle \frac{\partial \bar{I}}{\partial y} \right\rangle_{34} (x_4 - x_3) \right\} \\
\left. + \kappa_{41} (r_4 + r_1) \left\{ \left\langle \frac{\partial \bar{I}}{\partial x} \right\rangle_{41} (y_1 - y_4) - \left\langle \frac{\partial \bar{I}}{\partial y} \right\rangle_{41} (x_1 - x_4) \right\} \right] \quad (9)
\end{aligned}$$

where κ_{12} , for example, is the conduction coefficient given by Eq. (1) defined on face 12. The equation for Q is written in a form appropriate for both cylindrical coordinates, where $r \rightarrow x$, and Cartesian coordinates, where $r \rightarrow 1$.

The complete conduction equation is written as a stencil, that is as an equation of the form,

$$\rho_o \frac{\partial I_o}{\partial t} = \left\{ a_o \bar{I}_o + \sum_{l=a}^h a_l \bar{I}_l \right\}. \quad (10)$$

The coefficients of the stencil are obtained by evaluating the coefficient of each $\bar{I}$ appearing in the equation for Q . They are given by.

$$a_b = b_{1b} + b_{2b} \quad ,$$

$$a_d = b_{2d} + b_{3d} \quad ,$$

$$a_f = b_{3f} + b_{4f} \quad ,$$

$$a_h = b_{4h} + b_{1h} \quad ,$$

$$a_a = b_{1a} + b_{2a} + b_{4a} ,$$

$$a_c = b_{1c} + b_{2c} + b_{3c} ,$$

$$a_e = b_{2e} + b_{3e} + b_{4e} ,$$

$$a_g = b_{3g} + b_{4g} + b_{1g} ,$$

(11)

and finally,

$$a_0 = b_{10} + b_{20} + b_{30} + b_{40}$$

The b 's, which are called coupling coefficients, are given by,

$$b_{1a} = \kappa_{12} \left(\frac{r_1 + r_2}{2} \right) \left\{ (y_2 - y_1)^2 + (x_2 - x_1)^2 \right\} / 2 A_{12} ,$$

$$b_{1o} = - b_{1a}$$

$$b_{1b} = - \kappa_{12} \left(\frac{r_1 + r_2}{2} \right) \left\{ (y_a - y_o) (y_2 - y_1) + (x_a - x_o) (x_2 - x_1) \right\} / 8 A_{12} ,$$

$$b_{1c} = b_{1b}, \quad b_{1h} = - b_{1b}, \quad b_{1g} = b_{1h} ,$$

$$b_{2c} = \kappa_{23} \left(\frac{r_2 + r_3}{2} \right) \left\{ (y_3 - y_2)^2 + (x_3 - x_2)^2 \right\} / 2 A_{23} ,$$

$$b_{2o} = - b_{2c} ,$$

$$b_{2d} = - \kappa_{23} \left(\frac{r_2 + r_3}{2} \right) \left\{ (y_c - y_o) (y_3 - y_2) + (x_c - x_o) (x_3 - x_2) \right\} / 8 A_{23}$$

$$b_{2e} = b_{2d}, \quad b_{2a} = -b_{2d}, \quad b_{2b} = b_{2a} ;$$

$$b_{3e} = \kappa_{34} \left(\frac{r_3 + r_4}{2} \right) \left\{ (y_4 - y_3)^2 + (x_4 - x_3)^2 \right\} / 2 A_{34} ,$$

$$b_{3o} = -b_{3e} ,$$

$$b_{3g} = -\kappa_{34} \left(\frac{r_3 + r_4}{2} \right) \left\{ (y_e - y_o) (y_4 - y_3) + (x_e - x_o) (x_4 - x_3) \right\} / 8 A_{34}$$

$$b_{3f} = b_{3g}, \quad b_{3d} = -b_{3f}, \quad b_{3c} = b_{3d} ;$$

$$b_{4g} = \kappa_{41} \left(\frac{r_4 + r_1}{2} \right) \left\{ (y_1 - y_4)^2 + (x_1 - x_4)^2 \right\} / 2 A_{41} ,$$

$$b_{4o} = -b_{4g}$$

$$b_{4h} = -\kappa_{41} \left(\frac{r_4 + r_1}{2} \right) \left\{ (y_g - y_o) (y_1 - y_4) + (x_g - x_o) (x_1 - x_4) \right\} / 2 A_{41}$$

$$b_{4a} = b_{4h}, \quad b_{4e} = -b_{4h}, \quad b_{4f} = b_{4e} .$$

(12)

Because of the large number of symmetries, only eight of the coupling coefficients must be independently computed. When the mesh is rectilinear, the coupling coefficients for cell centers b, d, f, and h are zero, and the stencil reduces to a compact five-point form. The five-point stencil for a square, Cartesian mesh is shown in Fig. 2.

The matrix of coefficients corresponding to the system of spatial differences to be solved over the mesh is symmetric. That is, the coupling coefficient between two vertices is the same independent of the direction of the coupling. Thus, the spatial part of the difference equation is in conservation form.

The Dufort-Frankel algorithm is used to advance Eq. (10) in time. The advancement scheme is given by,

$$\rho_0 \left({}^{n+1}I_0 - {}^{n-1}I_0 \right) - \delta t a_0 {}^{n+1}I_0 = \delta t \left\{ a_0 {}^{n-1}I_0 + 2 \sum_{\ell=2}^h a_\ell {}^{n+1}I_\ell \right\}, \quad (13)$$

where the superscript denotes the time level of the term, as for example ${}^{n+1}I_0$ is evaluated at time level $n+1$. [Note that the time differencing introduces an asymmetry into the coupling. This produces errors in conservation of energy of $O(\delta t^2)$.] The polynomial equation for ${}^{n+1}I_0$ is solved by a simple Newton-Raphson iteration.

One notes first that Eq. (13), which can be written,

$${}^{n+1}I_0 + b \left({}^{n+1}I_0 \right)^{7/2} - c = 0, \quad (14)$$

where b and c are constants, is a one-parameter Eq. (9). If the substitution $I' = {}^{n+1}I_0/c$ is made,⁹ Eq. (14) becomes

$$I' + \alpha I'^{7/2} - 1 = 0, \quad (15)$$

where $\alpha = bc^{5/2}$. When α is small, I' is approximately equal to one, and when α is large, I' approaches $\alpha^{-2/7}$. Thus, a good approximation to I' for all values of α is given by

$$I' \approx \frac{1}{1 + \alpha^{2/7}}, \quad (16)$$

and ${}^{n+1}I_0$ is approximately given by

$$n+1_{I_o} \approx c / \left(1 + \alpha^{2/7} \right) . \quad (17)$$

To improve the accuracy of this result, several iterations of Eq. (18) are performed.

$$(\ell)n+1_{I_o} = (\ell-1)n+1_{I_o} - \frac{(\ell-1)_S}{(\ell-1)_S'} , \quad (18)$$

where the superscript, (ℓ) , denotes the iteration number, and where $(\ell-1)_S$ and $(\ell-1)_S'$ are given by,

$$(\ell-1)_S = (\ell-1)n+1_{I_o} + b^{(\ell-1)} \left(n+1_{I_o} \right)^{7/2} - c , \quad (19)$$

and

$$(\ell-1)_S' = 1 + b^{(\ell-1)} \left(\frac{7}{2} \right) \left(n+1_{I_o} \right)^{5/2} . \quad (20)$$

Presently only five iterations are allowed. However, no more than two are usually necessary for five place accuracy.

III. A TIME STEP FOR THE THERMAL CONDUCTION ALGORITHM

The Dufort-Frankel scheme is unconditionally stable for all values of the time step.⁴ Nevertheless, the relation between the time step and the error in the

numerical solution makes it advantageous to limit the time step to limit the error. When the maximum allowable error in the solution is prescribed, the corresponding maximum allowable time step can be computed. In the following discussion, a time-step criterion is derived based on the estimated error in the solution of a linearized, one-dimensional thermal conduction equation. In addition, the criterion is related to the concept of a Courant condition, and then compared with the similar error-bounding criterion which can be derived for an implicit solution algorithm. From this comparison, an estimate is made of the relative efficiency of the ordinary explicit, Dufort-Frankel, and implicit time advancement schemes for the thermal conduction equation.

Finally, the results of the analysis of the linearized equation are tested for their applicability to the nonlinear equation by the comparison of exact and computed solutions to a traveling wave problem.

On a one-dimensional array of equally spaced points with spacing δx , the Dufort-Frankel algorithm for a linearized diffusion equation is given by,

$$n+1 I_j = n-1 I_j + \frac{2\sigma_j \delta t}{\delta x^2} \{ n I_{j+1} + n I_{j-1} - n+1 I_j - n-1 I_j \} , \quad (21)$$

where σ_j is given by,

$$\sigma_j = \frac{7}{2} \bar{\kappa} (n I_j)^{5/2} / \rho_j . \quad (22)$$

It is assumed that the stability of this equation is a necessary condition for the stability of the nonlinear equation. A dispersion relation for this equation may be derived, and from this it is found that Eq. (21) is unconditionally stable for all δt . The limiting solution as δt increases without bound is a purely oscillating wave with an approximate phase velocity $\delta x / \delta t$.

The truncation errors in Eq. (21) can be found by expanding each term about $n I_j$, and retaining only the zeroth order term in δx and δt . The differential

equation which is obtained in this way,

$$\frac{\partial I}{\partial t} = \sigma \left[\frac{\partial^2 I}{\partial x^2} - \left(\frac{\delta t}{\delta x} \right)^2 \frac{\partial^2 I}{\partial t^2} \right], \quad (23)$$

is the one which the solution to Eq. (21) satisfies to zeroth order in δx and δt . The error in the time derivative relative to the exact derivative, obtained when $\delta t/\delta x \rightarrow 0$, is given by

$$\epsilon = \left(\frac{\delta t}{\delta x} \right)^2 \left(\frac{\partial^2 I}{\partial t^2} / \frac{\partial^2 I}{\partial x^2} \right). \quad (24)$$

When the numerator is evaluated by iterating the exact equation an estimate for ϵ is obtained,

$$\epsilon \approx \left(\sigma \frac{\delta t}{L \delta x} \right)^2 + O(\delta t, \delta x), \quad (25)$$

where L is the gradient length defined by

$$\frac{1}{L^2} = \frac{1}{I} \frac{\partial^2 I}{\partial x^2}. \quad (26)$$

A limit on δt is obtained by specifying the maximum allowable error,

$$\delta t_{D.F.} < \epsilon_{\max}^{1/2} \delta x L / \sigma. \quad (27)$$

This criterion can be related to the concept of a Courant condition where the time step is chosen so that a diffusion "wave" propagates no more than C cells per time step. To do this, a wave velocity is obtained by considering the rate at which the gradient length increases with time because of diffusion in a typical profile, given by

$$I(x,0) = I_0 \exp(-x^2/2L^2) , \quad (28)$$

where L is the gradient length. The gradient length is easily shown to depend on time as given by,

$$L^2(t) = [L^2(t=0) + \sigma t] , \quad (29)$$

and thus the velocity of a diffusion wave (i.e., the rate at which the gradient length increases) is given by,

$$V = \sigma/L . \quad (30)$$

Substitution of this velocity into Eq. (27) gives the result that C, the Courant number, is given by,

$$C = \epsilon_{\max}^{1/2} . \quad (31)$$

From this one concludes that the relative error in the solution is $O(1)$ when the Dufort-Frankel scheme is allowed to propagate information one or more cells in a time step. This result is comparable with the conditions obtained by similar reasoning for implicit hyperbolic equations.

A similar error analysis may be performed on the implicit algorithm,

$$\begin{aligned}
 {}^{n+1}I_j = {}^nI_j + \frac{2\sigma_j \delta t}{\delta x^2} & \left[\theta \left({}^{n+1}I_{j+1} - {}^{n+1}I_j + {}^{n+1}I_{j-1} \right) \right. \\
 & \left. + (1-\theta) \left({}^nI_{j+1} - {}^nI_j + {}^nI_{j-1} \right) \right] ,
 \end{aligned} \tag{32}$$

which is unconditionally stable for $1/2 \leq \theta \leq 1$. The solution to Eq. (32) satisfies the differential equation, written

$$\frac{\partial I}{\partial t} = \sigma \frac{\partial^2 I}{\partial x^2} + \sigma^2 \delta t \left(\theta - \frac{1}{2} \right) \frac{\partial^4 I}{\partial x^4} \tag{33}$$

to $O(\partial x, \partial t)$. From this equation, a relative error is obtained which is given by

$$\epsilon = \frac{\sigma \delta t \left(\theta - \frac{1}{2} \right)}{L^2} + O(\delta x^2, \delta t^2) . \tag{34}$$

If a maximum error bound is placed on the solution, a criterion on the time step is obtained which is written,

$$\delta t_{IMP} < \frac{\epsilon_{max} L^2}{\sigma \left(\theta - \frac{1}{2} \right)} , \tag{35}$$

and is valid for $\theta > 1/2$. The error is zero to this order when $\theta = 1/2$. In this case, the Courant number is given by,

$$C = \frac{L}{\delta x} \frac{\epsilon_{\max}}{\left(\theta - \frac{1}{2}\right)} . \quad (36)$$

When Eq. (36) is compared with Eq. (32), it can be seen that for $\epsilon_{\max} = O(1)$ the Dufort-Frankel scheme allows a diffusion wave to propagate only one cell and the implicit scheme allows it to propagate one gradient length in a time step. However, this apparent advantage of an implicit scheme may not lead to an increase in computation speed in practice because a costly matrix inversion must be performed to solve an implicit equation. For example, if the inversion were performed by a Jacobi iteration, each iteration would advance information one mesh point. Thus, $L/\delta x$ iterations would be necessary to propagate a wave C cells. The effective Courant number for each iteration is then approximately one, and as many operations are required to obtain comparable accuracy for the implicit algorithm over a given interval in time as for the Dufort-Frankel algorithm. (Clearly, more sophisticated matrix iterative techniques would alter this conclusion in favor of the implicit scheme.)

Both of these algorithms may now be compared with the ordinary explicit equation for which the time step is limited by the stability condition,

$$\frac{\sigma \delta t}{\delta x^2} < \frac{1}{2} . \quad (37)$$

This condition leads to a maximum Courant number given by the inequality,

$$C < \frac{1}{2} \left(\frac{\delta x}{L} \right) . \quad (38)$$

which is inversely proportional to the gradient length. This behavior contrasts sharply with the Dufort-Frankel algorithm, where C is independent of L for a given accuracy, and the implicit algorithm, where C is linear in L .

Essentially, because both the Dufort-Frankel and the implicit algorithm are unconditionally stable, the time step can be set to give accuracy for those modes which are dominant instead of, as must be done for an ordinary explicit scheme, setting the time step small enough to ensure the stability of all possible modes. This allows a larger time step for the Dufort-Frankel and implicit algorithms, that is one which propagates information through the mesh in fewer computation cycles, than for an ordinary explicit scheme when thermal gradient lengths are long compared with the mesh spacing.

Numerical and exact solutions of the nonlinear equations can be compared for the traveling wave problem.¹⁰ The errors in the computed solution as a function of the Courant number can thus be explicitly demonstrated.

A simplified nonlinear equation written,

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2}{\partial x^2} u^{7/2} , \quad (39)$$

is differenced. When $u(0,t)$ is prescribed at $x = 0$ by the equation

$$u(t) = \left(\frac{5}{7} \frac{V^2}{\sigma} t \right)^{2/5} , \quad (40)$$

a wave propagates in the positive x direction with speed V . The self-similar solution to the nonlinear diffusion equation is given by,

$$u(x,t) = \left[-\frac{5}{7} \frac{V}{\sigma} (x-Vt) \right]^{2/5} , \quad x \leq Vt , \quad (41)$$

and

$$u(x,t) = 0 , \quad x > Vt . \quad (42)$$

The exact solution is compared with the computed solution for various values of the Courant number. For $\sigma = 100$, the numerical solutions with $C = 0.25, 0.5, 1.0$, and 5.0 are compared with the theoretical solutions in Fig. 3. As C increases, the increasing error in the numerical solution manifests itself as a reduction in the speed of propagation of the wavefront, and in the area under the curve. The latter is a reflection of the nonconservative nature of the Dufort-Frankel algorithm.⁴ The scaling of the relative error in the propagation speed with the Courant number is shown to agree with the linearized analysis for $C < 1$ in Fig. 4.

An additional demonstration that the error estimate derived from an analysis of the linearized equations is applicable to the nonlinear equations as well is shown in Fig. 5. To obtain the results shown, C is held constant and σ is varied between 1 and 100. In every case, V is equal to 1, and the conductivity for the corresponding linearized equation,

$$\sigma' = \sigma u^{5/2} \quad , \quad (43)$$

is also the same in every case at the time shown. According to the linearized analysis, the error in the computed solution should be insensitive to changes in σ when all other parameters are held constant, and clearly that is true.

The time step used in these calculations can be compared with the maximum stable time step for an ordinary explicit scheme. The maximum numerical value for σ' can be computed for the case shown in Fig. 3, and is found to be 27.6. The time step for an explicit calculation obeys the inequality

$$\delta t < \frac{\delta x^2}{\sigma'_{\max}} \quad , \quad (44)$$

and is thus just 1/15 the time step used for the calculation shown. Moreover, the explicit time step decreases as $u(o,t)$ increases in time, while the Dufort-Frankel time step remains constant because $L = \sigma'/V$ is constant. These

Fig. 1. The diagram defines the labeling for the thermal conduction, difference equation. The circles denote cell vertices, x 's, cell centers.

Fig. 2. The difference equation reduces to the stencil illustrated above when the cells are square.

Fig. 3. The computed solutions for various values of C , the Courant number, are compared with the theoretical solution.

Fig. 4. The scaling of the error in the propagation speed ϵ , with the Courant number, C , is illustrated.

results clearly demonstrate the unconditional stability of the Dufort-Frankel scheme when applied to a nonlinear equation.

The time step criterion is generalized to two dimensions by computing the gradient length from the equation,

$$1/L^2 = 1/T^{7/2} \left(\frac{\partial^2 T^{7/2}}{\partial x^2} + \frac{\partial^2 T^{7/2}}{\partial y^2} \right), \quad (45)$$

or

$$L = \delta x, \quad (46)$$

whichever is greater. The time step which limits the relative error in the numerical solution of Eq (1) to less than $\epsilon_{\max}$ is given by

$$\delta t < CL\delta x/\kappa T^{5/2}, \quad (47)$$

where C, the Courant number, is equal to $\epsilon_{\max}^{1/2}$.

IV. APPLICATION TO LASER-INDUCED PLASMA FLOW

The discussion in this section includes a description of the physical model used in these calculations, some details of the inclusion of this model into the basic hydrodynamics code, and a description of the results of the calculations of flow in spherical targets and thin foils.

A. Physical Model

The motion of a target, often a small spherical pellet (diameter 50 μm) or thin foil (thickness 1000 $\text{\AA}$) which has been illuminated by intense, focused laser light is computed. The processes by which energy is absorbed in the target, such as inverse bremsstrahlung, resonant absorption, and the plasma instabilities, tend to heat electrons preferentially. The electrons stay hot because the effectiveness of collisions in equilibrating ion and electron temperatures decreases with temperature. A model which is sometimes used to represent the resulting coupled heat and fluid flow is discussed by Widner.¹¹ In this model the target material is assumed to be a completely ionized, charge-neutral fluid with weakly coupled electron and ion temperatures. Equilibration of ion and electron temperatures occurs by Coulomb collision processes, but on a time scale which is at least comparable to the laser pulse length. The ion thermal conduction is neglected, since it proceeds at a rate of the order of the square root of the ratio of the electron to the ion mass times the rate for electron thermal conduction even when ion and electron temperatures are equal. The transport coefficients for electron thermal conduction and equilibrium are those given by Spitzer.⁸ A numerical viscosity is computed which acts only upon the ions, despite the fact that the equations given by Braginskii¹² for the electron and ion viscosities indicate the electron viscosity is of the same order as the ion viscosity when the temperature of the electrons is only slightly higher than that of the ions. This is, however, common practice.¹¹

An additional assumption in the model is that the electron distribution is locally Maxwellian. The thermalization time for the electrons varies as $T^{3/2}$, where T is the electron temperature.⁸ When T is large, the thermalization time may be of the order of the characteristic times for hydrodynamic motion, in which case the assumption of local thermodynamic equilibrium is no longer valid. Thus, results obtained with this model should be distrusted to the degree that non-Maxwellian electron distributions are likely to occur.

The hydrodynamic flow is computed using an implicit algorithm for the solution of the continuity and momentum equations, and an arbitrary Lagrangian-Eulerian mesh.^{5,7} The thermal conduction and equilibration calculations are added by chaining them to the hydrodynamic algorithm. (Chaining means that separate, sequential calculations of the hydrodynamic and thermal processes are performed each computation cycle. Of course, hydrodynamic

and transport processes are coupled physically because for example, both thermal conduction and energy absorption alter the pressures which drive the hydrodynamic motion. If necessary, the size of the errors introduced by chaining can be checked by altering the order of the sequence in which calculations are performed. Any differences would be due to errors.) Chaining adds flexibility, for the numerical method used in each element of the sequence can be tailored to the special problems posed by the physical process being computed.

The basic hydrodynamics algorithm is modified to incorporate a two-temperature fluid. A single pressure, the sum of the ion and electron partial pressures, drives the fluid motion. Thus the basic algorithm for the equations of fluid motion is unchanged. The equations are written in Lagrangian form as,

$$\frac{d\rho_T}{dt} + \rho_T (\nabla \cdot \vec{u}) = 0, \text{ and} \quad (48)$$

$$\rho_T \frac{d\vec{u}}{dt} + \nabla P_T = 0, \quad (49)$$

where P_T is the sum of the partial pressures of the electrons and ions, ρ_T the total mass density, and $\vec{u}$ the total fluid velocity of ions and electrons. The internal energy equation must be altered slightly. Where I_T is the total specific internal energy, the total energy equation for adiabatic changes is written,

$$\rho_T \frac{dI_T}{dt} = - P_T (\nabla \cdot \vec{u}). \quad (50)$$

The separate ion and electron energy changes are in the ratios

$$\frac{\frac{dI_e}{dt}}{I_e} = \frac{\frac{dI_i}{dt}}{I_i} = \frac{\frac{dI_T}{dt}}{I_T}, \quad (51)$$

where I_e and I_i are the electron and ion specific energies.

In hydrodynamic calculations, the convection of total energy and momentum is often calculated, and the internal energy is obtained by subtracting the resulting kinetic energy from the total energy. In the present calculation there are two internal energies, one more than can be computed by subtraction. In this case, the smaller energy is computed from a separate convection equation and the larger energy is computed by subtraction to minimize the relative error in any given energy term and to avoid negative energies. In laser-induced hydrodynamic motion, the electron temperature is generally much higher than the ion temperature, and so the ion energy is computed directly.

The thermal equilibration between ions and electrons by means of Coulomb collisions is described by the Eq. (52).

$$\frac{\partial}{\partial t} (T_i - T_e) = -2 \frac{(T_i - T_e)}{\tau} , \quad (52)$$

where T_i and T_e are the ion and electron temperatures. The thermal equilibration time, τ is given by,

$$\tau = \frac{3 m_e m_i^2 k^{3/2}}{8 \sqrt{2} \pi \rho_i \bar{Z}^2 e^4 \ln \Lambda} \left(\frac{T_e}{m_e} + \frac{T_i}{m_i} \right)^{3/2} , \quad (53)$$

where m_i and m_e are the ion and electron masses, ρ_i the ion mass density, $\bar{Z}$ the average ionization state, e the electronic charge, k Boltzmann's constant, and Λ the Coulomb integral. Energy is conserved during the equilibration process so that the sum of ion and electron energies is constant,

$$\frac{\partial}{\partial t} (\rho_e I_e + \rho_i I_i) = 0 . \quad (54)$$

When the ions are stripped of electrons, both ions and electrons behave as perfect gases, and obey the equation of state,

$$kT_{\alpha} = (\gamma-1) m_{\alpha} I_{\alpha} , \quad (55)$$

With this equation of state, and assuming that temperature equilibration is occurring independently of all other processes, energy conservation implies that

$$\frac{\partial}{\partial t} (T_i + \bar{Z} T_e) = 0 . \quad (56)$$

A simple implicit numerical scheme is obtained when Eqs.(52) and (56) are approximated by the finite difference equations.

$$n_{\Delta}^{n+1} = n_{\Delta} / (1 + 2\delta t / n\tau) , \quad (57)$$

and

$$n_E^{n+1} = n_E , \quad (58)$$

where $\Delta = T_i - T_e$ and $E = T_i + \bar{Z}T_e$. The new temperatures are computed from the expressions,

$$n_{T_i}^{n+1} = n_{T_i}^{n+1} \left(\frac{E + \bar{Z}\Delta}{1 + \bar{Z}} \right) , \quad (59)$$

and

$$n_{T_e}^{n+1} = n_{T_e}^{n+1} \left(\frac{E - \Delta}{1 + \bar{Z}} \right) . \quad (60)$$

That τ is evaluated with time level n temperatures causes appreciable errors only when δt is comparable with τ . When δt is either much less than or much greater than τ , Eqs. (59) and (60) approach the correct asymptotic limits. Even when δt and τ are comparable, errors in equilibration are important only when the electrons are hot enough so that electron thermal conductivity is high and is also sensitively dependent on the electron temperature. It is not likely that this will ever occur because when the electrons are hot, δt , which varies as $T_e^{-5/2}$, will be small compared with τ .

B. Results

1. The Implosion of a Spherical Pellet. Results are presented from the numerical calculation of the coupled heat and fluid flow of a spherical pellet of polyethylene when laser energy is deposited in a thin layer of its surface. Two different problems have been computed. In the first, the energy is deposited uniformly over the surface of the pellet and, as a result, the subsequent motion of the pellet is spherically symmetric. In the second, more energy is deposited on the top than on the bottom of the pellet, approximately 30% more, and the subsequent motion of the pellet is axisymmetric.

A full description of the motion of a heated pellet is given in Nuckolls and Wood.¹ For our purposes, it is sufficient to list the principal phases of the dynamics. Briefly, the heated material at the surface will ablate while thermal conduction carries energy into the pellet. Associated with the thermal gradient at the front of the inward propagating thermal wave, there is a strong pressure gradient which drives a converging shock. The shock coalesces on the origin and creates a hot, dense core of material which persists until shock reflection and the inward propagating rarefaction wave from the surface ablation disassemble it.

In Figs. 6 and 7, radial plots of the density and electron temperature are shown which illustrate the dynamics described above. These plots represent data taken from a two-dimensional calculation with spherically symmetric initial energy deposition. The radius of the pellet initially is 25×10^{-4} cm, the density 0.9 g cm^{-3} , and the deposited energy approximately 40J. The curves in Fig. 6 show density and temperature at 8×10^{-8} s. The density maximum at a radius equal to 9×10^{-4} cm marks the converging shock. The underdense portion of the curve beyond 15×10^{-4} -cm radius lies in the ablation region. Some pellet material has already expanded beyond 35×10^{-4} -cm radius.

At 14×10^{-8} s as shown in Fig. 7, the converging shock has reflected from the center of the pellet and is now moving out. The density at the center has already dropped from its maximum value, which is presumably greater than the maximum of 12.9 g cm^{-3} associated with the diverging shock. On the other hand, the electron temperature is as high at the center as at the shock front. Evidently, electron thermal conduction is effective in keeping the central portion in thermal equilibrium even as the disassembly takes place.

Two-dimensional representations of the flow for a similar, spherically symmetric case are shown in Figs. 8-13. The deposited energy is now 70J, and the initial electron temperature is 2.5 eV. The computation of the electron thermal conduction was performed at a Courant number equal to 0.5 with 10 cycles of the thermal conduction equation per hydro time step. The resulting hydro time step was approximately one-half that which the normal hydrodynamic stability conditions would allow. The mesh was moved with the fluid as in a Lagrangian computation. The equations contained no viscosity beyond that due to truncation errors in the difference equations.

A portion of the computation mesh for this calculation is shown. Only the inner 10 radial zones are included in the plot, because otherwise the core compression occupies only a small fraction of plots at later times. In addition to the zones shown, there are 15 additional radial zones beyond for a total of 525 zones in the full mesh. The mesh is rotationally symmetric about the vertical axis.

The compression of the core of the pellet is illustrated in Fig. 8 where the mesh is shown at 5, 10, and 16×10^{-8} s. The inner 10 radial zones all compress until, at 16×10^{-8} s, the radius of the core is reduced from 10×10^{-4} cm to 5.9×10^{-4} cm. The compression is not uniform, however. The innermost radial zone is much more strongly compressed than any other zone. This differential compression of the pellet is illustrated more clearly in Fig. 9, where contours of constant density are plotted. The values assigned to each contour progress in steps of 1.23 from the value 3.6 g cm^{-3} assigned to the contour labelled 0 to 28.5 g cm^{-3} assigned to the innermost contour. Thus, although all of the region shown has been compressed, only the innermost core has been compressed strongly.

The motion of the pellet is illustrated in Fig. 10, where the velocities are plotted at times corresponding to those in Fig. 8. The velocity is represented by a line which begins at a cell vertex and points in the direction

Fig. 5. The independence of the error in the propagation speed, ϵ , from the value of σ is shown.

Fig. 6. Radial density and electron temperature profiles are plotted at the time 8×10^{-8} s for a symmetrically illuminated spherical pellet.

Fig. 7. Plots corresponding to those in Fig. 6 are plotted at 14×10^{-8} s.

(a)

(b)

(c)

Fig. 8. A portion of the computation mesh is plotted at $5, 10$, and 16×10^{-8} s in panels a, b, and c for a symmetrically illuminated, spherical pellet. An axis of symmetry coincides with the left edge of the mesh in this and all figures through Fig. 20, and the scale is the same for all plots.

(a)

(b)

(c)

Fig. 9. The isodensity contours are plotted. The times correspond to those in Fig. 8.

(a)

(b)

(c)

Fig. 10. The velocity vectors are plotted at times corresponding to those in Fig. 8. The vectors begin at a cell vertex, and extend in the direction of the flow. Their lengths relative to each other indicate the relative velocity.

(a)

(b)

(c)

Fig. 11. Contours of electron temperature at times corresponding to those in Fig. 8 are plotted.

(a)

(b)

(c)

Fig. 12. The computation mesh is plotted for an asymmetrically illuminated spherical pellet at 5, 10, and 12 x 10⁻⁸s in panels a, b, and c.

(a)

(b)

(c)

Fig. 13. The velocity vectors corresponding to the mesh in Fig. 12 are shown.

of the flow. In Fig. 10a, the shock has reached a radius of 9×10^{-4} cm, and continues to propagate inward until the time shown in Fig. 10d. In Fig. 10d, the end of the compression of the innermost zone is shown as the converging shock reflects from the center.

Some asymmetry has been introduced into the results by truncation errors in the hydrodynamic difference equations, which are apparent only in the innermost zones at the time of maximum compression. The accuracy of the equations has been improved and will be reported in a later paper.

In contrast with the spherically symmetric case, the energy deposition in this second problem is not spherically symmetric. It is axisymmetric, with a 30% greater temperature on the top than on the bottom. The total energy deposited is about 80 J.

The compression of the pellet is once again illustrated by the computation mesh in Fig. 12 at 5, 10, and 12×10^{-8} s. It is difficult to understand from the zone plots exactly what has happened to the innermost core, but clearly the compression at 12×10^{-8} s in Fig. 12c is much less than it was at the time of maximum compression in the symmetric case.

The dynamics in the axisymmetric case are more closely shown in Fig. 13 by the velocity vector plots at 5, 10, and 12×10^{-8} s. In Fig. 13a, at 5×10^{-8} s, the shock has arrived at a radius of 10^{-3} cm. By 10×10^{-8} s, as shown in Fig. 13b, the shock has propagated into the central zones. It is so much stronger on top than on the bottom that the flow is no longer radial. By 12×10^{-8} s, as shown in Fig. 13c, the flow is still inward on the top of the innermost ring, but it is outward on the bottom. Thus, instead of compressing the core of the pellet, the shock passes through the core from top to bottom. In addition, the center of compression seems to be slightly below the geometric center of the pellet. At least that is the conclusion one can draw from Fig. 13c, where the shock seems to be converging on a point 10^{-4} cm below the center. In fact, the entire core is displaced downward by this amount as though the stronger ablation on the top had exerted a net downward impulse. In these terms, one can now understand the distortion of the computation mesh as resulting from the displacement of the center of compression from the geometric center of the mesh.

A result of the asymmetric implosion is that the maximum compression of the core is reduced. In Fig. 14c, where density contours at 12×10^{-8} s are shown, the maximum density, corresponding to the innermost contour, is 13.2 g cm^{-3} , a factor of 2 smaller than in the symmetric case. That this maximum occurs at 12

(a)

(b)

(c)

Fig. 14. The isodensity contours at times corresponding to the mesh in Fig. 12 are shown.

(a)

(b)

(c)

Fig. 15. Contours of electron temperature at times corresponding to the mesh in Fig. 12 are plotted.

$\times 10^{-8}$ s rather than 16×10^{-8} s is a consequence of the shorter radial transit time for the stronger shock coming from the top of the pellet. Because it does not encounter an equally strong shock arriving from the bottom, the compression is not supported as long and thus the maximum density is attained sooner and is lower.

Electron temperature contours to 12×10^{-8} s are shown in Fig. 15, but the most interesting contours are at 15×10^{-8} s, which are shown in Fig. 16. In this plot, the inner contours appear to be symmetric about a center at about $Z = -1 \times 10^{-4}$ cm. At a radial distance of about 4×10^{-4} cm from this center, there is a transition region beyond which the contours appear to be concentric about the original geometric center of the pellet. One could conclude from this plot that electron thermal conduction is a symmetrizing factor in the ablation region, but, because of the inertial response of the pellet to the originally asymmetric energy deposition, the core compression is not symmetric about the original center of the pellet.

Fig. 16. Contours of constant electron temperature at 15×10^{-8} s are plotted. Note that the outer contours are symmetric about the geometric center of the pellet, and the inner contours are symmetric about the downward displaced center of the compression.

2. The Ablation of a Thin Foil. In this problem, a circular spot on each side of thin foil is illuminated by a laser. The foil is 5×10^{-5} cm thick and 0.1 cm in diameter. The energy is deposited in a spot with a Gaussian fall off in the illumination intensity from the center to the edge of the disc. The width of the Gaussian profile is 10^{-2} cm. All of the energy is assumed to be absorbed within 2.5×10^{-6} cm of the surface, but it is immediately conducted into the interior. The total energy absorbed is 10 J.

The results of the calculations are illustrated in Figs. 17-20, where the computation mesh, the electron temperature contours, the velocity vectors, and the density contours are plotted at 1, 2, and 4×10^{-6} s.

The computation mesh gives an accurate representation of the ablation of the heated foil because the top of the mesh is a Lagrangian boundary which moves with the fluid. In the first plot of the mesh at 1×10^{-6} s in Fig. 17a the expansion of the foil has begun. The radial variation of the upward displacement of the upper surface reflects the radial profile of the energy deposition in the foil. This continues to be true as the expansion progresses, for the radial displacement of the computation zones is small compared with their vertical displacement even as late as 4×10^{-6} s as shown in Fig. 17c.

A representation of the dynamics is given by the velocity vector plots in Fig. 18. In Fig. 18a, at a time corresponding to Fig. 17a, the motion is vertical. By 4×10^{-6} s, the radial component of the velocity is comparable to the vertical velocity, and so eventually there will be appreciable radial displacement of the plasma.

The reason for the essentially one-dimensional character of ablation process can be deduced from the electron temperature and mass density plots in Figs. 19 and 20. The electron temperature is nearly constant through the thickness of the foil as early as 1×10^{-6} s as shown in Fig. 19a. The temperature gradient is clearly radial with a gradient length of the order of the spot size, namely $1-2 \times 10^{-2}$ cm. On the other hand, the gradient length for the variation of the density is of the order of the thickness of the foil, which at 1×10^{-6} s appears to be about 4×10^{-3} cm. Thus, the pressure gradient in the vertical direction will be 2.5 to 5.0 times as great as in the radial direction. Not until sometime between 2 and 4×10^{-6} s is the thickness of the ablating foil as great as the radial size of the heated region. However, by this time the radial gradient is small for radial distances less than 2×10^{-2} cm, and the maximum temperature has dropped

(a)

(b)

(c)

Fig. 17. The computation mesh for the calculation of the ablation of a thin foil is plotted at 1, 2, and 4×10^{-6} s. Not only is there an axis of symmetry on the left, but the bottom of the mesh is a reflecting plane. Thus, the case corresponds to normal illumination from both sides. The kink in the top boundary at 4×10^{-6} s is due to truncation errors in the difference equations near the axis of symmetry.

(a)

(b)

(c)

Fig. 18. Velocity vectors corresponding to the mesh in Fig. 17 are plotted.

(a)

(b)

(c)

Fig. 19. Contours of electron temperature corresponding to the mesh in Fig. 17 are plotted. The minimum temperature region, in the lower left corner, is caused by the two-dimensional expansion of the foil material.

(a)

(b)

(c)

Fig. 20. Contours of constant density are plotted corresponding to the mesh in Fig. 16.

from 465 eV to 100 eV. Thus, the radial pressure gradient is much weaker than it was initially.

(Of course, if the energy were deposited continuously the radial temperature gradients would be sustained over a longer interval so that the dynamics would be quite different. It is even possible, that the ablating foil might partially shadow the cold foil beneath.)

V. CONCLUSIONS

The applications presented of the thermal conduction algorithm to computations of the coupled conduction and fluid flow encountered in laser target studies provide a practical demonstration of the usefulness of the algorithm. They also provide information useful for future evaluations of relative merits of alternative approaches to this same problem. In order to make this algorithm more useful in laser fusion applications, the laser energy deposition must be computed.

Nevertheless, continuing interest in this method is motivated by its possible application to problems associated with mass and energy loss from open ended theta pinches. For the end-loss problem, the thermal conduction coefficient is anisotropic with different values perpendicular and parallel to the magnetic field lines. Flux coordinates are useful in identifying the local field direction,^{2,14} and can be implemented within the context of the ALE method without too much difficulty. The algorithm for thermal conduction reported here can then be used to compute end loss without further modification.

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APPENDIX

A LAGRANGE MULTIPLIER ADJUSTMENT TO CONSERVE ENERGY

The Dufort-Frankel algorithm is inherently nonconservative, because the thermal gradient is computed using different time levels of the temperature on one side of a cell boundary than on the other. The algorithm can be made energy conservative by means of a Lagrange multiplier which is computed so that energy is conserved globally. A unique adjustment to the temperature at each point in the mesh is not determined uniquely by the single requirement that energy be conserved globally. Thus, some other constraint or desirable feature may be built into the prescription from which the adjustment is calculated. A prescription which minimizes the root mean square adjustment over the mesh is derived below.

Consider the sum, S , defined by

$$S \equiv \left\{ \sum_{i,j} \frac{M_1^j (n_{11}^{j+1} - \bar{n}_{11}^j)^2}{\Delta_1^j} \right\} - 2\lambda \left\{ \sum_{i,j} M_1^j n_{11}^{j+1} - n_E \right\}, \quad (61)$$

where M_i^j and $^{n+1}I_i^j$ are the mass and specific energy of cell (i,j) at the end of the complete thermal conduction process, $\tilde{I}_i^j$ is the preliminary specific energy at the end of the Dufort-Frankel calculation, nE is the total electron energy before conduction, and λ is an undetermined Lagrange multiplier. The adjustment to be made to the specific energy in cell (i,j), $^{n+1}I_i^j - I_i^j$, is weighted by the quantity Δ_i^j , defined by,

$$\Delta_i^j \equiv \left| ^{n+1}I_i^j - \tilde{I}_i^j \right| , \quad (62)$$

where $^nI_i^j$ is the specific energy of cell (i,j) before conduction occurs. The mean square adjustment to the energy, weighted by Δ_i^j , is minimized by minimizing S subject to the constraint that the electron energy be conserved. When the variation of S with respect to the adjustment in each cell is performed and the result equated to zero, the adjustment in each cell is given by an equation of the form,

$$\left(^{n+1}I_i^j - \tilde{I}_i^j \right) = \lambda \Delta_i^j . \quad (63)$$

The Lagrange multiplier is evaluated by solving an equation of constraint which is formed by summing Eq. (63) over the entire mesh,

$$\sum_{i,j} M_i^j \left(^{n+1}I_i^j - \tilde{I}_i^j \right) = \lambda \sum_{i,j} M_i^j \Delta_i^j . \quad (64)$$

This is an equation for λ in terms of the total energy at time $(n+1)\delta t$. Since the total energy can be determined from known boundary fluxes for von-Neumann problems, λ is always calculable from the equation,

$$\lambda = \frac{n+1 E - \tilde{E}}{\sum_{i,j} M_i^j \Delta_i^j} \quad (65)$$

The adjustment given by Eqs. (63) and (65) is a reasonable one in that it says that the correction to the energy at a point is to the total correction as the energy change at that point is to the total change. Unfortunately, the adjustment introduces an instability which reduces its usefulness.

This instability is illustrated for $\sigma = 10$, $c = 0.5$ in Fig. 21. The smooth curve is the theoretical curve for the traveling wave problem, the curve marked by squares is the result of a computation without adjustment to conserve the area under the curve, and the curve marked by asterisks is the result with adjustment. The feature which clearly distinguishes the adjusted curve from the others is the spatial oscillation whose wavelength is equal to $2 \times \delta x$, the mesh spacing. The relative amplitude of this oscillation, about 10%, remains constant between $t = 20$ and $t = 50$ as shown by comparing Figs. 21b and 21c. It can be shown, by a simple analysis, that the oscillation is caused by an instability for which the fastest growing mode has wavelength $2 \times \delta x$, and which nonlinearly saturates at a finite amplitude.

To understand the source of this instability, it is assumed that the amplification matrix for the Eq. (21) is known, and is given by,

$$\tilde{I}_k = \sum_{k'} A_{k'} {}^n I_{k'}, \quad (66)$$

where $\tilde{I}_k$ is the Fourier component of the solution to Eq. (26), and A_k is an eigenvalue of the difference operator. After $\tilde{I}_k$ is calculated, it is to be adjusted so that energy is conserved globally. The adjustment is obtained from Eq. (63), except that the weighting function is defined by,

$$\Delta_i^j \equiv \left({}^n I_i^j - \tilde{I}_i^j \right)^2, \quad (67)$$

(a)

(b)

(c)

Fig. 21. The effect is demonstrated of the adjustment to impose conservation of area on the numerical solution of the traveling wave problem. The unadjusted and adjusted numerical solutions, represented by the curves through the squares and asterisks, respectively, are compared with the theoretical solution, represented by the smooth curve, at 10, 20, and 47.5 problem time units in panels a, b, and c.

instead of Eq. (62) to simplify the analysis. The amplification factor for the combined time-advancement and adjustment is now obtained from the equation,

$$^{n+1}I_k = \sum_{k'} A_{k'} \cdot ^nI_{k'} + \lambda \Delta_k, \quad (68)$$

where Δ_k is the k th Fourier component of Δ_1^j . Where α_k is defined by

$$\alpha_k \equiv \tilde{I}_k - ^nI_k, \quad (69)$$

Δ_k is given by the convolution,

$$\Delta_k = \sum_{k'} \alpha_{k'} \alpha_{k-k'}. \quad (70)$$

The Lagrange multiplier is thus given by,

$$\lambda = \frac{M_0 \left(^{n+1}I_0 - \tilde{I}_0 \right)}{\sum_{k'} \sum_{k''} M_{k'} \alpha_{k''} \alpha_{-k'-k''}}; \quad (71)$$

where M_k is the Fourier component of M . A spectrum must be known for I_k to evaluate the overall amplification matrix in Eq. (68). The simplest spectrum which illustrates the properties of the scheme is one in which only one mode other than $k = 0$ is nonzero as when nI_k is given by,

$$^nI_k = I_0 \delta(k) + I_\ell \delta(k-\ell). \quad (72)$$

When M is independent of position one finds that Δ_ℓ is

$$\Delta_\ell = 2(A_0 - 1) (A_\ell - 1) n_{I_0} n_{I_\ell} , \quad (73)$$

and from this that the overall amplification factor is given by

$$A'_\ell \cong (2 - A_\ell) , \quad \text{when } I_\ell \ll I_0 . \quad (74)$$

If, instead, $I_\ell \gtrsim I_0$, the amplification factor is given by

$$A'_\ell = \left\{ A_\ell - 2 \frac{(A_0 - 1)^2}{(A_\ell - 1)^2} \frac{I_0^2}{I_\ell^2} \right\} . \quad (75)$$

When $A_\ell < 1$ so that Eq. (68) is stable, the overall scheme is unstable since $A'_\ell > 1$. Thus, I_ℓ grows each cycle until it is comparable to or greater than I_0 . At that time I_ℓ ceases to grow, for then A'_ℓ as determined from Eq. (75), is approximately equal to A_ℓ .

Since the highest modes are damped more strongly than lower ones by a diffusion equation, the highest representable mode will be the most unstable one initially. It will grow, saturate, and remain relatively constant in amplitude.

A number of modifications to the adjustment procedure have been examined to eliminate this instability, among them the imposition of additional constraints on the solution. None of them has proved satisfactory. However, acceptable results are obtained when the time step obeys the accuracy condition given previously, where acceptable means the saturation level of the instability is relatively small. One might conclude from this that the adjustment may prove the more successful the less it is needed, for when the time step satisfies the accuracy criterion, the errors in energy conservation are small.