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A Finite Difference Scheme for the Heat Conduction Equation

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A symmetrical semi-implicit (SSI) difference scheme is formulated for the heat conduction equation. The scheme is easy to code, fast and quite accurate. The advantage of the scheme appears mainly when used for large, complicated, multidimensional grids and for nonlinear problems.

1. INTRODUCTION

We use equations similar to the heat conduction equation to calulate heat transfer, radiation transfer and hydrostatical equilibrium in our stellar evolution programs. We tried various numerical schemes and found that the most convenient scheme for complicated calculations (nonlinear, multidimensional calculations) is a symmetrical semi-implicit (SSI) scheme. The (SSI) scheme is easy to code, very economical in computer time and in computer fast memory, and at the same time it is unconditionally stable and quite accurate.

2. FINITE SPATIAL DIFFERENCES

The heat conduction equation reads

$$\frac{\partial \varepsilon(x, t)}{\partial t} + \operatorname{div} j(x, t) = 0, \tag{1}$$

$j = -D(\tau) \operatorname{grad} \tau$. Here $\varepsilon(x, t)$ is the energy density distribution, τ is the temperature, D is the heat conduction coefficient, and j is the current density. A relation, often nonlinear, $\varepsilon(\tau)$ is assumed to be given.

Integrating this equation over any finite volume element, we obtain an equation of the form

$$\frac{de_i}{dt} = -J_i(e_i, e_{k'}, e_{k''}, \ldots), \qquad J_i = \sum_k J_{ik}, \tag{2}$$

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where k runs over all neighbors of cell i. Here, e_i is the energy of the volume element i and J_i is the heat flux leaving that element. The neighbors cells are enumerated by $k', k'',...$, so that J_{ik} is the heat flux flowing from cell i to neighbor cell k. Obviously one has,

$$J_{ik} = -J_{ki}. \tag{2'}$$

There exist many schemes for writing the space-difference equation (2). In the one dimensional case, J_{ik} depends usually only on the energy e_i and the energy of the neighbor e_k. In multidimensional cases, the flux J_{ik} depends on energies of several neighbors. We do not discuss here any specific space-difference scheme. We assume that the heat conduction equation for any grid has been reduced to the form (2) by differencing methods or by finite element methods.

3. Finite Time Differences

The simplest difference scheme for Eq. (2) is obviously the explicit scheme

$$\frac{e_i - \bar{e}_i}{\Delta t} = -J(\bar{e}_i, \bar{e}_{k'}, \bar{e}_{k''},...), \tag{3}$$

where e_i is the value of the energy at the end of a time step and $\bar{e}_i$ is the value at the beginning of a time step.[1] As is well known, this scheme is only conditional stable. In most practical cases the limitation on the time step size is so severe that this scheme becomes impractical.

An unconditional stable scheme (at least for the linear case) is the implicit scheme

$$\frac{e_i - \bar{e}_i}{\Delta t} = -J_i(e_i, e_{k'}, e_{k''},...). \tag{4}$$

In the nonlinear multidimensional case, this scheme is very inconvenient and expensive as one has to solve many coupled nonlinear equations.

An alternative unconditionally stable scheme is a semi-implicit scheme

$$\frac{e_i - \bar{e}_i}{\Delta t} = -J_i(e_i, \bar{e}_{k'}, \bar{e}_{k''},...). \tag{5}$$

This scheme has the advantage that we need to solve only one (nonlinear) equation with one unknown (e_i) at a time. The difficulty with this scheme is that it is not symmetrical in the variables e_i, e_k because in general $J_{ik} \neq -J_{ki}$, in contradiction with Eq. (2'). This means that if we use Eq. (5) in a straightforward way, the total

[1] The value of any variable from the end of the previous time step is designated by an overbar ($J_{ik}, \bar{e}_i, \Delta\bar{t},...$).

energy in the domain is not conserved. In some cases, one can use a semi-implicit scheme and still have energy conservation by modifying the scheme. Consider the one-dimensional case and define J_i^* as follows [1, 2]:

$$J_i^* = -J_{i-1,i}(e_{i-1}, \bar{e}_i) + J_{i,i+1}(e_i, \bar{e}_{i+1}). \tag{6}$$

As e_{i+1} does not appear in (6), we can solve the system of equations

$$\frac{e_i - \bar{e}_i}{\Delta t} = -J_i^*, \qquad i = 1,..., N \tag{7}$$

in the order $i = 1, 2,..., N$. This works very well, provided the fluxes at the end points $J_{0,1}, J_{N,N+1}$ depend only on the energies e_1 and e_N, respectively. In the case of a boundary condition $J_{N,N+1} = 0$, the last equation is explicit and the scheme is only conditionally stable. If we use Eq. (7) for all time steps, we introduce a left–right asymmetry and a truncation error of the order of $\Delta t/\Delta x^2$. The remedy, if the boundary conditions allow it, is to use the scheme (7) and its mirror-reflection on alternating time steps. Not only is the left–right asymmetry removed, but also the accuracy is improved and the truncation error becomes of the order of $(\Delta t/\Delta x)^2$.

The implementation of using different directions of calculations in alternating steps is in many cases exceedingly inconvenient. For example, take the case of a general grid of finite elements in the plane which has no rectangular order. Thus, Eq. (7) can be generalized and the semi-implicit method can be formulated for multidimensional grids but usually the asymmetry inherent in the method can not be eliminated.

We propose here a new SSI scheme which is symmetrical and unconditional stable.

First, we solve Eq. (5) for all cells. By doing this, an amount of energy

$$\delta e_{ik} = [J_{ik}(e_i, \bar{e}_k) + J_{ki}(e_k, \bar{e}_i)] \cdot \Delta t \tag{8}$$

is lost "at the interface" between cell (i) and cell (k).

This amount of energy must be replenished to the system. We chose to add δe_{ik} to cells (i) and (k) at the next time step dividing it between the two cells in proportion to their heat capacity. Thus, the equation to be solved for each cell reads as

$$\frac{e_i - \bar{e}_i}{\Delta t} = -J_i(e_i, \bar{e}_{k'}, \bar{e}_{k''},...) + q_i,$$

$$q_i = \sum_k f_{ik} \cdot \delta e_{ik}/\Delta t = \sum_k f_{ik} \cdot (\bar{J}_{ik} + \bar{J}_{ki}) \cdot \frac{\bar{\Delta t}}{\Delta t}, \tag{9}$$

$$f_{ik} + f_{ki} = 1;$$

f_{ik} is the fraction of the heat capacity of cell (i) to the sum of heat capacities of cells (i) and (k). Usually one can put $f_{ik} = \frac{1}{2}$ without loss of accuracy. We can see that (9)

is a three-steps difference scheme as values from three different time steps appears in the difference equation. In practice, one has to save only the residuals q_i when passing from one time step to the next one. It is clear that the solution of (9) is independent of the order of calculations so that no numerical asymmetry enters into the solution.

Before proceeding with a closer analysis of the SSI method a few remarks about our experience with the various methods when used in stellar-evolution calculations. In that application, both $\varepsilon(\tau)$ and $D(\tau)$ are complicated nonlinear functions. The time step in the implicit scheme is limited in practice by the nonlinear nature of the problem. The number of iterations needed to solve the coupled equations increases fast with the time step. It turned out that accuracy was never a factor in determining the time step. The experience with semi-implicit methods is essentially similar though it is much easier to solve a single (nonlinear) equation. It does not pay to use a big time step because (also in this case) the amount of work increases with the time step. In general, economy dictates a bigger time step for the semi-implicit schemes than for the completely implicit scheme. Still an "economic step" was usually enough to obtain excellent accuracy. In some cases, when we tried to use a big time step an anoying ripple developed; this was not ordinary instability in the sense that it did not grow with time.

4. Stability and Consistency of the SSI Scheme

To discuss the stability and consistency of our difference scheme we shall use the one-dimensional case with a fixed Δx, D constant, and linear relation $\tau(\varepsilon) = \varepsilon/C$.

Using upper index for enumerating time steps, one gets

$$J_j(e_j^{n+1}, e_{j+1}^n, e_{j-1}^n) = -(J_{j,j-1}^{n+1} + J_{j,j-1}^{n+1})$$

$$= -\left\{-\frac{D}{\Delta x}(\tau_{j+1}^n - \tau_j^{n+1}) + (\tau_j^{n+1} - \tau_{j-1}^n)\right\},$$

$$J_{j,j+1}^n = -\frac{D}{\Delta x}(\tau_{j+1}^{n-1} - \tau_j^n),$$

$$J_{j+1,j}^n = \frac{D}{\Delta x}(\tau_{j+1}^n - \tau_j^{n-1}),$$

$$J_{j,j-1}^n = \frac{D}{\Delta x}(\tau_j^n - \tau_{j-1}^{n-1}),$$

$$J_{j-1,j}^n = -\frac{D}{\Delta x}(\tau_j^{n-1} - \tau_{j-1}^n),$$

$$q_j = 0.5(J_{j,j+1}^n + J_{j+1,j}^n) + 0.5(J_{j,j-1}^n + J_{j-1,j}^n).$$

Using Eq. (9) and assuming that $\Delta t = \Delta \tilde{t}$, one gets after some algebra,

$$\tau_j^{n+1} - \tau_j^n = -\frac{D \cdot \Delta t}{C \cdot \Delta x^2} \left\{ 2\tau_j^{n+1} - \left(\frac{3}{2}\tau_{j+1}^n + \tau_j^n + \frac{3}{2}\tau_{j-1}^n \right) + \left(\frac{1}{2}\tau_{j+1}^{n-1} + \tau_j^{n-1} + \frac{1}{2}\tau_{j-1}^{n-1} \right) \right\}. \tag{10}$$

Inserting into (10) a solution of the form

$$\tau_j^n = A e^{pn\Delta t + iqj}, \tag{11}$$

we obtain between p and q the relation

$$\lambda - 1 = -\alpha \left\{ 2\lambda - \left(\frac{3}{2}e^{iq} + 1 + \frac{3}{2}e^{-iq} \right) + \frac{1}{\lambda}\left(\frac{1}{2}e^{iq} + 1 + \frac{1}{2}e^{-iq} \right) \right\}$$

or

$$\lambda - 1 = -\alpha \left\{ 2\lambda - (1 + 3\cos q) + \frac{1}{\lambda}(1 + \cos q) \right\} \tag{12}$$

where $\lambda = e^{p\Delta t}$; $\alpha = D \cdot \Delta t / C \cdot \Delta x^2$.

To prove the stability of the difference scheme we have to show that $|\lambda| \leqslant 1$ for any q, i.e., for any wave length $\Delta x/q$. The quadratic equation for λ can be rewritten in the form

$$\lambda^2 - (3\gamma c + 1 - 2\gamma)\lambda + \gamma c = 0, \tag{13}$$

where $c = \cos^2 q$ and $\gamma = 2\alpha/(1 + 2\alpha)$ $(0 \leqslant \gamma, c \leqslant 1)$. Denote $b = 3\gamma c + 1 - 2\gamma$ and $d = b^2 - 4\gamma c$. We can look at three cases:

Case a. $d \leqslant 0$.

Than the two roots of (13) are complex conjugates and we have

$$|\lambda_1|^2 = |\lambda_2|^2 = \lambda_1 \lambda_2 = \gamma c < 1.$$

Case b. $d \geqslant 0$ and $b < 0$, $\gamma c > 0$.

Since $d \leqslant b^2$ and $b \geqslant -1$ for all γ and c, we have

$$0 \geqslant \lambda_2 \geqslant \lambda_1 \geqslant (b - d^{1/2})/2 \geqslant b \geqslant -1.$$

Case c. $d > 0$ and $b \geqslant 0$, $\gamma c > 0$.

Then we have the inequality

$$d = (3\gamma c + 1 - 2\gamma)^2 - 4\gamma c \leqslant (3\gamma c + 1 - 2\gamma c)^2 - 4\gamma c$$
$$= (1 - \gamma c)^2,$$

so that

$$0 \cdot \leqslant \lambda_1 < \lambda_2 \leqslant \tfrac{1}{2}(3\gamma c + 1 - 2\gamma + 1 - \gamma c) = 1 + \gamma c - \gamma \leqslant 1.$$

This complete the proof.

To check the consistency of the difference scheme we calculate the truncation error. Assume $\tau(x, t)$ to be a solution of $\partial\tau/\partial t - (D/C)\,\partial^2\tau/\partial^2 x = 0$, and substitute the Taylor expansion of $\tau(x, t)$ into (10). The result is

$$\frac{1}{\Delta t}\{\tau_j^{n+1} - \tau_j^n\} + \frac{D}{c\,\Delta x^2}\left\{2\tau_j^{n+1} - \left(\frac{3}{2}\tau_{j+1}^n + \tau_j^n + \frac{3}{2}\tau_{j-1}^n\right)\right.$$
$$\left. + \left(\frac{1}{2}\tau_{j+1}^{n-1} + \tau_j^{n-1} - \frac{1}{2}\tau_{j-1}^{n-1}\right)\right\}$$
$$= O[\Delta t] + O[\Delta x^2] + O[(\Delta t/\Delta x)^2].$$

Consistency therefore requires that $\Delta t/\Delta x \to 0$ as Δx and Δt tend to zero. Theoretically the appearance of a term of order $(\Delta t/\Delta x)^2$ in the truncation error is a severe disadvantage of the scheme; for any given Δx the time step must be kept sufficiently small to maintain accuracy.

However, as mentioned above, there are practical reasons to keep the time step small enough. The "economic" time step for the implicit scheme, in which the truncation error does not contain a term of order $(\Delta t/\Delta x)^2$, is usually of the same size as the time step of the SSI scheme and even smaller.

5. Numerical Example

The one-dimensional difference scheme was tested by simulating the diffusion equation (see [2, p. 201])

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}(u^5). \tag{14}$$

The exact solution is given by an implicit equation

$$5/4(u-1)^4 + 20/3(u-1)^3 + 15(u-1)^2 + 20(u-1) + 5\,\mathrm{In}(u-1)$$
$$= v(v \cdot t - x + x_0),$$

where v and x_0 are arbitrary constants.

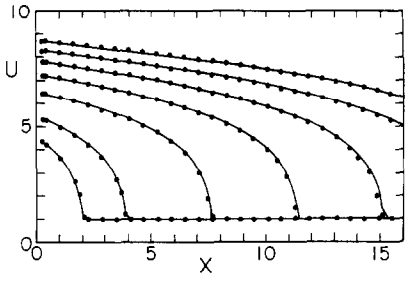

FIG. 1. Exact solution (—) versus numerical SSI solution (•) at equal time intervals; $\varepsilon_1 = 0.1$, $\varepsilon_2 = 0.01$.

The numerical simulation has been performed by imposing the exact flux on the left boundary, $x = 0$, and the exact solution (15) on the right boundary, $x = L$. Stability is proved for time steps up to steps that are 200 times bigger than the local maximal explicit time step (Fig. 3). Accuracy has been reached by limiting the time step according to two restrictions:

(1) $|e - \bar{e}|/|\bar{e}| \leqslant \varepsilon_1$,

(2) $|q|/|e| \leqslant \varepsilon_2$,

where e, $\bar{e}$, and q are defined by Eq. (9).

In Fig. 1, one can see that the numerical solution follows the exact solution almost accurately for $\varepsilon_1 = 0.1$ and $\varepsilon_2 = 0.01$. The two solutions are still in good agreement for $\varepsilon_1 = 0.1$ and $\varepsilon_2 = 0.08$ (Fig. 2). Accuracy is lost only for $\varepsilon_1 = \varepsilon_2 = 0.2$ (Fig. 3).

In the first case ($\varepsilon_2 = 0.01$), the size of the time step is on the average about 50 times greater than the maximal time step for which an explicit scheme is stable, whereas the computational time per step is almost the same. There is no need to say that for this one-dimensional test case an implicit scheme is very accurate and economic. The great advantage of the SSI scheme on an implicit scheme is seen in the two-dimensional case. For a grid with N-nodes and band width of size n, the

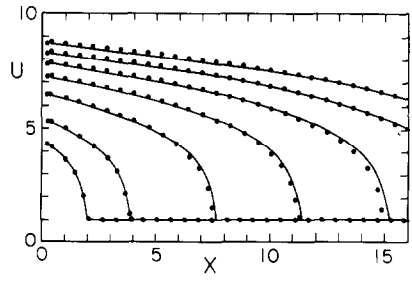

FIG. 2. Exact solution (—) versus numerical SSI solution (•) at equal time intervals; $\varepsilon_1 = 0.1$, $\varepsilon_2 = 0.08$.

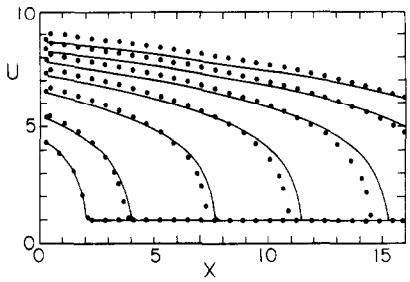

FIG. 3. Exact solution (—) versus numerical SSI solution (•) at equal time intervals; $\varepsilon_1 = 0.2$, $\varepsilon_2 = 0.2$.

cost of matrix factorization is of the order of $N \times n^2$. Iterative procedures may save some computational time but still the asymptotic cost grows like $N \times n^2$. Thus, implicit schemes may be very expensive for problems with large grids due to the factor of n^2. On the other hand using the SSI scheme one can compute the solution with quite big time steps whereas the cost grows only linearly with N.

6. SUMMARY

The SSI scheme is an efficient way to perform the time differencing in complicated large problems of heat conduction. It is unconditionally stable (in the linear case) and avoids the difficulties of large system of equations which arise by the fully implicit methods. The scheme may be used in any grid of cells and in any spatial difference method.

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