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NOTE

Time Step Size Selection for Radiation Diffusion Calculations[1]

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The purpose of this note is to describe a time step control technique as applied to radiation diffusion. Standard practice only provides a heuristic criteria related to the relative change in the dependent variables. We propose an alternative based on relatively simple physical principles. This time step control applies to methods of solution that are unconditionally stable and converges nonlinearities within a time step in the governing equations. Commonly, nonlinearities in the governing equations are evaluated using existing (old time) data. We refer to this as the semi-implicit (SI) method. When a method converges nonlinearities within a time step, the entire governing equation including all nonlinearities is self-consistently evaluated using advance time data (with appropriate time centering for accuracy).

This criteria grew out of our work using Newton–Krylov (NK) methods to solve radiation diffusion problems [2, 4]. We observed that standard time step control ideas were poorly correlated to our results with regards to efficiency and accuracy. Our results indicated that using a method that converged nonlinearities allows much larger time step sizes with acceptable accuracy.

Our governing equations are based on two temperature radiation diffusion,

$$\frac{\partial E}{\partial t} = \nabla \cdot \left(\frac{c}{3\kappa} \nabla E \right) + c\kappa (aT^4 - E) \tag{1a}$$

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and the material temperature equation

$$\frac{\partial C_v T}{\partial t} = c\kappa(E - aT^4), \tag{1b}$$

κ is the opacity, a is the Stefan–Boltzmann constant, and c is the speed of light. This can be reduced to one temperature radiation diffusion by assuming an equilibrium between the radiation and material temperatures, $E = aT^4$, and sum (1a) and (1b). The result is

$$\frac{\partial\left(aT^4 + C_v T\right)}{\partial t} = \nabla \cdot \left(\frac{c}{3\kappa}\nabla aT^4\right). \tag{2}$$

In the discussions below we will refer to (1a) and (1b) as the 2-T equations and (2) as the 1-T equation.

Time step control for (1) or (2) is traditionally based on the relative change in the dependent variables [1] when applied to problems which do not converge nonlinearities. Here, this is applied in the fashion

$$\eta = \frac{\left|E_j^n - E_j^{n-1}\right|}{E_j^n + E_{\text{floor}}},$$

where n is the time index, j is the space index, and E_{floor} is a prescribed constant usually set equal to a multiple of the lower bound for the energy in a given problem. The new time step size is then computed using

$$\Delta t_{\text{new}} = \Delta t_{\text{old}}\left(\frac{\eta_{\text{target}}}{\max_j \eta}\right)^{0.5},$$

in an attempt to smoothly approach η_{target}. The general thinking is that if the relative change in energy is kept small the linearization of the governing equations does not introduce significant errors and that the nonlinearities do not need to be converged. This quantity is typically chosen between 0.05 to 0.20.

We propose to use a criteria based on an estimate of the nonlinear wave speed present in the solution to be used. In one dimension this involves computing the ratio of temporal to spatial derivatives of the dependent variable(s). In principle, we are assuming that the hyperbolic PDE,

$$\frac{\partial E}{\partial t} + v_{\text{rad}}\frac{\partial E}{\partial x} = 0, \tag{3}$$

models the problem. This result is consistent with the construction of traveling wave similarity solutions. One generally assumes that the solution has the form $E(x - vt)$; upon such an assumption similarity forms for the Marshak wave are derived [6, 3]. Rearranging (3) gives the expression

$$v_{\text{rad}} = -\frac{\partial E/\partial t}{\partial E/\partial x}. \tag{4}$$

To avoid problems from lack of smoothness we compute this in a L_1 sense,

$$v_{\text{rad}} = \frac{\sum\left(\left|E_j^n - E_j^{n-1}\right|/\Delta t\right)}{(1/2)\sum\left(\left|E_{j+1}^n - E_{j-1}^n\right|/\Delta x\right)}.$$

With this estimate in hand, a Courant–Friedrichs–Lewy (CFL) condition can be used to provide a time step size,

$$\Delta t = \frac{C\|\Delta x\|}{v_{\text{rad}}}, \tag{5}$$

where $\|\Delta x\|$ uses the same norm as above (L_1). This can be simplified to

$$\Delta t_{\text{solution}} = \frac{(1/2)\sum \left|E_{j+1}^n - E_{j-1}^n\right|}{\sum\left(\left|E_j^n - E_j^{n-1}\right|/\Delta t\right)}. \tag{6}$$

In more than one dimension one can sum the spatial derivative to similar effect.

This will provide a time step commensurate with the dominant time scale in the problem. By using a L_1 norm in this estimate, the computed value will be smoothed and will provide an average of the dominant nonlinear time scale in a solution. Note that if the problem does not have any nonlinearity this estimate will reduce to an average of the explicit diffusion based time step limit over the grid. This can be demonstrated by substituting a linear diffusion equation into (4) and using the linearity to simplify (5) to

$$\Delta t = \frac{C\Delta x^2}{D},$$

where D is the linear diffusion coefficient. The result in (4) coincides with these results. Furthermore, as we show the results coincide with our observations regarding the accuracy and efficiency of solutions using NK methods for solving these equations.

We show three examples in support of our proposed time step control. In one dimension we will show the ability for a NK method to provide accurate, efficient solutions should the time step be selected by a Courant number defined by v_{rad} in (4). Our problems are selected from [4] for the 1-T equations and from [2] for the 2-T equations.

Previously, we have shown that through converging nonlinearities one can achieve higher order accuracy in radiation diffusion [4, 2]. Specifically, we have demonstrated nearly second-order (certainly super-linear) convergence on flux-limited radiation diffusion problems. This holds the promise of keeping the error from the solution fixed while taking significantly larger time steps. As the relative energy change criteria becomes larger it is no longer linearly related to the time step size. The Courant number requirement is linearly related to the time step size.

Specifically, we have run the earlier one dimensional, one temperature radiation diffusion benchmark [4], where a nonlinear flux-limited diffusion coefficient is used. The second-order method demonstrates a 1.70 convergence rate over the entire range of time step sizes investigated ($\Delta t = 1 \times 10^{-3}$ to $\Delta t = 0.5$) which corresponds to a CFL number range of 0.004–2, or a relative energy change range of 1.5–90%. It is notable that the method is stable, convergent, and efficient to much larger time step sizes (corresponding to a CFL number of 8). Present accepted practice would consider a 5% relative energy change a tight restriction in time step size selection. For the second-order (implicit midpoint) nonlinear integration method this corresponds to the error created by setting the CFL number to approximately 1/2. This would provide a solution of comparable quality with time step size nearly 70 times larger.

For a multidimensional implementation this provides a substantial savings. Using the method described in [4] we investigate the improvement in raw performance given by

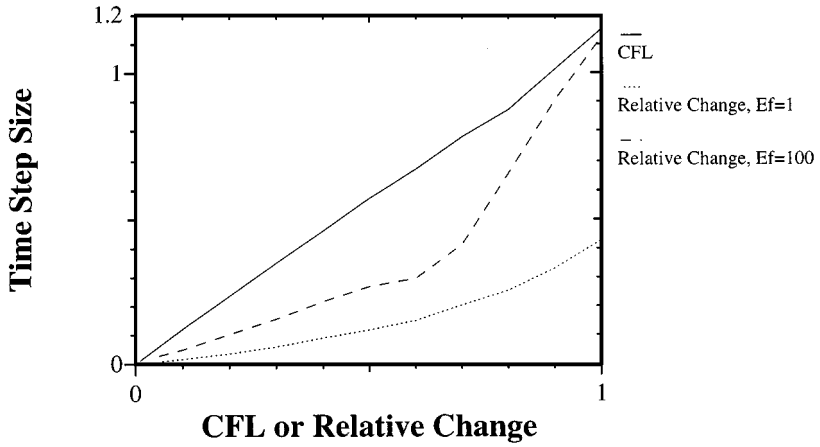

FIG. 1. The relation between the estimated Marshak wave CFL time step size and the time step size for a relative energy change based time step size control. Two floor energies are shown to demonstrate the effect of this modification in the relative energy change time step control.

the above described time step size criteria. We solve a multi-material problem with four distinct regions of differing mass number with an imposed radiation flux at one boundary. The Newton–Krylov (second-order, NK2) method uses an FGMRES algorithm [5] with a V-cycle multigrid preconditioner and the implicit midpoint rule time differencing. The nonlinear residual is converged to at least 1×10^{-4} with the ratio of linear to nonlinear residual kept at 1×10^{-2}. The linearized (semi-implicit, SI) method uses identical spatial differencing to the nonlinearly converged method except that the coefficients are linearized to old time values and the time differencing is backwards Euler. The linear convergence tolerance requires that the residual be converged below 1×10^{-6} using a multigrid V-cycle preconditioned conjugate gradient algorithm as a linear equation solver.

On a 64×64 grid, the NK2 method requires 50 times fewer time steps using a Courant number of $\frac{1}{2}$ as compared with the SI method using a relative energy change of 5%. For comparison, the differences between a CFL-based time step size and one based on relative energy change is shown in Fig. 1. While the CFL-based control retains a linear relation to time step size, the relative energy change based control has an exponential behavior with respect to time step size. In terms of overall use of CPU time, the NK2 method is 2.48 times faster using a CFL number of 0.25. A superiority in efficiency holds for time step sizes selected as low as a CFL number of 0.02. This reflects the complexity of Newton iteration as compared with the SI method.

On the other hand, if the time step size criteria imposed by the relative energy change limits the overall code, all other physics can be computed with a much larger time step size (assuming stability and accuracy in each case). Additionally, we demonstrated that NK2 method achieves better scaling with problem size than the SI scheme [4]. Thus, the disparity between the SI and NK methods will grow as the problem size is increased. On a 128×128 grid the ratio grows to 2.94 and on a 256×256 grid the ratio is 3.11.

The small time step size used in the SI method allows one to consider a simpler linear algebra solution. Using diagonally scaled conjugate gradient on the 64×64 grid yields savings over the multigrid solver, where it is 3.2 times faster. The poor scaling properties of the diagonal scaling preconditioner cause it to be 1.15 times slower than the multigrid

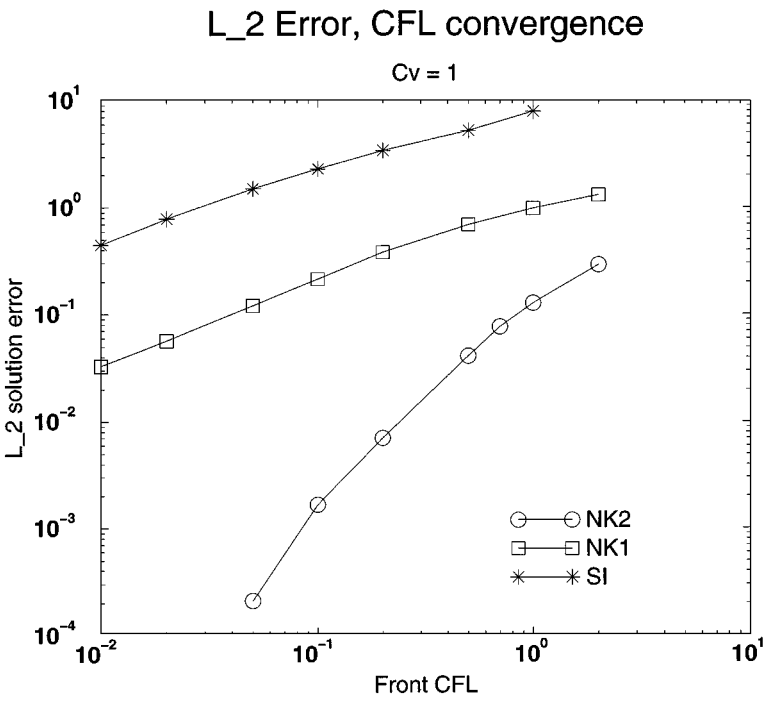

FIG. 2. A comparison of the L_2 norm of error as a function of the front CFL number and the various methods discussed in the text.

on the 256×256 grid and thus 3.58 times slower than the NK2 solver for a fixed level of solution accuracy.

Finally, we include results from a 2-T nonequilibrium model in one dimension from [2]. Here we use block symmetric Gauss–Seidel as the preconditioner with GMRES for the SI method and Newton–GMRES for the NK method. The linear and nonlinear convergence tolerances are the same as with the 1-T problems. The first model problem from [2] is run out to a time of 3 on a grid of 200 cells. The front CFL method is used to control the time step and a time step convergence is performed against the NK2 method with a time step of $\mathrm{CFL} = 10^{-3}$. We can see that NK2, $\mathrm{CFL} = 2.0$ is more accurate than SI, $\mathrm{CFL} = 0.01$. The relative energy error for SI, $\mathrm{CFL} = 0.01$, was 5 percent. First-order Newton–Krylov (NK1) achieves this same accuracy for $\mathrm{CFL} = 0.2$. In relative CPU performance NK1 is 4.16 times as fast as SI and NK2 is 7.25 times faster than SI all at the same accuracy. Figure 2 shows the accuracy of each of these methods as function of the computed front CFL number.

In summary, we have provided a physically motivated method to compute the size of the time step for the calculation of nonlinear diffusion phenomena. The overall consensus of our results seems to indicate that the use of second-order time differencing in conjunction with a NK method can yield high quality results with reduced cost if the CFL number is chosen in the range of 0.10–0.50.

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