Newton-Krylov Methods Applied to Nonequilibrium Radiation Diffusion

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March 13, 1998

1 Introduction

Radiation transport in astrophysical phenomena and inertial confinement fusion is often modeled using a diffusion approximation. When the radiation field is not in thermodynamic equilibrium with the material then a coupled set of time dependent reaction diffusion equations is used to simulate energy transport [1]. These equations are highly nonlinear and exhibit multiple time and space scales. Implicit integration methods are desired to overcome undesirable time step restrictions. Traditionally, the coupling of these systems has been handled via operator splitting, and the nonlinearities are seldom iterated on within a time step [1]. Both of these choices impose "effective" time step size restrictions for accuracy and nonlinear stability. Additionally, the nonlinear residual of the system is not formed, and thus it can not be used to monitor convergence within a time step.

We present results of applying a matrix-free Newton-Krylov method [2, 3] to a nonequilibrium radiation diffusion problem. Here, there is no use of operator splitting, and Newton's method is used to converged the nonlinearities within a time step. Since the nonlinear residual is formed, it is used to monitor convergence. It is demonstrated that a simple Picard-type linearization produces a sufficient preconditioning matrix for the Krylov method, thus eliminating the need to form or store a Jacobian matrix for Newton's method [4]. We discuss the possibility that the Newton-Krylov approach may allow

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larger time steps, with out loss of accuracy, as compared to an operator split approach where nonlinearities are not converged within a time step.

2 Physics Model

Ignoring hydrodynamics and thermal conduction and working in one dimension results in the following coupled system for radiation energy, E, and material temperature, T.
Radiation diffusion (grey approximation):

$$\frac{\partial E}{\partial t} - \frac{\partial}{\partial x}(cD_r \frac{\partial E}{\partial x}) = c\sigma_a(aT^4 - E) \tag{1}$$

Material energy balance:

$$C_v \frac{\partial T}{\partial t} = -c\sigma_a(aT^4 - E) \tag{2}$$

Here C_v is the material specific heat, c is the speed of light, a is the radiation constant, and σ_a is the photon absorption cross-section. In thermal equilibrium we have $E = aT^4$, and for the nonequilibrium case one can define a radiation temperature as, $T_r = (E/a)^{0.25}$. For simplicity, and to be consistent with the previous model problems of [5, 6] we will work in an arbitrary system of units where $C_v = c = a = 1.0$. We will also chose $\sigma_a = 1.0$ or $\sigma_a = T^{-3}$. From simple isotropic diffusion theory [1] we have the following form for the radiation diffusion coefficient,

$$D_r = \frac{1}{3\sigma_a}. \tag{3}$$

However, in regions of strong gradients simple diffusion theory can fail, resulting in a flux of energy moving faster than the speed of light. To prevent this artificial behavior the diffusion coefficient is augmented in the following heuristic fashion, referred to as flux limiting [1],

$$D_r = \frac{1}{(3\sigma_a + \frac{1}{E}\frac{\partial E}{\partial x})}. \tag{4}$$

Here, in the case of strong gradients in the radiation energy field the radiation energy flux is given by;

$$F = -cD_r \frac{\partial E}{\partial x} = cE, \tag{5}$$

which is the proper physical limit.

The model problem considered in this study is taken from [6] and consists of a unit radiation flux impinging on an initially cold slab of unit depth. This results in mixed, or Robin, boundary conditions at $L = 0$ and $L = 1$. Following [5], at $L = 0$ we use

$$\frac{1}{4}E - \frac{1}{6\sigma_a}\frac{\partial E}{\partial x} = 1, \tag{6}$$

and at $L = 1$ we use,

$$\frac{1}{4}E + \frac{1}{6\sigma_a}\frac{\partial E}{\partial x} = 0. \tag{7}$$

3 Time Integration and Nonlinear Iteration

We will use second order finite volumes to discretize the diffusion operator in the radiation diffusion equation on a uniform grid. The diffusion coefficient, D_r, is evaluated at cell faces by linearly interpolating T and E to cell faces and then evaluating D_r. Although this problem is very straightforward to solve we will use is to make quantitative comparisons between three implicit time integration methods. The first method is an operator split method where the diffusion term and the reaction term in the radiation equation are solved in 2 split steps. The reaction term here is solved coupled to the material energy equation in order to conserve energy. The second method is a fully coupled, linearized, semi-implicit technique which does not converged nonlinearities. By this we mean that D_r and σ_a are evaluated at previous time step solutions, and T^4 is linearized, such that we have a linear problem at each time step. The third method will be a matrix-free Newton-Krylov method [2, 3]. Here the nonlinearities will be converged at each time step, and we will consider a second order accurate time step. All linear systems are solved with a preconditioned GMRES [7] solver.

3.1 Operator Split Method (OS)

Here we split the solution of the radiation diffusion equation into its diffusion term and its reaction term. This is certainly not necessary for this problem, and in fact the discretized ODE for the material energy can be substituted directly into the descretized PDE for radiation energy. However for comparison we apply a splitting approach which might be considered typical when the material energy balance is a PDE (i.e. thermal conduction included). The reaction term is fully coupled to the material energy balance in order to conserve energy. n is the time level.

$$\frac{E^* - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^k \frac{\partial E^*}{\partial x}) = 0 \tag{8}$$

$$\frac{E^{n+1} - E^*}{\Delta t} = \sigma_a^n (T^{n+1}(T^n)^3 - E^{n+1}) \tag{9}$$

$$\frac{T^{n+1} - T^n}{\Delta t} = -\sigma_a^n (T^{n+1}(T^n)^3 - E^{n+1}) \tag{10}$$

We have been forced to define an intermediate variable, E^*, and the diffusion and reaction terms of the radiation diffusion equation are not evaluated with the same E field. The primary advantage here is the reduction in the size of the linear system to solve.

3.2 Coupled, Semi-Implicit, Method (SI)

Since there is no nonlinear iteration in this method, again we only require a time step index, n. Our system of equations becomes,

$$\frac{E^{n+1} - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^n \frac{\partial E^{n+1}}{\partial x}) = \sigma_a^n (T^{n+1}(T^n)^3 - E^{n+1}) \tag{11}$$

$$\frac{T^{n+1} - T^n}{\Delta t} = -\sigma_a^n (T^{n+1}(T^n)^3 - E^{n+1}) \tag{12}$$

As compared to the operator split method we have removed the temporary radiation energy variable E^* and thus the diffusion operator and the reaction term in the radiation energy equation are evaluated with the same E field. The cost for this has been solving a matrix equation with twice as many variables per grid cell. Still the nonlinearities are not converged within a time step.

3.3 Fully Implicit Newton Krylov Method (NK)

In this method we converge the nonlinearities within a time step thus we need both a time step index, n, and a nonlinear iteration (Newton) index, k. The first order accurate time integration method (NK1) is;

$$\frac{E^{n+1,k} - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^{n+1,k}\frac{\partial E^{n+1,k}}{\partial x}) = \sigma_a^{n+1,k}((T^{n+1,k})^4 - E^{n+1,k}) \quad (13)$$

$$\frac{T^{n+1,k} - T^n}{\Delta t} = -\sigma_a^{n+1,k}((T^{n+1,k})^4 - E^{n+1,k}) \quad (14)$$

The second order accurate time integration method (NK2) is;

$$\frac{E^{n+1,k} - E^n}{\Delta t} - \frac{1}{2}\frac{\partial}{\partial x}(D_r^{n+1,k}\frac{\partial E^{n+1,k}}{\partial x}) - \frac{1}{2}\frac{\partial}{\partial x}(D_r^n\frac{\partial E^n}{\partial x})$$
$$= \frac{1}{2}\sigma_a^{n+1,k}((T^{n+1,k})^4 - E^{n+1,k}) + \frac{1}{2}\sigma_a^n((T^n)^4 - E^n) \quad (15)$$

$$\frac{T^{n+1,k} - T^n}{\Delta t} = -\frac{1}{2}\sigma_a^{n+1,k}((T^{n+1,k})^4 - E^{n+1,k}) - \frac{1}{2}\sigma_a^n((T^n)^4 - E^n) \quad (16)$$

The nonlinear iteration is implemented with an inexact, Matrix-Free Newton-Krylov method. By inexact Newton we mean that the convergence tolerance of the linear solver (GMRES) is proportional to the current nonlinear residual. By matrix-free Newton-Krylov we mean that the required Jacobian-vector product in each GMRES iteration is replaced by a finite difference approximation to the true Jacobian-vector product [2]. Nonlinear convergence is declared when the residuals of the above discretized equations fall below a prescribed tolerance level.

While the matrix equation for the semi-implicit method is easy to form, the matrix equation for Newton's method may not be easy to form. Therefore we use the matrix resulting from the semi-implicit method linearization to precondition the Newton-Krylov method, and thus completely avoid the complexity of evaluating the true Jacobian [8] of the system. We refer to this as an implicit Picard linearization preconditioning Newton's method [4]. It should be emphasized that the effect of the true Jacobian of the system is felt in the Jacobian-vector product of GMRES.

4 Some Initial Results

First we compare results from the semi-implicit (SI) method and the Newton-Krylov (NK) method. For this problem we have a unit flux of radiation energy impinging on the left side (L=0) of a cold slab of unit width (L=1). 200 uniform finite volumes are use to discretize the problem in space. The initial conditions are $E^0 = 1.0 \times 10^{-5}$ and $T^0 = (E^0)^{0.25}$. We use $\sigma_a = T^{-3}$, and D_r is flux-limited. The problem is run out to time $t = 3.0$. We ramp our time step up through the first 8 time steps in a pre-defined fashion. The first time step is always equal to 0.1 times the final time step and the first 8 time steps are equal to 2 final time steps.

As a first, rough, measure of accuracy we define the front position as the center of the first cell to drop below $T_r = E^{0.25} = 0.1$. Here we define the second order NK method with a time step of 1.0e-3 as exact and measure the deviation of the other runs from this. For this "exact" solution the front position was x = 0.8325. The results in the table below indicate that there is a reduction in total linear solves to be had by converging the nonlinearities within a time step. This was accomplished by running the simulation at a larger time step, while maintaining accuracy through converging the nonlinearities. It should be noted that in practice, methods which do not converge nonlinearities within a time step monitor, and control, time step size by looking at maximum relative changes in E. In our results to date we have used a constant time step.

Additionally we plan to present results in the operator split algorithm, present results for the above problem at an earlier time, and analyze the accuracy with additional diagnostics. More detail will also be given on this specific problem and boundary conditions, including plots of physical results. We will make similar comparisons without flux-limiting and with a constant $\sigma_a = 1.0$.

5 Acknowledgments

This work was supported under the auspices of the U.S. Department of Energy under DOE contract W-7405-ENG-36 at Los Alamos National Laboratory.

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Table 1: Algorithm performance as a function of time step

Method and Time step	Number of time steps	Number of Nonlinear Its. per time step	Total Linear Solves	Front Position Error (Perct.)
NK2, dt=1.0e-3	3006	2	6012	0.0
NK2, dt=3.0e-2	106	6.5	689	0.6
NK1, dt=5.0e-3	606	3	1818	0.6
NK1, dt=3.0e-2	106	6.5	689	3.0
SI, dt=5.0e-4	6006	1	6006	1.2
SI, dt=5.0e-3	606	1	606	12.5
SI, dt=3.0e-2	106	1	106	40.0