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Title: NEWTON-KRYLOV METHODS APPLIED TO NONEQUILIBRIUM RADIATION DIFFUSION

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Newton-Krylov Methods Applied to Nonequilibrium Radiation Diffusion

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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 dependant 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 unwanted 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 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-based linearization produces a sufficient preconditioning matrix for the Krylov method, thus elevating the need to form or store a Jacobian matrix for Newton's method. We discuss the possibility that the Newton-Krylov approach may allow larger time steps, with out loss of accuracy, as compared to an operator split approach where nonlinearities are not converged within a time step.

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2 Physics Model

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:

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

For simplicity, and to be consistent with the previous model problems of [4, 5] we will work in an arbatray 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 coefficent is augmented in the following fashion [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 [5] and consists of a unit radiation flux impinging on an initicially cold slab of unit depth. This results in mixed, or Robin, bondary conditions at $L = 0$ and $L = 1$.

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 coeifficient , 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 straight forward to solve we will use is to make quantitative comparisions 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 eqation 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, linerized, semi-implcit technique which does not converged nonlinearities. By this we mean that D_r and σ_a are evaluated ate 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.

3.1 Operator Split Method

Here we split the solution of the radiation diffusion eqation into it diffusion term and its reaction term. The reaction term is fully coupled to the material energy balance in order to conserve energy.

$$\frac{E^* - E^k}{\Delta t} - \frac{\partial}{\partial x}(cD_r^k \frac{\partial E^*}{\partial x}) = 0 \tag{6}$$

$$\frac{E^{k+1} - E^*}{\Delta t} = \sigma_a^k (T^{k+1}(T^k)^3 - E^{k+1}) \tag{7}$$

$$\frac{T^{k+1} - T^k}{\Delta t} = -\sigma_a^k (T^{k+1}(T^k)^3 - E^{k+1}) \tag{8}$$

We have been forced to define an intermediate variable, E^*, and the diffusuin and reaction terms of the radiation diffusion eqation are not evaluated with the same E field.

3.2 Coupled, Semi-Implicit, Method

Since this is no nonlinear iteration in this method we only require a time step index, k. Our system of eqations becomes,

$$\frac{E^{k+1} - E^k}{\Delta t} - \frac{\partial}{\partial x}(cD_r^k \frac{\partial E^{k+1}}{\partial x}) = \sigma_a^k (T^{k+1}(T^k)^3 - E^{k+1}) \tag{9}$$

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

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 equationare 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

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

$$\frac{E^{k+1,n}-E^{k}}{\Delta t}-\frac{\partial}{\partial x}(cD_r^{k+1,n}\frac{\partial E^{k+1,n}}{\partial x})=\sigma_a^{k+1,n}((T^{k+1,n})^4-E^{k+1,n}) \quad (11)$$

$$\frac{T^{k+1,n}-T^{k}}{\Delta t}=-\sigma_a^{k+1,n}((T^{k+1,n})^4-E^{k+1,n}) \quad (12)$$

The second order accurate time integration method is;

$$\frac{E^{k+1,n}-E^{k}}{\Delta t}-\frac{\partial}{\partial x}(cD_r^{k+1/2,n}\frac{\partial E^{k+1/2,n}}{\partial x})=\sigma_a^{k+1/2,n}((T^{k+1/2,n})^4-E^{k+1/2,n}) \quad (13)$$

$$\frac{T^{k+1,n}-T^{k}}{\Delta t}=-\sigma_a^{k+1/2,n}((T^{k+1/2,n})^4-E^{k+1/1,n}) \quad (14)$$

The nonlinear iteration is implimented with and Inexact, Matrix-Free Newton-Krylov method. Convergence is declared when the residuals of the above discretized equations fall below a perscribed tolerence 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. We use the semi-implicit method to precondition a matrix-free Newton-Krylov method, and thus completeley avoid the complexity of evaluating the true Jacobian [6] of the system.

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 enrgy 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 flux-limiting is used. 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.

Additionally we plan to present resutls 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 comparisions without flux-limiting and with a constant $\sigma_a = 1.0$.

Table 1: Algorithm performance as a function of time step

Method and Time step	Number of time steps	Number of Nonliner 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

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References

[1] Richard L. Bowers and James R. Wilson. *Numerical Modeling in Applied Physics and Astrophysics.* Jones and Bartlett, Boston, 1991.

[2] P. N. Brown and Y. Saad. Hybrid Krylov methods for nonlinear systems of equations. *SIAM J. Sci. Stat. Comput.*, 11:450–481, 1990.

[3] D.A. Knoll and P.R. McHugh. Enhanced nonlinear iterative techniques applied to a nonequilibrium plasma flow. *SIAM J. Sci. Comput.*, 19(1), to appear,1998.

[4] R.H. Szilard and G.C. Pomraning. Numerical transport and diffusion methods in radiative transfer. *Nucl. Sci. Eng.*, 12:256, 1992.

[5] M. D'Amico and G.C. Pomraning. Treatment of nonlinearities in flux-limited diffusion calculations. *J. Quant. Spectrosc. Radiat. Transfer*, 49:457, 1993.

[6] M. D'Amico. A Newton-Raphson approach for nonlinear diffusion equations in radiation hydrodynamics. *J. Quant. Spectrosc. Radiat. Transfer*, 54:655, 1995.