A Multigrid Newton-Krylov Method for Flux-Limited Radiation Diffusion *

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Abstract

We focus on the implicit integration of radiation diffusion including flux-limited diffusion coefficients. The nonlinear integration is accomplished with a Newton-Krylov method. Preconditioning is achieved with a multigrid method on a Picard-type linearization of the governing equations. We investigate the efficiency of the linear and nonlinear iterative techniques.

1 Overview and Motivation

Radiation diffusion is a highly nonlinear phenomena. Despite this the integration of the governing equation numerically is typically accomplished with linearized PDEs where no attempt is made to converge the nonlinearities [1]. In addition to the simplicity of this approach there is a perception that effectively dealing with the nonlinearities with Newton's method is intractable. Even with methods which deal with some of the nonlinearities, there the often applied flux-limiters [1] are still dealt in a linearized fashion.

Radiation diffusion can be posed in many guises. For instance, both the material temperature and the radiation energy density can be considered as unknowns (the 2-T approximation considered elsewhere at this meeting [4]).

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Here, we focus on the simpler setting where the material temperature is in equilibrium with the radiation energy density and the governing equation is

$$\frac{\partial E}{\partial t} = \nabla \cdot D\left(E\right) \nabla E \, , \tag{1}$$

with E being the radiation energy density. and D is diffusion coefficient which is generally a nonlinear function of E [9, 5]. Additionally we have used a grey approximation where the energy density has been integrated in frequency. The energy dependence of D is found through the dependence of the opacity of the medium, $D = c/3\sigma$, as a function of temperature. In thermal equilibrium and with the speed of light, c, set to unity, we have $E = T^4$. A common form for the temperature dependence of the opacity is $\sigma \propto 1/T^3 \rightarrow D \propto T^3$.

Flux-limited diffusion was introduced to prevent transport faster than the maximum speed in the medium (the speed of light here). With flux-limited diffusion coefficients, the functional form of D will include the gradient of the energy density. The earliest form is due to Wilson [1] and contains the correct asymptotic behavior. Therefore as the gradients become small diffusion is recovered, while steep gradients recover the transport form of the equation. Wilson's form is

$$\mathbf{D}_L = \frac{1}{\frac{1}{\mathbf{D}(T)} + \frac{|\nabla E|}{E}} . \tag{2}$$

Further complications are imposed by multimaterial problems where the opacity is a function of the atomic (Z) number of the medium. This issue was addressed in a non-flux limited context in our earlier paper [7] where the multigrid preconditioning was shown to be quite effective. Below, we discuss our nonlinear integration technique and the multigrid/Picard-type preconditioning. Lastly, we show results that indicate that flux limited diffusion poses no significant new challenges to our methodology.

2 Multigrid Newton-Krylov Methods

We build upon our earlier efforts to combine multigrid as a preconditioner for Newton-Krylov methods [3]. Our goal is to execute an inexact Newton iteration within a time step. In order to calculate the updates to the dependent variables by approximately solving,

$$J\left(\mathbf{E}^k\right) \delta\mathbf{E} = -F\left(\mathbf{E}^k\right) , \tag{3}$$

where k is the iteration index and

$$\mathbf{E}^{k+1} = \mathbf{E}^{k} + \alpha\delta\mathbf{E} \tag{4}$$

to solve $F(\mathbf{E}) = 0$, here,

$$F(E) = \frac{\partial E}{\partial t} - \nabla \cdot D(E) \nabla E \, .$$

The under-relaxation factor α is defined by $\alpha = \min(1, 1/\|\delta E/E\|)$. We can do this in a matrix-free manner [2] without forming the full Jacobian via a finite difference approximation,

$$J\mathbf{v} \approx \frac{F(\mathbf{E} + \epsilon\mathbf{v}) - F(\mathbf{E})}{\epsilon} \tag{5}$$

where $\mathbf{v}$ is a Krylov vector and $\epsilon = \rho(1 + \|\mathbf{E}\|)$ and $\rho = 10^{-9}$ here.

The properties of GMRES make it advantageous for use as the Krylov method here (conversely the properties of other methods such as CGS, BiCGStab, and other similar methods are problematic). Additionally, GMRES has the property of finite termination and is more robust as a consequence. This is offset to some degree by the increased storage and work requirements imposed by GMRES. As noted before preconditioning the linear problem is essential for efficiency. Standard ILU(n) preconditioning becomes less efficient as the problem size grows and the corresponding growth in the number of GMRES iterations creates storage (and work) needs that limit problem size. We will employ a multigrid algorithm developed below to overcome this difficulty.

Our multigrid method was developed to both be simple, but robust for multimaterial problems [8, 6]. In keeping with these principles, we use simple piecewise constant interlevel transfer operators. Coarse grid equations are found through using control volume concepts to compute effective coarse grid diffusion coefficients from the previous fine grid. While this multigrid is simple its saving grace is that it is used to precondition a Krylov method. Previously, we have highlighted the degree to which the Krylov method returns this method to suitable robustness and scalability under the most severe circumstances.

Perhaps one of the most important, but subtle aspects of our method is the nonlinear preconditioning. It is this traditional linearization which, if applied iteratively to the same time step, constitutes a Picard-type nonlinear solver that forms the basis of the nonlinear preconditioning. The time differencing of this solver is

$$\frac{E^{n+1}+E^{n}}{\Delta t}=\nabla\cdot D\left(E^{n}\right)\nabla E^{n+1}\,, \tag{6}$$

where n is the time level index iteratively it takes the form

$$\frac{E^{n+1,k+1}+E^{n}}{\Delta t}=\nabla\cdot D\left(E^{n+1,k}\right)\nabla E^{n+1,k+1}\,, \tag{7}$$

again k is the iteration index. In other words, a convergent nonlinear Picard-type iteration preconditions Newton's method, which takes the finite difference form,

$$\frac{E^{n+1,k+1}+E^{n}}{\Delta t}=\nabla\cdot D\left(E^{n+1,k+1}\right)\nabla E^{n+1,k+1}\,. \tag{8}$$

Another way to look at the process is that the Newton-Krylov method accelerates the convergence of the multigrid Picard-type solver.

3 Results

Our principle objective in this paper is to describe how our approach handles the complication posed by flux-limited diffusion coefficients. This additional nonlinearity changes the character of both the linear and nonlinear iteration. Below, we address each issue separately. In keeping with our previous results, all of our results will use multigrid to precondition the Krylov method.

For a sample problem we compute the propagation of a Marshak wave [5, 9] through a multimaterial medium where two materials are present one with a mass number ten times the other. This provides the problem with a challenging multidimensional nature. A flux boundary condition is applied to the domain which is initialized to a uniform temperature. The asymptotic state of the boundary is a temperature ten times as large as the initial temperature. The small time step corresponds to a time step size of approximately 100 times the explicit stability limit while the large time step size is approximately 1000 times that limit.

First, we investigate the issue of multigrid/Krylov iterations (there is one V-cycle per Krylov iteration) where the time step size is relatively small (imbuing the linear problem with greater stability). This will provide evidence of the algorithm's behavior in a relatively benign case. As shown in Table 1 the efficiency of the multigrid-Krylov algorithm is quite good in all

Table 1: Average number of multigrid/Krylov iterations as a function of grid size and diffusion coefficient form. The time step size is small. Note that the notation D_L means the diffusion coefficient has been flux limited.

Grid	$D \propto T^0$	$D \propto T^3$	$D_L \propto T^0$	$D_L \propto T^3$
32^2	2.0	3.8	2.0	3.9
64^2	2.0	3.2	2.0	4.1
128^2	2.0	2.9	2.0	4.3
256^2	2.0	2.9	2.0	4.0
512^2	2.0	2.9	2.0	3.2

cases. The method exhibits rough linear scalability with modest sensitivity to the increasing nonlinearity of the diffusion coefficient.

Now the time step size will be much larger with the linear system more closely approximating a singular problem. Here again the scaling is roughly linear although the nonlinearity in both the temperature dependence and the flux limiting is more damaging to the performance of the algorithm. At worst the method becomes approximately two and half times as expensive per time step (which is amortized by the ten times larger time step size).

Next, the nonlinear iterative process is examined for both the flux-limited and non-flux-limited diffusion coefficients. When the diffusion coefficients are not flux-limited, the Picard-type solver is quite competitive, providing fewer linear iterations, but more nonlinear iterations as Table 3 shows. This is evidence of the modest nonlinearity associated with this problem, the diffusion coefficient has a nonlinear power of 3/4. When Wilson's flux-limiter is applied to the diffusion coefficients, Newton's method is far superior providing a significant advantage over the Picard-type method in both linear and nonlinear iterations. Furthermore, the difference between these methods grows as the grid is refined (holding Δt roughly constant).

3.1 Closing Remarks

We have demonstrated that the overall algorithm we propose while effected by the presence of flux limited diffusion is nevertheless robust. The

Table 2: Average number of multigrid/Krylov iterations as a function of grid size and diffusion coefficient form. The time step size is large.

Grid	$D \propto T^0$	$D \propto T^3$	$D_L \propto T^0$	$D_L \propto T^3$
32^2	4.3	5.6	5.0	11.5
64^2	4.0	4.9	5.8	11.0
128^2	4.0	4.8	5.8	10.9
256^2	4.0	4.8	5.8	11.4
512^2	4.0	4.0	5.8	12.9

Table 3: Average number of nonlinear/linear iterations for the nonlinear iterative techniques using the Picard-type and Newton methods. Non-flux-limited and Wilson's flux limiter are used.

Grid	Picard $D \propto T^3$	Picard $D_L \propto T^3$	Newton $D \propto T^3$	Newton $D_L \propto T^3$
32^2	5.67/4.67	8.94/11.00	3.90/5.52	2.50/2.94
64^2	5.69/4.69	10.95/18.55	4.00/6.00	2.36/3.41
128^2	5.19/4.19	17.39/41.48	3.26/4.46	2.42/5.13
256^2	5.20/6.26	27.07/92.90	3.27/4.57	2.65/9.36

multigrid-Krylov algorithm provides an effective means of solving both the linear and nonlinear problems in a scalable fashion. The nonlinear iteration provides a greatly increased efficiency when highly nonlinear flux-limited diffusion coefficients are employed.

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