Mixed Hybrid Finite Element Eddington Acceleration of Discrete Ordinates Source Iteration

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INTRODUCTION

One of the most challenging computational tasks is simulating the interaction of radiation with matter. A full description of a particle in flight includes three spatial variables (x,y and z), two angular or direction of flight variables (μ = the cosine of the polar angle and γ = the azimuthal angle), one energy variable (E) and one time variable (t). Numerical solutions require discretizing all seven variables leading to immense systems of algebraic equations. In addition, material properties can lead to vastly different solution behaviors making generalized numerical methods for radiation transport difficult to attain [1].

Lawrence Livermore National Laboratory (LLNL) is developing a high–order radiation–hydrodynamics code. The hydrodynamics portion is discretized using the Mixed Hybrid Finite Element Method (MHFEM), where values are taken to be constant within a cell with discontinuous jumps at both cell edges [2]. MHFEM is particularly suited for hydrodynamics but not for radiation transport. This work seeks to develop an acceleration scheme capable of robustly reducing the number of iterations in Discrete Ordinates Source Iteration calculations while being compatible with MHFEM multiphysics.

BACKGROUND

The steady–state, mono–energetic, isotropically–scattering, fixed–source Linear Boltzmann Equation in slab geometry is:

$$\mu \frac{\partial \psi}{\partial x}(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\int_{-1}^{1}\psi(x,\mu')d\mu' + \frac{Q(x)}{2} \quad (1)$$

where $\mu = \cos\theta$ is the cosine of the angle of flight θ relative to the x–axis, $\Sigma_t(x)$ and $\Sigma_s(x)$ the total and scattering macroscopic cross sections, $Q(x)$ the isotropic fixed–source and $\psi(x,\mu)$ the angular flux [1]. The factors of $\frac{1}{2}$ appear from normalization to

$$\int_{-1}^{1} \mathrm{d}\mu = 2. \quad (2)$$

This is an integro–differential equation due to the placement of the unknown, $\psi(x,\mu)$, under both a derivative and an integral.

The Discrete Ordinates (S_N) angular discretization sets μ to discrete values stipulated by an N–point Gauss quadrature rule. The scalar flux, $\phi(x)$, is then

$$\phi(x) = \int_{-1}^{1} \psi(x,\mu)\,\mathrm{d}\mu \xrightarrow{S_N} \sum_{n=1}^{N} w_n \psi_n(x) \quad (3)$$

where $\psi_n(x) = \psi(x,\mu_n)$ and the w_n are the quadrature weights corresponding to each μ_n [3]. The S_N equations are then

$$\mu_n \frac{\mathrm{d}\psi_n}{\mathrm{d}x}(x) + \Sigma_t(x)\psi_n(x) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2} \quad (4)$$

where $n = 1, 2, \dots, N$ and $\phi(x)$ is defined by Eq. 3. This is now a system of N coupled, ordinary differential equations.

The Source Iteration (SI) solution method decouples the S_N equations by lagging the right hand side of Eq. 5. In other words,

$$\mu_n \frac{\mathrm{d}\psi_n^{\ell+1}}{\mathrm{d}x}(x) + \Sigma_t(x)\psi_n^{\ell+1}(x) = \frac{\Sigma_s(x)}{2}\phi^{\ell}(x) + \frac{Q(x)}{2}, \; 1 \le n \le N \quad (5)$$

where the superscripts indicate iteration number. Equation 5 represents N independent, ordinary differential equations.

The iteration process begins with an initial guess for the scalar flux, $\phi^0(x)$. Equation 5 is then solved, using $\phi^0(x)$ on the right hand side, for the $\psi_n^1(x)$. $\phi^1(x)$ is then computed using Eq. 3. This process is repeated until

$$\frac{\|\phi^{\ell+1}(x) - \phi^{\ell}(x)\|}{\|\phi^{\ell+1}(x)\|} < \epsilon \quad (6)$$

where ϵ is a sufficiently small tolerance.

If $\phi^0(x) = 0$, then $\phi^{\ell}(x)$ is the scalar flux of particles that have undergone at most $\ell - 1$ collisions [1]. Thus, the number of iterations until convergence is directly linked to the number of collisions in a particle's lifetime. Typically, SI becomes increasingly slow to converge as the ratio of Σ_s to Σ_t approaches unity and the amount of particle leakage from the system goes to zero. SI is slowest in large, optically thick systems with small losses to absorption. In full radiation transport simulations each iteration could involve solving for hundreds of millions of unknowns. To minimize computational expense, acceleration schemes must be developed to rapidly increase the rate of convergence of SI.

Fortunately, the regime where SI is slow to converge is also the regime where Diffusion Theory is most accurate. A popular method for accelerating SI is Diffusion Synthetic Acceleration (DSA) where each source iteration involves both a transport sweep and a diffusion solve. DSA requires carefully differencing the S_N and diffusion steps in a consistent manner to prevent instability in highly scattering media with coarse spatial grids [4, 5]. DSA is not applicable in the setting of this presentation due to the incompatibility of MHFEM and S_N and the increased computational expense of solving consistently differenced diffusion. A new acceleration method is needed that avoids the consistency pitfall of DSA.

EDDINGTON ACCELERATION

The zeroth and first angular moments of Eq. 1 are

$$\frac{\mathrm{d}}{\mathrm{d}x}J(x) + \Sigma_a(x)\phi(x) = Q(x) \quad (7a)$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\langle\mu^2\rangle(x)\phi(x) + \Sigma_t(x)J(x) = 0 \quad (7b)$$

where $J(x) = \int_{-1}^{1} \mu\, \psi(x,\mu)\, \mathrm{d}\mu$ is the current and

$$\langle \mu^2 \rangle(x) = \frac{\int_{-1}^{1} \mu^2 \psi(x,\mu)\, \mathrm{d}\mu}{\int_{-1}^{1} \psi(x,\mu)\, \mathrm{d}\mu} \tag{8}$$

the Eddington factor. In S_N, the Eddington factor is

$$\langle \mu^2 \rangle(x) = \frac{\sum_{n=1}^{N} \mu_n^2 w_n \psi_n(x)}{\sum_{n=1}^{N} w_n \psi_n(x)}. \tag{9}$$

Note that no approximations have been made to arrive at Eqs. 7a and 7b. The Eddington factor is the true angular flux weighted average of μ^2 and therefore Eqs. 7a and 7b are just as accurate as Eq. 1.

This formulation is beneficial because Eq. 7a is a conservative balance equation and—if $\langle \mu^2 \rangle(x)$ is known—the moment equations' system of two first–order, ordinary differential equations can be solved directly with well–established methods. However, computing $\langle \mu^2 \rangle(x)$ requires already knowing the angular flux.

In Eddington Acceleration, S_N is used to compute the Eddington factor needed to solve the moment equations. Source iteration is then

1. Compute $\psi_n^{\ell+1/2}(x)$ with S_N
2. Compute $\langle \mu^2 \rangle^{\ell+1/2}(x)$ with Eq. 9
3. Solve the moment equations for $\phi^{\ell+1}(x)$ with the preconditioned $\langle \mu^2 \rangle^{\ell+1/2}(x)$
4. Use $\phi^{\ell+1}(x)$ on the right hand side of Eq. 5
5. Repeat until the scalar flux converges.

Acceleration occurs because the Eddington factor is a weak function of angular flux. This means that even poor angular flux solutions can accurately approximate the Eddington factor. In addition, the moment equations model the contributions of all scattering events at once, reducing the dependence on source iterations to introduce scattering information. The solution from the moment equations is then an approximation for the full flux and not the $\ell - 1$ collided flux as it was without acceleration.

In addition to acceleration, this scheme allows the S_N equations and moment equations to be solved with arbitrarily different spatial discretization methods. S_N can be spatially discretized using normal methods, such as Linear Discontinuous Galerkin or Diamond Difference, while the moment equations can be solved with MHFEM.

RESULTS

As a proof of concept for Eddington Acceleration, a Diamond Differenced S_N code was created along with an MHFEM solver for Eqs. 7a and 7b. The test problem of steady–state, one–group, isotropically–scattering, fixed–source radiation transport in slab geometry with a reflecting left boundary and vacuum right boundary was used to compare unaccelerated, Eddington accelerated, and DSA S_8 SI with 100 spatial cells

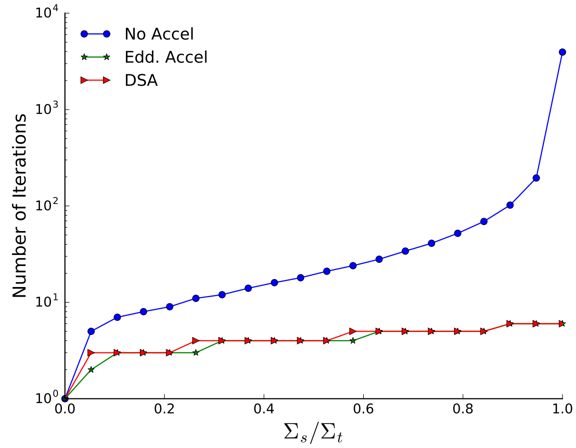

Fig. 1. A comparison of the number of iterations until convergence for unaccelerated, Eddington accelerated, and DSA S_8 SI.

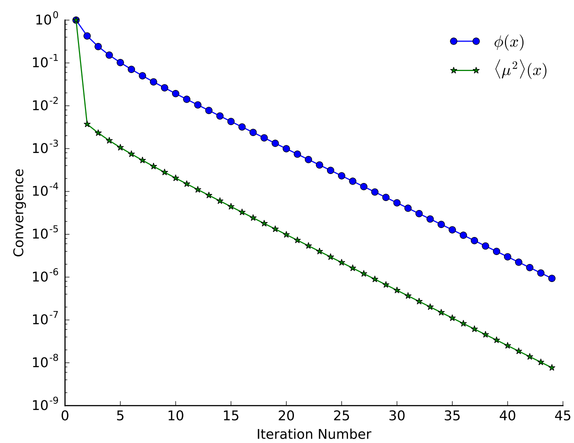

Fig. 2. The convergence rate of $\phi(x)$ compared to $\langle \mu^2 \rangle(x)$ for unaccelerated S_8 with $\Sigma_s/\Sigma_t = 0.75$.

and a domain length of 20 cm. The total macroscopic cross section was set to $1\,\mathrm{cm}^{-1}$ leading to a total optical thickness of 20 and an optical thickness per cell of 0.2.

Figure 1 shows the number of iterations until the convergence criterion in Eq. 6 was met with $\epsilon = 1 \times 10^{-6}$ for varying ratios of Σ_s to Σ_t. Aside from $\Sigma_s/\Sigma_t = 0$ where acceleration is not possible, the ratio of unaccelerated to Eddington accelerated iterations ranged between 2.5 and 750. This suggests that acceleration is occurring and that Eddington Acceleration does not just do twice the amount of work in each iteration.

Figure 2 shows the unaccelerated convergence criterion

$$\frac{\| f^{\ell+1} - f^{\ell} \|}{\| f^{\ell+1} \|} \tag{10}$$

as a function of iteration number for $f = \phi(x)$ and $f = \langle \mu^2 \rangle(x)$. The large drop in the convergence criterion between the first and second iterations supports the claim that $\langle \mu^2 \rangle(x)$ is a weak

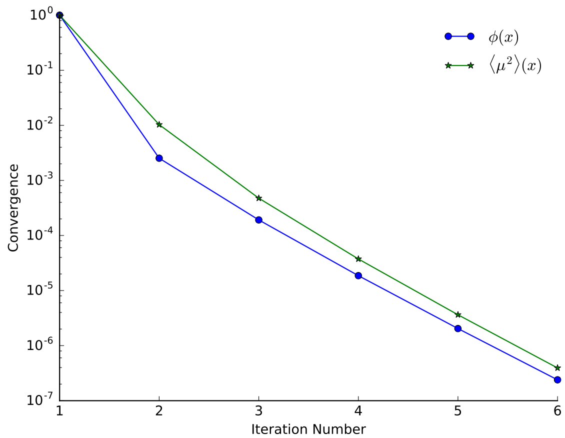

Fig. 3. The convergence rate of $\phi(x)$ compared to $\langle\mu^2\rangle(x)$ for Eddington accelerated S_8 with $\Sigma_s/\Sigma_t = 0.75$.

function of angular flux as it quickly converges despite a less convergent angular flux. When compared to Fig. 3, a plot of the convergence criterion versus number of iterations for Eddington accelerated S_8, it is clear that Eddington Acceleration transfers the fast rate of convergence of $\langle\mu^2\rangle(x)$ to $\phi(x)$.

CONCLUSIONS

The proposed acceleration scheme successfully accelerated S_8 source iteration calculations in slab geometry for a wide range of Σ_s/Σ_t. In the pure scattering regime ($\Sigma_s = \Sigma_t$), source iteration was accelerated by a factor of 750. This scheme is especially suited for multiphysics applications because the transport and acceleration steps do not need to be consistently differenced. In addition, the acceleration step produces a conservative solution that is computationally inexpensive compared to a transport sweep. Future work that will also be presented is the application of Eddington Acceleration to Linear Discontinuous Galerkin discretized S_N.

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