

Accelerating Discrete Ordinates Source Iteration with the Eddington Factor

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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 planar 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]. In the Discrete Ordinates (S_N) angular discretization, μ takes discrete values from an N -point Gauss quadrature rule. The scalar flux, $\phi(x)$, is then

$$\phi(x) = \int_{-1}^1 \psi(x, \mu) d\mu \xrightarrow{S_N} \sum_{n=1}^N w_n \psi_n(x) \quad (2)$$

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

$$\mu_n \frac{d\psi_n}{dx}(x) + \Sigma_t(x) \psi_n(x) = \frac{\Sigma_s(x)}{2} \phi(x) + \frac{Q(x)}{2} \quad (3)$$

for $n = 1, 2, \dots, N$ where $\phi(x)$ is defined by Eq. 2.

In the Source Iteration (SI) solution method, the right hand side of Eq. 3 is lagged. In other words,

$$\mu_n \frac{d\psi_n^{\ell+1}}{dx}(x) + \Sigma_t(x) \psi_n^{\ell+1}(x) = \frac{\Sigma_s(x)}{2} \phi^\ell(x) + \frac{Q(x)}{2}. \quad (4)$$

Equation 4 is iterated until

$$\frac{\|\phi^{\ell+1}(x) - \phi^\ell(x)\|}{\|\phi^{\ell+1}(x)\|} < \epsilon \quad (5)$$

where ϵ is a sufficiently small tolerance.

If the initial guess for the scalar flux, $\phi^0(x)$, is zero for all values of x , then $\phi^\ell(x)$ is the scalar flux of particles that have undergone $\ell - 1$ 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 highly scattering systems with small losses to absorption and particle leakage. In full radiation transport simulations with millions of unknowns, unneeded source iterations can be prohibitively expensive.

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

$$\frac{d}{dx} J(x) + \Sigma_a(x) \phi(x) = Q(x) \quad (6a)$$

$$\frac{d}{dx} \langle \mu^2 \rangle(x) \phi(x) + \Sigma_t(x) J(x) = 0 \quad (6b)$$

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

$$\langle \mu^2 \rangle(x) = \frac{\int_{-1}^1 \mu^2 \psi(x, \mu) d\mu}{\int_{-1}^1 \psi(x, \mu) d\mu} \quad (7)$$

the Eddington factor. Note that no approximations have been made to arrive at Eqs. 6a and 6b. The Eddington factor is the true angular flux weighted average of μ^2 and therefore Eqs. 6a and 6b are just as accurate as Eq. 1. In S_N , the Eddington factor is

$$\langle \mu^2 \rangle(x) = \frac{\sum_{n=1}^N \mu_n^2 w_n \psi_n(x)}{\sum_{n=1}^N w_n \psi_n(x)} \quad (8)$$

This formulation is beneficial because Eq. 6a 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.

The proposed acceleration scheme is:

1. Compute ψ_n with S_N and an arbitrary spatial discretization
2. Compute $\langle \mu^2 \rangle$ with Eq. 8
3. Interpolate $\langle \mu^2 \rangle$ onto the MHFEM grid
4. Solve the moment equations for $\phi(x)$ with the preconditioned $\langle \mu^2 \rangle$ using MHFEM.

This process is one source iteration consisting of an S_N transport step to compute the Eddington factor and an MHFEM acceleration step to compute $\phi(x)$. The scalar flux from the acceleration step is used in the right hand side of Eq. 4 and steps 1–4 are repeated until the acceleration step's $\phi(x)$ converges according to Eq. 5.

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 acceleration step is then an approximation for the full flux and not the $\ell - 1$ collided flux as it was without acceleration.

This scheme allows the S_N equations and moment equations to be solved with different spatial discretizations. S_N can be discretized using normal methods such as Linear Discontinuous Galerkin or Diamond Differencing while the moment equations can be solved on the same grid as the hydrodynamics.

RESULTS

As a proof of concept for Eddington acceleration, a Diamond Differenced S_N code was created in addition to an MHFEM solver for Eqs. 6a and 6b. 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.

Figure 1 shows the number of iterations until the convergence criterion in Eq. 5 was met with $\epsilon = 1 \times 10^{-6}$ for varying ratios of Σ_s/Σ_t . Aside from $\Sigma_s/\Sigma_t = 0$ where acceleration is not possible, the ratio of unaccelerated to Eddington accelerated iterations ranges between 2.5 and 700. 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

$$\frac{\|f^{\ell+1} - f^\ell\|}{\|f^{\ell+1}\|} \quad (9)$$

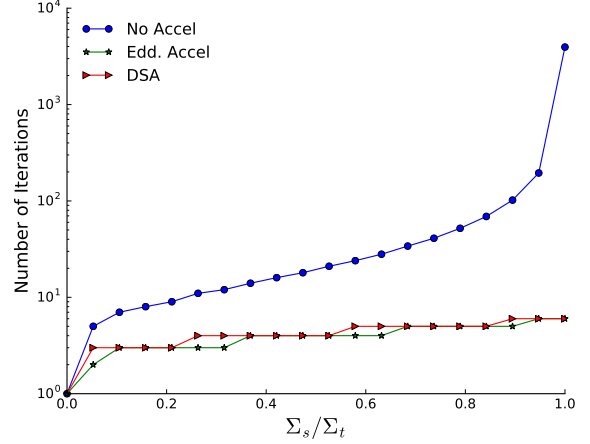


Fig. 1. A comparison of unaccelerated, Eddington accelerated and DSA S_8 .

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 function of angular flux. When compared to Fig. 3, 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 $\phi(x)$.

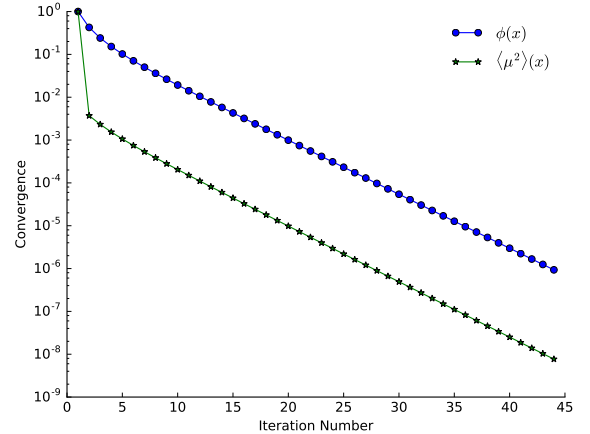


Fig. 2. The convergence rate of $\phi(x)$ compared to $\langle \mu^2 \rangle(x)$ for unaccelerated S_8 .

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

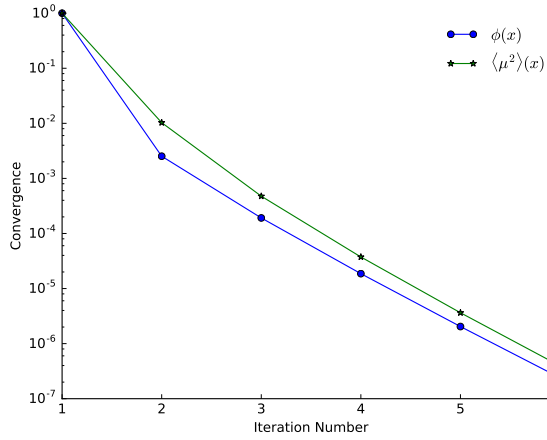


Fig. 3. The convergence rate of $\phi(x)$ compared to $\langle \mu^2 \rangle(x)$ for Eddington accelerated S_8 .

also be presented is the application of Eddington acceleration to Linear Discontinuous Galerkin discretized S_N .

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