Mixed Hybrid Finite Element Method Eddington Acceleration of Discrete Ordinates Source Iteration

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Overview

- 1. Motivation
- 2. Source Iteration Background
- 3. Eddington Acceleration
- 4. Results
- 5. Conclusions

Motivation

Motivation

Radiation Hydrodynamics

- Couple radiation transport and fluid dynamics
- Material temperatures so high that fluid momentum and energy are altered by release of thermal radiation
- Required in high energy density physics simulations (National Ignition Facility, astrophysics)

Radiation transport simulations are expensive and difficult to incorporate into hydrodynamics

Efficient methods developed independently

Mixed Hybrid Finite Element Method works well for hydrodynamics but is incompatible with radiation transport

Want to use MHFEM for hydrodynamics and Linear Discontinuous Galerkin for transport

Goal

Develop an acceleration scheme that

- 1. Robustly reduces the number of source iterations in Discrete Ordinates calculations
- 2. Increases compatibility with MHFEM multiphysics

Show that MHFEM can be used to accelerate lumped LDG radiation transport

Source Iteration Background

Boltzmann Equation

Steady-state, mono-energetic, istropically-scattering, fixed-source Linear Boltzmann Equation in 1D slab geometry:

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

 $\mu=\cos\theta$ the cosine of the angle of flight θ relative to the x-axis $\Sigma_t(x)$, $\Sigma_s(x)$ total and scattering macroscopic cross sections Q(x) the isotropic fixed-source $\psi(x,\mu)$ the angular flux

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Integro-differential equation

Discrete Ordinates Angular Discretization

Compute angular flux on ${\cal N}$ discrete angles defined by Gauss Quadrature

$$\psi(x,\mu) \xrightarrow{S_N} \begin{cases} \psi_1(x), & \mu = \mu_1 \\ \psi_2(x), & \mu = \mu_2 \\ \vdots \\ \psi_N, & \mu = \mu_N \end{cases}$$

 $\mu_1,\ \mu_2,\ \dots,\ \mu_N$ defined by N-point Gauss Quadrature Rule Integrate order N-1 polynomials exactly with

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

4

S_N Equations

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

N coupled, ordinary differential equations

All coupling in scattering term

Source Iteration

Decouple by lagging scattering term

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

N independent, first-order, ordinary differential equations

Solve each equation with well-known sweeping process

Source Iteration

- 1. Given previous estimate for $\phi^\ell(x),$ solve for $\psi_n^{\ell+1}$
- 2. Compute $\phi^{\ell+1}(x) = \sum_{n=1}^{N} w_n \psi_n^{\ell+1}(x)$
- 3. Update scattering term with $\phi^{\ell+1}(x)$ and repeat until:

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

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If
$$\phi^0(x) = 0$$

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Convergence rate is linked to the number of collisions in a particle's lifetime

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 $\phi^1(x)$ is the uncollided flux

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 $\phi^2(x)$ is uncollided and once collided flux

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- $\phi^1(x)$ is the uncollided flux
- $\phi^2(x)$ is uncollided and once collided flux
- $\phi^\ell(x)$ is the scalar flux of particles that have undergone at most $\ell-1$ collisions

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Slow to converge in optically thick systems with minimal losses to absorption and leakage

Diffusion Synthetic Acceleration

Large, highly scattering systems \Rightarrow Diffusion Theory is accurate!

Diffusion Synthetic Acceleration

- 1. Given previous estimate for $\phi^{\ell}(x)$, solve for $\psi_n^{\ell+1/2}$
- 2. Compute $\phi^{\ell+1/2}(x) = \sum_{n=1}^{N} w_n \psi_n^{\ell+1/2}(x)$
- 3. Solve diffusion equation for a correction factor, $f^{\ell+1}(x)$
- 4. Update scattering term with $\phi^{\ell+1}(x) = \phi^{\ell+1/2}(x) + f^{\ell+1}(x)$ and repeat until:

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

DSA Problems

Becomes non-convergent in highly scattering media with coarse spatial grids

Transport and Diffusion steps must be consistently differenced

Consistently differenced equations are more expensive to solve

Transport and MHFEM are not compatible

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Transport and MHFEM are not compatible

A new acceleration scheme is needed!

Eddington Acceleration

Zeroth Angular Moment

Boltzmann Equation

$$\mu \frac{\mathrm{d}\psi}{\mathrm{d}x}(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2}$$

Zeroth Angular Moment

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$$\mu \frac{\mathrm{d}\psi}{\mathrm{d}x}(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{\Sigma_s(x)}{2}\phi(x) + \frac{Q(x)}{2}$$

Integrate over all angles

$$\int_{-1}^{1} \mu \frac{\mathrm{d}\psi}{\mathrm{d}x}(x,\mu) \,\mathrm{d}\mu + \int_{-1}^{1} \Sigma_{t}(x)\psi(x,\mu) \,\mathrm{d}\mu = \int_{-1}^{1} \frac{\Sigma_{s}(x)}{2}\phi(x) \,\mathrm{d}\mu + \int_{-1}^{1} \frac{Q(x)}{2} \,\mathrm{d}\mu$$

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$$\int_{-1}^{1} \mu \frac{\mathrm{d} \psi}{\mathrm{d} x}(x, \mu) \, \mathrm{d} \mu \ + \int_{-1}^{1} \Sigma_{t}(x) \psi(x, \mu) \, \mathrm{d} \mu = \int_{-1}^{1} \frac{\Sigma_{s}(x)}{2} \phi(x) \, \mathrm{d} \mu \ + \int_{-1}^{1} \frac{Q(x)}{2} \, \mathrm{d} \mu$$

Use
$$J(x) = \int_{-1}^{1} \mu \psi(x, \mu) \, d\mu$$
, $\phi(x) = \int_{-1}^{1} \psi(x, \mu) \, d\mu$

Zeroth Angular Moment

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

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

$$\int_{-1}^1 \mu^2 \frac{\mathrm{d} \psi}{\mathrm{d} x}(x,\mu) \, \mathrm{d} \mu + \underbrace{\int_{-1}^1 \mu \Sigma_t(x) \psi(x,\mu) \, \mathrm{d} \mu}_{\Sigma_t(x)J(x)} = \int_{-1}^1 \mu \frac{\Sigma_s(x)}{2} \phi(x) \, \mathrm{d} \mu + \int_{-1}^1 \mu \frac{Q(x)}{2} \, \mathrm{d} \mu$$

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$$\int_{-1}^{1} \mu^2 \frac{\mathrm{d} \psi}{\mathrm{d} x}(x,\mu) \, \mathrm{d} \mu + \underbrace{\int_{-1}^{1} \mu \Sigma_t(x) \psi(x,\mu) \, \mathrm{d} \mu}_{\Sigma_t(x)J(x)} = \underbrace{\int_{-1}^{1} \mu \frac{\Sigma_s(x)}{2} \phi(x) \, \mathrm{d} \mu + \int_{-1}^{1} \mu \frac{Q(x)}{2} \, \mathrm{d} \mu}_{\text{Isotropic} \Rightarrow 0}$$

Rearrange derivative

$$\frac{\mathrm{d}}{\mathrm{d}x} \int_{-1}^{1} \mu^2 \psi(x,\mu) \,\mathrm{d}\mu$$

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Multiply and divide by $\int_{-1}^{1} \psi(x,\mu) d\mu$

$$\frac{\mathrm{d}}{\mathrm{d}x} \int_{-1}^{1} \psi(x,\mu) \,\mathrm{d}\mu \frac{\int_{-1}^{1} \mu^{2} \psi(x,\mu) \,\mathrm{d}\mu}{\int_{-1}^{1} \psi(x,\mu) \,\mathrm{d}\mu}$$

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$$\frac{\mathrm{d}}{\mathrm{d}x} \underbrace{\int_{-1}^{1} \psi(x,\mu) \, \mathrm{d}\mu}_{\phi(x)} \underbrace{\frac{\int_{-1}^{1} \mu^{2} \psi(x,\mu) \, \mathrm{d}\mu}{\int_{-1}^{1} \psi(x,\mu) \, \mathrm{d}\mu}}_{\text{Eddington Factor}}$$

Rearrange derivative

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Eddington Factor

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

Rearrange derivative

$$\frac{\mathrm{d}}{\mathrm{d}x} \int_{-1}^{1} \mu^2 \psi(x,\mu) \,\mathrm{d}\mu$$

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Shape function

Moment Equations

Moment Equations

$$\frac{\mathrm{d}}{\mathrm{d}x}J(x) + \Sigma_a(x)\phi(x) = Q(x) \tag{Zeroth Moment}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\langle\mu^2\rangle(x)\phi(x) + \Sigma_t(x)J(x) = 0 \tag{First Moment}$$

Solve First Moment for J(x)

$$J(x) = -\frac{1}{\Sigma_t(x)} \frac{\mathrm{d}}{\mathrm{d}x} \langle \mu^2 \rangle(x) \phi(x)$$

Combine Zero and First Moments ⇒ Drift Diffusion Equation

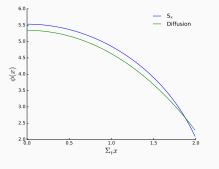
$$-\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{\Sigma_t(x)}\frac{\mathrm{d}}{\mathrm{d}x}\langle\mu^2\rangle(x)\phi(x) + \Sigma_a(x)\phi(x) = Q(x)$$

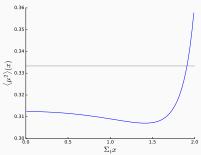
Fick's Law: set
$$\langle \mu^2 \rangle(x) = \frac{1}{3}$$

$$J(x) = -\frac{1}{3\Sigma_t(x)} \frac{\mathrm{d}}{\mathrm{d}x} \phi(x)$$

S₈ v. Diffusion

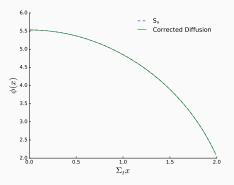
Small system \Rightarrow diffusion not expected to be accurate





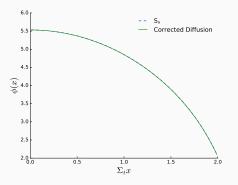
S₈ v. Drift Diffusion

Use $\langle \mu^2 \rangle(x)$ from S₈ in Moment Equations



S₈ v. Drift Diffusion

Use $\langle \mu^2 \rangle(x)$ from S₈ in Moment Equations



Drift Diffusion and S_N match!

Eddington Acceleration

Use S_N to compute $\langle \mu^2 \rangle(x)$ and Moment Equations to find $\phi(x)$

Eddington Acceleration

- 1. Given the previous estimate for the scalar flux, $\phi^\ell(x)$, solve for $\psi_n^{\ell+1/2}(x)$
- 2. Compute $\langle \mu^2 \rangle^{\ell+1/2}(x)$
- 3. Solve the Moment Equations for $\phi^{\ell+1}(x)$ using $\langle \mu^2 \rangle^{\ell+1/2}(x)$
- 4. Update the scalar flux estimate with $\phi^{\ell+1}(x)$ and repeat the iteration process until the scalar flux converges

Eddington Acceleration Properties

Acceleration occurs due to:

- 1. Angular shape of the angular flux converges quickly \Rightarrow Eddington factor quickly converges
- 2. Solution to moment equations models all scattering events at once
- 3. Dependence on source iterations to introduce scattering information is reduced

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Downside: produces 2 solutions (S_N and Drift Diffusion)

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Benefits

- 1. No need for consistent differencing \Rightarrow transport and acceleration steps can be differenced with arbitrarily different methods
- 2. Moment Equations are conservative
- 3. Accelerates source iterations
- 4. Difference between S_N and Drift Diffusion solution can be used as a measure of iteration uncertainty

Results

Test Problem

Slab with reflecting left boundary and vacuum right boundary

Thickness of 20 cm

$$\Sigma_t(x) = 1\,\mathrm{cm}^{-1}$$

100 cells \Rightarrow optical thickness of 20 and optical thickness per cell of 0.2

 S_8 solved with lumped Linear Discontinuous Galerkin

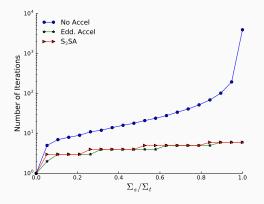
Moment Equations solved with Mixed Hybrid Finite Element

Compare to acceleration to constistently differenced S_2SA

Iterations to Convergence Comparison

Vary ratio of Σ_s to Σ_t

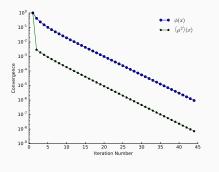
More scattering \Rightarrow more diffusive, harder for S_N to solve

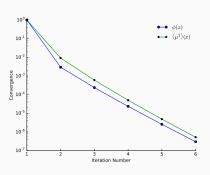


Accelerates between 2.5 and 650 times \Rightarrow acceleration is occurring

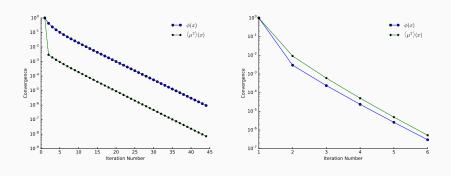
Performs similarly to consistent acceleration scheme

Convergence Rate Comparison





Convergence Rate Comparison



Fast rate of convergence of $\langle \mu^2 \rangle(x)$ is transferrd to $\phi(x)$

Conclusions

Summary

Conclusions

- Scheme successfully accelerated source iteration in 1D slab geometry
- Inherently compatible with rad-hydro multiphysics
 - Transport and acceleration steps can be discretized with arbitrarily different methods
 - Avoids consistency issues
 - Provides less expensive, conservative solution
- Proved Mixed Hybrid Finite Element Method can be used to accelerate lumped Linear Discontinuous Galerkin transport

Summary

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- Scheme successfully accelerated source iteration in 1D slab geometry
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Future Work

- Develop a rad-hydro algorithm
 - Make use of inexpensive Moment solution in operator split iterations
- Add discretization in energy
- Higher dimensions
- Anisotropic scattering

References

- M. L. ADAMS AND E. W. LARSEN, Fast Iterative Methods for Discrete-Ordinates Particle Transport Calculations, vol. 40, Progress in Nuclear Technology, 2002.
- [2] R. E. ALCOUFFE, Diffusion Synthetic Acceleration Methods for the Diamond–Differenced Discrete–Ordinates Equations, 1977.
- [3] F. BREZZI AND M. FORTIN, *Mixed and Hybdrid Finite Element Methods*, Springer, 1991.
- [4] J. I. CASTOR, Radiation Hydrodynamics, 2003.
- [5] S. N. SHORE, An Introduction to Astrophysicial Hydrodynamics, Academic Press, Inc., 1992.
- [6] J. S. WARSA, T. A. WAREING, AND J. E. MOREL, Fully Consistent Diffusion Synthetic Acceleration of Linear Discontinuous Transport Discretizations on Three–Dimensional Unstructured Meshes.

