# 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 is altered by release of thermal radiation
- Required in high energy density physics (National Ignition Facility, astrophysics)

Radiation transport simulations are expensive and difficult to incorporate into hydro

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

- 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  $\theta$  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

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

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# $S_N$ 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

#### Source Iteration

Decouple by lagging scattering term

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

N independent, first-order, ordinary differential equations

#### **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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#### **Need For Acceleration in Source Iteration**

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

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

$$\mu_n \frac{d\psi_n^1}{dx}(x) + \Sigma_t(x)\psi_n^1(x) = \frac{\Sigma_s(x)}{2}\phi^0(x) + \frac{Q(x)}{2}, 1 \le n \le N$$

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

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

Each source iteration adds scattering information

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

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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:

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

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

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Transport and MHFEM are not compatible

A new acceleration scheme is needed!

**Eddington Acceleration** 

# Zeroth Angular Moment

#### Boltzmann Equation

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

Integrate over all angles

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

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**

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

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

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

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

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

Rearrange derivative

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

Rearrange derivative

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

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

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

Rearrange derivative

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

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

Rearrange derivative

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

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

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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

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

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

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

**Eddington Factor** 

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

Shape function

# **Moment Equations**

#### **Moment Equations**

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

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

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  $\Rightarrow$  Drift Diffusion Equation

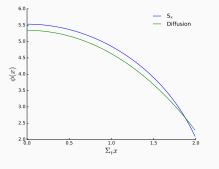
$$-\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{\Sigma_t(x)}\frac{\mathrm{d}}{\mathrm{d}x}\langle\mu^2\rangle(x)\phi(x) + \Sigma_a(x)\phi(x) = Q(x)$$

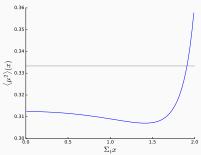
Fick's Law: set 
$$\langle \mu^2 \rangle(x) = \frac{1}{3}$$

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

# S<sub>8</sub> v. Diffusion

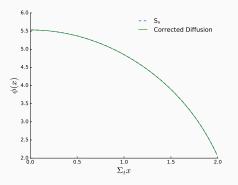
Small system  $\Rightarrow$  diffusion not expected to be accurate





# S<sub>8</sub> v. Drift Diffusion

Use  $\langle \mu^2 \rangle(x)$  from S<sub>8</sub> 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

Downside: produces 2 solutions ( $S_N$  and Drift Diffusion)

#### **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

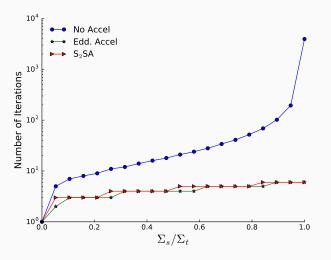
$$\Sigma_t(x) = 1\,\mathrm{cm}^{-1}$$

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

 $\mathsf{S}_8$  solved with lumped Linear Discontinuous Galerkin

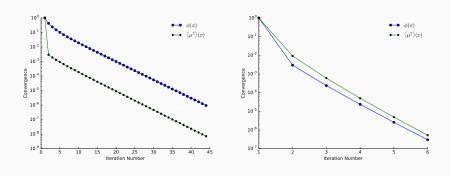
Moment Equations solved with Mixed Hybrid Finite Element

# **Iterations to Convergence Comparison**



Accelerates between 2.5 and 650 times  $\Rightarrow$  acceleration is occurring Performs similarly to consistent acceleration scheme

# **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

#### 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.

