

# Variable Eddington Factor Method with Hybrid Spatial Discretization

International Conference on Transport Theory  
Novel Numerical Methods

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# Overview

1. Background
2. Description of VEF Method
3. Discretizations
4. Scattering Update Methods
5. Computational Results
6. Conclusions and Future Work

# Background

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# Variable Eddington Factor Method Background

One of the first nonlinear methods for accelerating source iterations

Use  $S_N$  to create a transport informed drift diffusion solution

Produces 2 solutions: one from  $S_N$  and one from drift diffusion

- Do not necessarily become identical when the iterative process converges if not consistently differenced
- Solutions do converge as the mesh is refined  $\Rightarrow$  built in truncation estimator

Will show that the benefits outweigh producing 2 separate solutions

# Why Nonlinear Acceleration?

Classic discretizations (step, diamond) are not suitable for radiative transfer in High Energy Density Physics regime  $\Rightarrow$  Discontinuous Galerkin (DG)

Linear acceleration of Discontinuous Finite Element  $S_N$  is somewhat problematic

- Consistent differencing required (Adams and Martin NSE 1992)
- Requires the diffusion equation to be expressed in  $P_1$  form which is more difficult to solve (Warsa, Wareing, Morel NSE 2002)
- Partially consistent linear acceleration methods are generally difficult to develop (Wang and Ragusa NSE 2010)

## Why Nonlinear Acceleration? (cont.)

Nonlinear acceleration has relaxed consistency requirements

- Drift diffusion acceleration equation can be discretized in any valid manner without regard for consistency with  $S_N$
- Preserves the thick diffusion limit regardless of discretization consistency as long as  $S_N$  solution becomes isotropic

Can use VEF drift diffusion in multiphysics calculations

- VEF drift diffusion is conservative and inexpensive (compared to an  $S_N$  sweep)
- Couple drift diffusion to other physics components
- Can use discretization compatible with other physics while still retaining benefits of DG  $S_N$

# Motivation

Mixed Finite Element Method (MFEM) is being used for high order hydrodynamics calculations (Dobrev, Kolev, Rieben SIAM 2012)

MFEM is not appropriate for standard, first-order form of transport equation

⇒ VEF method with DG  $S_N$  discretization + MFEM drift diffusion discretization

## Goals

Show Lumped Linear Discontinuous Galerkin (LLDG)  $S_N$  can be efficiently and accurately paired with MFEM drift diffusion for one group, 1D neutron transport

## **Description of VEF Method**

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Planar geometry, fixed-source, 1-D, one group, neutron transport equation

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

# $S_N$ Equations

Planar geometry, fixed-source, 1-D, one group, neutron transport equation

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$S_N$  angular discretization

$$\mu_n \frac{d\psi_n}{dx}(x) + \sigma_t(x) \psi_n(x) = \frac{\sigma_s(x)}{2} \phi(x) + \frac{Q(x)}{2}, \quad 1 \leq n \leq N$$

where

$$\phi(x) = \sum_{n=1}^N w_n \psi_n(x), \quad \psi_n(x) = \psi(x, \mu_n)$$

Lag scattering term

$$\mu_n \frac{d}{dx} \psi_n^{\ell+1/2}(x) + \sigma_t(x) \psi_n^{\ell+1/2}(x) = \frac{\sigma_s(x)}{2} \phi^\ell(x) + \frac{Q(x)}{2}, \quad 1 \leq n \leq N$$

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Source Iteration

$$\phi^{\ell+1} = \phi^{\ell+1/2}$$

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Source Iteration

$$\phi^{\ell+1} = \phi^{\ell+1/2}$$

Slow to converge in optically thick and highly scattering systems

Instead, solve

$$-\frac{d}{dx} \frac{1}{\sigma_t(x)} \frac{d}{dx} \left[ \langle \mu^2 \rangle^{\ell+1/2}(x) \phi^{\ell+1}(x) \right] + \sigma_a(x) \phi^{\ell+1}(x) = Q(x),$$

for  $\phi^{\ell+1}(x)$  using transport information from iteration  $\ell + 1/2$

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Transport information passed through the **Variable Eddington Factor**:

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

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- Angular flux weighted average of  $\mu^2$



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- Angular flux weighted average of  $\mu^2$
- Depends on angular shape of the angular flux, not its magnitude

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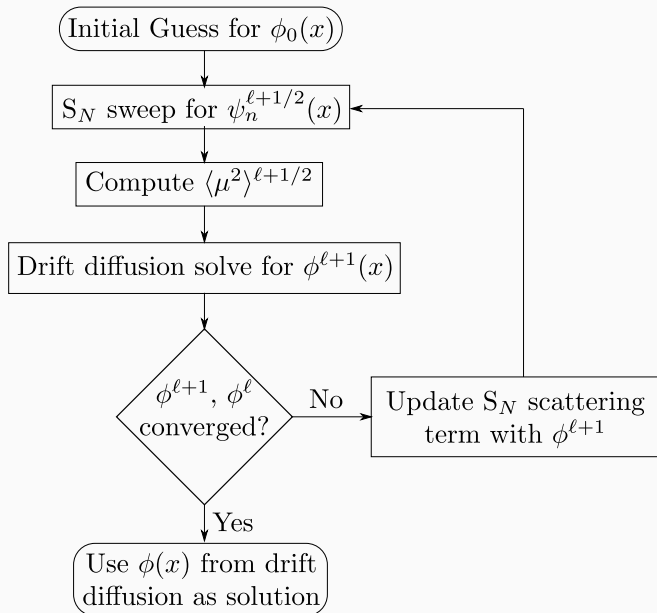
Use  $\phi^{\ell+1}$  to update scattering term in  $S_N$  sweep or as final solution if converged

# Acceleration Properties

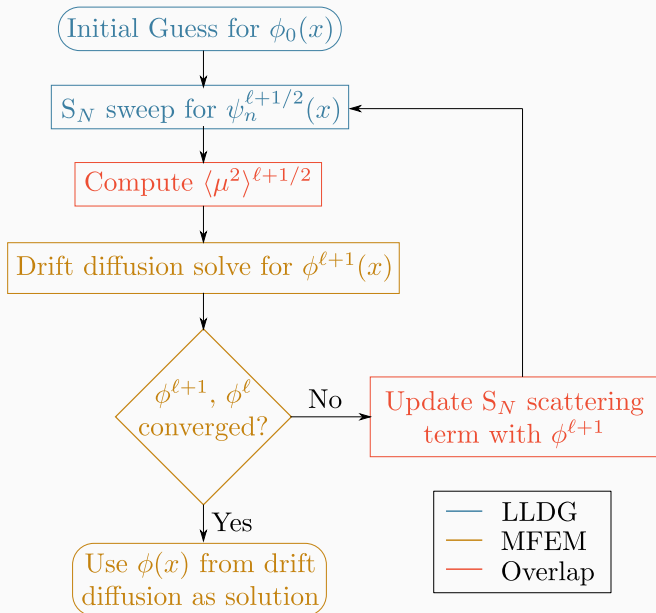
Angular shape of the angular flux, and thus the Eddington factor, converges much faster than the scalar flux

Drift diffusion includes scattering

# VEF Algorithm



# VEF Algorithm

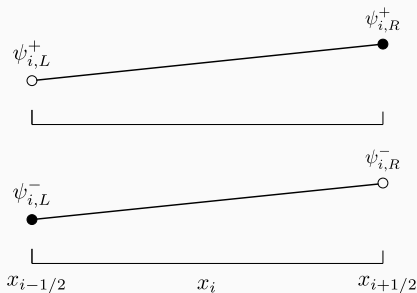


# Discretizations

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# Lumped Linear Discontinuous Galerkin $S_N$

- 2 discontinuous, linear basis functions
- Cell edges uniquely defined through upwinding



- Within the cell,  $\psi$  is a linear combination of the basis functions:

$$\psi_{n,i}(x) = \psi_{n,i,L} B_{i,L}(x) + \psi_{n,i,R} B_{i,R}(x), \quad x \in (x_{i-1/2}, x_{i+1/2})$$

- Cell centers through through polynomial interpolation (evaluate at  $x_i$ )
- Linear case: average of  $\psi_{n,i,L}$  and  $\psi_{n,i,R}$
- Sweep through local systems

# Handling Overlap in Eddington Factor

For integration by parts in MFEM weak form, need:

- $\langle \mu^2 \rangle$  on cell boundary
- $\langle \mu^2 \rangle(x)$  on interior of cell

Cell edges: use **uniquely defined, upwinded** cell edge values of  $\psi$  in Gauss Quadrature

$$\langle \mu^2 \rangle_{i \pm 1/2} = \frac{\sum_{n=1}^N \mu_n^2 \psi_{n,i \pm 1/2} w_n}{\sum_{n=1}^N \psi_{n,i \pm 1/2} w_n}$$

Cell centers: use polynomial interpolation function for the angular flux

$$\langle \mu^2 \rangle(x) = \frac{\sum_{n=1}^N \mu_n^2 \psi_n(x) w_n}{\sum_{n=1}^N \psi_n(x) w_n}, \quad x \in (x_{i-1/2}, x_{i+1/2}),$$

- Rational polynomial  $\Rightarrow$  can't be integrated analytically
- Preserves nonlinear spatial dependence of Eddington factor in MFEM formulation



# Constant-Linear Mixed Finite Element Drift Diffusion

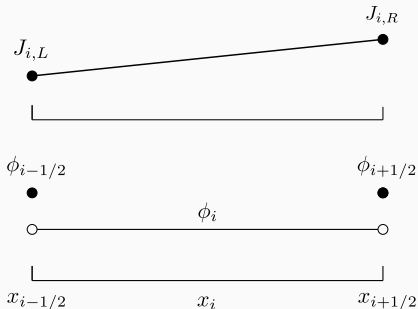
- Different basis functions for primary and secondary variables  $(\phi, J)$

- $\phi$ : constant with discontinuous jumps at the edges

- $J$ : linear discontinuous basis functions (same as in LLDG)

- 5 unknowns per cell

- $\phi$  and  $J$  are doubly defined on the edges but will later be made continuous through enforcing continuity of flux and current



System of first order equations equivalent to drift diffusion:

$$\frac{d}{dx} J(x) + \sigma_a(x) \phi(x) = Q(x)$$

$$\frac{d}{dx} [\langle \mu^2 \rangle(x) \phi(x)] + \sigma_t(x) J(x) = 0$$

# Weak Form

System of first order equations equivalent to drift diffusion:

$$\frac{d}{dx} J(x) + \sigma_a(x) \phi(x) = Q(x)$$

$$\frac{d}{dx} [\langle \mu^2 \rangle(x) \phi(x)] + \sigma_t(x) J(x) = 0$$

Multiply by  $\phi$  basis function and integrate over cell  $i$ :

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{d}{dx} J(x) + \sigma_a(x) \phi(x) \, dx = \int_{x_{i-1/2}}^{x_{i+1/2}} Q(x) \, dx$$

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Multiply by  $J$  basis functions ( $B_{i,L}$  and  $B_{i,R}$ ) and integrate:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} B_{i,L/R}(x) \frac{d}{dx} [\langle \mu^2 \rangle(x) \phi(x)] + B_{i,L/R}(x) \sigma_t(x) J(x) \, dx = 0$$

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## Weak Form (cont.)

Integrate by parts:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} B_{i,L/R}(x) \frac{d}{dx} [\langle \mu^2 \rangle(x) \phi(x)] dx =$$
$$\underbrace{\left[ B_{i,L/R}(x) \langle \mu^2 \rangle(x) \phi(x) \right]_{x_{i-1/2}}^{x_{i+1/2}}}_{\text{Edge Eddington Factors}} - \underbrace{\int_{x_{i-1/2}}^{x_{i+1/2}} \langle \mu^2 \rangle(x) \phi(x) \frac{dB_{i,L/R}}{dx} dx}_{\text{Interior Eddington Factors}}$$

## Weak Form (cont.)

Integrate by parts:

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On the interior:

- $\phi(x)$  and  $\frac{dB_{i,L/R}}{dx}$  are constant (for linear case)
- Use Gauss Quadrature to approximate

$$\langle \mu^2 \rangle_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \langle \mu^2 \rangle(x) dx$$

3 equations from weak form but 5 unknowns per cell

Enforce continuity of  $\phi$  and  $J$  at the interior cell edges:

$$\phi_{i+1/2} = \phi_{(i+1)-1/2}$$

$$J_{i,R} = J_{i+1,L}$$

Use transport consistent, Marshak-like boundary conditions

Can then eliminate  $J$  and assemble a system of equations of cell centers and edges of  $\phi$  only

Solve resulting **Symmetric Positive Definite Matrix** with a 5 band solver

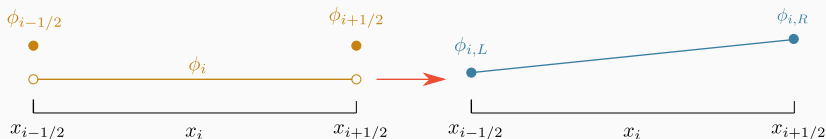


# Scattering Update Methods

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# Scattering Update Overlap

Must reconstruct an LLDG-like  $\phi$  from the MFEM drift diffusion  $\phi$



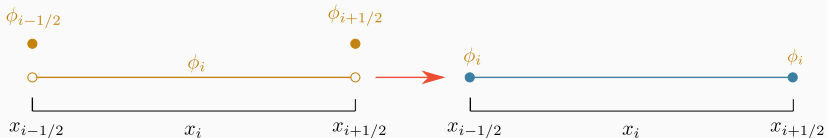
To remain general, reconstruct from cell centers only

- Temperature equation will not have cell edges (no continuity of temperature)

# Flat Scattering Update

Naive: flat update

$$\phi_{i,L/R} = \phi_i$$

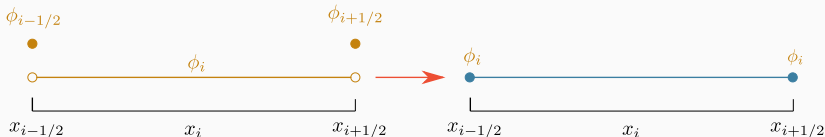


Converts constant MFEM to discontinuous constant in scattering term

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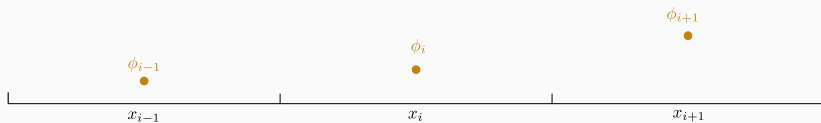
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Converts constant MFEM to discontinuous constant in scattering term

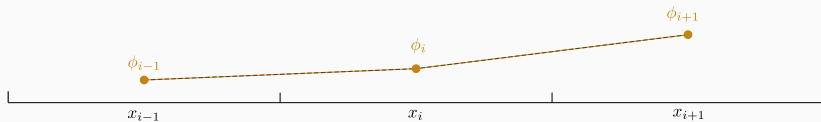
Better: construct a linear dependence from neighboring MFEM cell centers

# Linear Reconstruction



# Linear Reconstruction

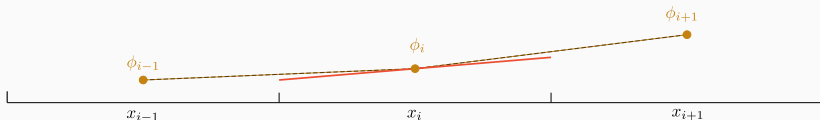
Compute slopes from neighboring cell centers



# Linear Reconstruction

Compute slopes from neighboring cell centers

Generate an average slope from left and right slopes, apply van Leer-type slope limiting

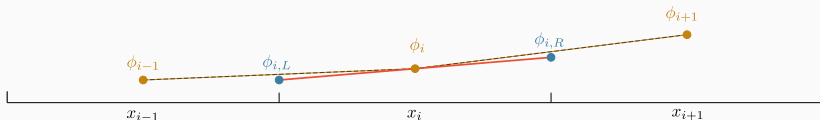


# Linear Reconstruction

Compute slopes from neighboring cell centers

Generate an average slope from left and right slopes, apply van Leer-type slope limiting

Interpolate to cell edge



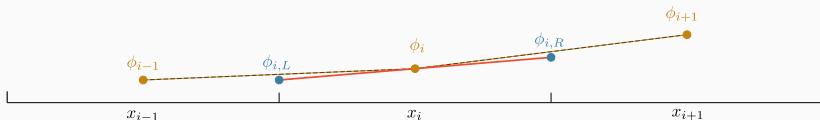


# Linear Reconstruction

Compute slopes from neighboring cell centers

Generate an average slope from left and right slopes, apply van Leer-type slope limiting

Interpolate to cell edge



This method:

- Preserves the cell center value from MFEM
- Reconstructs a linear, discontinuous  $\phi$  from MFEM cell centers only
- Uses slope limiting to prevent unphysical oscillations

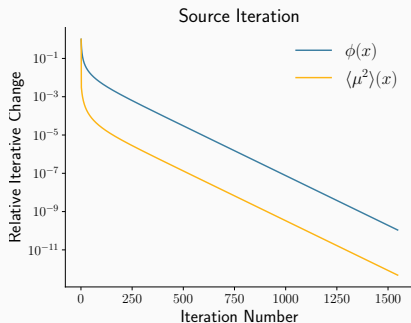
# Computational Results

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# Iterative Convergence Comparison

Relative iterative change (crude measure of iterative convergence)

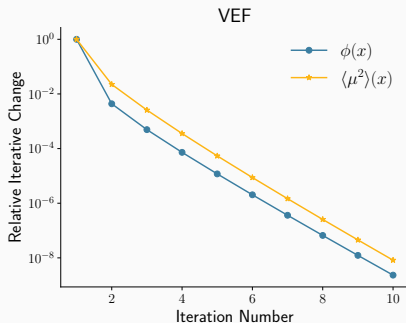
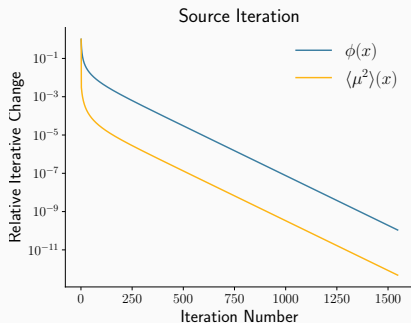
$$\frac{\|f^{\ell+1} - f^{\ell}\|_2}{\|f^{\ell+1}\|_2}$$



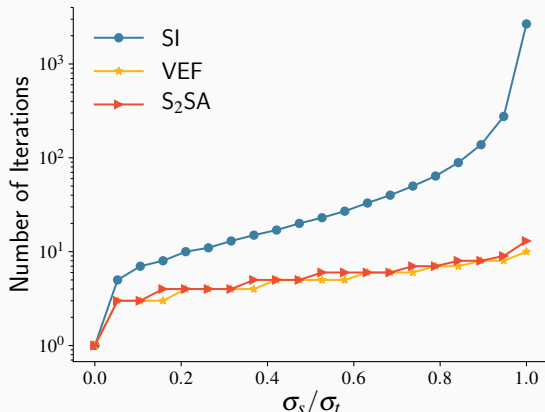
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# Comparison to SI and Consistently Differenced $S_2SA$



**Figure 1:** A comparison of the number of iterations required to converge for Source Iteration, VEF acceleration, and  $S_2SA$  for varying ratios of  $\sigma_s$  to  $\sigma_t$ .

# Method of Manufactured Solutions

Set  $Q(x, \mu_n)$  to force solution to

$$\phi(x) = \sin\left(\frac{\pi x}{x_b}\right)$$

Fit error to

$$E = Ch^p$$

| Update Method | $p$   | $C$   | $R^2$                   |
|---------------|-------|-------|-------------------------|
| Flat          | 1.979 | 1.18  | $9.9999 \times 10^{-1}$ |
| Linear        | 1.988 | 0.786 | $9.9887 \times 10^{-1}$ |

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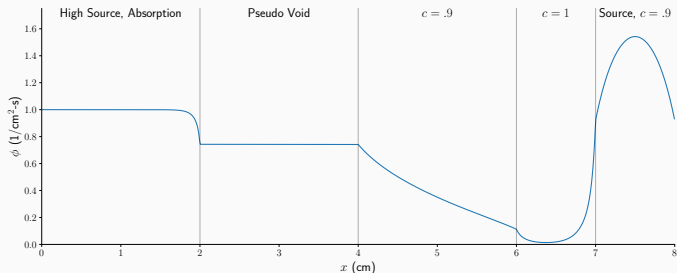
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| Linear        | 1.988 | 0.786 | $9.9887 \times 10^{-1}$ |

Same order of accuracy but linear reconstruction is more accurate

# VEF Drift Diffusion/ $S_N$ Solution Convergence

Compare the  $L_2$  norm of the difference between  $S_N$  and drift diffusion solutions for:

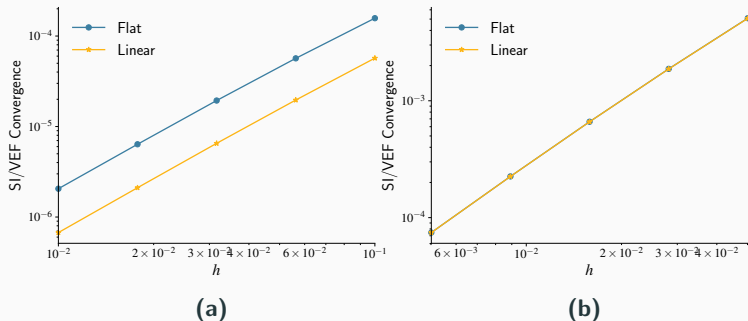
- Homogeneous system with  $\frac{\sigma_s}{\sigma_t} = .99$
- Reed's problem



**Figure 2:** VEF solution for Reed's problem.

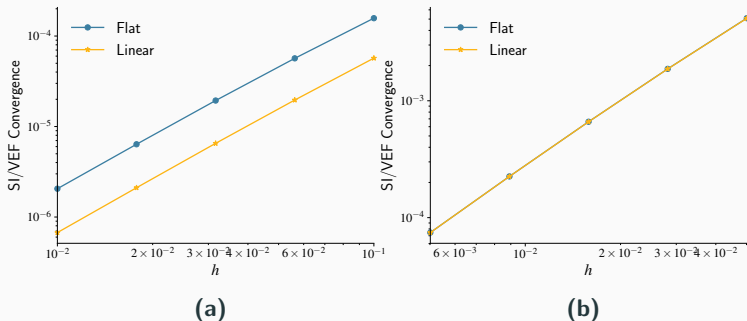


## VEF Drift Diffusion/ $S_N$ Solution Convergence (cont.)



**Figure 3:** Comparison of difference between solutions for both scattering update methods for (a) homogeneous problem and (b) Reed's problem.

## VEF Drift Diffusion/ $S_N$ Solution Convergence (cont.)



**Figure 3:** Comparison of difference between solutions for both scattering update methods for (a) homogeneous problem and (b) Reed's problem.

Linearly reconstructed solution is more accurate for homogeneous problem only

# Thick Diffusion Limit Test

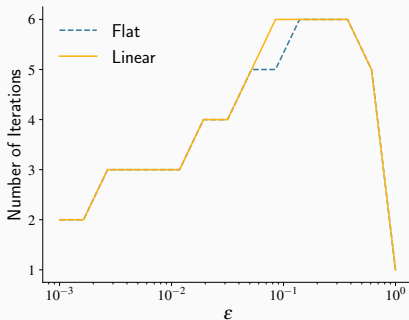
Scale cross sections and source according to:

$$\sigma_t(x) \rightarrow \sigma_t(x)/\epsilon, \quad \sigma_s(x) \rightarrow \epsilon\sigma_s(x), \quad Q(x) \rightarrow \epsilon Q(x)$$

Diffusion length is invariant

$$L^2 = \frac{D}{\sigma_a} = \frac{1}{3\sigma_t\sigma_a} \rightarrow \frac{1}{3\frac{\sigma_t}{\epsilon}\sigma_a\epsilon}$$

As  $\epsilon \rightarrow 0$ , the system becomes diffusive



## Conclusions and Future Work

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# Conclusions

Successfully paired Lumped Linear Discontinuous Galerkin  $S_N$  with constant-linear Mixed Finite Element drift diffusion

Acceleration is as effective as consistently differenced  $S_2SA$

Thick diffusion limit is preserved

Overlap between discretizations:

- Carried linear dependence from LLDG into MFEM
- Used slope reconstruction with limiting to regenerate a linear  $S_N$  source from MFEM

Conservative drift diffusion equation can be coupled to other physics components

Drift diffusion discretization can match other physics components while retaining benefits of DG  $S_N$

Built in error estimator

Extend to high order finite elements in 2/3D

Radiative transfer

Investigate the impact of the linear reconstruction method on the "teleportation effect"

# References

- [1] M. ADAMS AND E. LARSEN, *Fast iterative methods for discrete-ordinates particle transport calculations*, Progress in Nuclear Energy, 40 (2002), pp. 3–159.
- [2] M. L. ADAMS AND W. R. MARTIN, *Diffusion synthetic acceleration of discontinuous finite element transport iterations*, Nuclear Science and Engineering, 111 (1992), pp. 145–167.
- [3] R. ALCOUFFE, *Diffusion synthetic acceleration methods for the diamond-differenced discrete-ordinates equations*, Nuclear Science and Engineering, 64 (1977), pp. 344–355.
- [4] V. DOBREV, T. KOLEV, AND R. RIEBEN, *High-order curvilinear finite element methods for lagrangian hydrodynamics*, SIAM Journal on Scientific Computing, 34 (2012), pp. B606–B641.
- [5] E. W. LARSEN, J. MOREL, AND J. WARREN F. MILLER, *Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes*, Journal of Computational Physics, 69 (1987), pp. 283–324.
- [6] E. W. LARSEN, J. MOREL, AND WARREN F. MILLER, JR., *Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes*, Journal of Computational Physics, 69 (1987), pp. 283–324.
- [7] M. MIFTEN AND E. LARSEN, *The quasi-diffusion method for solving transport problems in planar and spherical geometries*, Journal of Transport Theory and Statistical Physics, 22(2-3) (1992), pp. 165–186.

# References

- [8] J. MOREL AND E. LARSEN, *A multiple balance approach for differencing the  $s_n$  equations*, Nuclear Science and Engineering, 105 (1990), pp. 1–15.
- [9] B. VAN LEER, *Towards the ultimate conservative difference scheme I: The quest for monotonicity*, Lecture Notes in Physics, 18 (1973), pp. 163–168.
- [10] Y. WANG AND J. C. RAGUSA, *Diffusion synthetic acceleration for high-order discontinuous finite element  $s_n$  transport schemes and application to locally refined unstructured meshes*, Nuclear Science and Engineering, 166 (2010), pp. 145–166.
- [11] J. WARSA, T. WAREING, AND J. MOREL, *Fully-consistent diffusion-synthetic acceleration of linear discontinuous  $s_n$  transport discretizations on unstructured tetrahedral meshes*, Nuclear Science and Engineering, 141 (2002), pp. 235–251.



**Questions?**