Variable Eddington Factor Method with Hybrid Spatial Discretization

International Conference on Transport Theory

Novel Numerical Methods

Samuel S. Olivier[1], Jim E. Morel[2]

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[1]Department of Nuclear Engineering, University of California, Berkeley
[2]Department of Nuclear Engineering, Texas A&M University

Berkeley
UNIVERSITY OF CALIFORNIA

Overview

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

Background

Variable Eddington Factor Method

One of the first nonlinear methods for accelerating source iterations

Use S_N to iteratively 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) S$_N$

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

$\Rightarrow$ 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

S_N Equations

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

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

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S_N angular discretization

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

where

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

Source Iteration

Lag scattering term

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

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

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Source Iteration

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

Slow to converge in optically thick and highly scattering systems

VEF Drift Diffusion

Instead, solve

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

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:

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

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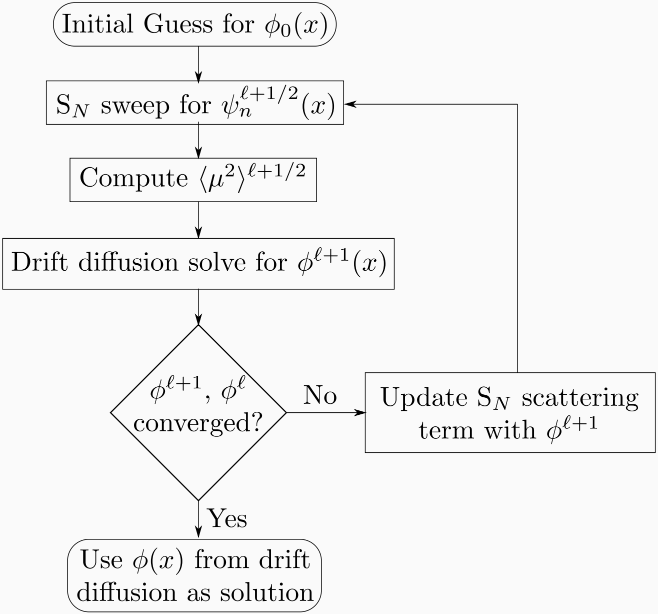
- Angular flux weighted average of μ^2
- Depends on angular shape of the angular flux, not its magnitude

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

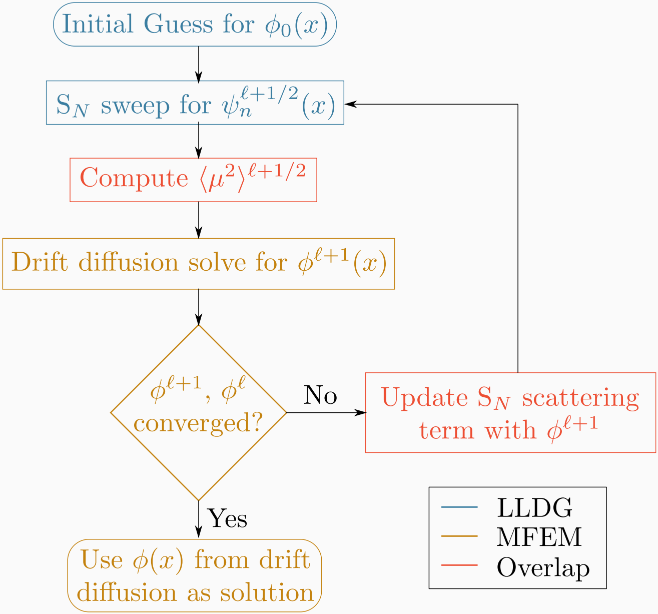
Acceleration Properties

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

Drift diffusion includes scattering


Initial Guess for $\phi_0(x)$
S_N sweep for $\psi_n^{\ell+1/2}(x)$
Compute $\langle \mu^2 \rangle^{\ell+1/2}$
Drift diffusion solve for $\phi^{\ell+1}(x)$
$\phi^{\ell+1}$, ϕ^{ℓ} converged?
No
Update S_N scattering term with $\phi^{\ell+1}$
Yes
Use $\phi(x)$ from drift diffusion as solution

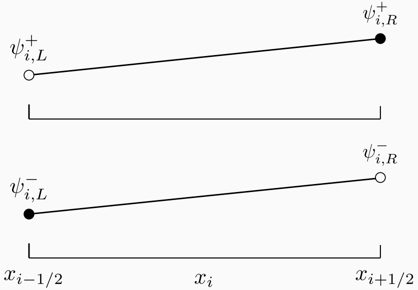
VEF Algorithm



Discretizations

Lumped Linear Discontinuous Galerkin S_N

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



- Within the cell, ψ 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 ψ in Gauss Quadrature

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

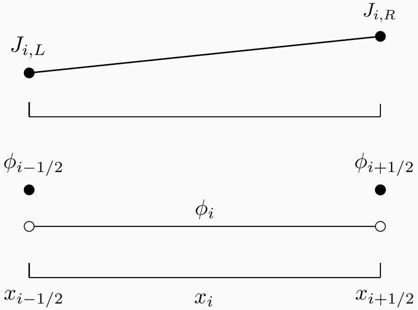
Cell centers: use polynomial interpolation function for the angular flux

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

- 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 (ϕ, J)
- ϕ: constant with discontinuous jumps at the edges
- J: linear discontinuous basis functions (same as in LLDG)



- 5 unknowns per cell
- ϕ and J are doubly defined on the edges but will later be made continuous through enforcing continuity of flux and current

Weak Form

System of first order equations equivalent to drift diffusion:

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

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

Weak Form

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Multiply by ϕ basis function and integrate over cell i:

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

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

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

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Weak Form (cont.)

Integrate by parts:

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

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

Weak Form (cont.)

Integrate by parts:

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

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On the interior:

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

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

where $\langle\mu^2\rangle(x)$ is the rational polynomial shown before

MFEM Closure

3 equations from weak form but 5 unknowns per cell

Enforce continuity of ϕ 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

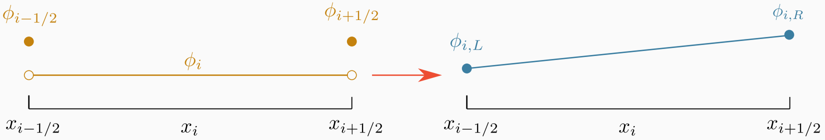
Can then eliminate J and assemble a system of equations of cell centers and edges of ϕ only

Solve resulting Symmetric Positive Definite Matrix with a 5 band solver

Scattering Update Methods

Scattering Update Overlap

Must reconstruct an LLDG-like ϕ from the MFEM drift diffusion ϕ

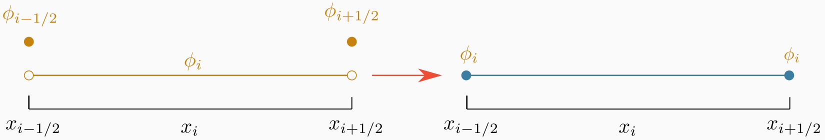


To remain general, reconstruct from cell centers only

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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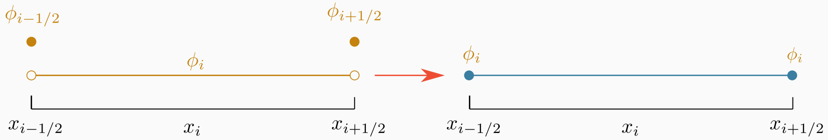
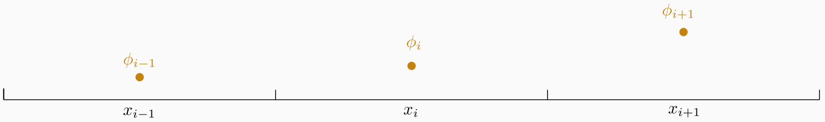


Converts constant MFEM to discontinuous constant in scattering term

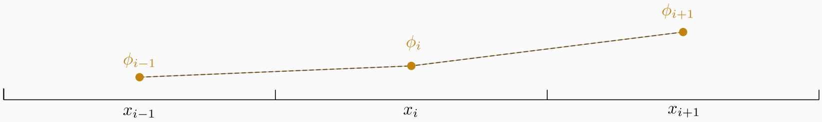
Better: construct a linear dependence from neighboring MFEM cell centers

Linear Reconstruction



Linear Reconstruction

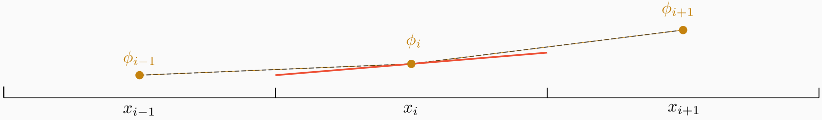
Compute slopes from neighboring cell centers



Linear Reconstruction

Compute slopes from neighboring cell centers

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



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Compute slopes from neighboring cell centers

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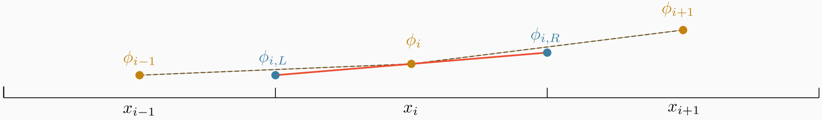
Interpolate to cell edge



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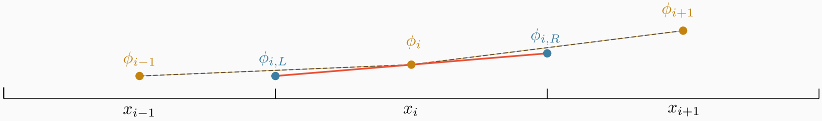


This method:

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

Computational Results

Homogeneous Test Problem

Homogeneous cross sections, source

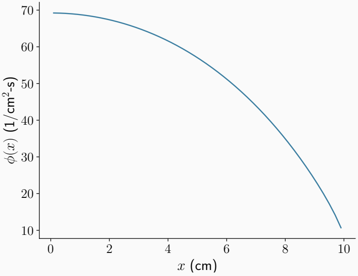
Left reflecting, right vacuum, total thickness of 10 cm

50 uniform spatial cells with S_8 quadrature

Scattering ratio of 0.99 ($\sigma_t = 1\,\frac{1}{\text{cm}}, \sigma_s = 0.99\,\frac{1}{\text{cm}}$)

Source set to $Q = 1\,\frac{\text{particles}}{\text{s}\cdot\text{cm}^3}$

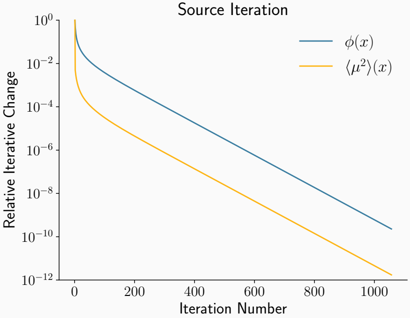
Implemented with Python



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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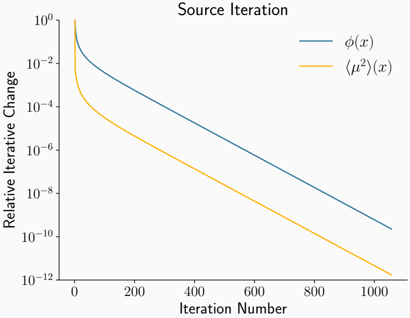

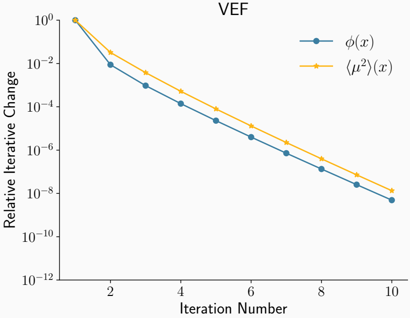

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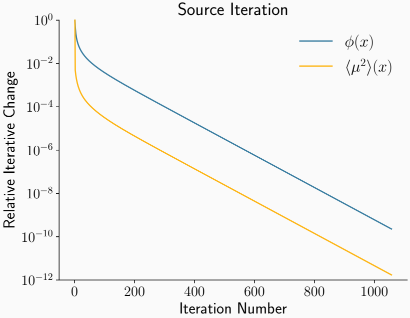
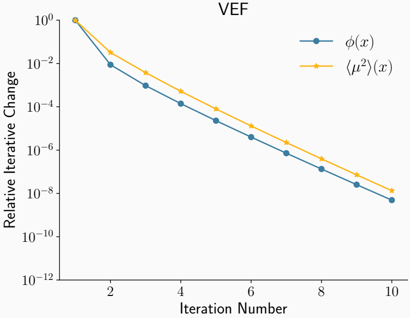
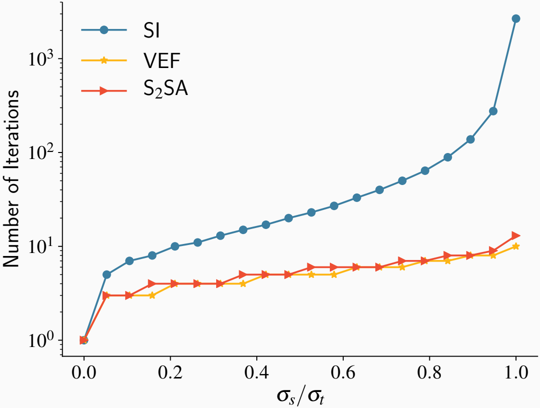




Fast rate of convergence of $\langle\mu^2\rangle(x)$ transfered to $\phi(x)$

Comparison to SI and Consistently Differenced S_2SA



VEF method performs similarly to consistently-differenced S_2SA

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
Flat	1.979	1.18
Linear	1.988	0.786

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Flat	1.979	1.18
Linear	1.988	0.786

Same order of accuracy but linear reconstruction is more accurate

VEF Drift Diffusion/S$_N$ Solution Convergence

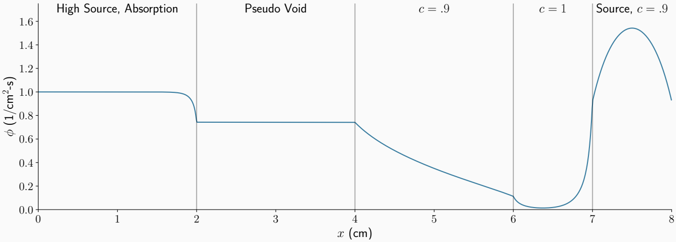
Compare the L$_2$ norm of the difference between S$_N$ and drift diffusion solutions for:

- Homogeneous system with $\frac{\sigma_s}{\sigma_t} = 0.99$

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 $\frac{\sigma_s}{\sigma_t} = 0.99$
- Reed's problem

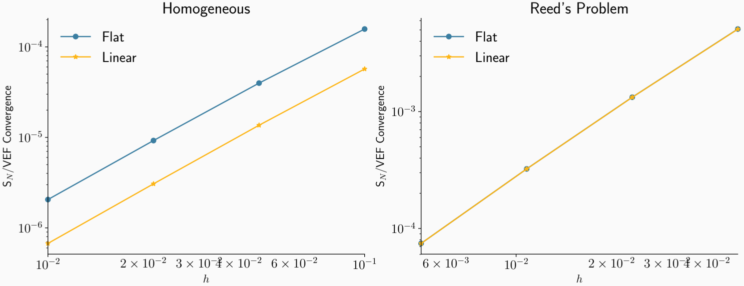


VEF Drift Diffusion/S$_N$ Solution Convergence (cont.)

Compare

$$\frac{\|\phi_{\mathsf{Sn}} - \phi_{\mathsf{VEF}}\|}{\|\phi_{\mathsf{Sn}}\|}$$

as cell spacing is decreased



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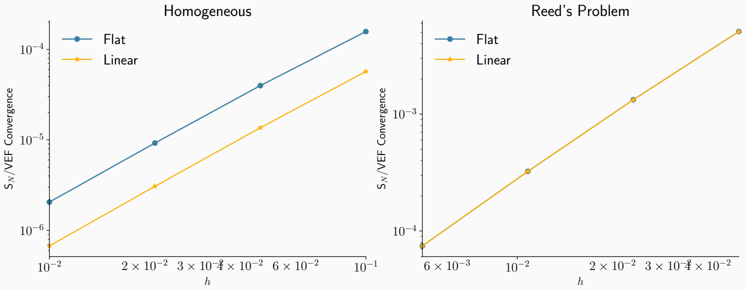


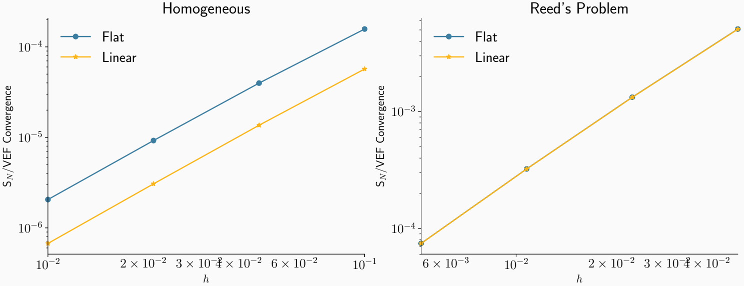
S$_N$ and VEF solutions converge as mesh is refined (difference is $\propto$ LTE)

VEF Drift Diffusion/S$_N$ Solution Convergence (cont.)

Compare

$$\frac{\|\phi_{\mathsf{Sn}} - \phi_{\mathsf{VEF}}\|}{\|\phi_{\mathsf{Sn}}\|}$$

as cell spacing is decreased



S$_N$ and VEF solutions converge as mesh is refined (difference is $\propto$ LTE)

Linear reconstruction was 3 times as convergent in homogeneous case but only 0.1% more convergent in Reed's problem

Thick Diffusion Limit Test

Scale cross sections and source according to:

$$\sigma_t(x) \to \sigma_t(x)/\epsilon,$$

$$\sigma_a(x) \to \epsilon\sigma_a(x),$$

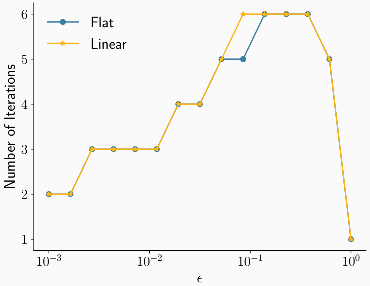
$$Q(x) \to \epsilon Q(x)$$

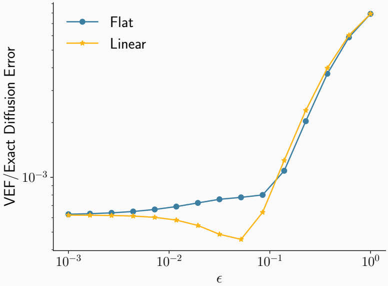
Diffusion length is invariant

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

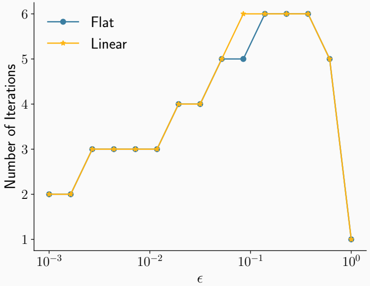
As $\epsilon \to 0$, the system becomes diffusive

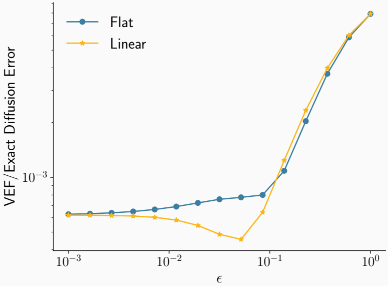
Thick Diffusion Limit Test (cont.)





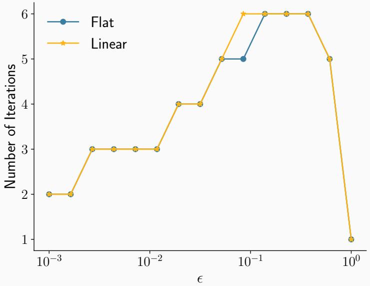
Thick Diffusion Limit Test (cont.)

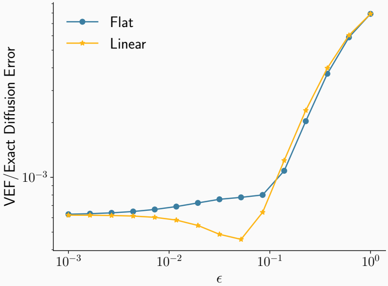




VEF solution $\to$ exact diffusion as $\epsilon \to 0$

Thick Diffusion Limit Test (cont.)





VEF solution $\to$ exact diffusion as $\epsilon \to 0$

Inconsistent discretization still preserves acceleration in thick diffusion limit

Conclusions and Future Work

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$_2$SA

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

Future Work

Extend to high order finite elements in 2/3D

Radiative transfer

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

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Questions?