Variable Eddington Factor Method with Hybrid Spatial Discretization

International Conference on Transport Theory Novel Numerical Methods

Samuel S. Olivier¹, Jim E. Morel² October 19, 2017



 $^{^{1}\}mathsf{Department}$ of Nuclear Engineering, University of California, Berkeley

²Department of Nuclear Engineering, Texas A&M University

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 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 ⇒ 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)
- ullet 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

- ullet VEF drift diffusion is conservative and inexpensive (compared to an S_N sweep)
- Couple drift diffusion to other physics components
- \bullet Can use discretization compatible with other physics while still retaining benefits of DG ${\rm S}_N$

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

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

S_N Equations

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

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

 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

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

Source Iteration

Lag scattering term

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

Source Iteration

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

Source Iteration

Lag scattering term

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

Source Iteration

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

Slow to converge in optically thick and highly scattering systems

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 $\ell+1/2$

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 $\ell+1/2$

Transport information passed through the Variable Eddington Factor:

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

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 $\ell+1/2$

Transport information passed through the Variable Eddington Factor:

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

 \bullet Angular flux weighted average of μ^2

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 $\ell+1/2$

Transport information passed through the Variable Eddington Factor:

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

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

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 $\ell+1/2$

Transport information passed through the Variable Eddington Factor:

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

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

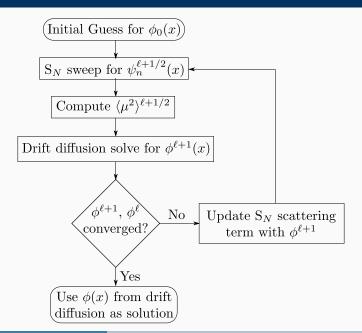
Use $\phi^{\ell+1}$ to update scattering term in S_N sweep or as final solution if converged

Acceleration Properties

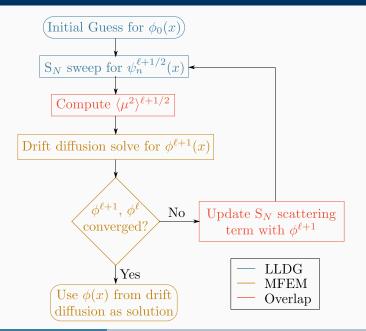
Angular shape of the angular flux, and thus the Eddington factor, converges much faster than the scalar flux $\,$

Drift diffusion includes scattering

VEF Algorithm



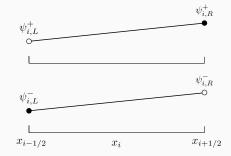
VEF Algorithm



Discretizations

Lumped Linear Discontinuous Galerkin S_N

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



ullet Within the cell, ψ is a linear combination of the basis functions:

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

- ullet 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

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

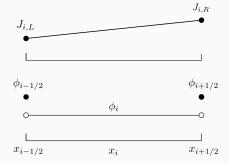
Cell centers: use polynomial interpolation function for the angular flux

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

- ullet 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
- ullet ϕ 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:

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

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

System of first order equations equivalent to drift diffusion:

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

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

Multiply by ϕ basis function and integrate over cell i:

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

System of first order equations equivalent to drift diffusion:

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

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

Multiply by ϕ basis function and integrate over cell i:

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

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

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

System of first order equations equivalent to drift diffusion:

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

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

Multiply by ϕ basis function and integrate over cell i:

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

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

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

Weak Form (cont.)

Integrate by parts:

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

Weak Form (cont.)

Integrate by parts:

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

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

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

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

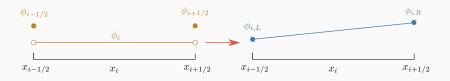
Can then eliminate J and assemble a system of equations of cell centers and edges of ϕ only

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



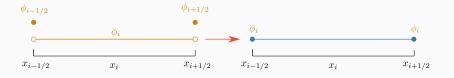
To remain general, reconstruct from cell centers only

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

Flat Scattering Update

Naive: flat update

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

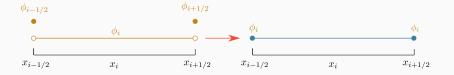


Converts constant MFEM to discontinuous constant in scattering term

Flat Scattering Update

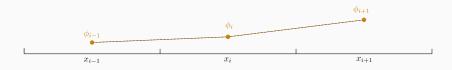
Naive: flat update

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



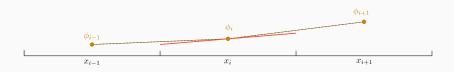
Converts constant MFEM to discontinuous constant in scattering term Better: construct a linear dependence from neighboring MFEM cell centers

Compute slopes from neighboring cell centers



Compute slopes from neighboring cell centers

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



Compute slopes from neighboring cell centers

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

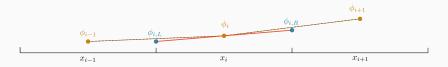
Interpolate to cell edge



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
- \bullet Reconstructs a linear, discontinuous ϕ from MFEM cell centers only
- Uses slope limiting to prevent unphysical oscillations

Computational Results

Iterative Convergence Comparison

Relative iterative change (crude measure of iterative convergence)

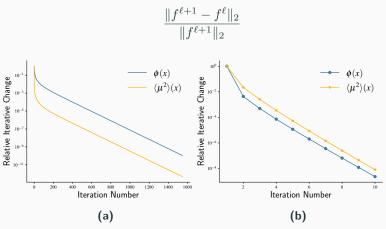


Figure 1: Relative iterative change for $\phi(x)$ and $\langle \mu^2 \rangle(x)$ for (a) unaccelerated and (b) VEF accelerated SI.

Comparison to SI and Consistently Differenced S₂SA

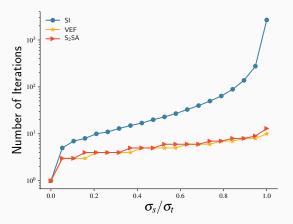


Figure 2: A comparison of the number of iterations required to converge for Source Iteration, VEF acceleration, and S_2SA for varying ratios of σ_s to σ_t .

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	9.9999×10^{-1}
Linear	1.988	0.786	9.9887×10^{-1}

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	9.9999×10^{-1}
Linear	1.988	0.786	9.9887×10^{-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:

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

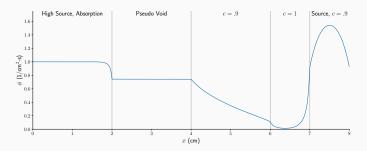


Figure 3: VEF solution for Reed's problem.

VEF Drift Diffusion/ S_N Solution Convergence (cont.)

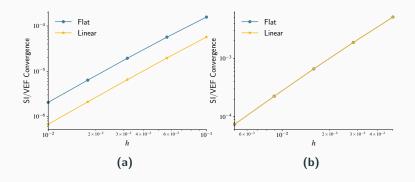


Figure 4: Comparison of difference between solutions for both scattering update methods for (a) homogeneous problem and (b) Reed's problem.

VEF Drift Diffusion/ S_N Solution Convergence (cont.)

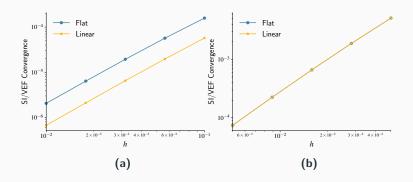


Figure 4: Comparison of difference between solutions for both scattering update methods for (a) homogeneous problem and (b) Reed's problem.

Linearly reconstructed solution is more accurate for homogeneous problem only

Thick Diffusion Limit Test

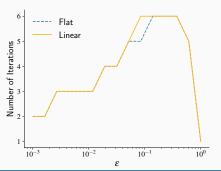
Scale cross sections and source according to:

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

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



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 S₂SA

Thick diffusion limit is preserved

Overlap between discretizations:

- Carried linear dependence from LLDG into MFEM
- ullet Used slope reconstruction with limiting to regenerate a linear ${\sf S}_N$ 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"

References

- 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.
- 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.

