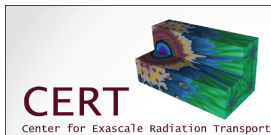


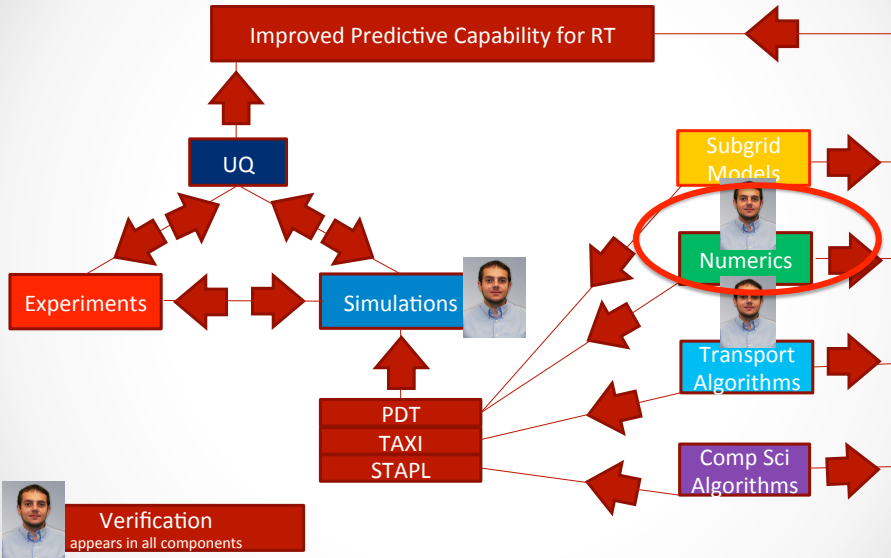
Diffusion Synthetic Acceleration for Massively-Parallel Transport Sweeps using a Discontinuous Finite element Method

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Project Components and Integration



- 1 Motivation for this Work
- 2 Diffusion Synthetic Acceleration on Polytopes using a DFEM technique
 - Brief review of DSA Theory
 - Symmetric Interior Penalty (SIP) Form for Diffusion
 - Modified Interior Penalty (MIP) form for DSA
 - 3D Fourier analysis results
 - MIP-DSA results with PDT
- 3 Acceleration of thermal upscattering iterations
 - Two-grid Acceleration of thermal upscattering
 - Two-grid Fourier analysis results
 - PDT results
- 4 Summary

Motivation

Parallel Transport Sweeps

- Massively-parallel transport sweeps is a mature technology
- PDT's weak scaling demonstrated up to **1.5 million cores** for **logically-block grids** (and ongoing work for parallel transport sweeps on **unstructured grids**)
- Enabling technologies:
 - ① **Discrete ordinates** angular discretization (decouples directions in the streaming+collision transport operator)
 - ② Discontinuous Finite Element Method (**DFEM**) for spatial discretization ("invert the transport operator in a given direction on a cell-by-cell basis")
 - ③ **Aggregation** of spatial cells and angular directions (and energy groups) into work-unit "tasks" and **task scheduling**

Typical Drawbacks of Transport Sweeps

Slow iterative convergence in optically thick configurations, $(\sigma_{t,g} \cdot \text{diam}(\mathcal{D})) \gg 1$

- ① **within an energy group**: $\sigma_s^{g \rightarrow g} / \sigma_{t,g} \approx 1$
- ② **thermal upscattering** when solved using a Gauss-Seidel approach for material with little thermal absorption

Iterative Procedure

Source Iteration

$$\psi^{(\ell+1)} = \mathbf{L}^{-1} \left(\mathbf{M} \boldsymbol{\Sigma} \phi^{(\ell)} + \mathbf{Q} \right)$$

$$\phi^{(\ell+1)} = \mathbf{D} \psi^{(\ell+1)}$$

The operation \mathbf{L}^{-1} is a transport sweep.

Operator Terms

\mathbf{L} - streaming + collision operator

\mathbf{M} - moment-to-discrete operator

$\boldsymbol{\Sigma}$ - scattering operator

$\mathbf{L} = \text{diag}(L_1, \dots, L_{n_\Omega})$

\mathbf{D} - discrete-to-moment operator

\mathbf{Q} - source operator

GMRES equivalent form

Sweep-Preconditioning

$$(\mathbf{I} - \mathbf{D} \mathbf{L}^{-1} \mathbf{M} \boldsymbol{\Sigma}) \boldsymbol{\Phi} = \mathbf{D} \mathbf{L}^{-1} \mathbf{Q}$$

Synthetic Acceleration

Transport sweep and iteration error

$$\mathbf{L}\psi = \mathbf{M}\Sigma\phi + \mathbf{Q}$$

$$\mathbf{L}\psi^{(\ell+1/2)} = \mathbf{M}\Sigma\phi^{(\ell)} + \mathbf{Q} + \mathbf{M}\Sigma(\phi^{(\ell+1/2)} - \phi^{(\ell+1/2)})$$

$$\delta\psi^{(\ell+1/2)} \equiv \psi - \psi^{(\ell+1/2)}$$

$$\delta\phi^{(\ell+1/2)} \equiv \mathbf{D}\delta\psi^{(\ell+1/2)}$$

$$\mathbf{L}\delta\psi^{(\ell+1/2)} - \mathbf{M}\Sigma\delta\phi^{(\ell+1/2)} = \mathbf{M}\Sigma(\phi^{(\ell+1/2)} - \phi^{(\ell)}) = \mathbf{R}^{(\ell+1/2)}$$

Error approximation and update

If we could exactly solve for the error, then the solution could be obtained immediately:

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

However, this is just as difficult as the original transport problem. Instead, we estimate the error using low-order operators:

$$\mathbf{A}\delta\phi^{(\ell+1/2)} = \tilde{\mathbf{R}}^{(\ell+1/2)}$$

\mathbf{A} is a low-order diffusion operator.

Diffusion Synthetic Acceleration

Desirable properties for the diffusion operator \mathbf{A}

- Symmetric Positive-Definite (SPD) in order to use efficient solvers (e.g., CG)
- Availability of suitable preconditioners (e.g., PCG with Algebraic MultiGrid)
- Can handle concave and degenerate polygonal/polyhedral cells
- Discontinuous FEM (same DFEM space as transport to avoid the need for a discontinuous update when using CFEM for diffusion)

$$-\nabla \cdot D \nabla \Phi(\mathbf{r}) + \sigma \Phi(\mathbf{r}) = q(\mathbf{r}), \quad \mathbf{r} \in \mathcal{D}$$

General Boundary Conditions:

$$\begin{aligned} \Phi(\mathbf{r}) &= \Phi_0(\mathbf{r}), & \mathbf{r} \in \partial \mathcal{D}^d \\ -D \partial_n \Phi(\mathbf{r}) &= J_0(\mathbf{r}), & \mathbf{r} \in \partial \mathcal{D}^n \\ \frac{1}{4} \Phi(\mathbf{r}) + \frac{1}{2} D \partial_n \Phi(\mathbf{r}) &= J^{inc}(\mathbf{r}), & \mathbf{r} \in \partial \mathcal{D}^r \end{aligned}$$

Symmetric Interior Penalty (SIP) Form for Diffusion

Weak form: $a(\Phi, b) = \ell(b)$

Bilinear Form

$$\begin{aligned}
 a(\Phi, b) = & \left\langle D \nabla \Phi, \nabla b \right\rangle_{\mathcal{D}} + \left\langle \sigma \Phi, b \right\rangle_{\mathcal{D}} \\
 & + \left\{ \kappa_e^{SIP} [\![\Phi]\!], [\![b]\!] \right\}_{E_h^i} - \left\{ [\![\Phi]\!], \{ \{ D \partial_n b \} \} \right\}_{E_h^i} - \left\{ \{ \{ D \partial_n \Phi \} \}, [\![b]\!] \right\}_{E_h^i} \\
 & + \left\{ \kappa_e^{SIP} \Phi, b \right\}_{\partial \mathcal{D}^d} - \left\{ \Phi, D \partial_n b \right\}_{\partial \mathcal{D}^d} - \left\{ D \partial_n \Phi, b \right\}_{\partial \mathcal{D}^d} + \frac{1}{2} \left\{ \Phi, b \right\}_{\partial \mathcal{D}^r}
 \end{aligned}$$

Linear Form

$$\begin{aligned}
 \ell(b) = & \left\langle q, b \right\rangle_{\mathcal{D}} - \left\{ J_0, b \right\}_{\partial \mathcal{D}^n} + 2 \left\{ J_{inc}, b \right\}_{\partial \mathcal{D}^r} \\
 & + \left\{ \kappa_e^{SIP} \Phi_0, b \right\}_{\partial \mathcal{D}^d} - \left\{ \Phi_0, D \partial_n b \right\}_{\partial \mathcal{D}^d}
 \end{aligned}$$

SIP Penalty Coefficient

$$\kappa_e^{SIP} \equiv \begin{cases} \frac{C_B}{2} \left(\frac{D^+}{h^+} + \frac{D^-}{h^-} \right) & , e \in E_h^i \\ C_B \frac{D^-}{h^-} & , e \in \partial\mathcal{D} \end{cases}$$

$$C_B = cp(p+1)$$

c - user defined constant ($c \geq 1$)

p - polynomial order of the finite element basis (1, 2, 3, ...)

$D^{(+/-)}$ - diffusion coefficient defined on the positive/negative side of a face

$h^{(+/-)}$ - orthogonal projection defined on the positive/negative side of a face

$$[[u]] := u^+ - u^- \quad \{\{u\}\} := \frac{u^+ + u^-}{2}$$

$$u^\pm = \lim_{s \rightarrow 0^\pm} u(\mathbf{r} + s\mathbf{n})$$

Modified Interior Penalty (MIP) Form

Recall the DSA equation:

$$\mathbf{A}\delta\phi^{(\ell+1/2)} = \tilde{\mathbf{R}}^{(\ell+1/2)}$$

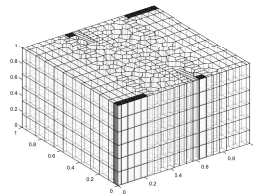
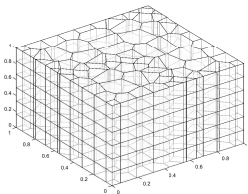
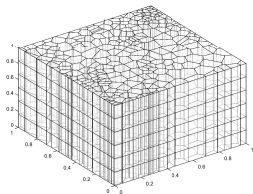
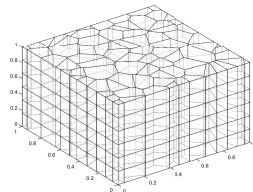
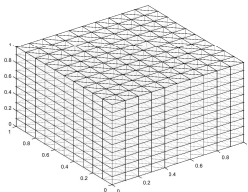
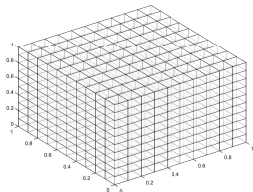
DSA Form

$$\begin{aligned} & \langle D\nabla\delta\Phi, \nabla b \rangle_{\mathcal{D}} + \langle \sigma\delta\Phi, b \rangle_{\mathcal{D}} \\ & + \left\{ \kappa_e^{MIP} \llbracket \delta\Phi \rrbracket, \llbracket b \rrbracket \right\}_{E_h^i} - \left\{ \llbracket \delta\Phi \rrbracket, \{ \{ D\partial_n b \} \} \right\}_{E_h^i} - \left\{ \{ \{ D\partial_n \delta\Phi \} \}, \llbracket b \rrbracket \right\}_{E_h^i} \\ & + \frac{1}{2} \left\{ \delta\Phi, b \right\}_{\partial\mathcal{D}^{vac}} = \langle R, b \rangle_{\mathcal{D}} - \left\{ \delta J_{inc}, b \right\}_{\partial\mathcal{D}^{ref}} \end{aligned}$$

MIP Penalty Term

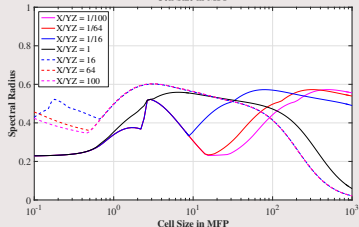
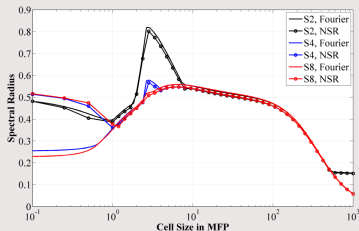
$$\kappa_e^{MIP} = \max \left(\frac{1}{4}, \kappa_e^{SIP} \right)$$

3D DFEM DSA Analysis

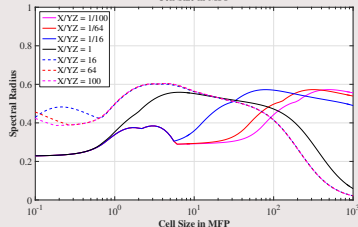
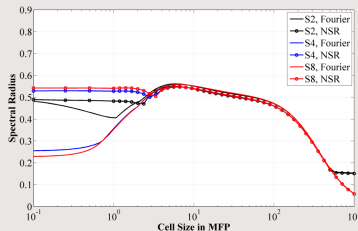


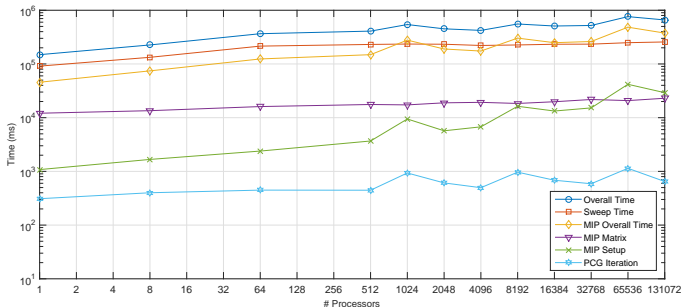
Fourier analysis - 3D PWL basis functions

$c = 1$



$c = 4$



MIP DSA Timing Data with PDT on Vulcan using **HYPRE**

Problem Description

- Modified Zerr problem - used optimal sweep aggregation parameters
 - homogeneous cube - about 500 mfp and $c=0.9999$
 - S_8 level-symmetric quadrature (80 directions total)
- pointwise convergence tolerance of $1e-8$
- SI precondition with MIP DSA using **HYPRE PCG and AMG** (~ 22 SI @ high core counts, and ~ 10 CG iters/DSA)

Two-Grid Acceleration - Ideal for graphite and heavy-water configurations

Multigroup system of equations

Gauss-Seidel iterations over thermal groups:

$$\mathbf{L}_{gg} \psi_g^{(k+1/2)} = \mathbf{M} \sum_{g'=0}^g \Sigma_{gg'} \phi_{g'}^{(k+1/2)} + \mathbf{M} \sum_{g'=g+1}^G \Sigma_{gg'} \phi_{g'}^{(k)} + \mathbf{Q}_g$$

Error and residual

$$\mathbf{L}_{gg} \delta \psi_g^{(k+1/2)} = \mathbf{M} \sum_{g'=0}^g \Sigma_{gg'} \delta \phi_{g'}^{(k+1/2)} + \mathbf{R}_g^{(k+1/2)}$$

$$\mathbf{R}_g^{(k+1/2)} = \mathbf{M} \sum_{g'=g+1}^G \Sigma_{gg'} \left(\phi_{g'}^{(k+1/2)} - \phi_{g'}^{(k)} \right)$$

Solution update

$$\delta \phi_g^{(k+1/2)} = \epsilon^{(k+1/2)} \xi_g, \quad \sum_{g=0}^G \xi_g = 1$$

$$(\Sigma_t - \text{tril}(\Sigma_s)^{-1}) \text{triu}(\Sigma_s) \xi = \rho \xi$$

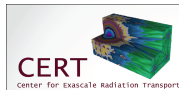
1G Error Diffusion System

$$\nabla \cdot \langle D \rangle \nabla \epsilon + \langle \sigma \rangle \epsilon = \langle R \rangle$$

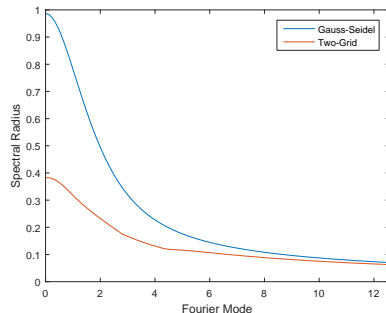
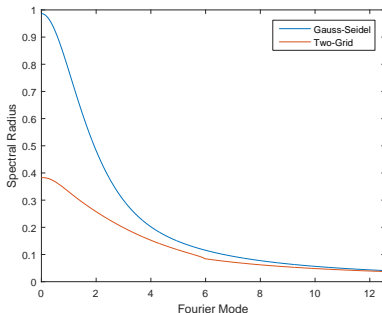
$$\langle D \rangle = \sum_{g=0}^G D_g \xi_g$$

$$\langle \sigma \rangle = \sum_{g=0}^G \left(\sigma_{t,g} \xi_g - \sum_{g'=0}^G \sigma_{s,0}^{gg'} \xi_{g'} \right)$$

$$\langle R \rangle = \sum_{g=0}^G R_g^{(k+1/2)} \xi_g$$



Two-Grid Acceleration - Fourier analysis results (P_0 and P_1 scattering)



Two-grid acceleration implementation in PDT

- Successfully implemented and debugged
 - Includes non-orthogonal mesh configurations
 - Includes multi-material configurations
- Have tested the two-grid methodology on a homogeneous graphite block as well as a block with an air duct
- Iteration counts for a very large configuration (very optically thick) are similar to simple infinite medium calculations

Example: S_8 level-symmetric quadratures, 64,000 spatial DOFs, 99 energy groups (IM1 XS-data), run locally on 8 procs.

Materials	Unaccelerated Iterations	Accelerated Iterations
Graphite Only	2027	21
Graphite + Air Duct	2138	23

Materials	Unaccelerated Solve Time	Accelerated Solve Time
Graphite Only	51.67 hours	31.23 minutes
Graphite + Air Duct	54.5 hours	35.56 minutes



Work Summary and Status

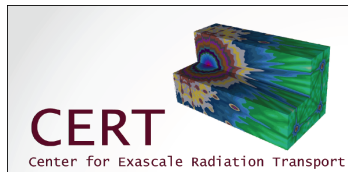
DFEM Diffusion as an accelerator

- Successfully developed and implemented an Modified Interior Penalty DFEM method as a diffusion synthetic accelerator for both
 - ① within group iterations and
 - ② thermal upscattering iterations
- MIP-DSA leads to symmetric positive definite matrices (PCG with AMG through HYPRE)
- Excellent initial scaling results with PDT up to 132,000 cores.

Next steps

- Push into PDT's trunk repository
- Further scaling tests
- Apply to IM-1 experiments

Questions?

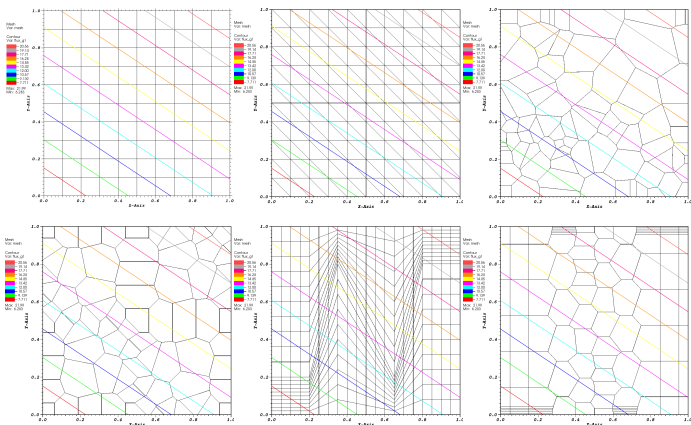


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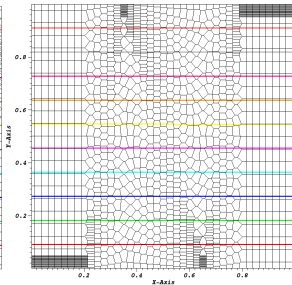
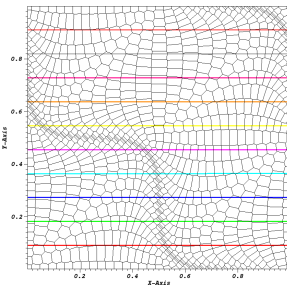
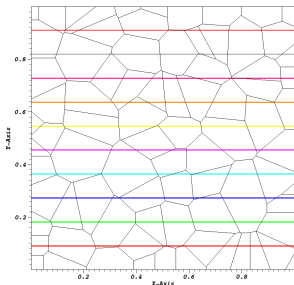
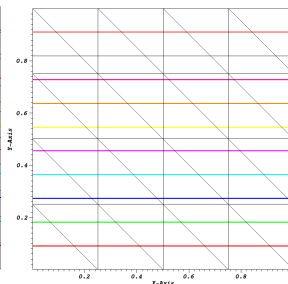
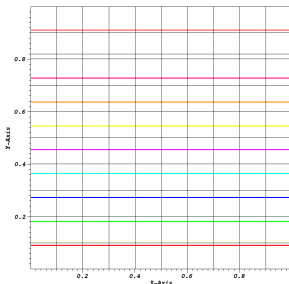
2D Exactly-Linear Transport Solutions - mean value coordinates

$$\mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \sigma_t \psi = Q(x, y, \mu, \eta)$$

$$\psi(x, y, \mu, \eta) = ax + by + c\mu + d\eta + e, \quad \phi(x, y) = 2\pi(ax + by + e)$$



SIP exactly linear solutions on 3D polyhedral meshes using the PWL basis functions



SIP convergence study - gaussian solution on 3D cube using the PWL basis functions

$$\Phi(x, y, z) = xyz(L_x - x)(L_y - y)(L_z - z) \exp(-(\mathbf{r} - \mathbf{r}_0) \cdot (\mathbf{r} - \mathbf{r}_0))$$

$$L_x = L_y = L_z = 1.0, \quad \mathbf{r}_0 = (3/4, 3/4, 3/4)$$

