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

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Outline

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, $(\sigma_{t,g} \cdot \mathrm{diam}(\mathcal{D})) \gg 1$

1. within an energy group: $\sigma_s^{g \to g} / \sigma_{t,g} \approx 1$
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
- $\mathbf{L} = diag(L_1, \ldots, L_{n_\Omega})$
- $\mathbf{D}$ - 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:

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

A is a low-order diffusion operator.

Diffusion Synthetic Acceleration

Desirable properties for the diffusion operator **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)

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

General Boundary Conditions:

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

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Symmetric Interior Penalty (SIP) Form for Diffusion

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

Bilinear Form

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

Linear Form

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

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

$$[\![u]\!] := u^+ - u^- \qquad \{\{u\}\} := \frac{u^+ + u^i}{2}$$

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

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Modified Interior Penalty (MIP) Form

Recall the DSA equation:

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

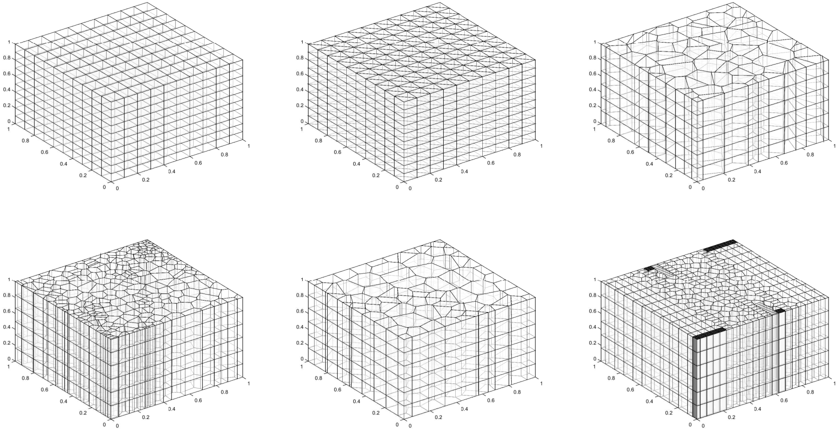
DSA Form

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

MIP Penalty Term

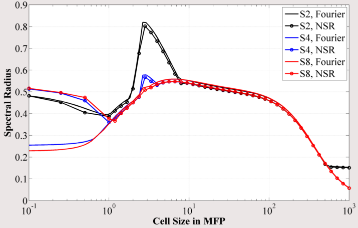
$$\kappa_e^{MIP} = \max\left(\frac{1}{4}, \kappa_e^{SIP}\right)$$

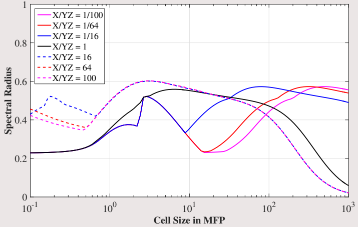
3D DFEM DSA Analysis



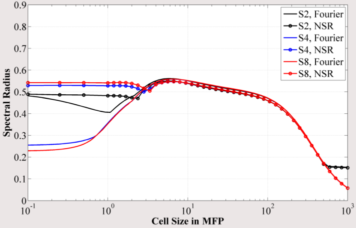
Fourier analysis - 3D PWL basis functions

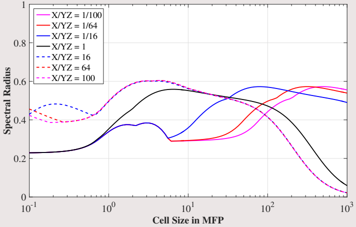
$c = 1$





$c = 4$





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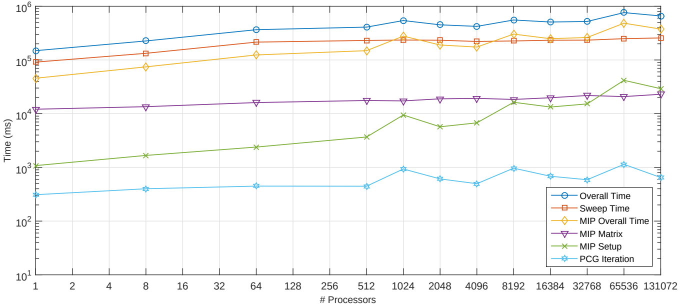
MIP DSA Timing Data with PDT on Vulcan using HYPRE



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:

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

Error and residual

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

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

Solution update

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

$$\left(\mathbf{\Sigma}_\mathbf{t} - tril(\mathbf{\Sigma}_\mathbf{s})^{-1}\right) triu(\mathbf{\Sigma}_\mathbf{s})\xi = \rho\xi$$

1G Error Diffusion System

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

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

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

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

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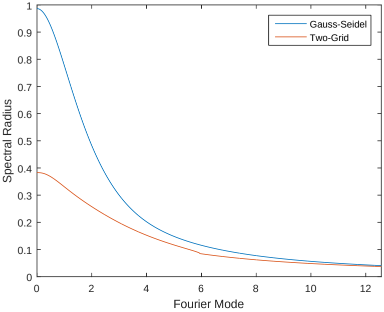
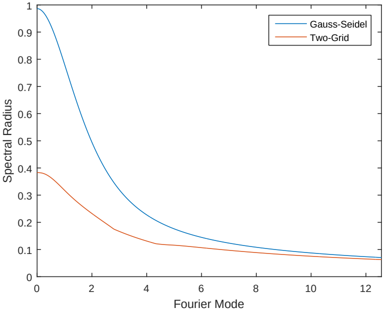
Two-Grid Acceleration - Fourier analysis results (P_0 and P_1 scattering)





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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

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Thank you

Questions?

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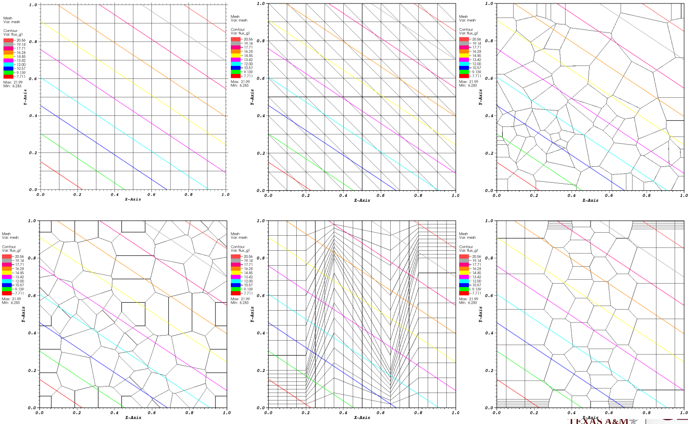
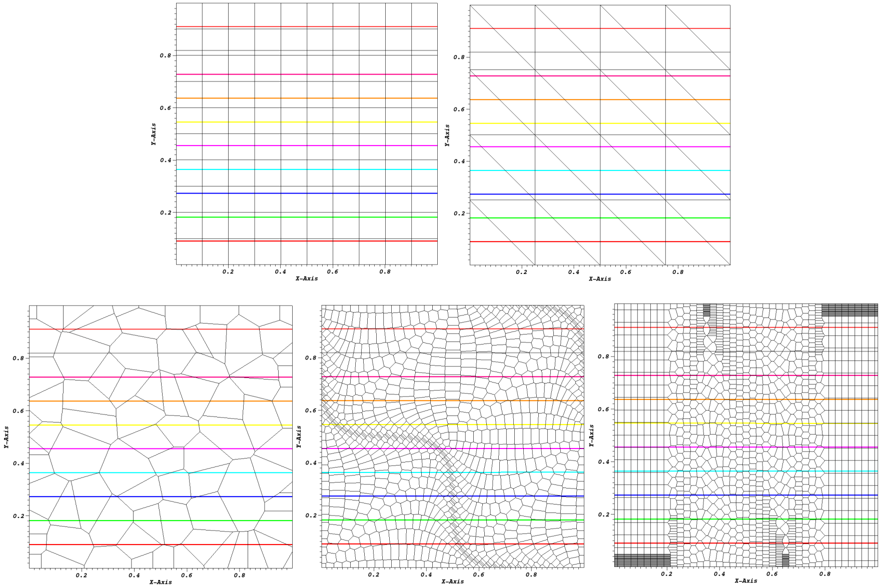
2D Exactly-Linear Transport Solutions - mean value coordinates

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

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

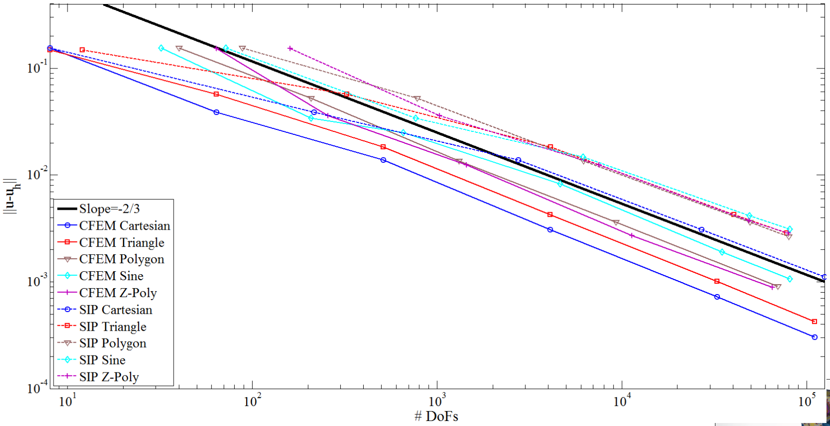


SIP exactly linear solutions on 3D polyhedral meshes using the PWL basis functions



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

$$\Phi(x,y,z) = xyz(L_x - x)(L_y - y)(L_z - z)\exp(-(\mathbf{r}-\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0))$$
$$L_x = L_x = L_x = 1.0, \qquad \mathbf{r}_0 = (3/4, 3/4, 3/4)$$



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