Higher-Order DGFEM Transport Calculations on Polytope Meshes for Massively-Parallel Architectures

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Outline

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   - Polytope Grid Motivation
2. Polytope Finite Element Basis Functions
   - Linear Basis Functions on 2D Polygons
   - Quadratic Serendipity Basis Functions on 2D Polygons
   - Linear Basis Functions on 3D Polyhedra
3. Diffusion Synthetic Acceleration on Polytopes
   - Theory
   - MIP Diffusion Form
4. Proposed Work and Current Status
5. Ongoing Work

The Continuous-Energy Transport Equation

Transport Equation

$$[\mathbf{\Omega} \cdot \nabla + \sigma_t(\mathbf{r}, E)]\, \psi(\mathbf{r}, E, \mathbf{\Omega}) = \int_{4\pi} \int_0^{\infty} \sigma_s(\mathbf{r}, E', E, \mathbf{\Omega}', \mathbf{\Omega}) \psi(\mathbf{r}, E', \mathbf{\Omega}') dE' d\Omega' + Q(\mathbf{r}, E, \mathbf{\Omega})$$

Boundary Conditions

$$\psi(\mathbf{r}, E, \mathbf{\Omega}) = \psi^{inc}(\mathbf{r}, E, \mathbf{\Omega}) + \int_{4\pi} \int_0^{\infty} \beta(\mathbf{r}, E', E, \mathbf{\Omega}', \mathbf{\Omega}) \psi(\mathbf{r}, E', \mathbf{\Omega}') dE' d\Omega'$$

Term Definitions

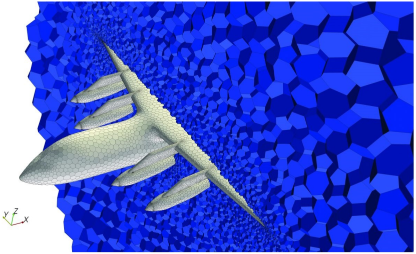
$\mathbf{r}$ - neutron position
E - neutron energy
$\mathbf{\Omega}$ - neutron solid angle
$\psi(\mathbf{r}, E, \mathbf{\Omega})$ - angular flux
$Q(\mathbf{r}, E, \mathbf{\Omega})$ - distributed neutron source
$\sigma_t(\mathbf{r}, E)$ - total macroscopic cross section
$\sigma_s(\mathbf{r}, E', E, \mathbf{\Omega}', \mathbf{\Omega})$ - total macroscopic scattering cross section
$\beta(\mathbf{r}, E', E, \mathbf{\Omega}', \mathbf{\Omega})$ - boundary albedo

Energy and Angular Discretization

Spatial Discretization

Polytope Grid Motivation

- Other physics communities are now employing polytope grids due to decreased cell/face counts (CFD in particular)
- They allow for transition elements between different domain regions
- Hanging nodes from non-conforming meshes are not necessary
- Independently-generated simplicial grids (*i.e.* created in parallel) can be stitched together with polytopes without communicating the whole mesh across processors



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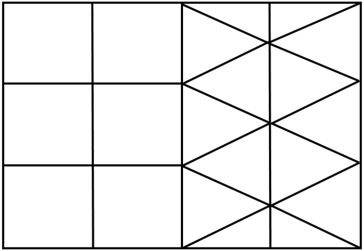

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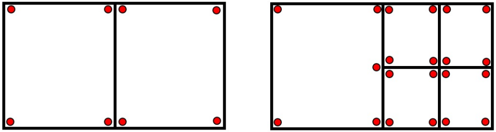

(a) (b)

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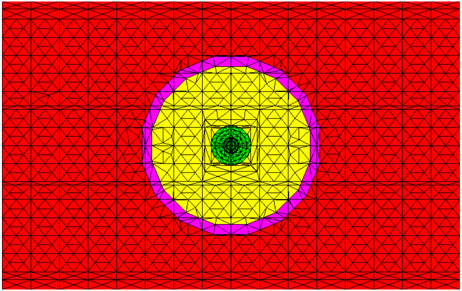
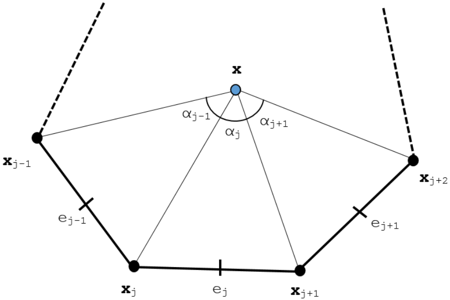


Arbitrary Polygon and Definitions



2D Linear Basis Function Properties - Barycentric Coordinates

1. $\lambda_i \geq 0$
2. $\sum_i \lambda_i = 1$
3. $\sum_i \mathbf{x}_i \lambda_i(\mathbf{x}) = \mathbf{x}$
4. $\lambda_i(\mathbf{x}_j) = \delta_{ij}$

Wachspress Rational Functions

Piecewise Linear Functions

Mean Value Coordinates

Maximum Entropy Coordinates

Quadratic Serendipity Basis Functions on 2D Polygons

Linear Basis Functions on 3D Polyhedra

The Diffusion Equation and Boundary Conditions

The Diffusion Equation

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

Boundary Conditions

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

Symmetric Interior Penalty (SIP) Form

Bilinear Form

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

Linear Form

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

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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

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

Modified Interior Penalty (MIP) Form

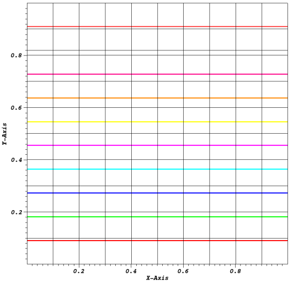
Diffusion Form

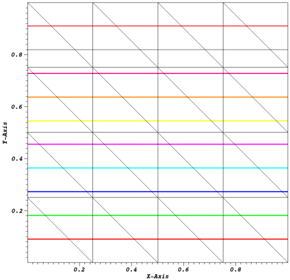
$$\left\langle D\nabla\Phi, \nabla b\right\rangle_{\mathcal{D}} + \left\langle \sigma\Phi, b\right\rangle_{\mathcal{D}}$$
$$+\left\{\kappa_e^{MIP}[\![\Phi]\!], [\![b]\!]\right\}_{E_h^i} - \left\{[\![\Phi]\!], \{\{D\partial_n b\}\}\right\}_{E_h^i} - \left\{\{\{D\partial_n\Phi\}\}, [\![b]\!]\right\}_{E_h^i}$$
$$+\left\{\kappa_e^{MIP}\Phi, b\right\}_{\partial\mathcal{D}^{vac}} - \frac{1}{2}\left\{\Phi, D\partial_n b\right\}_{\partial\mathcal{D}^{vac}} - \frac{1}{2}\left\{D\partial_n\Phi, b\right\}_{\partial\mathcal{D}^{vac}}$$
$$= \left\langle q, b\right\rangle_{\mathcal{D}}$$

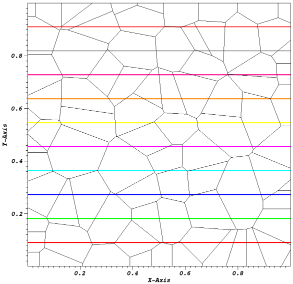
MIP Penalty Term

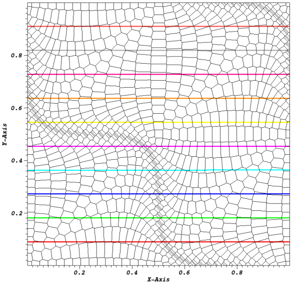
$$\kappa_e^{MIP} = \max(\frac{1}{4}, \kappa_e^{SIP})$$

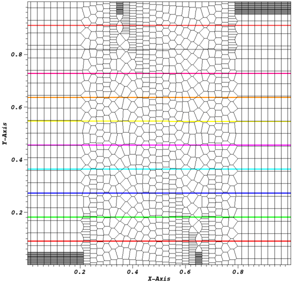
SIP exactly linear solutions on 3D polyhedral meshes using the PWL basis functions





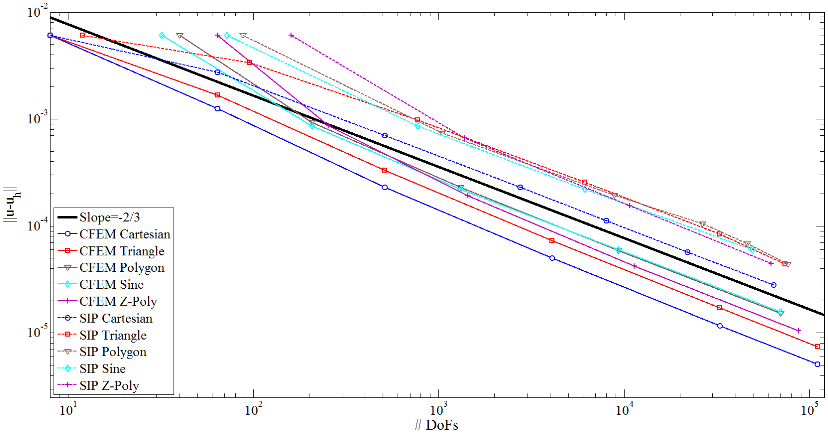






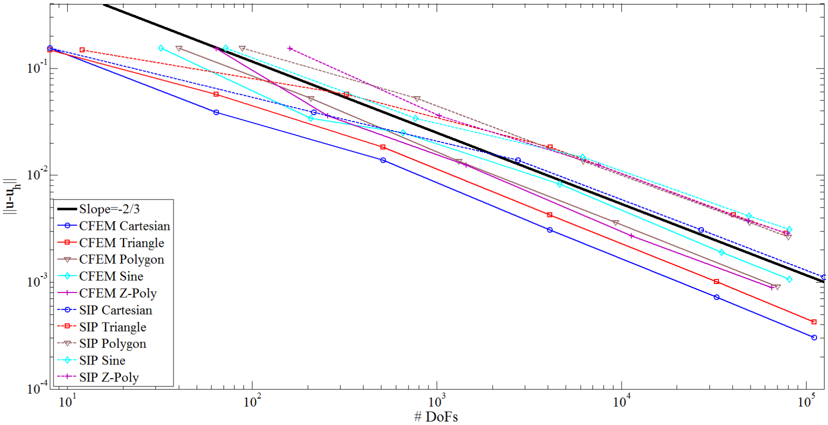
SIP convergence study - quadratic solution on 3D cube using the PWL basis functions

$$\Phi(x,y,z) = xyz(L_x - x)(L_y - y)(L_z - z)$$
$$L_x = L_x = L_x = 1.0$$

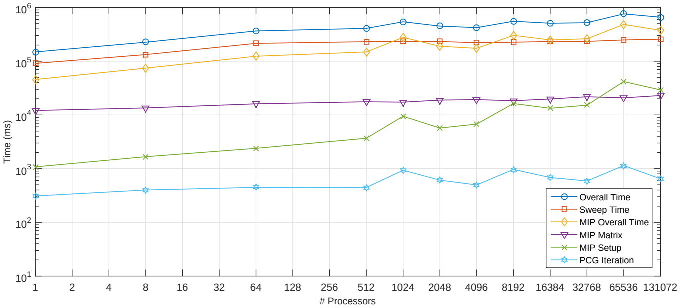


SIP convergence study - gaussian solution on 3D cube using the PWL basis functions

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



MIP DSA Timing Data with PDT on Vulcan using HYPRE



Problem Description

- Modified Zerr problem - used optimal sweep aggregation parameters
  - homogeneous cube - c=0.9999
  - $S8$ level-symmetric quadrature
- pointwise convergence tolerance of 1e-8
- precondition with MIP DSA using HYPRE PCG and AMG

Questions?

A special acknowledgment to the Department of Energy Rickover Fellowship Program in Nuclear Engineering, which provides strong support to its fellows and their professional development.

A stretch goal is to compare my method to Monte Carlo

I claim the following is the best way to show our method has practical importance, because continuous-energy Monte Carlo codes do exact particle tracking / kinematics and use very accurate cross sections. Such codes may attain higher fidelity in all respects than DRAGON.

Start with a 0-D problem to isolate energy discretization effects

1. Come up with a reactor-themed problem
2. Solve the same problem in PDT and MCNP or OpenMC
3. Choose QOI, such as k-eigenvalue, radial power profile, absorption/fission rates per nuclide, etc.
4. Quantify how errors in PDT's QOI change as energy resolution is increased

Build up problem complexity slowly: cylindricized pin cell with white boundary conditions, infinite lattice of pin cells, heterogeneous lattice of pin cells, etc.

1. Quantify how errors in PDT's QOI change as spatial / angular / scattering moment resolution is increased
2. Quantify how errors in PDT's QOI change as energy resolution is increased
3. ...
4. Profit

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