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

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Outline

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

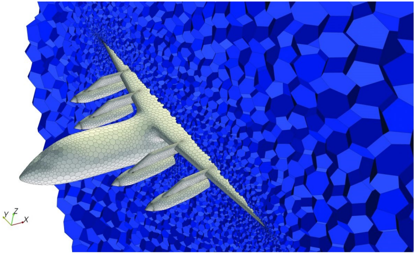
$\mathbf{r}$ - neutron position
E - neutron energy
$\mathbf{\Omega}$ - neutron solid angle
$\psi(\mathbf{r}, E, \mathbf{\Omega})$ - angular flux
$Q(\mathbf{r}, E, \mathbf{\Omega})$ - distributed neutron source
$\sigma_t(\mathbf{r}, E)$ - total macroscopic cross section
$\sigma_s(\mathbf{r}, E', E, \mathbf{\Omega}',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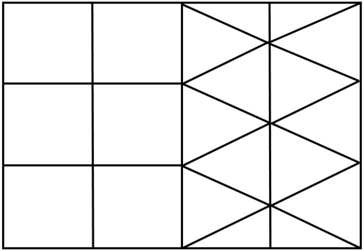

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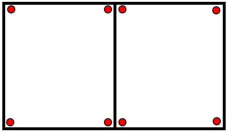
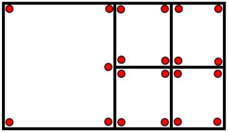


(a)



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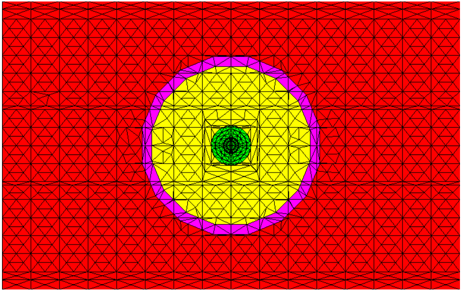
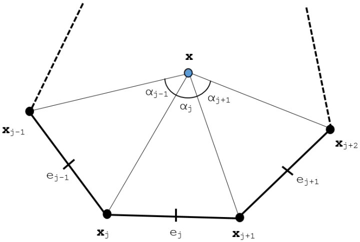


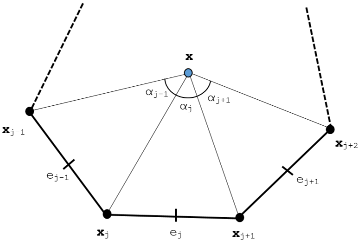
Arbitrary Polygon and Definitions



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. $\lambda_i(\mathbf{x}_j) = \delta_{ij}$

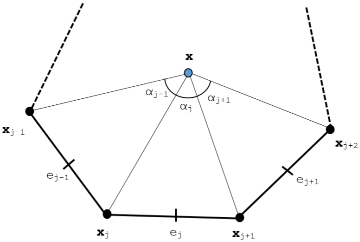
Wachspress Rational Functions



$$\lambda_i^W(\mathbf{x}) = \frac{w_i(\mathbf{x})}{\sum_j w_j(\mathbf{x})}, \qquad w_j(\mathbf{x}) = \frac{A(\mathbf{x}_{j-1}, \mathbf{x}_j, \mathbf{x}_{j+1})}{A(\mathbf{x}, \mathbf{x}_{j-1}, \mathbf{x}_j)\, A(\mathbf{x}, \mathbf{x}_j, \mathbf{x}_{j+1})}$$

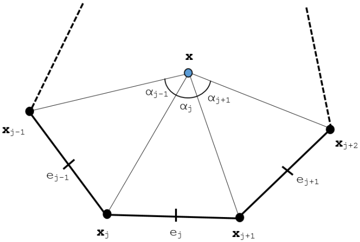
Piecewise Linear Functions

Mean Value Coordinates



$$\lambda_i^{MV}(\mathbf{x}) = \frac{w_i(\mathbf{x})}{\sum_j w_j(\mathbf{x})}, \qquad w_j(\mathbf{x}) = \frac{\tan(\alpha_{j-1}/2) + \tan(\alpha_j/2)}{|\mathbf{x}_j - \mathbf{x}|}$$

Maximum Entropy Coordinates



$$\lambda_i^{ME}(\mathbf{x}) = \frac{w_i(\mathbf{x})}{\sum_j w_j(\mathbf{x})}, \qquad w_j(\mathbf{x}) = m_j(\mathbf{x}) \exp(-\omega \cdot (\mathbf{x}_j - \mathbf{x}))$$

Summary of the 2D Linear Basis Functions

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

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

Linear Form

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

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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

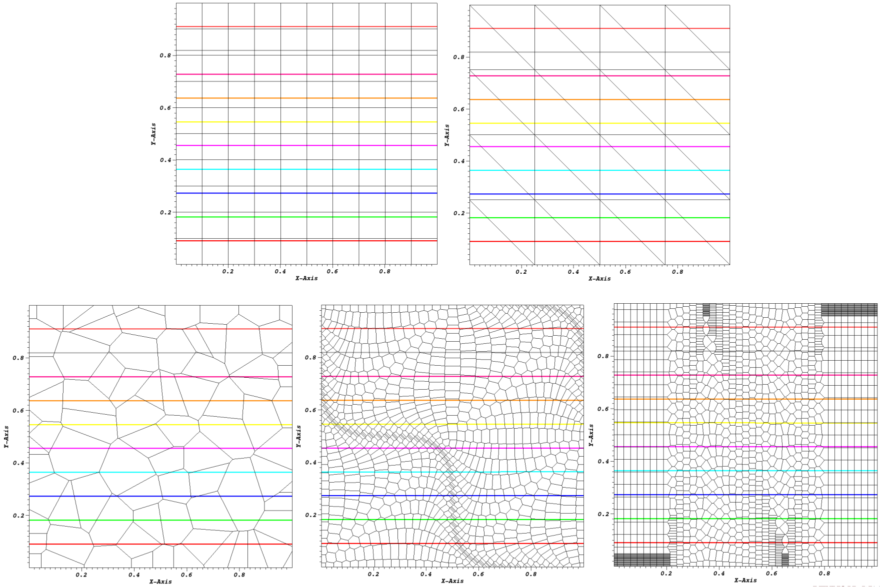
Diffusion Form

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

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



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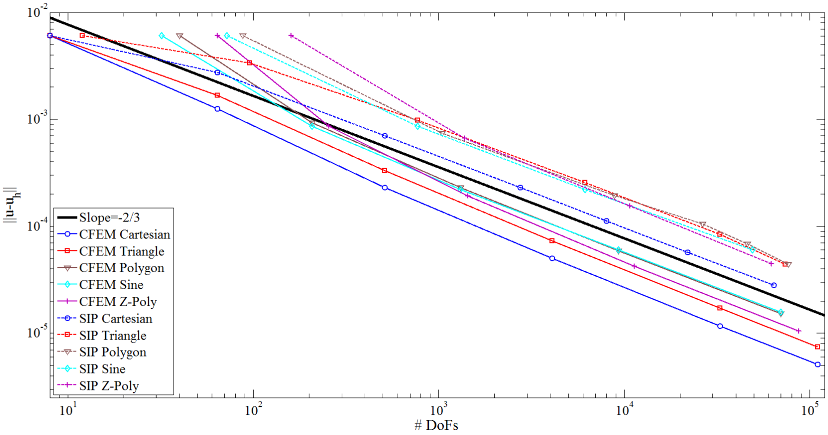
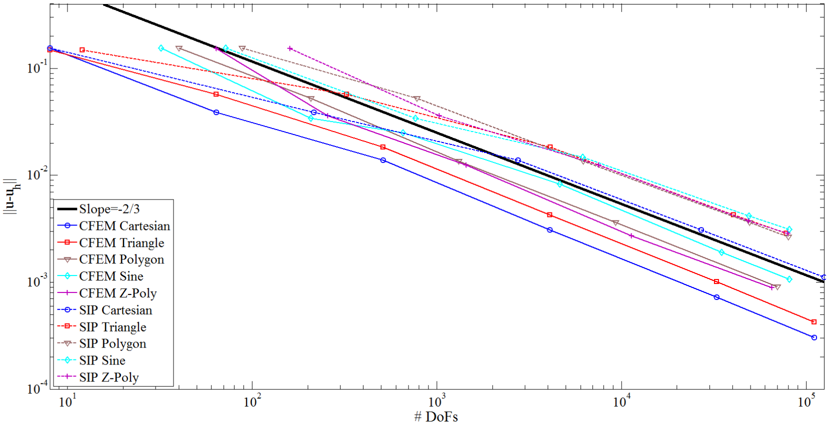
SIP convergence study - quadratic solution on 3D cube using the PWL basis functions

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



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

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



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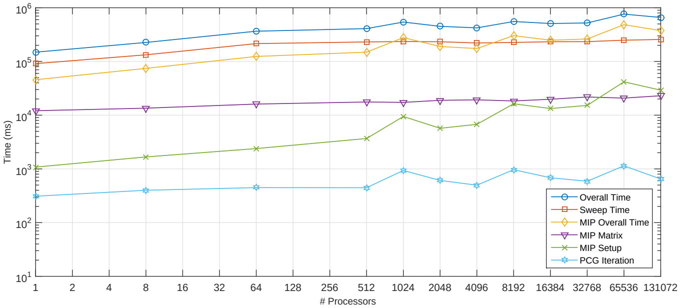
MIP DSA Timing Data with PDT on Vulcan using HYPRE



Problem Description

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

I look forward to your feedback regarding my PhD Proposal

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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