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

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Outline

The Continuous-Energy Transport Equation

Transport Equation

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

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

The multigroup S_N equations

$$\left(\mathbf{\Omega}_m \cdot \nabla + \sigma_{t,g}\right) \psi_{m,g} = \sum_{g'=1}^{G} \sum_{p=0}^{N_P} \frac{2p+1}{4\pi} \sigma_{s,p}^{g' \to g} \sum_{n=-p}^{p} \phi_{p,n,g'} Y_{p,n}(\mathbf{\Omega}_m) + Q_{m,g}$$

Multigroup Method

$$\psi_g = \int_{E_g}^{E_{g-1}} \psi(E)\, dE$$

cross sections goes here...

S_N Discretization

$$\phi_{p,n} \equiv \int_{4\pi} d\Omega\, \psi(\mathbf{\Omega})\, Y_{p,n}(\mathbf{\Omega}),$$

$$\sigma_{s,p} \equiv \int_{-1}^{1} d\mu\, \sigma_s(\mu_0) P_p(\mu_0)$$

$$\mu_0 \equiv \mathbf{\Omega}' \cdot \mathbf{\Omega}$$

$$\sigma_s(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \equiv \frac{1}{2\pi} \sigma_s(\mu)$$

$$P_p(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \equiv \frac{1}{2\pi} P_p(\mu)$$

Spatial Discretization

Iterative Procedure

Classic Source Iteration

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

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

$$\phi = \mathbf{D}\psi$$

Operator Terms

L - streaming + collision operator
M - moment-to-discrete operator
D - discrete-to-moment operator
Σ - scattering operator

Transport Sweep

The operation $\mathbf{L}^{-1}$ can be performed in different ways. For this work, we will use the matrix-free, full-domain transport sweep.

Optically thick problems can cause slow convergence rates

Source Iteration Approximate Spectral Radius

$$\rho^{(k+1)} \approx \frac{||\phi^{(k+1)} - \phi^{(k)}||}{||\phi^{(k)} - \phi^{(k-1)}||}$$

Optically Thick Cases - leakage/absorption does not dominate

- 1-group sense: $\frac{\sigma_s}{\sigma_t} \approx 1$ and $(\sigma_t \cdot \text{diam}(\mathcal{D})) \gg 1$
- MG sense:
  - Thermal upscattering into higher energy groups is significant
  - Single group iteration, g, with $\frac{\sigma_s^{g \to g}}{\sigma_{t,g}} \approx 1$ and $(\sigma_{t,g} \cdot \text{diam}(\mathcal{D})) \gg 1$
- TRT problem:
  - heat capacities tend to zero
  - time steps tend to infinity

Higher-Order FEM Motivation

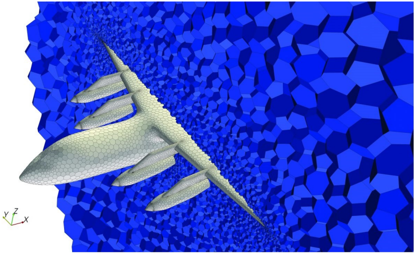
FEM convergence rate - no solution irregularity

$$||u - u_h||_{L_2} = C\, h^{p+1}, \qquad ||u - u_h||_{L_2} = C\, N_{dof}^{-\frac{p+1}{d}}$$

C - error constant dependent on mesh, and basis function polynomial order
h - maximum diameter for an element
p - polynomial order of the finite element basis
N_{dof} - total degrees of freedom: $N_{dof} \propto h^{-d}$
d - dimensionality of the problem (*i.e.*, 1,2,3)

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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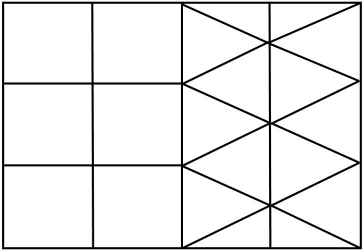

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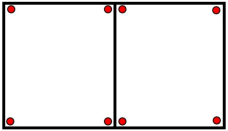
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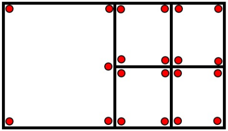
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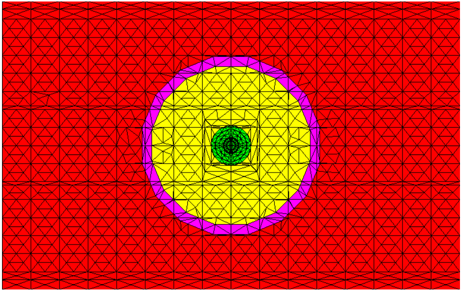
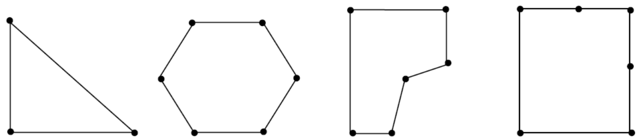
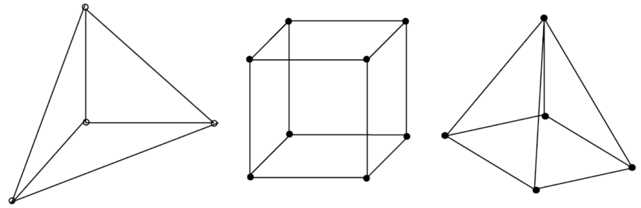


Polytope Finite Elements

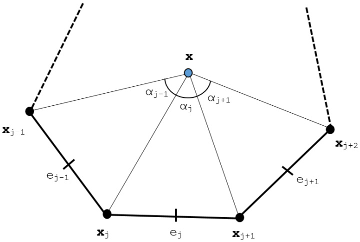
2D arbitrary convex/concave polygons



3D convex polyhedra



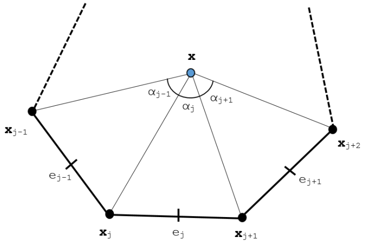
Linear Basis Functions on 2D Polygons



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

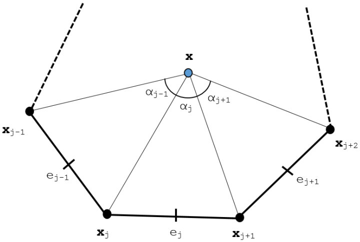
Wachspress Rational Functions



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

$$A(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \frac{1}{2} \begin{vmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{vmatrix}$$

Piecewise Linear (PWL) Functions



$$\lambda_i^{PWL}(\mathbf{x}) = t_i(\mathbf{x}) + \alpha_i t_c(\mathbf{x})$$

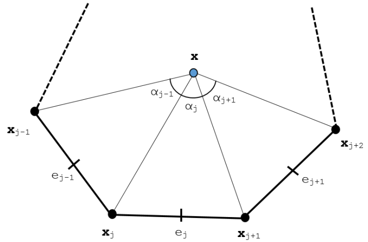
t_i - standard 2D linear function for a triangle $(i, i+1, K_c)$; 1 at vertex i that linearly decreases to 0 to the cell center and the adjoining vertices

t_c - 2D tent function; 1 at cell center and linearly decreases to 0 to each cell vertex

$\alpha_i = \frac{1}{N_V}$ - weight parameter for vertex i

N_V - number of cell vertices

Mean Value Coordinates

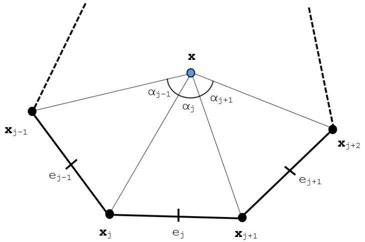


$$\lambda_i^{MV}(\mathbf{x}) = \frac{w_i(\mathbf{x})}{\sum_j w_j(\mathbf{x})}, \qquad w_j(\mathbf{x}) = \frac{\tan(\alpha_{j-1}/2) + \tan(\alpha_j/2)}{|\mathbf{x}_j - \mathbf{x}|}$$

Limit as $\mathbf{x} \to \mathbf{x}_j$

$$\lim_{\mathbf{x}\to\mathbf{x}_j} \tan(\alpha_{j-1}/2) + \tan(\alpha_j/2) = 0 \qquad \longrightarrow \qquad \lim_{\mathbf{x}\to\mathbf{x}_j} w_j(\mathbf{x}) = 1$$

Maximum Entropy Coordinates



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

$$\omega^* = \operatorname{argmin} F(\omega, \mathbf{x}) \qquad F(\omega, \mathbf{x}) = \ln \left(\sum_j w_j(\mathbf{x}) \right)$$

Summary of the 2D Linear Basis Functions

Basis Function	Dimension	Polytope Types	Analytical/Numerical	Direct/Iterative
Wachspress	2D/3D	Convex*	Numerical	Direct
PWL	1D/2D/3D	Convex/Concave	Analytical	Direct
Mean Value	2D**	Convex/Concave	Numerical	Direct
Max Entropy	1D/2D/3D	Convex/Concave	Numerical	Iterative***

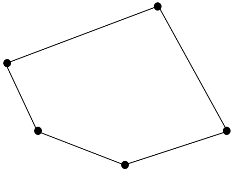
* - weak convexity for Wachspress coordinates does not cause blow up

** - mean value 3D analogue only applicable to tetrahedron

*** - maximum entropy minimization solved via Newton's Method

Quadratic Serendipity Basis Functions on 2D Polygons

1. Form the linear barycentric functions - $\{\lambda_i\}$
2. Construct the pairwise products - $\{\mu_{ab}\}$
3. Eliminate the interior nodes to form a serendipity basis - $\{\xi_{ij}\}$



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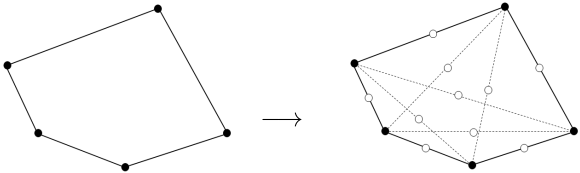

$\{\lambda_i\}$
Linear

$\{\mu_{ab}\}$
Quadratic

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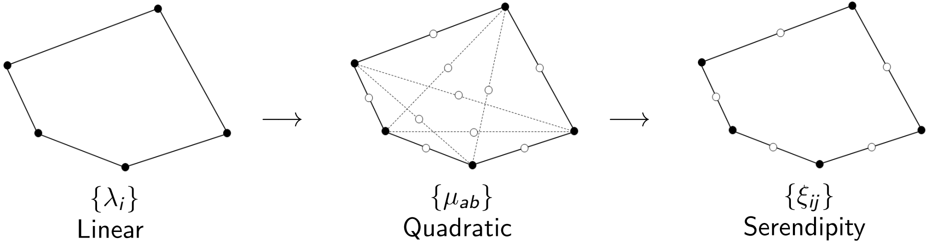


Pairwise products of the barycentric basis functions

Necessary Precision Properties

$$\sum_{aa \in V} \mu_{aa} + \sum_{ab \in E \cup D} 2\mu_{ab} = 1$$

$$\sum_{aa \in V} \mathbf{x}_{aa}\mu_{aa} + \sum_{ab \in E \cup D} 2\mathbf{x}_{ab}\mu_{ab} = \mathbf{x}$$

$$\sum_{aa \in V} \mathbf{x}_a\mathbf{x}_a^T\mu_{aa} + \sum_{ab \in E \cup D} \left(\mathbf{x}_a\mathbf{x}_b^T + \mathbf{x}_b\mathbf{x}_a^T\right)\mu_{ab} = \mathbf{x}\mathbf{x}^T$$

V - vertex nodes
E - face midpoint nodes
D - interior diagonal nodes

Further Notation/Notes

$$\mathbf{x}_{ab} = \frac{\mathbf{x}_a + \mathbf{x}_b}{2}, \qquad \mu_{ab} = \lambda_a\lambda_b$$

$$\mu_{ab}^K(\mathbf{r}) = 0, \qquad \{ab \in D,\, \mathbf{r} \in \partial K\}$$

Eliminate interior nodes to form serendipity basis

Reduction Problem - $[\xi] := \mathbb{A}\,[\mu]$

$$\mathbb{A} = \begin{bmatrix} c_{11}^{11} & \dots & c_{ab}^{11} & \dots & c_{(n-2)n}^{11} \\ \dots & \ddots & \vdots & \ddots & \vdots \\ c_{11}^{ij} & \dots & c_{ab}^{ij} & \dots & c_{(n-2)n}^{ij} \\ \dots & \ddots & \vdots & \ddots & \vdots \\ c_{11}^{n(n+1)} & \dots & c_{ab}^{n(n+1)} & \dots & c_{(n-2)n}^{n(n+1)} \end{bmatrix}$$

Serendipity Precision Properties

$$\sum_{ii \in V} \xi_{ii} + \sum_{i(i+1) \in E} 2\xi_{i(i+1)} = 1$$

$$\sum_{ii \in V} \mathbf{x}_{ii}\xi_{ii} + \sum_{i(i+1) \in E} 2\mathbf{x}_{i(i+1)}\xi_{i(i+1)} = \mathbf{x}$$

$$\sum_{ii \in V} \mathbf{x}_i \mathbf{x}_i^T \xi_{ii} + \sum_{i(i+1) \in E} \left(\mathbf{x}_i \mathbf{x}_{i+1}^T + \mathbf{x}_{i+1}\mathbf{x}_i^T \right) \xi_{i(i+1)} = \mathbf{x}\mathbf{x}^T$$

Special case - bilinear coordinates on the unit square

Bilinear coordinates and quadratic extension

$$\lambda_1 = (1-x)(1-y)$$
$$\lambda_2 = x(1-y)$$
$$\lambda_3 = xy$$
$$\lambda_4 = (1-x)y$$

$$\mu_{11} = (1-x)^2(1-y)^2 \qquad \mu_{12} = (1-x)x(1-y)^2$$
$$\mu_{22} = x^2(1-y)^2 \qquad \mu_{23} = x^2y(1-y)$$
$$\mu_{33} = x^2y^2 \qquad \mu_{34} = (1-x)xy^2$$
$$\mu_{44} = (1-x)^2y^2 \qquad \mu_{41} = (1-x)^2y(1-y)$$
$$\mu_{13} = (1-x)x(1-y)y \qquad \mu_{24} = (1-x)x(1-y)y$$

Reduction matrix

$$\mathbb{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1/2 & 1/2 \end{bmatrix}$$

Serendipity coordinates

$$\xi_{11} = (1-x)(1-y)(1-x-y)$$
$$\xi_{22} = x(1-y)(x-y)$$
$$\xi_{33} = xy(-1+x+y)$$
$$\xi_{44} = (1-x)y(y-x)$$
$$\xi_{12} = (1-x)x(1-y)$$
$$\xi_{23} = xy(1-y)$$
$$\xi_{34} = (1-x)xy$$
$$\xi_{41} = (1-x)y(1-y)$$

TEXAS A&M ENGINEERING

Linear Basis Functions on 3D Polyhedra

Linear basis functions and convex polyhedra only for 3D

- The 2D quadratic serendipity formulation is more arduous in 3D
- Intercell coupling is not straightforward for concave polyhedra
- Focus on 3D PWL functions - MAXENT only other function for arbitrary polyhedra
- Focus on 3D parallelepipeds and extruded convex polygons (convex prisms)

3D PWL basis functions

$$b_i(\mathbf{x}) = t_i(\mathbf{x}) + \sum_{f=1}^{F_i} \beta_f^i t_f(\mathbf{x}) + \alpha_i t_c(\mathbf{x})$$

t_i - standard 3D linear function for a tet $(i, i+1, f_c, K_c)$; 1 at vertex i, linearly decreases to 0 to the cell center, each adjoining face center, and each adjoining vertex

t_c - 3D tent function; 1 at cell center, linearly decreases to 0 at all vertices and face centers

t_f - face tent function; 1 at face center, linearly decreases to 0 at each face vertex and cell center

$\alpha_i = \frac{1}{N_V}$ - weight parameter for vertex i

$\beta_f^i = \frac{1}{N_f}$ - weight parameter for face f touching vertex i

Theory goes here...

Theory goes here...

The diffusion equation is used as our low-order operator

The Diffusion Equation

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

General Boundary Conditions

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

Desirable diffusion form properties

- Can handle concave and degenerate polytope cells
- Symmetric Positive-Definite (SPD)
- Availability of suitable preconditioners
- Agnostic of directionality of interior faces

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

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

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

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

MIP Penalty Term

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

Proposed Work

POLYFEM

1. Analyze the different 2D linear polygonal basis functions for use in DGFEM transport calculations
2. Perform the same analysis with the quadratic serendipity basis functions

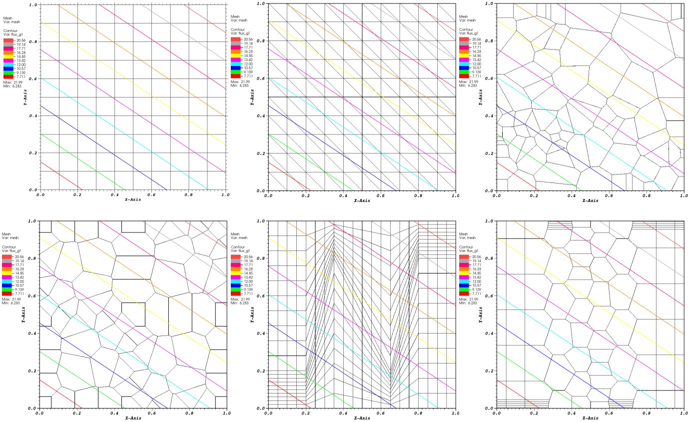
MIP DSA

1. Analyze the 2D linear/quadratic basis functions with DSA preconditioning through Fourier/numerical analysis
2. Extend the analysis of MIP DSA to arbitrary convex 3D polyhedra
3. Implement MIP DSA in PDT using HYPRE
   1. Analyze the scalability of the method to high process counts
   2. Perform parametric studies on aggregation/partitioning factors to generate a performance model of MIP DSA with HYPRE
   3. Implement and perform analysis of two-grid acceleration at scale
   4. Run reactor-type problem (*e.g.*, C5G7)
   5. Run real-world numerical experiments - IM1

2D Exactly-Linear Transport Solutions - mean value coordinates

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

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

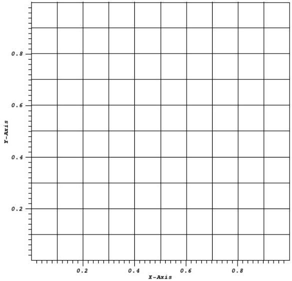


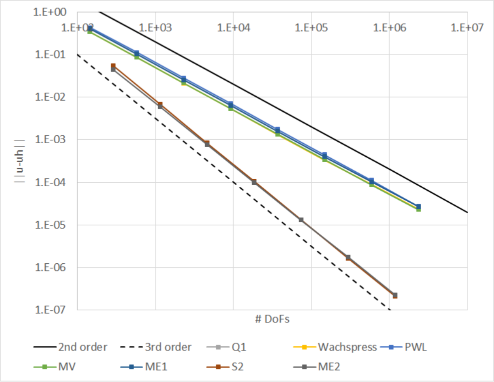
TEXAS A&M ENGINEERING

Convergence rates using MMS for the 2D polygonal basis functions

$$\psi(x,y) = \sin(\nu\frac{\pi x}{L_x})\sin(\nu\frac{\pi y}{L_y})$$

$$\phi(x,y) = 2\pi\sin(\nu\frac{\pi x}{L_x})\sin(\nu\frac{\pi y}{L_y})$$

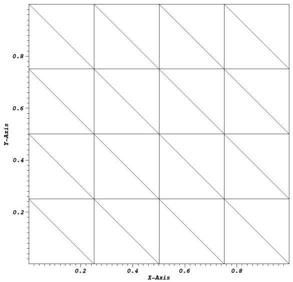


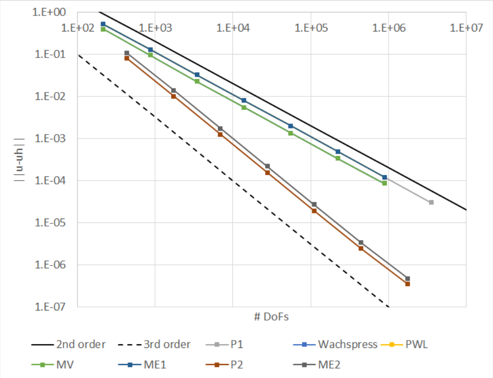


Convergence rates using MMS for the 2D polygonal basis functions

$$\psi(x,y) = \sin(\nu \frac{\pi x}{L_x}) \sin(\nu \frac{\pi y}{L_y})$$

$$\phi(x,y) = 2\pi \sin(\nu \frac{\pi x}{L_x}) \sin(\nu \frac{\pi y}{L_y})$$

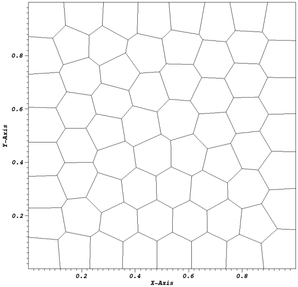


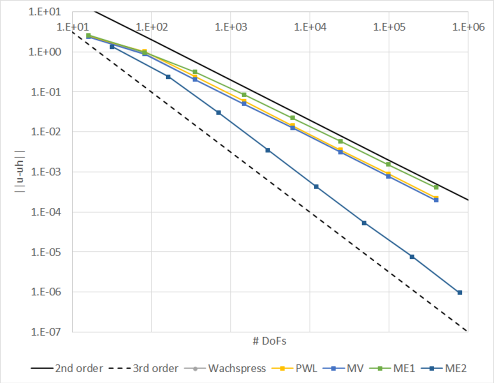


Convergence rates using MMS for the 2D polygonal basis functions

$$\psi(x,y) = \sin(\nu\frac{\pi x}{L_x})\sin(\nu\frac{\pi y}{L_y})$$

$$\phi(x,y) = 2\pi\sin(\nu\frac{\pi x}{L_x})\sin(\nu\frac{\pi y}{L_y})$$

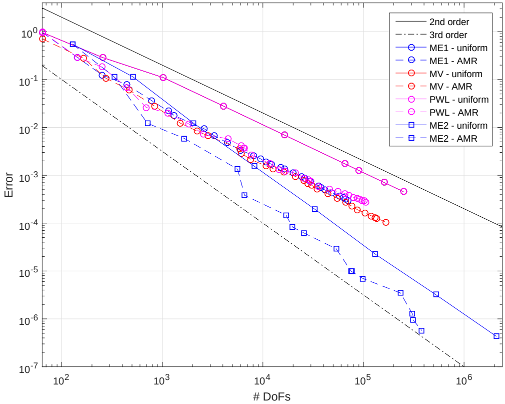




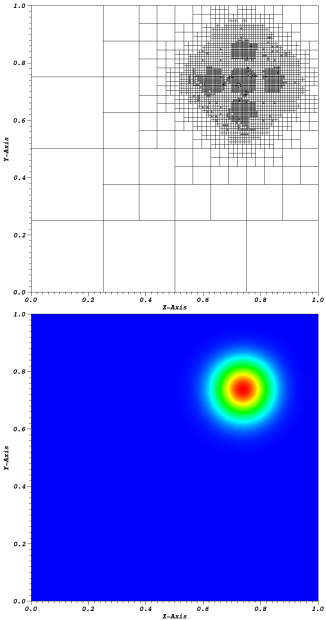
Convergence rates using MMS and AMR for the 2D polygonal basis functions

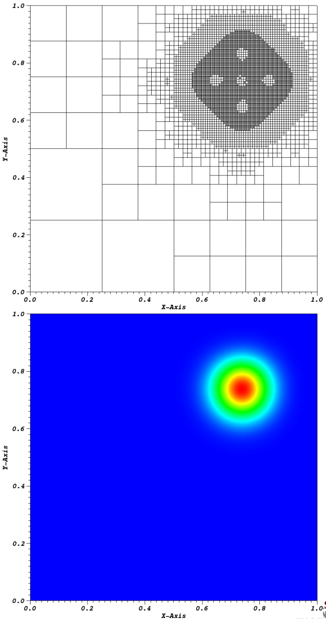
$$\psi(x,y) = x(L_x - x)y(L_y - y)\exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{\gamma}\right),$$

$$\phi(x,y) = 2\pi x(L_x - x)y(L_y - y)\exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{\gamma}\right)$$

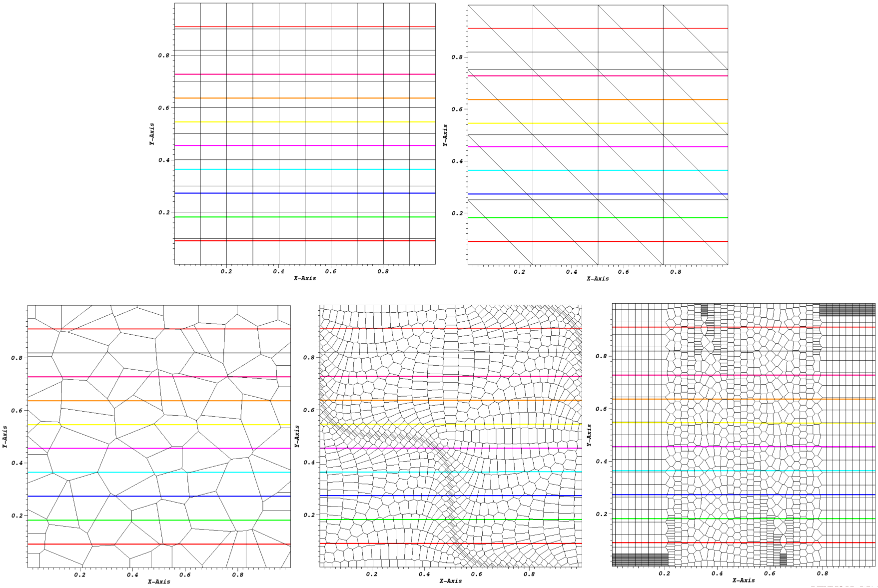


Linear ME cycle 15 (left) and quadratic ME cycle 08 (right)



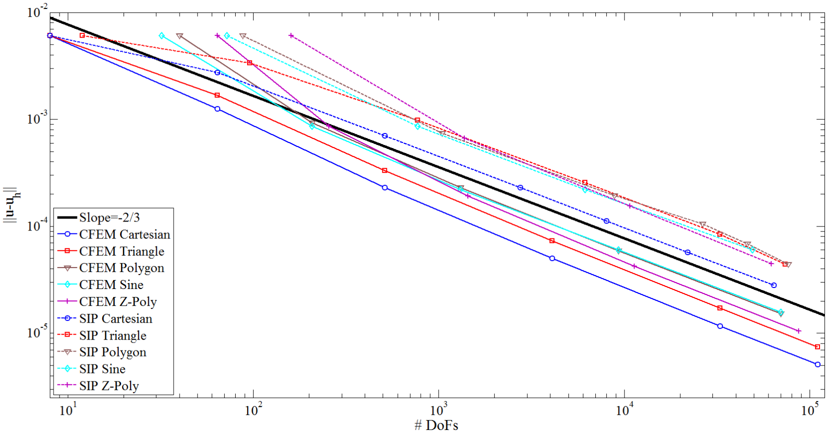


SIP exactly linear solutions on 3D polyhedral meshes using the PWL basis functions



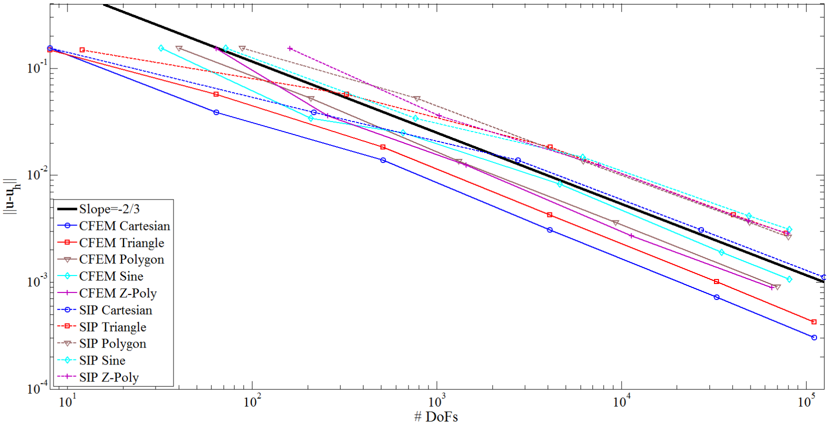
SIP convergence study - quadratic solution on 3D cube using the PWL basis functions

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



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

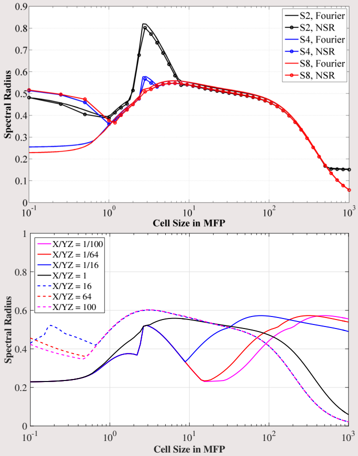
$$\Phi(x,y,z) = xyz(L_x - x)(L_y - y)(L_z - z)\exp(-(\mathbf{r}-\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0))$$
$$L_x = L_x = L_x = 1.0, \qquad \mathbf{r}_0 = (3/4, 3/4, 3/4)$$



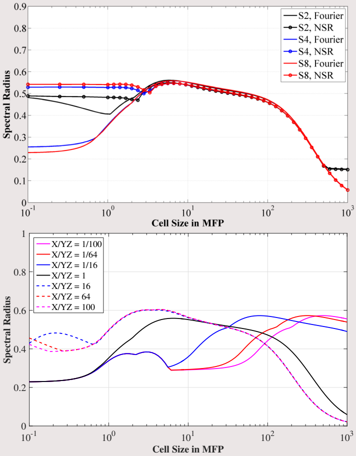
TEXAS A&M ENGINEERING

Fourier analysis - 3D PWL basis functions

$c = 1$

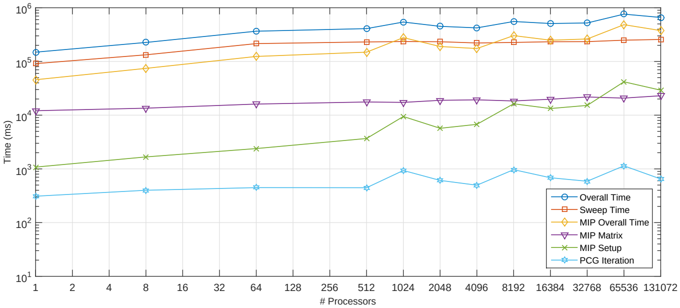


$c = 4$



TEXAS A&M ENGINEERING

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
- pointwise convergence tolerance of 1e-8
- SI precondition with MIP DSA using HYPRE PCG and AMG

Two-grid acceleration implementation in PDT

- Successfully implemented and deugged
  - 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

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

POLYFEM Ongoing Work

- Finish quadratic serendipity extension for polygonal finite elements to Wachspress, PWL, and mean value.
- Determine the effects of numerical integration strategies on highly-distorted polygonal elements
- Perform analysis on benchmark cases using AMR
  - Searchlight problem (partially completed)
  - IAEA-EIR-2 problem

MIP DSA Ongoing Work

- Finish the MIP DSA Fourier analysis for all the 2D polygonal basis functions (including the quadratic serendipity extension).
- Analyze the effects of AMR with polygonal basis functions on the MIP DSA PCG iteration counts (with and without bootstrapping)
- Remaining PDT work:
  - Complete parametric studies (a lot of the raw results have been compiled) of MIP DSA with HYPRE and generate a working performance model
  - Perform additional two-grid acceleration studies on simple geometries
  - Run IM1 problem with two-grid acceleration
  - Commit all acceleration additions to master for use in the CERT project

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.