

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

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# Outline

## 1 Overview

- The DGFEM  $S_N$  Transport Equation
- Motivation for this Work

## 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 Work Summary

# The Continuous-Energy Transport Equation

## Transport Equation

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

## Boundary Conditions

$$\psi(\mathbf{r}, E, \Omega) = \psi^{inc}(\mathbf{r}, E, \Omega) + \int_{\Omega' \cdot \mathbf{n} < 0} \int_0^\infty \beta(\mathbf{r}, E', E, \Omega', \Omega) \psi(\mathbf{r}, E', \Omega') dE' d\Omega'$$

## Term Definitions

$\mathbf{r}$  - neutron position

$E$  - neutron energy

$\Omega$  - neutron solid angle

$\psi(\mathbf{r}, E, \Omega)$  - angular flux

$Q(\mathbf{r}, E, \Omega)$  - distributed neutron source

$\sigma_t(\mathbf{r}, E)$  - total macroscopic cross section

$\sigma_s(\mathbf{r}, E', E, \Omega', \Omega)$  - total macroscopic scattering cross section

$\beta(\mathbf{r}, E', E, \Omega', \Omega)$  - boundary albedo

# Energy and Angular Discretization

## The multigroup $S_N$ equations

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

## Multigroup Method

$$\psi_g = \int_{\Delta E_g} \psi(E) dE, \quad \Delta E_g \in [E_g, E_{g-1}]$$

$$\sigma_{t,g} = \frac{\int_{\Delta E_g} \sigma_t(E) \psi(E) dE}{\int_{\Delta E_g} \psi(E) dE}$$

## Spherical Harmonics

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

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

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

$$\sigma_s(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \equiv \frac{1}{2\pi} \sigma_s(\mu_0)$$

$$P_k(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \equiv \frac{1}{2\pi} P_k(\mu_0)$$

## Spatial Discretization - 1 group/direction and general source

Multiply element  $K$  by basis functions and apply Gauss theorem

$$-(\boldsymbol{\Omega}_m \cdot \nabla b_m, \psi_m)_K + \sum_{f=1}^{N_f^K} \left\langle (\boldsymbol{\Omega}_m \cdot \mathbf{n}_f) b_m, \tilde{\psi}_m \right\rangle_f + (\sigma_t b_m, \psi_m)_K = (b_m, Q_m)_K$$

The upwind scheme

$$\tilde{\psi}_m(\mathbf{r}) = \begin{cases} \psi_m^-, & \partial K^+ \\ \psi_m^+, & \partial K^- \setminus \partial \mathcal{D} \\ \psi_m^{inc}, & \partial K^- \cap \partial \mathcal{D}^d \\ \psi_{m'}^-, & \partial K^- \cap \partial \mathcal{D}^r \end{cases} \quad \psi_m^\pm(\mathbf{r}) \equiv \lim_{s \rightarrow 0^\pm} \psi_m(\mathbf{r} + s(\boldsymbol{\Omega}_m \cdot \mathbf{n})\mathbf{n})$$

Full set of equations for element  $K$

$$\begin{aligned} & -(\boldsymbol{\Omega}_m \cdot \nabla b_m, \psi_m)_K + (\sigma_t b_m, \psi_m)_K + \left\langle (\boldsymbol{\Omega}_m \cdot \mathbf{n}) b_m, \psi_m^- \right\rangle_{\partial K^+} \\ & + \left\langle (\boldsymbol{\Omega}_m \cdot \mathbf{n}) b_m, \psi_m^+ \right\rangle_{\partial K^- \setminus \partial \mathcal{D}} + \left\langle (\boldsymbol{\Omega}_m \cdot \mathbf{n}) b_m, \psi_{m'}^- \right\rangle_{\partial K^- \cap \partial \mathcal{D}^r} \\ & = (b_m, Q_m)_K + \left\langle (\boldsymbol{\Omega}_m \cdot \mathbf{n}) b_m, \psi_m^{inc} \right\rangle_{\partial K^- \cap \partial \mathcal{D}^d} \end{aligned}$$

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## Iterative Procedure

### Classic Source Iteration

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

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

### Operator Terms

$\mathbf{L}$  - streaming + collision operator

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

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

$\boldsymbol{\Sigma}$  - scattering operator

$\mathbf{Q}$  - source 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

- $\sigma_s^{g \rightarrow g} / \sigma_{t,g} \approx 1$  and  $(\sigma_{t,g} \cdot \text{diam}(\mathcal{D})) \gg 1$
- Thermal upscattering into higher energy groups is significant

### Answer - Precondition the transport sweep

- Diffusion Synthetic Acceleration (DSA)
- Transport Synthetic Acceleration (TSA)
- Boundary Projection Acceleration (BPA)
- etc.

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# Higher-Order FEM Motivation

## FEM convergence rate - no solution irregularity

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

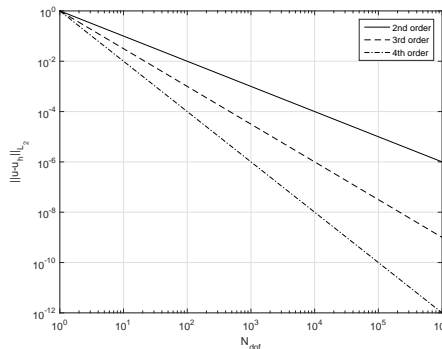
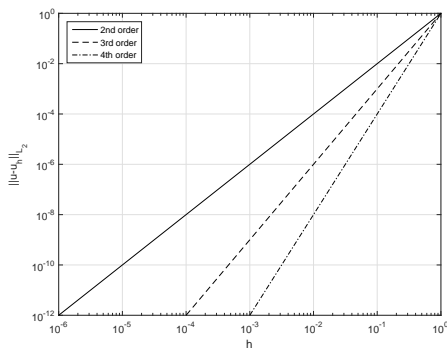
$C$  - error constant dependent on mesh, basis function, and polynomial order

$h$  - maximum diameter for an element

$p$  - polynomial order of the finite element basis

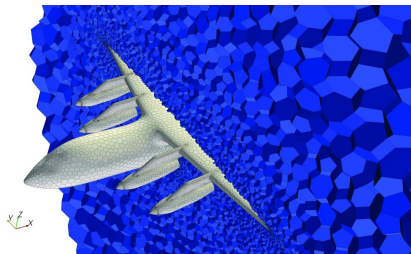
$N_{dof}$  - total degrees of freedom:  $N_{dof} \propto h^{-d}$

$d$  - dimensionality of the problem (i.e., 1,2,3)



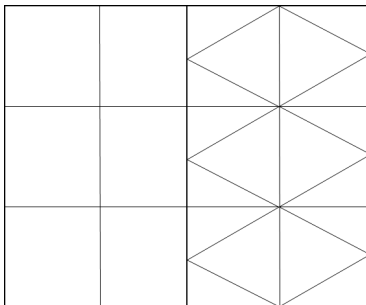
## Polytope Grid Motivation

- 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



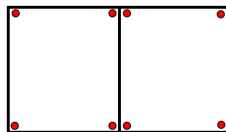
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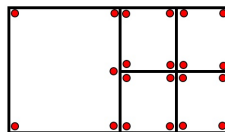


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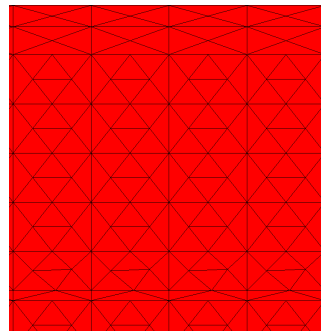
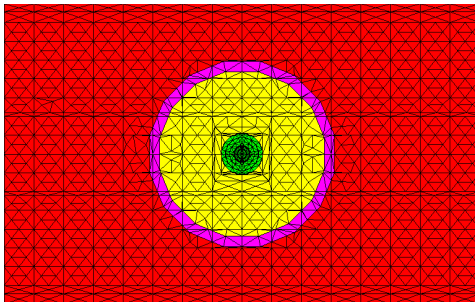
(a)



(b)

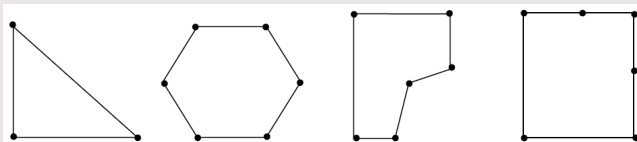
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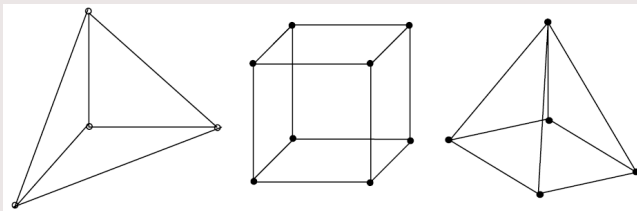


# Polytope Finite Elements

## 2D arbitrary convex/concave polygons



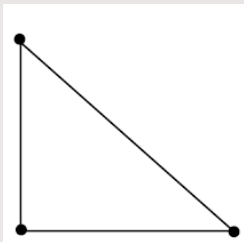
## 3D convex polyhedra





# A common class of linear finite elements - the $\mathbb{P}_1$ space

## 2D $\mathbb{P}_1$ space - reference element

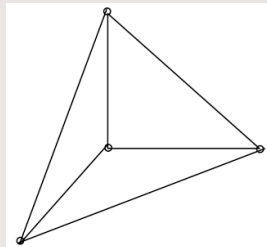


$$\lambda_1(r, s) = 1 - r - s$$

$$\lambda_2(r, s) = r$$

$$\lambda_3(r, s) = s$$

## 3D $\mathbb{P}_1$ space - reference element



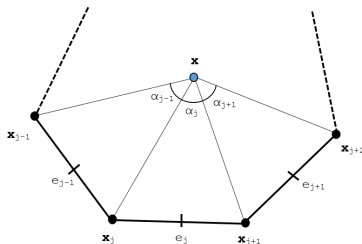
$$\lambda_1(r, s, t) = 1 - r - s - t$$

$$\lambda_2(r, s, t) = r$$

$$\lambda_3(r, s, t) = s$$

$$\lambda_4(r, s, t) = t$$

# Linear Basis Functions on 2D Polygons

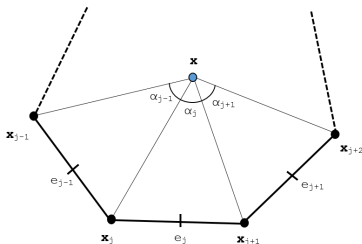


## Basis Function Properties - Barycentric Coordinates

$\lambda_i$  - linear basis function located at vertex  $i$

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

# Linear Basis Functions on 2D Polygons

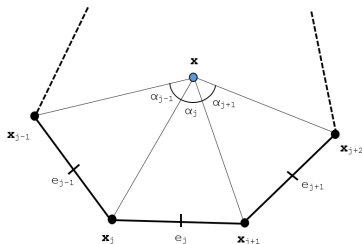


## Linear basis functions that we consider

- ① Wachspress rational coordinates\*
- ② Piecewise linear (PWL) coordinates\*
- ③ Mean value coordinates
- ④ Maximum entropy coordinates

\*have been previously analyzed for transport problems

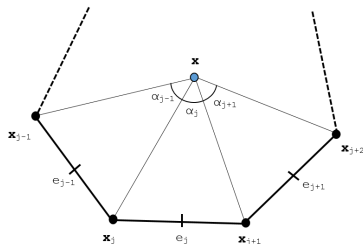
# Wachspress Rational Functions



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

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

# Piecewise Linear (PWL) Functions



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

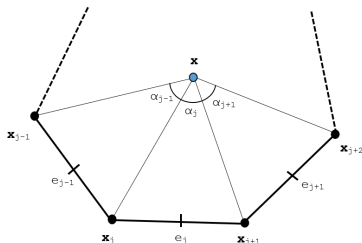
$t_i$  - standard 2D linear function for a triangle  $(i, i+1, C)$ ; 1 at vertex  $i$  that linearly decreases to 0 to the cell center and the adjoining vertices

$t_c$  - 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



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

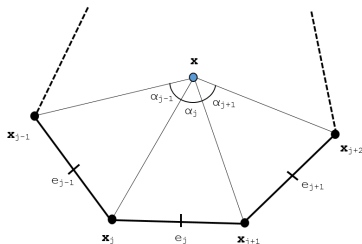
Limit as  $\mathbf{x} \rightarrow \mathbf{x}_j$

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

$\longrightarrow$

$$\lim_{\mathbf{x} \rightarrow \mathbf{x}_j} w_j(\mathbf{x}) = 1$$

# Maximum Entropy Coordinates



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

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

# Finite element architecture

## Mass Matrix - element $K$

$$\mathbf{M}^K = \int_K d\mathbf{r} \lambda(\mathbf{x}) \lambda^T(\mathbf{x}) = \sum_{q=1}^{N_q^K} w_q^K \lambda(\mathbf{x}_q^K) \lambda^T(\mathbf{x}_q^K)$$

## Advection Matrix - element $K$

$$\mathbf{G}^K = \int_K d\mathbf{r} \nabla \lambda(\mathbf{x}) \lambda^T(\mathbf{x}) = \sum_{q=1}^{N_q^K} w_q^K \nabla \lambda(\mathbf{x}_q^K) \lambda^T(\mathbf{x}_q^K)$$

## Surface Matrix - face $f$ for element $K$

$$\mathbf{N}_f^K = \int_f ds \lambda(\mathbf{x}) \lambda^T(\mathbf{x}) = \sum_{q=1}^{N_f} w_q^f \lambda(\mathbf{x}_q^f) \lambda^T(\mathbf{x}_q^f)$$



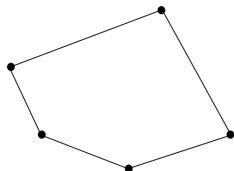
# Summary of the 2D Linear Basis Functions

Basis Function	Dimension	Polytope Types	Integration	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 triangular-faceted polyhedra
- \*\*\* - maximum entropy minimization solved via Newton's Method

# Quadratic Serendipity Basis Functions on 2D Polygons

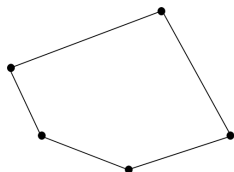
- 1 Form the linear barycentric functions -  $\{\lambda_i\}$
- 2 Construct the pairwise products -  $\{\mu_{ab}\}$
- 3 Eliminate the interior nodes to form a serendipity basis -  $\{\xi_{ij}\}$



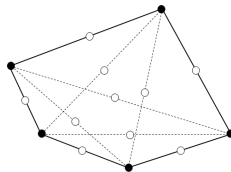
$\{\lambda_i\}$   
Linear

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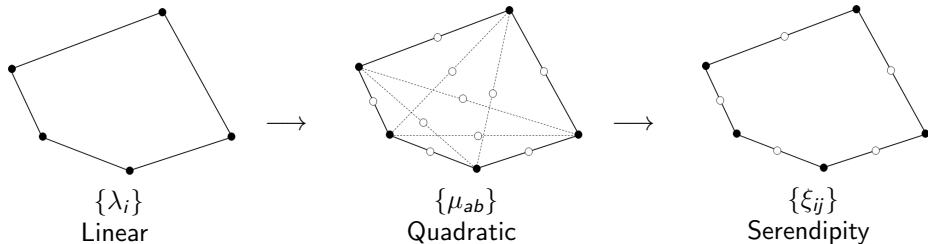
Linear

 $\{\mu_{ab}\}$ 

Quadratic

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# Pairwise products of the barycentric basis functions

## Necessary Precision Properties

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

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

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

$V$  - vertex nodes

$E$  - face midpoint nodes

$D$  - interior diagonal nodes

## Further Notation/Notes

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

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

# Eliminate interior nodes to form serendipity basis

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

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

## Serendipity Precision Properties

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

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

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

$\xi_{ii}$  - basis function at vertex  $i$

$\xi_{i(i+1)}$  - basis function at face midpoint between vertices  $(i, i+1)$

# Special case - bilinear coordinates on the unit square

## Bilinear coordinates and quadratic extension

$$\lambda_1 = (1-x)(1-y)$$

$$\lambda_2 = x(1-y)$$

$$\lambda_3 = xy$$

$$\lambda_4 = (1-x)y$$

$$\mu_{11} = (1-x)^2(1-y)^2 \quad \mu_{12} = (1-x)x(1-y)^2$$

$$\mu_{22} = x^2(1-y)^2 \quad \mu_{23} = x^2y(1-y)$$

$$\mu_{33} = x^2y^2 \quad \mu_{34} = (1-x)xy^2$$

$$\mu_{44} = (1-x)^2y^2 \quad \mu_{41} = (1-x)^2y(1-y)$$

$$\mu_{13} = (1-x)x(1-y)y \quad \mu_{24} = (1-x)x(1-y)y$$

## 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

$$\xi_{11} = (1-x)(1-y)(1-x-y)$$

$$\xi_{22} = x(1-y)(x-y)$$

$$\xi_{33} = xy(-1+x+y)$$

$$\xi_{44} = (1-x)y(y-x)$$

$$\xi_{12} = (1-x)x(1-y)$$

$$\xi_{23} = xy(1-y)$$

$$\xi_{34} = (1-x)xy$$

$$\xi_{41} = (1-x)y(1-y)$$

# 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
- 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  $i$



# Diffusion Synthetic Acceleration

## Transport iteration and error

$$\mathbf{L}\psi = \mathbf{B}\phi + \mathbf{C}\phi + \mathbf{Q}$$

$$\mathbf{L}\psi^{(\ell+1/2)} = \mathbf{B}\phi^{(\ell+1/2)} + \mathbf{C}\phi^{(\ell)} + \mathbf{Q}$$

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

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

---


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

## Error approximation and update

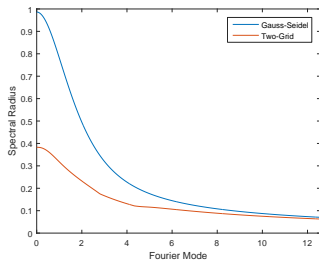
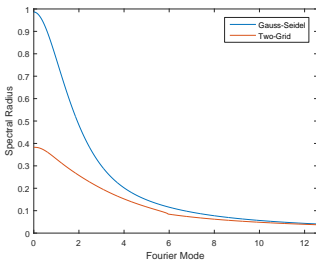
If we could exactly solve for the error, then the solution could be obtained immediately:

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

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

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

# Two-Grid Acceleration



The diffusion equation is used as our low-order operator

## The Diffusion Equation

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

## General Boundary Conditions

$$\Phi(\mathbf{r}) = \Phi_0(\mathbf{r}), \quad \mathbf{r} \in \partial \mathcal{D}^d$$

$$-D \partial_n \Phi(\mathbf{r}) = J_0(\mathbf{r}), \quad \mathbf{r} \in \partial \mathcal{D}^n$$

$$\frac{1}{4} \Phi(\mathbf{r}) + \frac{1}{2} D \partial_n \Phi(\mathbf{r}) = J^{inc}(\mathbf{r}), \quad \mathbf{r} \in \partial \mathcal{D}^r$$

## 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

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

## 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

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

## Modified Interior Penalty (MIP) Form

### Diffusion Form

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

### MIP Penalty Term

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

## Proposed Work

### POLYFEM

- ① Analyze the 2D linear polygonal basis functions for use in DGFEM transport calculations
- ② Perform the same analysis with the quadratic serendipity basis functions
- ③ Determine the effects of numerical integration on highly-distorted polygonal elements
- ④ Perform analysis on benchmark cases using polygonal meshes (including AMR)

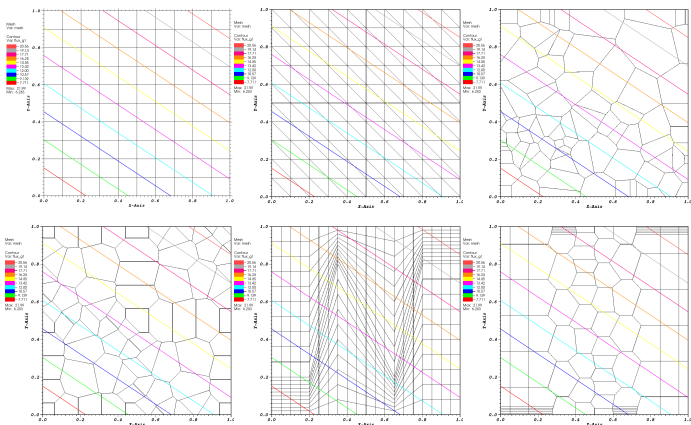
### MIP DSA

- ① Analyze the 2D polygonal basis functions with DSA preconditioning through Fourier/numerical analysis
- ② Analyze the effects of AMR with polygonal basis functions on the MIP DSA PCG iteration counts (with and without bootstrapping)
- ③ Extend the analysis of MIP DSA to arbitrary convex 3D polyhedra
- ④ Implement MIP DSA in PDT using HYPRE
  - ① Analyze the scalability of the method to high process counts
  - ② Implement and perform analysis of two-grid acceleration
  - ③ Perform parametric studies on aggregation/partitioning factors - generate a performance model of MIP DSA with HYPRE
  - ④ Run realistic numerical experiments - IM1 and reactor geometries

## 2D Exactly-Linear Transport Solutions - mean value coordinates

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

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

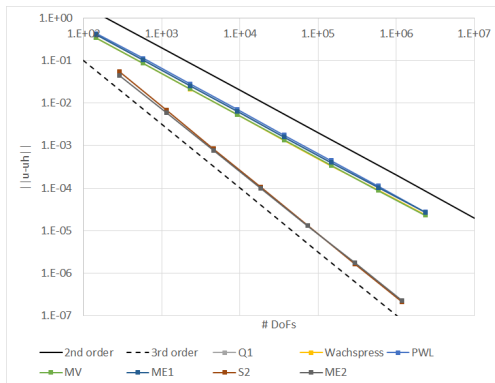
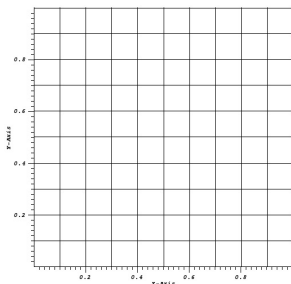




# Convergence rates using MMS for the 2D polygonal basis functions

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

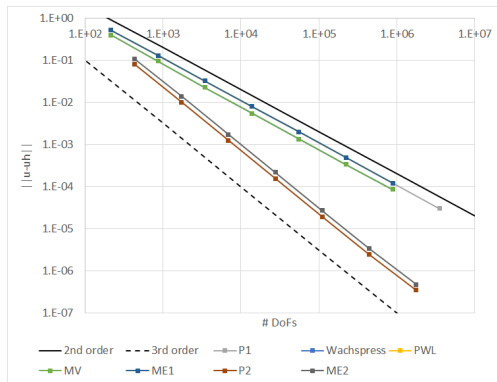
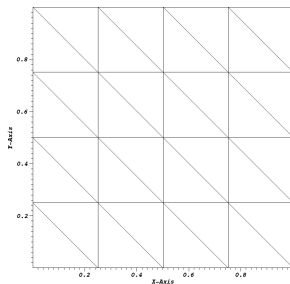
$$\phi(x, y) = 2\pi \sin\left(\nu \frac{\pi x}{L_x}\right) \sin\left(\nu \frac{\pi y}{L_y}\right)$$



# Convergence rates using MMS for the 2D polygonal basis functions

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

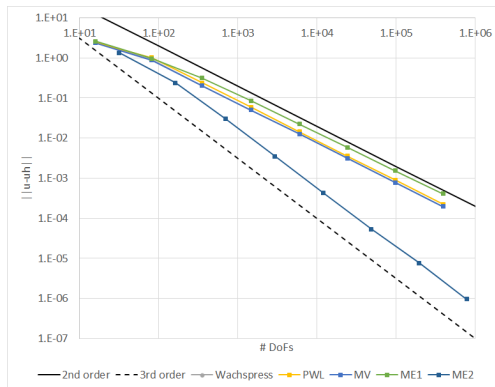
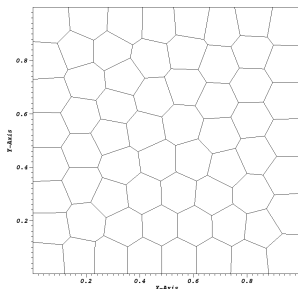
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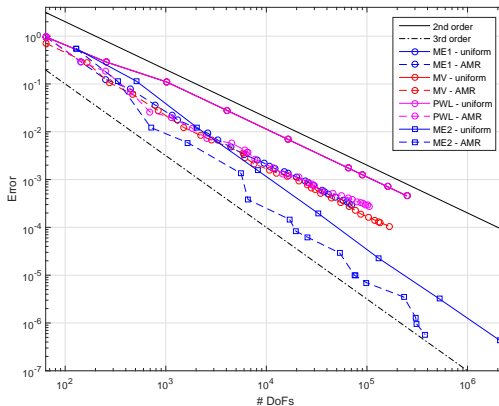
$$\phi(x, y) = 2\pi \sin\left(\nu \frac{\pi x}{L_x}\right) \sin\left(\nu \frac{\pi y}{L_y}\right)$$



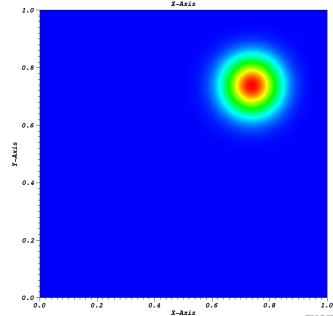
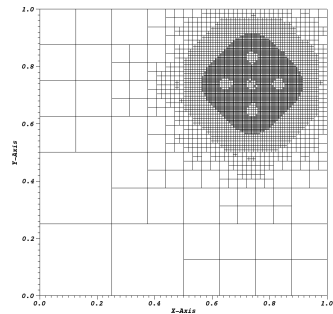
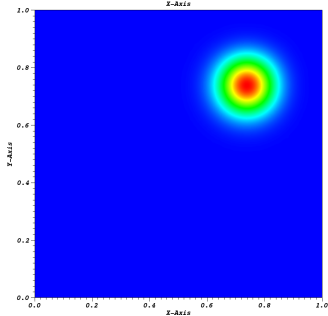
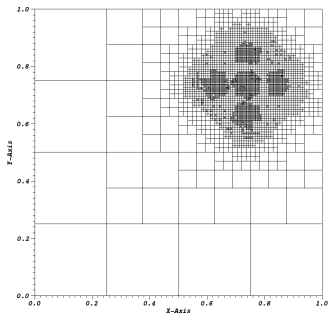
# Convergence rates using MMS and AMR for the 2D polygonal basis functions

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

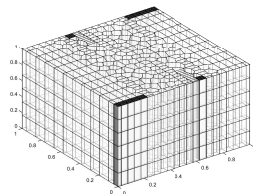
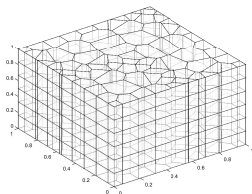
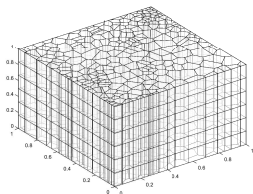
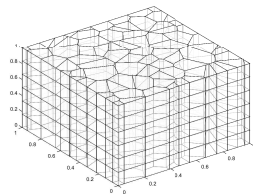
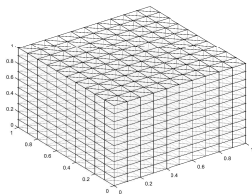
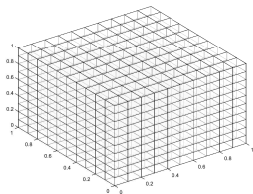
$$\phi(x, y) = 2\pi x(L_x - x)y(L_y - y) \exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{\gamma}\right)$$



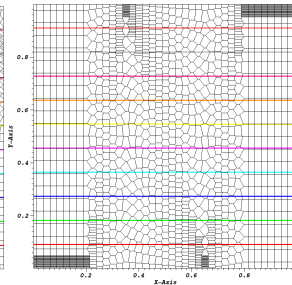
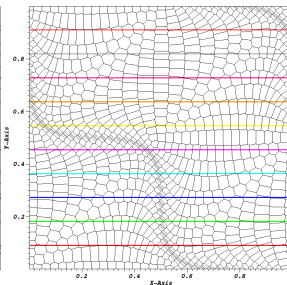
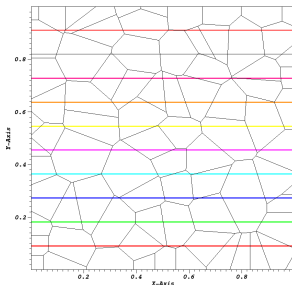
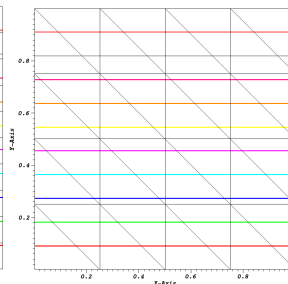
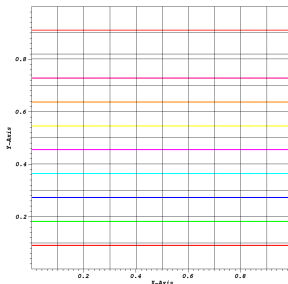
## Linear ME cycle 15 (left) and quadratic ME cycle 08 (right)



# 3D FEM/DSA Analysis



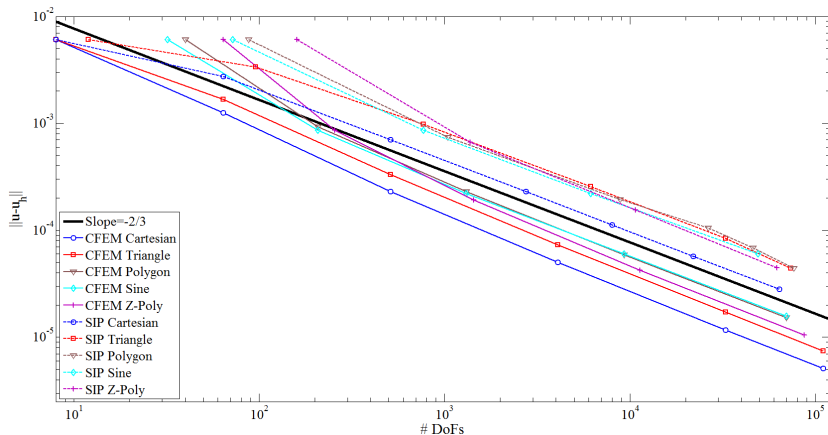
# SIP exactly linear solutions on 3D polyhedral meshes using the PWL basis functions



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

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

$$L_x = L_y = L_z = 1.0$$

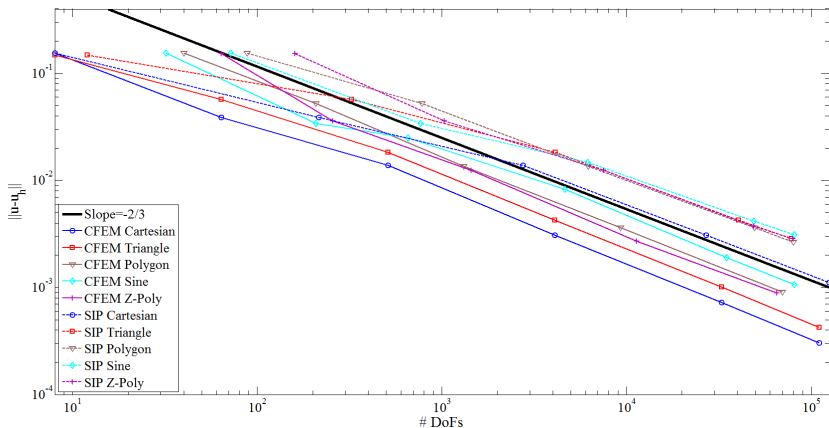




# SIP convergence study - gaussian solution on 3D cube using the PWL basis functions

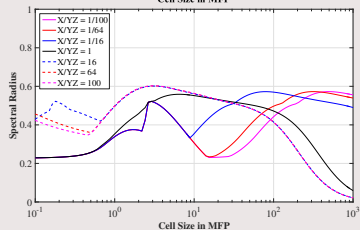
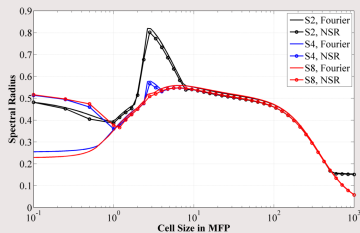
$$\Phi(x, y, z) = xyz(L_x - x)(L_y - y)(L_z - z) \exp(-(\mathbf{r} - \mathbf{r}_0) \cdot (\mathbf{r} - \mathbf{r}_0))$$

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

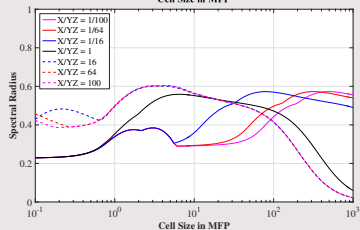
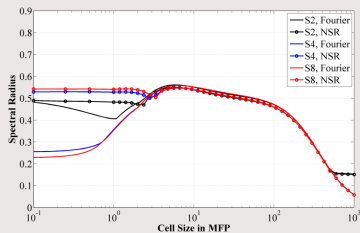


# Fourier analysis - 3D PWL basis functions

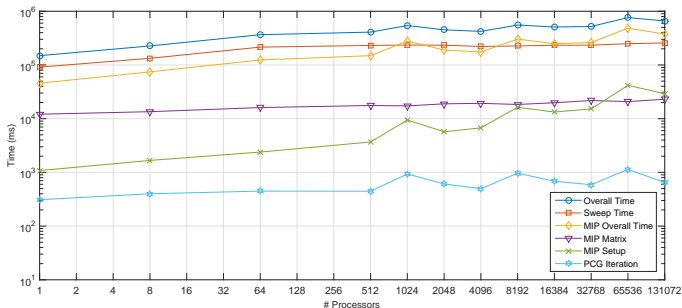
$c = 1$



$c = 4$



# 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  $c=0.9999$
  - S8 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 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

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

Work Summary and Status - completed (blue), in-progress (orange), and not-started (red)

## POLYFEM

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  - ④ Run realistic numerical experiments - IM1 and reactor geometries

## 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.



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# Stretch Goals

# Limits of the Wachspres coordinates



# Limits of the mean value coordinates

# Limits of the maximum entropy coordinates