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

Michael W. Hackemack

Chair: Jean C. Ragusa
Committee Members: Marvin L. Adams, Jim E. Morel, Nancy M. Amato
External Advisor: Troy Becker

Department of Nuclear Engineering
Texas A&M University
College Station, TX, USA 77843

mike_hack@tamu.edu

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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

Iterative Procedure

Classic Source Iteration

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

$$\Phi^{(\ell+1)} = \mathbf{DL}^{-1}\left(\mathbf{M\Sigma\Phi}^{(\ell)} + \mathbf{Q}\right)$$

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

Operator Terms

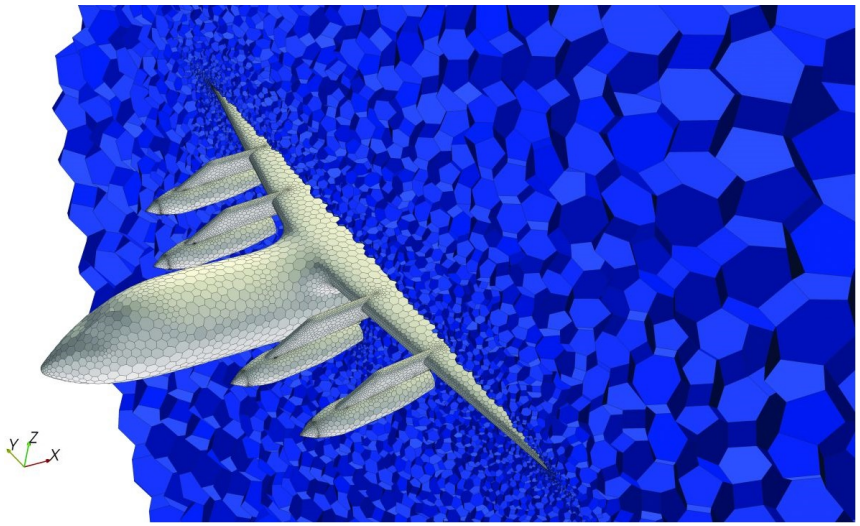
L - streaming + collision operator
M - moment-to-discrete operator
D - discrete-to-moment operator
Σ - scattering operator

Transport Sweep

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

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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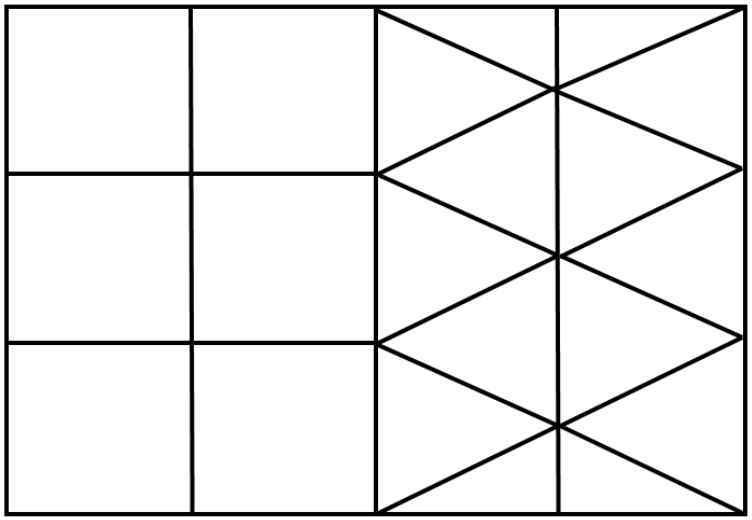

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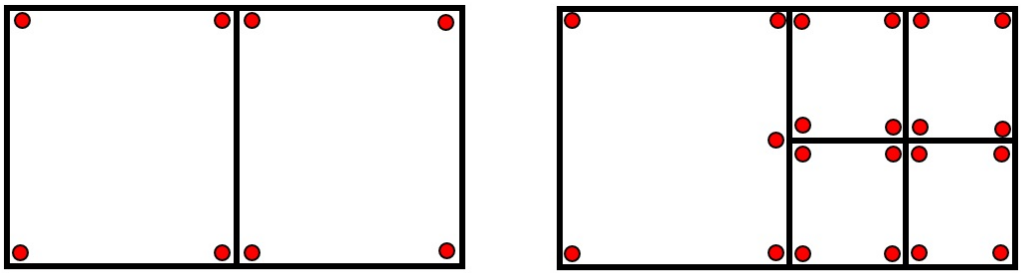

(a) (b)

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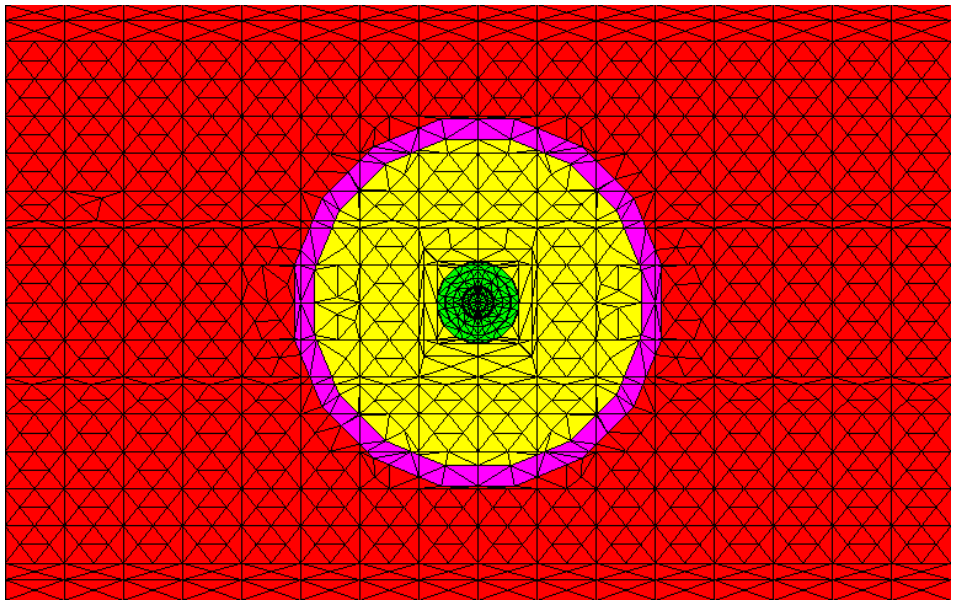
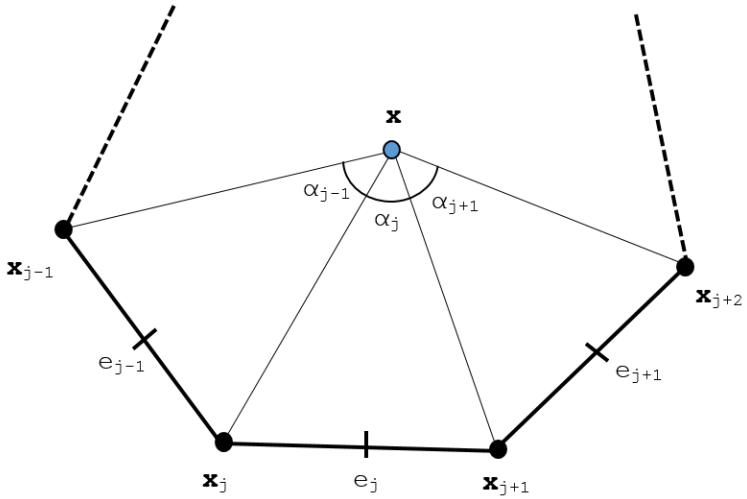


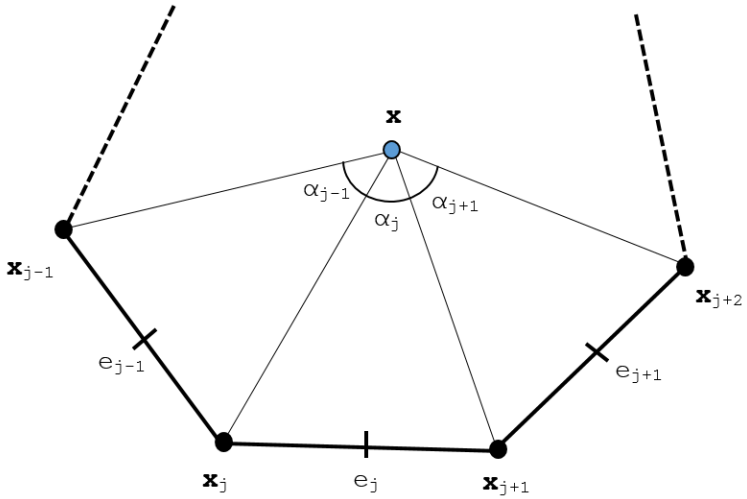
Linear Basis Functions on 2D Polygons



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



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

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

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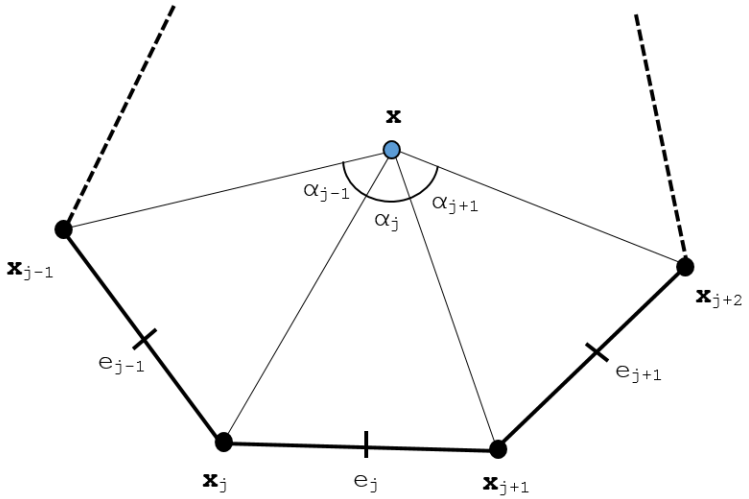
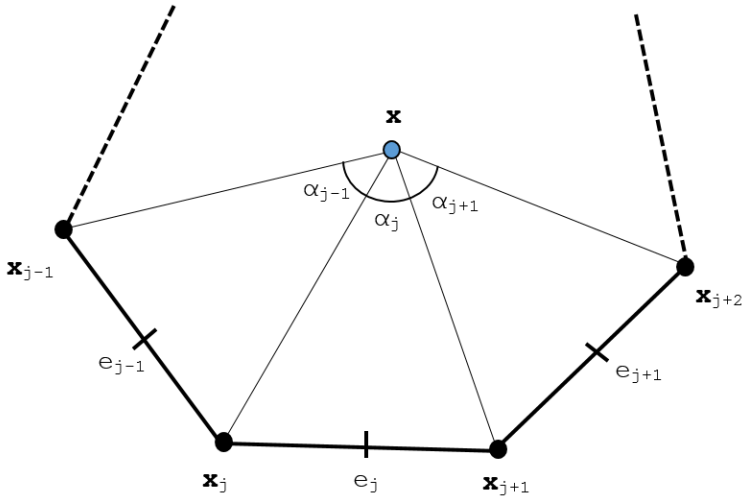
Piecewise Linear (PWL) Functions

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



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

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

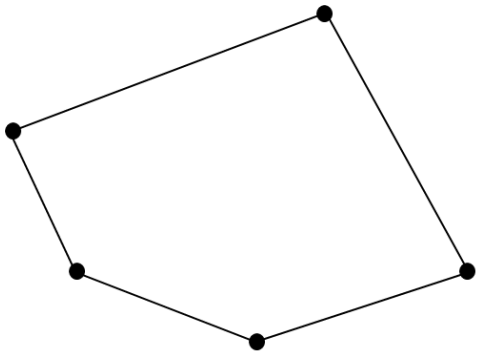
Summary of the 2D Linear Basis Functions

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 barycentrric 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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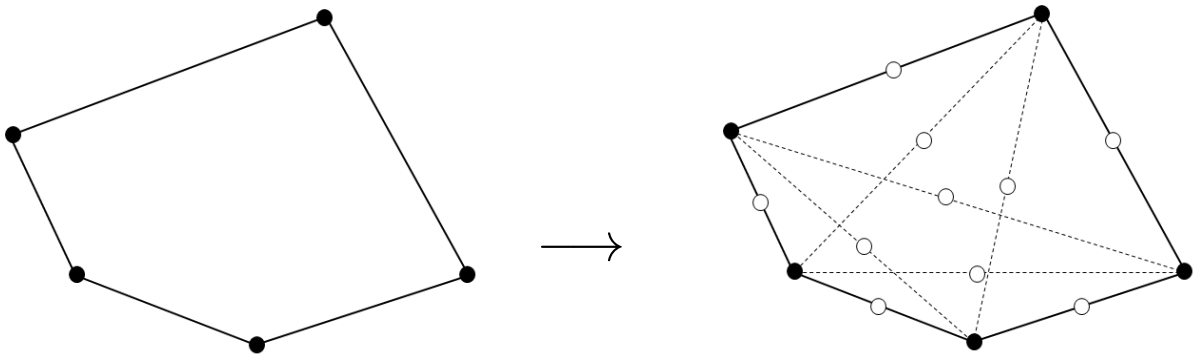

$\{\lambda_i\}$
Linear

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

Quadratic Serendipity Basis Functions on 2D Polygons

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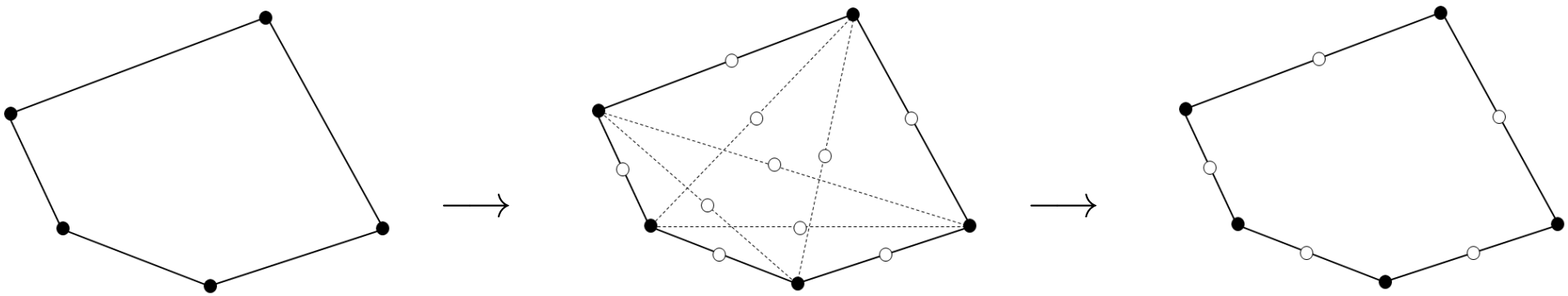

$\{\lambda_i\}$
Linear

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

$\{\xi_{ij}\}$
Serendipity

Pairwise products of the barycentric basis functions

Necessary Precision Properties

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

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

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

Further Notation

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

Eliminate interior nodes to form serendipity basis

Linear Basis Functions on 3D Polyhedra

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

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

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

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

Linear Form

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

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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

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

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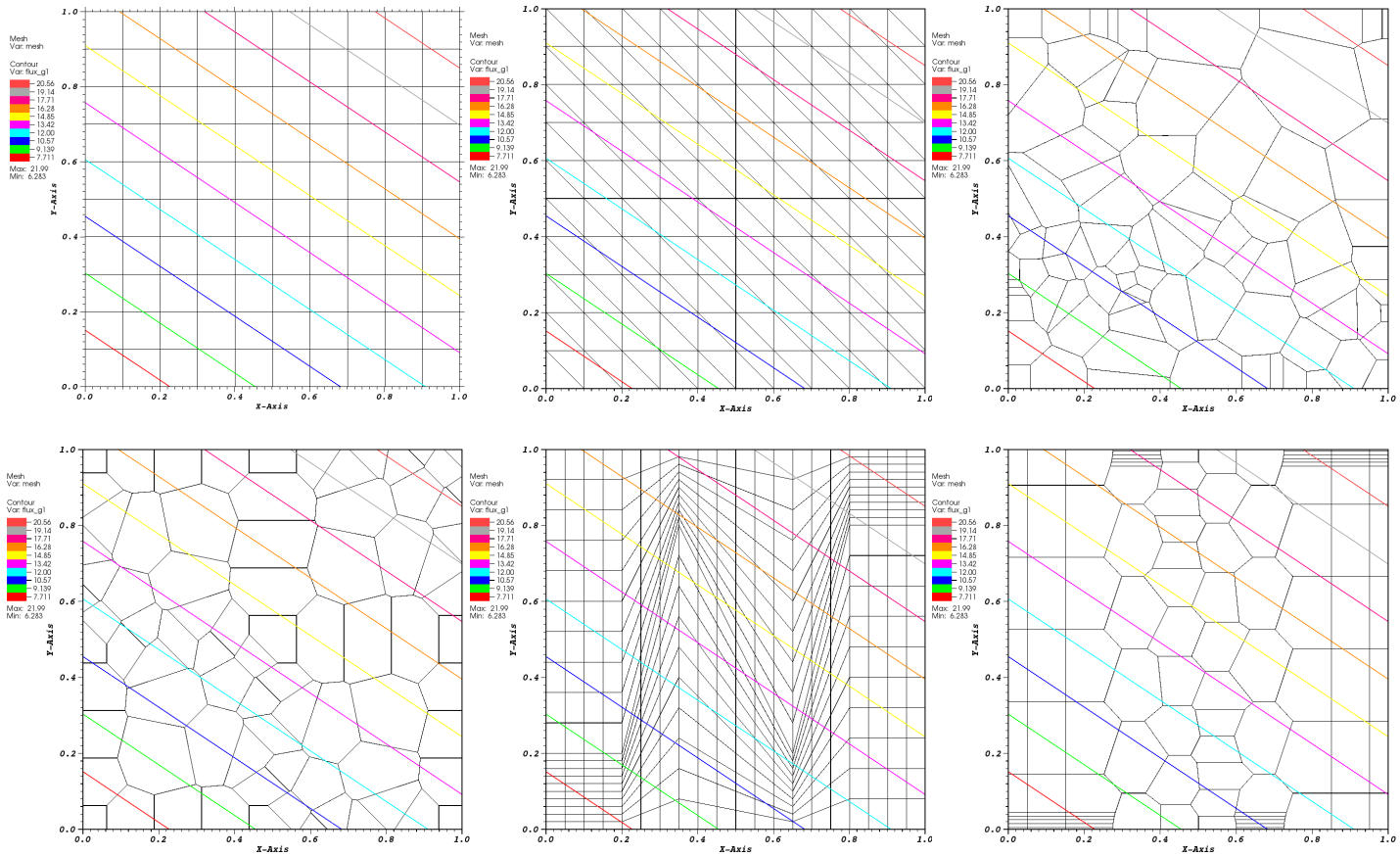
2D Exactly-Linear Transport Solutions - mean value coordinates

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

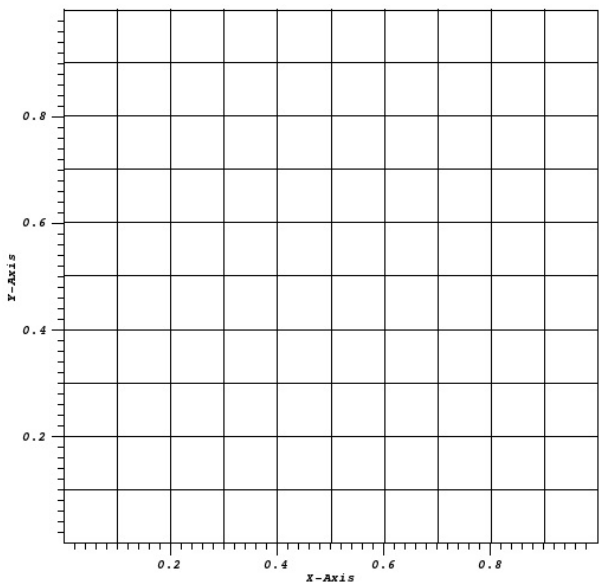
$$\psi(x,y,\mu,\eta)=ax+by+c\mu+d\eta+e,\qquad \phi(x,y)=2\pi\left(ax+by+e\right)$$

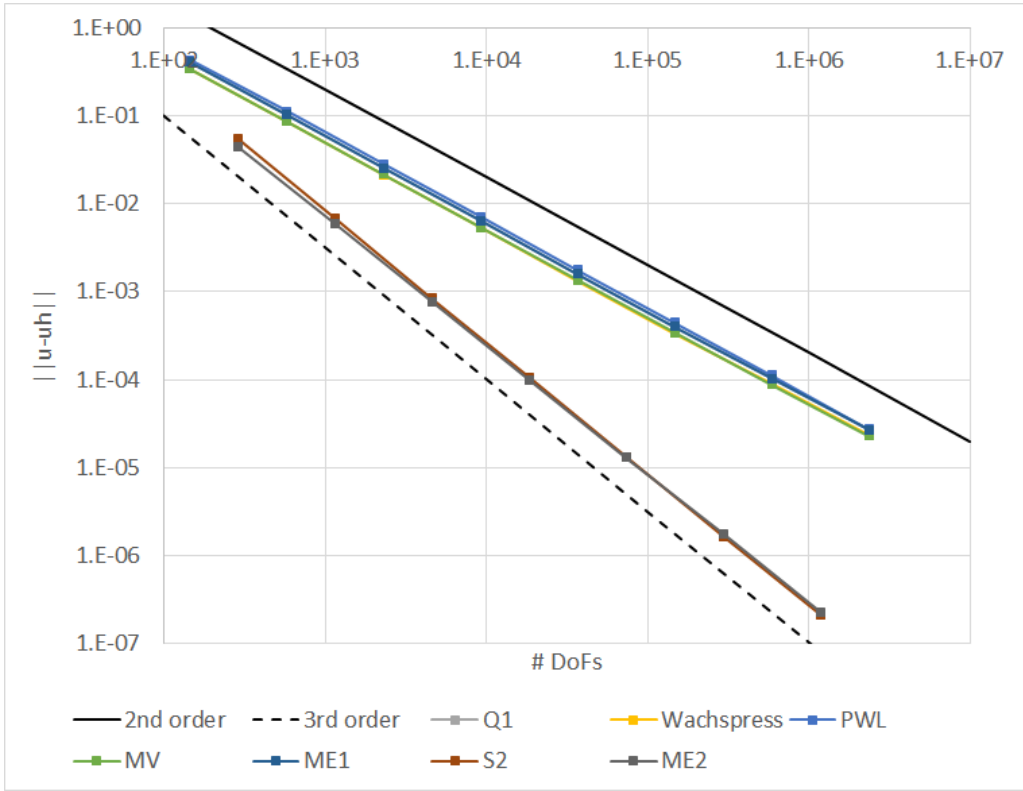


Convergence rates using MMS for the 2D polygonal basis functions

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

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





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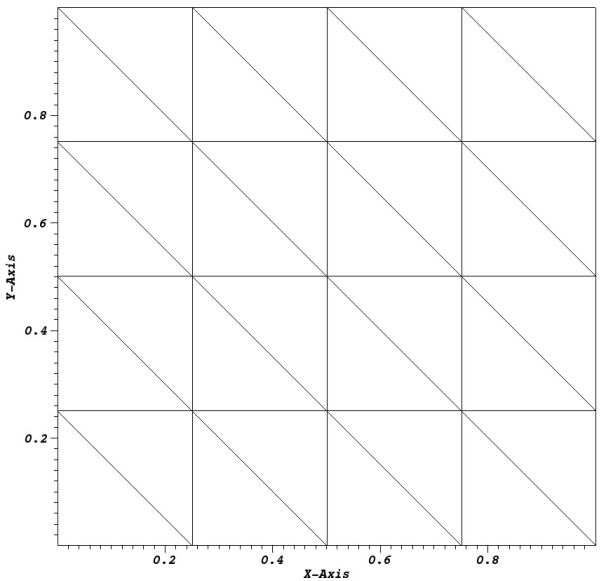

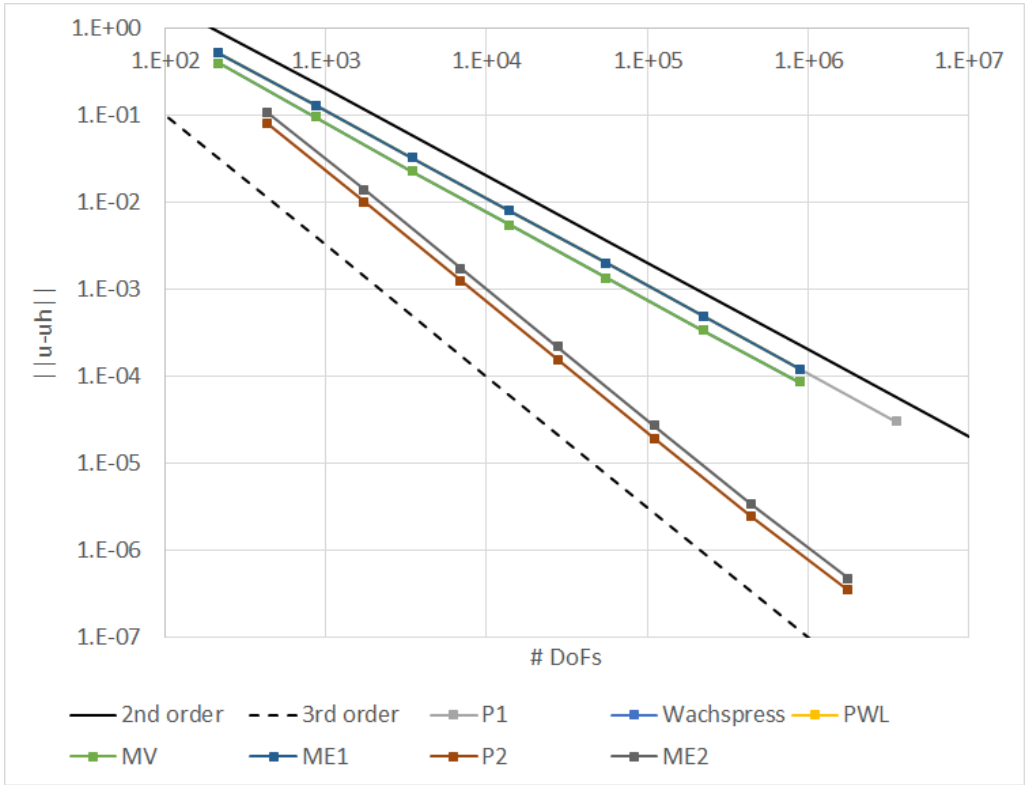

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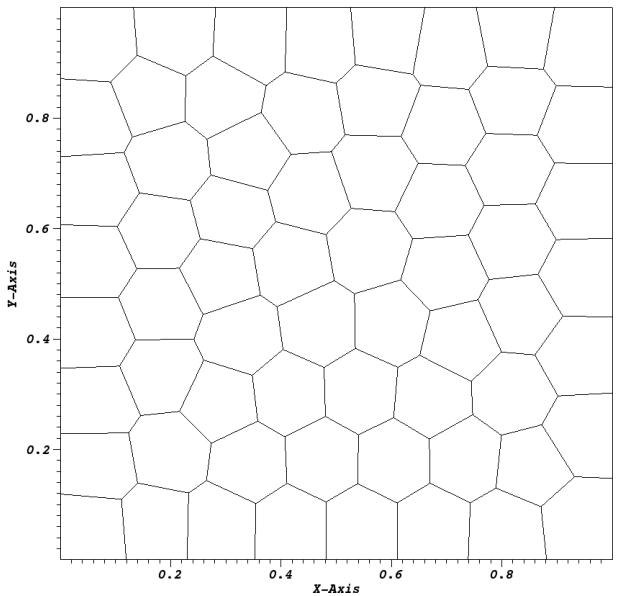
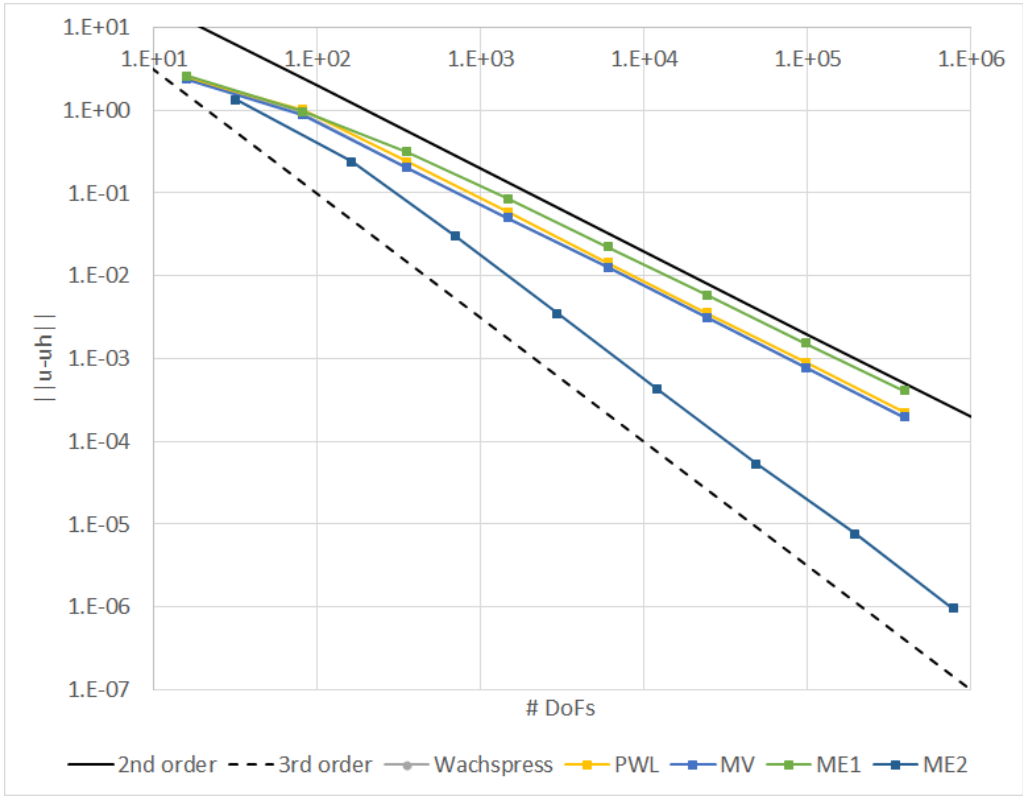
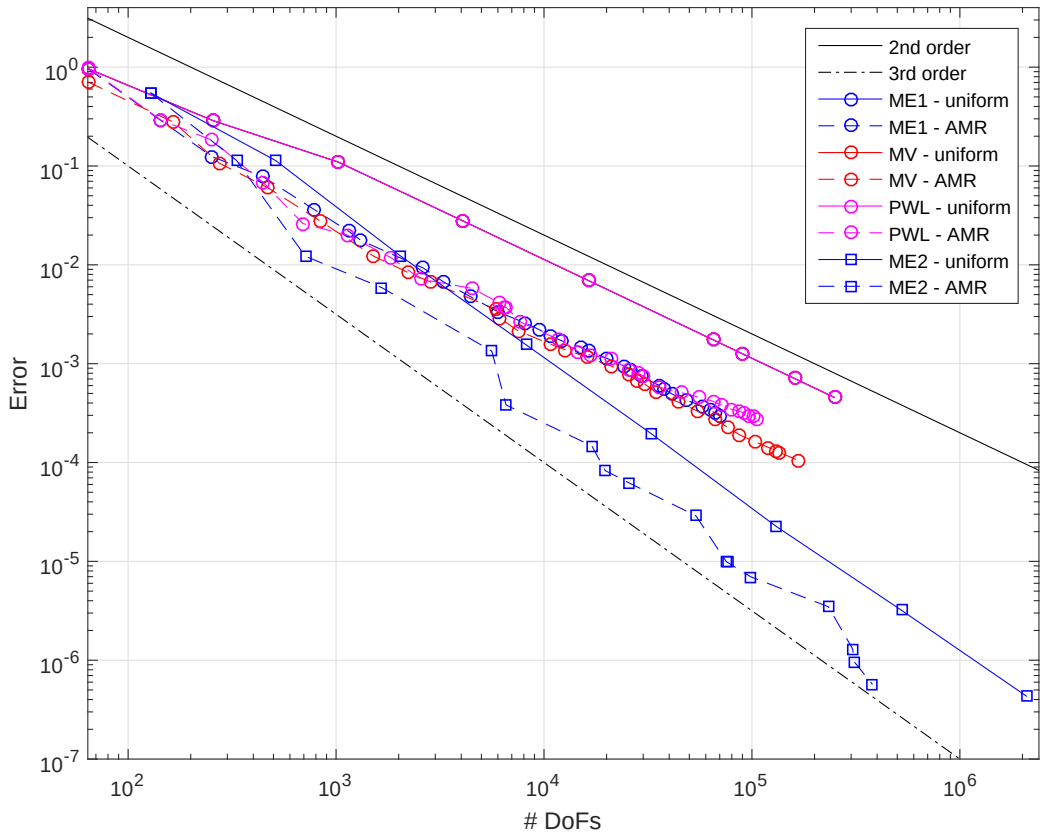




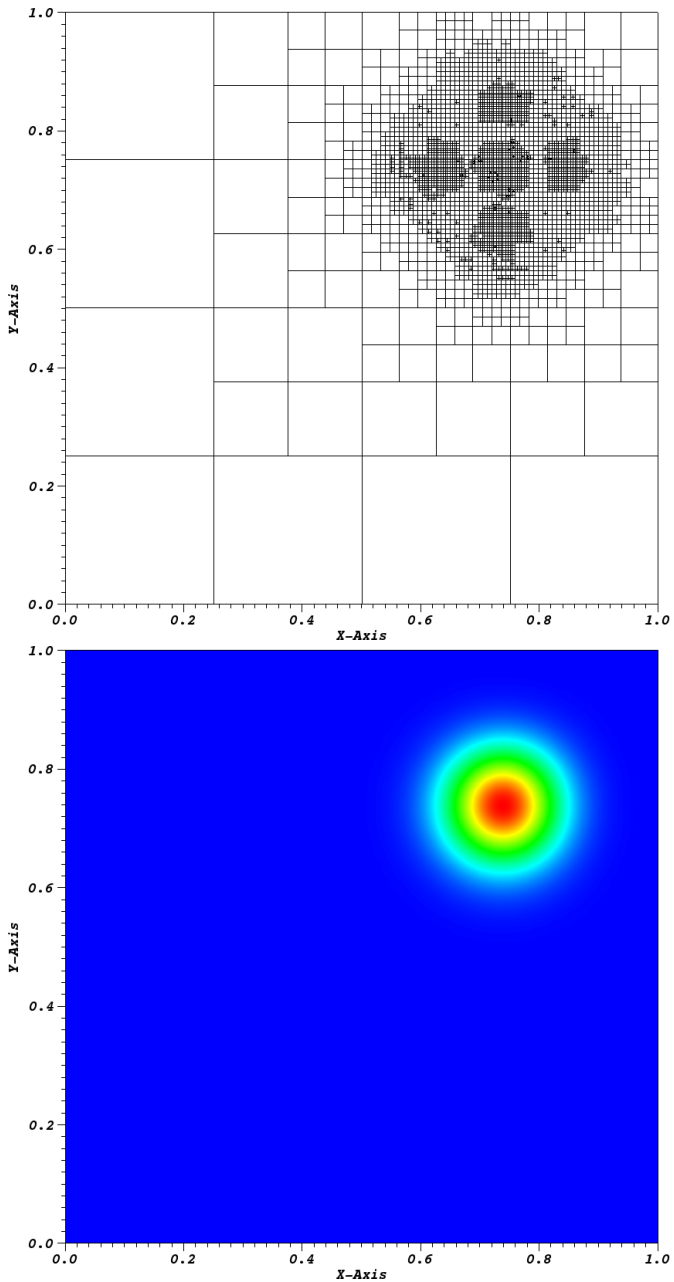
Convergence rates using MMS and AMR for the 2D polygonal basis functions

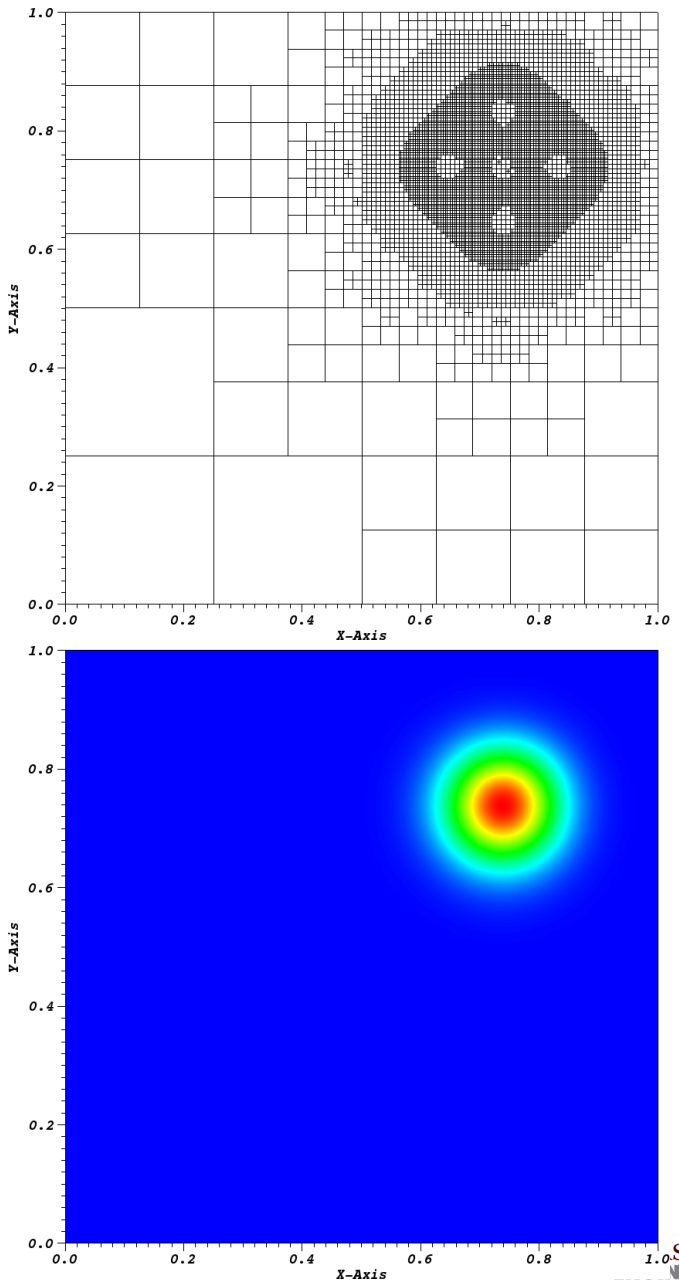
$$\psi(x,y) = x(L_x - x)y(L_y - y)\exp(-\frac{(x-x_0)^2 + (y-y_0)^2}{\gamma}),$$

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

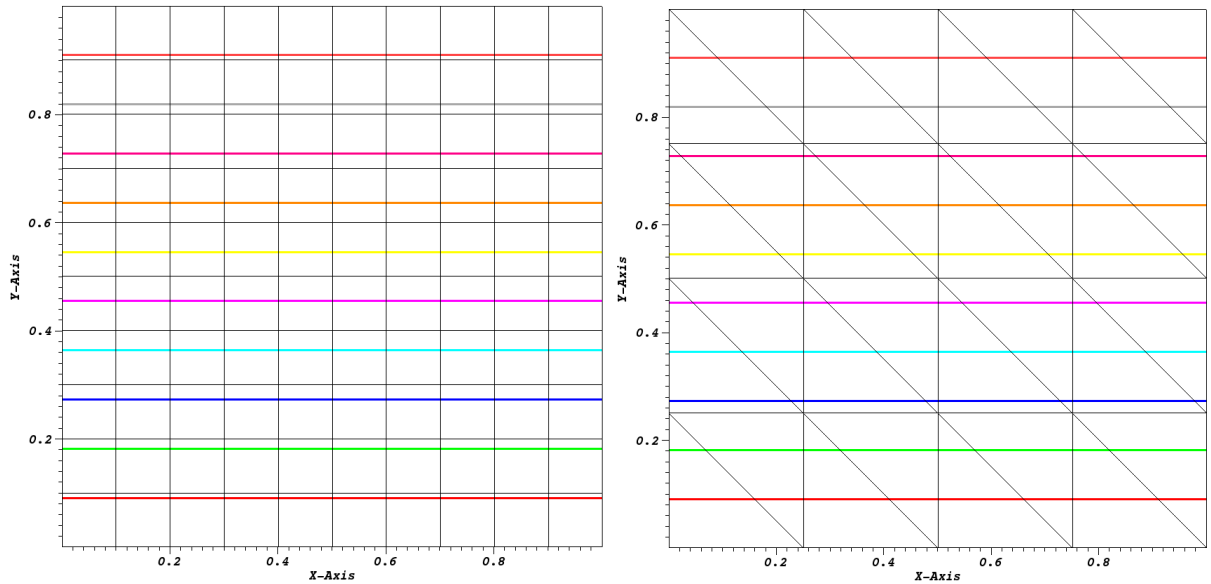


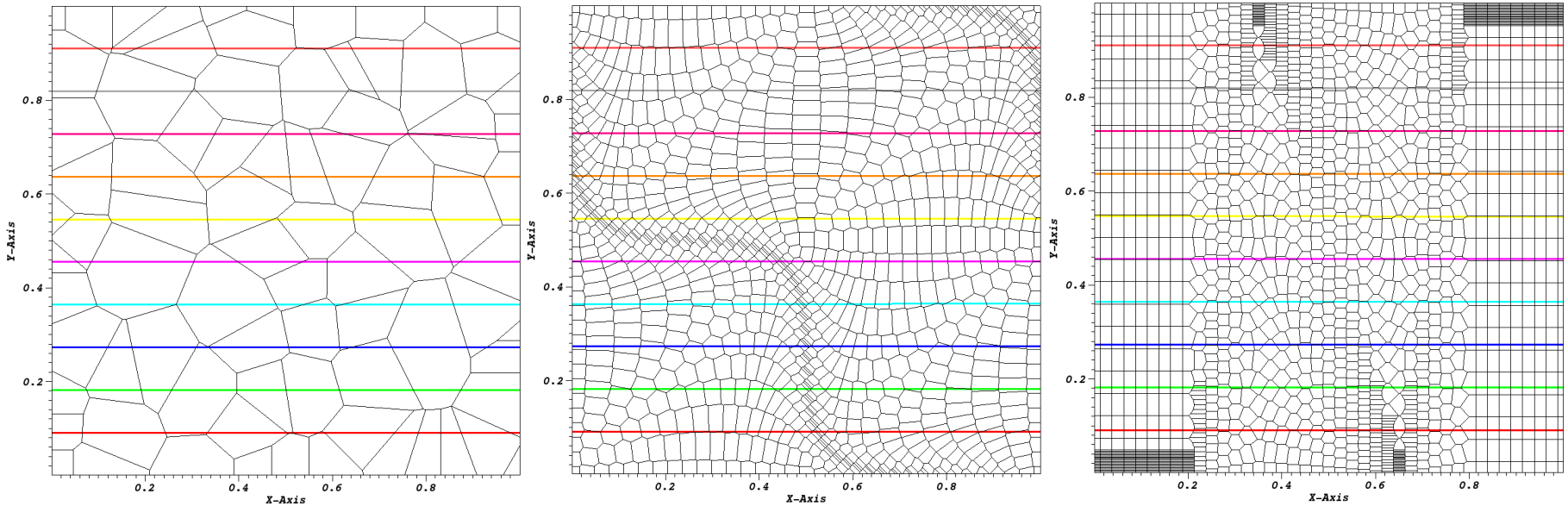
Linear ME cycle 15 (left) and quadratic ME cycle 08 (right)





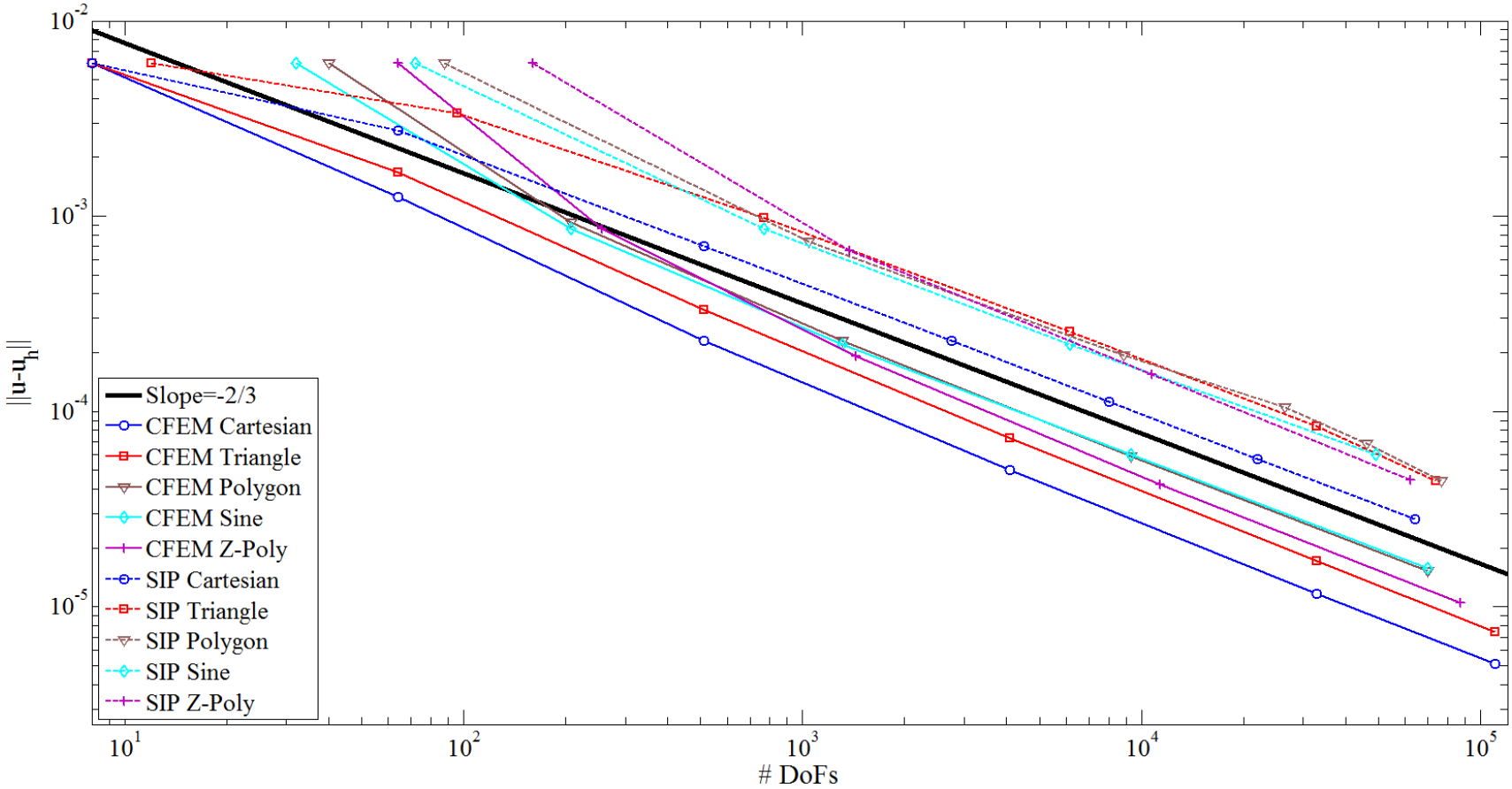
SIP exactly linear solutions on 3D polyhedral meshes using the PWL basis functions





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

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



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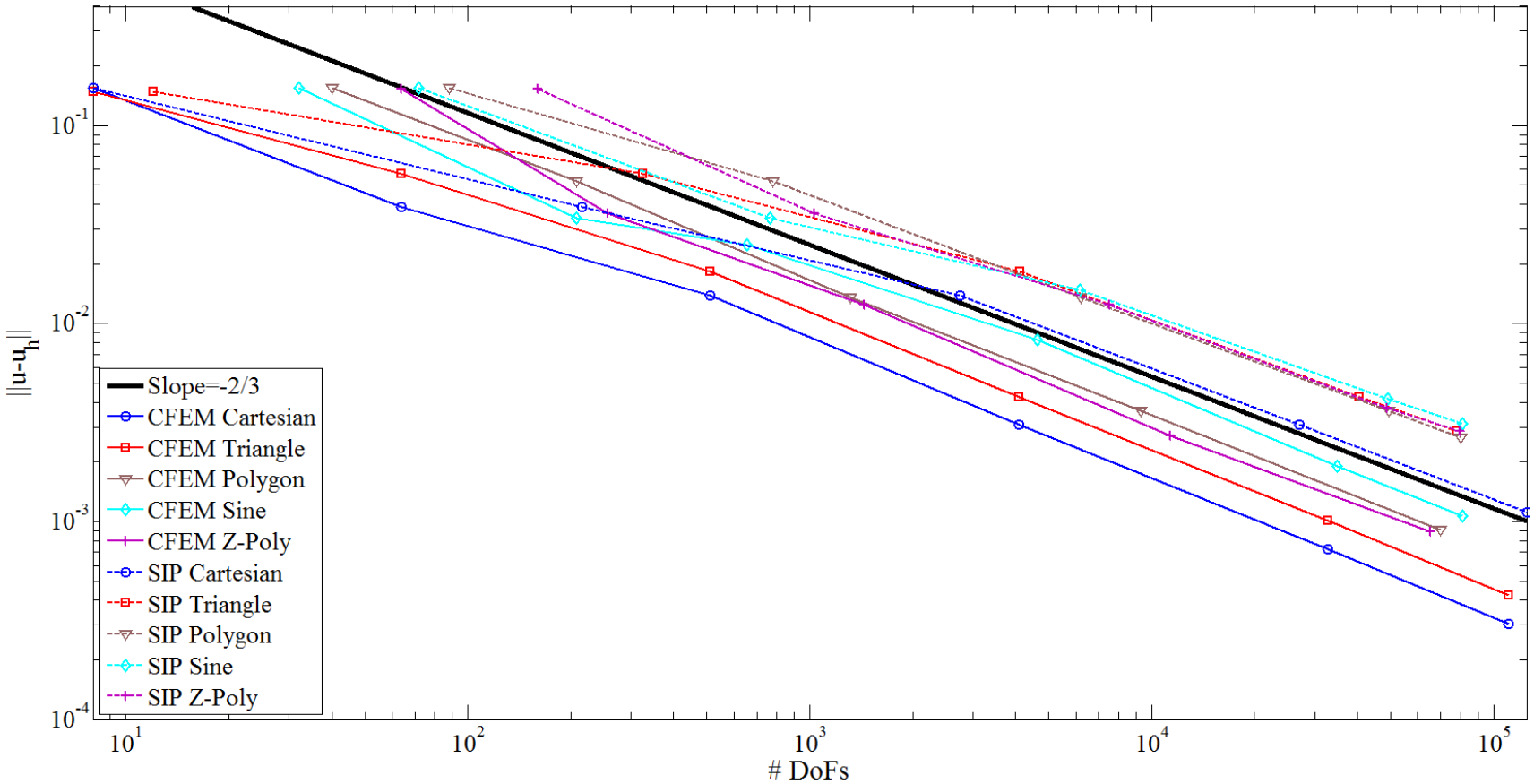
SIP convergence study - gaussian solution on 3D cube using the PWL basis functions

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



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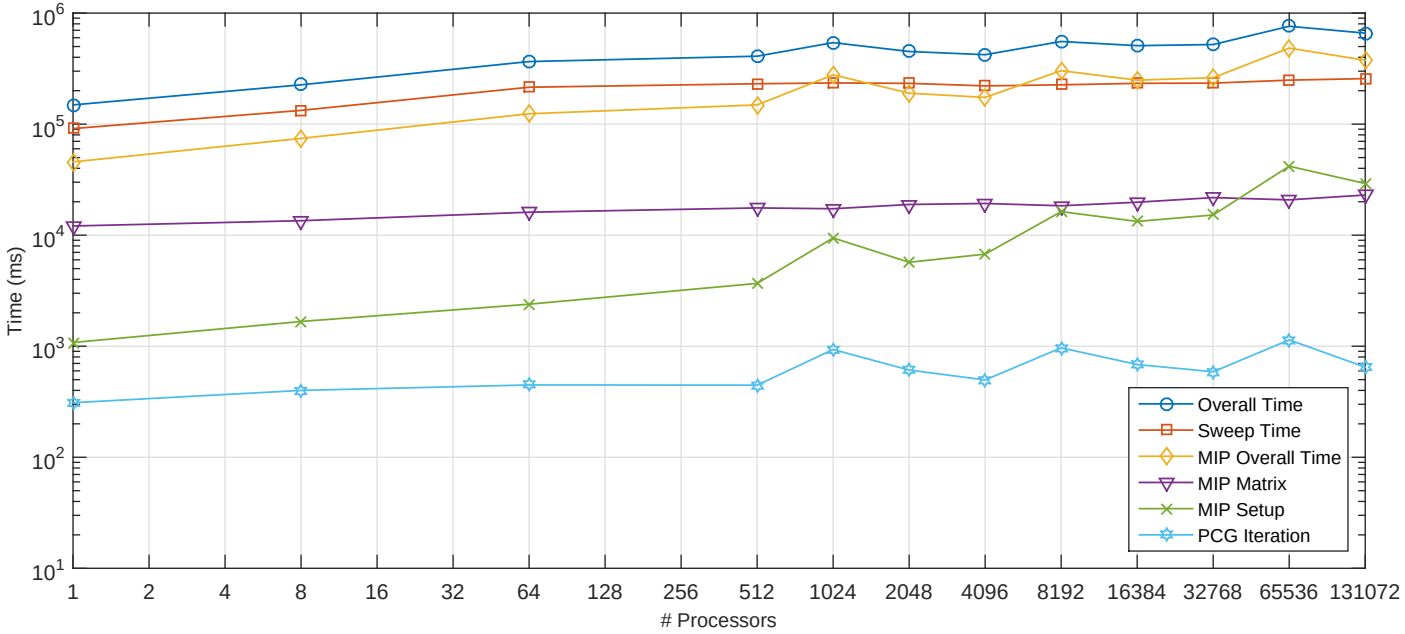
MIP DSA Timing Data with PDT on Vulcan using HYPRE



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

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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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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