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VERIFICATION OF DETERMINISTIC RADIATION TRANSPORT CODES

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PRESENTED BY

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SAND2020-

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Outline

- Description of radiation transport discretizations
- General verification definitions and techniques
- Special considerations for unstructured meshes
- Application to Sceptre transport code
- Results
- Conclusions

Continuous-Energy Boltzmann Transport Equation

The steady-state transport equation describes a six-dimensional phase space:

- 3 in space (r)
- 1 in energy (E)
- 2 in direction ($\vec{\Omega}$).

The fundamental unknown is the angular flux density ψ

$$\left[\vec{\Omega}\cdot\nabla + \sigma_t(r,E)\right]\psi\left(r,E,\vec{\Omega}\right) =$$

$$\int dE' \int d\vec{\Omega'}\sigma_s\left(r,E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega}\right)\psi\left(r,E',\vec{\Omega}'\right) + q\left(r,E,\vec{\Omega}\right)$$

$\vec{\Omega}\cdot\nabla$: “streaming” term

σ_t: “collision” (total) term

σ_s: double differential scattering term

Energy differencing: multigroup

SCEPTRE

If we integrate the energy-dependent Boltzmann equation over an energy range ("group"), we obtain a coupled system of within-group (or monoenergetic) equations, which are typically solved via "outer" (Richardson) iterations:

$$[\vec{\Omega} \cdot \nabla + \sigma_{t,g}(r)]\psi_g(r,\vec{\Omega}) =$$

$$\sum_{g\prime} \int d\vec{\Omega'} \sigma_{s,g\prime\to g}(r,\vec{\Omega}' \to \vec{\Omega})\psi_{g\prime}(r,\vec{\Omega}') + q_g(r,\vec{\Omega})$$

Note: assumptions about the spectral shape of the flux are made, which affects the multigroup cross sections. This is notoriously difficult for neutronics due to nuclear resonances. Such cross sections are usually supplied as an external database rather than embedded in the code.

(Takeaway lesson: Deterministic codes "solve" the cross section problem by defining it as someone else's problem.)

Forms of Monoenergetic Boltzmann Transport Equation

First-order: $$\left[\Omega\cdot\nabla+\sigma_t\right]\psi\left(r,\Omega\right)=M\Sigma D\,\psi\left(r,\Omega\right)+Q\left(r,\Omega\right)$$

Second-order:

$$\left[-\Omega\cdot\nabla\Re^{-1}\Omega\cdot\nabla+\Re\right]\psi\left(r,\Omega\right)=Q\left(r,\Omega\right)-\Omega\cdot\nabla\left[\Re^{-1}Q\left(r,\Omega\right)\right]$$

The two continuous forms above are equivalent.

Discretizations, however, yield different properties:

- Solutions
- Solvers

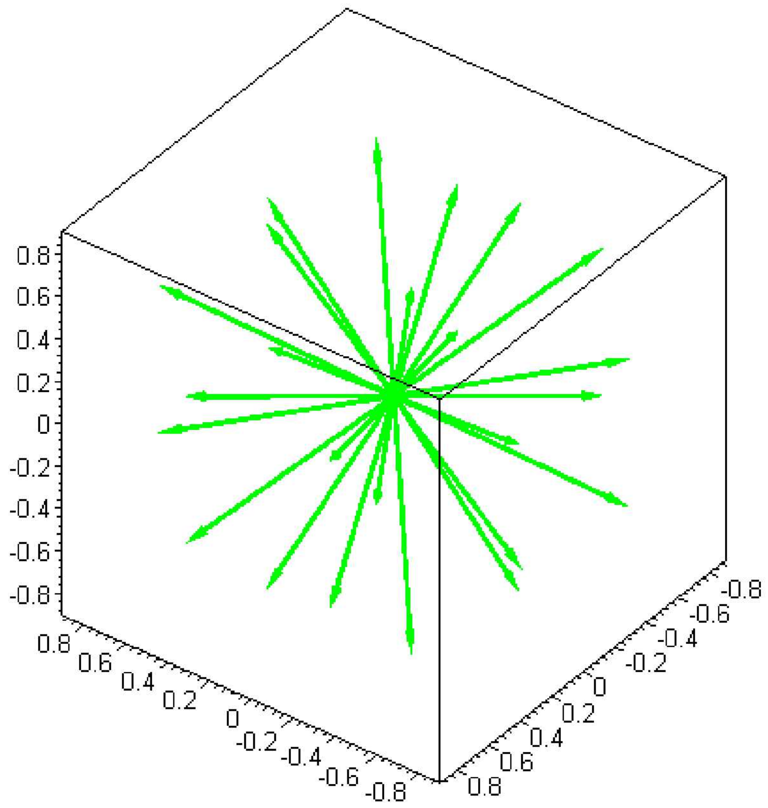
Spatial discretizations

There are various spatial discretizations that have been used for deterministic codes. We will focus on finite element methods

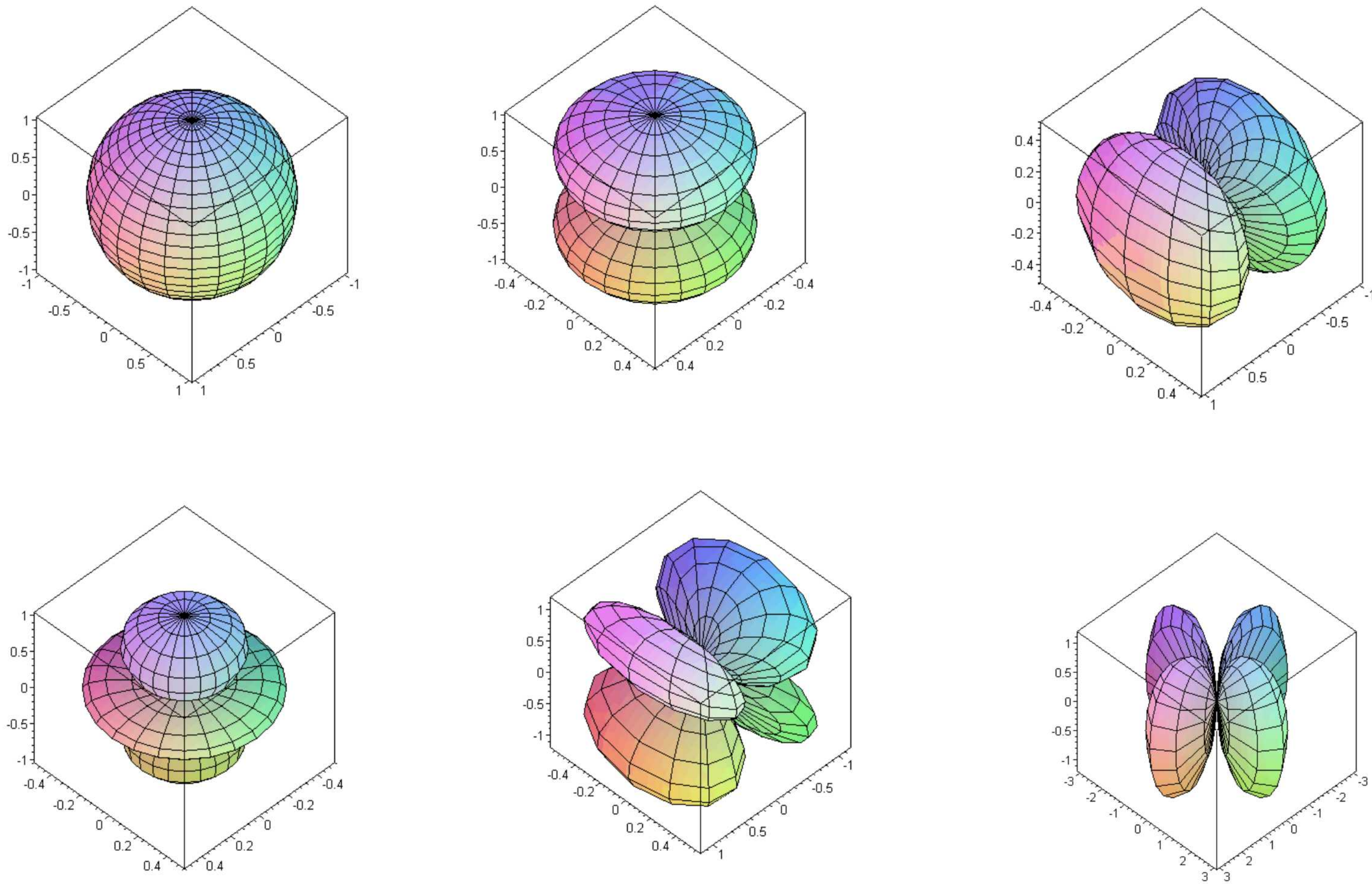
- Discontinuous Galerkin FEM for 1st-order form
- Continuous FEM for 2nd-order form
- Linear and quadratic basis functions
- Structured and unstructured meshes

Angular discretization: discrete ordinates (Sn)

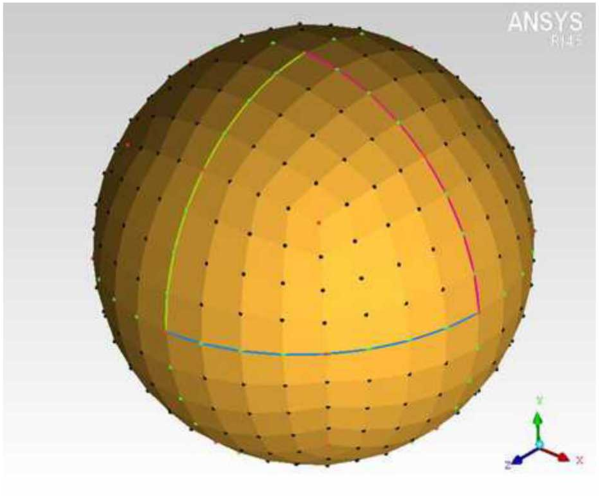
- Collocation in angle
- Compute solution in discrete directions
- Use numerical quadrature to compute angular integrations



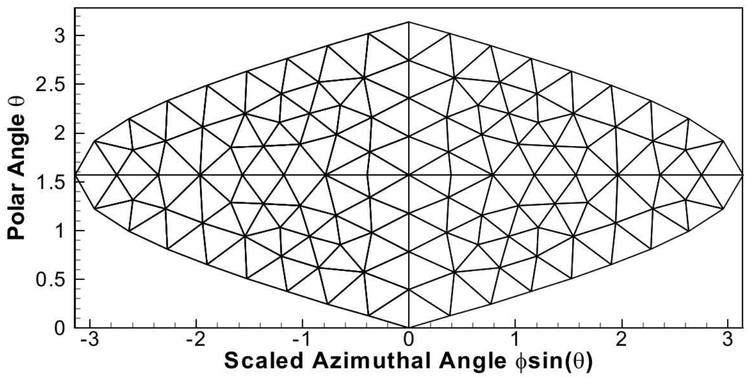
Angular discretization: spherical harmonics (Pn)



Angular discretization: finite elements



Unit sphere with surface mesh



Mesh of sphere mapped to planar region

Verification techniques: method of manufactured solutions

General equation to solve:

$$Du = q$$

Classic verification approach:

Set q → derive u; compare u_h to u

MMS verification approach:

Set u → derive q; compare u_h to u

Requires the code to accept a general source term

Verification techniques: method of manufactured solutions

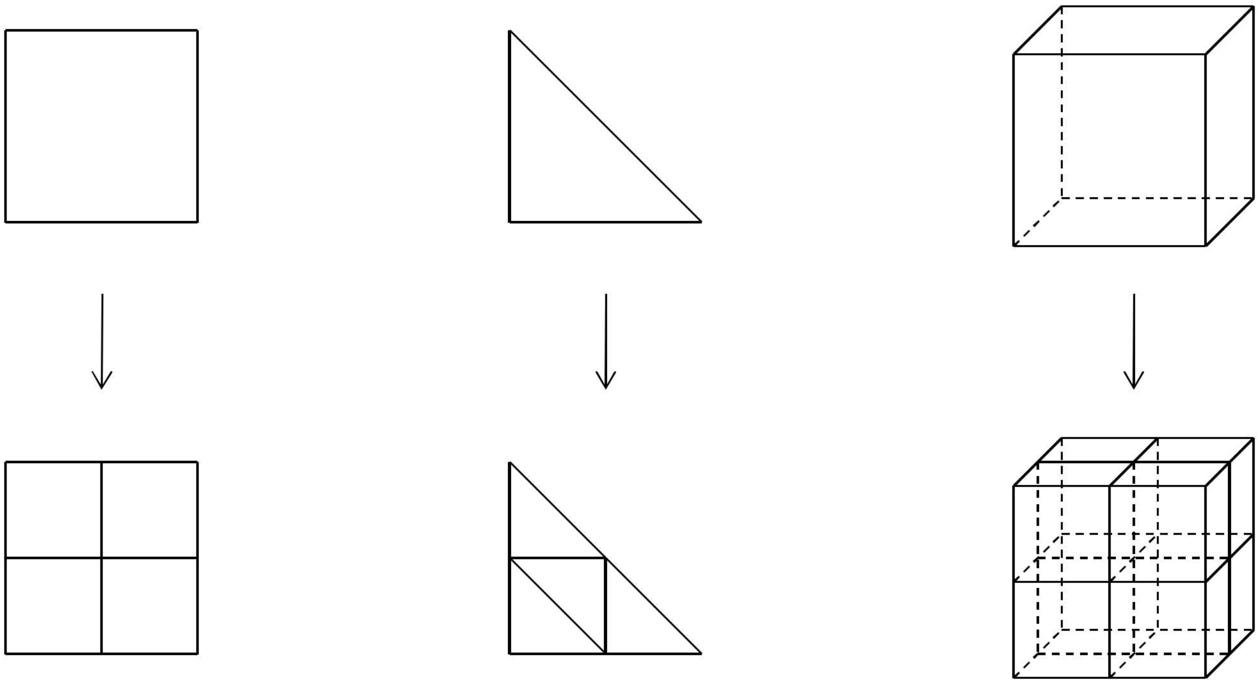
The method of manufactured solutions is used to verify error convergence rates.

$$\varepsilon_h = u_h - u = ch^p + c'h^{p+1} + \cdots$$

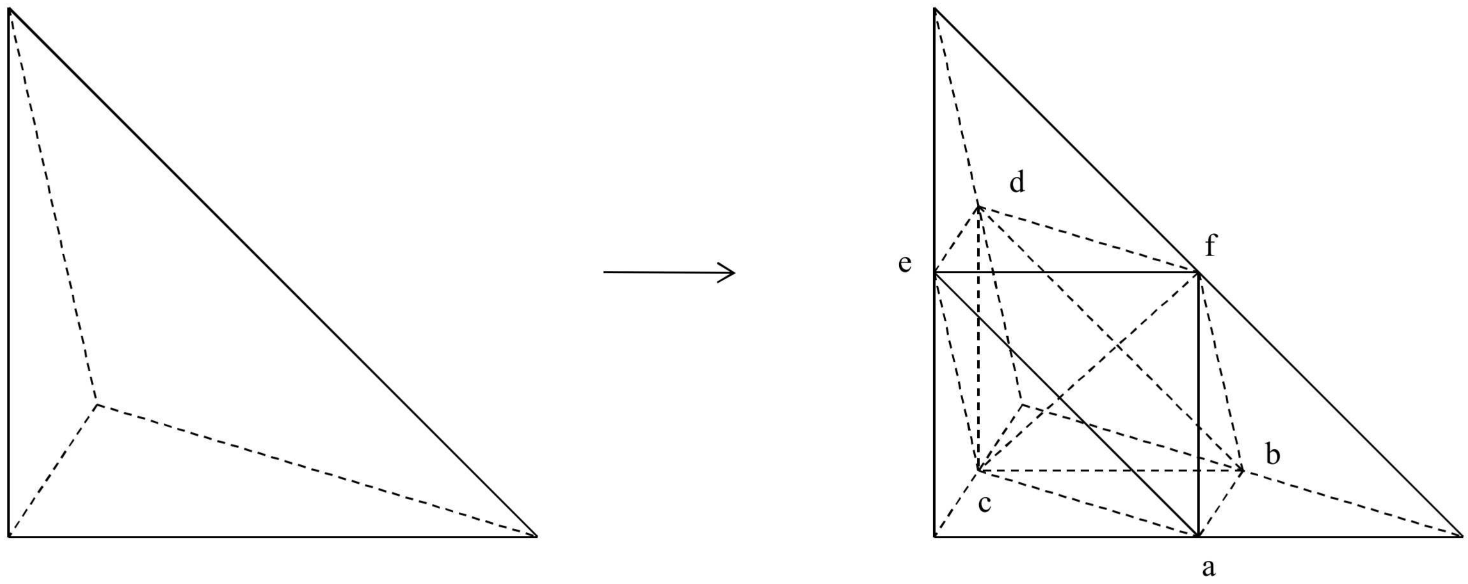
$$\rightarrow \quad p = \log_2\left(\frac{\varepsilon_h}{\varepsilon_{h/2}}\right)$$

We compare the observed convergence rate to the theoretical rate on a series of meshes to verify the code.

Unstructured meshes: refinement rules

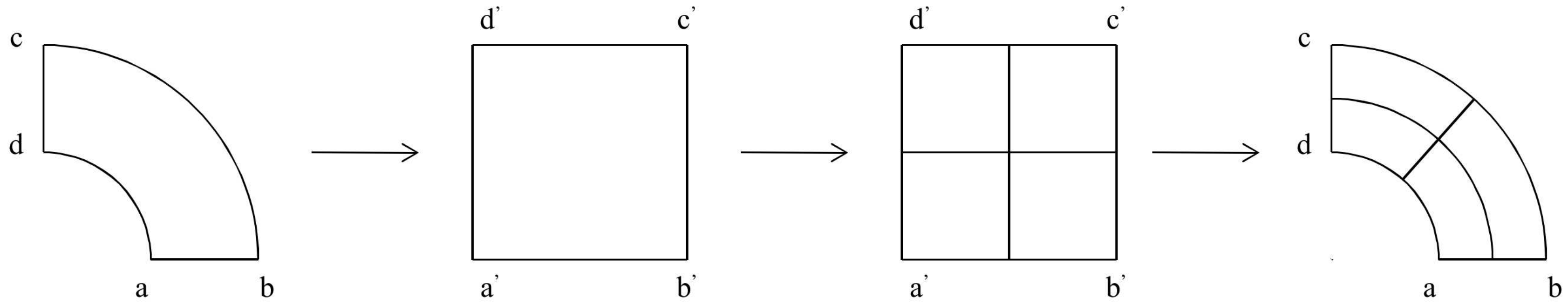


Unstructured meshes: refinement rules (tetrahedra)



The shortest diagonal *ad*, *be*, or *cf* should be used to subdivide each tetrahedron. Failure to do so can result in tetrahedra of increasingly poor quality.

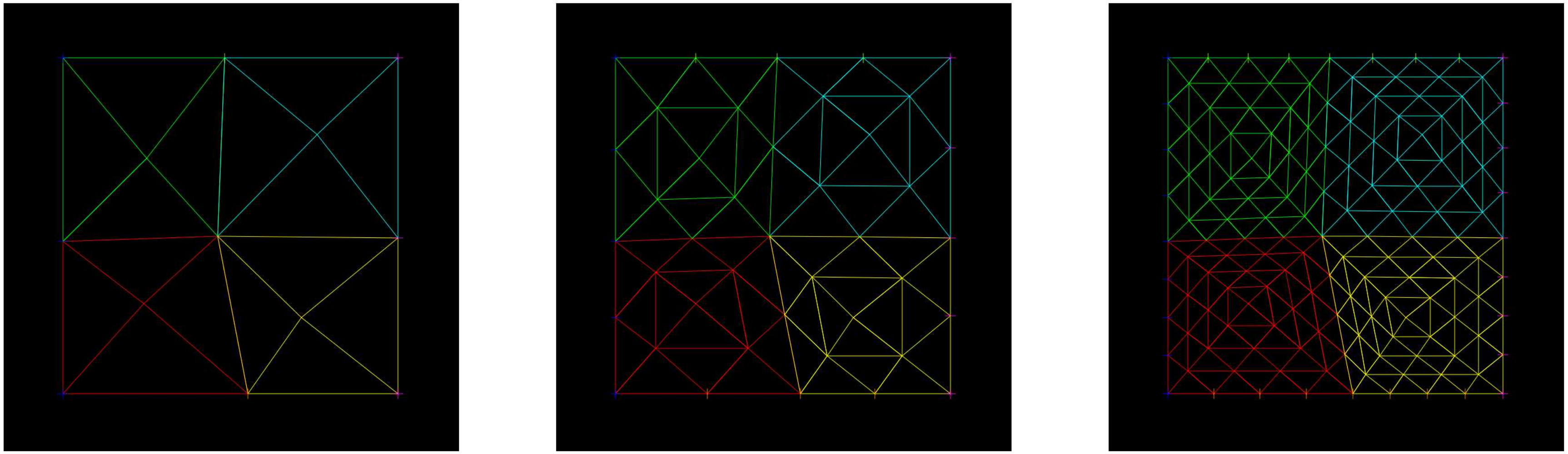
Mesh refinement rules for curved elements



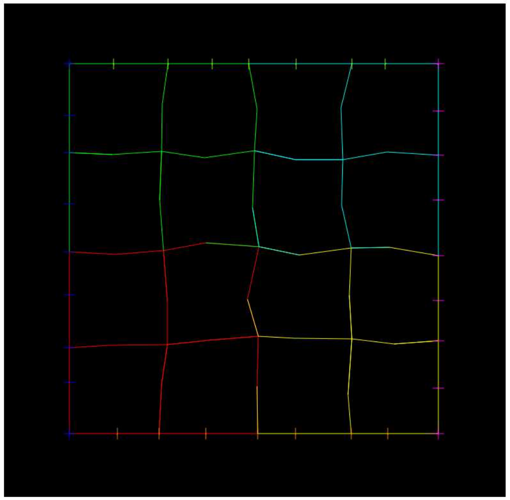
Element refinement should occur in interpolation space (i.e. “master element”).

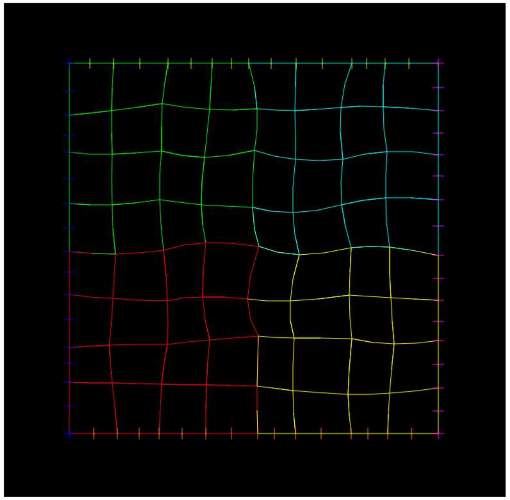
- ensures valid elements
- preserves Jacobians

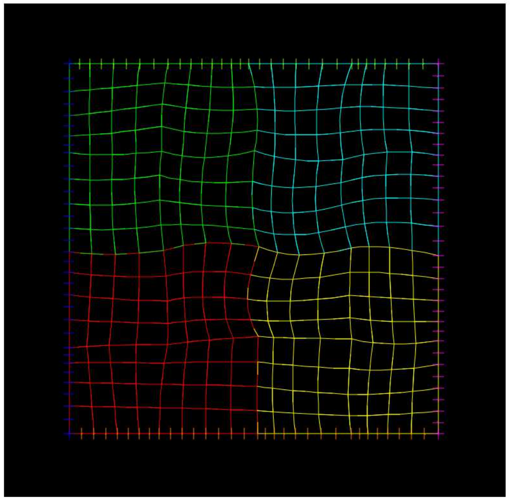
Example: triangular mesh refinement



Example: quadrilateral mesh refinement







SCEPTRE Code Description

SCEPTRE: Sandia's Computational Engine for Particle Transport for Radiation Effects

- Linear steady-state deterministic Boltzmann transport solver
- S_n, P_n, or FEM in angle
- Multigroup in energy
- Discontinuous FEM (1st order) and continuous FEM (2nd order) on unstructured meshes
- Second-order variants
  - Even/odd parity flux (EOPF)
  - Self-adjoint angular flux (SAAF)
  - Least-squares (LS)

Error metrics used by Sceptre

L-norm: $$\left[\int d\Omega \int dV \left|\psi^n\right|\right]^{1/n}$$

H-norm: $$\left[\int d\Omega \int dV \left\|\nabla \psi\right\|^n\right]^{1/n}$$

Streaming-norm: $$\left[\int d\Omega \int dV \left|\Omega \cdot \nabla \psi\right|^n\right]^{1/n}$$

Used to determine the difference between a computational result and a reference solution.

Test strategy

We generate tests in two different categories:

- "Exact" tests: The solution can be exactly computed/represented regardless of problem refinement (also called "patch" tests)
- "Inexact" tests: The discrete solution will contain discretization error, which hopefully decreases with problem refinement.

Exactly solvable problems (prediction)

	1	x	y	z	xy	xz	yz	xyz	x^2	y^2	z^2	x^2y	x^2z	y^2x	y^2z	z^2x	z^2y	x^2yz	y^2xz	z^2xy
edge2	SU	SU																		
edge3	SU	SU							S											
tri3	SU	SU	SU																	
tri6	SU	SU	SU		S				S	S										
quad4	SU	SU	SU		S															
quad8	SU	SU	SU		S				S	S		S		S						
tet4	SU	SU	SU	SU																
tet10	SU	SU	SU	SU	S	S	S		S	S	S									
hex8	SU	SU	SU	SU	S	S	S	S												
hex20	SU	SU	SU	SU	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S

S: Structured meshes

U: Unstructured meshes

Jacobians are generally non-constant in unstructured meshes, resulting in some finite element integrals that cannot be exactly computed with standard quadratures.

Structured mesh results, 2D

SCEPTRE

Element Type	Solver	L_{inf} error norm					
		1	x	x^2	xy	x^3	x^2y
tri3	Sn-1st	7.79×10^{-14}	3.70×10^{-14}	**1.06×10^{-2}**	**5.04×10^{-3}**	**2.73×10^{-2}**	**1.26×10^{-2}**
tri6	Sn-1st	7.74×10^{-13}	7.85×10^{-13}	7.43×10^{-13}	6.60×10^{-13}	**9.47×10^{-4}**	**2.79×10^{-4}**
quad4	Sn-1st	2.55×10^{-15}	1.67×10^{-15}	**1.18×10^{-2}**	1.22×10^{-15}	**3.13×10^{-2}**	**1.04×10^{-2}**
quad8	Sn-1st	1.05×10^{-14}	7.55×10^{-15}	7.33×10^{-15}	4.44×10^{-15}	**1.05×10^{-3}**	3.44×10^{-15}
tri3	Sn-EOP	2.29×10^{-14}	4.90×10^{-14}	**2.07×10^{-2}**	**5.32×10^{-3}**	**5.20×10^{-2}**	**2.46×10^{-2}**
tri6	Sn-EOP	8.06×10^{-14}	1.10×10^{-13}	1.14×10^{-13}	1.98×10^{-13}	**2.33×10^{-3}**	**5.61×10^{-4}**
quad4	Sn-EOP	3.66×10^{-15}	7.12×10^{-14}	**1.50×10^{-2}**	7.26×10^{-14}	**4.18×10^{-2}**	**1.31×10^{-2}**
quad8	Sn-EOP	5.63×10^{-14}	1.38×10^{-13}	1.13×10^{-13}	1.92×10^{-13}	**1.80×10^{-3}**	1.56×10^{-13}

Unstructured mesh results, 2D

Element Type	Solver	L_{inf} error norm					
		1	x	x^2	xy	x^3	x^2y
tri3	Sn-1st	1.03×10^{-13}	5.27×10^{-14}	**1.40×10^{-2}**	**6.83×10^{-3}**	**3.22×10^{-2}**	**1.60×10^{-2}**
tri6	Sn-1st	1.53×10^{-12}	1.05×10^{-12}	**7.40×10^{-3}**	**2.52×10^{-3}**	**2.14×10^{-2}**	**5.32×10^{-3}**
quad4	Sn-1st	4.11×10^{-15}	2.66×10^{-15}	**2.09×10^{-2}**	**6.12×10^{-3}**	**4.03×10^{-2}**	**1.85×10^{-2}**
quad8	Sn-1st	4.64×10^{-14}	2.76×10^{-14}	**3.04×10^{-2}**	**1.75×10^{-2}**	**5.72×10^{-2}**	**3.26×10^{-2}**
tri3	Sn-EOP	3.67×10^{-14}	7.75×10^{-14}	**2.34×10^{-2}**	**9.23×10^{-3}**	**5.39×10^{-2}**	**2.43×10^{-2}**
tri6	Sn-EOP	7.41×10^{-14}	9.03×10^{-14}	**6.83×10^{-3}**	**3.25×10^{-3}**	**1.97×10^{-2}**	**6.95×10^{-3}**
quad4	Sn-EOP	9.88×10^{-14}	6.87×10^{-14}	**3.34×10^{-2}**	**9.51×10^{-3}**	**6.12×10^{-2}**	**2.77×10^{-2}**
quad8	Sn-EOP	6.76×10^{-14}	9.76×10^{-14}	**1.57×10^{-2}**	**7.64×10^{-3}**	**3.60×10^{-2}**	**1.36×10^{-2}**

Structured mesh results, 3D

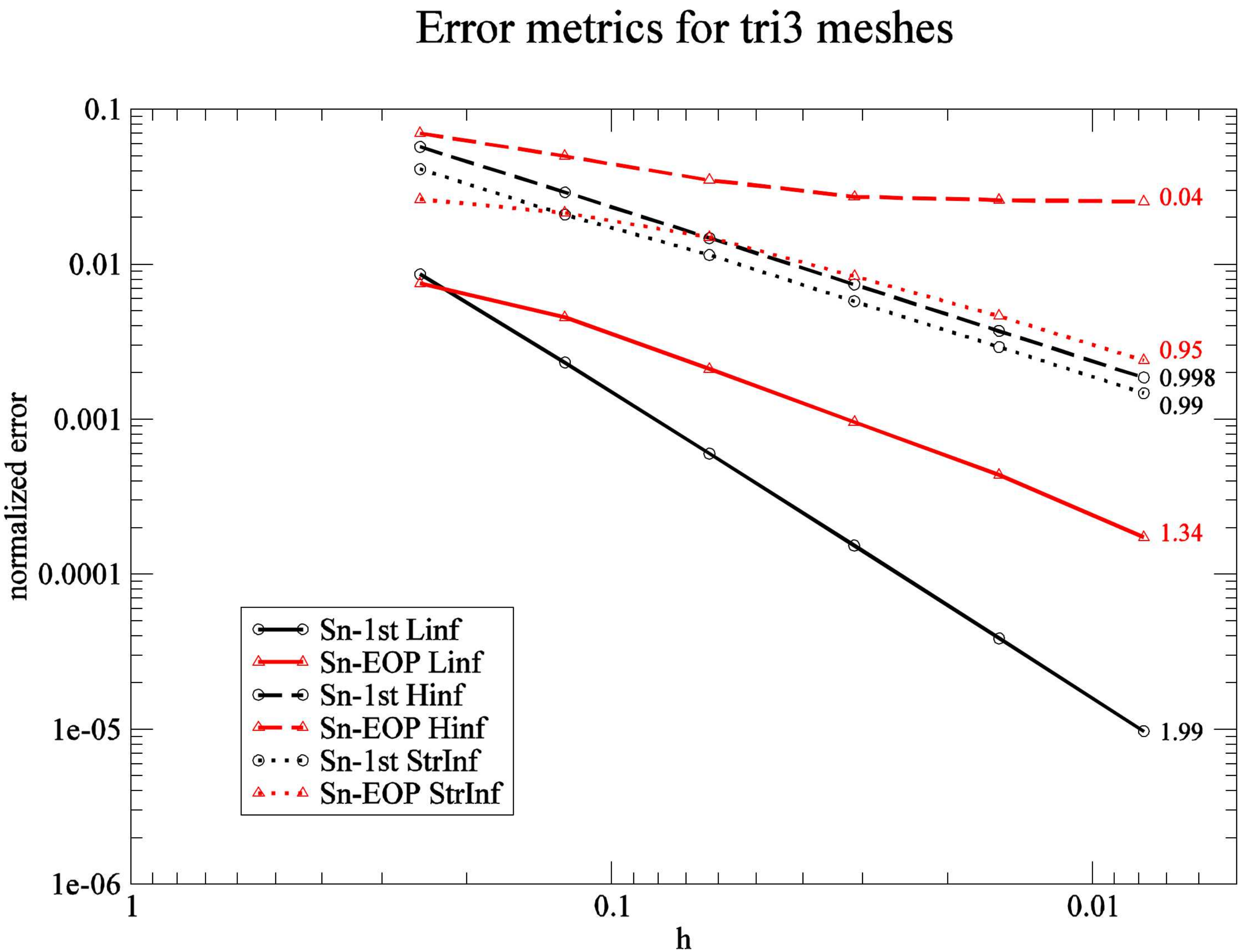
Element Type	Solver	L_{inf} error norm							
		1	x	x^2	xy	x^3	x^2y	xyz	x^2yz
tet4	Sn-1st	1.05×10^{-12}	5.01×10^{-13}	**9.81×10^{-3}**	**5.74×10^{-3}**	**2.53×10^{-2}**	**1.85×10^{-2}**	**8.57×10^{-3}**	**1.62×10^{-2}**
tet10	Sn-1st	3.08×10^{-12}	1.48×10^{-12}	1.14×10^{-12}	1.08×10^{-12}	**9.20×10^{-4}**	**4.36×10^{-4}**	**1.88×10^{-4}**	**7.82×10^{-4}**
hex8	Sn-1st	5.88×10^{-15}	4.88×10^{-15}	**1.33×10^{-2}**	5.22×10^{-15}	**3.46×10^{-2}**	**1.17×10^{-2}**	4.33×10^{-15}	**1.03×10^{-2}**
hex20	Sn-1st	6.11×10^{-14}	3.64×10^{-14}	4.25×10^{-14}	3.97×10^{-14}	**1.13×10^{-3}**	2.32×10^{-14}	2.24×10^{-14}	1.97×10^{-14}
tet4	Sn-EOP	2.87×10^{-13}	2.22×10^{-14}	**1.87×10^{-2}**	**9.42×10^{-3}**	**4.94×10^{-2}**	**2.65×10^{-2}**	**1.82×10^{-2}**	**3.67×10^{-2}**
tet10	Sn-EOP	6.80×10^{-13}	2.26×10^{-13}	1.90×10^{-13}	1.72×10^{-13}	**1.91×10^{-3}**	**6.91×10^{-4}**	**3.26×10^{-4}**	**1.21×10^{-3}**
hex8	Sn-EOP	9.17×10^{-14}	1.03×10^{-14}	**3.29×10^{-2}**	1.39×10^{-14}	**8.99×10^{-2}**	**3.08×10^{-2}**	9.27×10^{-15}	**2.88×10^{-2}**
hex20	Sn-EOP	8.46×10^{-14}	6.06×10^{-14}	5.64×10^{-14}	4.45×10^{-14}	**3.62×10^{-3}**	5.20×10^{-14}	4.76×10^{-14}	3.55×10^{-14}

Unstructured mesh results, 3D

SCEPTRE

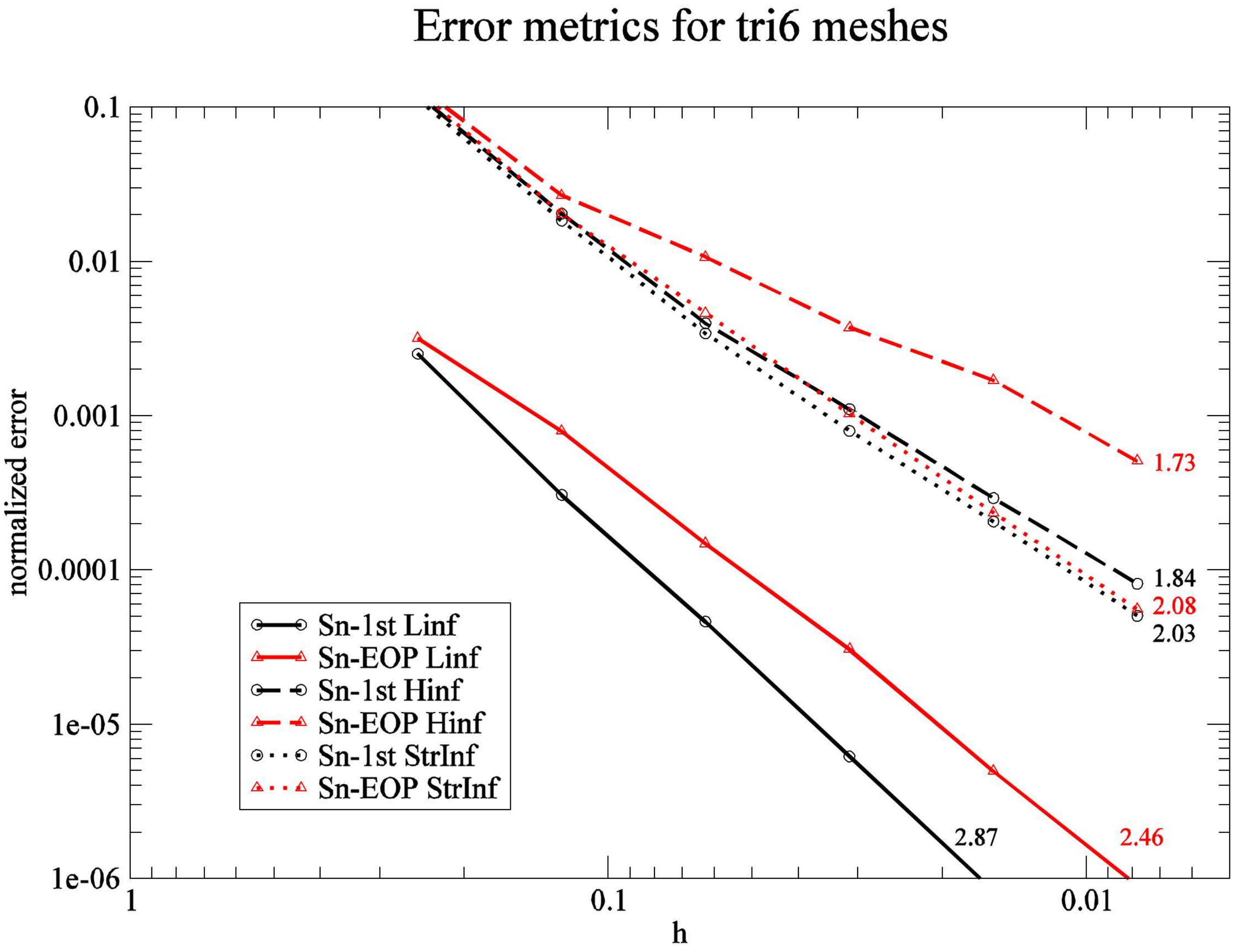
Element Type	Solver	L_{inf} error norm							
		1	x	x^2	xy	x^3	x^2y	xyz	x^2yz
tet4	Sn-1st	1.20×10^{-12}	5.82×10^{-13}	**1.88×10^{-2}**	**9.14×10^{-3}**	**4.89×10^{-2}**	**1.94×10^{-2}**	**1.13×10^{-2}**	**1.87×10^{-2}**
tet10	Sn-1st	4.20×10^{-12}	2.25×10^{-12}	**9.15×10^{-4}**	**6.30×10^{-4}**	**2.70×10^{-3}**	**1.63×10^{-3}**	**1.03×10^{-3}**	**1.36×10^{-3}**
hex8	Sn-1st	1.08×10^{-14}	9.77×10^{-15}	**2.35×10^{-2}**	**7.66×10^{-3}**	**6.15×10^{-2}**	**2.08×10^{-2}**	**1.01×10^{-2}**	**1.66×10^{-2}**
hex20	Sn-1st	6.38×10^{-14}	5.60×10^{-14}	**5.27×10^{-3}**	**3.14×10^{-3}**	**1.03×10^{-2}**	**4.20×10^{-3}**	**4.36×10^{-3}**	**5.26×10^{-3}**
tet4	Sn-EOP	4.40×10^{-13}	3.31×10^{-13}	**2.33×10^{-2}**	**1.53×10^{-2}**	**5.54×10^{-2}**	**3.24×10^{-2}**	**2.66×10^{-2}**	**4.91×10^{-2}**
tet10	Sn-EOP	1.41×10^{-13}	1.53×10^{-13}	**1.17×10^{-3}**	**9.17×10^{-4}**	**4.09×10^{-3}**	**1.67×10^{-3}**	**1.29×10^{-3}**	**1.94×10^{-3}**
hex8	Sn-EOP	3.55×10^{-13}	2.88×10^{-13}	**4.79×10^{-2}**	**9.16×10^{-3}**	**1.25×10^{-1}**	**4.55×10^{-2}**	**1.30×10^{-2}**	**5.14×10^{-2}**
hex20	Sn-EOP	1.10×10^{-13}	6.18×10^{-14}	**6.86×10^{-3}**	**6.07×10^{-3}**	**1.62×10^{-2}**	**6.78×10^{-3}**	**5.85×10^{-3}**	**7.28×10^{-3}**

Convergence rates for linear FEM



Convergence rates for quadratic FEM

SCEPTRE

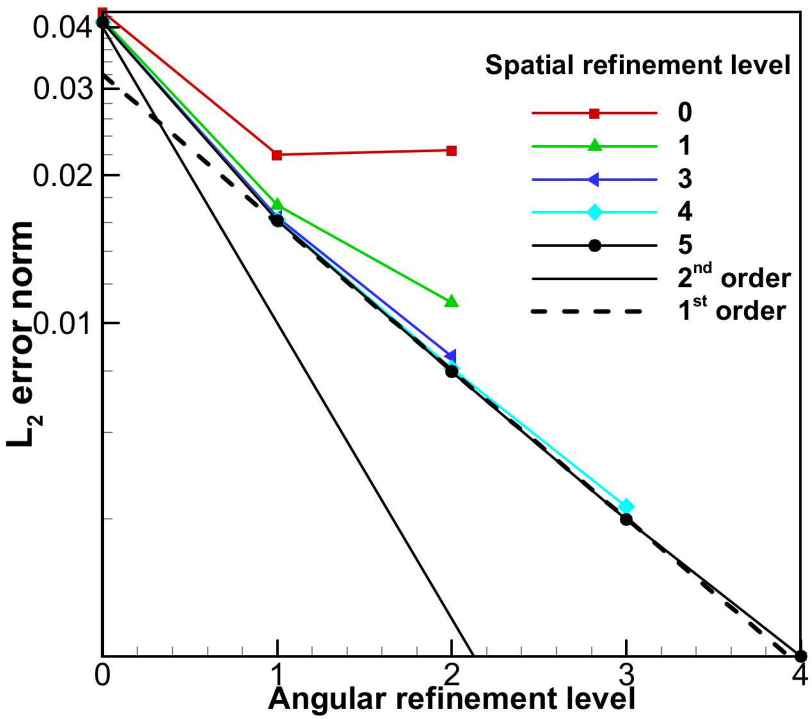


Sceptre bugs/issues identified by means of MMS testing

- 2^{nd}-order methods have inherent degradation of convergence order
- Element quadratures lose accuracy when Jacobians are non-constant, but do not affect convergence order
- MMS test generation incorrectly calculated gradients
- Inconsistent definitions of face rotations/mirroring
- Some solvers used 0 rather than previous iterate solutions for outer iteration
- Some solvers used incorrect scattering cross section functor

Angular FEM verification

We have a limited amount of verification data for FEM in angle



Angular refinement on series of fixed spatial meshes

Conclusions

- Radiation transport methods discretize in energy, angle, and space
- Robust verification activities for spatial discretizations
  - “Exact” and “inexact” problems
  - Structured and unstructured meshes
- Verification on angular differencing currently limited to exact problems for S_n and P_n discretizations; some convergence analysis for FEM in angle
- Verification of multigroup energy differencing for exact problems