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Verification of Radiation Transport Codes with Unstructured Meshes

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Outline

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

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V&V Definitions

Verification: Does the computer code faithfully implement the intended physical model?

"Are we solving the equations correctly?"

Validation: Is the physical model adequate for its intended use?

"Are we solving the correct equations?"

V&V Mappings

reality

Physical model $\qquad$ Validation

$$Du = q$$

Discretization $\qquad$ Verification

$$D_h u_h = q_h$$

Implementation $\qquad$ Verification

$$D_h^* u_h^* = q_h^*$$

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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

Verification techniques: method of manufactured solutions

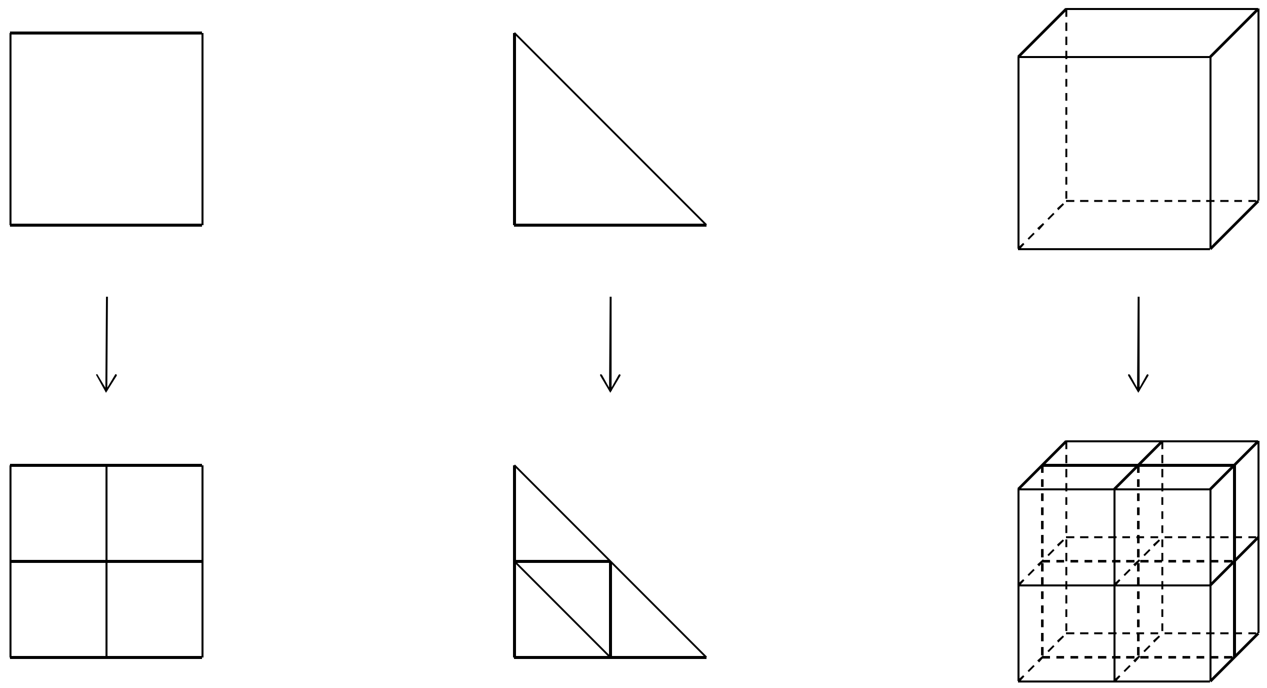
The method of manufactured solutions is used to verify error convergence rates.

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

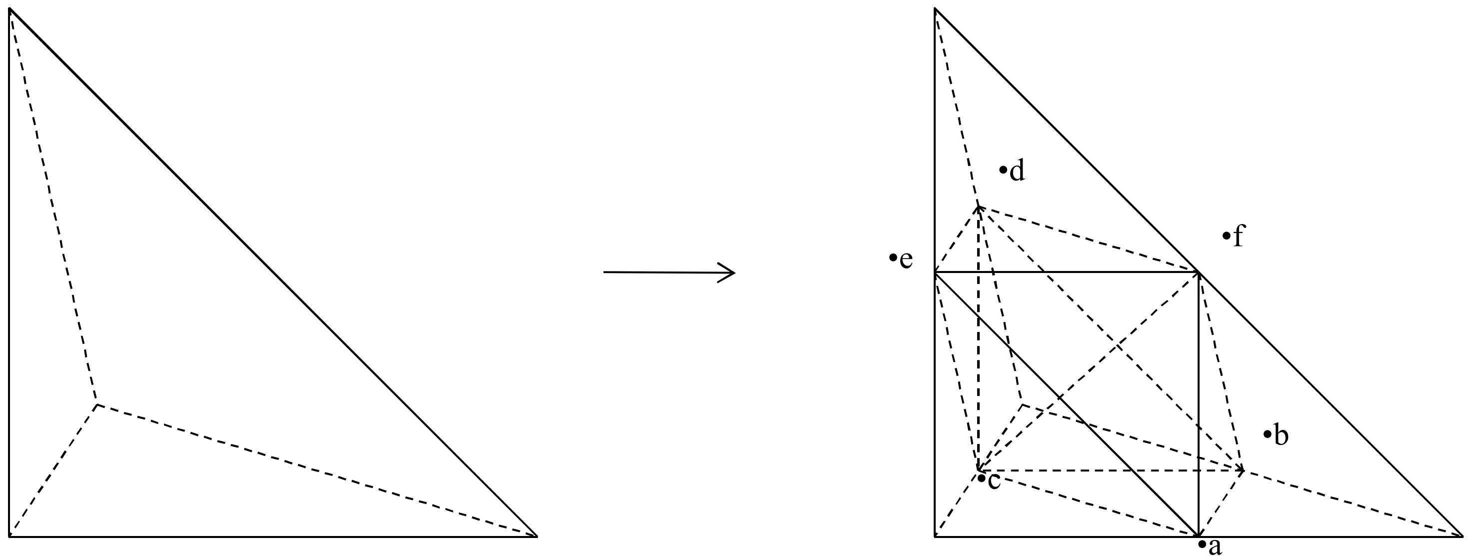
$$\rightarrow \quad p = \log_2\left(\frac{\varepsilon_h}{\varepsilon_{h/2}}\right)$$

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.

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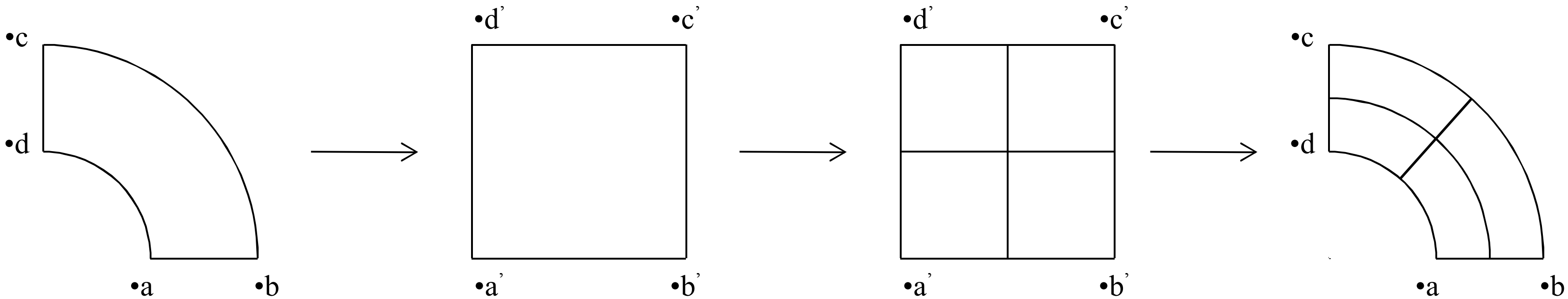
Mesh refinement rules for curved elements



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

- ensures valid elements
- preserves Jacobians

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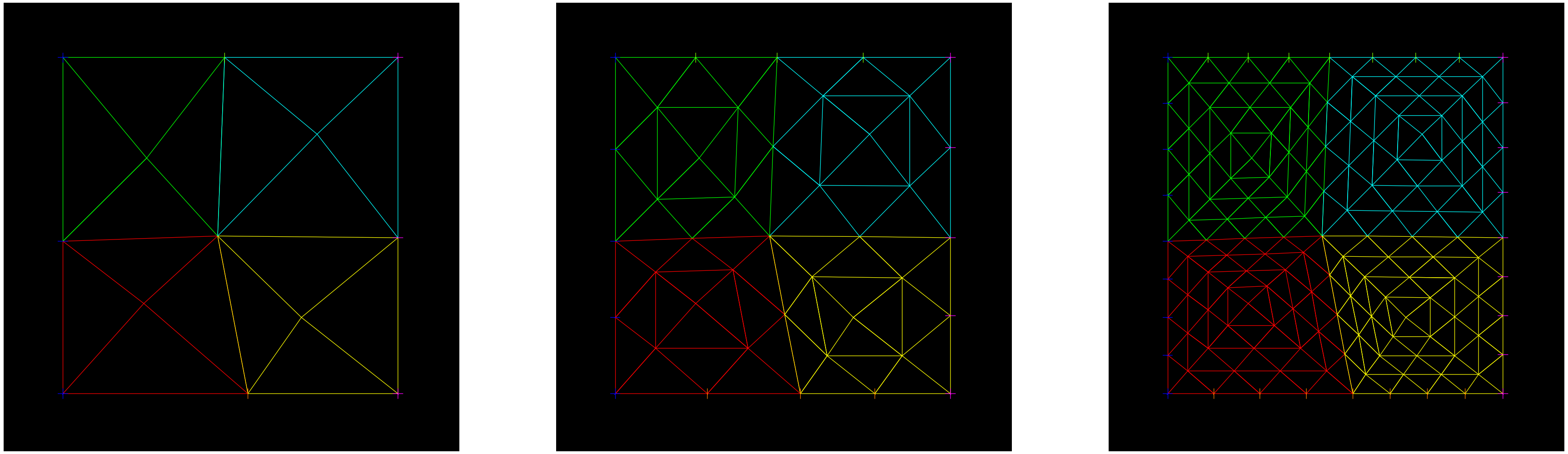
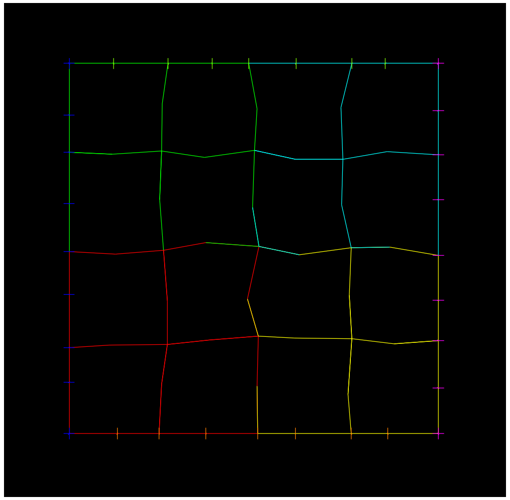
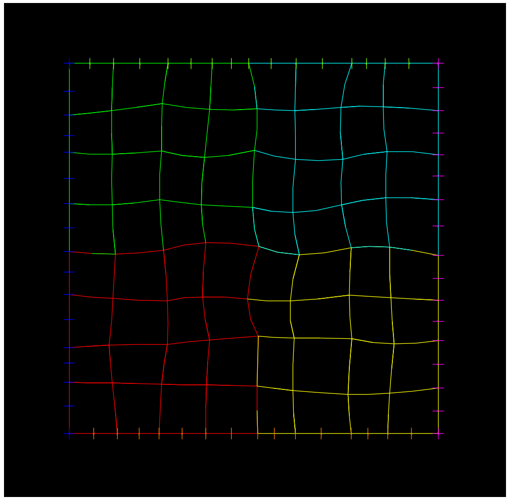
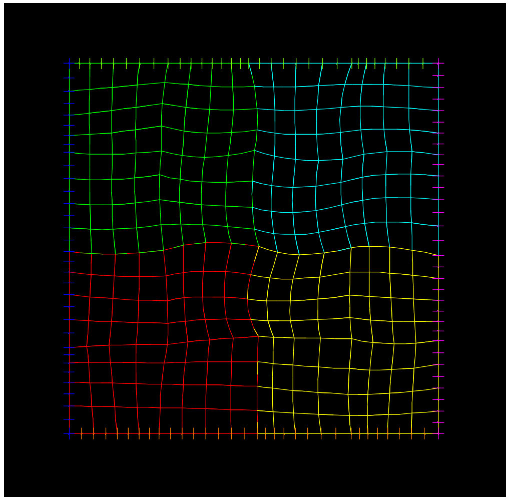
Example: triangular mesh refinement



Example: quadrilateral mesh refinement







Forms of Boltzmann Transport Equation

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

Second-order:

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

The two continuous forms above are equivalent.

Discretizations, however, yield different properties:

- Solutions
- Solvers

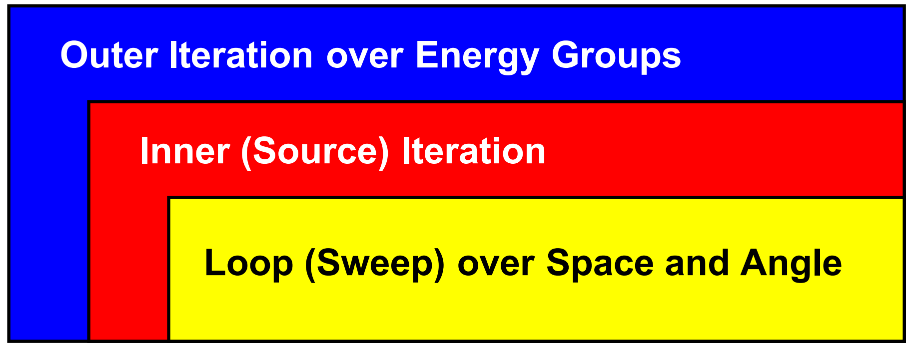
SCEPTRE Code Description

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

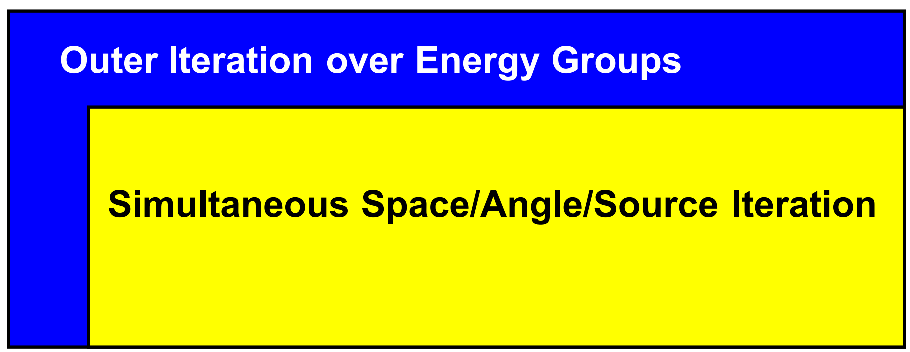
- Linear steady-state deterministic Boltzmann transport solver
- Discrete ordinates (S_n) in angle
- Multigroup in energy
- Discontinuous FEM (1st order) and continuous FEM (2nd order) on unstructured meshes
- Second-order variants
  - Even/odd parity flux (EOPF)
  - Self-adjoint angular flux (SAAF)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

Solvers for Boltzmann Transport Equation in Sceptre

First-order:



Second-order:



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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.

(In)Exactly solvable problems, 2D results
h = 0.25, structured mesh, isotropic scattering

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}

(In)Exactly solvable problems, 2D results
h = 0.25, unstructured mesh, isotropic scattering

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}**

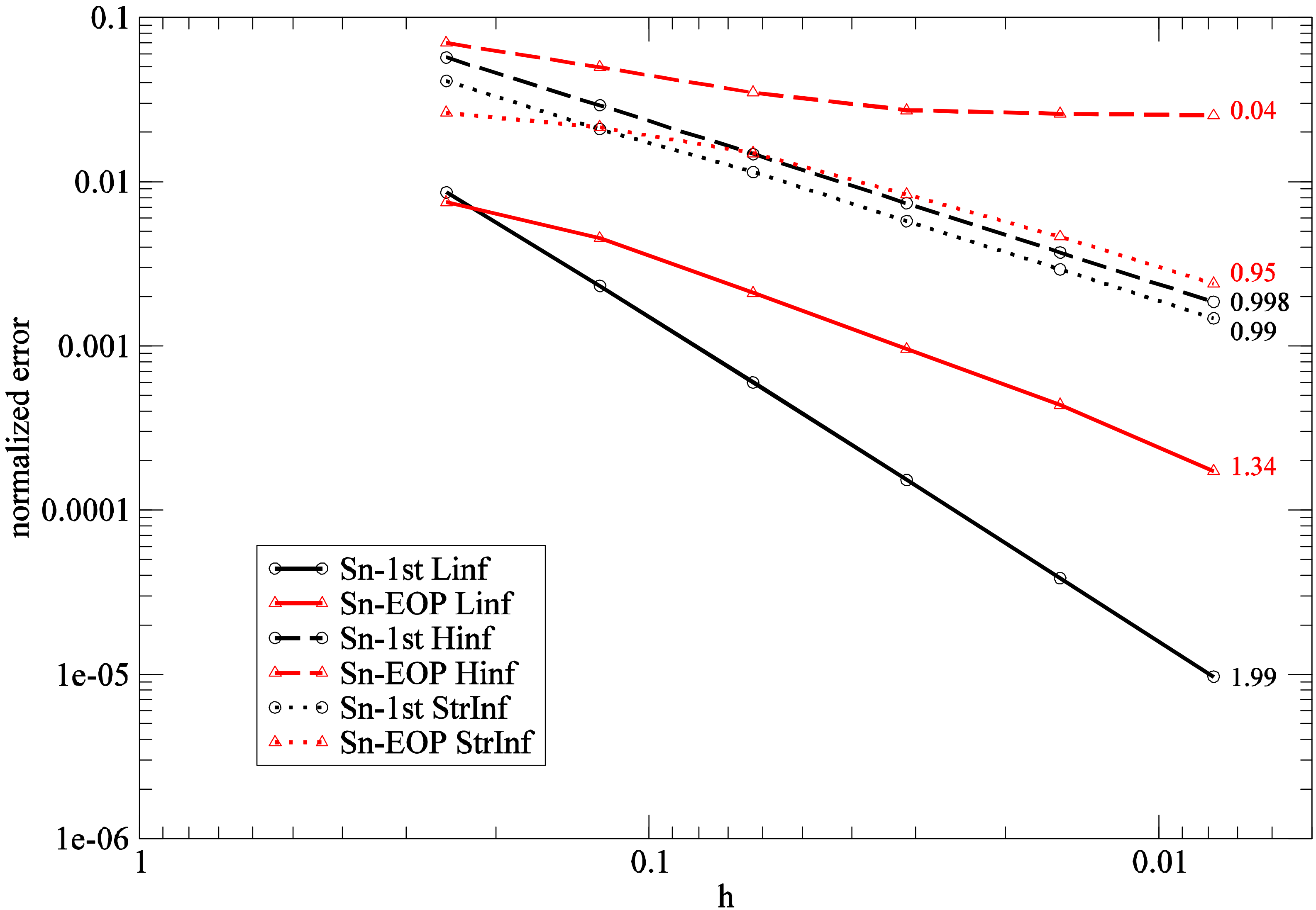
(In)Exactly solvable problems, 3D results
h = 0.25, structured mesh, isotropic scattering

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}

(In)Exactly solvable problems, 3D results
h = 0.25, unstructured mesh, isotropic scattering

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}**

Error metrics for tri3 meshes



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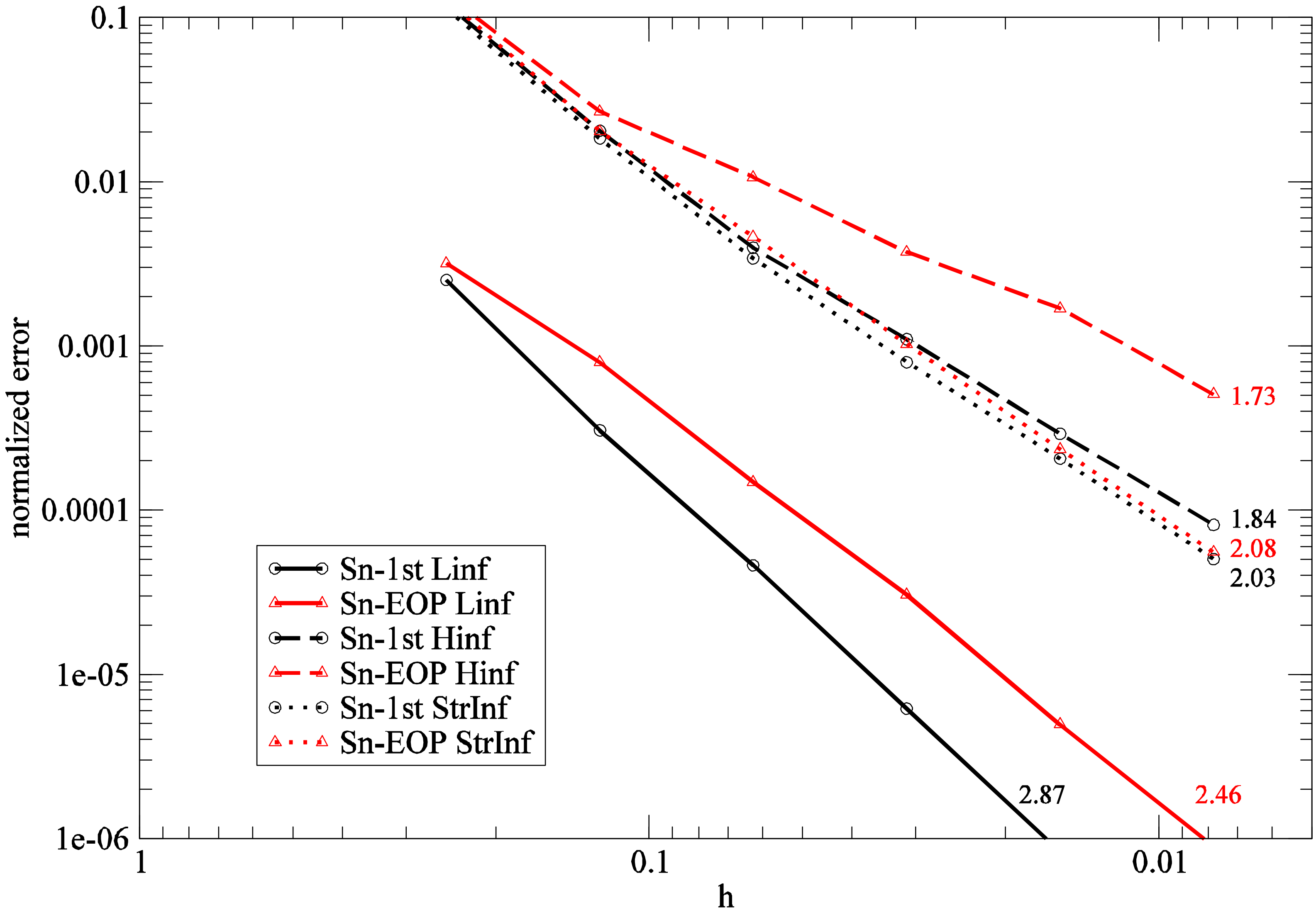
Error metrics for tri6 meshes



Why have we done all this?

The Sceptre code, of course, is completely bug-free. It always has been. Our testing is merely to demonstrate that fact to skeptics. ☺

Hypothetically speaking, though, if there had been bugs/issues with Sceptre…

…here's a partial list of what we would have found.

- 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

Future verification work

- Multigroup treatment
- Angular refinement (p-refinement)
- Discontinuous boundary conditions or solutions
- Reflecting/periodic boundary conditions

Conclusions

- Verification of transport codes with structured meshes is quite valuable and has been previously reported
- Verification with unstructured meshes introduces additional complexities
- We have successfully applied numerous verification tests with unstructured meshes to the Sceptre code
- Such testing helps to identify both code and algorithm issues
- The end result is a high and sustainable degree of confidence in the verified code

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