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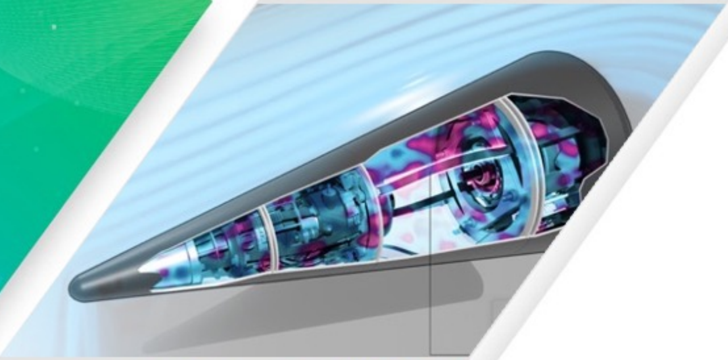
Verification and Validation of the Boltzmann-CSD Solver within the SCEPTRE package



Harley Hanes, Shawn Pautz, Brian Freno

2024 ASME VVUQ Symposium, 5/15/24, College Station, TX

U.S. DEPARTMENT OF ENERGY NNSA

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Overview

Verification and validation of FEM for energy implementation within SCEPTRE

Background

- Radiation Transport and Solver Approaches
- Boltzmann Equation

Numerical Model

- Standard discretization and energy limitations
- FEM for energy approach

V&V Progress

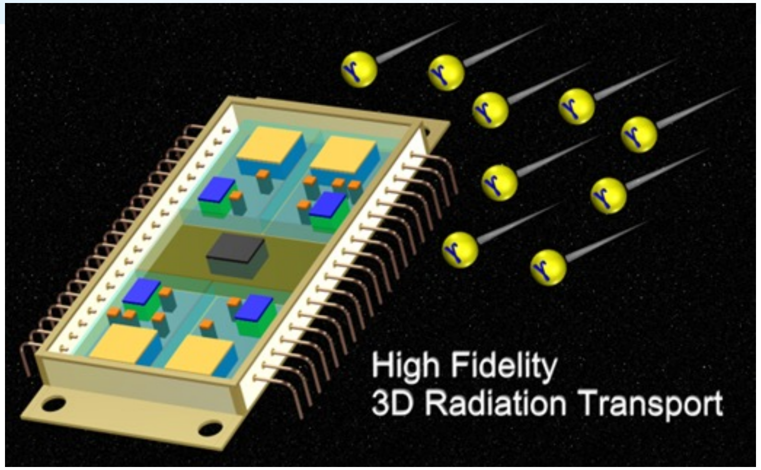
- Prior verification results
- FEM for energy verification results
- Future Work

Radiation Transport Applications

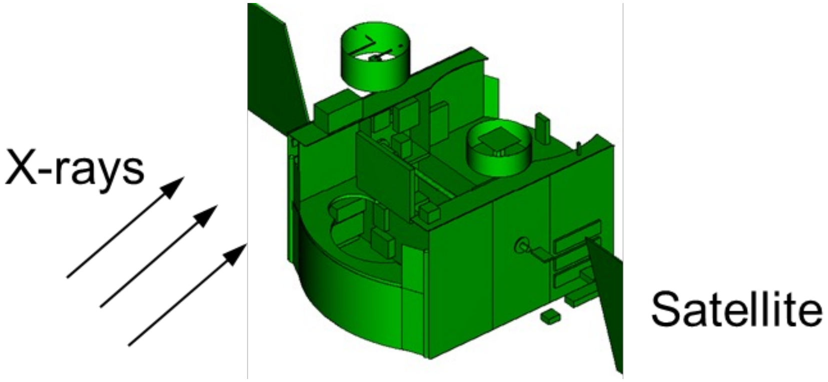
- Electrical components susceptible to damage from photon/electron radiation in high-radiation environments

- **Example:** Protection of sensors and processors on satellites requires radiation transport modeling to allocate sufficient shielding

- SCEPTRE (Sandia's Computational Engine for Particle Transport for Radiation Effects) models photon/electron radiation transport

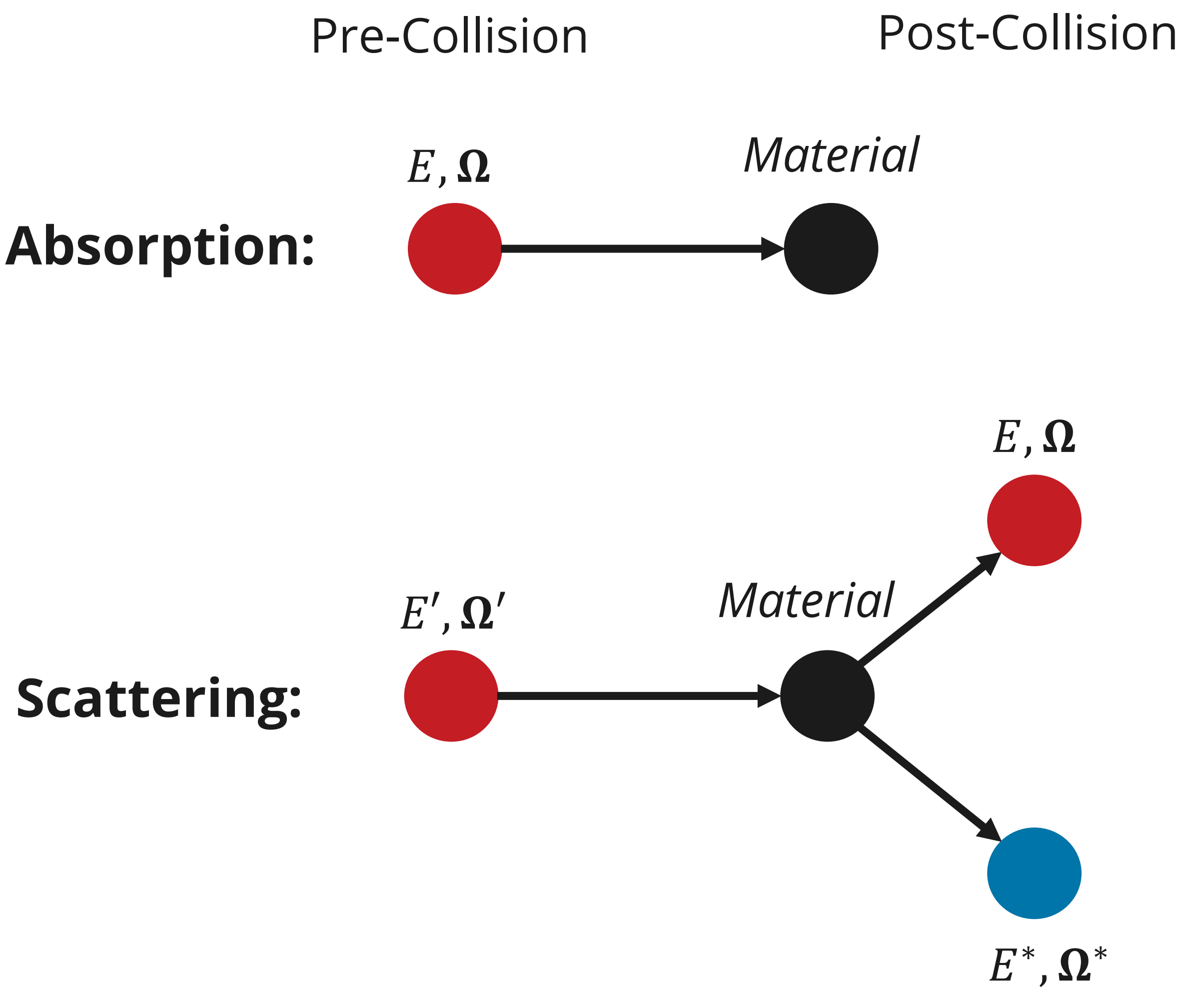


SCEPTRE



Radiation Transport Fundamentals

- Particles defined by,
  - $\boldsymbol{r}$: Position
  - E: Energy (MeV)
  - $\boldsymbol{\Omega}$: Unit vector for direction of travel
- Relevant material interactions:
  - Absorption
  - Scattering
- Interactions defined by cross sections: probability per unit path length an interaction occurs



Solver Approaches

Radiation transport solved with deterministic or Monte Carlo approaches

Deterministic Approach (SCEPTRE)

- Numerically solves governing equations for transport effects
- Memory and/or runtime limited
- Efficient for differential quantities
  - Charge/energy deposition distributions
  - Emission quantities
- Applications
  - X-ray induced EM fields in cables

Monte Carlo Approach

- Solves random walk of particles subject to transport effects
- Runtime limited
- Efficient for integral quantities
  - Total charge crossing a surface
  - Total dose in a region
- Applications
  - Non-meshed domains

Boltzmann Transport Equation

Boltzmann transport equation models particle flux $\psi(\boldsymbol{r}, E, \boldsymbol{\Omega})$ (density of particles as a function of space/energy/angle)

$$[\boldsymbol{\Omega} \cdot \nabla + \sigma_t(\boldsymbol{r}, E)]\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \int dE' \int d\overrightarrow{\Omega'} \sigma_s(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})\psi(\boldsymbol{r}, E', \boldsymbol{\Omega}') + Q(\boldsymbol{r}, E, \boldsymbol{\Omega})$$

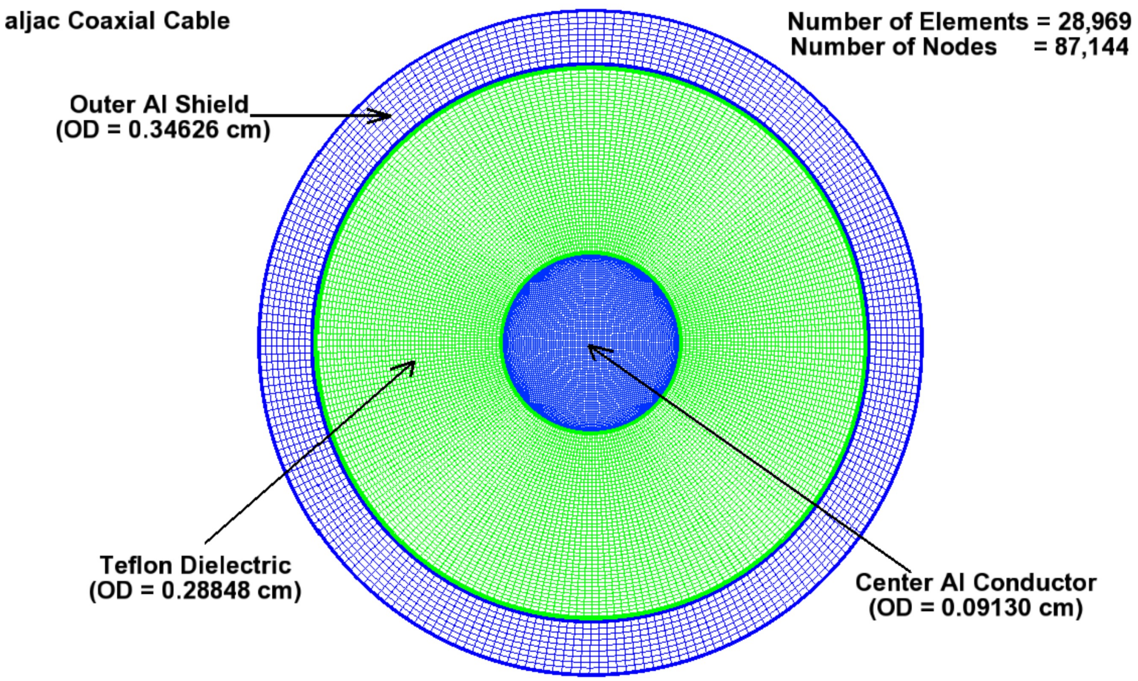
- $\boldsymbol{\Omega} \cdot \nabla$: Particle streaming
- $\sigma_t(\boldsymbol{r}, E)$: Total cross-section (losses due to absorption and scattering)
- $Q(\boldsymbol{r}, E, \boldsymbol{\Omega})$: Particle sources
- $\sigma_s(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})$**:** Scattering cross-section (Particles entering $(E, \boldsymbol{\Omega})$ from $(E', \boldsymbol{\Omega}')$)

Requires discretization of terms in space/energy/angle

Discretization Approaches

Spatial: Finite-element method (FEM)

Dimension	Element Type	Basis Order	Mesh Name
1D	Edge	Linear	edge2
		Quadratic	edge3
2D	Triangular	Linear	tri3
		Quadratic	tri6
	Quadrilateral	Linear	quad4
		Quadratic	quad8
3D	Tetrahedral	Linear	tet4
		Quadratic	tet10
	Hexahedral	Linear	hex8
		Quadratic	hex20



Liscum-Powell, J.L., Bohnhoff, W.J., Turner, D.C. (2007). *A Cable SGEMP Tutorial*. SAND2007-2548. https://www.osti.gov/servlets/purl

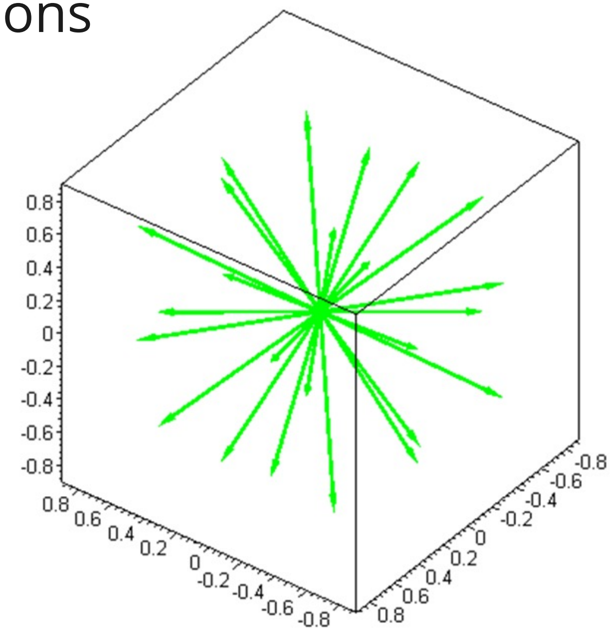
Discretization Approaches

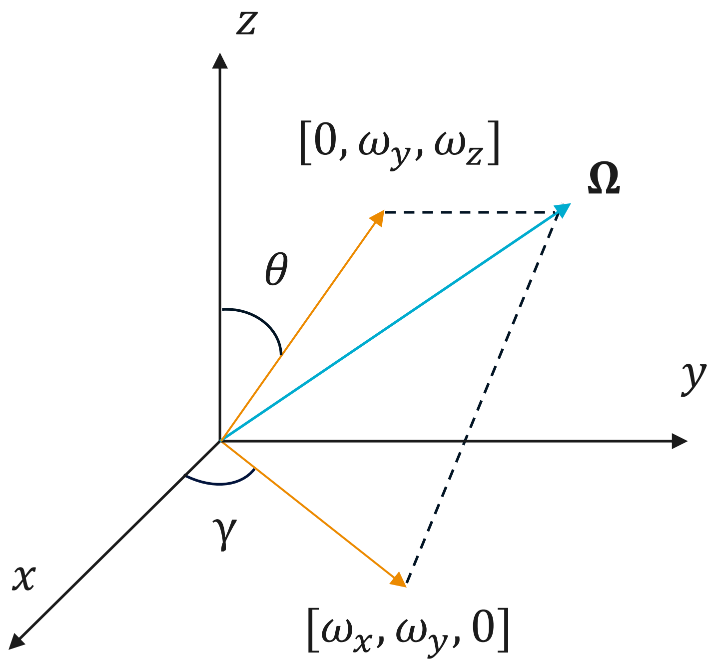
Angular: Discrete Ordinates

Note: $\mathbf{\Omega} = [\omega_x, \omega_y, \omega_z] = [\sin\theta\cos\gamma, \sin\theta\sin\gamma, \cos\theta]$

SCEPTRE collocates in discrete directions

Integrals approximated with quadrature using collocation directions





$\mathbf{\Omega}$: unit-vector for direction of travel

$[0, \omega_y, \omega_z]$: Projection onto $y - z$ plane

$[\omega_x, \omega_y, 0]$: Projection onto $x - y$ plane

Discretization Approaches

Energy: Multigroup approach

1. Energy Domain: $[E_{\min}, E_{\max}] = [E_0, E_G]$

   Groups: $[E_0, E_1], [E_1, E_2], \dots, [E_{G-1}, E_G]$

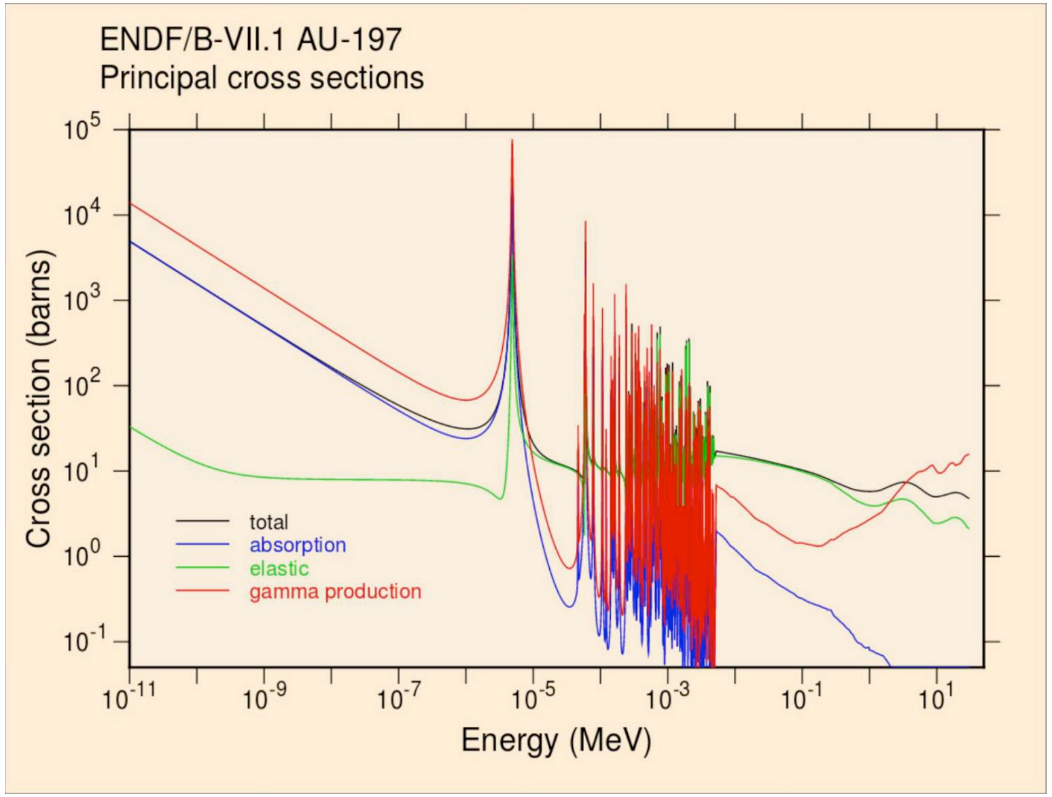
   Group g: $[E_{g-1}, E_g]$

2. Cross-section and source terms in group g approximated with weighted average

$$\sigma_t^{(g)}(\boldsymbol{r}) = \frac{\int_{E_{g-1}}^{E_g} \sigma_t(\boldsymbol{r}, E) w(\boldsymbol{r}, E) dE}{\int_{E_{g-1}}^{E_g} w(\boldsymbol{r}, E) dE}$$

3. System solved for averaged flux within each energy group

SCEPTRE uses CEPXS (Coupled Electron-Photon Cross Sections) to compute cross-sections



Total and constituent neutron cross sections for Au-197 (Los Alamos National Laboratory T-2 Nuclear Information Service, 2019)

Boltzmann-CSD Equation

Derivative with respect to energy presents complication for multigroup approach

Additionally models "soft" scattering that only changes particle energy:

$$[\boldsymbol{\Omega} \cdot \nabla + \sigma_t(\boldsymbol{r}, E)]\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \boxed{\frac{\partial(S\psi)}{\partial E}} + \int dE' \int d\overrightarrow{\Omega'} \sigma_s(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})\psi(\boldsymbol{r}, E', \boldsymbol{\Omega}') + Q(\boldsymbol{r}, E, \boldsymbol{\Omega})$$

Amount of CSD scattering determined by stopping power S

Two approaches to express energy derivative:

1. Scattering cross-section approximation:
   - Adjust σ_s for finite-difference approximation of expected energy derivative
   - Uses same solver formulation
2. FEM for energy discretization:
   - Implement FEM for energy discretization of $\psi(\boldsymbol{r}, E, \boldsymbol{\Omega})$
   - Allows direct computation of energy derivatives, **requires verification**

SCEPTRE Verification Approach

We use the method of manufactured solutions (MMS) for code verification

For a given spatial/angular/energy discretization

1. Manufacture arbitrary solution $\tilde{\psi}(\boldsymbol{r}, E, \boldsymbol{\Omega})$ and set of cross-section parameters (σ_t, σ_s, S)
2. Compute manufactured source term $Q(\boldsymbol{r}, E, \boldsymbol{\Omega})$ such that $\tilde{\psi}(\boldsymbol{r}, E, \boldsymbol{\Omega})$ satisfies Boltzmann-CSD equation
3. Provide SCEPTRE cross-section parameters and manufactured source term and assess two cases
   1. **Exact:** $\tilde{\psi}(\boldsymbol{r}, E, \boldsymbol{\Omega})$ exactly represented by discretization. SCEPTRE should have near-zero error at any discretization
   2. **Inexact:** $\tilde{\psi}(\boldsymbol{r}, E, \boldsymbol{\Omega})$ not exactly represented by discretization. SCEPTRE should converge to $\tilde{\psi}(\boldsymbol{r}, E, \boldsymbol{\Omega})$ at specific rate

Prior Work: Spatial FEM Verification for exact cases

Existing verification of SCEPTRE of multigroup approach

Exact monomials for **Structured (S)** and **Unstructured (U)** mesh types

	Element Type	Basis Order	Mesh Name	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
1D	Edge	Linear	edge2	SU	SU																		
		Quadratic	edge3	SU	SU							S											
2D	Triangular	Linear	tri3	SU	SU	SU																	
		Quadratic	tri6	SU	SU	SU		S				S	S										
	Quadrilateral	Linear	quad4	SU	SU	SU		S															
		Quadratic	quad8	SU	SU	SU		S				S	S		S		S						
3D	Tetrahedral	Linear	tet4	SU	SU	SU	SU																
		Quadratic	tet10	SU	SU	SU	SU	S	S	S		S	S	S									
	Hexahedral	Linear	hex8	SU	SU	SU	SU	S	S	S	S												
		Quadratic	hex20	SU	SU	SU	SU	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S

Unstructured meshes have non-constant Jacobians, lowering order of exactness

Pautz, S.D. (2011). Verification of Radiation Transport Codes with Unstructured Meshes.
International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering.

Spatial FEM Verification for Inexact Cases

1-D Results

Manufactured solutions

- One or two energy groups
- Sum of 5th order polynomials and exponentials in space

Cases

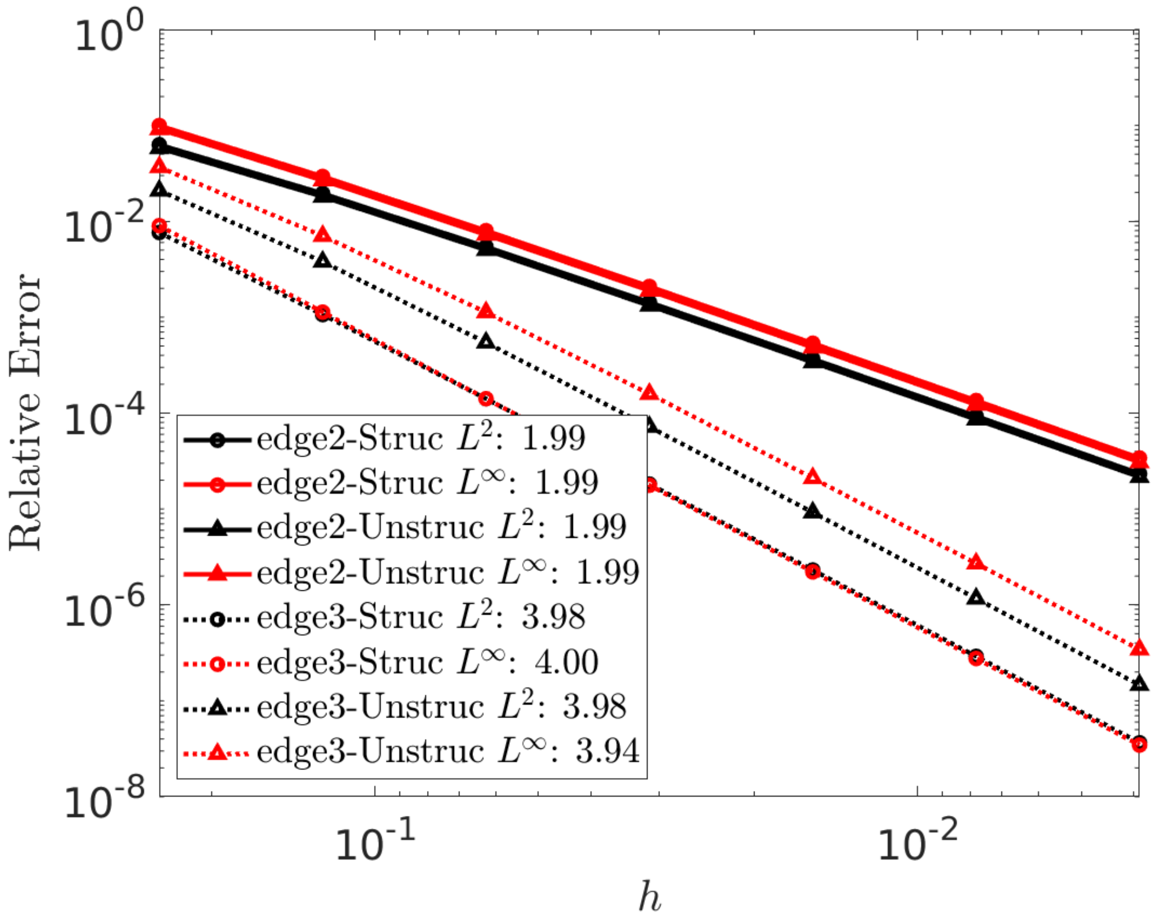
Test convergence in L^2 and L^∞ norms on all mesh cases

Expected Convergence

Linear: 2nd order

Quadratic: 4th order

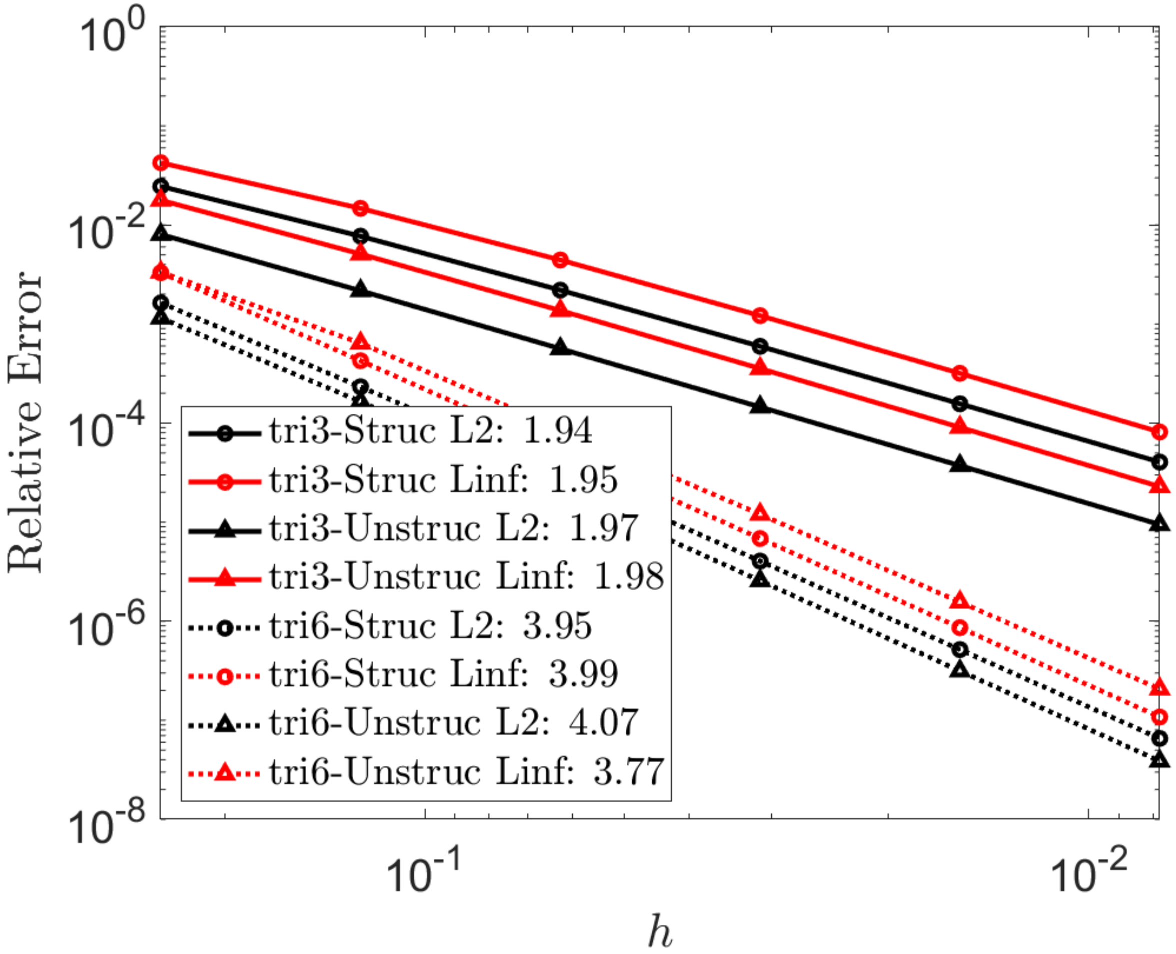
Edge Meshes



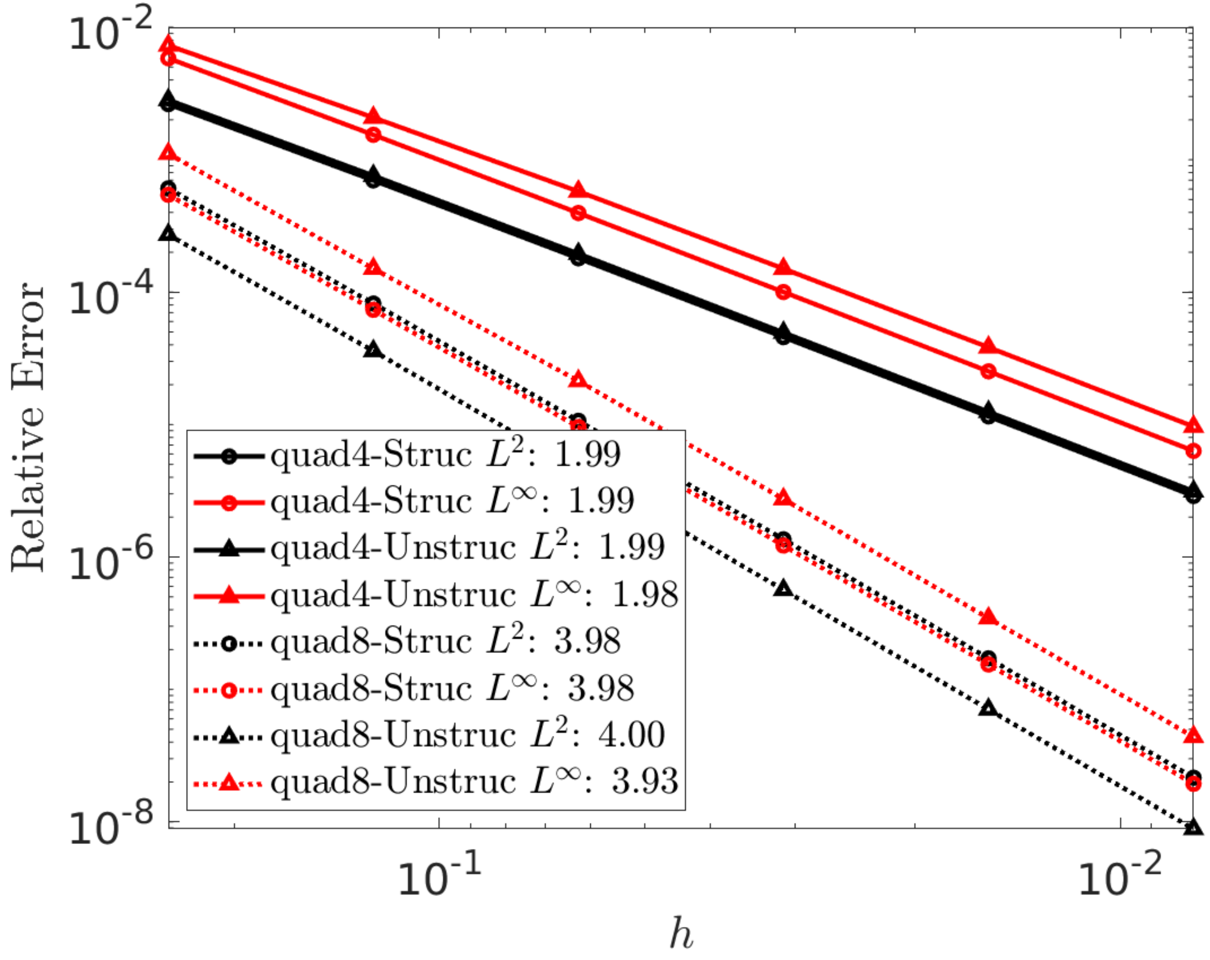
Spatial FEM Verification for Inexact Cases

2-D Results

Triangular Meshes



Quadrilateral Meshes



Joint Spatial-Energy Exact Verification

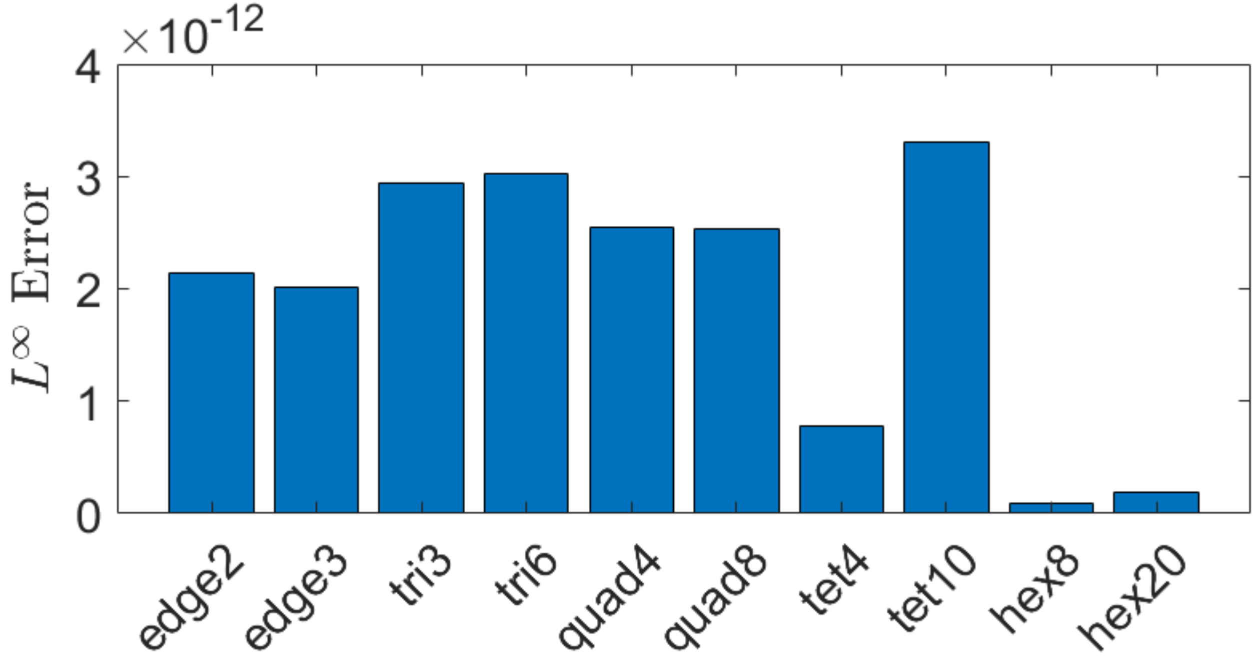
Verify FEM for energy discretization applied to Boltzmann-CSD

Test exact manufactured solutions to Boltzmann-CSD on all spatial meshes to test for any joint spatial/energy errors

Manufactured Solutions

$$\tilde{\psi}(\boldsymbol{r}, E, \boldsymbol{\Omega}) = (a + bE) f(\boldsymbol{r}, \boldsymbol{\Omega})$$

Used $f(\boldsymbol{r}, \boldsymbol{\Omega})$ up to order of exactness of spatial mesh.



Future Work: Inexact Tests

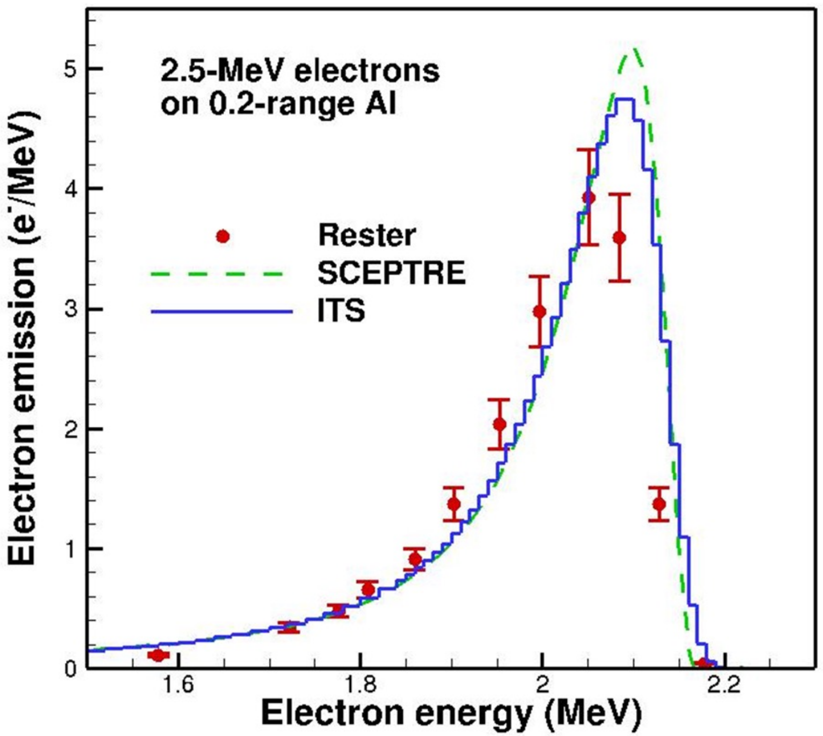
3 types of inexact discretization tests need to be performed

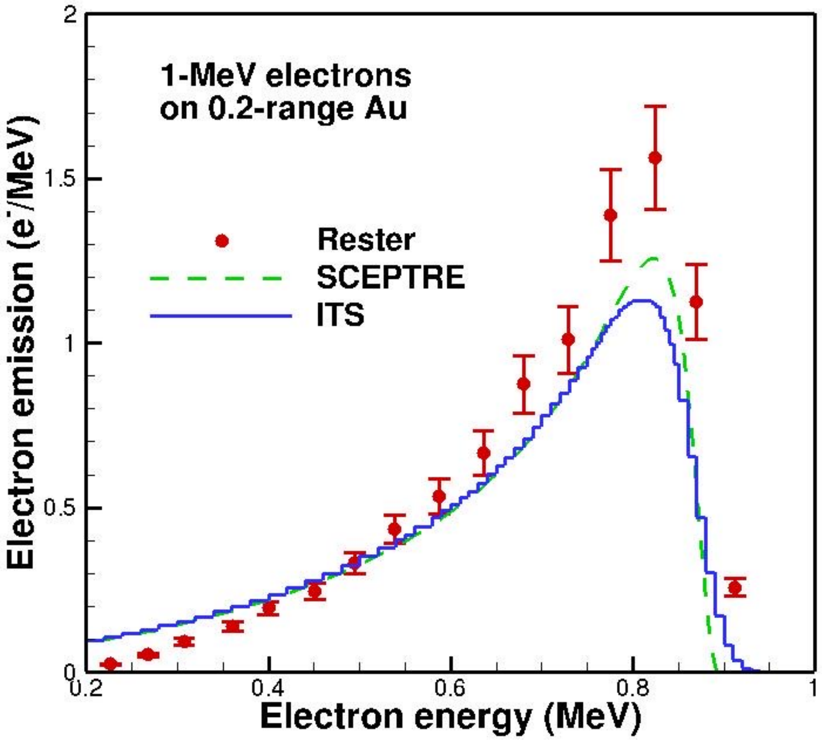
1. Inexact for energy, exact for space
   - Spatial MS component of joint exact tests, non-linear energy component
2. Exact for energy, inexact for space
   - Existing spatial inexact tests using FEM for energy
3. Inexact for energy and space
   - Test joint convergence for energy and space discretizations
   - Convergence rates are products of energy and spatial convergence rates

Future Work: Validation

Validate SCEPTRE FEM for energy solution to Boltzmann-CSD model of electron beams through aluminum/gold plates

- SCEPTRE multigroup approach and Monte Carlo ITS (Integrated Tiger Series) show moderate accuracy
- Anticipate SCEPTRE with FEM for energy to better model experimental data





Drumm, C.R, Fan, W.C. (2021). Validation of the SCEPTRE Boltzmann-CSD Solver. *Sandia National Laboratories.*

Conclusions

Background and Limitations

- Radiation transport modeling critical to protect electrical components in high-radiation environments
- SCEPTRE improves quantification of boundary layer/differential effects
- Traditional energy multigroup approach limits more complicated cases

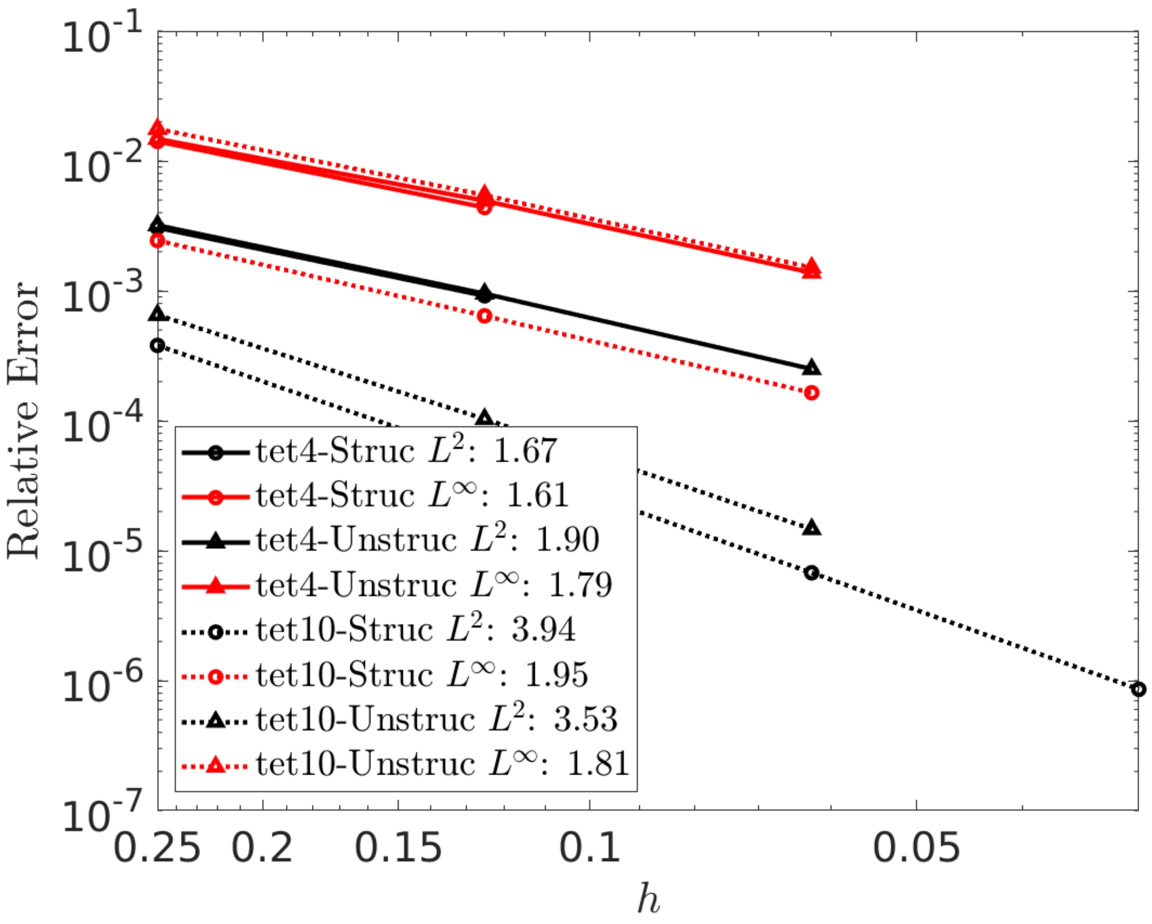
New Approach

- FEM for energy extends use cases of SCEPTRE
- Initial exact verification of FEM for energy complete
- Planned inexact verification will add verification evidence
- Planned validation results will quantify accuracy improvements of FEM for energy

Spatial FEM Verification for Inexact Cases

3-D Results

Tetrahedral Meshes



Hexahedral Meshes