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Verification of the Finite Element Method Energy Discretization in SCEPTRE

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Outline

Background

- Photon/Electron Transport and SCEPTRE
- Code Verification Using Method of Manufactured Solutions (MMS)

Verification Approach

- Manufactured Solutions
- Energy Discretizations and Cross-Sections

Verification Results

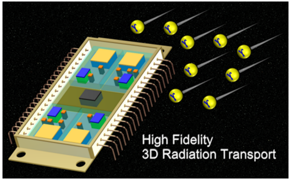
- Exact Verification
- Inexact Verification

Conclusions and Future Work

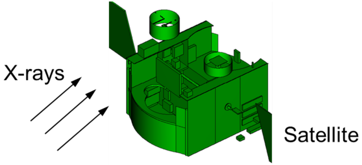
SCEPTRE

Photon/Electron Radiation Transport

- Electrical components suceptible to damage from photon/electron radiation
- **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



SCEPTRE

Boltzmann Transport Equation

Boltzmann transport equation models particle flux $\psi(\boldsymbol{r}, E, \boldsymbol{\Omega})$ (density of particles)

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

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

SCEPTRE solves Boltzmann equation using a deterministic transport algorithm

SCEPTRE

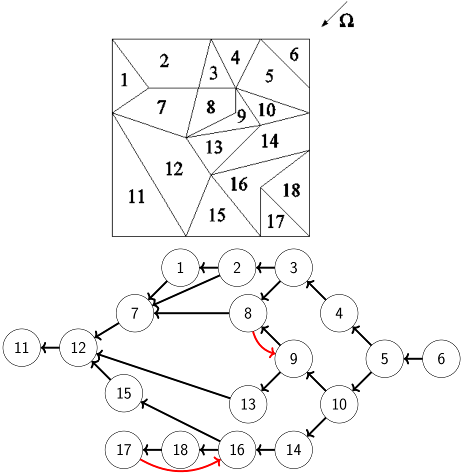
SCEPTRE Solver Approach

SCEPTRE Transport Algorithm

- Resolves loops in transport graphs
- Can solve transport on unstructured 2D and 3D meshes

SCEPTRE Discretizations

- Space: Finite element method (FEM)
- Angle: Discrete ordinates
- Energy: Multigroup, **linear FEM**



SCEPTRE

Boltzmann-CSD Equation

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

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

Continuous slowing down (CSD) scattering cross-section given by stopping power S

Two approaches to express energy derivative:

1. Approximate CSD by adjusting σ_s multigroup approximation
   - Uses same solver formulation as Boltzmann transport equation
2. FEM for energy discretization (**New Approach**):
   - Allows direct computation of energy derivatives, **requires verification**

Code Verification

Discretization Error Convergence

Continuous equations are numerically discretized to discretization size h

$$r(u) = 0 \quad \rightarrow \quad r_h(u_h) = 0$$

Discretization generally introduces error

$$e_h = u - u_h \neq 0$$

Error should converge to zero as discretization is refined

$$\lim_{h \to 0} e_h \rightarrow 0$$

Error norm should decrease at specific rate p

$$\|e_h\| \leq Ch^p$$

Problem: Measuring error requires a known solution

Code Verification

Method of Manufactured Solutions (MMS)

Approach

1. Manufacture arbitrary solution: u_M
2. Insert manufactured solution into continuous equations to get residual term

$$r(u_M) \neq 0$$

3. Set discretized equations equal to residual term and solve

$$r_h(u_h) = r(u_M)$$

4. We expect

$$u_h \to u_M$$

Error can now be computed since solution is known

Code Verification

Finite-Difference Example

Consider Laplace equation : $r(u) = \frac{\partial^2 u}{\partial x^2} = 0$

Discretize with finite differences: $\frac{\partial^2 u}{\partial x^2} \approx r_h(u_h) = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$

Manufacture arbitrary solution: $u_M(x) = c_0 + c_1 x + c_2 x^2$

Compute residual term: $r(u_M) = 2c_2$

Set discretized equations equal to residual term and solve:

$$r_h(u_h) = \frac{\partial^2 u_M}{\partial x^2} \quad \rightarrow \quad \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 2c_2$$

Two cases for error:

- **Exact:** If $c_2 = 0$, then $\|u_h - u_M\| = 0$ for all h
- **Inexact:** If $c_2 \neq 0$, then $\|u_h - u_M\| \leq Ch^2$ for some $C > 0$

MMS Formulation

Manufactured Solutions and Error Norms

Manufacture a solution $\psi_M(\boldsymbol{r}, E, \boldsymbol{\Omega}) = g(E)f(\boldsymbol{r}, \boldsymbol{\Omega})$ and use 2 cases for $g(E)$:

1. **Exact:** $g(E) = c_0 + c_1 E$
   SCEPTRE error should be near-zero (linear FEM)
2. **Inexact:** $g(E) = c_0 + c_1 E + c_2 E^2 + c_3 E^3 + c_4 \exp(c_5 E)$
   SCEPTRE error should be $\mathcal{O}(h_E^2)$

Compute relative error with L^2 and L^∞ norms:

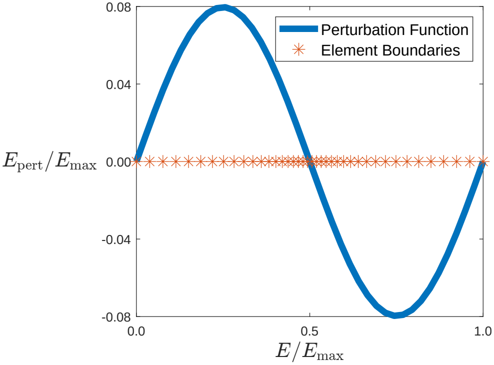
$$e_2(\tilde{\psi}, \psi) = \frac{\|\tilde{\psi} - \psi\|_2}{\|\psi\|_2} \qquad \|\psi\|_2 = \sqrt{\int_A \int_{E_{\min}}^{E_{\max}} \int_{4\pi} \psi^2(\boldsymbol{r}, E, \boldsymbol{\Omega}) d\boldsymbol{\Omega} dE d\boldsymbol{r}}$$

$$e_\infty(\tilde{\psi}, \psi) = \frac{\|\tilde{\psi} - \psi\|_\infty}{\|\psi\|_\infty} \qquad \|\psi\|_\infty = \max_{(\boldsymbol{r}, E, \boldsymbol{\Omega})} |\psi(\boldsymbol{r}, E, \boldsymbol{\Omega})|$$

MMS Formulation

Energy Discretization

- Test both uniform and non-uniform energy meshes
- Non-uniform
  - Non-smooth meshes can disrupt convergence
  - Generate non-uniform meshes with sinusoidal perturbation



MMS Formulation

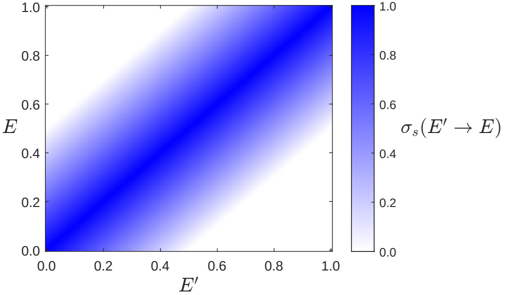
Manufactured Cross-Sections

Cross-sections must also be refined with energy mesh

- Define $\sigma_a(E)$, $S(E)$, $\sigma_s(E' \to E')$ to be 3^{rd} order polynomials
- Define scattering width w where $\sigma_s(E' \to E)$ decreases linearly to $\sigma_s(E' \to E' \pm w) = 0$

$$\sigma_s(E' \to E) = \max\left(m(E)\left(1 - \frac{|E' - E|}{w}\right), 0\right)$$

- Multigroup cross-sections computed exactly



Scattering cross-section with $\sigma_s(E' \to E') = 1$ and $w = 1/2$

Results

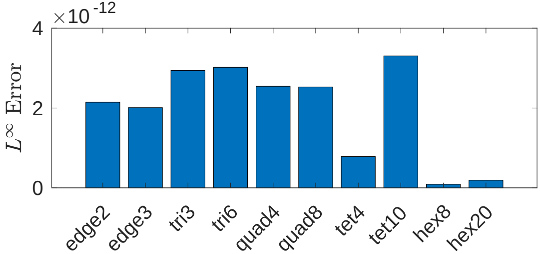
Exact Tests

Manufacture solutions for Boltzmann-CSD using exactly discretized fluxes on all spatial meshes to test for any joint spatial/energy errors

Manufactured Solution Form

$$\psi_M(\boldsymbol{r}, E, \boldsymbol{\Omega}) = (c_0 + c_1 E) f(\boldsymbol{r}, \boldsymbol{\Omega})$$

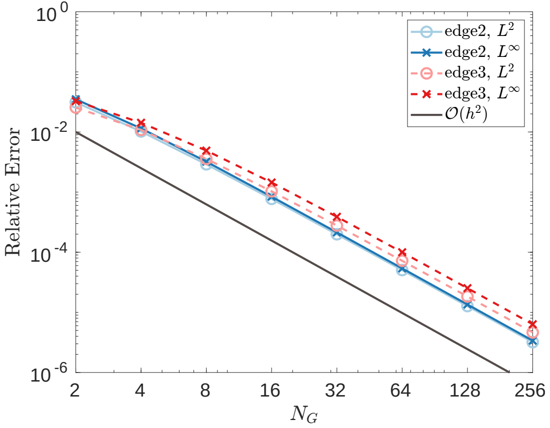
Test multiple $c_0, c_1 \in [0, 2]$ using 2 and 4 energy groups for each spatial mesh



Results

Uniform Energy Meshes with 1D Spatial Meshes

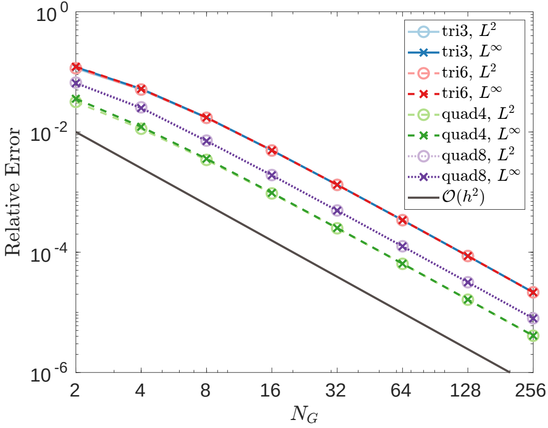
- Test convergence by doubling number of energy groups (N_G) each step
- Confirm expected energy convergence observed with all spatial meshes
- Energy discretization shows expected convergence for 1D spatial meshes



Results

Uniform Energy Meshes with 2D Spatial Meshes

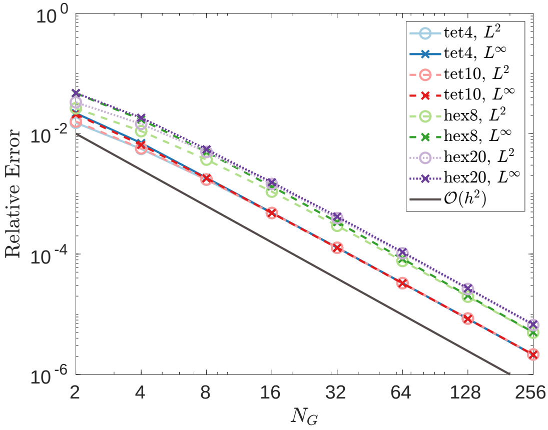
- Energy discretization shows expected convergence for 2D spatial meshes



Results

Uniform Energy Meshes with 3D Spatial Meshes

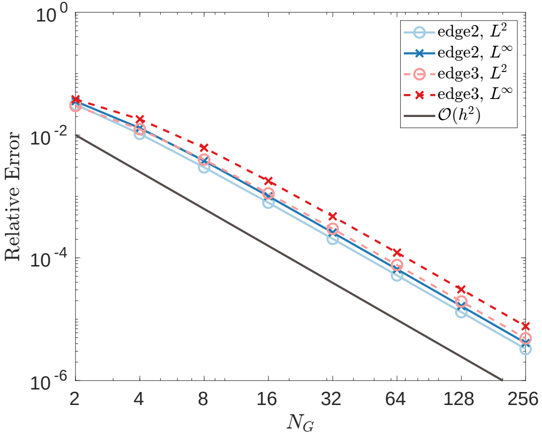
- Energy discretization shows expected convergence for 3D spatial meshes
- All cases for uniform energy meshes show expected convergence



Results

Non-Uniform Energy Meshes with 1D Spatial Meshes and only CSD Scattering

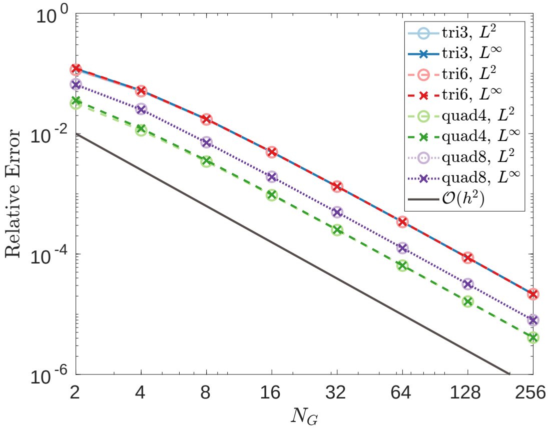
- Check convergence for non-uniform energy meshes without scattering
- Energy discretization shows expected convergence for 1D spatial meshes



Results

Non-Uniform Energy Meshes with 2D Spatial Meshes and only CSD Scattering

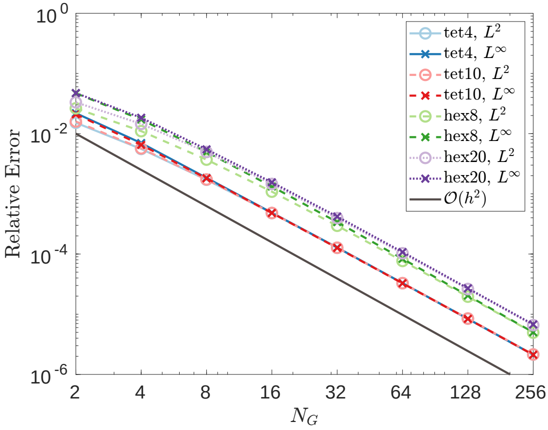
- Energy discretization shows expected convergence for 2D spatial meshes



Results

Non-Uniform Energy Meshes with 3D Spatial Meshes and only CSD Scattering

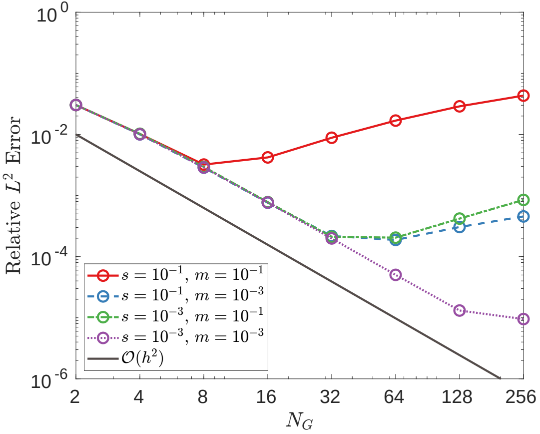
- Energy discretization shows expected convergence for 3D spatial meshes
- All cases for non-uniform energy meshes without scattering verified



Results

Non-Uniform Energy Meshes with Scattering

- Vary scattering magnitude (s) and nonuniform perturbation magnitude (m) with edge2 spatial mesh
- Non-decaying error proportional to smN_G
- Flexibility of MMS helps clarify implementation errors in addition to identifying them



Conclusions

- SCEPTRE is a deterministic photon/electron radiation transport code
- SCEPTRE discretizes energy with linear finite elements to solve more complex transport cases
- Code verification assesses whether numerical discretizations are implemented correctly
- MMS sets arbitrary functions as solutions to check exactness and convergence
- SCEPTRE shows anticipated convergence for uniform energy meshes with scattering and non-uniform energy meshes without scattering
- Verification of linear finite element scattering treatment on non-uniform energy meshes is ongoing

Future Work

Improving Credibility of Boltzmann-CSD Implementation

- Investigate convergence issues for scattering on non-uniform energy meshes
- Verify using physical cross-sections computed by CEPXS
- Check Boltzmann-CSD model against electron beam experimental data (validation)