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Phase-Space Finite Elements in a Least-Squares Solution of the Transport Equation

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Overview of the talk

- Background/motivation
- Creating a finite elements angular “mesh”
- Least-squares solution method
- Results
  - Convergence rate analysis
  - Ray-effect mitigation
  - Transport with electric fields
- Future work

Background/motivation

- Ray-effect mitigation
- Discontinuous (DFE) vs. continuous (CFE) space/angle
- Comparison with discrete ordinates (Sn) and spherical harmonics (Pn) methods for radiative transfer equation
  - L. L. Briggs, W. F. Miller, Jr., and E. E. Lewis, "Ray-Effect Mitigation in Discrete Ordinate-Like Angular Finite Element Approxi mation in Neutron Transport," *Nuclear Science and Engineering*, **57**, pp.205-217 (1975).
  - W. R. Martin, C. E. Yehnert, L. Lorence and J. J. Duderstadt, "Phase-Space Finite Element Methods Applied to the First-Order Form of the Transport Equation," *Annals of Nuclear Energy,* **8,** pp. 633-649 (1981).
  - G. G. M. Coppa, G. Lapenta, and P. Ravetto, "Angular Finite Element Techniques in Neutron Transport," *Annals of Nuclear E nergy*, **17**, pp.363-378 (1990).
  - R. Becker, R. Koch, H.-J. Bauer, and M. F. Modest, "A Finite Element Treatment of the Angular Dependency of the Even-Parit y Equation of Radiative Transfer," *Journal of Heat Transfer*, **132**, pp.1-13 (2010).
- Our motivation is to develop capability for transport of charged-particles in the presence of ElectroMagnetic (EM) fields

Transport with EM fields

- Adds energy and angular derivative terms to the transport operator

$$\boxed{\frac{1}{v}\frac{\partial\psi}{\partial t} + \vec{\Omega}\cdot\nabla\psi + \sigma\psi} \leftarrow \text{without fields}$$

$$+q(\vec{\mathcal{E}}\cdot\vec{\Omega})\left[\frac{\partial\psi}{\partial E} - \frac{1+4\beta^2}{\mathcal{D}(E)}\psi\right]$$

$$+\frac{q}{\mathcal{D}(E)}\left[\mathcal{E}_x(1-\mu^2) - \mathcal{E}_y\mu\eta - \mathcal{E}_z\mu\xi + v(\mathcal{B}_z\eta - \mathcal{B}_y\xi)\right]\frac{\partial\psi}{\partial\mu}$$

$$+\frac{q}{\mathcal{D}(E)(1-\mu^2)}\left[\mathcal{E}_z\eta - \mathcal{E}_y\xi + v\left[\mathcal{B}_y\mu\eta + \mathcal{B}_z\mu\xi - \mathcal{B}_x(1-\mu^2)\right]\right]\frac{\partial\psi}{\partial\varphi} = S$$

where E is the kinetic energy,

$$\mathcal{D}(E) = \frac{E(E+2m_o c^2)}{E+m_o c^2}$$

$$\vec{\mathcal{E}} = \mathcal{E}_x\mathbf{i} + \mathcal{E}_y\mathbf{j} + \mathcal{E}_z\mathbf{k}$$

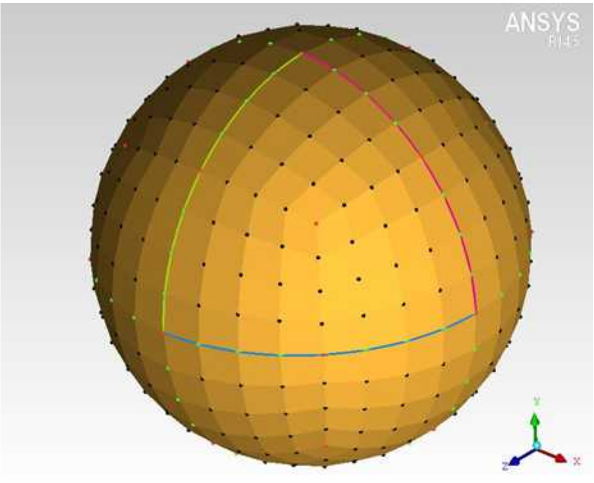
$$\vec{\mathcal{B}} = \mathcal{B}_x\mathbf{i} + \mathcal{B}_y\mathbf{j} + \mathcal{B}_z\mathbf{k}$$

Angular and energy FE builds on spatial FE

- Mesh database
- Element integrations
- FEM matrices
- Jacobians
- Mesh connectivity
- DFEM/CFEM transport fields
- Parallelism in angle/energy?
- Meshing/graphics capability

Energy/angular FE mesh

- Energy mesh (1D)
  - Use existing linear (edge2) and quadratic (edge3) capability
- Angular mesh
  - Triangular or quadrilateral mesh of the surface of a unit sphere
  - For 2D spatial geometry, mesh one hemisphere
- Resulting angular mesh is a 2D mesh with 3D coordinates
- Incompatible with current FEM database format
- Not an insurmountable difficulty, however



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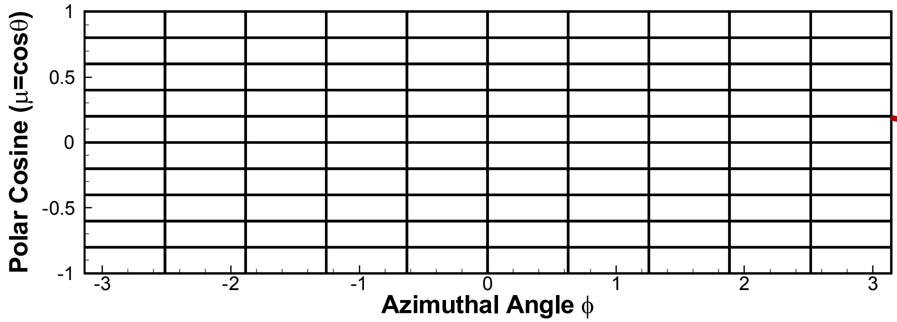
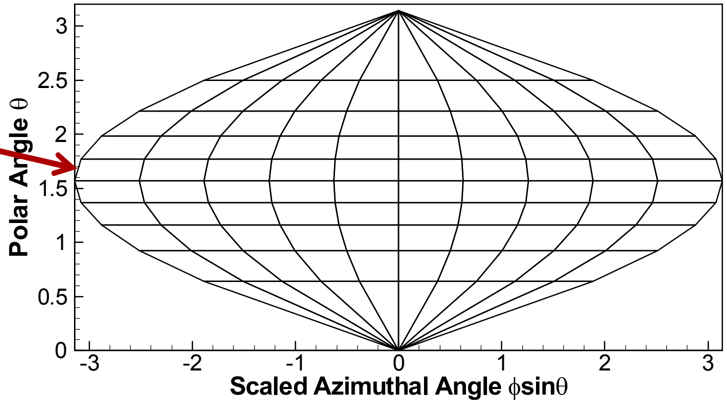
Alternative angular FE meshing

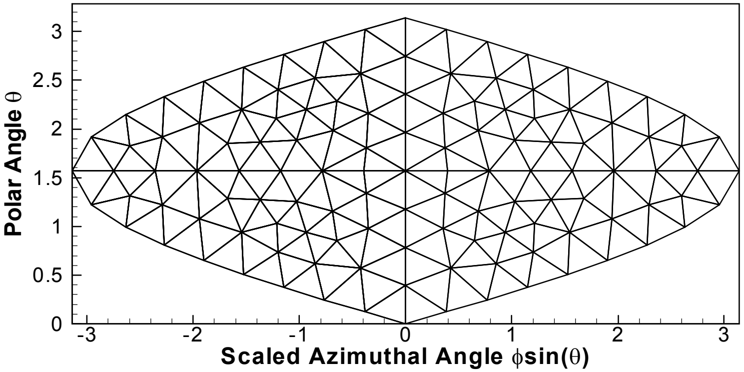


Regular mesh in μ-ϕ space



Mapped from μ-ϕ space mesh

- μ-ϕ space mesh difficulties
  - Elements mapped to a single point at the poles
  - Non-uniform mesh
- Alternative: map sphere to planar region and then mesh



Mesh of sphere mapped to planar region

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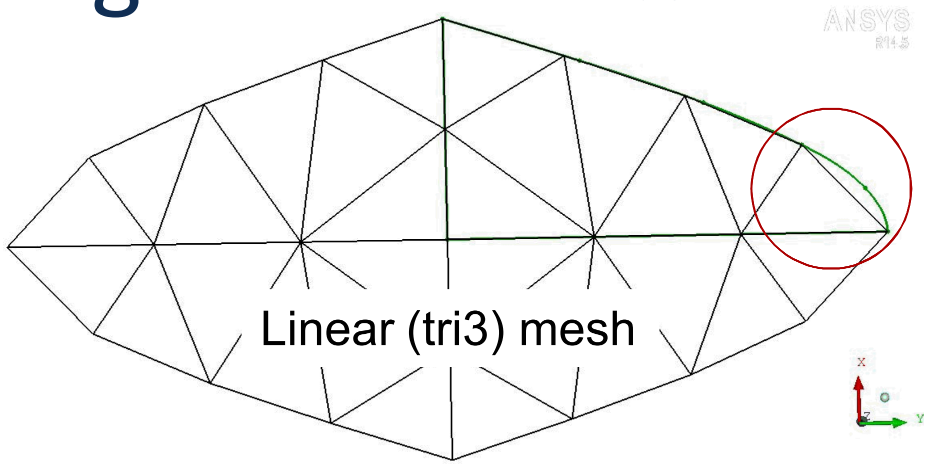
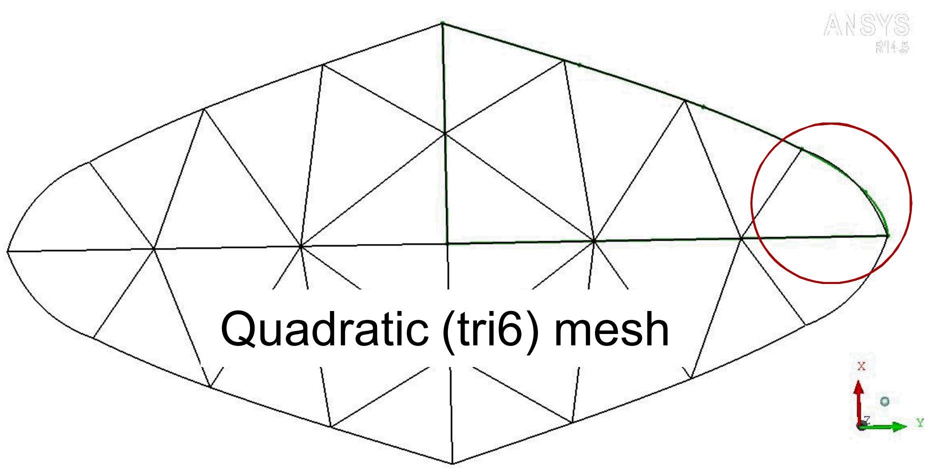
Multidimensional angular finite elements comparison

Angular mesh	Rotationally invariance possible?	Integral sum exactly to 4π?	Planar mesh?
Surface of unit sphere	fully	no	no
μ-ϕ regular mesh	partially	yes	yes
Sphere projected to plane	partially	no	yes
S_N	fully	yes	N/A
P_N	fully	yes	N/A

Mesh of projected region integrates to < 4π

SCEPTRE





- Linear mesh fails to capture curve near ends of region
- Quadratic mesh much better, with nodes projected to geometry (isoparametric)

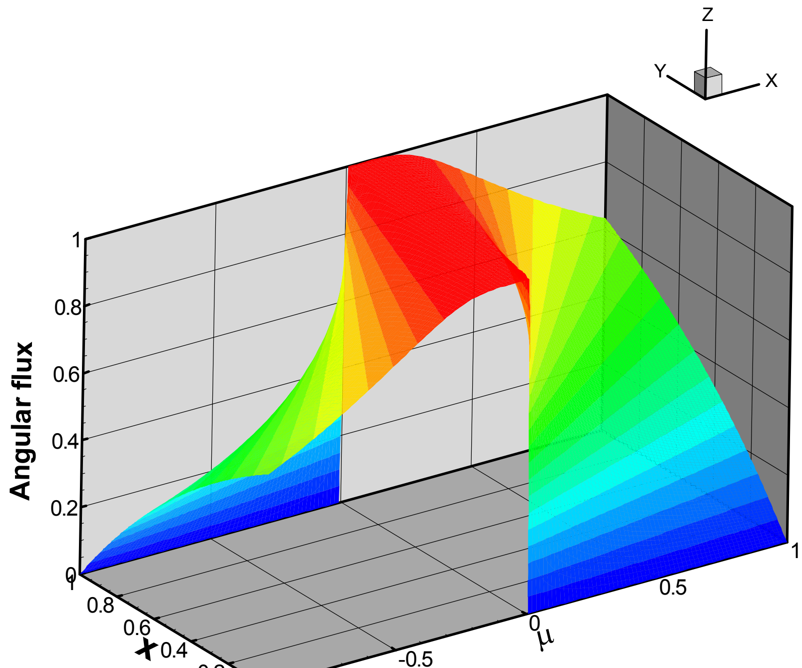
h-convergence of angular mesh refinement

- Unlike p-convergence of S_N and P_N methods
- 1D test problem
  - Unit total cross section
  - No scattering
  - Uniform isotropic source
  - Vacuum boundary conditions
- Analytic solution available:

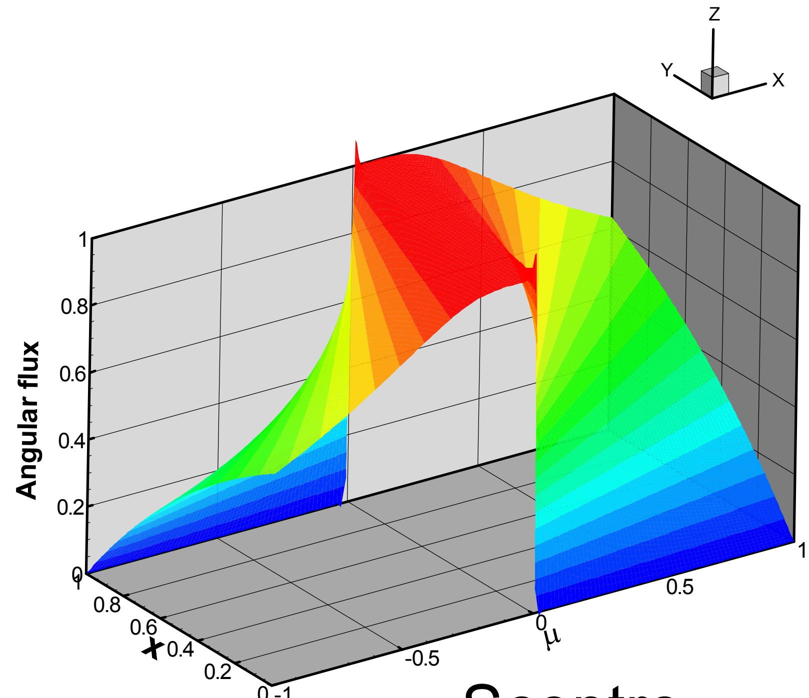
$$\psi(x,\mu) = 1 - e^{\frac{(1-x)}{\mu}}, \quad \mu < 0$$

$$\psi(x,\mu) = 1 - e^{-\frac{x}{\mu}}, \quad \mu > 0$$

Sceptre result compared with analytic solution



Analytic



Sceptre

- Good agreement except at discontinuity

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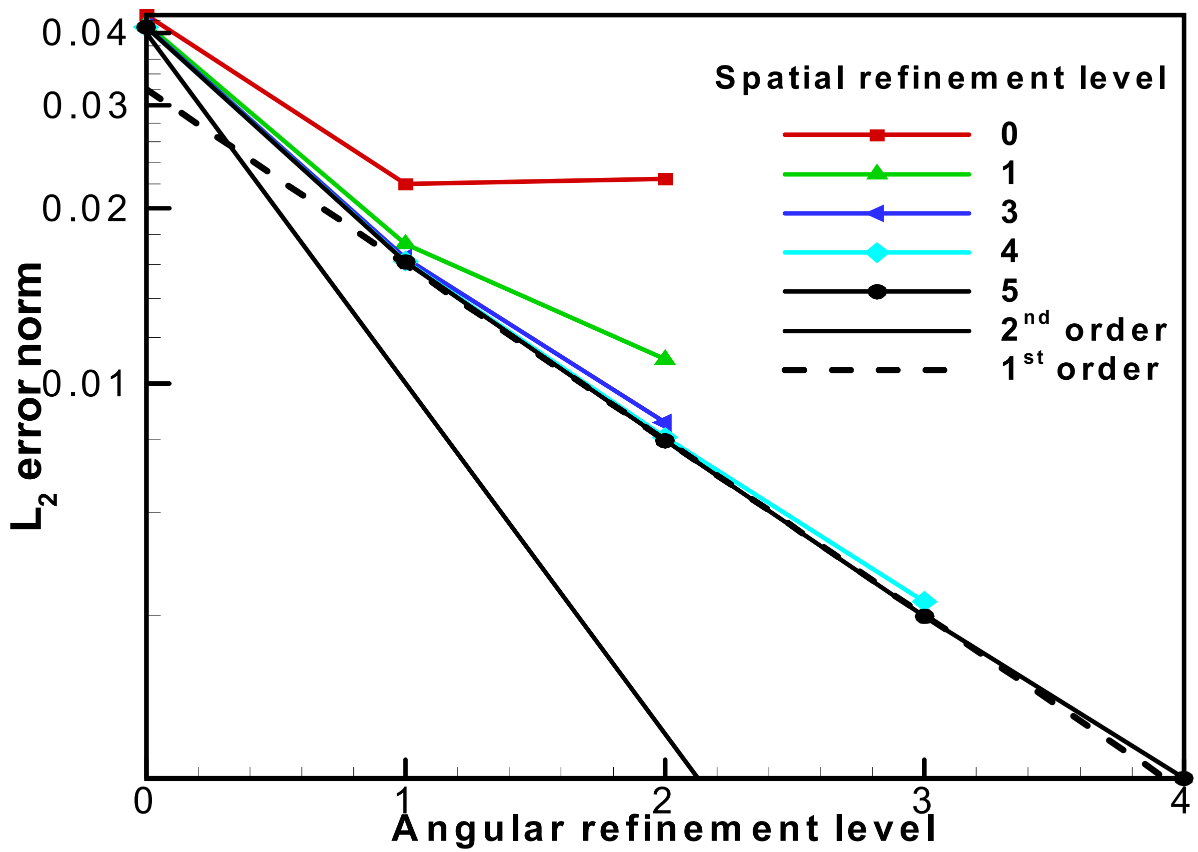
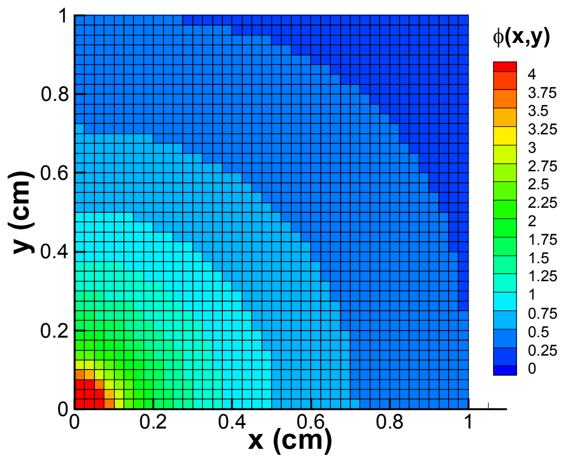
1^{st} order convergence rate observed



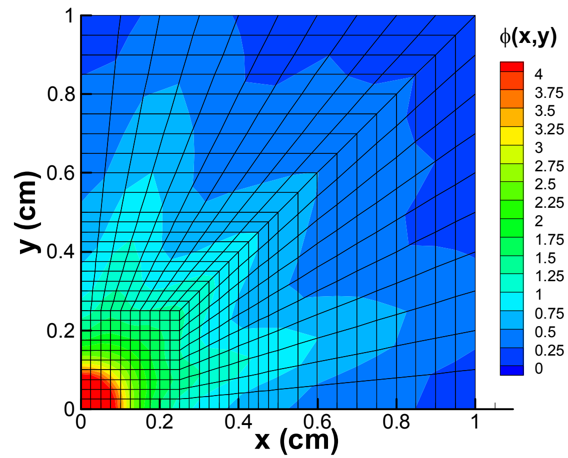
Ray-effects mitigation test problem

- Unit total cross section
- Scattering ratio 0.999
- Isotropic scattering
- Unit square region
- Reflective BC along x and y axes
- Point source at the origin

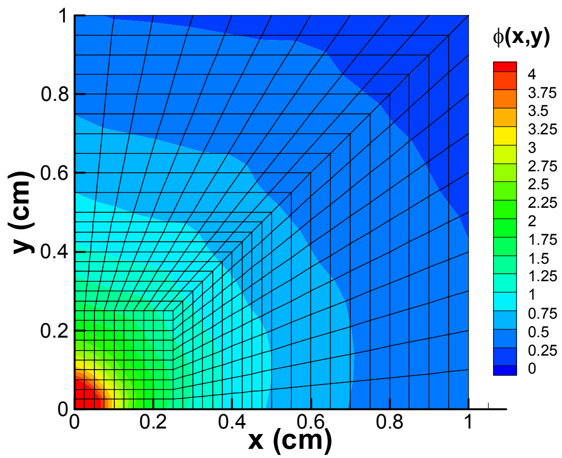
FE in angle reduces ray effects



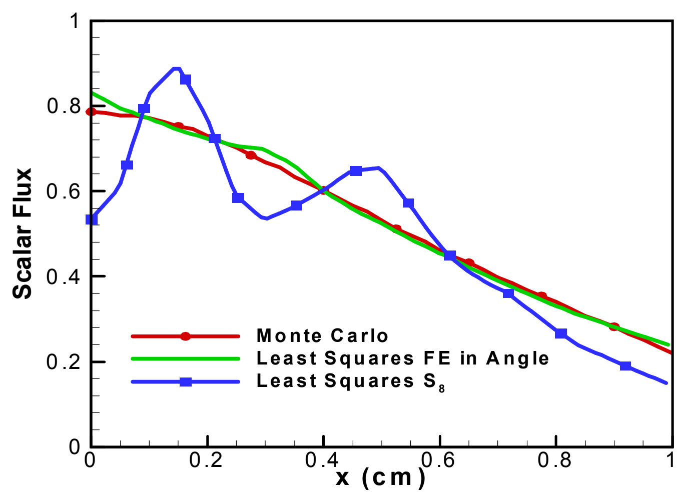
MITS Monte Carlo



Sceptre S_8 discrete ordinates



Sceptre FE in angle



Electron transport in void with electric field (non-relativistic)

SCEPTRE

$$\mu\frac{\partial\psi}{\partial x} + q\mathcal{E}_x\mu\frac{\partial\psi}{\partial E} - \frac{\mu}{2E}\psi(x,\mu,E) + \frac{q}{2E}\mathcal{E}_x\left(1-\mu^2\right)\frac{\partial\psi}{\partial\mu} = 0$$

- Family of analytic solutions available:

$$\psi(x,\mu,E) = \sqrt{E}f\left(E - q\mathcal{E}_x x, \mu^2 E - q\mathcal{E}_x x\right)$$

- Specific solution chosen for Sceptre comparison:

$$\psi(x,\mu,E) = \sqrt{E}\left(\mu^2 E - x\right)$$

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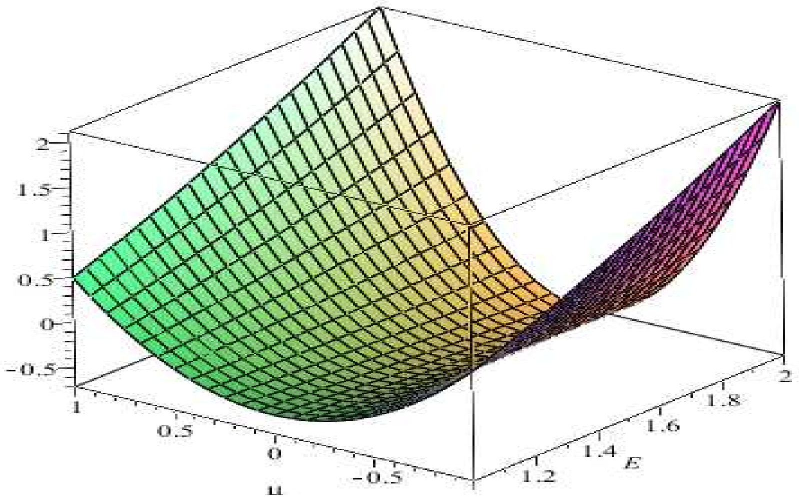
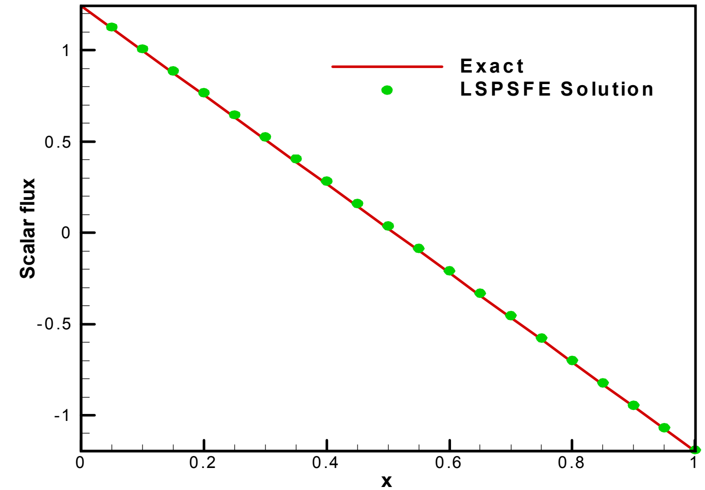
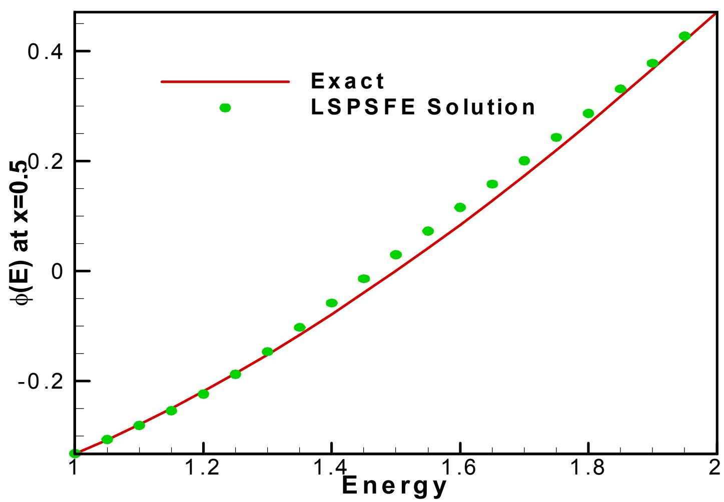
Boundary conditions for space/energy/angle

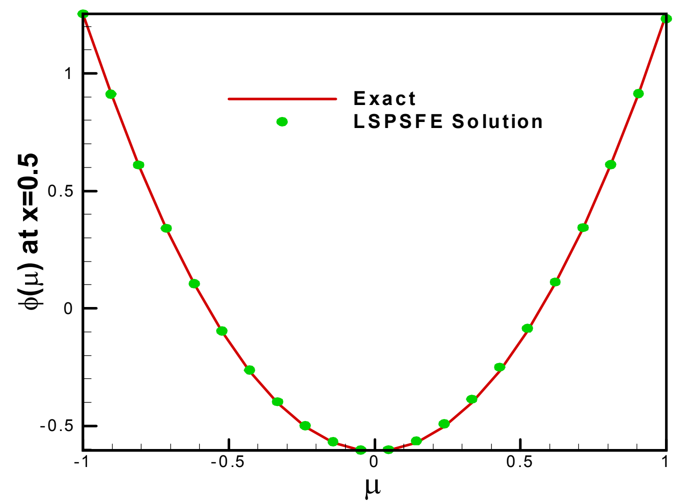
- Specify solution at spatial boundaries for incoming directions
- Specify solution a energy phase-space boundaries
  - At upper energy bound for $q\hat{\mathcal{E}} \cdot \mathbf{\Omega} < 0$
  - At lower energy bound for $q\hat{\mathcal{E}} \cdot \mathbf{\Omega} > 0$
- Specify solution at angular phase-space boundary
  - At μ=1 for $q\mathcal{E}_x < 0$
  - At μ=-1 for $q\mathcal{E}_x > 0$

Sceptre results compared with analytic solution









Future work

- Upwind differencing (space/angle/energy)
  - DFEM more accurate for problems with discontinuities (when does rad transport not have discontinuities)
  - Sceptre transport fields set up to handle DFEM
  - With LSFEM SPD matrix ensured (unlike SAAF and EOPF second-order methods)
  - Trilinos has tools for CFEM, more development needed for DFEM
- Periodic boundary conditions for projected angular mesh (or revisit using mesh of surface of unit sphere)
- Complete implementation of multi-D transport in material with EM fields
- Preconditioning/memory management