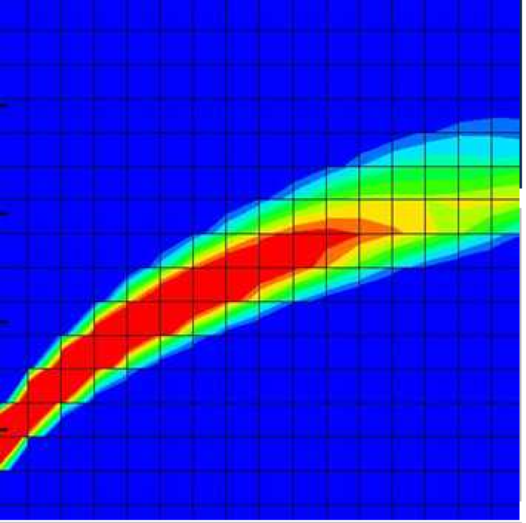

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A Discontinuous Phase-Space Finite Element Discretization of the Linear Boltzmann Equation with EM Fields for Charged Particle Transport

SCEPTRE

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Outline

- Background
- Incorporation of EM terms into Boltzmann equation
- Discretizations
- Results
- Conclusions

Background/motivation

- Some radiation transport problems involve charged particles within electromagnetic fields
- Much existing work on charged particle transport without EM field effects, or on plasma/EM modeling without certain transport effects
- ITS Monte Carlo code can handle transport of charged particles in materials without EM effects, or streaming in voids with EM effects
- LDRD project to develop deterministic solvers to handle EM effects in transport codes (e.g. Sceptre)

Challenges

- Various properties break paradigm of existing deterministic approaches/codes
  - Curved trajectories instead of straight-line path between collisions
  - Continuously changing energies rather than discrete changes
  - Relativistic effects – must be explicitly aware of energies, masses, etc.

Boltzmann equation with acceleration term

$$\frac{1}{c\beta}\frac{\partial\psi}{\partial t} + \left[\vec{\Omega}\cdot\nabla + \sigma_t(r,E)\right]\psi\left(r,E,\vec{\Omega},t\right) + \nabla_v\cdot\frac{\vec{a}}{v}\psi\left(r,E,\vec{\Omega},t\right)$$

$$= \int dE' \int d\vec{\Omega'}\sigma_s\left(r,E'\to E,\vec{\Omega}'\to\vec{\Omega}\right)\psi\left(r,E',\vec{\Omega}',t\right) + S\left(r,E,\vec{\Omega},t\right)$$

Expansion of acceleration term

$$\nabla_v \cdot \frac{\vec{a}}{v}\psi = \nabla_v \cdot \vec{a}N = \vec{a} \cdot \nabla_v N + (\nabla_v \cdot \vec{a})N$$

$$\vec{a} \cdot \nabla_v N = (\vec{a} \cdot \vec{\Omega})\frac{\partial N}{\partial v} + \frac{1}{v}\left[a_x - \mu(\vec{a} \cdot \vec{\Omega})\right]\frac{\partial N}{\partial \mu} + \frac{1}{v(1-\mu^2)}(\vec{\Omega} \times \vec{a})_x \frac{\partial N}{\partial \varphi}$$

$$\nabla_v \cdot \vec{a} = \frac{\partial(\vec{a} \cdot \vec{\Omega})}{\partial v} + \frac{1}{v}\left[(1-\mu^2)\frac{\partial a_x}{\partial \mu} - \mu\eta\frac{\partial a_y}{\partial \mu} - \mu\xi\frac{\partial a_z}{\partial \mu}\right] + \frac{1}{v(1-\mu^2)}\left[-\xi\frac{\partial a_y}{\partial \varphi} + \eta\frac{\partial a_z}{\partial \varphi}\right]$$

Boltzmann equation with acceleration term (change of variables)

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \vec{\Omega}\cdot\nabla\psi + \sigma\psi + \frac{\vec{a}\cdot\vec{\Omega}}{v}\left(\frac{\partial\psi}{\partial v} - \frac{1}{v}\psi\right)$$
$$+\frac{1}{v^2}\left[a_x - \mu(\vec{a}\cdot\vec{\Omega})\right]\frac{\partial\psi}{\partial\mu} + \frac{1}{v^2(1-\mu^2)}(\vec{\Omega}\times\vec{a})_x\frac{\partial\psi}{\partial\varphi} + (\nabla_v\cdot\vec{a})\frac{\psi}{v} = S$$

Dynamics of Lorentz force

$$\vec{F} = q\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right)$$

$$\vec{a} = \frac{1}{\gamma m_o}\left[\vec{F} - \beta^2\left(\vec{F} \cdot \vec{\Omega}\right)\vec{\Omega}\right]$$

$$= \frac{1}{\gamma m_o}\left\{q\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) - \beta^2\left[q\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) \cdot \vec{\Omega}\right]\vec{\Omega}\right\}$$

$$= \frac{q}{\gamma m_o}\left\{\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) - \left[\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) \cdot \frac{\vec{v}}{\mathrm{c}}\right]\frac{\vec{v}}{\mathrm{c}}\right\}$$

$$= \frac{q}{\gamma m_o}\left[\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}} - \frac{\vec{\mathcal{E}} \cdot \vec{v}}{\mathrm{c}}\frac{\vec{v}}{\mathrm{c}}\right]$$

$$= \frac{q}{\gamma m_o}\left[\vec{\mathcal{E}} + v\vec{\Omega} \times \vec{\mathcal{B}} - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\vec{\Omega}\right]$$

Components of Lorentz force

$$\frac{\vec{a}\cdot\vec{\Omega}}{v}\frac{\partial\psi}{\partial v} = q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\frac{\partial\psi}{\partial E}$$

$$\left(\vec{a}\cdot\vec{\Omega}\right)\frac{\psi}{v^2} = \frac{q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)}{E+m_o c^2}\frac{1-\beta^2(E)}{\beta^2(E)}\psi$$

$$\left(\boldsymbol{\nabla}_v\cdot\vec{a}\right)\frac{\psi}{v} = -\frac{5q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)}{E+m_o c^2}\,\psi$$

Components of Lorentz force

$$\frac{1}{v^2}\left[a_x - \mu(\vec{a}\cdot\vec{\Omega})\right]\frac{\partial\psi}{\partial\mu} + \frac{1}{v^2(1-\mu^2)}(\vec{\Omega}\times\vec{a})_x\frac{\partial\psi}{\partial\varphi}$$

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

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

$$\mathcal{D}(E) \equiv \frac{E(E+2m_oc^2)}{E+m_oc^2}$$

Final Boltzmann-EM equation

$$\frac{1}{c\beta}\frac{\partial\psi}{\partial t} + \left[\vec{\Omega}\cdot\nabla + \sigma_t(r,E)\right]\psi\left(r,E,\vec{\Omega},t\right) +$$

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

$$\frac{q}{D(E)}\left[\varepsilon_x(1-\mu^2) - \varepsilon_y\mu\eta - \varepsilon_z\mu\xi + v\left(B_z\eta - B_y\xi\right)\right]\frac{\partial\psi}{\partial\mu} +$$

$$\frac{q}{D(E)(1-\mu^2)}\left[\varepsilon_z\eta - \varepsilon_y\xi + v\left(B_y\mu\eta + B_z\mu\xi - B_x(1-\mu^2)\right)\right]\frac{\partial\psi}{\partial\varphi}$$

$$= \int dE' \int d\vec{\Omega'}\sigma_s\left(r,E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega}\right)\psi\left(r,E',\vec{\Omega}',t\right) + S\left(r,E,\vec{\Omega},t\right)$$

Spatial and energy discretization: discontinuous finite elements

- Spatial FEM well-known, already implemented in Sceptre
- Energy FEM relatively easy to implement in multigroup code

Angular discretization: discrete ordinates (?)

- Treat the *angular* redistribution terms from electromagnetic acceleration as "scattering":

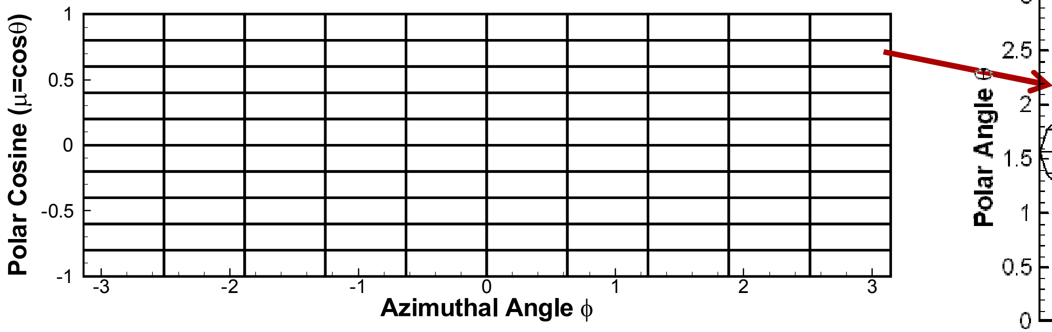
  Discretize the differential operators involving $\frac{\partial \psi}{\partial \mu}$ and $\frac{\partial \psi}{\partial \varphi}$ by

  - Expanding angular flux in terms of spherical harmonics in angle
  - Using properties of harmonics to create expansion of derivatives
  - Applying quadrature rule to evaluate the angular moments
- Allows us to leverage existing discrete ordinates codes
- Difficult to solve
  - Source iteration of these "scattering" terms is unstable
  - Full matrix is asymmetric

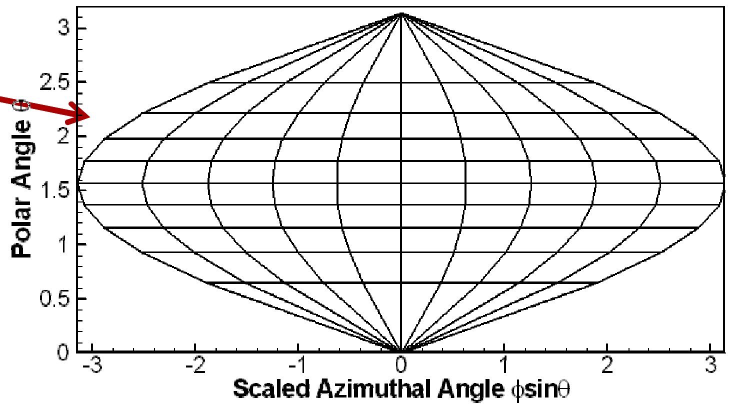
Angular discretization: finite elements

- Finite element in angle is not new but doesn't exist in any production transport codes
- Allows us to directly treat angular derivatives
- Need to create angular mesh

Angular meshes

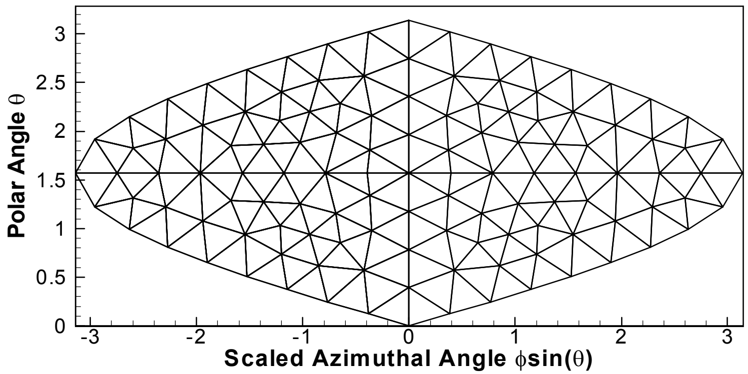


Regular mesh in μ-ϕ space



Mapped from μ-ϕ space mesh

- Problems with meshing μ-ϕ space:
  - Elements mapped to a single point at the poles
  - Non-uniform mesh
- Alternative: use sinusoidal projection and then mesh



Mesh of sphere mapped to planar region

Final method: fully discontinuous FEM in all phase-space variables

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$$\psi(\vec{r},E,\vec{\Omega}) = \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E) \sum_{k=1}^{K} W_j(\vec{\Omega}) \psi_{ijk}$$

- Large number of unknowns
  - $N_{spatial\ element}$ x $N_{spatial\ basis}$ x N_{group} x $N_{energy\ basis}$ x $N_{angular\ element}$ x $N_{angular\ basis}$
  - 10^4 x 4 X 50 x 2 X 100 x 3 = $O(10^9)$
- Extremely complex elemental equations and lots of new code
  - 800 new components
  - 100,000 lines of additional C++ code – split between Sceptre code base (“radlib”) and research code base (radlibEM)

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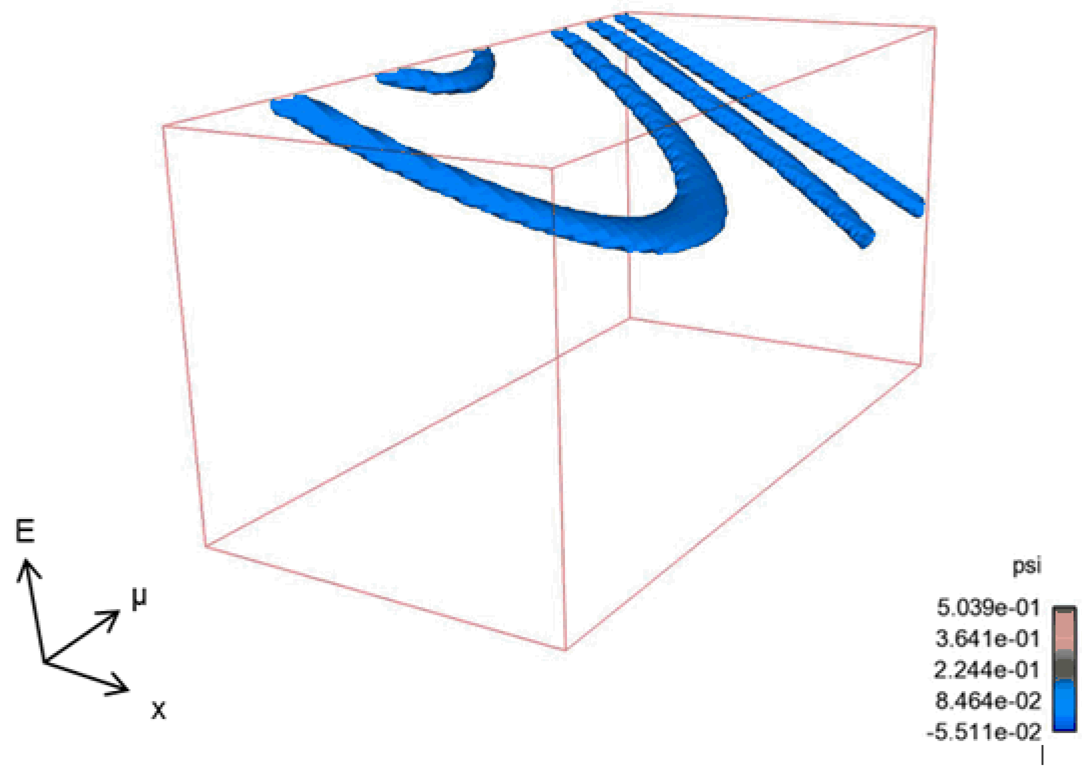
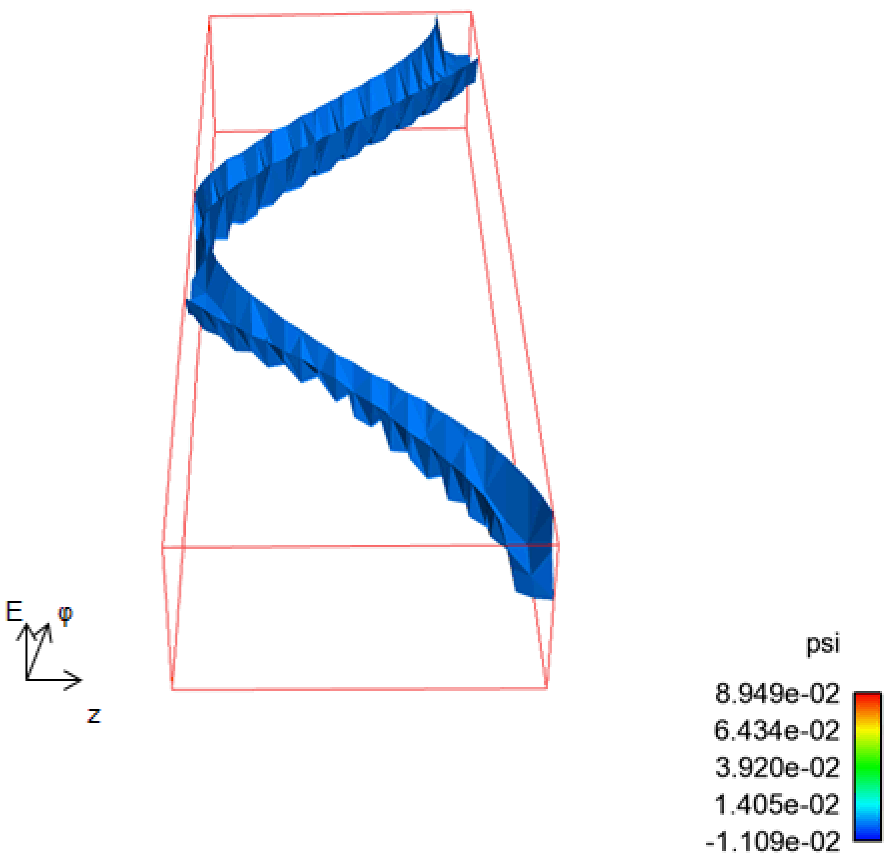
Results: Electron Transport in Void
Constant Electric Field

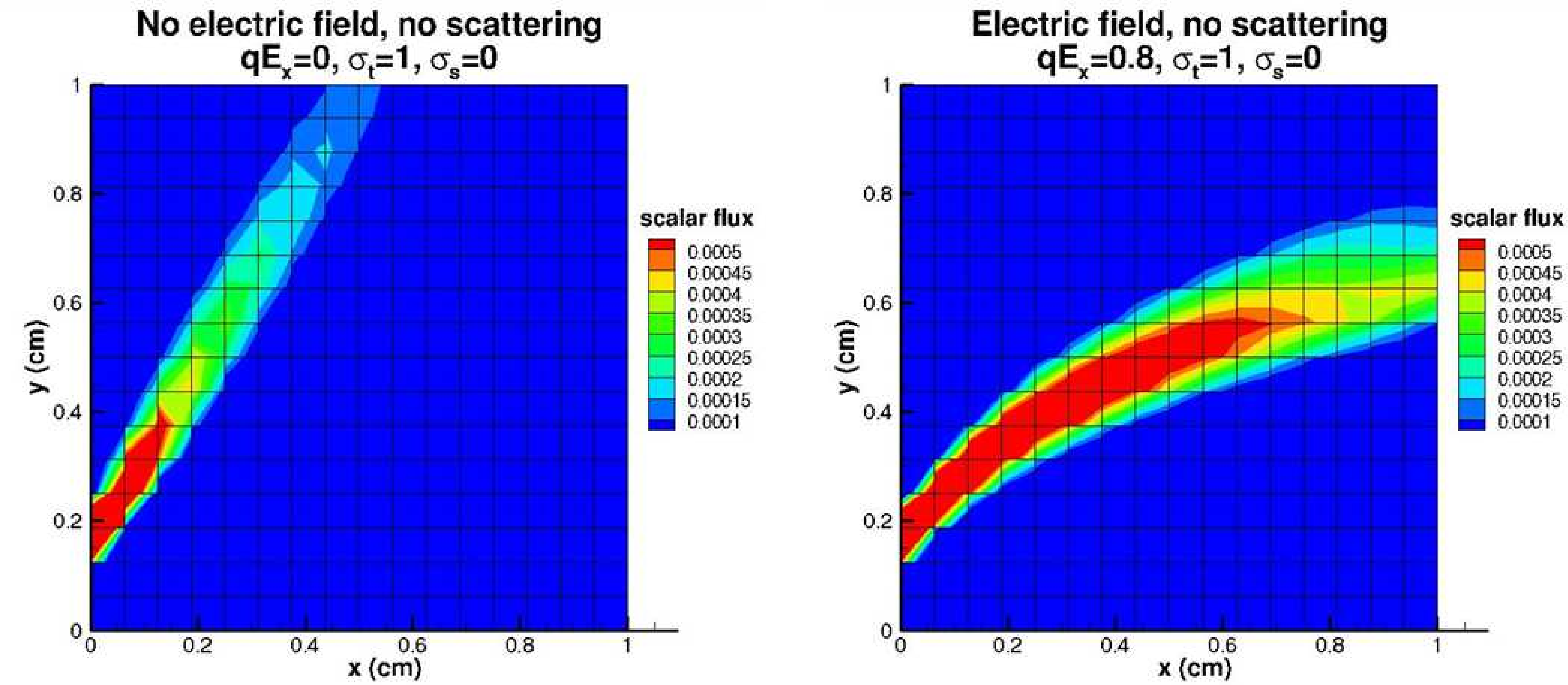


Results: Electron Transport in Void Constant Magnetic Field

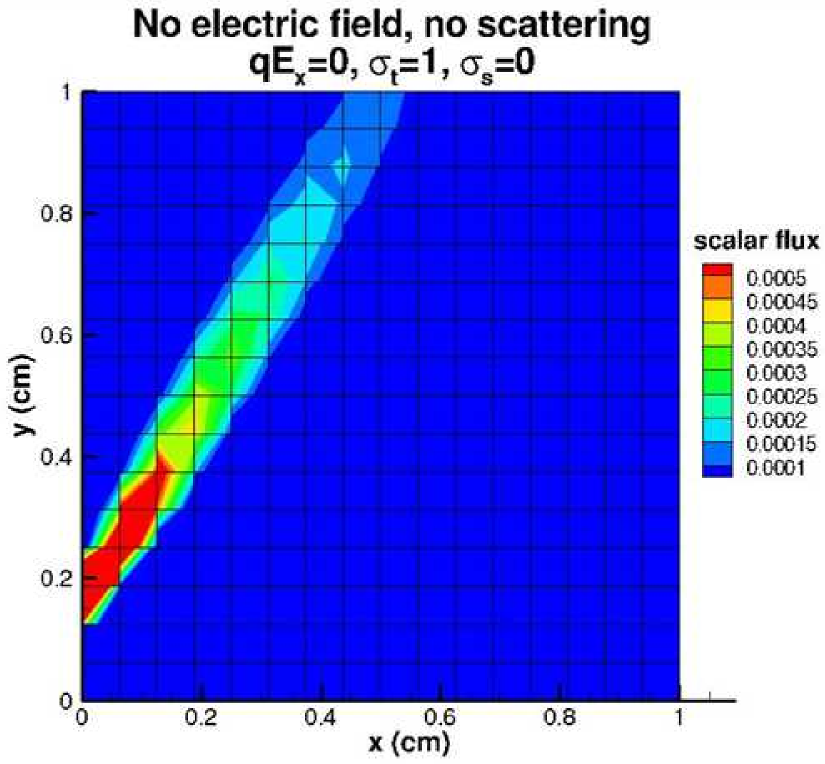


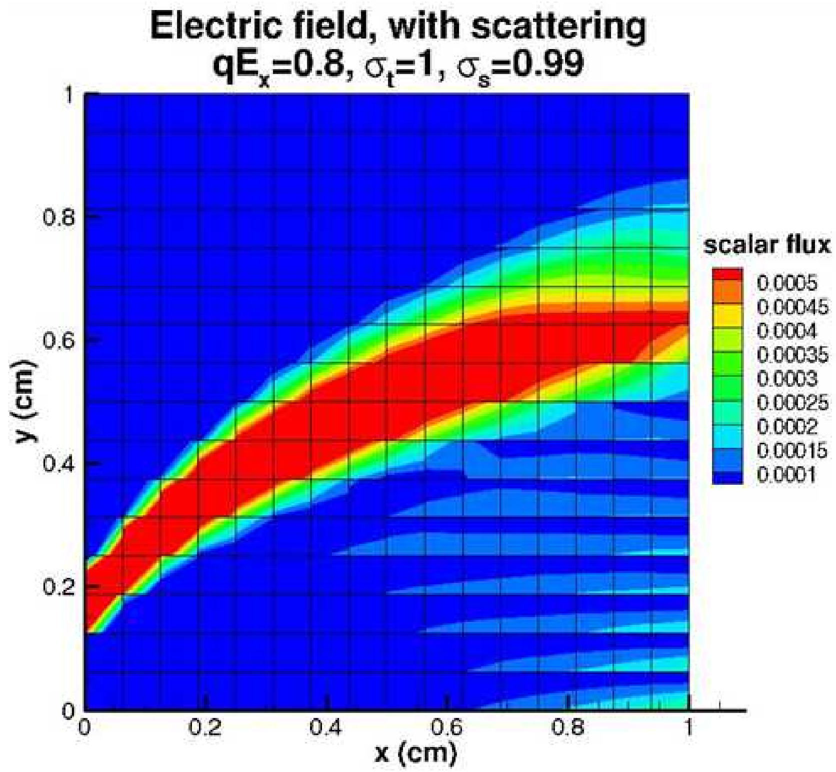
Results: Electron Transport in Pure Absorber

- Unit square region, unit total cross section, incident electron beam at an oblique angle



Result: Electron Transport with Scattering





Order of convergence tests

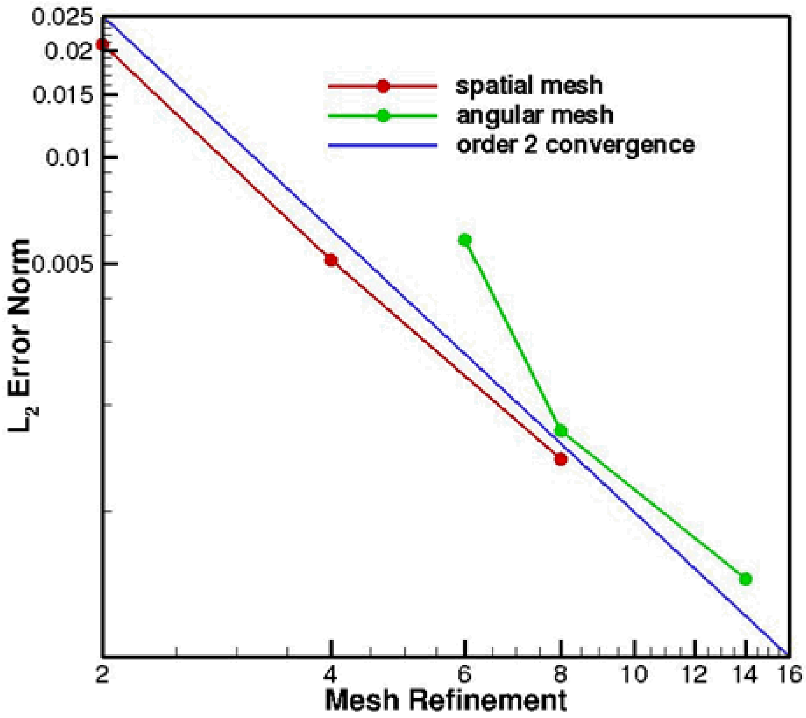
- Method of Manufactured Solutions (MMS)
- Convergence rate analyses for MMS test problem w.r.t. space/angle mesh refinement

$\sigma_t = 10, \sigma_s$=9.99, Isotropic scattering with Unit Electric Field in +X Direction

Analytic Solution

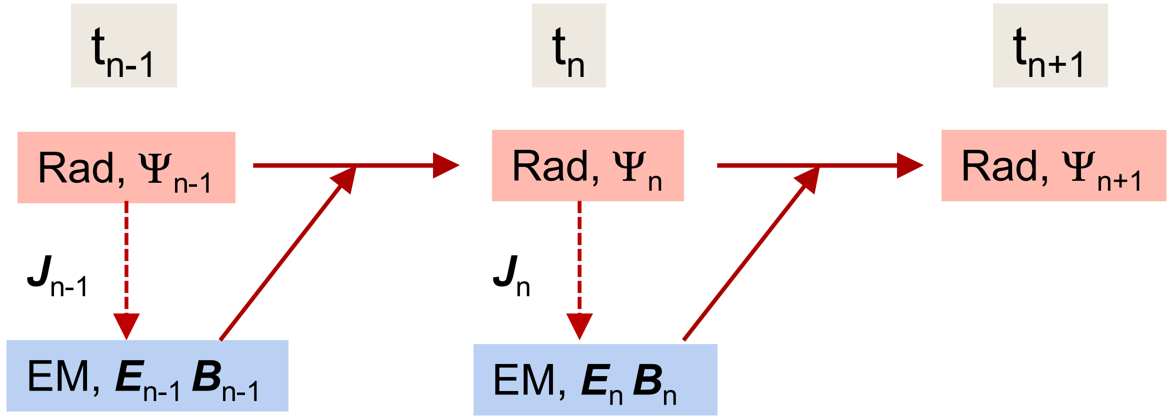
$$\psi(x, y, \mu, \varphi, E) = x^2(1+\mu)\sqrt{E}$$

Spatial Mesh	Angular Mesh	L_2 Error Norm
2x2	16x16	0.0207081
4x4	16x16	0.00512301
8x8	16x16	0.00140234
16x16	6x6	0.00582827
16x16	8x8	0.00168432
16x16	14x14	0.000646928



Time-dependent coupling with EM solver

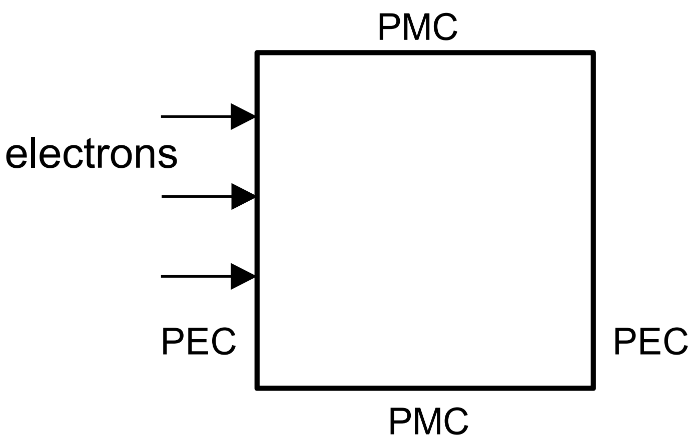
- Time advancement in a staggered order (Operator Split)
  - Fully implicit differencing for electron transport
  - Newmark beta method for electromagnetics
  - Limitation on time-step size

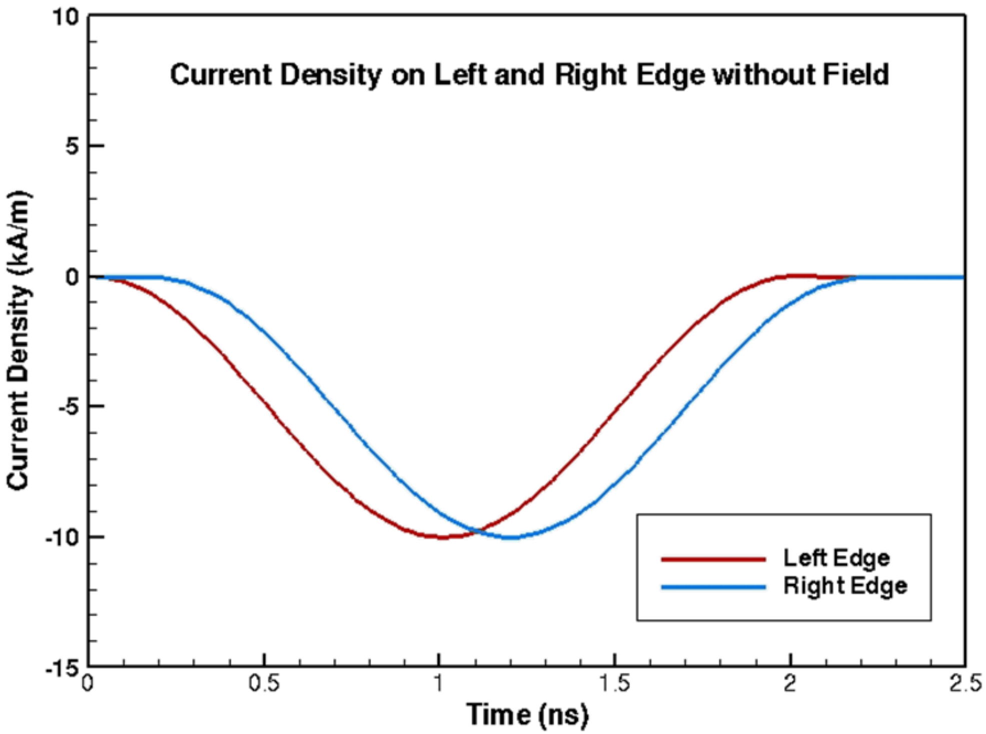


Ψ Electron Angular Flux
$\boldsymbol{J}$ Electron Current Density
$\boldsymbol{E}$ Electric Field
$\boldsymbol{B}$ Magnetic Flux Density

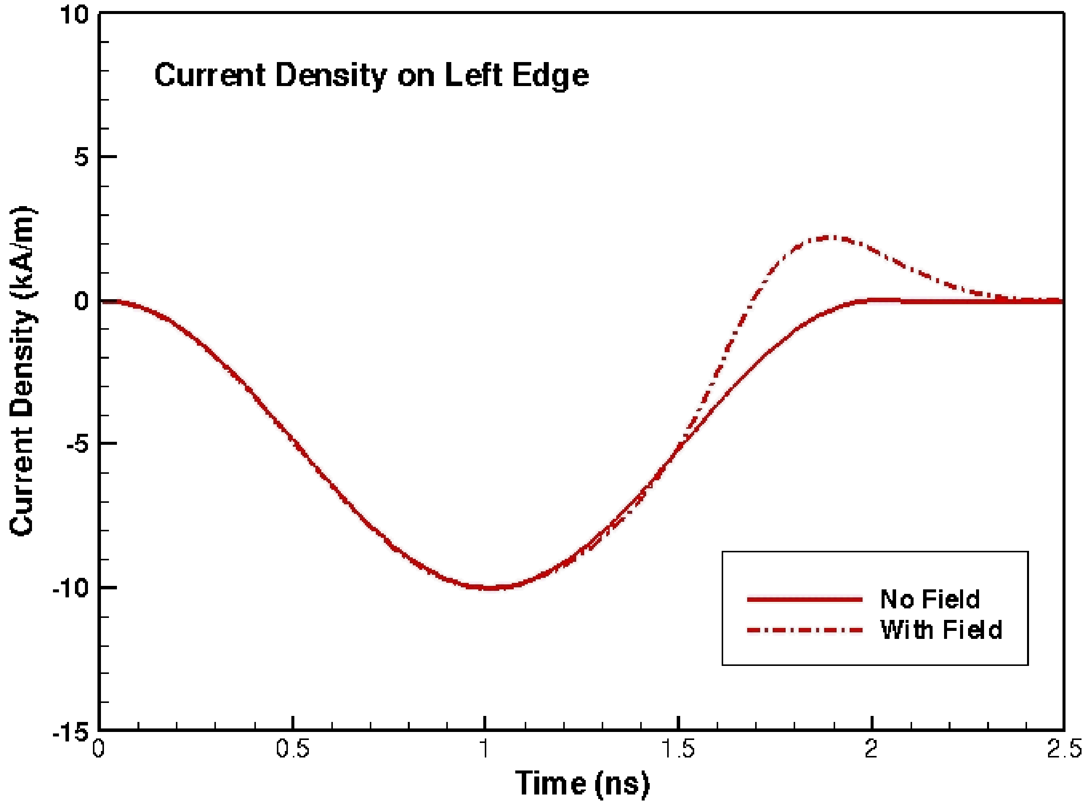
Result: Capacitor charging

- 1 cm x 1 cm square of void
- 10 kA/m peak current
- 2-ns wide sine-square pulse
- Electron energy = 10 keV

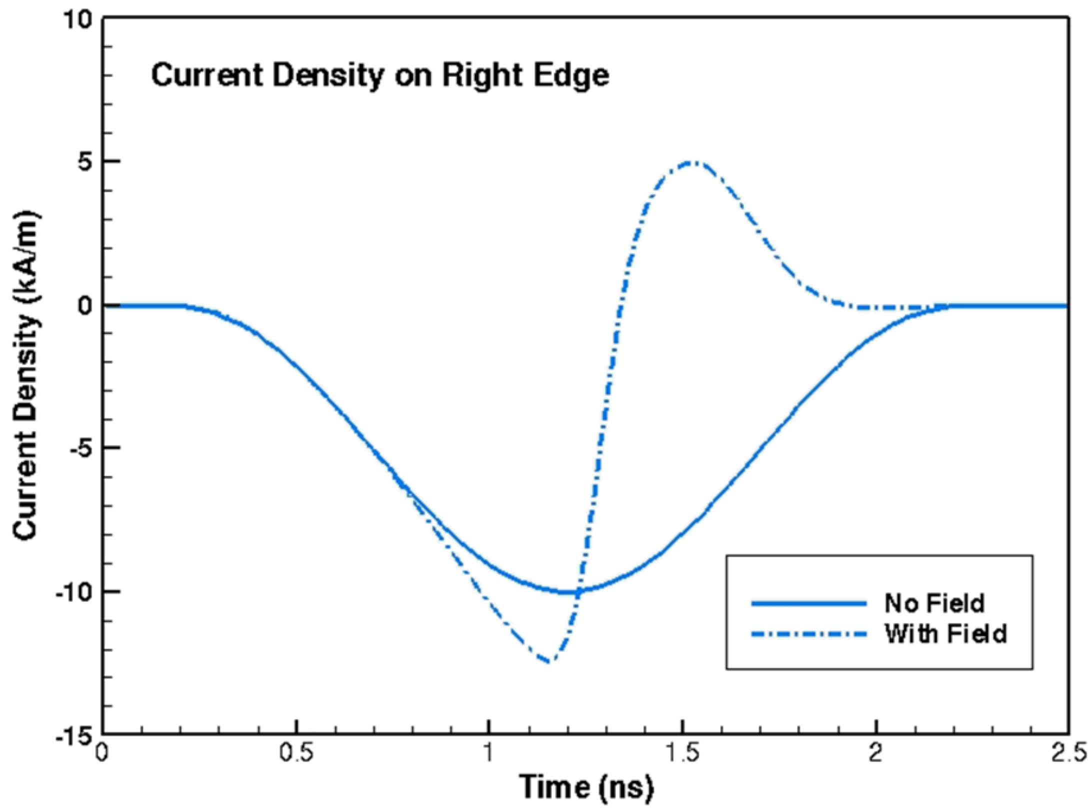




Result: Capacitor charging



Result: Capacitor charging



Future work

- **Need to "productize" the research code – packaging, refactoring, testing**
- **Desire to integrate with more sophisticated EM solvers**
- **Finite elements in energy can improve our transport even without EM fields, particularly for cross sections (e.g. CSD operator)**
- **Finite elements in angle can improve our transport for streaming-dominated problems (mitigate ray-effects)**

Conclusions

- **We have derived a form of the Boltzmann equation that includes the effects of electromagnetic fields on relativistic charged particle transport**
- **We have developed a deterministic discretization and solution technique to model charged particle transport with EM fields**
- **We have demonstrated coupled electron transport and consistent electric field with a simple time integration scheme**