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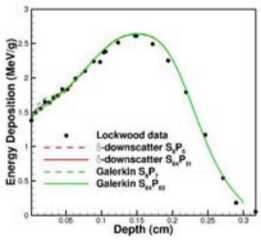

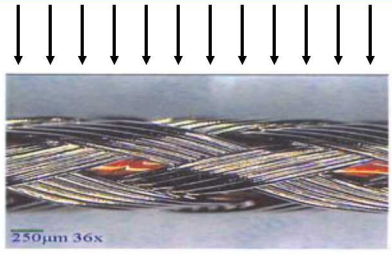

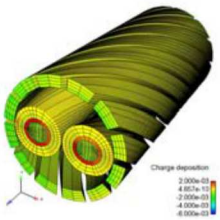

Specializations in the SCEPTRE Code for Charged-Particle Transport

Clif Drumm, Wesley Fan and Shawn Pautz

Radiation Effects Theory Dept. Sandia National Laboratories

RPSD 2018 Santa Fe, NM

27 August, 2018

U.S. DEPARTMENT OF ENERGY | NNSA

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Overview

- Methods for handling highly-forward-peaked scattering
- Methods for handling slow convergence of scattering source iterations
- Development activities
  - Discontinuous finite elements (DFE) in energy applied to the Continuous-Slowing-Down (CSD) term
  - Transport in the presence of ElectroMagnetic (EM) fields

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Methods for Handling Highly-Forward-Peaked Scattering

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- Legendre polynomial expansion alone inadequate
- Explicit δ-function down-scatter term (extended transport correction)
- Galerkin mapping between angular flux and angular moments

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Explicit δ-Function Downscatter

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$$\sigma_{g'\to g}(\mu_0) \cong \sum_{l=0}^{L} \tilde{\sigma}^{l}_{g'\to g}\, P_l(\mu_0) + \sigma^{L+1}_{g'\to g}\delta(1-\mu_0)$$

- Down-scatter source depends upon the angular moments *and* angular flux

$$\boldsymbol{\Omega}\cdot\nabla\psi_g + \sigma_{t,g}\psi_g = \sum\nolimits_{l,g'} \left\{ [M]\left[\tilde{\Sigma}^{l}_{g'\to g}\right]\phi_{g'} + \left[\Sigma^{L+1}_{g'\to g}\right]\psi_{g'} \right\} + Q_g$$

$[M]$ is the moment-to-discrete operator

$\left[\tilde{\Sigma}^{l}_{g'\to g}\right]$ and $\left[\Sigma^{L+1}_{g'\to g}\right]$ are the diagonal scattering cross section matrices

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Galerkin Mapping Between Angular Flux and Angular Moments

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- Discrete-to-moment operator $[D]$ is the inverse of the moment-to-discrete operator $[M]$
- Similarity transformation of the (diagonal) scattering moments matrix
- Requires that the number of scattering moments be equal to the number of angular quadrature directions

$$\boldsymbol{\Omega} \cdot \nabla \psi_g + \sigma_{t,g} \psi_g = \sum_{l,g'} [M] \left[\Sigma^l_{g' \to g} \right] [M]^{-1} \psi_{g'} + Q_g$$

J. MOREL, "A Hybrid Collocation-Galerkin-Sn Method for Solving the Boltzmann Transport Equation," *Nucl. Sci. Eng.,* **101**, 72 (1989).

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Energy Deposition Compared with Lockwood Data

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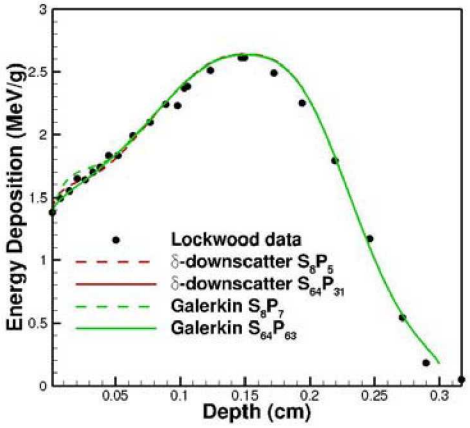

- 1-MeV electrons on range-thick Be
- Good agreement except for low-order Galerkin

G. LOCKWOOD, L. RUGGLES, G. MILLER and J. HALBLEIB, "Calorimetric Measurement of Electron Energy Deposition in Extended Media- Theory vs Experiment," Sandia National Laboratories report, SAND79-0414, Albuquerque, NM (reprinted 1987).

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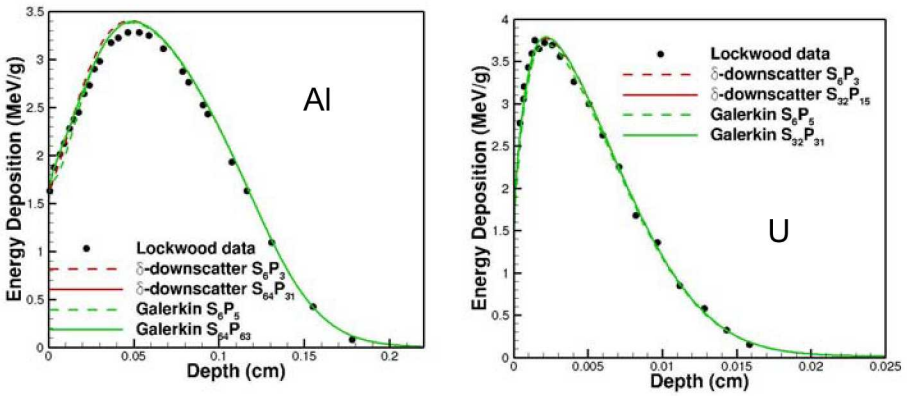
Energy Deposition Compared with Lockwood Data

- 1-MeV electrons on range-thick Al and U



Methods for Handling Slow Convergence of Scattering-Source Iterations

- Charged-particle cross sections have large scattering ratios resulting in slow convergence of source iterations
- SCEPTRE includes multiple solver options that perform well for problems including cross sections with large scattering ratios
- Alternative solvers perform well as accelerators (Transport Synthetic Acceleration, TSA)

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SCEPTRE Contains Multiple Solver Options

- Traditional sweeps-based solver using source iteration
  - Fast for photons
  - Slow for electrons
  - Small memory requirement
- Simultaneous space-angle Krylov solvers
  - Fast for electrons
  - Slow for photons
  - Large memory requirement
  - Multiple solver options
    - S_N or P_N angular treatment
    - Self-Adjoint Angular Flux (SAAF) or Least-Squares (LS) utilizing continuous spatial finite elements
    - 1st-order transport utilizing discontinuous spatial finite elements

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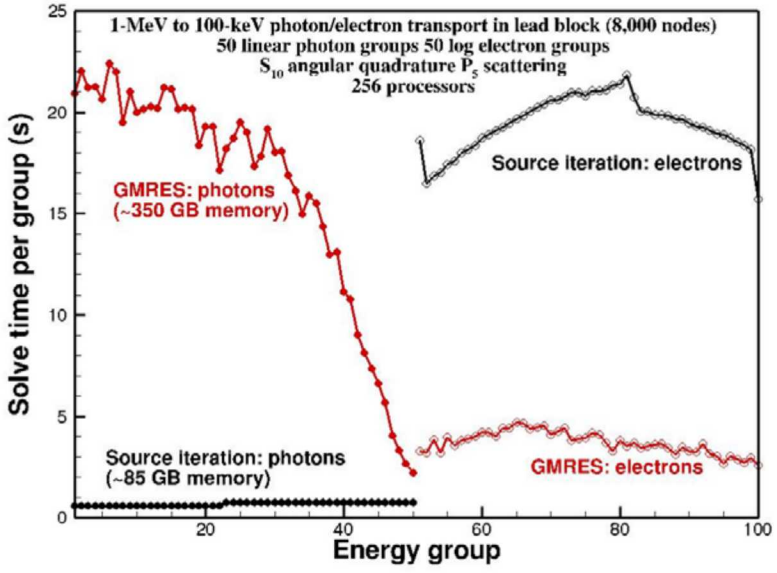
Comparison of Timing Results



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Test Problem: Photon/Electron Transport on Twisted-Pair Braided Shielded Cable

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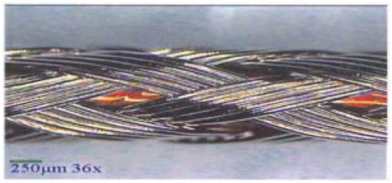
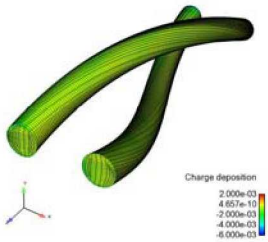
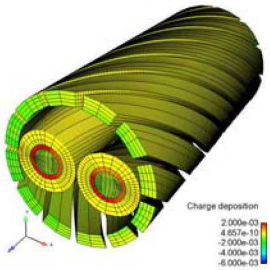
Planar photon source





~¼ million nodes



Twisted-pair with shield removed

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Convergence for Various TSA Preconditioners

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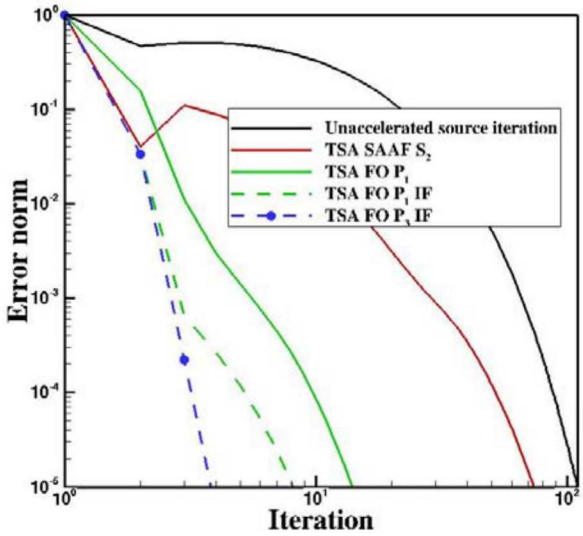

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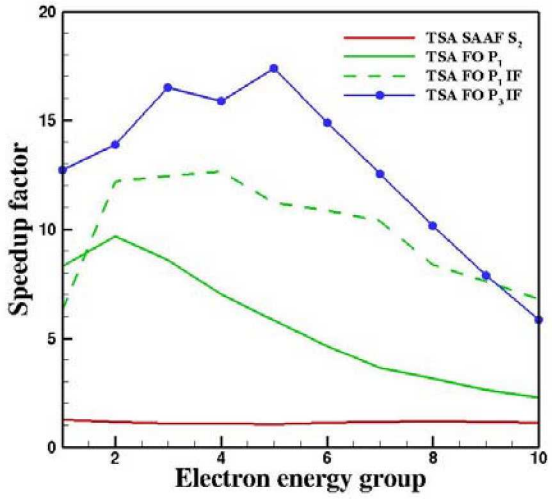
Speed-Up Factors for Various TSA Preconditioners



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Speed Up Depends on Details of the Coarse-Level Solves

TSA method	Coarse-level parameters			Total solve time of electron groups (s)	Speed up
	Preconditioner	Convergence tolerance	Max iterations		
none	-	-	-	3530	1
FO P_1	none	0.01	100	653	5.4
FO P_1	IF	0.01	10	365	9.7
FO P_3	IF	0.01	10	272	13.
SAAF S_2	none	10^{-4}	1000	3160	1.1

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Finite-Elements in Energy

- Effective for modeling the Continous-Slowing-Down (CSD) term
- Requires FE weighted cross sections and stopping powers
- SCEPTXS code is being developed to replace CEPXS to include FE weighted data

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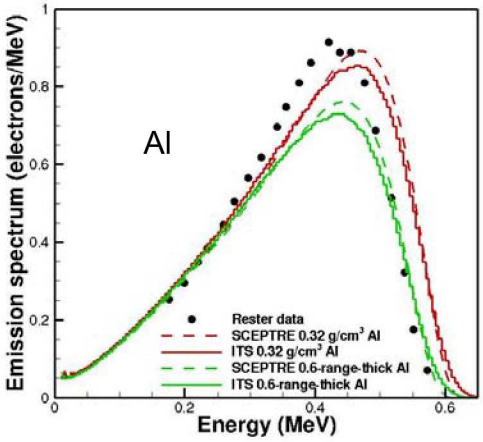
Electron Emission Spectrum (Rester Data)

- Electron emission spectrum sensitive to the aluminum thickness



D. RESTER and J. DERRICKSON, "Electron Transmission Measurements for Al, Sn, and Au Targets at Electron Bombarding Energies of 1.0 and 2.5 MeV," *J. App. Phys.*, **42**, 714 (1971).

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Charged-Particle Transport in the Presence of EM Fields

- Relativistic Vlasov equation

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \boldsymbol{\Omega}\cdot\nabla\psi + \sigma\psi + q(\boldsymbol{\mathcal{E}}\cdot\boldsymbol{\Omega})\left[\frac{\partial\psi}{\partial E} - \frac{1+4\beta^2}{\mathcal{D}(E)}\psi\right]$$
$$+\frac{q}{\mathcal{D}(E)}\left[\mathcal{E}_x(1-\mu^2) - \mathcal{E}_y\mu\eta - \mathcal{E}_z\mu\xi + v\left(\mathcal{B}_z\eta - \mathcal{B}_y\xi\right)\right]\frac{\partial\psi}{\partial\mu}$$
$$+\frac{q}{\mathcal{D}(E)(1-\mu^2)}\left[\mathcal{E}_z\eta - \mathcal{E}_y\xi + v\left[\mathcal{B}_y\mu\eta + \mathcal{B}_z\mu\xi - \mathcal{B}_x(1-\mu^2)\right]\right]\frac{\partial\psi}{\partial\varphi} = Q$$

$$\mathcal{D}(E) = \frac{E(E+2m_0c^2)}{E+2m_0c^2}$$

$$\boldsymbol{\mathcal{E}} = \mathcal{E}_x\boldsymbol{i} + \mathcal{E}_y\boldsymbol{j} + \mathcal{E}_z\boldsymbol{k}$$
$$\boldsymbol{\mathcal{B}} = \mathcal{B}_x\boldsymbol{i} + \mathcal{B}_y\boldsymbol{j} + \mathcal{B}_z\boldsymbol{k}$$

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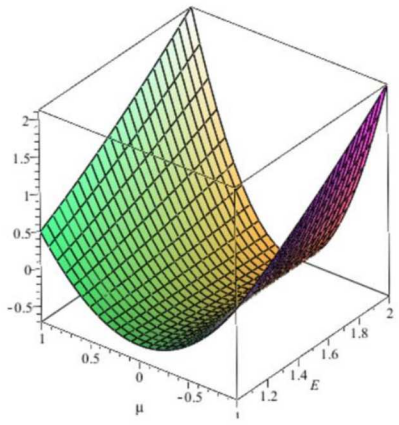
Simple Method of Manufactured Solutions (MMS) Test Problem

- 1D
- Void
- Uniform electric field
- No magnetic field

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



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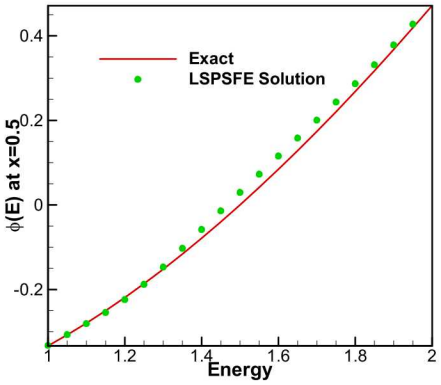
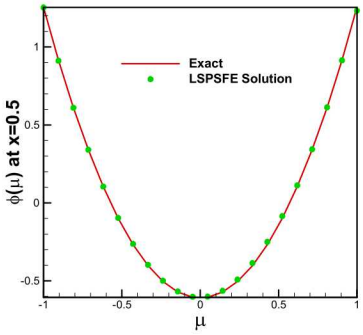
Least-Squares Phase-Space FE (LSPSFE) Solution





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Conclusions

- Productization of new capabilities
  - Finite-elements in energy
  - Finite elements in angle
  - Transport in the presence of EM fields
- More experience with acceleration/preconditioning methods
  - Some problems resist acceleration
  - Many knobs to turn to get effective speedup
- New weighted cross section/stopping power
  - Energy weighted for energy finite elements
  - Angular weighted for angular finite elements

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