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Scattering Cross Sections for Electron Transport Using Energy-Finite-Element Weighting

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Motivation

- Electron transport is characterized by frequent collisions resulting in small deflection and energy loss
  - Cross sections are large
  - Rapidly varying in energy
  - Extremely forward peaked
- The Multi-Group (MG) approximation introduces error that is hard to quantify
- Application of the Finite-Element in Energy (FE-E) method to electron transport results in:
  - More accurate cross-section modeling
  - Straight-forward characterization of error
- Two methods for handling extreme forward-peaked scattering
  - Continuous Slowing Down (CSD) model
  - δ-function down-scatter model

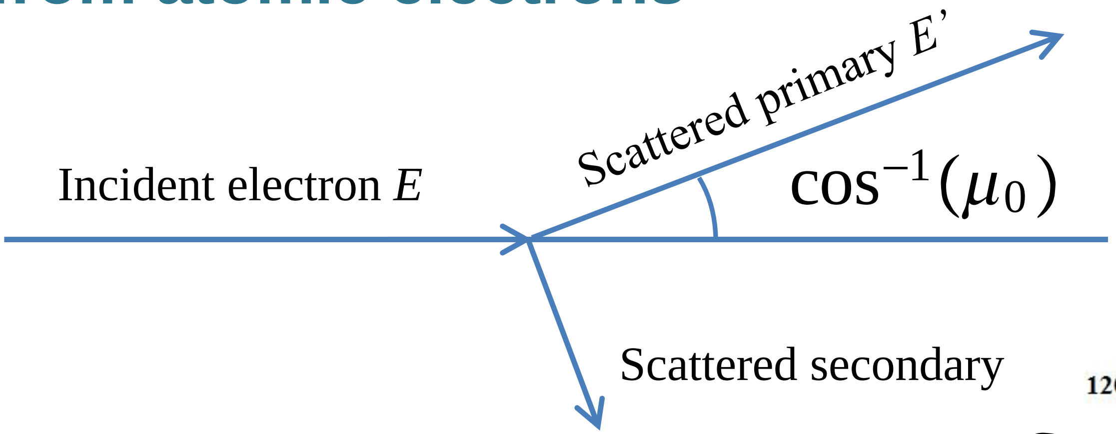
Overview

- Describe Boltzmann-CSD equation with δ-function down-scatter
- Develop Finite-Element in Energy (FE-E) capability
- Identify a scattering kernel that can be used to generate FE-E weighted cross sections and stopping powers
  - Apply scattering kernel to compute stopping powers and compare with experimental values
  - Add angular dependence for fully energy-angle differential cross section
- Apply the Method of Manufactured Solutions (MMS) to test the FE-E capability
  - "Exact" tests (to within round-off and iterative convergence tolerance)
    - *test using MG cross sections*
    - *test using FE-E weighted cross sections*
  - Inexact-in-energy test to measure a convergence rate with energy-mesh refinement ("exact" in space and angle)

Legacy CEPXS code to be replaced by new code for photon-electron cross section processing

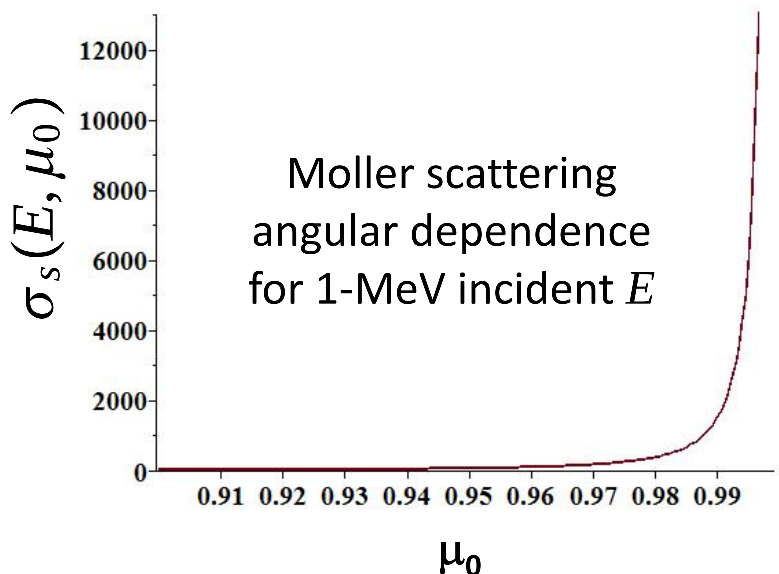
- **S**andia **C**omputational **E**ngine for **P**article **T**ransport **C**ross **S**ections (SCEPTXS)
- C++
- Photon/electron/positron cross sections for deterministic and MG Monte Carlo transport codes and continuous-energy Monte Carlo
- New cross section format
- Flexible partition between Continuous Slowing Down (CSD) model and multi-group Legendre (MG-L)
- Generate FE-E weighted and MG cross sections and stopping powers
- Add the capability to generate cross sections for energies below the current 1-keV cutoff
- Multi-year effort

Angular dependence of inelastic electron scattering from atomic electrons



$$\mu_0(E \rightarrow E') = \frac{\sqrt{E'(E+2m_0c^2)}}{\sqrt{E(E'+2m_0c^2)}}$$

- Compute μ_0 from scattering kinematics
- Neglect binding energy
- m_0c^2 is the electron rest mass
- Scattering extremely forward peaked for small energy transfer



Angle-energy differential scattering cross section:

$$\sigma_s(\mu_0, E \rightarrow E') = \delta\left(\mu_0 - \frac{\sqrt{E'(E+2m_0c^2)}}{\sqrt{E(E'+2m_0c^2)}}\right)\sigma_s(E \rightarrow E')$$

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Boltzmann-CSD equation

- Electron scattering cross sections are large and extremely forward peaked in the limit of small energy transfer
  - Neglect direction change for small energy transfer
  - Introduce Continuous-Slowing-Down (CSD) term to model energy loss

Boltzmann equation:

$$\mathbf{\Omega} \cdot \nabla\psi + \sigma_t \psi(\mathbf{r}, \mathbf{\Omega}, E) = \int_E^{E_{\max}} \int_{4\pi} \sigma_s(\mathbf{\Omega}' \to \mathbf{\Omega}, E' \to E) \psi(\mathbf{r}, \mathbf{\Omega}', E') d\mathbf{\Omega}' dE' + Q(\mathbf{r}, \mathbf{\Omega}, E)$$

Stopping power:

$$S(E) \equiv \int_{E/2}^{E} (E - E')\sigma_s(E \to E')dE'$$

Restricted stopping power:

$$S_R(E) \equiv \int_{E-\Delta}^{E} (E - E')\sigma_s(E \to E')dE'$$

Specified partition energy between CSD and non-CSD

Boltzmann-CSD equation:

$$\mathbf{\Omega} \cdot \nabla\psi + \sigma_t \psi(\mathbf{r}, \mathbf{\Omega}, E) - \frac{\partial(S_R\psi)}{\partial E} = \int_{E+\Delta}^{E_{\max}} \int_{4\pi} \sigma_s(\mu_0, E' \to E) \psi(\mathbf{r}, \mathbf{\Omega}', E') d\mathbf{\Omega}' dE' + Q(\mathbf{r}, \mathbf{\Omega}, E)$$

δ-function down scattering approximation

Even after removal of CSD component, scattering cross sections are still extremely forward peaked

Scattering moments

$$\sigma_{sl}(E' \to E) \equiv \int_{-1}^{1} P_l(\mu_0)\sigma_s(\mu_0, E' \to E)d\mu_0$$

Angular dependence can be more-accurately modeled by separating a forward δ-function component

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

Where modified scattering moments are

$$\tilde{\sigma}_{s,l}(E' \to E) \equiv \sigma_{s,l}(E' \to E) - \sigma_{s,L+1}(E' \to E)$$

Boltzmann-CSD equation

Forward δ-down-scatter source

$$\mathbf{\Omega} \bullet \nabla\psi + \sigma_t\psi(\mathbf{r}, \mathbf{\Omega}, E) - \frac{\partial(S_R\psi)}{\partial E} = \int_{E+\Delta}^{E_{\max}} \sigma_{s,L+1}(E' \to E)\psi(\mathbf{r}, \mathbf{\Omega}, E')dE'$$

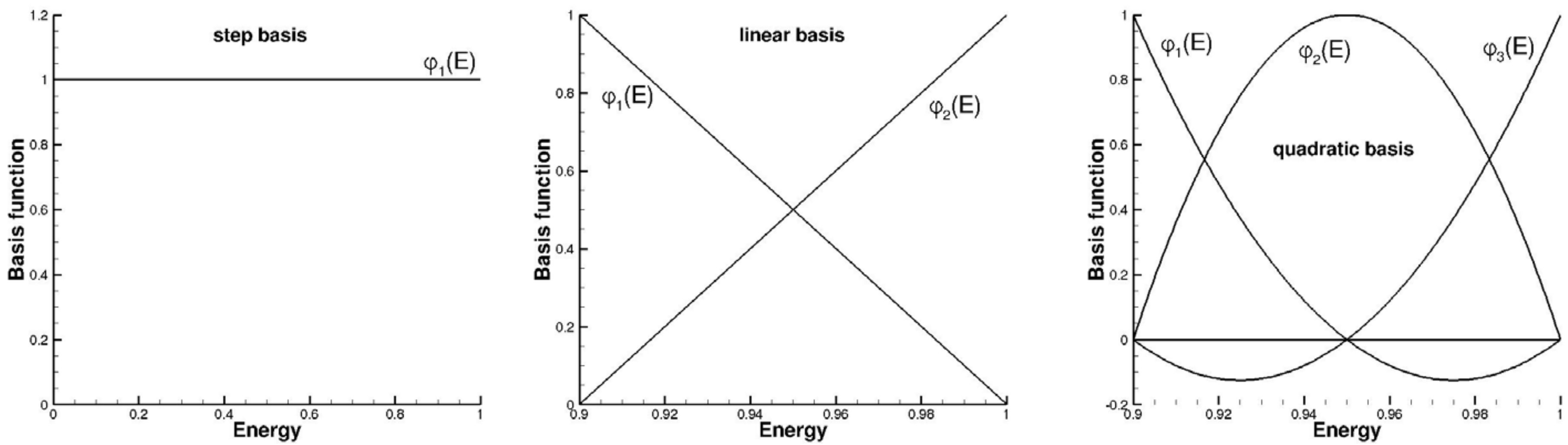
$$+\sum_{l,m} Y_{l,m}(\mathbf{\Omega}) \int_{E+\Delta}^{E_{\max}} \tilde{\sigma}_{s,l}(E' \to E)\phi_{l,m}(\mathbf{r}, E')dE' + Q(\mathbf{r}, \mathbf{\Omega}, E)$$

down-scatter source moments

FE-E Method: expand angular flux in energy basis functions

$$\psi(\mathbf{r},\mathbf{\Omega},E) \cong \sum_{i'} \psi_g^{i'}(\mathbf{r},\mathbf{\Omega})\varphi_g^{i'}(E), \quad E \in [E_{g,l}, E_{g,u}]$$

Using step basis results in MG cross sections



FE-E method applied to the Boltzmann-CSD equation

- Expand the angular flux and source terms in the energy basis functions
- Multiply by an energy basis function
- Integrate over an energy element
- Integrate CSD energy derivative term by parts
  - Use upwind differencing in energy for a Discontinuous-Finite-Element (DFE) approximation in energy

$$\mathbf{\Omega} \bullet \nabla\psi + \sigma_t \psi(\mathbf{r}, \mathbf{\Omega}, E) - \frac{\partial(S_R \psi)}{\partial E} = \int_{E+\Delta}^{E_{\max}} \sigma_{s,L+1}(E' \rightarrow E)\psi(\mathbf{r}, \mathbf{\Omega}, E')dE'$$

$$+\sum_{l,m} Y_{l,m}(\mathbf{\Omega}) \int_{E+\Delta}^{E_{\max}} \tilde{\sigma}_{s,l}(E' \rightarrow E)\phi_{l,m}(\mathbf{r}, E')dE' + Q(\mathbf{r}, \mathbf{\Omega}, E)$$

FE-E weighted cross sections and stopping power

Total cross section matrix

$$\sigma_{t,g}^{i,i'} = \left\langle \varphi_g^i(E), \sigma_t(E)\varphi_g^{i'}(E) \right\rangle$$

Restricted stopping power matrix

$$S_{R,g}^{i,i'} = \left\langle \frac{d\varphi_g^i}{dE}, S_R(E)\varphi_g^{i'}(E) \right\rangle$$

Scattering cross section array

$$\sigma_{sl,g'\to g}^{i,i'} = \left\langle \varphi_g^i(E), \left\langle \sigma_{sl}(E' \to E), \varphi_{g'}^{i'}(E') \right\rangle \right\rangle$$

FE-E implementation in SCEPTRE

- 1st-order form of the transport equation
- DFE method in space
- DFE method in energy
- S_N approximation in angle
- P_N scattering approximation
- Form linear system for all space, all directions and all energy basis functions for a single energy element
- Solve using GMRES iterations sequentially from highest energy element to lowest

Relativistic Binary-Encounter-Bethe (RBEB) kernel

Y-K. KIM, J. P. SANTOS and F PARENTE, "Extension of the binary-encounter-dipole model to relativistic incident electrons," *Phys. Rev. A*, **62**, 1-14 (2000).

$$\sigma_{RBEB}(E \rightarrow E') = \sum_j \frac{4 \cdot 10^{24} \pi a_0^2 \alpha^4 Z_j m_0 c^2 N}{(\beta_t^2 + \beta_u^2 + \beta_b^2) b_j^2}$$

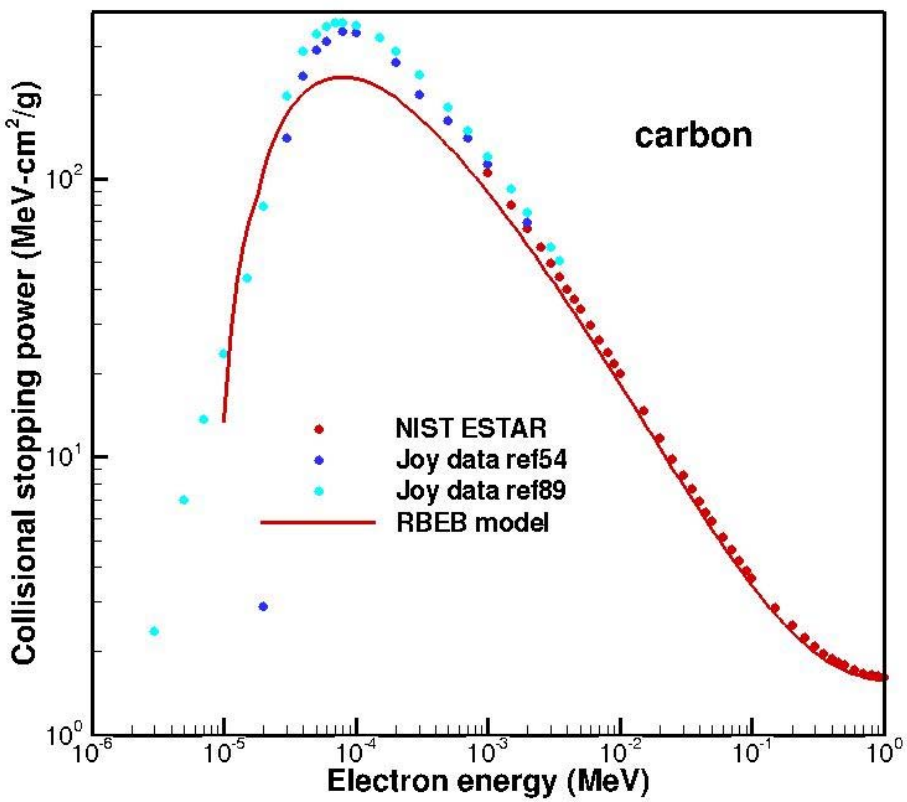
$$\left\{ -\frac{4 m_0 c^2 (2E + m_0 c^2) b_j^2}{(E + 2 m_0 c^2)^2 (E - E')(E' + b_j)} + \frac{b_j^2}{(E - E')^2} + \frac{b_j^2}{(E' + b_j)^2} + \frac{4 b_j^2}{(E + 2 m_0 c^2)^2} \right.$$

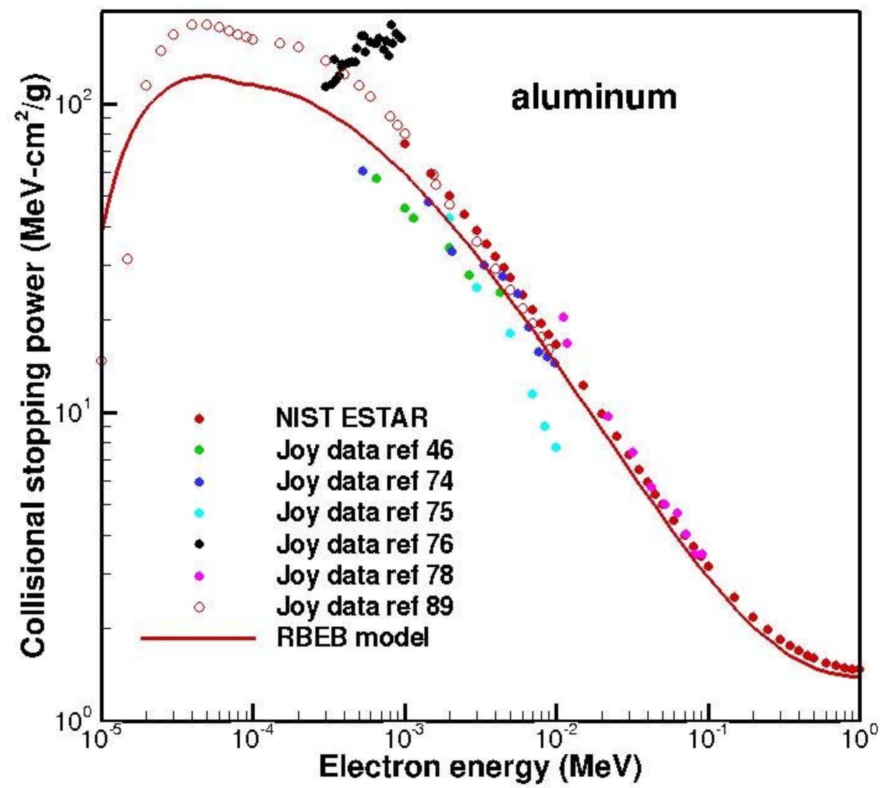
$$\left. + \frac{b_j^3}{(E' + b_j)^3} \left[\ln\left(\frac{E(E + 2 m_0 c^2)}{(m_0 c^2)^2} \right) - \frac{E(E + 2 m_0 c^2)}{(E + m_0 c^2)^2} - \ln\left(\frac{2 b_j}{m_0 c^2} \right) \right] \right\}$$

Apply an adaptive integration routine to compute stopping power from RBEB kernel: carbon and aluminum

$$S(E) \equiv \sum_j Z_j \int_{(E-b_j)/2}^{E-b_j} (E - E')\sigma_{RBEB,j}(E \to E')dE'$$

Z_j is the occupancy of the j^{th} level





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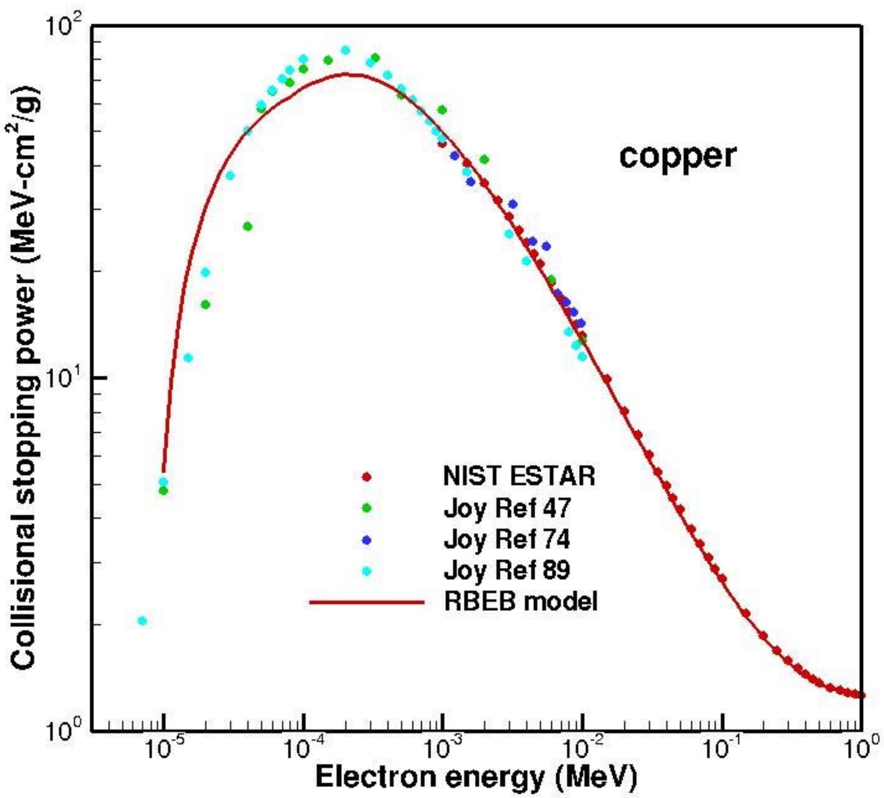
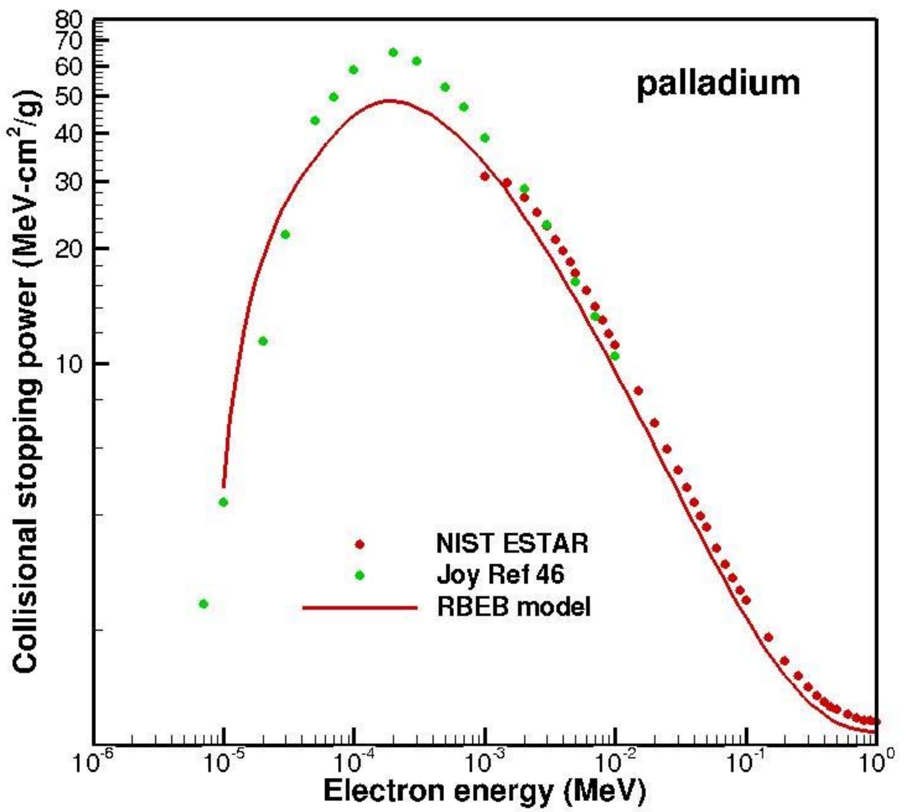
Apply an adaptive integration routine to compute stopping power from RBEB kernel: copper and palladium

- RBEB model under-estimates the peak stopping power
  - Measured data includes excitation cross section
  - RBEB model does not





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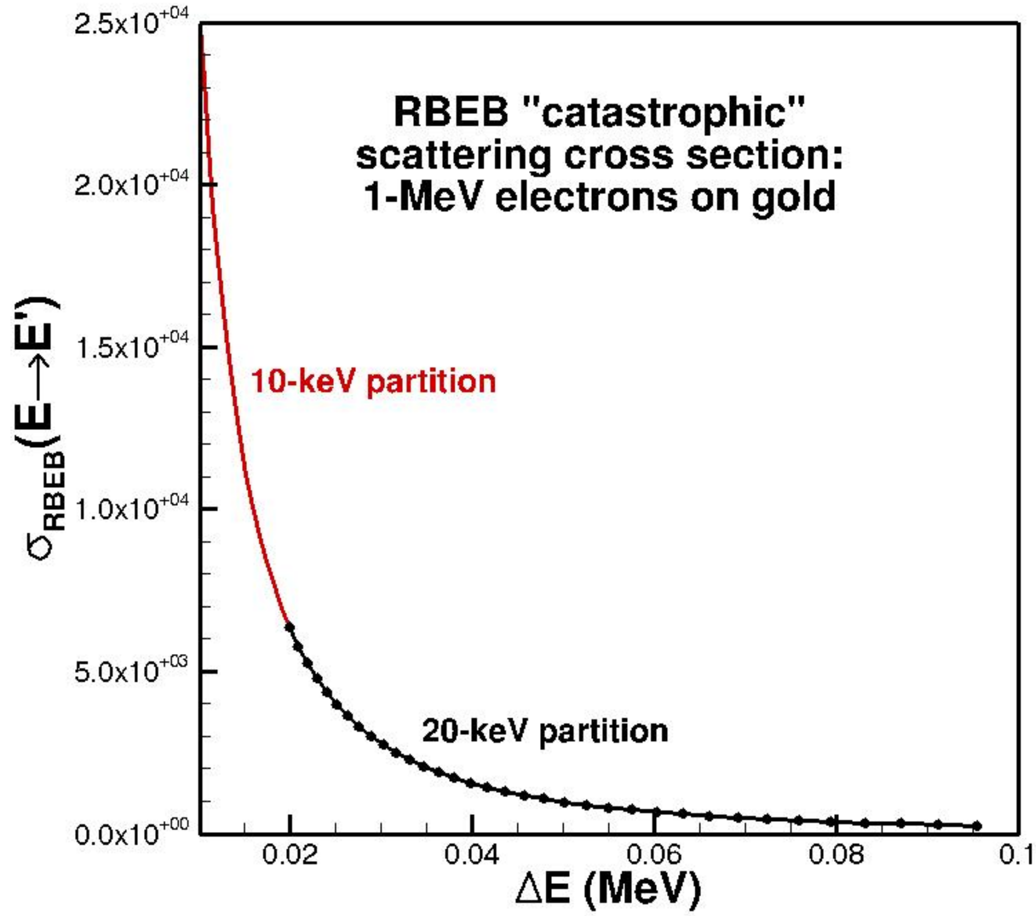
Energy gradient of the scattering cross section depends upon the partition between CSD and MG-L

$$S_R(E) \equiv \sum_j \int_{E-\Delta}^{E-b_j} (E - E')\sigma_{s,j}(E \rightarrow E')dE'$$

- Δ is the partition energy between the CSD and MG-L treatments
- A lower value of Δ increases the energy gradient in the cross section
- Δ can be either specified explicitly or computed from a specified scattering cosine



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Legendre polynomial expansion of the angular dependence of the cross sections

- Forward δ-function down-scatter approximation
  - Remove forward-peaked component from scattering cross section
  - Treat forward δ-function down-scatter explicitly in scattering-source term
  - Resulting modified cross section less forward peaked

Scattering moments

$$\sigma_{s,l}(E \to E') = P_l\left(\frac{\sqrt{E'(E+2m_0c^2)}}{\sqrt{E(E'+2m_0c^2)}}\right)\sigma_{RBEB}(E \to E')$$

Remove forward-scattering component

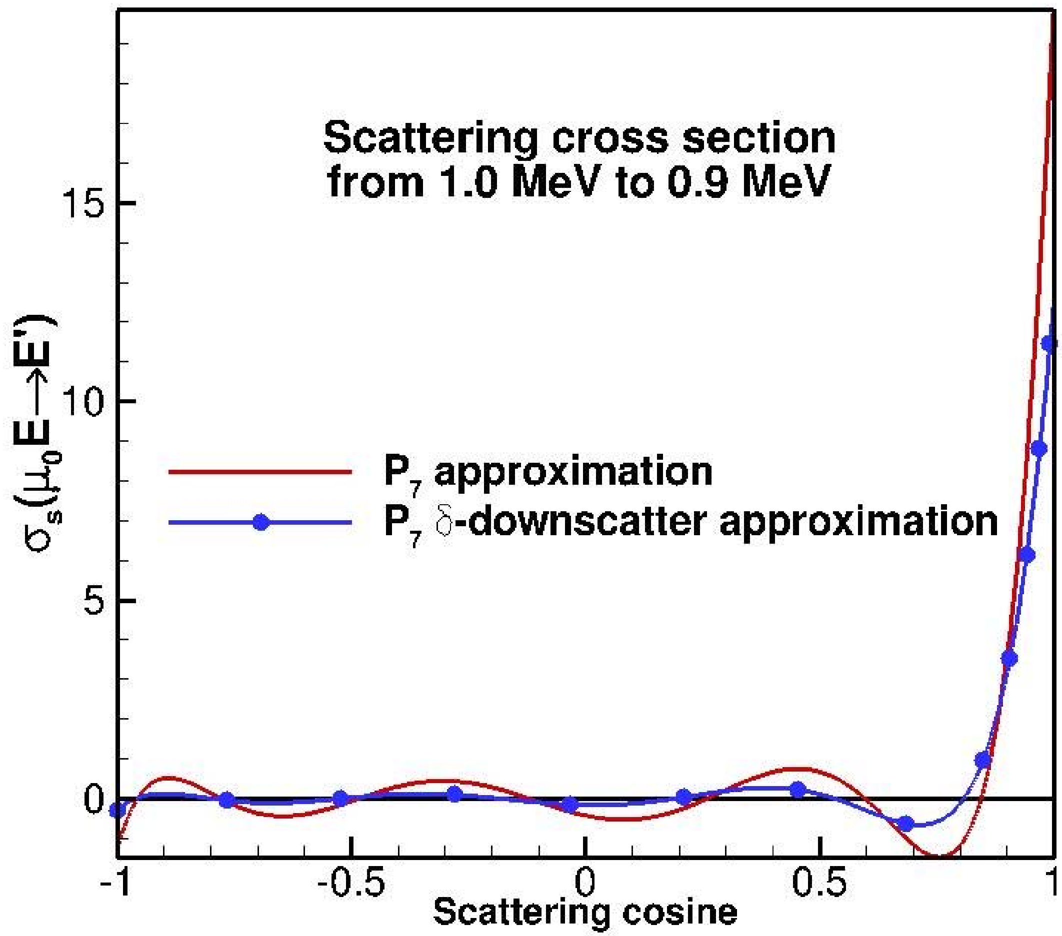
$$\sigma_s(\mu_0, E' \to E) \cong \sum_{l=0}^{L} P_l(\mu_0)\tilde{\sigma}_{s,l}(E' \to E) + \sigma_{s,L+1}(E' \to E)\delta(1-\mu_0)$$

Modified scattering moments

$$\tilde{\sigma}_{s,l}(E' \to E) \equiv \sigma_{s,l}(E' \to E) - \sigma_{s,L+1}(E' \to E)$$

Explicit treatment of forward δ-function down-scatter term reduces scattering anisotropy

- P_7 approximation of the electron scattering cross section from 1 MeV to 0.9 MeV
- Same cross section with δ-down-scatter term removed
  - More smooth
  - Less forward peaked



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"Exact" MMS test using RBEB MG cross sections

- 1-MeV electrons in aluminum/gold slab
- 40 uniformly-spaced energy groups
- CSD/MG-L partition: 20 keV
- S_8 quadrature P_1 scattering

$$\psi_{MMS}(x, \mu, E) = x(1 + \mu)E$$

restricted stopping power

$$Q_{MMS}(x, \mu, E) = (\mu + x\sigma_{t,g})(1 + \mu)E - x(1 + \mu)S_{R,g}$$

$$-xE(\sigma_{0,g} + 3\mu\sigma_{1,g}),\ E \in [E_{g,l}, E_{g,u}]$$

Error metric	L_2 error norm
Absolute	9.85×10^{-11}
Relative	1.97×10^{-10}

“Exact” MMS test using FE-E weighted RBEB cross sections

- 1-MeV electrons in aluminum slab
- 10 logarithmically-spaced energy elements
- CSD/MGL partition: μ_0=0.99
- S_{16} quadrature P_7 scattering

Boundary restricted stopping powers

$$\psi_{MMS}(x,\mu,E) = xE\sum_{n=0}^{7}\mu^n$$

FE weighted restricted stopping power

$$Q_{MMS}(x,\mu,E) = [\mu E + xE\langle\sigma_t\rangle + xE\langle S_R\rangle + xE^u S_R^u - xE^l S_R^l]\sum_{n=0}^{7}\mu^n$$

$$-xE[\tfrac{176}{105}\langle\sigma_{s,0}\rangle + \tfrac{248}{105}\mu\langle\sigma_{s,1}\rangle + (\tfrac{18}{7}\mu^2 - \tfrac{6}{7})\langle\sigma_{s,2}\rangle + (\tfrac{314}{99}\mu^3 - \tfrac{314}{165}\mu)\langle\sigma_{s,3}\rangle$$

$$+(\tfrac{26}{11}\mu^4 - \tfrac{156}{77}\mu^2 + \tfrac{78}{385})\langle\sigma_{s,4}\rangle + (\tfrac{34}{13}\mu^5 - \tfrac{340}{117}\mu^3 + \tfrac{170}{273}\mu)\langle\sigma_{s,5}\rangle$$

$$+(\mu^6 - \tfrac{15}{11}\mu^4 + \tfrac{5}{11}\mu^2 - \tfrac{5}{231})\langle\sigma_{s,6}\rangle + (\mu^7 - \tfrac{21}{13}\mu^5 + \tfrac{105}{143}\mu^3 - \tfrac{35}{429}\mu)\langle\sigma_{s,7}\rangle],\ E\in[E_{g,l},E_{g,u}]$$

Error metric	L_2 error norm
Absolute	$4.28\text{x}10^{-12}$
Relative	$1.02\text{x}10^{-11}$

Inexact MMS test using FE-E weighted cross sections (1)

Define simple scattering kernel

- Large for small energy loss
- Forward peaked for small energy loss

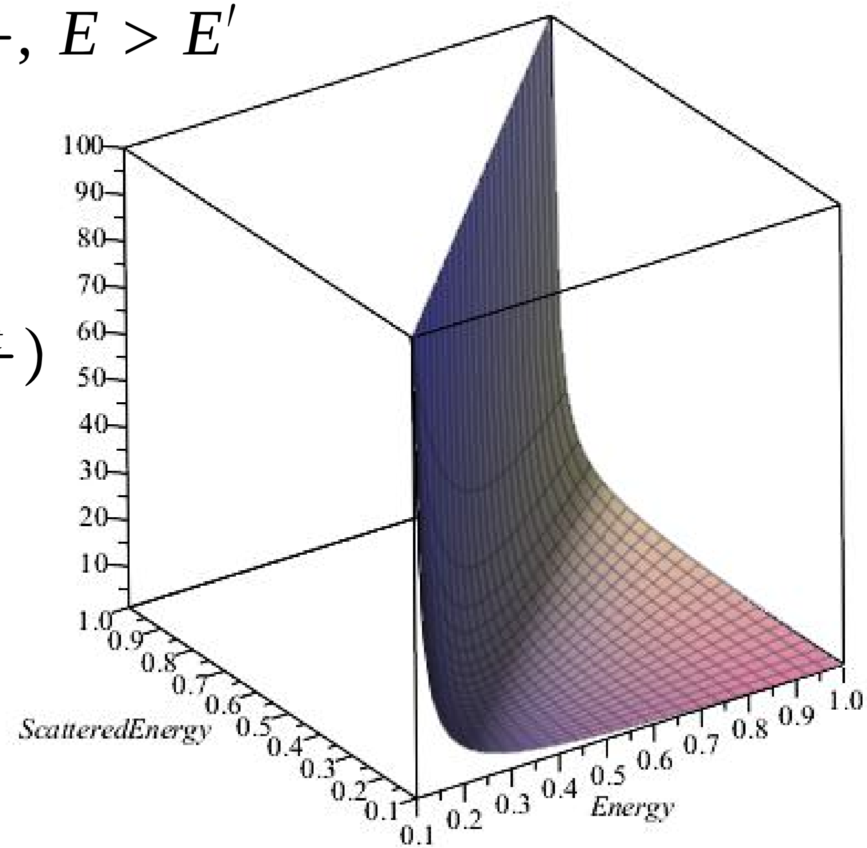
$$\sigma_s(\mu_0, E \rightarrow E') = \frac{\delta[\mu_0 - (1 - E + E')]}{E + \varepsilon - E'}, \; E > E'$$

Total cross section

$$\sigma_t(E) = \int_{E_{cut}}^{E} \frac{dE'}{E + \varepsilon - E'} = \ln\left(\frac{E + \varepsilon - E_{cut}}{\varepsilon}\right)$$

Scattering moments

$$\sigma_s^l(E' \rightarrow E) = \frac{P_l(1 - E' + E)}{E' + \varepsilon - E}$$



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Inexact MMS test using FE-E weighted cross sections (2)

- E_{max}=1.0 MeV, E_{cut} = 20 keV, ε=0.01
- Linearly- or logarithmically-spaced energy elements
- S_8 quadrature P_1 scattering

$$\psi_{MMS}(x,\mu,E) = \frac{x(1+\mu)}{E}$$

$$Q_{MMS}(x,\mu,E) = \ln\left(\frac{E+\varepsilon-E_{cut}}{\varepsilon}\right)\frac{x(1+\mu)}{E}$$

$$\frac{\mu(1+\mu)}{E} - \ln\left[\frac{E}{E_{\max}}\frac{E_{\max}+\varepsilon-E}{\varepsilon}\right]\frac{x}{E-\varepsilon}$$

$$-\frac{x\mu}{E-\varepsilon}\left[(E+1)\ln\left(\frac{E}{E_{\max}}\right)+(1+\varepsilon)\ln\left(\frac{E_{\max}+\varepsilon-E}{\varepsilon}\right)\right]$$

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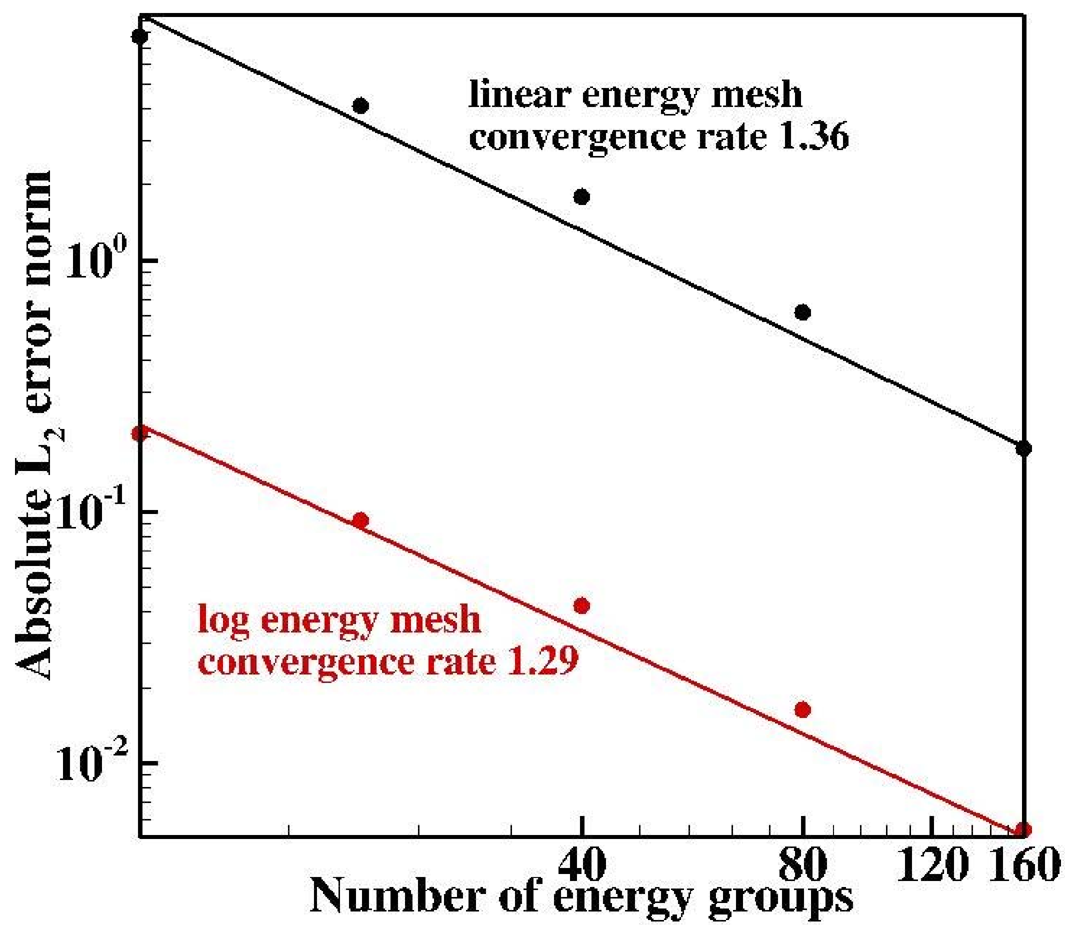
Inexact MMS test using FE-E weighted cross sections (3)

- Exact in space and angle
- Similar convergence rates for linear or logarithmic energy mesh
- Much lower absolute error for logarithmic energy mesh due to steep cross-section energy gradient at low energy
- Convergence rates less than 2.0 expected for DFE-E approximation



Summary and future work

- Generation and application of Finite-Element in Energy (FE-E) weighted scattering cross sections have been presented
- The Relativistic Binary-Encounter-Bethe (RBEB) scattering kernel was used and shown to provide reasonable agreement with measured stopping-power data
- The partition between CSD and MG-L modeling can be arbitrarily defined
  - As a specific scattering energy
  - As a specific scattering angle
- Investigate the relationship between CSD and forward δ-down-scatter terms
  - Both terms reduce energy without direction change
  - Determining the “optimal” partition between CSD and MG-L treatment requires further investigation
- Include additional physics
- Investigate convergence rate with energy-mesh refinement
- Apply FE-E weighted cross section to some multi-dimensional applications