Electron Mode in FRENSIE

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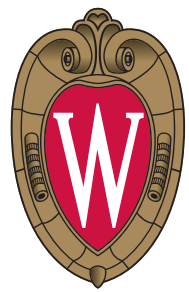

Electron Transport in FRENSIE

Forward Mode

- Condensed History
- Secondary Particles
- Atomic Relaxation
- Simulation of hard electron transport events
  - Atomic excitation
  - Hard elastic scattering
  - Electroionization
  - Bremmstrahlung

Adjoint Mode

- Hybrid Multigroup/Continuous-Energy Monte Carlo using Boltzmann-Fokker-Planck Equation (BFP)

Electron Transport in Monte Carlo Codes

MCNP

- Historically has only used a condensed-history approched with Goudsmit-Saunderson mutiple scattering techniques.
- MCNP6 implemented a single-event method for energies below 1 keV, were the condensed-history method no longer holds.

Penelope

- Implenments a mixed method that simulates soft (condensed-history) events below a cutoff energy/angle and hard (single-events) above.
- Uses Goudsmit-Saunderson Multiple Scattering

EGS

- Condensed History Method
- Historically used Molière Multiple Scattering Theory
- EGS5 implemented Goudsmit-Saunderson Multiple Scattering to take into account spin and relativistic effects needed in the MeV range

Electron Mode

Frensie

- Hard events implemented using cross-sectional data from MCNP6
- Condensed history method will be chosen in conjunction with an adjoint method
- Ultimately hope to implement a mixed method for forward transport

Current Capabilities

- Single Scattering Events from 100 GeV to 10 eV
- Elastic, Bremsstrahlung, Electroionization, Atomic Excitation
- Secondary particles created, but photons not tracked
- Atomic relaxation implemented

Problems

- Absorption at low energies
- Negative energy from Electroionization

Atomic Excitation

Reaction

- There is no angular deflection.
- There are no secondary particles.

Implementation

- Energy dependent electron energy loss are tabulated in ACE tables.
- No sampling is required for this process.

Hard Elastic Scattering

Reaction

- There is no energy loss.
- There are no secondary particles.

Implementation

- ACE tables provide histogram CDF of the outgoing angle cosine, μ, for $14 - 16$ energy groups.
- for $\mu > 0.999999$ an analytical function, $f(\mu)$, derived from Molière's screening factor is used to compute the scattering angle

$$f(\mu) = \frac{A}{(\eta + 1 - \mu)^2}$$

$$\eta(E, Z) = \frac{1}{4}\left(\frac{\alpha mc}{0.885p}\right)^2 Z^{2/3}[1.13 + 3.76(\alpha Z/\beta)^2]$$

Electroionization

Reaction

- The subshell is directly sampled.
- A knock-on electron is ejected.
- The incident electron energy is reduced by the $E_{knock} + E_{binding}$.

Implementation

- ACE tables provide CDF of the knock-on energy, E_{knock}, based on the incident electron energy.
- Conservation of momentum is used to find the scattering and ejection angles (which are sampled independently).
- The shell vacancy is handled using atomic relaxation data.

Electroionization Scattering Angle

Conservation of Momentum

$$(p_{knock}c + p_a c)^2 = (pc)^2 + (p'c)^2 - 2pp'cos(\theta)$$

$$cos(\theta) = \frac{(pc)^2 + (p'c)^2 - (p_{knock}c)^2}{2pp'}$$

Conservation of Energy

$$(T + m_e c^2) + (M_a c^2) = (T' + m_e c^2) + (T_a + M_a c^2 + T_{knock} + m_e c^2) + E_{Binding}$$

Assume the binding energy is negligible

$$T = T' + T_{knock}$$

Solving you obtain:

$$cos(\theta) = \frac{T'}{T}\frac{p}{p'} \quad \text{and} \quad cos(\phi) = \frac{T_{knock}}{T}\frac{p}{p_{knock}}$$

Sampling Electroionization

The original sampling routine implemented in FRENSIE differed slightly from MCNP6 which caused the sampling of negative electrons energies.

- ACE tables provide CDF of the knock-on energy, E_{knock}, based on the incident electron energy.
- The original implementation randomly selected whether to sample the upper or lower energy bin.
- A correlated sample must be made to avoid non physical values.

Bremmstrahlung

Reaction

- A photon is ejected.
- ACE tables provide CDF of the photon energy, E_γ, based on the incident electron energy.
- The incident electron energy is reduced by the E_γ.
- The electron direction is assumed to be essentially unchanged.

Implementation

- An analytical dipole function, $p(\mu)$, is used to sample the direction of the outgoing photon.
- MCNP6 also uses a table based scheme from their condensed history method.

$$p(\mu)d\mu = \frac{(1-\beta^2)}{2(1-\beta\mu)^2}d\mu$$

Known Problems

Absorption at low energies

- At energies near the cutoff (10 eV) the reaction cross section is dominated by elastic scattering (by order 10^7 for H)
- It is unlikely the electron will scatter below the cutoff energy
- A temporary fix is to raise the cutoff energy (to 15eV for H) to prevent indefinite elastic scattering
- MCNP notes this problem and suggests a minimum cutoff energy of 20eV

Adjoint Mode Outline

Hybrid Multigroup/Continuous-Energy BFP

- Advantages
- Boltzmann-Fokker-Planck Equation (BFP)
- Modifications to BFB
- Solution to Modified BFG
- Monte Carlo Method
- Adjoint
- Other Possible Adjoint Methods

Advantaged

- The same basic multigroup cross-section data can be used for forward and adjoint calculations.
- The adjoint transport model is nearly identical to the forward making implementation easy
- The transport equation is generalized for Monte Carlo transport of neutral and charged particles.
  They implement for electrons and photons.

Boltzmann-Fokker-Planck Equation

$$\Omega \cdot \nabla \psi + \sigma_t \psi = \int_0^{\infty} \int_0^{2\pi} \int_{-1}^{+1} \sigma_s(E' \to E, \mu_0) \times \psi(\mu', \phi', E') d\mu' d\phi' dE' + \frac{\alpha}{2} \left\{ \frac{\partial}{\partial \mu} \left[(1-\mu^2) \frac{\partial \psi}{\partial \mu} \right] + \frac{1}{1-\mu^2} \frac{\partial^2 \psi}{\partial \phi^2} \right\} + \frac{\partial}{\partial E}[S\psi] + Q$$

- The Boltzmann Operator treats the large-angled or "smooth" component of the cross-section
- The Fokker-Planck Opertor treats the forward-peaked or "singular" component of the cross-section

Fokker-Planck Operators

Continuous-Scattering Operator

$$F_\alpha \psi = \frac{\alpha}{2}\left\{\frac{\partial}{\partial \mu}\left[(1-\mu^2)\frac{\partial \psi}{\partial \mu}\right] + \frac{1}{1-\mu^2}\frac{\partial^2 \psi}{\partial \phi^2}\right\}$$

- Constructed so the mean change in angle cosine per path length is equal to the restricted momentum transfer

$$\Delta\mu/\text{path length} = \text{restricted momentum transfer}$$

Continuous-Slowing Down Operator

$$\frac{\partial}{\partial E}[S\psi]$$

- Constructed so the mean change in energy per path length is equal to the restricted stopping power

$$\Delta E/\text{path length} = \text{restricted stopping power}$$

Approximate Angular Fokker-Planck Operator

Let:

$$\lim_{\mu_s \to 1} B_\alpha \psi = F_\alpha \psi$$

Where:

$$B_\alpha \psi = \int_0^{2\pi} \int_{-1}^{+1} \sigma_a(E, \mu_0) \psi(\mu', \phi', E) d\mu' d\phi' - \sigma_a \psi$$

- Eigenvalues are equal at limit
- High-order eigenvalues become more approximate and are underestimated
- Error for higher order flux moments can be ignored if they are large compared to temporal and spatial scale lengths
- Holds for condensed history where the scale lengths are large compared to mfp

Legendre Cross-Section Expansion

Expand the cross-sections using Legendre polynomials

$$\hat{\sigma}_s(E' \to E, \mu_o) = \sum_{l=0}^{L} \frac{2l+1}{4\pi} \sigma_s^{(l)}(E' \to E) P_l(\mu_o)$$

Where:

$$\sigma_s^{(l)}(E' \to E) = 2\pi \int_{-1}^{+1} \sigma_s(E' \to E), \mu_o) P_l(\mu_o) d\mu_o$$

Hybrid Multigroup/Continuous-Energy Approximation

- Break energy up into N groups such that for group g:

$$E_{g+1/2} < E < E_{g-1/2}$$

- Radau quadratures are used to get the weighted least-squares fits in energy for:
  - The Smooth Component Cross-Sections (σ)
  - The Restricted Momentum Transfers (α)
  - The Restricted Stopping Power (S)

Replace the parameter, f with $\tilde{f}$

$$\tilde{f}(E) = \sum_{g=1}^{N} f_g B_g(E) \quad \text{Where} \quad B_g(E) = \begin{cases} 1 & E \in (E_{g+1/2}, E_{g-1/2}) \\ 0 & \textit{Otherwise} \end{cases}$$

f_g is the weighted group average of $f(E)$ using Radau quadratures

Multigroup/Continuous Energy BFP Equation

$$\Omega \cdot \nabla \psi + \tilde{\sigma}_t \psi = \int_E^{E_{1/2}} \int_0^{2\pi} \int_{-1}^{+1} \tilde{\sigma}_s(E' \to E, \mu_0) \psi(\mu', \phi', E') d\mu' d\phi' dE' + \int_0^{2\pi} \int_{-1}^{+1} \tilde{\sigma}_\alpha(\mu_o) \psi(\mu', \phi') d\mu' d\phi' - \tilde{\sigma}_\alpha(\mu_o) \psi + \frac{\partial}{\partial E}[\tilde{S}\psi] + Q$$

- The Boltzmann Operator reduces to Standard Multigroup method.
- Exponential distribution of path lengths (compared fixed path length for condensed history).
- Accuracy depends on: # of groups, Order of Legendre expansion, μ_s

Collision Algorithm: Location and Energy

Let E_p be the energy of a particle in group g

- The total group cross-section is the sum of the smooth-component Boltzmann and continuous-scattering cross-sections:

$$\sigma_g^{total} = \sigma_{t,g} + \sigma_{\alpha,g} \quad \text{Where} \quad \sigma_{\alpha,g} = \frac{\alpha}{1-\mu_s}$$

- σ_g^{total} is used to find the distance to next collision, D_c
- D_c is compared to the distance to material, D_m, and distance to energy, $D_e = \frac{E_p - E_{g+1/2}}{S_g}$
- The new energy is:

$$E_p^{new} = E_p^{old} - S_g D_c$$

Collision Algorithm: Reaction

Can either have a smooth-component Boltzmann or continuous-scattering reaction with probabilities:

$$P_B = \frac{\sigma_{t,g}}{\sigma_g^{total}} \quad \text{and} \quad P_\alpha = \frac{\sigma_{\alpha,g}}{\sigma_g^{total}}$$

- If P_α is selected a new direction for the particle is randomly sampled based on a polar scattering angle with cosine equal to μ_s.
- If P_B is selected the particle is removed and M new particle are generated at the collision site.
- Multiplication Factor

$$M = \frac{1}{\sigma_g^{total}} \int_{E_{g+1/2}}^{E_{g-1/2}} \sigma_s^{(0)}(E' \rightarrow E) dE' = \frac{1}{\sigma_{t,g}} \sum_{k=g}^{N} \sigma_{s,g\rightarrow k}^{(0)}$$

Collision Algorithm: Reaction (Continued)

Average M must be preserved

- Let $M = \text{Integer} + \text{Remainder} = I + R$
- Create I or $I + 1$ particles with probability $1.0 - R$ or R.

Energy

- Particles generated in group g has an energy range of $E_{g+1/2} < E < E_{g-1/2}$
- Randomly sample energy from a uniform distribution.

Angle

- Sample angle based on the discrete Radau distributions.
- Separate Radau distribution for each smooth-component Boltzmann group-to-group transfer.

Adjoint Multigroup/Continuous Energy BFP Equation

$$-\Omega \cdot \nabla \psi^{\dagger} + \tilde{\sigma}_t \psi^{\dagger} =$$
$$\int_{E_{N+1/2}}^{E} \int_0^{2\pi} \int_{-1}^{+1} \tilde{\sigma}_s(E \to E', \mu_0) \psi^{\dagger}(\mathbf{r}, \mu', \phi', E') d\mu' d\phi' d$$
$$+ \int_0^{2\pi} \int_{-1}^{+1} \tilde{\sigma}_\alpha(\mu_o) \psi^{\dagger}(\mu', \phi') d\mu' d\phi' - \tilde{\sigma}_\alpha(\mu_o) \psi^{\dagger}$$
$$- \frac{\partial}{\partial E}[\tilde{S} \psi^{\dagger}] + \frac{\partial S}{\partial E} \psi^{\dagger} + Q^{\dagger}$$

- Let the dot product be:

$$[f, h] = \sum_{g=1}^{N} f_g h_g \frac{1}{\Delta E_g}$$

- The adjoint cross-section is then:

$$\sigma_{s,k \to g}^{\dagger(l)} = \sigma_{s,g \to k}^{(l)} \frac{\Delta E_g}{\Delta E_k}$$

Other Possible Adjoint Methods

- 1980 - Adjoint Electron Transport in the CSDA
  - Goudsmit and Saunderson Scattering
- 1995 - Adjoint Elecrton-Photon Tansport using BFS in ITS
  - Multigroup/Continuous Energy
- 1996 - Adjoint Multigroup/Continuous Energy BFP Equation
- 2005 - Generalized Particle for Couple Adjoint γ - e^- - e^+ Transport
  - CSDA using Molière's multiple scattering