Review of Summer at Sandia National Lab

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Outline

- Interaction at Sandia
- Condensed History's History
- Moment Preserving Method
- Adjoint Analog Transport

Sandia

Condensed History Electron Transport

Challenges

- Electron charge increases scattering cross section
- Neutral Particles may scatter a couple dozen times over a distance
- Electrons may scatter 10,000 or more times over the same distance
- Purely analog transport is impractical at higher energies
- Approximations must be made to reduce computation costs
- Monte Carlo development lags behind

A Condensed Random Walk method was developed

- Electrons are moved a set step length
- A multiply scattering theory is sampled to find the outgoing direction
- The Continuous Slowing Down Approximation (CSDA) is used to calculate energy loss
- Production of secondary are averaged
- Approximations dont hold below 1 keV

Condensed History Step

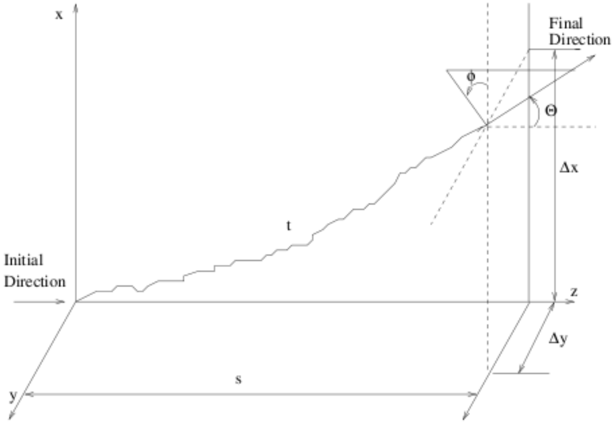


Figure : Schematic of electron transport mechanics model in EGS. Where s is the step length, t the total distance traveled, Δx and Δy are the lateral displacements, Θ and ϕ are the final polar and azimuthal angles.

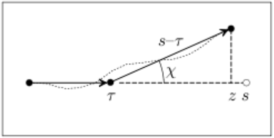
Improvements to Condensed History

Improving Transport Mechanics

- Random Hinge transport
- Modified Random Hinge transport
- More accurate Transport near boundaries

Mixed Analog/Condensed Simulation

- Hard events involving large angle scattering, secondary particles, and catastrophic interactions are analog
- Soft events involving small angle scattering are condensed
- Majority of electron cross section is due to soft elastic scattering
- Below 1 keV simulation becomes purely analog



Moment Preserving Method (MP)

Advantages

- Legendre moments of the cross section are preserved
  - mfps are reduced, increasing efficiency
  - Less forward peaked angular scattering distribution
  - Accuracy can be maintained by preserving some of the low-order moments
- Simplified physics that reflect the analog process are used
- Implementation simpler than Condensed History
- Distribution is no longer continuous but discrete

Reduced Order Physics (ROP)

The Boltzmann Collision Operator Approximated Using ROP

- Integral form maintained
- Keeps correct transport mechanics
- Allows single-event simulations

The analog cross section, Σ, is replaced with a ROP cross section, $\tilde{\Sigma}$

$\tilde{\Sigma}$ preserves a finite number of moments of the analog cross section

$$\Sigma_{el,l} = 2\pi \int_{-1}^{1} P_l(\mu) \Sigma_{el}(\mu) d\mu$$

$$\tilde{\Sigma}_{el,l} = \Sigma_{el,l} \text{ for } l = 1, 2, ..., L$$

ROP Elastic Cross Section

MP Method Only

$$\tilde{\Sigma}(E,\mu) = \sum_{n=1}^{N} \frac{\alpha_n(E)}{2\pi}\delta[\mu - \zeta_n] + \frac{\alpha N + 1(E)}{2\pi}\delta[\mu - 1]$$

- Where α_n and ζ_n are the weights and nodes of the Radau quadrature
- The $\zeta_{N+1} = 1$ node and weight are eliminated

Hybrid Method

$$\tilde{\Sigma}(E,\mu) = \Sigma^{Analog}(E,\mu) + \sum_{n=1}^{N} \frac{\alpha_n(E)}{2\pi}\delta[\mu - \zeta_n]$$

- Below a cutoff, $\mu*$, analog transport is used
- Where $\Sigma^{Analog}(E,\mu)$ is the analog cross section for $\mu \in [-1, \mu*)$
- Only have discrete angles above $\mu*$

Adjoint Transport

Adjoint Collision Kernel

$$C^{\dagger}(\mathbf{r'}, E' \rightarrow E, \mathbf{\Omega'} \rightarrow \mathbf{\Omega}) = \sum_{A} p_A^{\dagger}(\mathbf{r'}, E') \sum_{j} p_{j,A}^{\dagger}(E') \frac{\sigma_{j,A}(E) c_{j,A}(E) f_{j,A}(E \rightarrow E', \mathbf{\Omega} \rightarrow \mathbf{\Omega'})}{\sigma_{j,A}^{\dagger}(E')} \quad (1)$$

$$\sigma_{j,A}^{\dagger}(E') = \int \sigma_{j,A}(E) c_{j,A}(E) f_{j,A}(E \rightarrow E') dE \quad (2)$$

$$p_A^{\dagger}(\mathbf{r'}, E') = \frac{\Sigma_A^{\dagger}(\mathbf{r'}, E')}{\Sigma^{\dagger}(\mathbf{r'}, E')} \qquad p_{j,A}^{\dagger}(E') = \frac{\sigma_{j,A}^{\dagger}(E')}{\sigma_A^{\dagger}(E')}$$

Adjoint Transport

First the type of nuclide that the electron interacts with is sampled from:

$$p_A^\dagger(\mathbf{r'}, E') = \frac{\Sigma_A^\dagger(\mathbf{r'}, E')}{\Sigma\dagger(\mathbf{r'}, E')} \tag{3}$$

Then the reaction type is sampled from:

$$p_{j,A}^\dagger(E') = \frac{\sigma_{j,A}^\dagger(E')}{\sigma_A^\dagger(E')}$$

Finally, E and Ω are sampled from:

$$f_{j,A}^\dagger(E' \to E, \mathbf{\Omega'} \to \mathbf{\Omega}) = \frac{\sigma_{j,A}(E) c_{j,A}(E) f_{j,A}(E \to E', \mathbf{\Omega} \to \mathbf{\Omega'})}{\sigma_{j,A}^\dagger(E')}$$

Adjoint Cross-Sections

Electrons reactions are not specifically dependent on the incoming and outgoing angle, but instead on μ. Therefore the equations reduced to:

$$\sigma^{\dagger}(E') = \int \int \sigma(E)c(E)f(E \rightarrow E', \mu)dEd\mu \tag{4}$$

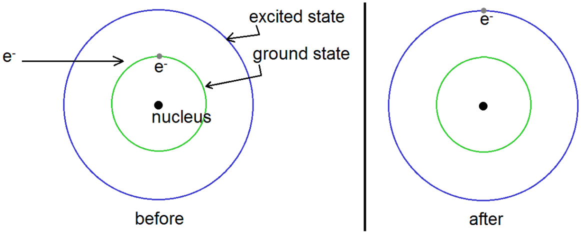
$$f^{\dagger}(E' \rightarrow E, \mu) = \frac{\sigma(E)c(E)f(E \rightarrow E', \mu)}{\sigma^{\dagger}(E')} \tag{5}$$

$$\sigma^{\dagger}(E' \rightarrow E, \mu) = \sigma(E \rightarrow E', \mu) \tag{6}$$

Atomic Excitation

An incident electron loses some energy by exciting an outer electron to higher energy states

- There is no angular deflection (interaction is considered distant)
- There are no secondary particles
- Energy loss to incident electron



Atomic Excitation

- Their is no angular deflection
- Cross-sections are independent of angle
- Each incoming energy will scatter into a unique outgoing energy
- There is a one-to-one correspondence between the incoming and outgoing energy

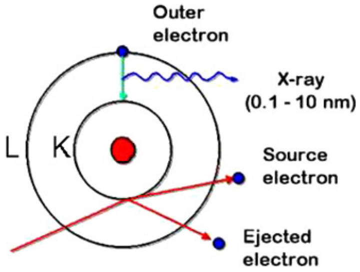
$$\begin{aligned} \sigma^{\dagger}(E' \to E, \mu) =& \sigma(E \to E', \mu) = \\ \sigma^{\dagger}(E') =& \sigma(E) \end{aligned} \tag{7}$$

$$f^{\dagger}(E', \mu) = \frac{\sigma(E) f(E, \mu)}{\sigma^{\dagger}(E')} = f(E, \mu) \tag{8}$$

Electroionization

An incident electron scatters off an atom, ionizing an electron from one of its subshells

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



Electroionization

- A second electron is produced
- There is a unique angle for each $E \rightarrow E'$ pair

$$p(E \rightarrow E', \mu) = f(E \rightarrow E') \tag{9}$$

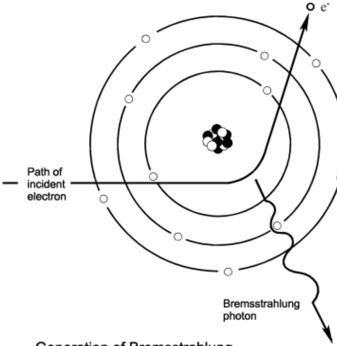
$$\sigma^\dagger(E') = \int \sigma(E) f(E \rightarrow E') dE \tag{10}$$

$$f^\dagger(E' \rightarrow E, \mu) = \frac{\sigma(E) f(E \rightarrow E')}{\sigma^\dagger(E')} \tag{11}$$

Bremsstrahlung

An incident electron interacts with an atom releasing electromagnetic radiation

- A photon is ejected
- Incident electron energy is reduced by E_{γ}
- The incident electron energy is reduced by $E_{Knock} + E_{Binding}$



Generation of Bremsstrahlung

Bremsstrahlung

- Angular deflection is assumed to be negligible
- Cross-sections are independent of angle

$$\begin{aligned}\sigma^\dagger(E' \to E, \mu) =& \sigma(E \to E', \mu) = \\ \sigma^\dagger(E' \to E) =& \sigma(E \to E') = \sigma(E) f(E \to E')\end{aligned} \tag{12}$$

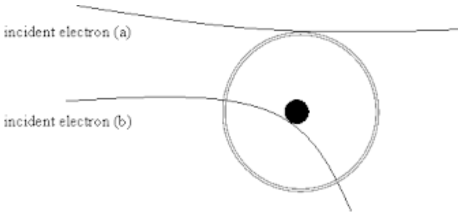
$$\sigma^\dagger(E') = \int \sigma(E) f(E \to E') dE \tag{13}$$

$$f^\dagger(E' \to E) = \frac{\sigma(E) f(E \to E')}{\sigma^\dagger(E')} \tag{14}$$

Elastic Scattering

An incident electron scatters off a nucleus retaining its energy

- Energy loss is assumed to be negligible
- There are no secondary particles
- Angular deflection occurs



Elastic Scattering

- Their is no energy loss ($E = E'$)
- Adjoint and Forward transport will be exactly the same

$$\begin{aligned}\sigma^{\dagger}(E' \rightarrow E, \mu) =& \sigma(E \rightarrow E', \mu) = \\ \sigma^{\dagger}(E, \mu) =& \sigma(E, \mu)\end{aligned} \tag{15}$$

Therefore equations (6) and (7) reduce to:

$$\sigma^{\dagger}(E') = \sigma(E) \tag{16}$$

$$f^{\dagger}(E, \mu) = f(E, \mu) \tag{17}$$