Electron Mode in FRENSIE

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Single-Event Adjoint Electron Transport

Goals

- Transform forward electron data to adjoint
- Use single-event ACE data in transformation
- Output usable adjoint single-event electron cross-sections and PDF's

Forward Transport

Time-Independent Boltzmann Equation

$$\Omega\nabla\phi(\mathbf{r},E,\mathbf{\Omega})+\Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E,\mathbf{\Omega})= \int\int\Sigma_t(\mathbf{r},E')C(\mathbf{r},E'\to E,\mathbf{\Omega'}\to\mathbf{\Omega})\phi(\mathbf{r},E',\mathbf{\Omega'})dE'd\Omega'+S(\mathbf{r},E,\mathbf{\Omega}) \quad (1)$$

Collision Kernel

$$C(\mathbf{r},E'\to E,\mathbf{\Omega'}\to\mathbf{\Omega})= \sum_A p_A(\mathbf{r},E')\sum_j p_{j,A}(E')c_{j,A}(E')f_{j,A}(E'\to E,\mathbf{\Omega'}\to\mathbf{\Omega}) \quad (2)$$

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

Adjoint Transport

Adjoint Collision Kernel

$$C^\dagger(\mathbf{r'}, E' \rightarrow E, \boldsymbol{\Omega'} \rightarrow \boldsymbol{\Omega}) = \sum_A p_A^\dagger(\mathbf{r'}, E') \sum_j p_{j,A}^\dagger(E') \frac{\sigma_{j,A}(E) c_{j,A}(E) f_{j,A}(E \rightarrow E', \boldsymbol{\Omega} \rightarrow \boldsymbol{\Omega'})}{\sigma_{j,A}^\dagger(E')} \quad (3)$$

$$\sigma_{j,A}^\dagger(E') = \int \sigma_{j,A}(E) c_{j,A}(E) f_{j,A}(E \rightarrow E') dE \quad (4)$$

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

Adjoint Transport

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

$$p_A^\dagger(\mathbf{r'}, E') = \frac{\Sigma_A^\dagger(\mathbf{r'}, E')}{\Sigma\dagger(\mathbf{r'}, E')} \tag{5}$$

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:

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

Adjoint Cross-Sections

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

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

$$f^{\dagger}(E' \rightarrow E, \mu) = \frac{\sigma(E)c(E)f(E \rightarrow E', \mu)}{\sigma^{\dagger}(E')} \tag{7}$$

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

Elastic Scattering

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

$$\begin{aligned} \sigma^\dagger(E' \rightarrow E, \mu) =& \sigma(E \rightarrow E', \mu) = \\ \sigma^\dagger(E, \mu) =& \sigma(E, \mu) \end{aligned} \tag{9}$$

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

$$\sigma^\dagger(E') = \sigma(E) \tag{10}$$

$$f^\dagger(E, \mu) = f(E, \mu) \tag{11}$$

Elastic Scattering

Implementation in FRENSIE

- Add the ability to take an adjoint particle to the forward class
- Add a scatter electron function

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

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

$$f^{\dagger}(E', \mu) = \frac{\sigma(E) f(E, \mu)}{\sigma^{\dagger}(E')} = f(E, \mu) \tag{13}$$

Atomic Excitation

Implementation in FRENSIE

- Create energy dependent electron energy gain data tables
  - Replace the incoming energy with the outgoing energy in the ACE energy loss tables
  - Use interpolation to create a more uniform energy bin structure
- Create Adjoint Atomic Excitation class similar to forward case

Bremsstrahlung

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

$$\begin{aligned}\sigma^\dagger(E' \to E, \mu) =&\sigma(E \to E', \mu) = \\ \sigma^\dagger(E' \to E) =&\sigma(E \to E') = \sigma(E) f(E \to E')\end{aligned} \tag{14}$$

$$\sigma^\dagger(E') = \int \sigma(E) f(E \to E') dE \tag{15}$$

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

Bremsstrahlung

Implementation in FRENSIE

- Create 2D electron energy gain pdf data tables
  - Numerically integrate the cross section for a given energy loss over all incident energies
  - Use interpolation to create a energy bin structure
  - Create a pdf for each outgoing energy bin
- Create new adjoint Bremsstrahlung class

Electroionization

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

$$p(E \to E', \mu) = f(E \to E') \tag{17}$$

$$\sigma^{\dagger}(E') = \int \sigma(E) f(E \to E') dE \tag{18}$$

$$f^{\dagger}(E' \to E, \mu) = \frac{\sigma(E) f(E \to E')}{\sigma^{\dagger}(E')} \tag{19}$$

Braking Down the Adjoint Electroionization Cross-Section

- The adjoint cross-section can be broken into two parts corresponding to the primary and secondary particle
- The primary particle has a energy range: $E/2 \leq E' \leq E$
- The secondary particle has a energy range: $E_{min} \leq E' \leq E/2$

$$\begin{aligned} \sigma^{\dagger}(E') =& \sigma^{\dagger}_{prim}(E') + \sigma^{\dagger}_{sec}(E') \\ =& \int \sigma(E)\Big(f_{prim}(E \rightarrow E') + f_{sec}(E \rightarrow E')\Big)dE \end{aligned} \tag{20}$$

Electroionization

Implementation in FRENSIE

- Create 2D electron energy gain pdf data tables
  - Numerically integrate the cross section for a given outgoing electron energy over all incident electron energies
  - Use interpolation to create a energy bin structure
  - Create a pdf for each knock-on energy bin
- Create new adjoint Electroionization template class