Update: Electron Mode in FRENSIE

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Outline

Hybrid Multigroup/Continuous-Energy Monte Carlo using Boltzmann-Fokker-Planck

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

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

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

- 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

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

Where:

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

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 $\tilde{f}$

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

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

Multigroup/Continuous Energy BFP Equation

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

- 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

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

- 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:

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