### 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
- 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

$$F_{lpha}\psi=rac{lpha}{2}\Big\{rac{\partial}{\partial\mu}\Big[(1-\mu^2)rac{\partial\psi}{\partial\mu}\Big]+rac{1}{1-\mu^2}rac{\partial^2\psi}{\partial\phi^2}\Big\}$$

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

 $\Delta\mu/{
m path}$  length = 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

$$\Delta E$$
/path length = 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:

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

## 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 ( $\sigma$ )

The Restricted Momentum Transfers ( $\alpha$ )

The Restricted Stopping Power (S)

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

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

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

# Multigroup/Continuous Energy BFP Equation



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

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

# 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:

$$\sigma_{g}^{total} = \sigma_{t,g} + \sigma_{\alpha,g}$$
 Where  $\sigma_{\alpha,g} = \frac{\alpha}{1 - \mu_{s}}$ 

- $\sigma_g^{total}$  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,  $D_e=rac{E_p-E_{g+1/2}}{S_\sigma}$
- 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:

$$P_B = rac{\sigma_{t,g}}{\sigma_g^{total}}$$
 and  $P_{lpha} = rac{\sigma_{lpha,g}}{\sigma_g^{total}}$ 

- If  $P_{\alpha}$  is selected a new direction for the particle is randomly sampled based on a polar scattering angle with cosine equal to  $\mu_s$ .
- If  $P_B$  is selected the particle is removed and M new particle are generated at the collision site.
- Multiplication Factor

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

# Collision Algorithm: Reaction (Continued)



#### Average M must be preserved

- Let M = Integer + 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

• 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:

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

## Other Possible Adjoint Methods



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