

# **Adjoint Discrete Scattering Models for Electron Dose Calculations**

**Thomas Quirk  
Sandia National Laboratories\***

**Sandia Student Symposium 2006  
Albuquerque, NM  
August 1, 2006**



# Overview

---

- Radiation Transport
- GBFP Method
  - Discrete Model
- Forward Transport
- Adjoint Transport
- Weight Correction
- Results



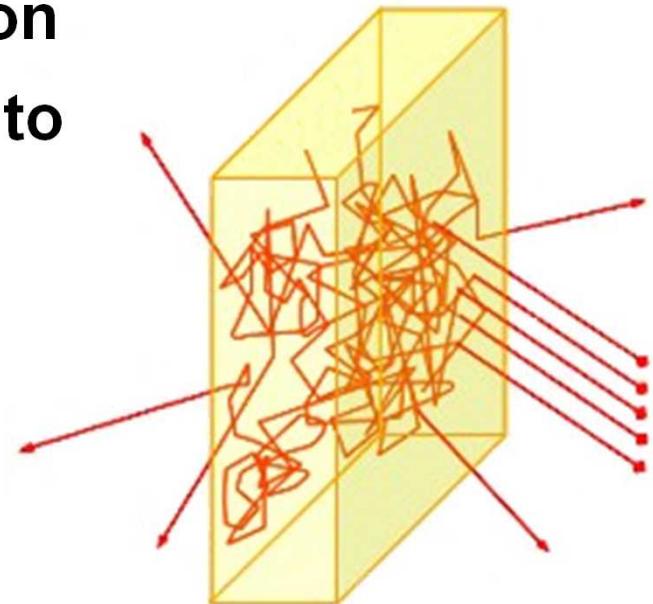


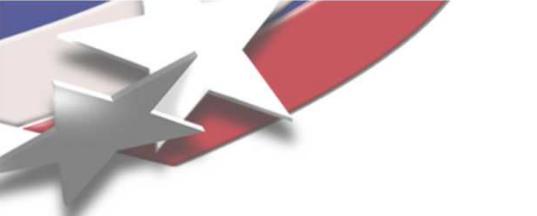
# Monte Carlo Method

---

For either adjoint or forward calculations:

1. Sample a distance to interaction
2. Sample an isotope with which to interact
3. Sample type of interaction
4. Sample result of interaction
5. Adjust Particle/Tally Statistics
6. Repeat upon survival

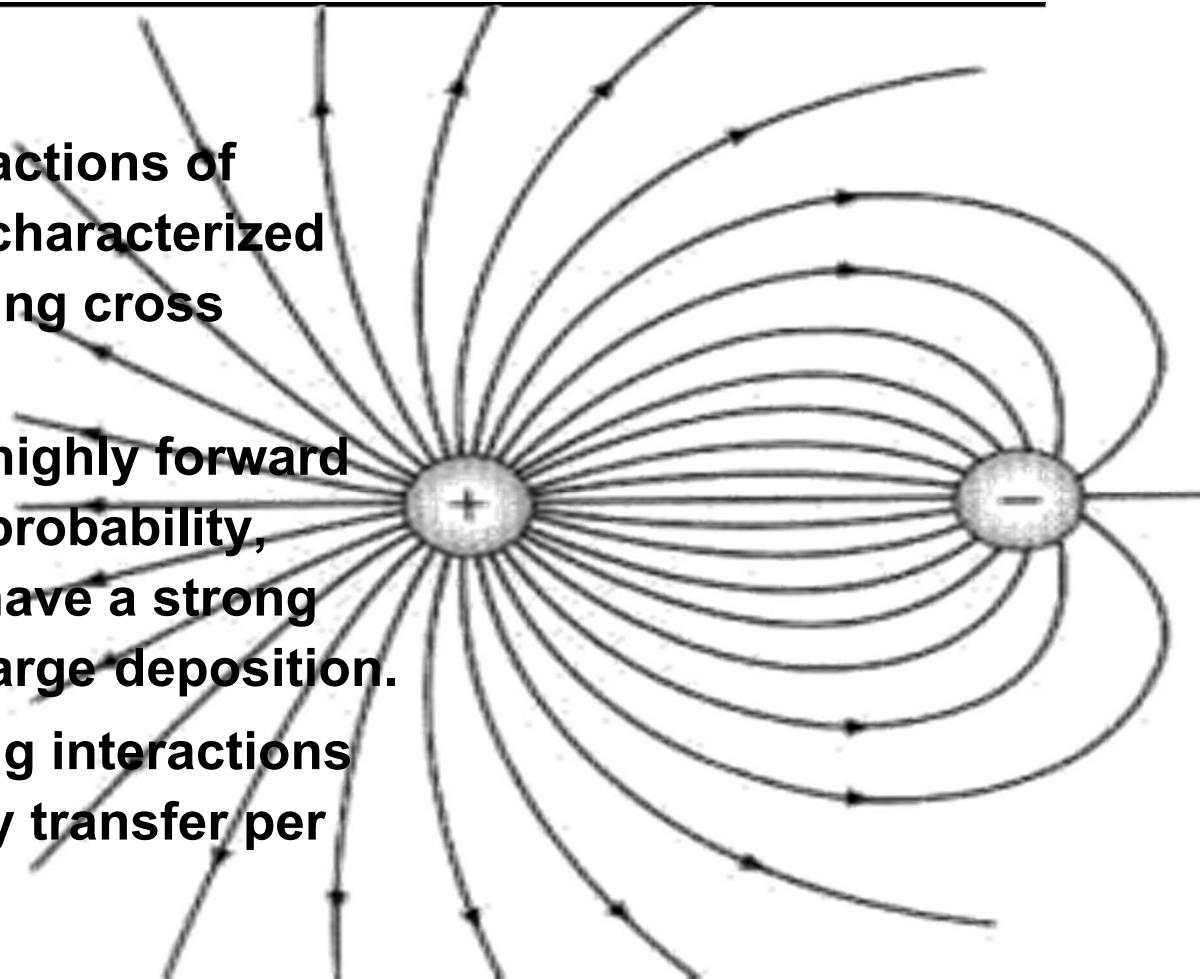




# Electron Transport

---

- The non-binary interactions of charged particles is characterized by large total scattering cross sections.
- Elastic scattering is highly forward peaked, but the low-probability, high-angle scatters have a strong impact on energy/charge deposition.
- Small-angle scattering interactions result in small energy transfer per interaction.



# Forward Radiation Transport

---

**Forward Linear Boltzmann Transport Equation:**

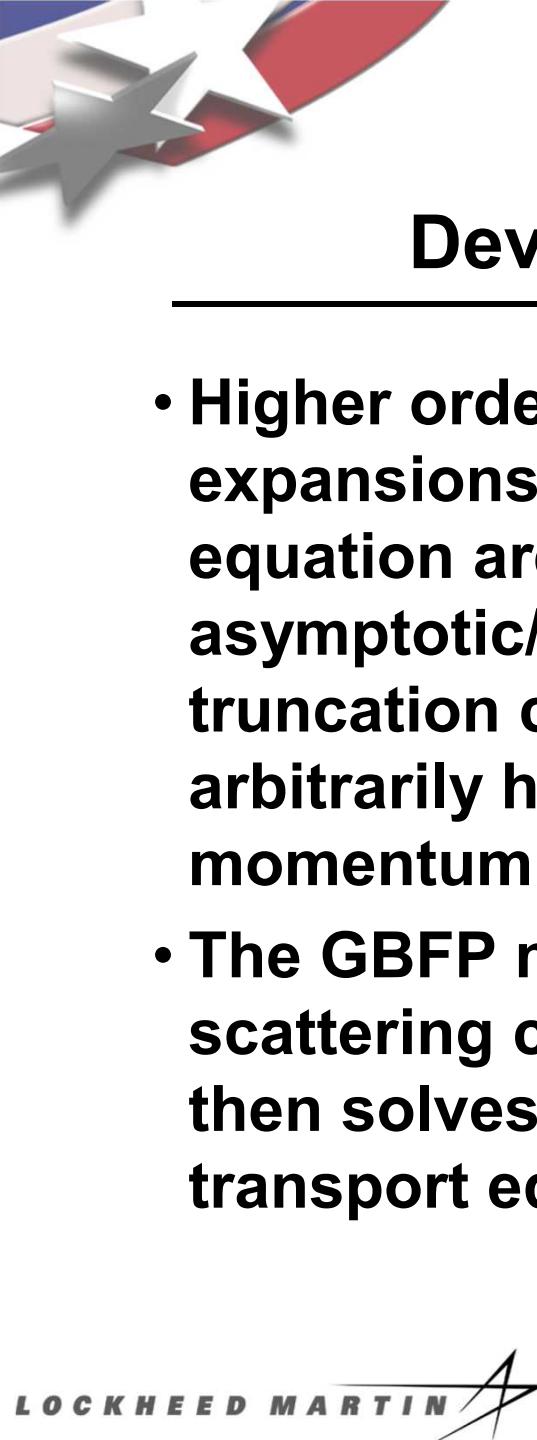
$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, E) + [\sigma_{s,el}(\vec{r}, E) + \sigma_{s,in}(\vec{r}, E)] \psi(\vec{r}, \vec{\Omega}, E) = \\ \int_{4\pi} \sigma_{s,el}(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}', E) \psi(\vec{r}, \vec{\Omega}', E) d\vec{\Omega}' + \int_0^\infty \sigma_{s,in}(\vec{r}, \vec{\Omega}, E' \rightarrow E) \psi(\vec{r}, \vec{\Omega}, E') dE'$$

Lewis theory suggests a direct correlation between preserving moments of the differential cross section (DCS) and the accuracy of the model as measured by space-angle moments of the infinite medium solution



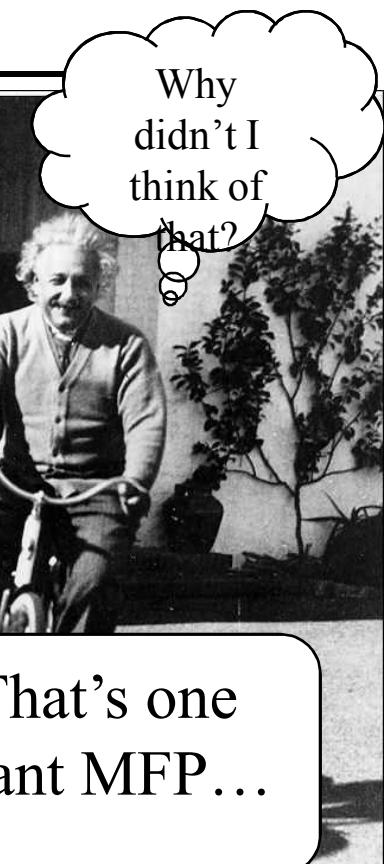
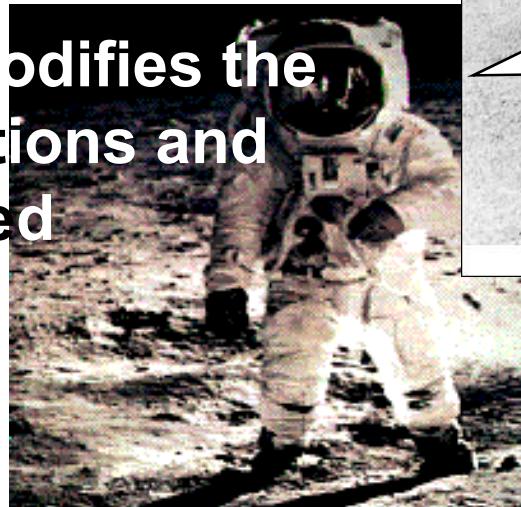
**Momentum-Transfer Moments:**

$$\sigma_n = 2\pi \int_{-1}^1 d\mu_0 (1-\mu)^n \sigma_s(\vec{r}, \mu_0, E)$$



# Development of Forward GBFP

- Higher order Fokker-Planck expansions of the transport equation are asymptotic/unstable. No finite truncation can preserve arbitrarily higher-order momentum transfer moments.
- The GBFP method modifies the scattering cross sections and then solves a modified transport equation.



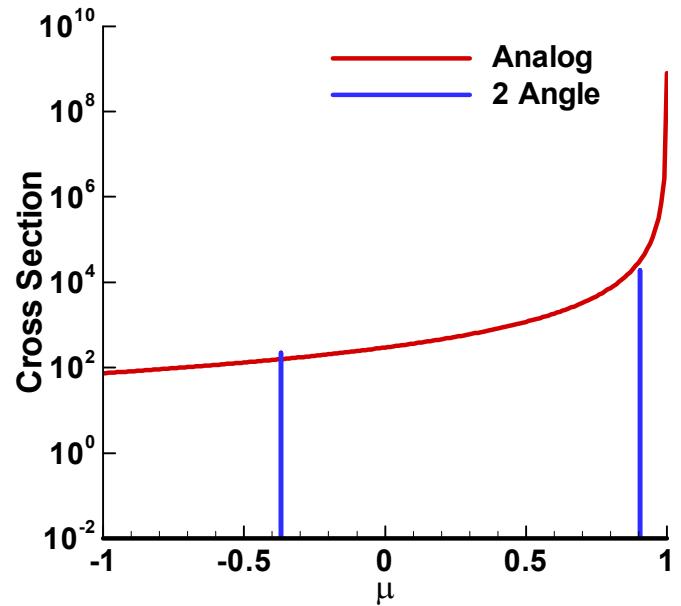
# Discrete Model for Electron Scattering

The discrete scattering kernel is:

$$\tilde{\sigma}_s(\vec{r}, \mu_0, E) = \sum_{n=1}^N \frac{\alpha_n(\vec{r}, E)}{2\pi} \delta[\mu_0 - \xi_n(\vec{r}, E)]$$

$\alpha_n$  are amplitudes

$\xi_n$  are scattering cosines



Requiring that  $\alpha_n$  and  $\xi_n$  preserve  $2N$  momentum transfer moments ( $\sigma_n$ ,  $n=1, \dots, 2N$ ) produces a nonlinear algebraic system, which is solved using Sloan's MORSE algorithm.

Sloan, D.P., "A New Multigroup Monte Carlo Scattering Algorithm for Neutral and Charged-Particle Boltzmann and Fokker-Planck Calculations," Technical Report SAND83-7094, Sandia National Laboratories (1983).



# Discrete Model for Electron Scattering

---

## ADVANTAGES

- Very fast, direct sampling
- Only requires moments (should be independent of DCS )
- Accuracy and speed depend on moment preservation, easily adjusted
- In practice, only 4-8 discrete angles provided excellent accuracy

## DISADVANTAGES

- Ray effects may skew angular tallies/integrated quantities of interest



# Adjoint Radiation Transport

## Adjoint Linear Boltzmann Transport Equation:

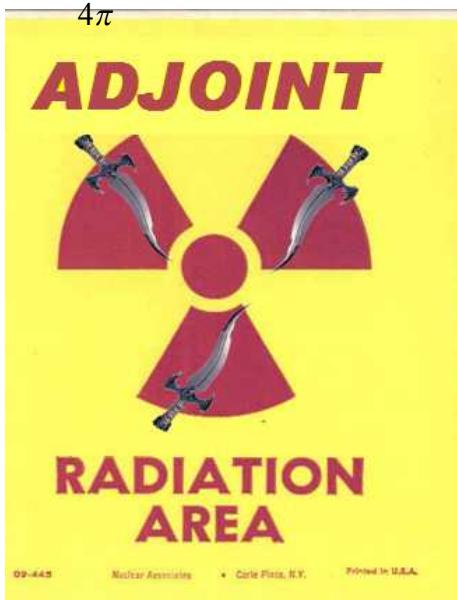
$$-\vec{\Omega} \cdot \nabla \psi^\dagger(\vec{r}, \vec{\Omega}, E) + [\sigma_{s,el}(\vec{r}, E) + \sigma_{s,in}(\vec{r}, E)] \psi^\dagger(\vec{r}, \vec{\Omega}, E) = \int_{4\pi} \sigma_{s,el}(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}', E) \psi^\dagger(\vec{r}, \vec{\Omega}', E) d\vec{\Omega}' + \int_0^\infty \sigma_{s,in}(\vec{r}, \vec{\Omega}, E \rightarrow E') \psi^\dagger(\vec{r}, \vec{\Omega}, E') dE'$$

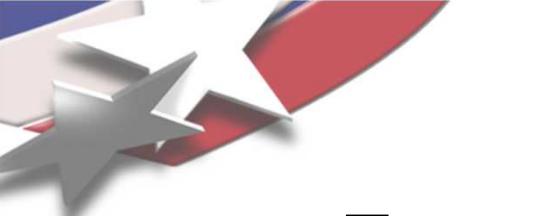
Anti-symmetry in the first operator makes the problem “backwards”

Notice the daggers, and the energetic changes

Angular DCS is unchanged by symmetry

Don't worry about boundary conditions...





# Transforming the Adjoint Equation

---

- Differences stem in the total and DCS:

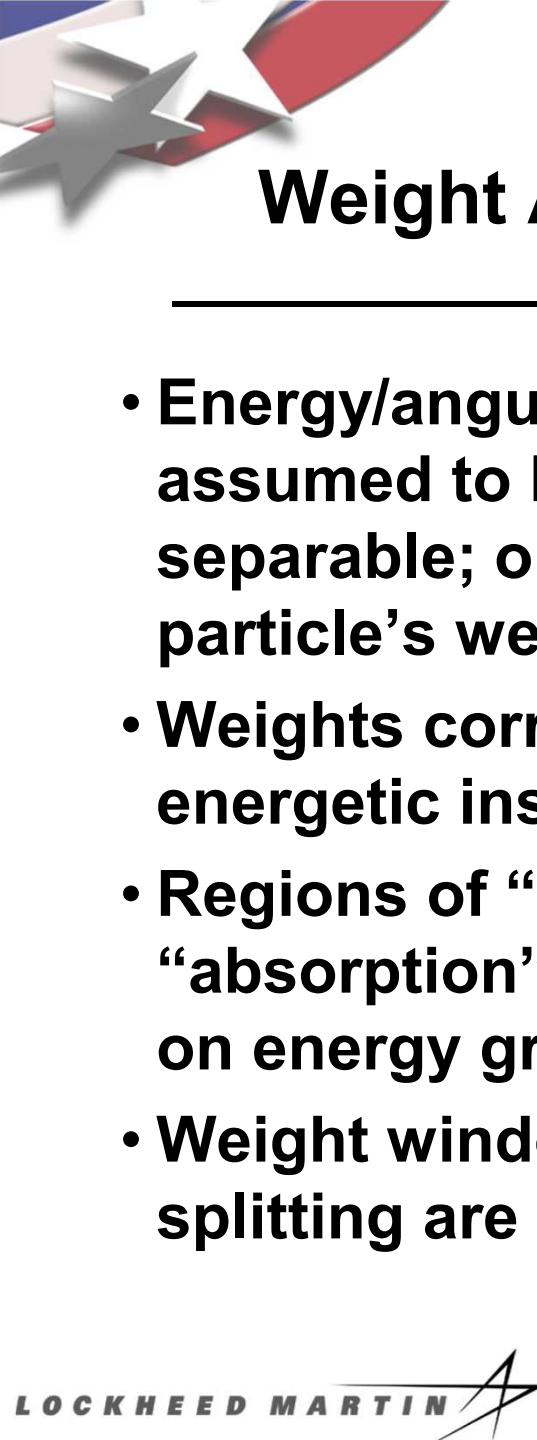
$$\sigma_{e,tot}(E) \neq \int_0^{\infty} \sigma_e(E \rightarrow E') \psi^\dagger(E') dE'$$

- Can the problem be made to look forward?
- Adjusting the DCS is akin to classical variance reduction techniques

YES

$$\int_0^{\infty} \sigma_e(E' \rightarrow E) \frac{\sigma_e(E \rightarrow E')}{\sigma_e(E' \rightarrow E)} dE'$$

↑  
Sample Interaction      ↑  
Tally this weight

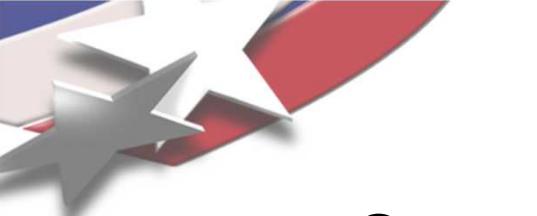


# Weight Adjustments: The Key to GBFP<sup>†</sup>

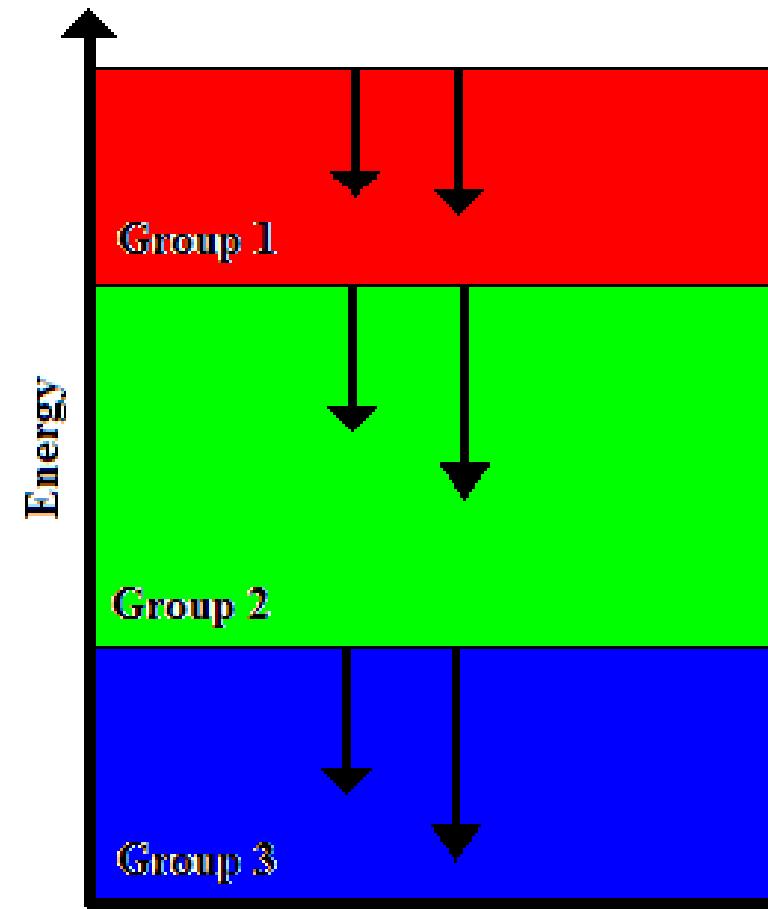
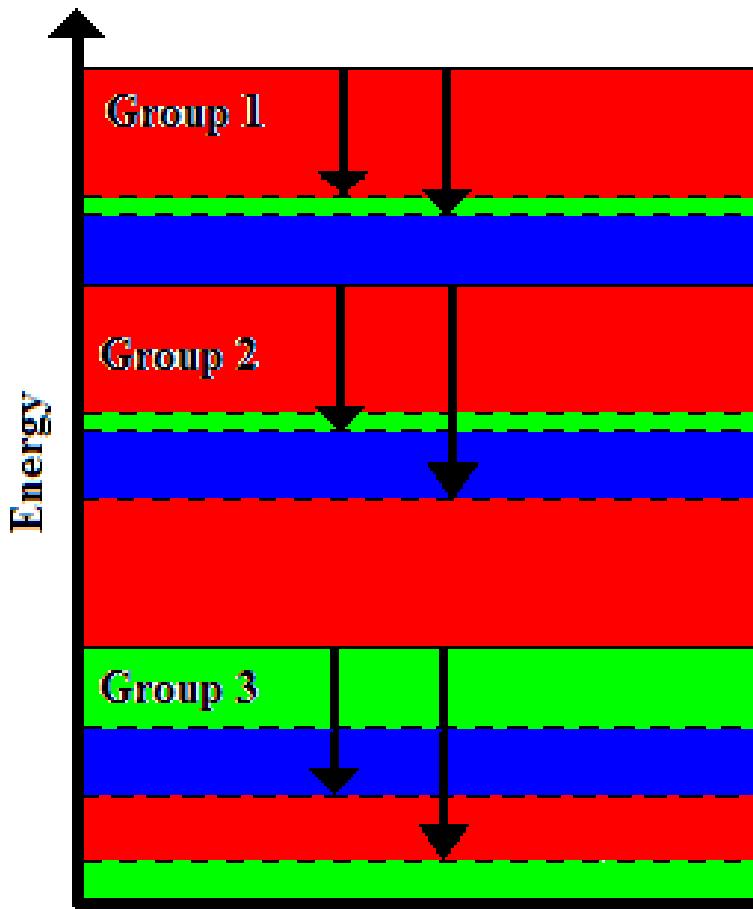
---

- Energy/angular scattering are assumed to be independent and separable; only energy affects the particle's weight
- Weights corrections are ratio of energetic inscatter to outscatter
- Regions of “multiplication” and “absorption” both occur and depend on energy group structure
- Weight windows, Russian roulette, and splitting are some obvious next steps





# Complexity of Adjoint Energy Grid





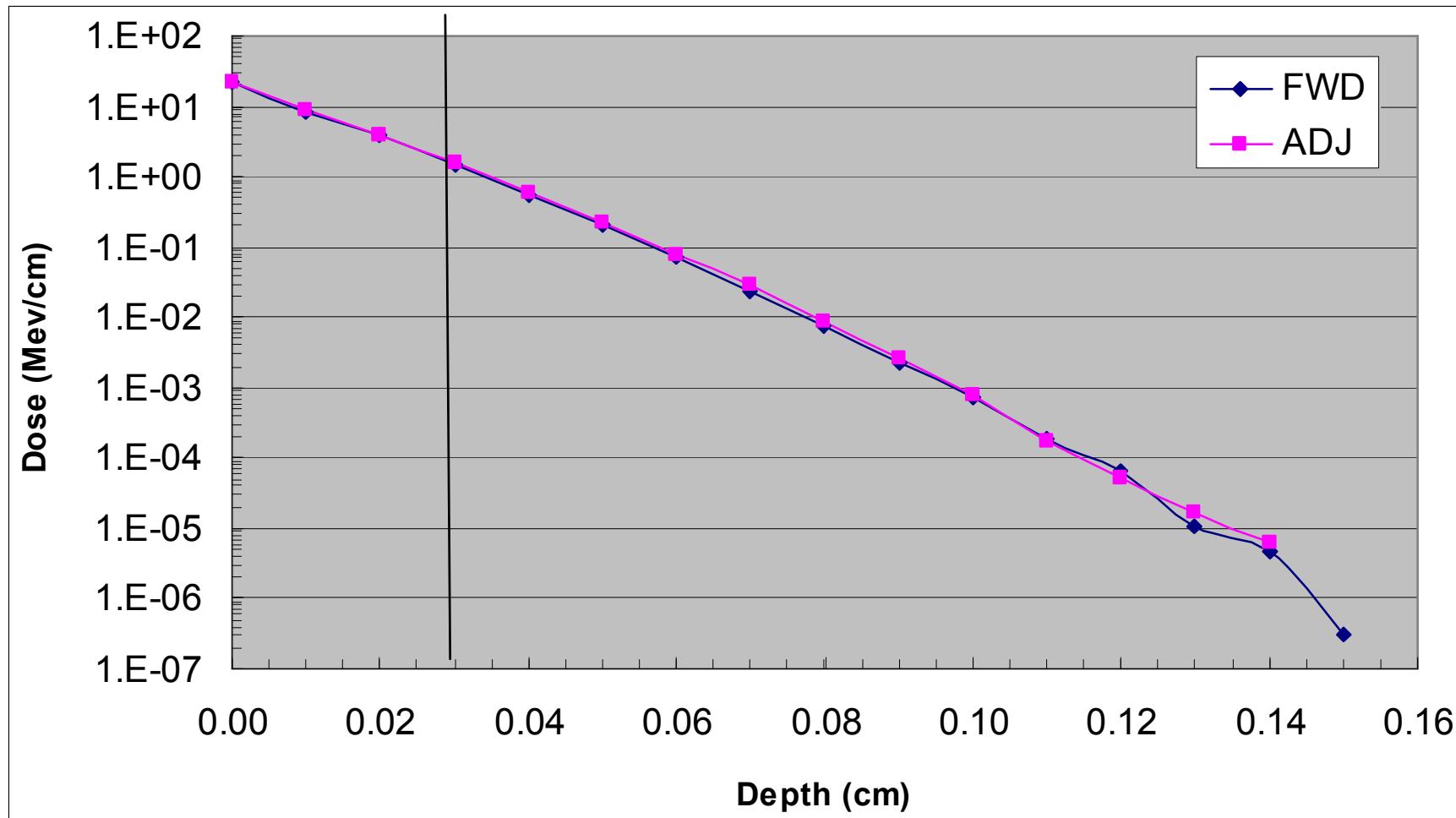
# Test Problem

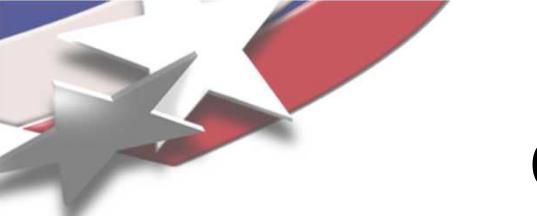
---

- **Slab geometry with source at left interface**
- **Two materials: 0.03 cm of Au followed by 0.47 cm of (*essentially* infinite) Si**
- **Source is isotropic in angle and uniform in energy [0, 1 MeV]**  
(all histories in prescribed energy range are tallied equally)
- **Simulation used two discrete angles and one discrete energy**
- **Results generated using  $10^6$  histories**

# Energy Deposition

Au/Si Slabs, 2 Angles, 1 Energy,  $10^6$  History, Uniform and Isotropic Source





# Questions? Comments? Unequivocal praise?

---

