Development of a Monte Carlo Code System with Continuous Energy Adjoint Transport Capabilities for Neutrons and Photons

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Preliminary Examination

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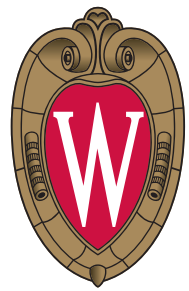

Outline

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The Monte Carlo method

- The Monte Carlo method is a stochastic method in which samples are drawn from a parent population through sampling procedures governed by a set of probability laws.
- From the samples, statistical data is acquired and analyzed to make inferences about the parent population.

Radiation Transport Problems

- **System of Interest:** collection of bounded regions containing a material, vacuum, source or detector
- **Parent Population:** set of all possible radiation histories
- **Sample:** radiation history drawn from set of all possible histories
- **Probability Laws:** related to material interaction cross sections
- **Sampling Process Variations**: forward and adjoint

The Forward Process vs. the Adjoint Process

The Forward Process

- Starting point of a history is sampled from the source
- Information about the history is recorded in the detector
- Probability laws used for sampling states of the history can be derived from the *transport equation*

The Adjoint Process

- Starting point of a history is sampled from the detector
- Information about the history is recorded in the source
- Probability laws used for sampling states of the history can be derived from the *adjoint transport equation*

Motivations for Using the Adjoint Process

1. Motivation 1: The source and detector phase space
   - Adjoint process generally more efficient than forward process when phase space of the source is larger than phase space of detector

2. Motivation 2: The adjoint flux interpretation
   - Adjoint process estimates a quantity called the adjoint flux
   - Physical interpretation of the adjoint flux is a source importance or sensitivity to the detector response
   - Adjoint flux can be invaluable when exact source distribution is not known (optimization problems)

Shutdown Dose Calculations Using the R2S Method

- Photon dose in a particular region of an experiment, fusion device or fission device resulting from neutron activation of material is desired
- This information is useful for planning maintenance on the experiment or device
- These problems are often solved using the rigorous 2-step method (R2S)

The R2S method

1. Neutron flux throughout the experiment or device is calculated
2. Activation code calculates the material activation and photon sources from neutron flux data
3. Photon dose calculated in areas of interest using a forward process

Shutdown Dose Calculations Using the R2SA Method

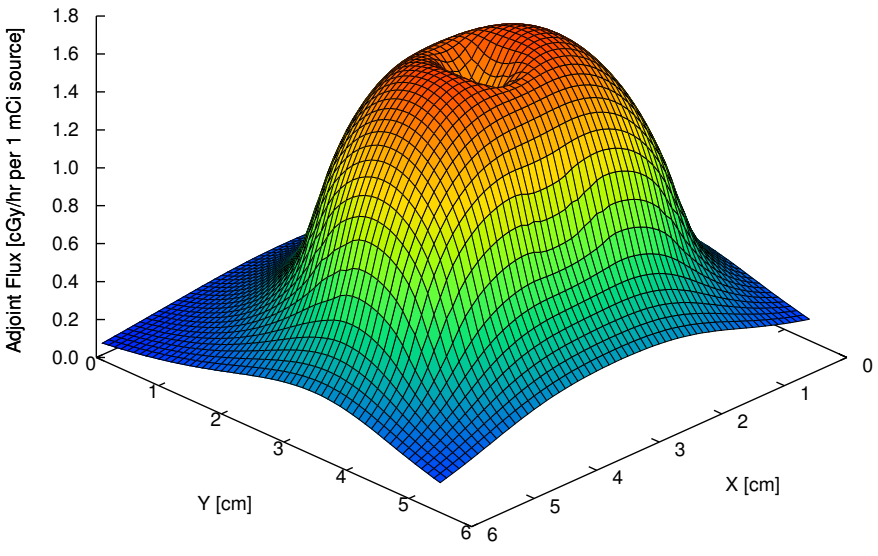
- Amount of activated material is often much larger than the region where the dose distribution is desired
- These problems could potentially benefit from the adjoint process for photons
- When the adjoint process is used, the solution method is called the rigorous 2-step adjoint method (R2SA)

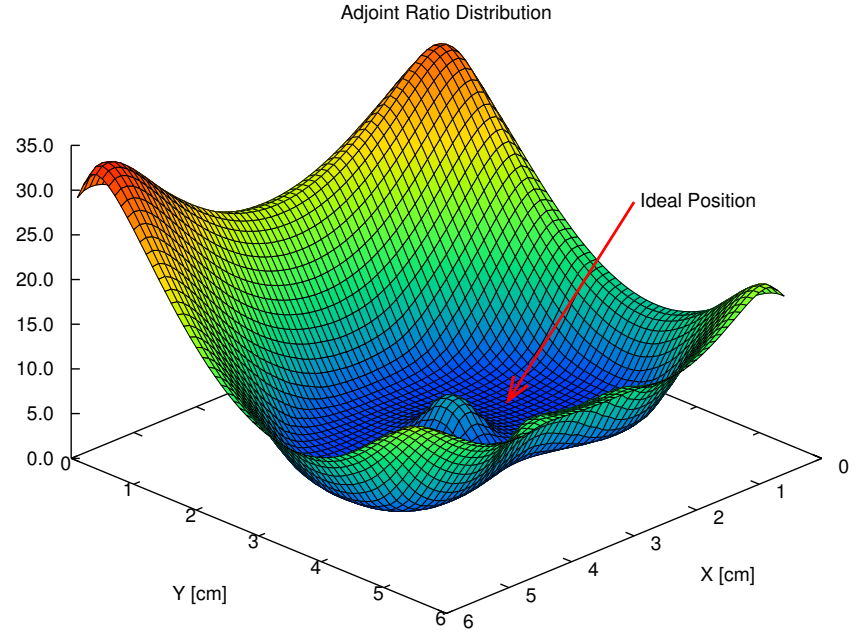
The R2SA method

1. Neutron flux throughout the experiment or device is calculated
2. Activation code calculates the material activation and photon sources from the neutron flux data
3. Photon dose is calculated in areas of interest using an adjoint process

Permanent Implant Brachytherapy

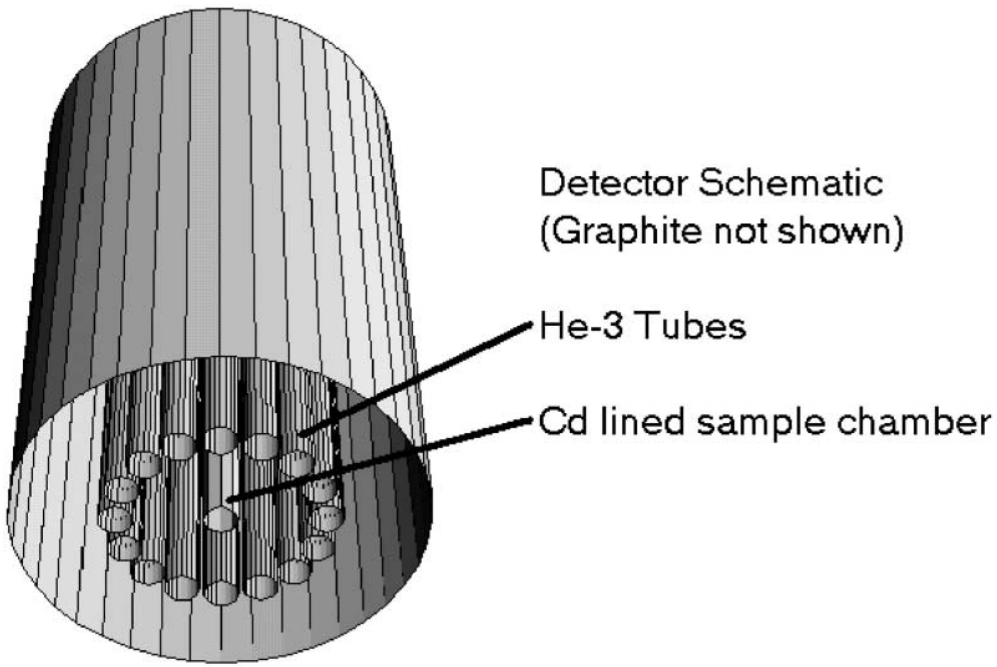
- **Optimization goal:** determine a source configuration that provides an optimal dose distribution to the target while minimizing the dose to sensitive structures
- Adjoint flux data allows one to eliminate source positions that result in a high dose to sensitive structures relative to the target
  - Shown to simplify and speed up optimization algorithms



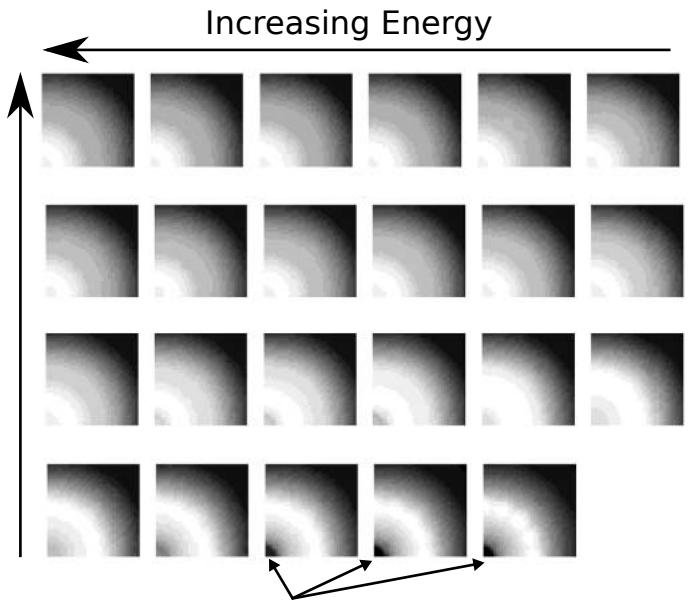


Detector Design

- Adjoint flux can allow for spectral performance of a detector to be predicted for an arbitrary source distribution
- Detector design can then be be optimized before it is constructed
  - Important for detectors with rare materials (e.g. He^3 neutron detectors)



Detector Adjoint Flux Data



Continuous Energy Capabilities of Popular Codes

Code	n	γ	$n^\dagger$	$\gamma^\dagger$
EGS4	-	$\surd$	-	-
EGSnrc	-	$\surd$	-	-
ITS6	-	$\surd$	-	-
PENELOPE	-	$\surd$	-	-
MORSE	-	-	-	-
TART2005	$\surd$	$\surd$	-	-
MCNP5/6	$\surd$	$\surd$	-	-
MCNPX	$\surd$	$\surd$	-	-
GEANT4	$\surd$	$\surd$	-	$\surd$
MCBEND	$\surd$	$\surd$	$\surd$	-
FACEMC	$\surd$	$\surd$	$\surd$	$\surd$

- A lack of necessary adjoint cross section data is a major deterrent to implementing the adjoint process on a continuous energy scale.

Outline

Fredholm Integral Equations of the Second Kind (FIESKs)

$$F(x) = S(x) + \lambda \int_a^b K(x, y) F(y) dy$$

- Important equation for radiation transport
- $S(x)$ is a forcing function
- $K(x, y)$ is the kernel of the integral equation
  - Characterizes the transition from some initial state y to the state x
  - Often written as $K(y \rightarrow x)$ to signify this interpretation

Volterra Integral Equations of the Second Kind

$$F(x) = S(x) + \lambda \int_a^x K(y \to x) F(y) dy$$

- Very similar to the FIESK except one limit of integration is variable
- Comes about whenever there is a preferred direction for the independent variable (i.e. particle scattering kinematics)
- Can be converted to a FIESK using a modified kernel

$$F(x) = S(x) + \lambda \int_a^b K'(y \to x) F(y) dy$$

$$K'(y \to x) = \begin{cases} K(y \to x) & \text{if } y < x \\ 0 & \text{if } y > x. \end{cases}$$

The Method of Successive Approximations

$$f_0(x) = S(x)$$

$$f_n(x) = S(x) + \lambda \int_a^b K(y \to x) f_{n-1}(y) dy$$

$$F(x) = \lim_{n \to \infty} f_n(x)$$

- The solution is more commonly expressed as a Neumann series:

$$F(x) = S(x) + \lambda \int_a^b K(y \to x) S(y) dy +$$
$$\lambda^2 \int_a^b \int_a^b K(y \to x) K(y_1 \to y) S(y_1) dy_1 dy +$$
$$\lambda^3 \int_a^b \int_a^b \int_a^b K(y \to x) K(y_1 \to y) K(y_2 \to y_1) S(y_2) dy_2 dy_1 dy +$$
$$\dots$$

The Monte Carlo Method

$$\text{Random Walk: } \begin{cases} p^1(x) & = \frac{S(x)}{\int S(x)dx} \\ p(y \to x) & = C(y)K(y \to x) \\ p(y) & = 1 - \int_a^b p(y \to x)dx. \end{cases}$$

- $p^1(x)$ represents the probability of a random walk starting in state x
- $p(y \to x)$ characterizes the probability of a transition from initial state y to new state x
- $p(y)$ represents the probability of termination in state y
- From these probability distribution functions (PDFs) random walks can be constructed
- Using special statistical rules, called estimators, the solution to the FIESK can be estimated from the random walks

The Transport Equation

$$\hat{\Omega} \cdot \vec{\bigtriangledown} \varphi(\vec{r}, E, \hat{\Omega}, t) \; + \; \Sigma_T(\vec{r}, E)\varphi(\vec{r}, E, \hat{\Omega}, t) = S(\vec{r}, E, \hat{\Omega}, t) \; + \int \int \Sigma_T(\vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega})\varphi(\vec{r}, E^{'}, \hat{\Omega}^{'}, t) dE^{'} d\hat{\Omega}^{'}$$

- The transport equation describes the expected behavior of particles in a medium
- The right side of this equation is called the emission density $\chi(\vec{r}, E, \hat{\Omega})$

$$\chi(\vec{r}, E, \hat{\Omega}) = S(\vec{r}, E, \hat{\Omega}) + \int \int \Sigma_T(\vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega})\varphi(\vec{r}, E^{'}, \hat{\Omega}^{'}) dE^{'} d\hat{\Omega}^{'}$$

- The transport equation must be converted to a FIESK to derive a Monte Carlo random walk process for radiation transport

The Transport Equation in Integral Form

- The method of characteristics is used to convert the transport equation to an ordinary differential equation (ODE)
- Subsequent solution of this ODE results in the integral transport equation

$$\varphi(\vec{r}, E, \hat{\Omega}) = \int_0^{\infty} \chi(\vec{r} - R\hat{\Omega}, E, \hat{\Omega}) \exp\left[-\int_0^{R} \Sigma_T(\vec{r} - R'\hat{\Omega}, E) dR'\right] dR$$
$$= \int \chi(\vec{r}', E, \hat{\Omega}) \tau(\vec{r}', \vec{r}, E, \hat{\Omega}) dV'.$$

- The function $\tau(\vec{r}', \vec{r}, E, \hat{\Omega})$ allows the line integral to be expressed as a volume integral

$$\tau(\vec{r}', \vec{r}, E, \hat{\Omega}) = \exp\left[-\int_0^{|\vec{r}-\vec{r}'|} \Sigma_T(\vec{r} - R'\hat{\Omega}, E) dR'\right] \frac{\delta\left(\hat{\Omega} - \left[\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right]\right)}{|\vec{r} - \vec{r}'|^2}$$

The Emission Density FIESK

- To construct the emission density FIESK, the integral transport equation is substituted into the equation for the emission density

$$\chi(\vec{r}, E, \hat{\Omega}) = S(\vec{r}, E, \hat{\Omega}) + \int \int \Sigma_T(\vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) \cdot \int \chi(\vec{r}^{'}, E', \hat{\Omega}^{'}) \tau(\vec{r}^{'}, \vec{r}, E^{'}, \hat{\Omega}^{'}) dV^{'} dE^{'} d\hat{\Omega}^{'}$$

$$= S(\vec{r}, E, \hat{\Omega}) + \int \int \int K(\vec{r}^{'} \rightarrow \vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) \cdot \chi(\vec{r}^{'}, E', \hat{\Omega}^{'}) dV^{'} dE^{'} d\hat{\Omega}^{'}$$

- The kernel of the emission density FIESK is

$$K(y \rightarrow x) = K(\vec{r}^{'} \rightarrow \vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) = \Sigma_T(\vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) \tau(\vec{r}^{'}, \vec{r}, E^{'}, \hat{\Omega}^{'})$$

- This kernel can be simplified by introducing two new kernels

The Transport Kernel

$$T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega}) = \Sigma_T(\vec{r}, E)\tau(\vec{r}', \vec{r}, E, \hat{\Omega})$$

$$= \Sigma_T(\vec{r}, E) \exp\left[-\int_0^{|\vec{r}-\vec{r}'|} \Sigma_T(\vec{r} - R'\hat{\Omega}, E)dR'\right] \frac{\delta\left(\hat{\Omega} - \left[\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right]\right)}{|\vec{r} - \vec{r}'|^2}$$

- Describes the movement of particles through space
- Quantity $T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega})dV$ is probability that a particle at $\vec{r}'$ with energy E and direction $\hat{\Omega}$ will have next collision in volume element dV at $\vec{r}$
- The factor $\Sigma_T(\vec{r}, E)$ prevents new positions $\vec{r}$ from being sampled in a vacuum

The Collision Kernel

$$C(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{\Sigma_T(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})}{\Sigma_T(\vec{r}, E')}$$

- Describes the movement of particles through energy and direction
- In a non-multiplying medium, this kernel integrates to

$$P_{NA}(E') = \frac{\Sigma_s(\vec{r}, E')}{\Sigma_T(\vec{r}, E')}$$

- Upon expansion, a procedure for sampling a new energy and direction from this kernel becomes clear

$$C(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \sum_j \frac{\Sigma_j(\vec{r}, E') c_i(\vec{r}, E') f_i(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})}{\Sigma_T(\vec{r}, E')}$$

$$= \sum_A \frac{\Sigma_A(\vec{r}, E')}{\Sigma_T(\vec{r}, E')} \sum_j \frac{\sigma_{A,j}(E')}{\sigma_A(E')} c_{A,j}(E') p_{A,j}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})$$

The Emission Density FIESK Revisited

- Using the transport kernel and the collision kernel, the state transition kernel for the emission density FIESK can be simplified:

$$
\begin{aligned}
K(y \to x) &= K(\vec{r}^{\,'} \to \vec{r}, E^{'} \to E, \hat{\Omega}^{'} \to \hat{\Omega}) \\
&= \Sigma_T(\vec{r}, E^{'} \to E, \hat{\Omega}^{'} \to \hat{\Omega}) \tau(\vec{r}^{\,'}, \vec{r}, E^{'}, \hat{\Omega}^{'}) \\
&= \left[\frac{\Sigma_T(\vec{r}, E^{'} \to E, \hat{\Omega}^{'} \to \hat{\Omega})}{\Sigma_T(\vec{r}, E^{'})} \right] \left[\Sigma_T(\vec{r}, E^{'}) \tau(\vec{r}^{\,'}, \vec{r}, E^{'}, \hat{\Omega}^{'}) \right] \\
&= C(\vec{r}, E^{'} \to E, \hat{\Omega}^{'} \to \hat{\Omega}) T(\vec{r}^{\,'} \to \vec{r}, E^{'}, \hat{\Omega}^{'})
\end{aligned}
$$

- Sampling a new state from the state transition kernel $K(y \to x)$ is now straightforward

The Collision Density FIESK

- The collision density and emission density are directly related

$$\psi(\vec{r}, E, \hat{\Omega}) = \int T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega}) \chi(\vec{r}', E, \hat{\Omega}) dV'$$

- The collision density FIESK is therefore

$$\psi(\vec{r}, E, \hat{\Omega}) = \int S(\vec{r}', E, \hat{\Omega}) T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega}) dV' + \int \int \int L(\vec{r}' \rightarrow \vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}', E', \hat{\Omega}') dE' d\hat{\Omega}' dV'$$

- The state transition kernel for this FIESK is

$$\begin{aligned} L(y \rightarrow x) &= L(\vec{r}' \rightarrow \vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \\ &= T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega}) C(\vec{r}', E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \end{aligned}$$

The Monte Carlo Process for Radiation Transport

- From the emission density FIESK and collision density FIESK, the random walk process for each quantity can be determined

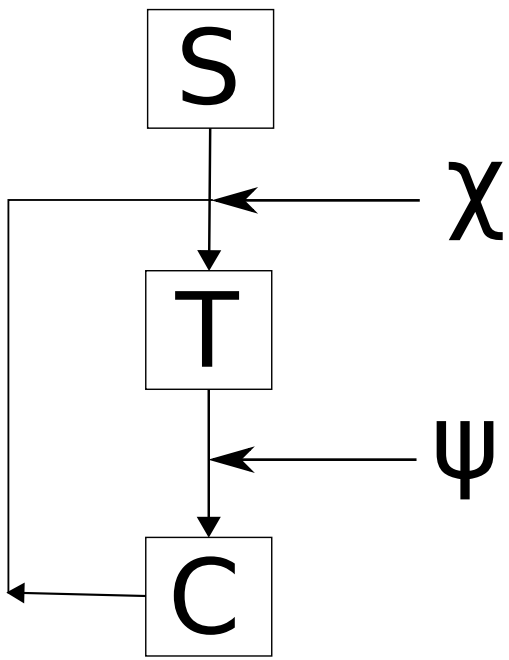
$$\chi(x) \text{ Random Walk: } \begin{cases} p^1(x) & = \frac{S(x)}{\int S(x)dx} \\ p(y \to x) & = K(y \to x) \\ p(x) & = 1 - \overline{P}_{NA}(x) \end{cases}$$

$$\psi(x) \text{ Random Walk: } \begin{cases} p^1(x) & = \frac{S_c(x)}{\int S_c(x)dx} \\ p(y \to x) & = L(y \to x) \\ p(x) & = 1 - P_{NA}(x) \end{cases}$$

- $\overline{P}_{NA}(x)$ is an average survival probability along the line from $\vec{r}'$ to $\vec{r}$
- $S_c(x)$ is the first collided source
- Both processes can be combined into a single process

The Combined Monte Carlo Process

- The kernels $K(y \rightarrow x)$ and $L(y \rightarrow x)$ only differ in the order of the collision and transport kernels
- The collision kernel and transport kernel will always be sampled from in succession
- Both densities can therefore be estimated during the same process



The Adjoint Transport Equation Forcing Function

- A material response can be calculated using the flux and a material response function $r(\vec{r}, E, \hat{\Omega})$

$$R = \langle \varphi r \rangle$$

- The flux is characterized by the transport equation

$$H_B \cdot \varphi(\vec{r}, E, \hat{\Omega}) = S(\vec{r}, E, \hat{\Omega})$$

- The adjoint operator is defined by the following relationship:

$$\langle \varphi^\dagger H_B \cdot \varphi \rangle = \langle \varphi H_B^\dagger \cdot \varphi^\dagger \rangle$$

- Want to calculate the same material response

$$R = \langle \varphi r \rangle = \langle \varphi H_B^\dagger \cdot \varphi^\dagger \rangle = \langle \varphi^\dagger H_B \cdot \varphi \rangle = \langle \varphi^\dagger S \rangle$$

- The forcing function for the adjoint transport equation must be the material response function

The Adjoint Transport Equation

- Using the definition of the adjoint operator, the adjoint transport equation can be derived

$$-\hat{\Omega} \cdot \vec{\nabla}\varphi^{\dagger}(\vec{r}, E, \hat{\Omega}) + \Sigma_T(\vec{r}, E)\varphi^{\dagger}(\vec{r}, E, \hat{\Omega}) = r(\vec{r}, E, \hat{\Omega}) + \int \int \Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')\varphi^{\dagger}(\vec{r}, E', \hat{\Omega}')dE'd\hat{\Omega}'$$

- The right side of this equation is called the adjoint emission density

$$\theta^{\dagger}(\vec{r}, E, \hat{\Omega}) = r(\vec{r}, E, \hat{\Omega}) + \int \int \Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')\varphi^{\dagger}(\vec{r}, E', \hat{\Omega}')dE'd\hat{\Omega}'$$

- This equation must be converted to a FIESK to derive a Monte Carlo random walk process for adjoint radiation transport

The Adjoint Transport Equation in Integral Form

- The method of characteristics is used to convert the adjoint transport equation to an ordinary differential equation (ODE)
- Subsequent solution of this ODE results in the integral adjoint transport equation

$$\begin{aligned}\varphi^{\dagger}(\vec{r},E,\hat{\Omega}) &= \int_0^{\infty}\theta^{\dagger}(\vec{r}+R\hat{\Omega},E,\hat{\Omega})exp\left[-\int_0^{R}\Sigma_T(\vec{r}+R^{'}\hat{\Omega},E)dR^{'}\right]dR \\ &= \int\theta^{\dagger}(\vec{r}^{\,'},E,\hat{\Omega})\tau^{\dagger}(\vec{r}^{\,'},\vec{r},E,\hat{\Omega})dV^{'}\end{aligned}$$

- The function $\tau^{\dagger}(\vec{r}^{\,'},\vec{r},E,\hat{\Omega})$ allows the line integral to be expressed as a volume integral

$$\tau^{\dagger}(\vec{r}^{\,'},\vec{r},E,\hat{\Omega}) = \exp\left[-\int_0^{|\vec{r}^{\,'}-\vec{r}|}\Sigma_T(\vec{r}+R^{'}\hat{\Omega},E)dR^{'}\right]\frac{\delta\left(\hat{\Omega}-\left[\frac{\vec{r}^{\,'}-\vec{r}}{|\vec{r}^{\,'}-\vec{r}|}\right]\right)}{|\vec{r}^{\,'}-\vec{r}|^2}$$

The Adjoint Emission Density FIESK

- To construct the adjoint emission density FIESK, the integral adjoint transport equation is substituted into the equation for the adjoint emission density:

$$\theta^{\dagger}(\vec{r},E,\hat{\Omega}) = r(\vec{r},E,\hat{\Omega}) + \int\int \Sigma_T(\vec{r},E\rightarrow E^{'},\hat{\Omega}\rightarrow\hat{\Omega}^{'}) \cdot \int \theta^{\dagger}(\vec{r}^{'},E^{'},\hat{\Omega}^{'})\tau^{\dagger}(\vec{r}^{'},\vec{r},E^{'},\hat{\Omega}^{'})dV^{'}dE^{'}d\hat{\Omega}^{'}$$

$$= r(\vec{r},E,\hat{\Omega}) + \int\int\int M^{\dagger}(\vec{r}^{'}\rightarrow\vec{r},E^{'}\rightarrow E,\hat{\Omega}^{'}\rightarrow\hat{\Omega}) \cdot \theta^{\dagger}(\vec{r}^{'},E^{'},\hat{\Omega}^{'})dV^{'}dE^{'}d\hat{\Omega}^{'}$$

- The kernel of the adjoint emission density FIESK is

$$M^{\dagger}(y\rightarrow x) = M^{\dagger}(\vec{r}^{'}\rightarrow\vec{r},E^{'}\rightarrow E,\hat{\Omega}^{'}\rightarrow\hat{\Omega}) = \Sigma_T(\vec{r},E\rightarrow E^{'},\hat{\Omega}\rightarrow\hat{\Omega}^{'})\tau^{\dagger}(\vec{r}^{'},\vec{r},E^{'},\hat{\Omega}^{'})$$

- This kernel can be simplified by introducing two new kernels

The Adjoint Transport Kernel

$$T^{\dagger}(\vec{r}^{\,\prime} \rightarrow \vec{r}, E, \hat{\Omega}) = \Sigma_T(\vec{r}, E)\tau^{\dagger}(\vec{r}^{\,\prime}, \vec{r}, E, \hat{\Omega})$$

$$= \Sigma_T(\vec{r}, E) \exp\left[-\int_0^{|\vec{r}^{\,\prime} - \vec{r}|} \Sigma_T(\vec{r} + R^{\prime}\hat{\Omega}, E) dR^{\prime}\right] \frac{\delta\left(\hat{\Omega} - \left[\frac{\vec{r}^{\,\prime} - \vec{r}}{|\vec{r}^{\,\prime} - \vec{r}|}\right]\right)}{|\vec{r}^{\,\prime} - \vec{r}|^2}$$

- Describes the movement of adjoint particles through space
- Quantity $T^{\dagger}(\vec{r}^{\,\prime} \rightarrow \vec{r}, E, \hat{\Omega})dV$ is probability that an adjoint particle at $\vec{r}^{\,\prime}$ with energy E and direction $\hat{\Omega}$ will have next collision in volume element dV at $\vec{r}$
- The factor $\Sigma_T(\vec{r}, E)$ prevents new positions $\vec{r}$ from begin sampled in a vacuum

The Adjoint Collision Kernel

$$C^{\dagger}(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{\Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\int \int \Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}') dE d\hat{\Omega}}$$
$$= \frac{\Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^{\dagger}(\vec{r}, E')}$$

- Describes the movement of adjoint particles through energy and direction
- Not immediately clear what this kernel should integrate to - force it to integrate to unity for simplicity
- Normalization factor is referred to simply as the total macroscopic adjoint cross section
- Expansion of this kernel is necessary to derive a sampling procedure

The Expanded Adjoint Collision Kernel

$$C^{\dagger}(\vec{r},E^{'} \rightarrow E,\hat{\Omega}^{'} \rightarrow \hat{\Omega}) = \frac{\Sigma_T(\vec{r},E \rightarrow E^{'},\hat{\Omega} \rightarrow \hat{\Omega}^{'})}{\Sigma^{\dagger}(\vec{r},E^{'})}$$

$$= \sum_j \frac{\Sigma_j(\vec{r},E)c_j(\vec{r},E)f_j(E \rightarrow E^{'},\hat{\Omega} \rightarrow \hat{\Omega}^{'})}{\Sigma^{\dagger}(\vec{r},E^{'})}$$

$$= \sum_A \frac{\Sigma_A^{\dagger}(\vec{r},E^{'})}{\Sigma^{\dagger}(\vec{r},E^{'})} \sum_j \frac{\sigma_{A,j}^{\dagger}(E^{'})}{\sigma_A^{\dagger}(E^{'})} \frac{\sigma_{A,j}(E)c_{A,j}(E)p_{A,j}(E \rightarrow E^{'},\hat{\Omega} \rightarrow \hat{\Omega}^{'})}{\sigma_{A,j}^{\dagger}(E^{'})}$$

- Through expansion the definition of the adjoint cross section also becomes clear

$$\sigma_{A,j}^{\dagger}(E^{'}) = \int \int \sigma_{A,j}(E)c_{A,j}(E)p_{A,j}(E \rightarrow E^{'},\hat{\Omega} \rightarrow \hat{\Omega}^{'})dEd\hat{\Omega}$$

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

The Adjoint Emission Density FIESK Revisited

- The state transition kernel for the adjoint emission density FIESK can be simplified using the previous two kernels

$$
\begin{aligned}
M^{\dagger}(y \rightarrow x) &= M^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) \\
&= \Sigma_T(\vec{r}, E \rightarrow E^{'}, \hat{\Omega} \rightarrow \hat{\Omega}^{'}) \tau^{\dagger}(\vec{r}^{\,'}, \vec{r}, E^{'}, \hat{\Omega}^{'}) \\
&= \left[\frac{\Sigma_T(\vec{r}, E \rightarrow E^{'}, \hat{\Omega} \rightarrow \hat{\Omega}^{'})}{\Sigma^{\dagger}(\vec{r}, E^{'})} \right] \left[\frac{\Sigma^{\dagger}(\vec{r}, E^{'})}{\Sigma_T(\vec{r}, E^{'})} \right] \left[\Sigma_T(\vec{r}, E^{'}) \tau^{\dagger}(\vec{r}^{\,'}, \vec{r}, E^{'}, \hat{\Omega}^{'}) \right] \\
&= C^{\dagger}(\vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) P^{\dagger}(\vec{r}, E^{'}) T^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E^{'}, \hat{\Omega}^{'})
\end{aligned}
$$

- This kernel also contains a factor $P^{\dagger}(\vec{r}, E^{'})$ called the adjoint weight factor
- This factor is bounded in the interval $(0, \infty)$.

The Adjoint Collision Density FIESK

- The adjoint collision density and emission density are directly related

$$\xi^{\dagger}(\vec{r}, E, \hat{\Omega}) = \int T^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E, \hat{\Omega}) \theta^{\dagger}(\vec{r}^{\,'}, E, \hat{\Omega}) dV^{'}$$

- The adjoint collision density FIESK is therefore

$$\xi^{\dagger}(\vec{r}, E, \hat{\Omega}) = \int r(\vec{r}^{\,'}, E, \hat{\Omega}) T^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E, \hat{\Omega}) dV^{'} + \int \int \int N^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) \xi^{\dagger}(\vec{r}^{\,'}, E^{'}, \hat{\Omega}^{'}) dE^{'} d\hat{\Omega}^{'} dV^{'}$$

- The state transition kernel for this FIESK is

$$\begin{aligned} N^{\dagger}(y \rightarrow x) &= N^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) \\ &= T^{\dagger}(\vec{r}^{\,'} \rightarrow \vec{r}, E, \hat{\Omega}) C^{\dagger}(\vec{r}^{\,'}, E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) P^{\dagger}(\vec{r}^{\,'}, E^{'}) \end{aligned}$$

The Monte Carlo Random Walk Process

- From the adjoint emission density FIESK and adjoint collision density FIESK, the random walk process can be determined

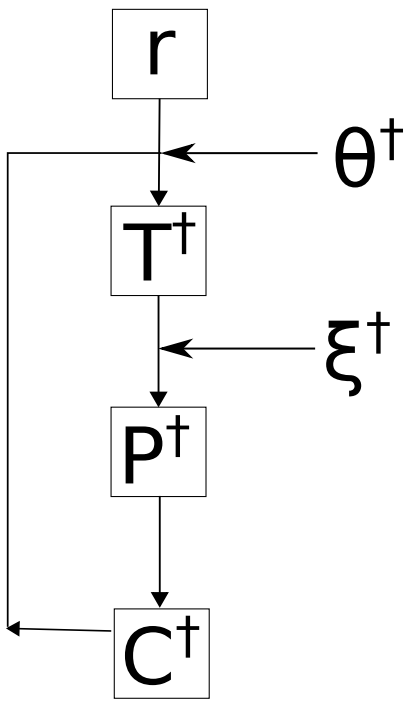
$$\theta^\dagger(x) \text{ Random Walk: } \begin{cases} p^1(x) & = \frac{a(x)}{\int a(x)dx} \\ p(y \rightarrow x) & = \frac{M^\dagger(y \rightarrow x)}{\overline{P}^\dagger(y)} \\ p(x) & = 0 \end{cases}$$

$$\xi^\dagger(x) \text{ Random Walk: } \begin{cases} p^1(x) & = \frac{S_c^\dagger(x)}{\int S_c^\dagger(x)dx} \\ p(y \rightarrow x) & = \frac{N^\dagger(y \rightarrow x)}{P^\dagger(y)} \\ p(x) & = 0 \end{cases}$$

- There is no absorption reaction for adjoint radiation
  - Due to the adjoint cross section definition
- Russian roulette must be used to end random walks
- Both processes can be combined into a single process

The Combined Monte Carlo Adjoint Process

- The kernels $M^{\dagger}(y \rightarrow x)$ and $N^{\dagger}(y \rightarrow x)$ only differ in the order of the adjoint collision kernel, adjoint transport kernel and adjoint weight factor
- Both densities can therefore be estimated during the same process



Outline

The Adjoint Incoherent Scattering Cross Section

- Use the definition of the adjoint double differential transfer probability to construct this cross section:

$$p^{\dagger}_{i.s}(E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) = \frac{\sigma_{i.s.}(E) c_{i.s.}(E) p_{i.s.}(E \rightarrow E^{'}, \hat{\Omega} \rightarrow \hat{\Omega}^{'})}{\sigma^{\dagger}_{i.s.}(E^{'})}$$

$$\sigma^{\dagger}_{i.s.}(E^{'}) p^{\dagger}_{i.s}(E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) = \sigma_{i.s.}(E) p_{i.s.}(E \rightarrow E^{'}, \hat{\Omega} \rightarrow \hat{\Omega}^{'})$$

$$\sigma^{\dagger}_{i.s}(E^{'} \rightarrow E, \hat{\Omega}^{'} \rightarrow \hat{\Omega}) = \sigma_{i.s.}(E \rightarrow E^{'}, \hat{\Omega} \rightarrow \hat{\Omega}^{'})$$

- Both the forward and adjoint cross sections are only dependent on the angle between the initial and final directions:

$$\sigma^{\dagger}_{i.s}(E^{'} \rightarrow E, \hat{\Omega}^{'} \cdot \hat{\Omega}) = \sigma_{i.s.}(E \rightarrow E^{'}, \hat{\Omega} \cdot \hat{\Omega}^{'})$$

$$\sigma^{\dagger}_{i.s}(E^{'} \rightarrow E, \mu) = \sigma_{i.s.}(E \rightarrow E^{'}, \mu)$$

The Adjoint Incoherent Scattering Cross Section

- The double differential incoherent scattering cross section is

$$\sigma_{i.s.}(E^{'} \rightarrow E, \mu) = \frac{d\sigma_{i.s.}(E^{'}, E, \mu, Z)}{dEd\mu}$$
$$= \frac{\pi r_e^2}{m_e c^2 \alpha'^2} \left[\frac{\alpha}{\alpha^{'}} + \frac{\alpha^{'}}{\alpha} - 1 + \mu^2 \right] S\left(y(\alpha^{'}, \mu), Z\right)$$
$$\cdot \delta\left(\mu - \left[1 - \frac{1}{\alpha} + \frac{1}{\alpha^{'}}\right]\right)$$

- The adjoint double differential incoherent scattering cross section is therefore

$$\sigma^{\dagger}_{i.s.}(E^{'} \rightarrow E, \mu) = \frac{\pi r_e^2}{m_e c^2 \alpha^2} \left[\frac{\alpha^{'}}{\alpha} + \frac{\alpha}{\alpha^{'}} - 1 + \mu^2 \right] S\left(y(\alpha, \mu), Z\right)$$
$$\cdot \delta\left(\mu - \left[1 - \frac{1}{\alpha^{'}} + \frac{1}{\alpha}\right]\right)$$

The Integrated Adjoint Incoherent Scattering Cross Section

- Limits of integration must be determined to compute the integrated adjoint incoherent cross section
- Use the kinematic equation for the adjoint process

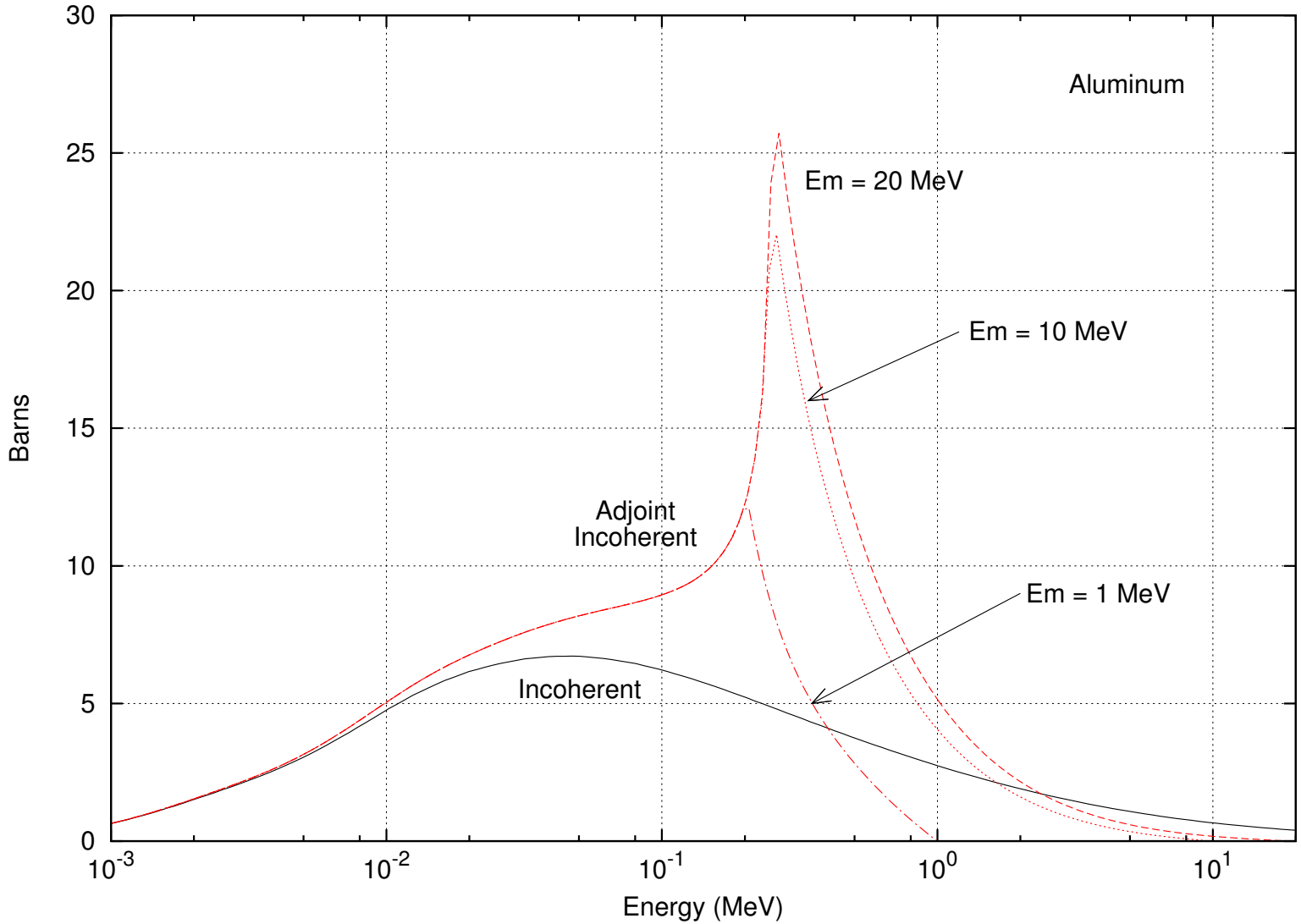
$$E = \frac{E^{'}}{1 - \alpha^{'}(1 - \mu)}$$

$$\mu = 1: \quad E_{low} = E^{'}$$

$$\mu = 1 - \frac{1}{\alpha^{'}}: \quad E_{high} = \infty$$

- The integrated cross section will be unbound unless a max problem energy is set

The Integrated Adjoint Incoherent Scattering Cross Section



The Adjoint Coherent Scattering Cross Section

- Use the definition of the adjoint double differential cross section

$$\sigma^{\dagger}_{c.s.}(E^{'} \rightarrow E, \hat{\Omega}^{'} \cdot \hat{\Omega}) = \sigma_{c.s.}(E \rightarrow E^{'}, \hat{\Omega} \cdot \hat{\Omega}^{'})$$

- In the forward interaction, the energy of the photon does not change:

$$\sigma^{\dagger}_{c.s.}(E^{'}, \hat{\Omega}^{'} \cdot \hat{\Omega}) = \sigma_{c.s.}(E^{'}, \hat{\Omega} \cdot \hat{\Omega}^{'})$$

$$\frac{\sigma^{\dagger}_{c.s.}(E^{'}, \mu)}{d\mu} = \frac{\sigma_{c.s.}(E^{'}, \mu)}{d\mu}$$

- Both the forward and adjoint differential coherent scattering cross section are therefore the same:

$$\frac{d\sigma^{\dagger}_{c.s.}(E^{'}, \mu, Z)}{d\mu} = \frac{d\sigma_{c.s.}(E^{'}, \mu, Z)}{d\mu}$$

$$= \pi r_e^2 (1 + \mu^2) F^2(y, Z)$$

The Adjoint Pair Production Cross Section

- Use the definition of the adjoint double differential cross section

$$\sigma^{\dagger}_{p.p.}(E^{'} \rightarrow E, \hat{\Omega}^{'} \cdot \hat{\Omega}) = 2\sigma_{p.p.}(E \rightarrow E^{'}, \hat{\Omega} \cdot \hat{\Omega}^{'})$$

- The simplified double differential pair production cross section is

$$\begin{aligned}\sigma_{p.p.}(E^{'} \rightarrow E, \mu) &= \frac{d^2\sigma_{p.p.}(E^{'}, Z)}{dEd\mu} \\ &= \frac{[\sigma_{p.p.}(E^{'}, Z) + \sigma_{t.p.}(E^{'}, Z)]\delta(E - m_e c^2)}{2}\end{aligned}$$

- The adjoint pair production cross section is therefore

$$\begin{aligned}\sigma^{\dagger}_{p.p.}(E^{'} \rightarrow E, \mu) &= \frac{d^2\sigma^{\dagger}_{p.p.}(E^{'}, E, Z)}{dEd\mu} \\ &= 2\left[\frac{[\sigma_{p.p.}(E, Z) + \sigma_{t.p.}(E, Z)]\,\delta(E^{'} - m_e c^2)}{2}\right]\end{aligned}$$

The Adjoint Pair Production Cross Section

$$\frac{d^2\sigma^{\dagger}_{p.p.}(E^{'},E,Z)}{dEd\mu} = 2\left[\frac{\left[\sigma_{p.p.}(E,Z)+\sigma_{t.p.}(E,Z)\right]\delta(E^{'}-m_ec^2)}{2}\right]$$

- The two annihilation photons are taken into account with the factor of 2
- Unless the adjoint photon energy is m_ec^2 this cross section is zero
- A modification to the adjoint random walk process is made which forces adjoint photons to have energy m_ec^2
- The modification is rather complicated but is fairly computationally inexpensive

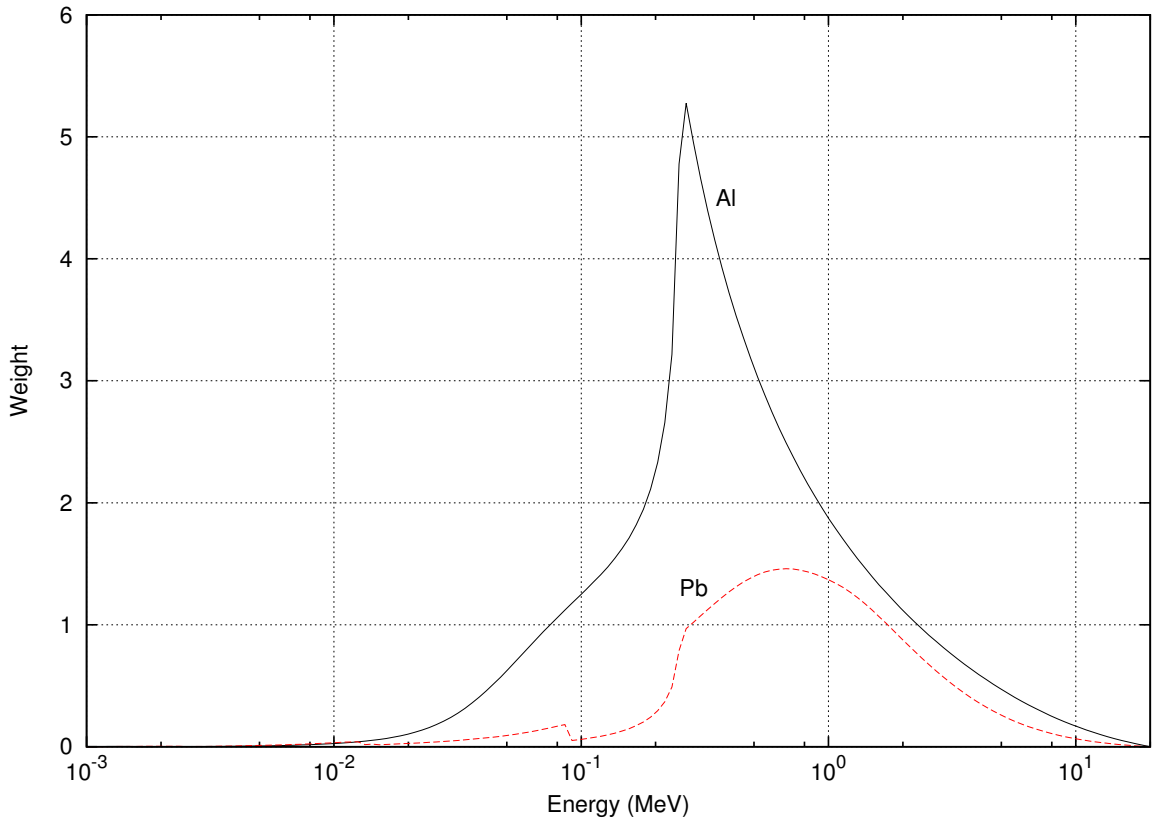
Current Limitation: The Photoelectric Effect

- **Problem:**
  - Photoelectric effect occurs when a photon is absorbed by an atom
  - An electron is ejected leaving an electron shell vacancy
  - Atomic relaxation occurs to fill the vacancy with x-rays potentially released
  - Emitted x-rays can be important for certain problems (e.g. brachytherapy seed characterization)
  - The adjoint process cannot currently take these x-rays into account

- **Possible Solution:** Compute x-ray production cross sections for which equivalent adjoint cross sections can be computed

The Adjoint Photon Weight Factor

- Important feature of the adjoint process.
- Bound to the interval $(0,\infty)$ instead of (0,1)
- Can negatively effect the statistics of the random walks.
- Thorough characterization of its effects must be completed.



Outline

FACEMC Code Requirements

- **Energy Range:**
  - 1 keV - 20 MeV for photons and adjoint photons
  - 10^{-5} eV - 20 MeV for neutrons and adjoint neutrons
- **Spatial Domain Modeling:** CAD based (primarily)
  - Accomplished with the direct accelerated geometry (DAG) package
- **Variance Reduction:** implicit capture, Russian roulette, splitting, forced collisions, weight windows
  - Weight windows must be user generated
- **Parallelism:** domain replication

FACEMC Validation Plan

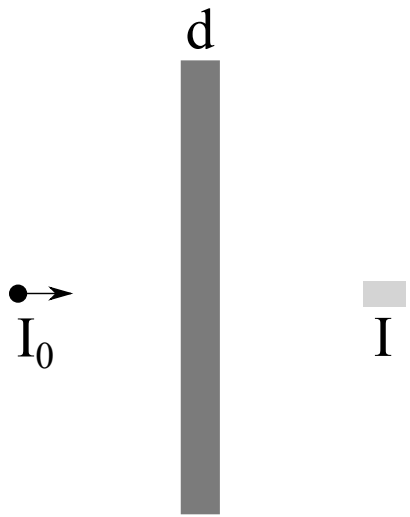
1. **Benchmarking:** simulation of benchmark test problems for photons and neutrons

2. **Code-to-Code Comparisons:** calculate integral quantities and spectra and compare against other validated Monte Carlo codes

3. **Intra-Code Comparisons:** calculate integral quantities and spectra using FACEMC forward and adjoint simulations

FACEMC Validation Plan: Step 1

- **GEANT4 Photon Benchmark Problem:** calculate mass attenuation coefficients and partial interaction coefficients
- Results will be compared to NIST values

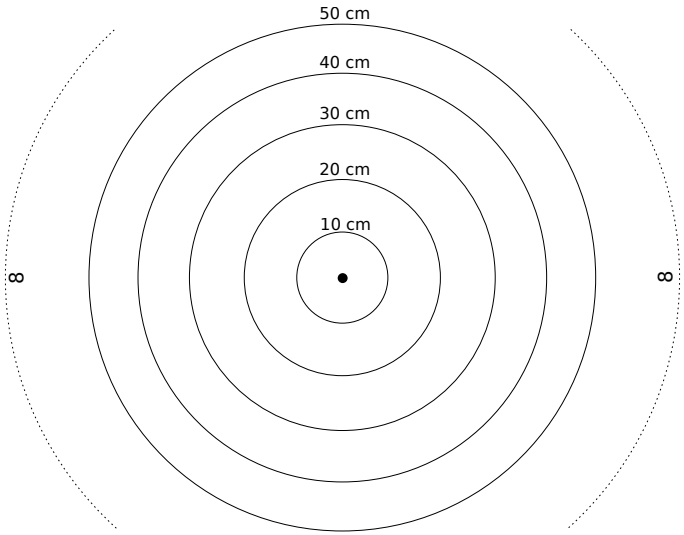


$$\left(\frac{\mu}{\rho}\right) = -\frac{1}{\rho d} \ln\left(\frac{I}{I_0}\right)$$

- For neutrons, several experiments from the Shielding Integral Benchmark Archive Database (SINBAD) will be modeled

FACEMC Validation Plan: Step 2

- **Problem Geometry:**



- **Source:**
  - isotropic point source with several discrete energies (photons)
  - isotropic point source with a fission spectrum (neutrons)
- **Quantities:** Flux spectrum and total flux at each spherical surface
- **Comparison Codes:** PENELOPE, MCNP5 and TART2005

FACEMC Validation Plan: Step 3

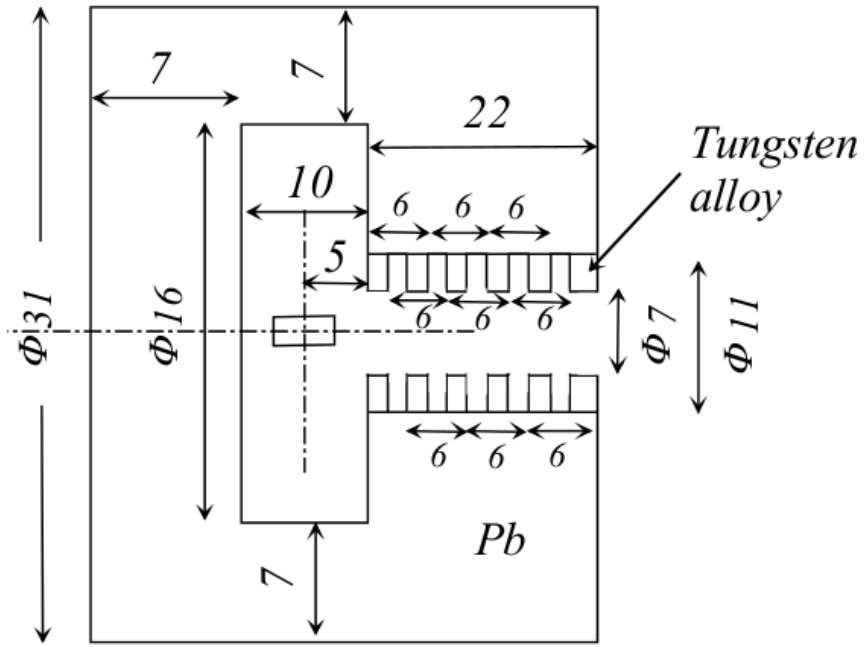
- **Problem Geometry:** same as FACEMC validation plan step 2
  - Due to unique symmetry, the adjoint problem can be constructed identically to the forward problem (point source)

- **Source:** isotropic point source with several discrete energies (photons and adjoint photons)

- **Quantities:** Flux spectrum and total flux at each spherical surface

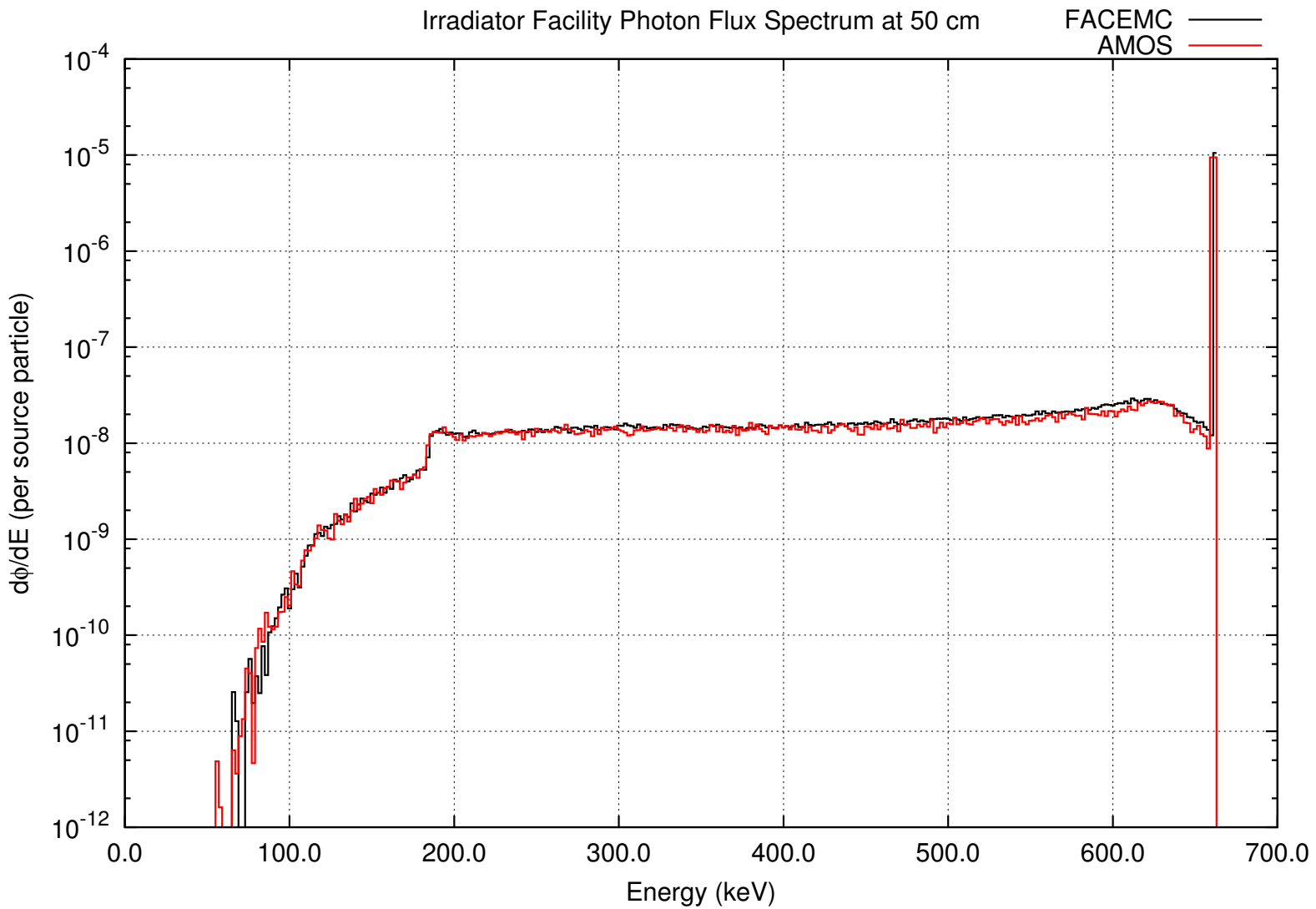
Preliminary Validation of FACEMC: AMOS Comparison

- **Problem Geometry:** simple irradiation facility
  - The source is located behind the tungsten alloy collimator.



- **Source:** isotropically emitting Cs-137 gamma source
- **Quantity:** flux spectrum 50 cm from center of source (on axis)
- **Comparison Code:** AMOS (TU Dresden research code)

AMOS Comparison Results

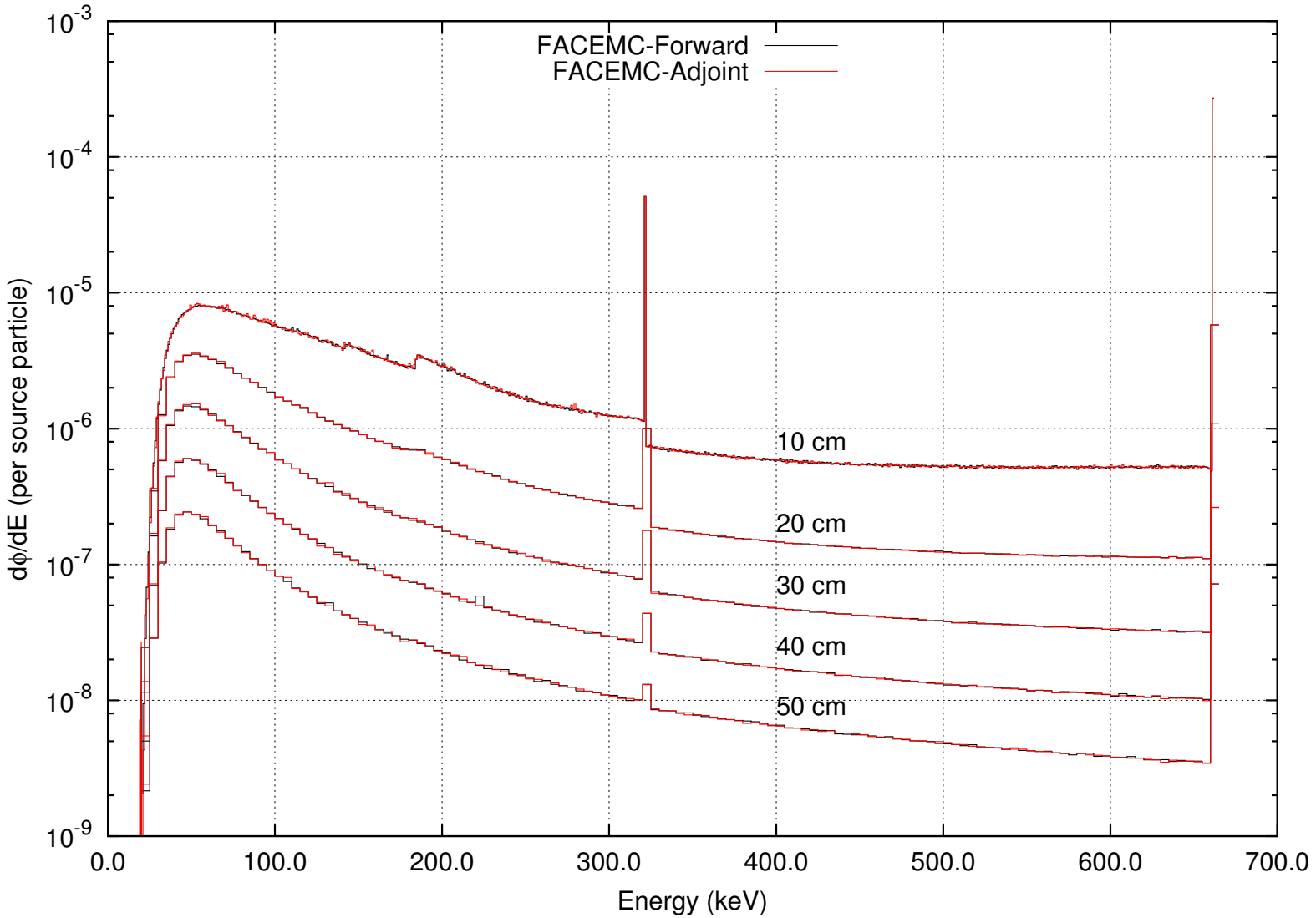


Preliminary Validation of FACEMC: Forward vs. Adjoint

- **Problem Geometry:** same as FACEMC validation step 3
- **Source:** isotropic point source emitting at 661.66 keV (80%) and 321.0 keV (20%)
- **Material:** water
- **Number of histories:** 10^7

Distance (cm)	Flux (for. mode)	Relative Error	Flux (adj. mode)	Relative Error	% Diff.
10	1.5748e-3	0.0007	1.5788e-3	0.0014	0.25
20	4.1291e-4	0.0007	4.1491e-4	0.0018	0.48
30	1.4150e-4	0.0007	1.4235e-4	0.0022	0.60
40	5.2255e-5	0.0011	5.2322e-5	0.0027	0.13
50	1.9963e-5	0.0014	2.0030e-5	0.0033	0.34

Forward vs. Adjoint Spectrum Results



Outline

Future work on FACEMC: Development

1. Solve the low energy x-ray emission problem for adjoint photons
2. Complete background work on neutron and adjoint neutron transport cross sections and sampling techniques
3. Complete coding of the second version of all major FACEMC components
4. Complete the computation of adjoint neutron cross sections and storage in an HDF5 format library
5. Complete the FACEMC validation plan
6. Characterize the effect of the adjoint weight factor on the variance of the adjoint process

Future work on FACEMC: Challenge Problems

1. Calculate the adjoint data required for brachytherapy treatment planning optimization using data from a patient
2. Calculate the adjoint data required for external beam treatment planning using a standard phantom
3. Run a full scale shutdown dose calculation for a fusion device using the R2SA method
4. Run a fusion shielding problem using the adjoint neutron transport capabilities of FACEMC

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