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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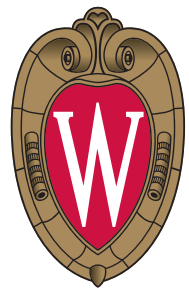

Outline

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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

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

The Adjoint Process

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

Motivations for using the adjoint process

- The motivation for using the adjoint process can separated into two catagories:
  1. One based on the phase space of the source and detector
  2. One based on the physical interpretation of the quantity that is estimated during the adjoint process

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

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

Shutdown dose calculations using the R2S method

- The 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

- The neutron flux throughout the experiment or device is calculated.
- An activation code calculates the material activation and photon sources from the neutron flux data.
- The photon dose is calculated in areas of interest using a forward process.

Shutdown dose calculations using the R2SA method

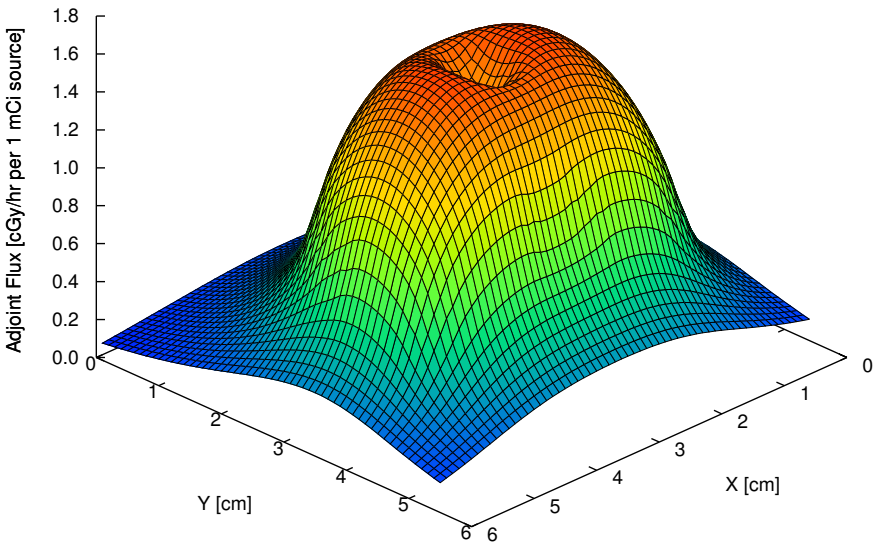
- In shutdown dose calculations, the amount of activated material is often much larger than the region where the dose distribution is desired.
- These problems could potentially benefit from the adjoint process for photons.
- When the adjoint process is used, the solution method is called the rigorous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

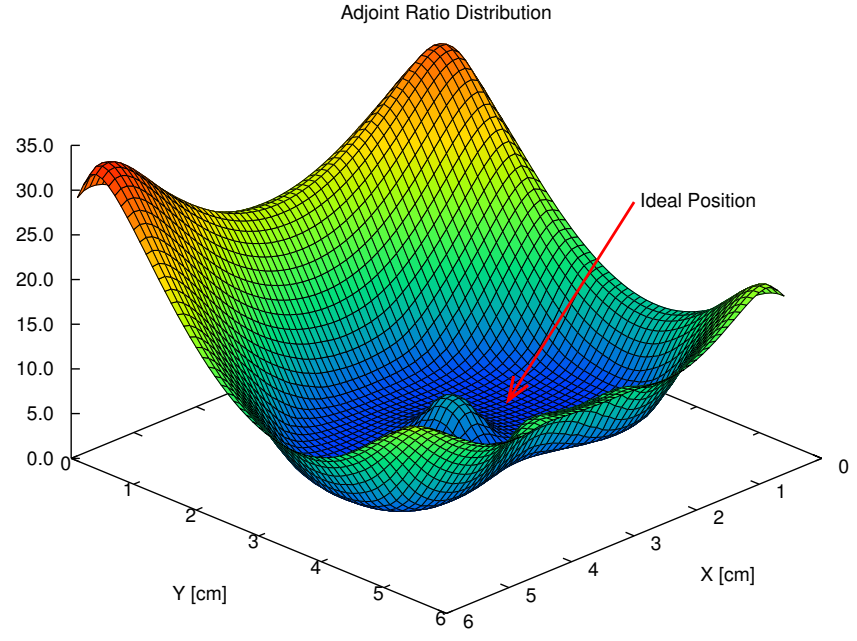
The R2SA method

- The neutron flux throughout the experiment or device is calculated.
- An activation code calculates the material activation and photon sources from the neutron flux data.
- The photon dose is calculated in areas of interest using an adjoint process

Permanent implant brachytherapy

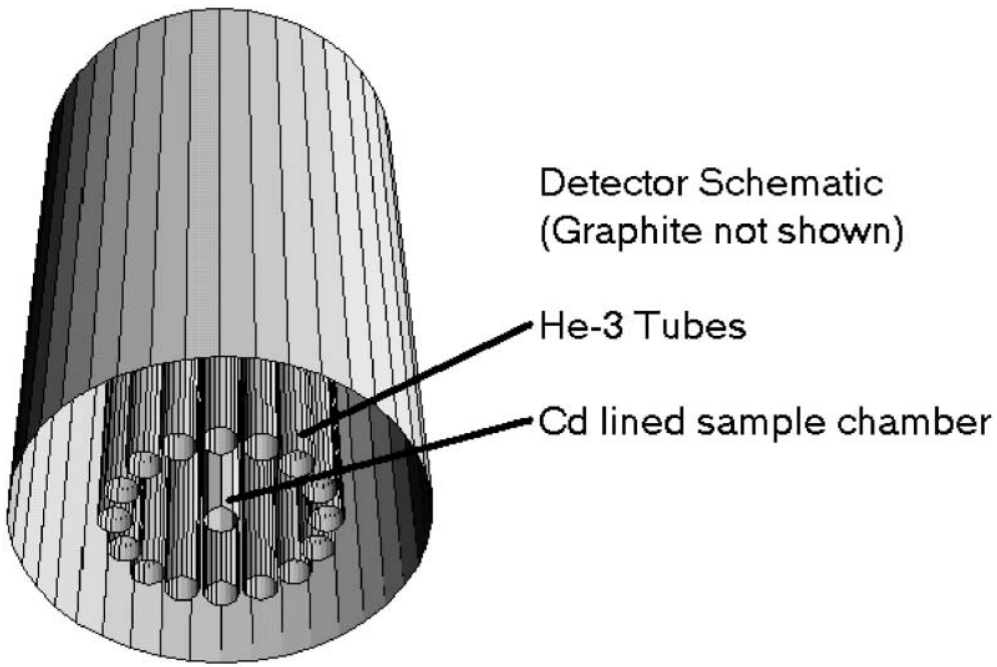
- **Optimization goal:** determine a source configuration that provides an optimal dose distribution to the target while minimizing the dose to sensitive structures.
- Adjoint flux data allows one to eliminate source positions that result in a high dose to sensitive structures relative to the target,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



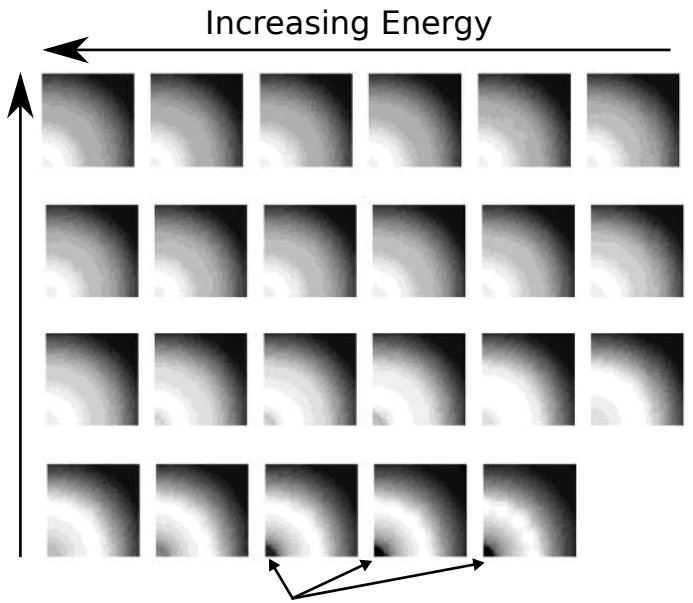


Detector design

- The adjoint flux can allow for the spectral performance of a detector to be predicted for an arbitrary source distribution.
- This data allows the detector design to be optimized before it is constructed, which is 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 deterent to implementing the adjoint process on a continouous energy scale.

Outline

Fredholm Integral Equations of the second kind (FIESKs)

The FIESK

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

- The function $S(x)$ is a forcing function.
- The function $K(x, y)$ is the kernel of the integral equation
- $K(x, y)$ characterizes the transition from some initial state y to the state x.
- It is often written as $K(y \to x)$ to signify this interpretation.

The Volterra integral equation of the second kind

- This equation is very similar to the FIESK except one limit of integration is variable.
- This equation comes about whenever there is a preferred direction for the independent variable (i.e. particle scattering kinematics)
- It can be written as a FIESK using a modified kernel

The Volterra integral equation of the second kind

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

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

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

Analytical solution method for a FIESK

The method of successive approximations

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

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

$$\begin{aligned} F(x) &= \lim_{n \to \infty} f_n(x) \\ &= S(x) + \lambda \int_a^b K(y \to x) S(y) dy + \\ &\quad \lambda^2 \int_a^b \int_a^b K(y \to x) K(y_1 \to y) S(y_1) dy_1 dy + \\ &\quad \lambda^3 \int_a^b \int_a^b \int_a^b K(y \to x) K(y_1 \to y) K(y_2 \to y_1) S(y_2) dy_2 dy_1 dy + \\ &\quad \dots \end{aligned}$$

Numerical solution method for a FIESK

The Monte Carlo random walk process

$$\text{Random Walk:} \begin{cases} p^1(x) & = p(x_1 = x) \\ p(y \to x) & = p(x_{n+1} = x | x_n = y, k > n) \\ p(x) & = p(k = n | x_n = x). \end{cases}$$

- $p^1(x)$ characterizes the probability that the first event of a random walk occurs in state x.
- $p(y \to x)$ characterizes the probability of a transition from an initial state y to a new state x.
- $p(x)$ represents the probability of termination in a state x.
- The above probability distribution functions (PDFs) must have the following properties:
  1. $p^1(x) \geq 0$
     $\int_\Gamma p^1(x) dx = 1$
  2. $p(y \to x) \geq 0$
     $\int_\Gamma p(y \to x) dx = q(y) = 1 - p(y).$

Proof that the Monte Carlo method recovers the solution

- First define the event density as the expected value of the number density of events that happen in state x:

$$P(x) = 1 \cdot P^1(x) + 1 \cdot P^2(x) + \ldots = \sum_{n=1}^{\infty} P^n(x)$$

$$P^1(x) = p^1(x)$$

$$P^n(x) = \int_\Gamma p(y \to x) P^{n-1}(y) dy.$$

- Using the event density and the Monte Carlo method, the solution to a FIESK is recovered:

$$P(x) = \sum_{n=1}^{\infty} P^n(x) = p^1(x) + \int_\Gamma p(y \to x) \sum_{n=2}^{\infty} P^{n-1}(y) dy$$

$$= p^1(x) + \int_\Gamma p(y \to x) P(y) dy.$$

The transport equation

$$\frac{1}{v}\frac{\partial\varphi(\vec{r},E,\hat{\Omega},t)}{\partial t}+\hat{\Omega}\cdot\vec{\bigtriangledown}\varphi(\vec{r},E,\hat{\Omega},t)+\Sigma_T(\vec{r},E)\varphi(\vec{r},E,\hat{\Omega},t)=$$
$$S(\vec{r},E,\hat{\Omega},t)+\int\int\Sigma_T(\vec{r},E^{'}\rightarrow E,\hat{\Omega}^{'}\rightarrow\hat{\Omega})\varphi(\vec{r},E^{'},\hat{\Omega}^{'},t)dE^{'}d\hat{\Omega}^{'}$$

- The transport equation describes the expected behavior of particles in a medium.
- This equation must be converted to a FIESK to derive a Monte Carlo random walk process.
- First define the emission density $\chi(\vec{r},E,\hat{\Omega})$, which is the expected density of particles exiting a collision or the source, as

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

Converting the transport equation to an integral form

- The method of characteristics will be used to convert the transport equation to an integral form:

$$\vec{r}^{\,\prime} = \vec{r} - R\hat{\Omega}.$$

- A directional derivative along the characteristic can be determined:

$$\begin{aligned}\frac{d}{dR} &= \frac{dx^{\prime}}{dR}\frac{\partial}{\partial x} + \frac{dy^{\prime}}{dR}\frac{\partial}{\partial y} + \frac{dz^{\prime}}{dR}\frac{\partial}{\partial z} \\ &= -\Omega_x\frac{\partial}{\partial x} - \Omega_y\frac{\partial}{\partial y} - \Omega_z\frac{\partial}{\partial z} \\ &= -\hat{\Omega}\cdot\vec{\nabla}.\end{aligned}$$

- The transport equation becomes

$$-\frac{d}{dR}\varphi(\vec{r}^{\,\prime}, E, \hat{\Omega}) + \Sigma_T(\vec{r}^{\,\prime}, E)\varphi(\vec{r}^{\,\prime}, E, \hat{\Omega}) = \chi(\vec{r}^{\,\prime}, E, \hat{\Omega}).$$

The transport equation in integral form

- Using the following integrating factor, the transport equation can be converted to an integral form:

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

- By integrating the equation from 0 to ∞ and assuming that the flux goes to zero as R goes to ∞, the integral equation is obtained:

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

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

The emission density FIESK

- To construct the emission density FIESK, the integral transport equation will be substituted into the equation for the emission density:

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

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

- The kernel of the emission density FIESK is

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

- This kernel can be simplified by introducing two new kernels.

The transport kernel

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

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

$$\cdot \frac{\delta\left(\hat{\Omega} - \left[\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}\right]\right)}{|\vec{r} - \vec{r}'|^2}$$

- This kernel describes the movement of particles through space.
- It is normalized to unity and can thus be used as a PDF for sampling new particle positions.
- The quantity $T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega})dV$ can be interpreted as the probability that a particle at $\vec{r}'$ with energy E and direction $\hat{\Omega}$ will have its next collision in volume element dV at $\vec{r}$.
- Due to the factor $\Sigma_T(\vec{r}, E)$, a new position $\vec{r}$ will never be sampled in a vacuum.

The collision kernel

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

- This kernel describes the movement of particles through energy and direction.
- 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 $\psi(\vec{r}, E, \hat{\Omega})$ is the expected density of particles entering a collision.
- It is related to the emission density by

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

- 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

- The following PDFs govern the Monte Carlo random walk process for the emission density and collision density:

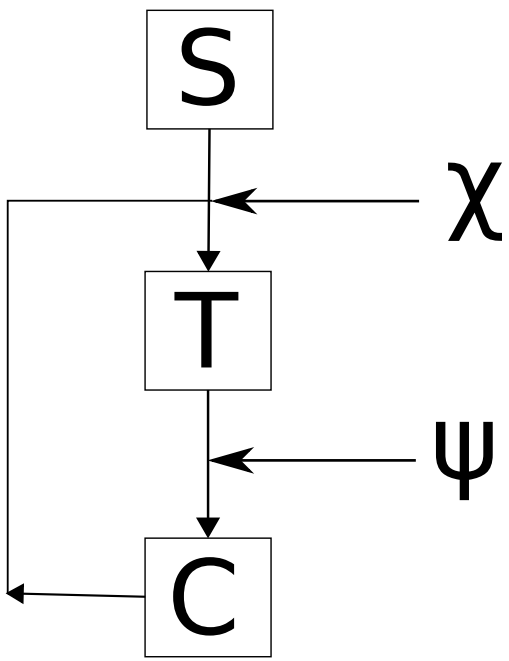
$$\chi(x) \text{ Random Walk: } \begin{cases} p^1(x) & = \frac{S(x)}{\int_\Gamma S(x)dx} \\ p(y \to x) & = K(y \to x) \\ p(x) & = 1 - \overline{P}_{NA}(x), \end{cases}$$

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

- $P_{NA}(x) = \frac{\Sigma_s(\vec{r},E')}{\Sigma_T(\vec{r},E')}$ is the non-absorption or survival probability.
- $\overline{P}_{NA}(x)$ 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 state transition kernels for the emission density and the collision density only differ in the ordering of the transport and collision kernels.
- They can therefore be estimated during the same random walk process.



Derivation of the adjoint transport equation

- An adjoint operator is defined by the following relationship:

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

- The transport equation can be written in an operator form:

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

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

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

- If $H_B^\dagger \cdot \varphi^\dagger$ is set equal to the response function, the material response becomes

$$\begin{aligned} R &= \langle \varphi r \rangle = \langle \varphi H_B^\dagger \cdot \varphi^\dagger \rangle \\ &= \langle \varphi^\dagger H_B \cdot \varphi \rangle = \langle \varphi^\dagger S \rangle. \end{aligned}$$

The adjoint transport equation

- Using the transport equation in operator form and the definition of the adjoint operator, the adjoint transport equation can be derived.
- The adjoint transport equation is

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

- The adjoint emission denisty will be defined as

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

- The simplified adjoint transport equation is

$$-\hat{\Omega}\cdot\vec{\bigtriangledown}\varphi^{\dagger}(\vec{r},E,\hat{\Omega})+\Sigma_T(\vec{r},E)\varphi^{\dagger}(\vec{r},E,\hat{\Omega})=\theta^{\dagger}(\vec{r},E,\hat{\Omega}).$$

The adjoint transport equation in integral form

- Using a very similar process to the one used for the transport equation the adjoint transport equation can be converted to an integral form:

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

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

The adjoint emission density FIESK

- To construct the adjoint emission density FIESK, the integral adjoint transport equation will be 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

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

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

$$\cdot \frac{\delta\left(\Omega - \left[\frac{\vec{r}'-\vec{r}}{|\vec{r}'-\vec{r}|}\right]\right)}{|\vec{r}' - \vec{r}|^2}$$

- This kernel describes the movement of adjoint particles through space.
- It is normalized to unity and can thus be used as a PDF for sampling new particle positions.
- The quantity $T^{\dagger}(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega})dV$ can be interpreted as the probability that an adjoint particle at $\vec{r}'$ with energy E and direction $\hat{\Omega}$ will have its next collision in volume element dV at $\vec{r}$.

The adjoint collision kernel

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

- This kernel describes the movement of adjoint particles through energy and direction.
- The normalization factor for this kernel will be referred to simply as the total macroscopic adjoint cross section.
- To derive a sampling procedure for this kernel, it must be expanded into its constituent reactions.

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 of this kernel, 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

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

$$
\begin{aligned}
M^{\dagger}(y \rightarrow x) &= M^{\dagger}(\vec{r}^{\,\prime} \rightarrow \vec{r}, E^{\prime} \rightarrow E, \hat{\Omega}^{\prime} \rightarrow \hat{\Omega}) \\
&= \Sigma_T(\vec{r}, E \rightarrow E^{\prime}, \hat{\Omega} \rightarrow \hat{\Omega}^{\prime}) \tau^{\dagger}(\vec{r}^{\,\prime}, \vec{r}, E^{\prime}, \hat{\Omega}^{\prime}) \\
&= \left[\frac{\Sigma_T(\vec{r}, E \rightarrow E^{\prime}, \hat{\Omega} \rightarrow \hat{\Omega}^{\prime})}{\Sigma^{\dagger}(\vec{r}, E^{\prime})} \right] \left[\frac{\Sigma^{\dagger}(\vec{r}, E^{\prime})}{\Sigma_T(\vec{r}, E^{\prime})} \right] \\
&\quad \cdot \left[\Sigma_T(\vec{r}, E^{\prime}) \tau^{\dagger}(\vec{r}^{\,\prime}, \vec{r}, E^{\prime}, \hat{\Omega}^{\prime}) \right] \\
&= C^{\dagger}(\vec{r}, E^{\prime} \rightarrow E, \hat{\Omega}^{\prime} \rightarrow \hat{\Omega}) P^{\dagger}(\vec{r}, E^{\prime}) T^{\dagger}(\vec{r}^{\,\prime} \rightarrow \vec{r}, E^{\prime}, \hat{\Omega}^{\prime}).
\end{aligned}
$$

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

The adjoint collision density FIESK

- The adjoint collision density $\xi^\dagger(\vec{r}, E, \hat{\Omega})$ is the expected density of adjoint particles entering a collision.
- It is related to the adjoint emission density by

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

- 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 for adjoint radiation

- The following PDFs govern the Monte Carlo random walk process for the adjoint emission density and the adjoint collision density:

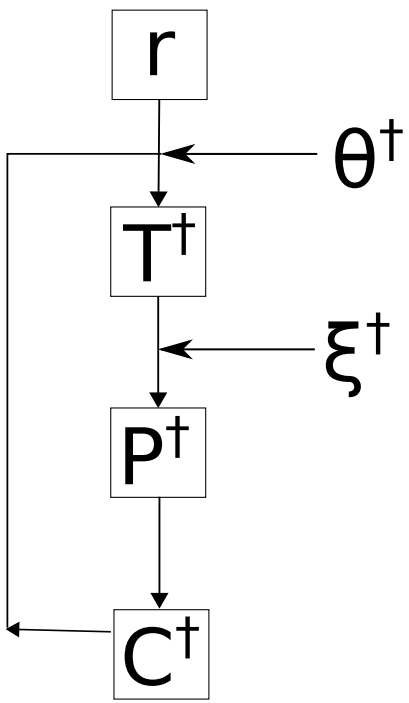
$$\theta^\dagger(x) \text{ Random Walk: } \begin{cases} p^1(x) & = \frac{a(x)}{\int_\Gamma a(x)dx} \\ p(y \to x) & = \frac{M^\dagger(y \to x)}{\overline{P}^\dagger(y)} \\ p(x) & = 0 \end{cases}$$

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

- Due to the definition of the adjoint cross section, there is no absorption reaction for adjoint radiation.
- 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 state transition kernels for the emission density and the collision density only differ in the ordering of the adjoint transport kernel, adjoint collision kernel, and adjoint weight factor.
- They can therefore be estimated during the same random walk process.



Outline

Developing the adjoint incoherent scattering cross section

- To conduct adjoint incoherent scattering, the cross section for this interaction must be derived:

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

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

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

- 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

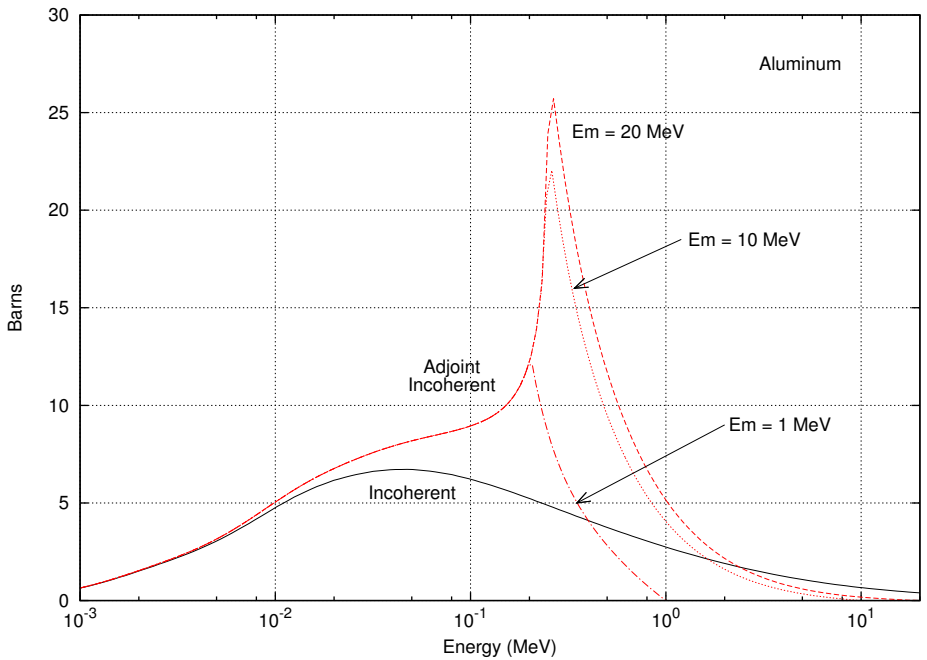
$$\sigma^{\dagger}_{i.s.}(E^{'} \rightarrow E, \mu) = \frac{\pi r_e^2}{m_e c^2 \alpha^2} \left[\frac{\alpha^{'}}{\alpha} + \frac{\alpha}{\alpha^{'}} - 1 + \mu^2 \right] S\left(y(\alpha, \mu), Z\right)$$
$$\cdot \delta\left(\mu - \left[1 - \frac{1}{\alpha^{'}} + \frac{1}{\alpha}\right]\right).$$

The integrated adjoint incoherent scattering cross section

- The scattering kinematics of the adjoint interaction have an interesting property:

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

- There is a discontinuity when $\mu = 1 - \frac{1}{\alpha'}$, which results in an unbound integrated cross section.
- A max problem energy must be set to bound the integrated cross section.



The adjoint coherent scattering cross section

- To conduct adjoint coherent scattering, the cross section for this interaction must be derived.
- The forward and adjoint cross sections are only dependent on the angle between the initial and final directions.
- In addition, the energy of the photon does not change in a forward coherent scatter:

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

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

$$\frac{d\sigma_{c.s.}(\alpha^{'}, \mu, Z)}{d\mu} = \frac{d\sigma^{\dagger}_{c.s.}(\alpha^{'}, \mu, Z)}{d\mu}$$
$$= \pi r_e^2 (1 + \mu^2) F^2(y, Z).$$

Developing the adjoint pair production cross section

- To conduct adjoint pair production, the cross section for this interaction must be derived.
- As with all other photon cross sections, these cross sections are only depenedent on the angle between the initial and final directions:

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

- The simplified double differential pair production cross section is

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

The adjoint pair production cross section

- The adjoint pair production cross section is

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

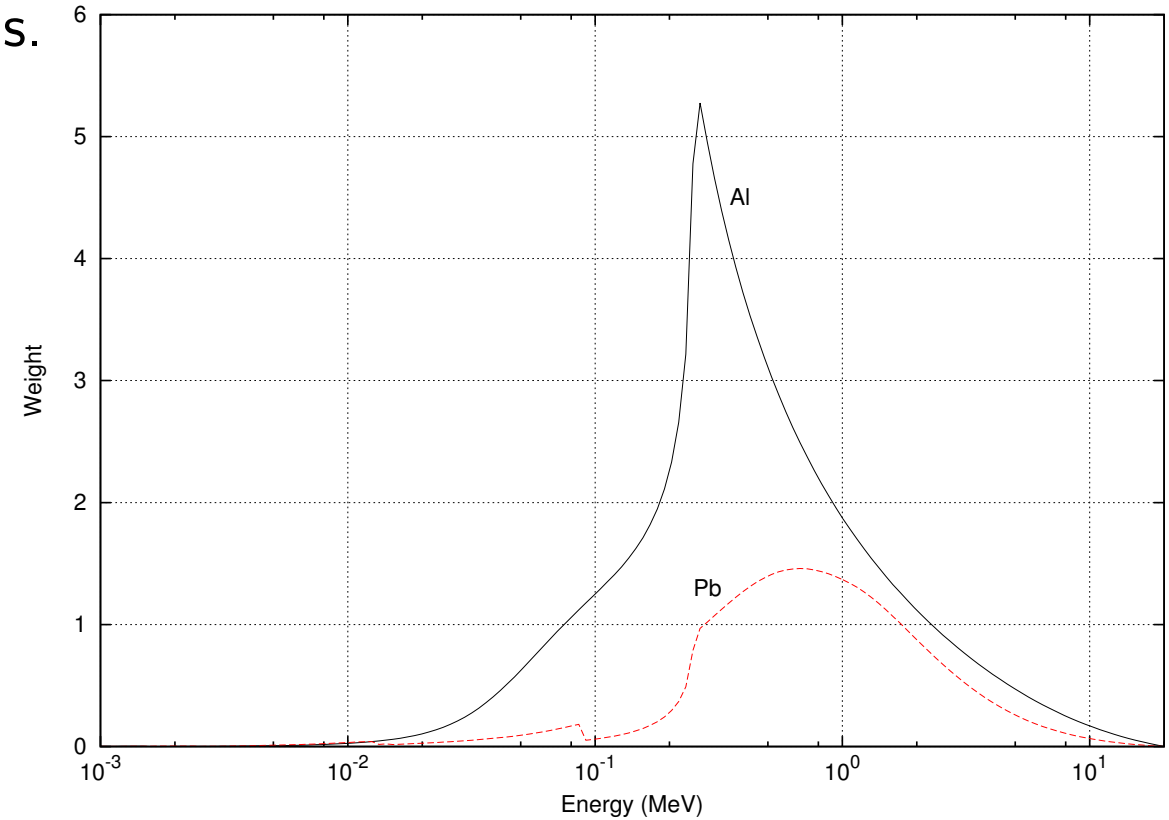
- The adjoint double differential pair production cross section will be zero unless the initial energy of the adjoint photon is equal to $m_e c^2$.
- A modification to the adjoint Monte Carlo random walk process must be made for adjoint photons to model adjoint pair production.
- The modification is rather complicated and will not be discussed further in this presentation.

The photoelectric effect

- The photoelectric effect occurs when a photon of energy E is absorbed by a target atom.
- An electron will be ejected leaving an electron shell vacancy.
- Atomic relaxation will occur to fill the vacancy, which has the potential to release x-rays.
- These x-rays can be important for certain problems (e.g. brachytherapy seed characterization).
- The adjoint process cannot currently take these x-rays into account since there is not an equivalent adjoint reaction.

The adjoint photon weight factor

- The adjoint weight factor is an important feature of the adjoint process.
- Because it is bound to the interval $(0,\infty)$ instead of $(0,1)$ it can negatively effect the statistics of the random walks.
- Many test problems will need to be run to characterize the effect for adjoint photons.

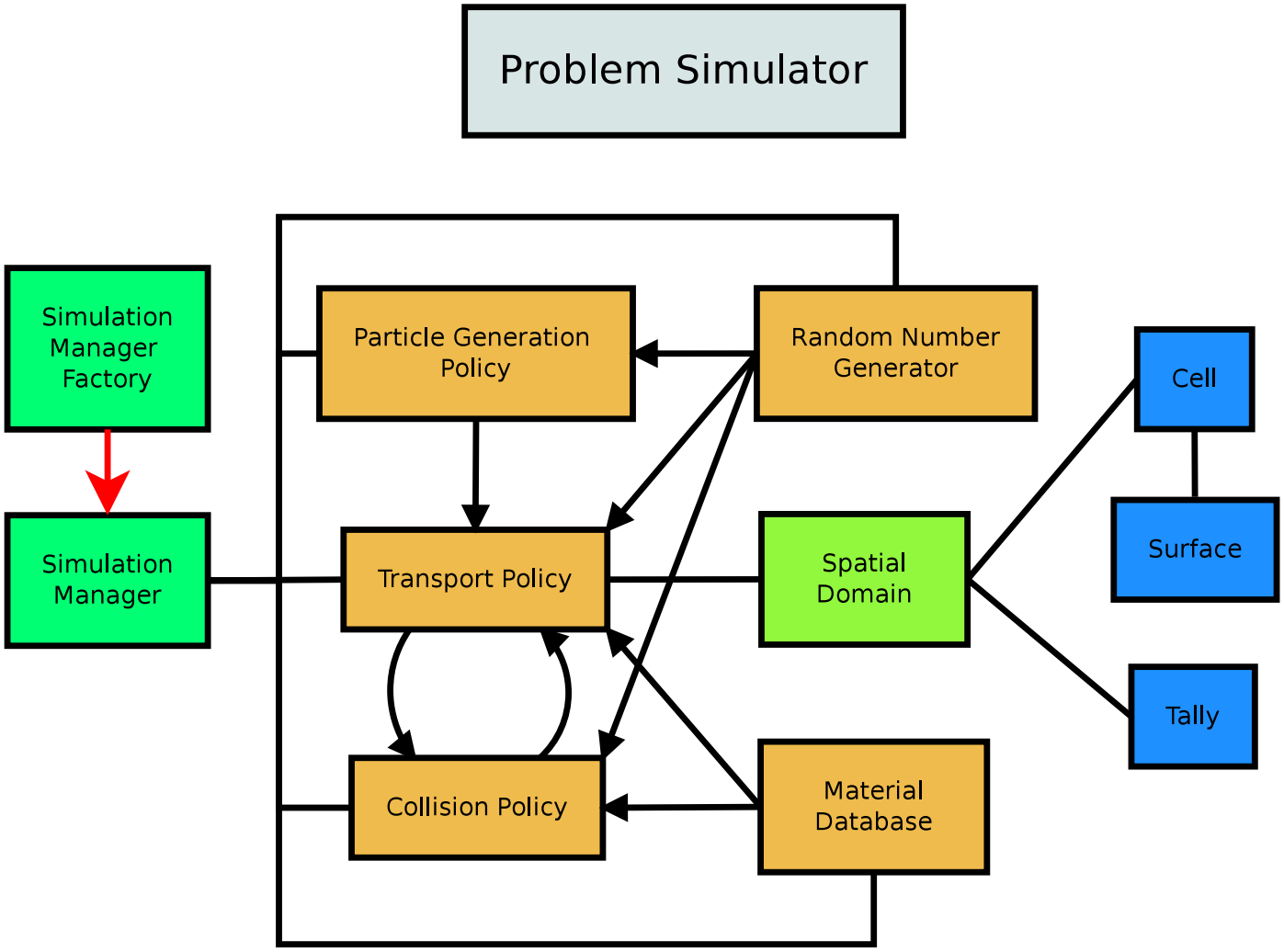


Outline

FACEMC code requirements

- The FACEMC code will be able to model photons and adjoint photons in the energy range of 1 keV to 20 MeV.
- The FACEMC code will also be able to model neutrons and adjoint neutrons in the energy range of 10^{-5} eV to 20 MeV.
- The direct accelerated geometry (DAG) package will primarily used for spatial domain modeling.
- The main variance reduction techniques that will be available are Russian roulette, splitting, and weight windows.
- The code will be able to run in parallel using domain replication only.

Major Components of FACEMC



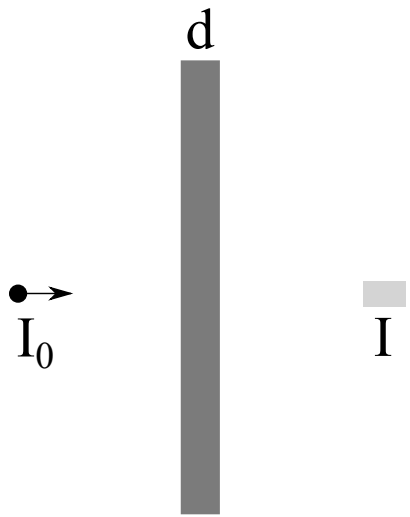
- FACEMC version 1.0 is currently complete.

FACEMC validation plan

- The following validation plan has been created to ensure that FACEMC functions properly:
  1. Calculation of benchmark test problems for photons and neutrons
  2. Code-to-code comparisons of integral quantities and photon or neutron spectra against other Monte Carlo codes that have been previously validated
  3. Comparison of integral quantities and spectra from forward and reverse simulations
- Each step will be elaborated upon.

FACEMC validation plan step 1

- The same benchmark problem that was used to validate GEANT4 photon simulations will be used with FACEMC.
- In this problem, photon mass attenuation coefficients and partial interaction coefficients will be calculated and compared to NIST values

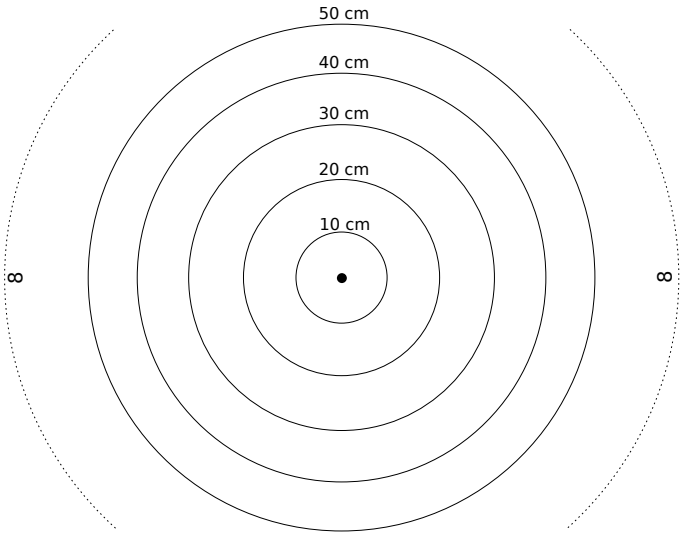


$$\left(\frac{\mu}{\rho}\right) = -\frac{1}{\rho d}\ln\left(\frac{I}{I_0}\right)$$

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

FACEMC validation plan step 2

- A code-to-code comparison problem has been created to test FACEMC agains codes that have already been validated:



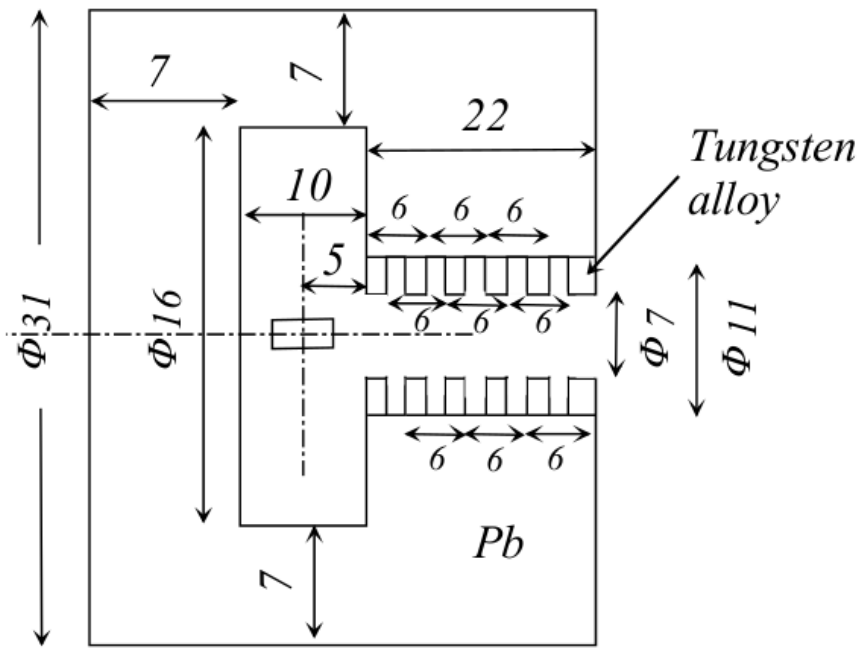
- For photons, an isotropic point source with two discrete energies will be modeled.
- For neutrons, an isotropic point source with a fission spectrum will be modeled.
- PENELOPE, MCNP5 and TART2005 will be the codes that are tested against.

FACEMC validation plan step 3

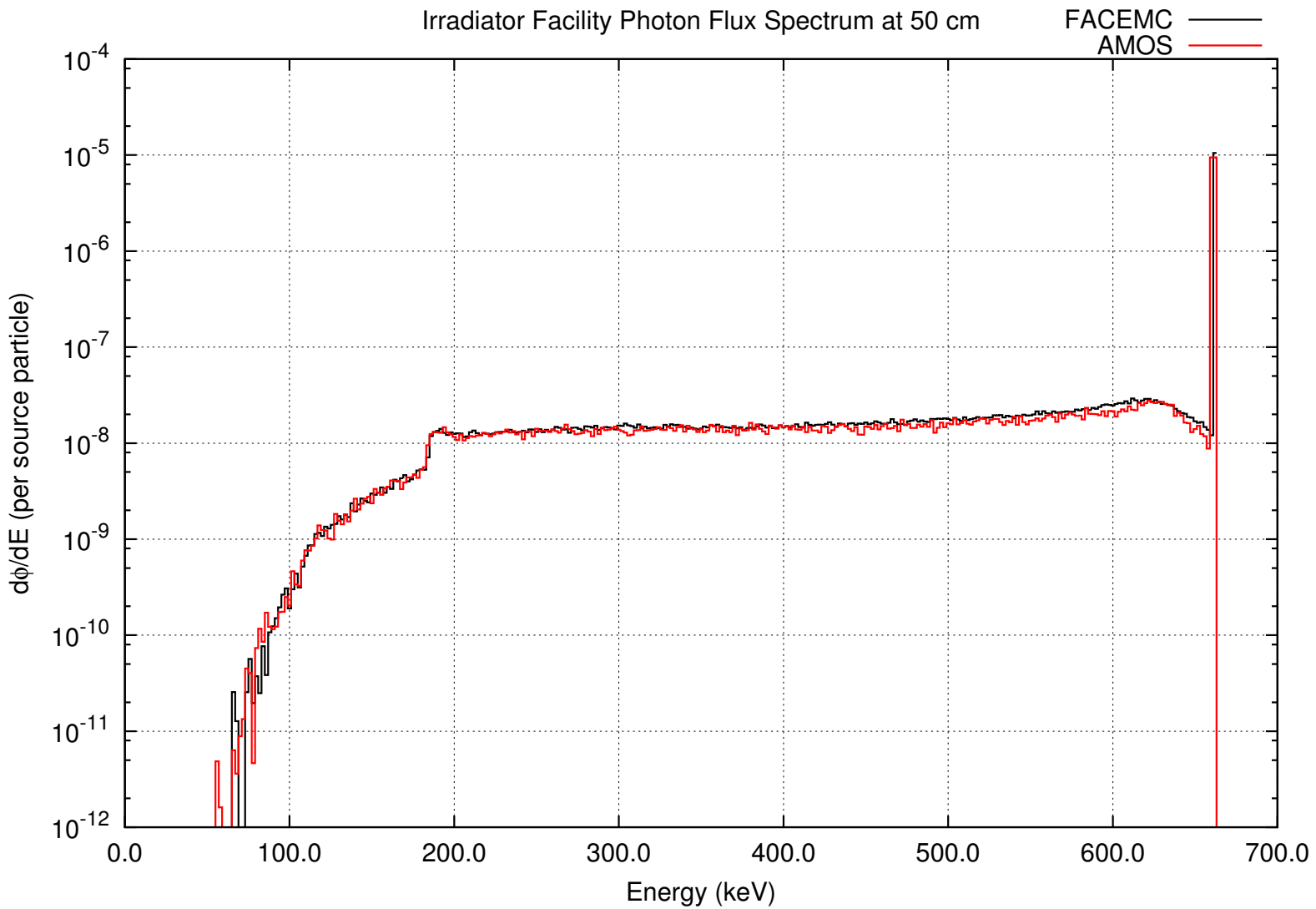
- The third step of the validation plan will focus on comparisons between forward and adjoin calculations using FACEMC only.
- The problem from step 2 will be used.
- Due to unique symmetry in that problem, the adjoint problem can be constructed identically to the forward problem.
- A proof of this symmetry is lengthy and will not be shown in this presentation.

Preliminary validation of FACEMC: AMOS comparison

- A comparison to the AMOS code was made using a simple model of an irradiation facility.
- A Cs-137 gamma source is located behind the tungsten alloy collimator.
- The flux spectrum 50 cm from the center of the source on the axis of the source was calculated.



AMOS comparison results

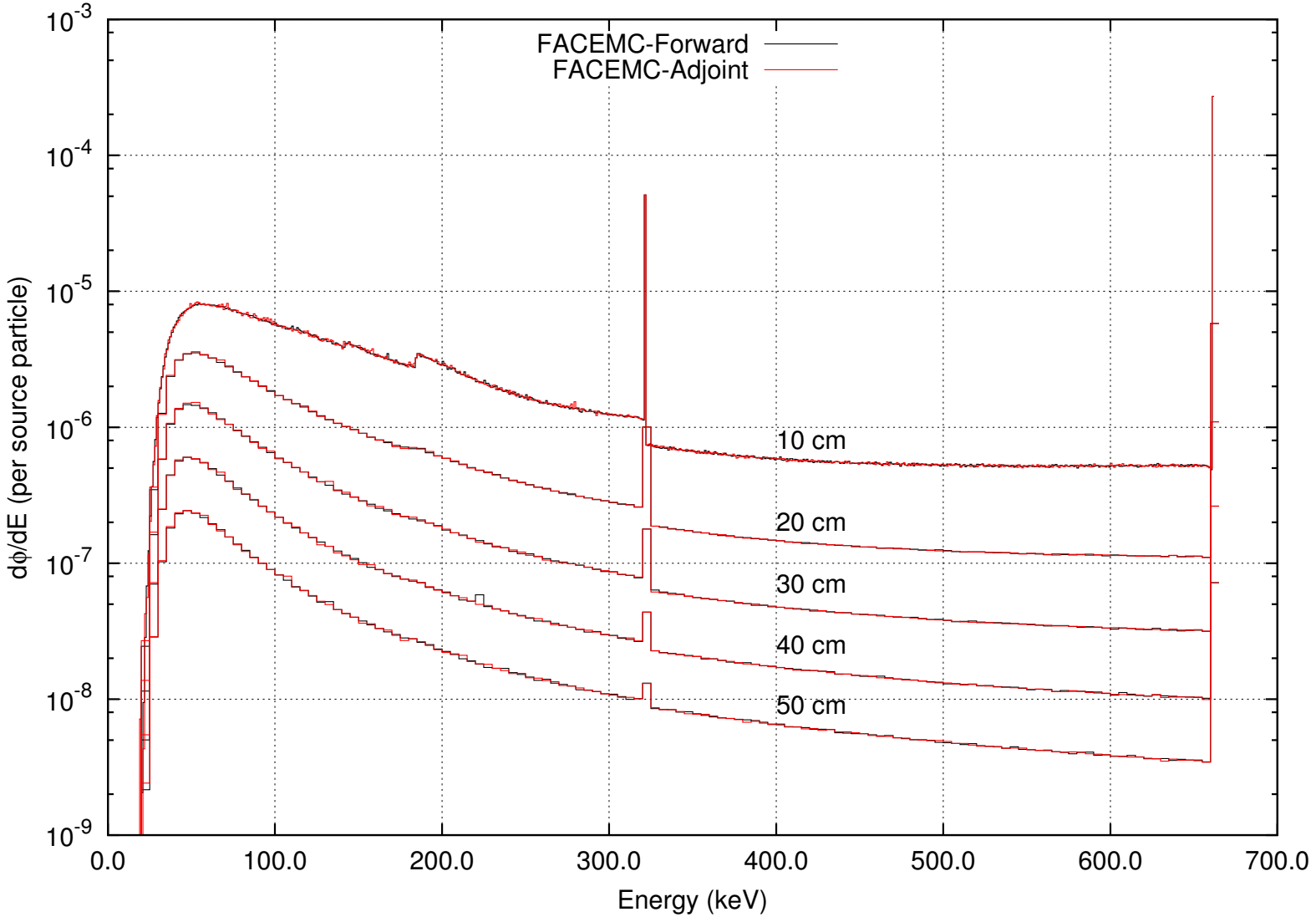


Preliminary validation of FACEMC: forward vs. adjoint

- The problem from validation step 3 was used.
- **Source energies:** 661.66 keV, 321.0 keV
- **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 work:**
  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.
- **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 shielding problem using the adjoint neutron transport capabilities of FACEMC.