

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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1 Introduction

- The Monte Carlo Method

- Motivations for using the adjoint process

- Monte Carlo codes available today

2 The Monte Carlo Random Walk Process

- General Monte Carlo theory

- The Monte Carlo random walk process for radiation transport

- The Monte Carlo random walk process for adjoint radiation transport

3 Adjoint Photon Cross Sections

- Adjoint photon incoherent scattering

- Adjoint photon coherent scattering

- Adjoint photon pair production

- The adjoint photon weight factor

4 Forward-Adjoint Continuous Energy Monte Carlo (FACEMC) Code

- Code overview

- Validation plan

5 Future Work

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- 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

- 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*

① Motivation 1: The source and detector phase space

- Adjoint process generally more efficient than forward process when phase space of 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)
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- Three classes of problems will be discussed that can benefit from the adjoint process

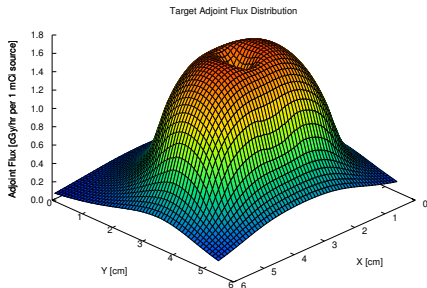
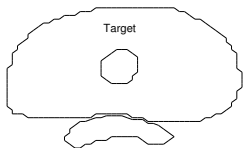
Shutdown Dose Calculations Using the R2S(A) Method

- Photon dose in a region of a nuclear system resulting from neutron activation of material is desired
- This information is useful for planning maintenance on the system
- These problems are often solved using the rigorous 2-step method (R2S)
- The adjoint process can be useful for small regions of interest

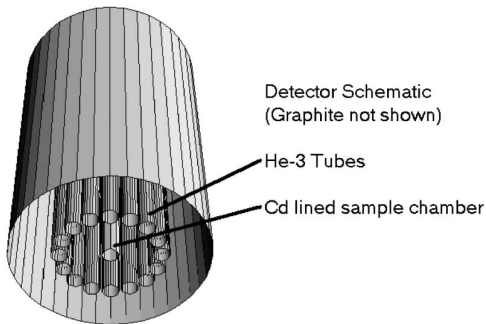
The R2S(A) method

- ① Neutron flux throughout the system 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 or an adjoint process (A)

- **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

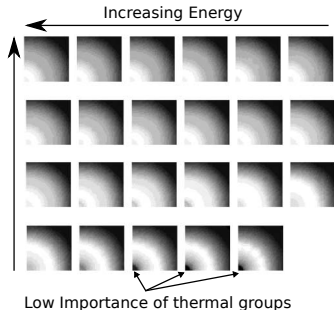


- Adjoint flux can allow for spectral performance of a detector to be predicted for an arbitrary source distribution
- Detector design can then be optimized before it is constructed
 - Important for detectors with rare materials (e.g. He^3 neutron detectors)



(Sjoden, 2002)

Detector Adjoint Flux Data



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

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

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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

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

- 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

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

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

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

- $p^1(x)$ represents the probability of a random walk starting in state x
- $p(y \rightarrow x)$ 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

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

- The transport equation 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

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

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

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

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

$$\begin{aligned}\chi(\vec{r}, E, \hat{\Omega}) &= S(\vec{r}, E, \hat{\Omega}) + \int \int \Sigma_T(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \\ &\quad \cdot \int \chi(\vec{r}', E', \hat{\Omega}') \tau(\vec{r}', \vec{r}, E', \hat{\Omega}') dV' dE' d\hat{\Omega}' \\ &= S(\vec{r}, E, \hat{\Omega}) + \int \int \int K(\vec{r}' \rightarrow \vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \\ &\quad \cdot \chi(\vec{r}', E', \hat{\Omega}') dV' dE' d\hat{\Omega}'\end{aligned}$$

- The kernel of the emission density FIESK is

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

- This kernel can be simplified by introducing two new kernels

$$\begin{aligned} T(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega}) &= \Sigma_T(\vec{r}, E) \tau(\vec{r}', \vec{r}, E, \hat{\Omega}) \\ &= \Sigma_T(\vec{r}, E) \exp \left[- \int_0^{|\vec{r}-\vec{r}'|} \Sigma_T(\vec{r} - R' \hat{\Omega}, E) dR' \right] \frac{\delta \left(\hat{\Omega} - \left[\frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|} \right] \right)}{|\vec{r} - \vec{r}'|^2} \end{aligned}$$

- 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 its 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

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

- 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

$$\begin{aligned} C(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) &= \sum_j \frac{\Sigma_j(\vec{r}, E') c_j(\vec{r}, E') f_j(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})}{\Sigma_T(\vec{r}, E')} \\ &= \sum_A \frac{\Sigma_A(\vec{r}, E')}{\Sigma_T(\vec{r}, E')} \sum_j \frac{\sigma_{A,j}(E')}{\sigma_A(E')} c_{A,j}(E') p_{A,j}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \end{aligned}$$

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

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

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

- 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

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

- The state transition kernel for this FIESK is

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

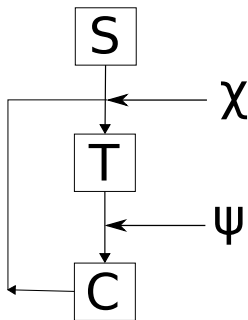
- From the emission density FIESK and collision density FIESK, the random walk process for each quantity can be determined

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

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

- $\bar{P}_{NA}(x)$ 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 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



- 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

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

- The adjoint operator is defined by the following relationship:

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

- Want to calculate the same material response

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

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

- 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 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

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

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

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

- The kernel of the adjoint emission density FIESK is

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

- This kernel can be simplified by introducing two new kernels

$$\begin{aligned} T^\dagger(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega}) &= \Sigma_T(\vec{r}, E) \tau^\dagger(\vec{r}', \vec{r}, E, \hat{\Omega}) \\ &= \Sigma_T(\vec{r}, E) \exp \left[- \int_0^{|\vec{r}' - \vec{r}|} \Sigma_T(\vec{r} + R' \hat{\Omega}, E) dR' \right] \frac{\delta \left(\hat{\Omega} - \left[\frac{\vec{r}' - \vec{r}}{|\vec{r}' - \vec{r}|} \right] \right)}{|\vec{r}' - \vec{r}|^2} \end{aligned}$$

- Describes the movement of adjoint particles through space
- Quantity $T^\dagger(\vec{r}' \rightarrow \vec{r}, E, \hat{\Omega})dV$ is probability that an adjoint 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 begin sampled in a vacuum

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

- 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

$$\begin{aligned}
 C^\dagger(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) &= \frac{\Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\
 &= \sum_j \frac{\Sigma_j(\vec{r}, E) c_j(\vec{r}, E) f_j(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\
 &= \sum_A \frac{\Sigma_A^\dagger(\vec{r}, E')}{\Sigma^\dagger(\vec{r}, E')} \sum_j \frac{\sigma_{A,j}^\dagger(E')}{\sigma_A^\dagger(E')} \frac{\sigma_{A,j}(E) c_{A,j}(E) p_{A,j}(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\sigma_{A,j}^\dagger(E')}
 \end{aligned}$$

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 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(\vec{r}, 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,j}(E) c_{A,j}(E) p_{A,j}(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\sigma_A^\dagger(E') \sigma_{A,j}^\dagger(E')}
 \end{aligned}$$

$$\begin{aligned}
 C^\dagger(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) &= \frac{\Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\
 &= \sum_j \frac{\Sigma_j(\vec{r}, E) c_j(\vec{r}, E) f_j(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\
 &= \sum_A \frac{\Sigma_A^\dagger(\vec{r}, E')}{\Sigma^\dagger(\vec{r}, E')} \left(\sum_j \frac{\sigma_{A,j}^\dagger(E')}{\sigma_A^\dagger(E')} \sigma_{A,j}(E) c_{A,j}(E) p_{A,j}(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}') \right) \frac{1}{\sigma_{A,j}^\dagger(E')}
 \end{aligned}$$

$$\begin{aligned} C^\dagger(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) &= \frac{\Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\ &= \sum_j \frac{\Sigma_j(\vec{r}, E) c_j(\vec{r}, E) f_j(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\ &= \sum_A \frac{\Sigma_A^\dagger(\vec{r}, E')}{\Sigma^\dagger(\vec{r}, E')} \sum_j \frac{\sigma_{A,j}^\dagger(E')}{\sigma_A^\dagger(E')} \frac{\sigma_{A,j}(E) c_{A,j}(E) p_{A,j}(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\sigma_{A,j}^\dagger(E')} \end{aligned}$$

$$\begin{aligned}
 C^\dagger(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) &= \frac{\Sigma_T(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\
 &= \sum_j \frac{\Sigma_j(\vec{r}, E) c_j(\vec{r}, E) f_j(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\Sigma^\dagger(\vec{r}, E')} \\
 &= \sum_A \frac{\Sigma_A^\dagger(\vec{r}, E')}{\Sigma^\dagger(\vec{r}, E')} \sum_j \frac{\sigma_{A,j}^\dagger(E')}{\sigma_A^\dagger(E')} \underbrace{\frac{\sigma_{A,j}(E) c_{A,j}(E) p_{A,j}(E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')}{\sigma_{A,j}^\dagger(E')}}_{\text{highlighted}}
 \end{aligned}$$

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

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

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

- 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 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

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

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

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

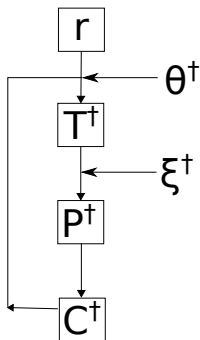
$$\xi^\dagger(x) \text{ Random Walk: } \begin{cases} p^1(x) &= \frac{S_c^\dagger(x)}{\int S_c^\dagger(x) dx} \\ p(y \rightarrow x) &= \frac{N^\dagger(y \rightarrow x)}{\bar{P}^\dagger(y)} \\ p(x) &= 0 \end{cases}$$

- 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



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3 Adjoint Photon Cross Sections

- Adjoint photon incoherent scattering

- Adjoint photon coherent scattering

- Adjoint photon pair production

- The adjoint photon weight factor

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5 Future Work

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

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

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

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

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

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

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

The Adjoint Incoherent Scattering Cross Section



- The double differential incoherent scattering cross section is the following, where $S(y, Z)$ is the scattering function:

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

- The adjoint double differential incoherent scattering cross section is therefore

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

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

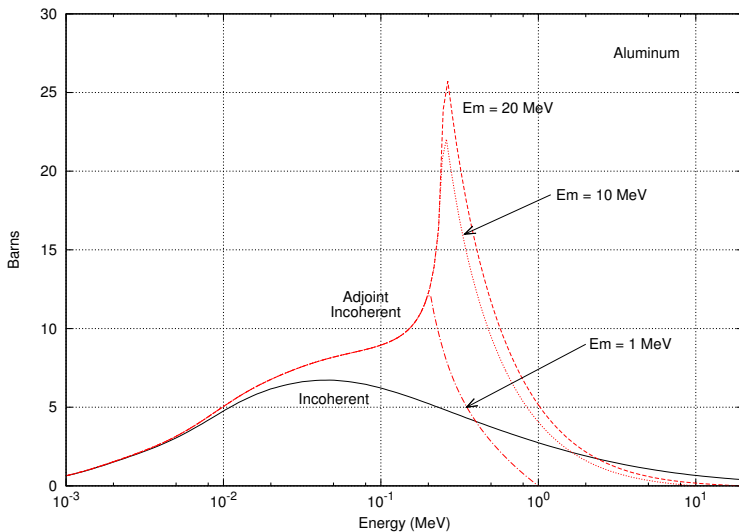
$$E = \frac{E'}{1 - \alpha'(1 - \mu)}$$

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

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

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

The Integrated Adjoint Incoherent Scattering Cross Section



- Use the definition of the adjoint double differential cross section

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

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

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

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

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

$$\begin{aligned} \frac{d\sigma_{c.s.}^{\dagger}(E', \mu, Z)}{d\mu} &= \frac{d\sigma_{c.s.}(E', \mu, Z)}{d\mu} \\ &= \pi r_e^2 (1 + \mu^2) F^2(y, Z) \end{aligned}$$

- $F(y, Z)$ is the atomic form factor

The Adjoint Pair Production Cross Section



- Use the definition of the adjoint double differential cross section

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

- 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

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

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

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



- **Problem:**

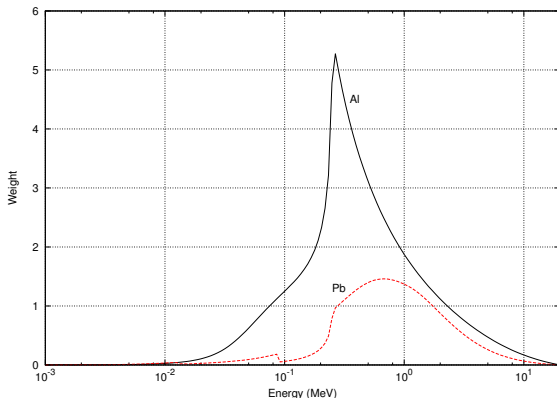
- Photoelectric effect occurs when a photon is absorbed by an atom
- An electron is ejected leaving an electron shell vacancy
- Atomic relaxation occurs to fill the vacancy with x-rays potentially released
- Emitted x-rays can be important for certain problems (e.g. brachytherapy seed characterization)
- 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.



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- Validation plan

5 Future Work

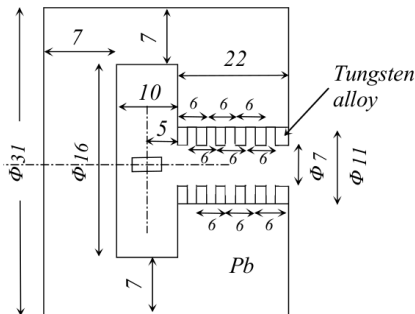


- **Energy Range:**
 - 1 keV - 20 MeV for photons and adjoint photons
 - 10^{-5} eV - 20 MeV for neutrons and adjoint neutrons
- **Spatial Domain Modeling:** CAD based (primarily)
 - Accomplished with the direct accelerated geometry (DAG) package
- **Variance Reduction:** implicit capture, Russian roulette,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

- ➊ **Benchmarking:** simulation of benchmark test problems for photons and neutrons
- ➋ **Code-to-Code Comparisons:** calculate integral quantities and spectra and compare against other validated Monte Carlo codes
- ➌ **Intra-Code Comparisons:** calculate integral quantities and spectra using FACEMC forward and adjoint simulations

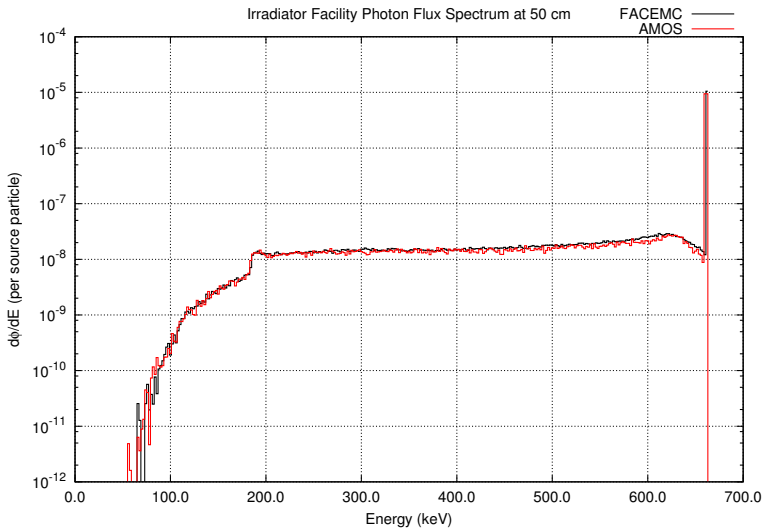
Preliminary Validation of FACEMC: AMOS Comparison

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



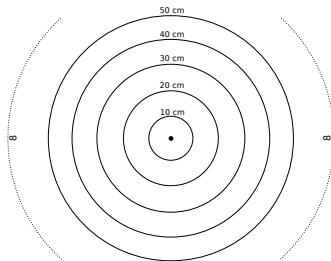
- **Source:** isotropically emitting Cs-137 gamma source
- **Quantity:** flux spectrum 50 cm from center of source (on axis)
- **Comparison Code:** AMOS (TU Dresden research code)

AMOS Comparison Results



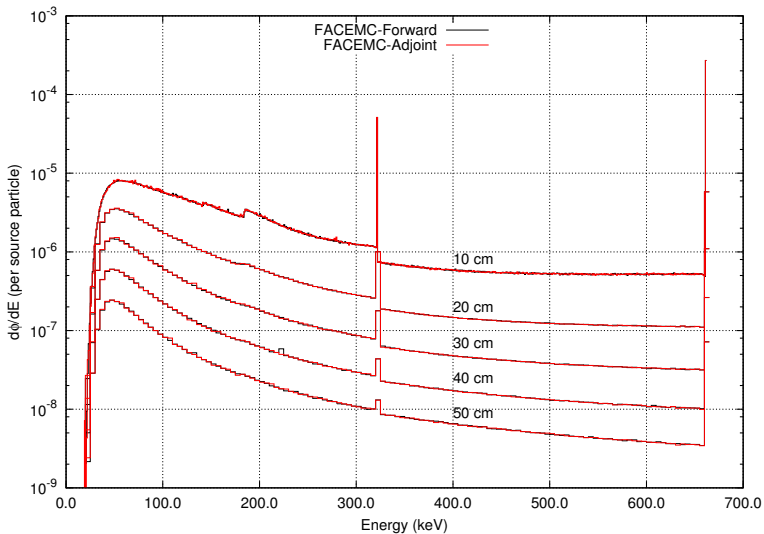
Preliminary Validation of FACEMC: Forward vs. Adjoint

- **Problem Geometry:**
- **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



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- Code overview

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5 Future 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
- 6 Characterize the effect of the adjoint weight factor on the variance of the adjoint process



- 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

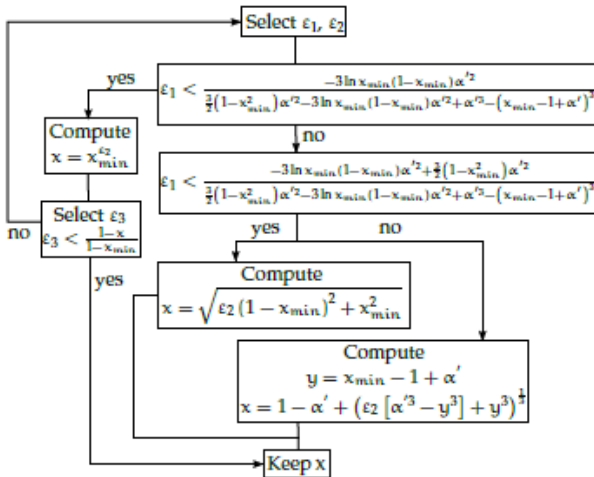
Thanks to...

- Douglass Henderson
- Bruce Thomadsen
- TU Dresden
- The NRC

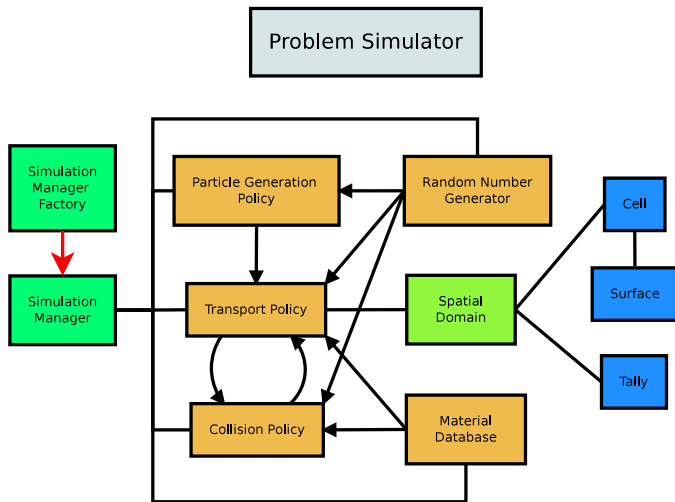
Support

This work was performed under appointment to the Nuclear Regulatory Commission Fellowship program at the University of Wisconsin - Madison Department of Engineering Physics.

Adjoint K.N. Rejection Sampling Procedure

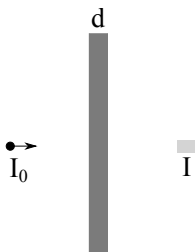


Major Components of FACEMC



- FACEMC version 1.0 is currently complete.

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

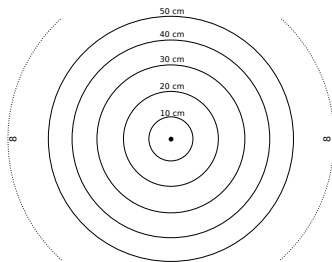


The diagram shows a horizontal arrow representing a beam of particles (photons) moving from left to right. The arrow is labeled I_0 at its tail. It passes through a vertical grey bar representing a material of thickness d . The bar is labeled d at its top. After passing through the bar, the beam is represented by a shorter horizontal arrow labeled I at its tail.

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

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

- **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



- **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:** same as FACEMC validation plan step 2
- **Quantities:** Flux spectrum and total flux at each spherical surface

- ① Complete all theoretical work by September 1st, 2013
- ② Complete all coding work by March 1st, 2014
- ③ Complete the validation plan by April 1st, 2014
- ④ Complete all of the the challenge problems by June 1st, 2014
- ⑤ Ideal thesis completion date: August 1st, 2014 - September 1st, 2014