



Office of Defense Nuclear Nonproliferation
Research and Development

**University and Industry Technical Interchange
(UITI2013) Review Meeting**

**An Innovative Hybrid Deterministic/Monte
Carlo Radiation Transport Method for
Modeling Radiation Sensor Systems**

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Research Team



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- Georgia Tech
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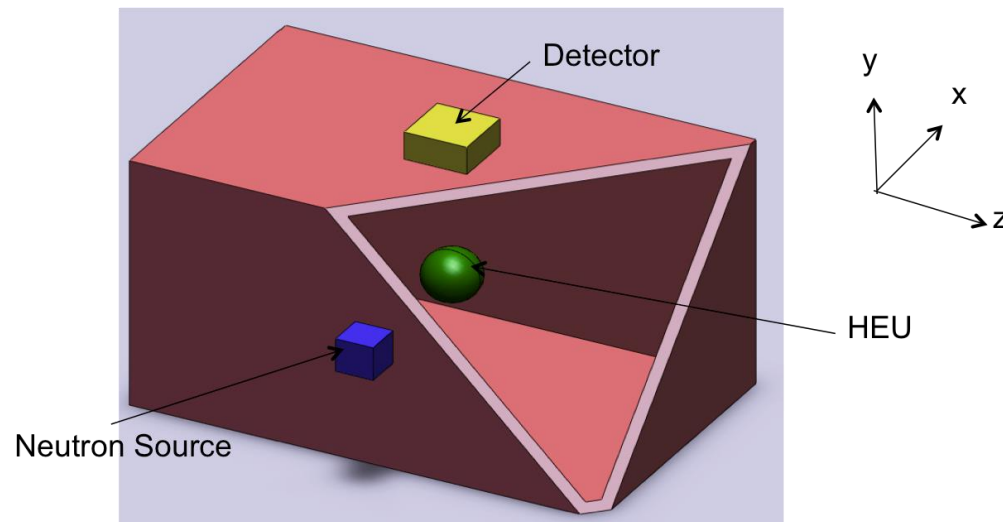
Summary



- **A hybrid Monte Carlo and deterministic methodology has been developed for application to active interrogation systems.**

- **The methodology in Part 2 consists of three steps:**
 1. Calculation of neutron flux distribution due to neutron source transport and subcritical multiplication
 2. Generation of gamma source distribution from (n, γ) interactions
 3. Determination of gamma current at a detector window

- Development of an hybrid transport methodology that quickly yields gamma current at a detector window of an active interrogation system
- Testing of methodology for a cargo container with third-density water cargo and a highly enriched uranium (HEU) sphere



Cargo Container: $243.84 \times 259.08 \times 283.456 \text{ cm}^3$
Neutron Source: D-T (14.1 MeV), $13.5 \times 13.5 \text{ cm}^2$
SNM: 25 kg sphere of HEU, radius = 6.75 cm
Detector Window: $13.5 \times 13.5 \text{ cm}^2$



Objectives



- **Create a database of response coefficients and adjoint functions to model a cargo container**
- **Develop software to quickly determine the gamma current at the detector window**
- **Benchmark (accuracy & computation time) the software against the MCNP5 Monte Carlo calculations**



Deliverables



- **Novel particle transport techniques for simulation of active interrogation systems**
- **Reports on development of methodologies and results**
- **Conference and journal publications on novel particle transport methodologies and benchmarking of the AIMS software**



Theory



Discussion on the three-step methodology



Theory

Step 1: Calculation of neutron flux distribution



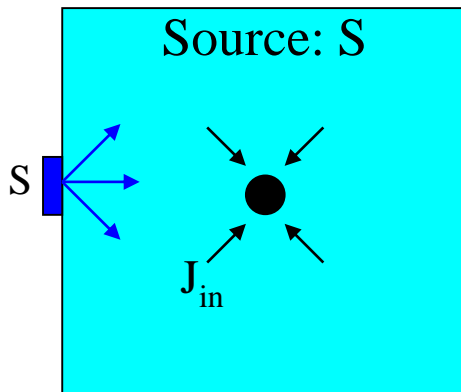
- A response function methodology was developed for neutron transport within the cargo container and subcritical multiplication as well as determination of fission neutron source density
- The model is split into two regions: cargo and region-of-interest (ROI)

S = external source

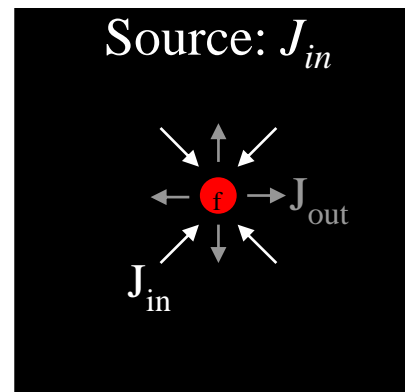
J_{in} = total integrated (over energy and area) current entering ROI

J_{out} = total integrated (over energy and area) current exiting ROI

- HEU
- Cargo
- Not Modeled

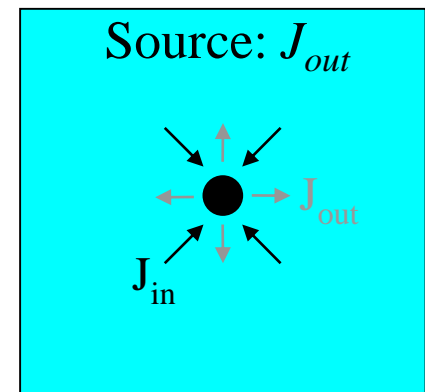


$$\alpha_{s,in} = \frac{J_{in}}{S}$$



$$\alpha_{in,out} = J_{out} / J_{in}$$

$$\alpha_{in,f} = f / J_{in}$$



$$\alpha_{out,in} = \frac{J'_{in}}{J_{out}}$$



Theory

Step 1: Calculation of neutron flux distribution



By combining the information from the 5 problems, we obtain the following system of equations

$$J_{in} = S\alpha_{s,in}$$

Flux entering ROI from source

$$J_{out} = J_{in}\alpha_{in,out} + J_{in}'\alpha'_{in,out}$$

Flux exiting ROI, from each incoming spectrum

$$J_{in}' = J_{out}\alpha'_{out,in}$$

Flux reflected back into ROI

$$F = J_{in}\alpha_{in,f} + J_{in}'\alpha'_{in,f}$$

Fission Rate in ROI

Using above equations, we solve F

$$F = S\alpha_{s,in} \left(\alpha_{in,f} + \frac{\alpha'_{in,f} \alpha_{in,out} \alpha_{out,in}}{1 - \alpha'_{in,out} \alpha'_{out,in}} \right)$$



Theory

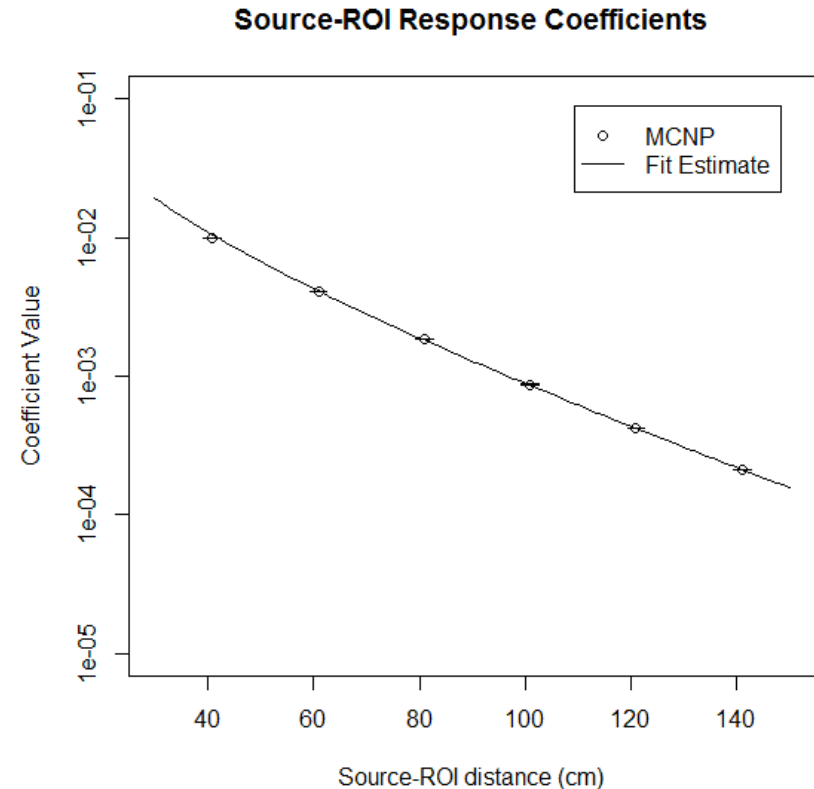
Step 1: Calculation of neutron flux distribution



- Of the coefficients, only $\alpha_{s,in}$ should change significantly with HEU location.
- Use a fit of the form:

$$\alpha(r) = \frac{\alpha_0}{r} \exp(-\sigma r)$$

- r is the source-ROI distance
- α_0 and σ are coefficients determined by a least squares fit to a series of MCNP calculations at varying r





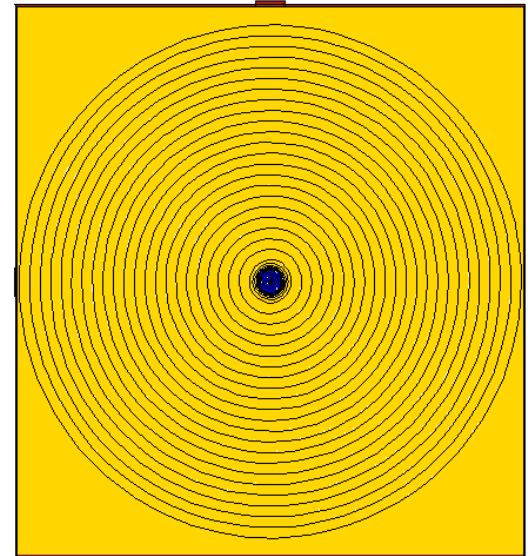
Theory

Step 1: Calculation of neutron flux distribution



- The fission rate has been calculated, now the flux distribution is needed
- Assume the flux distribution is radially symmetric around the HEU
- MCNP calculation to tally fission neutron flux as a function of distance $\tilde{\phi}_g^n(r)$
- Flux at any point (x,y,z) can now be calculated as:

$$\phi_g^n(x,y,z) = F \tilde{\phi}_g^n \left(\sqrt{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2} \right)$$





Theory

Step 2: Determine gamma source distribution



- Calculate the gamma source distribution $S_{i,g}^\gamma$ due to subcritical multiplication in the HEU

$$S_{i,g}^\gamma = \sum_{g'} \phi_{i,g'}^n \sigma(n, \gamma)_{i,g' \rightarrow g}$$

- The neutron flux $\phi_{i,g}^n$ in Step 1 is found to match the adjoint function mesh to be used in Step 3
- Using the Bugle-96 neutron-gamma cross-section $\sigma(n, \gamma)_{i,g' \rightarrow g}$



Theory

Step 3: Determine gamma current at detector window



- Define the angular gamma flux ψ^γ and angular adjoint function $\psi^{\gamma,\dagger}$ with boundary conditions:

$$H\psi^\gamma = S^\gamma \text{ where } \psi^\gamma = 0 \text{ for } \hat{n} \cdot \hat{\Omega} < 0$$

$$H^\dagger \psi^{\gamma,\dagger} = S^{\gamma,\dagger} \text{ where } \psi^{\gamma,\dagger} = \delta(E - E_g) \delta(r - r_d) \text{ for } \hat{n} \cdot \hat{\Omega} > 0$$

- Form the commutation relation between the forward and adjoint equations, noting that $S^{\gamma,\dagger} = 0$

$$\langle \psi^{\gamma,\dagger} H \psi^\gamma \rangle - \langle \psi^\gamma H^\dagger \psi^{\gamma,\dagger} \rangle = \langle \psi^{\gamma,\dagger} S^\gamma \rangle - \langle \psi^\gamma S^{\gamma,\dagger} \rangle$$

- On the left only the leakage term remains and using the divergence theorem and the boundary conditions gives:

$$\int_{\hat{n} \cdot \hat{\Omega} > 0} dE \int d\Omega \int d\Gamma (\hat{n} \cdot \hat{\Omega}) \psi^\gamma(r, E, \hat{\Omega}) \delta(E - E_g) \delta(r - r_d) = \langle \psi^{\gamma,\dagger} S^\gamma \rangle$$

$$J_+^\gamma(r_d, E_g) = \langle \psi^{\gamma,\dagger} S^\gamma \rangle = \sum_i \sum_{g'} \phi_{i,g'}^{\gamma,\dagger} S_{i,g'}^\gamma \Delta V_i$$

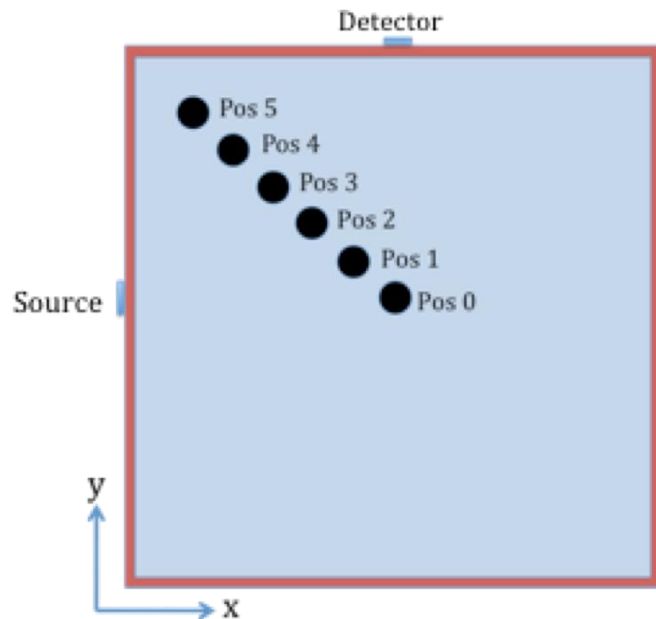
- Compute the adjoint function for a boundary adjoint flux at the detector window using the TITAN 3-D parallel transport code to obtain $\phi^{\gamma,\dagger}$



Results



- Consider 6 different HEU positions within the cargo container
- For each HEU position, simulate scanning the source-detector assembly along the long axis of the container starting from the center
- Compare the hybrid method calculated current with a reference MCNP5 solution



HEU Position	(x cm, y cm)
0	(0,0)
1	(-20,20)
2	(-40,40)
3	(-60,60)
4	(-80,80)
5	(-100,100)



Results



- **AIMS (Active Interrogation for Monitoring Special-nuclear-materials) software tool developed to use a pre-calculated database to determine the gamma current at the detector window**
 1. Uses pre-calculated response coefficients from Step 1 and determines the neutron flux distribution
 2. Completes Step 2 to obtain the gamma distribution
 3. Uses pre-calculated adjoint function to complete Step 3
- **Note: the response coefficient calculation assumes the HEU is at position 0 (container center) and the adjoint function calculation does not model the HEU**
- **Compare the group 8 (2-3 MeV) gamma current because it has the largest magnitude due to fission neutrons**



Results



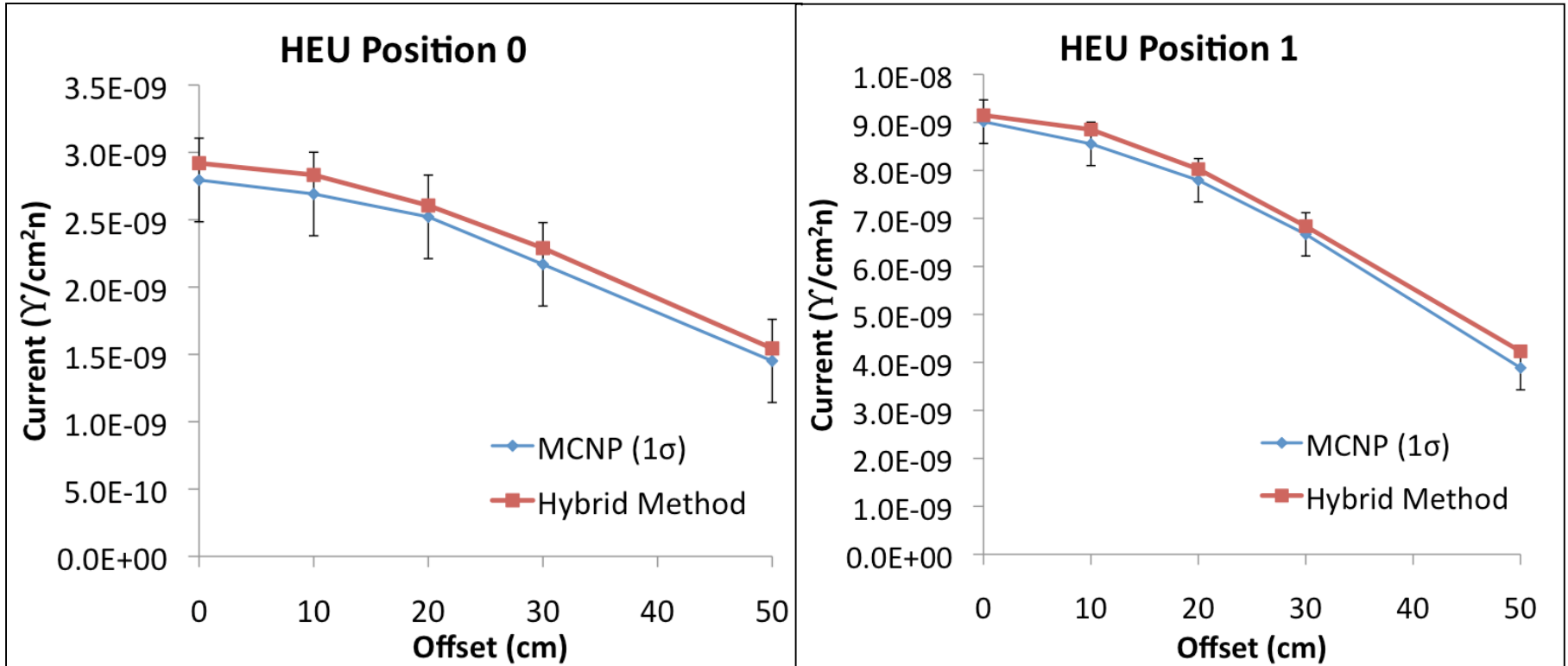
Total fission rate: Response method vs. MCNP5

ROI Position	Fission Rate		
	MCNP (1 σ)	Response Method	Difference
0	5.55E-03 (0.09%)	5.60E-03	1.01%
1	1.07E-02 (0.09%)	1.03E-02	-1.88%
2	1.72E-02 (0.15%)	1.66E-02	-3.16%
3	2.00E-02 (0.14%)	1.99E-02	-0.74%
4	1.54E-02 (0.16%)	1.69E-02	9.42%
5	7.18E-03 (0.08%)	1.08E-02	50.31%

Note that the response coefficients were calculated for an HEU sphere located at the container center.

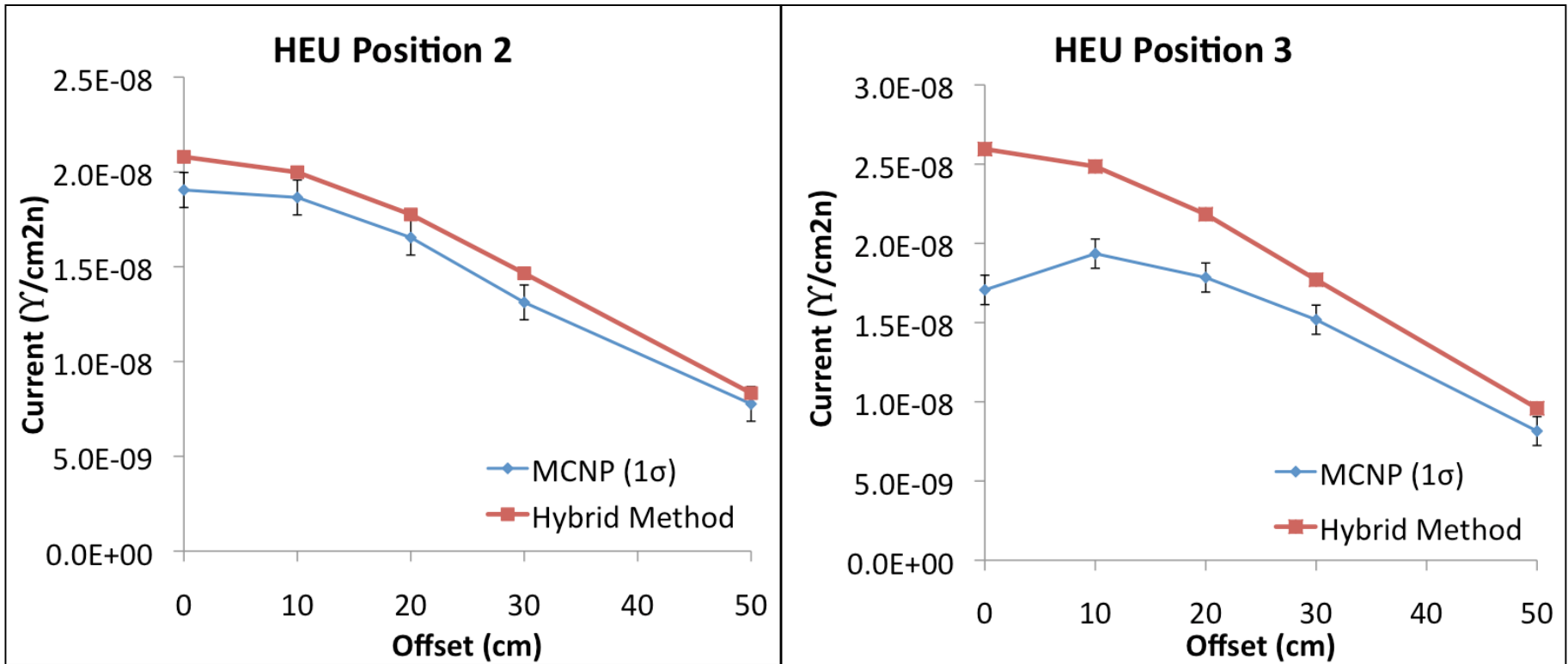


Results





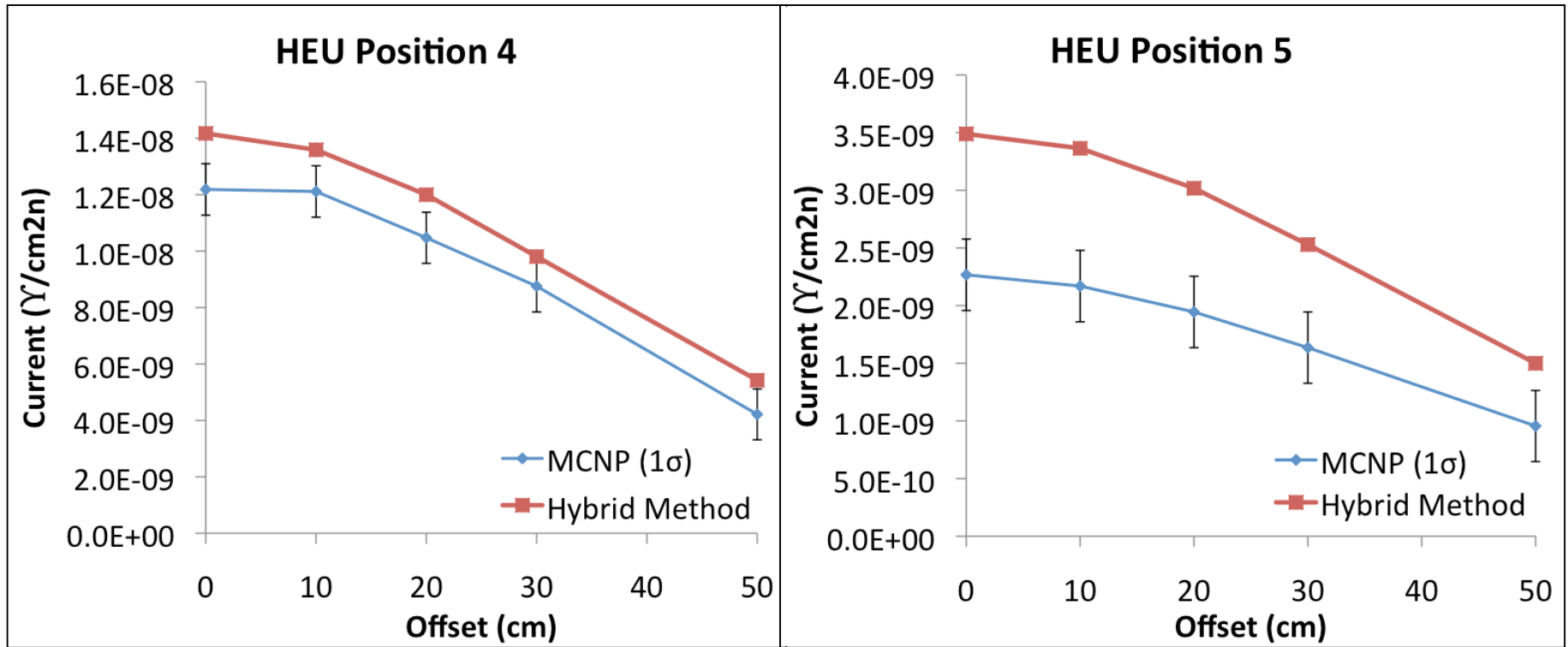
Results



In position 3, the HEU is almost exactly centered between the source and detector and this results in a reduction in detector current until the source-detector assembly is off-set.



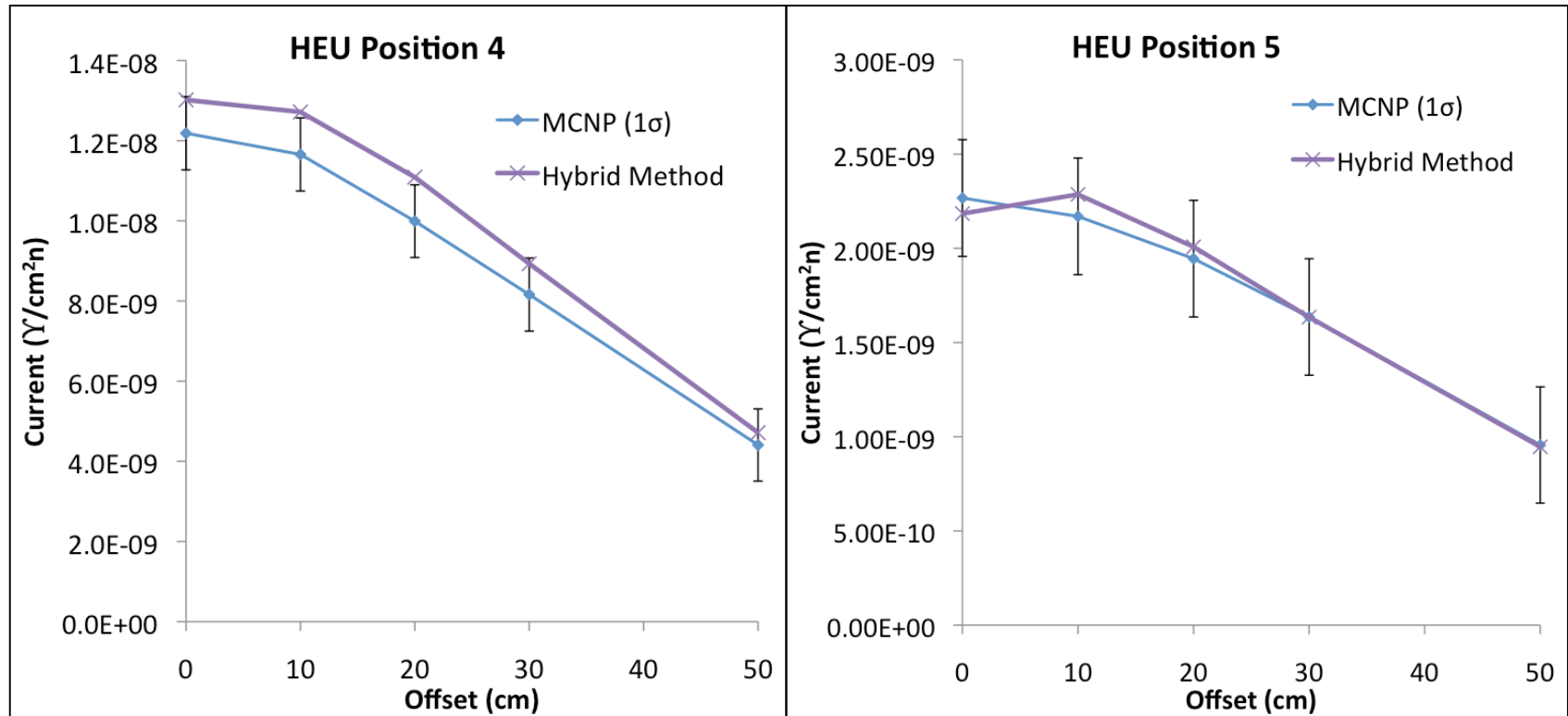
Results



In positions 4 & 5, the HEU is approaching the cargo container wall and the hybrid solutions are consistently higher than the reference solution as a result. The database would have to be expanded with more accurate model representations to improve the accuracy of the AIMS solution.



Results



Expanded database with recalculated fission rate coefficients for specific HEU locations to improve AIMS accuracy.



Results



Computation time comparison:

Pre-calculated Database Computation Times	
Response coefficients (serial)	60 hours
Group 8 adjoint function (8 proc)	5.9 hours

Computation Time for 5 Scanning Locations		
	AIMS per HEU Position (serial)	0.053 hours
MCNP5* (8 processors)	HEU Position 0 or 5	495 hours
	HEU Position 1	254 hours
	HEU Position 2, 3, or 4	63 hours

*Times are for the MCNP5 uncertainties given in plots (4.8%-32.3%)



Conclusions



- **A hybrid Monte Carlo and deterministic radiation transport methodology and corresponding computation tool (AIMS) have been developed to quickly model an active interrogation system**
- **The fission rate calculation step showed excellent agreement with MCNP5 until the HEU neared the wall in positions 4 & 5**
- **The hybrid method was compared with MCNP5 for a scanning source-detector assembly and several HEU locations to determine the sensitivity to the database accuracy**
- **The AIMS software was found to be in excellent agreement with MCNP5 when the HEU is within about 56 cm of the container center**
- **AIMS accuracy is reduced when the HEU is located directly between the source and detector or near the container wall**
- **The AIMS software is several orders of magnitude faster than MCNP5 for this model**



Future Work



- **Include the detector response function (IFLEX-incident flux response expansion) algorithm from Part 1 of this project developed by Georgia Tech into the AIMS software into the AIMS software**
- **Prepare databases for other cargo materials (e.g., wood)**
- **Perform further benchmarking of the AIMS software, including expanding the database where needed (e.g., near the container wall)**