Propagation of Uncertainty from a Source Computed with Monte Carlo

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Introduction

• Multi-step Monte Carlo problems
  – Step one constructs a source
  – Step two uses the source
  – Propagation of uncertainty usually not done

• Examples
  – Dose rates from neutron activation
  – Active interrogation
  – Reactor fuel depletion
Introduction

• How to handle the uncertainty?
  – Run step one a really really long time
    • Until it is “smooth”
    • But how long is long enough?
  – Use multiple clones
    • Run both steps with different seeds in step one
    • Run step two calculations for very long times
    • Determine at variance in the step two answer - due to step one
    • Costly!

• Need a way to quickly estimate the uncertainty in the step two answer due to the uncertainty in the step one answer
Theory

• For a single source of strength $S \pm \sigma_S$ from Step One,

• Used in a source/detector problem to compute a response

$$ R = \int f(E') \phi(\vec{r}, E') dE $$

• Uncertainty in detector response is then

$$ \sigma_{\text{total}}^2 = \sigma_S^2 + \sigma_{\text{MC}}^2 $$
Theory

• Now consider a mesh source, with voxel strength \( S_i \pm \sigma_i \) and normalized energy distribution of \( q_i(E) \).

• \( R_i(E) \) is the response due to a unit source of \( E \) in voxel \( i \).

• Response is the sum of the response from each source

\[
R = \sum S_i R_i \quad R_i = \int q_i(E) R_i(E) \, dE
\]

• Using standard propagation of uncertainty

\[
\sigma_S^2 = \sum \left( \frac{\partial R}{\partial S_i} \right)^2 \sigma_i^2 + 2 \sum_{i \neq j} \left( \frac{\partial R}{\partial S_i} \right) \left( \frac{\partial R}{\partial S_j} \right) \rho_{ij} \sigma_i \sigma_j
\]
Theory

• Using standard propagation of uncertainty

\[
\sigma_S^2 = \sum \left( \frac{\partial R}{\partial S_i} \right)^2 \sigma_i^2 + 2 \sum_{i \neq j} \left( \frac{\partial R}{\partial S_i} \right) \left( \frac{\partial R}{\partial S_j} \right) \rho_{ij} \sigma_i \sigma_j
\]

• Ignoring correlations, then a lower bound to \( \sigma_S^2 \) can be found

\[
\sigma_S^2 \approx \sum \left( \frac{\partial R}{\partial S_i} \right)^2 \sigma_i^2 \\
\approx \sum \left( \int q_i(E) R_i(E) \, dE \right)^2 \sigma_i^2
\]
Theory

- Estimate of uncertainty is then

\[ \sigma_S^2 = \sum \left( \int q_i(E) R_i(E) \, dE \right)^2 \sigma_i^2 \]

- So, we just need \( R_i(E) \) - the response due to a unit source of energy \( E \) located in voxel \( i \), for every voxel and energy.

- That is a large number of forward calculations.

- \( R_i(E) \) is the definition of the adjoint flux \( \phi_i^+(E) \), for an adjoint calculation using a source of \( Q^+(E) = f(E) \).
Theory

• With one adjoint calculation, we can estimate $\sigma_S^2$.

$$\sigma_S^2 = \sum \left( \int q_i(E) \phi_i^+(E) \, dE \right)^2 \sigma_i^2$$

• Then the total uncertainty is

$$\sigma_{total}^2 = \sigma_S^2 + \sigma_{MC}^2$$
Example Problem 1

- Consider the problem of computing the photon dose rate from neutron activation (inspired by the ITER SDDR)

- Very simplified:
  - Steel slab (gray) with 0.005% $^{59}\text{Co}$ impurity
  - 14.1 MeV neutrons, uniform (yellow)
  - Compute dose rate at 100 cm from slab

- Activation cross section $\Sigma(E_n)$
  - $^{59}\text{Co}(n,\gamma)^{60}\text{Co}$
  - Activation time is short
  - No initial amount of $^{60}\text{Co}$
Example Problem 1

- Activation rate density

\[ R(\vec{r}) = \int \Sigma(E_n) \phi_n(\vec{r}, E_n) \, dE_n \]

- $^{60}\text{Co}$ density after activation time $T$

\[ N_{60}(\vec{r}) = R(\vec{r}) \, N_{59}^0 \, T \]

- Photon source strength

\[ S_\gamma(\vec{r}) = 1.9985 \, \lambda \, N_{60}(\vec{r}) \]

1.173 MeV (49.96%) 1.332 MeV (50.03%)
Example Problem 1

• Step One – determine photon source
  - Neutron transport problem
  - Compute $^{59}\text{Co}$ activation rate

- Compute $^{60}\text{Co}$ source strength
Example Problem 1

- Step Two – determine photon dose rate (rem/hr) at detector

### Photon Point Detector 1.

<table>
<thead>
<tr>
<th>tally/quantity</th>
<th>average</th>
<th>standard deviation</th>
<th>relation uncert</th>
</tr>
</thead>
<tbody>
<tr>
<td>uncollided flux</td>
<td>2.01366E+04</td>
<td>2.18563E+00</td>
<td>0.00011</td>
</tr>
<tr>
<td>total flux</td>
<td>6.80372E+04</td>
<td>2.05406E+01</td>
<td>0.00030</td>
</tr>
<tr>
<td>response 5</td>
<td>1.06167E-01</td>
<td>2.75416E-05</td>
<td>0.00026</td>
</tr>
</tbody>
</table>

Total Monaco cpu time for this problem was 61.5 minutes

\[106.167 \pm 0.027 \text{ mrem/hr}\]
Example Problem 1

• Estimate uncertainty due to ‘noisy’ source using brute force

• 64 clones of Step One and Step Two
  – Average dose rate 103.4 mrem/hr
  – Average reported uncertainty 0.029 mrem/hr
  – Observed standard deviation 3.05 mrem/hr

• Observed is combination of source uncertainty and transport uncertainty in Step Two – almost entirely due to source
  – $\sigma_S = 3.05$ mrem/hr
Example Problem 1

• Estimate uncertainty due to ‘noisy’ source using adjoint

• Coarse fast adjoint (84×100×100, 19g, $S_4/P_1$)
  – Estimate of response: 153 mrem/hr
  – Estimate of uncertainty: 1.89 mrem/hr
  – From clones: $103.4 \pm 3.05$ mrem/hr

• Better adjoint (104×100×100, 47g, $S_8/P_3$)
  – Estimate of response: 99 mrem/hr
  – Estimate of uncertainty: 1.52 mrem/hr

• Estimate is factor of 2 lower than observed
## Example Problem 1

- With different adjoint calculations

<table>
<thead>
<tr>
<th>Adjoint Parameters</th>
<th>Response</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_n/P_l$ (cm)</td>
<td>Value (mrem/hr)</td>
</tr>
<tr>
<td>Mesh (min)</td>
<td></td>
</tr>
<tr>
<td>(cm) (min)</td>
<td></td>
</tr>
<tr>
<td>$4/1$</td>
<td></td>
</tr>
<tr>
<td>2.0 6.4</td>
<td>153</td>
</tr>
<tr>
<td>1.0 7.2</td>
<td>125</td>
</tr>
<tr>
<td>0.5 8.1</td>
<td>118</td>
</tr>
<tr>
<td>$8/3$</td>
<td></td>
</tr>
<tr>
<td>2.0 30.6</td>
<td>149</td>
</tr>
<tr>
<td>1.0 33.4</td>
<td>116</td>
</tr>
<tr>
<td>0.5 37.5</td>
<td>107</td>
</tr>
<tr>
<td>$4/1$</td>
<td></td>
</tr>
<tr>
<td>2.0 15.3</td>
<td>146</td>
</tr>
<tr>
<td>1.0 17.5</td>
<td>116</td>
</tr>
<tr>
<td>0.5 19.4</td>
<td>109</td>
</tr>
<tr>
<td>$8/3$</td>
<td></td>
</tr>
<tr>
<td>2.0 72.3</td>
<td>140</td>
</tr>
<tr>
<td>1.0 80.7</td>
<td>107</td>
</tr>
<tr>
<td>0.5 90.8</td>
<td>99</td>
</tr>
</tbody>
</table>

Better adjoint calculations give closer response estimate.

Estimate of uncertainty due to source is half of observed in clones.
Example Problem 1

- Different amounts of source uncertainty
  - Used different run times for Step One: 15, 30, 60, 120 minutes

![Graph showing relative uncertainty vs. run time](image-url)
Example Problem 2

- Cylcotron Vault (Carroll, 2000)
  - High energy protons can create neutrons
  - Neutrons can activate concrete floor/walls
  - Activations products can build up over time
    - Co-60 (1 Bq/g), Cs-134, Eu-152 (3 Bq/g), Eu-154
  - Concrete requires rad-waste disposal

- Example Problem 2
  - Fission neutrons 1 m above floor
  - Activate floor for 10 years
  - Shutdown, wait 10 years
  - Compute dose 1 m above floor
Example Problem 2

- **Step One**
  - Neutron transport
  - Fission neutron source above floor
  - Compute mesh tally of 4 activation rates
  - Convert to mesh sources
    - Activate/Decay using reaction rates

- **Step Two**
  - Use 4 mesh sources
  - Compute photon dose rate above floor

- **Dose Uncertainty due to Mesh Sources**
  - Compare adjoint estimate to clone approach
Example Problem 2

- Step One - Reaction Rates (/target/sec)

- $\text{Co}^{59}(n,\gamma)\text{Co}^{60}$
- $\text{Cs}^{133}(n,\gamma)\text{Cs}^{134}$
- $\text{Eu}^{151}(n,\gamma)\text{Eu}^{152}$
- $\text{Eu}^{153}(n,\gamma)\text{Eu}^{154}$
Example Problem 2

- Step One - Reaction Rates, Relative Uncertainties

- $^{59}\text{Co}(n,\gamma)^{60}\text{Co}$
- $^{133}\text{Cs}(n,\gamma)^{134}\text{Cs}$
- $^{151}\text{Eu}(n,\gamma)^{152}\text{Eu}$
- $^{153}\text{Eu}(n,\gamma)^{154}\text{Eu}$
Example Problem 2

**Use reaction rate to compute activity after 20 years**

<table>
<thead>
<tr>
<th>Initial condition</th>
<th>During irradiation ( (0 \leq t \leq T) )</th>
<th>After irradiation ( (T &lt; t) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M(0) = M_0 )</td>
<td>( \frac{d}{dt} M(t) = -RM(t) )</td>
<td>( \frac{d}{dt} M(t) = 0 )</td>
</tr>
<tr>
<td>( N(0) = 0 )</td>
<td>( \frac{d}{dt} N(t) = +RM(t) - \lambda N(t) )</td>
<td>( \frac{d}{dt} N(t) = -\lambda N(t) )</td>
</tr>
</tbody>
</table>

During irradiation \( (0 < t \leq T) \)

\[
M(t) = M_0 e^{-Rt}
\]

\[
N(t) = \frac{RM_0}{\lambda - R} \left( e^{-Rt} - e^{-\lambda t} \right)
\]

After irradiation \( (T < t) \)

\[
M(t) = M_0 e^{-RT}
\]

\[
N(t) = \frac{RM_0}{\lambda - R} \left( e^{-RT} - e^{-\lambda T} \right) e^{-\lambda (t-T)}
\]
Example Problem 2

• Step Two Source - Activity (Bq/cm$^3$)

- Co$^{60}$
- Cs$^{134}$
- Eu$^{152}$
- Eu$^{154}$
Example Problem 2

- Cobalt-60, 1.9985 gammas/decay
- Cesium-134, 2.2280 gammas/decay
- Europium-152, 0.9426 gammas/decay
- Europium-154, 1.6526 gammas/decay
Example Problem 2

• Step Two – determine photon dose rate (rem/hr) above floor

Photon Point Detector 1.

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<th>average value</th>
<th>standard deviation</th>
<th>relat uncert</th>
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<tr>
<td>uncollided flux</td>
<td>3.36069E-01</td>
<td>1.03766E-04</td>
<td>0.00031</td>
</tr>
<tr>
<td>total flux</td>
<td>1.29852E+00</td>
<td>4.87784E-04</td>
<td>0.00038</td>
</tr>
<tr>
<td>response 6</td>
<td>3.07876E+00</td>
<td>1.18726E-03</td>
<td>0.00039</td>
</tr>
</tbody>
</table>

Total Monaco cpu time for this problem was 2.01 hours

3.07876 ± 0.00119 mrem/yr
Example Problem 2

• Estimate uncertainty due to ‘noisy’ source using brute force

• 64 clones of Step One and Step Two
  – Average dose rate \( 3.07524 \text{ mrem/yr} \)
  – Average reported uncertainty \( 0.00125 \text{ mrem/yr} \)

  – Observed standard deviation \( 0.00625 \text{ mrem/yr} \)

• Observed is combination of source uncertainty and transport uncertainty in Step Two – almost entirely due to source
  – \( \sigma_S = 0.00612 \text{ mrem/yr} \)
Example Problem 2

• Estimate uncertainty due to ‘noisy’ source using adjoint

• Adjoint calculation (160×160×72, 47g, $S_8$/$P_3$, 3 hrs)

  – Estimate of response: 2.91687 mrem/hr
  – Estimate of uncertainty: 0.00084 mrem/hr

  – From clones: $3.07524 \pm 0.00612$ mrem/hr

• Estimate is a factor of 7.3 lower than observed value
Summary

• Using an adjoint calculation may provide a basis for computing the uncertainty in the step two answer due to the uncertainty in step one

• Estimate is a lower bound, ignores correlations in uncertainty

\[ \sigma_s^2 = \sum \left( \frac{\partial R}{\partial S_i} \right)^2 \sigma_i^2 + 2 \sum_{i \neq j} \left( \frac{\partial R}{\partial S_i} \right) \left( \frac{\partial R}{\partial S_j} \right) \rho_{ij} \sigma_i \sigma_j \]

  – Example 1: estimate was factor of 2 low
  – Example 2: estimate was factor of 7.3 low

• Some further study needed to determine if this is worth pursuing