Perturbation/sensitivity calculations with Serpent

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A collision history-based approach to GPT calculations

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Perturbation/sensitivity calculations with Serpent
Considered response functions

Effect of a perturbation of the parameter $x$ on the response $R$:

$$S_x^R \equiv \frac{dR/R}{dx/x}$$

Considered response functions:

- $R = k_{\text{eff}}$  Effective multiplication factor
  (Iterated Fission Probability method, Politecnico di Milano – PSI collaboration)

- $R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle}$  Reaction rate ratios

- $R = \frac{\langle \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle}$  Bilinear ratios (Adjoint-weighted quantities)

- $R = ?$  Something else
A collision history-based approach to GPT calculations
Reactor rate ratios
Adjoint-weighted quantities (bilinear ratios)

Particle’s weight perturbation

All the cross sections (and probability distributions) are artificially increased by a factor \( f \).

Events are rejected with a probability of \( (1 - 1/f) \).

\[ f = 0.5 \]

\[
 w^* \approx w^0 \cdot \left( 1 + \frac{d\Sigma_{n,2n}}{\Sigma_{n,2n}} \right) \cdot \left( 1 + \frac{d\Sigma_{s}}{\Sigma_{s}} \right) \cdot \left( 1 - \frac{d\Sigma_{f}}{\Sigma_{f}} \right) \cdot \left( 1 + \frac{d\Sigma_{s}}{\Sigma_{s}} \right) \cdot \left( 1 - \frac{d\Sigma_{c}}{\Sigma_{c}} \right) \cdot \left( 1 + \frac{d\Sigma_{f}}{\Sigma_{f}} \right) \cdot \left( 1 + \frac{d\Sigma_{s}}{\Sigma_{s}} \right) \cdot \left( 1 + \frac{d\Sigma_{f}}{\Sigma_{f}} \right) \ldots
\]
Adopting the distribution of the corrected particles weight in the reference system as unbiased estimator of the “exact” neutron flux distribution in the perturbed system.

Re-normalization of the total population weight.

Convergence of the propagation (latent?) generations.
A collision history-based approach to GPT calculations
Reaction rate ratios
Adjoint-weighted quantities (bilinear ratios)

Particle’s weight perturbation

\[ x = \text{nuclear data} \] for reaction \( r \), on the isotope \( i \), in the material \( m \), in the incident neutron energy bin \( e \), in the volume \( s \) (outgoing neutron energy bin \( e' \) and scattering cosine bin \( l \))

\[
\frac{\partial w_n}{\partial x/x} \approx w_n \cdot \sum_{g=(\alpha-\lambda)}^{\alpha} \left( (n,g) \text{ACC}_x - (n,g) \text{REJ}_x \right)
\]

\( \alpha \) = present generation
\( \lambda \) = number of propagation generations

\( \text{ACC}_x \) = accepted events \( x \) in the history of the particle \( n \)
\( \text{REJ}_x \) = rejected events \( x \)
Reaction rate ratios (method)

\[ R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle} \]

\[ R' = \frac{\langle \Sigma_1 + \Delta \Sigma_1, \phi + \Delta \phi \rangle}{\langle \Sigma_2 + \Delta \Sigma_2, \phi + \Delta \phi \rangle} \]

Neglecting cross terms...

\[ \frac{\Delta R}{R} = \frac{\langle \Delta \Sigma_1, \phi \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \Delta \Sigma_2, \phi \rangle}{\langle \Sigma_2, \phi \rangle} + \frac{\langle \Sigma_1, \Delta \phi \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \Sigma_2, \Delta \phi \rangle}{\langle \Sigma_2, \phi \rangle} \]

\[ S^R_x = \frac{\langle \frac{\partial \Sigma_1}{\partial x/x}, \phi \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \frac{\partial \Sigma_2}{\partial x/x}, \phi \rangle}{\langle \Sigma_2, \phi \rangle} + \frac{\langle \Sigma_1, \frac{\partial \phi}{\partial x/x} \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \Sigma_2, \frac{\partial \phi}{\partial x/x} \rangle}{\langle \Sigma_2, \phi \rangle} \]

\[ S^R_x \underbrace{=} \frac{\langle \frac{\partial \Sigma_1}{\partial x/x}, \phi \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \frac{\partial \Sigma_2}{\partial x/x}, \phi \rangle}{\langle \Sigma_2, \phi \rangle} \underbrace{\text{direct terms}} + \frac{\langle \Sigma_1, \frac{\partial \phi}{\partial x/x} \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \Sigma_2, \frac{\partial \phi}{\partial x/x} \rangle}{\langle \Sigma_2, \phi \rangle} \underbrace{\text{indirect terms}} \]
Reaction rate ratios (method)

Considering track-length estimators (for simplicity)...

\[
\langle \Sigma_1, \phi \rangle = q \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \ell_t \Sigma_1
\]

\[
\langle \Sigma_1, \frac{\partial \phi}{\partial x} \rangle = q \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \frac{\partial w_n}{w_n} \cdot \frac{\partial x}{x} \cdot \ell_t \Sigma_1
\]

\[
\langle \Sigma_1, \frac{\partial \phi}{\partial x} \rangle = q \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \left[ \sum_{g = (\alpha - \lambda)}^{\alpha} \left( ACC_{x}^{(n,g)} - REJ_{x}^{(n,g)} \right) \right] \ell_t \Sigma_1
\]
Indirect terms:

\[
\frac{\langle \Sigma_1, \frac{\partial \phi}{\partial x} / x \rangle}{\langle \Sigma_1, \phi \rangle} = \frac{q \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \left[ \sum_{g=(\alpha-\lambda)}^{\alpha} \left( ACC_x^{(n,g)} - REJ_x^{(n,g)} \right) \right] \ell_t \Sigma_1}{q \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \ell_t \Sigma_1}
\]

Average net number of \( x \) events (i.e., real - virtual) in the last \( \lambda \) generations, weighted on the contributions to the track length estimator of \( \langle \Sigma_1, \phi \rangle \)

Indirect part of \( S_x^R \) is obtained as the difference between the average number of net \( x \) events in the last \( \lambda \) generations, weighted on the tally contributions for two generic detectors \( \langle \Sigma_1, \phi \rangle \) and \( \langle \Sigma_2, \phi \rangle \)
A collision history-based approach to GPT calculations

Reaction rate ratios
Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)

\[ R = \frac{\iiint \phi(r, E) \cdot \sigma_f^{238} U(E) \, dE \, dr}{\iiint \phi(r, E) \cdot \sigma_f^{235} U(E) \, dE \, dr} \]

Jezebel (Pu sphere)
PU-MET-FAST-001

\(^{238}\text{U} / ^{235}\text{U}\) fission rate ratio
(measured in the center of the system)
A collision history-based approach to GPT calculations
Reaction rate ratios
Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)

Flattop-Pu (Popsy)
PU-MET-FAST-006

$^{238}$U/$^{235}$U fission rate ratio
(measured in the center of the system)

(not in scale)
A collision history-based approach to GPT calculations

Reaction rate ratios

Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)

\[ R = \frac{\iiint \phi(r, E) \cdot \sigma_{238}^U(E) \, dE \, dr}{\iiint \phi(r, E) \cdot \sigma_{235}^U(E) \, dE \, dr} \]

UAM TMI-1 PWR pin-cell

\(^{238}\text{U}/^{235}\text{U}\) fission rate ratio in the fuel pellet

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Perturbation/sensitivity calculations with Serpent
A collision history-based approach to GPT calculations

Reaction rate ratios

Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)

ERANOS results from Sandro Pelloni @ PSI

Jezebel - F28/F25 - Pu-239 - elastic scattering

F28/F25 sensitivity - 10 generations

- Sensitivity per lethargy unit
- Energy (eV)

Extended SERPENT-2 (JEFF-3.1)
Extended SERPENT-2 (ENDF/B-VII)
ERANOS
TSUNAMI-1D

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Perturbation/sensitivity calculations with Serpent
A collision history-based approach to GPT calculations

Reaction rate ratios

Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)

ERANOS results from Sandro Pelloni @ PSI

Jezebel - F28/F25 - Pu-239 - inelastic scattering

F28/F25 sensitivity - 10 generations
A collision history-based approach to GPT calculations
Reaction rate ratios
Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)
ERANOS results from Sandro Pelloni @ PSI
A collision history-based approach to GPT calculations

Reaction rate ratios
Adjoint-weighted quantities (bilinear ratios)

Reaction rate ratios (results)
ERANOS results from Sandro Pelloni @ PSI

Popsy (Flattop) - F28/F25 - Pu-239 - chi total
F28/F25 sensitivity - 10 generations - ENDF/B-VII

Sensitivity per lethargy unit
Extended SERPENT-2
TSUNAMI-1D

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Perturbation/sensitivity calculations with Serpent
Reaction rate ratios (results)
ERANOS results from Sandro Pelloni @ PSI

Popsy (Flattop) - F28/F25 - Pu-239 - fission
F28/F25 sensitivity - 10 generations - JEFF-3.1

Energy (eV)
Sensitivity per lethargy unit
Extended SERPENT-2
ERANOS

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Perturbation/sensitivity calculations with Serpent
A collision history-based approach to GPT calculations

**Reaction rate ratios**

Adjoint-weighted quantities (bilinear ratios)

**Reaction rate ratios (results)**

ERANOS results from Sandro Pelloni @ PSI

### UAM TMI-1 PWR cell - F28/F25 - H - total

F28/F25 sensitivity - 10 generations - ENDF/B-VII

**Perturbation/sensitivity calculations with Serpent**

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UAM TMI-1 PWR cell - F28/F25 - U-238 - disappearance

F28/F25 sensitivity - 10 generations - ENDF/B-VII

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Perturbation/sensitivity calculations with Serpent
## Reaction rate ratios (results)

ERANOS results from Sandro Pelloni @ PSI

Energy integrated sensitivity coefficients for Jezebel for the response function \( R = F_{28}/F_{25} \).

<table>
<thead>
<tr>
<th>( x )</th>
<th>( S_x^R )</th>
<th>JEFF-3.1</th>
<th>Serpent</th>
<th>Eranos</th>
<th>Rel. diff</th>
<th>ENDF/B-VII</th>
<th>Serpent</th>
<th>TSUNAMI-1D</th>
<th>Rel. diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ^{239}\text{Pu} ) ( \sigma_{\text{tot}} )</td>
<td>-0.14856 ( \pm ) 0.1%</td>
<td>-0.14923</td>
<td>-0.5%</td>
<td>-0.16404 ( \pm ) 0.1%</td>
<td>-0.16477</td>
<td>-0.4%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{239}\text{Pu} ) ( \sigma_{\text{inl}} )</td>
<td>-0.13475 ( \pm ) 0.0%</td>
<td>-0.13308</td>
<td>1.2%</td>
<td>-0.15996 ( \pm ) 0.0%</td>
<td>-0.15898</td>
<td>0.6%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{239}\text{Pu} ) ( \sigma_{\text{ela}} )</td>
<td>-0.06844 ( \pm ) 0.2%</td>
<td>-0.06854</td>
<td>-0.1%</td>
<td>-0.06386 ( \pm ) 0.2%</td>
<td>-0.06396</td>
<td>-0.2%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{239}\text{Pu} ) ( \sigma_{\text{fis}} )</td>
<td>+0.04750 ( \pm ) 0.1%</td>
<td>+0.04607</td>
<td>3.0%</td>
<td>+0.05173 ( \pm ) 0.1%</td>
<td>+0.05002</td>
<td>3.3%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{240}\text{Pu} ) ( \sigma_{\text{tot}} )</td>
<td>-0.01255 ( \pm ) 0.3%</td>
<td>-0.01243</td>
<td>1.0%</td>
<td>-0.01407 ( \pm ) 0.3%</td>
<td>-0.01405</td>
<td>0.1%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{239}\text{Pu} ) ( \sigma_{\text{dis}} )</td>
<td>+0.00995 ( \pm ) 0.1%</td>
<td>+0.01005</td>
<td>-1.0%</td>
<td>+0.01006 ( \pm ) 0.1%</td>
<td>+0.01008</td>
<td>-0.2%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{240}\text{Pu} ) ( \sigma_{\text{inl}} )</td>
<td>-0.00822 ( \pm ) 0.2%</td>
<td>-0.00820</td>
<td>0.2%</td>
<td>-0.00803 ( \pm ) 0.2%</td>
<td>-0.00798</td>
<td>0.6%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{240}\text{Pu} ) ( \sigma_{\text{ela}} )</td>
<td>-0.00387 ( \pm ) 0.7%</td>
<td>-0.00384</td>
<td>0.8%</td>
<td>-0.00403 ( \pm ) 0.7%</td>
<td>-0.00409</td>
<td>-1.5%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{239}\text{Pu} ) ( \sigma_{n,xn} )</td>
<td>-0.00278 ( \pm ) 0.2%</td>
<td>-0.00251</td>
<td>9.7%</td>
<td>-0.00201 ( \pm ) 0.2%</td>
<td>-0.00193</td>
<td>4.0%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{240}\text{Pu} ) ( \sigma_{\text{fis}} )</td>
<td>-0.00103 ( \pm ) 1.9%</td>
<td>-0.00097</td>
<td>5.8%</td>
<td>-0.00256 ( \pm ) 0.7%</td>
<td>-0.00253</td>
<td>1.2%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{240}\text{Pu} ) ( \sigma_{\text{dis}} )</td>
<td>+0.00066 ( \pm ) 0.4%</td>
<td>+0.00066</td>
<td>0.0%</td>
<td>+0.00062 ( \pm ) 0.5%</td>
<td>+0.00062</td>
<td>0.0%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{241}\text{Pu} ) ( \sigma_{\text{tot}} )</td>
<td>-0.00061 ( \pm ) 1.6%</td>
<td>-0.00045</td>
<td>26.2%</td>
<td>-0.00069 ( \pm ) 1.5%</td>
<td>-0.00068</td>
<td>1.4%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^{241}\text{Pu} ) ( \sigma_{\text{inl}} )</td>
<td>-0.00046 ( \pm ) 0.9%</td>
<td>-0.00047</td>
<td>-2.2%</td>
<td>-0.00061 ( \pm ) 0.8%</td>
<td>-0.00060</td>
<td>1.6%</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Bilinear ratios (method)

\[ R = \frac{\langle \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle} \]

Examples:

\[ \beta_{\text{eff}} = \frac{\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_d \bar{\nu}_d \Sigma_f \phi \rangle}{\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \rangle} \]
\[ \ell_{\text{eff}} = \frac{\langle \phi^\dagger, \frac{1}{\nu} \phi \rangle}{\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \rangle} \]
\[ \alpha_{\text{coolant}} = -\frac{\langle \phi^\dagger, \Sigma_{t,\text{coolant}} \phi \rangle}{\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \rangle} \]
Bilinear ratios (method)

\[
R' = \frac{\langle \phi^\dagger + \Delta \phi^\dagger, (\Sigma_1 + \Delta \Sigma_1)(\phi + \Delta \phi) \rangle}{\langle \phi^\dagger + \Delta \phi^\dagger, (\Sigma_2 + \Delta \Sigma_2)(\phi + \Delta \phi) \rangle}
\]

\[
\frac{\Delta R}{R} = \frac{\langle \phi^\dagger, \Delta \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_1 \phi \rangle} - \frac{\langle \phi^\dagger, \Delta \Sigma_2 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle} + \frac{\langle \phi^\dagger, \Sigma_1 \Delta \phi \rangle}{\langle \phi^\dagger, \Sigma_1 \phi \rangle} - \frac{\langle \phi^\dagger, \Sigma_2 \Delta \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle} + \frac{\langle \Delta \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_1 \phi \rangle} - \frac{\langle \Delta \phi^\dagger, \Sigma_2 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle}
\]

\[
S_x^R = \frac{\langle \phi^\dagger, \frac{\partial \Sigma_1}{\partial x/x} \phi \rangle}{\langle \phi^\dagger, \Sigma_1 \phi \rangle} - \frac{\langle \phi^\dagger, \frac{\partial \Sigma_2}{\partial x/x} \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle} + \frac{\langle \phi^\dagger, \Sigma_1 \frac{\partial \phi}{\partial x/x} \rangle}{\langle \phi^\dagger, \Sigma_1 \phi \rangle} - \frac{\langle \phi^\dagger, \Sigma_2 \frac{\partial \phi}{\partial x/x} \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle} + \frac{\langle \frac{\partial \phi^\dagger}{\partial x/x}, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_1 \phi \rangle} - \frac{\langle \frac{\partial \phi^\dagger}{\partial x/x}, \Sigma_2 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle}
\]
Bilinear ratios (method)

Adopting Iterated Fission Probability importance estimators:

\[
I_{n}^{(\gamma)} = \frac{1}{q'} \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} w_k
\]

Importance of neutrons in generation \(\alpha\) is calculated as function of the neutron descendants in generation \(\alpha + \gamma\).

Effect of perturbation on neutron importance:

\[
\frac{\partial I_{n}^{(\gamma)}}{\partial x/x} = \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} \frac{\partial w_k}{\partial x/x} - \frac{1}{w_n^2} \frac{\partial w_n}{\partial x/x} \sum_{k \in d_n^{(\gamma)}} w_k
\]
Bilinear ratios (method)

Indirect terms...

Effect of perturbation on the forward flux:

\[
\langle \phi^\dagger, \Sigma_1 \frac{\partial \phi}{\partial x/x} \rangle = \sum_{n \in \alpha} \sum_{t \in n} \frac{\partial w_n}{\partial x/x} \cdot \ell_t \Sigma_1 \cdot \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} w_k
\]

Effect of perturbation on the adjoint flux:

\[
\langle \frac{\partial \phi^\dagger}{\partial x/x}, \Sigma_1 \phi \rangle = \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \ell_t \Sigma_1 \left( \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} \frac{\partial w_k}{\partial x/x} - \frac{1}{w_n^2} \frac{\partial w_n}{\partial x/x} \sum_{k \in d_n^{(\gamma)}} w_k \right)
\]

Sum of indirect terms (rewritten as function of neutrons in generation $\alpha + \gamma$):

\[
\langle \phi^\dagger, \Sigma_1 \frac{\partial \phi}{\partial x/x} \rangle + \langle \frac{\partial \phi^\dagger}{\partial x/x}, \Sigma_1 \phi \rangle = \sum_{k \in (\alpha+\gamma)} \left[ w_k \left( \sum_{t \in (-\gamma)_k} \ell_t \Sigma_1 \right) \frac{\partial w_k}{w_k} \right]
\]
Example: effective prompt lifetime

\[
R = \frac{\left\langle \phi^\dagger, \frac{1}{v} \phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \Xi_t \Sigma_f \phi \right\rangle}
\]

Simple IFP estimator for the numerator:

\[
\left\langle \phi^\dagger, \frac{1}{v} \phi \right\rangle = \frac{1}{q'} \sum_{k \in (\alpha+\gamma)} w_k \cdot (-\gamma) l_k
\]

Numerator terms of the perturbation:

\[
\frac{\left\langle \phi^\dagger, \frac{1}{v} \frac{\partial \phi}{\partial x/x} \right\rangle}{\left\langle \phi^\dagger, \frac{1}{v} \phi \right\rangle} + \frac{\left\langle \frac{\partial \phi^\dagger}{\partial x/x}, \frac{1}{v} \phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{v} \phi \right\rangle} = \sum_{k \in (\alpha+\gamma)} w_k \left[ \sum_{g=(\alpha-\lambda)} \left( (n,g)^{ACC_x} - (n,g)^{REJ_x} \right) \right] (-\gamma) l_k
\]
Bilinear ratios (method)

Denominator terms:

\[
\frac{\langle \phi^\dagger, F \frac{\partial \phi}{\partial x/x} \rangle}{\langle \phi^\dagger, F \phi \rangle} + \frac{\langle \phi^\dagger, \frac{\partial F}{\partial x/x} \phi \rangle}{\langle \phi^\dagger, F \phi \rangle} + \frac{\langle \frac{\partial \phi^\dagger}{\partial x/x}, F \phi \rangle}{\langle \phi^\dagger, F \phi \rangle} = \sum_{k \in (\alpha+\gamma)} w_k \left[ \frac{\sum_{g=(\alpha-\lambda)} (\alpha+\gamma) \left( (n,g) ACC - (n,g) REJ \right)}{\sum_{g=(\alpha-\lambda)}} \right]
\]

We finally obtain the sensitivity coefficient for \( \ell_{\text{eff}} \):

\[
S_{x \ell_{\text{eff}}} = \frac{E \left[ \sum_{\text{history}} (ACC - REJ) \right] - E \left[ \sum \left( ACC - REJ \right) \right]}{E \left[ (-\gamma) I \right]} = \frac{\text{COV} \left[ (-\gamma) I, \sum_{\text{history}} (ACC - REJ) \right]}{E \left[ (-\gamma) I \right]}
\]
Bilinear ratios (method)

Everything is much more simple...

If the quantity $R$ can be estimated as the ratio of two generic Monte Carlo responses

$$R = \frac{E[e_1]}{E[e_2]}$$

the sensitivity coefficient of $R$ with respect to $x$ can be obtained as:

$$S_x^R = \frac{COV\left[e_1, \sum_{\text{history}} (ACC_x - REJ_x)\right]}{E[e_1]} - \frac{COV\left[e_2, \sum_{\text{history}} (ACC_x - REJ_x)\right]}{E[e_2]}$$
Bilinear ratios (results)

Jezebel - Leff - Pu-239 - elastic scattering
Effective prompt lifetime sensitivity - 4-8 generations - ENDF/B-VII

Sensitivity per lethargy unit

- Extended SERPENT-2
- TSUNAMI-1D (EGPT)

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Perturbation/sensitivity calculations with Serpent
Bilinear ratios (results)

Jezebel - Leff - Pu-239 - disappearance
Effective prompt lifetime sensitivity - 4-8 generations - ENDF/B-VII

![Graph showing bilinear ratios and sensitivity per lethargy unit against energy (eV)].

-2×10^{-3}
-4×10^{-3}
-6×10^{-3}
-8×10^{-3}
-1×10^{-2}

Energy (eV)

0

-2×10^{-3}
-4×10^{-3}
-6×10^{-3}
-8×10^{-3}
-1×10^{-2}

Sensitivity per lethargy unit

Extended SERPENT-2
TSUNAMI-1D (EGPT)
Bilinear ratios (results)

Popsy (Flattop) - Leff - Pu-239 - fission
Effective prompt lifetime sensitivity - 8-16 generations - ENDF/B-VII
Bilinear ratios (results)

Popsy (Flattop) - Leff - U-238 - inelastic scattering
Effective prompt lifetime sensitivity - 8-16 generations - ENDF/B-VII
Bilinear ratios (results)

UAM TMI-1 PWR cell - $\alpha_{\text{coolant}}$ - U-238 - disappearance

coolant void reactivity coeff. sensitivity - 4 generations - ENDF/B-VII

Sensitivity per lethargy unit

Energy (eV)

Extended SERPENT-2
TSUNAMI-1D
Difference (S-T)
Bilinear ratios (results)

UAM TMI-1 PWR cell - $\alpha_{\text{coolant}}$ - U-235 - nubar total
coolant void reactivity coeff. sensitivity - 4 generations - ENDF/B-VII

Energy (eV)

Sensitivity per lethargy unit

Extended SERPENT-2
TSUNAMI-1D
Difference (S-T)
The method can be extended to scattering distribution sensitivities:

At each scattering event, two pairs of outgoing energy/scattering angle are sampled.

One is accepted as real event, the other is rejected as virtual.

Implicit and constraining of the sensitivity profiles adopting a **continuous method** (in energy and angle).
Scattering distributions

The un constrained $k_{\text{eff}}$ sensitivity to scattering distributions can be obtained adopting Iterated Fission Probability methods as:

$$S^k_{\text{eff}}(\mu, E) = E \left[ \sum \left( (-\gamma) ACC_{\text{f}}(\mu|E) \right) \right]$$

In practice, bin-integrated quantities are of interest:

$$S^k_{\text{f}}(\mu, E) = \int_{\mu}^{\mu+1} \int_{E}^{E+1} S^k_{\text{f}}(\mu, E) \, d\mu \, dE$$

The constraint in $k_{\text{eff}}$ sensitivities to scattering functions can be introduced in a discretized form, starting from the bin-integrated unconstrained sensitivity coefficients ($S^k_{\text{f}, j, i}$), as done in deterministic codes.
Scattering distributions

The normalization constraint can be introduced as a continuous (non discretized) relationship:

$$\hat{S}_{f^x}^{k_{\text{eff}}} (\mu, E) = S_{f^x}^{k_{\text{eff}}} (\mu, E) - f^x(\mu|E) \int_{-1}^{1} S_{f^x}^{k_{\text{eff}}} (\mu^*, E) \, d\mu^*$$

In the present collision-history approach, the second term of the RHS of the Eq. above can be estimated as the density of rejected scattering events with $$(\mu|E)$$:

$$f(\mu|E) \int_{-1}^{1} S_{f^x}^{k_{\text{eff}}} (\mu^*, E) \, d\mu^* = E \left[ \sum \left( (-\gamma) \, \text{REJ}_{f(\mu|E)} \right) \right]$$

A continuous (in energy and angle) Monte Carlo estimator for the constrained sensitivity to scattering distribution is available:

$$\hat{S}_{f^x}^{k_{\text{eff}}} (\mu, E) = E \left[ \sum \left( (-\gamma) \, \text{ACC}_{f^x(\mu|E)} - (-\gamma) \, \text{REJ}_{f^x(\mu|E)} \right) \right]$$
Scattering distributions

**Jezebel - Pu-239 - elastic scattering**

Sensitivity to scattering cosine in CoM frame (constrained) - 6 generations - ENDF/B-VII

![Graph showing sensitivity to scattering cosine in CoM frame for Jezebel - Pu-239 - elastic scattering with sensitivity per cosine width on the y-axis and scattering cosine on the x-axis.]

- Effective prompt lifetime -- Extended SERPENT-2
- Keff -- Extended SERPENT-2
- Keff -- MCNP
Scattering distributions

Jezebel, $k_{\text{eff}}$ sensitivity to elastic scattering distribution
Scattering distributions

Jezebel, $\ell_{\text{eff}}$ sensitivity to elastic scattering distribution
Scattering distributions

Jezebel, $F_{28}/F_{25}$ sensitivity to elastic scattering distribution
A collision history-based approach to GPT calculations
Reaction rate ratios
Adjoint-weighted quantities (bilinear ratios)

Legendre moments

Scattering distributions are often expressed as an expansion of Legendre polynomials:

\[ f^x(\mu|E) \approx \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(\mu) f^x_n(E) \]

The sensitivity of \( R \) to the \( n^{th} \) Legendre moment of a given scattering distribution can be defined as follows:

\[ S_{f_n^x}^R \equiv \frac{dR}{df_n^x / f_n^x} \]

\[ S_{f_n^x}^R(E) = \int_{-1}^{1} \frac{dR}{R} \cdot \frac{df^x(\mu|E)}{f^x(\mu|E)} \cdot \frac{df^x_n(E)}{df^x_n(E)} \cdot f^x_n(E) \cdot \frac{1}{f^x(\mu|E)} \cdot d\mu \]

\[ \frac{2n+1}{2} P_n(\mu) \]
Legendre moments

All the terms in $G_{f_n^x}$ can be calculated on-the-fly:

$$G_{f_n^x} = \frac{2n+1}{2} P_n(\mu) \cdot f_n^x(E) \cdot 1/f^x(\mu|E)$$

Continuous Monte Carlo estimator for the sensitivity to the Legendre moments of the scattering distributions:

$$S_{f_n^x}^R = \frac{\text{COV} \left[ e_1 , \sum \text{history } G_{f_n^x} \right]}{E[e_1]} - \frac{\text{COV} \left[ e_2 , \sum \text{history } G_{f_n^x} \right]}{E[e_2]}$$
Scattering distributions

Jezebel - Keff - Pu-239 - elastic scattering - P1

Keff sensitivity - 3 generations - ENDF/B-VII

Incident energy (MeV)

Sensitivity (0.1 MeV energy bins)

Extended SERPENT-2 (-0.1007)
MCNP (-0.0896)
Kiedrowski, B. C., 2013. (LA-UR-13-27498)

Keff sensitivity - 3 generations - ENDF/B-VII

Perturbation/sensitivity calculations with Serpent
Scattering distributions

Jezebel - $k_{\text{eff}}$ - Pu-239 - elastic scattering

Effective multiplication factor sensitivity - 3 generations - ENDF/B-VII

- Sensitivity per lethargy unit
- Scattering XS ($f_0$) -- Ext. Serpent
- 1st Legendre moment -- Ext. Serpent
- Scatt. XS (G. Palmiotti)
- 1st Leg. moment (G. Palmiotti)
- MCNP 1st Leg. moment
- Kiedrowski, B. C., (LA-UR-13-27498)
Scattering distributions

Jezebel - $l_{\text{eff}}$ - Pu-239 - elastic scattering

Effective prompt lifetime sensitivity - 2-4 generations - ENDF/B-VII
Scattering distributions

Jezebel - F28/F25 - Pu-239 - elastic scattering

Central F28/F25 ratio sensitivity - 6 generations - ENDF/B-VII
Latent generations convergence
ERANOS results from Sandro Pelloni @PSI

Flattop (Pu239 configuration) - U238 Inelastic scattering
Extended Serpent2 (LPSC version) - adj-weighted sensitivity - 10 latent generations
Serpent results for sensitivities to scattering distributions have not been fully tested/verified yet!
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QUESTIONS? SUGGESTIONS? NEW IDEAS?