Continuous-Energy
TSUNAMI Sensitivity
Capabilities in SCALE 6.2

\[ S_{R,\Sigma} = \frac{\delta R/R}{\delta \Sigma/\Sigma} \]

Dr. Christopher M. Perfetti
Radiation Transport Group
Reactor and Nuclear Systems Division
Oak Ridge National Laboratory
Introduction to Sensitivity Coefficients

- Sensitivity coefficients provide insight on the sources and impact of uncertainty in nuclear engineering models.

Input Information:
- Nuclear Data ($\Sigma$)
- Number Densities ($N$)
- Material Densities ($\rho$)

Input Uncertainty:
- $\Delta \Sigma$, $\Delta N$, $\Delta \rho$

Monte Carlo Code

Output Information:
- $k_{\text{eff}}$, Dose Rate, Fission Rate, etc...

Output Uncertainty:
- $\Delta k_{\text{eff}}$, $\Delta$ Dose Rate, $\Delta$ Fission Rate

$$S_{R,\Sigma x} = \frac{\delta R/R}{\delta \Sigma x / \Sigma x}$$
Introduction to Sensitivity Coefficients

• Sensitivity coefficients describe the fractional change in a response that is due to perturbations, or uncertainties, in system parameters.

\[ S_{R,\Sigma_x} = \frac{\delta R / R}{\delta \Sigma_x / \Sigma_x} \]

• The SCALE TSUNAMI code calculates sensitivity coefficients for critical eigenvalue or reaction rate ratio responses:

\[ R = k_{eff} \]
\[ R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle} \]
TSUNAMI Sensitivity Methods

1. TSUNAMI-1D
   Deterministic, Multigroup

2. TSUNAMI-2D
   Deterministic, Multigroup

3. TSUNAMI-3D
   - Multigroup TSUNAMI-3D
     Monte Carlo, Multigroup
   - Iterated Fission Probability (IFP) Method
     Monte Carlo, Continuous-Energy
   - CLUTCH Method
     Monte Carlo, Continuous-Energy

• TSUNAMI offers several options for sensitivity calculations based on the desired level of accuracy and runtime.
Continuous-Energy Resolution

- Continuous-energy capabilities allow for a better understanding of the phenomena that contribute to system uncertainty.

![Graph showing sensitivity per unit lethargy versus energy (eV). The graph compares O-16 capture sensitivity for 238-group Multigroup VS Microgroup CLUTCH.]
Applications for Sensitivity Analysis

• Design Optimization
  Reactor Design, Isotope Production

• Uncertainty Propagation and Quantification
  Criticality Safety, Reactor Design

• Identifying Relevant Benchmarks for Licensing Applications
  Criticality Safety, Reactor Design

• Anticipating Modeling and Simulation Code Biases
  Criticality Safety, Reactor Design, etc.
Sensitivity Applications: Design Optimization

The Long Road to $^{252}$Cf

- Less than 1% of all heavy curium feedstock in HFIR is transmuted into $^{252}$Cf.
- An ORNL LDRD by Perfetti et. al used capture-to-fission sensitivity coefficients to improve the efficiency of $^{252}$Cf transmutation.
- This work achieved a greater than 10x improvement in $^{252}$Cf production efficiency.
Sensitivity Applications: Uncertainty Propagation

- Sensitivity coefficients can be combined with cross section uncertainties to quantify the uncertainty in a response.

\[
S_{k,\Sigma_x} \cdot \text{Cov}_{\Sigma_x,\Sigma_y} \cdot S_{k,\Sigma_y}^T = \sigma_k^2
\]

\[
\begin{align*}
\left(\frac{\delta k}{k}\right) & \cdot \left(\frac{\Delta \Sigma}{\Sigma}\right)^2 & \cdot \left(\frac{\delta k}{k}\right) & = \sigma_k^2 \\
\left(\frac{\delta \Sigma}{\Sigma}\right) & \cdot \left(\frac{\delta \Sigma}{\Sigma}\right) & \cdot \left(\frac{\Delta k}{k}\right)^2
\end{align*}
\]

The Sandwich Equation
Sensitivity Applications: Benchmark Similarity Assessment

- The similarity coefficient, $c(k)$ or $c_k$, describes the amount of nuclear data-induced uncertainty that is shared by two systems.

$$S_{R_1,\Sigma_x} \cdot \text{Cov}_{\Sigma_x,\Sigma_y} \cdot S^T_{R_2,\Sigma_y} = \sigma^2_{R_1,R_2}$$

$$c_k = \frac{\sigma^2_{R_1,R_2}}{\sigma_{R_1} \sigma_{R_2}}$$

- The TSUNAMI-IP code calculates $c_k$ values between a target application and reference benchmark experiments.
Integrating Nuclear Criticality Experiments into Differential Nuclear Data Evaluations

U.S. Nuclear Regulatory Commission
  Nuclear Materials Safety and Safeguards, Nuclear Reactor Regulation, Office of New Reactors

U.S. DOE / Areva / Duke Energy
  Mixed Oxide Fuel Fabrication Facility

Candu Energy
  ACR-1000 Design Validation

Atomic Energy of Canada, Ltd.
  ACR-700 NRC Review/PIRT

U.S. DOE
  Yucca Mountain post-closure criticality safety

Global Nuclear Fuels
  Transportation package licensing

Svensk Kärnbränslehantering AB
  Swedish used fuel repository

Organization for Economic Cooperation and Development, Nuclear Energy Agency
  International Expert Groups

TSUNAMI in Practice
• Experimental benchmark data is used to improve the accuracy of the initial computed responses.
• This assimilation consistently adjusts the underlying nuclear data.
• This capability will be discussed further in the TSURFER presentation.
Calculating Sensitivity Coefficients

Relative sensitivity of $k_{\text{eff}}$ to single energy group of a particular nuclide-reaction pair cross section, $S_{x,g}$, is expressed as:

$$S_{k,\Sigma_{x,g}} = \frac{\partial k_{\text{eff}}}{\partial \Sigma_{x,g}} \left/ \frac{k_{\text{eff}}}{\Sigma_{x,g}} \right.$$ 

$$S_{k,\Sigma(r)} = \frac{\partial k}{\partial \Sigma(r)} \left/ \Sigma(r) \right.$$ 

where

- $\phi$ = neutron flux;
- $\phi^*$ = adjoint neutron flux;
- $k = k_{\text{eff}}$, the largest of the eigenvalues;
- $A$ = operator that represents all of the transport equation except for the fission term;
- $B$ = operator that represents the fission term of the transport equation;
- $\Sigma$ = problem-dependent resonance self-shield macroscopic cross sections;
- $\xi$ = phase space vector; and
- $\langle \rangle$ indicate integration over space, direction and energy variables.
Calculating Sensitivity Coefficients

• For a sample capture reaction \((cap.)\), the First-Order Perturbation Equation reduces to something like:

\[
S_{k,\Sigma_{cap.}} = \frac{\delta k/k}{\delta \Sigma_{cap}/\Sigma_{cap}} = \frac{\langle \Phi^\dagger \Sigma_{cap} \Phi \rangle}{\frac{1}{k} \langle \Phi^\dagger \Sigma_{fis.} \Phi \rangle}
\]

• Tallying reaction rates is relatively straightforward for a Monte Carlo code.

• The challenge is therefore tallying the forward and adjoint fluxes as a function of space, energy, and angle.
Calculating Sensitivity Coefficients

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• Tallying reaction rates is relatively straightforward for a Monte Carlo code.

• The challenge is therefore tallying the forward and adjoint fluxes as a function of space, energy, and angle.
CE TSUNAMI-3D Sensitivity Methods

Eigenvalue Sensitivity Calculations

• CLUTCH Method (cet=1)
• IFP Method (cet=2)

Generalized Perturbation Theory Sensitivities

• GEAR-MC Method: CLUTCH only (cet=4)
• GEAR-MC Method: CLUTCH + IFP (cet=5)
Things you need for a multigroup TSUNAMI-3D Calculation:

- Spatial Flux Mesh
- Flux Moments
- Separate Adjoint Transport Solution
- Volume Calculations
- Cross Section Self-Shielding
- Expert Judgment

\[ \tilde{\phi}_j = \int \phi(\hat{\Omega}) R_j(\hat{\Omega}) d\hat{\Omega} \]

points = \( \frac{\text{volume}}{\ln(\text{volume}/5000)} \)
Why use Continuous Energy?

• CE TSUNAMI-3D uses cutting-edge Monte Carlo methods to calculate sensitivity coefficients, and requires:
  – No flux moment calculations
  – No spatial flux mesh (sort of)
  – No volume calculations
  – No problem-dependent cross section self-shielding
  – No implicit sensitivity effects
  – No adjoint transport simulation, just one forward simulation

• CE TSUNAMI-3D avoids the large memory footprints that can be required by multigroup TSUNAMI-3D.

• Use of continuous-energy physics more accurately models the physics of neutron interactions (see: the read energy input block ).
H-1 Elastic Scatter Sensitivity
238-group CLUTCH VS Microgroup CLUTCH

U-238 Capture Sensitivity
238-group CLUTCH VS Microgroup CLUTCH

Energy (eV)

Sensitivity per Unit Lethargy
Why NOT use Continuous Energy?

• The simulation runtimes are usually longer than for multigroup TSUNAMI-3D.

• In many applications multigroup TSUNAMI-3D calculations already provide sufficient accuracy.

• Some problems may still require a spatial flux mesh, significant computational memory, and/or expert judgment.
CE TSUNAMI-3D Sensitivity Methods

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Generalized Perturbation Theory Sensitivities

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Iterated Fission Probability Method

- The Iterated Fission Probability (IFP) method calculates adjoint-weighted tallies using the notion that the importance of an event is proportional to the population of neutrons present in the system during some future generation.

- In practice, the IFP method can require storing reaction rate tallies for a significant number of generations.

- In CE TSUNAMI-3D, the IFP method is used by setting: \( \text{cet}=2 \)

- The number of “latent generations” is set using the \( \text{cfp}=# \) parameter.

Illustration of the IFP process. Image courtesy of Brian Kiedrowski.
How Many Latent Generations Do We Need?

• IFP calculations should use somewhere between 2 and 20 latent generations to obtain accurate sensitivity tallies.
  – In practice, most simulations require between 5 and 10 latent generations.

• The memory footprint of SCALE IFP calculations scales linearly with the number of latent generations.
  – Users should use enough latent generations to obtain accurate sensitivity coefficients, but also as few as possible to minimize the simulation’s memory footprint.
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Let’s Try CE TSUNAMI-3D
Let’s Try CE TSUNAMI-3D
IFP Method Memory Requirements

- The IFP method allows for very accurate sensitivity coefficient calculations, but sometimes encounters large computational memory footprints and long problem runtimes.
- For a model of a typical PWR with depletion isotopics...

\[
38,000 \text{ unique isotope-regions} \times 12 \text{ reactions per isotope} \times 44 \text{ energy groups} \times 11 \text{ generations of storage} \times 10,000 \text{ particles per generation} \times 8 \text{ bytes per double} = 17,656 \text{ gigabytes of memory}
\]
CE TSUNAMI-3D Sensitivity Methods

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• CLUTCH Method \((\text{cet}=1)\)
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CLUTCH/Contributon Methodology

- The CLUTCH method calculates the importance of collisions by tallying how many fission neutrons are created by a particle after it leaves the collision:

\[
\phi^+(\tau_s) = \int_V G(\tau_s \rightarrow r)F^+(r) \, dr,
\]

...where:

\[ G(\tau_s \rightarrow r) = \text{The number of fission neutrons created at } r \text{ by the neutron originating in the phase space } \tau_s. \]

\[ F^*(r) = \text{The average importance of fission neutrons born at } r, \text{ or:} \]

\[
F^+(r) = \int_{E} \int_{\Omega} \frac{\chi(r, E)}{4\pi} \phi^+(r, E, \Omega) \, d\Omega \, dE.
\]
CLUTCH VS IFP

- The CLUTCH method is more efficient than IFP (both in terms of speed and memory usage).
- The downside to CLUTCH is that you need to compute $F^*(r)$.

**Sensitivity Method Memory Usage**

<table>
<thead>
<tr>
<th>Model</th>
<th>IFP</th>
<th>CLUTCH</th>
<th>Memory Reduction Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Pin</td>
<td>2,113 MB</td>
<td>1.06 MB</td>
<td>1,990</td>
</tr>
<tr>
<td>Godiva</td>
<td>26 MB</td>
<td>0.12 MB</td>
<td>220</td>
</tr>
<tr>
<td>HMF-025-005</td>
<td>1,675 MB</td>
<td>0.16 MB</td>
<td>10,470</td>
</tr>
<tr>
<td>LCT-010-014</td>
<td>19,509 MB</td>
<td>25 MB</td>
<td>780</td>
</tr>
<tr>
<td>NAC-UMS</td>
<td>21,201 MB</td>
<td>3,416 MB</td>
<td>6.2</td>
</tr>
</tbody>
</table>

**Figure of Merit (min\(^{-1}\))**

- **H-1**: 1.0E+01
- **O-16**: 1.0E+02
- **U-235**: 1.0E+05
- **U-238**: 1.0E+06
- **Pu-239**: 1.0E+07

**Nuclide Sensitivity**

- **IFP**
- **CLUTCH**
The F*(r) Function

- The CLUTCH Method uses an importance weighting function, F*(r), to compute multi-generational sensitivity effects.
- The F*(r) function describes the average response importance generated by fission neutrons born at location r.
- The F*(r) function can be calculated using the IFP method during inactive generations with no significant loss of accuracy and with significant memory savings.
The F*(r) Function

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How to use CLUTCH with an $F^*(r)$ Mesh

- Set $cet=1$ to enable CLUTCH.

- Set $cfp=#$ to set the number of latent generations for the IFP calculation that populates the $F^*(r)$ mesh.

- Consider increasing the number of inactive generations to allow the $F^*(r)$ mesh to converge.

- Set $cgd=#$ to tell CE TSUNAMI-3D the ID of the GridGeometry mesh for $F^*(r)$.

- Make the GridGeometry mesh for $F^*(r)$. 
Let’s Try CE TSUNAMI-3D...with CLUTCH!

Note: a 1cm-2cm mesh is sufficiently resolved for most CLUTCH $F^*(r)$ calculations.
Let's Compare our IFP and CLUTCH Sensitivities

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>IFP Sensitivity</th>
<th>CLUTCH Sensitivity</th>
<th>Difference (# Standard Dev.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-234</td>
<td>6.92E-03 ± 6.71E-04</td>
<td>6.37E-03 ± 2.68E-04</td>
<td>-0.76</td>
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<tr>
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<td>8.09E-01 ± 5.18E-03</td>
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</tr>
<tr>
<td>U-238</td>
<td>1.69E-02 ± 1.50E-03</td>
<td>1.61E-02 ± 5.43E-04</td>
<td>-0.46</td>
</tr>
</tbody>
</table>
Best Practices for F*(r) Mesh Generation

- An F*(r) mesh with 1cm – 2cm mesh intervals is generally sufficiently resolved to generate accurate sensitivity coefficients.
- The F*(r) mesh must only cover all fissionable regions in a problem.
- Setting $\text{cfp}=-1$ will run CLUTCH assuming that $F*(r)=1$ everywhere.
  - Useful for models of infinitely-reflected systems.
- Since the F*(r) mesh is generated during skipped generations, NSK should be adjusted so that the F*(r) tallies can converge.
  - In general, simulating between 1 and 100 inactive particle histories per F*(r) mesh interval will produce an accurate F*(r) tally.
  - Our Godiva problem used a mesh with 5,832 intervals (18×18×18); 5,832 mesh intervals × 100 histories per interval / 1,000 particles per gen. = ~500 skipped generations.
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Improving the CLUTCH Input
Best Practices for F*(r) Mesh Generation

• Setting the FST=yes parameter will produce a .3dmap file showing the F*(r) mesh that was calculated.

• At the end of the inactive generations, SCALE will summarize the convergence of your F*(r) mesh in a warning message.

F*(r) Convergence Statistics:
WARNING: Of the 3682 F*(r) mesh intervals that scored tallies...
99.19% of the F*(r) tallies contain more than 5% uncertainty;
61.46% of the F*(r) tallies contain more than 10% uncertainty;
23.76% of the F*(r) tallies contain more than 20% uncertainty; and
5.38% of the F*(r) tallies contain more than 50% uncertainty.
Updated Sensitivity Coefficients

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>IFP Sensitivity</th>
<th>CLUTCH Sensitivity</th>
<th>Improved CLUTCH Run</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-234</td>
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</tr>
</tbody>
</table>
## TSUNAMI-3D Sensitivity Method Summary

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<thead>
<tr>
<th></th>
<th>Multigroup TSUNAMI</th>
<th>IFP</th>
<th>CLUTCH</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Accuracy</strong></td>
<td>Good</td>
<td>Excellent</td>
<td>Excellent</td>
</tr>
<tr>
<td><strong>Speed</strong></td>
<td>Good</td>
<td>Good</td>
<td>Excellent</td>
</tr>
<tr>
<td><strong>Efficiency</strong></td>
<td>Excellent</td>
<td>Good</td>
<td>Excellent</td>
</tr>
<tr>
<td><strong>Memory Requirements</strong></td>
<td>Limiting</td>
<td>Limiting</td>
<td>Typically Fine</td>
</tr>
<tr>
<td><strong>Ease of Use</strong></td>
<td>Requires a Flux Mesh</td>
<td>Very Easy</td>
<td>Must Calculate $F^*(r)$</td>
</tr>
</tbody>
</table>
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Generalized Perturbation Theory

- Generalized Perturbation Theory (GPT) estimates sensitivity coefficients for any system response that can be expressed as the ratio of reaction rates.

\[ S_{R,\Sigma} = \frac{\delta R/R}{\delta\Sigma/\Sigma} = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle} \]

- Calculating generalized sensitivity coefficients requires solving an inhomogeneous, or generalized, adjoint equation:

\[ L^\dagger \Gamma^\dagger = \lambda P^\dagger \Gamma^\dagger + S^\dagger \]

\[ S^\dagger = \frac{1}{R} \frac{\partial R}{\partial \phi} = \frac{\Sigma_1}{\langle \Sigma_1 \phi \rangle} - \frac{\Sigma_2}{\langle \Sigma_2 \phi \rangle} \]

- TSUNAMI offers several tools for performing GPT sensitivity analysis:
  - TSUNAMI-1D: Multigroup analysis using the XSDRN code.
  - TSUNAMI-2D: Multigroup analysis using the NEWT code.
  - TSUNAMI-3D: Continuous-energy analysis using the KENO-Va/VI codes.

Sensitivity of \(^{235}\text{U}\) thermal fission cross section
Generalized Perturbation Theory

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Sensitivity of 235U thermal fission cross section
Generalized Perturbation Theory

- GPT sensitivities can be used to understand the sources and impact of nuclear data uncertainty in responses such as:
  - Relative powers
  - Isotope Conversion ratios
  - Multigroup cross sections
  - Fission ratios
    - Example: $^{239}\text{Pu}(n,f)/^{235}\text{U}(n,f)$
- Experimental parameters
  - Example: $^{28}\rho$
    (ratio of epithermal/thermal $^{238}\text{U}$ capture rates in irradiation foils)

<table>
<thead>
<tr>
<th>NUMBER</th>
<th>EXPERIMENT</th>
<th>Type</th>
<th>Format</th>
<th>Value</th>
<th>Xsec Uncert</th>
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<tbody>
<tr>
<td>1</td>
<td>k_infinity</td>
<td>keff</td>
<td>Relative</td>
<td>1.1083E+0</td>
<td>4.98551E-1 % dk/k</td>
</tr>
<tr>
<td>2</td>
<td>fission grp_1</td>
<td>gpt</td>
<td>Relative</td>
<td>1.9155E-3</td>
<td>6.91925E-1 % dR/R</td>
</tr>
<tr>
<td>3</td>
<td>fission grp_2</td>
<td>gpt</td>
<td>Relative</td>
<td>2.7748E+2</td>
<td>3.23440E-1 % dR/R</td>
</tr>
<tr>
<td>4</td>
<td>absorpt grp_1</td>
<td>gpt</td>
<td>Relative</td>
<td>7.1637E-3</td>
<td>8.36728E-1 % dR/R</td>
</tr>
<tr>
<td>5</td>
<td>absorpt grp_2</td>
<td>gpt</td>
<td>Relative</td>
<td>5.3702E-2</td>
<td>2.38082E-1 % dR/R</td>
</tr>
<tr>
<td>6</td>
<td>cornerrod fpf</td>
<td>gpt</td>
<td>Relative</td>
<td>1.1458E+0</td>
<td>1.67147E-1 % dR/R</td>
</tr>
</tbody>
</table>
## CE TSUNAMI-3D GPT Response Extension

### Original GPT Responses

<table>
<thead>
<tr>
<th>Response</th>
<th>MT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total cross section</td>
<td>1</td>
</tr>
<tr>
<td>Fission cross section</td>
<td>18</td>
</tr>
<tr>
<td>$(n,\gamma)$ abs. cross section</td>
<td>102</td>
</tr>
<tr>
<td>Neutron prod. cross section</td>
<td>1452</td>
</tr>
<tr>
<td>Neutron flux</td>
<td></td>
</tr>
</tbody>
</table>

Original GPT Responses
## CE TSUNAMI-3D GPT Response Extension

<table>
<thead>
<tr>
<th>Original GPT Responses</th>
<th>Updated GPT Responses</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Total cross section</td>
<td>(MT = 1)</td>
</tr>
<tr>
<td>• Fission cross section</td>
<td>(MT = 18)</td>
</tr>
<tr>
<td>• $(n,\gamma)$ abs. cross section</td>
<td>(MT = 102)</td>
</tr>
<tr>
<td>• Neutron prod. cross section</td>
<td>(MT = 1452)</td>
</tr>
<tr>
<td>• Neutron flux</td>
<td></td>
</tr>
<tr>
<td>• Total cross section</td>
<td>(MT = 1)</td>
</tr>
<tr>
<td>• Total scatter cross section</td>
<td>(MT = 0)</td>
</tr>
<tr>
<td>• Elastic scatter cross section</td>
<td>(MT = 2)</td>
</tr>
<tr>
<td>• Inelastic scatter cross section</td>
<td>(MT = 4)</td>
</tr>
<tr>
<td>• $(n,2n)$ scatter cross section</td>
<td>(MT = 16)</td>
</tr>
<tr>
<td>• Fission cross section</td>
<td>(MT = 18)</td>
</tr>
<tr>
<td>• Total absorption cross section</td>
<td>(MT = 101)</td>
</tr>
<tr>
<td>• $(n,\gamma)$ absorption cross section</td>
<td>(MT = 102)</td>
</tr>
<tr>
<td>• $(n,p)$ absorption cross section</td>
<td>(MT = 103)</td>
</tr>
<tr>
<td>• $(n,d)$ absorption cross section</td>
<td>(MT = 104)</td>
</tr>
<tr>
<td>• $(n,t)$ absorption cross section</td>
<td>(MT = 105)</td>
</tr>
<tr>
<td>• $(n,^3\text{He})$ absorption cross section</td>
<td>(MT = 106)</td>
</tr>
<tr>
<td>• $(n,\alpha)$ absorption cross section</td>
<td>(MT = 107)</td>
</tr>
<tr>
<td>• Neutron production cross section</td>
<td>(MT = 1452)</td>
</tr>
<tr>
<td>• Flux-weighted CMM diffusion coefficient</td>
<td></td>
</tr>
<tr>
<td>• Neutron flux</td>
<td></td>
</tr>
</tbody>
</table>
Diffusion Coefficient Sensitivity Calculations: Cumulative Migration Method

- Developed by Liu in 2016 [1], the Cumulative Migration Method (CMM) allows for highly accurate diffusion coefficient calculations using the concept of “Migration Area”:

\[
M^2 = \frac{D}{\Sigma_r} = \frac{1}{6} \bar{r}^2
\]

\[
R(D_{CMM}) = \frac{\langle M^2 \Sigma_r \phi \rangle}{\langle \phi \rangle}
\]

- This method can face challenges when confronted with non-unit cell systems or non-cuboidal reflecting boundaries.

GPT Calculations in CE TSUNAMI-3D

- The generalized importance function for a response can be expressed as the sum of two terms: the intra-generation effect term and the inter-generational effect term.
  - The **intra-generation** effect describes how much importance a neutron generates after an event occurs.
  - The **inter-generational** effect describes the importance that is generated by the daughter fission neutrons of the original particle.

\[
\Gamma^\dagger(\tau_s) = \frac{1}{Q_s} \left\{ \frac{1}{R} \frac{\partial R}{\partial \phi}(r) \phi(\tau_s \rightarrow r) \right\} + \frac{\lambda}{Q_s} \left\langle \Gamma^\dagger(r) P(r) \phi(\tau_s \rightarrow r) \right\rangle
\]

- CE TSUNAMI-3D uses the **CLUTCH** sensitivity method to calculate the intra-generation term, and an Iterated Fission Probability-based approach to calculate the inter-generational term.

- For more background on this methodology, see:
  
The generalized importance function for a response can be expressed as the sum of two terms: the intra-generation effect term and the inter-generational effect term.

- The **intra-generation** effect describes how much importance a neutron generates after an event occurs.
- The **inter-generational** effect describes the importance that is generated by the daughter fission neutrons of the original particle.

\[
\Gamma^\dagger(\tau_s) = \frac{1}{Q_s} \left( \frac{1}{R} \frac{\partial R}{\partial \Phi} (r) \Phi(\tau_s \rightarrow r) \right) + \frac{\lambda}{Q_s} \left\langle \Gamma^\dagger(r)P(r)\Phi(\tau_s \rightarrow r) \right\rangle
\]

CE TSUNAMI-3D uses the **CLUTCH** sensitivity method to calculate the intra-generation term, and an **Iterated Fission Probability**-based approach to calculate the inter-generational term.

For more background on this methodology, see:

### GPT Flattop foil response sensitivity coefficients

#### F28/F25 Pu-239

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Response</th>
<th>Isotope</th>
<th>Direct Pert.</th>
<th>TSUNAMI-1D</th>
<th>GEAR-MC</th>
</tr>
</thead>
<tbody>
<tr>
<td>F28 / F25</td>
<td></td>
<td>$^{238}\text{U}$</td>
<td>$0.8006 \pm 0.0533$</td>
<td>$0.8024$ ($0.03 \sigma$)</td>
<td>$0.7954 \pm 0.0018$ ($-0.10 \sigma$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$^{239}\text{Pu}$</td>
<td>$0.0528 \pm 0.0043$</td>
<td>$0.0657$ ($2.99 \sigma$)</td>
<td>$0.0561 \pm 0.0012$ ($0.73 \sigma$)</td>
</tr>
</tbody>
</table>

#### F37/F25 U-238

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Response</th>
<th>Isotope</th>
<th>Direct Pert.</th>
<th>TSUNAMI-1D</th>
<th>GEAR-MC</th>
</tr>
</thead>
<tbody>
<tr>
<td>F37 / F25</td>
<td></td>
<td>$^{238}\text{U}$</td>
<td>$-0.1540 \pm 0.0102$</td>
<td>$-0.1551$ ($-0.11 \sigma$)</td>
<td>$-0.1608 \pm 0.0016$ ($-0.66 \sigma$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$^{239}\text{Pu}$</td>
<td>$0.0543 \pm 0.0048$</td>
<td>$0.0736$ ($3.99 \sigma$)</td>
<td>$0.0489 \pm 0.0010$ ($-1.10 \sigma$)</td>
</tr>
</tbody>
</table>

### Flattop total nuclide foil response sensitivities
How does the CE TSUNAMI-3D approach differ from other methods?

- Generalized Perturbation Theory Monte Carlo methods have been developed by Abdel-Khalik et al. for calculating generalized sensitivity coefficients in 3D, continuous-energy Monte Carlo applications, but these methods require performing multiple direct perturbation calculations and can require a large number of runs to calculate generalized sensitivity coefficients.

- This approach differs in that it:
  - Requires no perturbation calculations and no knowledge of nuclear covariance data.
  - Because our approach is not perturbation-based, we can easily calculate energy-dependent sensitivity coefficients for multiple responses to all input nuclear data parameters in one continuous-energy Monte Carlo transport calculation.
  - The deterministic, sensitivity-based TSUNAMI-1D and TSUNAMI-2D GPT methods require at least one transport calculation per generalized response.
Continuous-Energy TSUNAMI Sensitivity Capabilities in SCALE 6.2

TSUNAMI-1D/2D GPT Sequences

Input

BONAMIST / CENTRM / PMC or BONAMIST / NITAWLST

Resonance cross-section processing (repeated for all cells)

YES

NO

End

2D discrete ordinates
2D discrete ordinates adjoint calculation
S/U calculation for $k_{\text{eff}}$
2D discrete ordinates inhomogeneous adjoint calculation for each response
S/U calculation for a user-defined response

Substitute XSDRNPM in place of NEWT for TSUNAMI-1D

\[
L \phi = \lambda P\phi \\
L^\dagger \phi^\dagger = \lambda P^\dagger \phi^\dagger \\
L^\dagger \Gamma^\dagger = \lambda P^\dagger \Gamma^\dagger + S^\dagger
\]
CE TSUNAMI-3D GPT Sequence

SCALE Driver

Input

CE KENO

3D Monte Carlo

\[ L \phi = \lambda P \phi \]
\[ L^\dagger \phi^\dagger = \lambda P^\dagger \phi^\dagger \]
\[ L^\dagger \Gamma^\dagger = \lambda P^\dagger \Gamma^\dagger + S^\dagger \]

S/U calculation for \( k_{\text{eff}} \) and user-defined responses

SAMS

End
Definitions Block

- Used to define reaction rates, or responses, for GPT sensitivities.

- `mixture=#` is used to define the material for the response.
  - `multimix=#1 #2 #3 end` is used to define responses containing multiple materials.

- `ehigh=#1` and `elow=#2` will create an energy window for this response.

```
read definitions
response 5
  nuclide=92235
  reaction=fission
  mixture=10 micro
  ehigh=0.625
end response
response 6
  unity mixture=10
end response
end definitions
```
Definitions Block

- **reaction=#** keyword is used to define the reaction of interest.
  - Omitting this keyword and entering “unity” will result in a flux response.
  - Reactions available in CE TSUNAMI-3D:
    - mt=1 (total XS)
    - mt=18 (fission)
    - mt=102 (n, gamma)
    - mt=452 (nu-bar)
- **nuclide=ZZAAA** will tally the response for only one nuclide.

```plaintext
read definitions
response 5
  nuclide=92235
  reaction=fission
  mixture=10 micro
  ehigh=0.625
end response
response 6
  unity mixture=10
end response
end definitions
```
SystemResponses Block

read systemresponses
  ratio 1 title='U235-fis'
    numer 5 end
    denom 6 end
  end ratio
end systemresponses

• Each response must have its own ratio # and end ratio input lines.

• The numer keyword is used to specify which Definition is in the response numerator.

• The denom keyword is used to specify which Definition is in the response denominator.
Summary

• The CE TSUNAMI-3D code within the SCALE 6.2 code package offers a variety of approaches for calculating sensitivity coefficients for both eigenvalue and GPT responses.

• The GPT TSUNAMI capabilities expand the range of applicability for SCALE S/U analyses.
Questions?

Please contact:

Chris Perfetti
perfetticm@ornl.gov