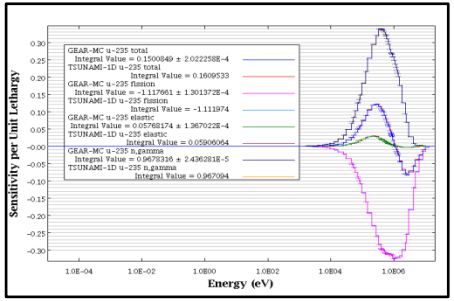
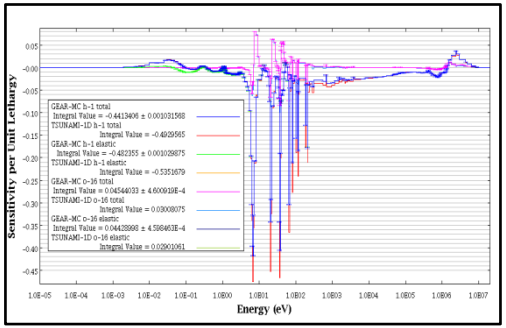
SCALE GPT Capabilities for S/U Analyses

$$S_{R,\Sigma} = \frac{\delta R/R}{\delta \Sigma/\Sigma}$$





ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

Overview

- The TSUNAMI (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) capabilities within the SCALE code system make use of sensitivity coefficients for an extensive number of criticality safety applications, including:
  - Quantifying the data-induced uncertainty in the eigenvalue of critical systems,
  - Assessing the neutronic similarity between different systems,
  - Quantifying computational biases, and
  - Guiding nuclear data adjustment studies.
- This presentation will provide a brief overview of the sensitivity analysis methods in SCALE 6.2 in CE TSUNAMI-3D.
- Recent improvements will be discussed that allow CE TSUNAMI-3D to calculate sensitivity coefficients for multiple GPT responses within a single simulation.
- This presentation will conclude with some recommendations for comparing sensitivity coefficient calculation methods between different codes and institutions.

OAK RIDGE National Laboratory

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)

OAK RIDGE National Laboratory

Introduction to Sensitivity Coefficients

- Sensitivity coefficient calculations in TSUNAMI are calculated using the First-Order Perturbation Equation, which requires adjoint-weighted reaction rate tallies…

$$S_{k,\Sigma_x} = \Sigma_x \frac{< \Phi^\dagger \left(\lambda \frac{\delta F}{\delta \Sigma_x} - \frac{\delta B}{\delta \Sigma_x} \right) \Phi >}{\lambda < \Phi^\dagger F \Phi >}$$

OAK RIDGE National Laboratory

Introduction to Sensitivity Coefficients

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

$$S_{k,\Sigma_{cap.}} = \frac{< \Phi^{\dagger} \Sigma_{cap.} \Phi >}{\frac{1}{k} < \Phi^{\dagger} \Sigma_{fis.} \Phi >}$$

- 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.

OAK RIDGE National Laboratory

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.

- The IFP method is very easy to use, requiring minimal user input/expertise to generate accurate sensitivity coefficient estimates.
- In practice, the IFP method can require storing reaction rate tallies for a significant number (2–20) of latent generations, resulting in a significant computational memory footprint.

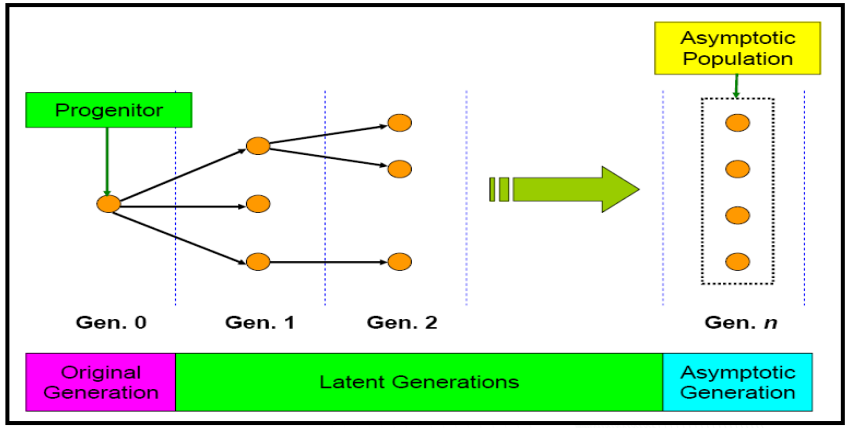
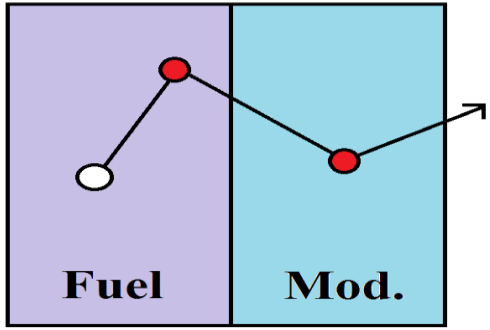


Illustration of the IFP process. Image courtesy of Brian Kiedrowski.

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:

$$\phi^{\dagger}(\tau_s) = \int_V G(\tau_s \rightarrow r) F^{\dagger}(r)\, dr,$$



…where:

G($\tau_s \rightarrow$ r) = The number of fission neutrons created at r by the neutron originating in the phase space τ_s.

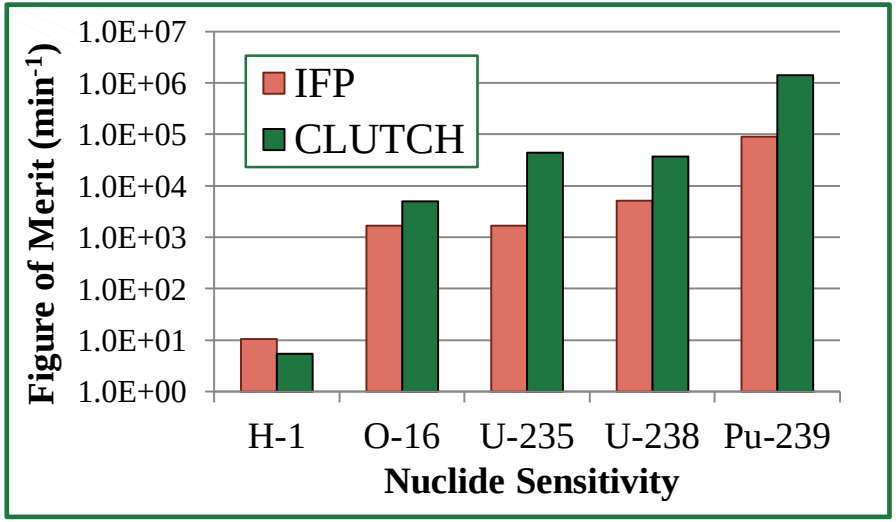
F*(r) = The average importance of fission neutrons born at r, or:

$$F^{\dagger}(r) = \int_E \int_\Omega \frac{\chi(r,E)}{4\pi}\, \phi^{\dagger}(r,E,\Omega) d\Omega dE.$$

OAK RIDGE National Laboratory

Comparing Eigenvalue Sensitivity Methods

- The CLUTCH method is typically 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			
Model	**IFP**	**CLUTCH**	**Memory Reduction Factor**
Fuel Pin	2,113 MB	1.06 MB	1,990
Godiva	26 MB	0.12 MB	220
HMF-025-005	1,675 MB	0.16 MB	10,470
LCT-010-014	19,509 MB	25 MB	780
NAC-UMS	21,201 MB	3,416 MB	6.2

National Laboratory

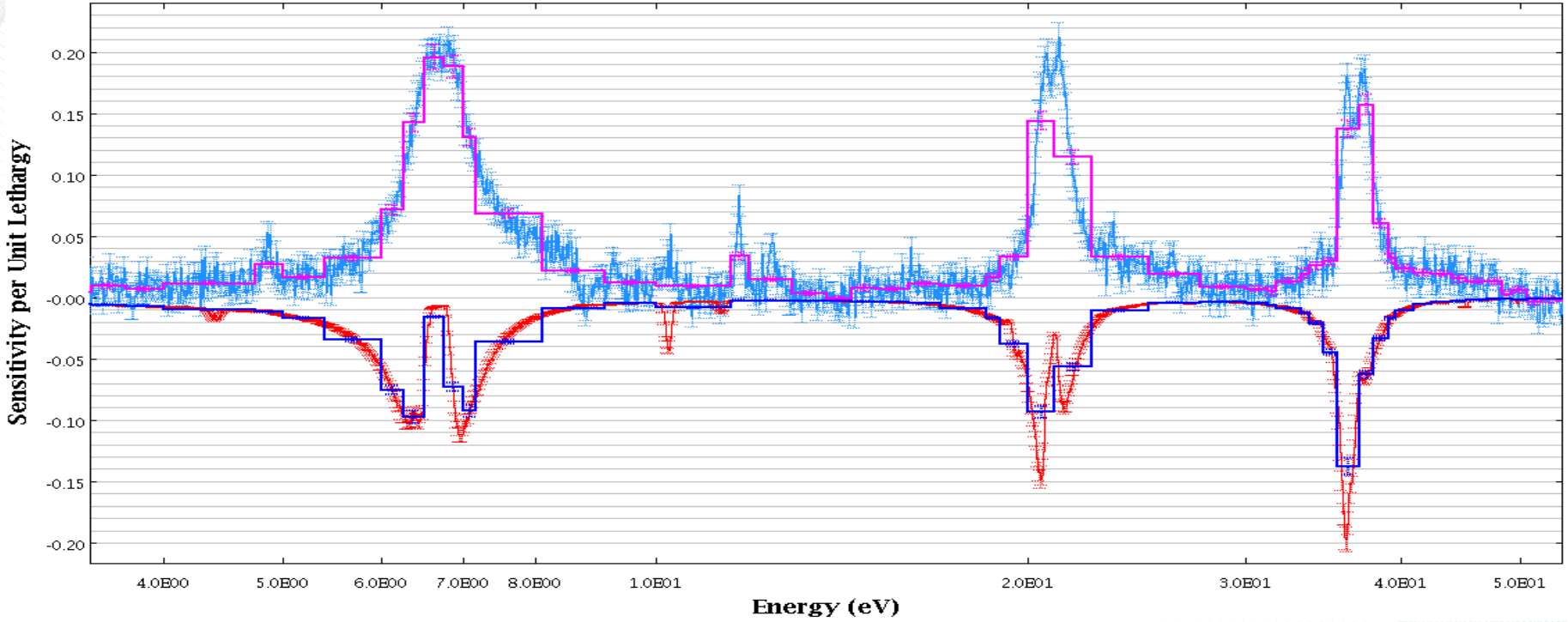
Why use Continuous Energy?

- 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 produced by multigroup TSUNAMI-3D.
- Use of continuous-energy physics more accurately models the physics of neutron interactions.

OAK RIDGE National Laboratory

H-1 Elastic Scatter Sensitivity
238-group CLUTCH VS
Microgroup CLUTCH

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



OAK RIDGE National Laboratory

Why NOT use Continuous Energy?

- The simulation runtimes are usually longer for CE TSUNAMI-3D than 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 when using CE TSUNAMI-3D's CLUTCH method.

OAK RIDGE National Laboratory

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)

OAK RIDGE National Laboratory

Generalized Perturbation Theory

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

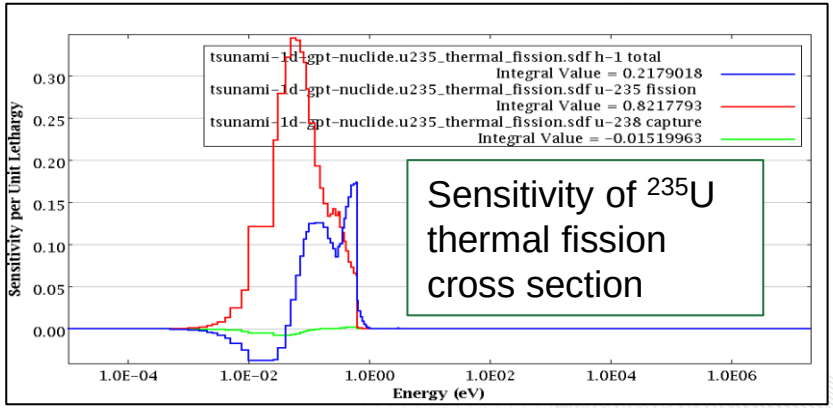
$$S_{R,\Sigma} = \frac{\delta R/R}{\delta\Sigma/\Sigma} \qquad R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

- 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.

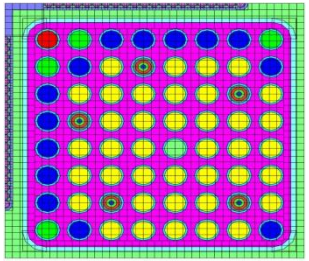


Generalized Perturbation Theory

- 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}Pu(n,f)/^{235}U(n,f)
  - Experimental parameters
    - Example: $^{28}\rho$

      (ratio of epithermal/thermal ^{238}U capture rates in irradiation foils)

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

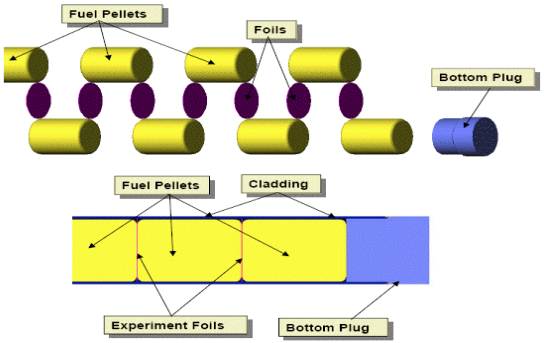


OECD UAM GPT Benchmark Phase 1-2 Results

NUMBER	EXPERIMENT	Type	Format	Value	Xsec Uncert
1	k_infinity	keff	Relative	1.1083E+0	4.98551E-1 % dk/k
2	fission_grp_1	gpt	Relative	1.9155E-3	6.91925E-1 % dR/R
3	fission_grp_2	gpt	Relative	2.7748E-2	3.23440E-1 % dR/R
4	absorpt_grp_1	gpt	Relative	7.1637E-3	8.36728E-1 % dR/R
5	absorpt_grp_2	gpt	Relative	5.3702E-2	2.38082E-1 % dR/R
6	cornerrod_fpf	gpt	Relative	1.1458E+0	1.67147E-1 % dR/R

Why should we care about GPT Sensitivities?

- GPT analysis may reveal biases in nuclear data for materials that do not contribute strongly to the eigenvalue of critical experiments.
  - Useful for isotopes/reaction rates whose real-world impact cannot be easily assessed with critical experiments, i.e. using Rh-103 foils to model the impact of Rh-103 distributed in spent fuel.



LEU-COMP-THERM-079

OAK RIDGE National Laboratory

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.

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

- 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.

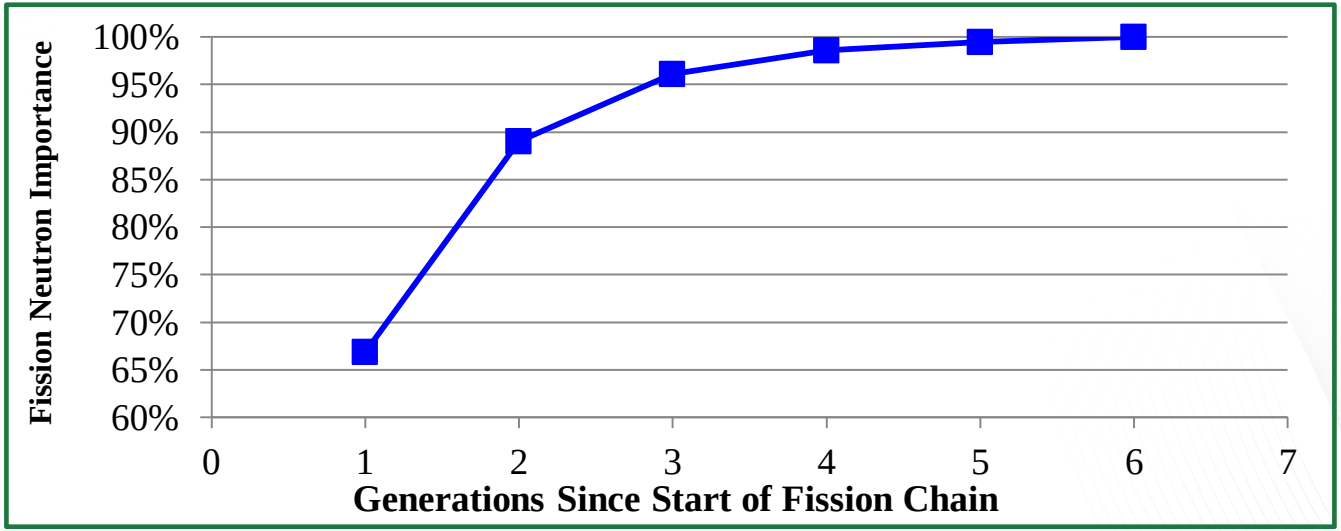
- For more background on this methodology, see:

C. M. Perfetti, B. T. Rearden, "Continuous-Energy Monte Carlo Methods for calculating Generalized Response Sensitivities using TSUNAMI-3D," in *Proc. of the 2014 International Conference on the Physics of Reactors (PHYSOR 2014),* Kyoto, Japan, September 28 – October 3, 2014.

OAK RIDGE National Laboratory

Inter-generational Importance

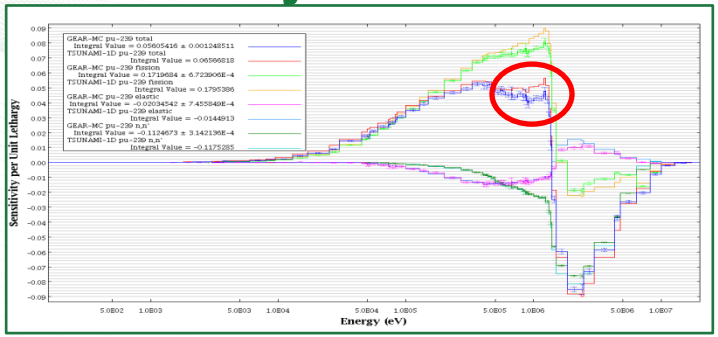
- The inter-generational term is calculated by tallying the intra-generational importance generated by neutrons in a fission chain as that importance approaches zero.



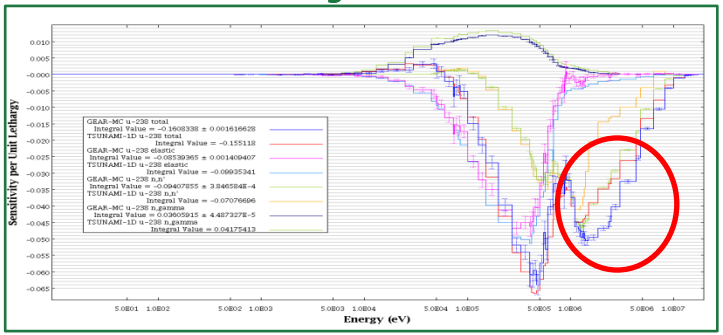
OAK RIDGE National Laboratory

GPT Flattop Foil Response Sensitivity Coefficients

F28/F25 Pu-239 Sensitivity Coefficients



F37/F25 U-238 Sensitivity Coefficients



Flattop Total Nuclide Foil Response Sensitivities

Experiment	Response	Isotope	Direct Pert.	TSUNAMI-1D	GEAR-MC
Flattop	F28 / F25	^{238}U	0.8006 ± 0.0533	0.8024 (**0.03 σ**)	0.7954 ± 0.0018 (**-0.10 σ**)
		^{239}Pu	0.0528 ± 0.0043	0.0657 (**2.99 σ**)	0.0561 ± 0.0012 (**0.73 σ**)
	F37 / F25	^{238}U	-0.1540 ± 0.0102	-0.1551 (**-0.11 σ**)	-0.1608 ± 0.0016 (**-0.66 σ**)
		^{239}Pu	0.0543 ± 0.0048	0.0736 (**3.99 σ**)	0.0489 ± 0.0010 (**-1.10 σ**)

IDGE National Laboratory

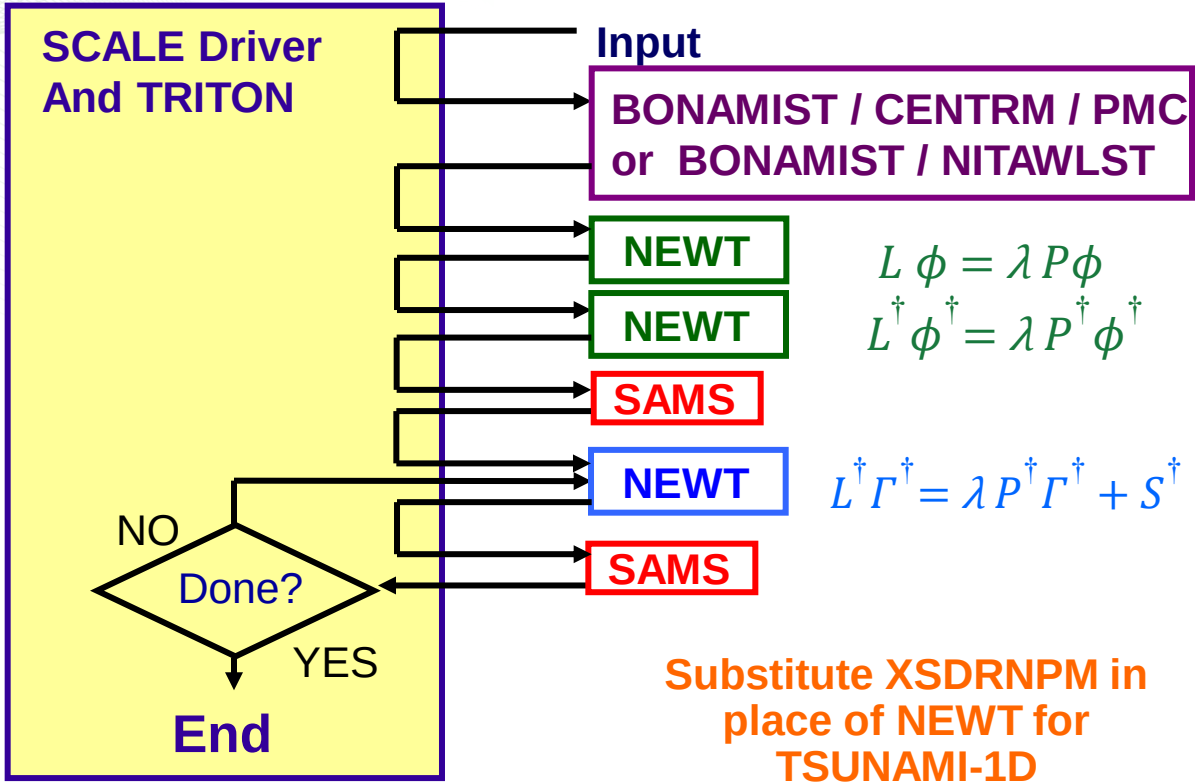
How does the CE TSUNAMI-3D approach differ from other methods?

- 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.

OAK RIDGE National Laboratory

TSUNAMI-1D/2D GPT Sequences



$$L\phi = \lambda P\phi$$

$$L^{\dagger}\phi^{\dagger} = \lambda P^{\dagger}\phi^{\dagger}$$

$$L^{\dagger}\Gamma^{\dagger} = \lambda P^{\dagger}\Gamma^{\dagger} + S^{\dagger}$$

Resonance cross-section processing (repeated for all cells)

2D discrete ordinates

2D discrete ordinates adjoint calculation

S/U calculation for k_{eff}

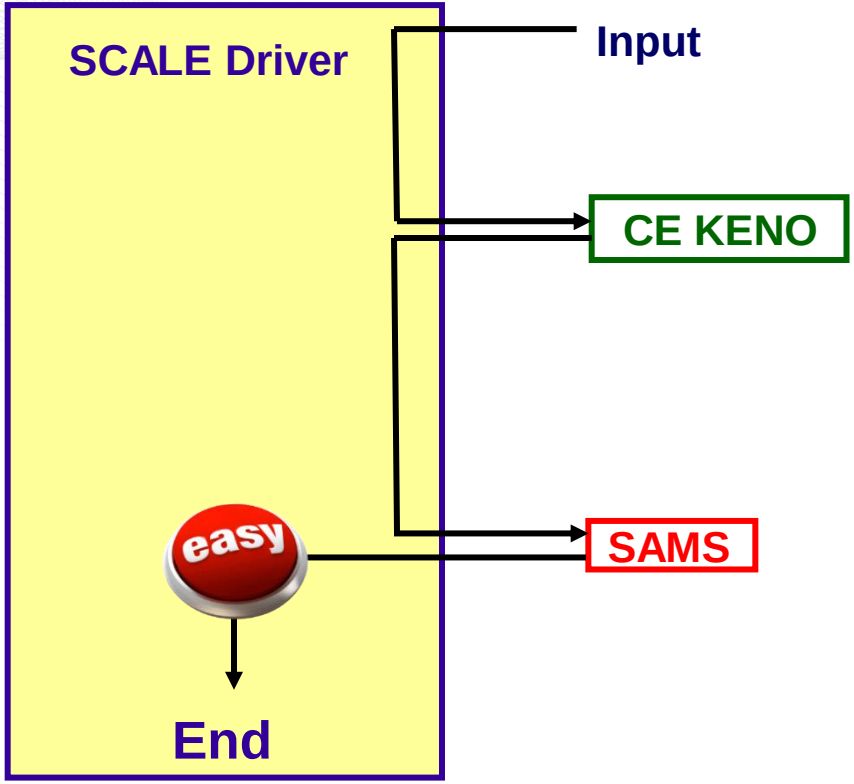
2D discrete ordinates inhomogeneous adjoint calculation for each response

S/U calculation for a user-defined response

Substitute XSDRNPM in place of NEWT for TSUNAMI-1D

OAK RIDGE National Laboratory

CE TSUNAMI-3D GPT Sequence



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_{eff} and user-defined responses

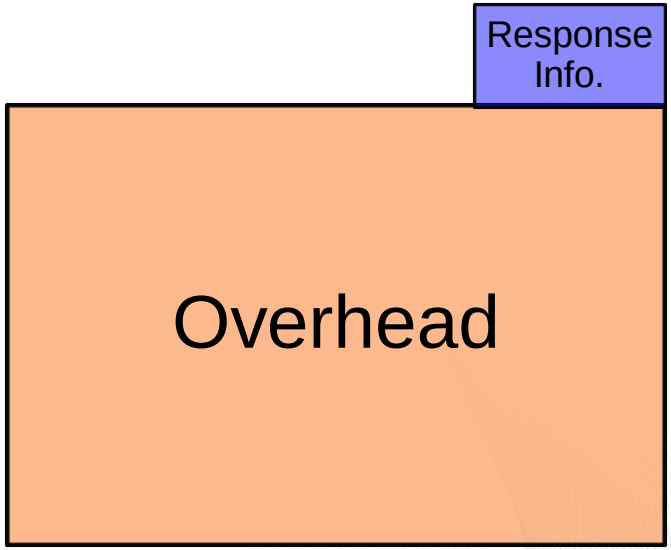
OAK RIDGE National Laboratory

Multi-response CE TSUNAMI-3D GPT Calculations

- The CE TSUNAMI-3D GPT capability has been improved to allow for multiple GPT response sensitivity calculations within a single simulation.
- Performing sensitivity calculations for additional GPT responses generally requires a modest increase in the problem's runtime and memory footprint.
- The input for entering GPT responses in CE TSUNAMI-3D is consistent with the format for GPT TSUNAMI-1D/2D.

IFP Sensitivity Methods:

Large Initial Overhead,
Low Additional Memory per Response



OAK RIDGE National Laboratory

Sensitivity Calculations: Memory Footprint

- Multi-response GEAR-MC calculations require a small increase in the computational memory footprint and simulation runtime.

Model	One GPT Response	Two GPT Responses	Three GPT Responses	Four GPT Responses
Flattop	502 MB	505 MB (+0.60%)	512 MB (+1.99%)	517 MB (+2.99%)
Fuel Pin	2,014 MB	2,020 MB (+0.30%)	2,016 MB (+0.10%)	2,019 MB (+0.25%)
MCT–004–001	3,609 MB	3,652 MB (+1.19%)	3,658 MB (+1.36%)	3,684 MB (+2.08%)
EGAMCT Fuel Assembly	16,497 MB	17,025 MB (+3.20%)	17,548 MB (+6.37%)	18,081 MB (+9.60%)

National Laboratory

Sensitivity Calculations: Runtime per Gen.

- Multi-response GEAR-MC calculations require a small increase in the computational memory footprint and simulation runtime.

Model	One GPT Response	Two GPT Responses	Three GPT Responses	Four GPT Responses
Flattop	0.574 min/Gen.	0.586 min/Gen. (+2.09%)	0.590 min/Gen. (+2.79%)	0.598 min/Gen. (+4.18%)
Fuel Pin	0.704 min/Gen.	0.720 min/Gen. (+2.27%)	0.727 min/Gen. (+3.27%)	0.744 min/Gen. (+5.68%)
MCT–004–001	0.963 min/Gen.	0.967 min/Gen. (+0.42%)	0.991 min/Gen. (+2.91%)	1.000 min/Gen. (+3.84%)
EGAMCT Fuel Assembly	2.609 min/Gen.	2.608 min/Gen. (-0.04%)	2.681 min/Gen. (+2.76%)	2.764 min/Gen. (+5.94%)

National Laboratory

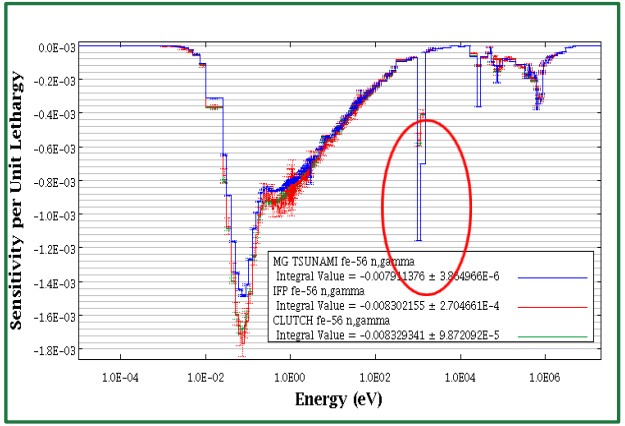
Summary

- The CE TSUNAMI-3D code within the SCALE 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.
- Recent improvements allow CE-TSUNAMI-3D to calculate sensitivity coefficients for multiple GPT responses within a single simulation with a modest, O(1%), increase in runtime and memory footprint.

OAK RIDGE National Laboratory

Thoughts on Comparing Various Sensitivity Methods

- Examining the c_k correlation coefficient may be an effective and fast means for assessing agreement between two sensitivity analysis methods.
- A stochastic cross section perturbation tool (i.e. XSUSA, Sampler, etc.) can generate reference uncertainty analysis information for sensitivity method comparisons.



^{56}Fe (n,γ) k_{eff} Sensitivity Coeff.
LEU-COMP-THERM-010-014

- Differences between multigroup and CE sensitivity coefficients are typically visible at resonance energies – even when accounting for implicit effects.
- Any cross-code comparison should also analyze the computational efficiency of sensitivity methods to provide insight on the most efficient sensitivity methods and implementation strategies.

OAK RIDGE National Laboratory

Bonus Slide: c_k Correlation Coefficient

- c_k is a single-valued parameter used to assess similarity of uncertainty weighted sensitivity profiles between a design system and a criticality experiment for all nuclide-reactions.
  - Practical interpretation: what fraction of the data-induced uncertainty is shared by two systems.
  - Normalized such that c_k of 1.0 indicates systems are neutronically identical; 0.0 indicates systems are completely different.
- Current guidance: if c_k is 0.9 or higher, 90% of the uncertainty is shared between the two systems – the experiment is applicable for the criticality code validation of the design system.
- Marginal applicability for c_k between 0.8 and 0.9.

OAK RIDGE National Laboratory

Questions???

Please contact:

Chris Perfetti
perfetticm@ornl.gov

OAK RIDGE National Laboratory