Use of SCALE Continuous-Energy Tools for Eigenvalue Sensitivity Coefficient Calculations

October 1, 2013

NCSD 2013

Wilmington, North Carolina, USA

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Introduction

• Eigenvalue sensitivity coefficients describe the change in the eigenvalue of a system that occurs due to uncertainty or perturbations in system parameters.



- The SCALE code contains a suite of uncertainty analysis tools including the TSUNAMI-3D code, which calculates eigenvalue sensitivity coefficients for 3D, multigroup Monte Carlo problems.
- The SCALE TSUNAMI methodology has recently been extended to enable eigenvalue sensitivity coefficients calculations using continuous-energy (CE) Monte Carlo methods.
- This both improves the fidelity of sensitivity coefficient calculations and expands the range of applications for sensitivity and uncertainty analyses.



Scope of this Study

- This study examines two International Criticality Safety Benchmark Evaluation Project (ICSBEP) critical benchmarks that produced poor multigroup (MG) eigenvalue and eigenvalue sensitivity results.
- These systems were modeled using the SCALE CE KENO and CE TSUNAMI tools to quantify the improvements in accuracy offered by the CE methods.



KENO-3D Model of HEU-MET-FAST-025-005 KENO-3D Model of LEU-COMP-THERM-010-014

- Sensitivity coefficients were also calculated for these test problems using the multigroup TSUNAMI-3D code, and the sensitivity methods were compared in terms of accuracy, efficiency, and memory requirements.
- Direct perturbation calculations were used to obtain reference sensitivity coefficients for the most important nuclides in each test problem.



Iterated Fission Probability Method

• The Iterated Fission Probability (IFP) method calculates adjointweighted 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 that are descendants of the original event.



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

- In practice, the IFP method requires storing reaction rate tallies for some number of generations until the importance of these tallies is determined.
- Although the memory requirements for storing these reaction rate tallies can be large, the IFP method allows for accurate sensitivity coefficient calculations with a reasonable increase in problem runtime.



CLUTCH Method

- The Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization (CLUTCH) method calculates the importance of events during a particle's lifetime by examining how many fission neutrons are created by that particle after the those events occur.
- The importance of an event given by:

$$\phi^*(\tau_s) = \frac{\lambda}{Q_s} \int_V G(\tau_s \to r) F^*(r) dr$$

where...

- $G(\tau_s \rightarrow r) =$ The number of fission neutrons created at r by a neutron originating in phase space τ_s .
- $F^*(r)$ = The average importance of a fission neutron born at *r*.



HEU-MET-FAST-025-005 Results

V Elastic Scattering Sensitivity

 $V(n,\gamma)$ Sensitivity



Eigenvalue Comparison

Reference	MG KENO	CE KENO	
0.9991 ± 0.0016	1.0132 ± 0.0001 (1.41% diff.)	1.0040 ± 0.0001 (0.49% diff.)	



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HEU-MET-FAST-025-005 Results

- Moving to CE calculations significantly improved the predicted eigenvalue.
- Significant differences were observed in the sensitivity coefficients at energies corresponding to those of large capture resonances.
- The CE total nuclide sensitivity coefficients were not significantly more accurate than the MG total nuclide sensitivity coefficients.

Nuclide	Direct Perturbation	MG TSUNAMI	IFP	CLUTCH
V	0.0883 ± 0.0063	$\begin{array}{c} 0.1000 \pm 0.0012 \\ (\textbf{1.834 \sigma}) \end{array}$	0.0904 ± 0.0002 (0.338 σ)	$\begin{array}{c} 0.0919 \pm 0.0002 \\ \textbf{(0.581 \sigma)} \end{array}$
U-234	0.0073 ± 0.0005	$0.0074 \pm 0.00001 \\ (0.155 \sigma)$	$\begin{array}{c} 0.0074 \pm 0.00004 \\ \textbf{(0.266 \sigma)} \end{array}$	$\begin{array}{c} 0.0074 \pm 0.00002 \\ \textbf{(0.191 \sigma)} \end{array}$
U-235	0.7147 ± 0.0467	$0.7358 \pm 0.0013 \\ (0.451 \sigma)$	$\begin{array}{c} 0.7383 \pm 0.0003 \\ \textbf{(0.505 \sigma)} \end{array}$	$\begin{array}{c} 0.7393 \pm 0.0002 \\ \textbf{(0.527 \sigma)} \end{array}$
U-238	0.0073 ± 0.0005	$0.0078 \pm 0.00004 \\ (0.863 \sigma)$	$\begin{array}{c} 0.0076 \pm 0.0001 \\ \textbf{(0.455 \sigma)} \end{array}$	$0.0076 \pm 0.00004 \\ (0.551 \sigma)$

HEU-MET-FAST-025-005 Total Nuclide Sensitivity Coefficient Comparison



LEU-COMP-THERM-010-014 Results

U-238 Total Nuclide Sensitivity

Fe-56 (n, γ) Sensitivity



Eigenvalue Comparison

Reference	MG KENO	CE KENO	
1.0000 ± 0.0028	1.0014 ± 0.0001 (0.14% diff.)	1.0021 ± 0.0001 (0.21% diff.)	



LEU-COMP-THERM-010-014 Results

- Moving to CE calculations did not significantly affect the predicted eigenvalue.
- Significant differences were again observed in the sensitivity coefficients at energies corresponding to those of large capture resonances.
- The CE total nuclide sensitivity coefficients were significantly more accurate than the MG total nuclide sensitivity coefficients.

Nuclide	Reference	MG TSUNAMI	IFP	CLUTCH	
H-1 (Mod.)	0.3062 ± 0.0032	0.3191 ± 0.0011 (3.825 σ)	0.3124 ± 0.0105 (0.562 σ)	0.3144 ± 0.0051 (1.357 σ)	
O-16	0.0632 ± 0.0039	0.0593 ± 0.0002 (-0.992 σ)	0.0576 ± 0.0025 (-1.204 σ)	0.0585 ± 0.0010 (-1.161 σ)	
Fe-56	0.0263 ± 0.0017	0.0262 ± 0.0001 (-0.023 σ)	0.0247 ± 0.0011 (-0.766 σ)	$\begin{array}{c} 0.0249 \pm 0.0007 \\ \textbf{(-0.710 \sigma)} \end{array}$	
U-235	0.1723 ± 0.0105	0.1550 ± 0.0001 (-1.639 σ)	0.1531 ± 0.0049 (-1.654 σ)	0.1540 ± 0.0018 (-1.709 s)	
U-238	-0.0761 ± 0.0011	$\begin{array}{c} -0.0769 \pm 0.0001 \\ (\textbf{-0.764 } \sigma) \end{array}$	$\begin{array}{c} -0.0769 \pm 0.0027 \\ (\textbf{-0.276 } \sigma) \end{array}$	$\begin{array}{c} -0.0762 \pm 0.0010 \\ (\textbf{-0.097 } \sigma) \end{array}$	

LEU-COMP-THERM-010-014 Total Nuclide Sensitivity Coefficient Comparison



CE TSUNAMI Performance Metrics





HEU-MET-FAST-025-005 FoM Comparison

LEU-COMP-THERM-010-014 FoM Comparison

Memory Increase Compared to Eigenvalue-only Calculation

Experiment	MG TSUNAMI	IFP	CLUTCH	
HEU-MET-FAST- 025-005	5,007 MB	1,675 MB	0.16 MB	
LEU-COMP- THERM-010-014	15,131 MB	19,509 MB	0.29 MB	

- The CLUTCH method is consistently more efficient than the IFP method.
- CE TSUNAMI is sometimes more efficient than MG TSUNAMI.
- CLUTCH produces a minimal memory footprint.



Conclusions and Future Work

- Moving to CE physics significantly improved the HEU-MET-FAST-025-005 eigenvalue estimates and the LEU-COMP-THERM-010-014 eigenvalue sensitivity coefficient estimates.
- Significant differences were observed in both systems for sensitivity coefficients near energies corresponding to those of large capture resonances. These differences did not always translate into significant differences in the energy-integrated total nuclide sensitivity coefficients.
- The CLUTCH method was found to be consistently more efficient than the IFP method, offering as much as an order of magnitude gain in efficiency.
- CE TSUNAMI produced higher FoMs than the MG TSUNAMI for several sensitivity coefficients, which was surprising because CE TSUNAMI calculations use continuous-energy physics.
- CE TSUNAMI is available in the SCALE 6.2 Beta2.
- Future work includes:
 - > Implementing a deterministic approach to pre-calculate the $F^*(r)$ mesh.
 - > Adding a capability to calculate angular scattering sensitivity coefficients.
 - > Developing the CE TSUNAMI generalized response sensitivity capability.



The authors would like to thank Kursat Bekar and Lester Petrie for their advice and assistance in implementing the CE TSUNAMI sequence.

The U.S. Department of Energy Nuclear Criticality Safety Program sponsored the preparation of this work.



References

- 1. SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee (June 2011). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.
- 2. C. M. Perfetti, Advanced Monte Carlo Methods for Eigenvalue Sensitivity Coefficient Calculations, doctoral dissertation, University of Michigan (2012).
- 3. B. T. Rearden, C. M. Perfetti, M. L. Williams, "SCALE Sensitivity Calculations using Contributon Theory," Proceedings of the *Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*, Tokyo, Japan, October 17–21, 2010.
- 4. B. C. Kiedrowski, F. B. Brown, P. P. H. Wilson, "Adjoint-Weighted Tallies for *k*-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nuclear Science and Engineering*, 168(3), pp.226–241 (2011).
- 5. C. M. Perfetti, W. R. Martin, B. T. Rearden, M. Williams, "Determining Importance Weighting Functions for Contributon Theory Eigenvalue Sensitivity Coefficient Methodologies," *Proc. PHYSOR 2012*, Knoxville, Tennessee, April 15–20, 2012, American Nuclear Society (2012) (CD-ROM).
- 6. M. Nakagawa, T. Mori, "Whole core calculations of power reactors by use of Monte Carlo method," *Journal of Nuclear Science and Technology*, 30 [7], pp. 692–701 (1993).
- 7. International Handbook of Evaluated Criticality Safety Benchmark Experiments, Nuclear Energy Agency Nuclear Science Committee of the Organization for Economic Co-operation and Development, NEA/NSC/DOC(95)03 (2010).
- 8. E. E. Lewis, W. F. Miller, Jr., *Computational Methods of Neutron Transport*, p. 329, American Nuclear Society, La Grange Park, Illinois, USA (1993).
- 9. J. M. Scaglione, W. J. Marshall, Assessment of Critical Benchmark Applicability to Potential Spent Fuel Configurations, ORNL/LTR-2011/376, Oak Ridge National Laboratory, Oak Ridge, TN, September 2011.



O-16 Capture Sensitivity 238-group CLUTCH VS Microgroup CLUTCH



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

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





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GPT Flattop Foil Sensitivity Coefficients

F37/F25 Foil Sensitivities 0.05 0.7 GEAR-MC u-235 total Sensitivity per Unit Lethargy Sensitivity per Unit Lethargy -0.00 Integral Value = $-1.002207 \pm 2.949901E-4$ 0.6 TSUNAMI-1D u-235 total Integral Value = -1.0053020.5 -0.05 GEAR-MC u-238 total GEAR-MC u-235 total Integral Value = 0.7954226 ± 0.001831639 0.4 Integral Value = $-0.9996065 \pm 2.451606E$ TSUNAMI-1D u-238 total -0.10TSUNAMI-1D u-235 total 0.3 Integral Value = 0.8024246Integral Value = -1.003709 GEAR-MC pu-239 total GEAR-MC u-238 total 0.2 Integral Value = $0.05605416 \pm 0.001248511$ -0.15Integral Value = $-0.1608338 \pm 0.001616628$ TSUNAMI-1D pu-239 total TSUNAMI-1D u-238 total 0.1 Integral Value = 0.06566818Integral Value = -0.155118 -0.20 GEAR-MC pu-239 total -0.0 Integral Value = $0.04891361 \pm 0.001025733$ TSUNAMI-1D pu-239 total -0.25 -0.1 Integral Value = 0.07362587-0.2 -0.30 -0.3 1.0E-04 1.0E-02 1.0E00 1.0E02 1.0E04 1.0E06 1.0E00 1.0E02 1.0E04 1.0E-04 1.0E-02 1.0E06 Energy (eV) Energy (eV)

Flattop Total Nuclide Foil Response Sensitivities

Experiment	Response	Isotope	Direct Pert.	GEAR-MC	T1D
Flattop	F28 / F25	U-238	0.8006 ± 0.0533	0.7954 ± 0.0018	0.8024
				(-0.097 σ)	(0.034 σ)
		Pu-239	0.0528 ± 0.0043	0.0561 ± 0.0012	0.0657
				(0.727 σ)	(2.993 σ)
	F37 / F25	U-238	-0.1540 ± 0.0102	-0.1608 ± 0.0016	-0.1551
				(-0.664 σ)	(-0.112 σ)
		Pu-239	0.0543 ± 0.0048	0.0489 ± 0.0010	0.0736
				(-1.097 σ)	(3.991 σ)

F28/F25 Foil Sensitivities