LA-UR-12-25949
Approved for public release; distribution is unlimited.

Title: Continuous-Energy Sensitivity Coefficient Capability in MCNP6

Author(s): Kiedrowski, Brian C.
Brown, Forrest B.

Intended for: 2012 ANS Winter Meeting & Nuclear Technology Expo, 2012-11-11 (San Diego, California, United States)

Continuous-Energy Sensitivity Coefficient Capability in MCNP6

Brian C. Kiedrowski and Forrest B. Brown

Los Alamos National Laboratory

November 12, 2012

Abstract

MCNP6 has the capability to compute *k*-eigenvalue sensitivity coefficients using continuous-energy physics. The methdology is presented. Verification is performed with an analytic solution, and results agree. Results are shown for a MOX lattice benchmark, and comparisons with TSUNAMI-3D and MONK are given. Direct perturbations are also performed, and results show general agreement. Sensitivity profiles are also shown for copper-reflected Zeus.

Introduction

- MCNP6 Status
- Methodology
- Verification & Results
- Outlook

MCNP6 Status

- Merger of MCNP5 and MCNPX complete!
- MCNP6 = merged codes + new features
- MCNP6-Beta2 currently available from RSICC.
- MCNP6-Beta3 being tested and available soon.
- Hopefully, production version of MCNP6 to follow.

k-Eigenvalue Sensitivity Capability

- New to MCNP6 (available in Beta3).
- Uses continuous-energy, adjoint-based methodologies in MCNP5-1.60.
- Computes sensitivity coefficients for cross sections, fission ν and χ, and scattering laws.
- User-defined energy resolution for results or tallies – no discretization in method.
- Nuclear Science & Engineering paper accepted and in publication (2013).

Sensitivity Methodology

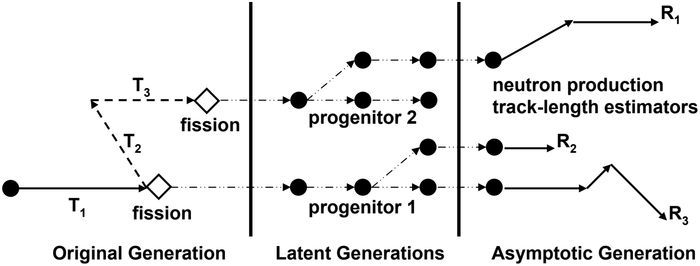
- Uses adjont-based approach:

$$S_{k,x} = -\frac{\langle \psi^{\dagger}, (\Sigma_x - \mathcal{S}_x - \lambda \mathcal{F}_x)\psi \rangle}{\langle \psi^{\dagger}, \lambda \mathcal{F} \psi \rangle}.$$

- Adjoint function computed by Iterated Fission Probability Method.
- No space-energy mesh required.
- One user parameter (to be explained), but default is conservative for almost all problems.

Iterated Fission Probabaility

- Divide active cycles or generations into "blocks" of some size (default 10).
- First cycle: accumulate scores and tag neutrons.
- Follow neutrons through generations, preserving tags.
- Last cycle: multiply scores by neutron production of corresponding progeny.



Tally Scores

$$S_{k,x} = -\frac{\langle \psi^\dagger, (\Sigma_x - \mathcal{S}_x - \lambda \mathcal{F}_x)\psi \rangle}{\langle \psi^\dagger, \lambda \mathcal{F} \psi \rangle}.$$

- Track-length estimator for Σ_x term.
- Analog collision estimator for scattering source term.
- Expected-value collision estimator for fission source term.

Constraining Sensitivities

- Fission χ and scattering laws are constrained:

$$\hat{S}_{k,x}(E,\mu|E_i) = S_{k,x}(E,\mu|E_i) - x(E,\mu|E_i)S_{k.x}(E_i).$$

- Incident energy binning needs to be fine enough to capture change in x with E_i or constraining will be biased.
- Small issue for fission χ, but important for scattering laws.
- For now, up to the user to pick E_i resolution, future work will automate this.

- Note: Outgoing energies E and angles μ used are those of the table; typically center-of-mass for MCNP.

Analytic Test Case

- Infinite-medium, multigroup problem with following data:

g	σ_t	σ_c	σ_f	ν	χ	σ_{sg1}	σ_{sg2}	σ_{sg3}
1	2	1/2	0	–	5/8	1	1/2	0
2	4	1	0	–	1/4	0	1	2
3	4	1/2	3/2	8/3	1/8	0	0	2

Analytic Test Case Results

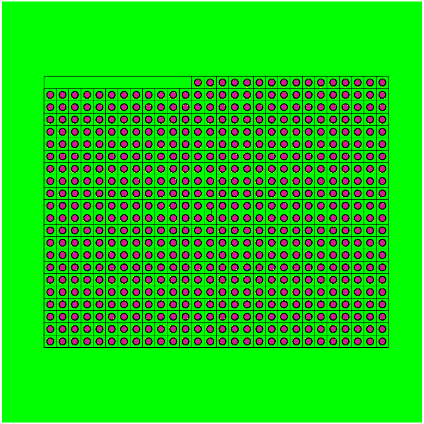
x	Exact $S_{k,x}$	MCNP6 $S_{k,x}$	C/E
σ_{c1}	$-5/24$	$-0.20868 \pm 0.10\%$	1.002
σ_{c2}	$-1/4$	$-0.24993 \pm 0.07\%$	0.999
σ_{c3}	$-1/4$	$-0.24985 \pm 0.05\%$	0.999
σ_{s12}	$+5/24$	$+0.20810 \pm 0.16\%$	0.999
σ_{s23}	$+1/4$	$+0.25083 \pm 0.15\%$	1.003
σ_{f3}	$+1/4$	$+0.25045 \pm 0.16\%$	1.002
ν_3	$+1$	$+1.00000 \pm 0.00\%$	1.000

Analytic Test Case Results

	$S_{k,x}$		
x	Exact	MCNP6 Adjoint	C/E
χ_1	$+5/12$	$+0.4169 \pm 0.09\%$	1.001
χ_2	$+1/3$	$+0.3334 \pm 0.07\%$	1.000
χ_3	$+1/4$	$+0.2497 \pm 0.06\%$	0.999
	$\hat{S}_{k,x}$		
x	Exact	MCNP6 Adjoint	C/E
χ_1	$-5/24$	$-0.2080 \pm 0.12\%$	0.999
χ_2	$-5/24$	$-0.2080 \pm 0.12\%$	0.999
χ_3	$+1/8$	$+0.1246 \pm 0.17\%$	0.997

MOX Lattice Benchmark

- Array of mixed-oxide (MOX) fuel pins submerged in water.
- ENDF/B-VII.0 data used.
- $k = 0.99899 \pm 0.00012$



MOX Lattice: Sensitivities Calculated

- The following sensitivities were calculated:
  - Total (with and without $S(\alpha, \beta)$).
  - Capture.
  - Components of capture: (n,γ), (n,p), (n,α), ...
  - Elastic scattering (with and without $S(\alpha, \beta)$).
  - Inelastic scattering.
  - Components of inelastic: 40 discrete levels + continuum.
  - n,2n
  - Fission ν.
  - Selected fission χ and scatter laws.
- Energy-integrated and energy-resolved.
- SCALE 238-group energy grid used for all isotopes in problem.

MOX Lattice: Top 10 Sensitivities

Isotope	Data	$S_{k,x}$	% Unc.
Pu-239	ν	+9.247E-01	0.02
H-1	Elastic	+4.144E-01	0.31
Pu-239	Fission	+3.776E-01	0.08
Pu-239	n,γ	−2.610E-01	0.06
O-16	Elastic	+8.674E-02	0.43
H-1	n,γ	−7.986E-02	0.13
H-1	$S(\alpha, \beta)$	+6.111E-02	0.87
Pu-240	n,γ	−5.901E-02	0.12
U-238	n,γ	−5.026E-02	0.12
Pu-241	ν	+2.828E-02	0.09

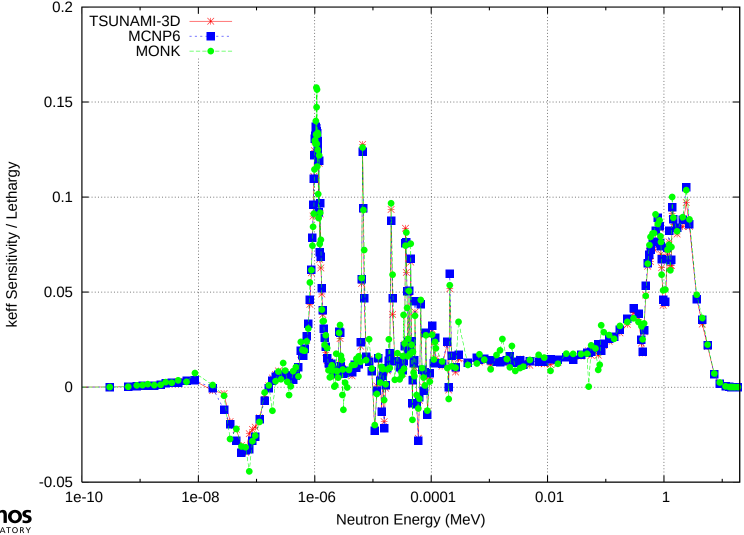
- Excluding total and combined capture.
- $S(\alpha, \beta)$ included for H-1 elastic.

MOX Lattice: Top 10 Total-XS Sensitivities

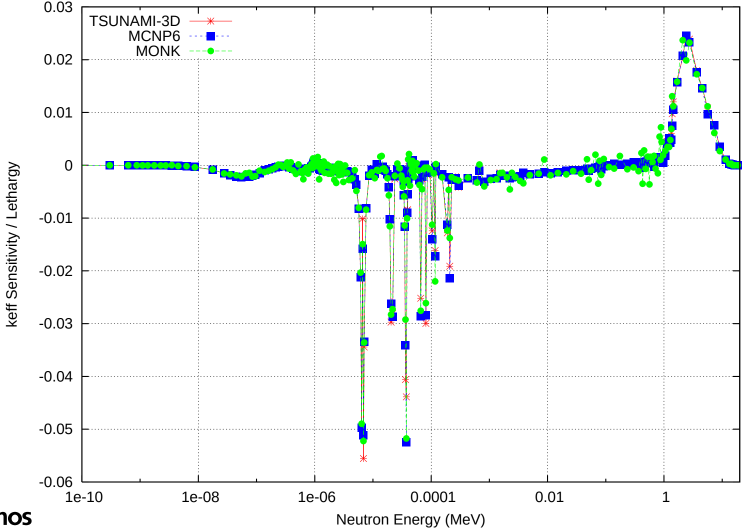
Isotope	$S_{k,x}$	% Unc.
H-1	+3.345E-01	0.35
Pu-239	+1.197E-01	0.25
O-16	+8.556E-02	0.44
Pu-240	−5.460E-02	0.16
U-238	−8.984E-03	1.16
Pu-241	+7.474E-03	0.30
Am-241	−6.761E-03	0.19
Fe-56	−2.599E-03	2.00
U-235	+2.598E-03	0.59
Pu-242	−2.012E-03	0.43

- $S(\alpha, \beta)$ included for H-1.

MOX Lattice: H-1 Elastic + $S(\alpha, \beta)$

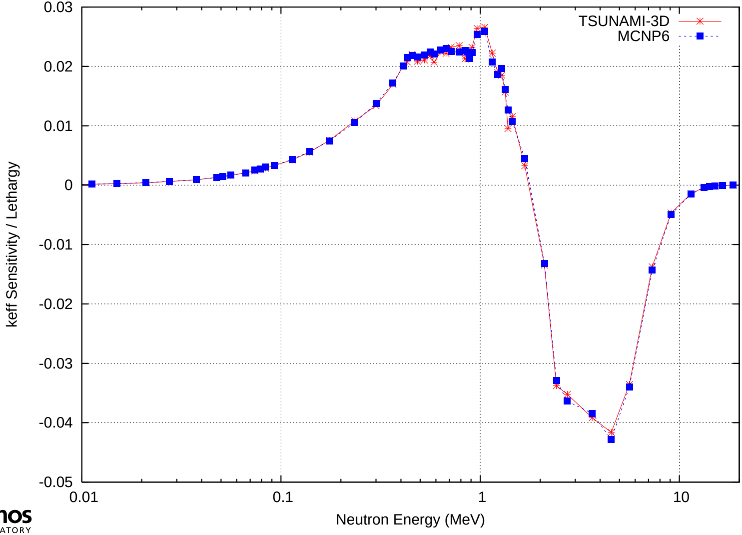


MOX Lattice: U-238 Total



UNCLASSIFIED

MOX Lattice: Pu-239 Fission-χ (Constrained)

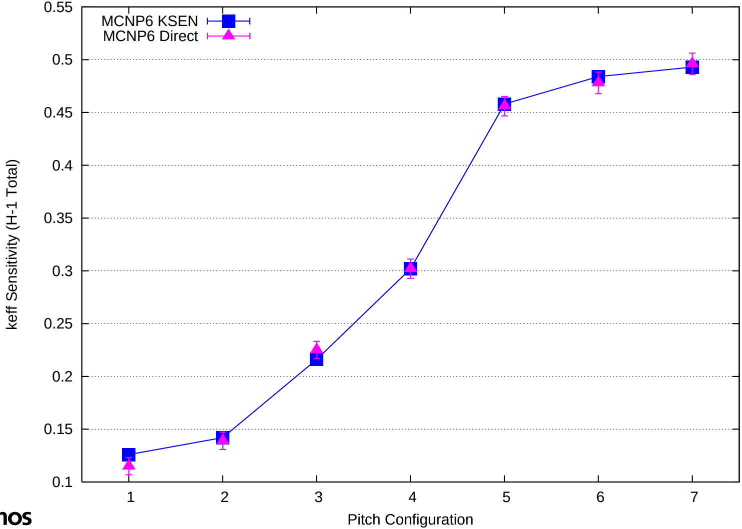


Infinite Pin-Cell Lattices

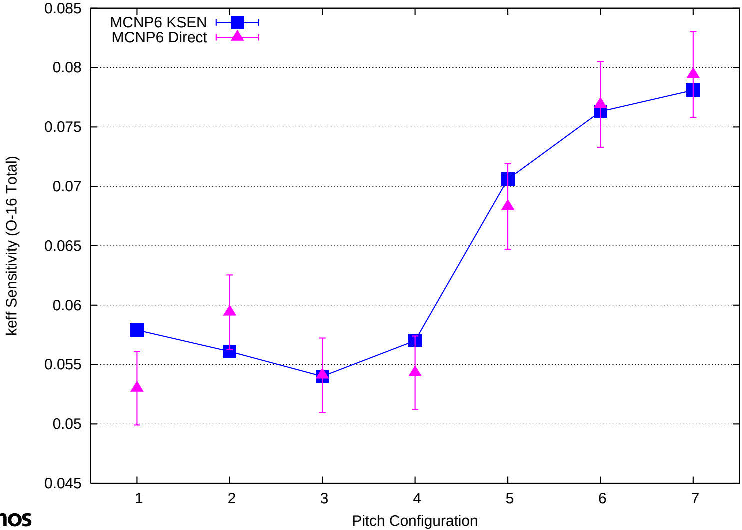
- 7 infinite arrays of MOX pins with varied pitches.
- Pin height chosen to make infinite lattice critical.
- MCNP6 versus direct density perturbations.

Config.	Pitch (cm)	Height (cm)
1	0.586	28.3
2	0.600	28.0
3	0.660	26.9
4	0.730	25.04
5	0.953	20.52
6	1.050	19.5
7	1.150	18.84

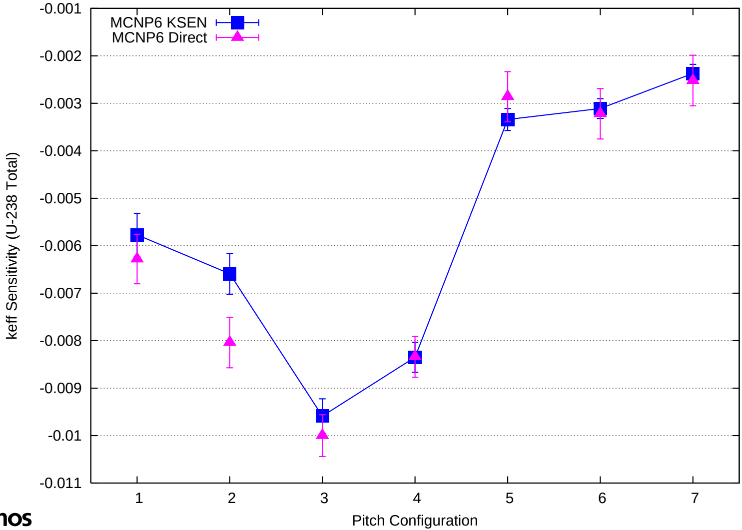
Infinite Array: H-1 Total



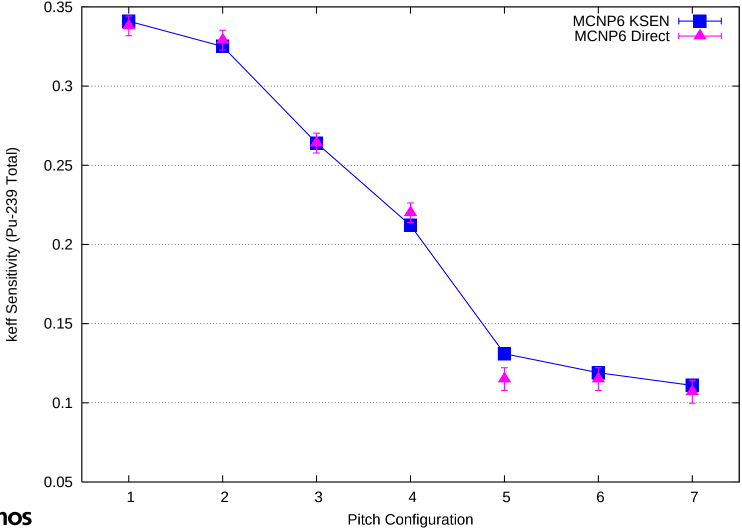
Infinite Array: O-16 Total



Infinite Array: U-238 Total



Infinite Array: Pu-239 Total



Copper-Reflected Zeus

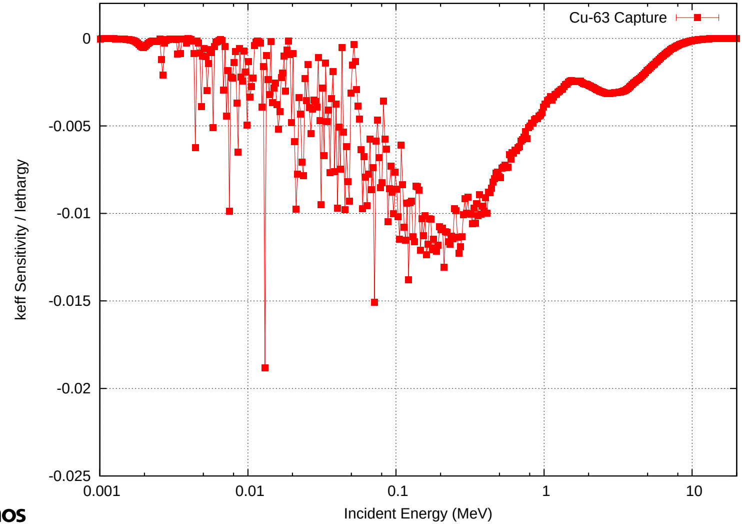
- HEU plates surrounded by a copper reflector.
- Performed at LACEF, recently redone at NCERC.

04-GA50001-183

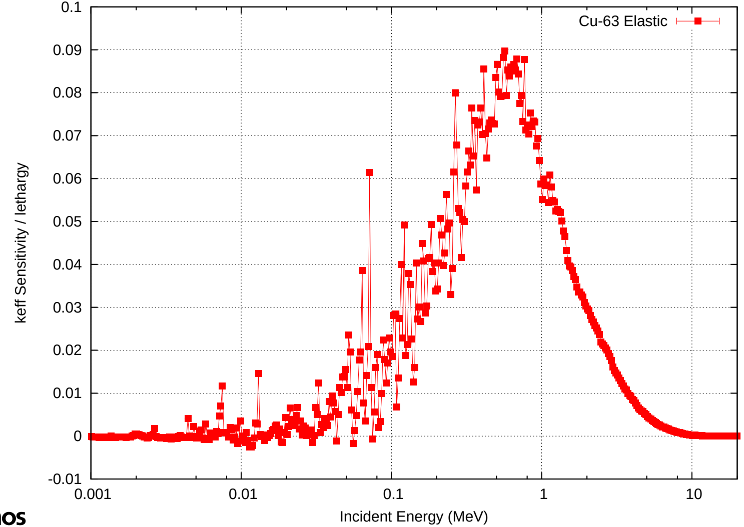
Copper-Reflected Zeus: Top Sensitivities

Isotope	Data	$S_{k,x}$
U-235	ν	$+9.874$E-01 $\pm$ 0.00%
U-235	Fission	$+5.771$E-01 $\pm$ 0.03%
Cu-63	Elastic	$+1.937$E-01 $\pm$ 0.22%
Cu-65	Elastic	$+9.576$E-02 $\pm$ 0.28%
U-235	n,γ	-6.734E-02 $\pm$ 0.05%
Cu-63	n,γ	-3.555E-02 $\pm$ 0.07%
Cu-63	n,n' Level 2	$+1.012$E-02 $\pm$ 0.32%
Cu-65	n,γ	-9.767E-03 $\pm$ 0.08%
Al-27	Elastic	$+8.951$E-03 $\pm$ 0.43%
Cu-63	n,n' Level 1	$+8.021$E-03 $\pm$ 0.36%
U-235	n,n' Continuum	$+6.713$E-03 $\pm$ 0.57%
Cu-63	n,n' Continuum	$+6.221$E-03 $\pm$ 0.31%
U-234	ν	$+6.044$E-03 $\pm$ 0.04%

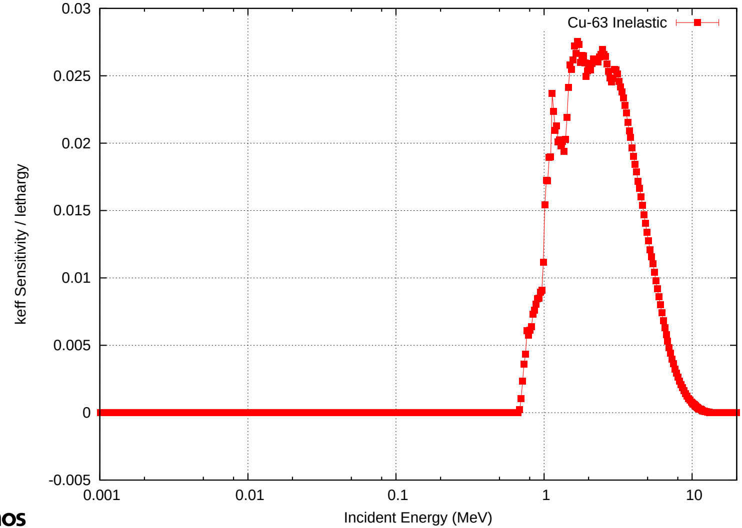
Zeus: Cu-63 Capture Cross-Section Sensitivity



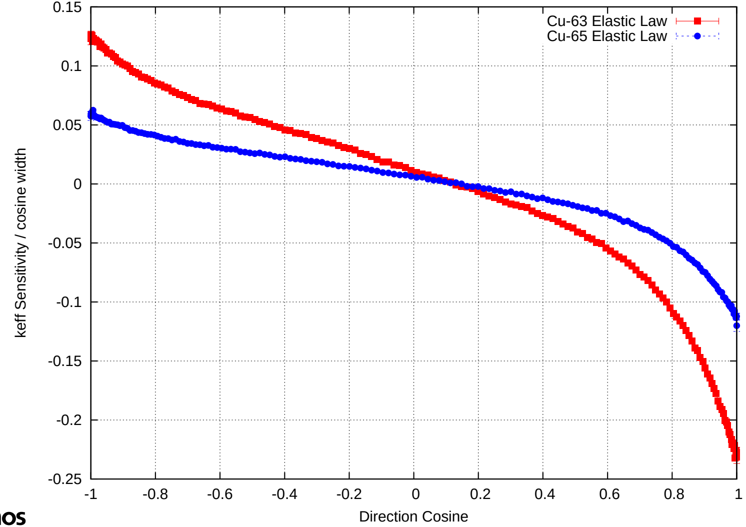
Zeus: Cu-63 Elastic Cross-Section Sensitivity



Zeus: Cu-63 Inelastic Cross-Section Sensitivity



Zeus: Cu Elastic Scattering Law Sensitivity



Summary

- MCNP6 was used to generate energy-integrated and energy-resolved sensitivity coefficients to k.
- Calculations were performed using continuous-energy ENDF/B-VII.0 data.
- **Results appear to agree** with continuous-energy MONK, and TSUNAMI-3D with implicit sensitivities.

- **Capability will be publicly available later this year in MCNP6-Beta3.**

MCNP6 Sensitivity/Uncertainty – Future Developments

- Development of ACE covariance libraries for uncertainty analysis (funded by DOE NCSP over next three years).
- Output file format in SCALE sdf format (high priority).
- Improvements to scatter law sensitivities; robust incident energy dependence (FY 2013).
- Sensitivities to system dimensions or interface locations (prototyped, coming in next few years).
- Gridless (no energy binning) sensitivity results with kernel-density estimators (future research).
- Sensitivities for criticality excursions (future research).

Acknowledgments

- Funding provided by the U.S. DOE/NNSA Nuclear Criticality Safety Program.
- Benchmark specifications and results provided by:
    - Tatiana Ivanova (IRSN)
    - Keith Bledose (ORNL)
    - James Dryda (AWE)

Questions?