Use of Direct Perturbation Calculations to Confirm the Accuracy of TSUNAMI-3D

T. M. Greene

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Outline

1. Introduction
2. Sensitivity and direct perturbation (DP) calculations
3. Experiment descriptions and results
4. Conclusion

Introduction

- Sensitivity coefficients provide insight on the sources and impact of uncertainty in nuclear engineering models
- Clearly identifies processes that are important to validate: Materials, Nuclides, Reactions, Energy
- TSUNAMI: sensitivity and uncertainty tool suite within SCALE that has capabilities with multigroup and continuous energy

Nuclear Data ($\mathbf{\Sigma}$, $\mathbf{\Delta\Sigma}$)
Number Densities ($\mathbf{N}$, $\mathbf{\Delta N}$)
Material Densities ($\mathbf{M}$, $\mathbf{\Delta M}$)

$$S_{R,\Sigma_x} = \frac{\frac{\delta R}{R}}{\frac{\delta \Sigma_x}{\Sigma_x}}$$

k_{eff}, $\Delta\, k_{eff}$

Sensitivity calculations

- TSUNAMI uses linear adjoint perturbation theory to compute sensitivity coefficients
- Predict the expected change in a response (R) due to a change in some input parameter (Σ)
- Sensitivity data file (SDF) created
  - MG uses forward and adjoint transport calculations
  - CE methods are Iterated fission probability (IFP) or Contributon methodology (CLUTCH)

Sensitivity calculations

- Sensitivities and uncertainty

$$S_{R,\Sigma_x} = \frac{\frac{\delta R}{R}}{\frac{\delta \Sigma_x}{\Sigma_x}} \Rightarrow S_{k,\Sigma_x} = \frac{\frac{\delta k_{eff}}{k_{eff}}}{\frac{\delta \Sigma_x}{\Sigma_x}} \Rightarrow$$

$$S_{k,\Sigma(\vec{r})} = -\frac{\Sigma(\vec{r})}{k} \frac{\left\langle \tilde{\phi}(\vec{\xi}) \left(\frac{\partial A[\Sigma(\vec{\xi})]}{\partial \Sigma(\vec{r})} - \frac{1}{k} \frac{\partial B[\Sigma(\vec{\xi})]}{\partial \Sigma(\vec{r})} \right) \phi(\vec{\xi}) \right\rangle}{\left\langle \tilde{\phi}(\vec{\xi}) \frac{1}{k^2} B[\Sigma(\vec{\xi})] \phi(\vec{\xi}) \right\rangle}$$

$$S_{k,\Sigma_x} \cdot \underbrace{Cov_{\Sigma_x,\Sigma_y}}_{\left(\frac{\Delta\Sigma}{\Sigma}\right)^2} \cdot S^T_{k,\Sigma_y} = \underbrace{\sigma_k^2}_{\left(\frac{\Delta k}{k}\right)^2}$$

Direct perturbation calculations

- DP sensitivity = reference sensitivity (total)
- Select important isotopes, elements, and/or materials of interest from the TSUNAMI sensitivities (greater than 0.01)
- Perturbation selected to cause ±0.5% Δk change
  - Perturbation large enough to yield accurate results and small enough to generate a linear response
  - $\Delta\rho = \frac{0.005}{S_{Total}}$

Direct perturbation calculations (continued)

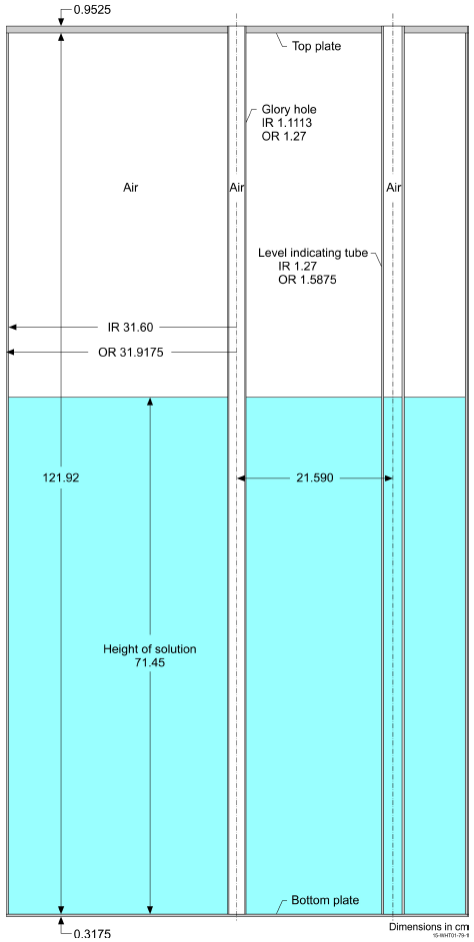
- Uncertainty-weighted linear least squares fit of k_{eff} points used to determine the DP sensitivity
  - Slope of the trend line is the sensitivity
- Desirable for the differences between TSUNAMI and DP sensitivities to be:
  - 1) less than 5%
  - 2) less than 0.01 in absolute sensitivity
  - 3) less than 2 standard deviations using the combined uncertainties
- Multi-point DP method
  - Calculate k_{eff} (k_i) at various densities (ρ_i)
  - Plot k_i/k_{nom} versus ρ_i/ρ_{nom}
  - Inspect plot for linearity
    - Slope of linear fit is DP sensitivity
    - Method yields small S_{DP} uncertainties

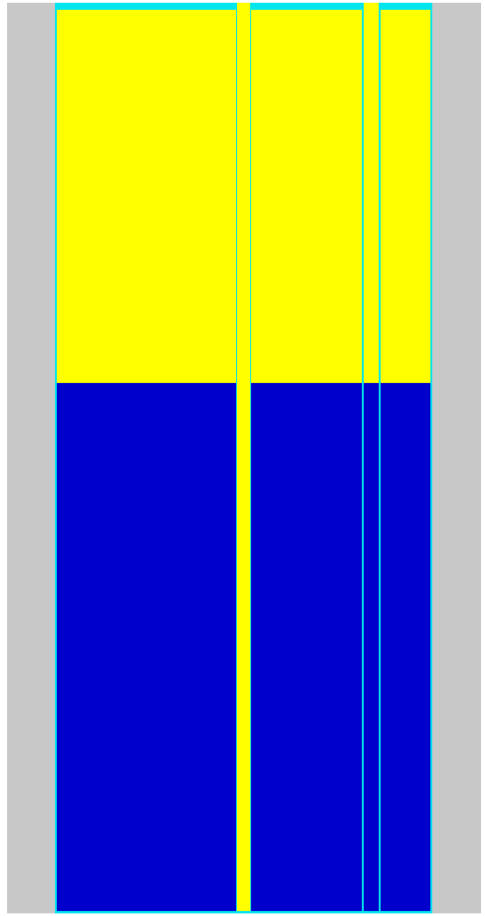
Direct perturbation calculations (continued)

- TSUNAMI sensitivities improved by increasing:
  - CLUTCH and IFP:
    - Increasing number of latent generations (generations between an event and the assessment of importance)
  - CLUTCH only:
    - Increasing the number of histories used to calculate F*(*r*)
    - Resolution of the F*(*r*) mesh grid
  - MG:
    - Generally refining mesh for flux moment tallies
    - Subdividing regions in geometry can also improve tallies

Multigroup experiment case study

- HEU-SOL-THERM-020
  - Experiment from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook
  - 5 cases
  - Cylindrical tank containing a solution of uranyl nitrate and heavy water





Results for HEU-SOL-THERM-020-005

- Examine sensitivity results from TSUNAMI
- Identify sensitivity values above 0.01
- Make sure fissile isotopes and moderator species are examined
- Also include materials/isotopes of interest

Total Sensitivity Coefficients by Nuclide

Mixture	Nuclide	Atom Density	Sensitivity		Std. Dev.	% Std. Dev.
1	h-1	6.6114E-04	3.2213E-02	+/-	5.5539E-05	(0.17%)
1	h-2	6.5453E-02	7.3842E-01	+/-	7.6791E-04	(0.10%)
3	n-14	3.2152E-05	2.7054E-05	+/-	6.8242E-08	(0.25%)
3	n-15	1.1746E-07	6.8019E-08	+/-	7.5769E-11	(0.11%)
1	o-16	3.3045E-02	2.4588E-01	+/-	3.2311E-04	(0.13%)
3	o-16	8.6359E-06	4.5724E-06	+/-	6.4137E-09	(0.14%)
1	o-17	1.2587E-05	-4.3868E-05	+/-	1.2055E-07	(0.27%)
3	o-17	3.2896E-09	1.4277E-09	+/-	1.8357E-14	(0.00%)
1	o-18	6.7906E-05	-9.6257E-10	+/-	1.3361E-12	(0.14%)
3	o-18	1.7747E-08	5.0171E-11	+/-	1.0022E-13	(0.20%)
1	f-19	6.7806E-05	5.5356E-04	+/-	6.9041E-07	(0.12%)
4	al-27	6.0262E-02	-3.3911E-04	+/-	9.5525E-06	(2.82%)
2	si-28	1.5661E-03	9.5541E-05	+/-	1.3836E-07	(0.14%)
2	si-29	7.9561E-05	5.6635E-06	+/-	7.9596E-09	(0.14%)
2	si-30	5.2508E-05	3.5439E-06	+/-	6.0653E-09	(0.17%)
2	cr-50	7.1740E-04	-6.7976E-06	+/-	7.2666E-07	(10.69%)
2	cr-52	1.3834E-02	9.9682E-04	+/-	1.7824E-06	(0.18%)
2	cr-53	1.5687E-03	8.0787E-05	+/-	1.6141E-06	(2.00%)
2	cr-54	3.9049E-04	2.8722E-05	+/-	3.7013E-08	(0.13%)
2	mn-55	1.7363E-03	4.7831E-04	+/-	3.0833E-06	(0.64%)
2	fe-54	3.4693E-03	3.8543E-04	+/-	1.4287E-06	(0.37%)
2	fe-56	5.4461E-02	1.0762E-02	+/-	2.2698E-05	(0.21%)
2	fe-57	1.2577E-03	1.4505E-04	+/-	4.1144E-07	(0.28%)
2	fe-58	1.6738E-04	1.5945E-05	+/-	2.7695E-08	(0.17%)
2	ni-58	5.2557E-03	2.3955E-03	+/-	4.3713E-06	(0.18%)
2	ni-60	2.0245E-03	1.7922E-04	+/-	6.2559E-07	(0.35%)
2	ni-61	8.8004E-05	1.5312E-05	+/-	2.8715E-08	(0.19%)
2	ni-62	2.8059E-04	9.7220E-05	+/-	3.8250E-07	(0.39%)
2	ni-64	7.1459E-05	9.0064E-06	+/-	2.1290E-08	(0.24%)
1	u-234	3.4751E-07	-2.2438E-03	+/-	2.5067E-07	(0.01%)
1	u-235	3.1770E-05	1.8224E-01	+/-	5.5473E-05	(0.03%)
1	u-238	1.7853E-06	-2.3804E-03	+/-	4.0028E-07	(0.02%)

Results for HEU-SOL-THERM-020-005 (continued)

Nuclide	TSUNAMI Results			Direct Perturbation Results					Results Comparison		
	S	σ_S	$\%\sigma_S$	S	σ_S	$\%\sigma_S$	#pts	R^2	DS (%)	DS (σ)	DS
^{1}H	3.22E-02	5.55E-05	0.17%	0.0322	0.0005	1.54%	3	0.9997	-0.01%	0.01	0.0000
^{2}H	7.38E-01	7.68E-04	0.10%	0.7272	0.0114	1.57%	3	1.0000	1.54%	0.98	0.0112
^{16}O	2.46E-01	3.23E-04	0.13%	0.2526	0.0038	1.50%	3	0.9994	-2.66%	1.77	-0.0067
^{56}Fe	1.08E-02	2.27E-05	0.21%	0.0108	0.0002	1.54%	3	0.9999	-0.07%	0.05	0.0000
^{235}U	1.82E-01	5.55E-05	0.03%	0.1810	0.0028	1.54%	3	0.9999	0.71%	0.46	0.0013

- Forward k_{eff} = 1.010255 ± 0.000052
- Adjoint k_{eff} = 1.01002 ± 0.00056

- Mesh interval size: 2 cm
- GEN=10000, NPG=50000, NSK=100
- AGN=13000, APG=50000, ASK=300
- Runtime: 6.8 days

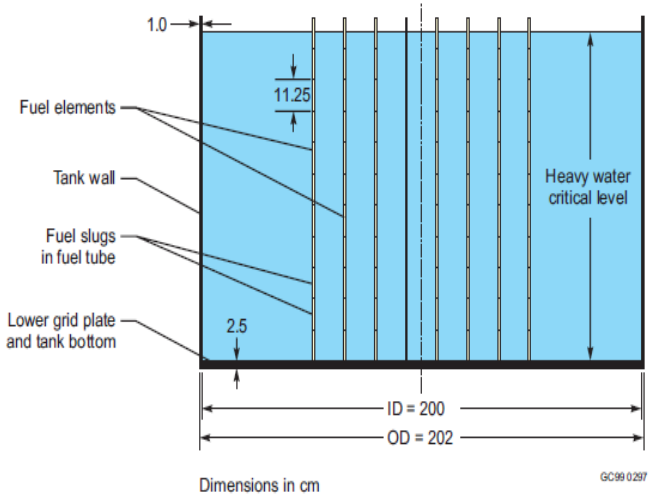
Results for HEU-SOL-THERM-020-005 (continued)

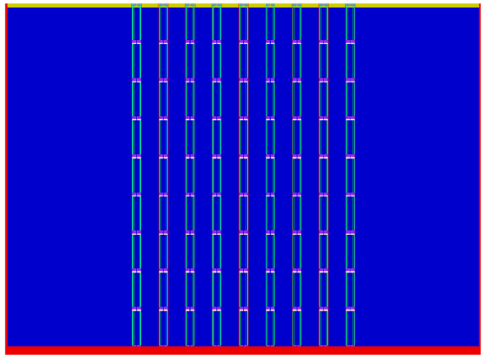
Nuclide	TSUNAMI Results			Direct Perturbation Results					Results Comparison		
	S	σ_S	$\%\sigma_S$	S	σ_S	$\%\sigma_S$	#pts	R^2	DS (%)	DS (σ)	DS
^{1}H	3.22E-02	5.55E-05	0.17%	0.0322	0.0005	1.54%	3	0.9997	-0.01%	0.01	0.0000
^{2}H	7.38E-01	7.68E-04	0.10%	0.7364	0.0102	1.38%	5	0.9987	0.27%	0.20	0.0020
^{16}O	2.46E-01	3.23E-04	0.13%	0.2526	0.0038	1.50%	3	0.9994	-2.66%	1.77	-0.0067
^{56}Fe	1.08E-02	2.27E-05	0.21%	0.0108	0.0002	1.54%	3	0.9999	-0.07%	0.05	0.0000
^{235}U	1.82E-01	5.55E-05	0.03%	0.1810	0.0028	1.54%	3	0.9999	0.71%	0.46	0.0013

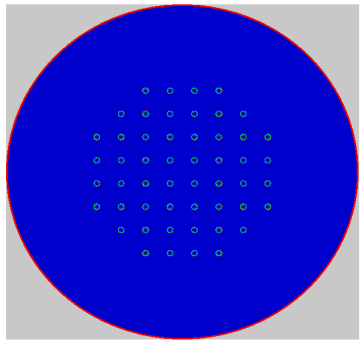
- Additional DP points for ^{2}H resulted in acceptable sensitivity differences

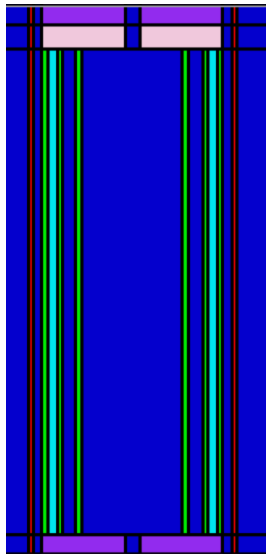
Continuous energy experiment case study

- HEU-COMP-THERM-017
  - Experiment from the ICSBEP Handbook
  - 9 cases
  - Cylindrical tank filled with fuel slugs arranged in lattices filled with heavy water moderator
  - Not a good candidate for multigroup treatment based on fuel slugs









Results for HEU-COMP-THERM-017-001

- Examine sensitivity results from TSUNAMI with IFP and CLUTCH
- Identify sensitivity values above 0.01
- Make sure fissile isotopes and moderator species are examined
- Also include materials/isotopes of interest

Results for HEU-COMP-THERM-017-001 (continued)

Nuclide	TSUNAMI CLUTCH Results			Results Comparison		
	S	σ_S	$\%\sigma_S$	DS (%)	DS (σ)	DS
^{2}H	5.60E-01	5.57E-02	9.95%	20.53%	1.70	0.0954
^{10}B	-2.41E-02	1.29E-05	-0.05%	-1.56%	1.13	0.0004
^{16}O	2.11E-01	2.21E-02	10.48%	26.22%	1.97	0.0438
^{27}Al(2)	-1.13E-02	3.24E-04	-2.87%	2.48%	0.76	-0.0003
^{27}Al(3)	-2.27E-02	4.54E-04	-2.00%	0.47%	0.19	-0.0001
^{235}U	2.94E-01	2.49E-04	0.08%	-1.33%	0.96	-0.0039

- Mesh interval size: 2 cm
- GEN=1000, NPG=10000, NSK=100
- CET=1 CFP=3
- k_{eff} = 1.00779 ± 0.00037

Nuclide	TSUNAMI IFP Results			Results Comparison		
	S	σ_S	$\%\sigma_S$	DS (%)	DS (σ)	DS
^{2}H	4.55E-01	7.60E-03	1.67%	-2.17%	1.06	-0.0101
^{10}B	-2.41E-02	2.38E-05	-0.10%	-1.27%	0.91	0.0003
^{16}O	1.58E-01	4.92E-03	3.12%	-5.52%	1.71	-0.0092
^{27}Al(2)	-1.14E-02	4.17E-04	-3.67%	2.97%	0.73	-0.0003
^{27}Al(3)	-2.25E-02	5.52E-04	-2.46%	-0.39%	0.14	0.0001
^{235}U	2.92E-01	6.02E-04	0.21%	-1.84%	1.33	-0.0055

- Mesh interval size: 2 cm
- GEN=1000, NPG=10000, NSK=100
- CET=2 CFP=3
- k_{eff} = 1.00745 ± 0.00033

Results for HEU-COMP-THERM-017-001 (continued)

Nuclide	TSUNAMI CLUTCH Results			Results Comparison		
	S	σ_S	$\%\sigma_S$	DS (%)	DS (σ)	DS
^{2}H	4.65E-01	1.72E-02	3.70%	0.02%	0.00	0.0001
^{10}B	-2.41E-02	3.84E-06	-0.02%	-1.35%	0.97	0.0003
^{16}O	1.67E-01	6.80E-03	4.08%	-0.09%	0.02	-0.0002
^{27}Al(2)	-1.10E-02	1.01E-04	-0.91%	-0.07%	0.04	0.0000
^{27}Al(3)	-2.21E-02	1.40E-04	-0.63%	-2.18%	1.43	0.0005
^{235}U	2.93E-01	7.68E-05	0.03%	-1.45%	1.05	-0.0043

- Mesh interval size: 2 cm
- GEN=10000, NPG=10000, NSK=100, SIG=0.00010
- CET=1 CFP=3
- k_{eff} = 1.00786 ± 0.00010

Nuclide	TSUNAMI IFP Results			Results Comparison		
	S	σ_S	$\%\sigma_S$	DS (%)	DS (σ)	DS
^{2}H	4.55E-01	8.75E-03	1.92%	-2.05%	0.91	-0.0095
^{10}B	-2.41E-02	2.88E-05	-0.12%	-1.30%	0.94	0.0003
^{16}O	1.62E-01	5.79E-03	3.57%	-2.76%	0.74	-0.0046
^{27}Al(2)	-1.13E-02	5.10E-04	-4.53%	1.94%	0.40	-0.0002
^{27}Al(3)	-2.29E-02	6.44E-04	-2.81%	1.51%	0.47	-0.0003
^{235}U	2.93E-01	7.03E-04	0.24%	-1.66%	1.19	-0.0049

- Mesh interval size: 2 cm
- GEN=1000, NPG=10000, NSK=100
- CET=2 CFP=5
- k_{eff} = 1.00745 ± 0.00033

Results for HEU-COMP-THERM-017-001 (continued)

- Improved results
  - IFP: increased number of latent generations to 5 (cfp=5)
  - CLUTCH: increased number of generations to 10000 (gen=10000)

- All result differences are below guideline parameters

Conclusions

- Use of DP calculations provides confidence in calculated sensitivities
  - Essentially confirms settings yield correct results
- HST-020-005 provides approach for multigroup sensitivity calculation
- HCT-017-001 provides two approaches for continuous energy calculations: IFP and CLUTCH

Questions?

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