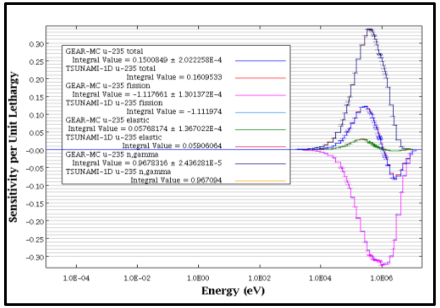
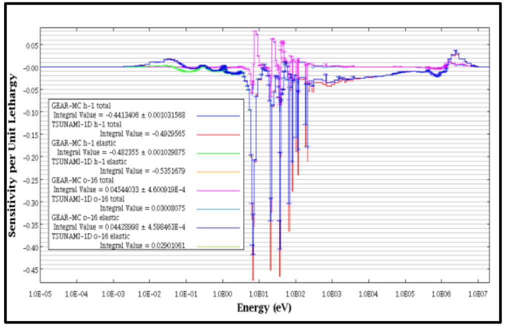
Continuous-Energy TSUNAMI Sensitivity Capabilities in SCALE 6.2

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





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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.

Calculating Sensitivity Coefficients

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

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

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

where

ϕ = neutron flux;
$\phi^{\dagger}$ = adjoint neutron flux
k = k_{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
Σ = problem-dependent resonance self-shield macroscopic cross sections
$\vec{\xi}$ = phase space vector; and
$\langle \; \rangle$ indicate integration over space, direction and energy variables.

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Calculating Sensitivity Coefficients

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

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

- 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.

Calculating Sensitivity Coefficients

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

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

- 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.

CE TSUNAMI-3D Sensitivity Methods

Eigenvalue Sensitivity Calculations

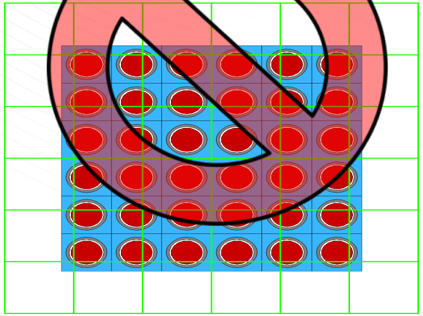
- CLUTCH Method (cet=1)
- IFP Method (cet=2)

Generalized Perturbation Theory Sensitivities

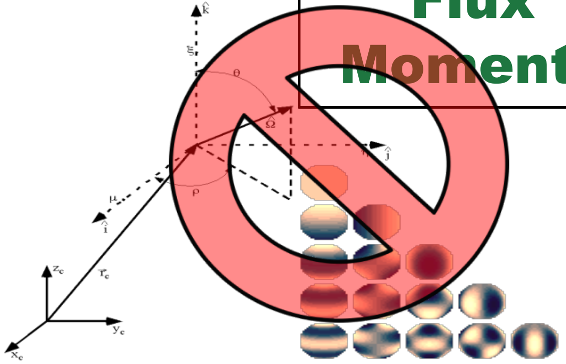
- GEAR-MC Method: CLUTCH only (cet=4)
- GEAR-MC Method: CLUTCH + IFP (cet=5)

Things you need for a multigroup TSUNAMI-3D Calculation:

Spatial Flux Mesh

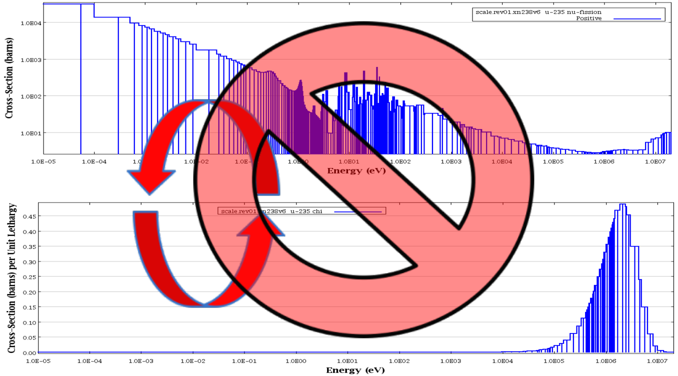


Flux Moments



$$\tilde{\phi}_j = \int \phi\left(\hat{\Omega}\right) R_j\left(\hat{\Omega}\right) d\hat{\Omega}$$

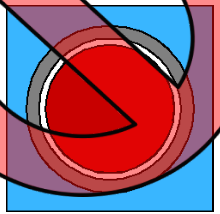
Separate Adjoint Transport Solution



Volume Calculations

$$points = \frac{volume}{ln\left(volume/5000\right)}$$

Cross Section Self-Shielding



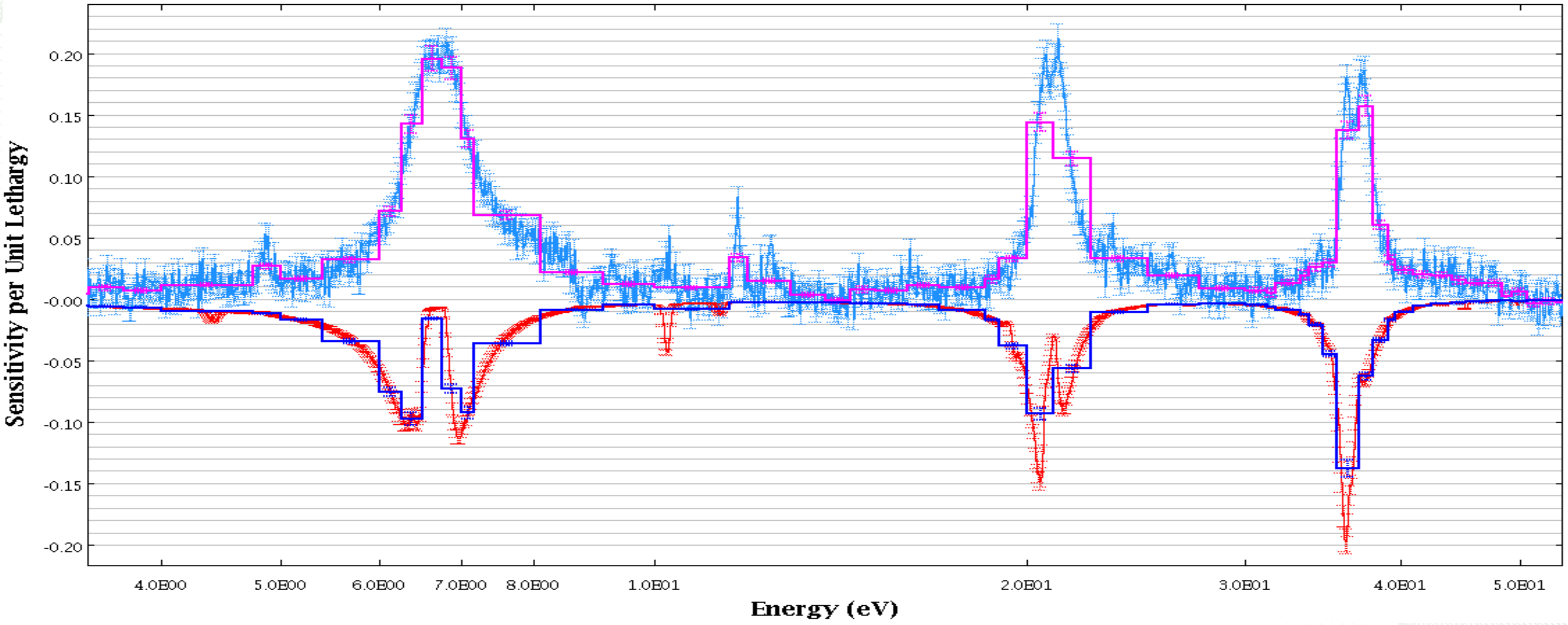
Expert Judgment

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



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

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)

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: **cet=2**
- The number of "latent generations" is set using the **cfp=#** parameter.

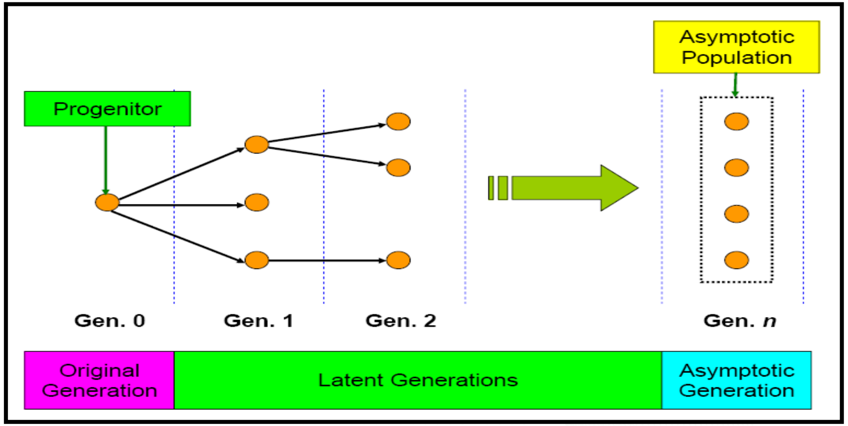


Illustration of the IFP process. Image courtesy of Brian Kiedrowski.

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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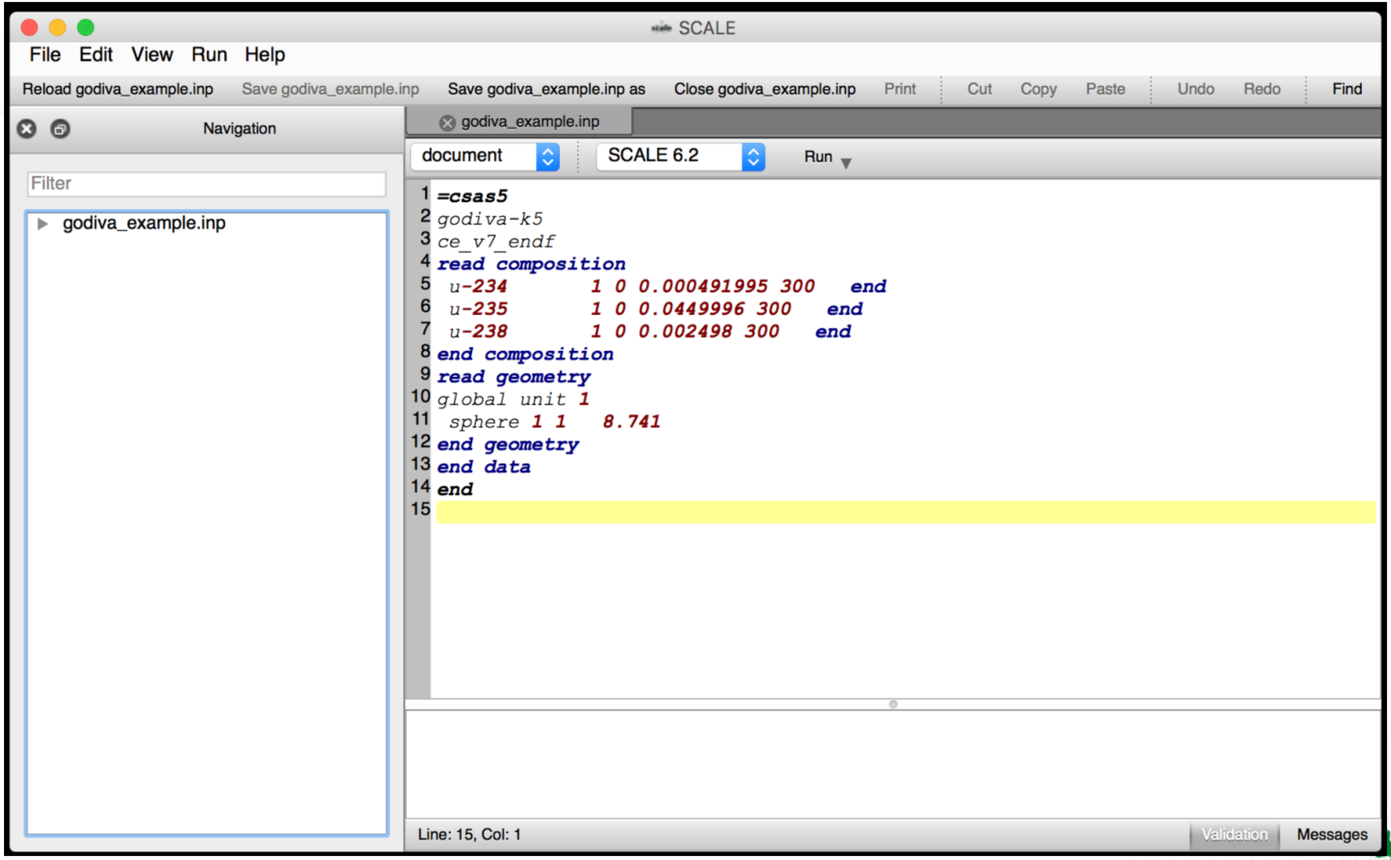
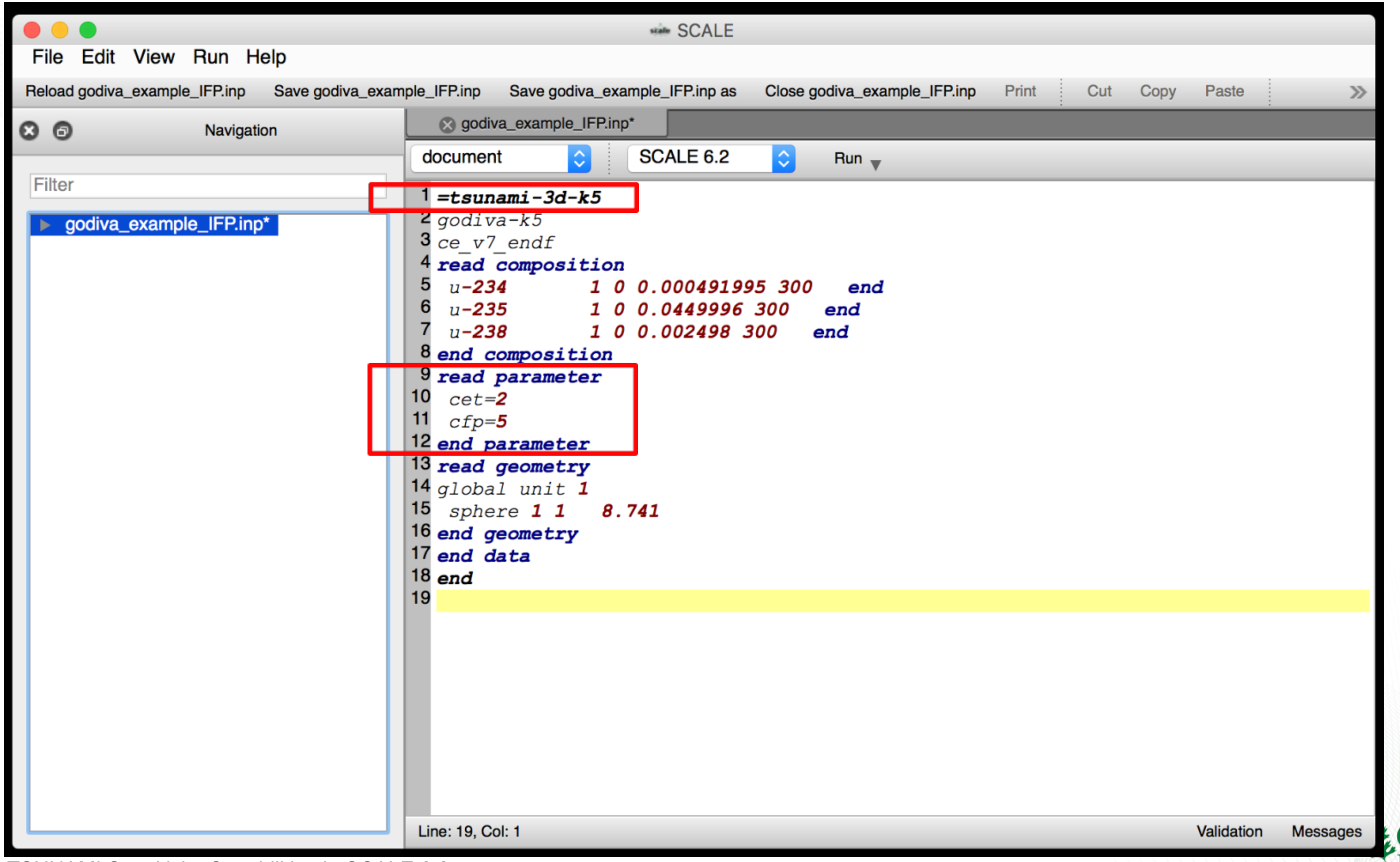
Let’s Try CE TSUNAMI-3D



Let's Try CE TSUNAMI-3D



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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 *unique isotope-regions*
× **12** *reactions per isotope*
× **44** *energy groups*
× **11** *generations of storage*
× **10,000** *particles per generation*
× **8** *bytes per double*
= **17,656** *gigabytes of memory*

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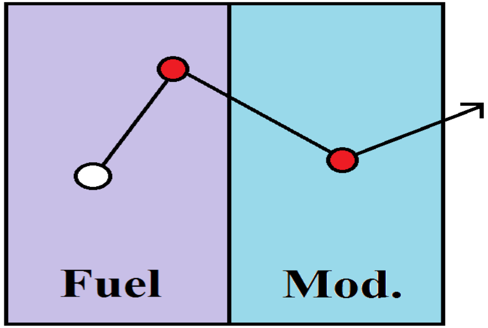
CLUTCH/Contributon Methodology

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



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

…where:

G(τ_s → 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:

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

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CLUTCH Memory Requirements

- The CLUTCH method requires one to store reaction rate tallies for every collision a particle sees from birth until death.
- Unlike the IFP method, this information is freed after a particle dies and is not carried for multiple generations.

38,000 *unique isotope-regions*
× **12** *reactions per isotope*
× **4,000** *collisions per history*
× **8** *bytes per double*
= **14.6** *gigabytes of memory*

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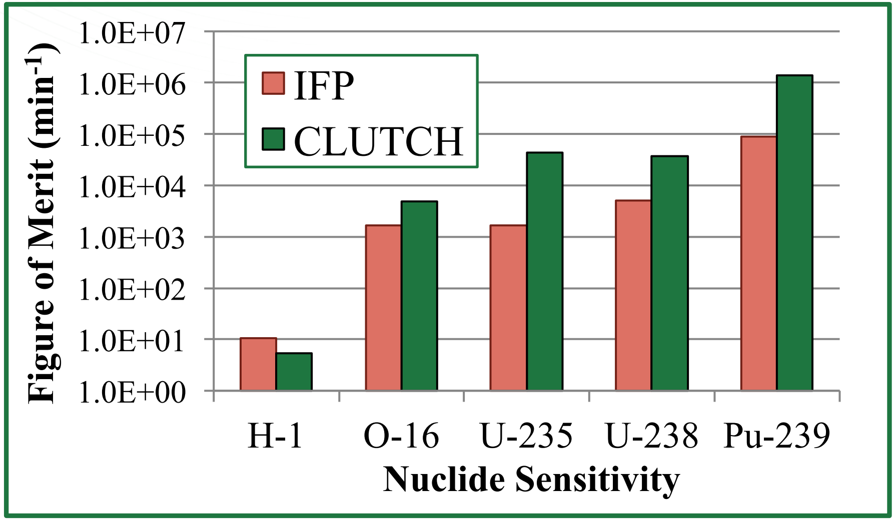
CLUTCH VS IFP

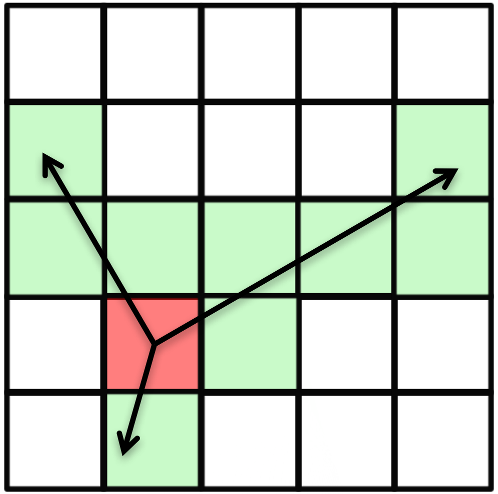
- The CLUTCH method is more efficient than IFP (both in terms of speed and memory usage).
- The downside to CLUTCH is that you need to compute F*(r).



Sensitivity Method Memory Usage			
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

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.



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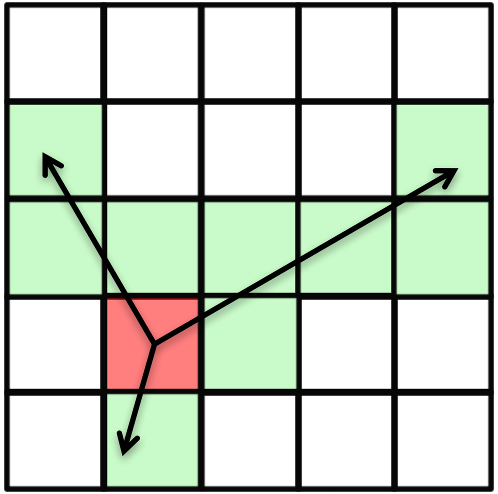

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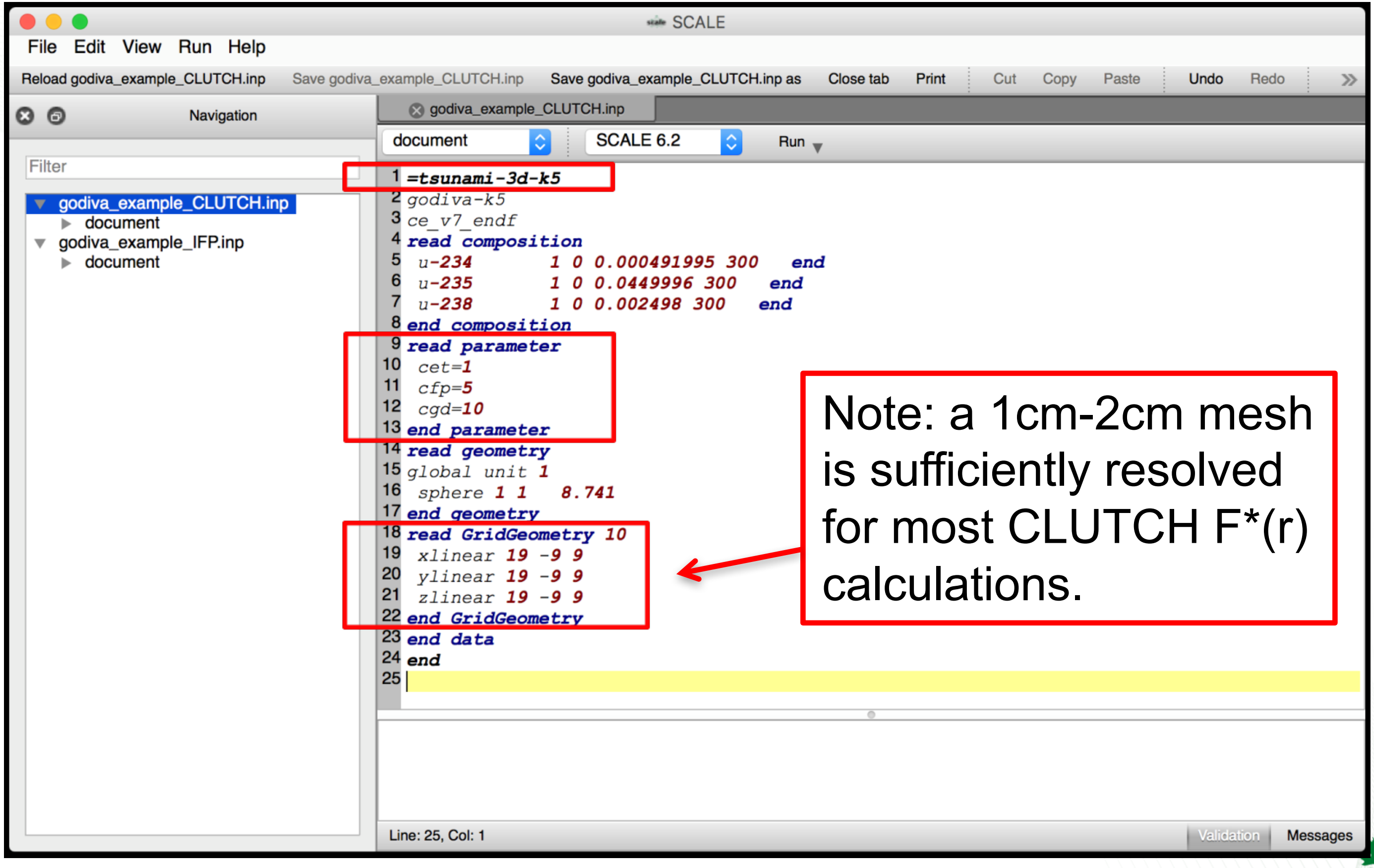
How to use CLUTCH with an F*(r) Mesh

- 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

Nuclide	IFP Sensitivity	CLUTCH Sensitivity	Difference (# Standard Dev.)
U-234	6.92E-03 ± 6.71E-04	6.37E-03 ± 2.68E-04	-0.76
U-235	8.09E-01 ± 5.18E-03	7.89E-01 ± 1.97E-03	**-3.67**
U-238	1.69E-02 ± 1.50E-03	1.61E-02 ± 5.43E-04	-0.46

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 **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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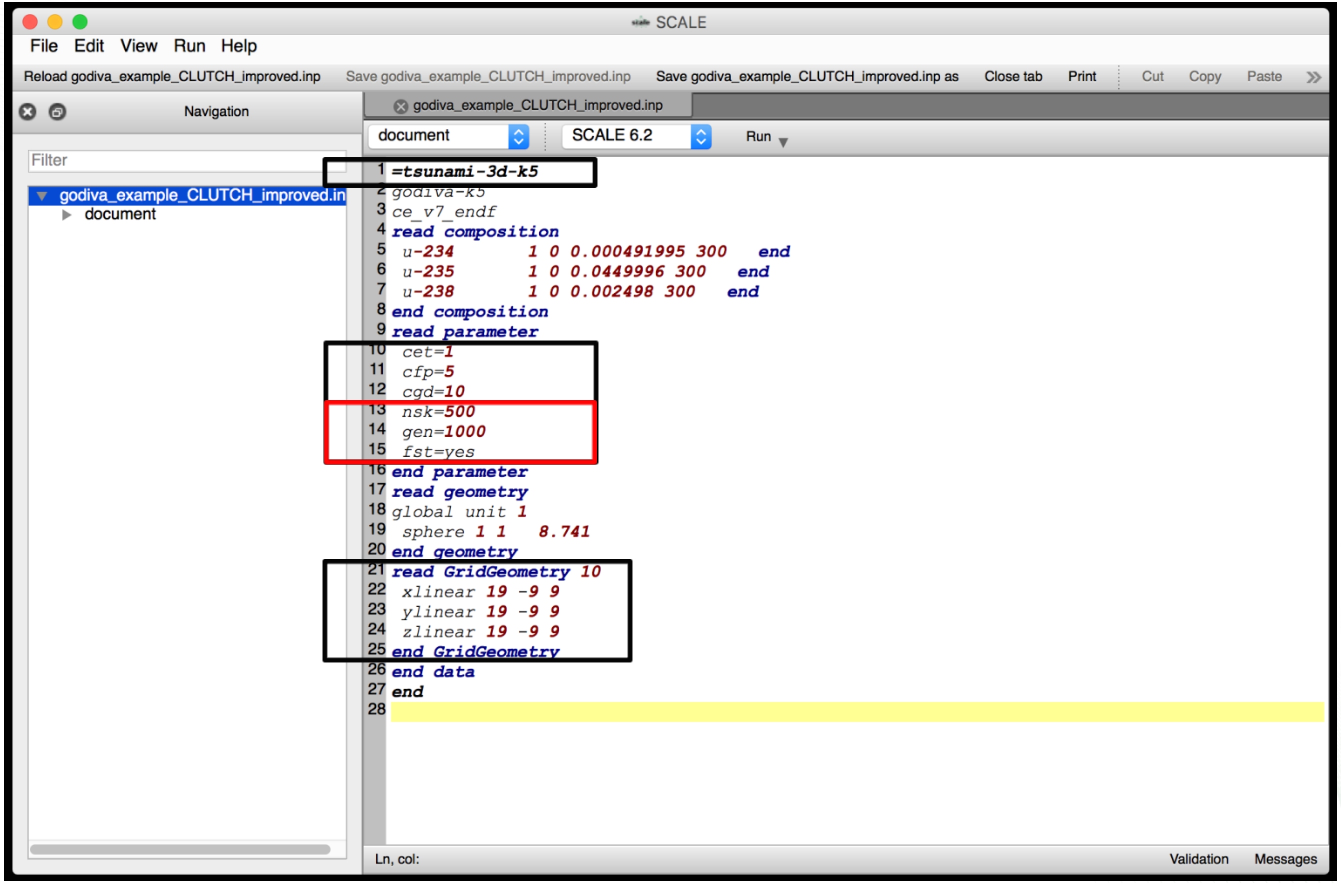
Improving the CLUTCH Input



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.

```
499      1.03074E+00   1.00056E+00   1.05296E-03   6.11893E+00   6.45500E-01
500      1.05307E+00   1.00067E+00   1.05612E-03   6.09369E+00   6.46667E-01


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.


501      9.82646E-01   1.00063E+00   1.05461E-03   6.04676E+00   6.49000E-01
502      9.64969E-01   1.00056E+00   1.05492E-03   6.17351E+00   6.51167E-01
```

Updated Sensitivity Coefficients

Nuclide	IFP Sensitivity	CLUTCH Sensitivity	Improved CLUTCH Run
U-234	6.92E-03 ± 6.71E-04	6.37E-03 ± 2.68E-04 (**-0.76 σ**)	7.73E-03 ± 2.71E-04 (**1.13 σ**)
U-235	8.09E-01 ± 5.18E-03	7.89E-01 ± 1.97E-03 (**-3.67 σ**)	8.01E-01 ± 1.81E-03 (**-1.46 σ**)
U-238	1.69E-02 ± 1.50E-03	1.61E-02 ± 5.43E-04 (**-0.46 σ**)	1.80E-02 ± 5.68E-04 (**0.71 σ**)

TSUNAMI-3D Sensitivity Method Summary

	Multigroup TSUNAMI	IFP	CLUTCH
Accuracy	Good	Excellent	Excellent
Speed	Good	Good	Excellent
Efficiency	Excellent	Good	Excellent
Memory Requirements	Limiting	Limiting	Typically Fine
Ease of Use	Requires a Flux Mesh	Very Easy	Must Calculate $F^*(r)$

CE TSUNAMI-3D Sensitivity Methods

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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.

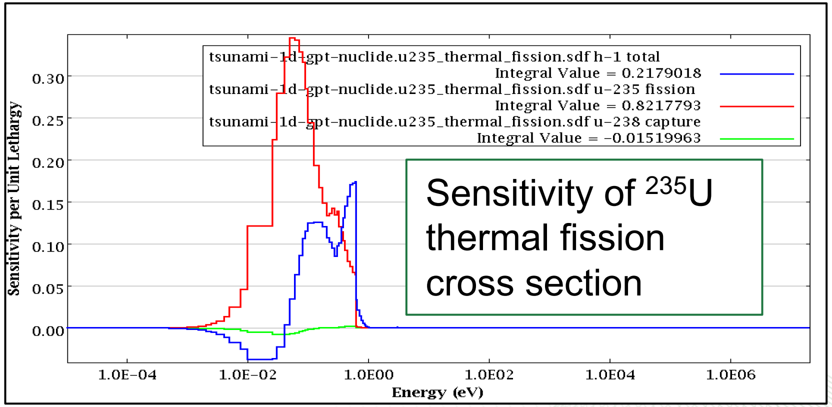
$$S_{R,\Sigma} = \frac{\delta R/R}{\delta\Sigma/\Sigma} \qquad R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

- 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.



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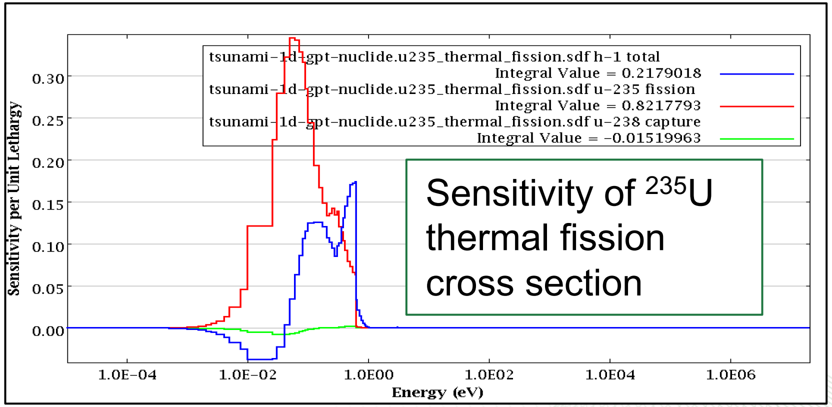
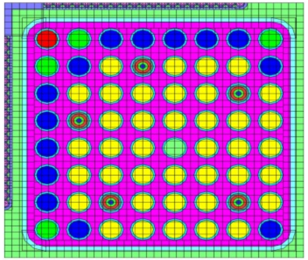


Generalized Perturbation Theory

- 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)



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

CE TSUNAMI-3D GPT Response Extension

Original GPT Responses

- Total cross section (MT = 1)
- Fission cross section (MT = 18)
- (*n*,γ) abs. cross section (MT = 102)
- Neutron prod. cross section (MT = 1452)
- Neutron flux

CE TSUNAMI-3D GPT Response Extension

Original GPT Responses	
Total cross section	(MT = 1)
Fission cross section	(MT = 18)
(*n*,γ) abs. cross section	(MT = 102)
Neutron prod. cross section	(MT = 1452)
Neutron flux	

Updated GPT Responses	
Total cross section	(MT = 1)
Total scatter cross section	(MT = 0)
Elastic scatter cross section	(MT = 2)
Inelastic scatter cross section	(MT = 4)
(*n,2n*) scatter cross section	(MT = 16)
Fission cross section	(MT = 18)
Total absorption cross section	(MT = 101)
(*n*,γ) absorption cross section	(MT = 102)
(*n*,p) absorption cross section	(MT = 103)
(*n*,d) absorption cross section	(MT = 104)
(*n*,t) absorption cross section	(MT = 105)
(*n*,^{3}He) absorption cross section	(MT = 106)
(*n*,α) absorption cross section	(MT = 107)
Neutron production cross section	(MT = 1452)
Flux-weighted CMM diffusion coefficient	
Neutron flux	

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":

$$M^2 = \frac{D}{\Sigma_r} = \frac{1}{6}\bar{r}^2 \qquad R(D_{CMM}) = \frac{\langle M^2 \Sigma_r \phi \rangle}{\langle \phi \rangle}$$

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

[1] Z. Liu, K. Smith, and B. Forget, "A Cumulative Migration Method for Computing Rigorous Transport Cross Sections and Diffusion Coefficients for LWR Lattices with Monte Carlo," *Proc. PHYSOR 2016*, Sun Valley, Idaho, May 1–5, 2016.

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.

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

- 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.

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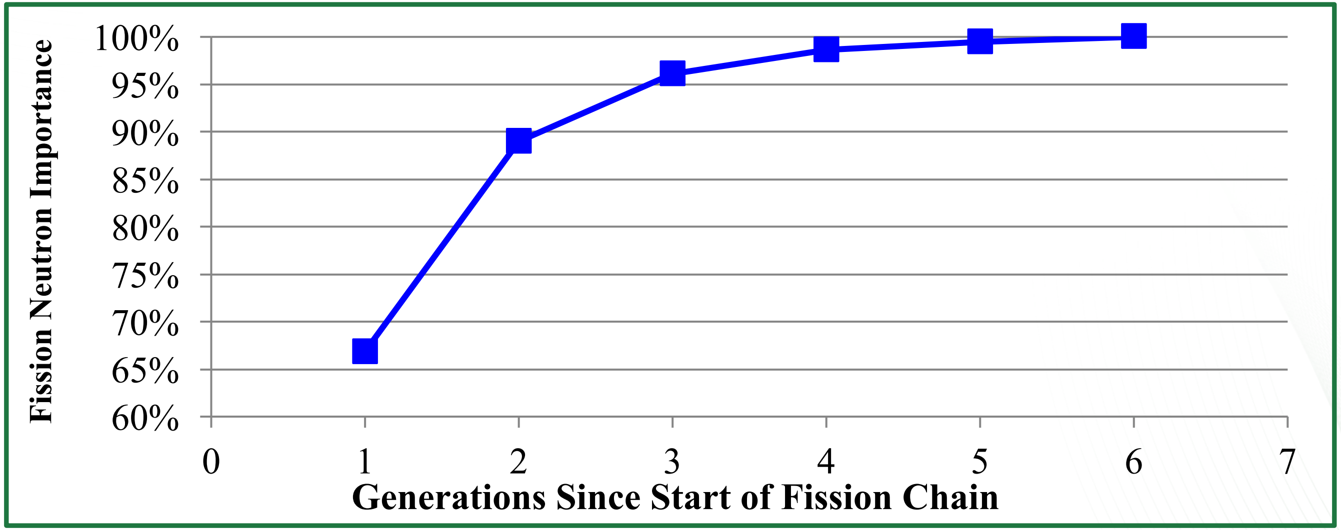
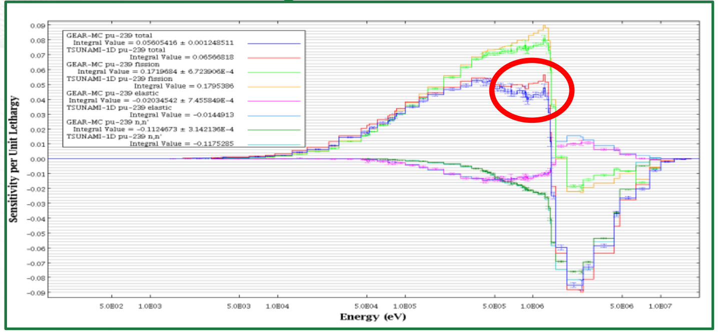
Inter-generational Importance

- The inter-generational term is calculated by tallying the intra-generational importance generated by neutrons in a fission chain as that importance approaches zero.
  - This term is tallied using the IFP method.
  - The number of "latent" generations used for tallying the inter-generational effect is specified using the **cfp=#** keyword.

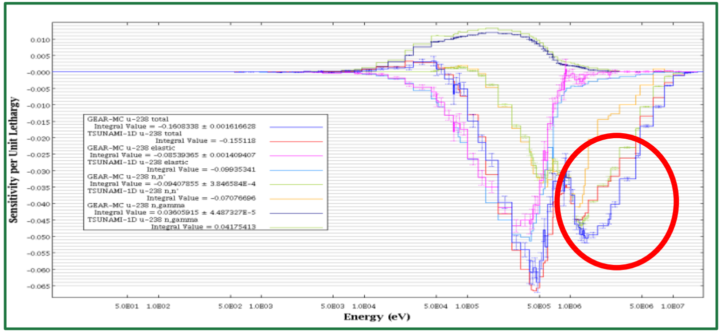


GPT Flattop Foil Response Sensitivity Coefficients

F28/F25 Pu-239 Sensitivity Coefficients



F37/F25 U-238 Sensitivity Coefficients



Flattop Total Nuclide Foil Response Sensitivities

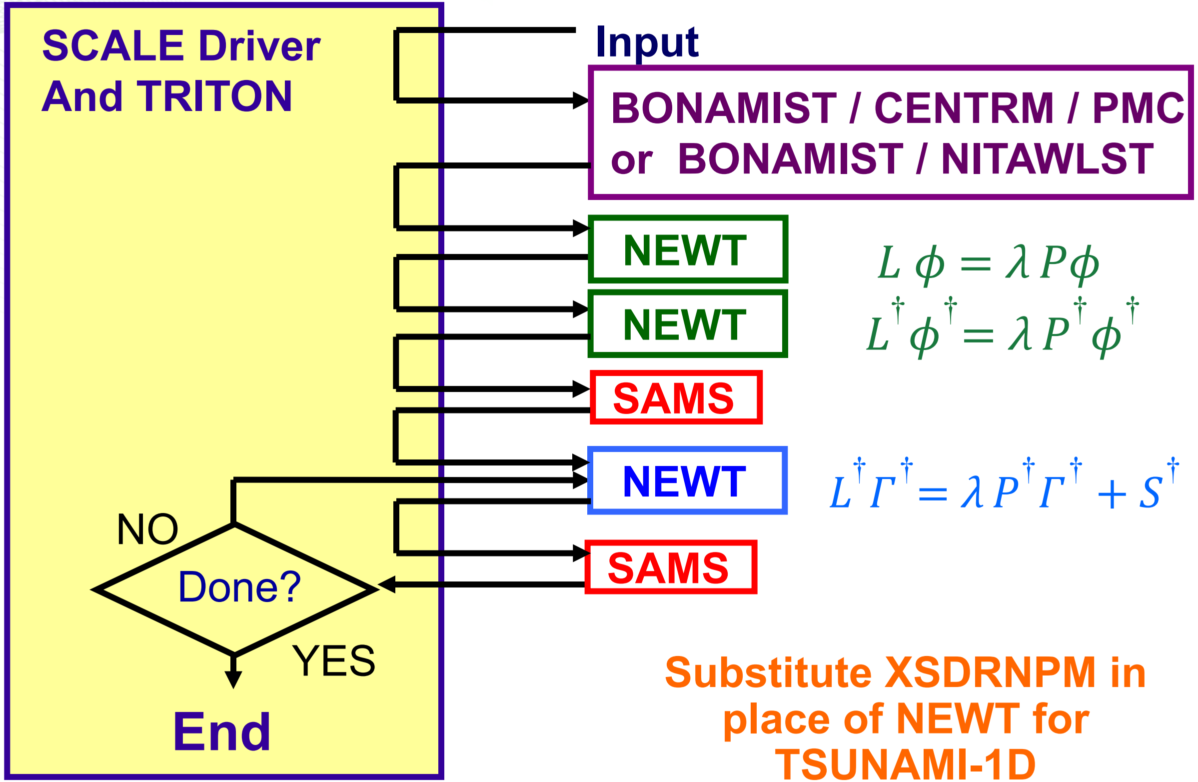
Experiment	Response	Isotope	Direct Pert.	TSUNAMI-1D	GEAR-MC
Flattop	F28 / F25	^{238}U	0.8006 ± 0.0533	0.8024 **(0.03 σ)**	0.7954 ± 0.0018 **(-0.10 σ)**
		^{239}Pu	0.0528 ± 0.0043	0.0657 **(2.99 σ)**	0.0561 ± 0.0012 **(0.73 σ)**
	F37 / F25	^{238}U	-0.1540 ± 0.0102	-0.1551 **(-0.11 σ)**	-0.1608 ± 0.0016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

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.

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

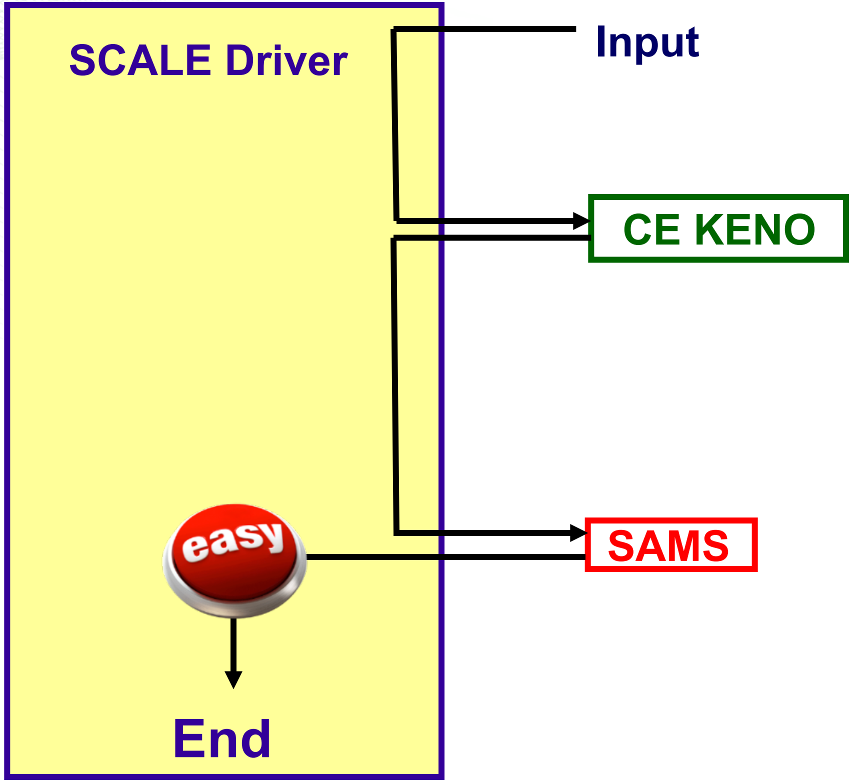
S/U calculation for k_{eff}

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

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

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.

```
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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?

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