

TSUNAMI-3D

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Learning goals

- Understand Multigroup TSUNAMI-3D
- Understand Continuous Energy TSUNAMI-3D
- Understand and complete workshop examples using Multigroup and Continuous Energy TSUNAMI-3D

Multigroup TSUNAMI-3D



Objectives

- Survey adjoint-based sensitivity theory for multigroup Monte Carlo eigenvalue sensitivity calculations
- Examine primary multigroup TSUNAMI-3D options
- Examine advanced options
- Discuss adjoint Monte Carlo eigenvalue calculations

Introduction

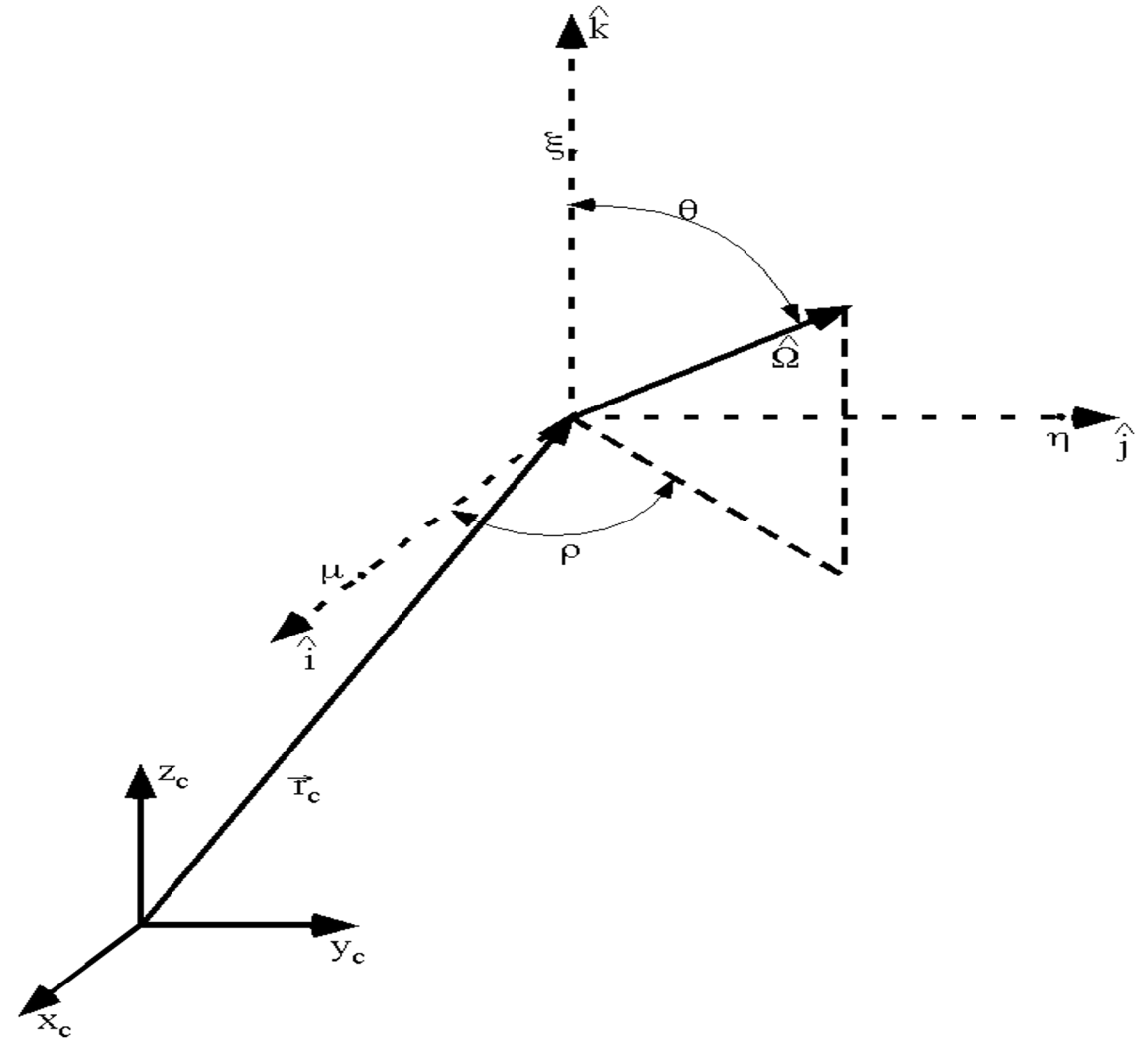
- TSUNAMI-3D: SCALE sequences that computes the k_{eff} sensitivities to nuclear data
- Input is largely the same as CSAS input
- The TSUNAMI-3D-K5 sequence uses KENO V.a for the transport solution, whereas TSUNAMI-3D-K6 uses KENO-VI
- Can assess uncertainty in k_{eff} due to nuclear covariance data

Monte Carlo techniques

- 3D Monte Carlo analysis is frequently used for accurate modeling of complex systems
- KENO is a widely used Monte Carlo code for criticality safety analysis that:
 - Operates within SCALE
 - Performs forward and adjoint calculations
 - Tallies angular flux moments

What are angular flux moments?

- Mathematical expression for the directional dependence of the flux
 - Which way is the flux going?
- Varies as a function of position
 - Where is the flux?



Flux moments

- Mathematically expressed as integral over all angles of angular flux with spherical harmonics

$$\tilde{\phi}_j = \int \phi(\hat{\Omega}) R_j(\hat{\Omega}) d\hat{\Omega}$$
- In other words, allows reconstruction of angular flux
- Computed for each energy and position
- Having more moments improves accuracy but requires more memory

Real-valued Spherical Harmonics Functions		
j	ℓ	$R_j(\hat{\Omega})$
0	0	1
1	1	$\cos \theta$
2	1	$-\sin \theta \cos \rho$
3	1	$-\sin \theta \sin \rho$
4	2	$\frac{1}{2}(3\cos^2 \theta - 1)$
5	2	$-\frac{\sqrt{3}}{3} 3 \sin \theta \cos \theta \cos \rho$
6	2	$-\frac{\sqrt{3}}{3} 3 \sin \theta \cos \theta \sin \rho$
7	2	$\frac{\sqrt{3}}{6} \sin^2 \theta \cos(2\rho)$
8	2	$\frac{\sqrt{3}}{6} \sin^2 \theta \sin(2\rho)$
9	3	$\frac{1}{2}(3\cos^3 \theta - 3\cos \theta)$
10	3	$-\frac{3\sqrt{6}}{12} \sin \theta (5\cos^2 \theta - 1) \cos \rho$
11	3	$-\frac{3\sqrt{6}}{12} \sin \theta (5\cos^2 \theta - 1) \sin \rho$
12	3	$\frac{\sqrt{15}}{2} \sin^2 \theta \cos \theta \cos(2\rho)$
13	3	$\frac{\sqrt{15}}{2} \sin^2 \theta \cos \theta \sin(2\rho)$
14	3	$-\frac{\sqrt{10}}{4} \sin^3 \theta \cos(3\rho)$
15	3	$-\frac{\sqrt{10}}{4} \sin^3 \theta \sin(3\rho)$

P₀

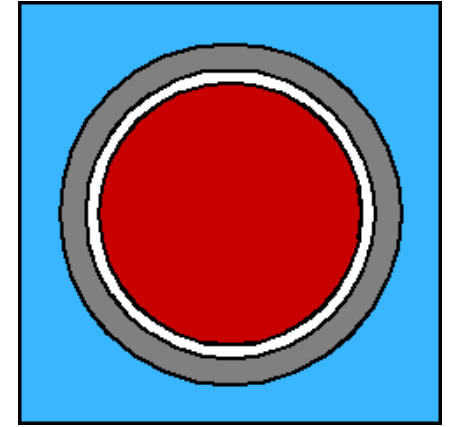
P₁

P₂

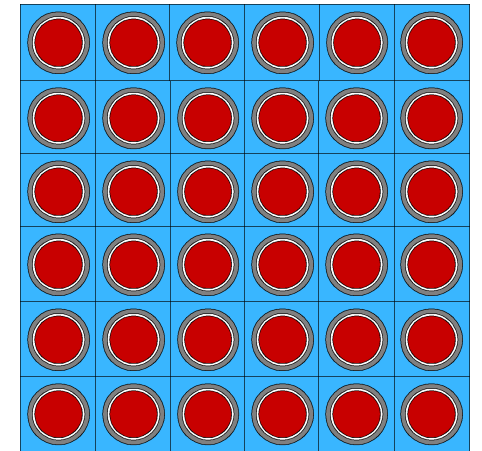
P₃

Array flux tallies in KENO

- KENO tallies flux by region
 1. Pellet
 2. Gap
 3. Clad
 4. Moderator
- Values are averaged across all instances of a UNIT in a problem: average flux over array or for all instances of a UNIT used as a HOLE



4 flux regions
fuel, gap, clad, mod.



6×6 Array of 4-region cell
for 144 regions

Sensitivity calculation

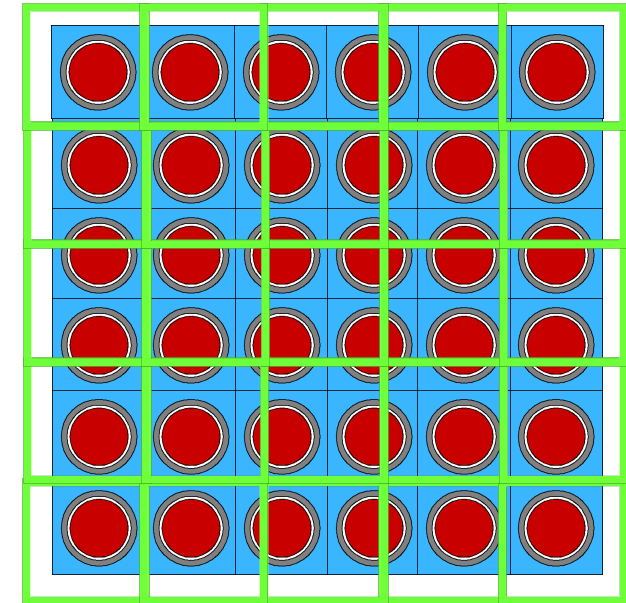
- Forward and adjoint flux moments are accumulated, multiplied, and summed over a region
- Region sensitivities are computed based on these fluxes
- Nuclide/mixture sensitivities are calculated by summing sensitivities over all regions in which the nuclide occurs in each mixture
- Total nuclide sensitivities are calculated by summing over all instances of a nuclide
- Total mixture sensitivities are calculated by summing all nuclides in each mixture
- Sensitivity coefficient generation is performed in SAMS

Spatial mesh for flux moment collection

- Use mesh to refine flux solution
- Automated spatial mesh option generates a uniform mesh over entire model
- Alternatively, the user can define the mesh
- Monte Carlo tracking is the same with or without the mesh, but flux solutions are refined within the mesh
 - Tallying generally does not impact distance to collision, reaction selection, or related physics

Array flux tallies in KENO with mesh

- Mesh accumulator modifies KENO behavior to tally flux by region **in each voxel**
- Still averaging in multiple instances of the same UNIT, but only within a voxel
- Provides significant spatial resolution without necessitating geometry changes
 - Same array with a single unit



Sensitivity calculation with mesh

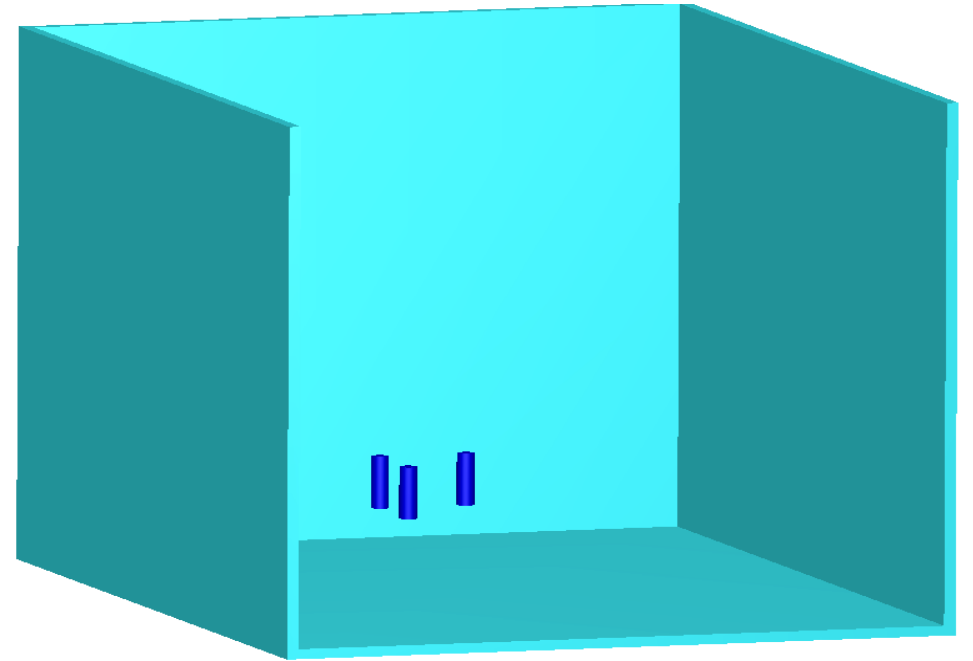
- Same process, but flux solutions are refined and better capture gradients
- SAMS output is the same
- Longer KENO calculations
 - More memory – can limit problem size and complexity
- Longer processing time in SAMS
- More accurate sensitivity calculations

Automated mesh

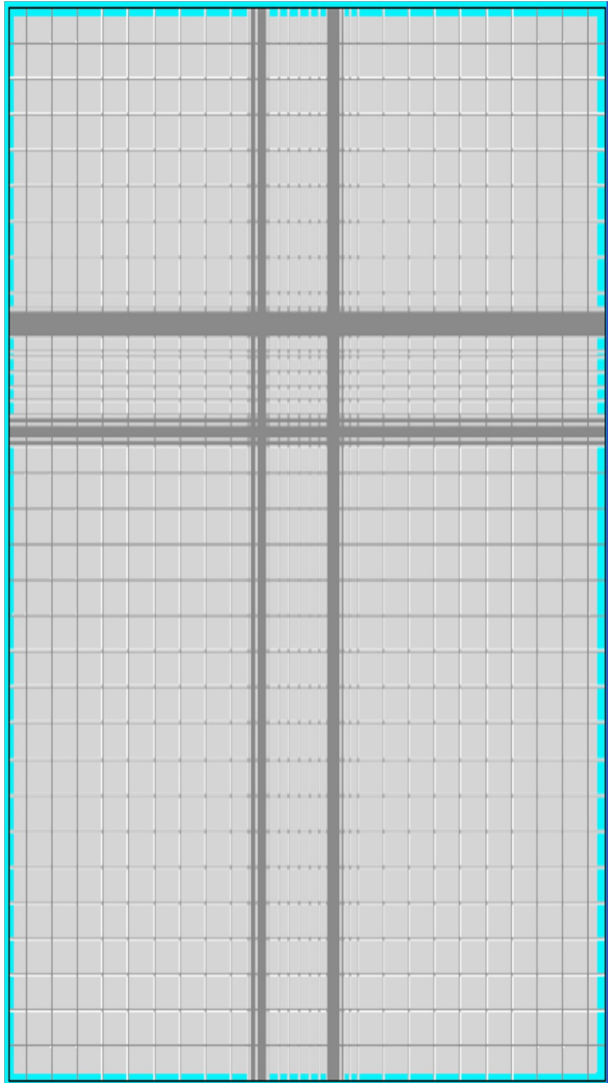
- Volumes of each region within each mesh interval must be computed
- Forward and adjoint fluxes are accumulated over same mesh, then multiplied before summing over a region
- Can be used with or without coordinate transform
- Sensitivities are computed for each user-input region, not over the mesh
- `mfx=yes msh=##` length of side of cube
- `mfx=##` can be used for inputs containing gridGeometry specification

Example: PU-SOL-THERM-014

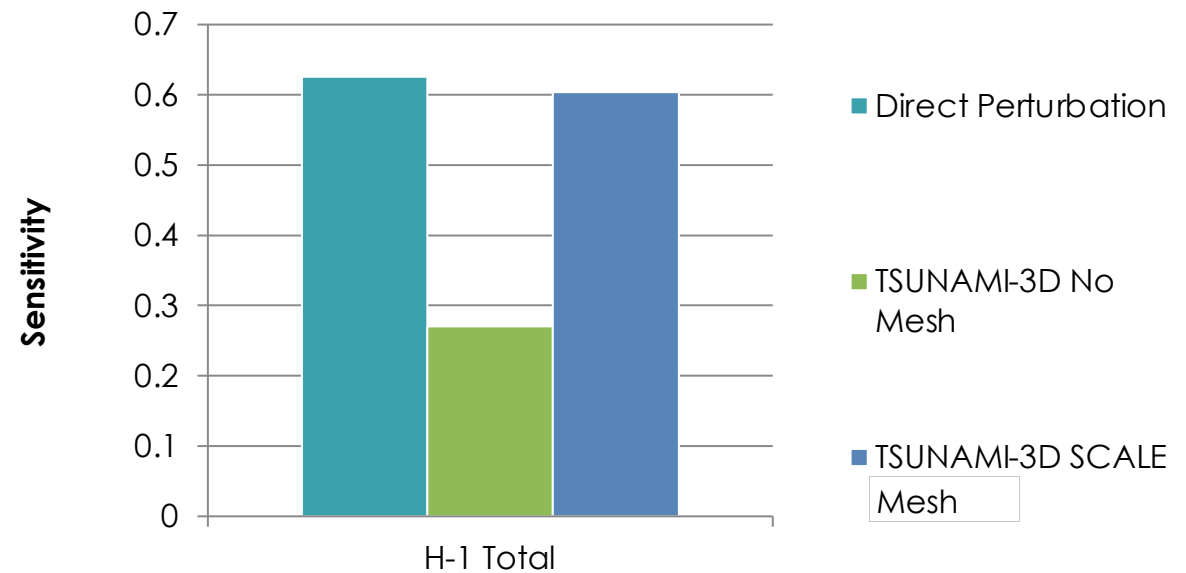
- Plutonium solution cans (~30 cm)
- Large room (~15 m)
- Desire 3 cm mesh for fissile solution
- Uniform mesh would create ~80,000,000 mesh intervals and require ~300 GB of RAM



User-defined variable mesh



- Mesh refined across fissile solution
- Requires ~140,000 mesh intervals
- ~500 MB of RAM



SCALE user-defined meshes: Two input options

List all planes explicitly

```
read gridgeometry 1
  xplanes
-750 -700 -650 -600 -550 -500 -450 -400 -350 -331 -325 -322 -319
-316 -313 -311 -310 -307 -304 -301 -298 -295 -292 -291 -271 -261
-241 -221 -201 -180 -175 -172 -169 -166 -163 -160 -160 -157 -154
-151 -148 -145 -142 -139 -100 -50 0 50 100 150 200 250 300 350
400 450 500 550 600 650 700 750
end
  yplanes
-585 -550 -500 -450 -400 -350 -300 -250 -200 -150 -116 -110 -107
-104 -101 -98 -96 -95 -92 -89 -86 -83 -80 -77 -76 -56 -36 -16 4
24 40 43 44 46 49 52 55 58 61 64 64 67 70 84 100 150 200 250 300
350 400 450 500 550 585
end
  zplanes
-540 -500 -450 -406 -386 -366 -346 -345 -342 -339 -336 -333 -330
-327 -326 -324 -321 -319 -316 -313 -310 -307 -306 -304 -300 -286
-250 -200 -150 -100 -50 0 50 100 150 200 250 300 350 400 450 500
550 570
end
end gridgeometry
```

Uniform plane generation

```
read gridgeometry 1
  xlinear 30 -750 750
  xlinear 15 -331 -291
  xlinear 15 -179 -139
  ylinear 24 -585 585
  ylinear 15 -116 -76
  ylinear 15 44 84
  zlinear 22 -540 570
end gridgeometry
```

SCALE flexible mesh – Explicit planes

- READ GRID *MESH GRID DATA* END GRID
- XPLANES= *xplanes* the cell boundaries in the x direction followed by end
- YPLANES= *yplanes* the cell boundaries in the y direction followed by end
- ZPLANES= *zplanes* the cell boundaries in the z direction followed by end

SCALE flexible mesh – Interpolated planes

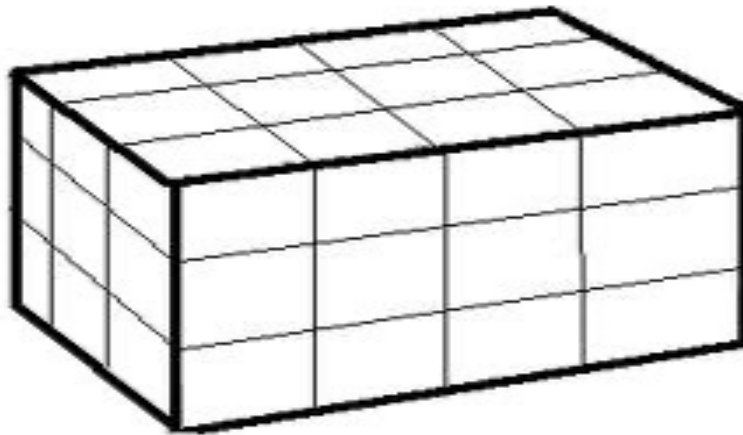
- XLINEAR *intervals xmin xmax*
- YLINEAR *intervals ymin ymax*
- ZLINEAR *intervals zmin zmax*

NOTE: The user must set the range in each direction so that the actual geometry is totally covered by the mesh for MG TSUNAMI. This is not a requirement in CSAS/KENO MG or CE TSUNAMI.

Mesh volume

- The volume of each region within each mesh interval must be known to compute sensitivity coefficients in MG TSUNAMI
- The sequence computes the volume through a stochastic sampling process
- SCALE 6.3.1 defaults:
 - 5000 points if volume < 13,600 cm³
 - For larger volumes:
$$points = \frac{volume}{\ln(volume/5000)}$$
- These defaults can lead to a long calculation time at the beginning of the calculation in “tsunami-3d-k5” or “tsunami-3d-k6”

Volume Block – Review



Monte Carlo Volume Calculation

- The Volume Block is used to control volume calculations in the CSAS6 (and TSUNAMI-3D) sequences
- Options described in [Section 8.1.3.13](#) of the SCALE manual
- Simplest approach:
 - Set type=random (Not supported in Shift)
 - Define cuboid over volume region to calculate volumes
 - (XP, YP, ZP) and (XM, YM, ZM) are corners
 - Set batches and number of points per batch (like for GEN and NPG)
 - No NSK analog as there is no source convergence
 - Can also specify sample_den to ensure density of points per batch instead
 - Volume and uncertainty for each region are printed in output

Monte Carlo Volume Calculation: Example

```
read volume  
  type=random points=1000000  batches=10000  
  xp=60.10 xm=-60.10 yp=60.10 ym=-60.10 zp=115.640 zm=-16.20  
end volume
```

Other Volume Block Options

- Other volume input options include:
 - Manually inputting vol= on media records.
 - Specify total volume if unit is used multiple times.
 - Take care to account for parts of the volume that are clipped by other regions.
 - Using Fulcrum to calculate volumes.
 - Calculated using SCALE ray tracing algorithm.
 - Executed using Run → Calculate Volumes.
 - User can then specify number of rays to trace in X, Y, and Z dimensions.
 - Volumes are then listed by Fulcrum in “Messages”.
 - Shift can calculate volumes using `type=trace`

Volume input examples

With SCALE 6.3.1 defaults, PU-SOL-THERM-014 mesh volumes are computed with
~150,000,000 points for 1000 batches

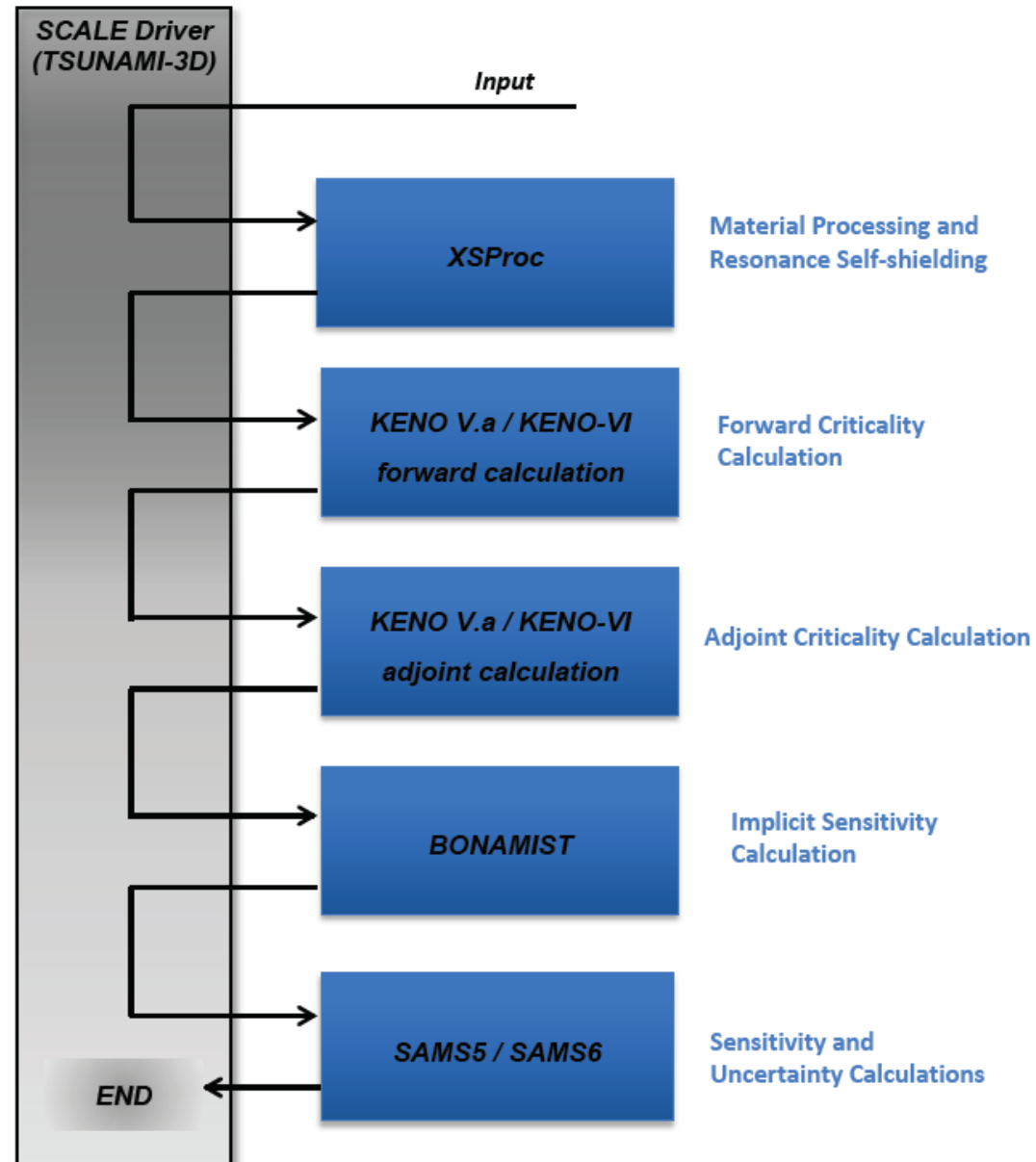
- Input sampling directly

```
read volume
  type=random
  batches=4000
  points=25000
end volume
```

- Input sampling density:

```
read volume
  sample_den=0.1
  batches=4000
end volume
```

Multigroup TSUNAMI-3D analysis sequence



TSUNAMI-3D input

Composition and Cell Data

```
=tsunami-3d-k5
U(2)F4 H/X=294 rafferty and mihalczo u(2)f4-2 unreflected (case 14)
v7.1-252
read comp
u-235 1 0 1.3303e-4 end
u-238 1 0 6.4370e-3 end
h 1 0 3.9097e-2 end
c 1 0 1.8797e-2 end
f 1 0 2.6280e-2 end
end comp
read cell
inhommedium 1 end
end cell
```

KENO V.a Data

```
read param npg=500 gen=200 apg=2000 tfm=no end param
read geom
global unit 1
cuboid 1 1 4p28.110 2p61.235
end geom
end data
```

Optional SAMS Data

```
read sams
prtgeom prtimp nocovar
end sams
end
```

TSUNAMI-3D input parameters

KENO V.a Parameter Data for TSUNAMI-3D

Parameter	Allowed Values	Default Value	Definition
*htm=	*no	yes	*must be included and set to no if using mfx= for MG only
nqd=	0,2,4,6,8,10,12,14,16	0	order of angular quadrature
pnm=	Non-negative integers	3	order of flux moment computed in KENO V.a
tfm=	yes/no	yes	compute angular fluxes and/or flux moments in transformed coordinate system
apg=	integer	$\text{ngp} \times 3$	number of neutrons per generation for adjoint calculation
abk=	integer	$\text{apg} \times 2$	number of neutron bank positions for the adjoint case
agn=	integer	gen	number of generations for the adjoint case
asg=	number	0	convergence criteria for k_{eff} to stop adjoint calculation
pmf=	yes/no	no	print more fluxes. prints angular flux and/or flux moment edits
mfx=	yes/no	no	compute mesh fluxes on mesh defined by msh
msh=	number	0	size of mesh used for mesh flux calculations
pms=	yes/no	no	print mesh fluxes

TSUNAMI-3D input parameters (cont.)

Optional SAMS Data for TSUNAMI-3D

Keyword	Default Value	Description
prtgeom	F	Flag to cause the sensitivities to be output for each geometry region
Prtmp	T	Prints explicit sensitivities coefficients, implicit sensitivity coefficients and complete sensitivity coefficients.
nohtml	F	Prevents generation of HTML output
largeimp=	100.0	Filter implicit sensitivities with value greater than largeimp
coverx=	56groupcov7.1	Name of covariance data file
pn=	3	Legendre order for moment calculations
prtflx	F	Print angular fluxes and flux moments (long edits)
prtvols	F	Flag to cause the volumes of the regions to be printed by SAMS
nomix	F	Flag to cause the sensitivities by mixture to be turned off
unconstrainedchi	F	Flag to generate pre-SCALE 6 unconstrained chi sensitivities

Example problem

- Homogeneous system
- LEU-COMP-THERM-033 from ICSBEP Handbook
 - case 45
 - $H/X=972$
 - 81.45 cm × 86.70 cm
× 88.22 cm



LEU-COMP-THERM-033-045

=CSAS5

LEU-COMP-THERM-033-045

v7.1-252

read comp

' U(2)F4-6

h-poly	6	0	6.0586E-02	300.0	END
--------	---	---	------------	-------	-----

f	6	0	1.2302E-02	300.0	END
---	---	---	------------	-------	-----

c	6	0	2.9128E-02	300.0	END
---	---	---	------------	-------	-----

u-235	6	0	6.2282E-05	300.0	END
-------	---	---	------------	-------	-----

u-238	6	0	3.0126E-03	300.0	END
-------	---	---	------------	-------	-----

u-234	6	0	6.2548E-07	300.0	END
-------	---	---	------------	-------	-----

end comp

read parameter end parameter ←

read geometry

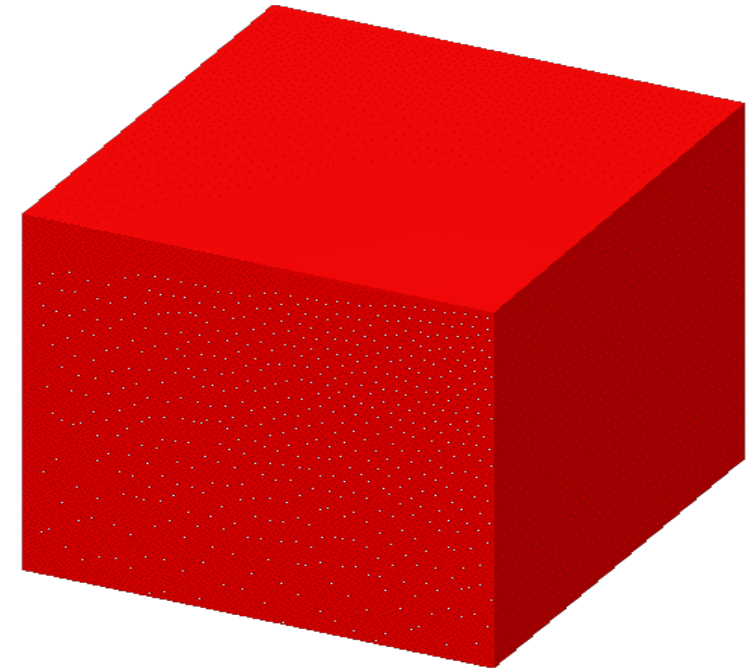
global unit 1

cuboid 6 1	40.725	-40.725	43.350	-43.350	44.110	-44.110
------------	--------	---------	--------	---------	--------	---------

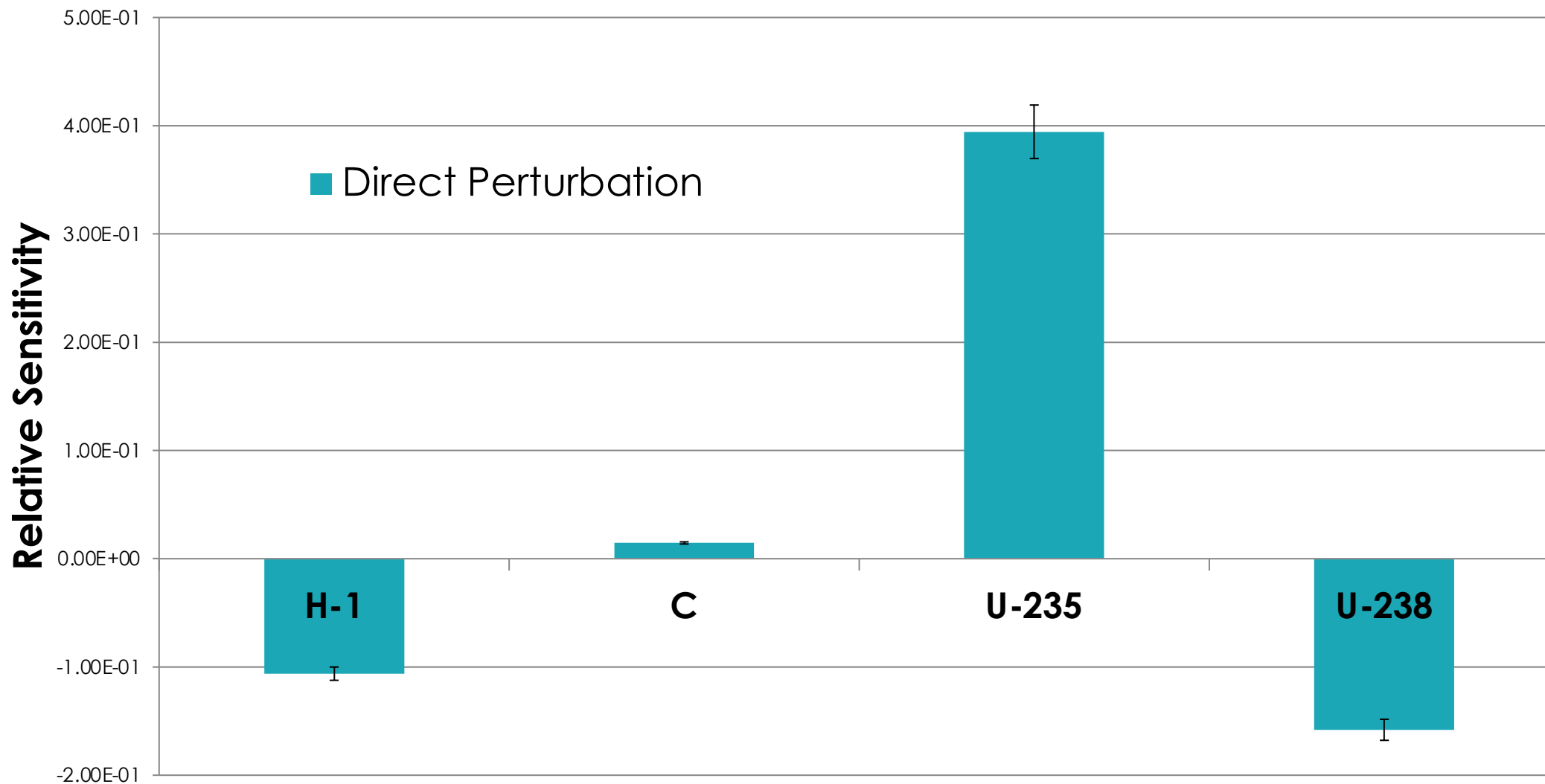
end geometry

end data

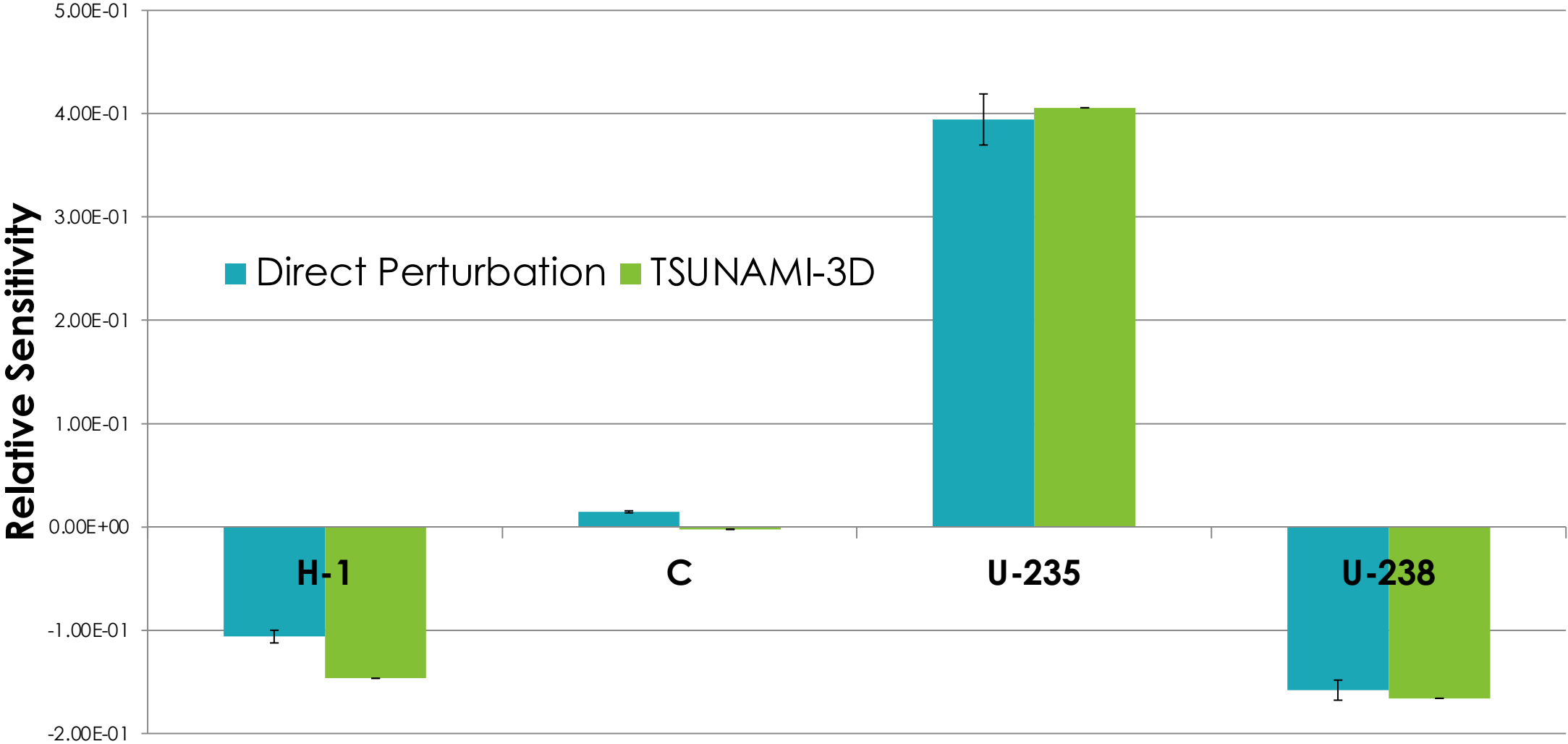
end



Reference sensitivity coefficients

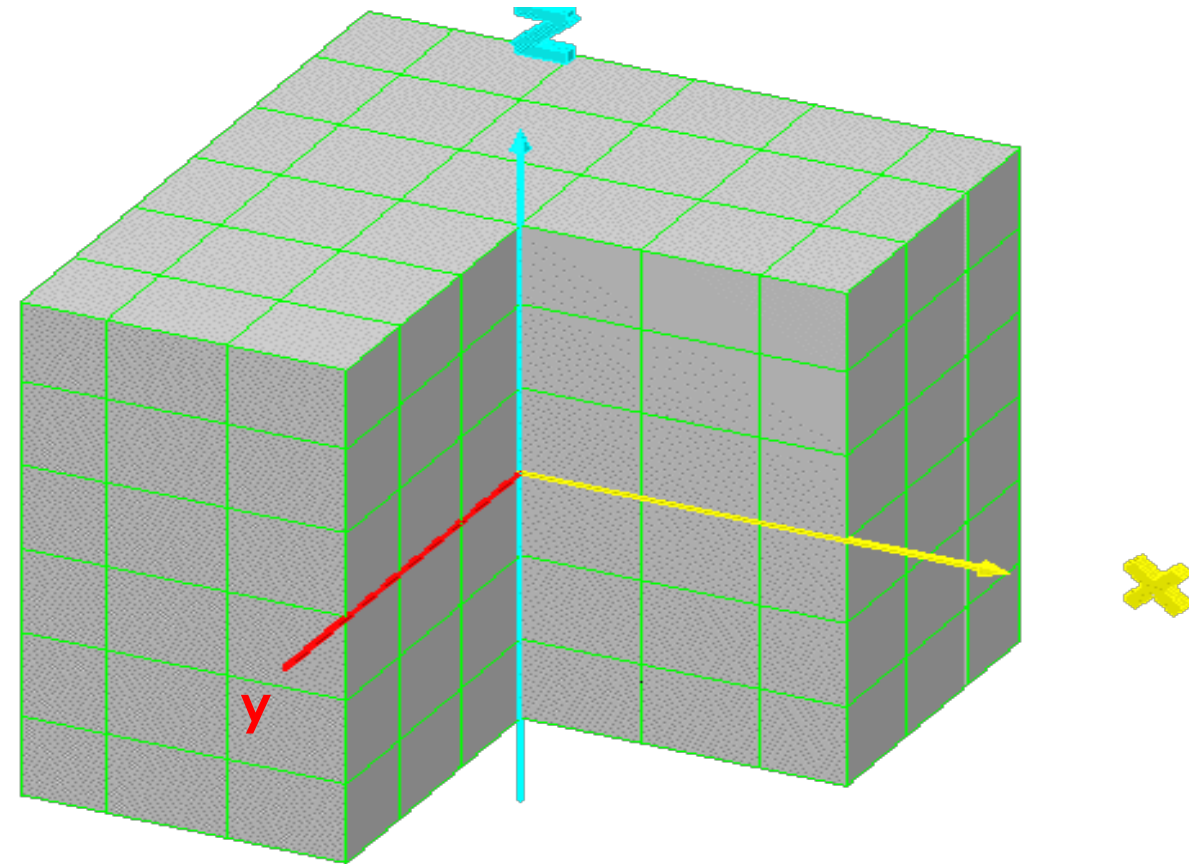
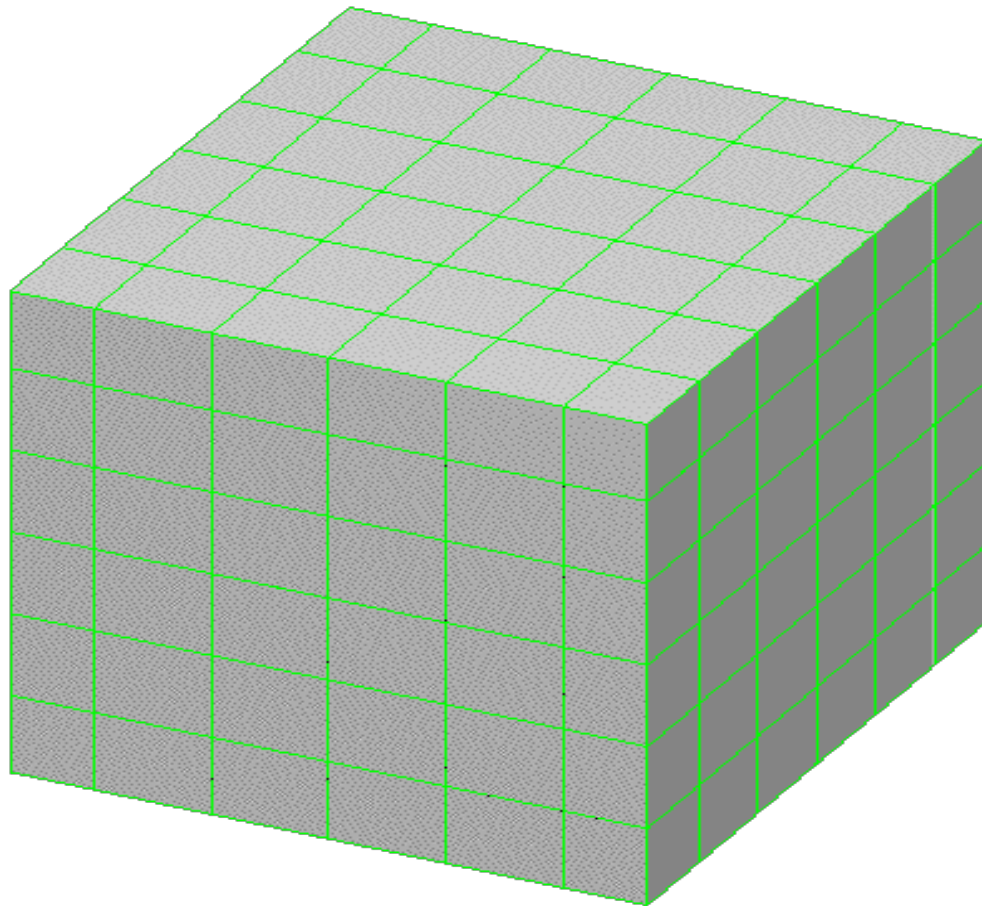


Sensitivity coefficient comparison



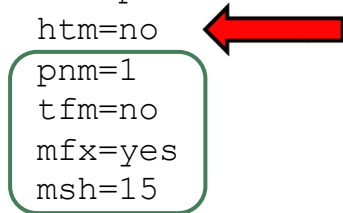
Sensitivity coefficient comparison

- Let's use an automated mesh to improve the spatially dependent flux solution

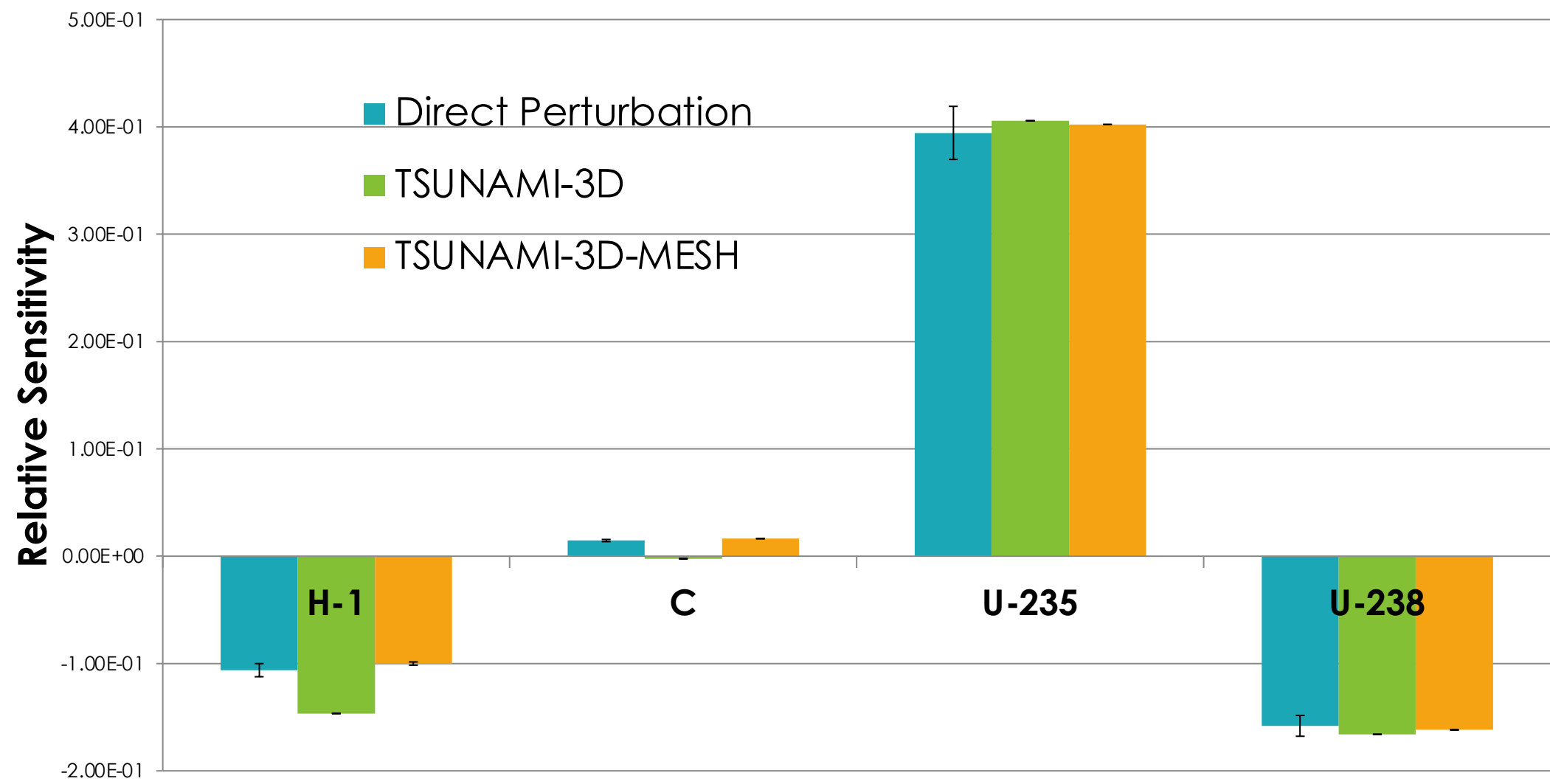


LEU-COMP-THERM-033-45: Enhanced input

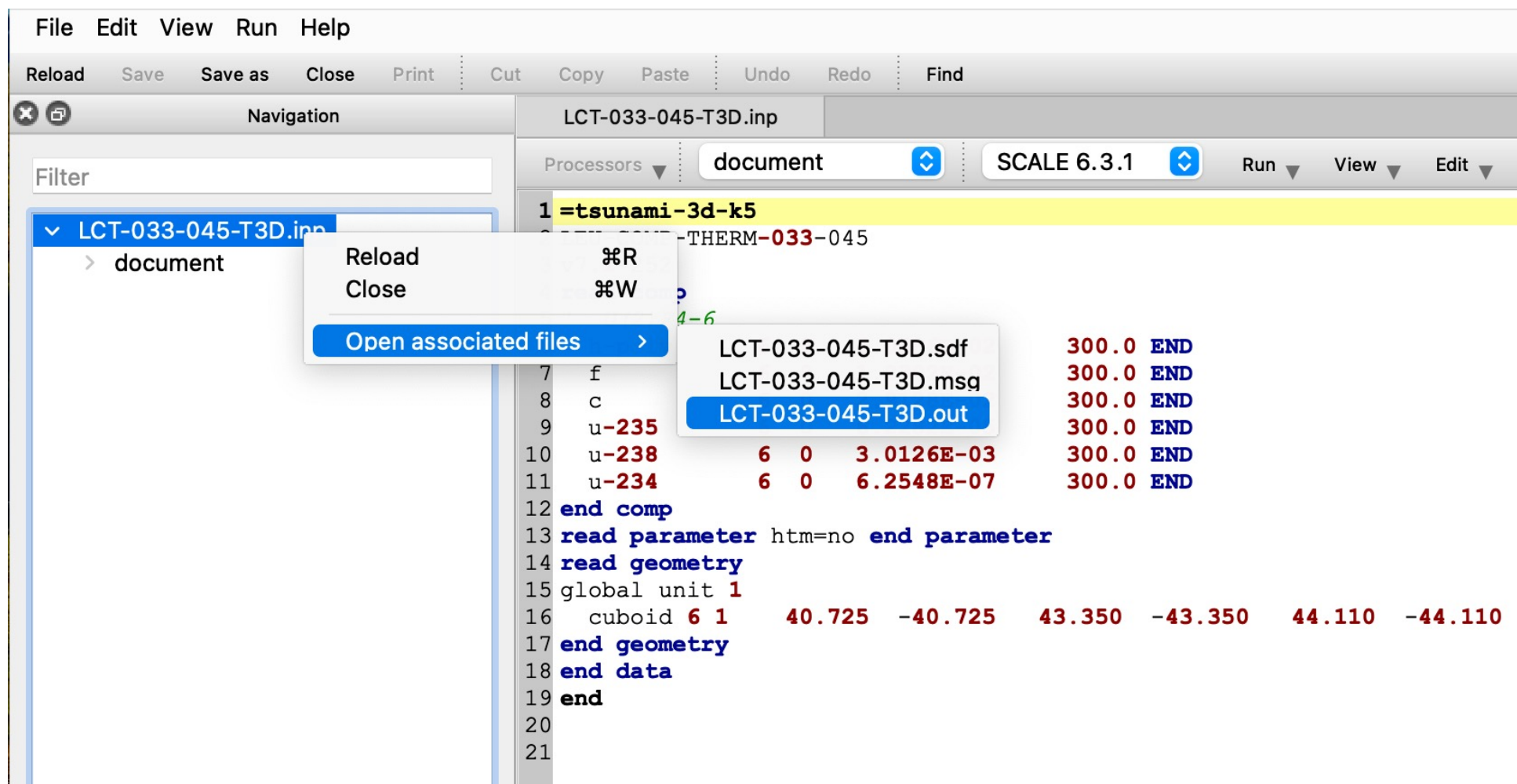
```
=tsunami-3d-k5
leu-comp-therm-033-045
v7.1-252
read composition
  h-poly      6 0 0.060586 300   end
  f           6 0 0.012302 300   end
  c           6 0 0.029128 300   end
  u-235       6 0 6.2282e-05 300   end
  u-238       6 0 0.0030126 300   end
  u-234       6 0 6.2548e-07 300   end
end composition
read parameter
  htm=no
  pnm=1
  tfm=no
  mfx=yes
  msh=15
end parameter
read geometry
global unit 1
  cuboid 6 1 40.725 -40.725 43.35 -43.35 44.11 -44.11
end geometry
end data
read sams
  makeimp
  prtimp
  usemom
end sams
end
```



Sensitivity coefficient comparison



Text output



Check k_{eff} results

```
1 *****
*** leu-comp-therm-033-045 ***
***
***          ***** final results table *****          ***
*** best estimate system k-eff          0.9940 + or - 0.0017 ***
*** Energy of average lethargy of Fission (eV) 5.13678E-02 + or - 4.78271E-05 ***
*** system nu bar 2.44390E+00 + or - 2.26600E-05 ***
*** system mean free path (cm) 5.61619E-01 + or - 1.79196E-04 ***
*** number of warning messages 7 ***
*** number of error messages 0 ***
*** k-effective satisfies the chi**2 test for normality at the 95 % level ***
***
*** there are 125 source meshes ***
*** source convergence tests failed ***
***
*****
```

```
*****
Congratulatory! You have successfully traversed the perilous path through KENO-V.a in 1.44267 minutes
*****
```

Forward Calculation

```
1 *****
*** leu-comp-therm-033-045 ***
***
***          ***** final results table *****          ***
*** best estimate system k-eff          0.994 + or - 0.017 ***
*** Energy of average lethargy of Fission (eV) 2.27579E-03 + or - 7.48153E-06 ***
*** system nu bar 1.99849E+00 + or - 6.78649E-03 ***
*** system mean free path (cm) 5.38069E-01 + or - 3.56783E-04 ***
*** number of warning messages 309 ***
*** number of error messages 0 ***
*** k-effective fails the chi**2 test for normality at the 99 % level ***
***
*** there are 125 source meshes ***
*** source convergence tests failed ***
***
*****
```

```
*****
Congratulatory! You have successfully traversed the perilous path through KENO-V.a in 8.23567 minutes
*****
```

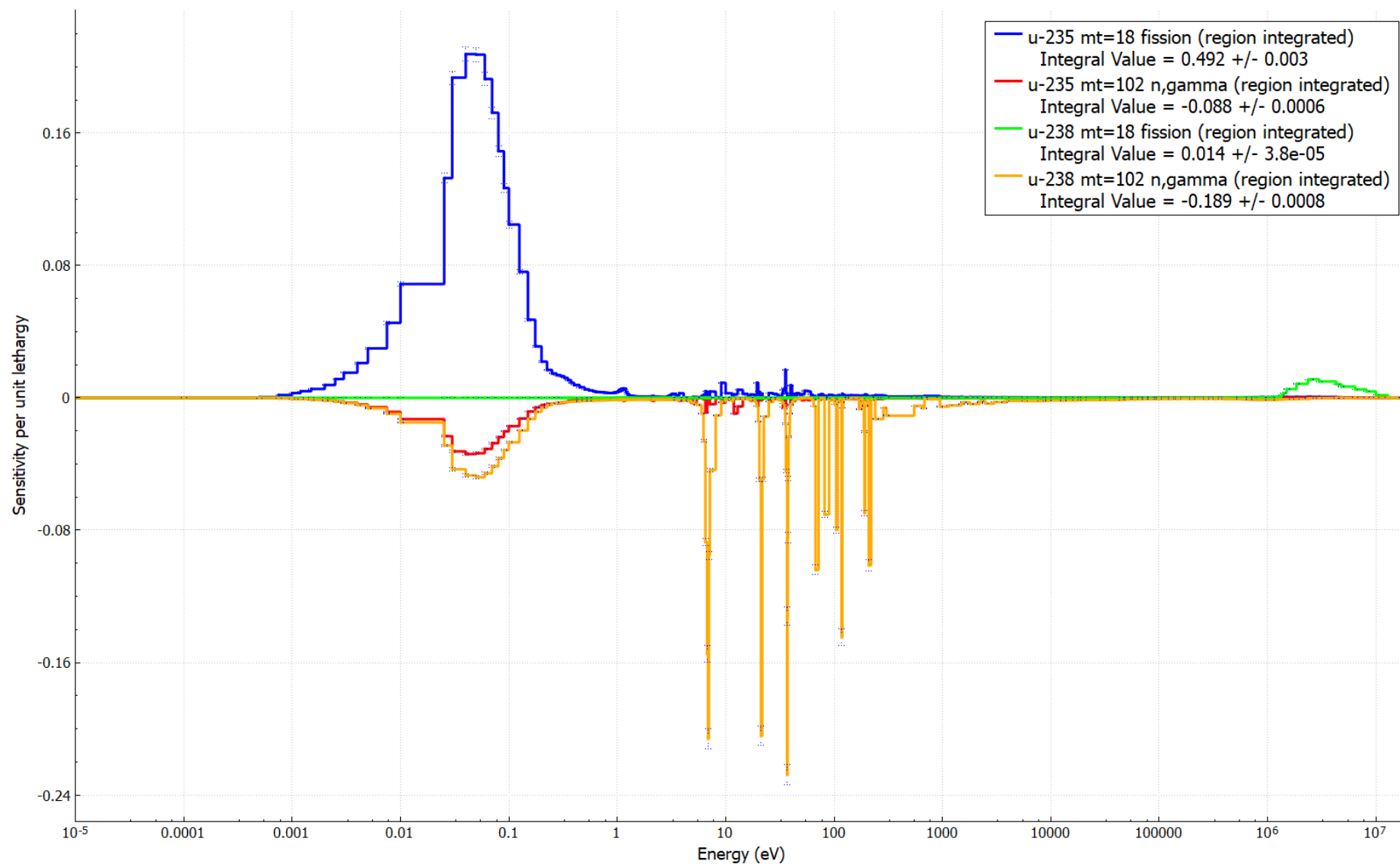
Adjoint Calculation

Check sensitivity results

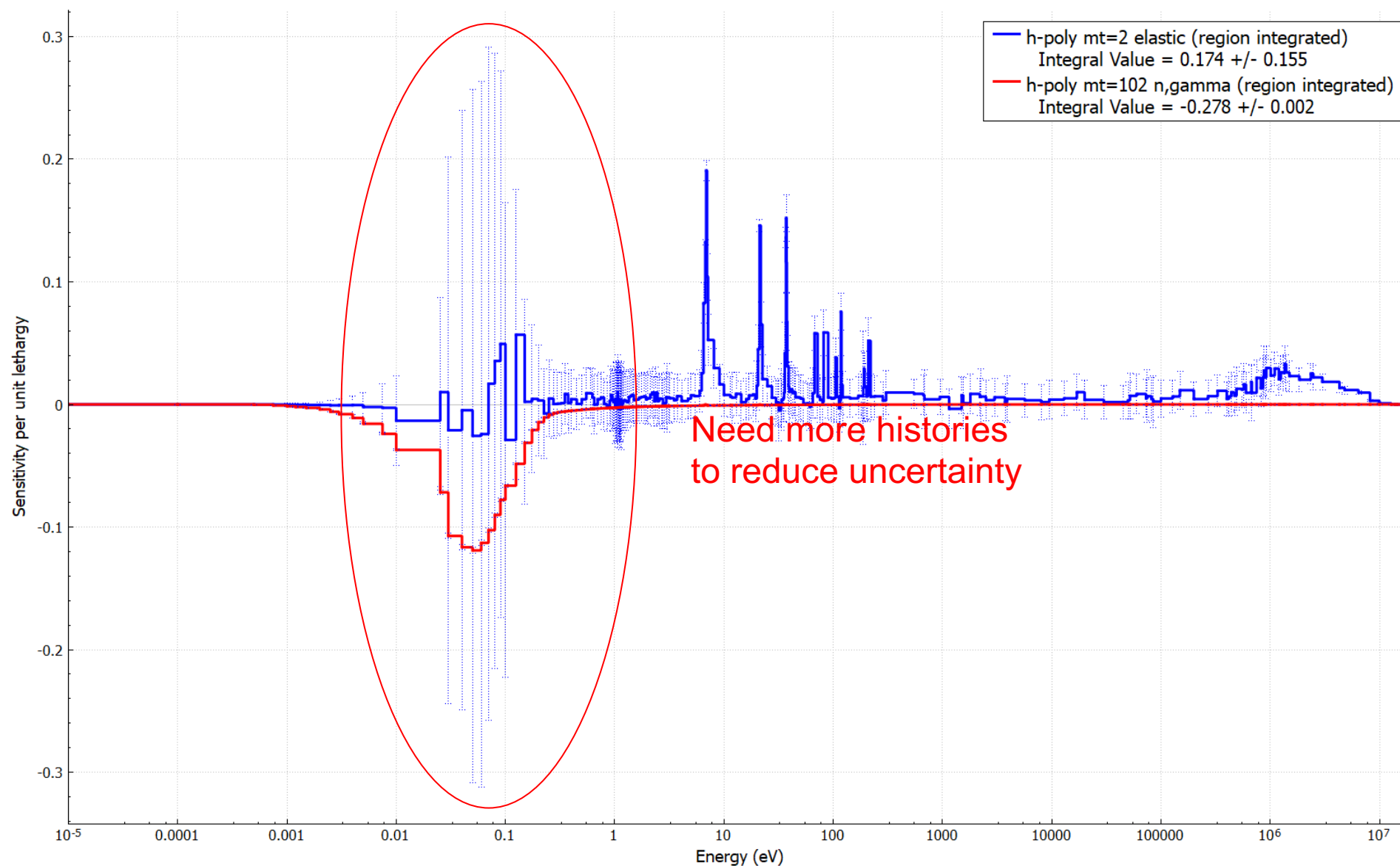
Total Sensitivity Coefficients by Nuclide

Mixture	Nuclide	Atom Density	Sensitivity	Std. Dev. %	Std. Dev.	
6	c	2.9128E-02	1.5518E-02 +/-	9.7536E-03	(62.85%)	
6	f-19	1.2302E-02	6.9213E-03 +/-	3.1659E-03	(45.74%)	
6	u-234	6.2548E-07	-1.1160E-03 +/-	7.1583E-06	(0.64%)	
6	u-235	6.2282E-05	4.0177E-01 +/-	3.7445E-03	(0.93%)	D.P. Value ~0.4
6	u-238	3.0126E-03	-1.5870E-01 +/-	1.5579E-03	(0.98%)	
6	h-poly	6.0586E-02	-1.0184E-01 +/-	1.4640E-01	(143.76%)	D.P. Value ~ -0.1

Energy-dependent sensitivities: ^{235}U and ^{238}U



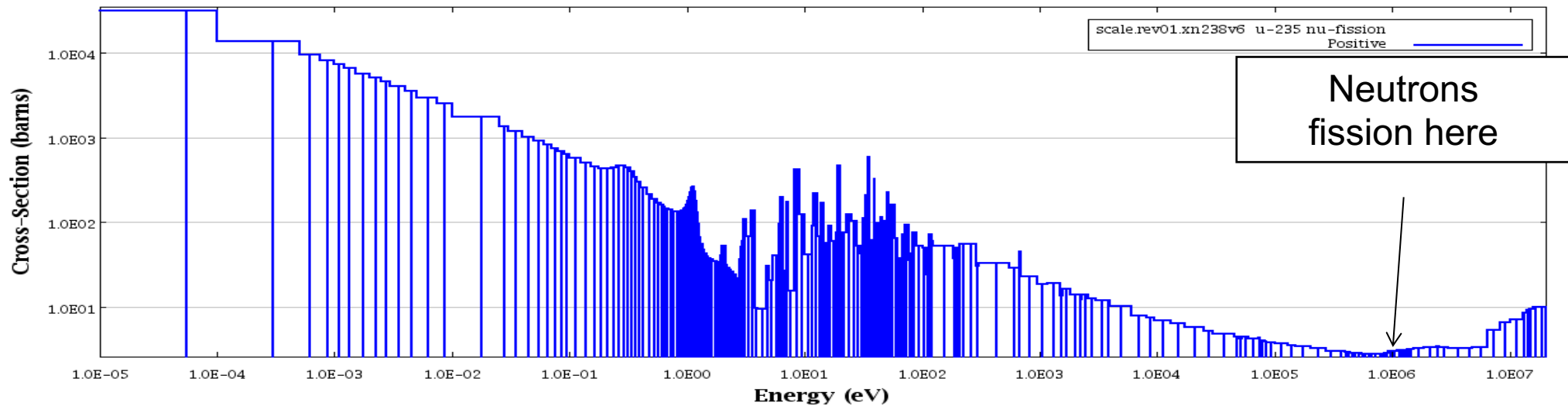
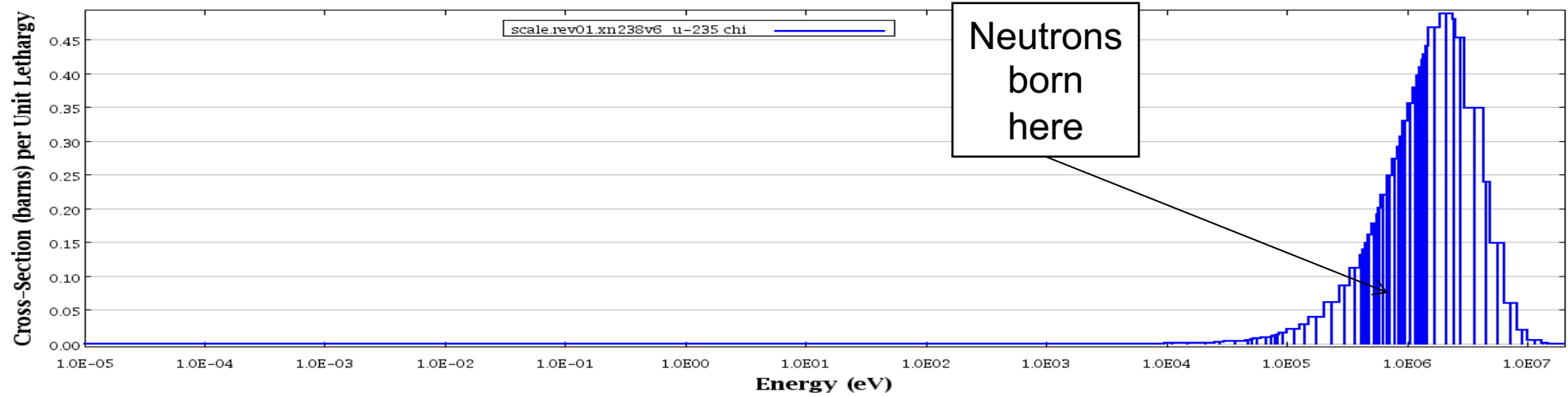
Energy-dependent sensitivities: ^1H



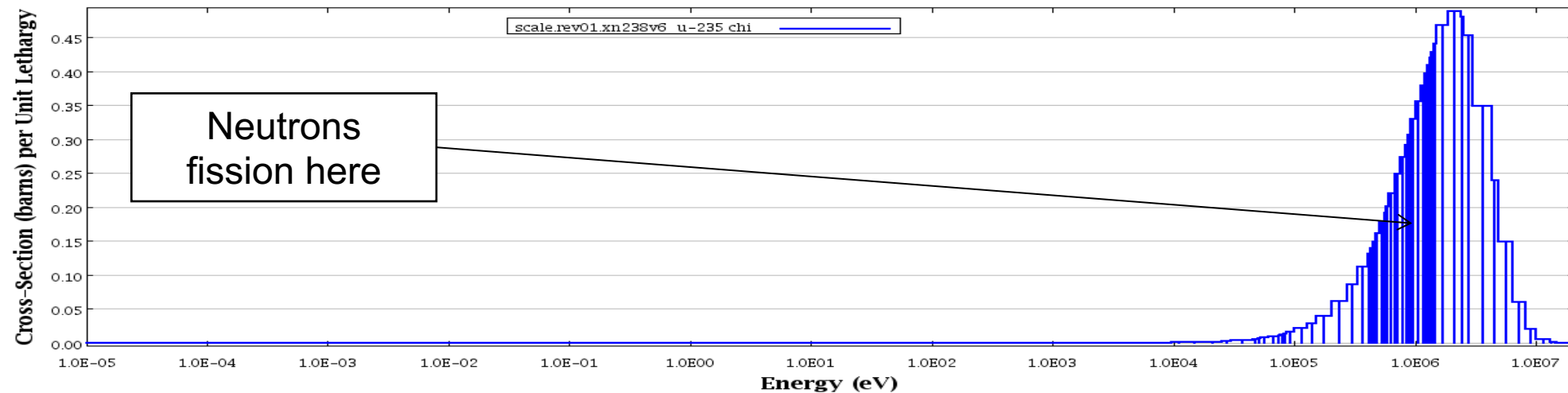
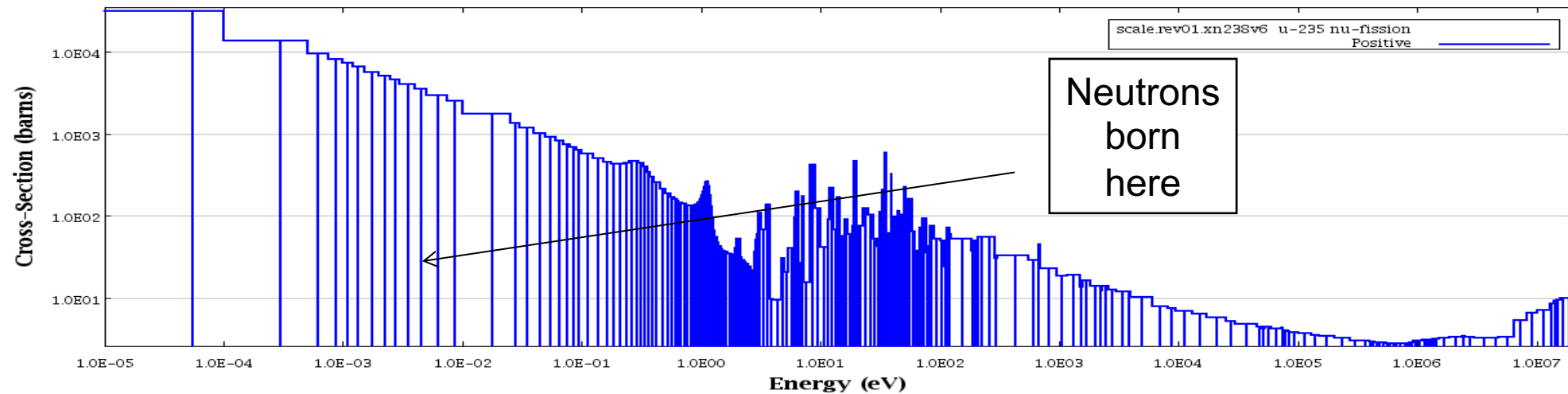
Solving the adjoint transport equation with MG Monte Carlo

- Adjoint solution is much more difficult with multigroup Monte Carlo than forward solution
 - Energy distributions from χ and fission cross sections are interchanged
 - Scattering matrix is inverted
- Neutrons are born per distribution of σ_f and must scatter to χ

Forward calculation for fast system



Adjoint calculation for fast system



Adjoint solution strategies

- Increase the number of particles per generation for adjoint solution (apg=) for intermediate and fast spectra systems
 - Default apg= 3 x NPG
- KENO will stop running due to lack of fission source in the system
- Check k_{eff} results to ensure that forward and adjoint solutions agree ($\Delta k < 0.01$)
- Lady Godiva problem: minimum apg=15000 to allow system to run

Multigroup TSUNAMI-3D recipe

- Start with CSAS5/CSAS6 model
- Change sequence to TSUNAMI-3D-K5/K6
- Consider special circumstances in resonance self-shielding for TSUNAMI analysis, especially for non-fuel materials
- Add TSUNAMI parameters to the *Parameter* block (apg, agn, asg, ask, mfx, msh)
 - Define flux mesh with *Grid* block if not using a uniform mesh (MSH=)
 - With mesh flux on, set tfm=no to disable the coordinate transform
- Execute TSUNAMI-3D
- Test with direct perturbations
- Examine results with Fulcrum

Appendix

- Equations and details for the interested attendee



Perturbation theory

Recall that sensitivity coefficients are computed from the product of forward and adjoint flux and its angular moments

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

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

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.

Spatial refinement of flux solutions

- Perturbation theory requires the product of the forward and adjoint flux moment solutions
- This is a sum-of-the-products quantity

Sum of products (correct)

$$P_{g,g',z}^{\ell} = \sum_j \left(\sum_{r \in Z} \tilde{\phi}_{g',r}^{\dagger j} \tilde{\phi}_{g,r}^j \right)$$

Product of sums (incorrect)

$$P_{g,g',z}^{\ell} = \sum_j \left(\sum_{r \in Z} \tilde{\phi}_{g',r}^{\dagger j} \sum_{r \in Z} \tilde{\phi}_{g,r}^j \right)$$

Calculation of flux moments

- Deterministic codes calculate flux moments from the angular flux over a fine mesh as

$$\tilde{\phi}_{g,z}^j = \sum_{n=1}^N w_n R_n^j \phi_{g,z}^n$$

w = angular weight; R = spherical harmonics; n = direction;

j = moment index (order); z = region; g = energy group

Flux moments in Monte Carlo

- Scalar fluxes are computed in Monte Carlo codes from a track length estimator

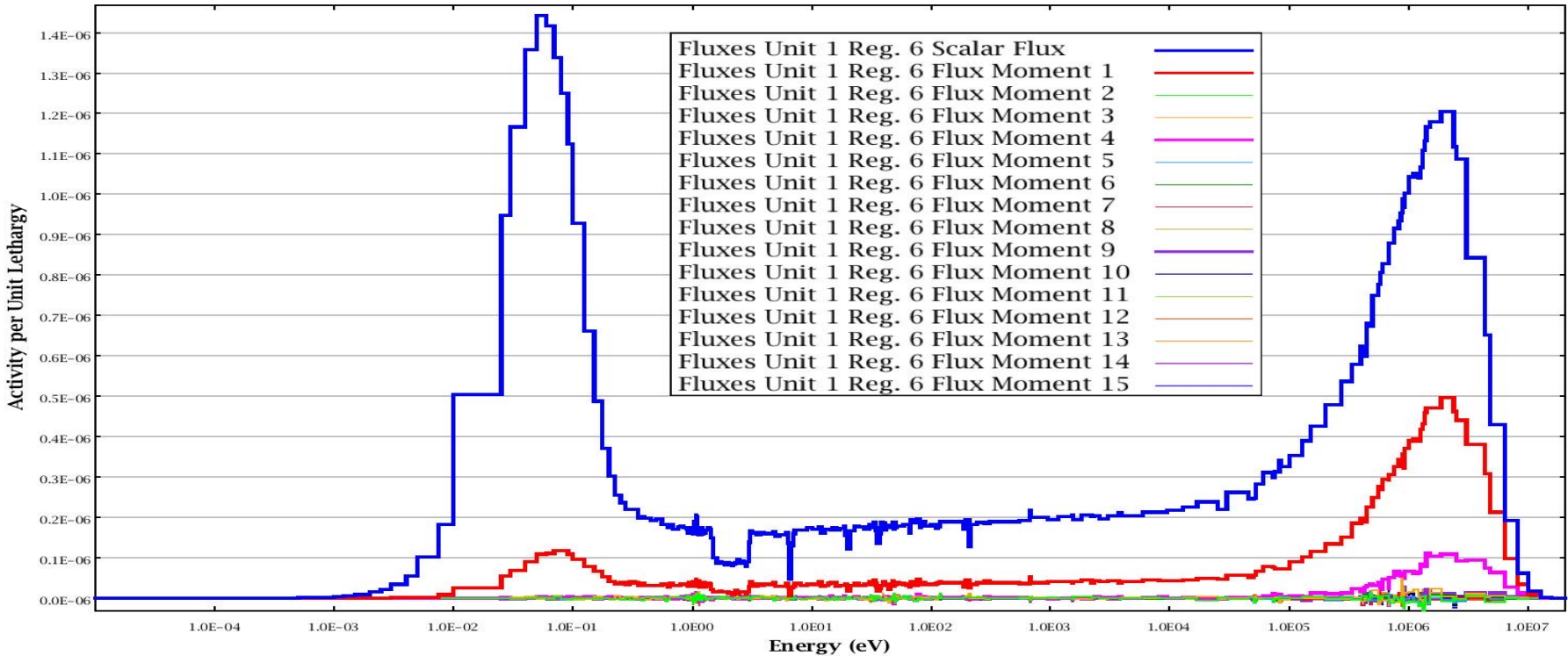
$$\phi_{g,z} = \frac{\sum_{k=1}^K wt_{k,z} l_{k,z}}{V_z \sum_{k=1}^K wt_{k,0}}$$

l = track length of neutron
 wt = neutron weight
 k = neutron number
 V = volume

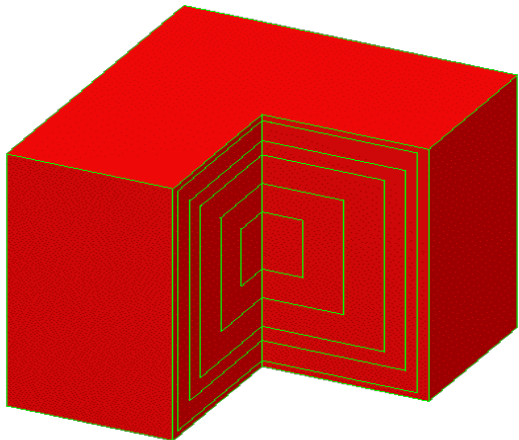
- KENO V.a track-length estimator for angular flux moments:

$$\tilde{\phi}_{g,z}^j = \frac{\sum_{k=1}^K R_k^j wt_{k,z} l_{k,z}}{V_z \sum_{k=1}^K wt_{k,0}}$$

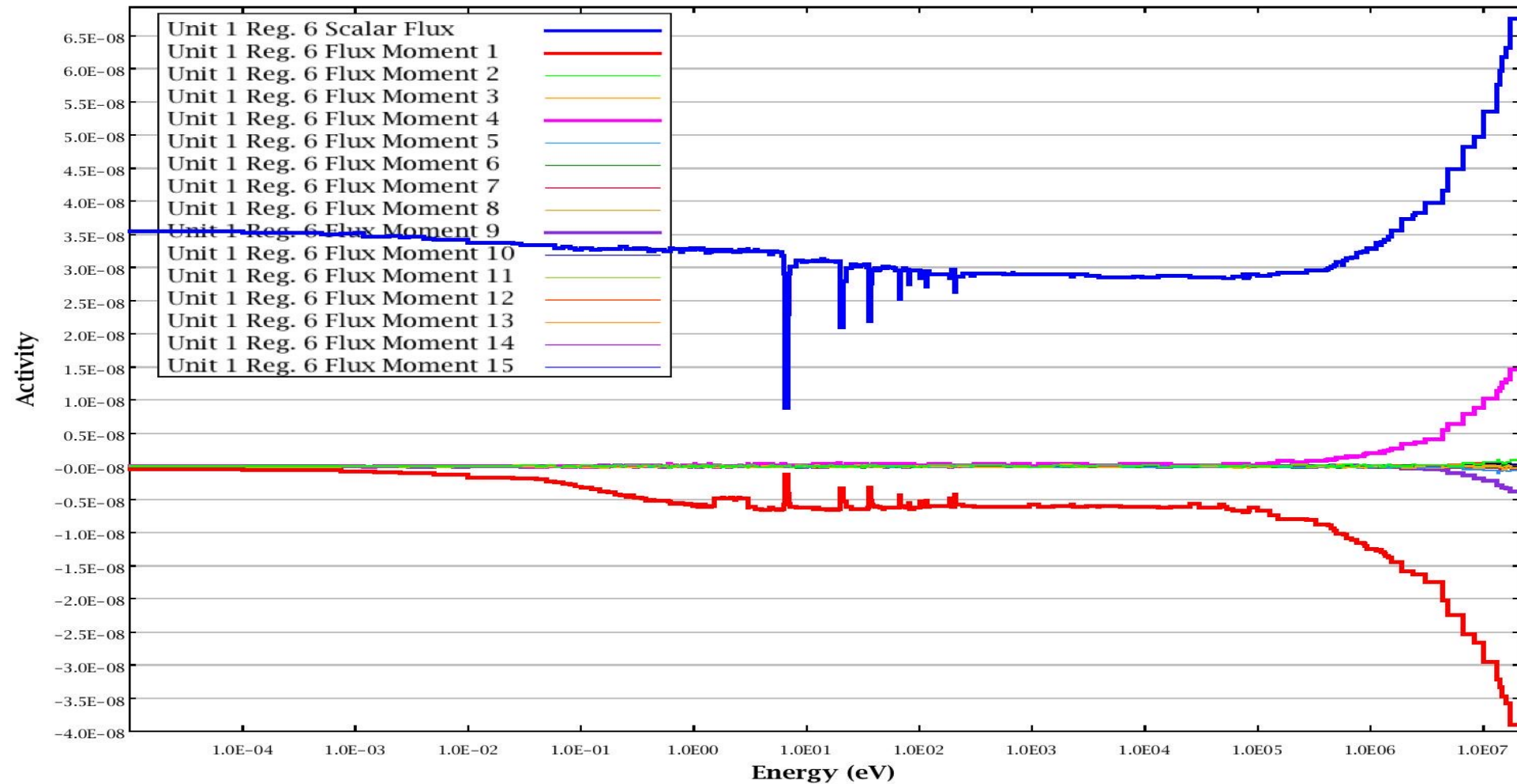
Flux moments in outer ~1 cm of ~80 cm moderated UF₄ critical cube

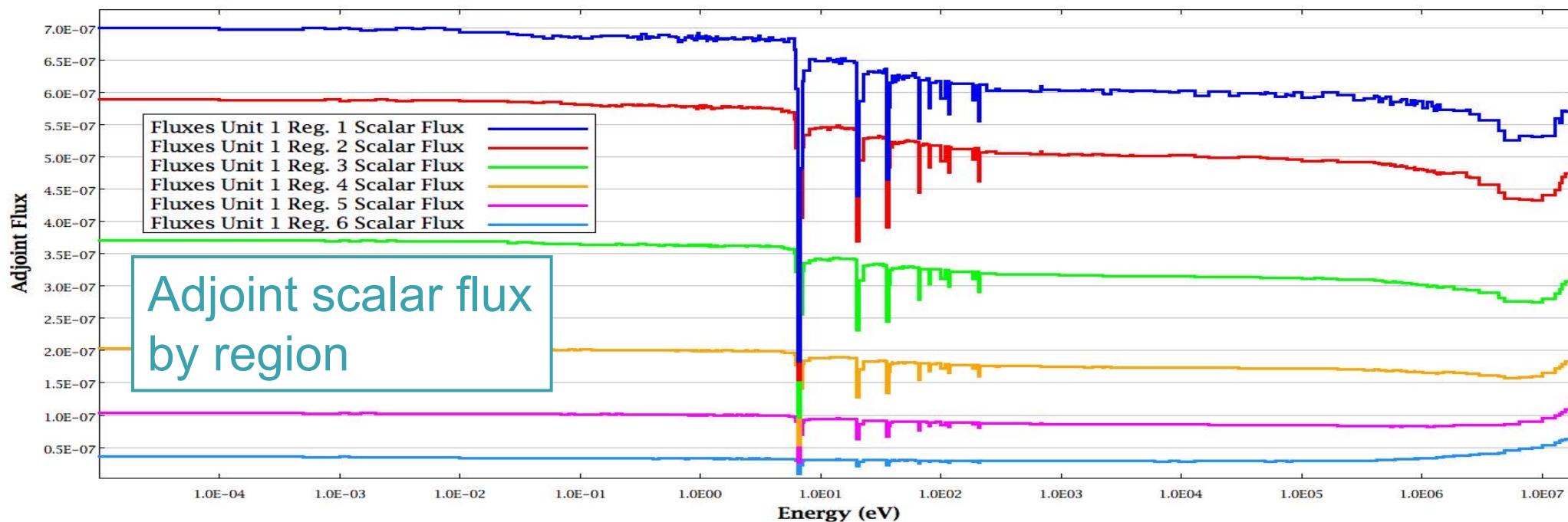
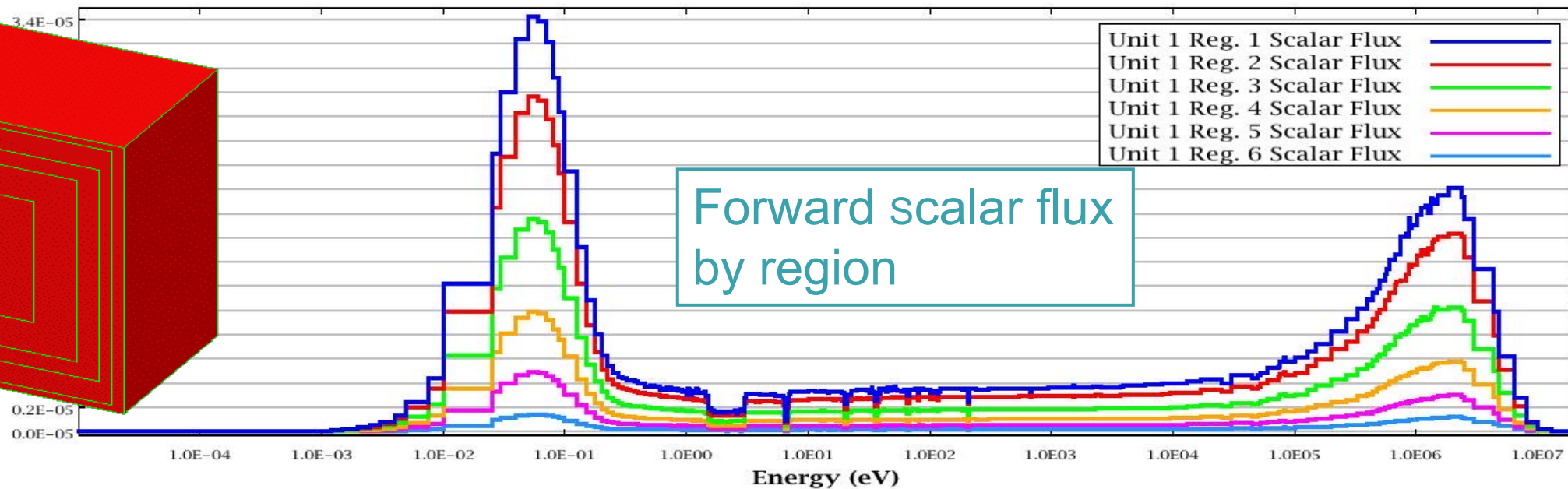
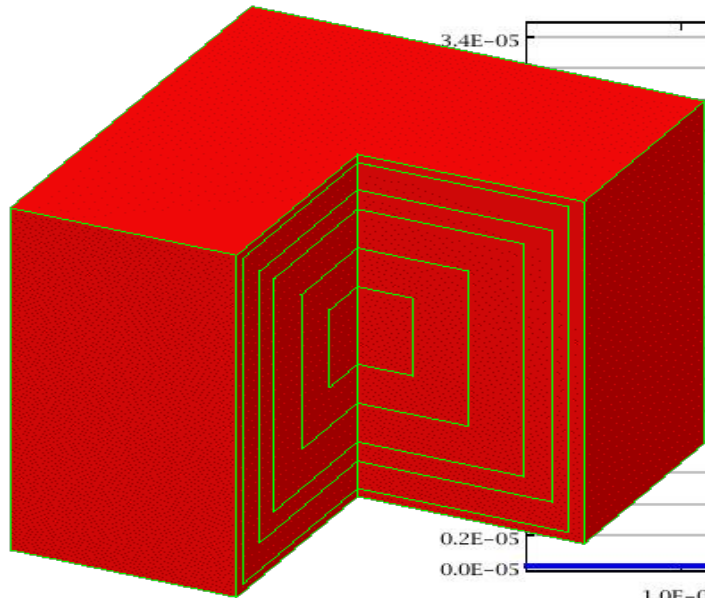


Real-valued Spherical Harmonics Functions		
j	ℓ	$R_j(\hat{\Omega})$
0	0	1
1	1	$\cos \theta$
2	1	$-\sin \theta \cos \rho$
3	1	$-\sin \theta \sin \rho$
4	2	$\frac{1}{2}(3\cos^2 \theta - 1)$
5	2	$-\frac{\sqrt{3}}{3} 3 \sin \theta \cos \theta \cos \rho$
6	2	$-\frac{\sqrt{3}}{3} 3 \sin \theta \cos \theta \sin \rho$
7	2	$\frac{\sqrt{3}}{6} \sin^2 \theta \cos(2\rho)$
8	2	$\frac{\sqrt{3}}{6} \sin^2 \theta \sin(2\rho)$
9	3	$\frac{1}{2}(3\cos^3 \theta - 3\cos \theta)$
10	3	$-\frac{3\sqrt{6}}{12} \sin \theta (5\cos^2 \theta - 1) \cos \rho$
11	3	$-\frac{3\sqrt{6}}{12} \sin \theta (5\cos^2 \theta - 1) \sin \rho$
12	3	$\frac{\sqrt{15}}{2} \sin^2 \theta \cos \theta \cos(2\rho)$
13	3	$\frac{\sqrt{15}}{2} \sin^2 \theta \cos \theta \sin(2\rho)$
14	3	$-\frac{\sqrt{10}}{4} \sin^3 \theta \cos(3\rho)$
15	3	$-\frac{\sqrt{10}}{4} \sin^3 \theta \sin(3\rho)$



Adjoint flux in outer region





Continuous-energy TSUNAMI-3D

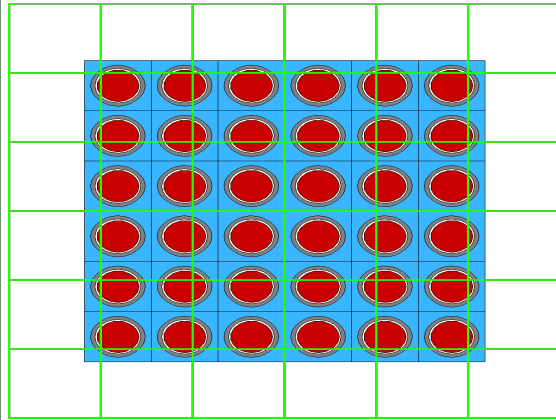


Objectives

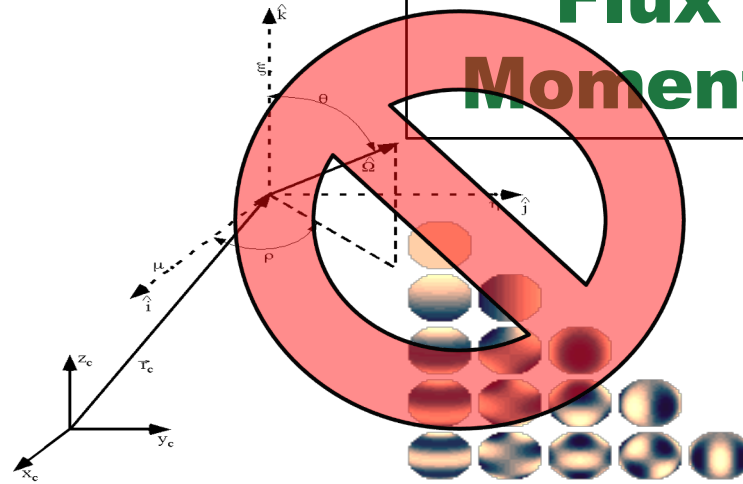
- Survey adjoint-based sensitivity theory for continuous-energy (CE) Monte Carlo eigenvalue sensitivity calculations
- Understand differences between MG and CE TSUNAMI methods
- Examine CE TSUNAMI-3D input options
- Perform example calculation

Some differences between MG and CE TSUNAMI-3D calculations:

Spatial Flux Mesh

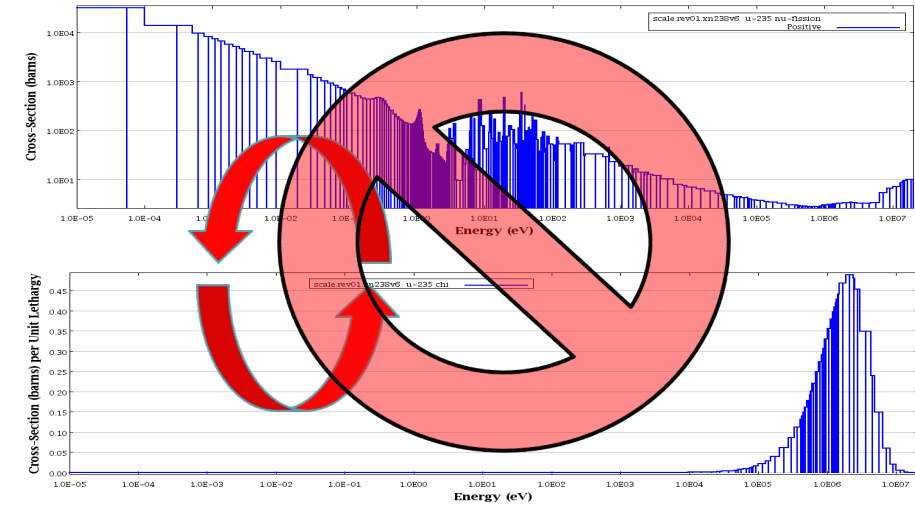


Flux Moments



 The image part with relationship ID rld4 was not found in the file.

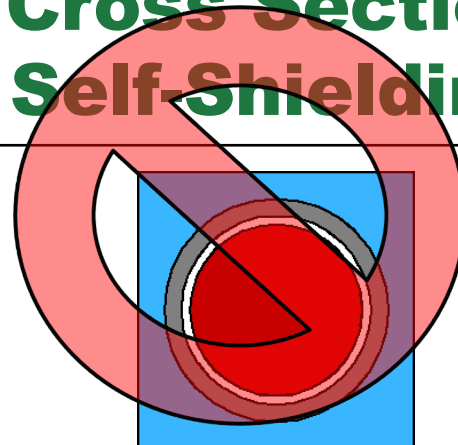
Separate Adjoint Transport Solution



Volume Calculations

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

Cross Section Self-Shielding



Expert Judgment



Why use CE?

- CE TSUNAMI-3D uses Monte Carlo to calculate sensitivity coefficients and does not require:
 - Flux moment calculations
 - Volume calculations
 - Problem-dependent cross section self-shielding or implicit sensitivity effects
 - Adjoint transport simulation
 - One method does not require a spatial mesh
- CE TSUNAMI-3D can avoid the large memory footprints that can be required by MG TSUNAMI-3D
- Use of CE physics more accurately models the physics of neutron interactions

Why NOT use CE?

- Simulation runtimes are usually longer for CE TSUNAMI-3D than those for MG TSUNAMI-3D
 - MG TSUNAMI-3D is generally more efficient (high figure of merit) than CE TSUNAMI-3D for thermal systems
- In many applications, multigroup TSUNAMI-3D calculations already provide sufficient accuracy
- CE calculations may still require a spatial mesh, large computational memory, and/or expert judgment

CE TSUNAMI-3D sensitivity methods

Eigenvalue Sensitivity Calculations

- **CLUTCH Method** (cet=1)
 - Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization
 - Available only with KENO V.a and KENO-VI
- **IFP Method** (cet=2)
 - Iterated Fission Probability
 - Available with KENO V.a, KENO-VI, and Shift

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

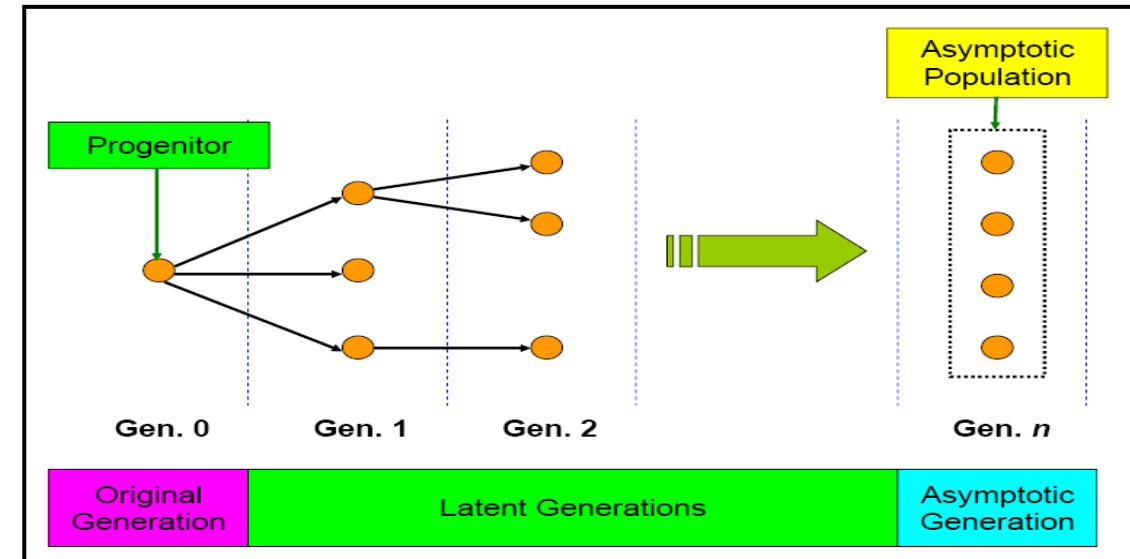


Illustration of the IFP process. Image courtesy of Brian Kiedrowski.

How many latent generations do we need?

- IFP calculations should use somewhere between 2 and 20 latent generations to obtain accurate sensitivities
 - In practice, most simulations require between 5 and 10 latent generations
- Memory footprint of SCALE IFP calculations increases 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
 - Shift's IFP implementation is realized with MPI support, and the memory footprint is spread across a node
 - Confirm results with direct perturbations!

Let's try CE TSUNAMI-3D

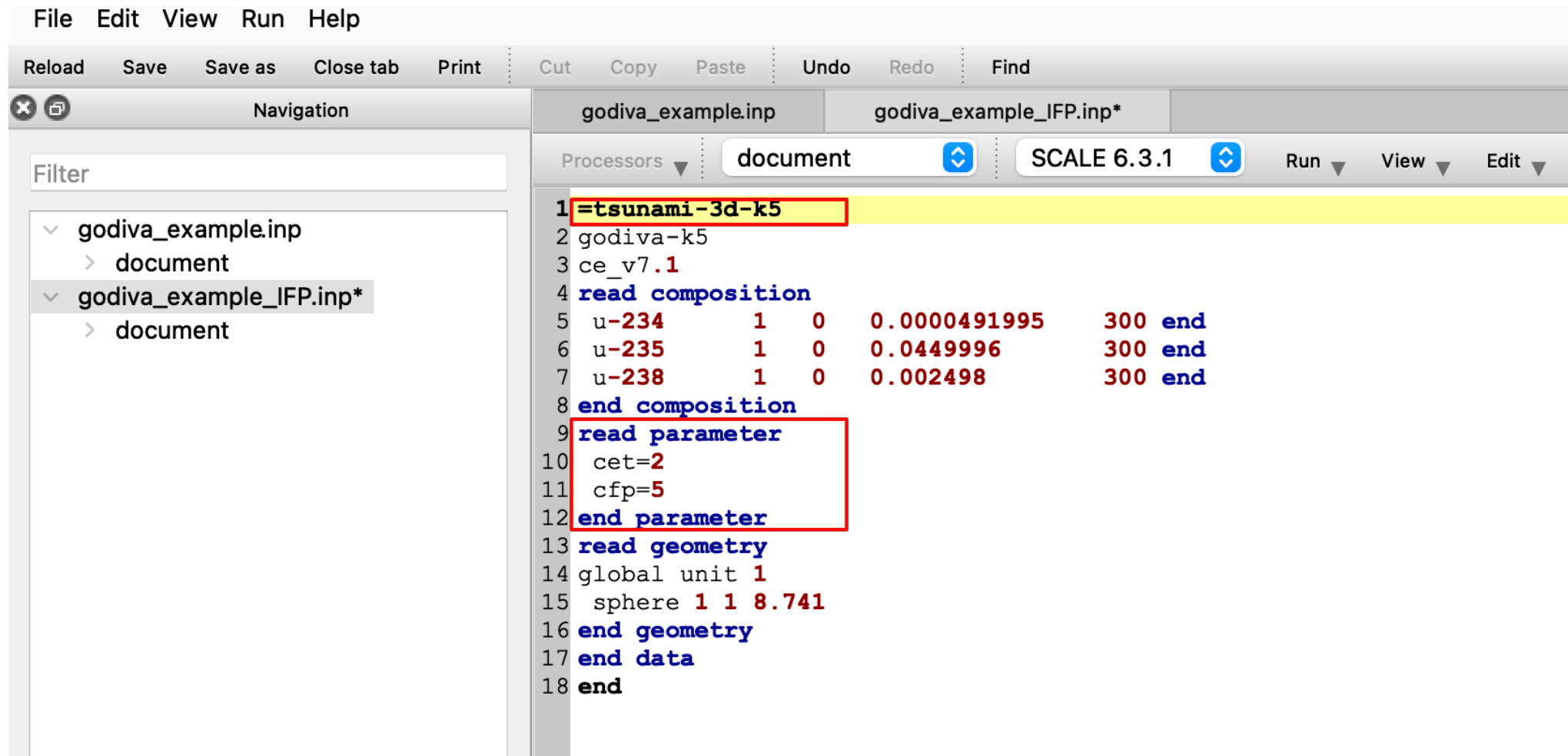
- Open the file:
workshops → class_demo → godiva_example.inp
- Add the CE TSUNAMI-3D parameters:
 - cet=2 (Enables the IFP method)
 - cfp=5 (Sets the number of latent generations to 5)

Let's try CE TSUNAMI-3D

The screenshot shows the SCALE 6.3.1 software interface. The top menu bar includes File, Edit, View, Run, and Help. Below this is a toolbar with buttons for Reload, Save, Save as, Close tab, Print, Cut, Copy, Paste, Undo, Redo, and Find. The main window is divided into two panes. The left pane, titled 'Navigation', shows a tree view with 'godiva_example.inp' expanded, revealing a sub-entry 'document'. The right pane displays the contents of 'godiva_example.inp' in a text editor. The text is as follows:

```
1 =csas5
2 godiva-k5
3 ce_v7.1
4 read composition
5 u-234      1  0  0.0000491995  300 end
6 u-235      1  0  0.0449996    300 end
7 u-238      1  0  0.002498     300 end
8 end composition
9 read geometry
10 global unit 1
11 sphere 1 1 8.741
12 end geometry
13 end data
14 end
15
```

Let's try CE TSUNAMI-3D



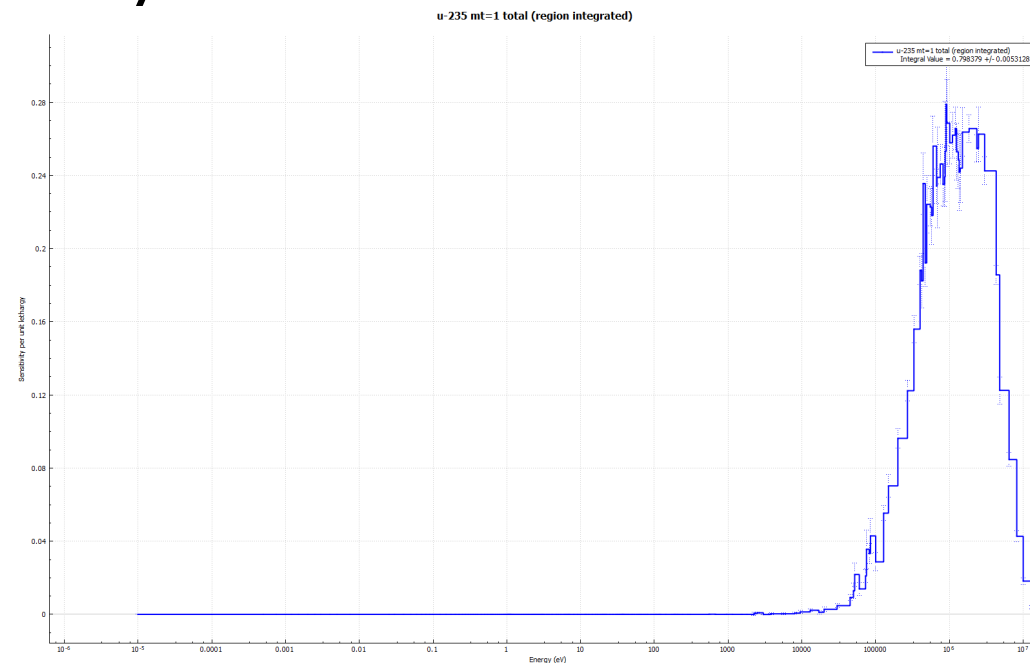
The screenshot shows the SCALE 6.3.1 interface. The left sidebar displays a file tree with 'godiva_example.inp' and 'godiva_example_IFP.inp*'. The main editor window shows the input file 'godiva_example_IFP.inp*' with the following content:

```
1 =tsunami-3d-k5
2 godiva-k5
3 ce_v7.1
4 read composition
5 u-234 1 0 0.0000491995 300 end
6 u-235 1 0 0.0449996 300 end
7 u-238 1 0 0.002498 300 end
8 end composition
9 read parameter
10 cet=2
11 cfp=5
12 end parameter
13 read geometry
14 global unit 1
15 sphere 1 1 8.741
16 end geometry
17 end data
18 end
```

Two sections are highlighted with red boxes: the first line '1 =tsunami-3d-k5' and the parameter block from line 9 to 12.

Let's try CE TSUNAMI-3D

- Run your input and then open the SDF
 - Right click on input in navigation panel in Fulcrum → open associated files → `godiva_example_IFP.sdf`
- Examine sensitivity coefficients:



IFP method memory requirements

- IFP frequently results in accurate sensitivity coefficients but requires large memory footprints and long runtimes
- A model of a typical pressurized water reactor spent nuclear fuel storage configuration with depleted isotopics might require as much as **706 GB** of memory with CFP=5
- IFP-Shift helps to reduce this requirement by taking advantage of its parallel computing capability

CE TSUNAMI-3D sensitivity methods

Eigenvalue Sensitivity Calculations

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

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:

$$\boxed{\phi^*(\tau_S)} = \int_V G(\tau_S \rightarrow r) F^*(r) dr,$$

Neutron
importance

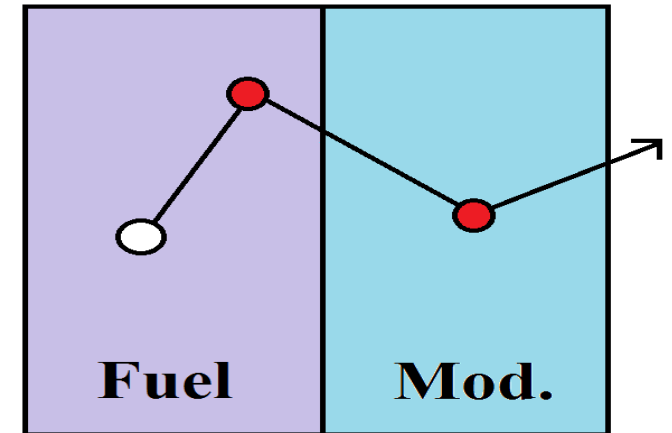
where:

$G(\tau_S \rightarrow r)$ = 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:

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

Adjoint flux

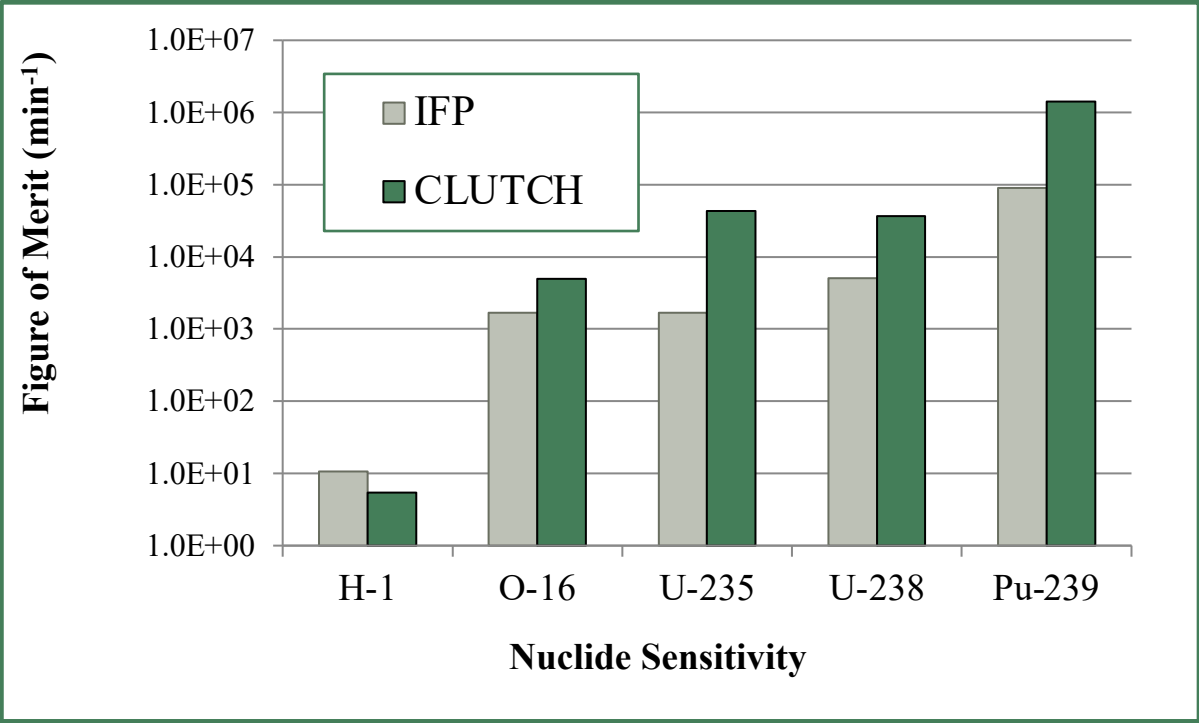


CLUTCH memory requirements

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

CLUTCH vs. IFP

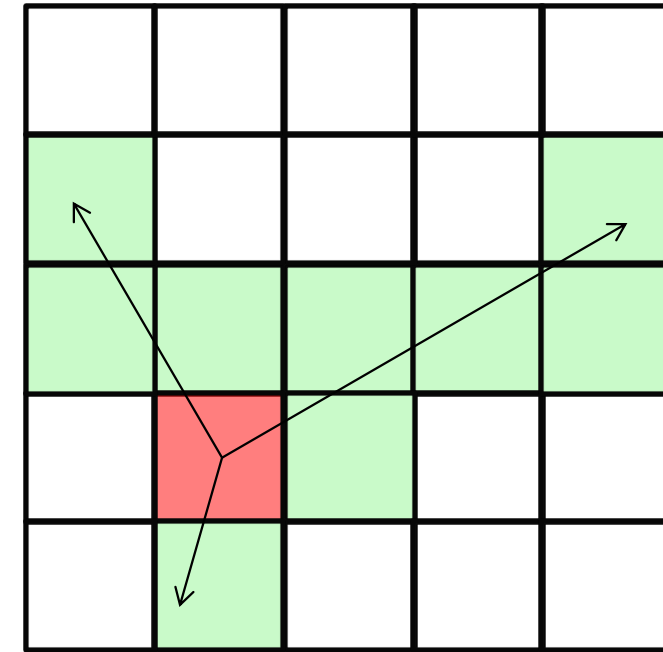
- The CLUTCH method is more efficient than IFP (both in terms of speed and memory usage)
- CLUTCH downside: $F^*(r)$ must be computed



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
- The $F^*(r)$ function can be calculated using the IFP method during inactive generations with no significant loss of accuracy and with significant memory savings
 - This requires a significant increase in the number of inactive generations: up to hundreds or more



Best practices for $F^*(r)$ mesh generation

- Experience has shown that an $F^*(r)$ mesh with 1–2 cm intervals often yields accurate sensitivity coefficients
 - Much larger meshes have been used successfully in some applications
- The $F^*(r)$ mesh must cover all regions in a problem containing **fissionable** material
- The $F^*(r)$ function is tallied during skipped generations, so NSK must be adjusted to allow for $F^*(r)$ convergence
 - In general, simulating between 1 and 100 inactive particle histories per $F^*(r)$ mesh interval will produce an accurate $F^*(r)$ tally
 - Lady Godiva with a 1 cm cubic mesh has 5,832 intervals ($18 \times 18 \times 18$)
 - 5,832 mesh intervals $\times$ 100 histories per interval / 1,000 particles per gen. = ~580 skipped generations

Uncertainty in $F^*(r)$ function

- Distribution of uncertainties in $F^*(r)$ function is provided

$F^*(r)$ Convergence Statistics:

```
WARNING: Of the      1170  $F^*(r)$  mesh intervals that scored tallies...  
    40.51% of the  $F^*(r)$  tallies contain more than 5% uncertainty;  
    26.50% of the  $F^*(r)$  tallies contain more than 10% uncertainty;  
    13.33% of the  $F^*(r)$  tallies contain more than 20% uncertainty; and  
     3.08% of the  $F^*(r)$  tallies contain more than 50% uncertainty.
```

- No reliable correlation has been established between the uncertainty distribution and the accuracy of CLUTCH-calculated sensitivity coefficients
- It may be essentially impossible to generate an accurate $F^*(r)$ function for a fissionable reflector

Best practices for $F^*(r)$ mesh generation

- Setting the FST=yes parameter will produce a .3dmap file showing the $F^*(r)$ function that was calculated
- The convergence summary of the $F^*(r)$ function is printed as a warning message at the end of the table of generations

```
SCALE
File Edit View Run Help
Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find
Navigat... godiva_example_CLUTCH.inp godiva_example_CLUTCH_improved.inp godiva_example_CLUTCH_improved.out
Filter
godiva_e
> docu
godiva_e
> docu
godiva_e
1627 996 9.94089E-01 1.00013E+00 1.23867E-03 6.12178E+00 0.00000E+00 0.00000E+00
1628 997 1.01021E+00 1.00015E+00 1.23601E-03 6.09216E+00 0.00000E+00 0.00000E+00
1629 998 9.84993E-01 1.00012E+00 1.23243E-03 6.13806E+00 0.00000E+00 0.00000E+00
1630 999 9.65236E-01 1.00005E+00 1.23283E-03 6.13328E+00 0.00000E+00 0.00000E+00
1631 1000 1.01908E+00 1.00009E+00 1.22989E-03 6.10306E+00 0.00000E+00 0.00000E+00
1632 restart data was written for generation 1000 random number=41C80DA78C5BDEAA
1633
1634 keno message number k5-123 execution terminated due to completion of the specified number of generations.
1635
1636
1637 F*(r) Convergence Statistics:
1638 WARNING: Of the 3161 F*(r) mesh intervals that scored tallies...
1639 97.56% of the F*(r) tallies contain more than 5% uncertainty;
1640 56.72% of the F*(r) tallies contain more than 10% uncertainty;
1641 21.42% of the F*(r) tallies contain more than 20% uncertainty; and
1642 4.56% of the F*(r) tallies contain more than 50% uncertainty.
1643
1644
1645 1 godiva-k5
1646
1647 lifetime = 6.25089E-09 + or - 7.31724E-12 generation time = 5.71364E-09 + or - 8.89061E-12
1648 nu bar = 2.59857E+00 + or - 2.02081E-04 average fission group = 2.59601E+01 + or - 1.28625E-02
1649 energy(ev) of the average lethargy causing fission = 8.19742E+05 + or - 1.03123E+03
1650 custom mean free path (cm) = 2.55070E+00 + or - 4.02267E-04
Line: 4437, Col: 42
```

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

- Set **cet=1** to enable CLUTCH
- Set **cfp=#** for the number of latent generations for the IFP calculation of the $F^*(r)$ function
- Increase the number of inactive generations to allow the $F^*(r)$ function to converge
- Set **cgd=#** to tell CE TSUNAMI-3D the ID of the GridGeometry mesh for $F^*(r)$ or **cgd=yes** and **msh=#** for uniform mesh
- Make the GridGeometry mesh for $F^*(r)$, if necessary

CLUTCH input

The screenshot displays the CLUTCH input editor interface. The top menu bar includes 'File', 'Edit', 'View', 'Run', and 'Help'. Below this is a toolbar with buttons for 'Reload', 'Save', 'Save as', 'Close tab', 'Print', 'Cut', 'Copy', 'Paste', 'Undo', 'Redo', and 'Find'. The main window is titled 'godiva_example_CLUTCH_improved.inp' and shows a list of processors on the left and a code editor on the right. The code editor contains the following text:

```
1 =tsunami-3d-k5
2 godiva-k5
3 ce_v7.1
4 read composition
5 u-234      1  0  0.0000491995  300 end
6 u-235      1  0  0.0449996    300 end
7 u-238      1  0  0.002498     300 end
8 end composition
9 read parameter
10 cet=1
11 cfp=5
12 nsk=500 gen=1000
13 cgd=yes msh=1
14 fst=yes
15 end parameter
16 read geometry
17 global unit 1
18 sphere 1 1 8.741
19 end geometry
20 end data
21 end
```

Several lines of code are highlighted with boxes: line 1 is boxed in black, lines 10 and 11 are boxed in black, lines 12 and 13 are boxed in red, and line 14 is highlighted in yellow. The interface also shows a 'Navigation' pane on the left with a 'Filter' field and a tree view showing 'godiva_example_CLUTCH_improved.i' and 'document'.

Sensitivity coefficients: Impact of $F^*(r)$

Nuclide	IFP Sensitivity	CLUTCH Sensitivity without $F^*(r)$	CLUTCH Sensitivity with $F^*(r)$
U-234	$7.06\text{E-}03$ $\pm 6.78\text{E-}04$	$6.88\text{E-}03$ $\pm 2.64\text{E-}04$ (-0.25 σ)	$7.32\text{E-}03$ $\pm 2.72\text{E-}04$ (-0.36 σ)
U-235	$7.98\text{E-}01$ $\pm 5.31\text{E-}03$	$7.88\text{E-}01$ $\pm 2.13\text{E-}03$ (-1.75 σ)	$8.02\text{E-}01$ $\pm 1.84\text{E-}03$ (-0.71 σ)
U-238	$1.74\text{E-}02$ $\pm 1.49\text{E-}03$	$1.62\text{E-}02$ $\pm 5.71\text{E-}04$ (-0.75 σ)	$1.80\text{E-}02$ $\pm 5.68\text{E-}04$ (-0.38 σ)

SAMS parameters

- Options for SAMS parameters are limited in CE TSUNAMI-3D
- Most of the limited SAMS parameters deal with processing sensitivity coefficients for MG TSUNAMI-3D
- The available SAMS options are as follows:
 - nomix *Does not print sensitivities by mixture*
 - unconstrainedchi *Does not constrain chi sensitivities*
 - ❑ *This is not a recommended option*

CLUTCH vs IFP

CLUTCH

- Advantages:
 - More efficient than IFP both in terms of speed and memory usage
 - Implemented in KENO in parallel
 - Often useful for fast-spectrum systems
- Disadvantages:
 - Known issues with sensitivities in reflectors
 - Unknown relationship between $F^*(r)$ convergence and sensitivity accuracy

IFP

- Advantages:
 - Generally accurate
- Disadvantages:
 - Memory use can make some problems impossible for real computers
 - No parallel implementation in KENO
 - Parallel implementation using SHIFT

TSUNAMI sensitivity methods

TSUNAMI Method		Accuracy	Runtime	Memory Footprint	Ease of Use
TSUNAMI-1D		Deterministic, Multigroup	Seconds	Negligible	Very Easy
TSUNAMI-2D		Deterministic, Multigroup	Seconds – Minutes	Negligible	Very Easy
TSUNAMI-3D	Multigroup Approach	Monte Carlo, Multigroup	Minutes – 1 Week	Mesh drives, can be considerable	Driven by mesh and XS processing
	IFP	Monte Carlo, Continuous-Energy	Minutes – Several Weeks [†]	Model and CFP drive, can be considerable	Easy
	CLUTCH	Monte Carlo, Continuous-Energy	Minutes – 1 Week*	Generally Negligible	Generally Easy

*CLUTCH is implemented in parallel in KENO and [†]IFP is implemented in parallel in Shift, allowing feasible runtimes.

The parallel executables are not distributed and must be built by the user. In serial, run times are hours to a month or more.

SAMS parameters

- Options for SAMS parameters are limited in CE TSUNAMI-3D
- Most of the limited SAMS parameters deal with processing sensitivity coefficients for MG TSUNAMI-3D
- The available SAMS options are as follows:
 - nomix *Does not print sensitivities by mixture*
 - unconstrainedchi *Does not constrain chi sensitivities*
 - ❑ *This is not a recommended option*

CE TSUNAMI-3D summary

- CE TSUNAMI-3D contains two methods for calculating eigenvalue sensitivity coefficients
- CE TSUNAMI-3D usually does not require as much input as multigroup TSUNAMI-3D, and it calculates sensitivity coefficients in a single forward simulation
- CLUTCH can be more efficient and may require less memory than IFP, but it requires generating an $F^*(r)$ mesh and running a sufficient number of “skipped” generations to tally the function
- The IFP sensitivity method (**cet=2**) requires inputting some number of latent generations (**cfp=#**)
 - Between 2 and 20 latent generations is recommended; 5 to 10 is generally sufficient
- The CLUTCH method (**cet=1**) requires:
 - Creating a mesh for tallying $F^*(r)$ → start with 1–2 cm uniform intervals or define a GridGeometry to use for $F^*(r)$ (**cgd=#**)
 - Some number of latent generations (**cfp=#**) → usually between 5 and 10 generations
 - Increase **NSK** so that the problem simulates between 1 and 100 histories per mesh interval

Appendix

- More equations and details for the interested attendee



Calculating sensitivity coefficients

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

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

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

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.

Calculating sensitivity coefficients (cont.)

- For a sample capture reaction (*cap.*), the first-order perturbation equation reduces to something like the following:

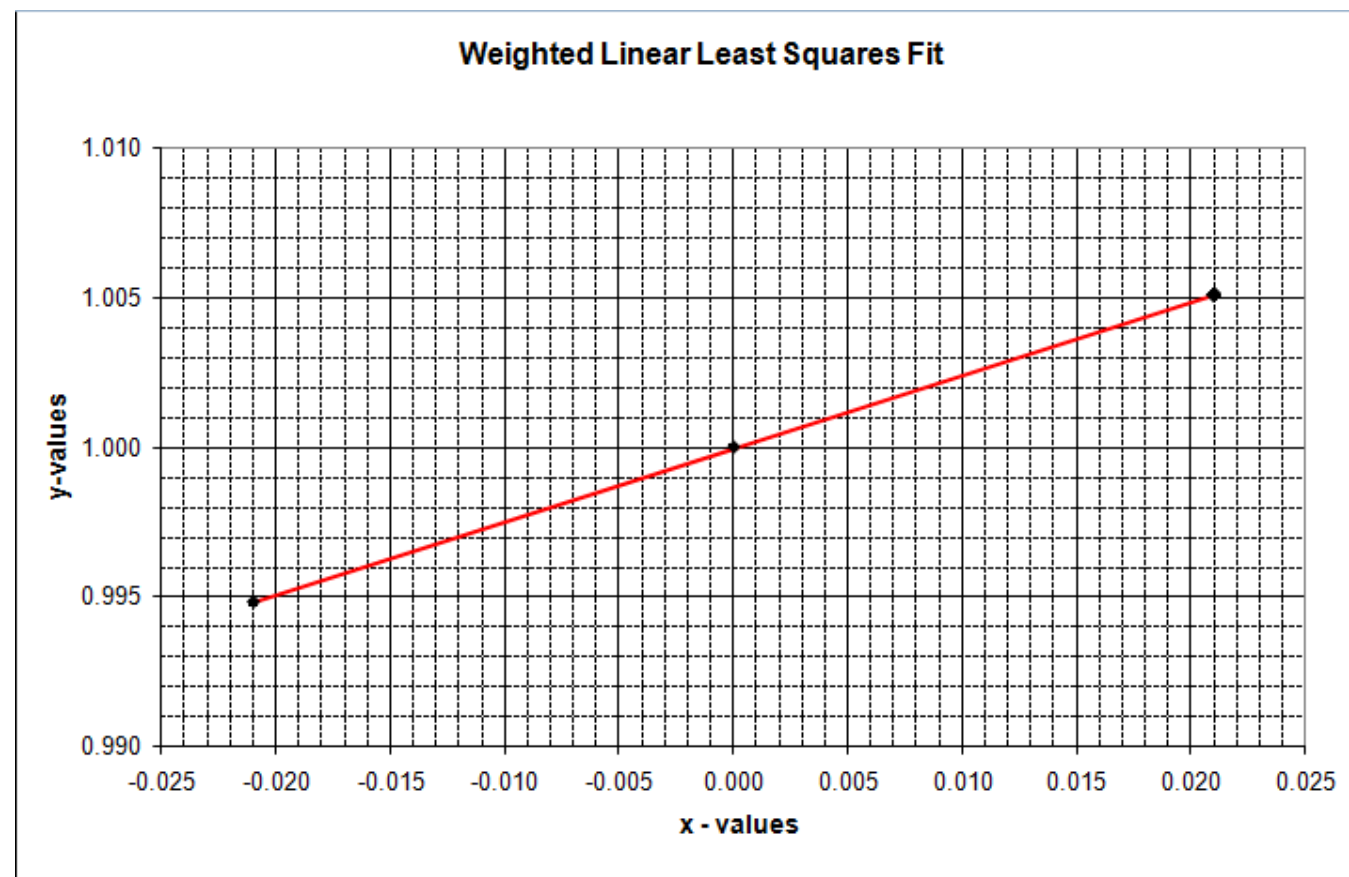
$$S_{k,\Sigma_{cap.}} = \frac{\langle \Phi^\dagger \Sigma_{cap.} \Phi \rangle}{\frac{1}{k} \langle \Phi^\dagger \Sigma_{fis.} \Phi \rangle}$$

- 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

Direct Perturbation Review – Three Point Method

- Use TSUNAMI Sensitivity to estimate $\Delta\rho = \frac{\left(\frac{0.005}{k_{eff}}\right)}{S_{Total}}$
- Example $S=0.25$ and $k_{eff}=1$: $\Delta\rho = 0.02$
 - The impact of k_{eff} on $\Delta\rho$ is pronounced for deeply subcritical application systems, but negligible for critical experiments
- For total sensitivities of 0.02 or higher, $\Delta\rho$ will be 25% or less
- Larger perturbations may depart from linear behavior

Direct Perturbation Plot



S_{DP}

S	σ	% σ	n	R ²
0.2446	0.0023	0.92%	3	1.0000

n = number of points used for the linear fit
R² = goodness of fit parameter, R² = unity means a perfect fit
S = slope of the line, = direct perturbation sensitivity estimate based on the linear fit
 σ = the uncertainty of the slope, = uncertainty of the DP estimate
% σ = the uncertainty of the slope as a percentage of the slope

σ_{SDP}

TSUNAMI-3D workshop



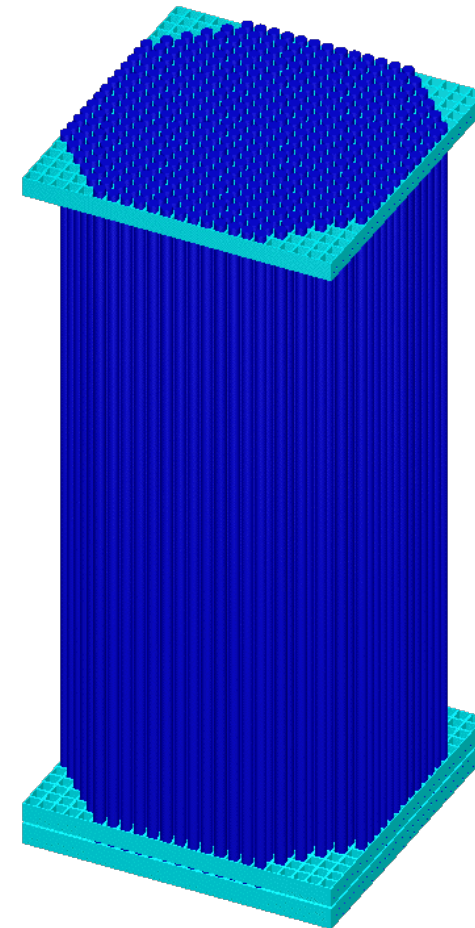
TSUNAMI-3D workshop

- As with TSUNAMI-1D workshop, the first problem is a class exercise, then other problems on your own
- While the class exercise problem is running, we will discuss recommended approaches for production calculations
- Then you'll have time on your own to work problems
- Starter KENO models are provided for all cases
- Review problems and select cases that would be most applicable to the systems you deal with, to maximize the usefulness of the workshop
 - Beware volume calculation defaults and memory size for fine mesh descriptions

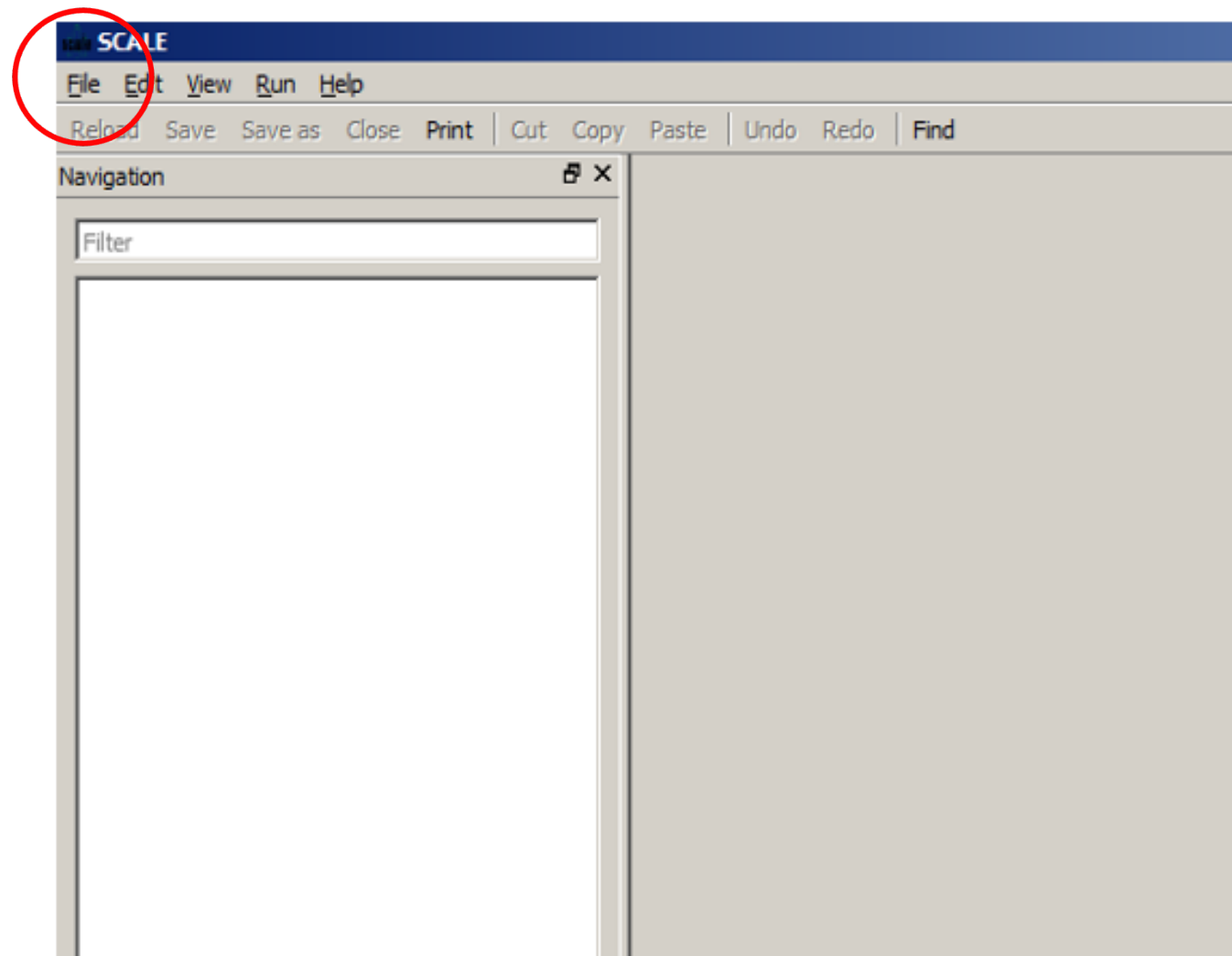
MIX-COMP-THERM-002-001

- Found in \workshops\inputs\kenova
- Rectangular arrays of water-moderated UO_2 -2 wt% PuO_2 (8% ^{240}Pu) fuel rods
- $\text{H}/(\text{U}+\text{Pu})=1.1946$
- $\text{EALF}=0.579$ eV
- $\text{Pu}/(\text{U}+\text{Pu})=0.0204$

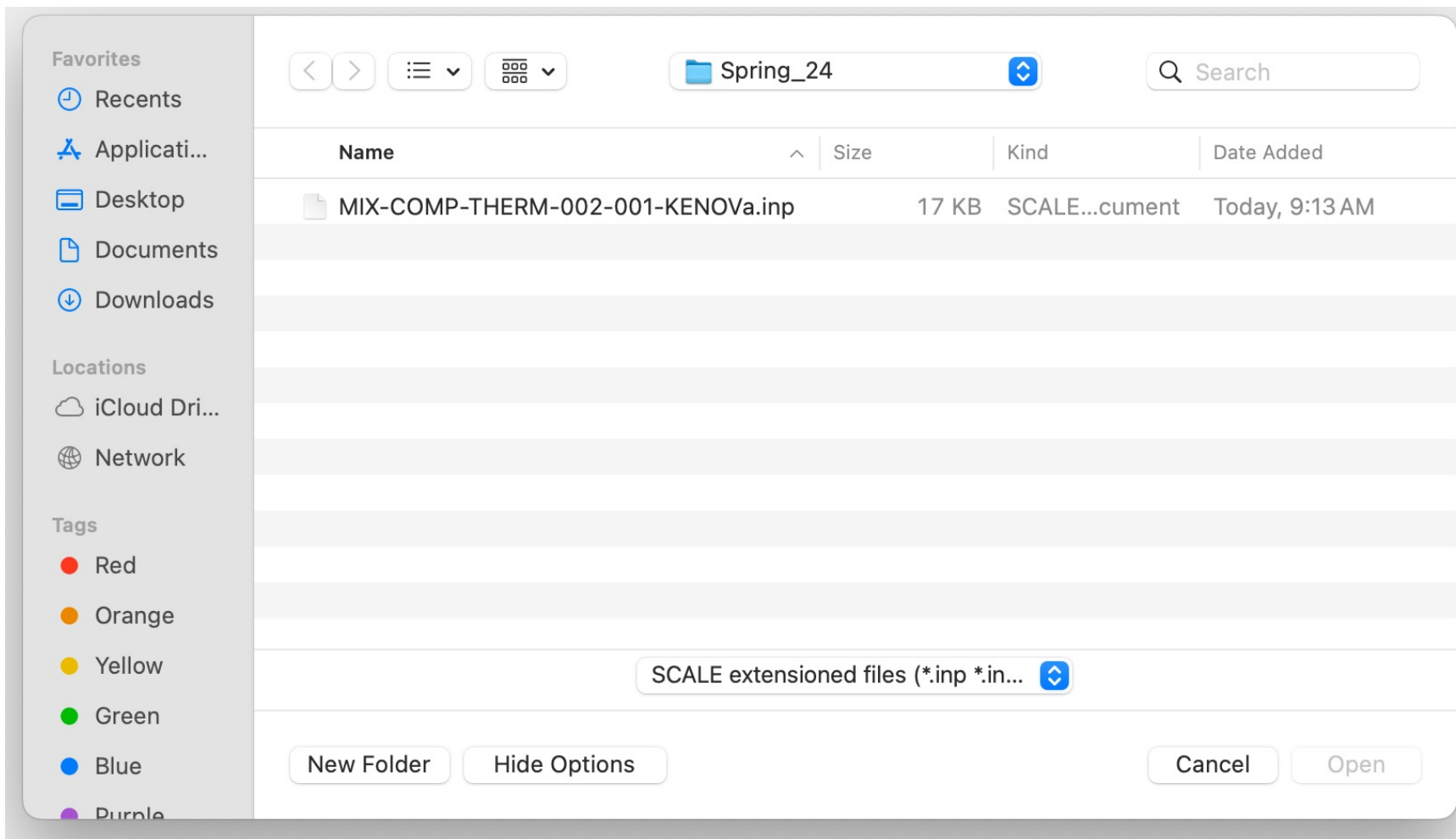
Nuclide	Direct Perturbation	TSUNAMI-3D
^{239}Pu	0.10 ± 0.01	
^1H Mix 4	0.34 ± 0.01	



Launch Fulcrum



Open CSAS5 file MIX-COMP-THERM-002-001-KENOVa.inp



Save as... new file MIX-COMP-THERM-002-001.inp

File Edit View Run Help

Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find

Navigation

Filter

MIX-COMP-THERM-002-001-KENOVa

document

Processors

document

SCALE 6.3.1

Run

View

Edit

1 'Input generated by GeeWiz SCALE 6.0.10.30 Compiled on October 30, 2009

2 =tsunami-3d-k5

3 epri .70 inch

4 ce_v7.1

5 read composition

6 u-234 1

7 u-235 1

8 u-236 1

9 u-238 1

10 pu-238 1

11 pu-239 1

12 pu-240 1

13 pu-241 1

14 pu-242 1

15 am-241 1

16 o 1

17 sn 2

18 fe 2

19 cr 2

20 ni 2

21 zr 2

22 al 3

23 h 4

24 o 4

25 b-10 4

26 b-11 4

27 pb 5

28 h 6

29 o 6

30 b-10 6

31 b-11 6

32 end composition

33 read celldata

Favorites

Applications

Desktop

Documents

Downloads

Locations

iCloud Drive

Network

Tags

Red

Orange

Yellow

Green

Blue

Purple

Gray

Save As: MIX-COMP-THERM-002-001.inp

Tags:

< > ⋮ ☰

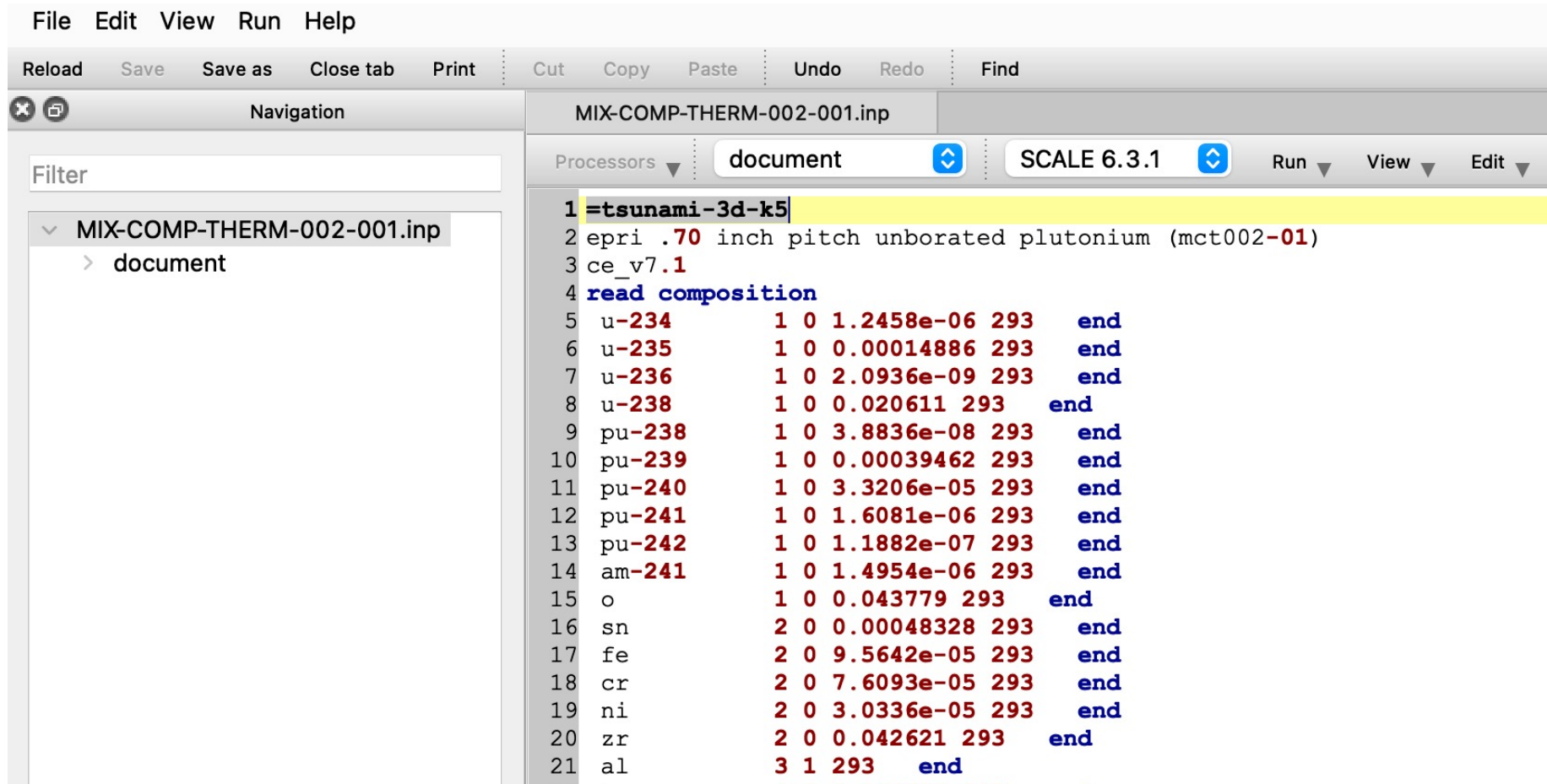
Spring_24

Search

Name	Size	Kind	Date Added
MIX-COMP-THE...001-KENOVa.inp	17 KB	SCALE...cument	Today, 9:13 AM

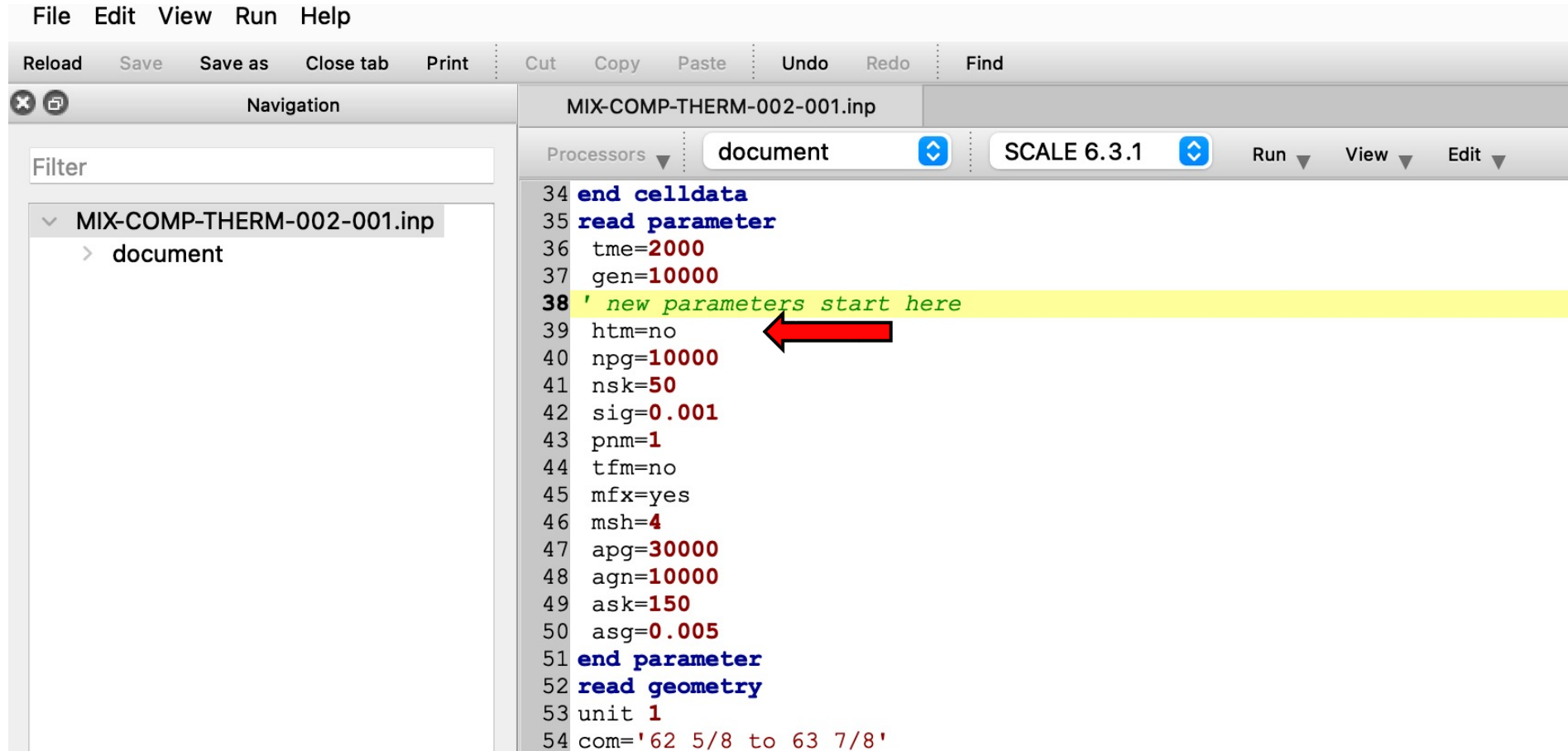
New Folder Cancel Save

Change sequence to TSUNAMI-3D-K5



```
File Edit View Run Help
Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find
Navigation
Filter
MIX-COMP-THERM-002-001.inp
> document
Processors document SCALE 6.3.1 Run View Edit
1 =tsunami-3d-k5
2 epri .70 inch pitch unborated plutonium (mct002-01)
3 ce_v7.1
4 read composition
5 u-234 1 0 1.2458e-06 293 end
6 u-235 1 0 0.00014886 293 end
7 u-236 1 0 2.0936e-09 293 end
8 u-238 1 0 0.020611 293 end
9 pu-238 1 0 3.8836e-08 293 end
10 pu-239 1 0 0.00039462 293 end
11 pu-240 1 0 3.3206e-05 293 end
12 pu-241 1 0 1.6081e-06 293 end
13 pu-242 1 0 1.1882e-07 293 end
14 am-241 1 0 1.4954e-06 293 end
15 o 1 0 0.043779 293 end
16 sn 2 0 0.00048328 293 end
17 fe 2 0 9.5642e-05 293 end
18 cr 2 0 7.6093e-05 293 end
19 ni 2 0 3.0336e-05 293 end
20 zr 2 0 0.042621 293 end
21 al 3 1 293 end
```

Set key parameters for long run



```
34 end celldata
35 read parameter
36 tme=2000
37 gen=10000
38 ' new parameters start here
39 htm=no
40 npg=10000
41 nsk=50
42 sig=0.001
43 pnm=1
44 tfm=no
45 mfx=yes
46 msh=4
47 apg=30000
48 agn=10000
49 ask=150
50 asg=0.005
51 end parameter
52 read geometry
53 unit 1
54 com='62 5/8 to 63 7/8'
```

*Remember to add htm=no since mfx=yes is present for MG.

Add SAMS block to print implicit sensitivity coefficients

```
221      10      10      10      10      5
222      10      10      10      10      10
223 end array
224 end data
225 read sams
226 prtimp
227 end sams
228 end
229
```

Line: 223, Col: 10 /tsunami_3dk5/arrays/term

Save and run SCALE

FileEditViewRunHelp

ReloadSaveSave asClosePrintCutCopyPasteUndoRedoFind

Navigation

Filter

MIX-COMP-THERM-002-001.inp

> document

MIX-COMP-THERM-002-001.inp

Processors

document

SCALE 6.3.1

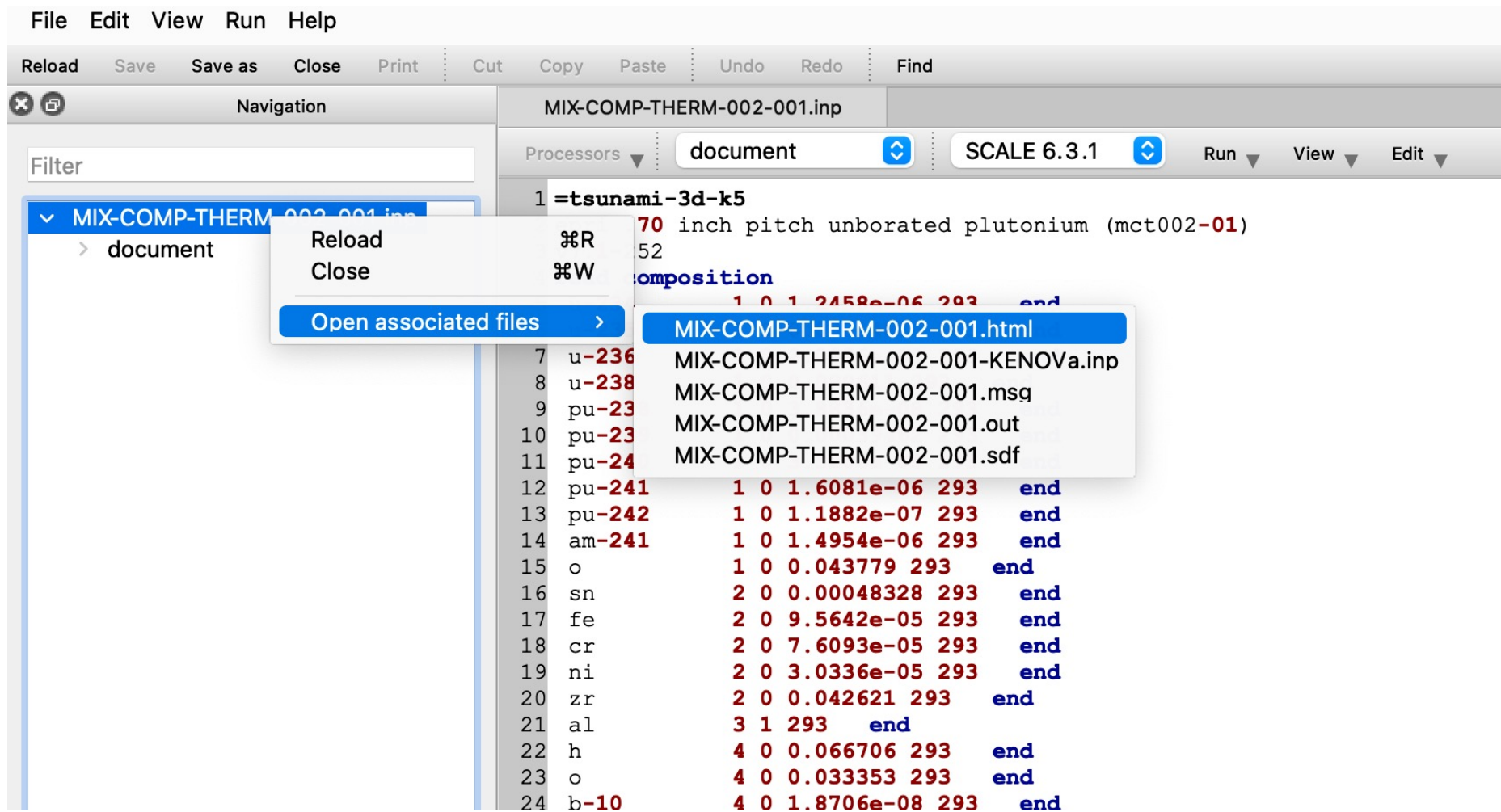
Run

View

Edit

175	8	8	8	3	3	3	3	3	3	3	3	3	3	3
176	8	8	8	8	3	3	3	3	3	3	3	3	3	3
177	8	8	8	8	8	3	3	3	3	3	3	3	3	3
178	9	9	9	9	9	4	4	4	4	4	4	4	4	4
179	9	9	9	9	4	4	4	4	4	4	4	4	4	4
180	9	9	9	4	4	4	4	4	4	4	4	4	4	4
181	9	9	4	4	4	4	4	4	4	4	4	4	4	4
182	9	4	4	4	4	4	4	4	4	4	4	4	4	4
183	4	4	4	4	4	4	4	4	4	4	4	4	4	4
184	4	4	4	4	4	4	4	4	4	4	4	4	4	4
185	4	4	4	4	4	4	4	4	4	4	4	4	4	4

Open HTML output



Main HTML page

The screenshot shows a web browser window with the title 'SCALE OUTPUT'. The address bar displays a file path: `file:///romulus-nas/users/wm4/scale_training/IFE/T3D_exercise/MIX-COMP-THERM-002-001_IFP.html`. The page content is as follows:

- Header: 'SCALE OUTPUT' with the SCALE logo on the right.
- Section: 'Select an Output Below'.
- Text: 'epri .70 inch pitch unborated plutonium (mct002-01)'.
- List:
 - 1. KENO-V.a[Forward]
 - 2. SAMS
- Section: 'Comments, Suggestions, User Assistance:'.
- Text: 'Contact SCALE Help', 'scalehelp@ornl.gov', 'or visit the SCALE website', and 'http://scale.ornl.gov/'.

Annotations on the image include:

- Red text 'Go to SCALE Website' with an arrow pointing to the SCALE logo.
- A red circle around the SCALE logo.
- A red circle around the '2. SAMS' option.
- Red text 'Sensitivity results' next to the '2. SAMS' option.

SAMS main page

General Information

Messages

Input Data

Derived Data

Results

 KENO-V.a - Program Verification Information
epri .70 inch pitch unborated plutonium (mct002-01) 

Return to
Main HTML
Page

Program Verification Information

code system	SCALE
version	6.3.1
program	kenova
creation date	10_feb_2023
library	/scale/release/6.3.1/serial/bin
prod	kenova
version	6.3.1
jobname	6tg
machine name	node37
date of execution	02_feb_2024
time of execution	13:20:12.68

Comments, Suggestions, User Assistance:

Contact SCALE Help

scalehelp@ornl.gov

or visit the SCALE website

http://scale.ornl.gov

 OAK RIDGE
National Laboratory

SCALE 6.3.1| Last Updated: February 2024

101

Sensitivity results by nuclide and reaction – Integrated over energy

General Information Input Data - Input Parameters - HTML Format Options - Summary of Transport Calculations Results - Energy, Region and Mixture Integrated Sensitivity Coefficients for this Problem - Energy and Region Integrated Sensitivity Coefficients for this Problem - Total Sensitivity Coefficients by Nuclide - Total Sensitivity Coefficients by Mixture - Sensitivity Data Plot - Uncertainty Information	scale SAMS - Energy, Region and Mixture Integrated Sensitivity Coefficients for this Problem scale				
	Sensitivity Coefficients for each Nuclide and Reaction				
Nuclide		Reaction	Sensitivity	Std. Dev.	% Std. Dev.
¹ H		total	3.0599E-01	± 1.5758E-02	5.15%
		elastic	3.8674E-01	± 1.5718E-02	4.06%
¹ H		capture	-8.0751E-02	± 2.5041E-04	0.31%
¹ H		n,gamma	-8.0751E-02	± 2.5041E-04	0.31%
² H		total	7.1515E-05	± 7.3195E-05	102.35%
		elastic	6.9997E-05	± 7.2859E-05	104.09%
² H		n,2n	1.5323E-06	± 1.6946E-06	110.59%
² H		capture	-1.4466E-08	± 4.3874E-11	0.30%
² H		n,gamma	-1.4466E-08	± 4.3874E-11	0.30%
¹⁰ B		total	-2.6290E-04	± 8.1319E-07	0.31%
		elastic	-8.4280E-07	± 1.0206E-09	0.12%
¹⁰ B		n,n'	-2.9309E-09	± 2.1617E-11	0.74%
¹⁰ B		capture	-2.6206E-04	± 8.1268E-07	0.31%
¹⁰ B		n,gamma	-3.4068E-08	± 1.0572E-10	0.31%
¹⁰ B		n,p	-8.8748E-10	± 4.6213E-12	0.52%
¹⁰ B		n,d	-9.3159E-11	± 1.9761E-12	2.12%
¹⁰ B		n,alpha	-2.6202E-04	± 8.1257E-07	0.31%
¹¹ B		total	-3.9138E-06	± 2.1112E-06	53.94%
		elastic	-3.9024E-06	± 2.1112E-06	54.10%

Sensitivity of k_{eff} to total cross section of each nuclide – Integrated over energy: equivalent number density perturbation

General Information

Input Data

- Input Parameters
- HTML Format Options
- Summary of Transport Calculations

Results

- Energy, Region and Mixture Integrated Sensitivity Coefficients for this Problem
- Energy and Region Integrated Sensitivity Coefficients for this Problem
- Total Sensitivity Coefficients by Nuclide
- Total Sensitivity Coefficients by Mixture
- Sensitivity Data Plot
- Uncertainty Information



Sensitivity Coefficients for Total Reaction for each Nuclide

These values are equivalent to the sensitivity of k_{eff} to the number density of each nuclide

Sort sensitivities

Good agreement with DP results

Mixture	Nuclide	Atom Density	Sensitivity ↑	Std. Dev.	% Std. Dev.
4	¹ H	6.6698E-02	3.2190E-01	± 1.3947E-02	4.33%
1	²³⁹ Pu	3.9462E-04	1.1311E-01	± 3.6970E-03	3.27%
1	²³⁵ U	1.4886E-04	2.6420E-02	± 1.3956E-03	5.28%
4	¹⁶ O	3.3272E-02	2.3652E-02	± 4.5331E-03	19.17%
6	¹⁶ O	3.3272E-02	2.0378E-02	± 1.7829E-03	8.75%
1	¹⁶ O	4.3673E-02	5.6240E-03	± 4.5115E-03	80.22%
2	⁹⁰ Zr	2.1929E-02	4.3854E-03	± 2.2133E-03	50.47%
2	⁹² Zr	7.3095E-03	2.5382E-03	± 1.3908E-03	54.79%
3	²⁷ Al	6.0307E-02	1.2103E-03	± 4.6389E-04	38.33%
1	²⁴¹ Pu	1.6081E-06	1.0616E-03	± 2.2780E-04	21.46%
2	⁹⁴ Zr	7.4075E-03	8.1863E-04	± 1.4454E-03	176.57%
2	¹²⁰ Sn	1.5745E-04	5.4627E-04	± 1.9977E-04	36.57%
5	²⁰⁸ Pb	1.7275E-02	3.9669E-04	± 2.5056E-04	63.16%
5	²⁰⁶ Pb	7.9453E-03	2.7820E-04	± 1.5061E-04	54.13%
5	²⁰⁷ Pb	7.2859E-03	2.2112E-04	± 1.5543E-04	70.29%
2	⁵⁸ Ni	2.0652E-05	1.2617E-04	± 1.0790E-04	85.52%
2	¹¹⁸ Sn	1.1705E-04	8.7688E-05	± 1.5519E-04	176.97%
2	⁵⁴ Fe	5.5903E-06	6.1594E-05	± 4.5489E-05	73.85%

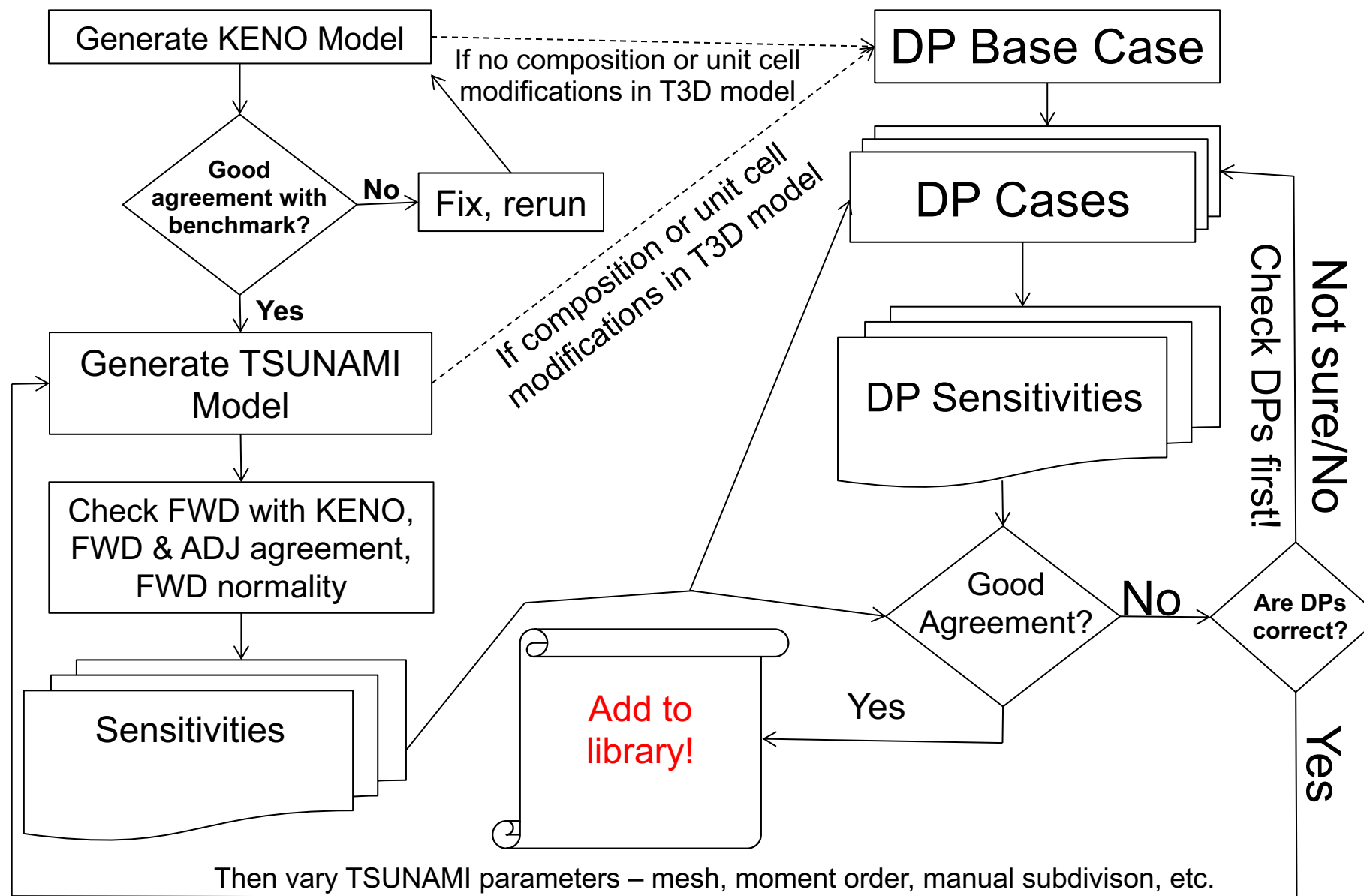
CLUTCH results

Mixture	Nuclide	Atom Density	Sensitivity ↑	Std. Dev.	% Std. Dev.
4	¹ H	6.6698E-02	2.6666E-01	± 1.4204E-02	5.33%
1	²³⁹ Pu	3.9462E-04	1.1297E-01	± 2.2213E-03	1.97%

Calculation notes:

- On a 3.6 GHz Windows PC, forward calculation takes ~3.5 minutes, adjoint ~20 minutes.
- Total runtime ~27 minutes
- KENO calculations require ~1 GB of RAM
- PNM=1 was set to speed up runtime and reduce storage
- NPG, APG, SIG, ASG were also reduced from recommended production values

SDF generation/verification process



Production calculations with TSUNAMI-3D

- Verify input model
 - Verify number densities against benchmark specification for exact match
 - Application system may not have exact number densities for matching, but compositions should be correct
 - Verify dimensions against benchmark specification for exact match
 - Again, for application system, appropriate dimensions may need to be determined
 - Review modeling assumptions and approximations to ensure they are reasonable

Production calculations with TSUNAMI-3D (cont.)

- Unit cell data (MG only)
 - Verify proper use of multiple unit cell specifications to reduce modeling approximations
 - Remove use of More Data with input Dancoff factors to specify multiple fuel types (SCALE 4 style input)
 - Consider necessity of separate unit cell input for wet/dry portions of fuel rods
 - Consider necessity of multiregion unit cells to properly account for implicit effects in interacting materials
 - Explicitly specify inhommedium individually for each mixture that does not appear in other unit cells
 - ex: *inf 12 end*

Production calculations with TSUNAMI-3D (cont.)

- MG parameters
 - Use mesh fluxes where possible and turn off transform. Initial mesh size is $1/10^{\text{th}}$ of smaller outer dimension of active fuel *msh=xxx mfx=yes tfm=no*
 - Consider starting with pitch as mesh size, potentially offset so each mesh cell is quartered
 - Set tight convergence criteria with *sig* and *asg* parameters with large numbers of generations for forward and adjoint calculations:
gen=10000 npg=10000 sig=0.0005 asg=0.001
 - For fast systems, set *apg* to a larger number as needed. Default *apg* is $3 \times npg$
 - Leave *pnm* at default value of 3, unless excess storage is needed for mesh fluxes, then set *pnm=1*
 - Increasing to *pnm=5* may help agreement between TSUNAMI and direct perturbations

Production calculations with TSUNAMI-3D (cont.)

- CE parameters
 - IFP and CLUTCH
 - Ensure an appropriate number of latent generations
 - More latent generations leads to a more accurate, but higher uncertainty, result
 - High-leakage systems are particularly susceptible to this due to short fission chains
 - CLUTCH only
 - Select a mesh
 - 1–2 cm has been shown to be adequate in most cases
 - NSK will likely need to increase significantly (hundreds to perhaps 1,000)
 - The importance function is tallied during these generations

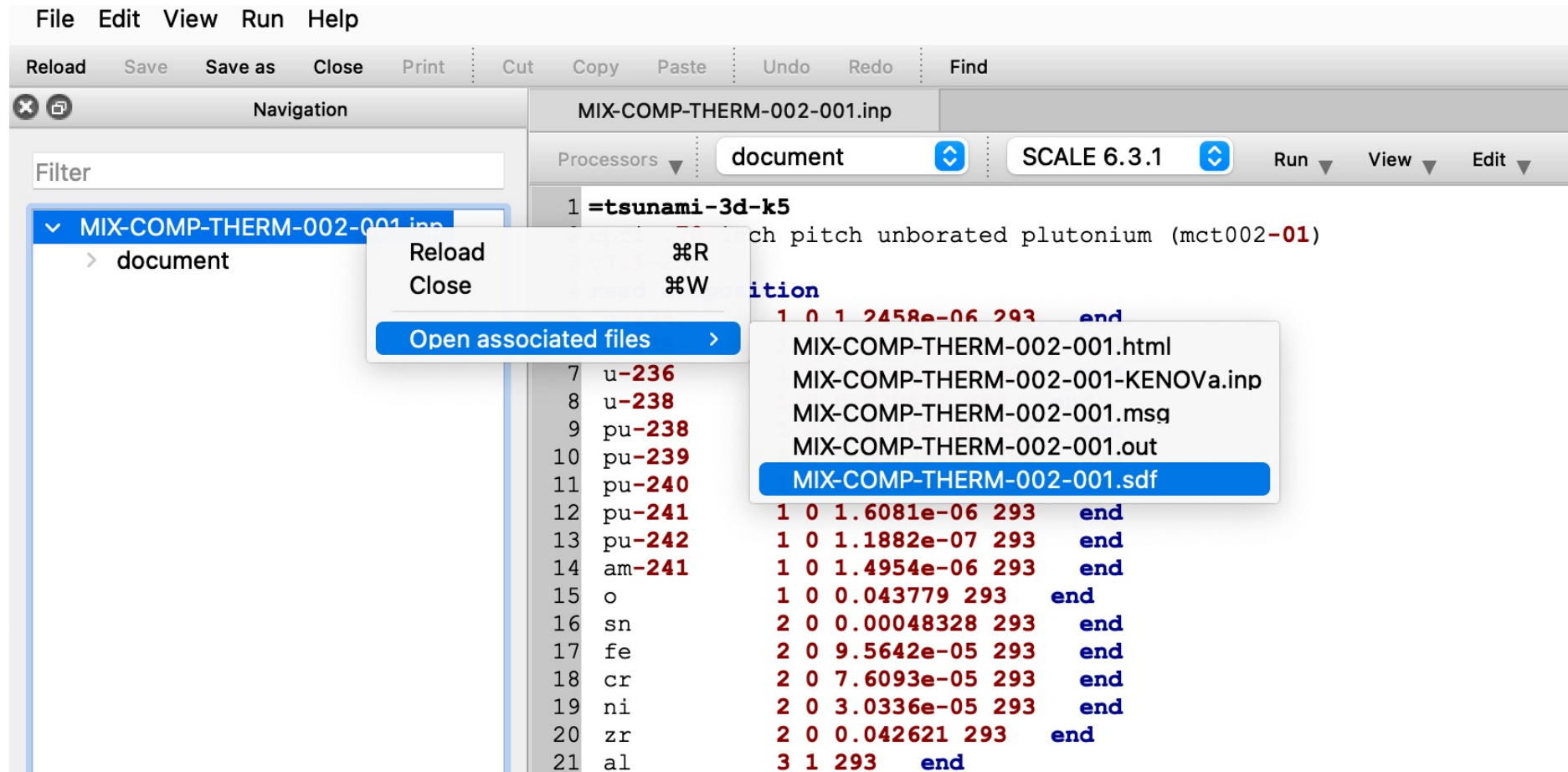
Production calculations with TSUNAMI-3D (con't)

- Verification of proper execution
 - MG and CE
 - Examine forward case for k_{eff} normality
 - Ensure forward calculation is well converged by examining plot of average k_{eff} by generations skipped (second KENO plot)
 - Verify forward k_{eff} is close to the expectation from measured/CSAS results
 - Inconsistent k_{eff} values require investigation
 - Inexplicable inconsistent results should be noted and discarded
 - MG only
 - Ensure forward and adjoint k_{eff} values are in good agreement, < 0.5% difference

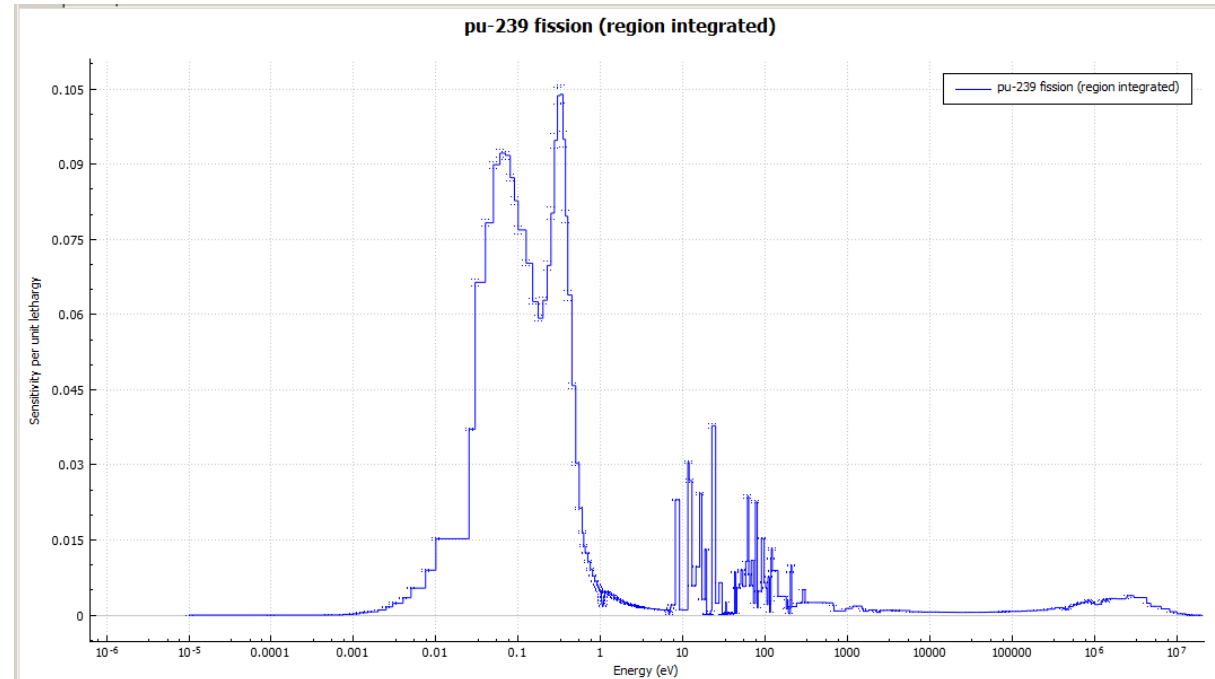
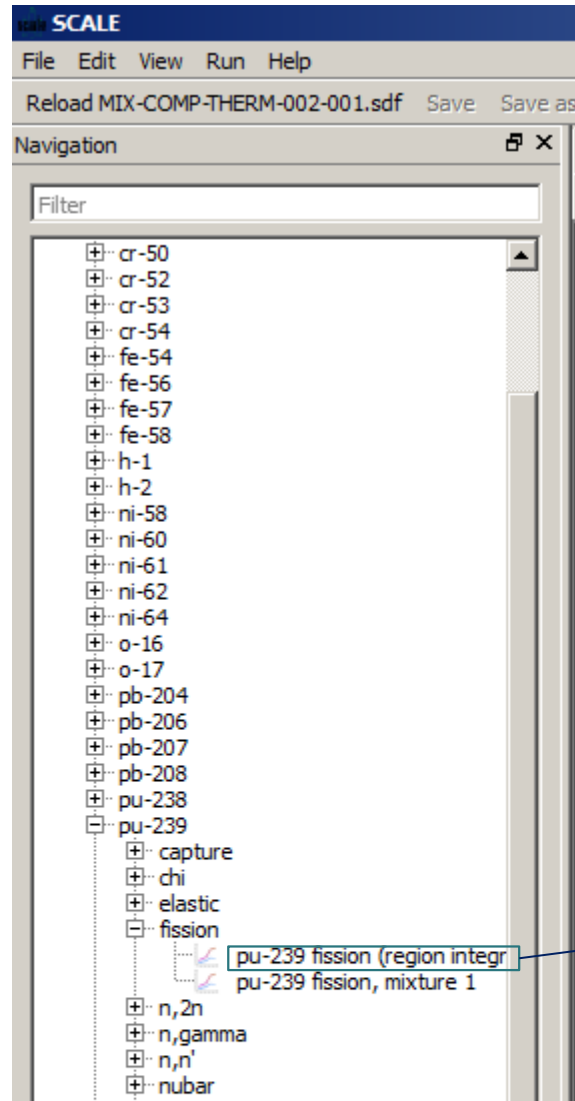
Production calculations with TSUNAMI-3D (cont.)

- Direct perturbation
 - Verify sensitivities of important nuclides with direct perturbations for each distinct model type with CSAS calculations
 - Verify at least the most important fissile nuclide and the most important moderating nuclide
 - If model is intended to validate a specific component, then test those nuclides as well (e.g., absorber materials, fission products, reflector materials)
 - Set tight convergence criteria to see effect of perturbation $gen=10000$
 $npg=10000$ $sig=0.0001$

Integrated plotting with Fulcrum



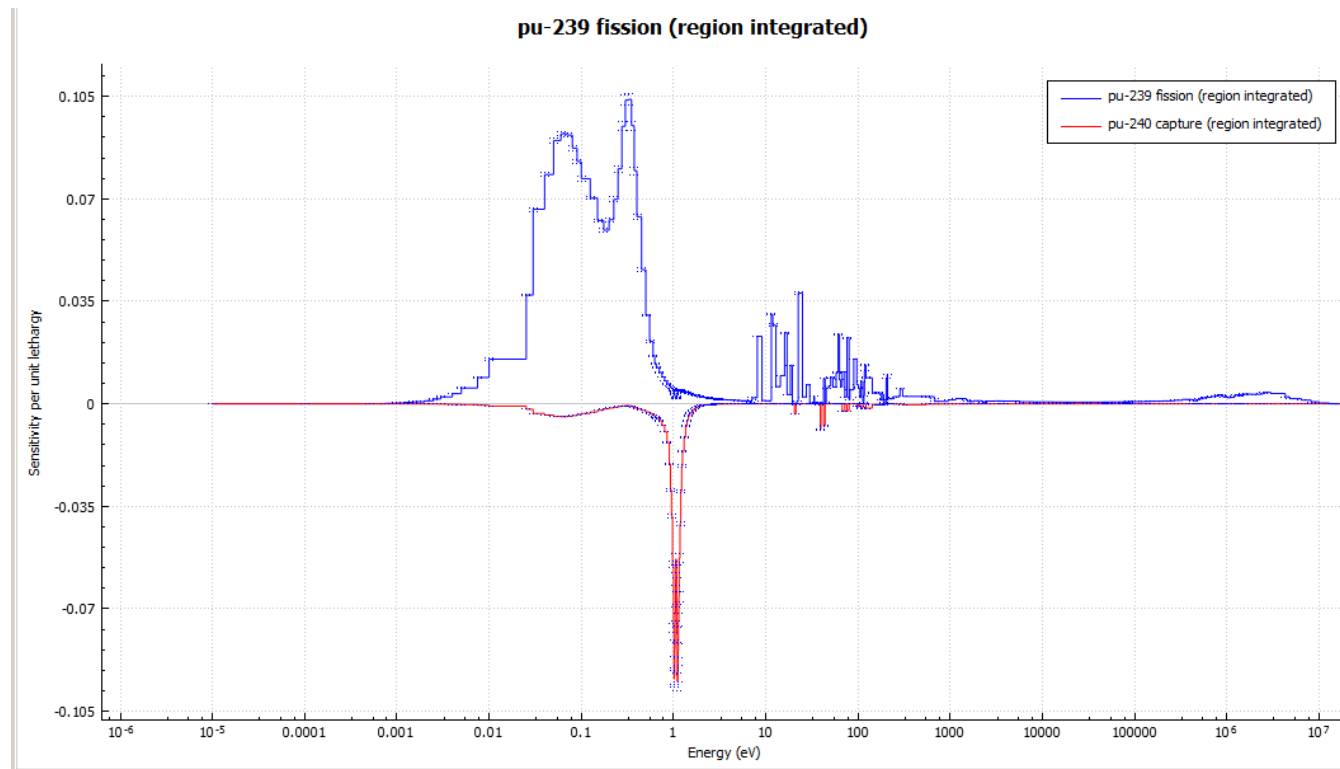
Navigate to Pu-239 fission



Double click

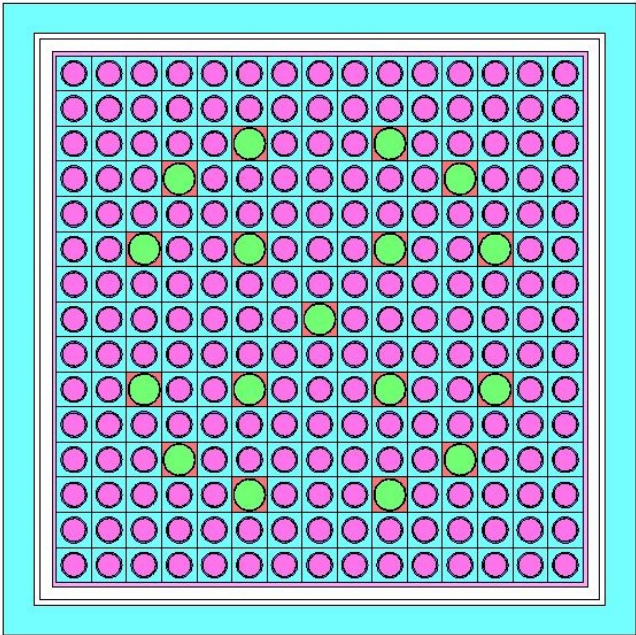
Show plots on same graph

- Right-click on other sensitivity
 - For example, Pu-240 capture
- “Add Graph to ...”



Questions before workshop time?

MOX fuel storage rack



Storage Tube
Inner dim 22 cm
0.5 cm thick SS-304
0.25 cm borated SS
7.9 g/cm³
2 wt% boron

Water with 300 ppm boron

Storage Tube Pitch 13 cm

15x15 Assy

Fuel Pins
Zirc-4 clad MOX fuel
Pu/(U+Pu) 6 wt%
0.3 wt% ²³⁵U, 99.7wt%²³⁸U
96 wt% ²³⁹Pu, 4 wt% ²⁴⁰Pu
Pellet Radius 0.47525 cm
Gap Radius 0.48515 cm
Clad Radius 0.54355 cm

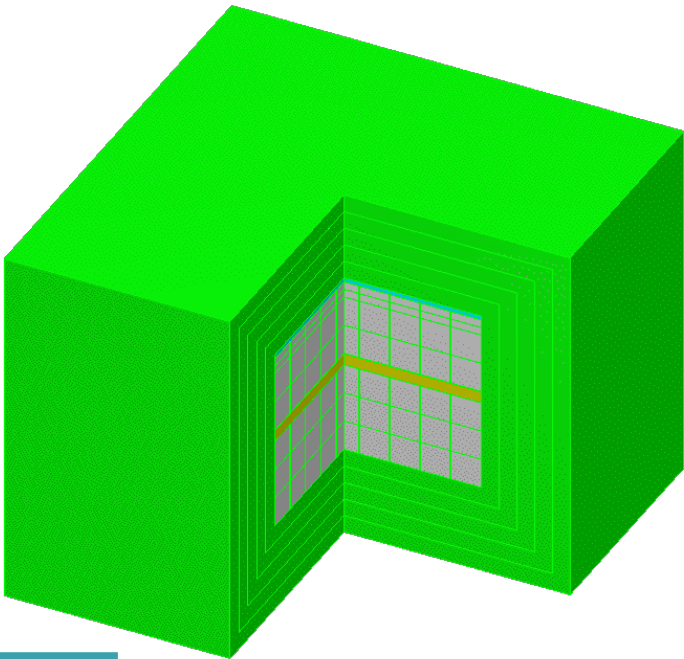
Guide Tubes
Zirc-4
Inner Radius 0.635 cm
Outer Radius 0.67055 cm

Length: 365 cm
Pin Pitch 1.4427 cm

Material	Direct Perturbation	TSUNAMI-3D
Mix 1	0.096 ± 0.007	
Mix 3	0.205 ± 0.007	

Critical experiments

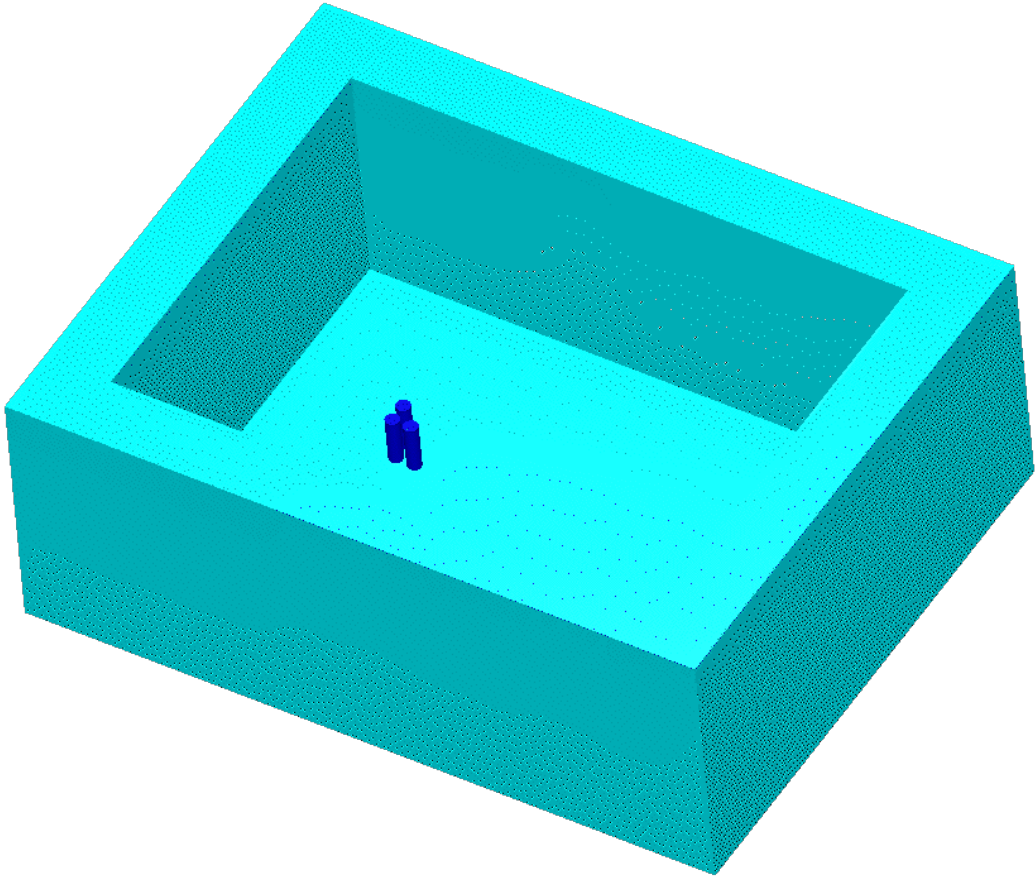
- MOX-Polystyrene compacts published in NS&E Vol. 55.
- Table 5, Case 4
 - $H/(U+Pu)=2.8$
 - $EALF=39.7\text{ eV}$
 - $Pu/(U+Pu)=0.303$



Nuclide	Direct Perturbation	TSUNAMI-3D
²³⁹ Pu Mix 1	0.243 ± 0.005	
¹ H Mix 1	0.103 ± 0.004	

PU-SOL-THERM-014-019

- 10 cm surface-to-surface separation.
- Create model that accurately computes sensitivity coefficients for ^1H and ^{239}Pu

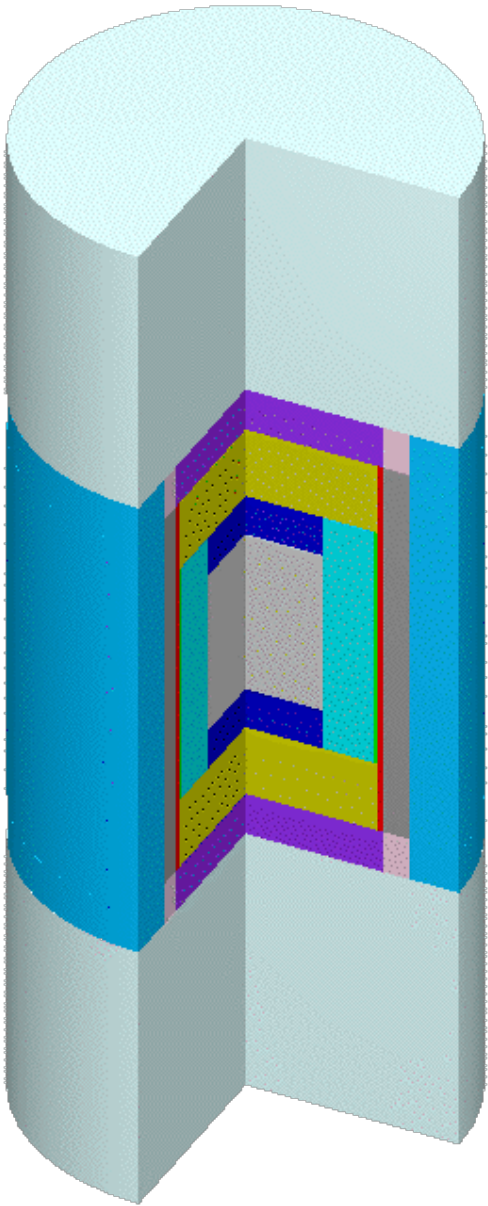


Nuclide	Direct Perturbation	TSUNAMI-3D
^{239}Pu	0.074 ± 0.003	
^1H Mix 1	0.595 ± 0.007	

MIX-MET-FAST-001-001

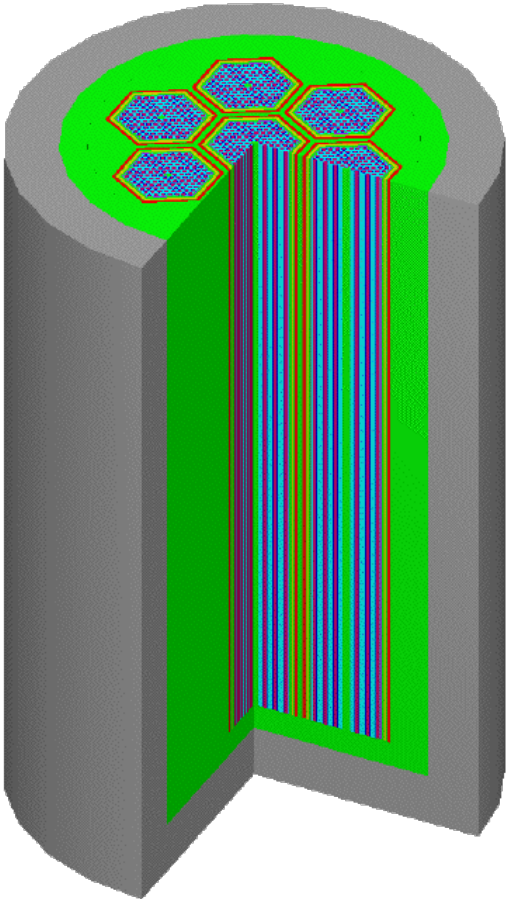
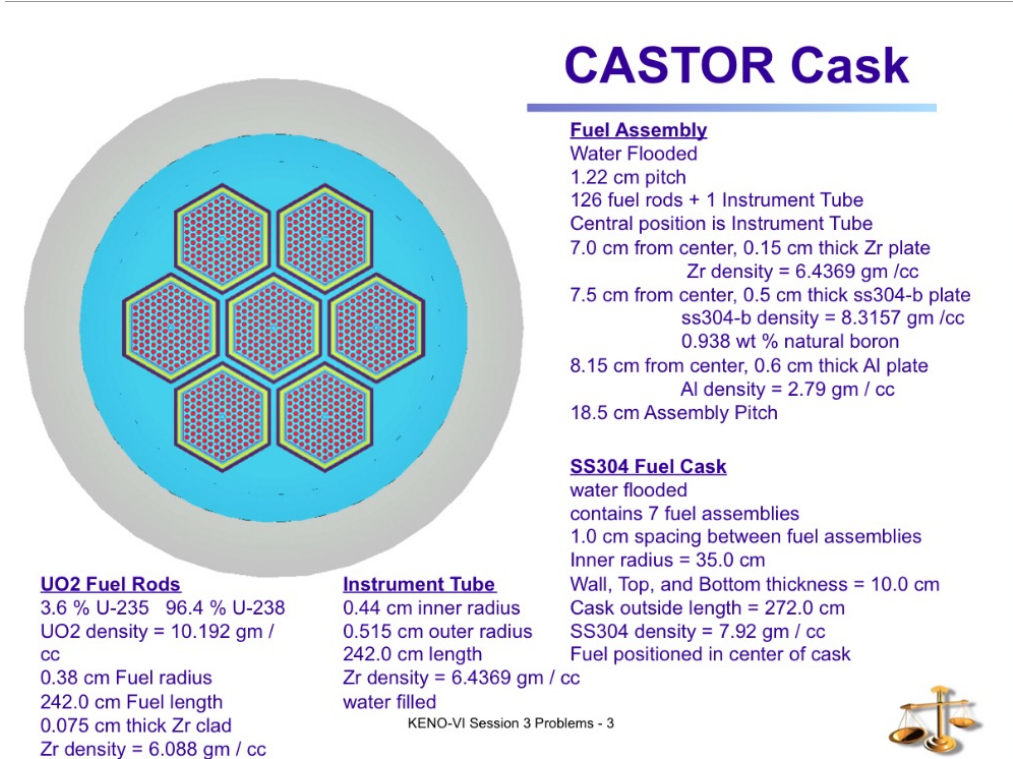
- ZPPR-21: Cylindrical assemblies of mixed fissile Pu and U metal reflected by graphite
 - $H/(U+Pu)=0$
 - $EALF=279,000\text{ eV}$
 - $Pu/(U+Pu)=0.414$

Nuclide	Direct Perturbation	TSUNAMI-3D
^{239}Pu	0.49 ± 0.009	
C Mix 3	0.19 ± 0.008	



Castor cask

KENO-VI model of VVER-440 shipping cask

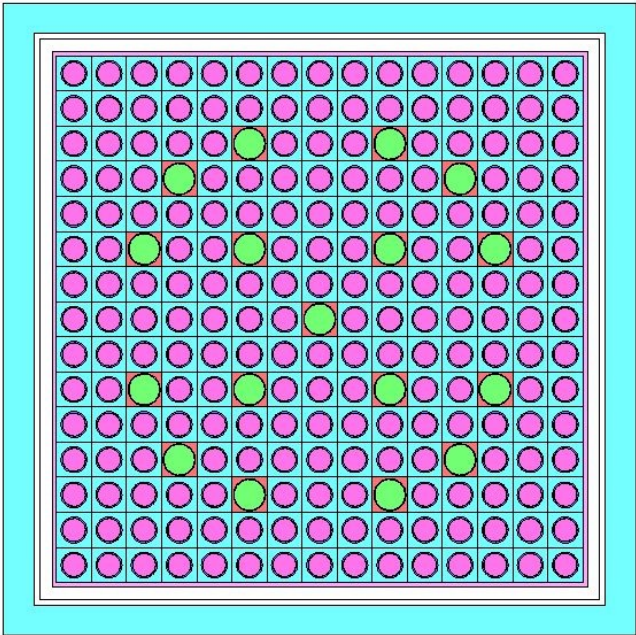


Material	Direct Perturbation	TSUNAMI-3D
Mix 1 - fuel	0.214 ± 0.010	
Mix 3 - moderator	0.499 ± 0.010	

TSUNAMI-3D workshop review



MOX fuel storage rack



Storage Tube
Inner dim 22 cm
0.5 cm thick SS-304
0.25 cm borated SS
7.9 g/cm³
2 wt% boron

Water with 300 ppm boron

Storage Tube Pitch 13 cm

15x15 Assembly Description

Fuel Pins

Zirc-4 clad MOX fuel
Pu/(U+Pu) 6 wt%
0.3 wt% ²³⁵U, 99.7wt%²³⁸U
96 wt% ²³⁹Pu, 4 wt% ²⁴⁰Pu
Pellet Radius 0.47525 cm
Gap Radius 0.48515 cm
Clad Radius 0.54355 cm

Guide Tubes

Zirc-4
Inner Radius 0.635 cm
Outer Radius 0.67055 cm
Length: 365 cm
Pin Pitch 1.4427 cm

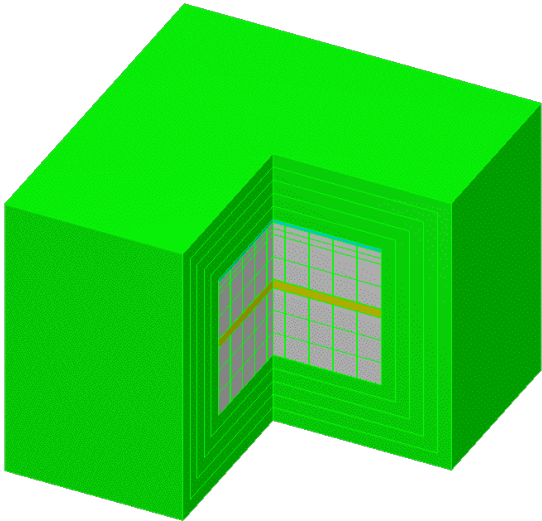
MG TSUNAMI Parameters			IFP/Shift	CLUTCH	
Run time =	36.5 minutes		96.0 min/ 2.90 min on 16 cores	14.6 min on 16 cores	
gen=10000	agn=10000	ffm=no	cet=2	cet=1	sig=0.002
npg=10000	apg=30000	mfx=yes	cfp=7	cfp=5	cgd=yes
sig=0.002	asg=0.005	msh=4	npg=10000	nsk=100	msh=2
nsk=50	ask=100		sig=0.0025		

Material	Direct Perturbation	MG TSUNAMI-3D	IFP	IFP-Shift	CLUTCH
Mix 1	0.096 ± 0.007	0.103 ± 0.003	0.083 ± 0.007	0.094 ± 0.011	0.094 ± 0.003
Mix 3	0.205 ± 0.007	0.209 ± 0.011	0.185 ± 0.012	0.217 ± 0.020	0.206 ± 0.006

Critical experiments

- MOX-Polystyrene compacts published in NS&E Vol. 55.
- Table 5, Case 4

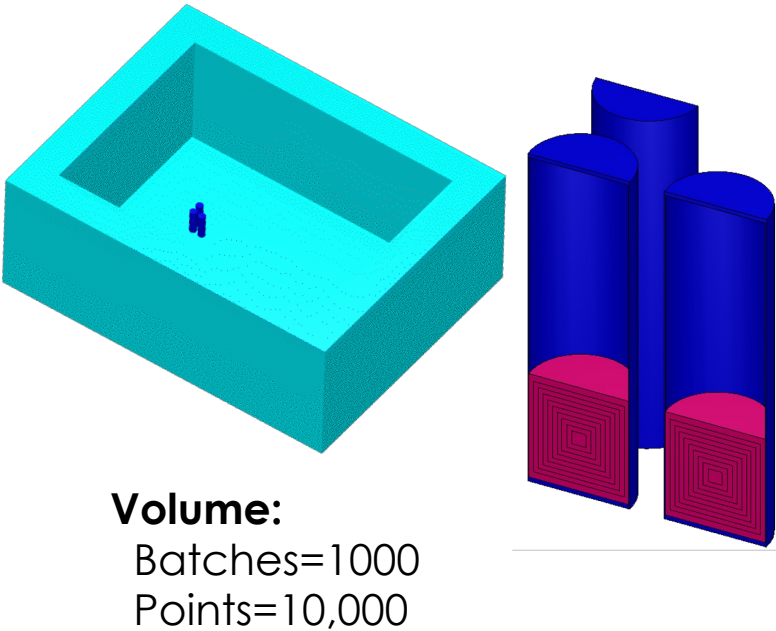
MG TSUNAMI Parameters			IFP/Shift	CLUTCH	
Run time	21.4 min		58.3 min/ 3.71 min on 16 cores	22.9 min on 16 cores	
gen=10050	agn=10150	tfm=no	cet=2	cet=1	sig=0.002
npg=10000	apg=30000	mfx=yes	cfp=5	cfp=5	cgd=yes
sig=0.002	asg=0.01	msh=7	npg=10000	nsk=200	msh=2
nsk=50	ask=150		nsk=40		



Nuclide	Direct Perturbation	MG TSUNAMI-3D	IFP	IFP-Shift	CLUTCH
²³⁹ Pu Mix 1	0.243 ± 0.005	0.231 ± 0.001	0.242 ± 0.004	0.241 ± 0.005	0.242 ± 0.001
¹ H Mix 1	0.103 ± 0.004	0.109 ± 0.008	0.115 ± 0.004	0.098 ± 0.009	0.109 ± 0.002

PU-SOL-THERM-014-019

MG TSUNAMI		CET IFP/Shift	CET CLUTCH
Run time	2.03 h	2.83 h/ 16.7 min (16 cores)	13.4 min (16 cores)
npg=15000 nsk=5 sig=100e-5 tfm=yes 10x10x10 mesh in each can	apg=15000 ask=145 asg=200e-5 mfx=yes	cet=2 cfp=5	cet=1 cfp=5 15x15x15 mesh in each can

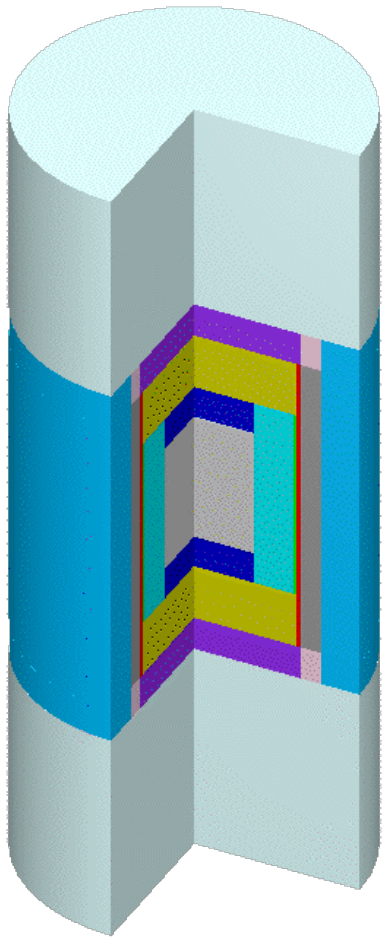


Nuclide	Direct Perturbation	MG TSUNAMI-3D	IFP	IFP-Shift	CLUTCH
²³⁹ Pu	0.074 ± 0.003	0.088 ± 0.022	0.069 ± 0.004	0.072 ± 0.003	0.083 ± 0.002
¹ H Mix 1	0.595 ± 0.007	0.614 ± 0.021	0.606 ± 0.014	0.614 ± 0.011	0.610 ± 0.010

MIX-MET-FAST-001-001

- Parameters

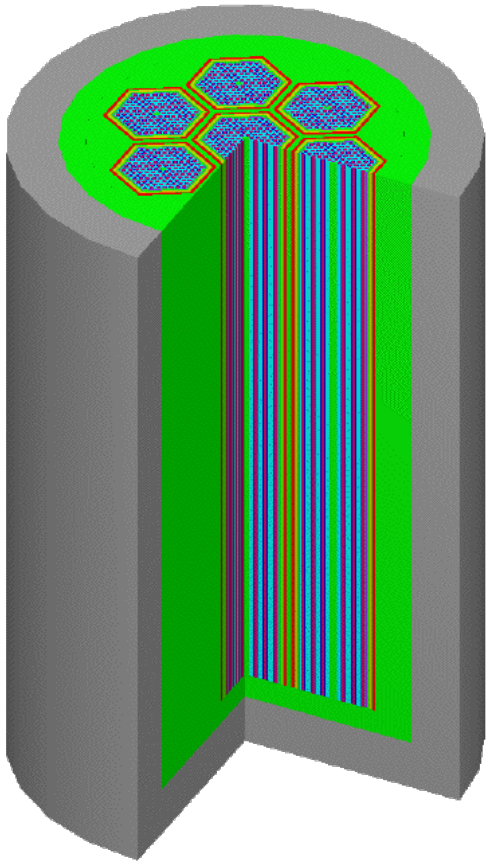
MG TSUNAMI		CET IFP/Shift	CET CLUTCH
Run time	3.21 h	3.02 h/ 9.22 min (16 cores)	22.8 min (16 cores)
npg=10000 nsk=50 sig=0.001 tfm=no msh=10	apg=50000 ask=150 asg=0.003 mfx=yes	cet=2 cfp=5	cet=1 cfp=5 msh=2



Nuclide	Direct Perturbation	MG TSUNAMI-3D	IFP	IFP-Shift	CLUTCH
²³⁹ Pu	0.49 ± 0.008	0.490 ± 0.001	0.503 ± 0.004	0.497 ± 0.004	0.496 ± 0.002
C Mix 3	0.19 ± 0.008	0.187 ± 0.002	0.199 ± 0.005	0.191 ± 0.005	0.198 ± 0.002

CASTOR cask

MG TSUNAMI		CET IFP/Shift	CET CLUTCH
Run time	1.86 h	1.16 h/ 6.08 min (16 cores)	5.67 min (16 cores)
npg=10000 sig=100e-5 tfm=no msh=6	apg=30000 asg=200e-5 mfx=yes	cet=2 cfp=5	cet=1 cfp=10 msh=5



Nuclide	Direct Perturbation	MG TSUNAMI-3D	IFP	IFP-Shift	CLUTCH
Fuel (Mix 1)	0.214 ± 0.010	0.220 ± 0.002	0.225 ± 0.007	0.235 ± 0.007	0.229 ± 0.004
Moderator (Mix 3)	0.499 ± 0.010	0.502 ± 0.009	0.519 ± 0.013	0.480 ± 0.013	0.526 ± 0.010

On your own

- Work other exercises
- Remember:
 - Pick the ones most applicable to your work!