SCALE 6.2 and AMPX Development and Modernization for the NCSP

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Nuclear Criticality Safety Program
Technical Program Review
Sandia National Laboratories

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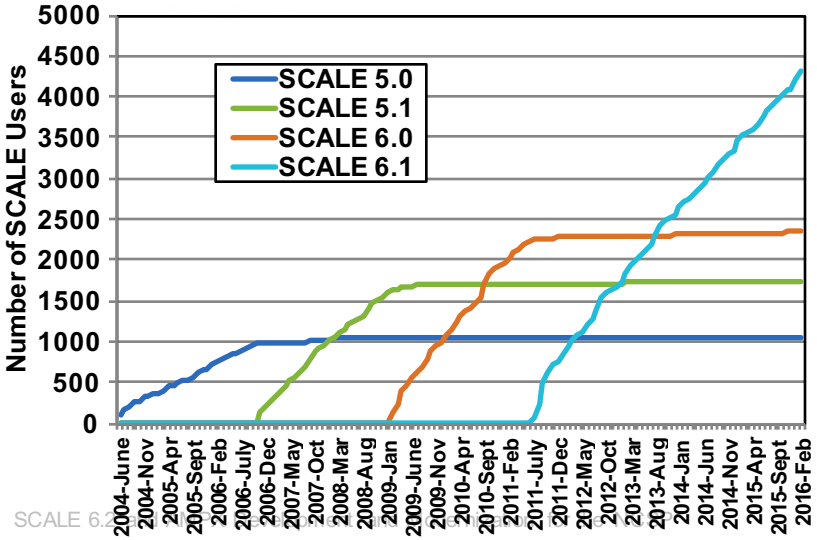
SCALE 6.1

- Released in 2011
- 4306 licenses issued through February 2016
- 3521 new users that had never used any previous version of SCALE
  - (2500 total SCALE users in 2009)
- Technical patches – 2 issued:
  - first for rarely encountered code error
  - second for error in ENDF decay data
  - (10 patches issued for SCALE 6.0 over 2 years)



SCALE 6.2 Goals

- Continued focus on quality, consistency and reliability
- Modernization for reduced runtime and memory requirements
- Improved nuclear data and uncertainty data
- Improved continuous-energy physics
- Advanced analysis techniques
- Consolidation of features
- New user interface
- Distribution of AMPX

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Modernized AMPX Modules

X10 – Multigroup library generation

- Complete rewrite in C++ to take advantage of
  - In-memory MG library resource shared with SCALE (this removes the restriction on maximum number of groups)
  - Integration routines shared within AMPX
  - A SCALE/AMPX class that defines sum rules for redundant cross sections and functions that apply the rules for MG data
- Apply more rigorous consistency, i.e. 2D are renormalized 1D to avoid numerical problems. (Integration of group-averaged 1D data is analytical, of 2D numerical)

Fabulous – Generates Bondarenko factors for unresolved resonance region (used in BONAMI and Polaris)

- Completely rewritten in C++
- Calculate problem independent cross section data as a function of background cross section σ_0 and temperature T; divide by a reference cross section to get F-Factors

$$\sigma_{x,g}^{(j)}(\sigma_0,T) = \frac{\int_g \sigma_x^{(j)}(E,T)\,\varphi(E,\sigma_0,T)\,\mathrm{dE}}{\int_g \varphi(E,\sigma_0,T)\,\mathrm{dE}}$$

- Tabulated as function of background cross section for application-specific use
- All integration are done with subclasses of NumIntegrate
- Enhanced features (next slides)

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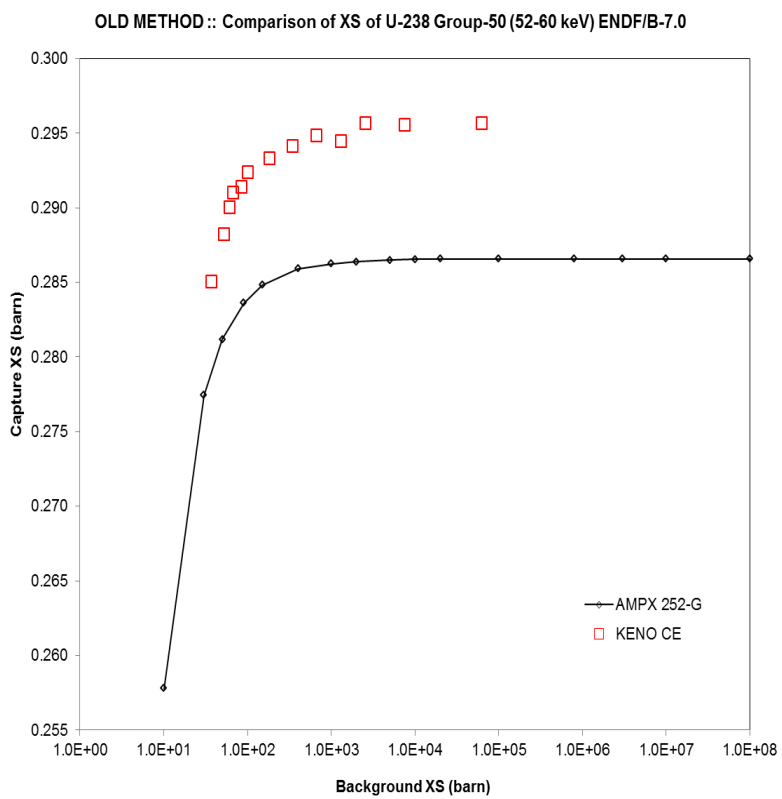
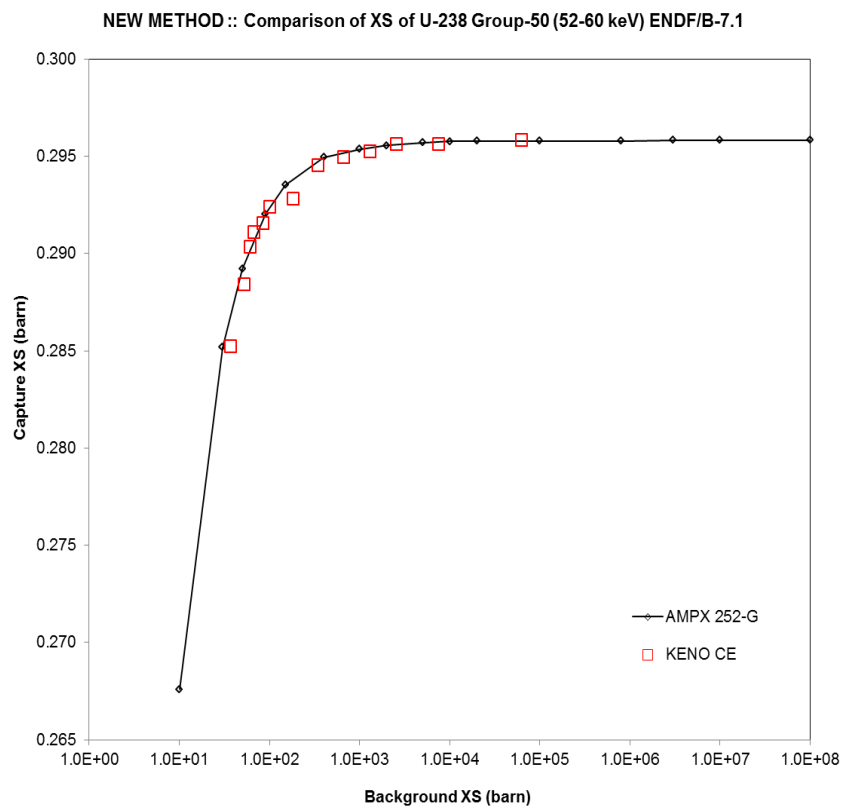
F-Factors now generated using probability tables typically used for continuous-energy Monte Carlo analysis

Prude



Probability table



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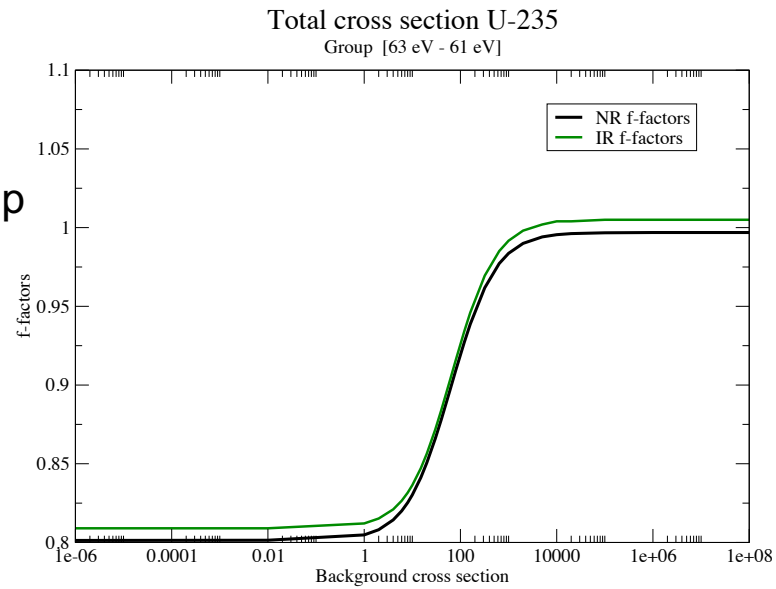
Homogenous F-Factor for Intermediate Resonance Treatment

- SCALE MG libraries provide F-factors for the full energy range.
- Intermediate resonance (IR) parameters account for overlap of resonances.
- Our MG libraries contain homogenous IR F-factors for nuclides with A>40 in the resolved resonance range. Otherwise narrow resonance (NR) f-factors are used.
- Use modules PMC and CENTRM to calculate a shielded cross section, with a CE flux for a homogenous model



$$\left(\sigma_t^{(j)}(E,T)+\sigma_0\right)\varphi(\mathrm{E},\sigma_0,T)=\int_E^{E/\alpha^{(j)}}\frac{\sigma_s^{(j)}(E',\mathrm{T})\varphi(E',\sigma_0,\mathrm{T})}{(1-\alpha^{(j)})E'}dE'+\sigma_0\int_E^{\infty}\frac{\varphi(E',\sigma_0\,\mathrm{T})}{E'}dE'$$

$1-\alpha^{(j)}$ = the maximum fractional energy loss in an elastic collision with nuclide j;

$\sigma_0=\frac{N^{(H)}}{N^{(j)}}\sigma_p^{(H)}$ (the background cross section);

$\sigma_p^{(H)}$ = the potential cross section for hydrogen;

If the desired scattering nuclide is not fissionable, a small amount of U-235 is added to the homogenous model

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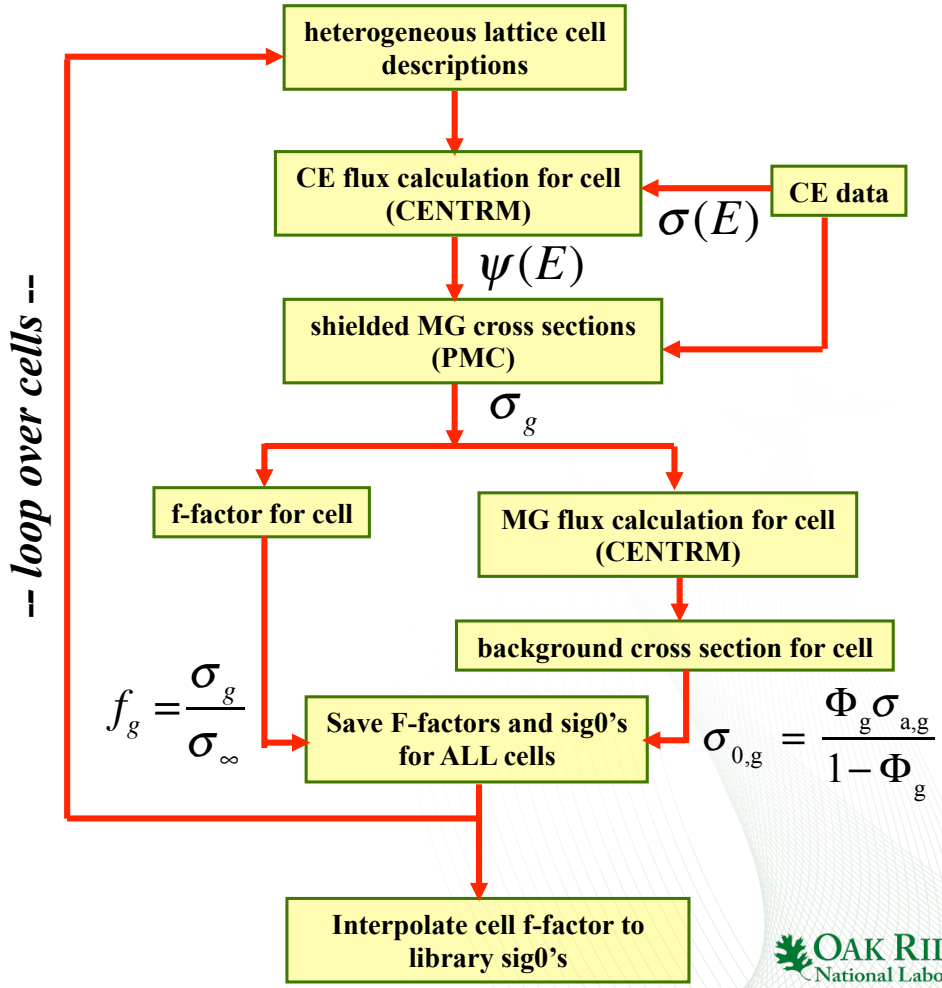
Heterogenous F-Factor for Intermediate Resonance Treatment

Similar to homogeneous f-factors, but:

- Heterogeneous models are used
- Background cross section can not be determined in advance
- A suite of heterogeneous models were developed for most common analysis scenarios



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Within Group Scattering F-Factors

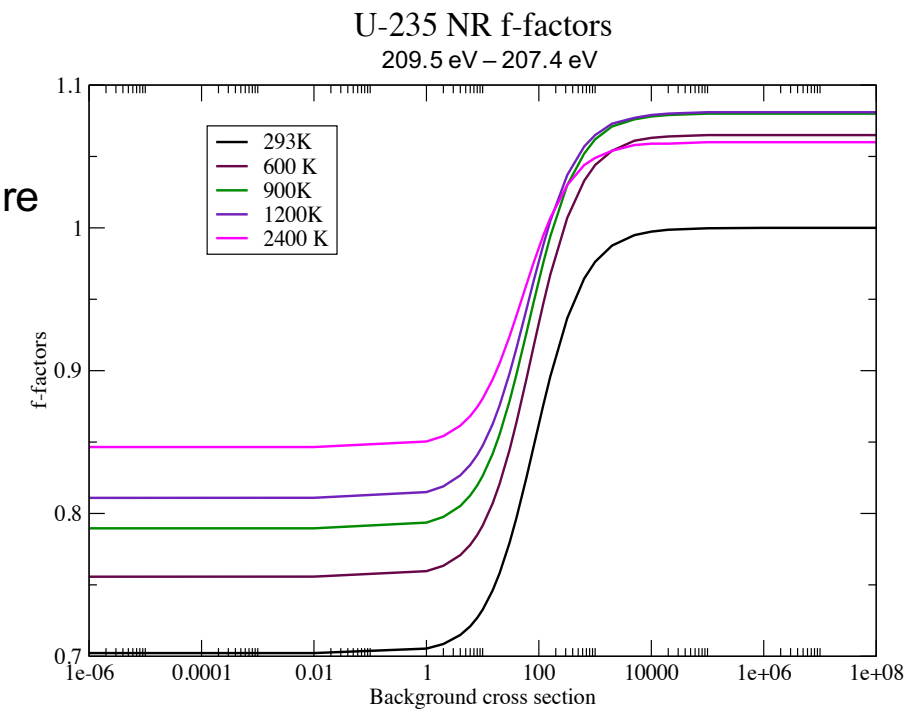
In order to account better for in-group elastic scattering, f-factors (NR and IR) are added to the MG library

For NR:

- Calculate the diagonal elements of the elastic scattering matrix, using the NR flux and temperature dependent 1D elastic point-data
- Calculate f-factor using the diagonal element of the elastic scattering matrix as a reference factor, i.e. infinite-dilute flux and 1D elastic at 293K

For IR:

- The same procedure is used as for other homogeneous or heterogeneous f-factors
- PMC generates a model dependent scattering matrix
- Calculate f-factors using the diagonal element of the shielded matrix and the the elastic scattering matrix as a reference factor



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Improvements in Polaris results due to new within-group scattering cross section

(Polaris is a new lattice physics depletion code developed for NRC)

Cross-section processing based on Bondarenko factors

- Improved Embedded Self-Shielding Methodology (ESSM) for resonance treatment
- New resonance self-shielding factors for within-group scattering cross section
- Removed reactivity bias as a function of temperature

PWR BOL Pin cell eigenvalue difference

Fuel T (K)	CE-KENO k-eff	Polaris (beta3)	Polaris (beta4)
600	1.18215	-82	-11
900	1.17172	-139	-8
1200	1.16260	-178	-8

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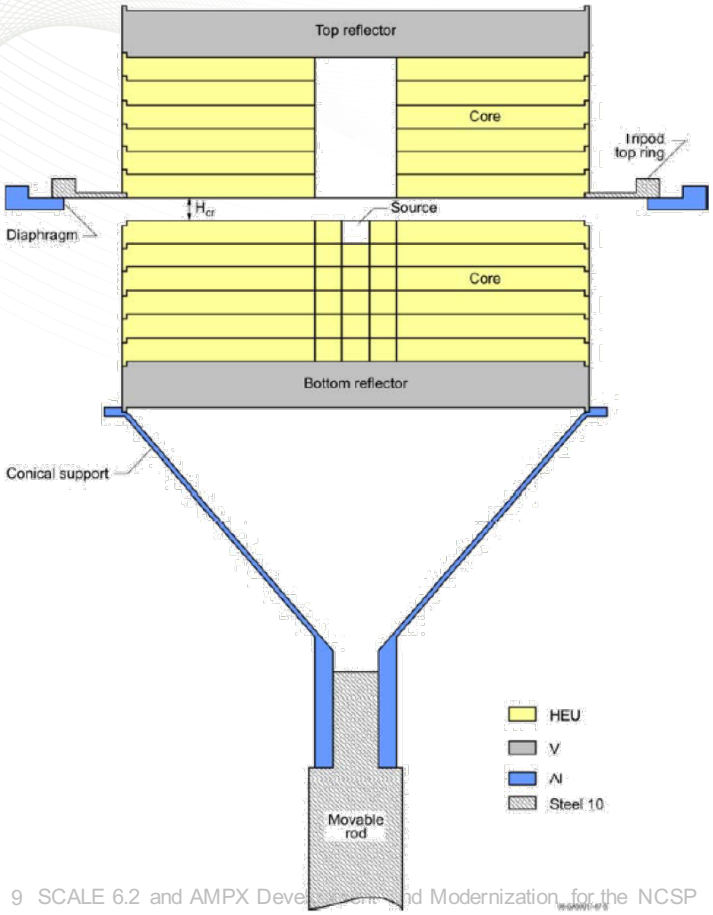
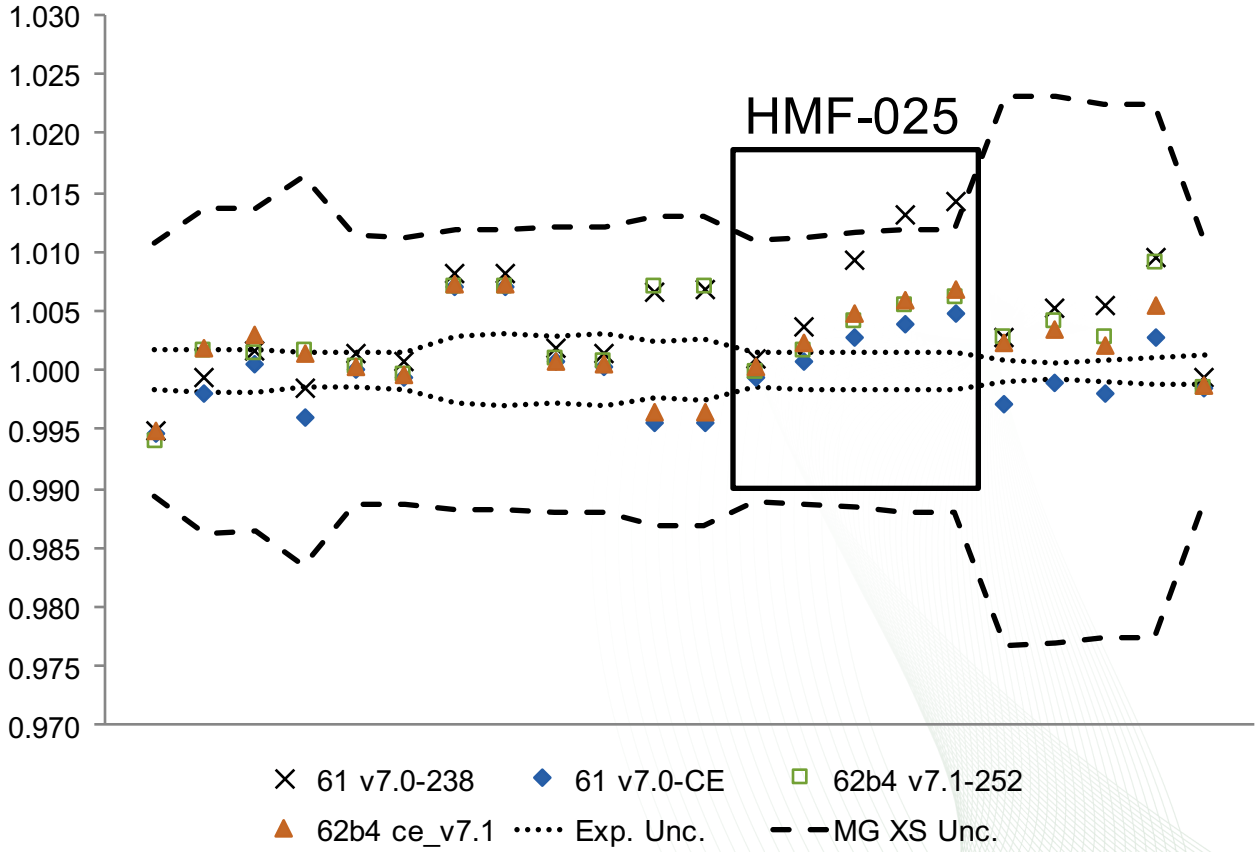
Improved KENO results for HEU-MET-FAST-025

Five Vanadium-Reflected HEU Cylinders





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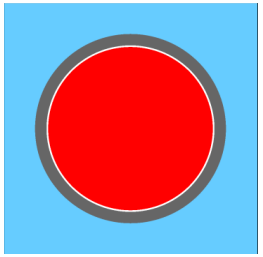
XSProc integrated with SCALE sequences

- Preparation of cross-sections for multigroup depletion and/or used fuel criticality analysis
- 18 fuel zones for infinite lattice calculation with axial burnup profile



Options	SCALE 6.1 (minutes)	SCALE 6.2 (minutes)	Speedup (6.1/6.2)
238 group CENTRM	112.1	27.4	**4.1**
252 group CENTRM	n/a	33.4	**3.4**
252 group BONAMI-IR	n/a	6.3	**17.9**

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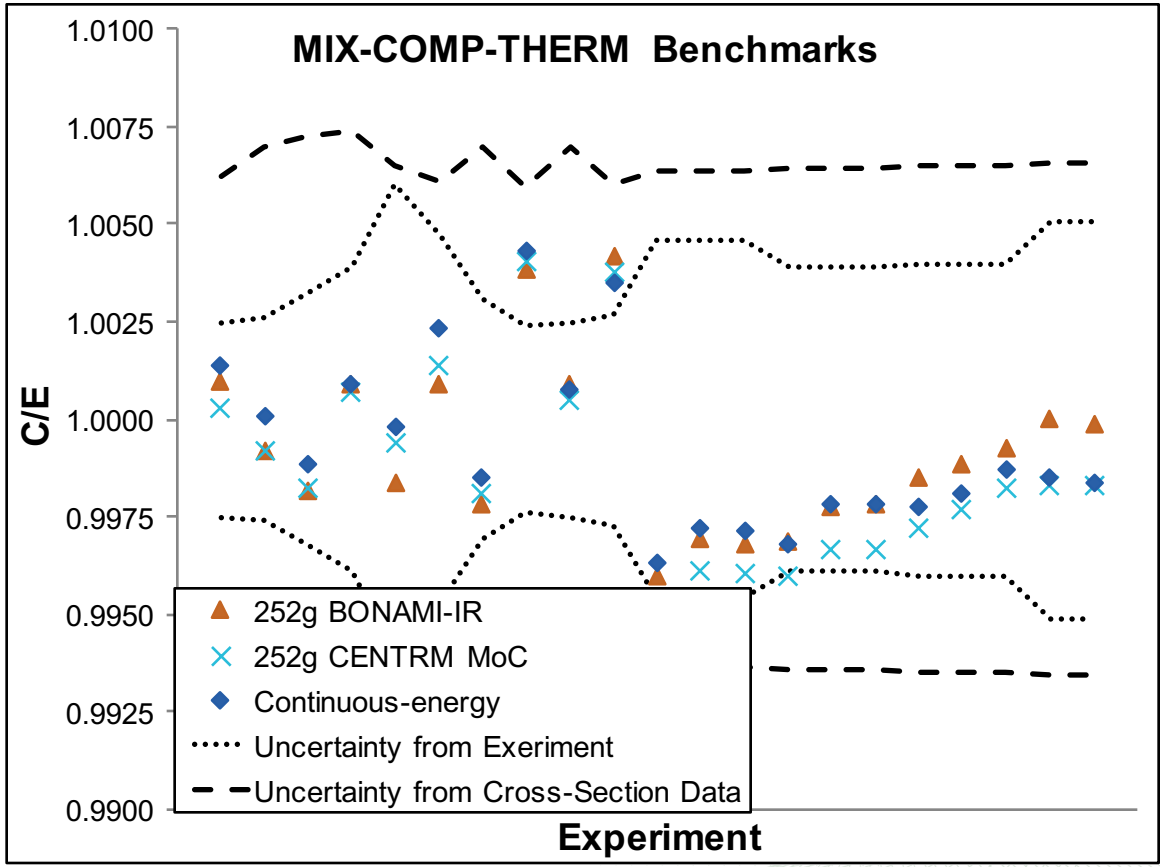
SCALE 6.2 Cross Section Data

- New CE cross-section data for neutron interactions, gamma yield, and gamma interactions
- ENDF/B-VII.1 nuclear data
- New MG neutron libraries
  - 252-group energy structure
  - 56-group energy structure
  - Intermediate resonance parameters
- Extensive test suite
  - ~400 VALID benchmarks
  - 7000 transmission tests
  - 5000 infinite medium tests
- New binary format replacing 40+ year-old AMPX format

AMPX now included with SCALE distribution so users can create their own libraries!



SCALE 6.2 Nuclear Data Libraries

Mnemonic names	Primary data source/format
v7-238 ; v7-238n ; v7.0-238n	ENDF/B-VII.0 238-group neutron library
v7.1-252n	ENDF/B-VII.1 252-group neutron library
v7.1-56n	ENDF/B-VII.1 56-group neutron library
v7.1-200n47g	ENDF/B-VII.1 200-group neutron/47-group gamma library
v7-200n47g ; v7.0-200n47g ; v7-200g47	ENDF/B-VII.0 200-group neutron/47-group gamma library
v7.1-28n19g	ENDF/B-VII.1 28-group neutron/19-group gamma library
v7-27n19g ; v7.0-27n19g	ENDF/B-VII.0 27-group neutron/19-group gamma library
ce_v7.1_endf	ENDF/B-VII.1 Continuous-energy neutron and gamma library
ce_v7 ; ce_v7_endf ; ce_v7.0_endf	ENDF/B-VII.0 Continuous-energy neutron and gamma library

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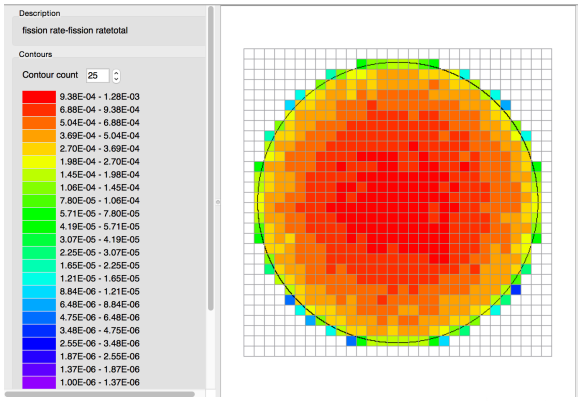
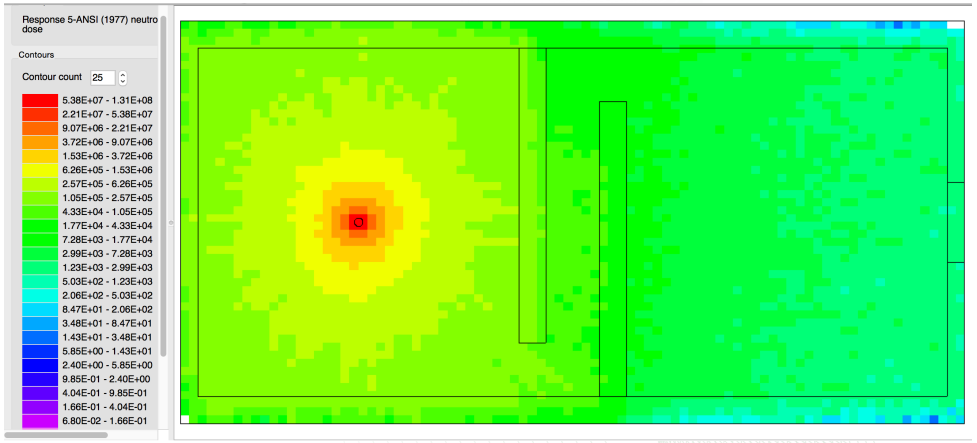
MAVRIC/Monaco Enhancements

- Continuous energy treatment
  - physics, dose responses, tallies
- More/better links to ORIGEN for source terms
  - Read spectrum from binary concentration file
  - Read in photon lines/intensities from ORIGEN data
- Improved statistical tests on tallies
- New statistical tests for mesh tallies
- Improvements on linking with Denovo
  - Macromaterials for better deterministic models
  - Denovo – more parameters, double precision output
- Improved link with KENO-VI for CAAS Problems
- MAVRIC Utilities – for post-processing





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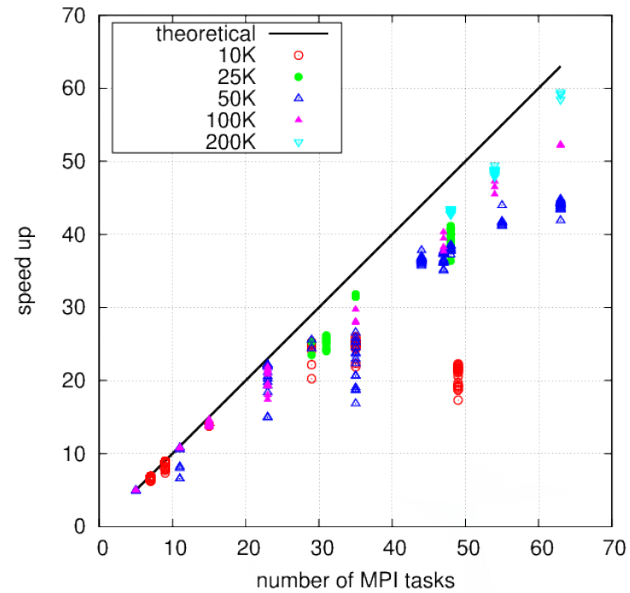
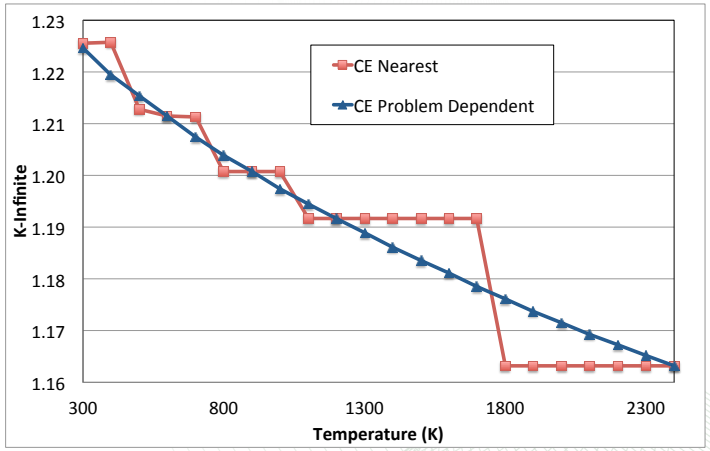
KENO Improvements

- Substantial reduction in memory requirements – over 99% improvement in many cases
- Accuracy improvements through comprehensive review and testing
- Parallel Computations
  - Significant speedups with MPI on Linux clusters
- Source Convergence
  - Sourcerer – Hybrid sequence to deterministic converge fission source
  - Shannon Entropy diagnostics
- Problem-Dependent Doppler broadening for CE calculations for thermal, resolved, and unresolved energy ranges
- Resonance upscatter treatment
  - Significant improvement in elevated temperature CE Monte Carlo





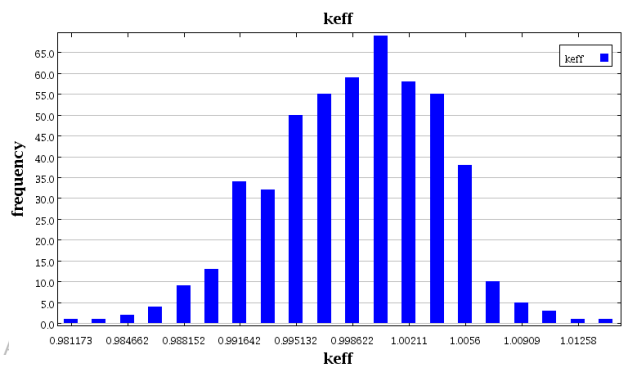
Enhanced Sensitivity and Uncertainty Analysis Tools

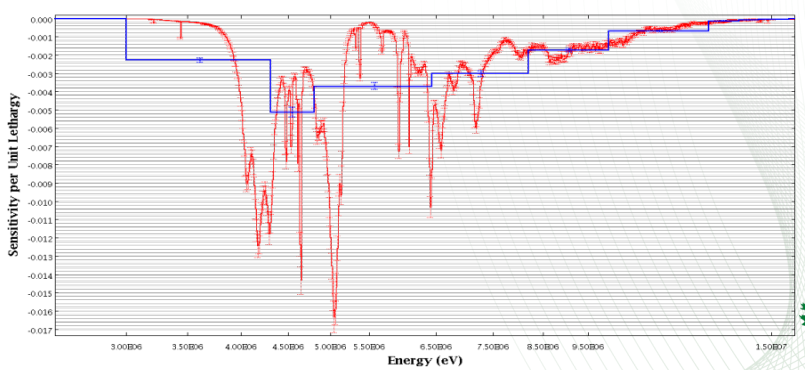
Sampler: Stochastic Uncertainty and Correlation Analysis

- Sampler provides uncertainties and correlation in any computed result from any SCALE sequence due to uncertainties in:
  - neutron cross sections
  - fission yield and decay data
  - geometry and composition

TSUNAMI: Adjoint-based Sensitivity Analysis

- Continuous-energy TSUNAMI-3D enhanced for improved runtime performance and improved stability.
- Generalized responses such as reaction rate ratios move to production capability.
- Multigroup group TSUNAMI-3D integrated with modern XSProc SCALE sequences





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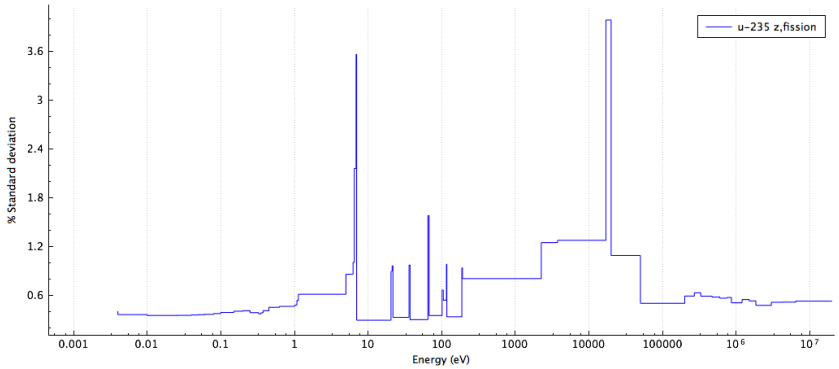
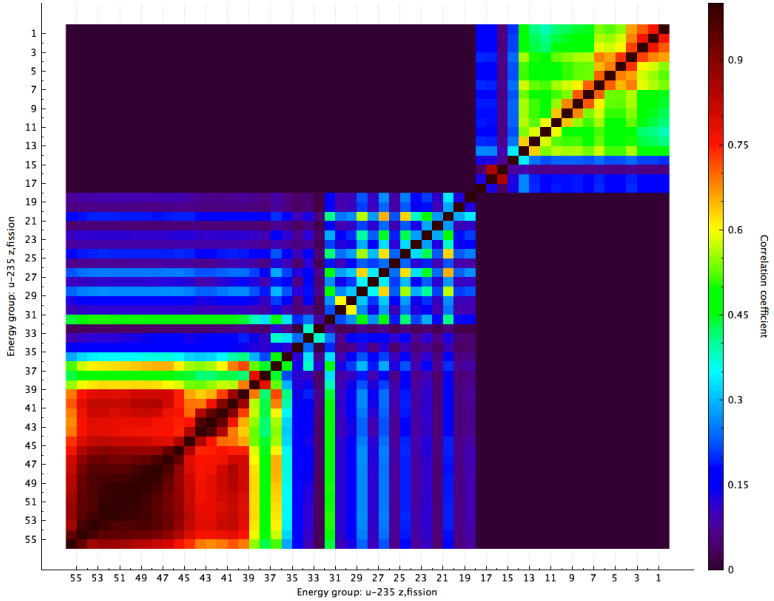
SCALE 6.2 Covariance Library

- ENDF/B-VII.1 for 187 isotopes
- SCALE 6.1 data retained for ~215 missing nuclides
- Modified ENDF/B-VII.1 ^{239}Pu nubar, ^{235}U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF/A repository
- Fission spectrum (chi) uncertainties processed from ENDF/B-VII.1 and from JENDL 4.0 (minor actinides)
  - Previous SCALE chi uncertainties were generated from Watt spectrum data and data were missing for minor actinides
- 56- and 252-group energy structures





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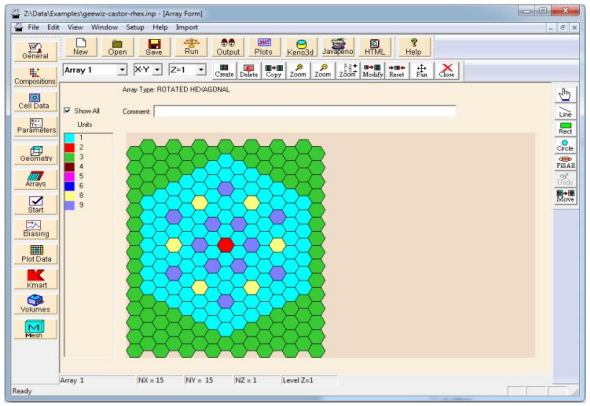
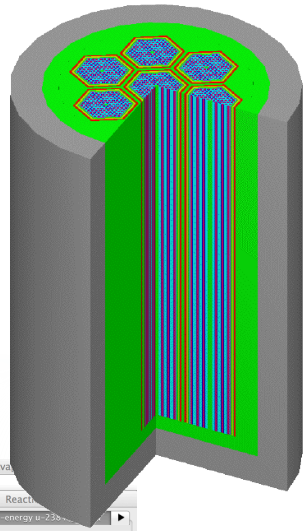
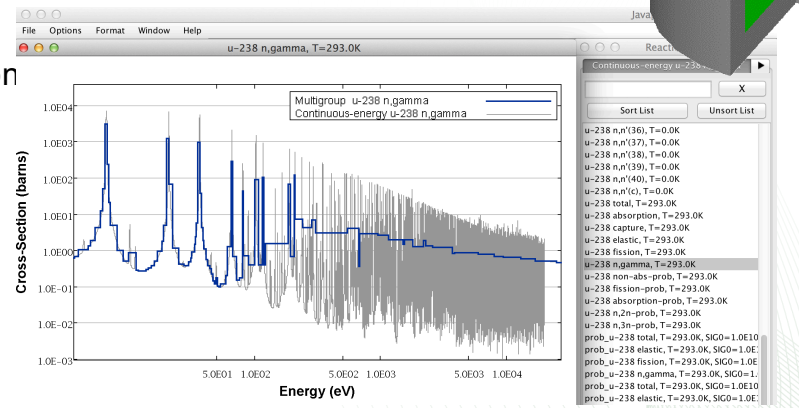
Previous User-Interfaces – Memory Lane

- **GEEWiz** (Graphically Enhanced Editor Wizard)
  - ~2000, Windows only, technology
  - was THE SCALE input editor supporting most Control Modules
- **Javapeño** (Java Plots Especially Nice Output)
  - Cross platform (Java) plotting program
  - Plots most SCALE data formats
- **Meshview**
  - Plots mesh tallies from Monaco and KENO
- **ChartPlot**
  - Plots tallies from Monaco
- **KENO3D – still available in 6.2**
  - KenoVa/VI (approximate) 3D Geometry Visualization+Verification
  - ~2000, Windows only, technology
- **OrigenArp**
  - ~2000, Windows only, technology
  - Convenience front-end for Origen-Arp
- **PlotOPUS**
  - ~2000, Windows only, technology
  - Plots Origen-Arp generated, OPUS post-processed results







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Fulcrum – Text-based input Creation, Visualization, and Review

SCALE

File Edit View Run Help

Reload MIX-COMP-THERM-004-001.inp | Save MIX-COMP-THERM-004-001.inp | Save MIX-COMP-THERM-004-001.inp as | Close tab | Print | Cut | Copy | Paste | Undo | Redo | Find

MIX-COMP-THERM-004-001.inp*

document | SCALE 6.2 | Run

```
99    cds=yes
100   flx=yes
101   fdn=yes
102 end parm
103 '
104 read geometry
105 'fuel cell
106 unit 1
107 array 1 3r0.0
108 'empty cell proximate to fuel array (immediate three cells)
109 unit 2
110 array 2 3r0.0
111 'empty cell removed from fuel array (beyond three cells)
112 unit 3
113 array 3 3r0.0
114 'units 101 thru 107 stack to make the fuel cell
115 unit 101
116 cylinder   6 1    0.5325    4.445  0.0
117 cylinder   19 1    0.6115    4.445  0.0
118 cuboid     8 1  4p0.9125    4.445  0.0
119 unit 102
120 cylinder   6 1    0.5325    0.6    0.0
121 cylinder   9 1    0.6115    0.6    0.0
122 cuboid     6 1  4p0.9125    0.6    0.0
123 unit 103
124 cylinder   6 1    0.5325   11.785  0.0
125 cylinder   9 1    0.6115   11.785  0.0
126 cuboid     8 1  4p0.9125   11.785  0.0
127 unit 104
128 cylinder   1 1    0.5325   59.55   0.0
129 cylinder   2 1    0.6115   59.55   0.0
130 cuboid     3 1  4p0.9125   59.55   0.0
```

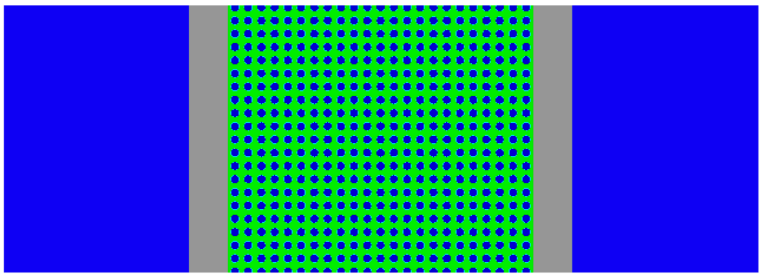
```
117:12: mixture value "19" does not exist in set: [ ../../../../comps/stdcomp/mixture
    ../../../../comps/stdcomp/alias
    ../../../../comps/atomcomp/mixture
    ../../../../comps/atomcomp/alias
    ../../../../comps/wtptcomp/mixture
    ../../../../comps/wtptcomp/alias
    ../../../../comps/arbmcomp/mixture
    ../../../../comps/arbmcomp/alias
    ../../../../comps/solution/mix/mixture
    ../../../../comps/solution/mix/alias
    ../../../../cells/infhommed/cellmix/mixture
    ../../../../cells/infhommed/cellmix/alias
    ../../../../cells/lattice/cellmix/mixture
```

Line: 117, Col: 12 /tsunami_3dk5/geometry/unit/cylinder/mixture | Validation | Messages

energy | pu-239-fission to pu-239-fission - Correlation coefficient matrix | MIX-COMP-THERM-004-001.inp : geometry (Line 104)

Top (X-Y) | Front (X-Z) | Side (Y-Z) | 3D | Meshes

Material | 2.8070x zoom

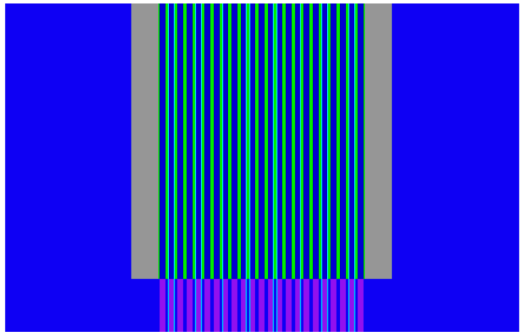


Origin: (4.61853e-14, 4.61853e-14, 22.5063)

MIX-COMP-THERM-004-001.inp : geometry (Line 104)

Top (X-Y) | Front (X-Z) | Side (Y-Z) | 3D | Meshes

Material | 2.2938x zoom



Origin: (4.61853e-14, 4.61853e-14, 22.5063)

Fulcrum – Input Autocompletion

SCALE

File Edit View Run Help

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MIX-COMP-THERM-004-001.inp*

document | SCALE 6.2 | Run

```
115 unit 101
116 cylinder   6 1    0.5325    4.445  0.0
117 cylinder   9 1    0.6115    4.445  0.0
118
119 sphere          - kenova (configurable)
120 sphere
121 hemisphere      - kenova (configurable)
122 hemisphere
123 hemisphe+x
124 hemisphe-x
125 hemisphe+y
126 hemisphe-y
127 hemisphe+z
128 hemisphe-z
129 xcylinder       - kenova (configurable)
130 xcylinder
131 xhemicyl+y
132 xhemicyl-y
133 xhemicyl+z
134 xhemicyl-z
135 ycylinder       - kenova (configurable)
136 ycylinder
137 yhemicyl+x
138 yhemicyl-x
139 yhemicyl+z
140 yhemicyl-z
141 cylinder
142 zcylinder       - kenova (configurable)
143 zcylinder
144 zhemicyl+x
145 zhemicyl-x
146 zhemicyl+y
    zhemicyl-y
    cube            - kenova (configurable)
    cube
    cuboid          - kenova (configurable)
    cuboid
    array           - kenova (configurable)
    array
    hole            - kenova (configurable)
    hole
```

Line: 118, Col: 1 /tsunami_3dk5/geometry/unit/cuboid/decl | Validation | Messages

energy | pu-239-fission to pu-239-fission - Correlation coefficient matrix | MIX-COMP-THERM-004-001.inp : geometry (Line 104)

Top (X-Y) | Front (X-Z) | Side (Y-Z) | 3D | Meshes

Material | 2.8070x zoom

Origin: (4.61853e-14, 4.61853e-14, 22.5063)

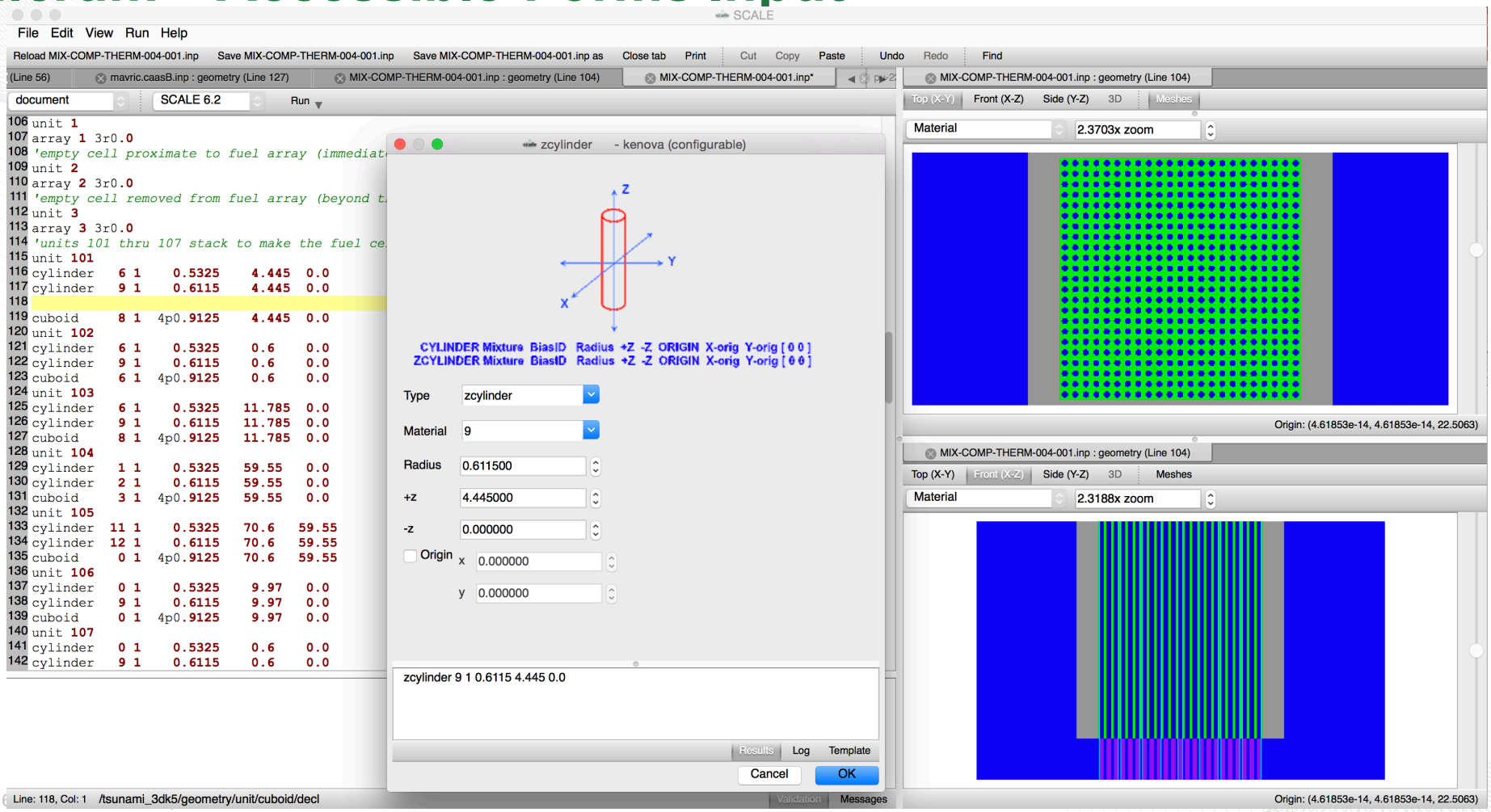
MIX-COMP-THERM-004-001.inp : geometry (Line 104)

Top (X-Y) | Front (X-Z) | Side (Y-Z) | 3D | Meshes

Material | 2.2938x zoom

Origin: (4.61853e-14, 4.61853e-14, 22.5063)

Fulcrum – Accessible Forms Input



Fulcrum – Job Execution and Results Review

SCALE

File Edit View Run Help

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Navigation

Filter

- ce_v7.1_endf.xml
- mavric.caasB.inp
  - document
- MIX-COMP-THERM-004-001
  - document
- MIX-COMP-THERM-00
- MIX-COMP-THERM-00
- MIX-COMP-THERM-00
- scale.rev08.252groupcov
- test1.inp*
  - document

Reload
Close
Open associated files ▸
- MIX-COMP-THERM-004-001.fissionSource.3dmap
- MIX-COMP-THERM-004-001.html
- MIX-COMP-THERM-004-001.inp.fulcrum.autosave
- MIX-COMP-THERM-004-001.kenoNuBar.txt
- MIX-COMP-THERM-004-001.msg
- MIX-COMP-THERM-004-001.out
- MIX-COMP-THERM-004-001.sdf

MIX-COMP-THERM-004-001.inp*

document | SCALE 6.2 | Run

```
114 'units 101 thru 107 stack to make the fuel cell
115 unit 101
116 cylinder    6 1     0.5325     4.445   0.0
117 cylinder    9 1     0.6115     4.445   0.0
118 cuboid      8 1   4p0.9125     4.445   0.0
                1     0.5325     0.6     0.0
                1     0.6115     0.6     0.0
123 unit 103
124 cylinder    6
```

43 13:12:34 2016

```
720      294                                                  13228E+0
721
722      295      9.98794E-01   9.96018E-01   5.79824E-04   4.14942E+0
723
724      296      9.99152E-01   9.96034E-01   5.77463E-04   4.15096E+0
725
726      297      9.92096E-01   9.96014E-01   5.74272E-04   4.12909E+0
727
728      298      1.00478E+00   9.96058E-01   5.71518E-04   4.10371E+0
729
730      299      9.98205E-01   9.96069E-01   5.69572E-04   4.11293E+0
731
732      300      9.89361E-01   9.96036E-01   5.67037E-04   4.13145E+0
733
734
735  mix-comp-therm-004-001
736                generation      average       avg k-eff      generati
737   generation  k-effective    k-effective     deviation        entrop
738
739      301      9.86169E-01   9.95986E-01   5.69295E-04   4.12618E+0
740
741
742  mix-comp-therm-004-001
743          ******      final results table      ******
744  best estimate system k-eff 0.99594 + or - 0.00056
745
746  Energy of average lethargy of Fission (eV) 1.42167E-01 + or -  2.
747  k-effective satisfies the chi**2 test for normality at the 95 % l
748
```

Line: 117, Col: 39 /tsunami_3dk5/geometry/unit/cylinder/dimensions/zb Validation Messages

energy | pu-239-fission to pu-239-fission - Correlation coefficient matrix | MIX-COMP-THERM-004-001.inp : geometry (Line 104)

Top (X-Y) | Front (X-Z) | Side (Y-Z) | 3D | Meshes

Available meshes	Min bound	Max bound	Custom min bound	Custom m
group 252 - rel. uncert.	4.758684672657654e-02	1.000004538615941e+00		
fission rate - total	4.423782739276514e-10	1.337129179263576e-05		
fission rate - total, abs. uncert.	4.423783104879541e-10	9.840817476974088e-07		
fission rate - total, rel. uncert.	4.758689377984851e-02	1.000000117029994e+00		

Overlay | 2.8194x zoom

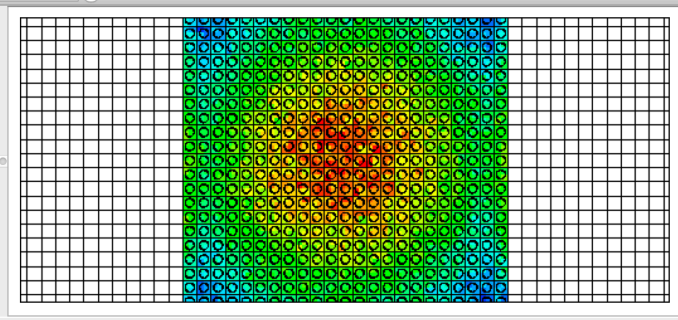
Description

fission rate-fission ratetotal

Contours

Contour count 25

- 1.28E-05 - 1.34E-05
- 1.23E-05 - 1.28E-05
- 1.18E-05 - 1.23E-05
- 1.12E-05 - 1.18E-05
- 1.07E-05 - 1.12E-05
- 1.02E-05 - 1.07E-05



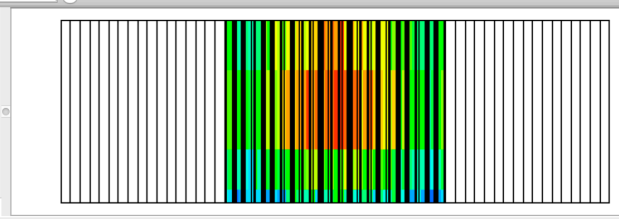
Origin: (4.61853e-14, 4.61853e-14, 22.5063)

MIX-COMP-THERM-004-001.inp : geometry (Line 104)

Top (X-Y) | Front (X-Z) | Side (Y-Z) | 3D | Meshes

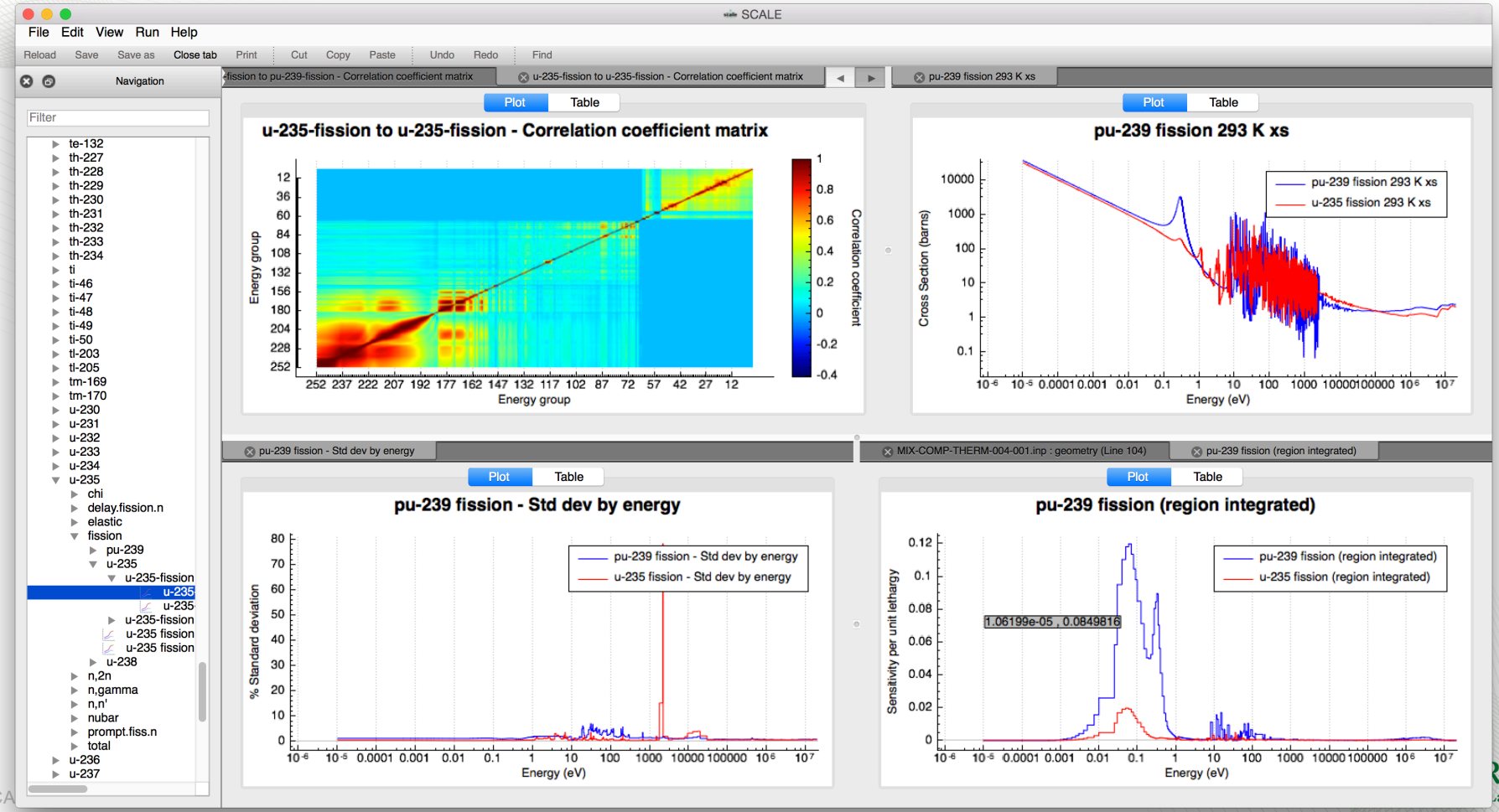
Overlay | 4.3834x zoom

- 1.28E-05 - 1.34E-05
- 1.23E-05 - 1.28E-05
- 1.18E-05 - 1.23E-05
- 1.12E-05 - 1.18E-05
- 1.07E-05 - 1.12E-05
- 1.02E-05 - 1.07E-05
- 9.63E-06 - 1.02E-05



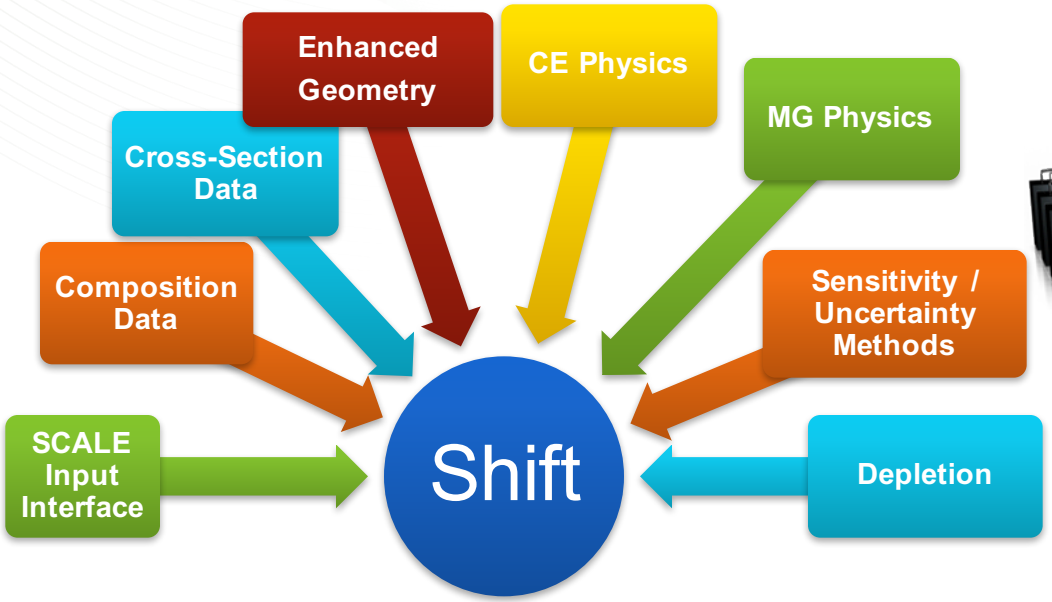
Origin: (4.61853e-14, 4.61853e-14, 22.5063)

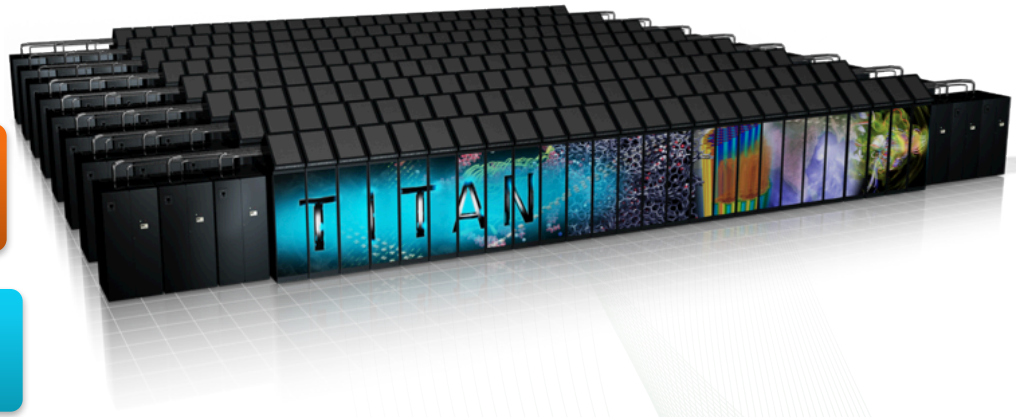
Fulcrum – Data Visualization



Beyond SCALE 6.2: Modular Capabilities Integrated for High-Performance Computing

Future SCALE Monte Carlo Code - Shift





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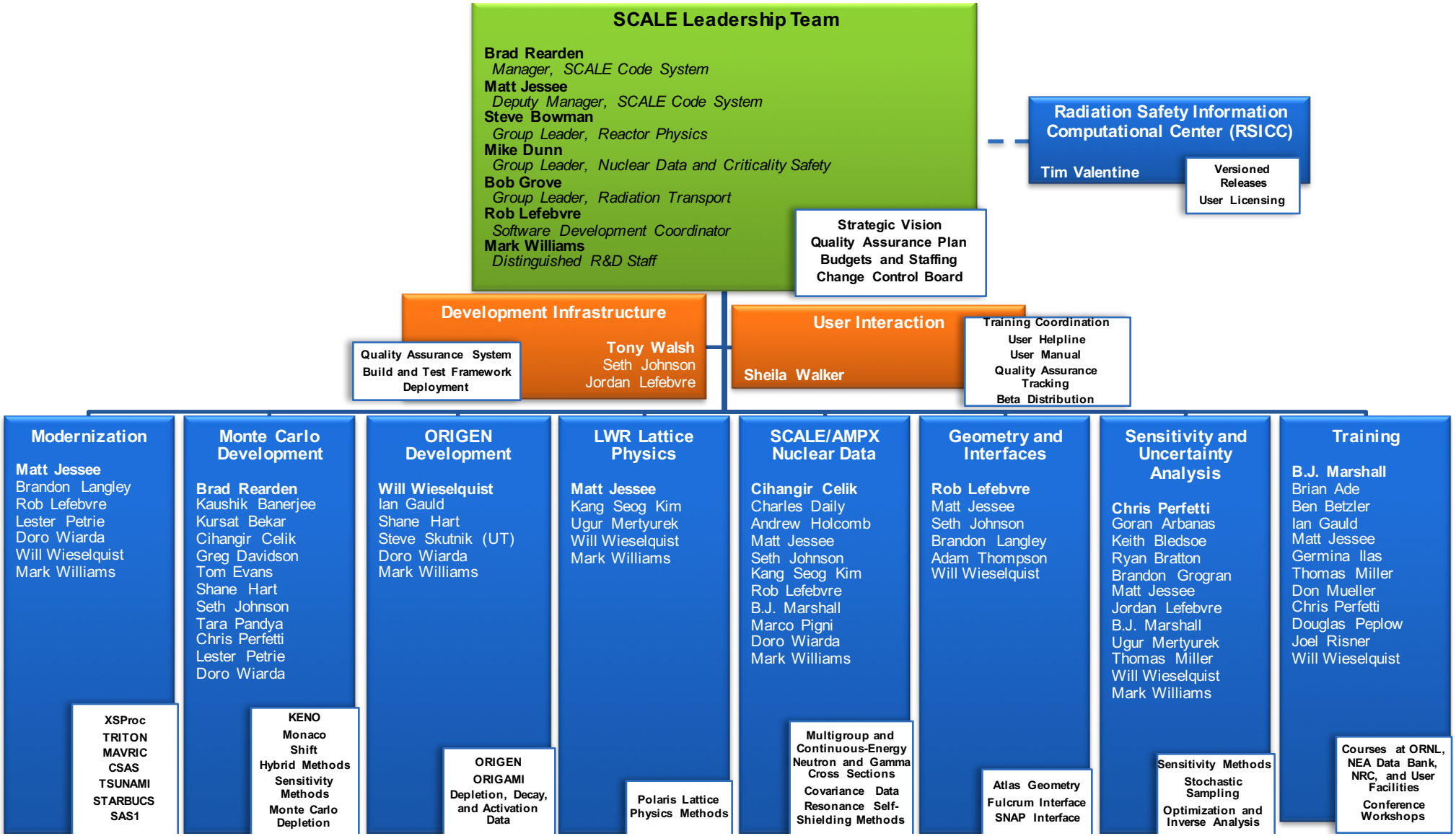
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