OAK RIDGE National Laboratory

SCALE 6.3 Overview

2021 SCALE Users' Group Workshop

Presenter: W. Wieselquist

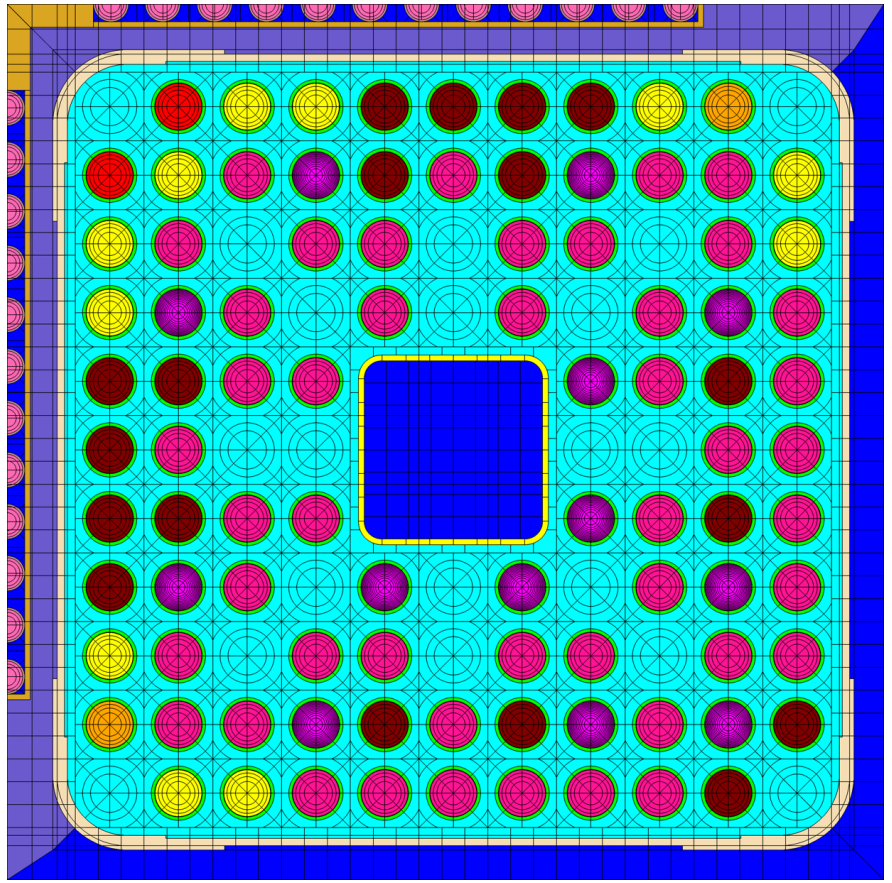
ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

Polaris in 6.3.0

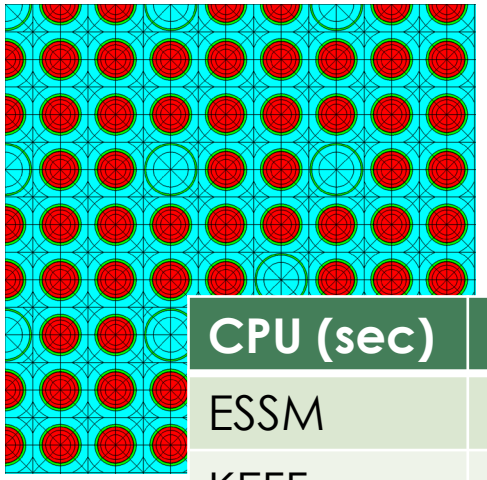
Product Owner: Matthew Jessee
Contributors: Kang Seog Kim, Shane Hart, Will Wieselquist, Jin Whan Bae, Ugur Mertyurek, Andrew Holcomb

- **Major Features**
  - Enhanced calculation archives
    - Reactor Libraries (F33) - new in 6.3
    - Nuclide Inventories (F71) - enhanced in 6.3
    - FG Nodal Cross sections – initial HDF5 in 6.3
    - Improved output summaries for each
  - Run-time improvement (>3x)
    - Faster transport solver (Next Slide)
    - New cell-based self-shielding method
- **Other improvements**
  - Enhanced BWR geometry modeling (channel geometry)
  - Time-dependent operating history with depletion
  - Easy to use input options for ATF materials
  - Improved Geometry robustness
- **All 6.3 enhancements driven by HALEU/HBU/ATF**



Polaris Speedups in Detail

- Polaris use cases investigated
  - 10-100 statepoint calculations for depletion/source term analysis
  - 100-1000 statepoint calculations for two-step core neutronics analysis
  - Statepoint: Self-Shelding (ESSM) + Eigenvalue (MOC) + Depletion (ORIGEN)
- Speedup investigations findings:
  - ESSM calculation takes too long
  - MOC calculation anisotropic source treatment could be optimized
- Resolution
  - Modified ESSM inner iteration to use fixed number of source iterations rather than BICGSTAB
  - Modified anisotopic source treatment to compute angular flux source pre-sweep



CPU (sec)	6.2.4	6.3.0*	Speedup
ESSM	158	28	5.6x
KEFF	251	79	3.1x
SUM	409	107	3.8x

- Additional 6.3 Improvements
  - Spurious geometry error defect has been resolved
  - Unnecessary BiCGSTAB warnings have been removed
  - Cell-based ESSM implemented (~30X speedup in ESSM) is implemented but not the default until library improvements
- Beyond 6.3
  - Additional reduction of energy groups on the fly (KEFF run-time reduction of 3X-5X
  - Octant symmetry (2X)
  - Branch-level parallelism

ORIGEN in 6.3.0

Product Owner: W. Wieselquist
Contributors: S. Hart, A. Holcomb, S. Skutnik,

- **Major Features**
  - Sensitivity coefficient
  - Overhaul of COUPLE (modernization)
  - Recoverable energy data updates
- **Other improvements**
  - Read ENDF decay/fission product yield data directly
  - OBIWAN command line utility
  - Isotopics interface file (e.g. for downstream MELCOR simulations)
- **Recent use in NRC Projects/Applications**
  - Decay heat for non-LWR severe accident
  - Decay heat, activity during decay for HALEU+HBU+ATF
  - Internal depletion solver for TRITON and Polaris

Sensitivity coefficient response table of change in number of atoms of Pu239 at EOL

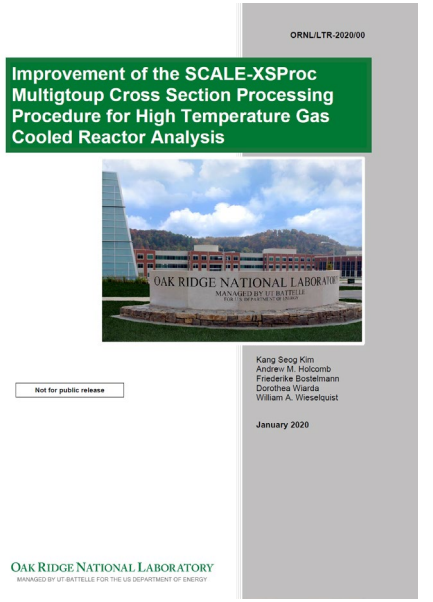
Parent	Daughter	MT	Type	Sens. Coeff.
Pu239	-	18	xs	-0.69
U238	Np239	102	xs	0.54
U239	-	-	decay	0.47
Pu239	Pu240	102	xs	-0.39
Pu238	Pu239	102	xs	0.02

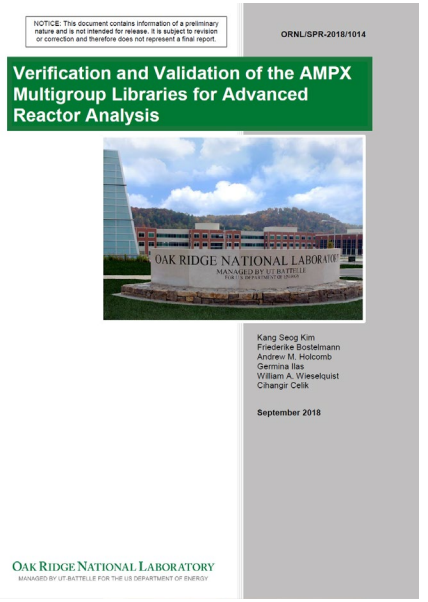
- A 1% increase in Pu239 fission cross section leads to a 0.69% DECREASE in Pu239
- A 1% increase in the total (n,g) for U-238, leads to a 0.54% INCREASE in Pu239

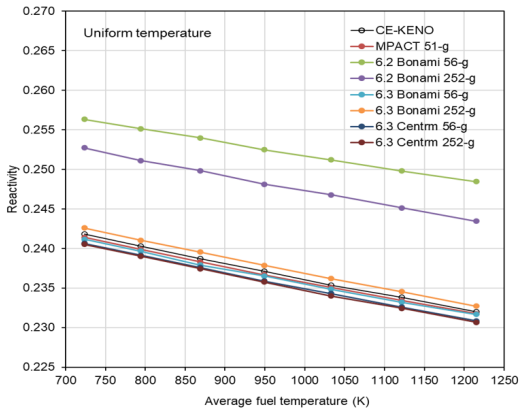
XSProc in 6.3.0

Product Owner: Kang Seog Kim
Contributors: Andrew Holcomb, Dorothea Wiarda, Rike Bostelmann, Will Wieselquist, Matthew Jessee

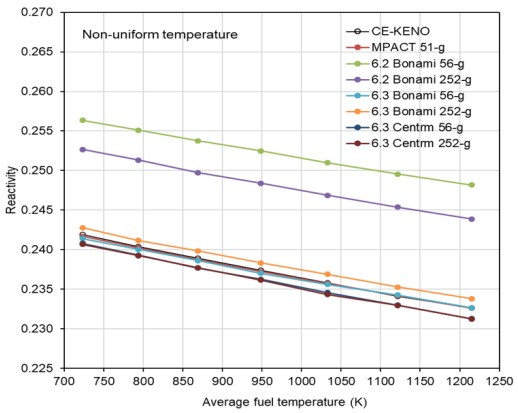
- **Major Features**
  - Enhanced accuracy
    - High temperature gas cooled reactor analysis
  - Multigroup library for advanced reactors
    - 1597-g library (all) & 302-g library (fast)
    - ENDF/B-VII.1 1-g library for MCDancoff
    - MADRE benchmark suite
  - Cell-based ESSM (>x30 speedup) next slide
- **Other improvements**
  - Intra-pin self-shielding method in BONAMI
    - M&C 2021 paper
- **Recent use in NRC Projects/Applications**
  - Pebble system depletion for HTGR/FHR
  - FHR special annular pebble







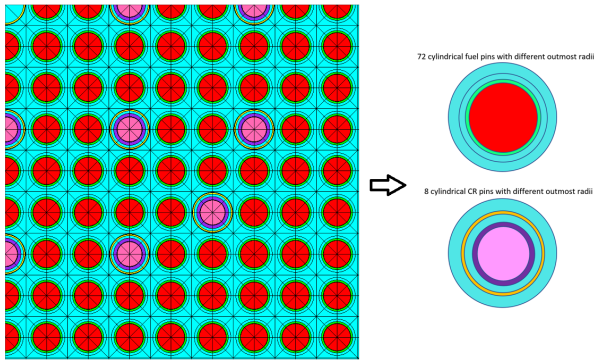
(a) Uniform temperature



(b) Nonuniform temperature

Cell-based Self-Shielding Speedups in Detail

- Cell-based ESSM (Embedded Self-shielding)
  - Dancoff calculation for fuel and control rods
  - Decompose Domain into 1D cylindrical cells to have same Dancoff factors



  - Solve the ESSM equations using 1D cylindrical collision probability
- Intra-pin self-shielding method
  - Same as the BONAMI intra-pin method
- Cell-based ESSM + Intra-pin self-shielding method
  - Precise intra-pin self-shielded cross sections

Case	CE-KENO	Polaris							
		k_{eff}	Δk	Time(sec)		k_{eff}	Δk	Time(sec)	
				ASSM-ESSM	transport			CELL-ESSM	transport
vera_ornl_1a	1.18700	1.18548	152	**0.69**	2.77	1.18550	150	**0.05**	2.68
vera_ornl_1b	1.18214	1.18050	164	**0.58**	2.61	1.18062	152	**0.04**	2.62
vera_ornl_1c	1.17144	1.17005	139	**0.59**	2.60	1.17017	127	**0.04**	2.78
vera_ornl_1d	1.16258	1.16108	150	**0.62**	2.73	1.16120	138	**0.04**	2.48
vera_ornl_1e	0.77127	0.77078	49	**0.64**	10.19	0.77079	48	**0.05**	9.36
vera_ornl_2a	1.18187	1.18097	90	**128.40**	222.00	1.18105	82	**1.40**	169.10
vera_ornl_2b	1.18323	1.18202	121	**162.50**	209.00	1.18216	107	**2.35**	199.50
vera_ornl_2c	1.17362	1.17248	114	**157.00**	163.40	1.17263	99	**2.27**	208.70
vera_ornl_2d	1.16556	1.16427	129	**137.40**	162.60	1.16442	114	**2.06**	153.40
vera_ornl_2e	1.06953	1.06869	84	**130.70**	168.00	1.06871	82	**1.66**	179.20
vera_ornl_2f	0.97569	0.97528	40	**167.70**	214.70	0.97525	44	**1.72**	170.20
vera_ornl_2g	0.84766	0.84784	-18	**109.70**	230.00	0.84548	218	**2.19**	208.20
vera_ornl_2h	0.78793	0.78615	178	**141.40**	171.80	0.78646	147	**2.02**	207.40
vera_ornl_2i	1.17962	1.17877	85	**122.80**	159.40	1.17885	77	**1.53**	173.00
vera_ornl_2j	0.97496	0.97452	44	**162.30**	216.10	0.97449	47	**2.20**	170.30
vera_ornl_2k	1.01977	1.01922	55	**138.40**	150.90	1.01914	63	**1.97**	170.50
vera_ornl_2l	1.01868	1.01694	174	**134.20**	601.00	1.01700	168	**1.69**	612.40
vera_ornl_2m	0.93855	0.93679	176	**116.20**	589.60	0.93684	171	**1.54**	568.00
vera_ornl_2n	0.86944	0.86774	170	**155.50**	629.10	0.86779	165	**1.87**	619.50
vera_ornl_2o	1.04717	1.04615	102	**106.00**	196.90	1.04651	66	**1.48**	190.80
vera_ornl_2p	0.92670	0.92586	84	**95.53**	162.70	0.92642	28	**1.31**	151.30

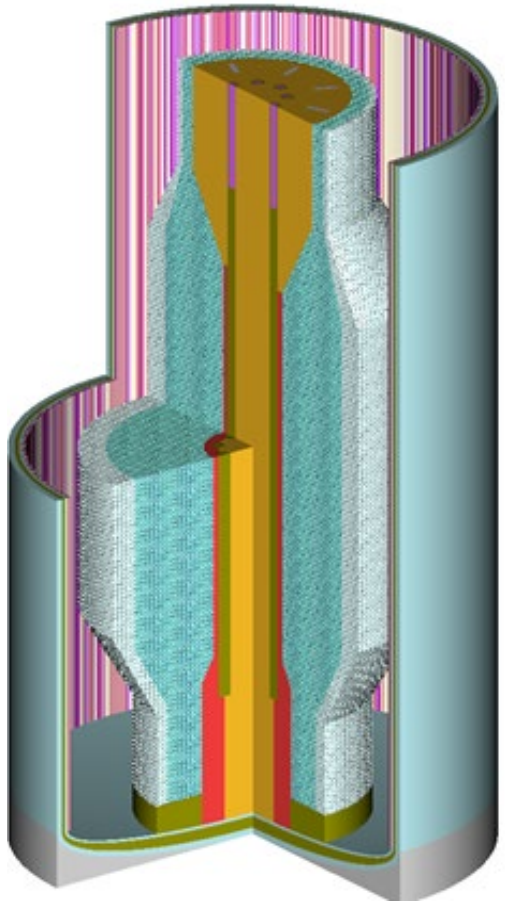
TRITON in 6.3.0

Product Owner: Rike Bostelmann
Contributors: Kursat Bekar, Brandon Langley, Shane Hart, Greg Davidson, Ben Betzler, Brian Ade, Ugur Mertyurek, Matt Jessee, Will Wieselquist

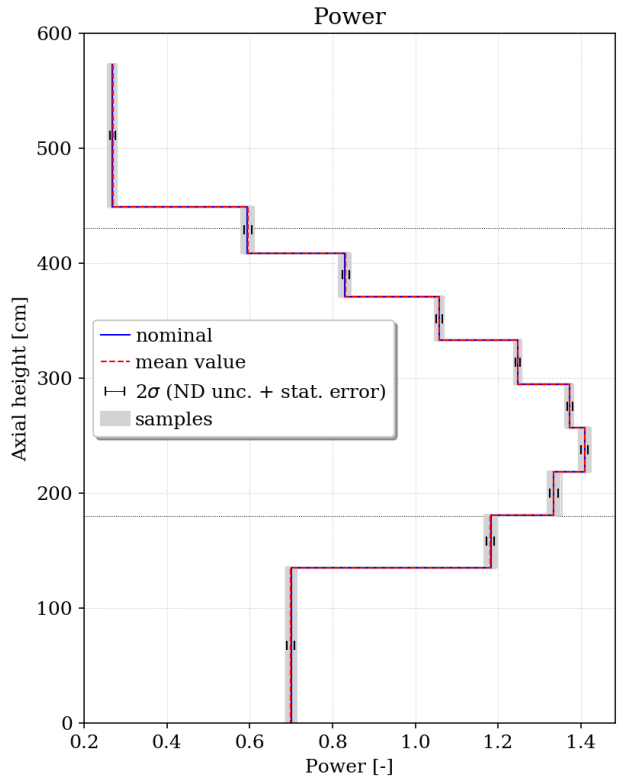
- **Major Features**
  - TRITON-Shift transport and depletion (CE and MG)
  - TRITON-Shift nodal data on cartesian mesh and global hexagonal mesh
  - Transport-only calculation
- **Other improvements**
  - Initial capability for feed and removal for MSR systems
  - Flexible, user-friendly tallying of flux, fission rate in TRITON-Shift with different (cartesian) meshes and group structures
  - Minor changes to parameter defaults
- **Recent use in NRC Projects/Applications**

  Non-LWR depletion calculations in Severe Accident and Nuclear Data Performance Assessment projects:
  - generation of representative isotopics
  - power profiles

Berkeley pebble-bed FHR



SCALE model

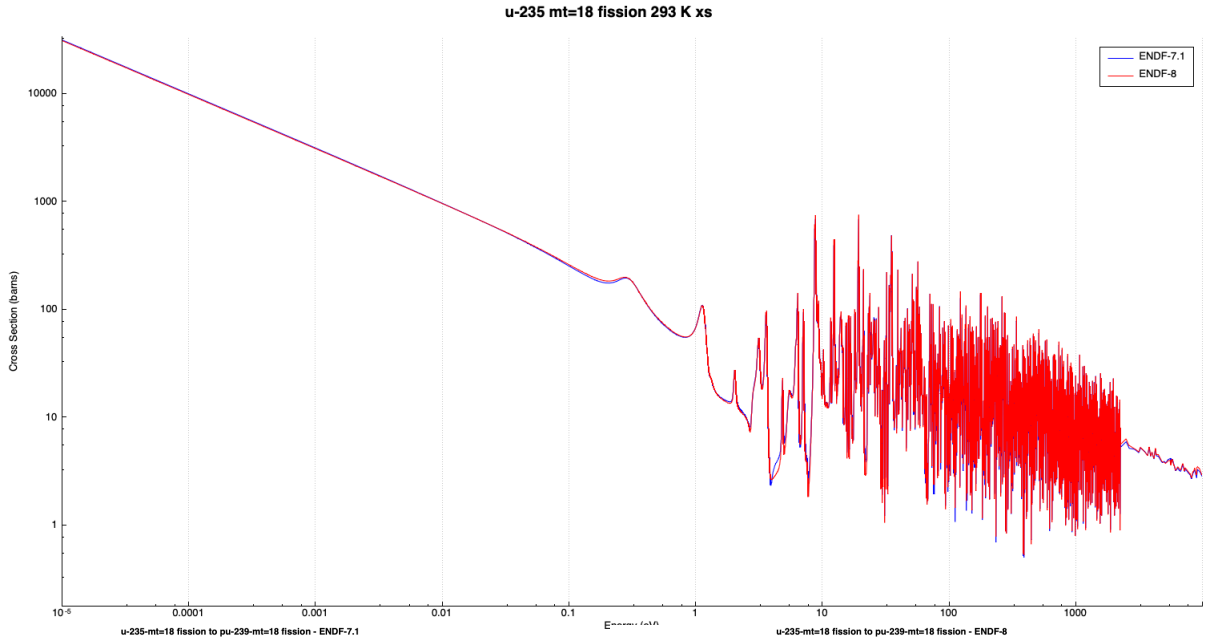


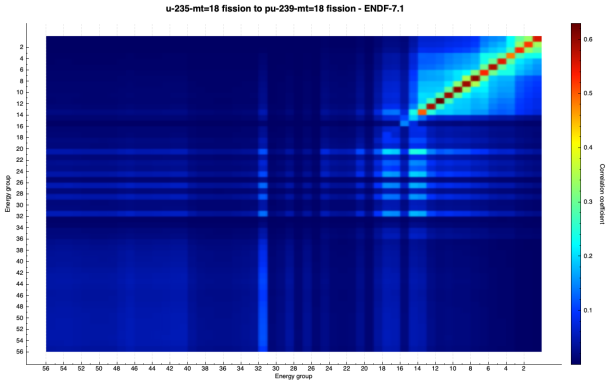
Axial power profile using transport-only

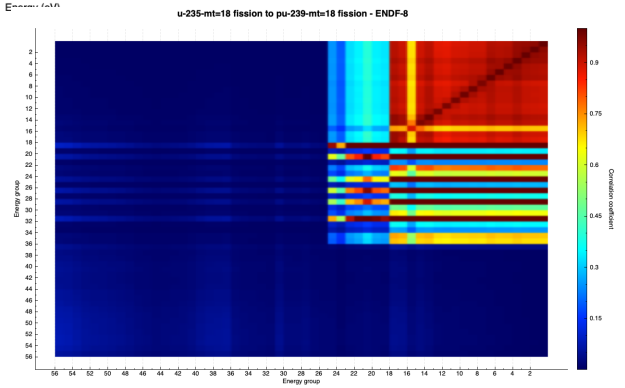
DATA in 6.3.0

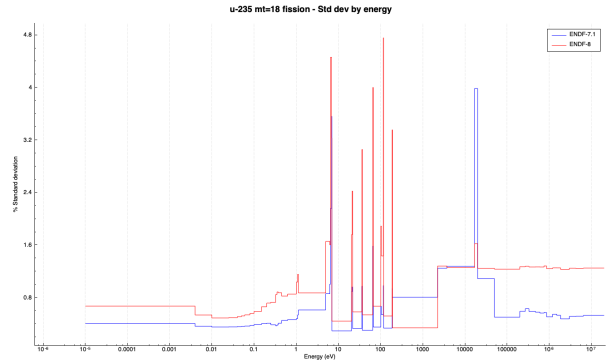
Product Owner: Andrew Holcomb
Contributors: Doro Wiarda, Rike Bostelmann, Kang Seog Kim

- **Major Features**
  - ENDF/B-VII.1 fixed probability tables
  - ENDF/B-VIII.0 (CE, MG in 56, 252, 302, 1597 groups)
  - Patched covariance data
- **Other improvements**
  - Migrating data resources to HDF5 format
  - Coupled libraries (56n19g, 252n47g)
  - Kinetics data with perturbations
- **Recent use in NRC Projects/Applications**
  - Every SCALE application
  - Sampler (estimate uncertainty in beta effective)
  - Nuclear data gap analysis







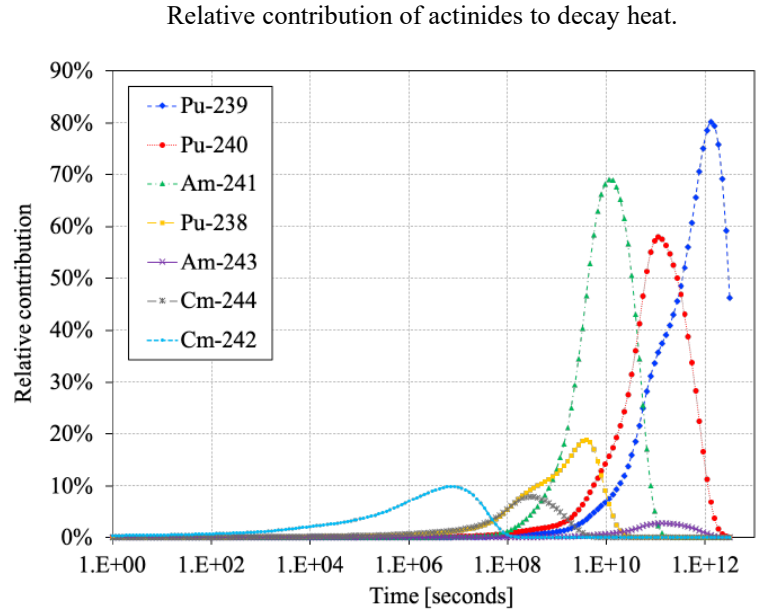


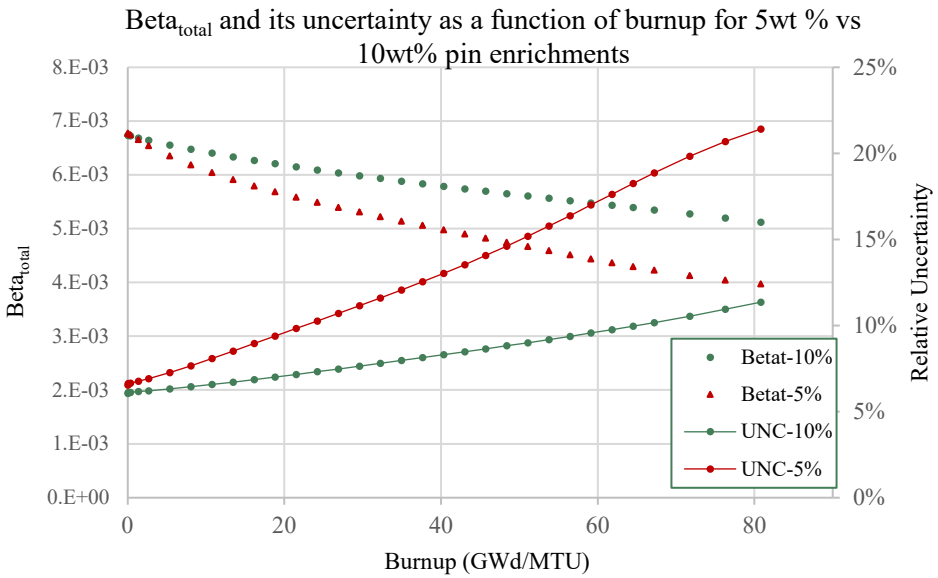
OAK RIDGE National Laboratory

Sampler in 6.3.0

Product Owner: Ugur Mertyurek
Contributors: Andrew Holcomb, Rike Bostelmann, Rob Lefebvre, Brandon Langley

- **Major Features**
  - Uncertainty quantification for kinetics parameters
  - Sensitivity Index calculation
  - Standardized distribution functions
- **Other improvements**
  - Multi-thread run capability (lost in 6.2.3)
  - Fulcrum integration and input error checking
  - Various parametric study improvements (mainly for NCSP applications)
- **Recent use in NRC Projects/Applications**
  - RP investigations on HALEU/HBU fuel
    - Decay heat and kinetic parameter trends
  - Regal RCA measurements
    - Uncertainty contributions to Gd isotopes C/M



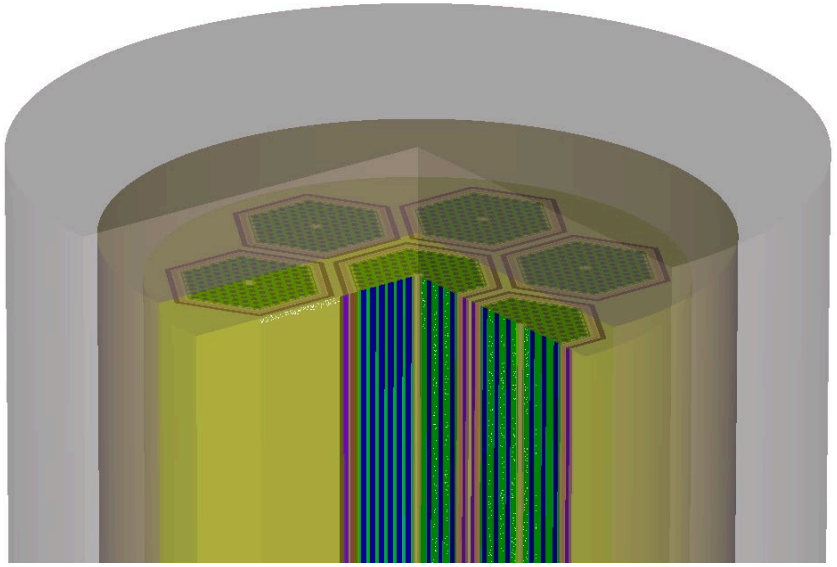


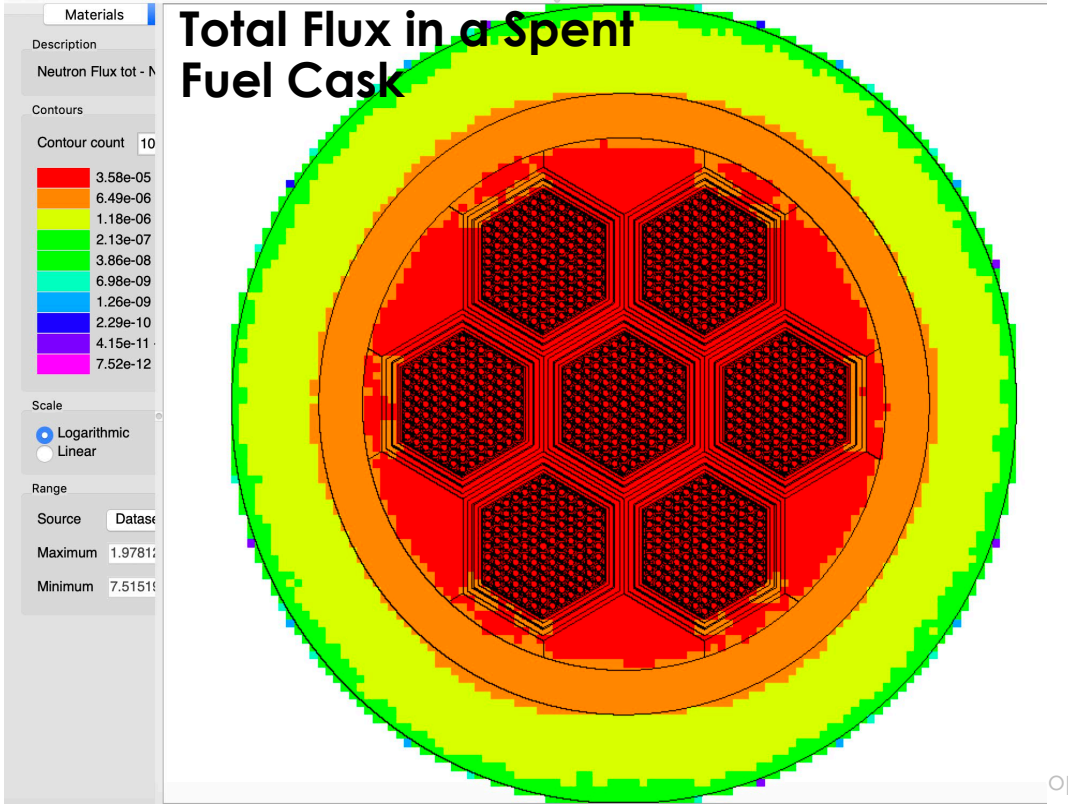
OAK RIDGE National Laboratory

CSAS in 6.3.0

Product Owner: Kursat Bekar
Contributors: Brandon Langley, Greg Davidson, B.J. Marshall

- **Major Features**
  - CSAS_Shift transport (both MG and CE)
- **Other improvements**
  - Capability to support the specification and use of multiple energy group boundaries in KENO
  - New input blocks to provide flexible/user-friendly tally specification (currently only flux, fission rate, fission source distribution mesh tallies are available) with both KENO and Shift
  - Reaction tallies with Shift transport
  - Diagnostic tallies with Shift transport
- **Recent use in Projects/Applications**
  - NRC Non-LWR Severe Accident Modeling & HALEU/HBU/ATF
  - NCSP experiment design



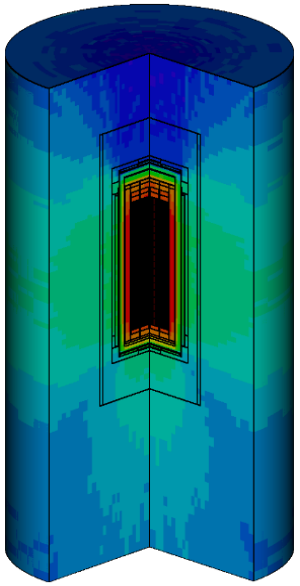


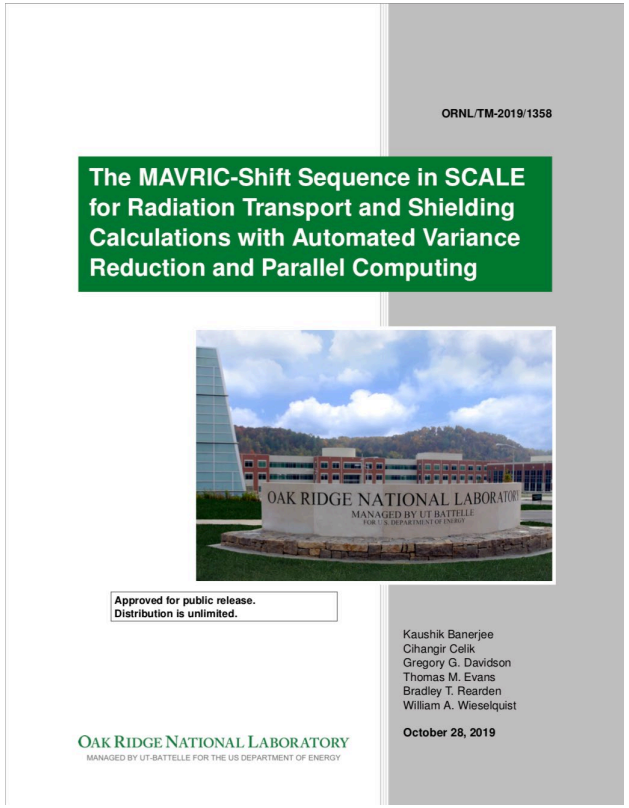
MAVRIC in 6.3.0

Product Owner: Cihangir Celik
Contributors: Gregory Davidson, Kaushik Banarjee, Kursat Bekar, Brandon Langley, and more.

- **Major Features**
  - parallel processing via Shift
- **Other improvements**
  - expanded flux-to-dose conversion factors
  - maintenance and bug fixes
  - Fulcrum integration
- **Recent use in Projects/Applications**
  - UNF&STANDARDS
  - storage and transportation of spent fuels
  - HALEU/HBU/ATF

Shift





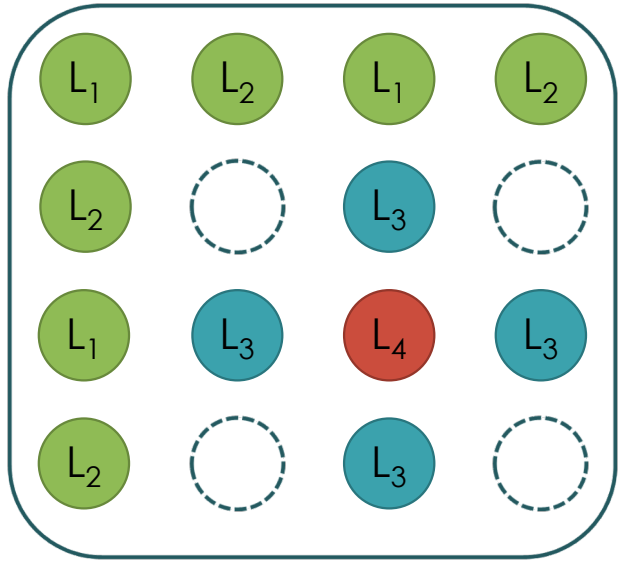
AOS-100 Dose Calculation Comparison

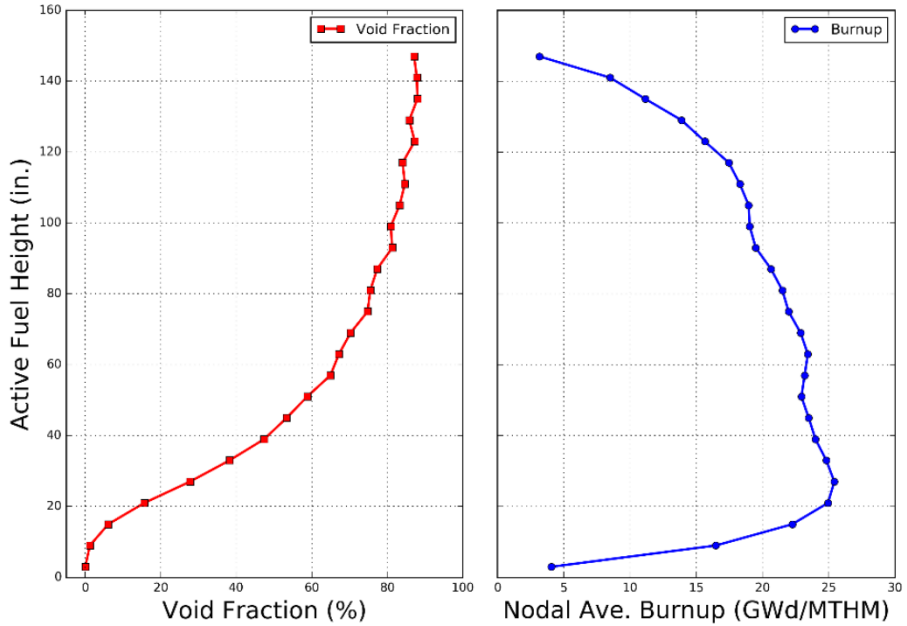
Sequence	Number of Processors	Wall Time (min)	FOM (1/min)
mavric	1	2340	1080
mavric-shift	1	1941	892
mavric-shift	4	967	436
mavric-shift	16	190	586
mavric-shift	256	18	372

ORIGAMI in 6.3.0

Product Owner: Steve Skutnik
Contributors: Rob Lefebvre, Will Wieselquist

- **No major changes to ORIGAMI core**
- **Related improvements**
  - New standard ORIGEN library format in HDF5, paving way for generality for LWR & non-LWR modeling
- **Recent use in Projects/Applications**
  - OBIWAN is used to post-process standard ORIGEN "f71" output files into "Inventory Interface" files which provide streamlined data transfer to MELCOR
  - ORIGAMI and OBIWAN are used by UNF-ST&NDARDS to add data to the database (using OBIWAN CSV output option)
  - Polaris now generates ORIGEN libraries which may be used in ORIGAMI



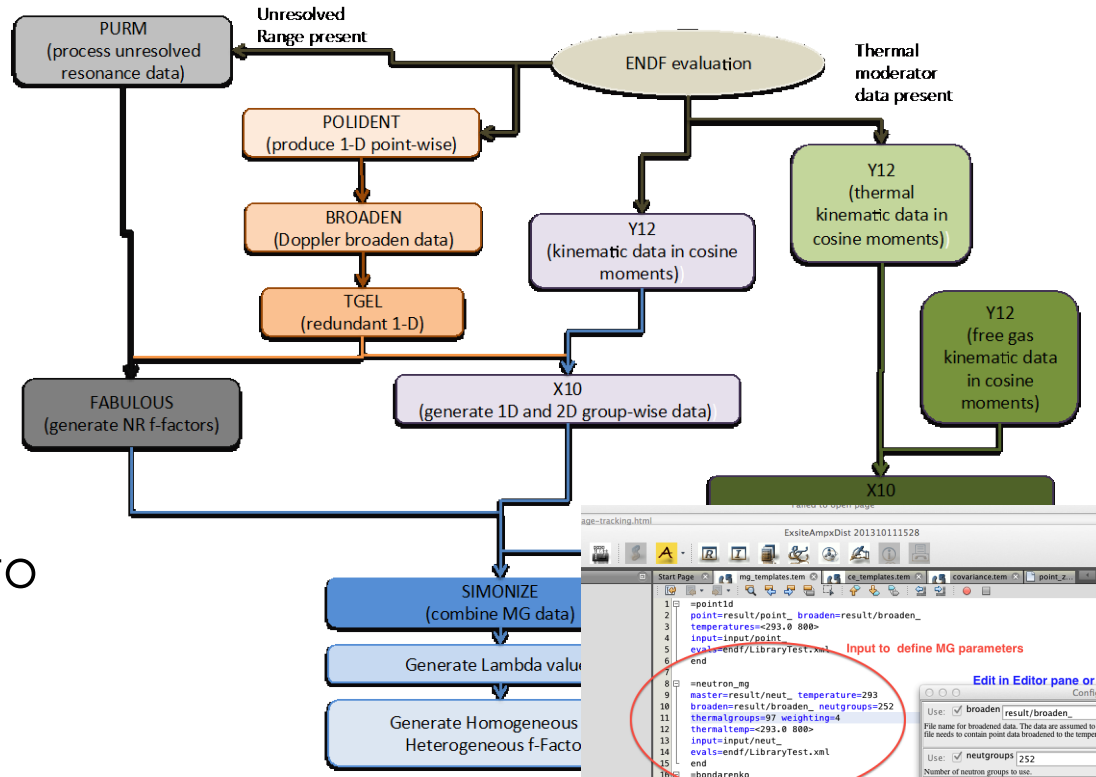


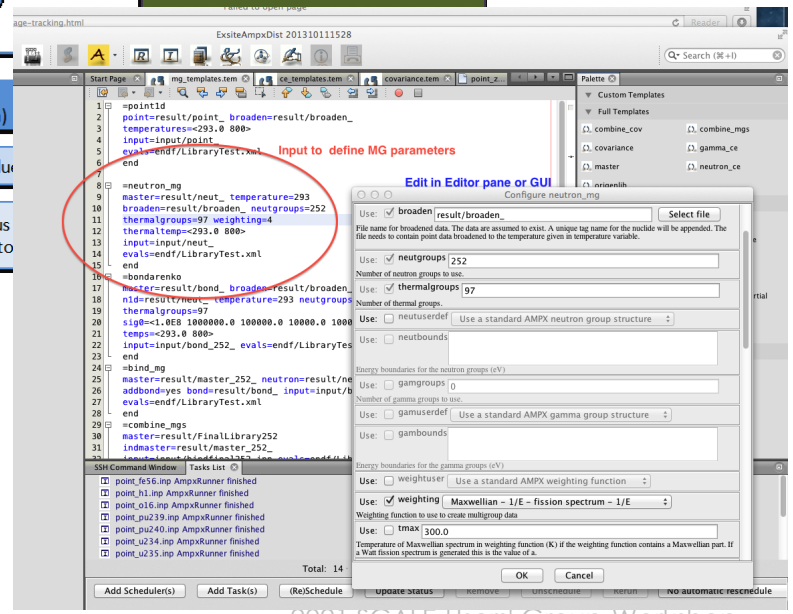
Void fraction and discharge burnup profile for a representative BWR assembly (from NUREG/CR-7240)

AMPX in 6.3.0

Product Owner: Andrew Holcomb
Contributors: Dorothea Wiarda, Cihangir Celik, Kang Seog Kim, Rike Bostelmann and more

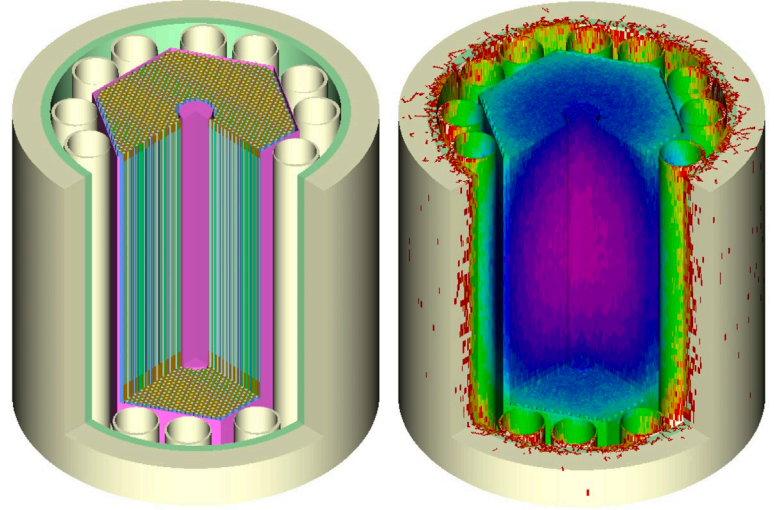
- **Major Features**
  - Generate MG, CE and covariance libraries for use in SCALE
  - Supports all ENDF formats
  - GUI to add use in making input files
- **Other improvements**
  - Support for the new GNDS format
  - Updates to covariance processing to correct for bad ENDF data
  - Improvements for the f-factors
- **Recent use in Projects/Applications**
  - Updated Data libraries for ENDF/B-VIII.0
  - Updated covariance libraries



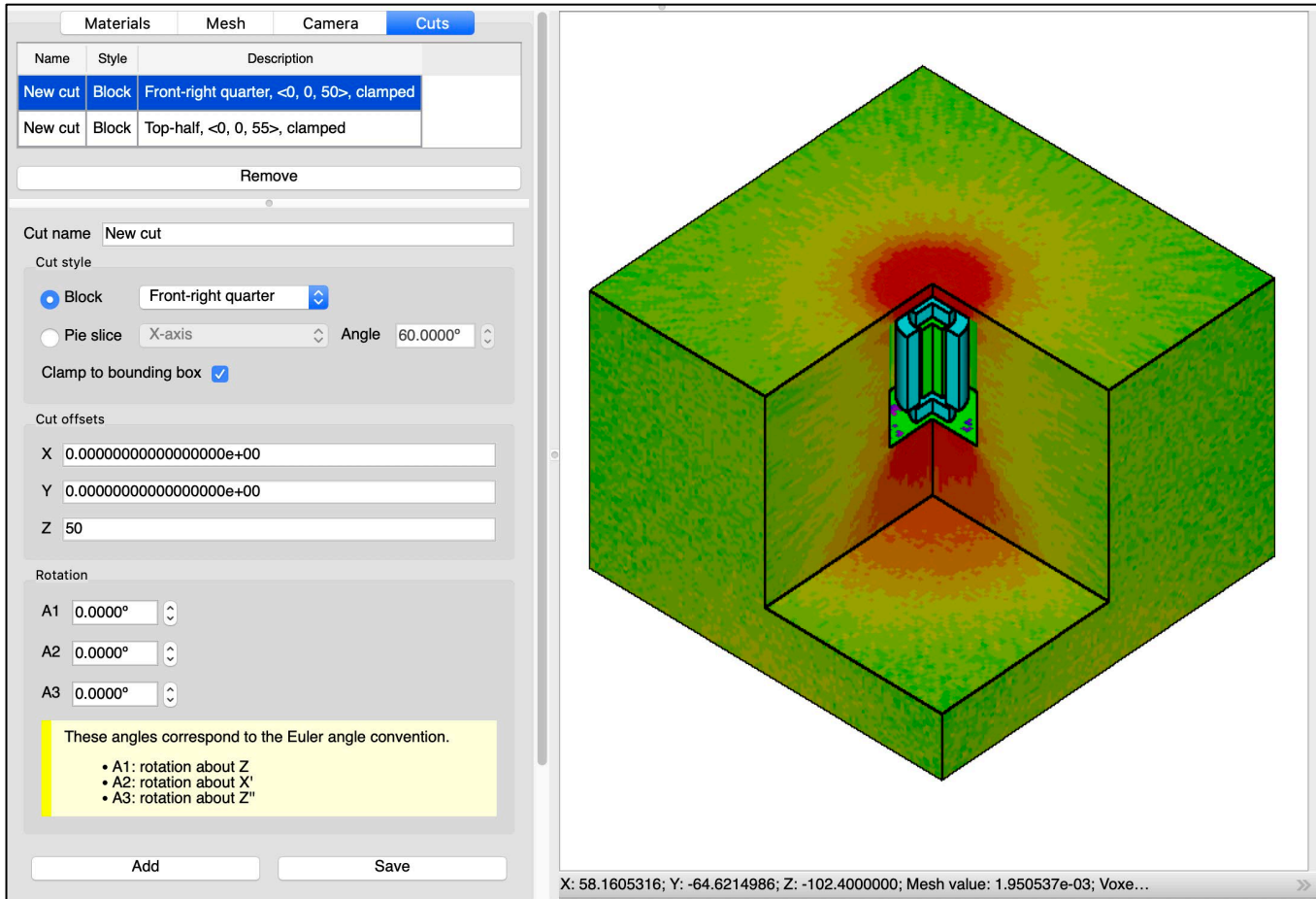


Fulcrum in 6.3.0

Product Owner: Rob Lefebvre
Contributors: Cihangir Celik, Andrew Holcomb, Brandon Langley, and Everyone else



- **Major Features**
  - 3D geometry and mesh data overlay visualization
    - Including geometry opacity and cut controls
- **Other improvements**
  - Interactive MAVRIC source distribution forms
  - Data plotting usability improvements
    - Large MG library handling
    - Preserve plot ranges while adding/removing data
  - Autocompletion of cross-section names
  - Over a dozen bug fixes
- **Recent use in Projects/Applications**
  - All the illustrative 3D geometry and mesh data plots

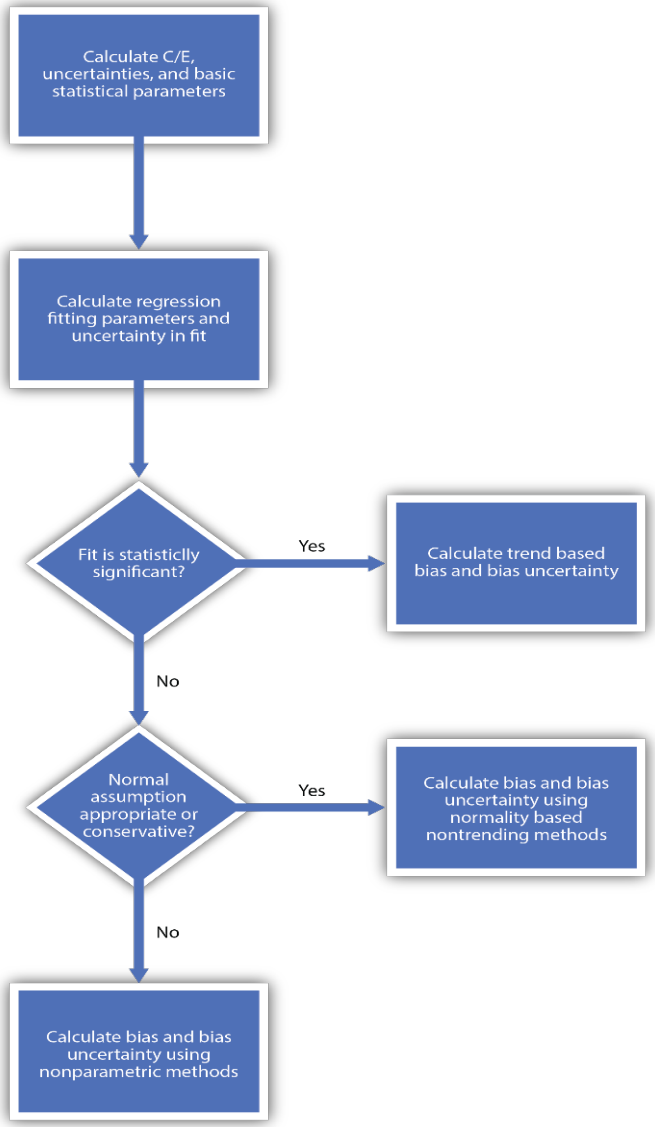


VADER in 6.3.0

Product Owner: Justin Clarity and Shane Hart
Contributors: B. J. Marshall, Will Wieselquist, Seth Johnson

- **Major Features**
  - Maintains old USLSTATS functionality
  - NUREG/CR-6698 trending methods
  - Parametric and Nonparametric methods
  - Chi-square Normality testing
  - Written in C++ to improve extensibility
  - TSUNAMI-IP produces VADER compatible inputs
- **Other improvements**
  - Expand the number of normality tests
  - Trend significance testing
- **Recent use in Projects/Applications**

  - Incorporates a significant number of validation methods to align with report released last year

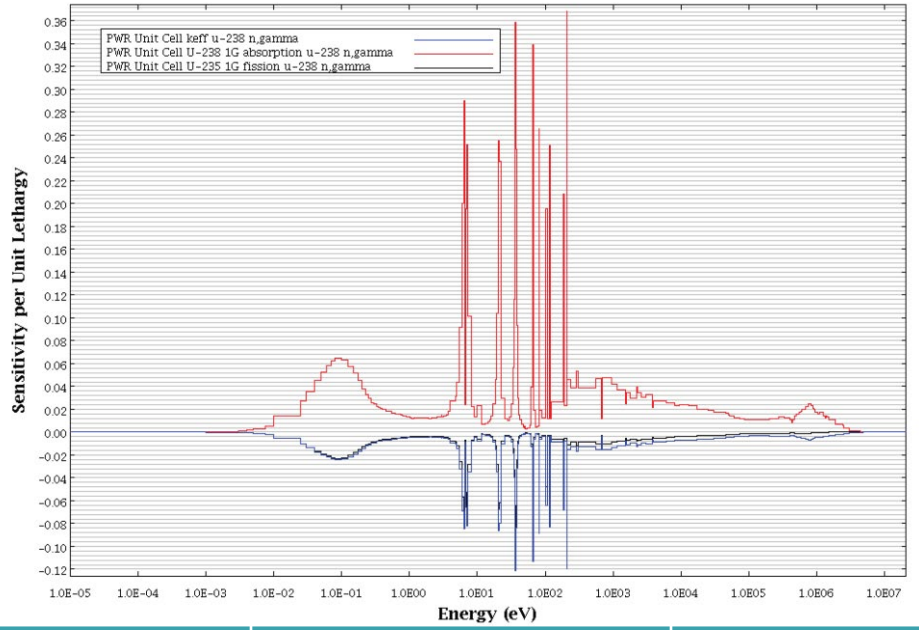



```
=vader

data=[
1.9947003 0.97978 0.00666
2.3125354 0.97862 0.00519
2.0489823 0.98018 0.00559
1.4951488 0.98123 0.00893
1.6272778 0.98207 0.00697
1.6992786 0.98000 0.00735
0.9360934 0.98848 0.00544
1.7664417 0.97843 0.00558
1.8082888 0.97523 0.00810
1.1019401 0.97965 0.00549
1.8500284 0.97295 0.00487
1.8733395 0.97805 0.00479
]

trend_values=[-2.995732274 0 3.912023005]

methods {
  USL1=[confidence=0.95 proportion=0.95
        extrapolate=Yes]
  LTB=[confidence=0.95 proportion=0.95]
  LTL=[confidence=0.95 proportion=0.95]
}

tests{
    trend_signicance[confidence=0.95]
    shapiro_wilk[confidence=0.95]
}
end
```

TSUNAMI in 6.3.0

Product Owner: Jordan McDonnell
Contributors: Kursat Bekar, Seth Johnson, B.J. Marshall, Rike Bostelmann, Travis Greene, Will A. Wieselquist

- **Major Features**
  - Sensitivity computations integrated into high performance Monte Carlo transport code, Shift
    - Distributed memory enables more accurate calculations with Iterated Fission Probability method
- **Other improvements**
  - Performance improvements
    - 45% speedup in TSUNAMI-IP
    - Reduced time-to-solution for TSURFER runs with large number of cases
  - HDF5 format for Sensitivity Data Files
- **Recent use in Projects/Applications**
  - Assessment of Existing Transportation Packages for Use with HALEU
  - Nuclear Data Gap Analysis



Number of SDFs	TSURFER run time, 6.2.4	TSURFER run time, 6.3.0
128	14 min	13 min
512	3.5 hours	1.5 hours
929	47.5 hours	2 hours
1229	~10 days	7.25 hours

Summary

- Many thanks to all the developers and beta testers inside and outside of lab
- Final stretch is closing out QA and doing final performance testing & improvements