Overview of SCALE 6.2

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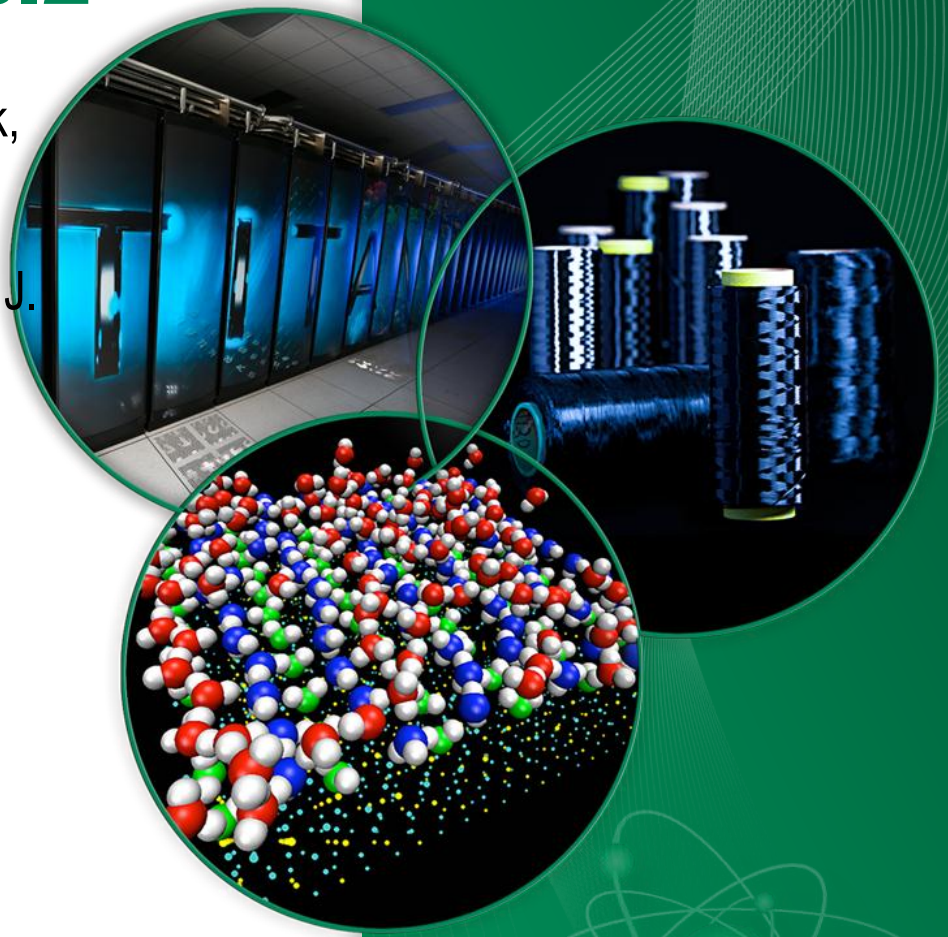
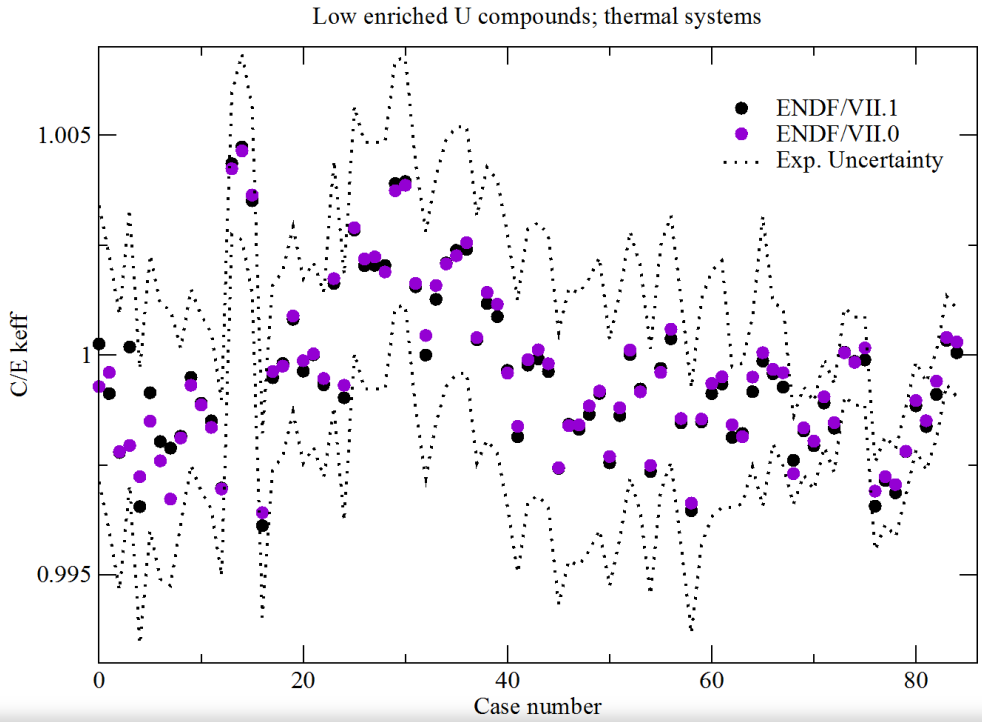


SCALE 6.2 Preview

- Significant updates since SCALE 6.1 in June 2011
- Focus on improved fidelity of solutions
- New nuclear data libraries in MG and CE
- Significant improvements in Monte Carlo capabilities
  - Comprehensive review and update of CE nuclear data, with orders of magnitude increase in testing for improved quality (sponsored by NRC)
  - CE TSUNAMI (sponsored by NCSP)
  - CE MAVRIC/Monaco (sponsored by NRC)
  - CE TRITON (other sponsor)
  - Hybrid source convergence tool (sponsored by DOE NE)
- Modular development, parallel computing, and integration with other code packages (NEAMS, CASL, external development)
- New sampling methods for uncertainty analysis and generation of experimental correlations (joint NCSP and DOE NE support)
- Modernized resonance self-shielding tools
- New lattice physics tool

New Data Libraries

- New CE cross-section data for neutron interactions, gamma yield, and gamma interactions (sponsored by NRC)
- New MG neutron libraries
  - Provides parameters for intermediate resonance approximation for rapid resonance self-shielding techniques
  - 252-group energy structure (sponsored by NRC)
  - 56-group energy structure (sponsored by NRC and DOE NE)
- Extensive test suite
  - 381 VALID benchmarks
  - 6300 transmission tests
  - 5000 infinite medium tests
- ENDF/B-VII.0 libraries released with SCALE 6.2 beta1
- ENDF/B-VII.1 libraries under QA review for release with SCALE 6.2 beta2



Improved Collision Kinematics Processing in AMPX

Since primarily used for MG:

Y12
File 7 -> cosine moments

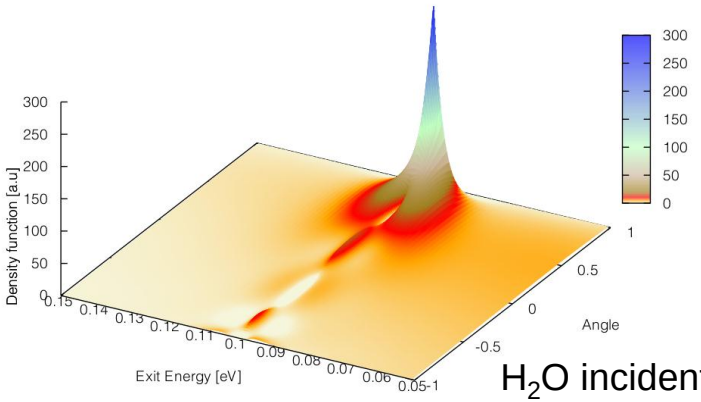
→

MONTEGO
cosine moments -> point-wise

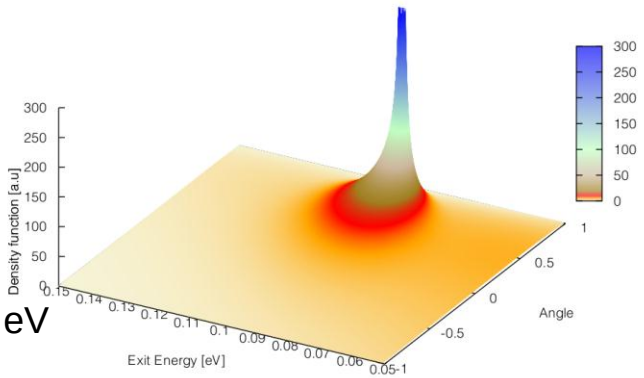
→

JAMAICAN
point-wise -> probability distr.

Y12->MONTEGO



Y12_GAM



H_2O incident energy 0.1 eV

Updated for CE library

Y12_GAM
File 7 ->point-wise

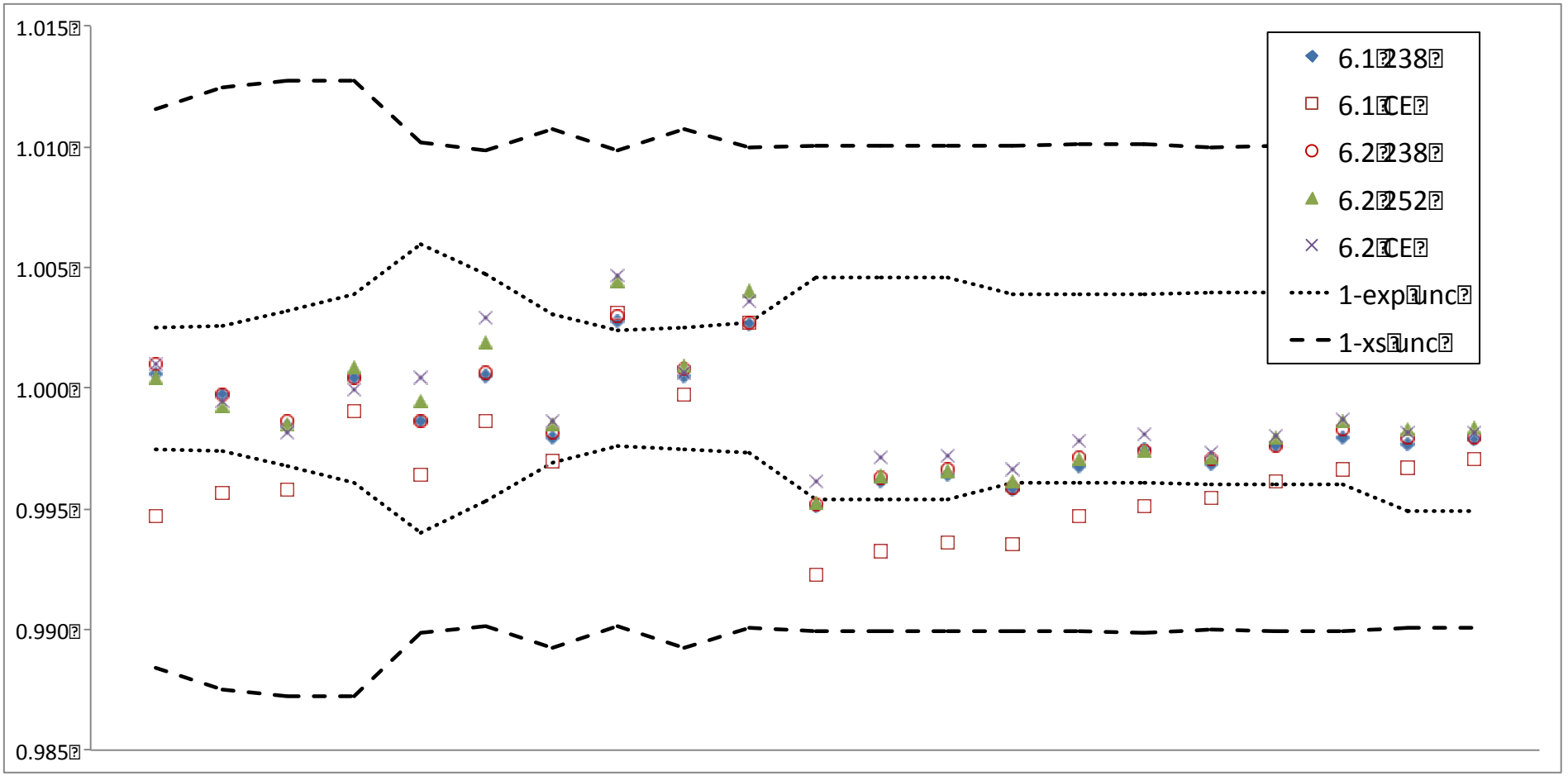
→

JAMAICAN
point-wise -> probability distr.

Refined energy grid is used → thinned to keep library size manageable

AMPX Processing Improvements Provide Improved C/E Especially for CE Calculations for MOX Benchmarks

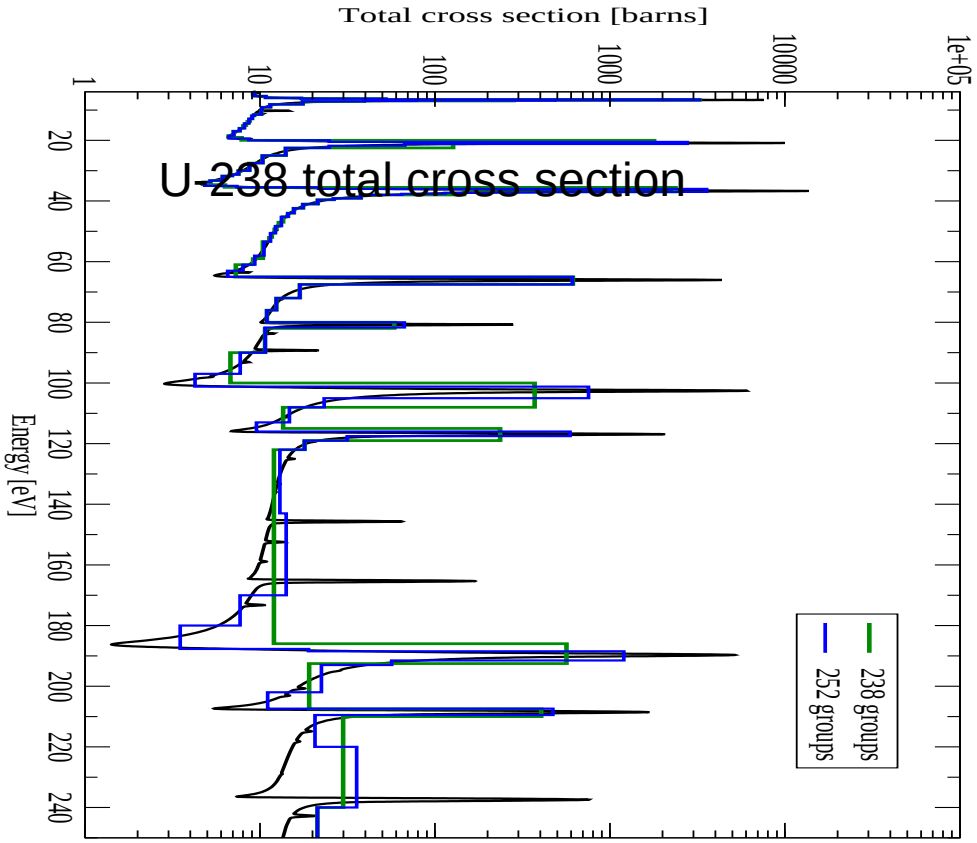
Up to 1000 pcm improvement for burned fuel



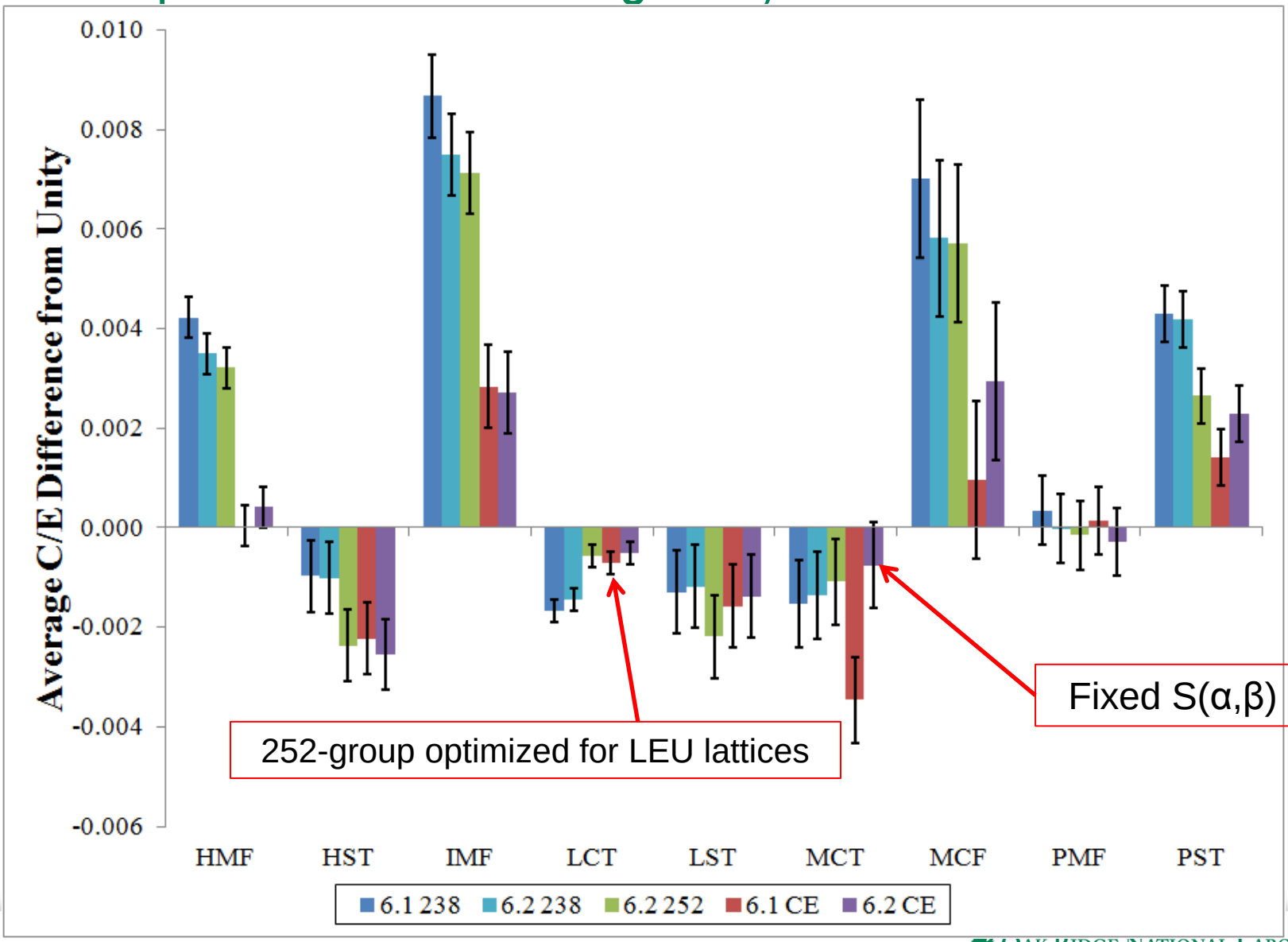
New 252-Group Library for SCALE

- 252 instead of 238 neutron groups, refined for LWRs
- Implements data needed for *Intermediate Resonance* approximation rapid self-shielding calculations with Bondarenko and Embedded Self-Shielding Methodology (SCALE and CASL)

- Weighted with CE flux for actinides and thermal H_2O
- Add Lambda-factors for all isotopes
- Add heterogeneous IR-factors for actinides
- Homogeneous IR-factors for other materials



SCALE 6.1 – 6.2 Validation
(Same experiments in all categories)



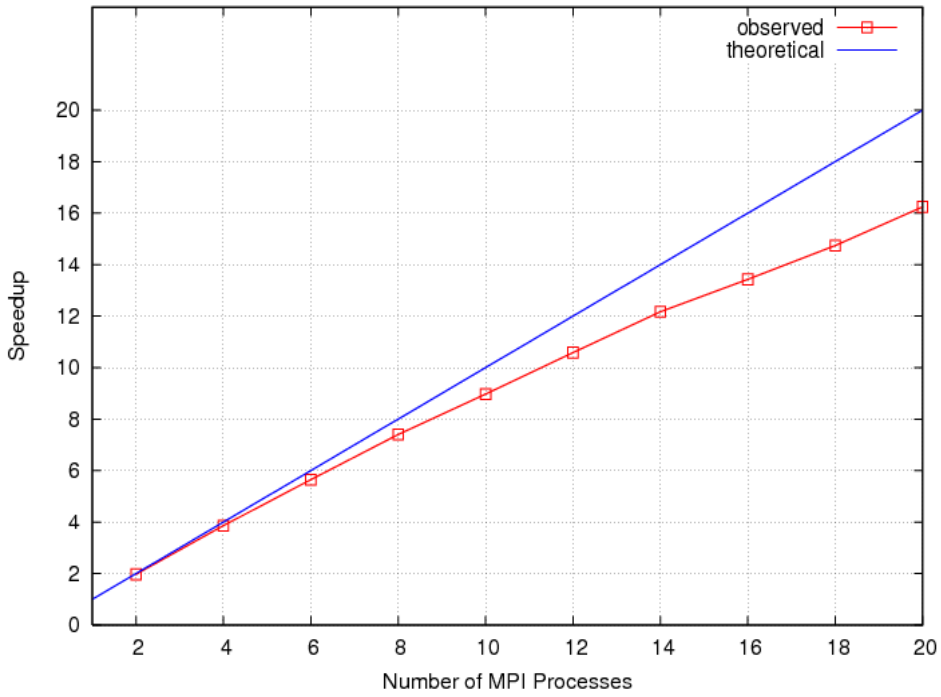
SCALE 6.2 beta1 Data Libraries

Alphanumeric name	Primary data source/format
v7-238	ENDF/B-VII.0 238-group neutron library
v7-252	ENDF/B-VII.0 252-group neutron library
v7-56	ENDF/B-VII.0 56-group neutron library
v7-200n47g	ENDF/B-VII.0 200 neutron/47 gamma library
v7-27n19g	ENDF/B-VII.0 27 neutron/19 gamma library
ce_v7_endf[b]	ENDF/B-VII.0 Continuous-energy neutron and gamma library

New KENO Features (available in SCALE 6.2):

Parallel KENO

- KENO joined parallel MC codes family
- Simple master-slave approach via MPI
- Domain replication
- Reproducible results
- Updating fission banks and tallies at the end of each generation
- Communication overhead due to these frequent updates



Parallel speed up of KENO-VI code in a depletion calculation.

- Parallel performance is strongly dependent on problem size and parameters
- Good scaling observed in CASL reference solution calculations with CE KENO (120-384 MPI processes)

New KENO Features (available in SCALE 6.2):

Multiple Mesh Support

- Previous KENO versions support only one mesh with a single mesh-based quantity
- This new feature enables multiple mesh definitions for tallying several mesh-based quantities

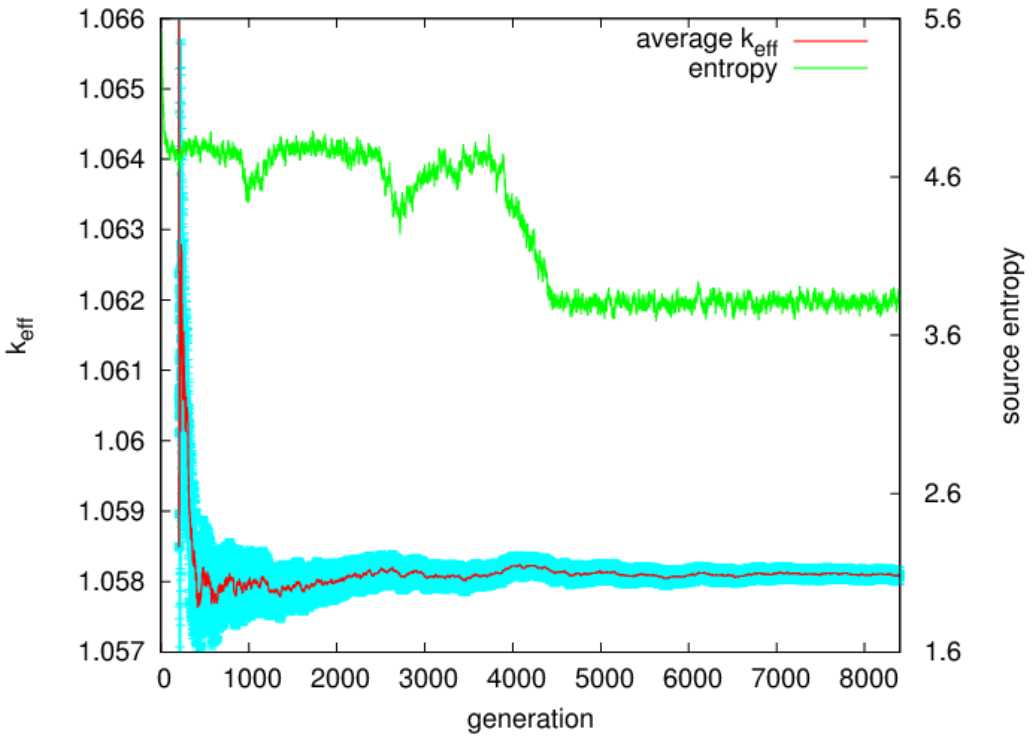
➔Enables:

- Mesh-based Source Convergence Diagnostics
- CE-TSUNAMI F*(r) mesh
- Mesh-based fission matrix approach
- Fission source tally (CADIS)
- Mesh fluxes
- …

New KENO Features (available in SCALE 6.2):

Source Convergence Diagnostics

- Relies on Shannon Entropy statistics[1,2,3]
- Accumulates fission source at each generation on a user-defined Cartesian mesh (default mesh size 5x5x5, covers entire geometry)
- Post-processes the accumulated fission source and computes entropy, relative entropy, average entropy, etc for three tests:
  - Test-1: Final Convergence
  - Test-2: First Converged Generation
  - Test-3: Adequate Active Generation

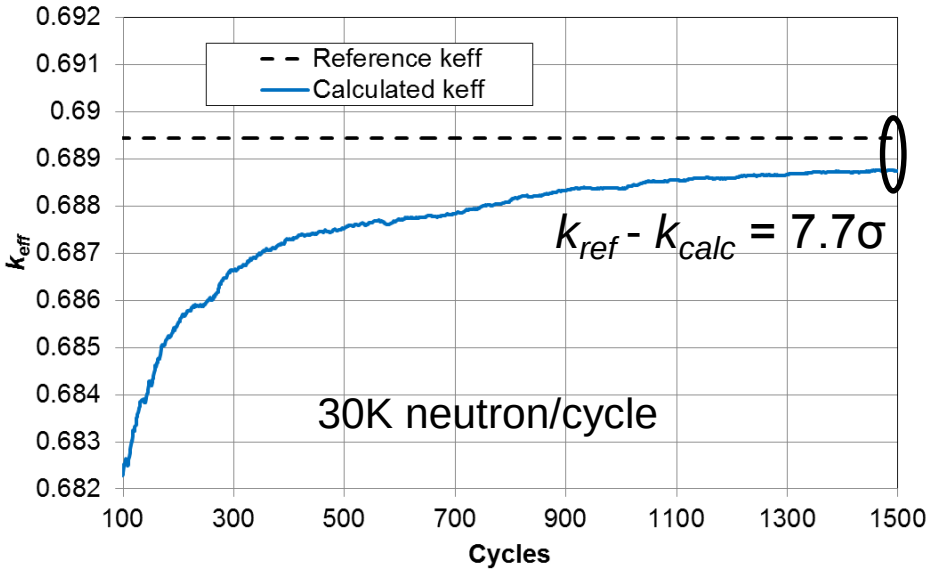


1. T. Ueki and Forrest B. Brown, "Stationarity and Source Convergence Diagnostics in Monte Carlo Criticality Calculation," Nuclear Mathematical and Computational Sciences Conference (M&C 2003), Gatlinburg, Tenn., April 6–10, 2003.
2. T. Ueki and F. B. Brown, "Stationary Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations," *Nuclear Science & Engineering* **149**, 38 (2005).
3. M. Wenner and A. Haghighat, "Study of Methods of Stationarity Detection for Monte Carlo Criticality Analysis with KENOV.a," *Trans. Am. Nucl. Soc.*, ***97***, 647–651 (2007).

Convergence problems of NAC-UMS-TSC-24

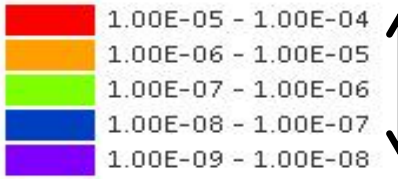
- Difficult to capture most reactive regions
- Decoupling due to water and flux traps

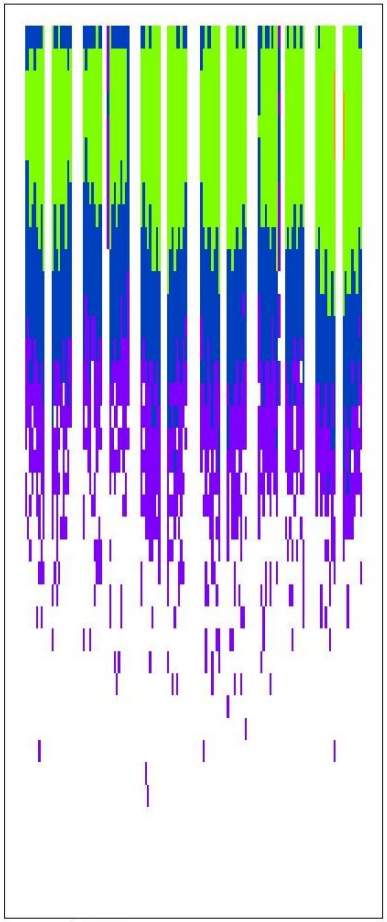
k_{eff} with uniform starting source



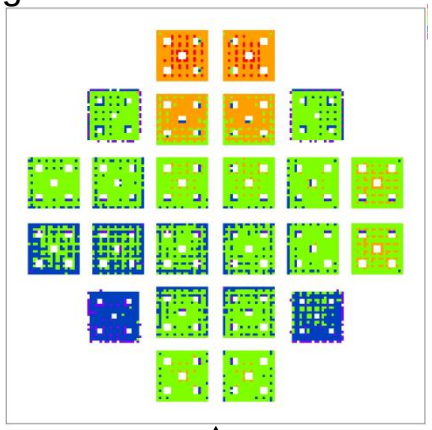
Unaffordable computer and human resources required to ensure reliability of canister-specific calculations

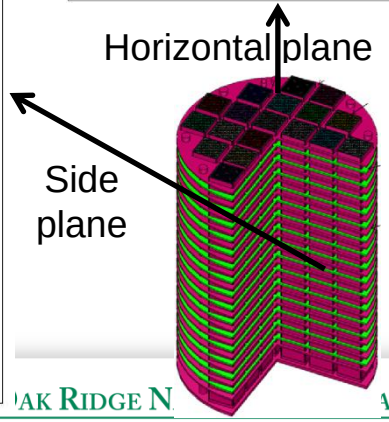
Reference fission source distribution



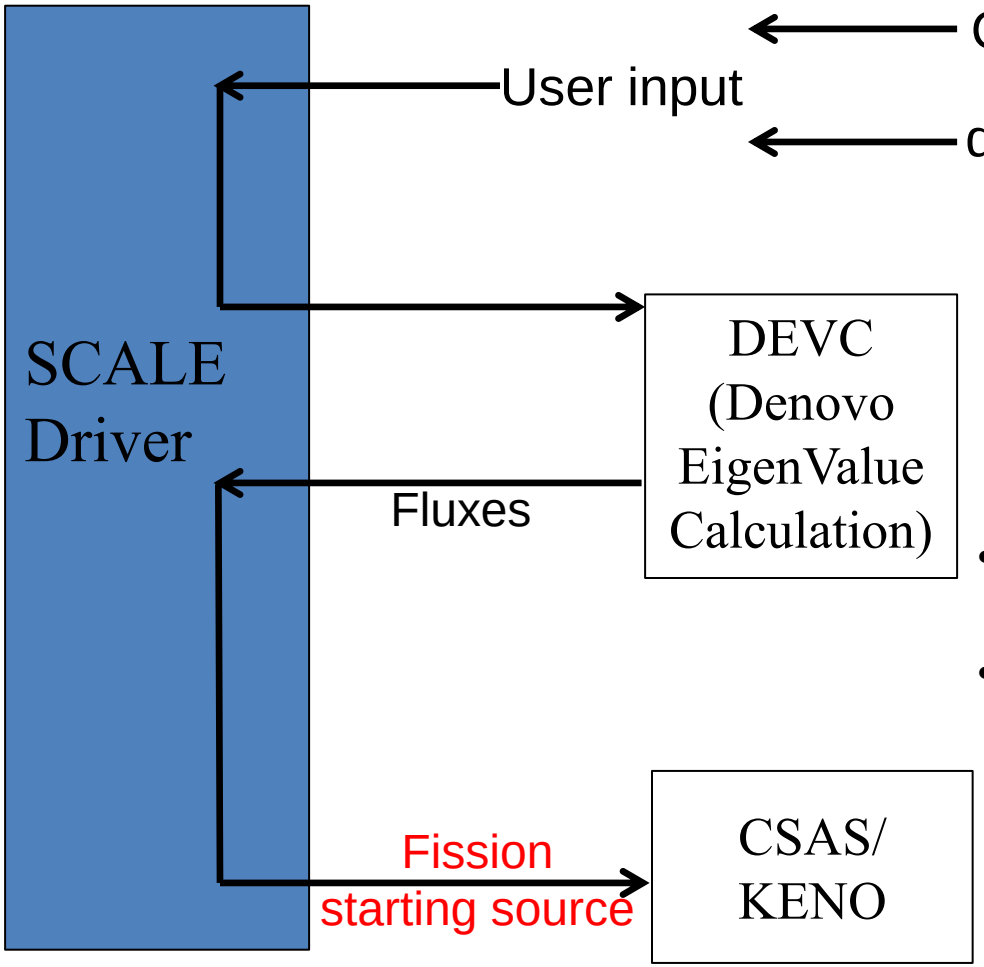


Difficulties in adequately sampling most reactive regions





Sourcerer



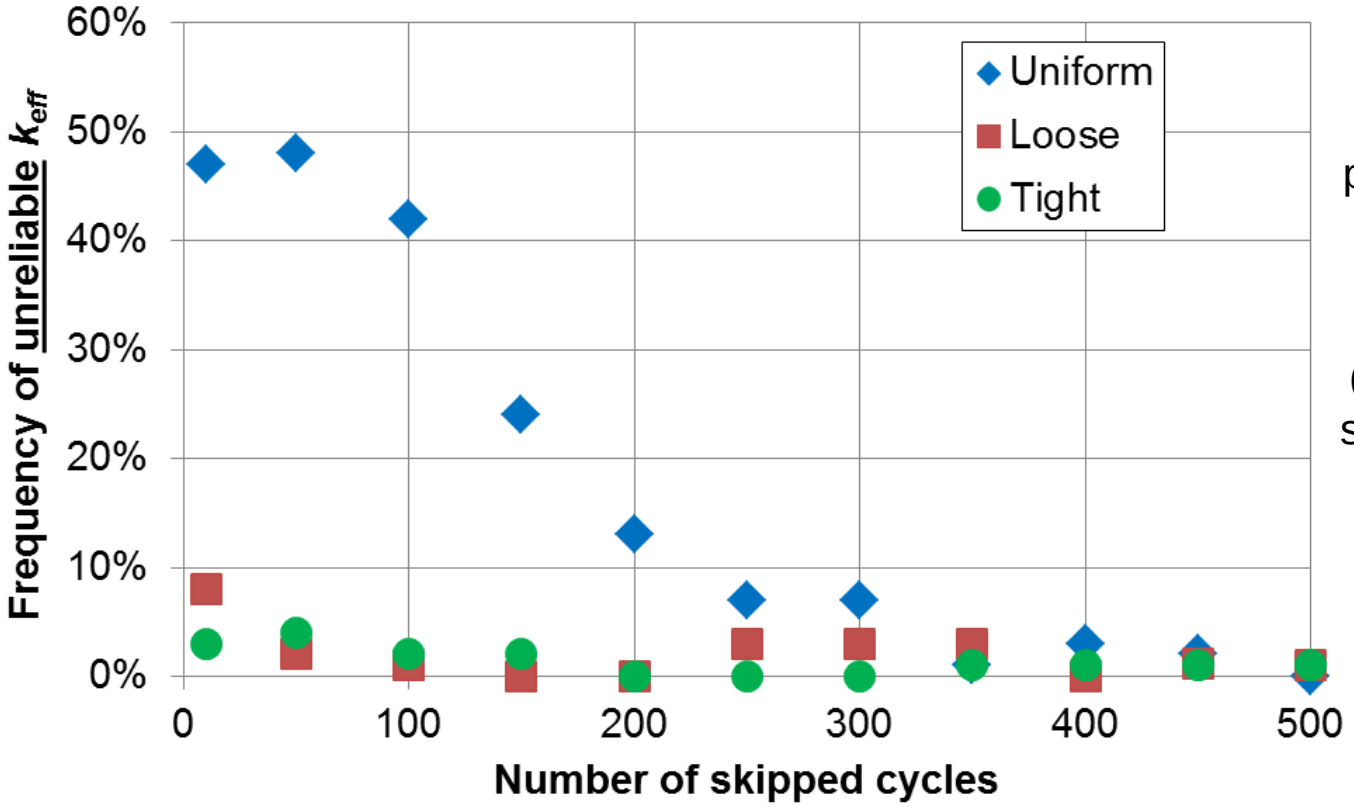
detSource block
- Denovo library
- Denovo mesh
- Denovo parameters

- Automatic mapping of KENO geometry on user-defined grid
- Materials mixing (macromaterials) using a volume weighted average of the materials in the MC model

Ibrahim et. al, "Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources," PHYSOR 2012

Reliability

Frequency of **not** calculating k_{eff} inside confidence interval
$k_{ref} - 3\sigma < k_{calc} < k_{ref} + 3\sigma$



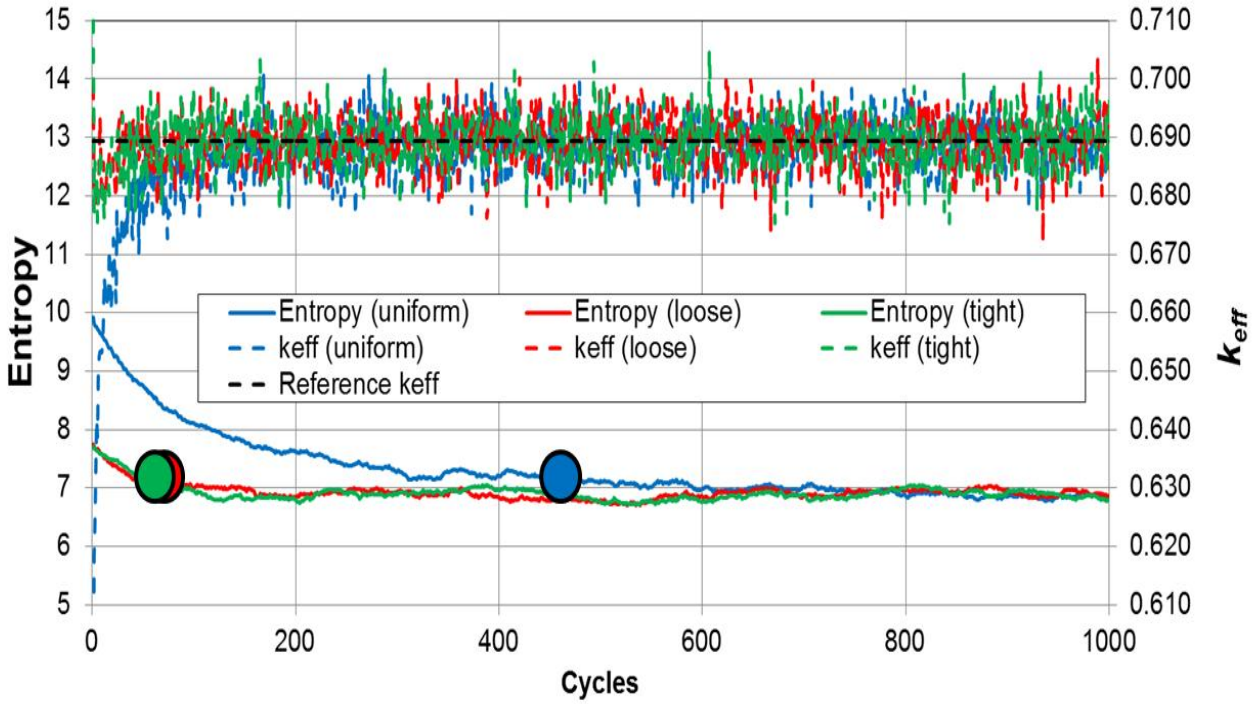
30,000 Neutrons per cycle and 500 active cycles

100 independent (different random seed) calculations for each point

Reliability of uniform source is comparable with the reliability of deterministic source after skipping 350 cycles

Efficiency

Step 1: Determination of number of skipped cycle



Skipped cycles are determined from the number of cycles after which the entropy falls inside a band determined by the average and the population standard deviation of the entropy of 1000 cycles. These 1000 cycles are counted after 750 cycles for uniform and 200 cycles for deterministic source.

Efficiency

Step 2: skipped cycle from step 1 and uncertainty threshold of 0.00025 is used to determine the active cycles.

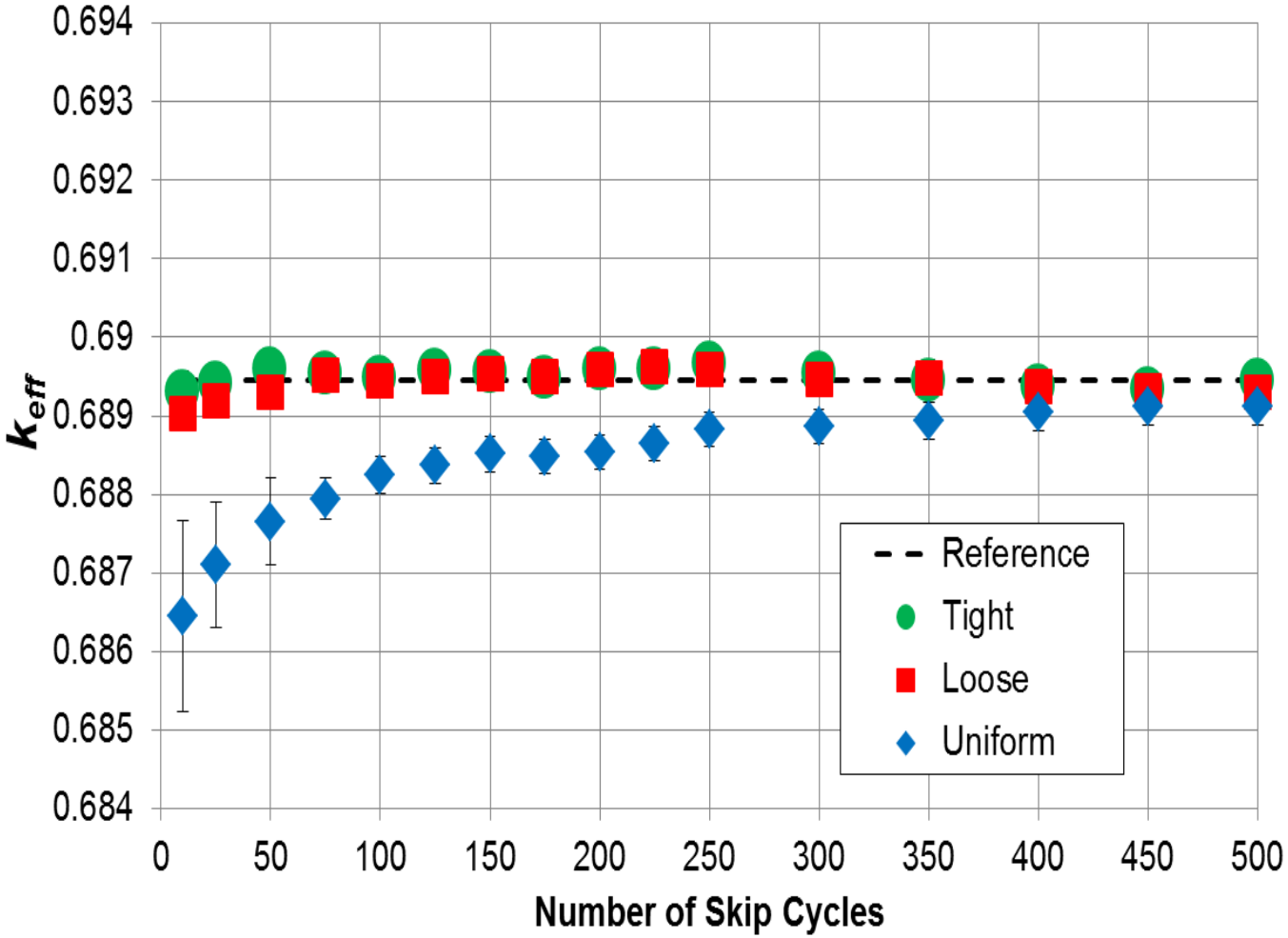
Speedup =(MC Time)/(MC Time + Deterministic Time)

Starting source	k_{eff}	Speedup
Uniform	0.68977 ± 0.00025	1.00
Loose	0.68944 ± 0.00024	**1.71**
Tight	0.68900 ± 0.00024	1.36

- 70% speedup
- Deterministic accuracy not critical

Efficiency

k_{eff} with 500 active cycles



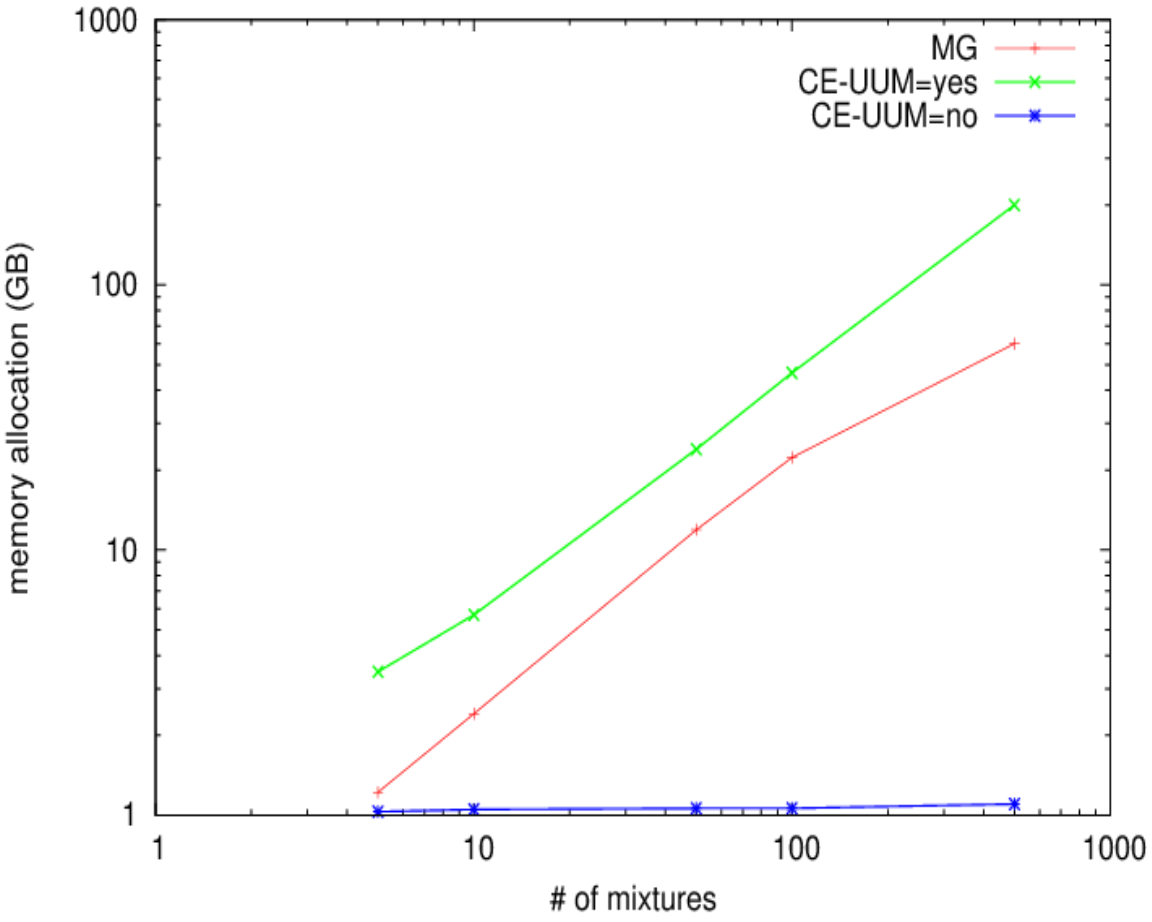
New KENO Features (available in SCALE 6.2):

Non-unionized energy grid for total and absorption cross-section calculations

- CE calculations in KENO through SCALE 6.1 uses "unionized energy grid," where material-dependent cross-section data are generated and stored for each user-defined mixture
  - Memory allocation increases with the number of mixtures
- Alternative approach: on-request mixture cross-section calculation
  - Memory requirement is almost independent from the number of mixtures in the model
  - Up to 40 % additional computational overhead ➔ but makes CE-TRITON, CE-TSUNAMI, CSAS6 calculations viable for the models with several mixtures

New KENO Features (available in SCALE 6.2):

- ➔ CE-UUM=yes refers the CE transport with unionized energy grid model
- ➔ CE-UUM=no refers CE transport with on-the-fly mixture cross-section calculations
- ➔ Memory allocation for MG KENO-VI calculation also includes the memory requirement of cross-section processing tools



MG & CE-UUM=yes requires >> 60 GB memory for the model with 500 mixtures

CE Performance Improvements

Observations/Issues:

- CE neutron data for KENO through SCALE 6.1 requires ~ 11.4 GB physical memory if all nuclides in the library are loaded (+430 nuclides)
- Size of CE data and additional memory requirement due to the newly added features limit both the serial and parallel KENO code performance

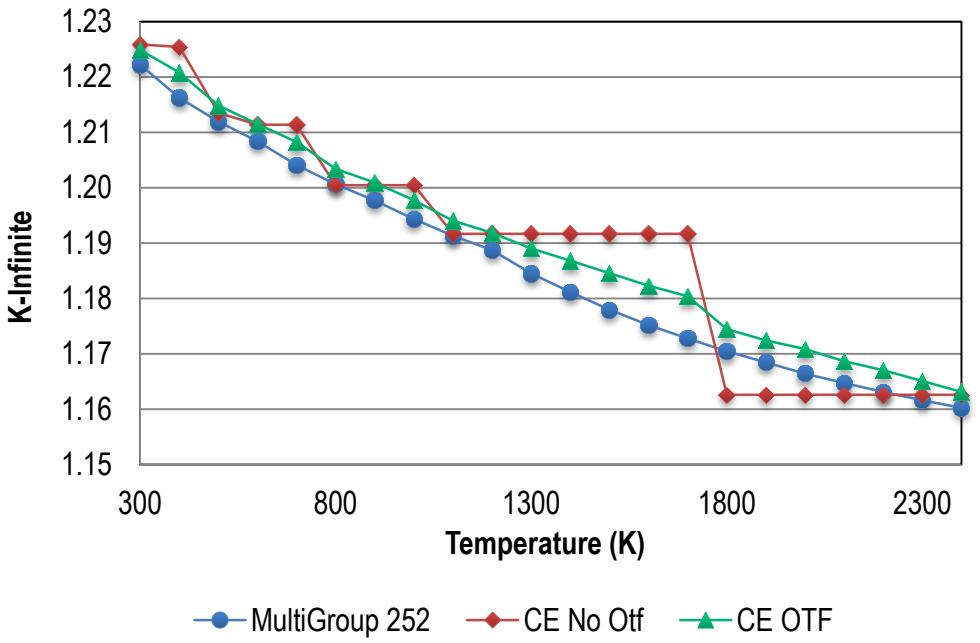
Memory footprint of CE data in CE transport has been reduced significantly by redesigning our codes and data!!!

Action	Memory Reduction (%)
Changed format of internal data storage arrays (double precision to single precision conversion)	15-45
Revisited 2D collision kinematics data and redesigned data containers for this data	5-30
Revised unionization at reaction level within a nuclide	5-10
Optimized nuclide object (data container)	3-15
TOTAL	20-95

New KENO Features (available in SCALE 6.2):

Cross-section Temperature Correction (pre-broadening)

- Libraries contain cross-section data typically broadened to a few temperatures
- If temperatures in the model are different than those present in the library ➔
  - MG KENO allows temperature correction through linear interpolation
  - CE KENO uses the closest temperature ➔ ~ a few hundred pcm differences



- 1D cross sections corrected using a finite difference method
  - Can pre-broaden cross sections before transport calculation
  - The same methodology can be used for true on-the-fly Doppler Broadening
- Planning to extend for the probability tables for unresolved resonance range
- Planning to determine ways to pre-broaden S(α,β) data

New KENO Features (available in SCALE 6.2):

Doppler Broadening Rejection Correction Method (DBRC)

- Thermal motion of target nuclides can significantly affect the collision between a neutron and nucleus in the epithermal energy range
- CE KENO uses free-gas scattering model to simulate this thermal motion
- DBRC method introduces corrections to the Doppler broadening of the scattering kernel with a new sampling equation
- Implementing this method can have significant impact on eigenvalue calculations due to the increase of neutrons being upscattered into absorption resonances
- Temperature increases ➔ more neutrons upscattered into the resonances, resulting in more absorptions and a lower eigenvalue (*keff*)
- Especially significant in reactor applications rather than criticality safety

Temperature (K)	CE KENO	CE KENO with DBRC	Difference (pcm)
293.6	1.34460	1.34451	-9
600.0	1.33053	1.32932	-121
900.0	1.31759	1.31759	-182
1200.0	1.31029	1.30730	-299
1400.0	1.28113	1.27478	-635

New KENO Features (available in SCALE 6.2):

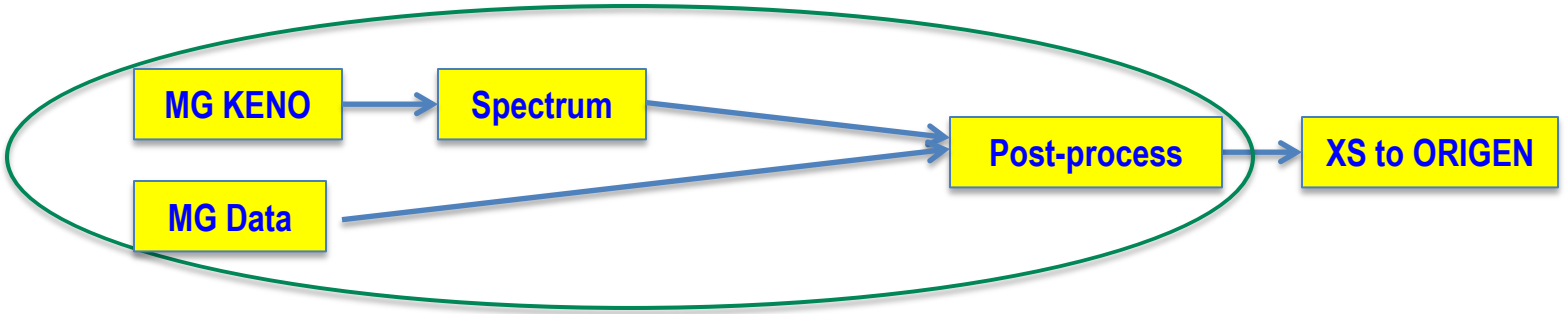
Few-group microscopic reaction cross-section calculations

- For all/selected mixtures in the model
- Uses track-length estimator for reaction rate tallies
- Uses track-length estimator for fluxes
- Uses reaction rate tallies and fluxes to compute microscopic reaction cross-sections
- User can specify energy group structure for tallying(Default 238 groups)

➔ **enables: CE-TRITON**

(new CE depletion module)

TRITON (MG):

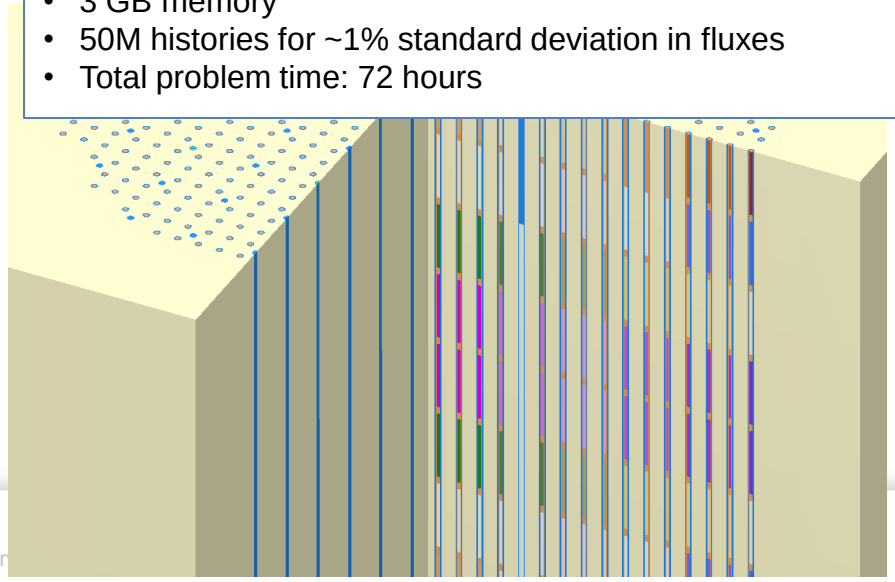


CE-TRITON:

CE Monte Carlo Depletion

- Designed for high-fidelity analysis of full core reactors
- MG reaction and flux tallies from CE data
- Efficient memory management
- Coupling with ORIGEN

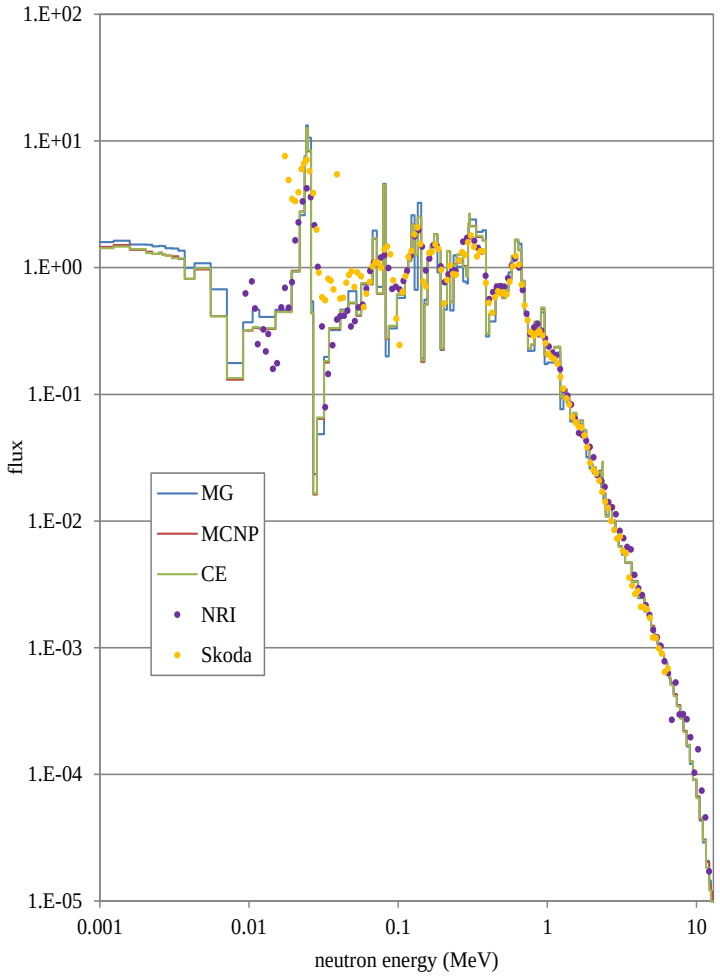
Graphite Reactor Benchmark Calculation
- 7,930 depletion zones
- ~10,000 units, ~32,000 regions
- 3 GB memory
- 50M histories for ~1% standard deviation in fluxes
- Total problem time: 72 hours



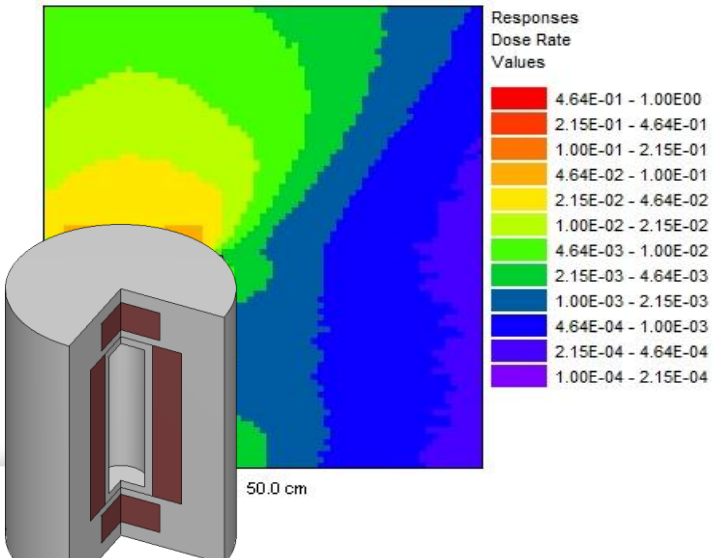
CE Shielding with MAVRIC/Monaco

- All hybrid capabilities supported with CE fidelity
- SCALE Continuous-Energy Modular Physics Package (SCEMPP)
  - Application Programmer Interface (API) for CE physics for next-generation Monte Carlo codes
- 6300 fixed-source transmission tests used in V&V

Flux results for iron sphere transmission experiment



Dose rate from ^{60}Co source in transportation package

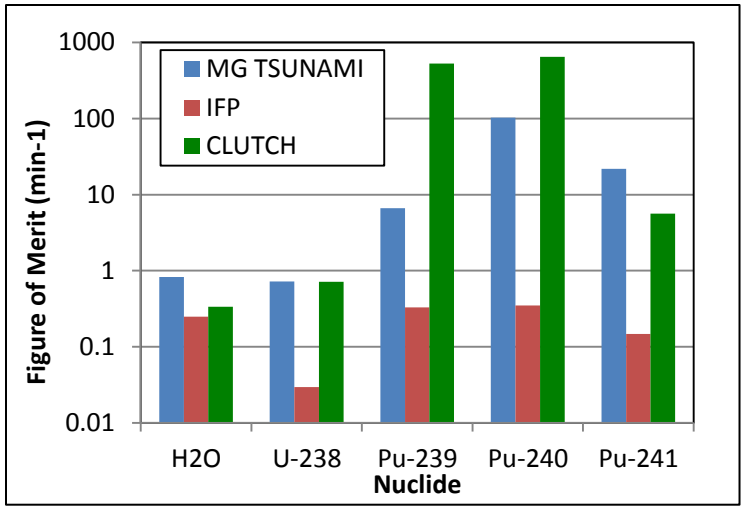


Enhancements in CE transport

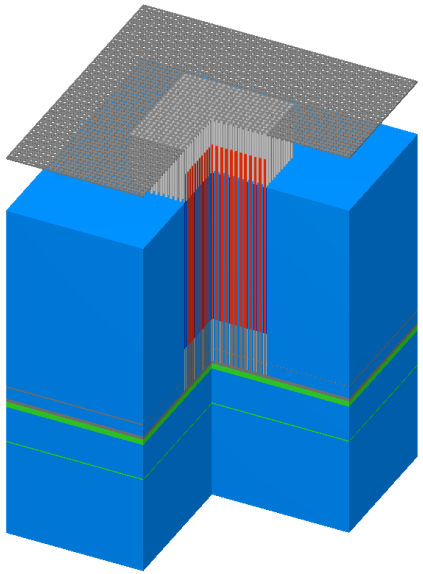
- A new CE physics engine, SCEMPP (Scale CE Modular Physics Package) was designed to support all MC transport codes in SCALE
  - Fortran and C++ APIs to support both legacy and future developments
  - Models particle collisions in a material and generates the particle(s) resulting from a collision
  - Also provides non-transport data, such as reaction responses and point detector data
  - Integrated to the Monaco code and MAVRIC sequence to provide CE particle transport for shielding and CAAS analyses (CE-Monaco/MAVRIC)
  - Will be integrated in KENO after adding fission treatment

Continuous-Energy Sensitivity Analysis

- Two new methods integrated into TSUNAMI / KENO for CE Calculations
  - Iterated Fission Probability
  - CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance Characterization)



Sensitivity	Reference	MG TSUNAMI	CE TSUNAMI	
			IFP	CLUTCH
H_2O	0.2935 ± 0.0179	0.2805 ± 0.0088 (-0.65 σ_{eff})	0.2733 ± 0.0052 (-1.08 σ_{eff})	0.2793 ± 0.0065 (-0.75 σ_{eff})
^{238}U	-0.0061 ± 0.0003	-0.0050 ± 0.0002 (2.80 σ_{eff})	-0.0055 ± 0.0003 (1.16 σ_{eff})	-0.0057 ± 0.0001 (1.14 σ_{eff})
^{239}Pu	0.1262 ± 0.0087	0.1264 ± 0.0014 (0.02 σ_{eff})	0.1188 ± 0.0020 (-0.83 σ_{eff})	0.1190 ± 0.0001 (-0.83 σ_{eff})
^{240}Pu	-0.03777 ± 0.00350	-0.03750 ± 0.00011 (0.08 σ_{eff})	-0.03738 ± 0.00060 (0.11 σ_{eff})	-0.03743 ± 0.00002 (0.10 σ_{eff})
^{241}Pu	0.00589 ± 0.00042	0.00599 ± 0.00004 (0.24 σ_{eff})	0.00567 ± 0.00014 (-0.50 σ_{eff})	0.00579 ± 0.00003 (-0.24 σ_{eff})
Memory Requirements (increase from Eigenvalue Analysis)		13 GB	11 GB	0.06 GB

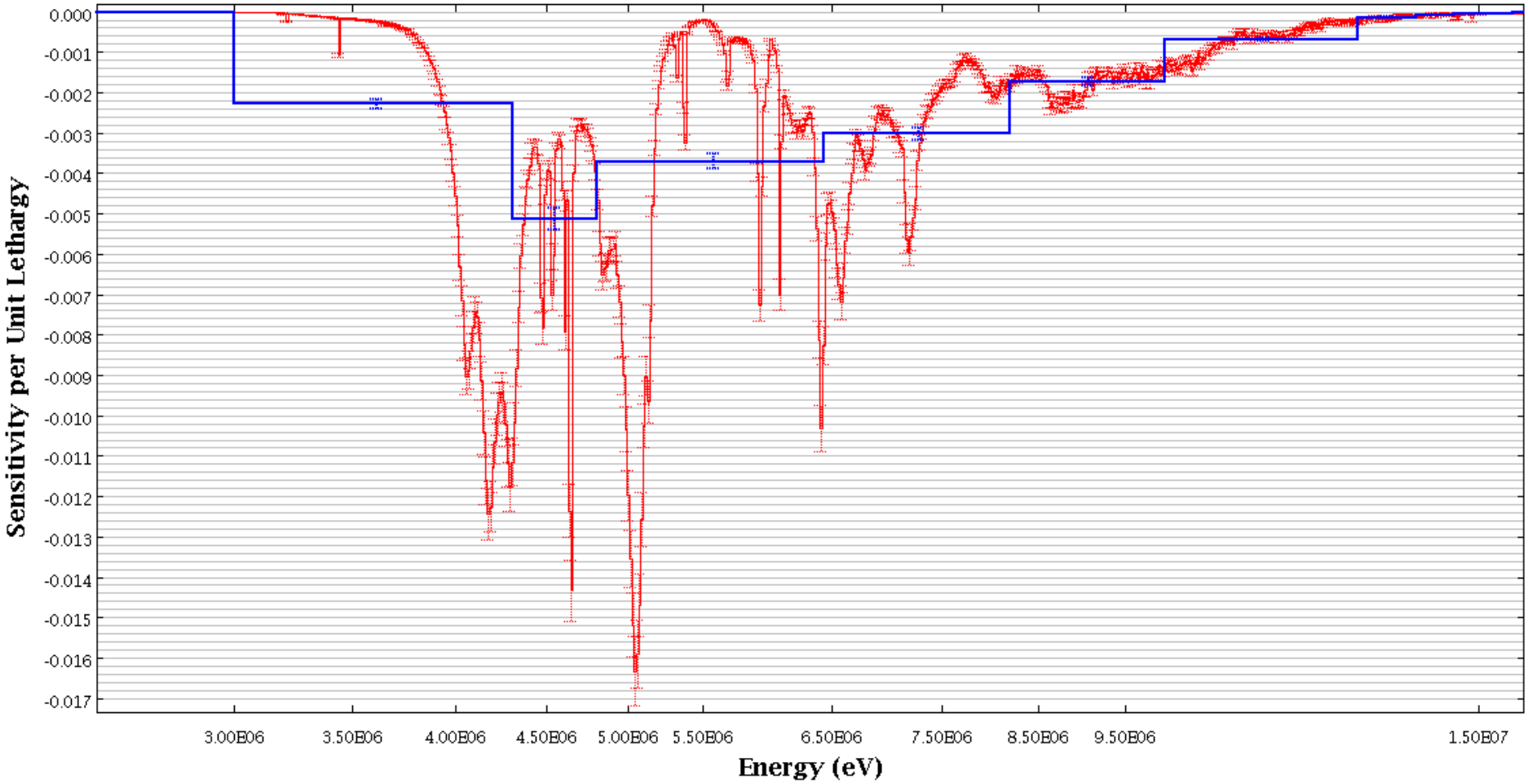


MIX-COMP-THERM-004 Critical Experiment

O-16 Capture Sensitivity

238-group CLUTCH VS

Microgroup CLUTCH



H-1 Elastic Scatter Sensitivity

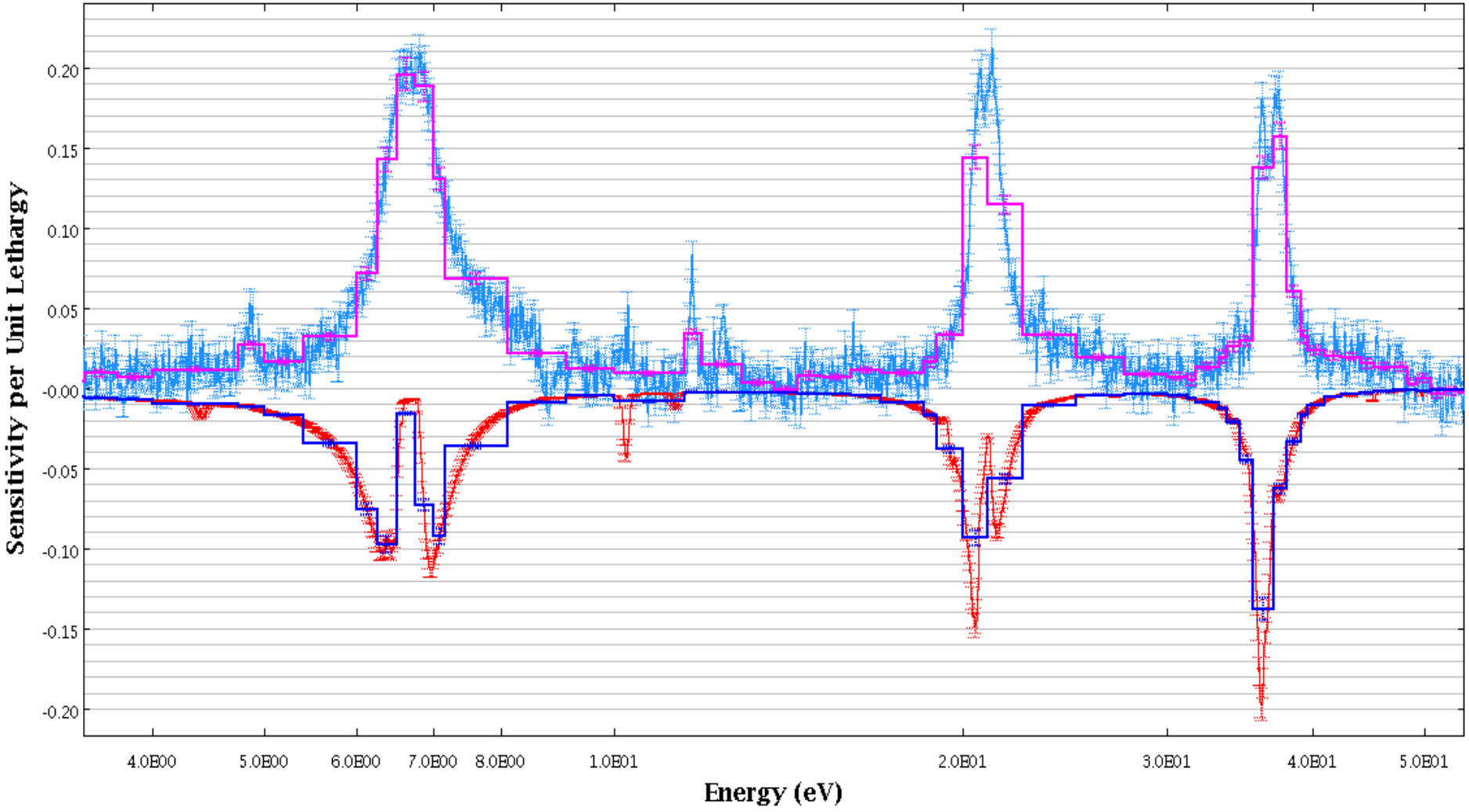
238-group CLUTCH VS

Microgroup CLUTCH

U-238 Capture Sensitivity

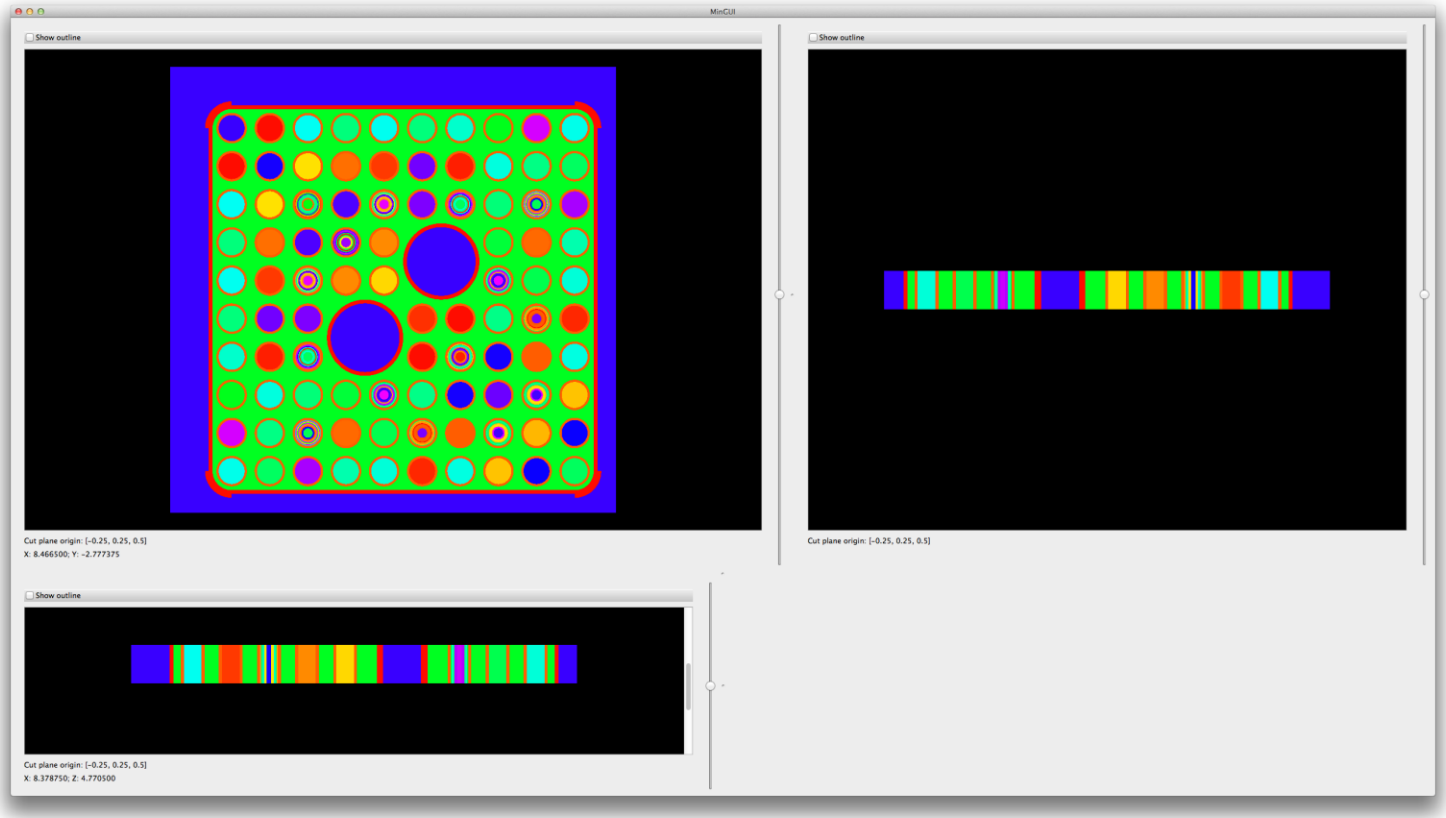
238-group CLUTCH VS

Microgroup CLUTCH



Atlas Geometry

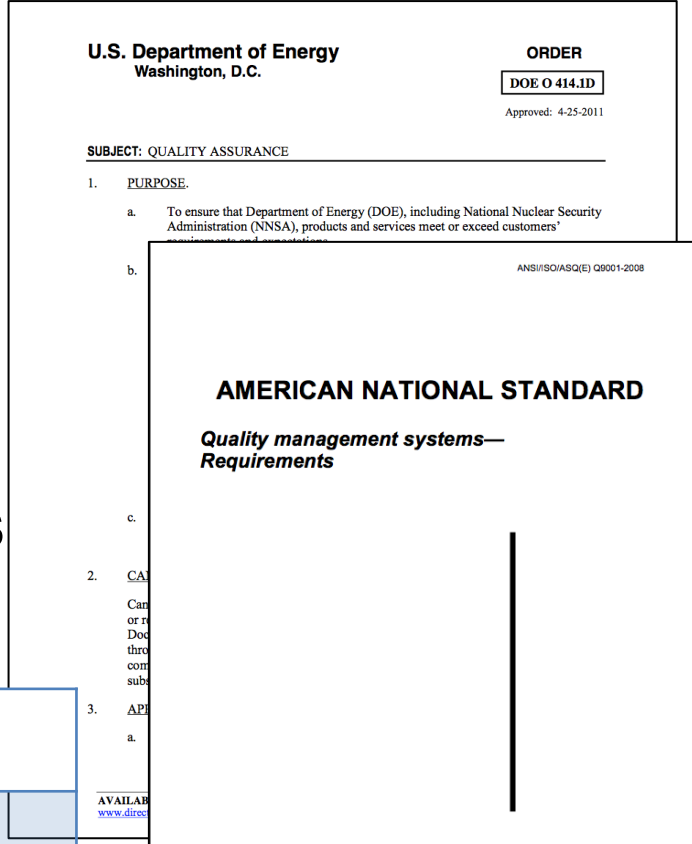
- Flexible new modular geometry engine for Monte Carlo and MOC calculations
- KENO V.a and KENO-VI plus Templated scenes



Updated QA Program

- Designed for Compliance with:
  - ISO 9001-2008
  - DOE 414.1D
  - ORNL SBMS
  - Consistent with ASME NQA-1
- Capabilities are tracked with the *Kanban* process through the *FogBugz* electronic *collaborative development environment*

Kanban Category	Meaning
Proposed	Task has been proposed for management approval
Approved	Task has been approved by management and assigned to a developer for implementation
In Progress	Developer is actively working to implement the feature
Ready for Testing	Developer has completed the implementation and the feature is ready for comprehensive testing
Ready to Ship	Item has passed all tests and is a candidate feature for quality assurance implementation
Shipped	Feature is implemented in quality-assured version


U.S. Department of Energy
Washington, D.C.

ORDER
DOE O 414.1D
Approved: 4-25-2011

SUBJECT: QUALITY ASSURANCE

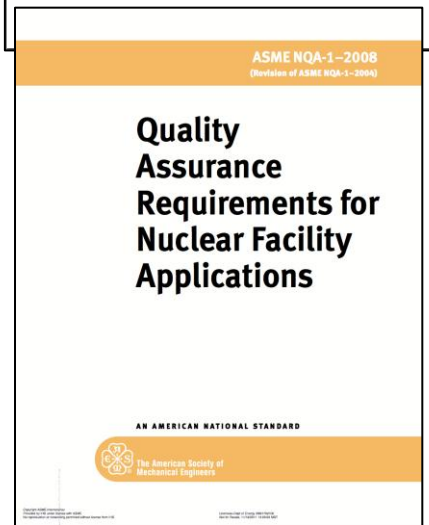
1. PURPOSE.
   a. To ensure that Department of Energy (DOE), including National Nuclear Security Administration (NNSA), products and services meet or exceed customers'

ANSI/ISO/ASQ(E) Q9001-2008

AMERICAN NATIONAL STANDARD

Quality management systems—Requirements

AMERICAN SOCIETY FOR QUALITY
P.O. BOX 3005
MILWAUKEE, WI 53201-3005



Improved SCALE V&V

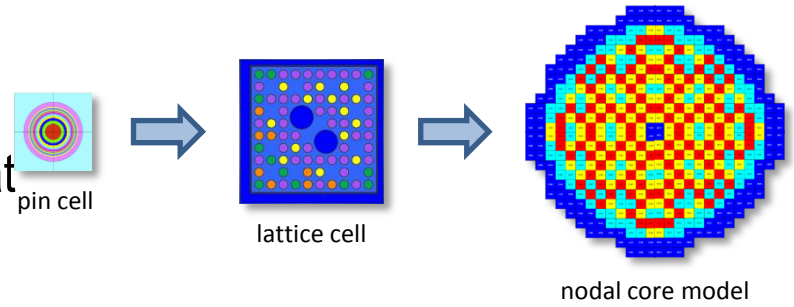
- Routine Test Suite
  - Run dozens of times each day
  - 263 Sample Problems
  - 379 Regression Problems
  - ~1000 Unit Tests
  - 381 VALID Benchmarks
- Supported Platforms:
  - Linux, Mac, Windows
    - Intel Release
    - Intel Debug
    - GNU Release
    - GNU Debug
  - Suite repeated with MPI on Linux and Mac

SCALE 6.2 Tentative Schedule

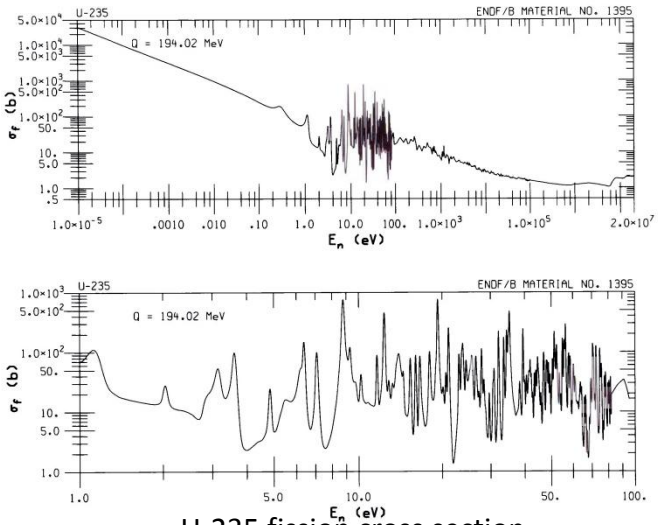
- Beta1 – currently under limited release
- Beta2 – broader release expected by December 2013
- Beta3 – expected in Spring 2014
- Production release – expected in Summer 2014

Shift Goal: Enable efficient full-core Monte Carlo reactor simulations on HPC platforms

- Current state-of-the-art methodology
  - Based on nodal framework (late 1970's)
  - High-order transport at small scale, diffusion at large scale
  - Single workstation paradigm



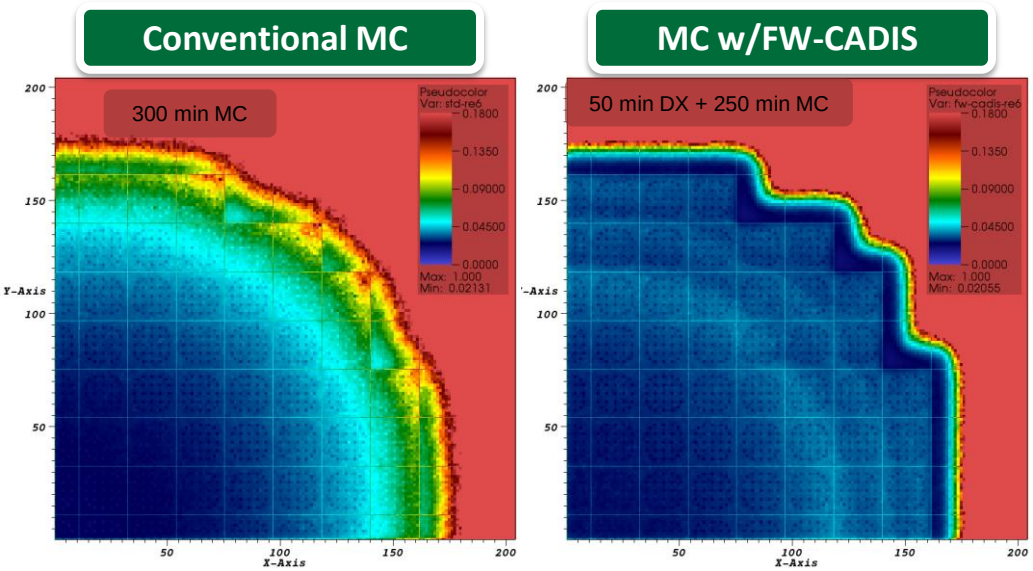
- Continuous-energy Monte Carlo (MC)
  - Explicit geometric, angular and nuclear data representation – highly accurate
  - Avoids problem-dependent multigroup xs processing – easy to use
  - Computationally intensive – considered prohibitive for "real" reactor analyses



U-235 fission cross section

CHALLENGE: Prohibitive computational TIME and MEMORY requirements

FW-CADIS method helps to overcome prohibitive computational TIME requirements



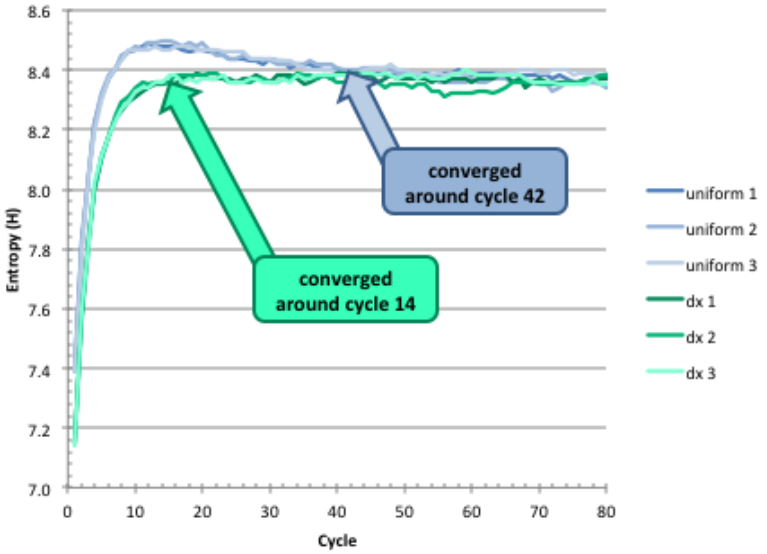
Statistical uncertainties in group 6 fluxes (0.15 to 0.275eV)

	MCNP	FW-CADIS
Uncertainty range	0.6 – 16.2%	1.0 – 6.6%
Time to < 2% uncertainty	323 hrs	45 hrs
Speed up (includes Denovo run time)	-	7.1*

*depending on computational parameters, the speed-up varied between 6 and 10

FW-CADIS deterministic solution can be exploited in other ways:

- Generate initial fission source and *k* for MC
  - accelerate source convergence
  - Improve convergence reliability



- Select domain boundaries
  - improve parallel load balancing
  - reduce Monte Carlo run time

Questions?

http://scale.ornl.gov

scalehelp@ornl.gov