SCALE and AMPX Advancements to Support NCS Applications

B. T. Rearden, M. E. Dunn, D. Wiarda, C. Celik, K. Bekar, M. L. Williams, D. E. Peplow, C. M. Perfetti, J. P. Lefebvre, and R. A. Lefebvre

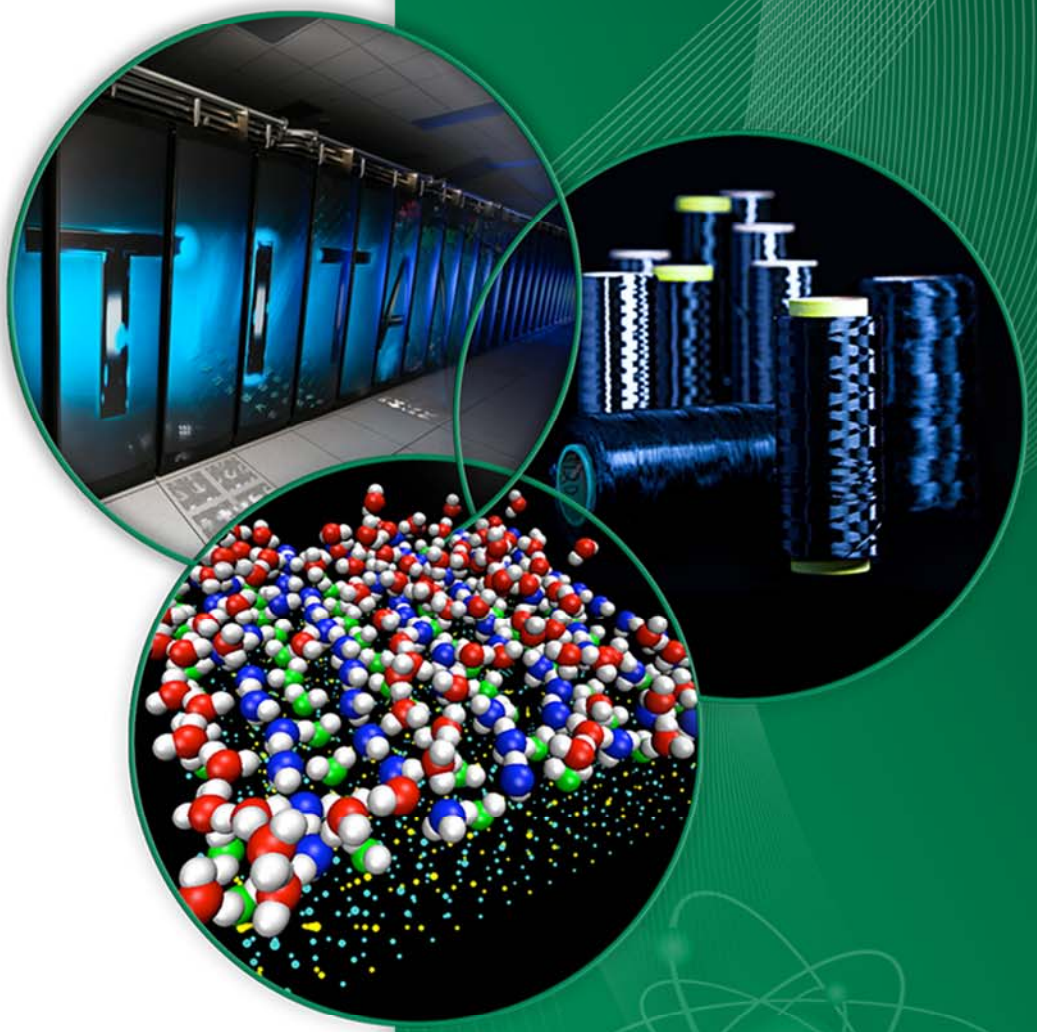
Oak Ridge National Laboratory

F. Havlůj

Nuclear Research Institute at Řež

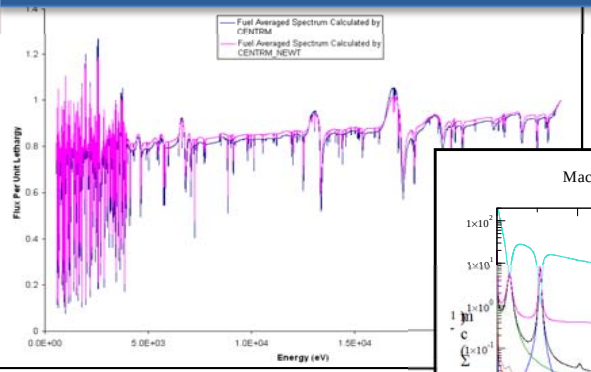
K. J. Dugan

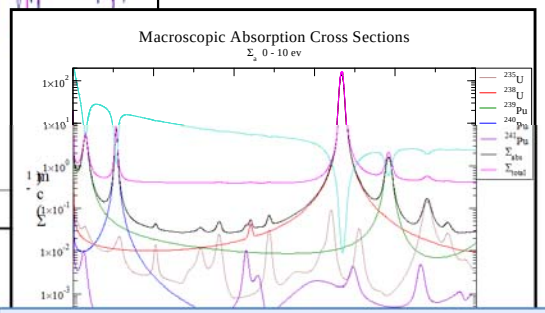
Texas A&M University



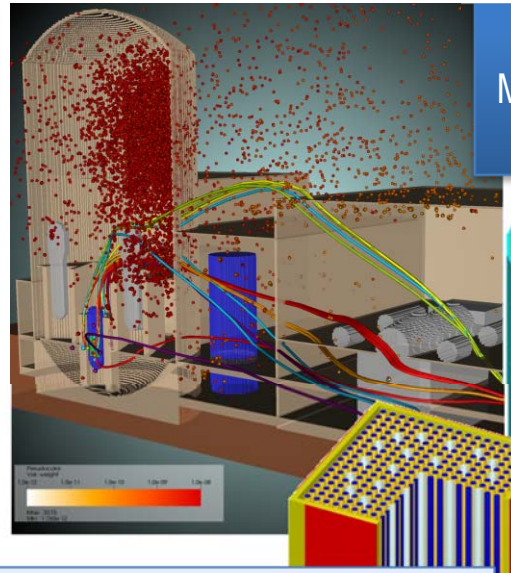
ANS Winter Meeting
Washington, DC
November 13, 2013

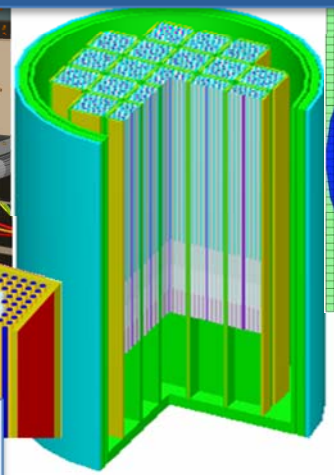
Convenient Material Input and Current Nuclear Data with Continuous-Energy Resonance Processing

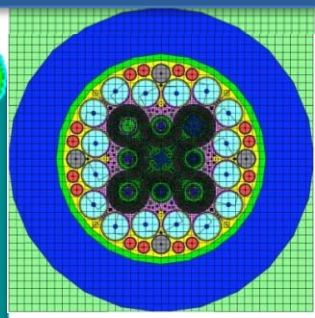




High-Resolution Geometry Modeling in Monte Carlo and Deterministic Transport for Criticality, Shielding, and Depletion





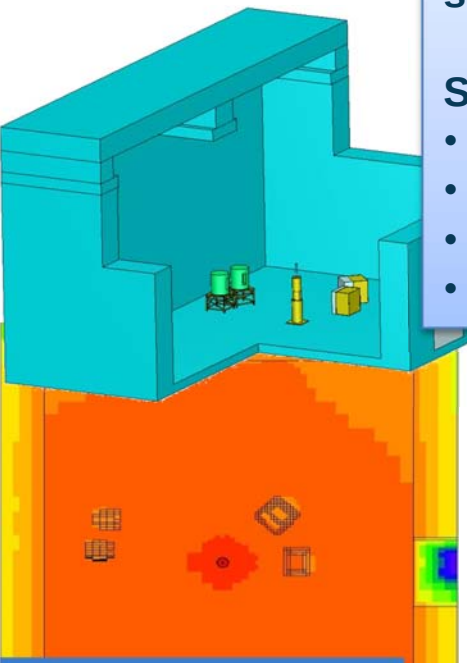


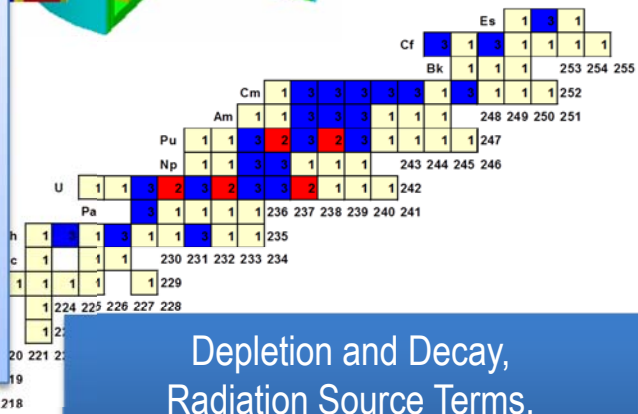
SCALE – A multipurpose nuclear modeling and simulation suite

Supported by multiple sponsors

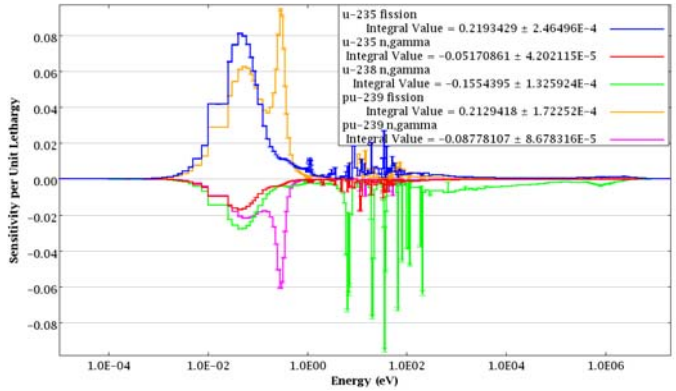
- **DOE/NNSA NCSP**
- **NRC**
- **DOE/NE**
- **DOE/EM**

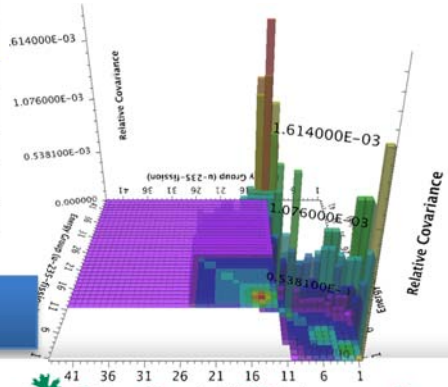
scale





Depletion and Decay, Radiation Source Terms, and Decay Heat



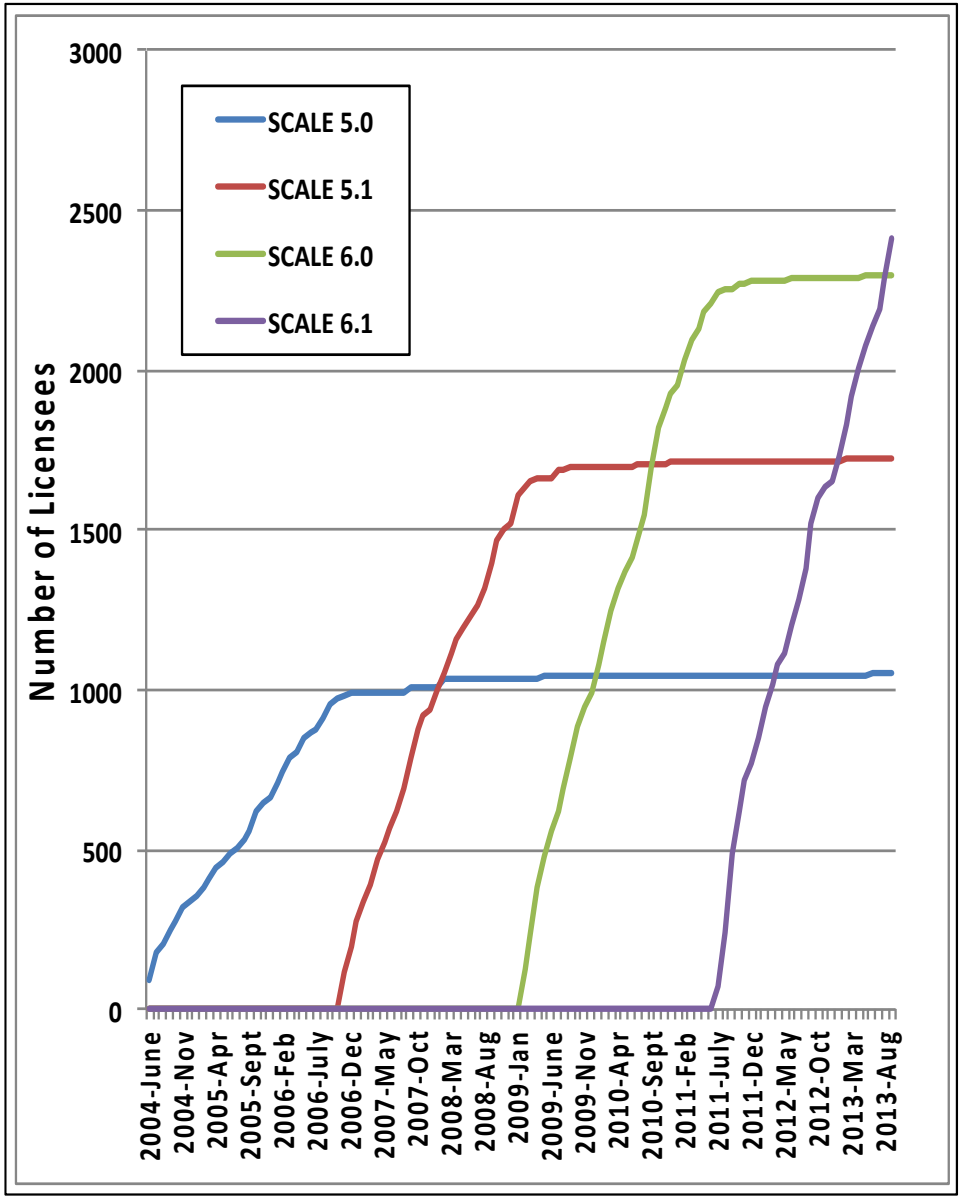


Radiation Shielding with Automated Variance Reduction

Sensitivity and Uncertainty Analysis

SCALE by the Numbers

- 7497
  - Distributions since 2004
- 5504
  - Unique users
- 40
  - Nations where SCALE is licensed



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MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

SCALE 6.2 Preview

- Significant updates since SCALE 6.1 in June 2011
- Focus on improved fidelity of solutions
- New nuclear data libraries in multigroup (MG) and continuous-energy (CE)
- Significant improvements in CE Monte Carlo capabilities
- 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
- Modernized resonance self-shielding tools
- Improved QA and V&V

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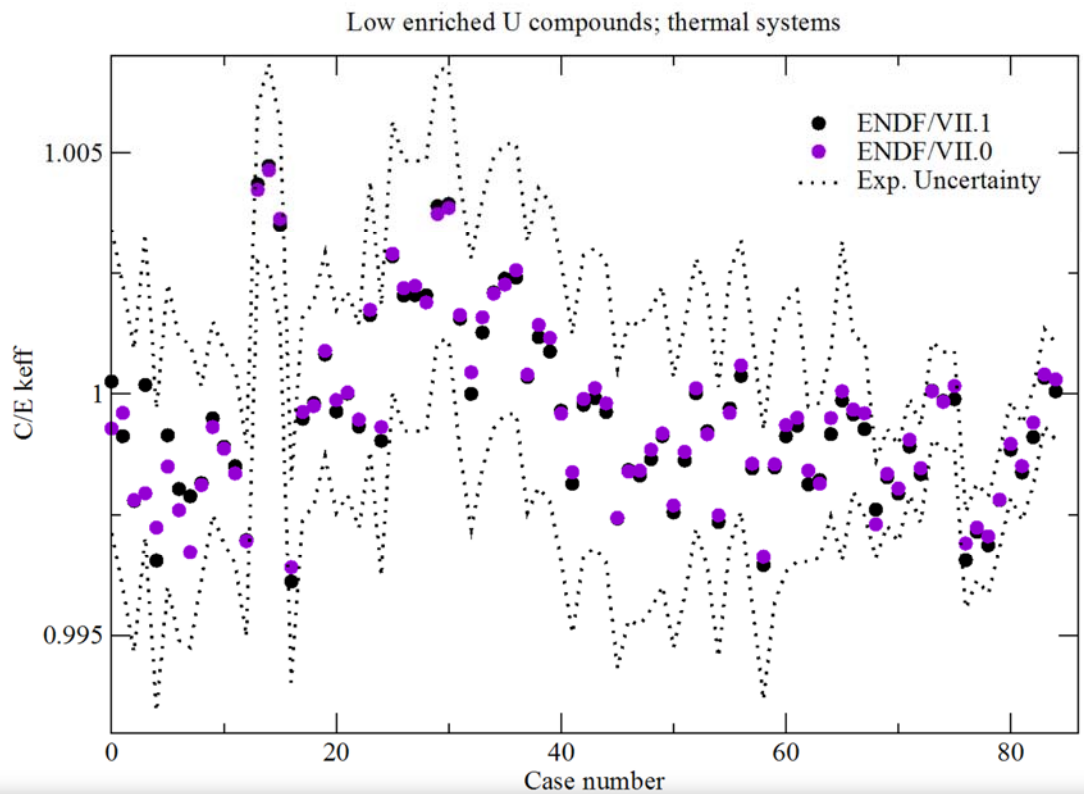
New Data Libraries

- New CE cross-section data for neutron interactions, gamma yield, and gamma interactions (sponsored by NRC, NCSP)
- 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, 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



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Improved Collision Kinematics Processing in AMPX

SCALE 6.0 and 6.1:

Y12
File 7 -> cosine moments

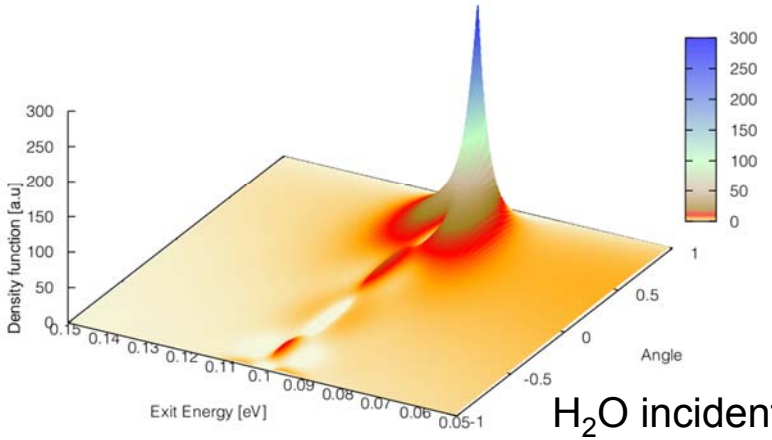
→

MONTEGO
cosine moments -> point-wise

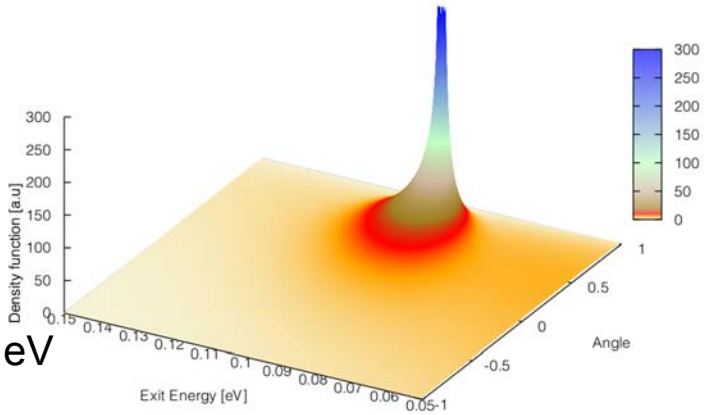
→

JAMAICAN
point-wise -> probability distr.

SCALE 6.0-6.1



SCALE 6.2



H_2O incident energy 0.1 eV

SCALE 6.2:

Y12_GAM
File 7 ->point-wise

→

JAMAICAN
point-wise -> probability distr.

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

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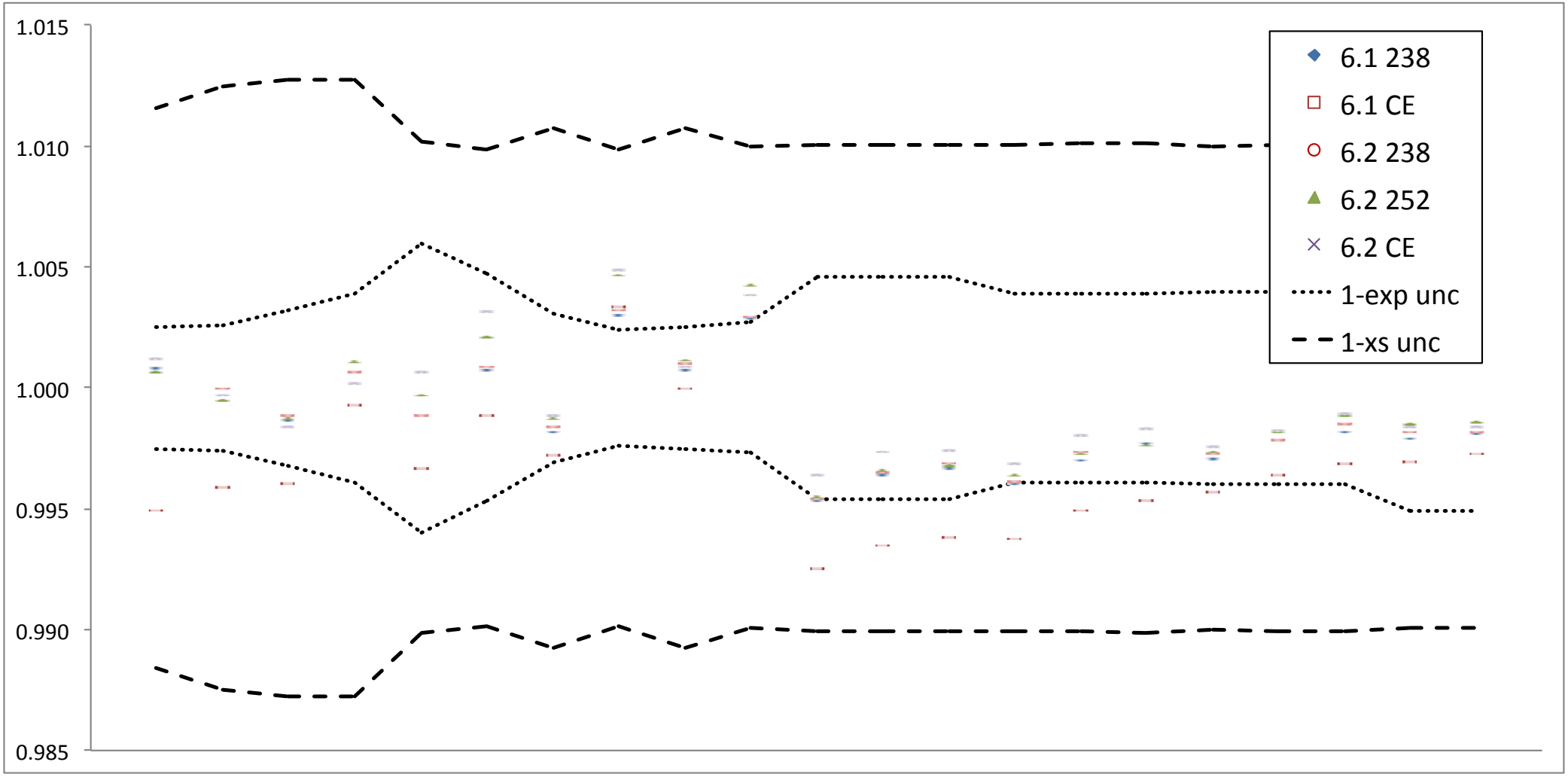
AMPX Processing Improvements Provide Improved C/E Especially for CE Calculations for MOX Benchmarks

Up to 1000 pcm improvement for burned fuel



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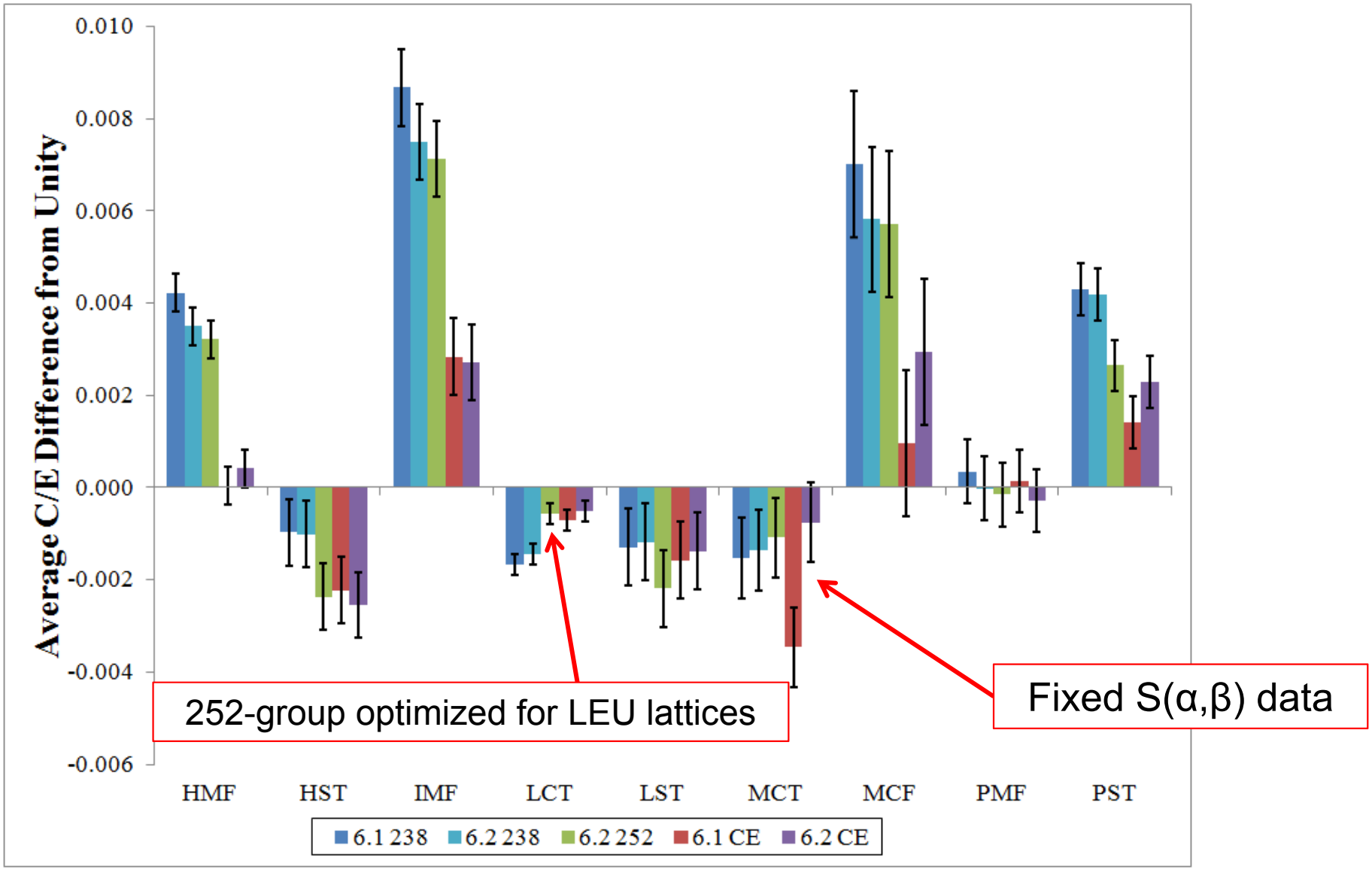
SCALE 6.1 and 6.2 C/E for ~400 VALID Benchmarks

(Same experiments in all categories)



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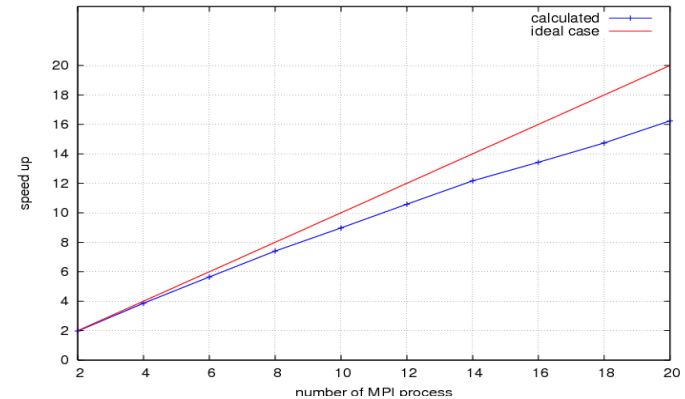
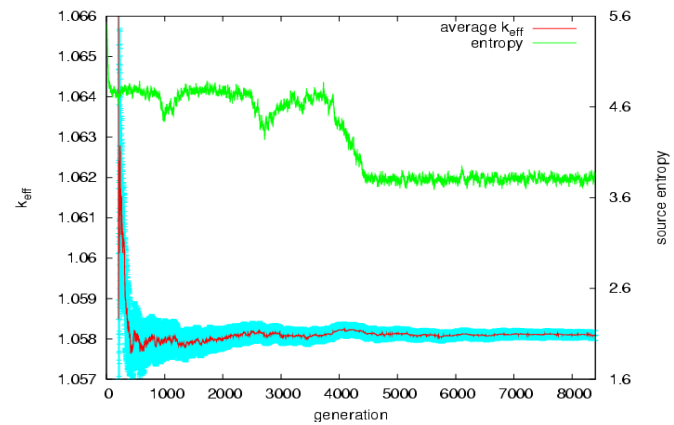
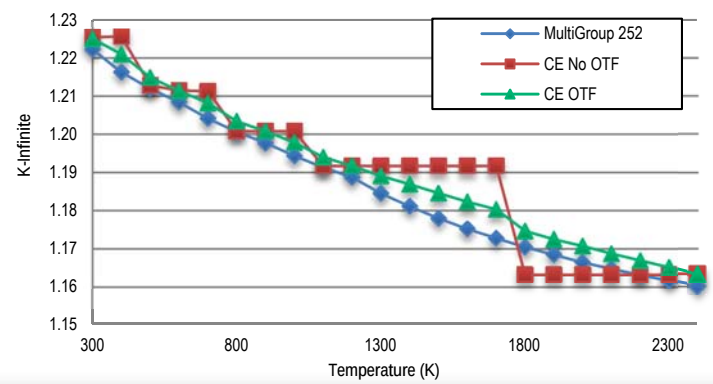
Monte Carlo Improvements for Criticality

- Parallel KENO (NRC and NCSP)
  - Significant speedups with MPI on Linux clusters
- Improved CE efficiency (ORNL)
  - Memory footprint reduced by 20-95%, depending on problem
  - Coding revised to provide improved consistency across platforms
- Source Convergence (NRC, NCSP, DOE NE)
  - Shannon Entropy diagnostics
  - Hybrid deterministic starting source methodology in Sourcerer for improved k_{eff} reliability
- Problem-Dependent Doppler broadening for CE calculations for resolved and unresolved (probability table) energy ranges (PhD)
- Doppler Broadened Rejection Correction (PhD)
  - Significant improvement in elevated temperature CE Monte Carlo







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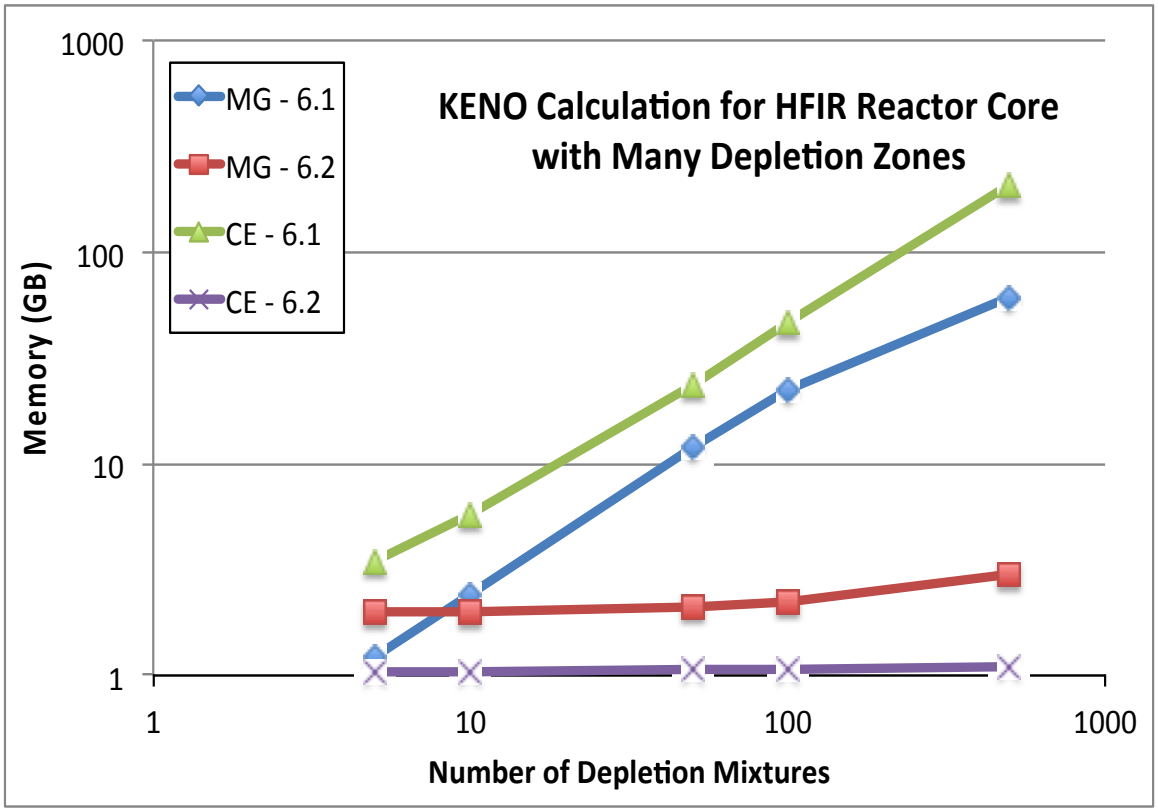
Memory Footprint

- Extensive rework of everything CE in SCALE and AMPX
- Introduction of efficient, XSProc module for MG calculations



CE Memory Improvements for Each Material	% Reduction in Memory
Conversion of internal data storage from double- to single-precision	15–45
Redesign of 2D collision kinematics data	5–30
Optimize nuclide object (in memory access to data)	3–15
Optional within-nuclide unionized reaction energy grid	10–20
TOTAL	40–95

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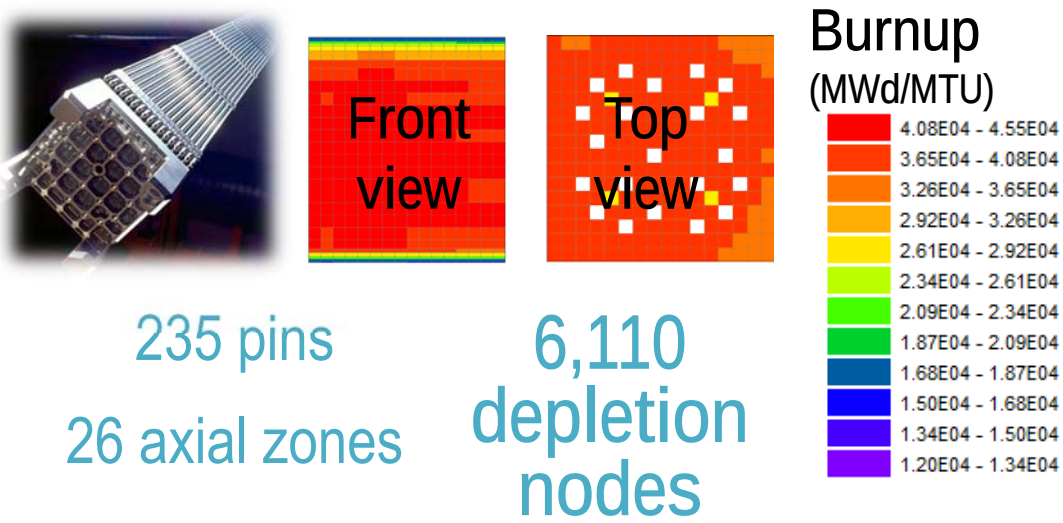
Modular Interfaces

- SCALE Continuous-Energy Modular Physics Package (SCEMPP) (NRC, ORNL)
  - Coupled neutron/gamma physics
  - Application Programmer Interface (API) for CE physics for next-generation Monte Carlo codes
  - Implemented for shielding in Monaco
  - HPC Monte Carlo with Shift (125K processors)
- 6300 fixed-source transmission tests used in V&V

- ORIGEN restructured to provide API and parallel capabilities (DOE NE)
- New ORIGAMI tool developed to rapidly characterize spent fuel.
- MPI with (near)-linear speedup



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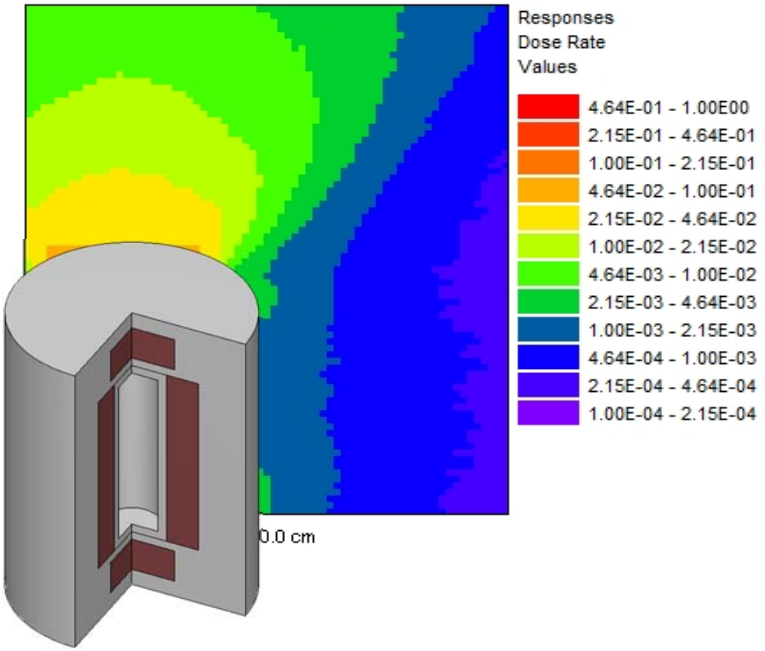
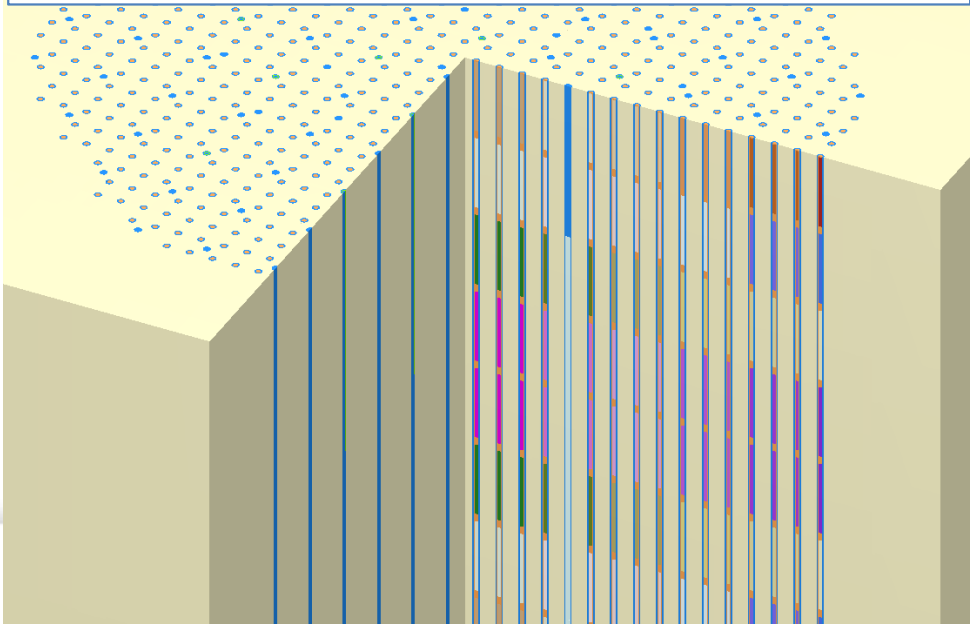
Capability Advancements

- CE Capabilities with MAVRIC/Monaco (NRC)
  - All hybrid capabilities supported with CE fidelity
  - Up to 50% improved results for dose rate calculations



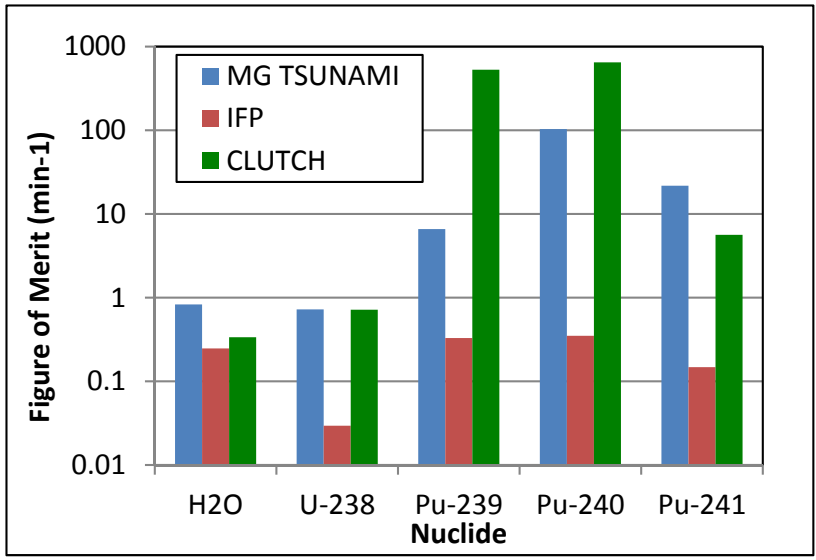
- CE Monte Carlo Depletion
  - Designed for high-fidelity analysis of full core reactors
  - Efficient memory management
  - MG reaction and flux tallies from CE data
  - Coupling with ORIGEN

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



Continuous-Energy Sensitivity Analysis

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



Sensitivity	Reference	MG TSUNAMI	CE TSUNAMI IFP	CE TSUNAMI 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

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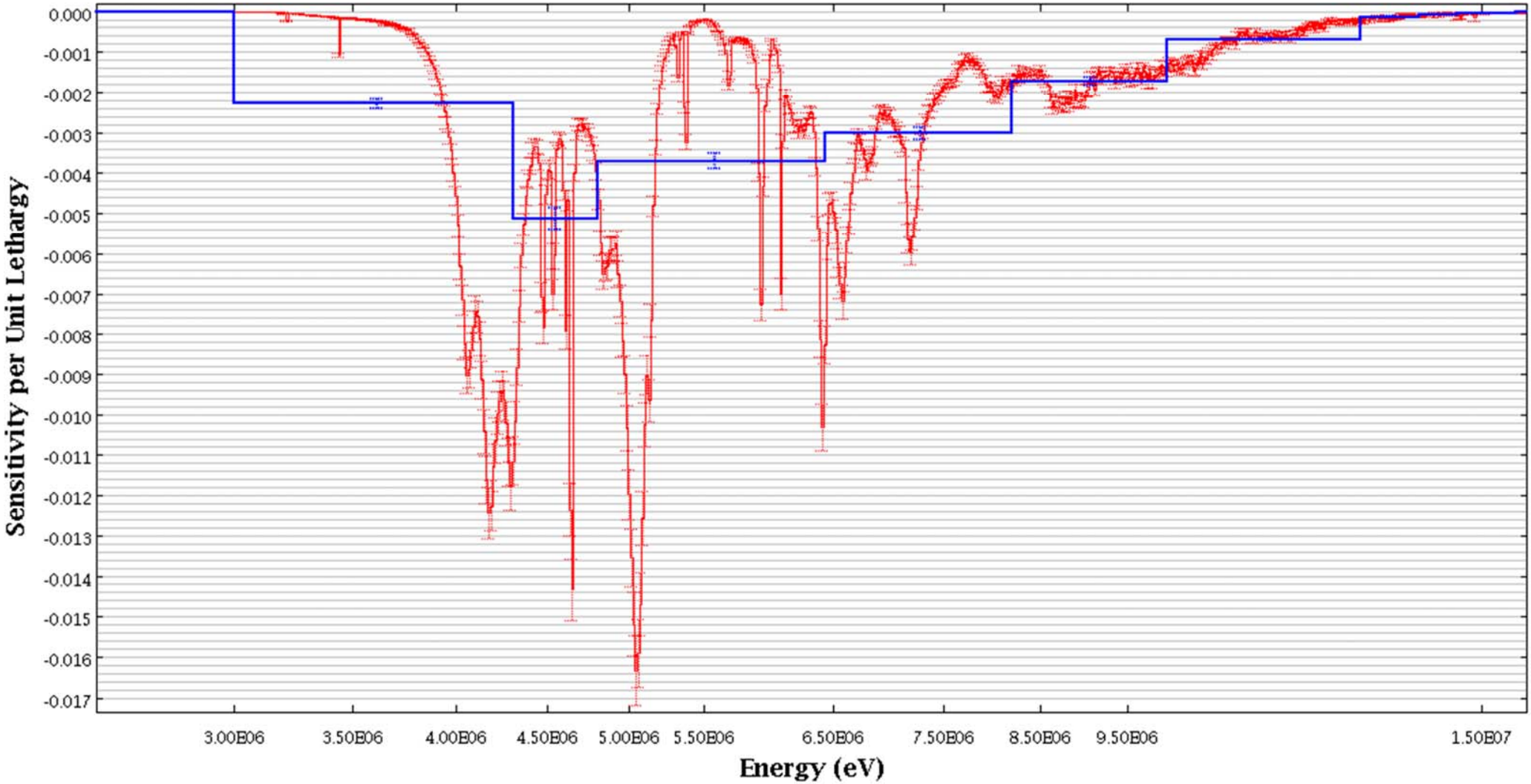
O-16 Capture Sensitivity

238-group CLUTCH VS

Microgroup CLUTCH



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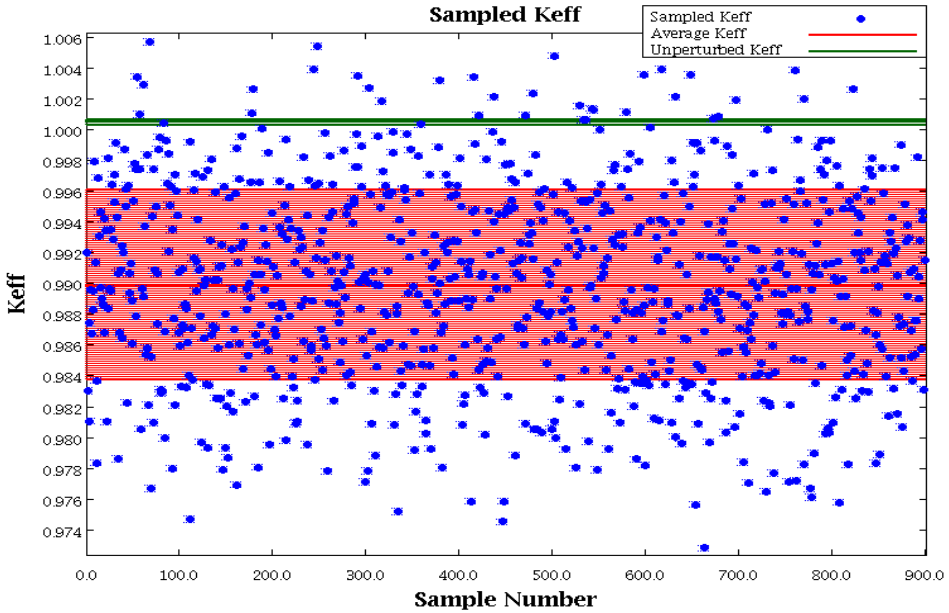
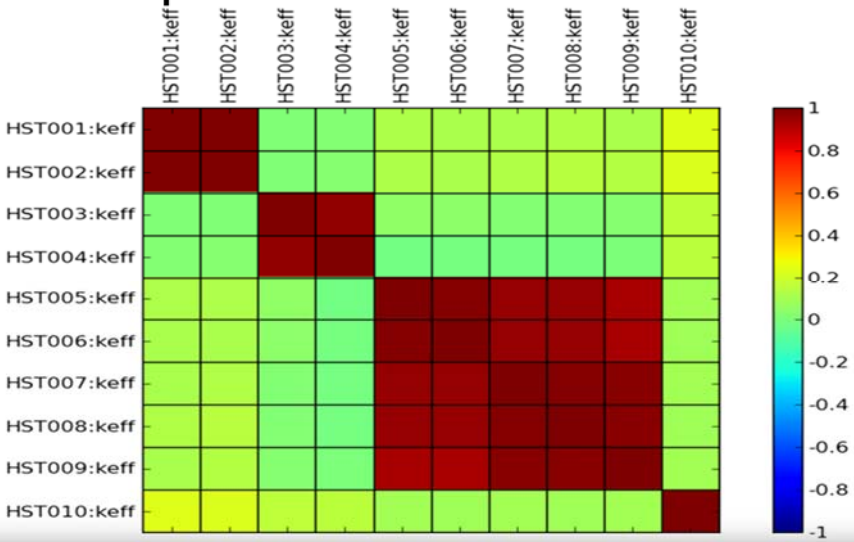
Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences (NRC, NCSP, DOE NE)

- Sampler provides uncertainty in any computed result from any SCALE sequence due to uncertainties in:
  - neutron cross sections
  - fission yield and decay data
  - geometry and composition
- Sampler propagates uncertainties through complex analysis sequences such depletion calculations
- Correlations between systems are also computed



Experimental Correlations



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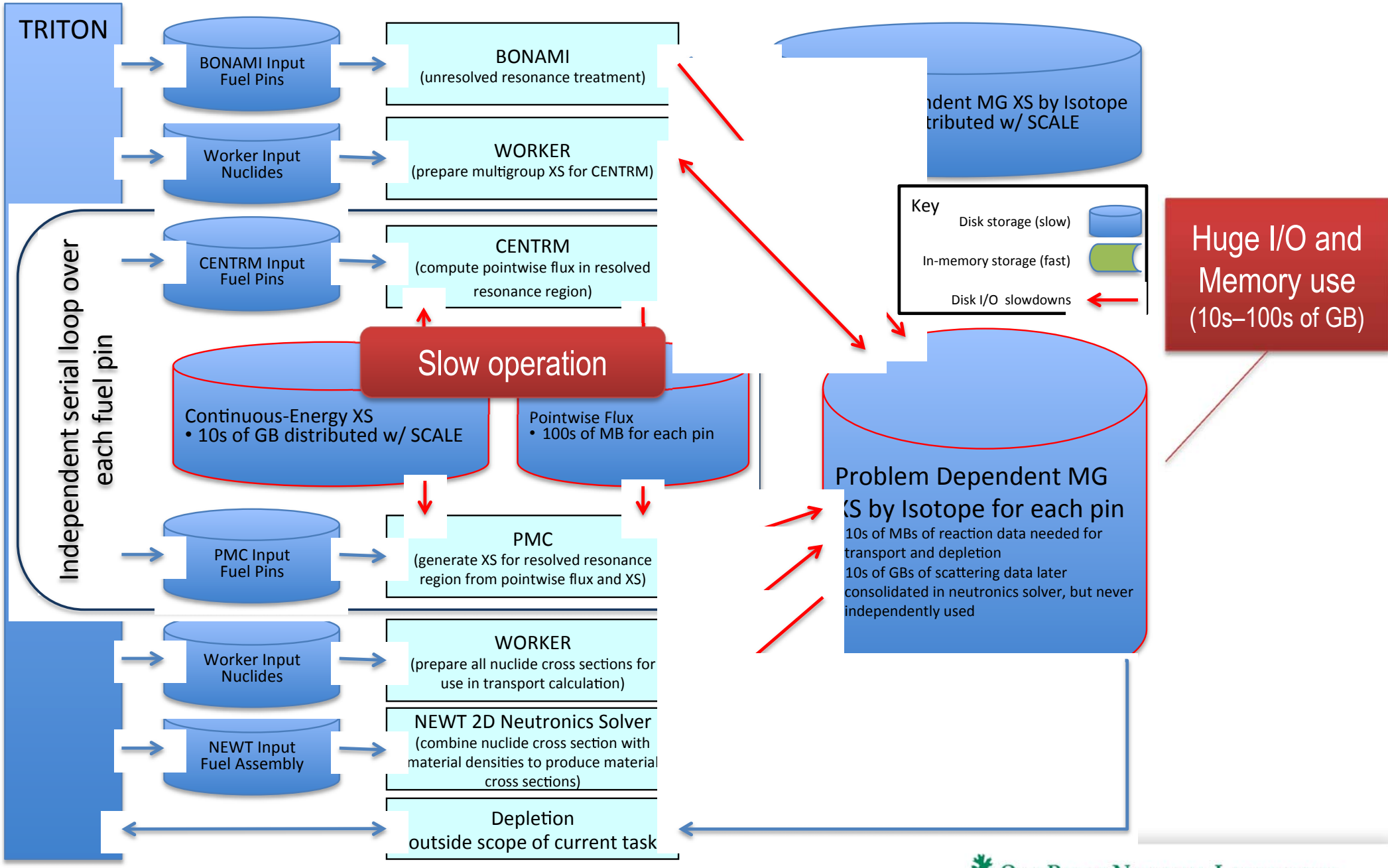
SCALE 5.0–6.1 Resonance Self-Shielding

(somewhat simplified view)



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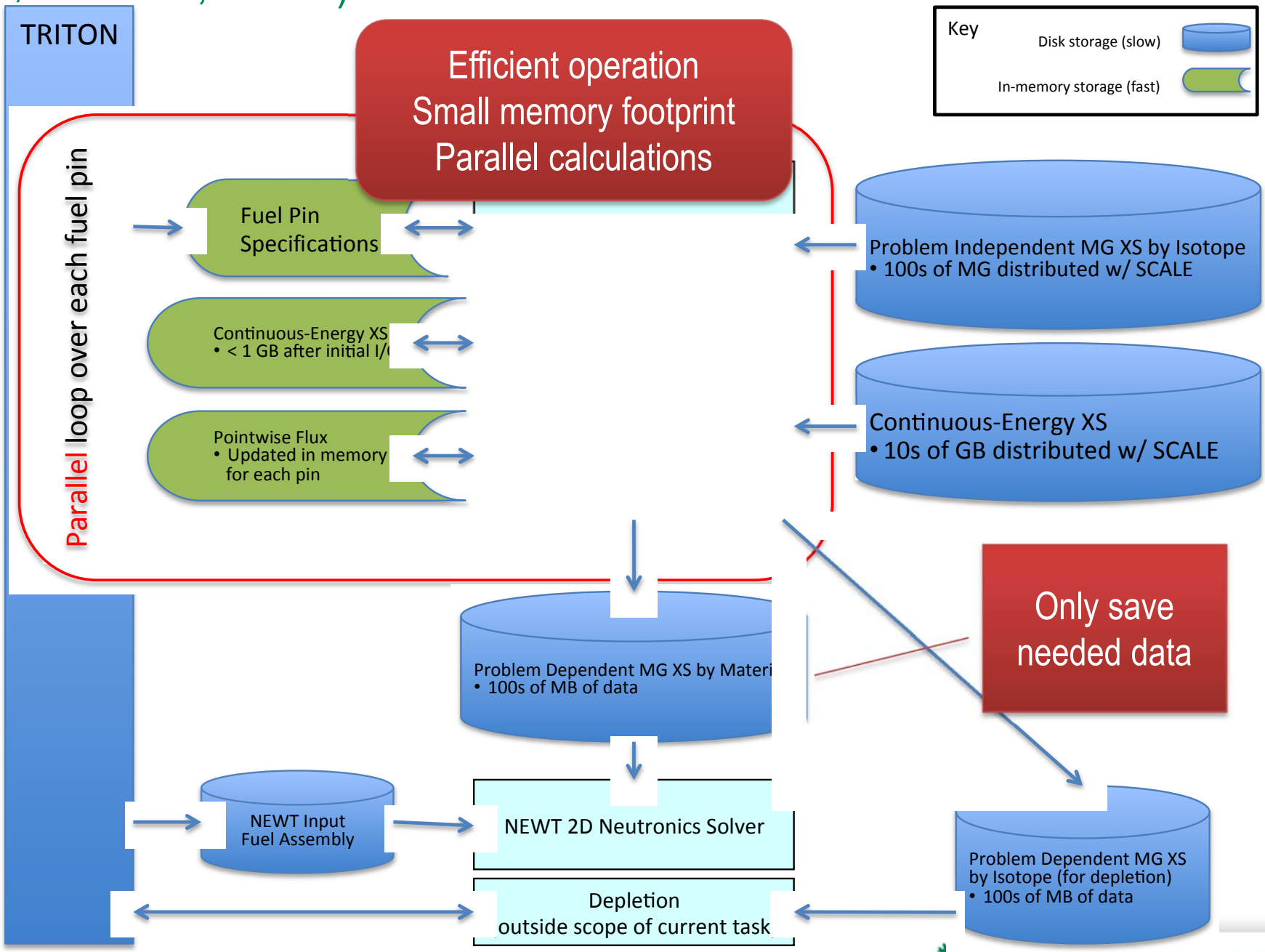
SCALE 6.2 Resonance Self-Shielding
(NRC, DOE NE, NCSP)



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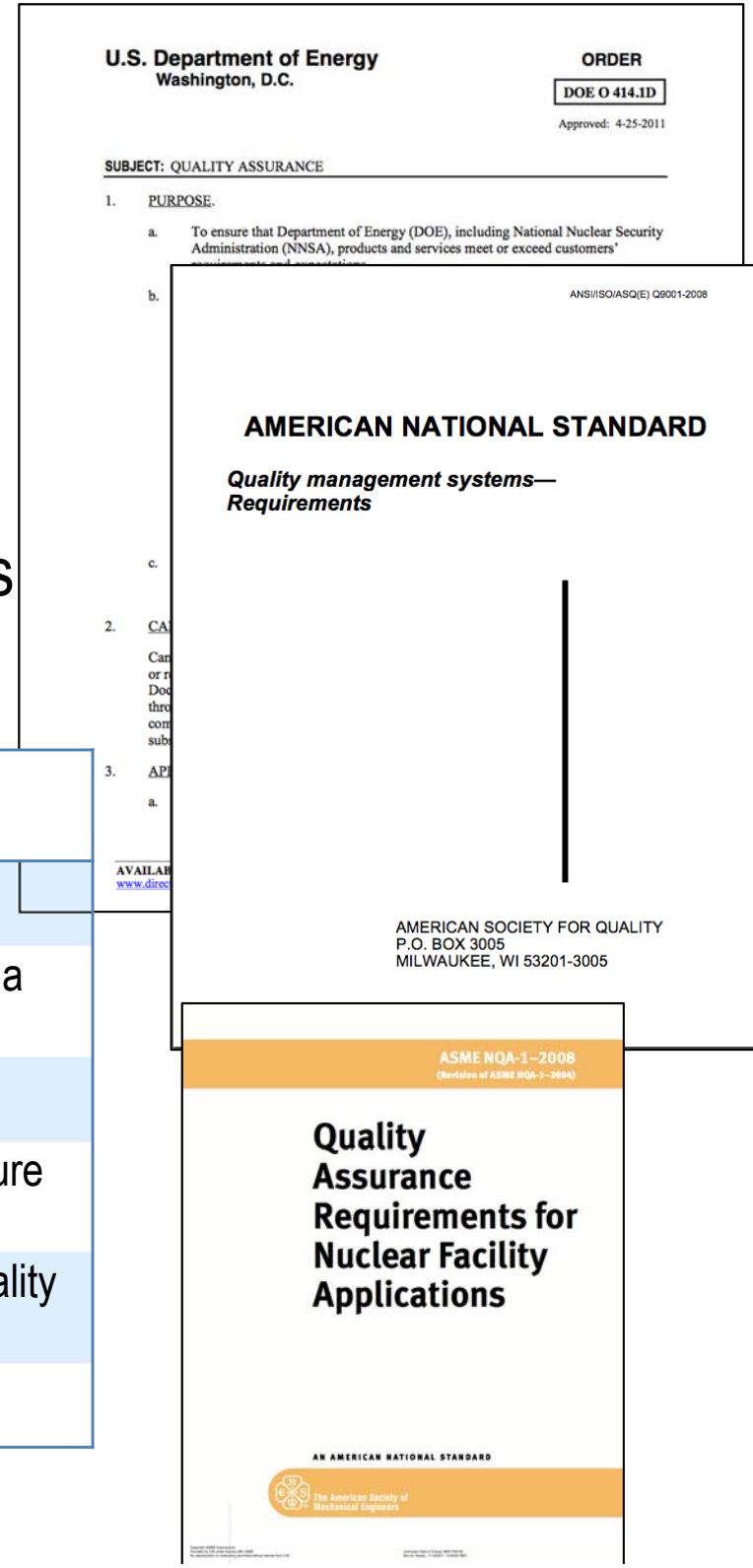
Updated QA Program (NCSP, NRC)

- 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

ASME NQA-1–2008
(Revision of ASME NQA-1–2004)

Quality Assurance Requirements for Nuclear Facility Applications

AN AMERICAN NATIONAL STANDARD

The American Society of Mechanical Engineers

Improved SCALE V&V (All Sponsors)

- 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

My CDash All Dashboards Log Out Thursday, May 23 2013 17:08:49 EDT

SCALE

Dashboard Calendar Previous Current Next Project

No file changed as of **Sunday, May 19 2013 - 21:00 EDT**

Show Filters Advanced View Auto-refresh Help

Nightly

Site	Build Name	Update	Configure		Build		Test			Build Time
		Files	Error	Warn	Error	Warn	Not Run	Fail	Pass	
dev1.ornl.gov	Release-Intel-12.0.3.174									Expected build
dev6.ornl.gov	Debug-Intel-12.0.3.174-openmpi-1.4.3									Expected build
dev6.ornl.gov	Release-Intel-12.0.3.174-openmpi-1.4.3									Expected build
dev1.ornl.gov	Debug-Intel-13.0.1.117									Expected build
dev2.ornl.gov	Debug-Intel-13.0.1.117-regression	10	0	3	0	50	0	18^{+1}_{-7}	354^{+6}_{-1}	May 20, 2013 - 09:37 EDT
dev1.ornl.gov	Release-Intel-13.0.1.117	2	0	1	0	50^{+50}	0	4^{+4}	676^{+676}	May 20, 2013 - 09:52 EDT
dev2.ornl.gov	Release-Intel-13.0.1.117-regression	10	0	3	0	50	0	1^{+1}	377_{-1}	May 20, 2013 - 09:37 EDT
dev2.ornl.gov	Release-Intel-13.0.1.117-regression	10	0	3	0	50	0	0_{-1}	378^{+1}	May 20, 2013 - 17:40 EDT

Continuous - Linux

Site	Build Name	Update	Configure		Build		Test			Build Time
		Files	Error	Warn	Error	Warn	Not Run	Fail	Pass	
dev4.ornl.gov	Release-GNU-4.6.1-samples	10	0	3	0	50	0	11	252	May 20, 2013 - 19:05 EDT
dev2.ornl.gov	Release-GNU-4.6.1-regression	10	0	3	0	50	0	5	373	May 20, 2013 - 18:24 EDT
dev4.ornl.gov	Release-Intel-13.0.1.117-samples	10	0	3	0	50	0	0	263	May 20, 2013 - 17:22 EDT
dev1.ornl.gov										2013 - 14:56 EDT
dev1.ornl.gov										2013 - 14:55 EDT
dev5.ornl.gov										2013 - 14:55 EDT
dev5.ornl.gov	Release-GNU-4.6.1-openmpi-1.4.3	10	0	3	0	50	0	4	944	May 20, 2013 - 14:55 EDT
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dev4.ornl.gov	Release-Intel-13.0.1.117-samples	10	0	3	0	50	0	0	263	May 20, 2013 - 09:36 EDT
dev2.ornl.gov	Debug-GNU-4.6.1-regression	10	0	3	0	50	0	10^{+1}	362_{-1}	May 20, 2013 - 09:35 EDT
dev2.ornl.gov	Release-GNU-4.6.1-regression	10	0	3	0	50	0	5	373	May 20, 2013 - 09:35 EDT
dev1.ornl.gov	Release-GNU-4.6.1	2	0	3	0	50	0	4	676	May 20, 2013 - 09:35 EDT

ctest-2.8.8

Total of ~70,000 tests run every day

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Conclusions

- SCALE 6.2 continues a 30-year legacy of nuclear systems modeling and simulation by providing comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, spent fuel and radioactive source term characterization, radiation shielding, and sensitivity/uncertainty analysis.
- The new capabilities within SCALE 6.2 provide significant advances over previous versions
  - Improved CE and MG data
  - CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity/uncertainty analysis,
  - Modularity for CE physics and depletion
  - Stochastic sampling with Sampler
  - Improved resonance self-shielding, QA, and V&V

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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

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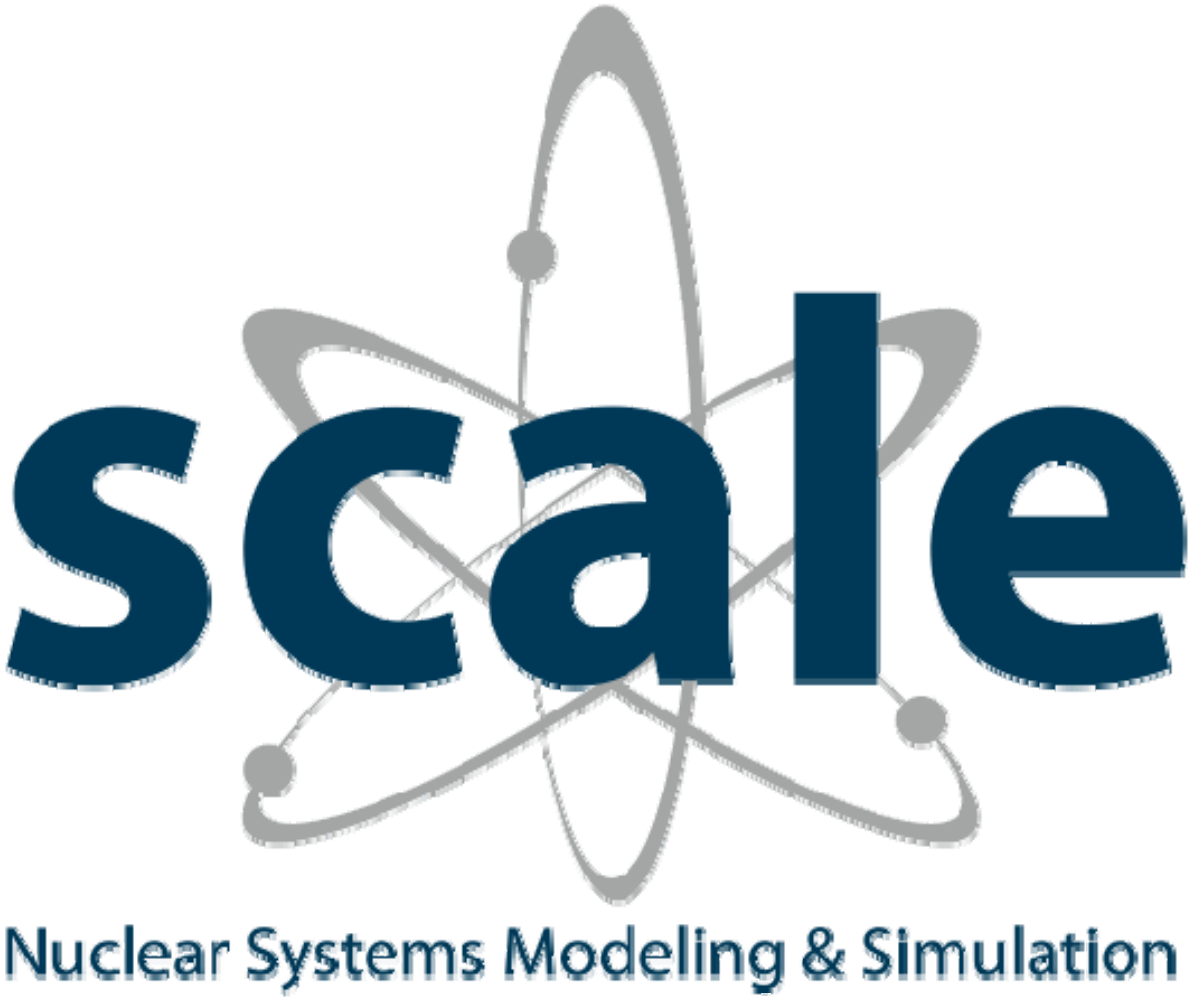
Questions?

http://scale.ornl.gov

scalehelp@ornl.gov



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