Accuracy and Runtime Improvements with SCALE 6.2

Presented to:

SCALE Users' Group Workshop

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SCALE 6.2 – April 2016

Innovative

- Modernized architecture for efficiency and quality
- Enhanced sensitivity and uncertainty analysis
- Problem-dependent temperature treatments for continuous-energy Monte Carlo
- Reference continuous-energy depletion

Efficient

- Accelerated lattice physics capabilities
- Reduced memory requirements
- Parallel calculations

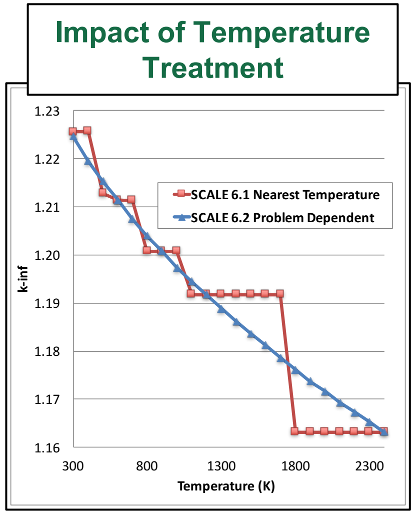
Accurate

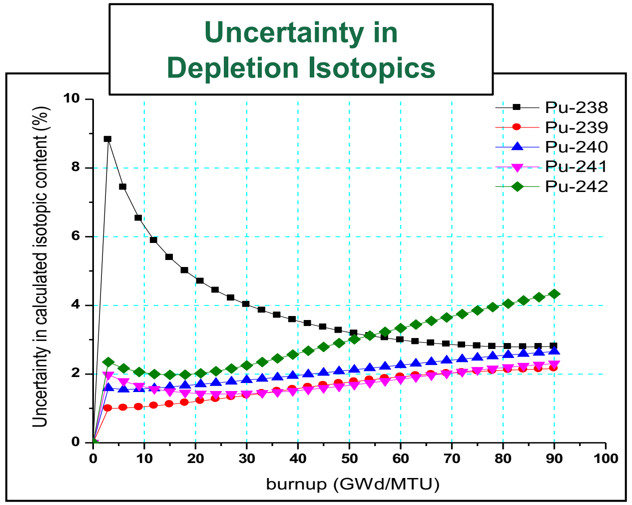
- Code and data enhancements to minimize historical biases
- Greatly expanded test suites for validation and verification

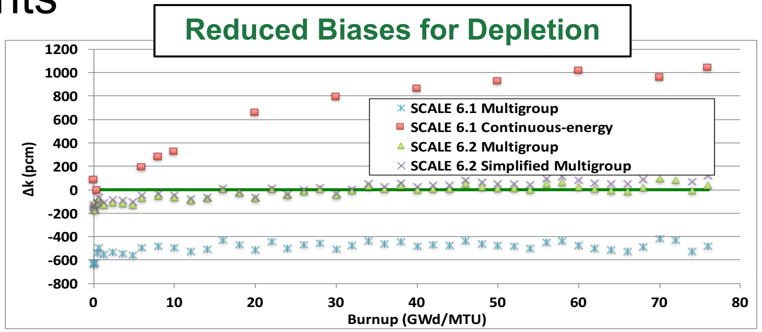
Easy to Use

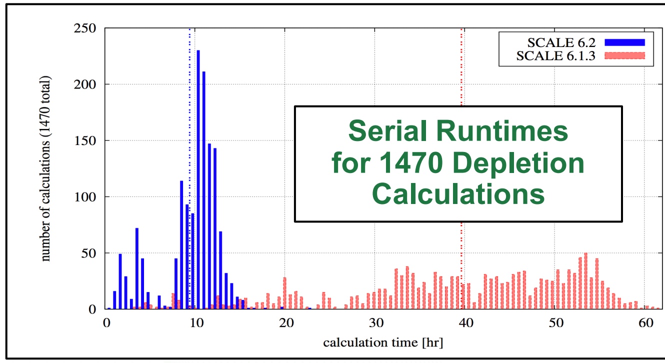
- Integrated user interface
- Simplified input

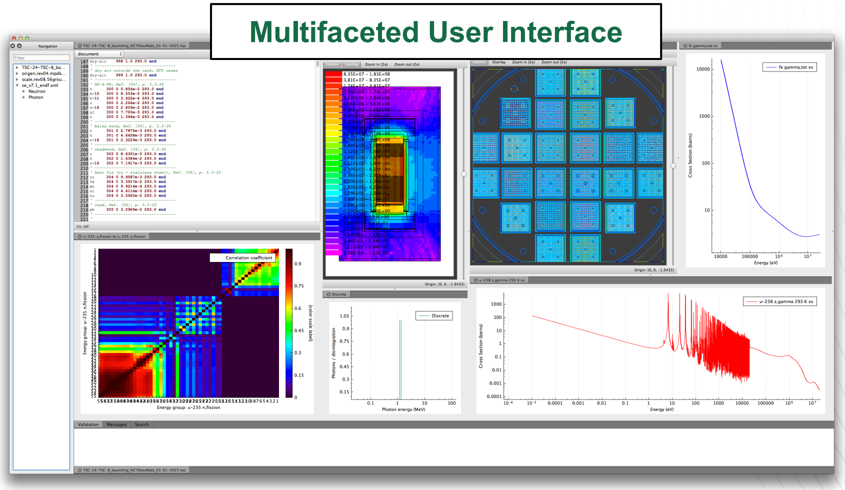
2000 licenses issued through March 2016

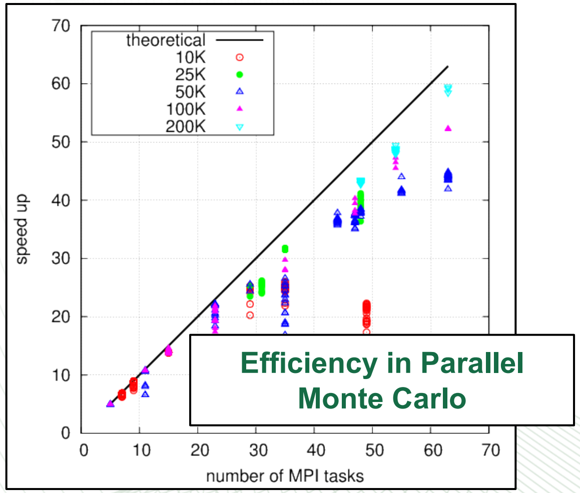




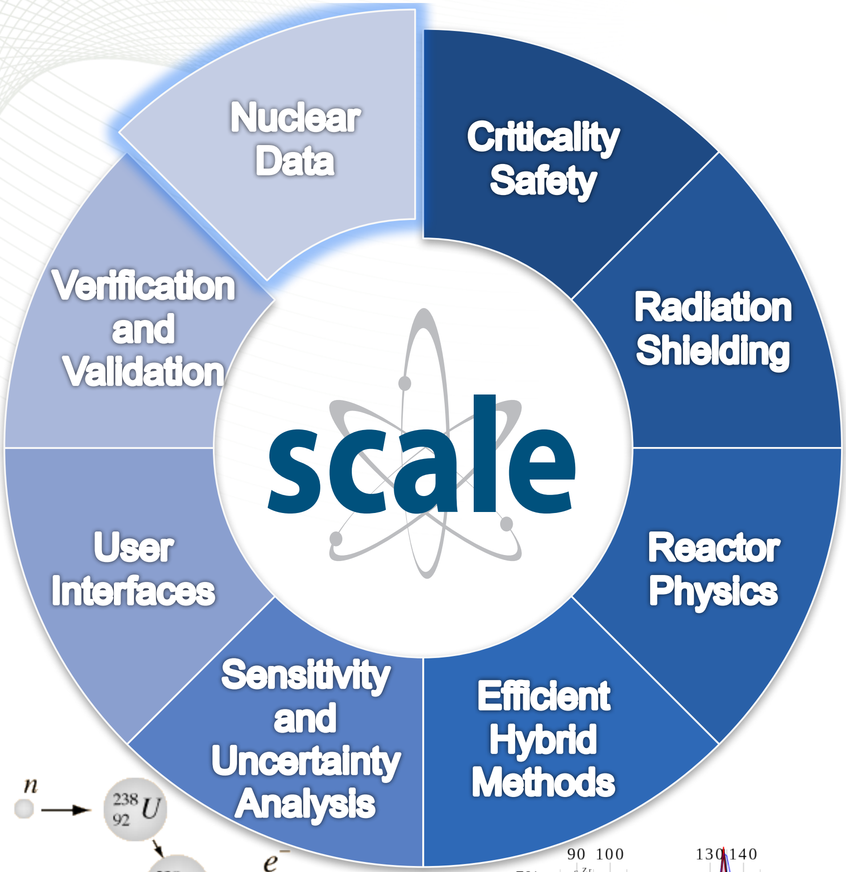


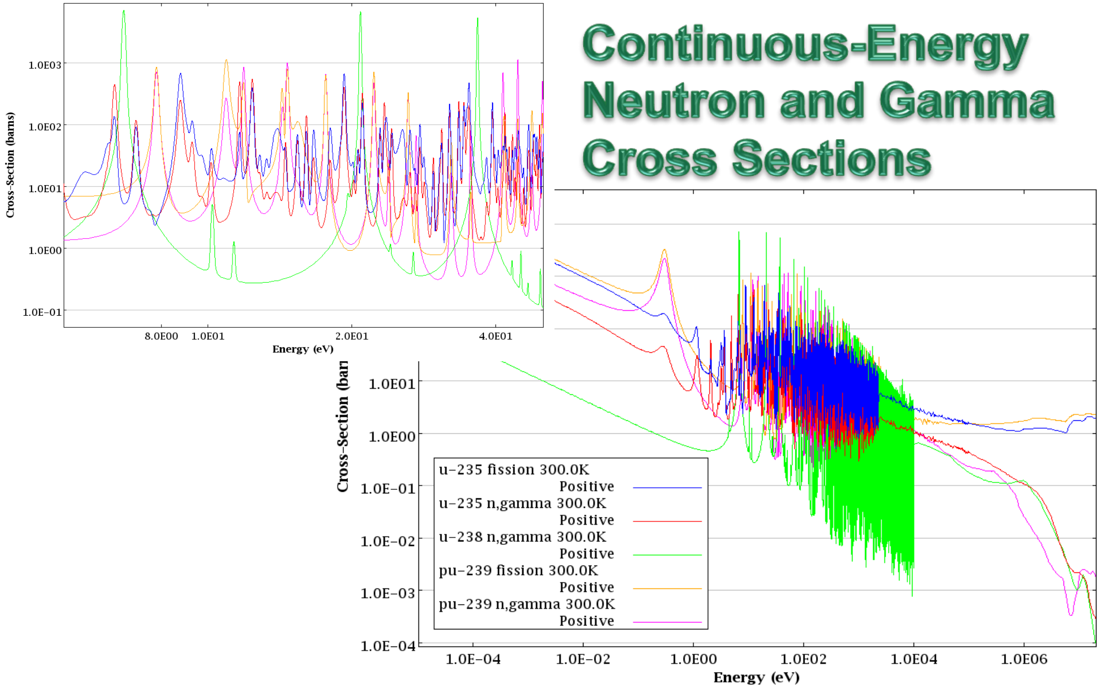






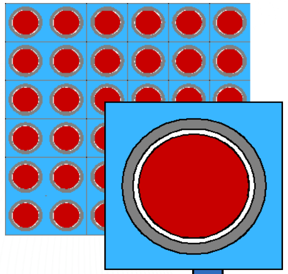
Nuclear Data from ORNL AMPX Tools

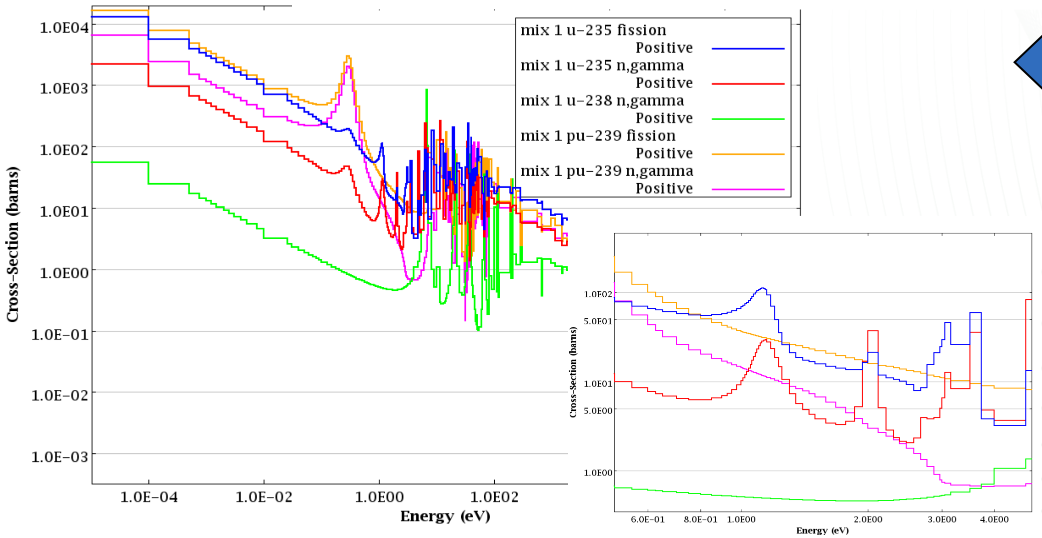




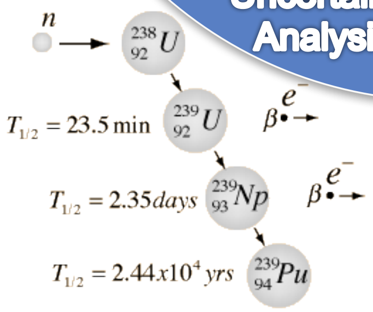
Continuous-Energy Neutron and Gamma Cross Sections

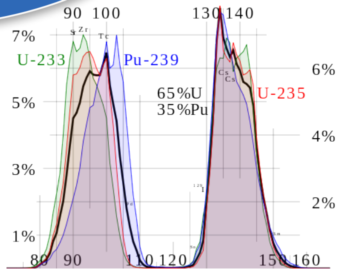
Resonance Self-Shielding





Multigroup Neutron and Gamma Cross Sections



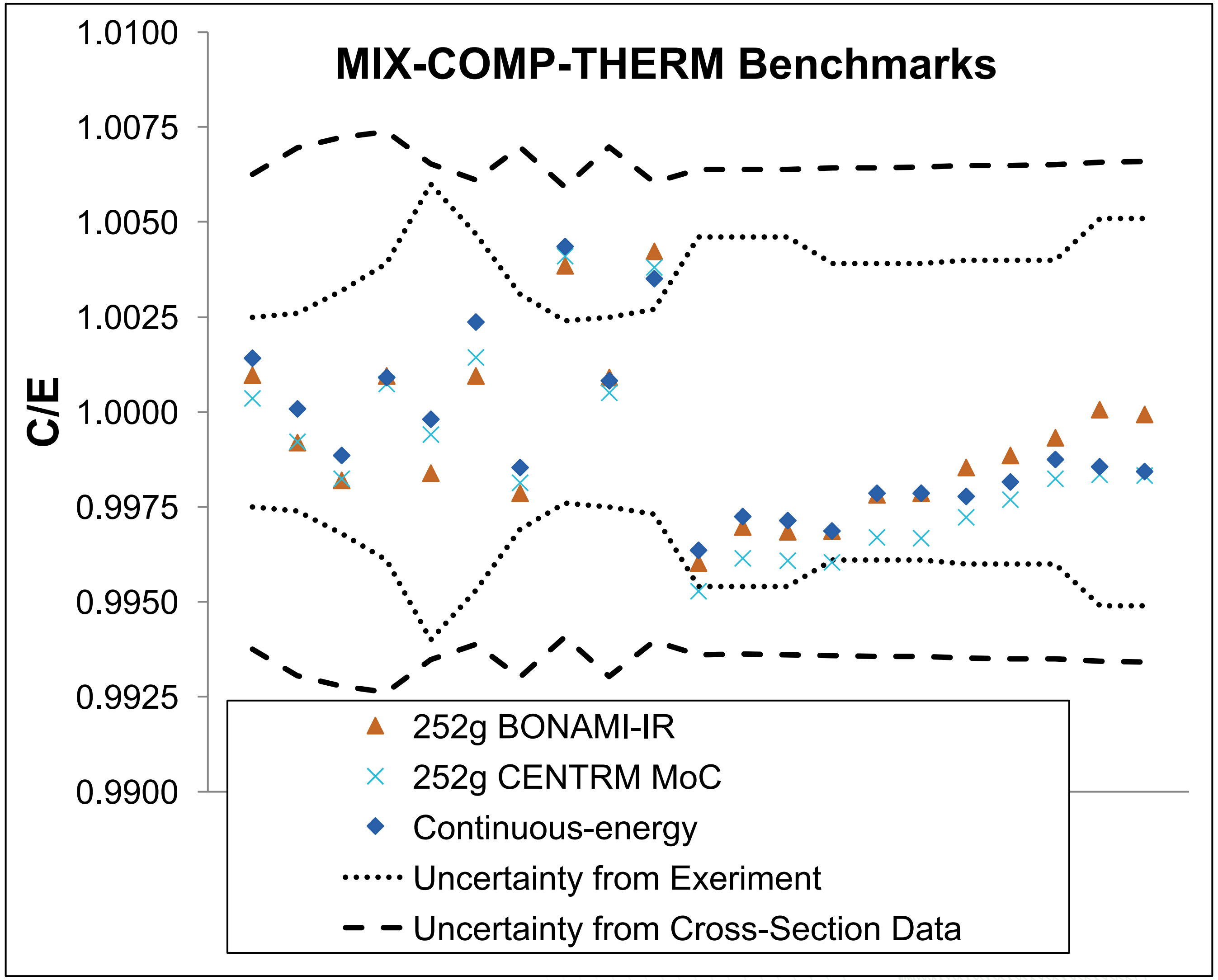


Depletion, Decay, and Activation Data

OAK RIDGE National Laboratory

Cross Section Data

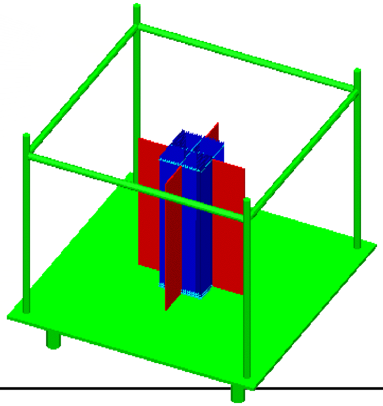
- New CE cross-section data for neutron interactions, gamma yield, and gamma interactions
- ENDF/B-VII.1 nuclear data
- New MG neutron libraries
  - 252-group energy structure
  - 56-group energy structure
  - Intermediate resonance parameters
- Extensive test suite
  - 411 VALID benchmarks
  - 7000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

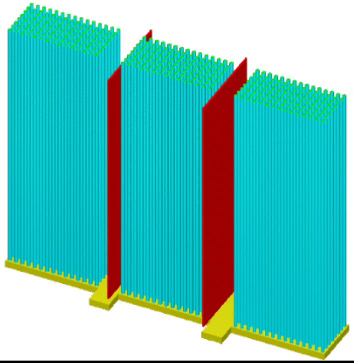
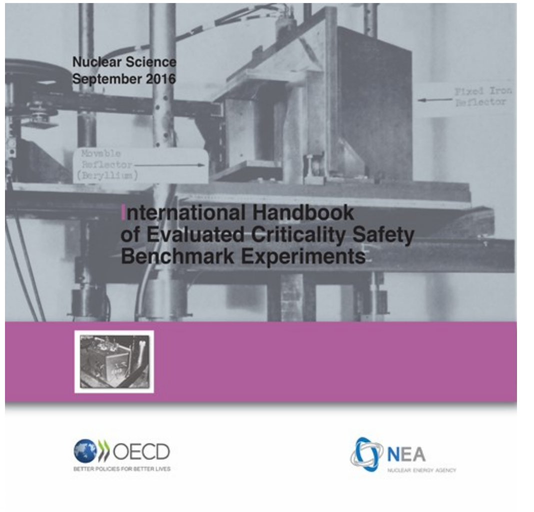


AMPX now included with SCALE distribution so users can create their own libraries!

Validation with critical benchmarks for many types of systems – VALID suite

- 411 configurations from International Criticality Safety Benchmark Evaluation Project (ICSBEP)

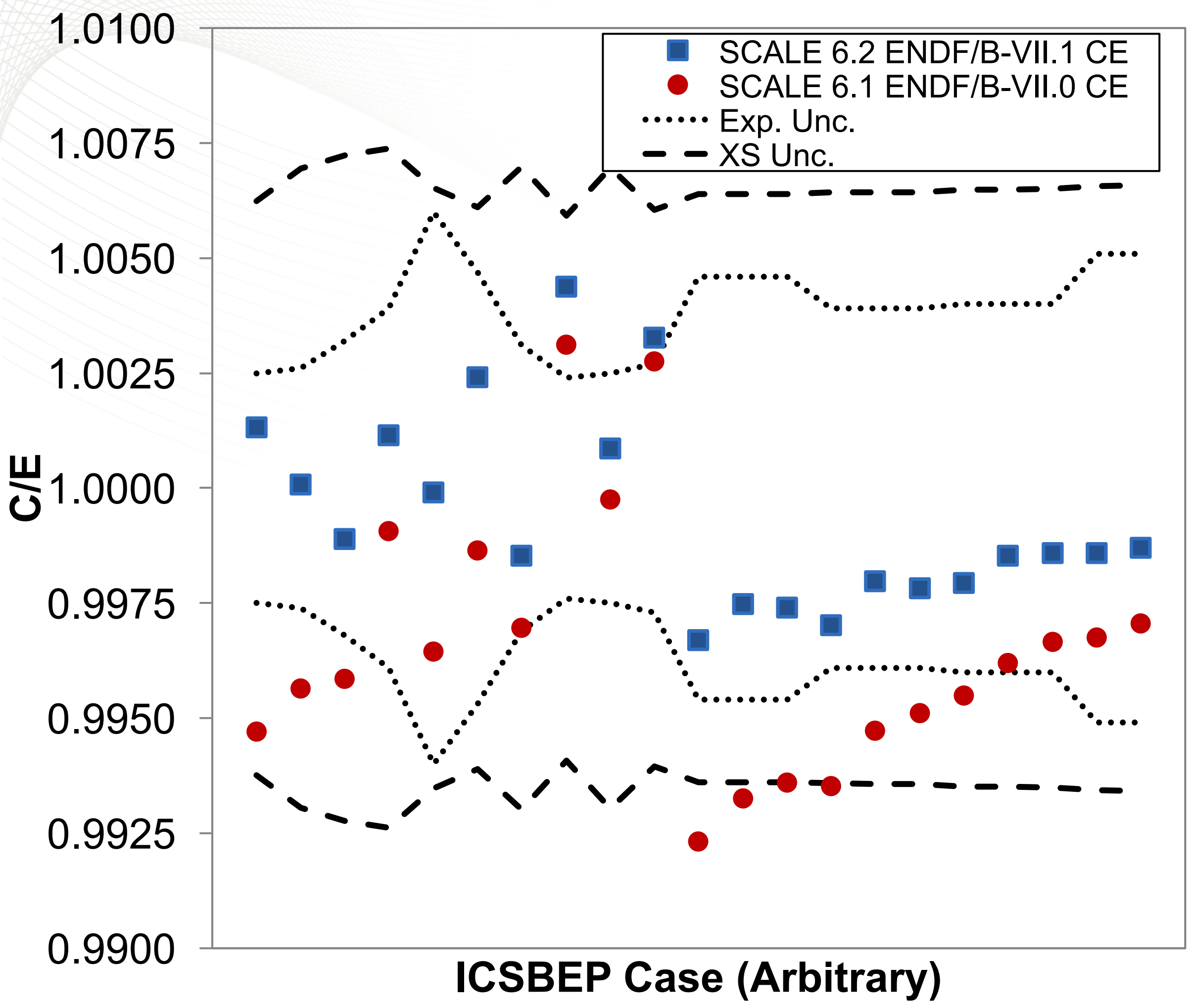



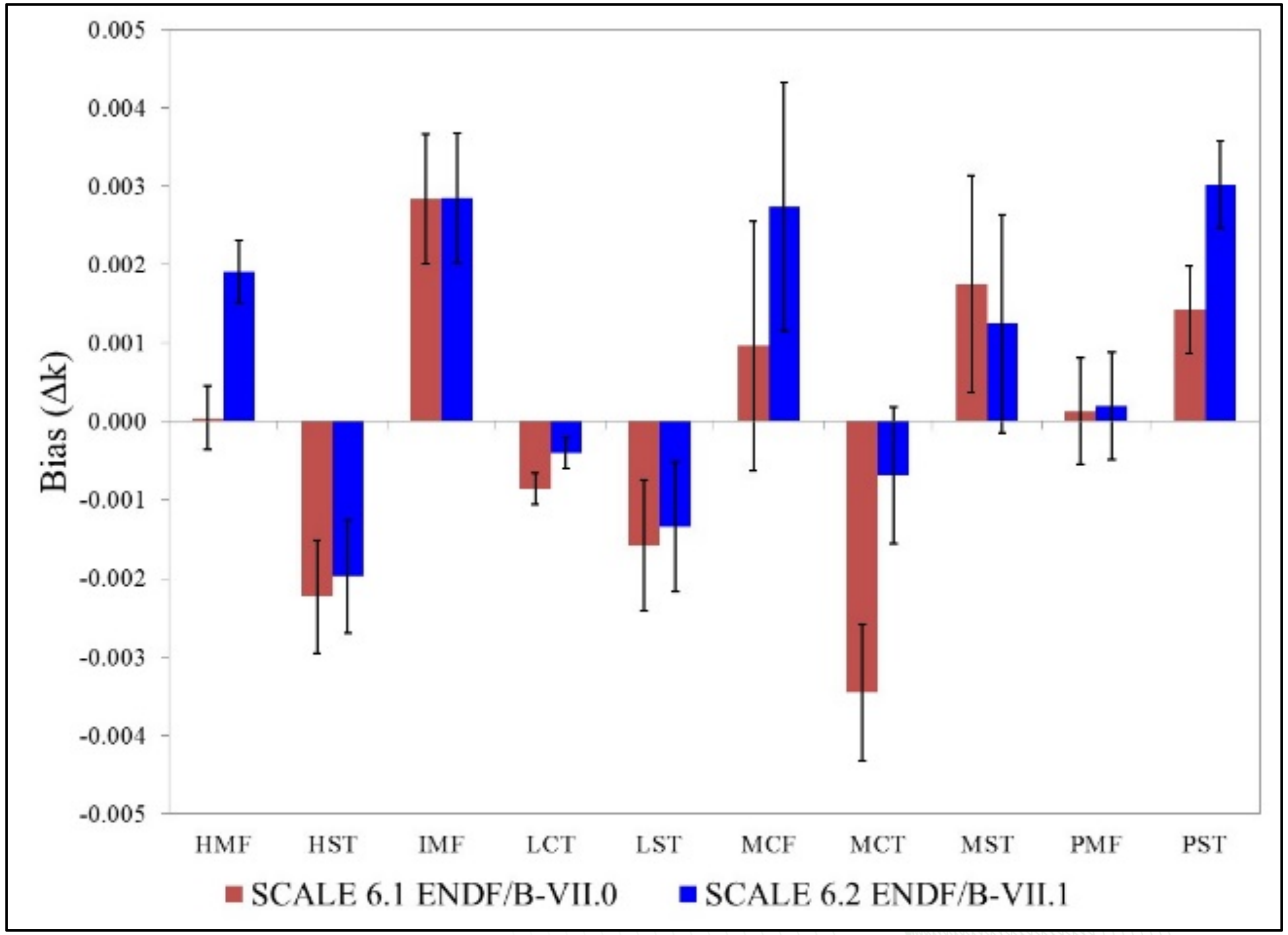



Sequence / Geometry	Experiment class	ICSBEP case numbers	Number of configurations
CSAS5 / KENO V.a	HEU-MET-FAST	15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 65	18
	HEU-SOL-THERM	1, 13, 14, 16, 28, 29, 30	52
	IEU-MET-FAST	2, 3, 4, 5, 6, 7, 8, 9	8
	LEU-COMP-THERM	1, 2, 8, 10, 17, 42, 50, 78, 80	140
	LEU-SOL-THERM	2, 3, 4	19
	MIX-MET-FAST	5, 6	2
	MIX-COMP-THERM	1, 2, 4	21
	MIX-SOL-THERM	2	3
	PU-MET-FAST	1, 2, 5, 6, 8, 10, 18, 22, 23, 24	10
	PU-SOL-THERM	1, 2, 3, 4, 5, 6, 7, 11, 20	81
CSAS6 / KENO-VI	HEU-MET-FAST	5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93	27
	IEU-MET-FAST	19	2
	MIX-COMP-THERM	8	28

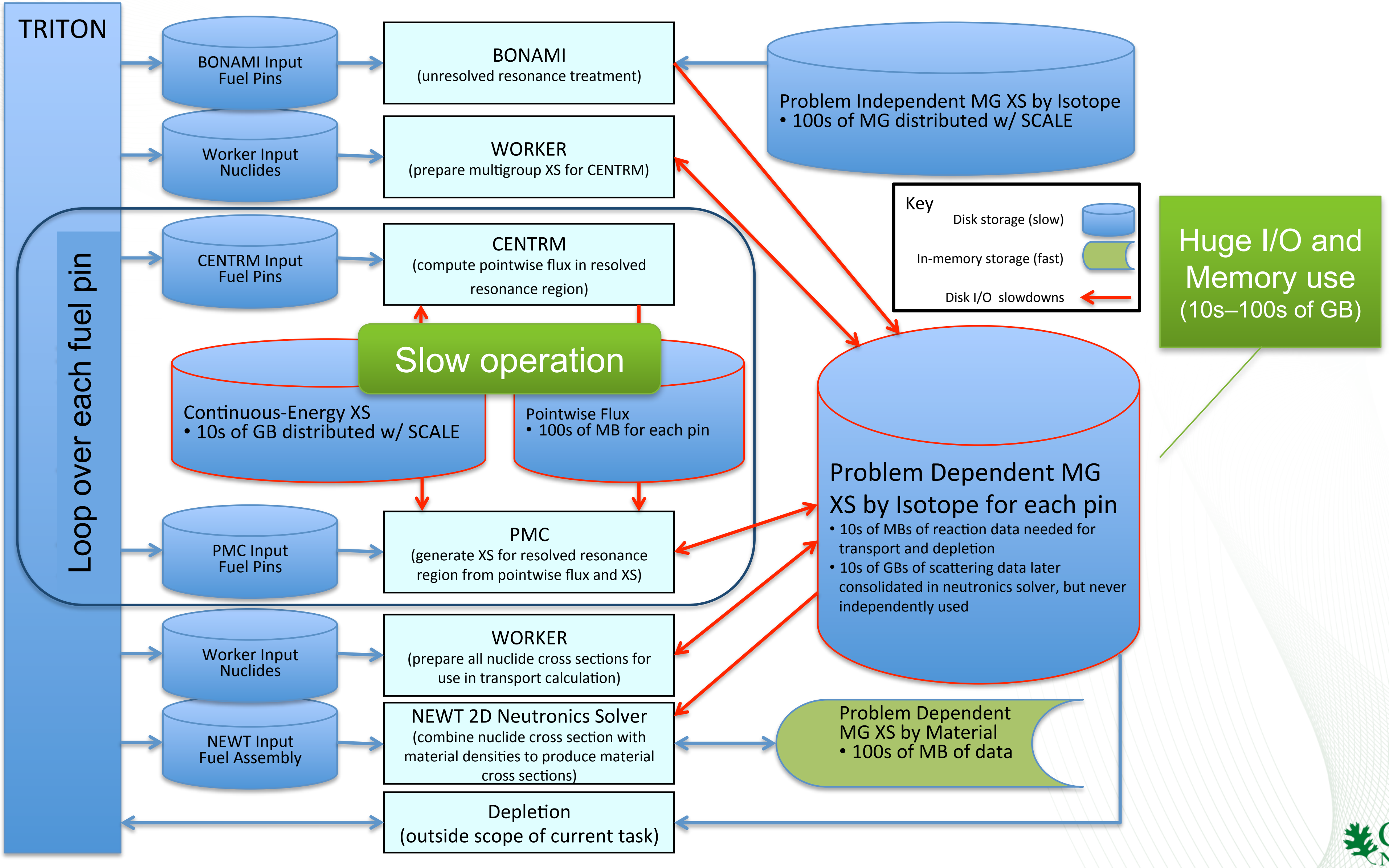
- **Fissile materials**
  - High-enriched uranium (HEU),
  - Intermediate-enriched uranium (IEU)
  - Low-enriched uranium (LEU)
  - Plutonium (Pu)
  - Mixed uranium/plutonium oxides (MOX)
- **Fuel form**
  - Metal (MET),
  - Fissile solution (SOL)
  - Multi-material composition (e.g. fuel pins – COMP)
- **Neutron spectra**
  - Fast
  - Thermal

Comparison SCALE 6.1 - 6.2 results for VALID benchmarks





SCALE 6.1 Resonance Self-Shielding (somewhat simplified view)



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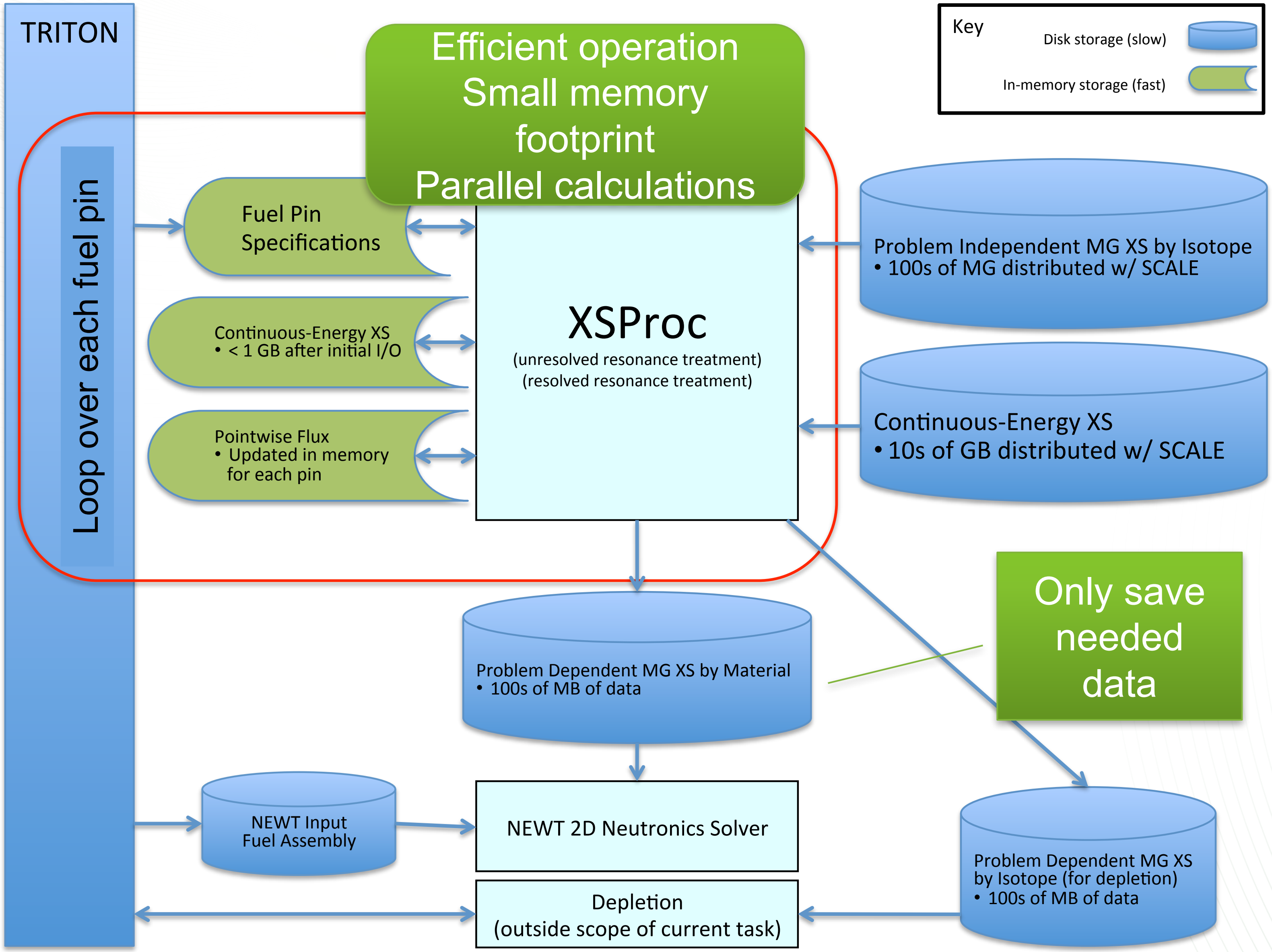
SCALE 6.2 Resonance Self-Shielding

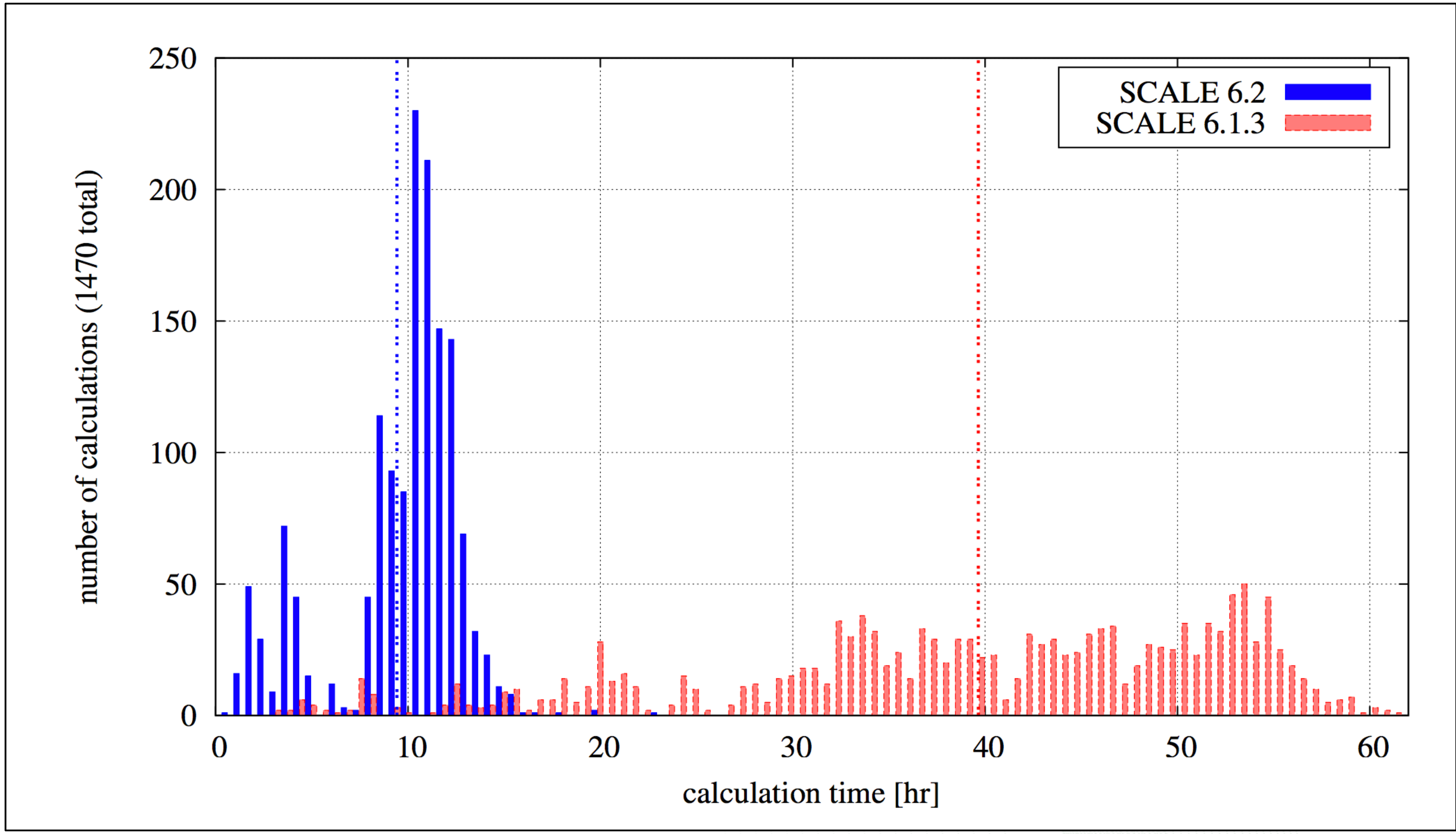


XSProc features

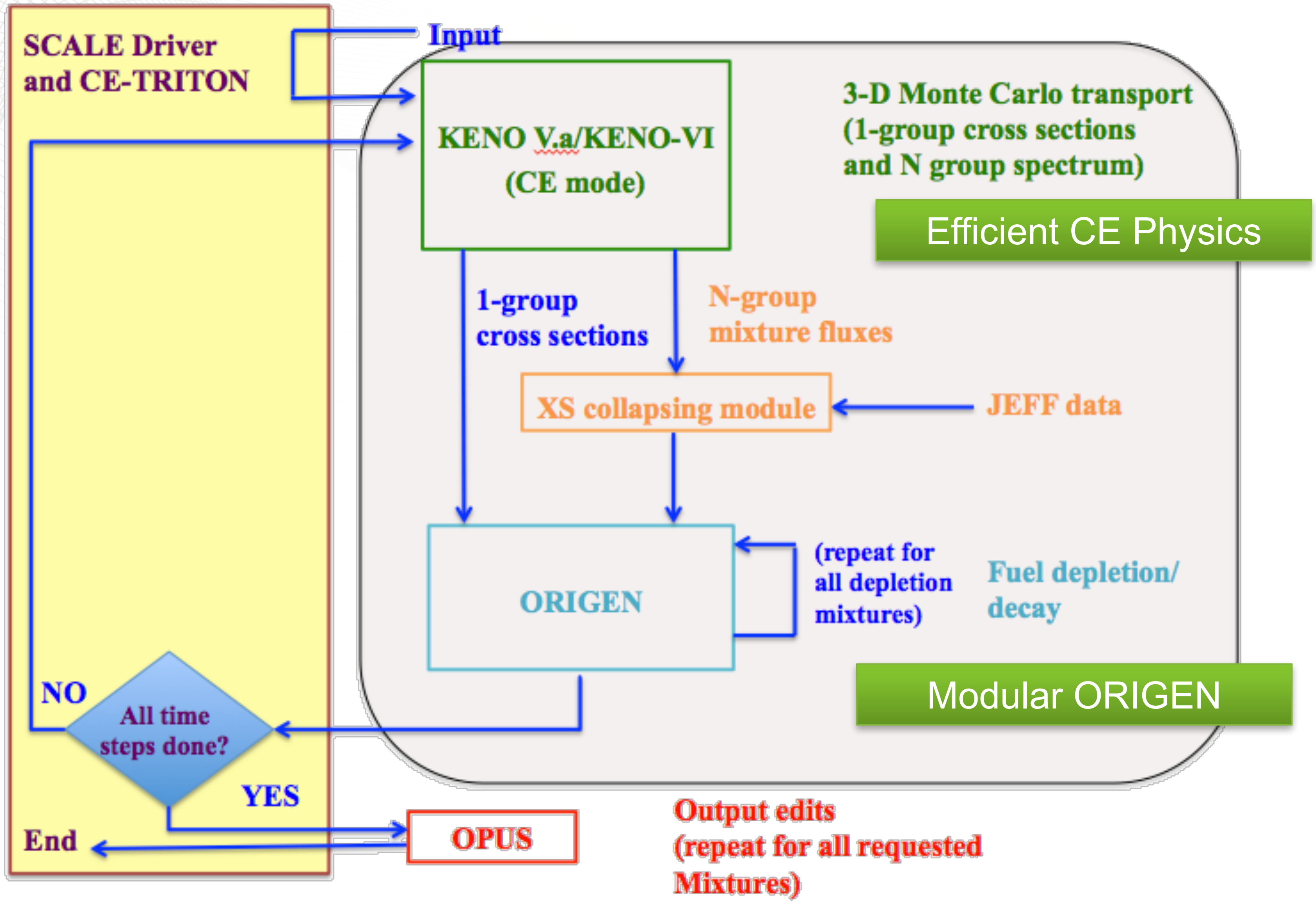
- XSProc provides capabilities for
  - resonance self-shielding of microscopic data,
  - macroscopic cross sections for mixtures,
  - one-dimension MG transport calculations to calculate eigenvalues and flux-weighting functions,
  - group collapsing of cross sections using flux spectra from the one-dimensional eigenvalue calculation or user input fixed source spectra, and
  - spatial homogenization of cross sections across material zones.
- Supported unit cell types
  - repeated lattices without need for Wigner-Seitz approximation
  - double-heterogeniety for HTGR, FHR, and FCM analysis
  - arbitrary slab, cylindrical, or spherical geometry
- Modern C++ architecture with API

TRITON Runtimes for 1470 ORIGEN Reactor Libraries

Assembly type (Libraries)		Lattice types
PWR	Babcock & Wilcox	15×15
	Westinghouse	14×14, 15×15, 17×17, 17×17-OFA
	Combustion Engineering	14×14, 16×16
	Siemens	14×14, 18×18
BWR	ABB	8×8-1
	Atrium	9×9-9, 10×10-9
	General Electric	8×8-4, 9×9-7, 7×7-0, 8×8-1, 8×8-2, 9×9-2, 10×10-8
	SVEA	64(8×8-1), 96(10×10-4), 100(10×10-0)
MOX	BWR Lattices	8×8-2, 9×9-1, 9×9-9, 10×10-9
	PWR Lattices	14×14, 15×15, 16×16, 17×17, 18×18
	BWR Lattices (×75)	ABB 8×8-1, Atrium 9×9-9, 10×10-9; GE 7×7-0, 8×8-1, 8×8-2, 9×9-2, 10×10-8; SVEA-64, 96, 100
	PWR Lattices (×15)	Siemens 14×14, 18×18; CE 14×14, 16×16; B&W 15×15; Westinghouse 14×14, 15×15, 17×17, 17×17-OFA
Other	AGR (×6)	
	CANDU (×1)	19-pin, 28-pin, 37-pin
	Magnox (×4)	
	RBMK (×24)	
	VVER-440 (×3)	flat, radial enrichments (3.82, 4.25, 4.38)
	VVER-1000 (×7)	flat enrichment



SCALE 6.2
Depletion with Continuous-Energy KENO

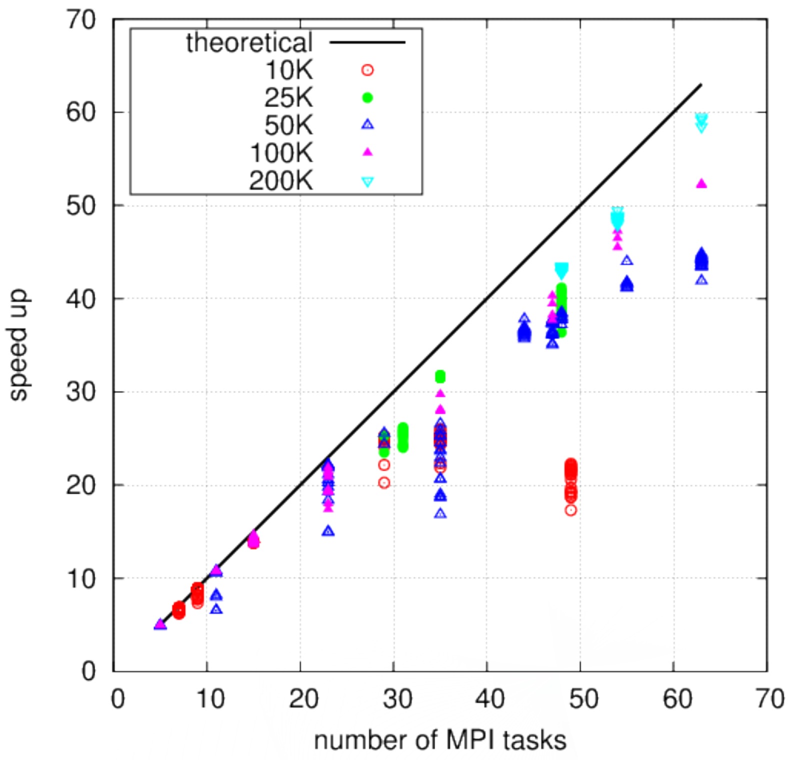


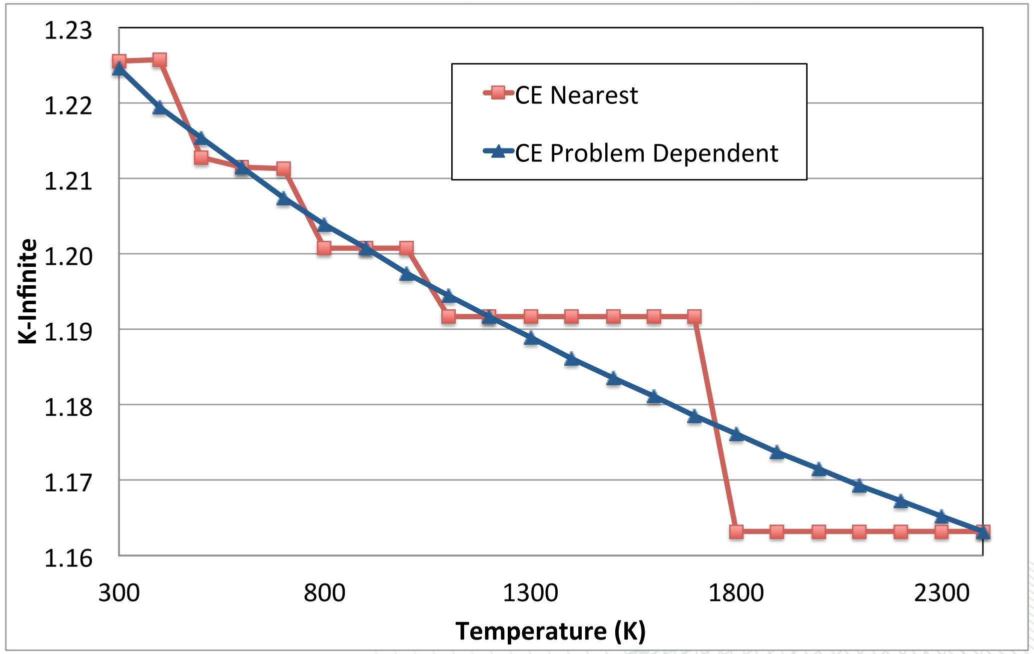
	MG	CE
^{234}U	4.03	3.37
^{235}U	5.34	5.04
^{236}U	1.82	1.65
^{238}U	-0.15	-0.15
^{238}Pu	-10.38	-10.15
^{239}Pu	7.05	5.70
^{240}Pu	3.15	2.82
^{241}Pu	0.72	-0.05
^{242}Pu	-7.40	-6.91
^{237}Np	2.33	2.39
^{241}Am	-6.56	-7.35
^{133}Cs	0.67	0.53
^{135}Cs	4.42	4.32
^{137}Cs	-2.76	-2.76
^{143}Nd	2.09	1.98
^{144}Nd	-3.22	-3.15
^{145}Nd	-3.01	-3.09
^{146}Nd	0.18	0.29
^{147}Nd	-0.03	-0.01
^{150}Nd	2.58	2.60

C/E -1 (%) for Spent Fuel Assay Data for a PWR Assembly

KENO Improvements

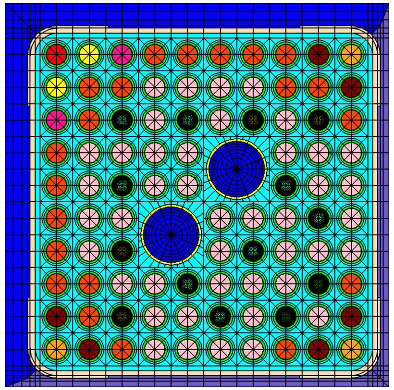
- Substantial reduction in memory requirements – over 99% improvement in many cases
- Accuracy improvements through comprehensive review and testing
- Parallel Computations
  - Significant speedups with MPI on Linux clusters
- Problem-Dependent Doppler broadening for CE calculations for thermal, resolved,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



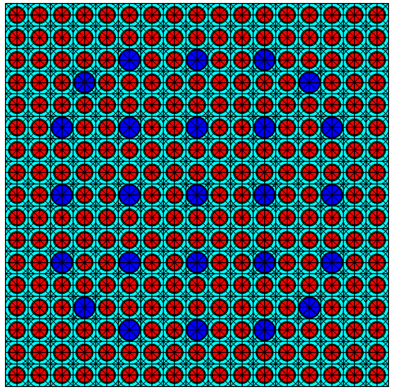


Polaris: Fast 2D lattice physics

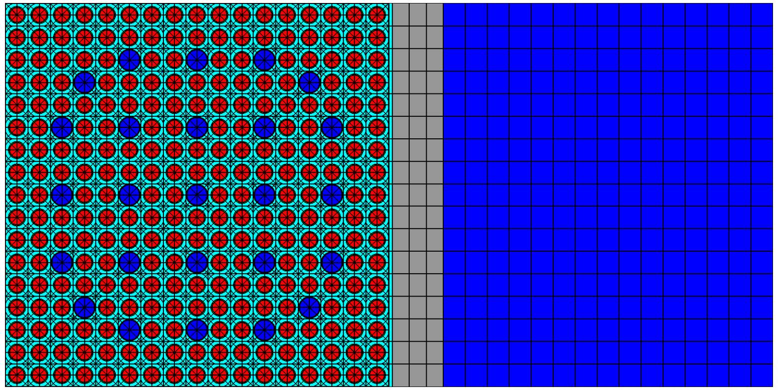
- **Simple Input**
  - Assembly geometry
  - Material definitions
  - Range of system conditions
- **Output**
  - Lattice physics parameters (.t16 file)
  - GENPMAXS converts .t16 file to .PMAX file
  - Spent Fuel Isotopics file (.f71 file)
- **Goals**
  - Fast: < 1 CPU minute per statepoint
  - Simple Input: 100 - 200 lines
  - Target accuracy compared to Monte Carlo:
    - 200 pcm dk
    - BWR: 1% RMS, 1.5% Max pin fission rate error
    - PWR: 0.5% RMS, 1.0% Max pin fission rate error
  - Good agreement with radiochemical assay data



BWR GE 10x10



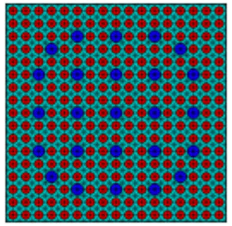
PWR W 17x17



Reflector Model

Pin power prediction

17×17 PWR lattice pin fission rate differences at nominal conditions for TRITON and Polaris

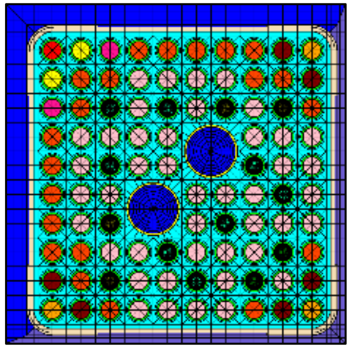


NEWT	
Polaris	

N/A								
0.08% 0.07%	-0.07% -0.09%							
0.09% 0.08%	-0.05% -0.07%	-0.13% -0.16%						
N/A	-0.06% -0.07%	0.01% -0.02%	N/A					
-0.01% -0.04%	0.04% 0.01%	0.00% -0.04%	0.05% 0.01%	0.19% 0.11%				
0.17% 0.16%	-0.09% -0.11%	-0.04% -0.06%	0.09% 0.07%	0.13% 0.04%	N/A			
N/A	0.16% 0.13%	0.23% 0.19%	N/A	0.10% 0.03%	0.12% 0.07%	0.01% 0.03%		
-0.01% -0.01%	-0.07% -0.08%	0.00% 0.00%	0.06% 0.04%	0.06% 0.05%	0.03% 0.07%	-0.06% 0.00%	-0.16% -0.11%	
-0.07% 0.00%	-0.10% -0.05%	-0.03% 0.02%	-0.10% -0.03%	-0.04% 0.00%	-0.12% -0.05%	-0.13% -0.05%	-0.13% -0.06%	-0.20% -0.11%

RMS	0.09 % 0.07 %
max	0.23 % 0.19 %

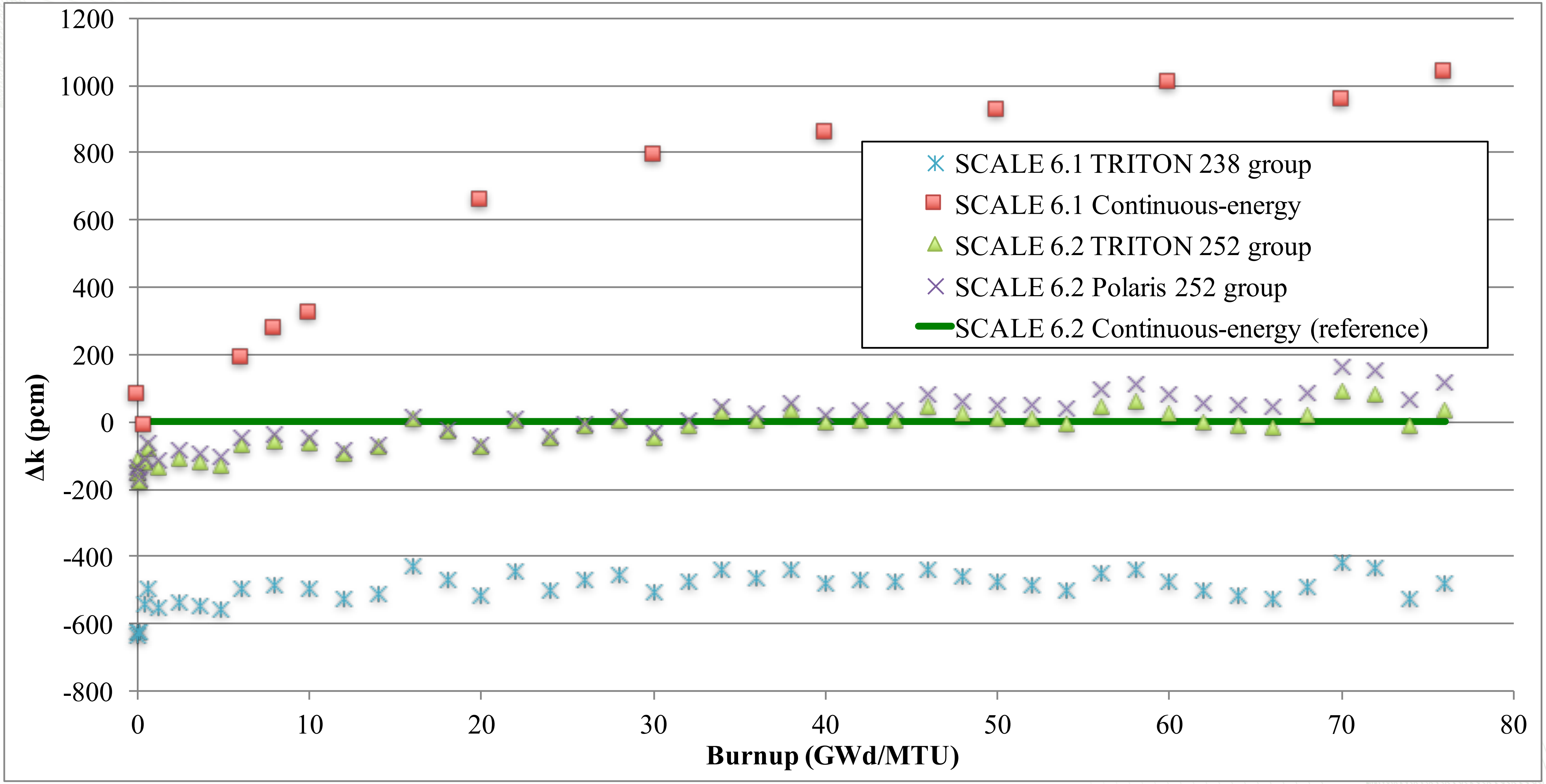
10×10 BWR lattice dominant zone pin power differences at 40% void fraction for TRITON and Polaris



0.84% 0.84%									
0.90% 0.67%	0.30% 0.45%								
0.64% 0.11%	-0.05% 0.18%	-0.13% -0.07%							
0.51% -0.10%	-0.02% 0.00%	-0.49% -0.09%	-0.13% -0.10%						
0.45% -0.36%	-0.31% -0.16%	-0.14% -0.16%	-0.35% 0.05%	0.04% 0.17%					
0.30% -0.30%	-0.08% -0.08%	-0.40% -0.14%			-0.01% 0.32%				
0.37% -0.32%	-0.23% -0.08%	-0.08% -0.10%			-0.03% 0.19%	-0.44% 0.04%			
0.21% -0.18%	-0.02% -0.03%	-0.59% -0.31%	-0.19% 0.00%	-0.37% -0.09%	-0.36% -0.08%	-0.20% -0.16%	-0.60% -0.23%		
0.87% 0.52%	0.01% 0.24%	-0.12% -0.09%	-0.43% -0.17%	-0.22% -0.10%	-0.14% -0.13%	-0.43% -0.13%	-0.05% -0.03%	-0.26% 0.07%	
0.78% 0.76%	0.35% 0.15%	0.06% -0.02%	0.08% -0.01%	-0.12% -0.18%	-0.19% -0.22%	-0.23% -0.31%	0.03% 0.05%	0.19% 0.18%	0.52% 0.66%

RMS	0.50 % 0.23 %
max	0.90 % 0.84 %

Eigenvalue prediction for PWR fuel depletion



Conclusions

- SCALE 6.2 provides many improvements in accuracy and runtime, especially for reactor physics calculations.
- CE Monte Carlo biases for MOX or burned-fuel calculations have been minimized with numerous revisions to the CE data and physics implementation in the codes.
- Monte Carlo innovations enable CE depletion with parallel Monte Carlo and integrated problem-dependent Doppler broadening.
- Historical biases in MG LWR calculations have reduced to approximately 100 pcm through many improvements in the nuclear data, group structures, and resonance self-shielding techniques.
- Runtimes for lattice physics calculations are greatly improved with the availability of the new Polaris tool as well as numerous enhancements in XSProc and NEWT as applied in TRITON.
- Custom nuclear data libraries can now be created with the inclusion of AMPX.