Overview of SCALE 6.2

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ANS NCSD 2013 Criticality Safety in the Modern Era: Raising the Bar Wilmington, NC





SCALE 6.2 Preview

- Significant updates since SCALE 6.1 in June 2011
- Focus on improved fidelity of solutions
- 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
- 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)
- New nuclear data libraries in MG and CE
- Modernized resonance self-shielding tools



Monte Carlo Improvements for Criticality

- Parallel KENO
 - Significant speedups with MPI on Linux clusters
- Improved CE efficiency
 - Memory footprint reduced by 20-95%, depending on problem
 - Coding revised to provide improved consistency across platforms
- Source Convergence
 - Shannon Entropy test in KENO
 - Hybrid deterministic starting source methodology in Sourcerer for improved k_{eff} reliability
- Problem-Dependent Doppler broadening for CE calculations
- Doppler Broadened Rejection Correction
 - Significant improvement in elevated temperature CE Monte Carlo







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
- 1.2GB memory
- 50M histories for ~1% standard deviation in fluxes
- Total problem time: 72 hours



C/E -1 (%) for Calvert Cliffs sample MKP109-P

	MG KENO	CE KENO
U-234	3.0	3.2
U-235	3.1	4.6
U-236	0.1	1.4
U-238	-1.7	-0.1
Pu-238	-10.5	-10.2
Pu-239	4.9	9.1
Pu-240	1.5	1.8
Pu-241	-1.1	1.5
Pu-242	-9.1	-8.2
Np-237	2.7	3.1
Am-241	-8.2	-5.8
Cs-133	-0.8	0.7
Cs-135	3.0	4.2
Cs-137	-4.3	-3.3
Nd-143	0.5	2.1
Nd-144	-4.7	-3.1
Nd-145	-4.4	-3.1
Nd-146	-1.5	0.3
Nd-148	-1.5	-0.1
Nd-150	1.0	2.5



CE Sensitivity Analysis with TSUNAMI

CLUTCH and MG-TSUNAMI Sensitivity Profiles for an Infinitely-Reflected Fuel Pin Problem







[→] The CE-KENO + CLUTCH run was faster than the MG-KENO + TSUNAMI run and it had a small memory footprint!

Energy-Integrated Sensitivity Coefficient Comparison

Nuclide	Direct Pert.	MG-TSUNAMI	CLUTCH
U-235	0.1660	0.1595	0.1642
U-238	-0.2207	-0.2264	-0.2126
H-1	0.0946	0.0785	0.0993
O-16	-0.0147	-0.0250	-0.0139

Energy-Integrated Sensitivity Coefficient

Differences (in number of $\sigma_{effective}$)

Nuclide	MG-TSUNAMI	CLUTCH
U-235	-0.79	-0.22
U-238	-0.64	0.91
H-1	-4.39	1.18
O-16	-7.49	0.51

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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

Dose rate from ⁶⁰Co source in transportation package



Flux results for iron sphere transmission experiment



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6 Overview of SCALE 6.2

Modular ORIGEN

- ORIGEN restructured to provide Application Programmer Interface (API) and parallel capabilities
- New ORIGAMI tool developed to rapidly characterize spent fuel.



235 pins, 26 axial zones **6,110 depletion nodes**

- ~50 hours runtime
- OpenMPI implementation with (near)-linear speed-up



Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences

- 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







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



Low enriched U compounds; thermal systems

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

Up to 1000 pcm improvement for burned fuel





SCALE 6.2 beta1 Data Libraries

Primary data source/format
ENDF/B-VII.0
238-group neutron library
ENDF/B-VII.0
252-group neutron library
ENDF/B-VII.0
56-group neutron library
ENDF/B-VII.0
200 neutron/47 gamma library
ENDF/B-VII.0
27 neutron/19 gamma library
ENDF/B-VII.0
Continuous-energy neutron and gamma library



SCALE 6.1 Resonance Self-Shielding

(somewhat simplified view)



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SCALE 6.2 Resonance Self-Shielding



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Ready to Ship	Item has passed all tests and is a candidate feature for quality assurance implementation		Applicatio	ns
Shipped	Feature is implemented in quality-assured version		AN ANERICAN MATIONAL STARS	1017

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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

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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
 - CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity/uncertainty analysis,
 - Modularity for CE physics and depletion
 - Stochastic sampling with Sampler
 - Improved CE and MG data.



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





http://scale.ornl.gov

scalehelp@ornl.gov



Nuclear Systems Modeling & Simulation



Improved Collision Kinematics Processing in AMPX

Since primarily used for MG:



Refined energy grid is used \rightarrow thinned to keep library size manageable



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 H₂O
- Add Lambda-factors for all isotopes
- Add heterogeneous IRfactors for actinides
- Homogeneous IR-factors for other materials

