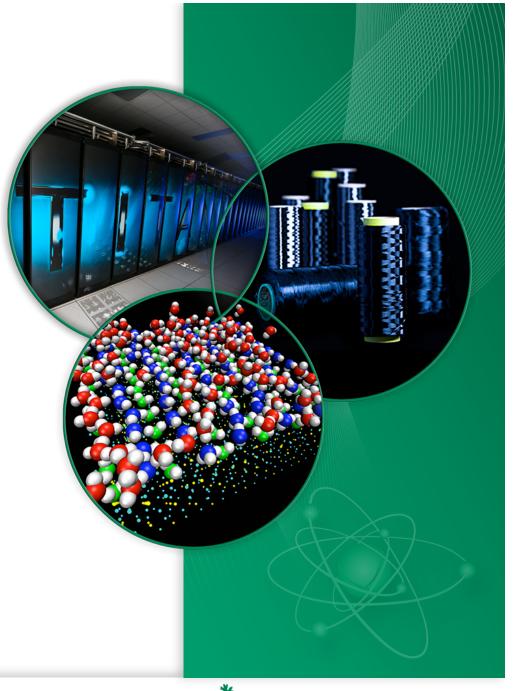# ORNL Analytical Methods Advancements to Support NCS Applications

Michael Dunn, Brad Rearden,
Dorothea Wiarda, Cihangir Celik,
Kursat Bekar, and Mark Williams

NCSP Technical Program Review Meeting
Washington, DC
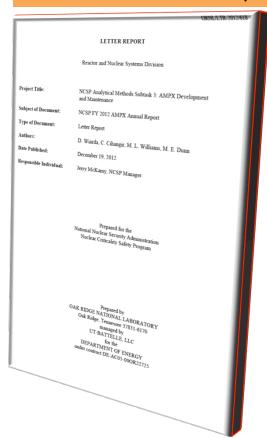May 30, 2013

Outline

- AMPX Cross-Section Processing Improvements

- SCALE Status
  - Quality Assurance Plan Update
  - SCALE 6.1.1 and 6.1.2 Patches

- Development for SCALE 6.2—Preview of NCS Advancements

- Summary

Key Improvements in AMPX Nuclear Data Generation Capabilities for SCALE

FY12 AMPX Annual Report

- Improved collision kinematics processing to support MG and CE library production

- Developed new CE and 252-group libraries for SCALE 6.2

- Generated new ENDF/B-VII.1 CE, MG, and covariance data libraries for testing with SCALE
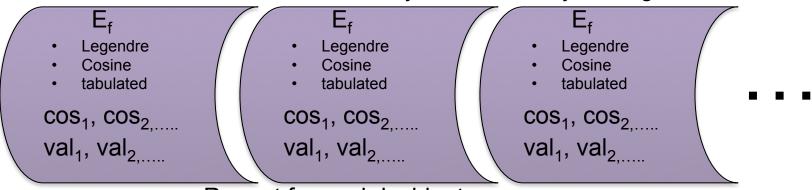
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Improved Collision Kinematics Processing

FORTRAN derived types for kinematic data
+functions to handle and add dynamic memory management

E_f
• Legendre
• Cosine
• tabulated
$\cos_1, \cos_2,.....$
$val_1, val_2,.....$

Repeat for each incident energy

New modules using the types

- KINZEST: combine kinematic files and select on AWP and ZAP
- KINKOS: convert between all supported formats
- MG_TO_KIN: convert MG scattering matrices to double differential form
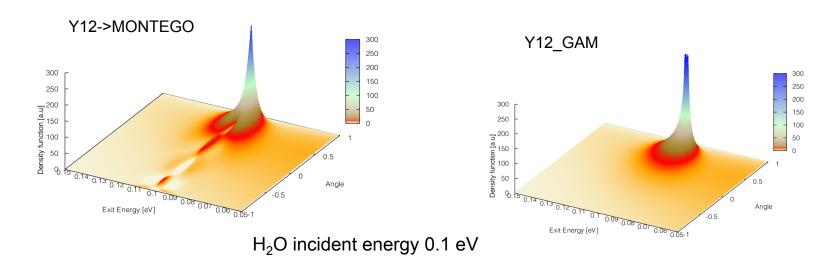
Supporting subroutines

- Insert additional exit energies or incident energies
- Test whether exit energies, exit angles or incident energies can be interpolated
- Thin exit energy or exit angles as needed.
- Convert between tabulated and moment formats, adding extra angles and exit energies as needed

Improved Collision Kinematics Processing

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.

In addition a much finer grid is used -> thinned in updated JAMAICAN to keep library size manageable

New 252-Group Library for SCALE

Key MG Library Improvements

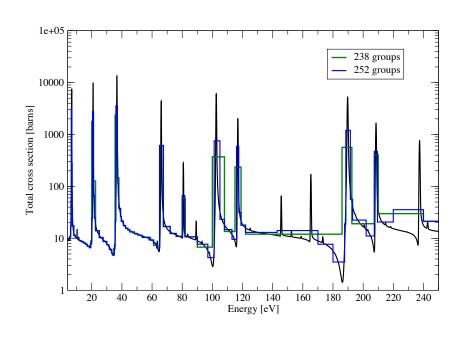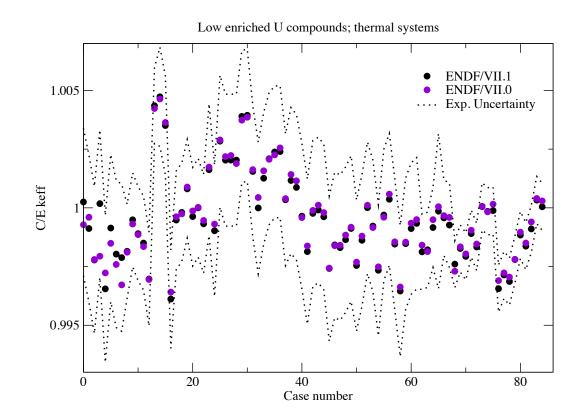- 252 instead of 238 neutron groups

- Use special centrm generated flux for actinides and thermal H_2O

- Add Lambda-factors for all isotopes

- Add homogenous IR-factors for actinides

U-238 total cross section

New CE Libraries for SCALE

- Process both ENDF/VII.0 and ENDF/B-VII.1 evaluations

- CE libraries generated by using all updated AMPX processing capabilities

- Extensive V&V testing of ENDF/B-VII.0 library using benchmark and regression test cases—library will be released with SCALE 6.2

- ENDF/B-VII.1 library produced at end of FY12—testing needed to QA ENDF/B-VII.1 library for release with SCALE

Low enriched U compounds; thermal systems

Legend:
- ● ENDF/VII.1
- ● ENDF/VII.0
- ⋯ Exp. Uncertainty

X axis: Case number
Y axis: C/E keff

SCALE User Statistics

- ## 7076
  - Distributions since 2004

- ## 5113
  - Unique users

- ## 40
  - Nations using SCALE

Updated QA Program

- Designed for Compliance with:
  - ISO 9001 (formal registration with ISO desired)
  - DOE 414.1D
  - ORNL SBMS
  - Consistent with ASME NQA-1

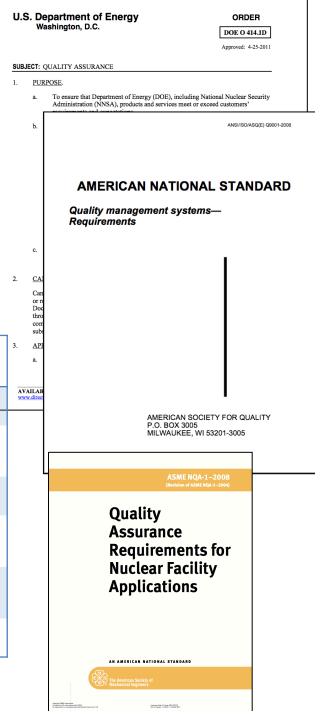- Capabilities are tracked with the *Kanban* process through the *FogBugz* electronic *collaborative development environment*

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'

   b.

ANSI/ISO/ASQ(E) Q9001-2008

AMERICAN NATIONAL STANDARD

Quality management systems— Requirements

c.

2. CA

Car
or r
Doc
thro
com
subs

3. API

   a.

AVAILAB
www.direc

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

SCALE 6.1.1 and SCALE 6.1.2 Patches

- SCALE 6.1.1 (May 2012)
  - Update to CENTRM for trace quantities of materials
  - Several lattice physics bug fixes
  - Updates to MAVRIC/Monaco to address minor issues
  - Updates to ORIGEN for JEFF data for fission products, fission product yields, and decay data
  - Update to KENO for hexagonally-pitched arrays
  - Other minor updates

- SCALE 6.1.2 (February 2013)
  - ENDF/B-VII.1 data for ORIGEN to address flaws in ENDF/B-VII.0
  - Update in ORIGEN for irradiation calculation with small time steps
  - Updated parallel branch calculations for lattice physics
  - Update for critical spectrum calculations with NEWT
  - Update to implicit sensitivity treatment with TSUNAMI
  - Update for double heterogeneous calculations

- http://scale.ornl.gov/downloads_scale6-1.shtml
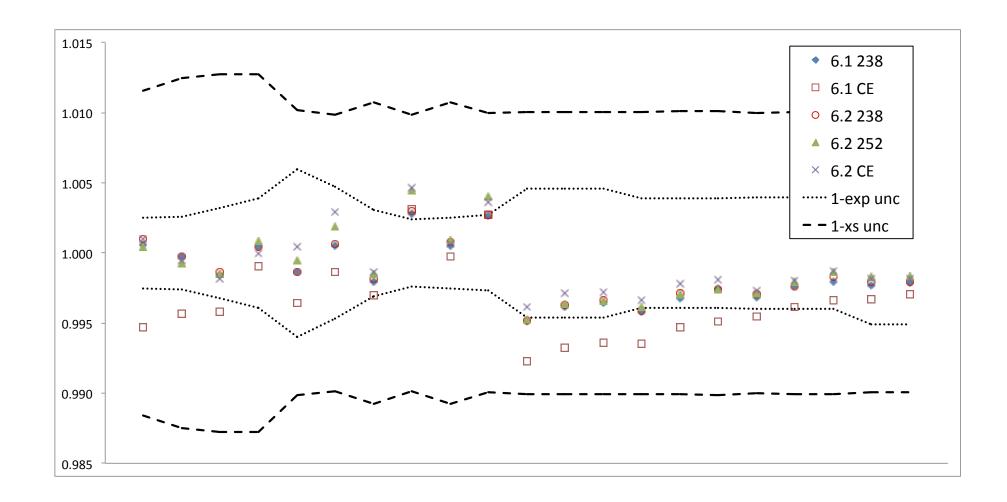
SCALE 6.2 Preview

- Focus on improved fidelity of solutions

- Significant improvements in CE Monte Carlo capabilities
  - Complete review and update of CE nuclear data, with orders of magnitude increase in testing for improved quality (funded by NRC)
  - CE TSUNAMI (funded by NCSP)
  - CE MAVRIC/Monaco (funded by NRC)
  - CE TRITON (other funding)

- New sampling methods for uncertainty analysis and generation of experimental correlations (joint NCSP and DOE NE support)

Data Libraries for SCALE 6.2

- **New Continuous-energy cross-section data for neutron interactions, gamma yield, and gamma interactions** (sponsored by NRC)

- **New Multigroup neutron libraries**
  - 252-group energy structure (sponsored by NRC)
  - 64-group energy structure (sponsored by NRC and DOE NE)

Mnemonic 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
v7-64	ENDF/B-VII.0 64-group neutron library
test-8grp	TEST LIBRARY 8-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

Improved C/E Especially for LEU and MOX Benchmarks

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Improved SCALE V&V

- ## Test Suite

  – 263 Sample Problems

  – 379 Regression Problems

  – 681 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
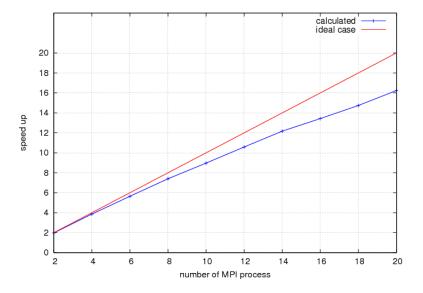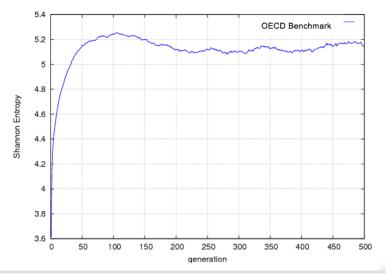
- Total of ~50,000 tests every day

Improved Analytical Capabilities for Nuclear Criticality Safety Analysis

- ## 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 Diagnostics
  - Implemented Shannon Entropy test in KENO

- ## Doppler Broadening Rejection Correction
  - Significant improvement in elevated temperature CE Monte Carlo

Table 1. Impact of DBRC as a Function of Temperature

Temperature (K)	Normal	DBRC	Difference (pcm)
293.6	1.34460	1.34451	-9
600.0	1.33053	1.32932	-121
900.0	1.31941	1.31759	-182
1200.0	1.31029	1.30730	-299
2400.0	1.28113	1.27478	-635

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Continuous-Energy TSUNAMI

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

MG-TSUNAMI u-235 nubar
  Integral Value = 0.9321769 ± 3.762369E-5
CLUTCH u-235 nubar
  Integral Value = 0.9321025 ± 4.057596E-4
MG-TSUNAMI u-235 fission
  Integral Value = 0.2904609 ± 2.558262E-4
CLUTCH u-235 fission
  Integral Value = 0.2938319 ± 4.150841E-4
MG-TSUNAMI u-238 total
  Integral Value = -0.2263954 ± 1.835341E-4
CLUTCH u-238 total
  Integral Value = -0.2125807 ± 8.246308E-4
MG-TSUNAMI h-1 total
  Integral Value = 0.07847114 ± 0.002209569
CLUTCH h-1 total
  Integral Value = 0.09928282 ± 0.002666733

Difficult convergence of MG adjoint

Runtime Parameter Comparison for the Fuel Pin Problem

	CLUTCH	MG-TSUNAMI
Memory Increase over Eigenvalue Calculation	2 MB	305 MB
Runtime	352.3 min	626.9 min

→ The CE-KENO + CLUTCH run was faster than the MG-KENO + TSUNAMI run and it had a small memory footprint!
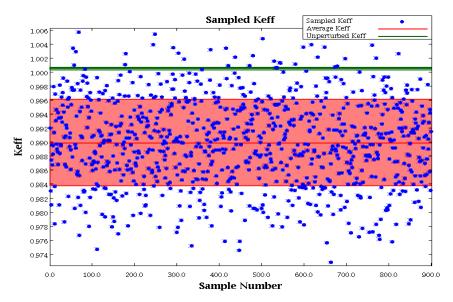
Energy-Integrated Sensitivity Coefficient Comparison

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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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

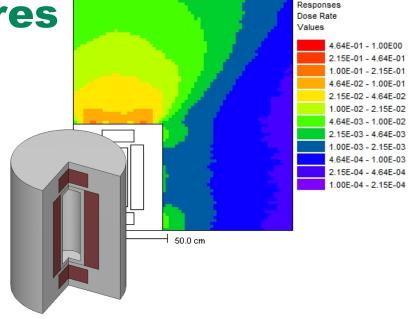- Correlations between systems are also computed
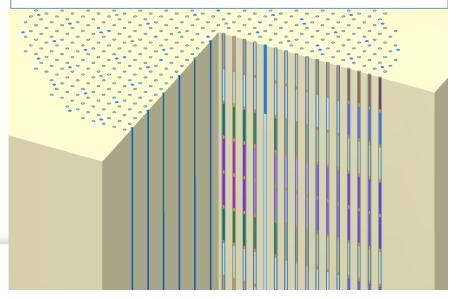

Sampled Keff

Experimental Correlations

	HST-001	HST-002	HST-003	HST-004	HST-005	HST-006	HST-007	HST-008	HST-009	HST-010
HST-001	1.00E+00	9.77E-01	2.68E-02	4.31E-02	6.02E-02	2.98E-02	5.74E-02	6.86E-02	4.59E-02	-4.97E-02
HST-002	9.77E-01	1.00E+00	7.50E-03	2.15E-02	7.55E-02	3.67E-02	6.37E-02	7.84E-02	5.07E-02	-5.11E-02
HST-003	2.68E-02	7.50E-03	1.00E+00	9.33E-01	9.60E-03	-2.20E-03	-1.40E-03	-1.49E-02	1.70E-03	3.21E-02
HST-004	4.31E-02	2.15E-02	9.33E-01	1.00E+00	2.16E-02	-5.30E-03	4.30E-03	-1.23E-02	7.20E-03	2.70E-02
HST-005	6.02E-02	7.55E-02	9.60E-03	2.16E-02	1.00E+00	7.53E-01	7.65E-01	8.26E-01	8.52E-01	-5.13E-02
HST-006	2.98E-02	3.67E-02	-2.20E-03	-5.30E-03	7.53E-01	1.00E+00	6.88E-01	7.50E-01	7.62E-01	-1.05E-01
HST-007	5.74E-02	6.37E-02	-1.40E-03	4.30E-03	7.65E-01	6.88E-01	1.00E+00	7.85E-01	8.29E-01	-9.24E-02
HST-008	6.86E-02	7.84E-02	-1.49E-02	-1.23E-02	8.26E-01	7.50E-01	7.85E-01	1.00E+00	8.72E-01	-1.10E-01
HST-009	4.59E-02	5.07E-02	1.70E-03	7.20E-03	8.52E-01	7.62E-01	8.29E-01	8.72E-01	1.00E+00	-6.44E-02
HST-010	-4.97E-02	-5.11E-02	3.21E-02	2.70E-02	-5.13E-02	-1.05E-01	-9.24E-02	-1.10E-01	-6.44E-02	1.00E+00

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Other Significant Features

- CE Capabilities with MAVRIC/ Monaco
  - All hybrid capabilities supported with CE fidelity
  - 6000 fixed-source transmission tests used in V&V

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

Responses
Dose Rate
Values

■	4.64E-01 - 1.00E00
■	2.15E-01 - 4.64E-01
■	1.00E-01 - 2.15E-01
■	4.64E-02 - 1.00E-01
■	2.15E-02 - 4.64E-02
■	1.00E-02 - 2.15E-02
■	4.64E-03 - 1.00E-02
■	2.15E-03 - 4.64E-03
■	1.00E-03 - 2.15E-03
■	4.64E-04 - 1.00E-03
■	2.15E-04 - 4.64E-04
■	1.00E-04 - 2.15E-04

50.0 cm

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

Summary

- Significant improvements in AMPX processing capabilities—collision kinematics

- Produced new CE and MG libraries for SCALE 6.2 based on ENDF/B-VII.0—also have ENDF/B-VII.1 libraries available that can be tested for deployment with SCALE

- SCALE
  - Developed and implemented new ISO 9001 compliant QAP
  - Released SCALE 6.1.1 and 6.1.2 patches
  - Implemented modern software development workflow management system with extensive testing (unit, regression, and benchmark testing)
  - SCALE 6.2 beta deployed for testing
  - Significant improvements in CE Monte Carlo capabilities for NCS