

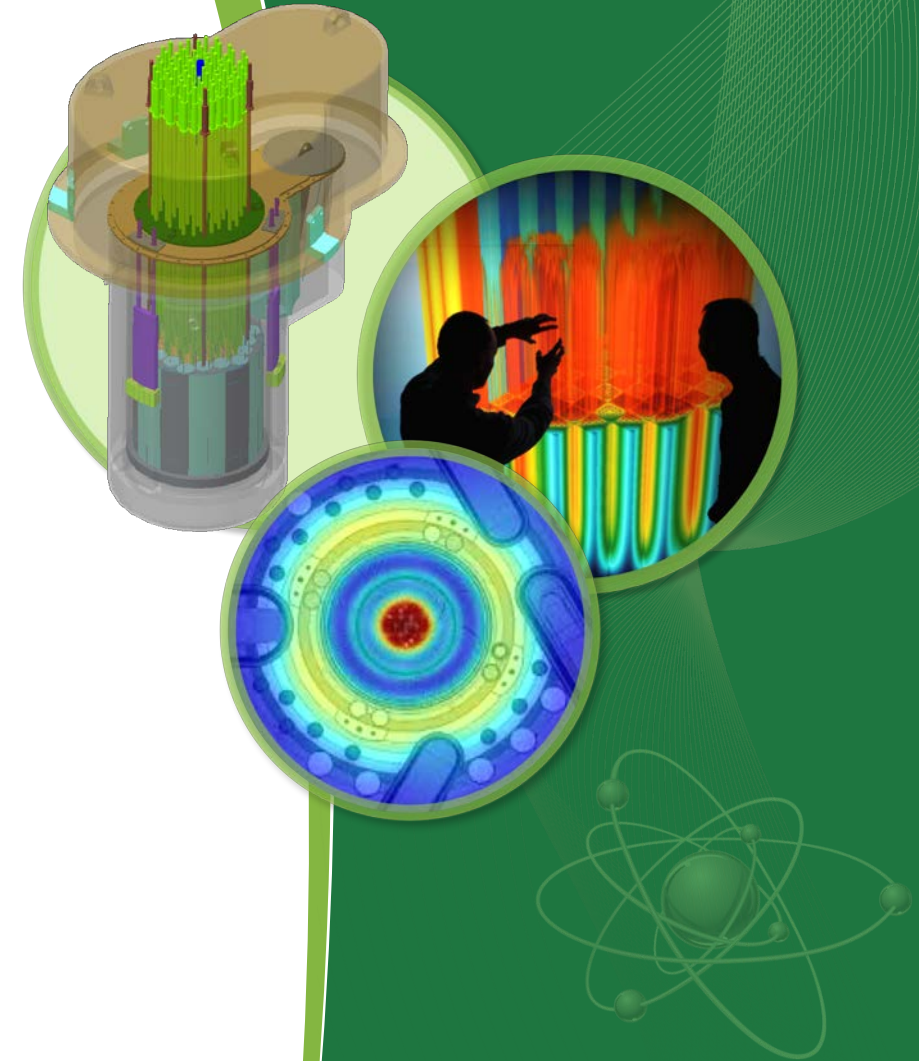
SCALE 6.2 and AMPX Development and Modernization for the NCSP

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**Nuclear Criticality Safety Program
Technical Program Review**

March 14, 2017



SCALE Leadership Team

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Group Leader, Reactor Physics

Mike Dunn
Group Leader, Nuclear Data and Criticality Safety

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Group Leader, Radiation Transport

Rob Lefebvre
Software Development Coordinator

Mark Williams
Distinguished R&D Staff

**Radiation Safety Information
Computational Center (RSICC)**

Tim Valentine

**Versioned
Releases
User Licensing**

**Strategic Vision
Quality Assurance Plan
Budgets and Staffing
Change Control Board**

**Infrastructure and
Support**

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Brandon Langley
Jordan Lefebvre
Rob Lefebvre
Adam Thompson
Sheila Walker

**Quality Assurance
System
Build and Test
Framework
Deployment**

**Monte Carlo
Development**

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Cihangir Celik
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Tom Evans
Shane Hart
Seth Johnson
Tara Pandya
Chris Perfetti
Doro Wiarda

**KENO/CSAS
MAVRIC/Monaco
Shift
Sourcerer**

**Decay, Depletion,
and Activation
Methods**

Will Wieselquist
Ian Gauld
Shane Hart
Germina Ilas
Thomas Miller
Steve Skutnik (UT)
Doro Wiarda
Mark Williams

**ORIGEN
ORIGAMI
Depletion, Decay,
and Activation
Data**

**Reactor Physics
Methods**

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Kursat Bekar
Ben Betzler
Greg Davidson
Tom Evans
Cole Gentry
Steven Hamilton
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**TRITON
Polaris
Advanced
Reactor R&D**

**Nuclear Data and
Methods**

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Charles Daily
Andrew Holcomb
Matt Jessee
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Kang Seog Kim
Rob Lefebvre
B.J. Marshall
Marco Pigni
Doro Wiarda
Mark Williams

**XSPROC
Neutron and Gamma
Cross Section Data
(MG&CE)
Covariance Data**

User Interfaces

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Brandon Langley
BJ Marshall
Josh Peterson
Adam Thompson
Will Wieselquist

**Fulcrum
SNAP
Geometry and
Data Visualization**

**Sensitivity and
Uncertainty
Analysis**

Chris Perfetti
Goran Arbanas
Aaron Bevill
Keith Bledsoe
Matt Jessee
Elizabeth Jones
Jordan Lefebvre
B.J. Marshall
Ugur Mertuyrek
Thomas Miller
Vladimir Sobes
Will Wieselquist
Mark Williams

**TSUNAMI
TSURFER
SAMPLER
Optimization and
Inverse Analysis**

**User Interaction
and Training**

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Brian Ade
Ben Betzler
Justin Clarity
Ian Gauld
Shane Hart
Matt Jessee
Henrik Liljenfeldt
B.J. Marshall
Thomas Miller
Don Mueller
Douglas Peplow
Chris Perfetti
Joel Risner
Sheila Walker
Will Wieselquist

**Courses at ORNL, NEA
Data Bank, NRC, and User
Facilities
Conference Workshops
Helpline, User Groups
Documentation**

Outline

- SCALE 6.2 and AMPX Release
- 2016 AMPX Highlights
- 2016 SCALE Highlights
- On-going activities

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

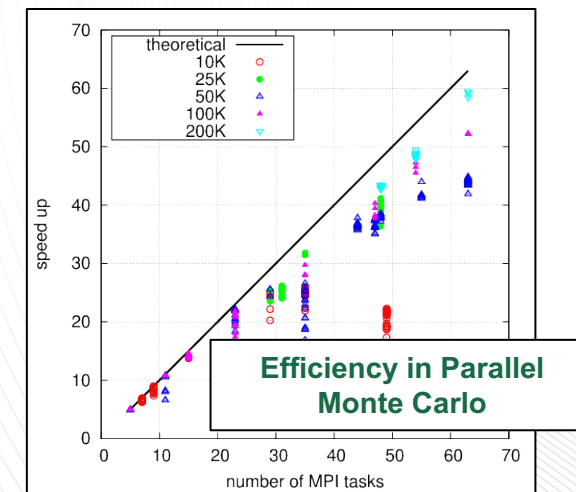
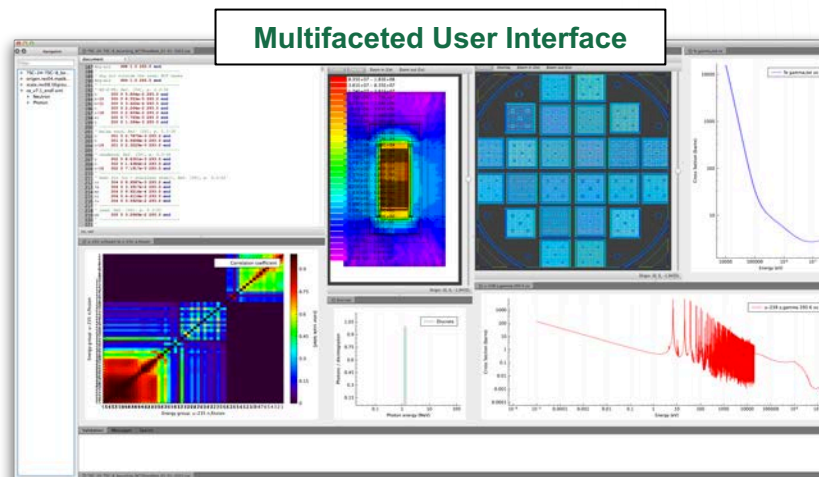
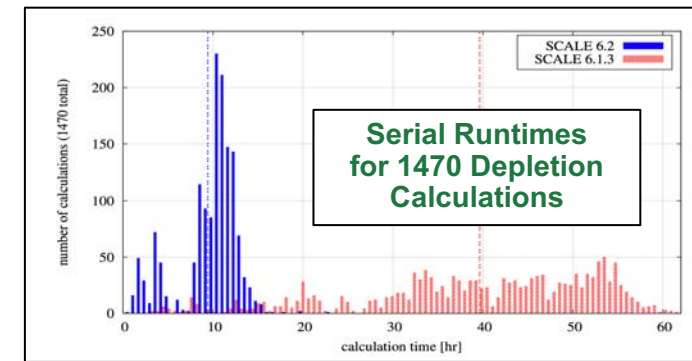
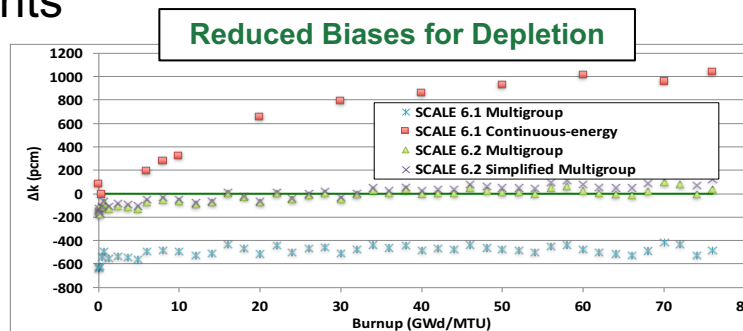
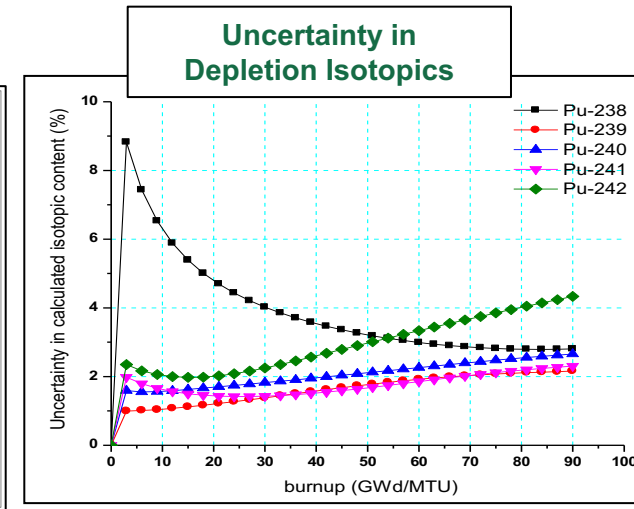
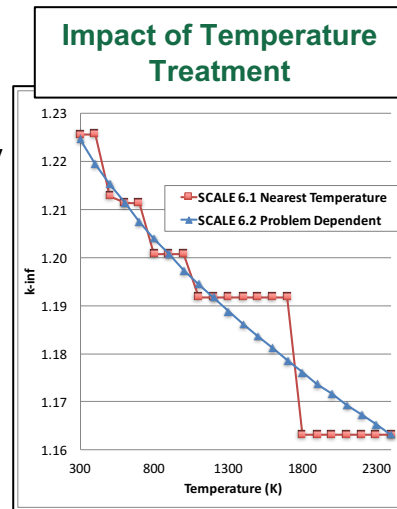
Accurate

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

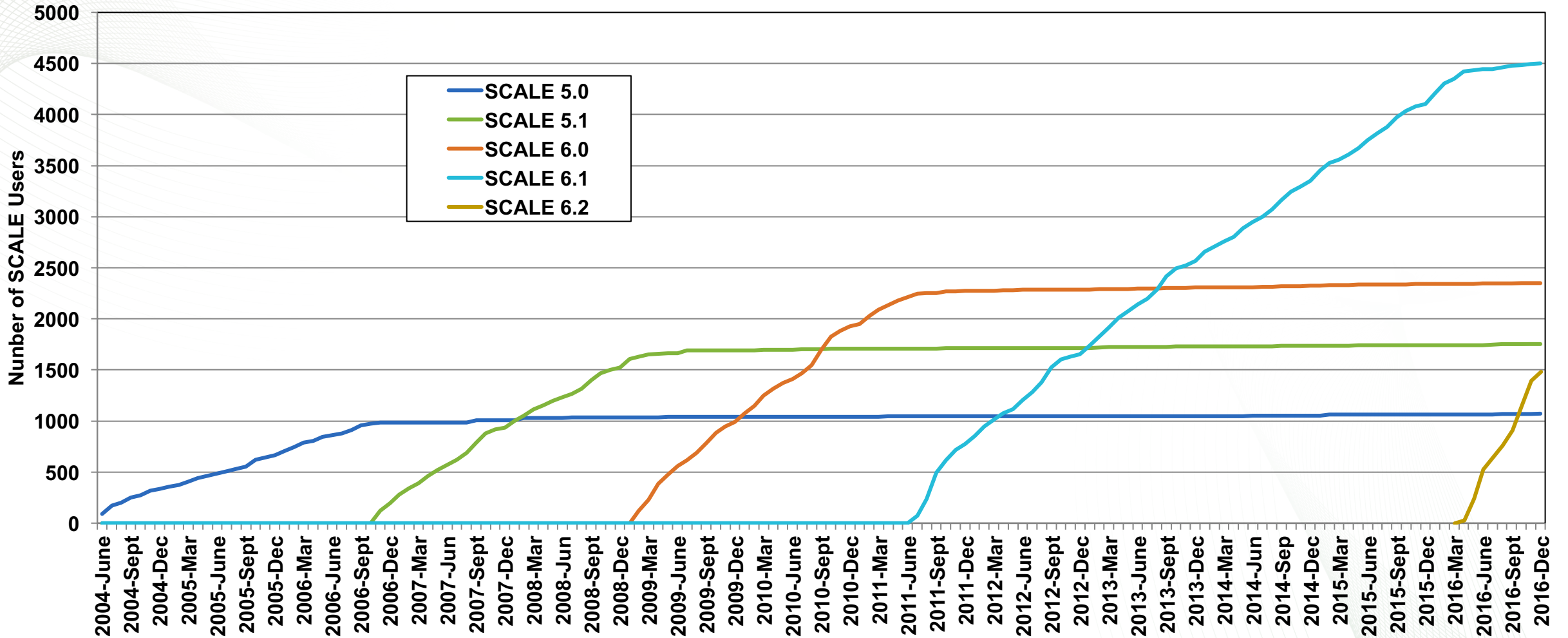
Easy to Use

- Integrated user interface
- Simplified input














1500 licenses issues through December 2016



SCALE licenses issued by version




SCALE Manual: reorganized, condensed, public download

- ▶  SCALE Code System
- ▶  README SCALE6.2
- ▶  1.0 Introduction
- ▶  2.0 Criticality Safety
- ▶  3.0 Reactor Physics
- ▶  4.0 Radiation Shielding
- ▶  5.0 Depletion, Activation, and Spent Fuel Source Terms
- ▶  6.0 Sensitivity and Uncertainty Analysis
- ▶  7.0 Material Specification and Cross Section Processing
- ▶  8.0 Monte Carlo Transport
- ▶  9.0 Deterministic Transport
- ▶  10.0 SCALE Nuclear Data Libraries
- ▶  11.0 SCALE Utilities Modules for SCALE Libraries

<http://scale.ornl.gov>
AMPX Manual available for download

ORNL/TM-2005/39
Version 6.2

SCALE Code System



B. T. Rearden and
M. A. Jessee, Editors

April 2016

SCALE 6.1: 4894 pages
SCALE 6.2: 2715 pages

SCALE 6.2 Updates (details on website)

SCALE 6.2.1

- Released July 2016
- Several Fulcrum Updates
- Minor bug fixes
- Modernized PUFF module in AMPX
- Lattice physics enhancements

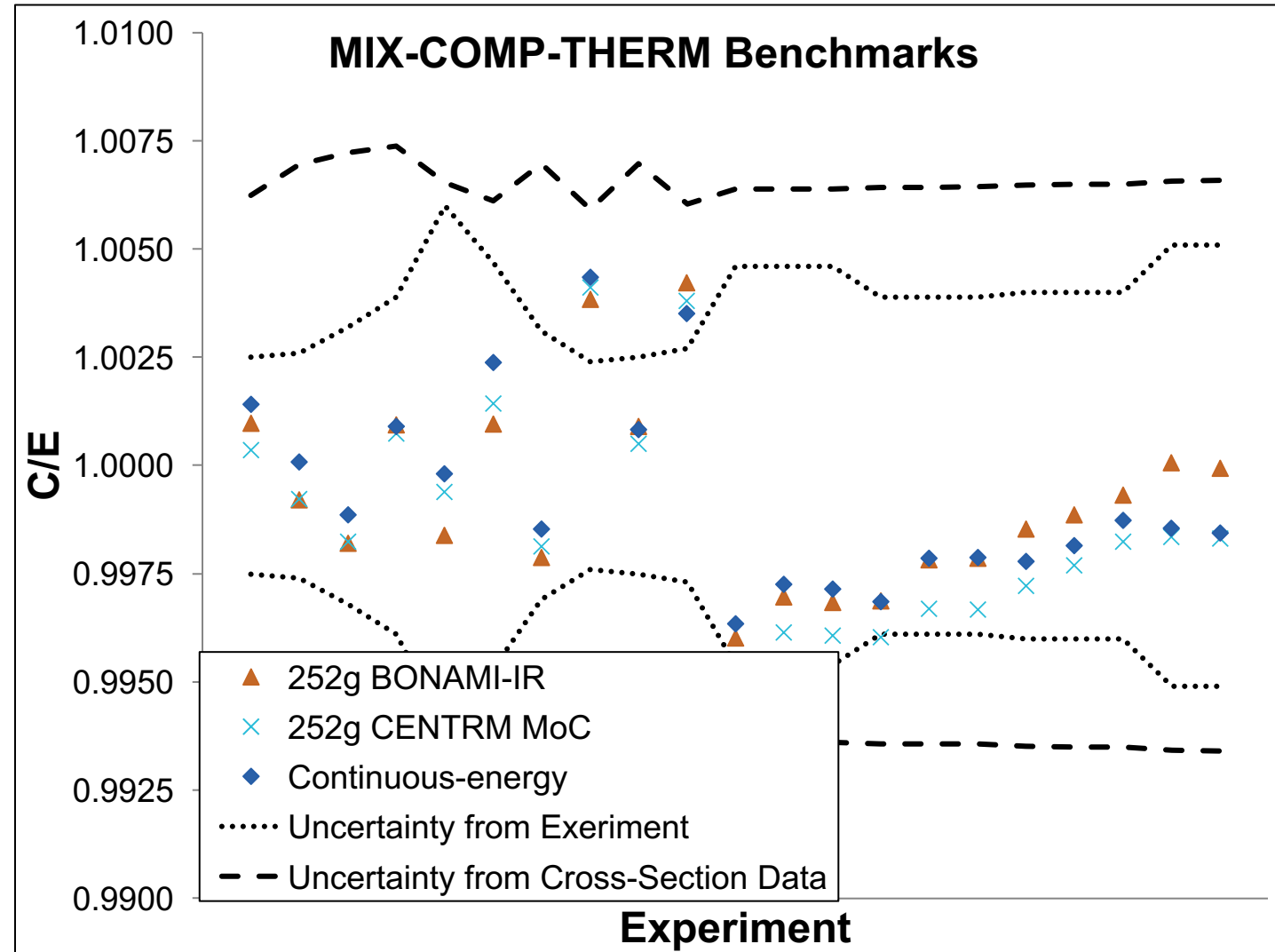
SCALE 6.2.2

- Released March 2017
- Minor bug fixes
- Lattice physics enhancements

SCALE 6.2 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
 - ~400 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!

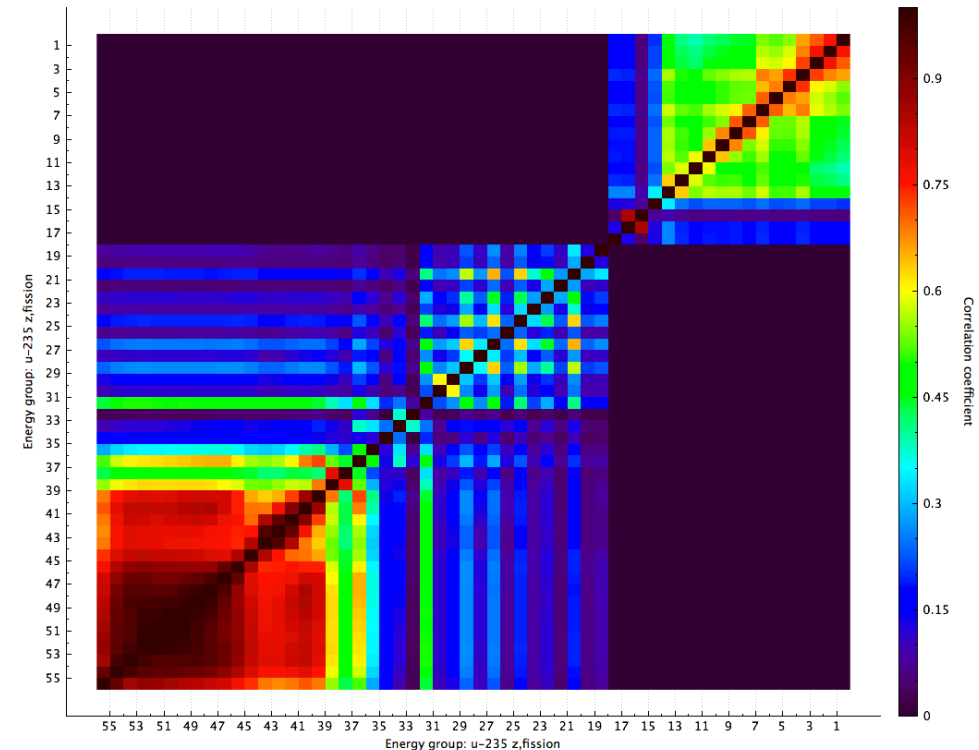
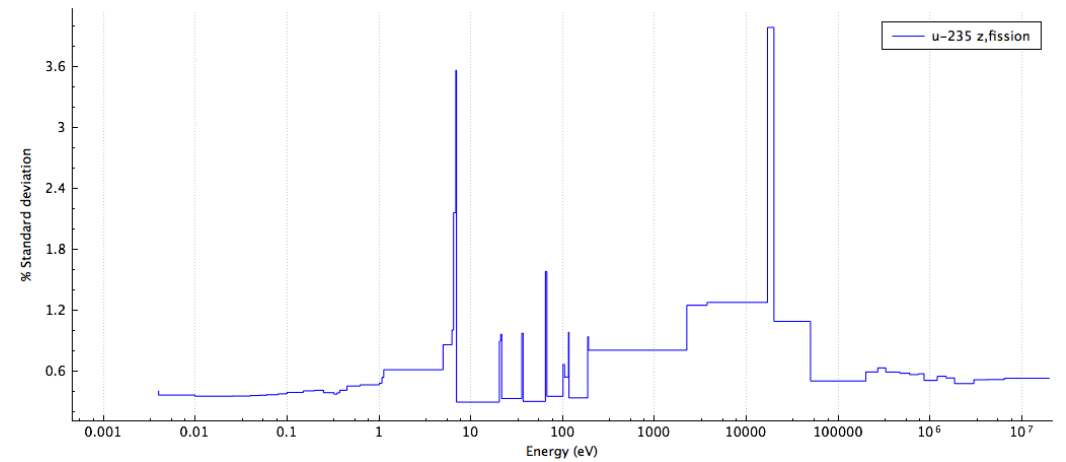


SCALE 6.2 Nuclear Data Libraries

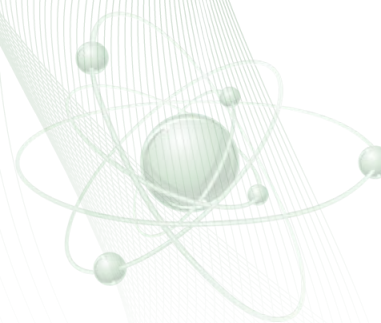
Mnemonic names	Primary data source/format
v7-238 ; v7-238n ; v7.0-238n	ENDF/B-VII.0 238-group neutron library
v7.1-252n	ENDF/B-VII.1 252-group neutron library
v7.1-56n	ENDF/B-VII.1 56-group neutron library
v7.1-200n47g	ENDF/B-VII.1 200-group neutron/47-group gamma library
v7-200n47g ; v7.0-200n47g ; v7-200g47	ENDF/B-VII.0 200-group neutron/47-group gamma library
v7.1-28n19g	ENDF/B-VII.1 28-group neutron/19-group gamma library
v7-27n19g ; v7.0-27n19g	ENDF/B-VII.0 27-group neutron/19-group gamma library
ce_v7.1_endf	ENDF/B-VII.1 Continuous-energy neutron and gamma library
ce_v7 ; ce_v7_endf ; ce_v7.0_endf	ENDF/B-VII.0 Continuous-energy neutron and gamma library

SCALE 6.2 Covariance Library

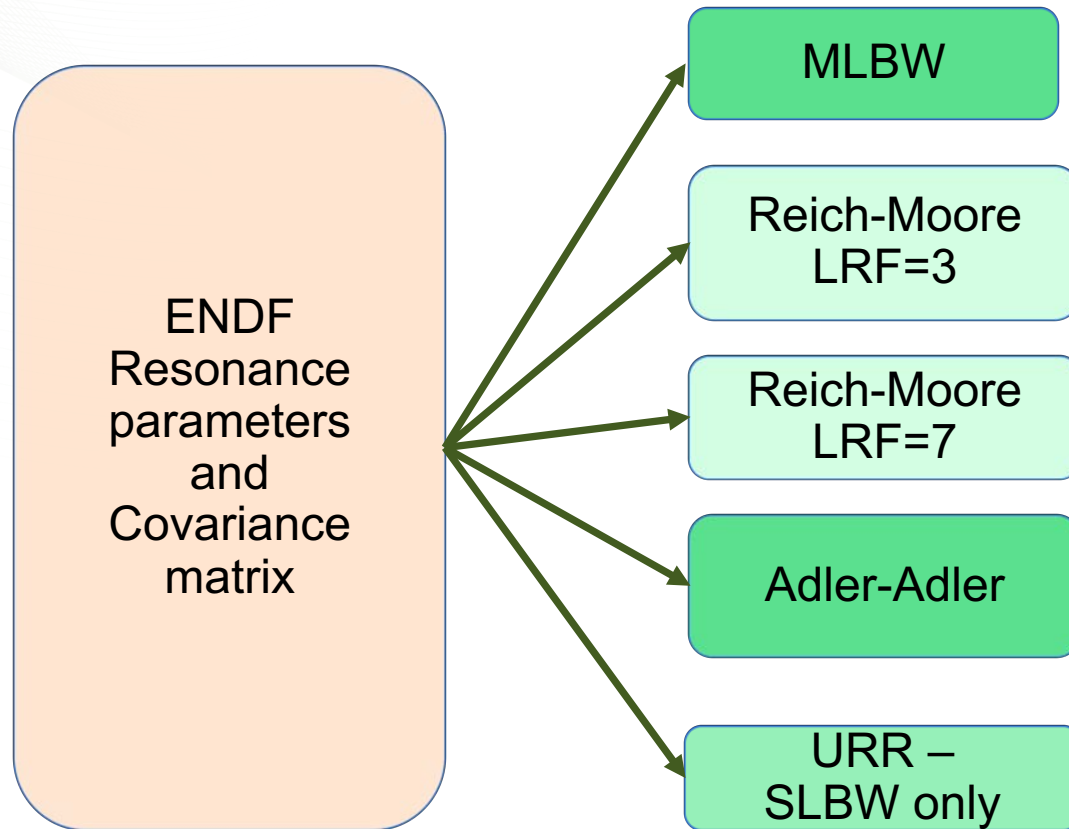
- ENDF/B-VII.1 for 187 isotopes
- SCALE 6.1 data retained for ~215 missing nuclides
- Modified ENDF/B-VII.1 ^{239}Pu nubar, ^{235}U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF/A repository
- Fission spectrum (chi) uncertainties processed from ENDF/B-VII.1 and from JENDL 4.0 (minor actinides)
 - Previous SCALE chi uncertainties were generated from Watt spectrum data and data were missing for minor actinides
- 56- and 252-group energy structures



AMPX Development



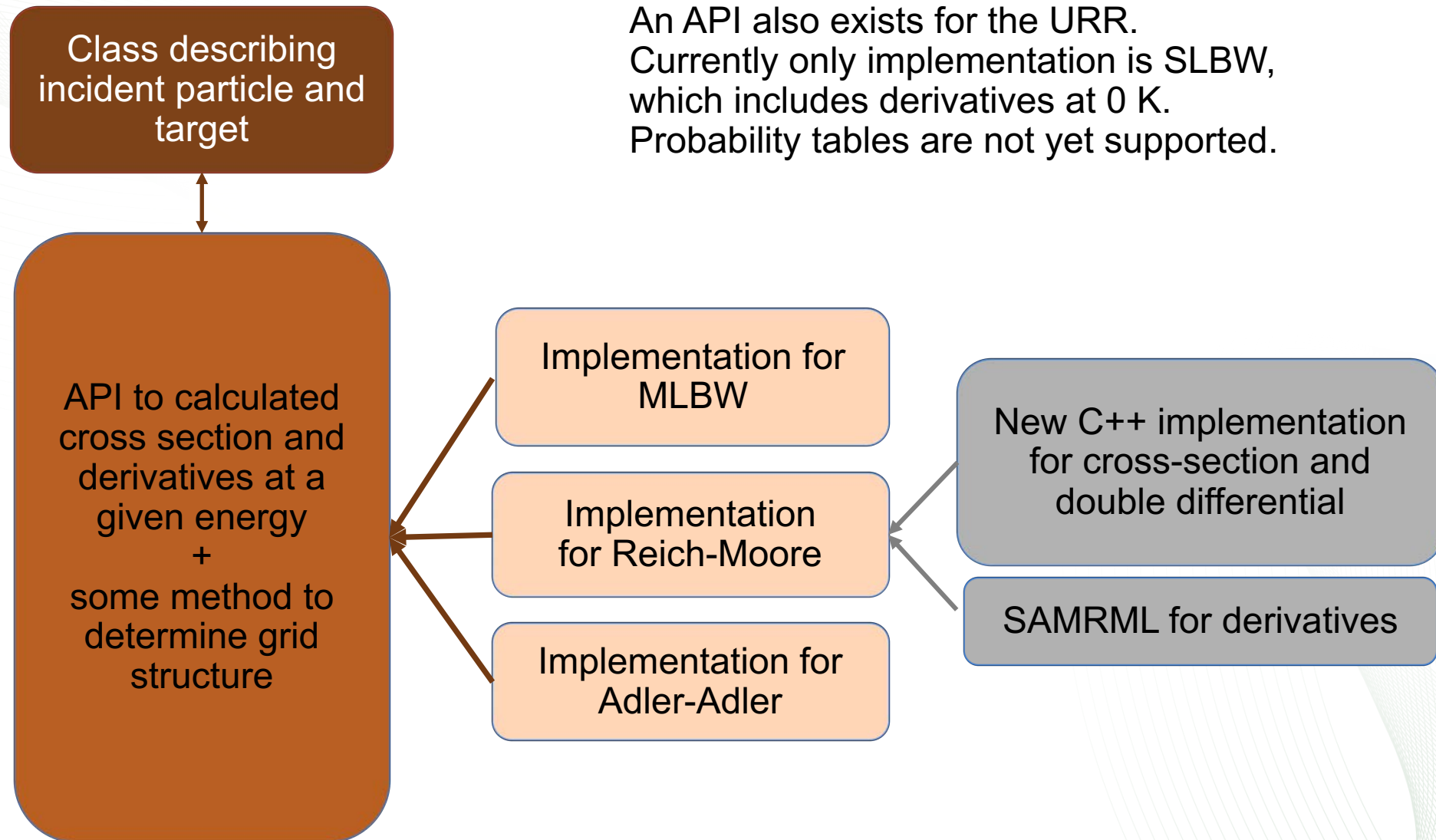
Resonance API



- SLBW and MLBW parameter are stored in the same class with a flag indicating which formalism to use
- Resonance parameters for Reich-Moore for LRF=3 are initially stored in a different class, but are converted to a LRF=7 class before calculation
- If derivatives are desired, all formalisms (except URR) are converted to LRF=7 so SAMRML can be used under the hood
- All resonance parameter classes can contain a covariance matrix. If converting to a different formalism, the covariance matrix is re-organized accordingly

A GND reader will be added to read the resonance parameters into memory

Resonance API classes



API to calculate group averaged derivatives and point-wise cross section from Resonance Parameters

- Read the ENDF data into the in-memory resonance parameter class
- A helper function returns an implementation of the resonance API class based on the resonance parameters passed in
- Calculate the point-wise reconstructed cross section at a given energy.
- An implementation of the AMPX integration routine (using fourth-order Runge–Kutta) with the function that returns values at a given E overridden.
- PUFF calls the above implementation with a flux and implementation of the resonance API class
- Apply the sandwich formula to get the covariance matrix with respect to the cross section on the user desired group structure.
- The API has been used in the modernized versions of PUFF (generate covariance library) and POLIDENT (reconstruct 1D cross section from ENDF files)

In-memory resource for COVERX data

- Data are read into memory
- File format (ascii, binary) is automatically detected, endianness no longer matters
- Methods to retrieve, add, delete cross section and matrices by material and reaction or by index
- Methods to convert between absolute and relative uncertainties and matrices
- Methods to convert to correlation matrices
- Class is written in C++ with Fortran bindings.
- Writer class that saves the data in ascii or binary format to disk

Dictionary
Energy bounds
Cross section + uncertainty MAT1, MT1
Cross section + uncertainty MAT2, MT2
..
Matrix <MAT1,MT1, MAT2, MT2>
Matrix <MAT3,MT3, MAT4, MT4>
...

Updated PUFF

- Resonance parameter covariance matrices use the resonance API
- New keyword based user input (old input is still supported)
- Better error reporting (done in the ENDF reading level)
- More output information
- Add redundant cross section if not present in ENDF
- Use the COVERX resource throughout the code to handle all temporary covariance matrices
- Add additional unit tests and keep old regression tests.
- Easier handling of cross-material covariance data

POLIDENT (point-wise 0K data) update

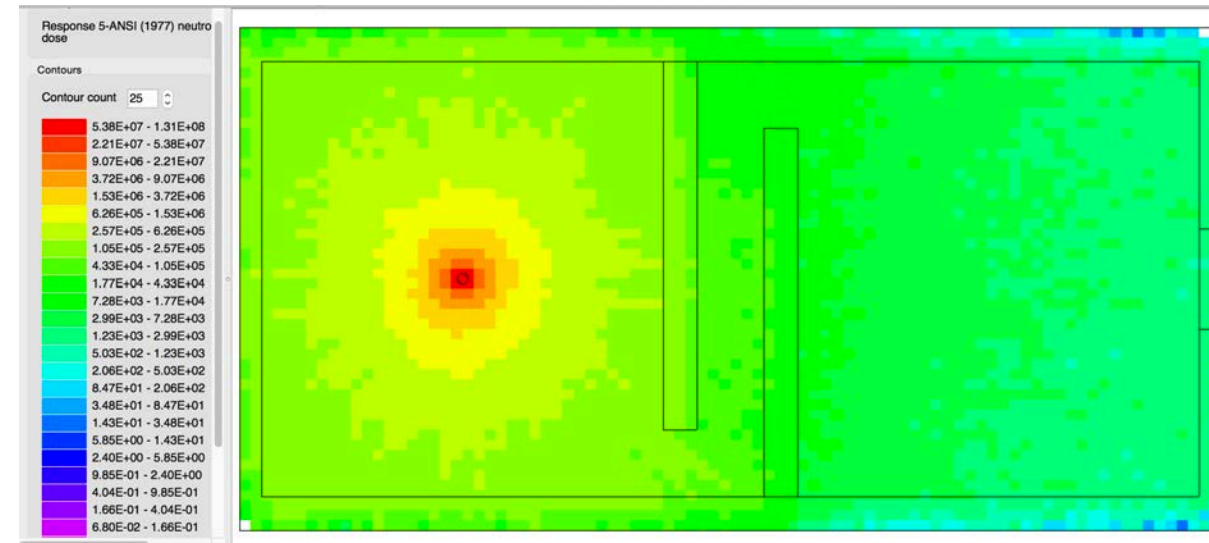
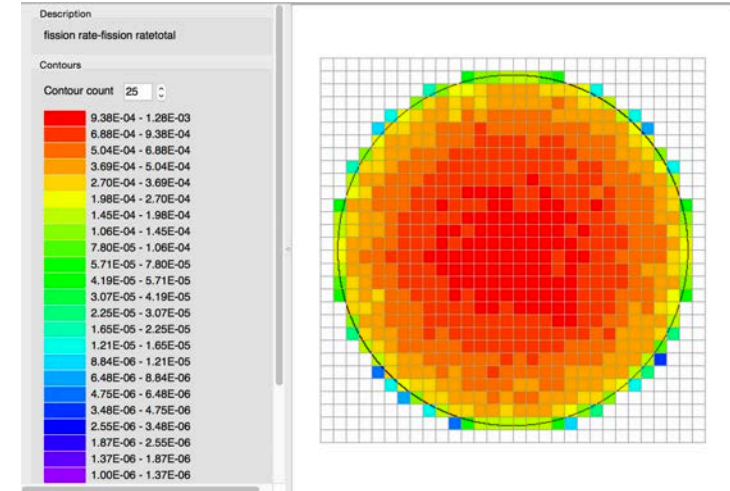
- POLIDENT was updated to take advantage of all the new API code:
 - Use the new C++ ENDF reading routines
 - Use the new resonance API
 - Use the API to determine the gridding in the RR and URR
 - Use templated classes to combine File 2 and File 3 data
- New keyword based user input (old input still supported)
- Use the new SCALE sequence/module architecture
- More consistent handling of discontinuities at the end of the RR and URR.
- Better error reporting

SCALE Development



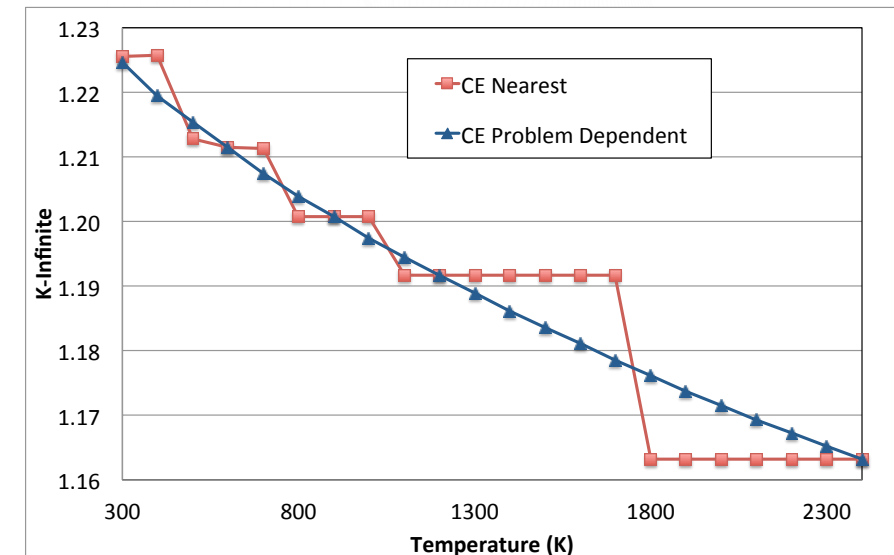
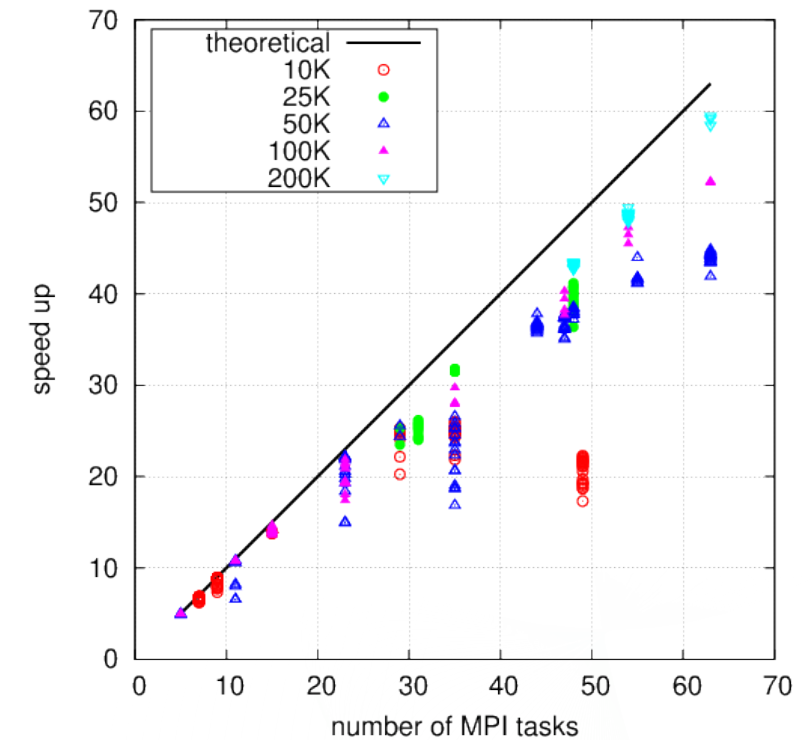
MAVRIC/Monaco Enhancements

- Continuous energy treatment
 - physics, dose responses, tallies
- More/better links to ORIGEN for source terms
 - Read spectrum from binary concentration file
 - Read in photon lines/intensities from ORIGEN data
- Improved statistical tests on tallies
- New statistical tests for mesh tallies
- Improvements on linking with Denovo
 - Macromaterials for better deterministic models
 - Denovo – more parameters, double precision output
- Improved link with KENO-VI for CAAS Problems
- MAVRIC Utilities – for post-processing



KENO Improvements

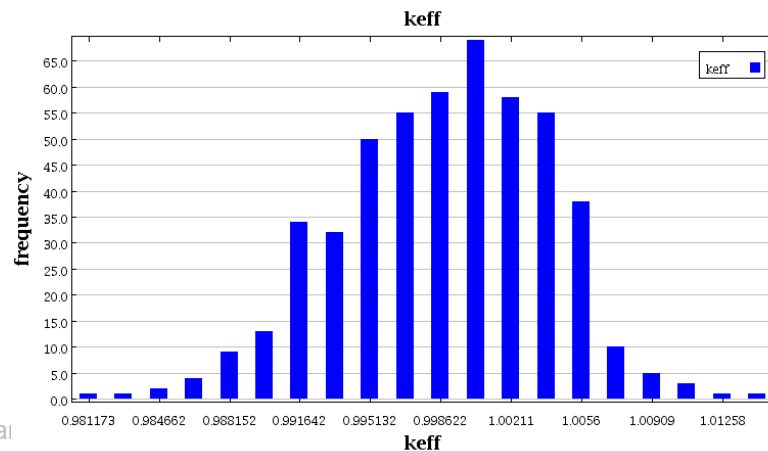
- Substantial **reduction in memory requirements** – over 99% improvement in many cases
- **Accuracy** improvements through comprehensive review and testing
- **Parallel Computations**
 - Significant speedups with MPI on Linux clusters
- **Source Convergence**
 - **Sourcerer** – Hybrid sequence to deterministic converge fission source
 - Shannon Entropy diagnostics
- **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



Enhanced Sensitivity and Uncertainty Analysis Tools

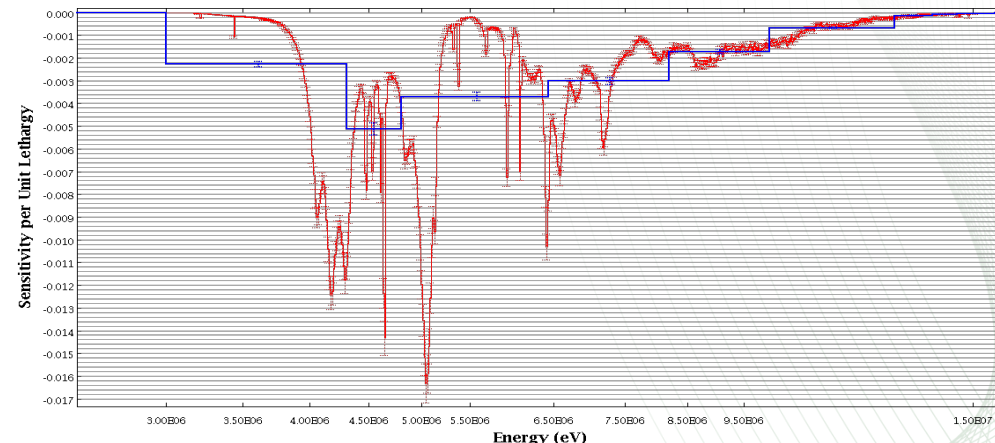
Sampler: Stochastic Uncertainty and Correlation Analysis

- Sampler provides uncertainties and correlation in **any computed result** from **any SCALE** sequence due to uncertainties in:
 - neutron cross sections
 - fission yield and decay data
 - geometry and composition

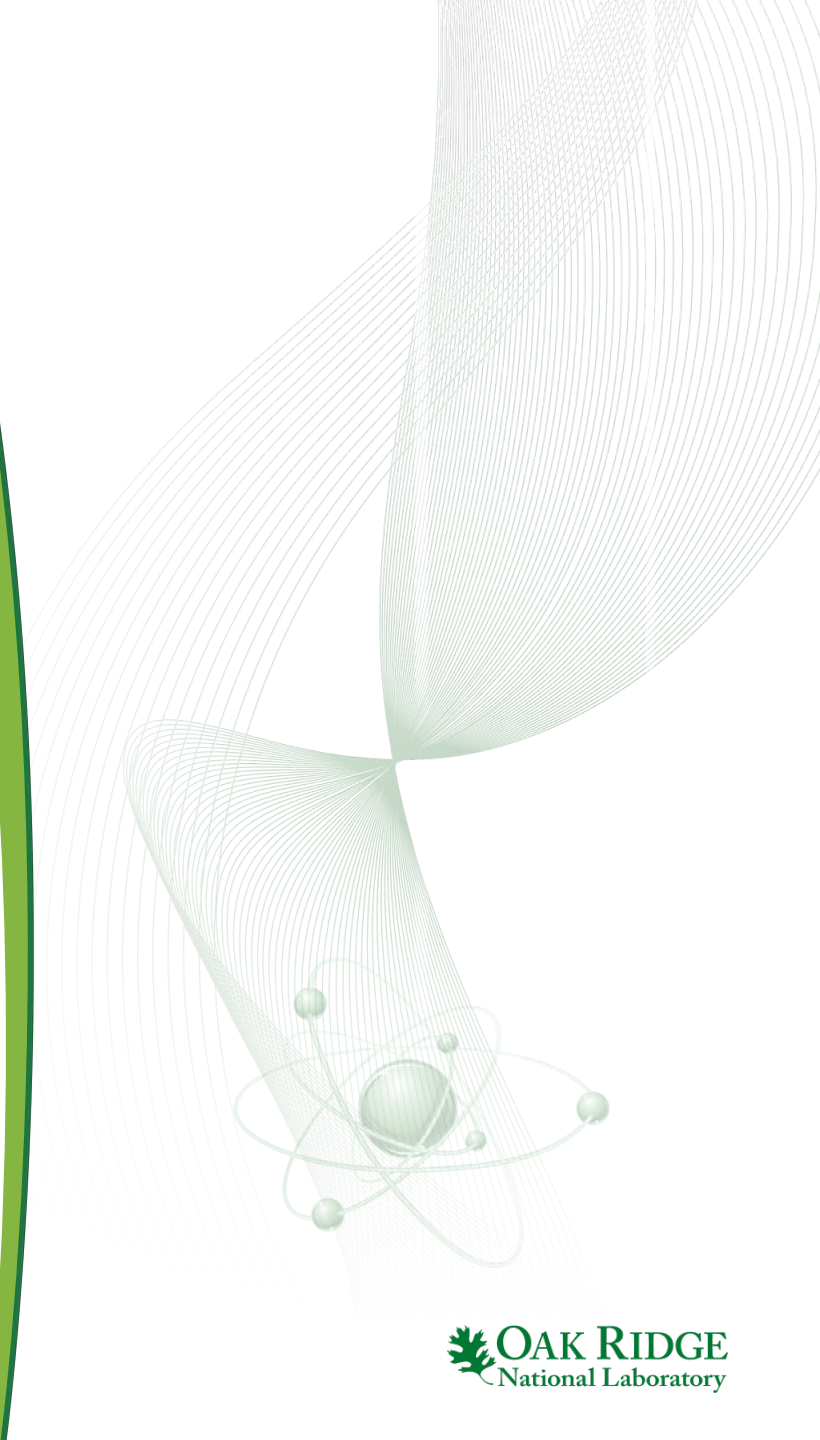


TSUNAMI: Adjoint-based Sensitivity Analysis

- Continuous-energy TSUNAMI-3D enhanced for improved runtime performance and improved stability.
- Generalized responses such as reaction rate ratios move to production capability.
- Multigroup group TSUNAMI-3D integrated with modern XSPROC SCALE sequences



2017 and beyond



SCALE/AMPX Modernization Plan

- Transition to modern infrastructure over several releases
 - 6.2 Begin process
 - 6.3 Enhanced capabilities
 - 7.0 Fully modern framework
- AMPX
 - Modernization of several modules
 - Ongoing implementation of GND format

SCALE Modernization Plan

August 26, 2012

Bradley T. Rearden

1. Introduction

SCALE provides a robust toolkit for lattice physics, nuclear criticality safety, source term characterization, radiation shielding, sensitivity and uncertainty analysis, and many other features essential for license reviews. However, the overall architecture of SCALE is based a 40-year old design where text files are used to control the logical flow of the analysis and data are passed between individual computational codes using binary files that are read from and written to the hard disk. Due to this legacy infrastructure, SCALE 6.1 only operates in serial mode, utilizing one computer processor for the entire calculation sequence, even when most users are performing their analysis on multi-core PCs or multi-node Linux clusters. Additionally, it is difficult to apply modern software development tools, testing, and deployment strategies to legacy Fortran code, which leads to inefficiencies in integrating new features, resolving possible code or data discrepancies, and rapidly deploying new SCALE features to end-users. Additionally, each SCALE component contains its own implementation of output formatting. Some, but not all, codes include a convenient HTML formatted output. As such, users are presented with various forms of output from each functional module, even when viewing a single output file from a single code execution.

A NRC/RES contract that recently concluded (N6823) provided the foundational modern framework for SCALE 7. The SCALE 7 framework provides an object-oriented parallel enabled software infrastructure with reusable components, such as centralized tools for cross-section data and output generation.

Currently, the first feature enabled in the modern SCALE 7 framework provides resonance self-shielded cross sections using Bondarenko factors with intermediate-resonance theory for use in subsequent analyses. Even when executed in serial mode, the modular design of SCALE 7 with reduced internal file I/O is about a factor of 4 faster than SCALE 6.1 for the same calculation. When parallel calculations are performed, more substantial speedups are realized. The SCALE 7 infrastructure provides the foundation for new projects, such as the Embedded Self-Shielding Methodology, but it lacks numerous features that are essential for an efficient, integrated product. However, most key capabilities (e.g., lattice physics, criticality, source terms, shielding, depletion, sensitivity and uncertainty analysis) necessary for licensing review have not been modernized.

Path Forward

- Continue to enhance test suite, with focus on nuclear data testing, integrated unit testing, and generation of V&V reports
- Review modernization plan and QA plan
- Continue to improve innovation, accuracy, efficiency, and ease-of-use
- Integrate all components into modern parallel framework with shared data resources
- Complete Shift to consolidate Monte Carlo capabilities
- Consider open source software model for expanded collaboration opportunities

Beyond SCALE 6.2: Modular Capabilities Integrated for High-Performance Computing Future SCALE Monte Carlo Code - **Shift**

