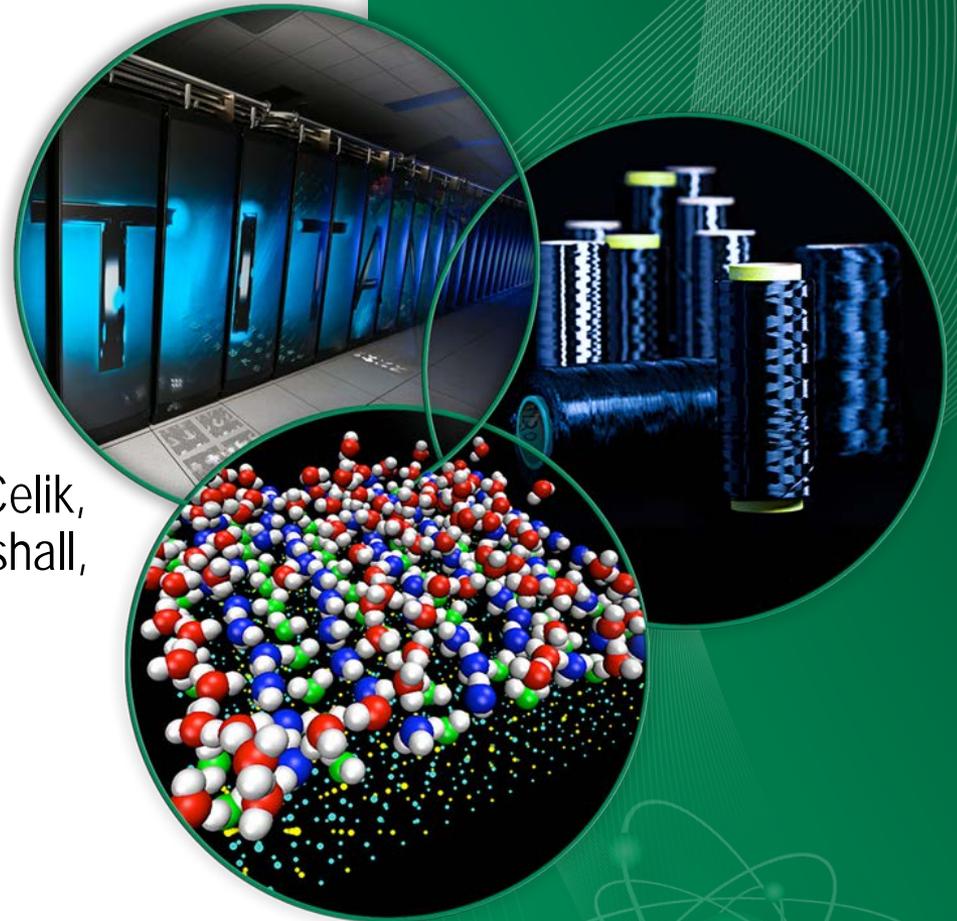


# AMPX Development and Modernization Status

Michael Dunn, Dorothea Wiarda, Cihangir Celik,  
Kursat Bekar, Charles Daily, William J. Marshall,  
Mark Williams, and Brad Rearden

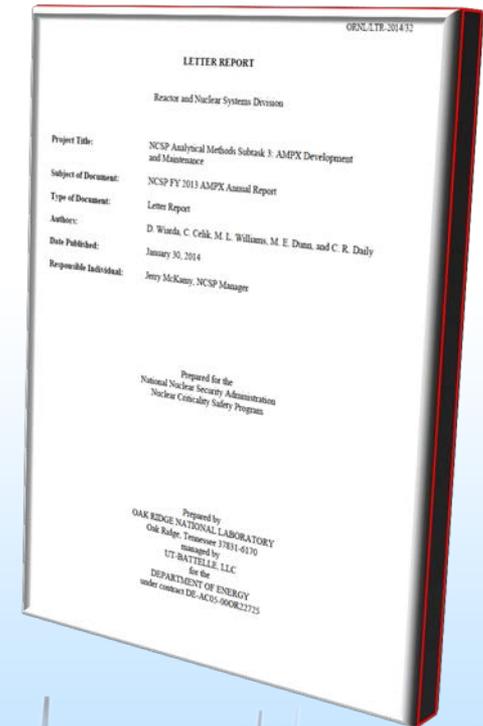
NCSP Technical Program Review Meeting  
Los Alamos, NM  
March 26-27, 2014



# Outline

- Background
- AMPX Modernization
  - AMPX / SCALE development merger and SQA
  - Status of code refactoring effort
- Status of ENDF/B-VII.1 libraries for SCALE
- Summary

FY13 AMPX Annual Report

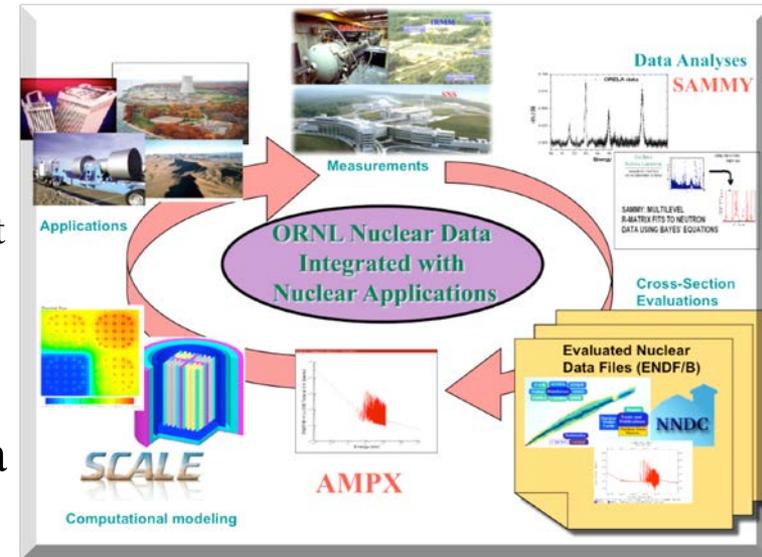


# AMPX Processing Capabilities Vital for SCALE

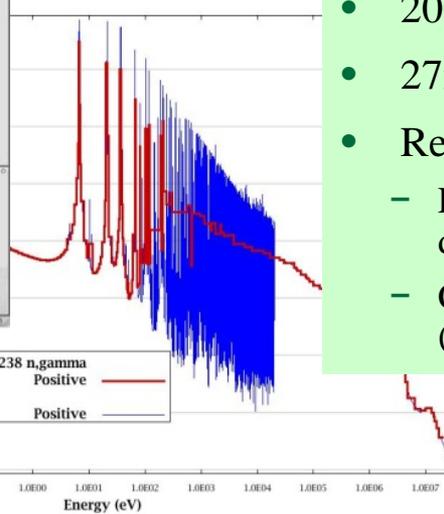
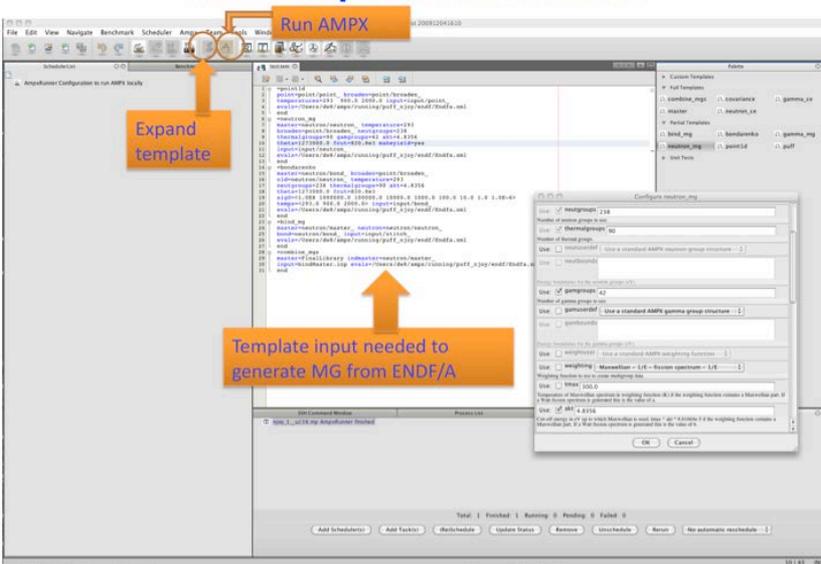
## ➤ SCALE relies upon AMPX for CE, MG, and Covariance Data Libraries

- MG and CE cross-section data
- Data processing procedures including problem-dependent resonance self-shielding
- Cross-section uncertainty data to support S/U methods in SCALE

## ➤ AMPX processes ENDF/B-formatted nuclear data evaluations to produce cross-section libraries



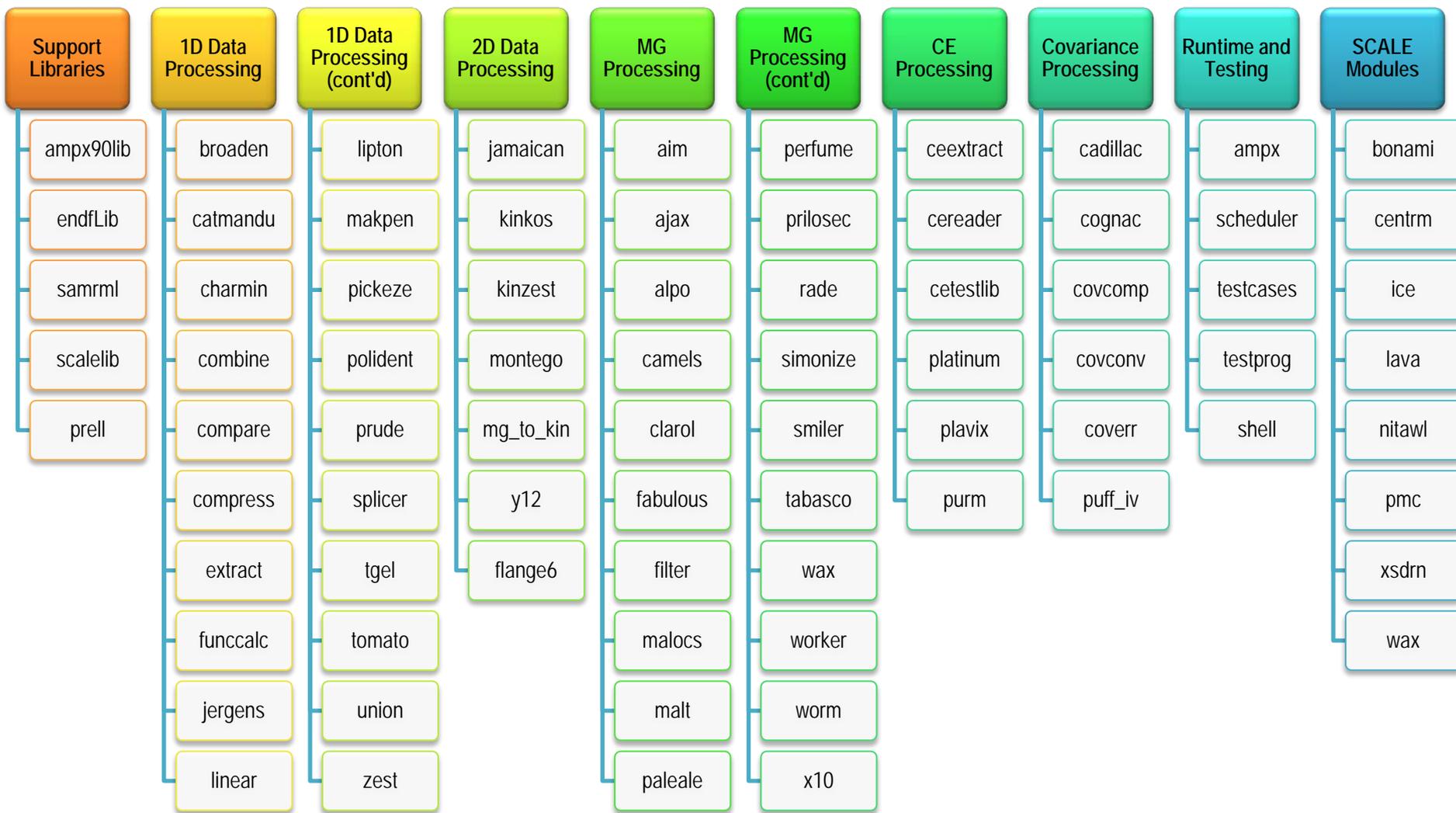
### AMPX Graphical User Interface



## Data Libraries Released with SCALE 6.1:

- CE ENDF/B-VI.8 and ENDF/B-VII.0
- 238-group ENDF/B-VI.8 and B-VII.0
- 200n47g ENDF/B-VI.8 and B-VII.0
- 27n19g ENDF/B-VII.0
- Recommended covariance data library
  - Evaluated and approximate covariance data
  - Covariance data for all ENDF/B nuclides (neutron)

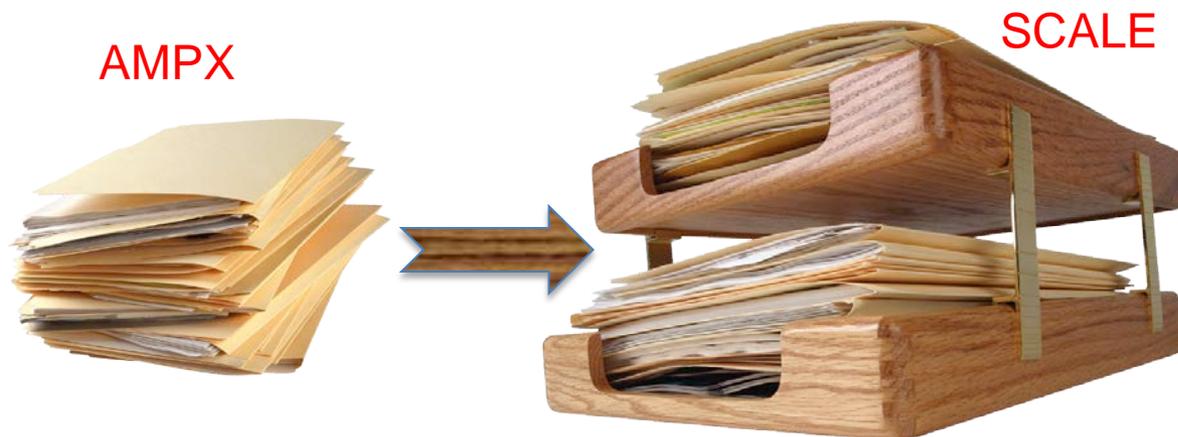
# AMPX Modular Code System (pre-Modernization Effort)





# AMPX/SCALE Development Merger

- **AMPX and SCALE remain separate code packages but developed under common infrastructure**
- Merge AMPX into the SCALE repository
- Convert to use the same build system.  
This allows developers to develop in the same framework
- Easier to share components that are the same for AMPX and SCALE
- Can now use SCALE continuous-integration test harness
- AMPX development performed under the SCALE QA procedure



# SCALE QA Program

- Designed for Compliance with:
  - ISO 9001 (ORNL registered with ISO)
  - 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

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. ANSII/ISO/ASQ(E) Q9001-2008

**AMERICAN NATIONAL STANDARD**

**Quality management systems—  
Requirements**

c.

2. CA

Can  
or r  
Doc  
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com  
sub

3. AP

a.

AVAILAR  
[www.ditree](http://www.ditree)

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



# Build and Test Infrastructure

- **FogBugz System**
  - QA and feature development tracking
  - Helpline tickets and email
- **After every update, SCALE and AMPX automatically built and tested to ensure functionality of all tested features**
  - ~1500 test cases (still need more)
  - Results of tests post to internal “dashboard” website

The screenshot shows the FogBugz interface. The top part displays a project overview for 'scale' with a history of updates and a Kanban board. The Kanban board has columns for Proposed (6), Approved (0), In Progress (6), In Testing (1), Ready to Ship (1), and Deployed (0). The 'In Progress' column contains several items, including '2972: (MLW) CENTRM 2D Moc Option' and '2976: (MLW) Sampler'. The 'In Testing' column contains '3053: (WBM) STARBUCS Updates'. The 'Ready to Ship' column contains '2962: (SW) CENTRM dependency on Legacy XSDRN'. The bottom part shows a detailed view of bug 6352, 'AMPX driver/Beta release', assigned to Dorothea Wiarda. It includes a table with Level (L2), Charge Number (35304154), and Sponsor (NCSP). The 'Functional Specification' section describes the requirements for the AMPX beta release.

Linux Regression															
Site	Build Name	Update		Configure			Build			Test				Build Time	Labels
		Files	Min	Error	Warn	Min	Error	Warn	Min	NotRun	Fail	Pass	Min		
<a href="#">node16.ornl.gov</a>	<a href="#">LEGACY-RELEASE-Intel-12.0.3.174</a>	13	0.2	0	0	1.3	0	0 <sub>10</sub>	5.6	0	4	477	221.6	2012-03-07T11:50:42 EST	(none)
<a href="#">node16.ornl.gov</a>	<a href="#">LEGACY-RELEASE-Intel-12.0.3.174</a>	11	0.4	0	0	3.4	0	16 <sup>+10</sup> <sub>20</sub>	14.1	0	4	477	223.8	2012-03-07T07:48:54 EST	(none)

Current Subscribers:  
[Dorothea Wiarda](#)  
[Jordan P. Lefebvre](#)

AMPX does not need the data directory - we need to be sure it can configure without it.  
 Functional Tests changed to 'AMPX can be installed and all unit test run from a source tree ready for the beta release.'

# SCALE Continuous Integration Testing

- 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

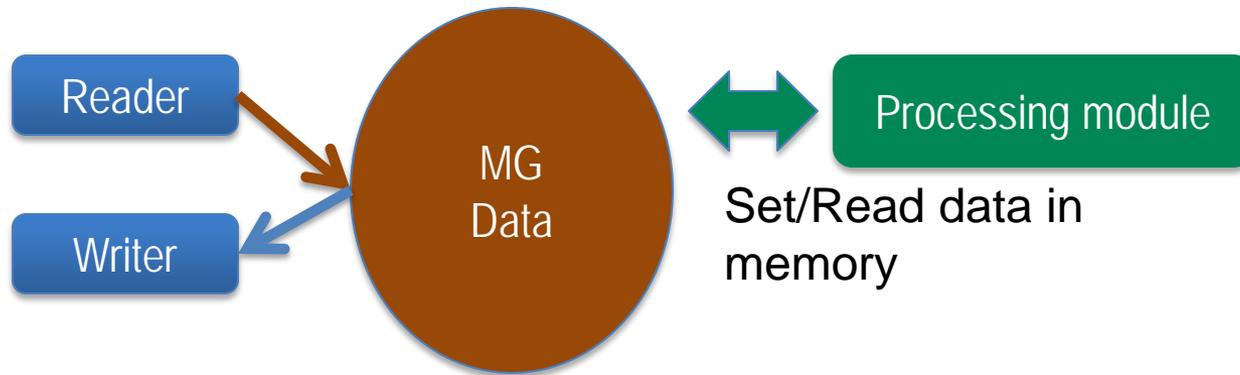
- Total of ~50,000 tests every day

The screenshot shows the SCALE Continuous Integration Testing dashboard. At the top, it displays 'My CDash All Dashboards Log Out' and 'SCALE' with navigation tabs for 'Dashboard', 'Calendar', 'Previous', 'Current', 'Next', and 'Project'. Below this, it indicates 'No file changed as of Sunday, May 19 2013 - 21:00 EDT' and provides options for 'Show Filters', 'Advanced View', 'Auto-refresh', and 'Help'. The main content is divided into two sections: 'Nightly' and 'Continuous - Linux'. Each section contains a table with columns for 'Site', 'Build Name', 'Update', 'Configure', 'Build', 'Test', and 'Build Time'. The 'Update' and 'Configure' columns are further subdivided into 'Files', 'Error', and 'Warn'. The 'Build' column is subdivided into 'Error' and 'Warn'. The 'Test' column is subdivided into 'Not Run', 'Fail', and 'Pass'. The 'Build Time' column shows the date and time of the build. The 'Nightly' section shows builds for sites dev1.ornl.gov and dev2.ornl.gov. The 'Continuous - Linux' section shows builds for sites dev1.ornl.gov through dev5.ornl.gov. A tooltip for 'ctest-2.6.8' is visible over the 'Files' column of the last row in the 'Continuous - Linux' section.

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	354				May 20, 2013 - 09:37 EDT
dev1.ornl.gov	Release-Intel-13.0.1.117	2	0	1	0	50	0	4	676				May 20, 2013 - 09:52 EDT
dev2.ornl.gov	Release-Intel-13.0.1.117-regression	10	0	3	0	50	0	1	377				May 20, 2013 - 09:37 EDT
dev2.ornl.gov	Release-Intel-13.0.1.117-regression	10	0	3	0	50	0	0	378				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	Debug-GNU-4.6.1	10	0	3	0	50	0	4	676				May 20, 2013 - 14:56 EDT
dev1.ornl.gov	Release-GNU-4.6.1	10	0	3	0	50	0	4	676				May 20, 2013 - 14:55 EDT
dev5.ornl.gov	Debug-GNU-4.6.1-openmpi-1.4.3	10	0	3	0	50	0	4	944				May 20, 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
dev3.ornl.gov	GCC-4.6.1-ANALYSIS	10	0	1	0	50	0	4	676				May 20, 2013 - 14:46 EDT
dev3.ornl.gov	Linux-DBC-GCC-4.7.2-RELEASE	10	0	1	0	50	0	5	675				May 20, 2013 - 14:46 EDT
dev5.ornl.gov	Debug-GNU-4.6.1-openmpi-1.4.3	10	0	3	0	50	0	4	944				May 20, 2013 - 09:36 EDT
dev5.ornl.gov	Release-GNU-4.6.1-openmpi-1.4.3	10	0	3	0	50	0	4	944				May 20, 2013 - 09:36 EDT
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	382				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

# Implementation of Shared SCALE/AMPX MG In-Memory Library Resource

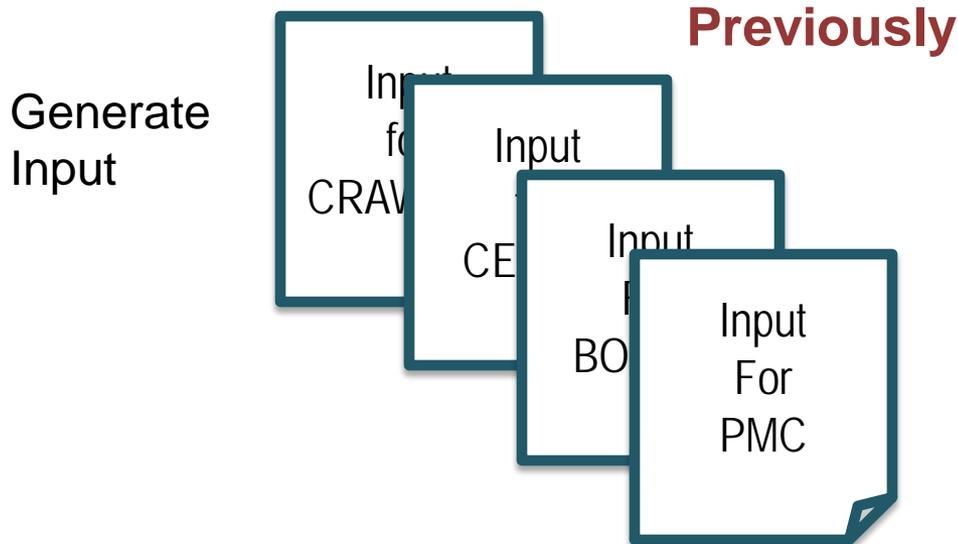
- SCALE developed a C++ in-memory resource to access MG library data. Reader and Writer classes are provided.
- Fortran bindings are provided.



- After the repository merge, AMPX can easily share the resource.
- If file format changes, it “automatically” changes in SCALE and AMPX.
- In-memory resource already allows for additional MG data (Subgroup data) and more than 999 groups.
- Most of the AMPX modules have been changed to use the new resource—X10 multi-group production module in the process of being changed.

# SCALE/AMPX Development Merger Allows Better Integration of Computational Tools

Calculation of “intermediate” resonance self-shielding factors for MG libraries requires use of AMPX and SCALE modules



- Run each module as separate program using system calls
- Very cumbersome and inefficient MG library generation procedure

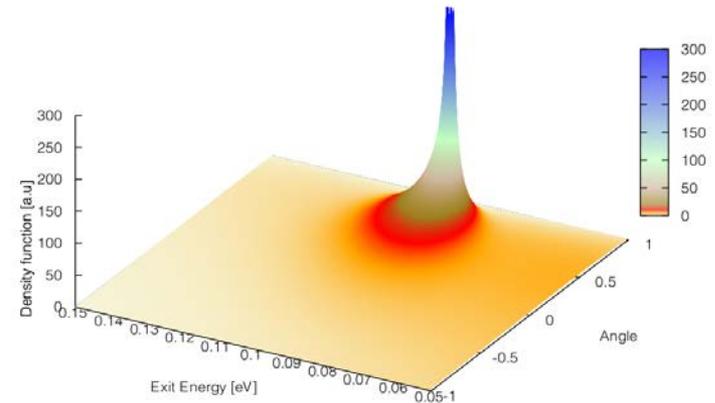
## Updated version



- SCALE added new sequence concept where processing is done in memory.
- AMPX now takes advantage of the new shielding cross section module.
- All data are passed in memory
- Changes in module input will be propagated at compile time – no more writing input for each program

# AMPX Modernization Efforts – Status of Code Refactoring Effort

- Initiated refactoring effort for AMPX processing modules
- Re-writing in C++ to allow easy code reuse
- Initial effort focused on AMPX collision kinematics module “Y12”
- Y12 needs many of the basic functionality given in the AMPX library functions, so many of the basic functionalities were rewritten in C++—will streamline refactoring efforts of other AMPX modules

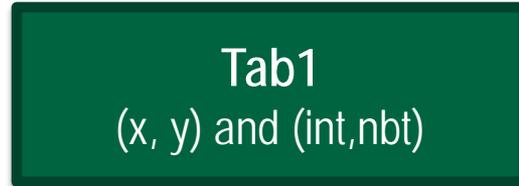


H<sub>2</sub>O incident energy 0.1 eV

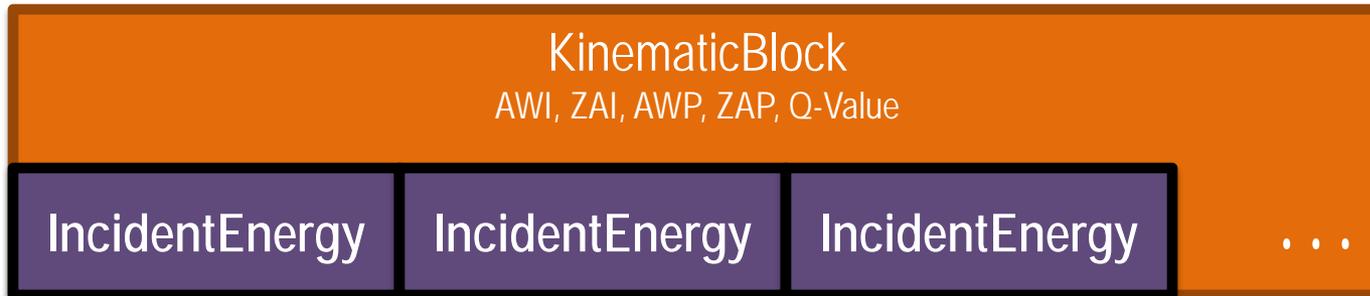
# Improved Data Management

## Basic Data Containers Translated from Fortran to C++

### 1-D data



### 2-D data



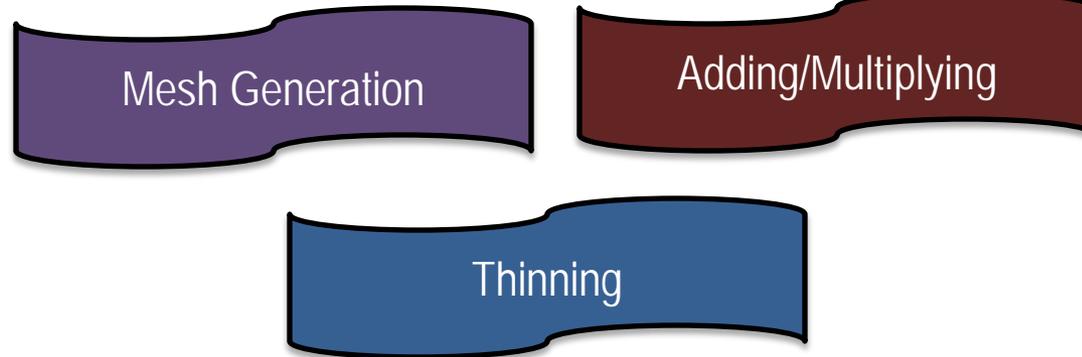
- Used in all new code
- Basic methods for integration and data access provided in the class
- Unit tests incorporated as code is refactored

# Improved Handling of Collision Kinematics Data

- C++ allows use of templates and functions that operate on them (used templates instead of inheritance to ensure type safety)

“Iterator”  
Class  
Remove  
Insert  
Interpolate

- Can define template functions to do the coding once.
- Hard part is interpolation and equality check (see next slide)



- Provided an Iterator class for all data containers:
  - Tab1
  - ExitEnergy
  - IncidentEnergy
  - KinematicBlock
- Do most of the unit test on the template functions using 1-D data, as it is easy to test.

# Improved Data Testing within AMPX: Interpolation and Equality Testing for Collision Kinematics Data

- On Energy in Tab1 (x,y) or angular cosine in tabulated angular distributions interpolate or compare on union grid – refine mesh as needed
- On Exit energy:
  - Only compare exit energy objects given at the same exit energy. Now we only need to compare on angular cosine value or Legendre order.
  - Interpolate if needed before comparison.
- On Incident Energy:
  - Interpolate using unit-based interpolation. Corresponding point interpolation is supported, but internally AMPX uses Unit-based
  - Only compare for the same incident energy. Interpolate before comparison if needed.

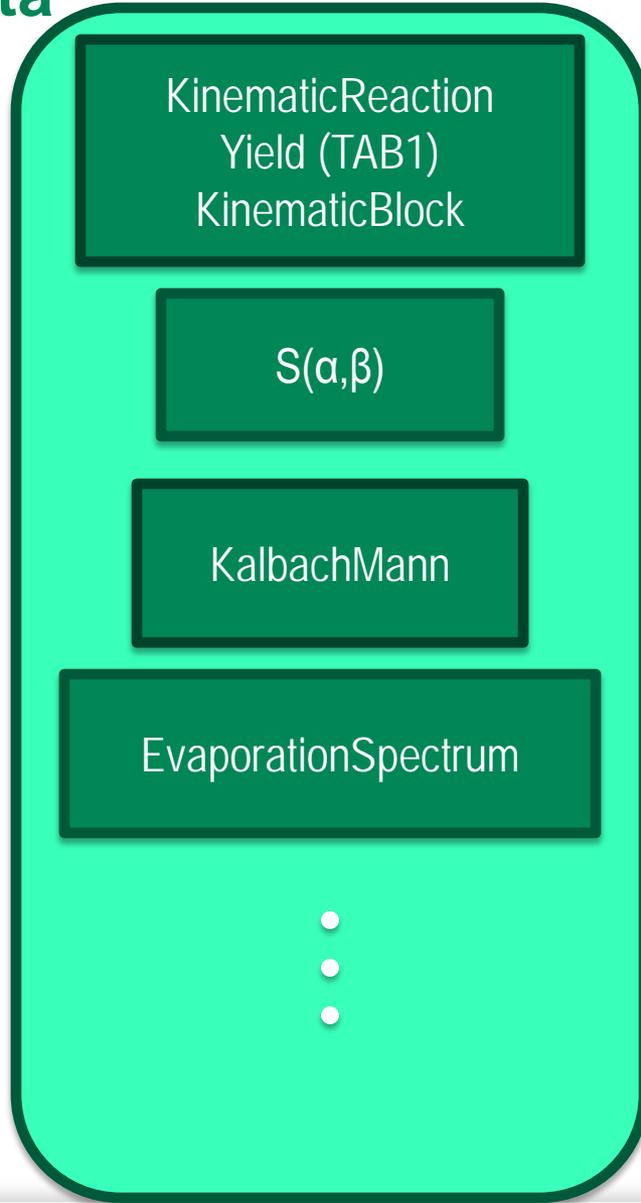
**Note:** Filling a mesh of incident energies based on a halving scheme can lead to an extremely dense mesh. Therefore we also allow a equality test based on exit energy range only.

# Improved Interface and Operations with ENDF Kinematics Data

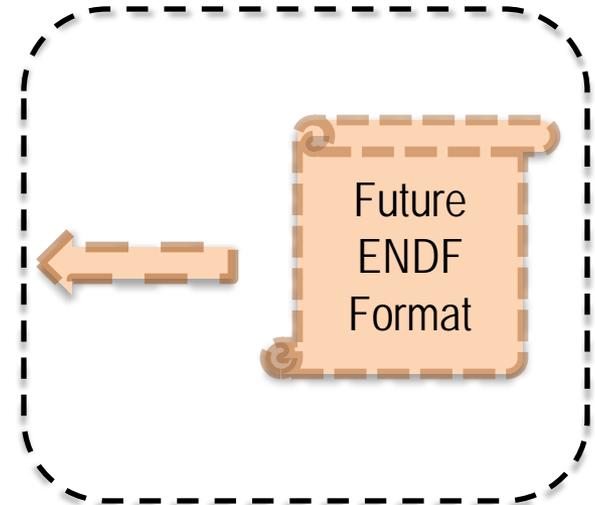
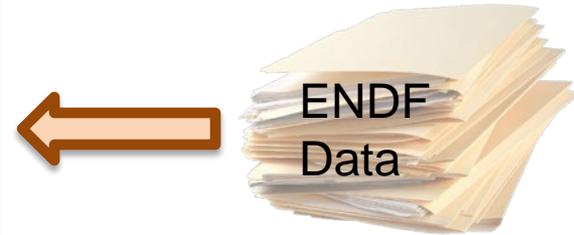
Y12 never reads ENDF data directly.



Produces:  
Tab1  
KinematicBlock



Processing code never reads ENDF formatted files directly



Plan to implement as part of AMPX modernization effort

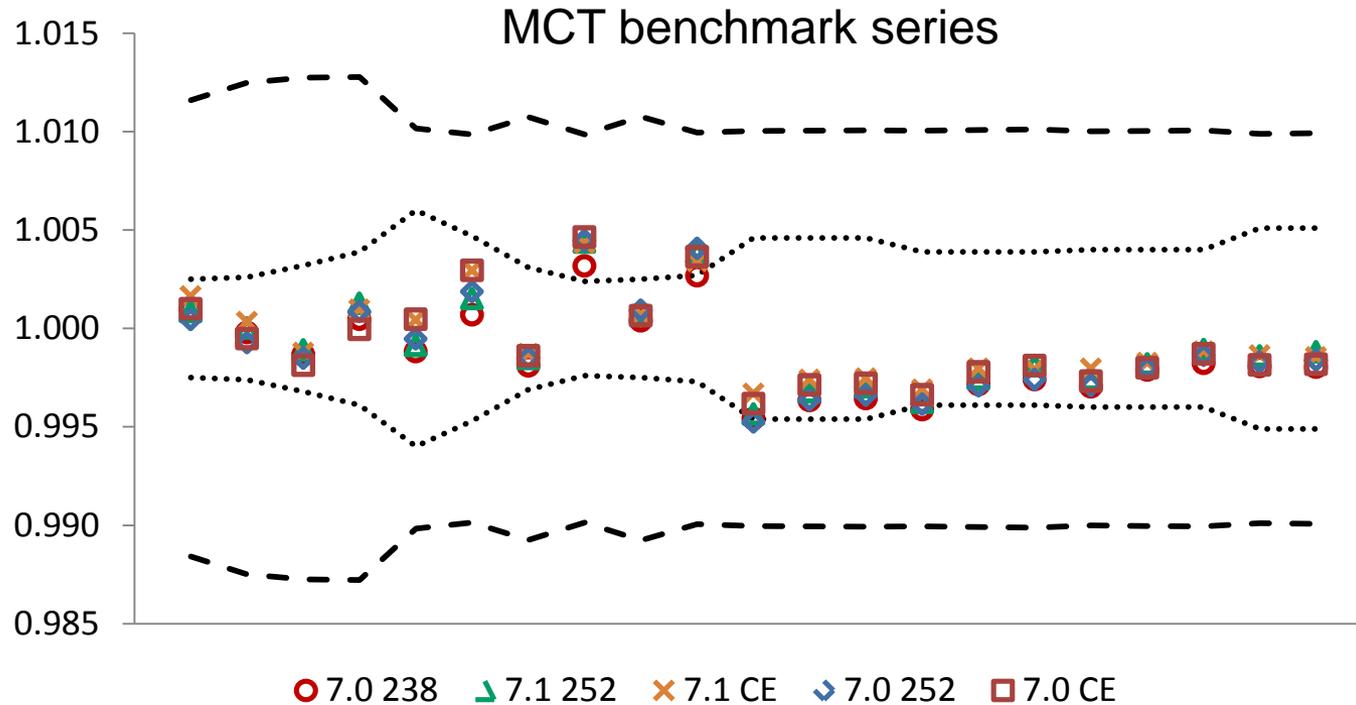
# Updated Processing of Elastic and Discrete Inelastic 2D Data

- Given in ENDF as angular distribution for a given incident energy in COM—exit energy given by kinematic formulas
- SCALE needs the data in LAB
- AMPX converts Legendre to tabulated if needed and then converts to LAB, finding a suitable exit energy mesh
- Additional incident energies are added for discrete inelastic reactions:
  - Add 10 additional incident energy values between threshold and first incident energy given in ENDF (equal lethargy spacing)
  - Refine the mesh (based on a halving scheme) over WHOLE incident energy range. HOWEVER, only ensure that the exit energy range can be interpolated in a unit-based interpolation
  - Thin the mesh, but compare for each incident energy, exit energy, and angle, i.e. the FULL distribution.

# Generate and Testing ENDF/VII.1 library for SCALE—Benchmark Testing

- Use the new Y12 to generate the kinematic data
- Use merged AMPX/SCALE repository version
- Generate CE libraries, MG, and covariance libraries

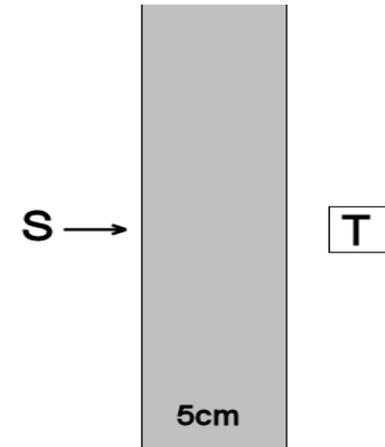
Example Validation Testing



- Run extensive tests on the library (transmission and benchmark cases)

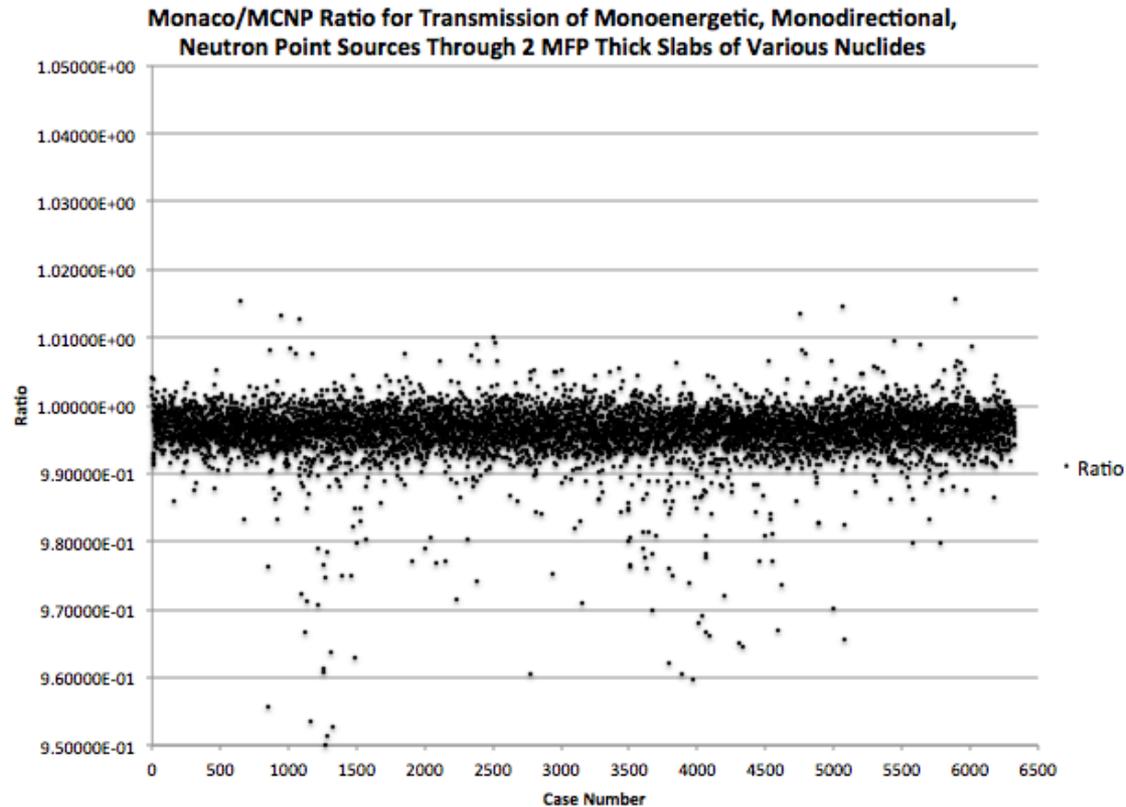
# Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries—Regression Tests

- Compared MONACO with AMPX-Generated CE Library to MCNP6 with NJOY-Generated ACE Library
  - Transmission Test Suite (7215 total cases)
    - Mono-energetic, Mono-directional, Point Source
    - 2 MFP slab of attenuating material
    - Compares total flux transmitted through slab to 2x2x2cm detector
    - Neutron-only (15 energies) and Gamma-only (9 energies) test suites
  - Leakage Test Suite (421 cases)
    - $^{252}\text{Cf}$  S.F. Neutron Spectrum, Point Source in center of 25cm sphere of attenuating material
    - Run in Coupled n- $\gamma$  mode
    - Compares neutron and gamma leakage spectra at outer radius of sphere for all converged (R.E. < 5%) groups



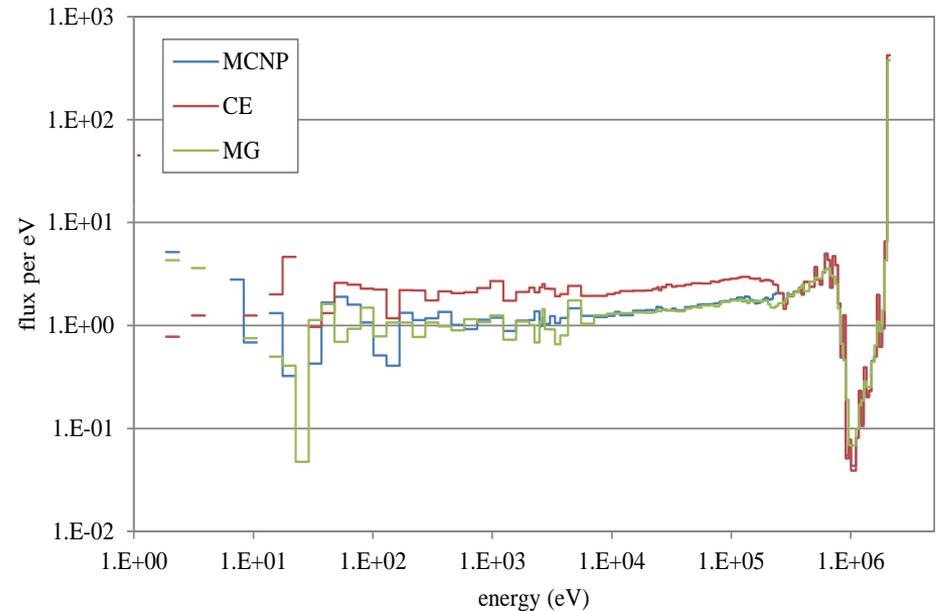
# Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries

- Overall, acceptable agreement between SCALE and MCNP for CE transmission cases
- ~90% of cases within +/- 1%
- Investigated differences for cases outside of 1% agreement—understand differences
- Some differences attributed to insufficient tally statistics
- Differences for some cases attributed to possible non-physical kinematics distributions in the base ENDF data and subsequent interpretation of data by processing codes (see next slide)



# Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries

- $^{182}\text{W}$  Investigation
- ENDF evaluation reveals up-scatter allowed for inelastic scattering to continuum reaction (MT=91 in ENDF)
- Up-scatter from stable isotope does not appear to be physical
- SCALE/CE-Monaco kinematics distributions are “faithful” to ENDF/B evaluation
- SCALE/MG does not allow up-scatter for non-thermal reactions
- MCNP & SCALE/MG agree—appears MCNP not allowing up-scatter to occur for inelastic scattering

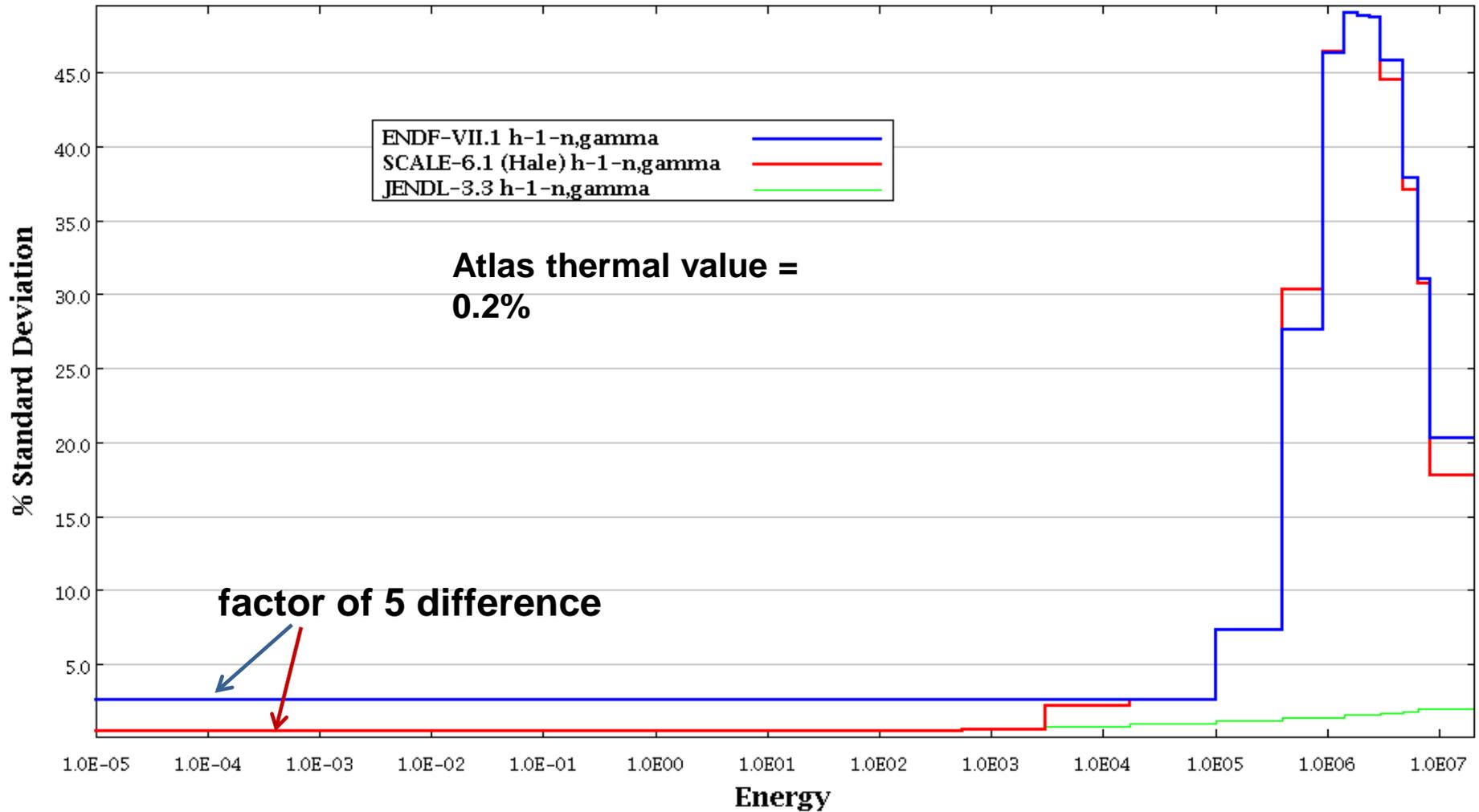


# ENDF/B-VII.1 Covariance Data Processed from ENDF/B-VII.1

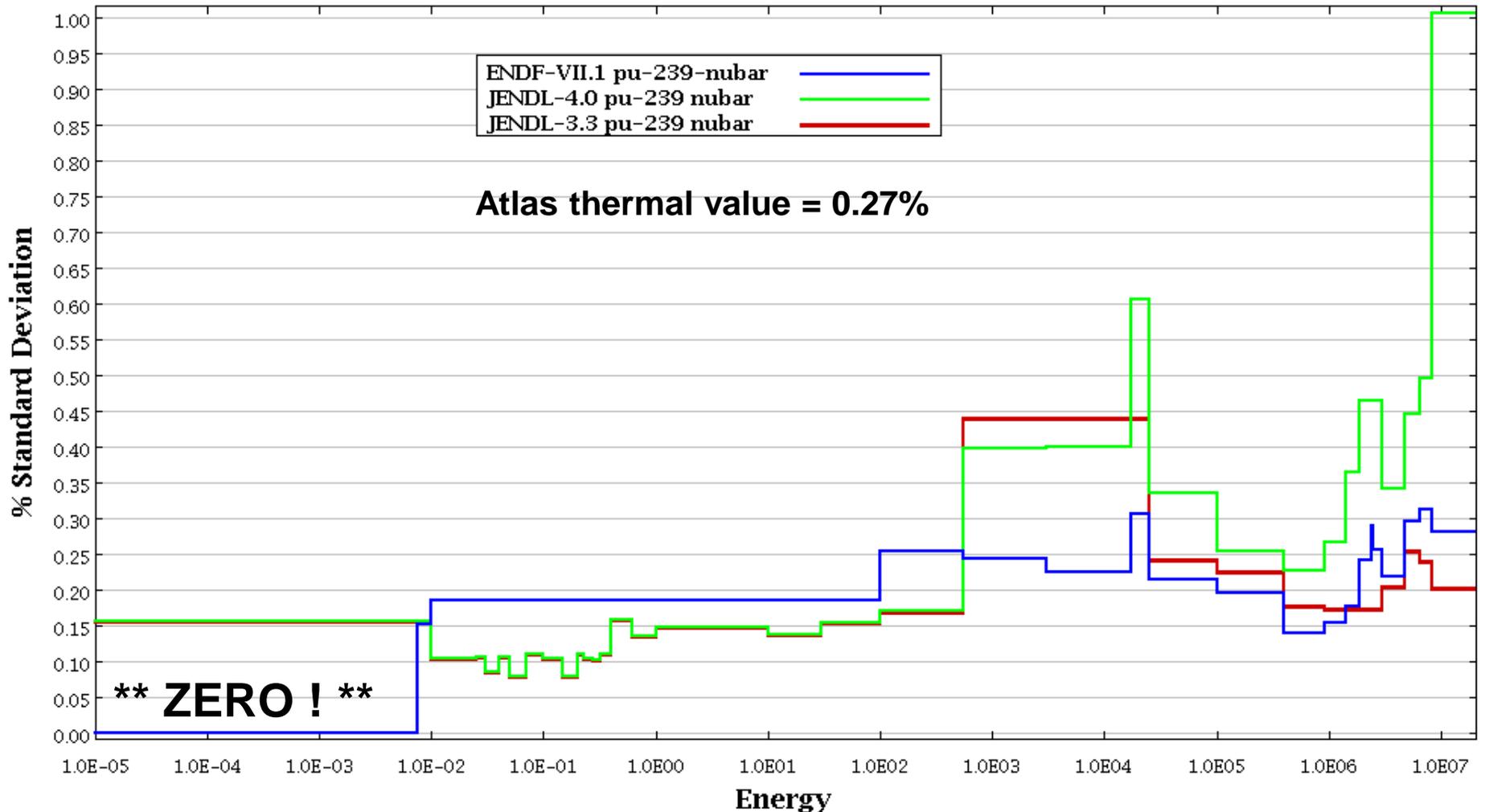
*Validation studies were performed for 320 benchmark experiments*

- Continuous energy (CE), 252g multigroup, and covariance data were processed using AMPX
- Critical eigenvalues computed with Keno Monte Carlo code using both 252g and CE data
- S/U calculations done with 252g TSUNAMI-3D (Keno) using:
  - ENDF-VII.1 covariance library
  - Modified ENDF-VII.1 library (“Mod covar”) with H capture uncertainty from SCALE-6.1 (Hale evaluation);  $^{235}\text{U}$  and  $^{239}\text{Pu}$  nubar uncertainties from JENDL

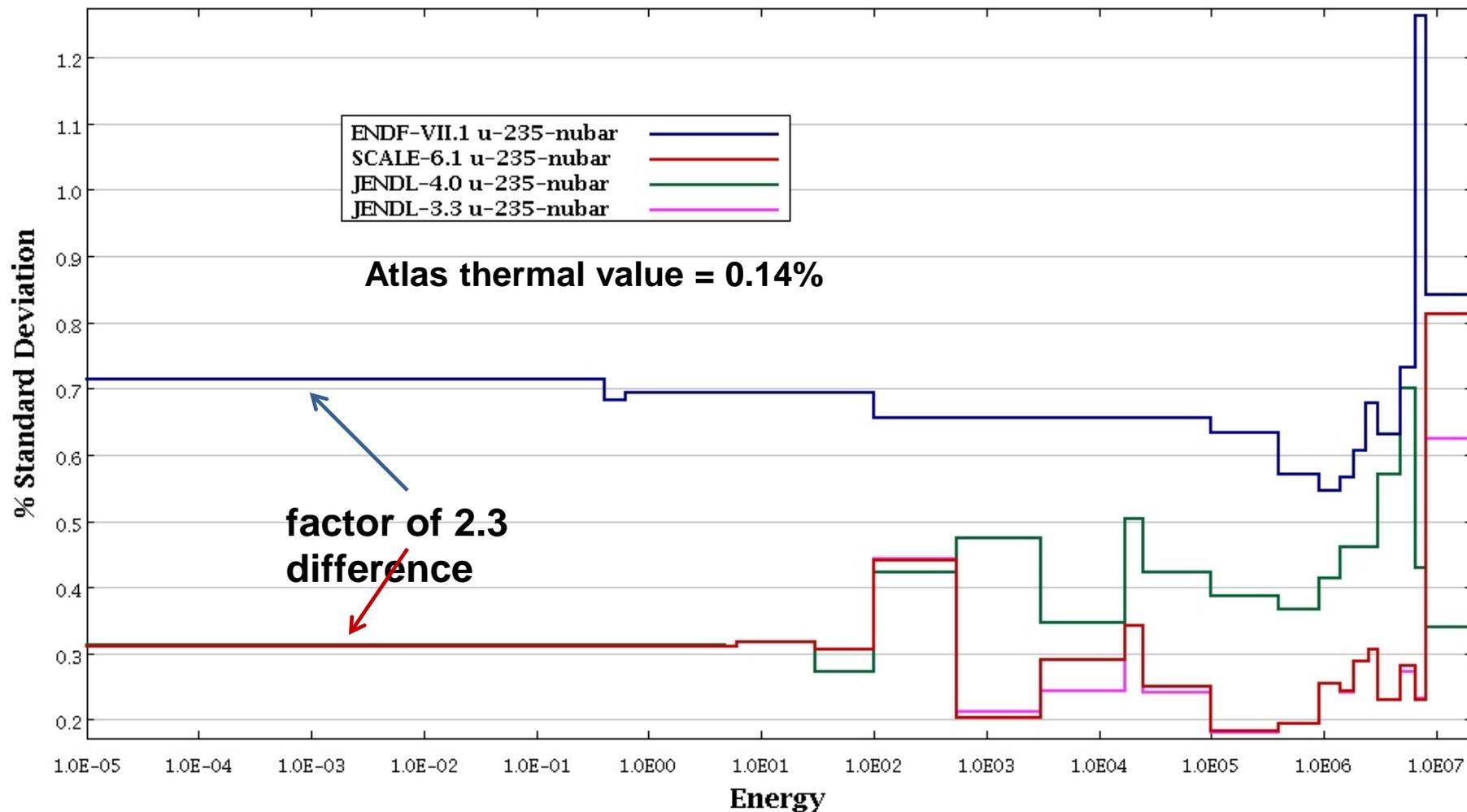
# H Capture Uncertainty (a problem)



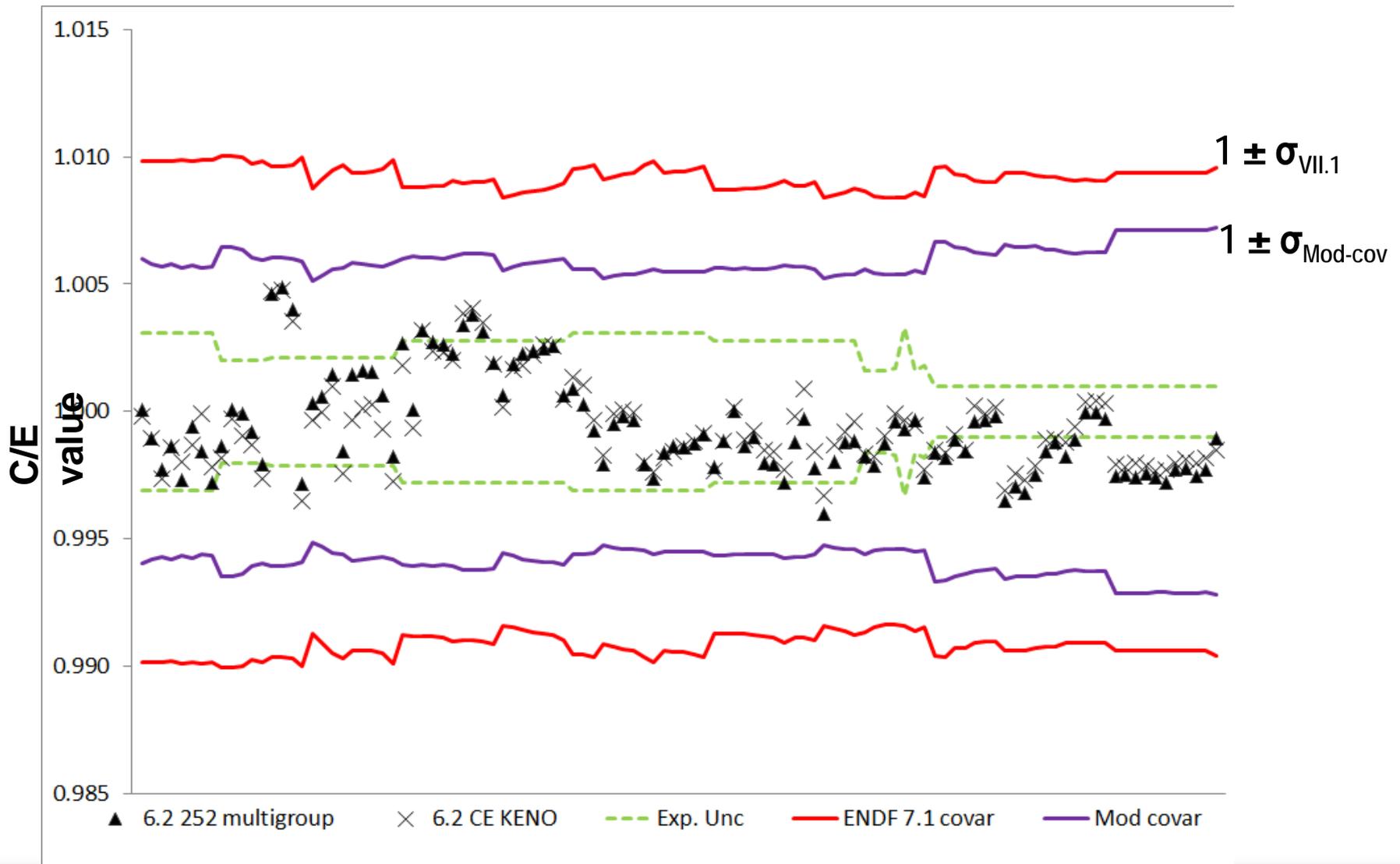
# Pu239 Nu-Bar Uncertainty (a problem)



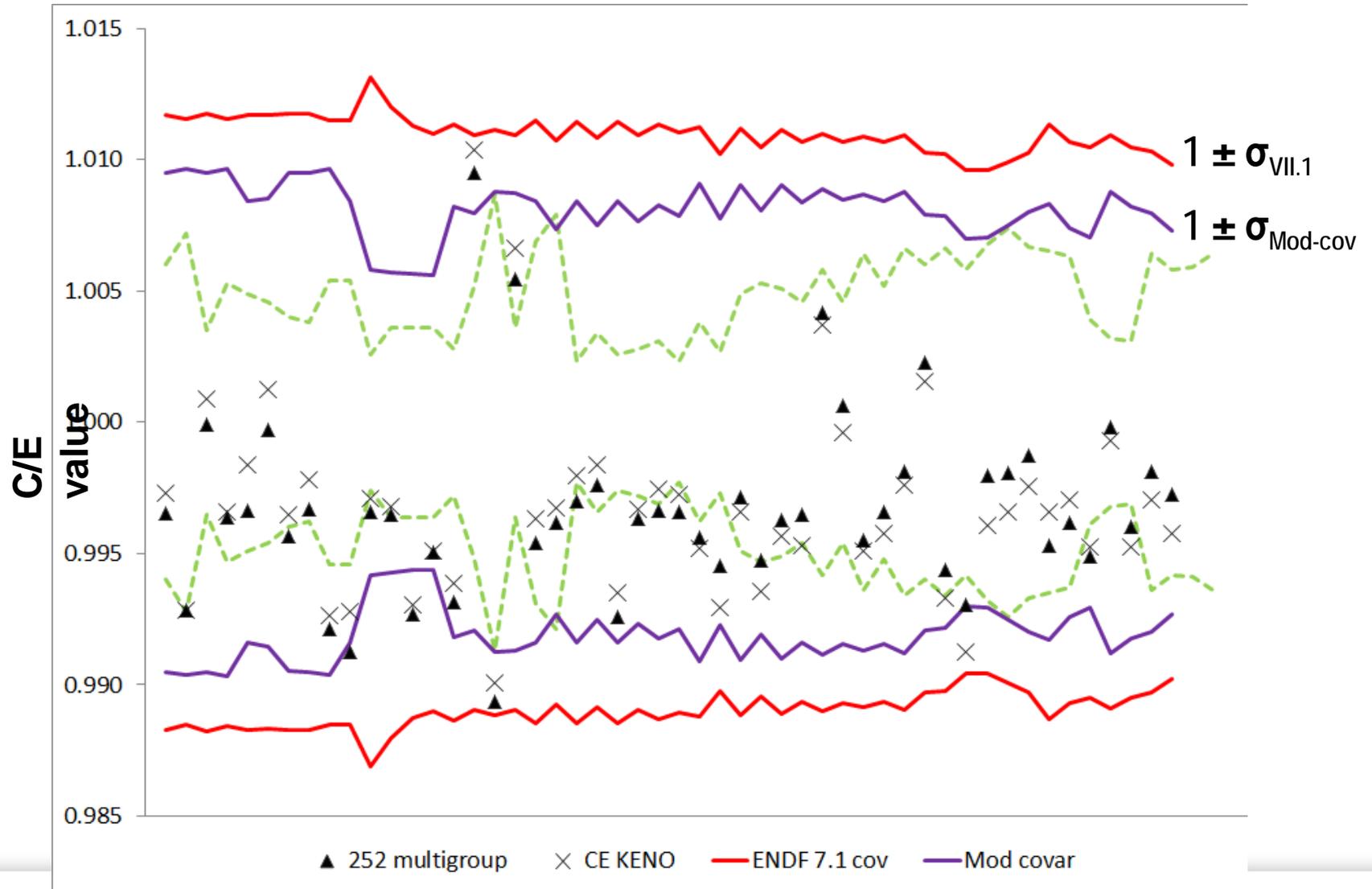
# U235 Nu-Bar Uncertainty (a problem)



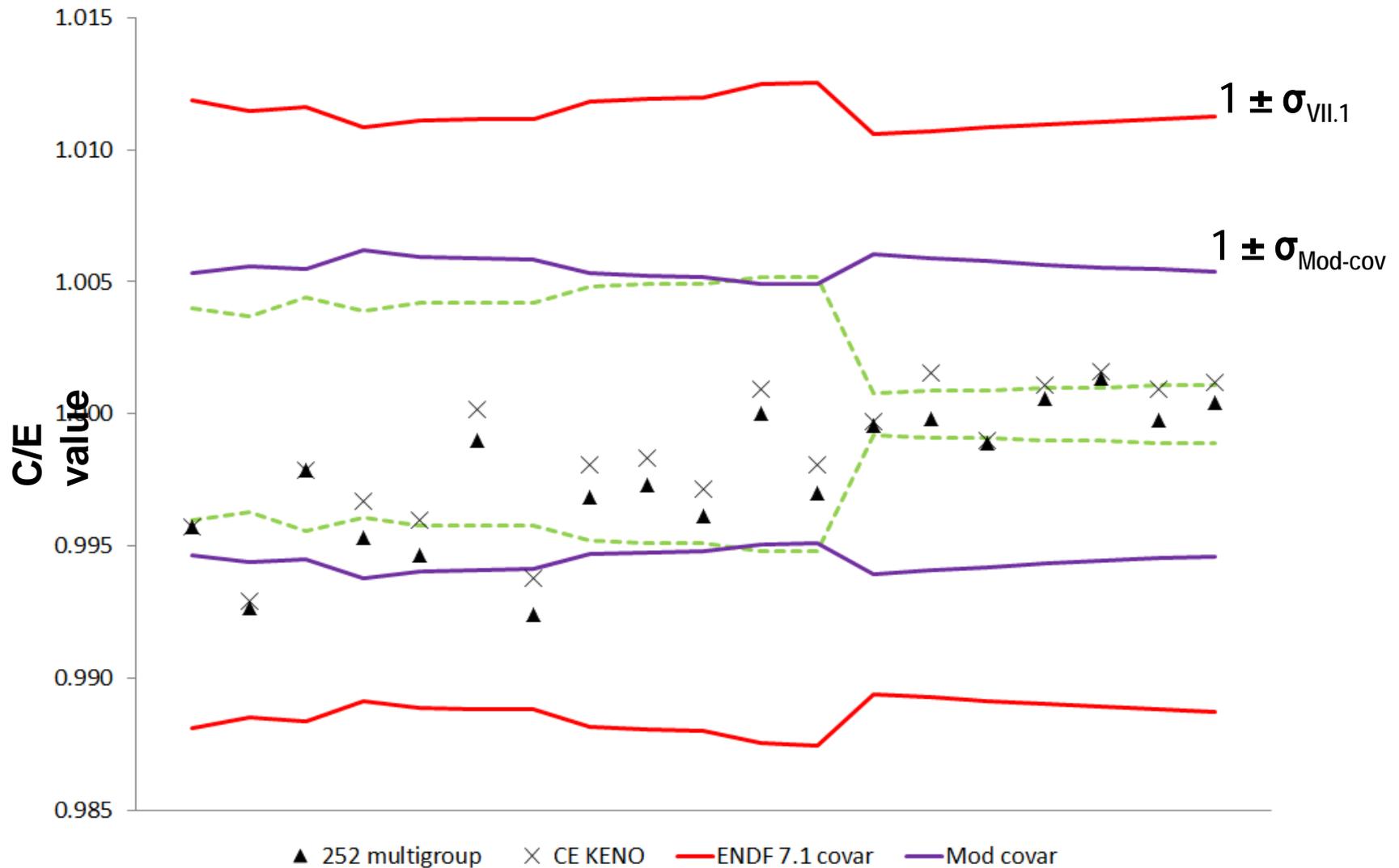
# Uncertainties for LEU-COMP-THERM Benchmarks



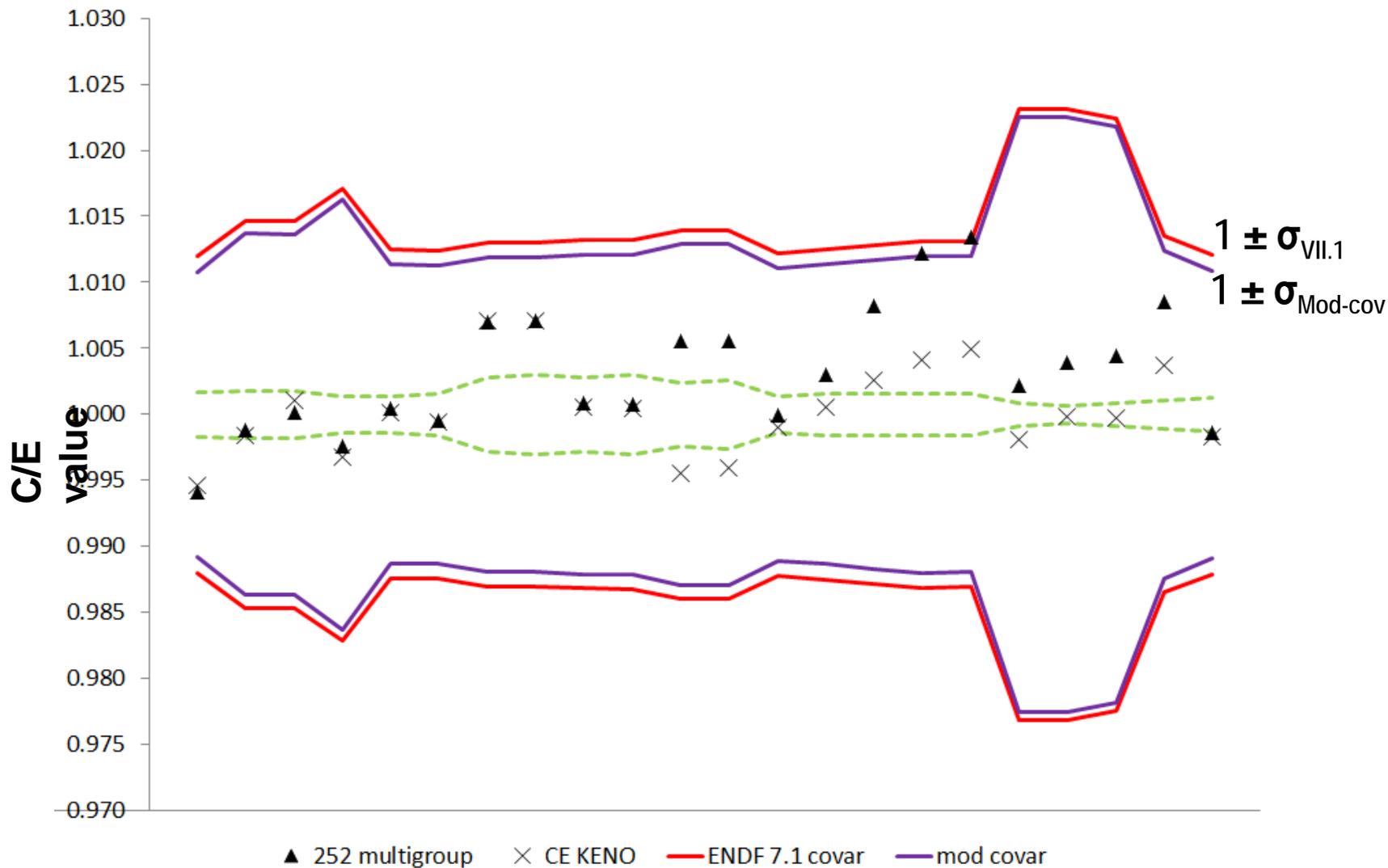
# Uncertainties for HEU-SOL-THERM Benchmarks



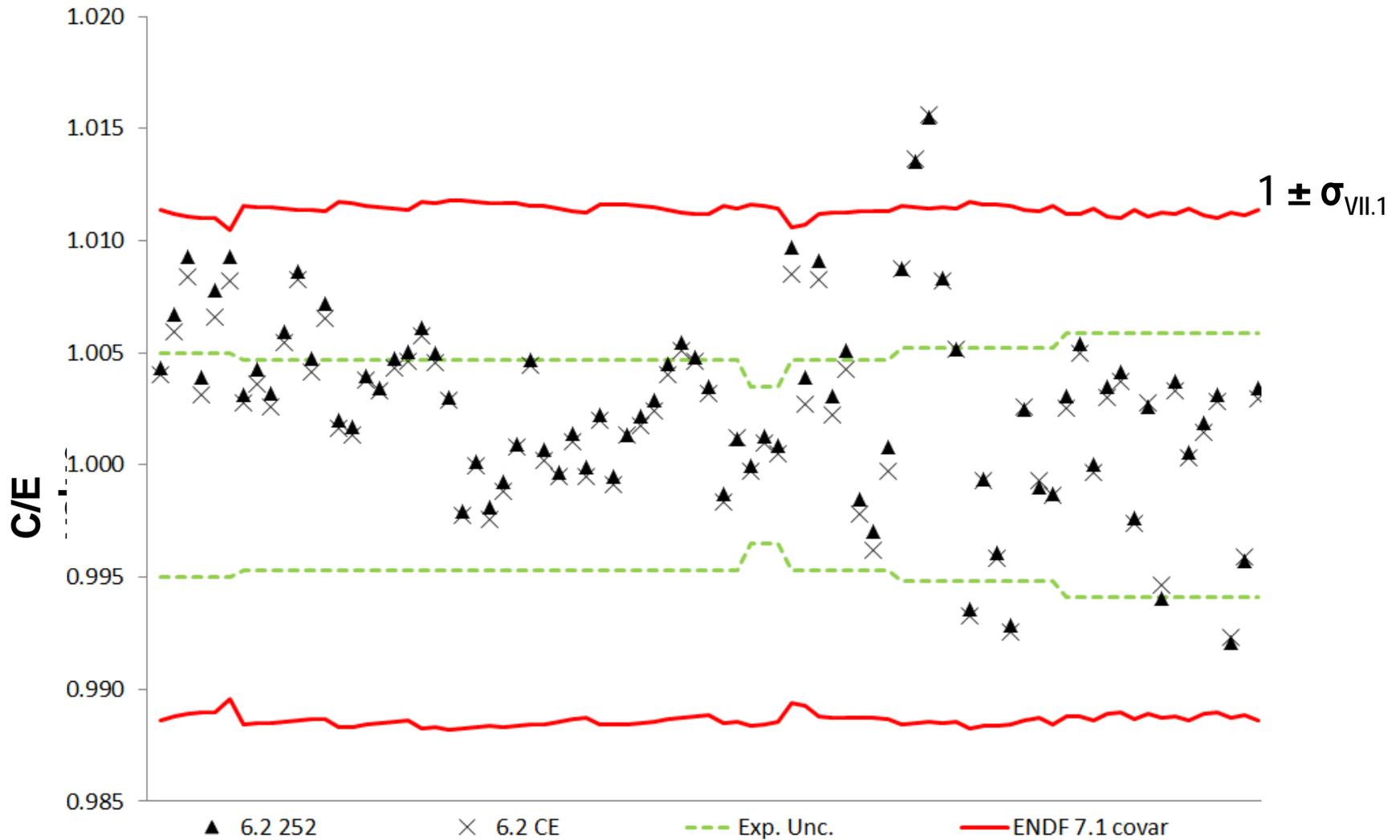
# Uncertainties for LEU-SOL-THERM Benchmarks



# Uncertainties for HEU-MET-FAST Benchmarks



# Uncertainties for PU-SOL-THERM Benchmarks



# Observed Standard Deviations are Less Than Predicted from Nuclear Data Covariances

Cases	St. Dev (pcm ) from C/E Values	St. Dev (pcm ) from S/U
HST	590	800
LST	259	556
LCT	185	583

# Results of ENDF/B-VII.1 Covariance Library Investigation—reported to CSEWG November 2013

- ENDF/B-VII.1 provides new covariance data for many nuclides—expands S/U capability
- Many VII.1 covariances are consistent with data in SCALE-6.1 library tested for applications
- Some problems seem to exist with  $^{235}\text{U}$  and  $^{239}\text{Pu}$  thermal nubar data
- H-1 thermal capture data has 5X larger uncertainty than SCALE-6.1, JENDL, and Atlas of Neutron Resonances
- Structure materials and fission products require further investigation
- Further investigation of ENDF/B-VII.1 is needed before moving to production use in SCALE

# Summary

- Significant progress in AMPX development and modernization
  - Converted AMPX build system to SCALE build system
  - Merged AMPX and SCALE repositories
  - Initiated AMPX module refactoring effort
    - Updated many of the foundation functionality to C++
    - Rewrote Y12 in C++ using the new foundation functionality
- Created CE and MG ENDF/VII.1 libraries using modernized, merged AMPX software
- Produced new CE and MG libraries for SCALE 6.2 based on ENDF/B-VII.1—testing in progress