

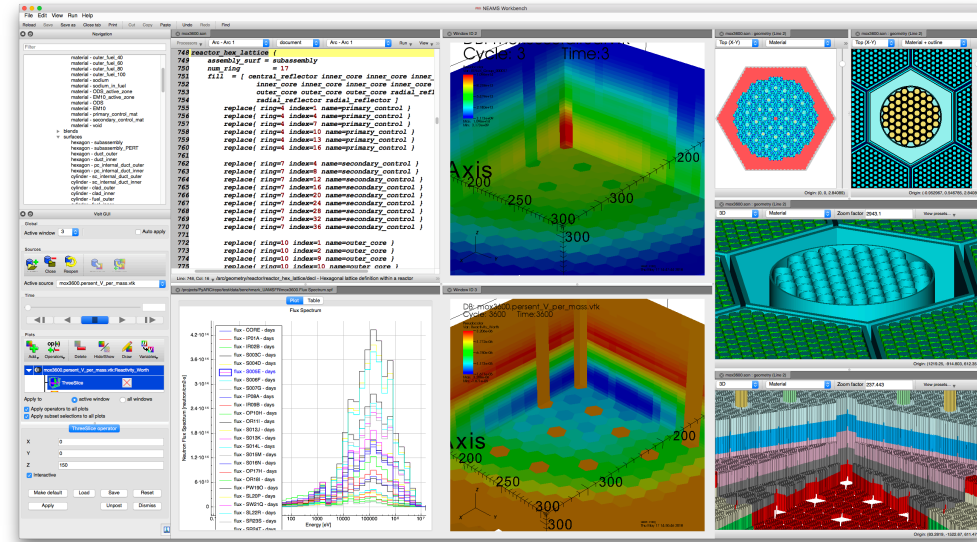
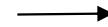
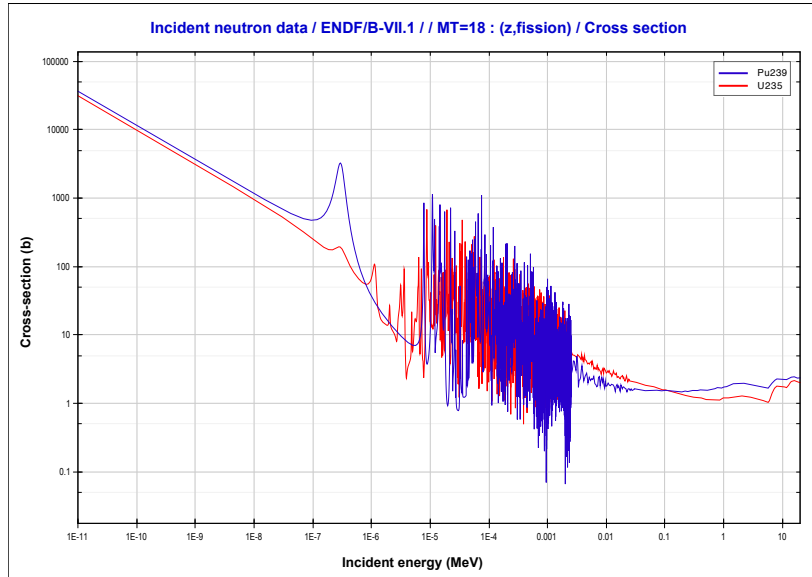
ENDF/B-VIII.0 Augmented Covariance Data

The first iteration

V. Sobes, B.J. Marshall, D. Wiarda
F. Bostelmann, A. Holcomb, B. T. Rearden

31st WPEC Meetings
24-28 June, 2019
NEA Headquarters
Boulogne-Billancourt, France

Nuclear data is necessary for reliable modeling and simulation of the next generation of nuclear reactors



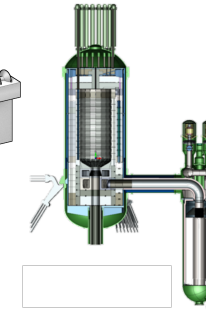
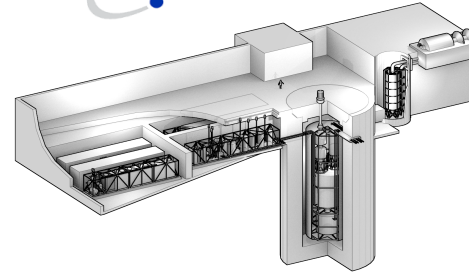
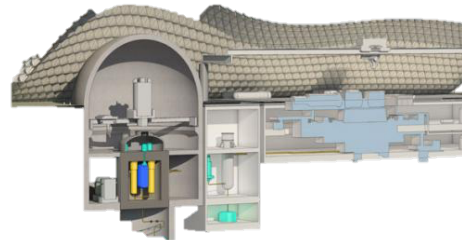
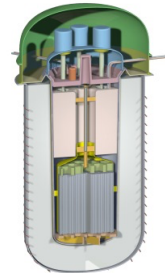
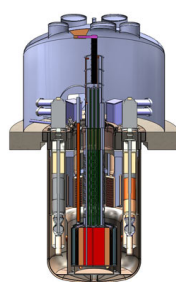
TerraPower

TERRESTRIAL ENERGY

TRANSATOMIC

Flibe ENERGY

Xenergy



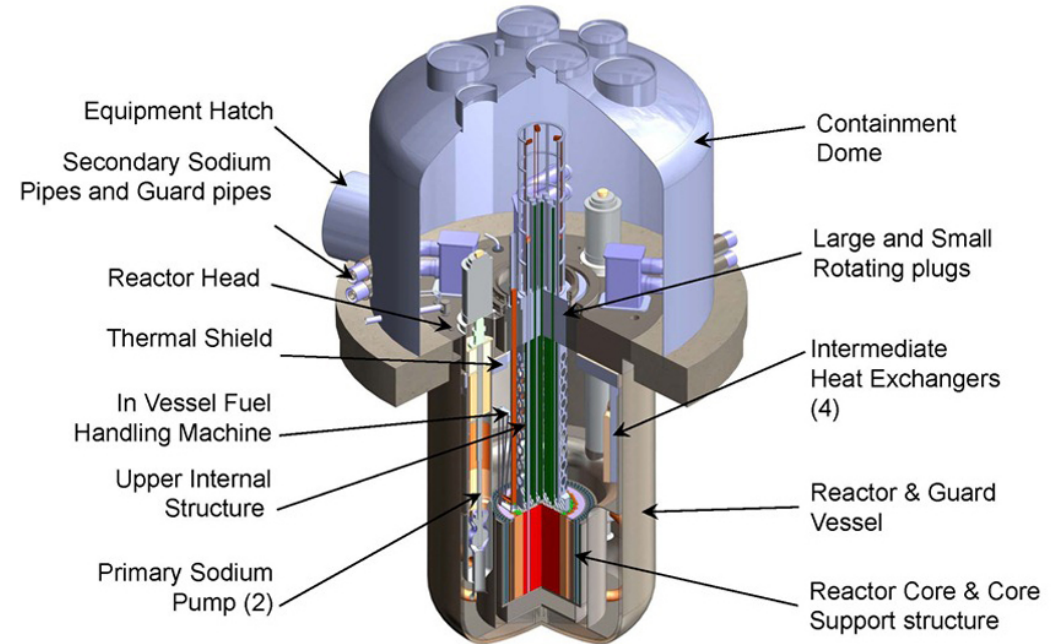
Nuclear data effecting reactor design (1/2)

Traveling Wave Reactor

Nuclear data uncertainty dominates:

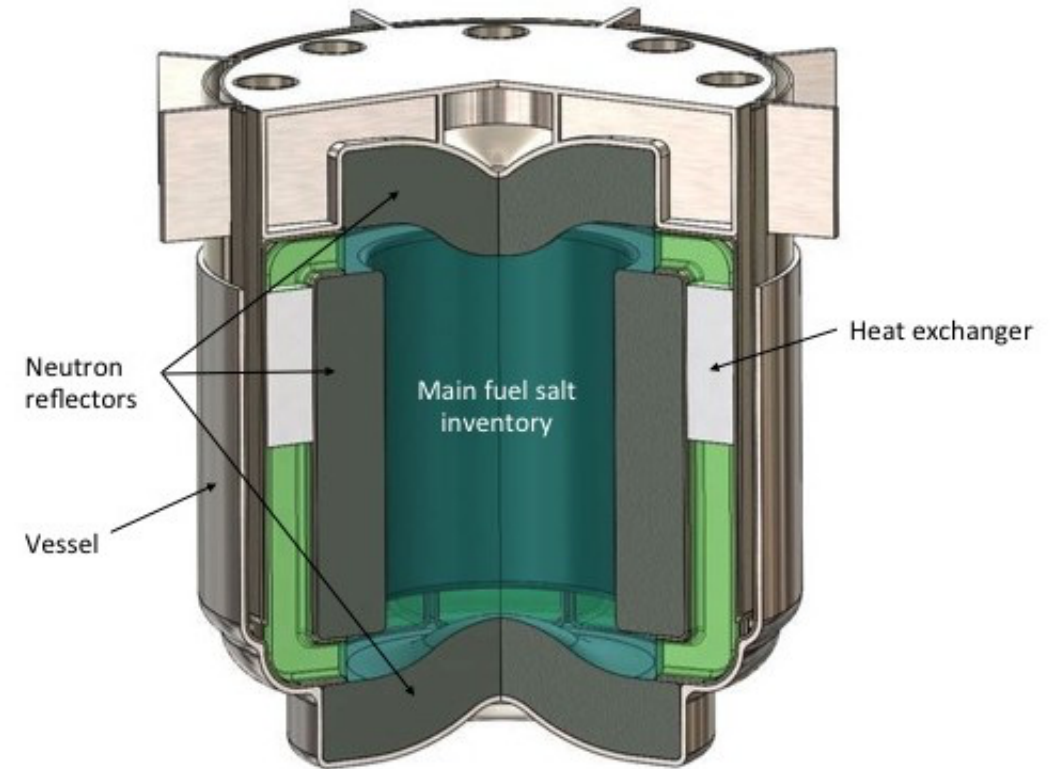
- Beginning-of-Life (BOL) k_{eff}
- Coolant temp. feedback
- Doppler feedback
- Control rod worth
- Void worth

Traveling Wave Reactor (TWR)



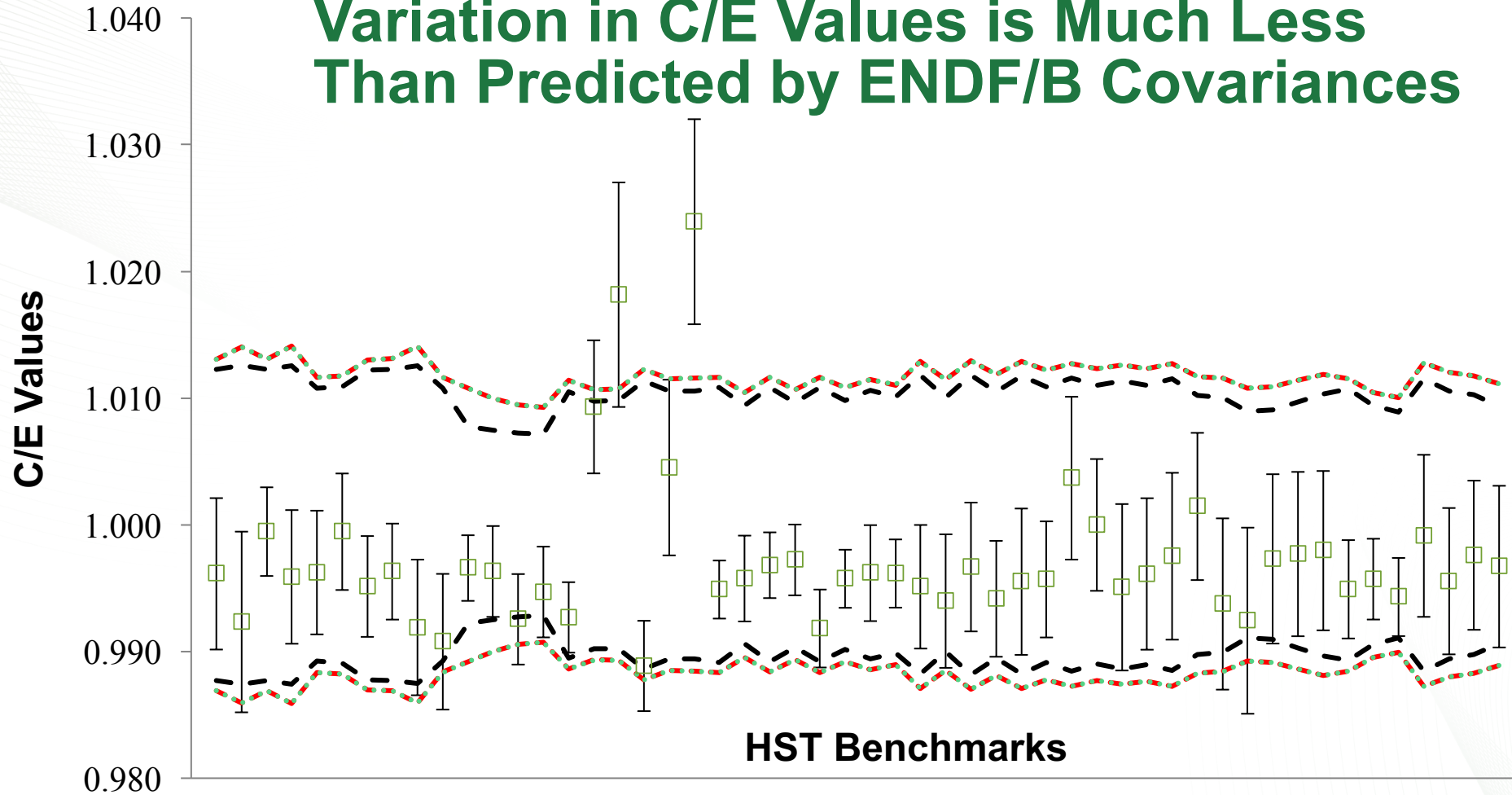
Nuclear data effecting reactor design (2/2)

Molten Chloride Fast Reactor



A change in absorption cross section of ^{35}Cl resulted in 2000 pcm change in BOL k_{eff}

Variation in C/E Values is Much Less Than Predicted by ENDF/B Covariances



- C/E
- - SCALE 6.2 Covariance Library
- - ENDF/B-VIII Beta 5 Covariance Library
- ENDF/B-VIII Beta 5 Covariance with SCALE 6.2

The response from the European nuclear data community to large propagated uncertainties



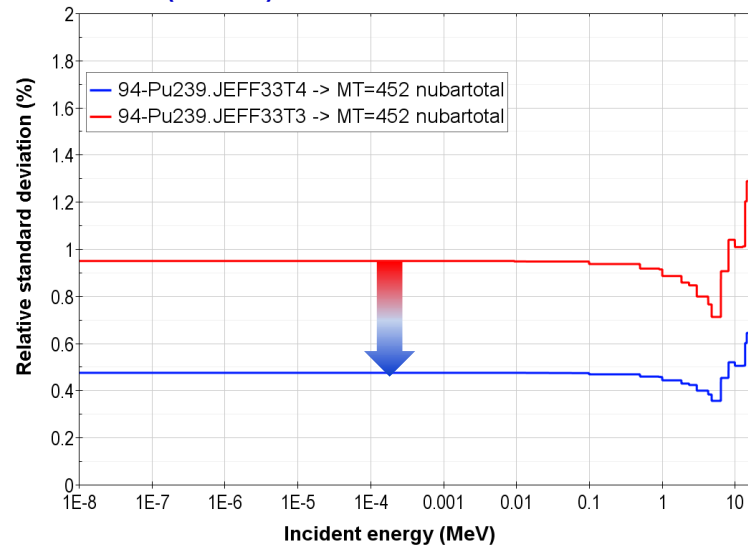
Nuclear Energy Agency



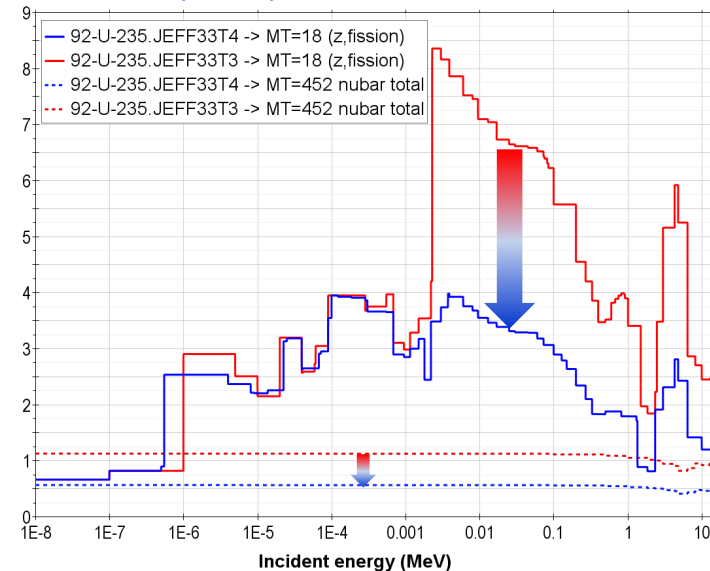
□ Differences between JEFF-3.3T4 and JEFF-3.3T3

- **JEFF-3.3T3**: uncertainty in the fast range was based on microscopic experiment only.
See files at: <http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T3/neutrons/>
- **JEFF-3.3T4**: reduced uncertainties to reflect adjustment (e.g. fast range to JEZEBEL).
See files at: <http://www.oecd-nea.org/dbdata/jeff-beta/JEFF33T4/neutrons/>

Incident neutron data // MAT9437 /
MT=452 : nubar total / Covariances data
(BOXER) Relative standard deviation

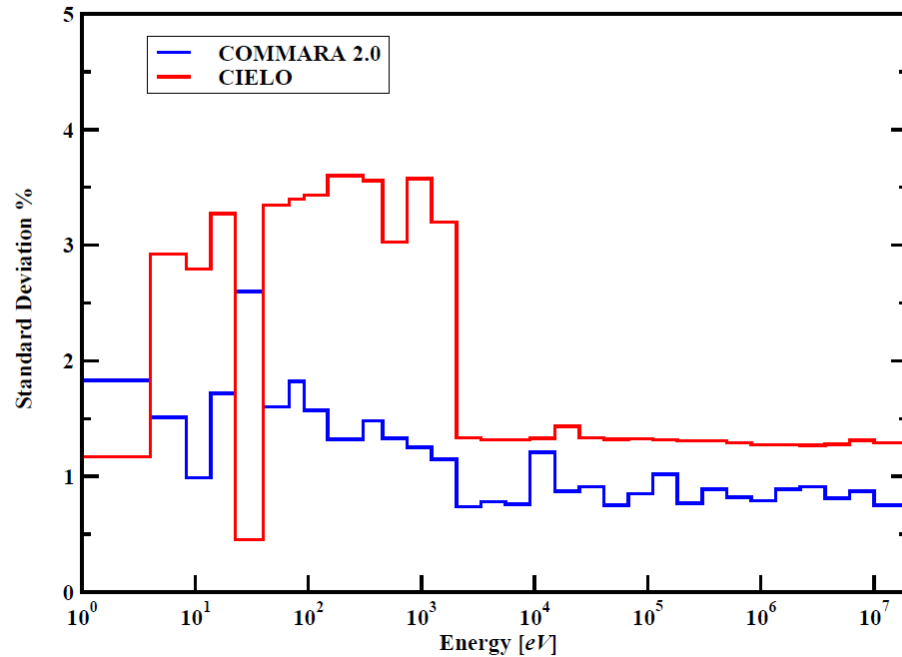


Incident neutron data // MAT9228 // Covariances
data (BOXER) Relative standard deviation

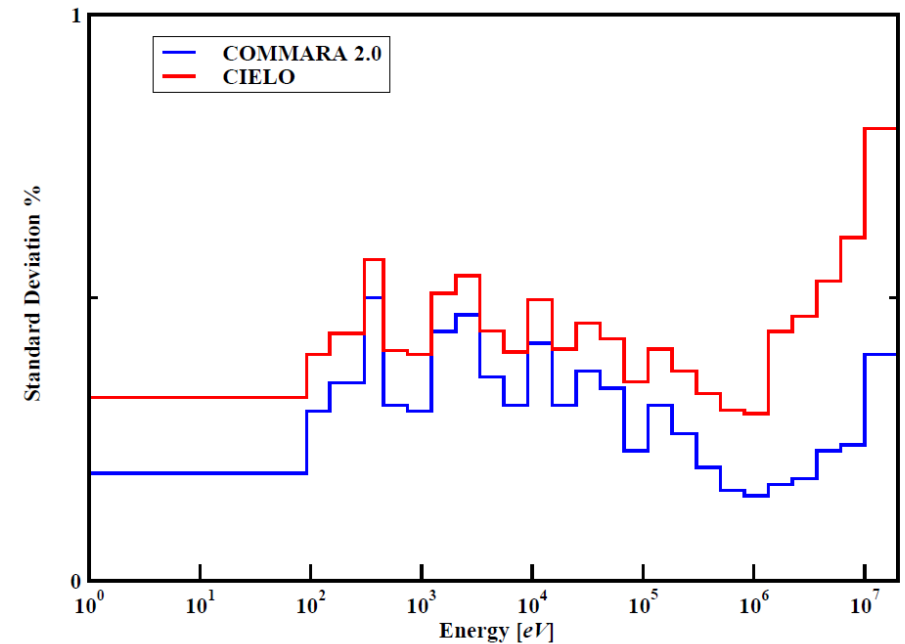


The US nuclear data community has (generally) increased uncertainties in the new library (red)

^{239}Pu σ Fission Standard Deviation %



^{239}Pu ν Bar Standard Deviation %



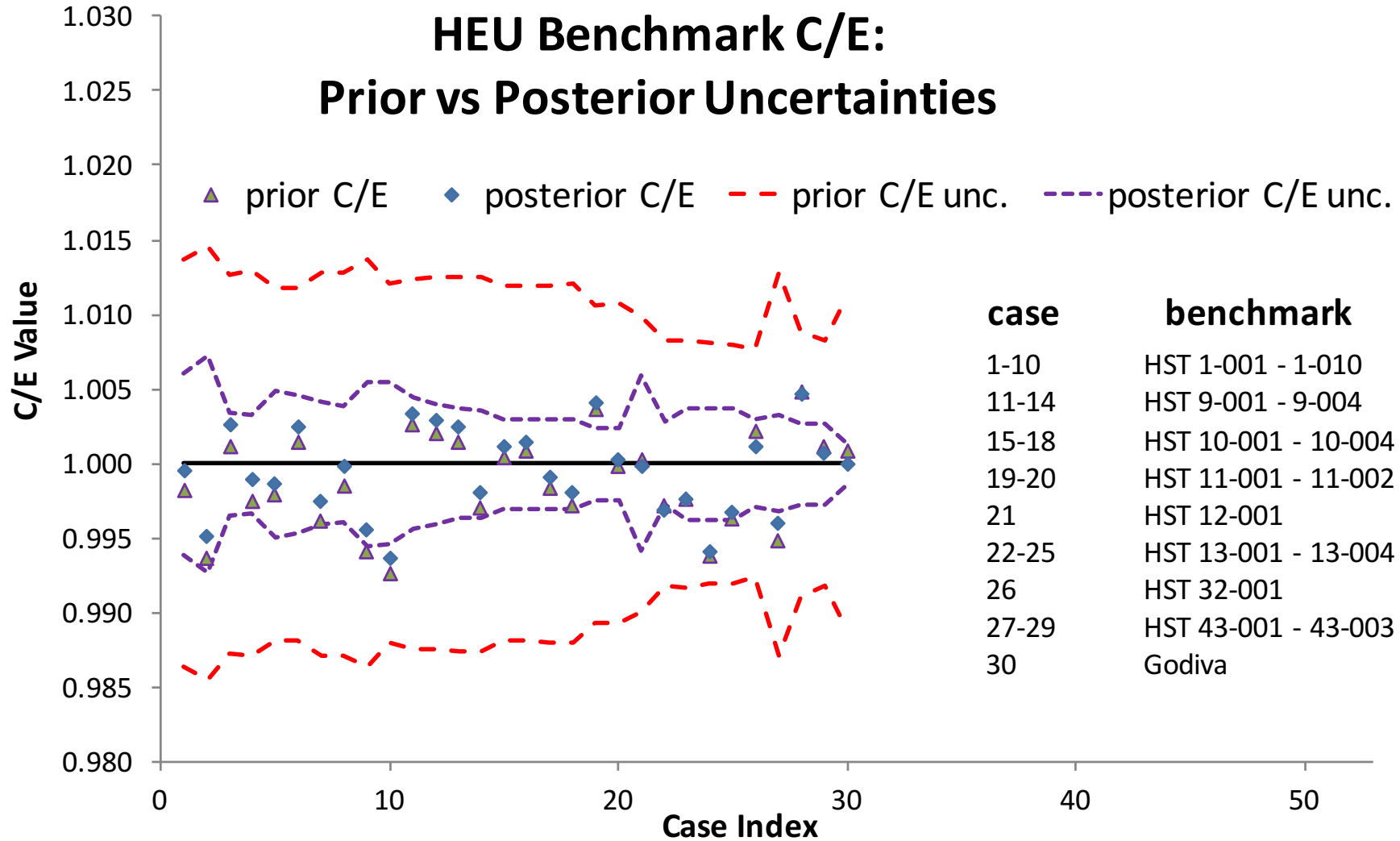
Slides from P. Palmiotti, WPEC 2018

The current official guidance from the US nuclear data center

Comments about the covariance in current ENDF evaluations

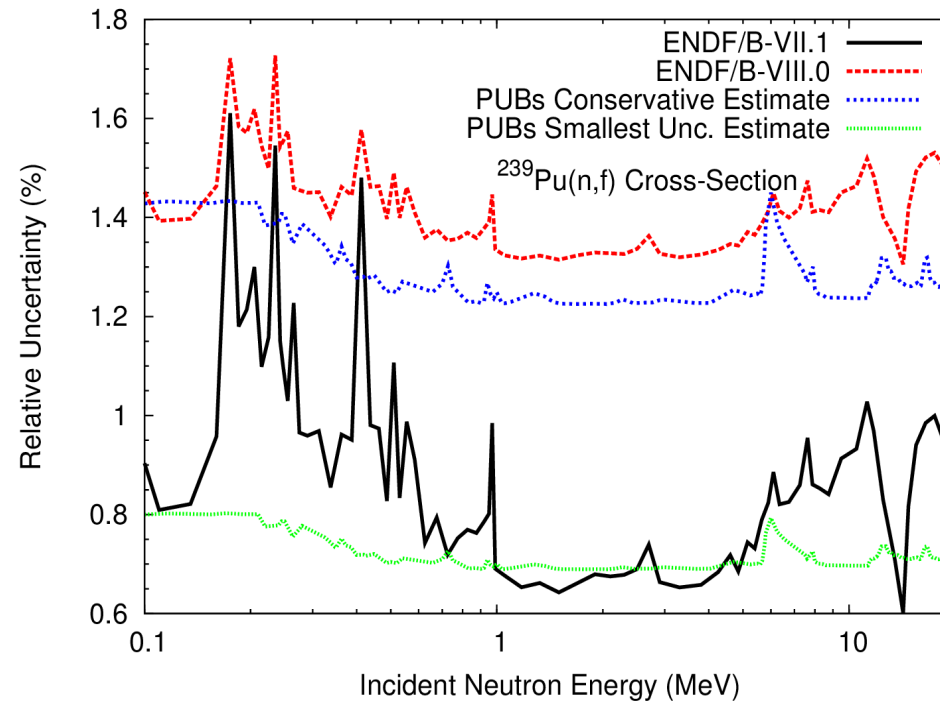
1. The covariance data in the ENDF evaluations represents uncertainties and correlations in differential data.
2. The use of this covariance to calculate uncertainties for integral quantities such as K_{eff} will **usually result in an overestimate of the uncertainty**. That said, comparisons to integral data are essential during the evaluation process and users should not be surprised if the *mean value* nuclear data allow for the accurate prediction of K_{eff} , **even if the covariances do not reflect this consideration**.
3. The recommended methodology to overcome this problem is to adjust the covariance to add information from set of integral data that represents the physics of the system for which the adjusted covariance will be used.
4. More information on this topic: <https://www.oecd-nea.org/science/wpec/sg33/>
5. **CSEWG is currently studying the best covariance representation for future releases.**

HEU Benchmark C/E: Prior vs Posterior Uncertainties



There are minimum bounds on realistic uncertainty estimates and adjustment methodologies often violate these

(5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.



PUBs: Physical Uncertainty Boundaries

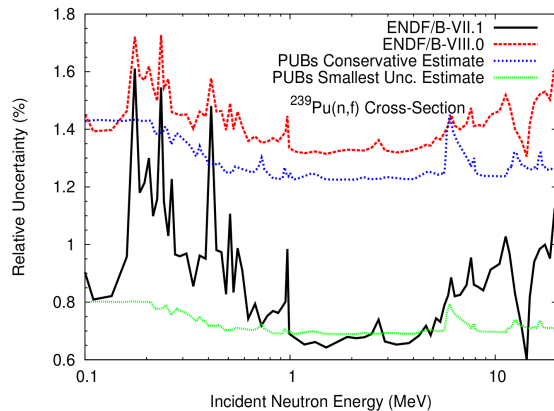
UNCLASSIFIED

Slide

The problem of too small uncertainties on differential data and too large uncertainties on integral data

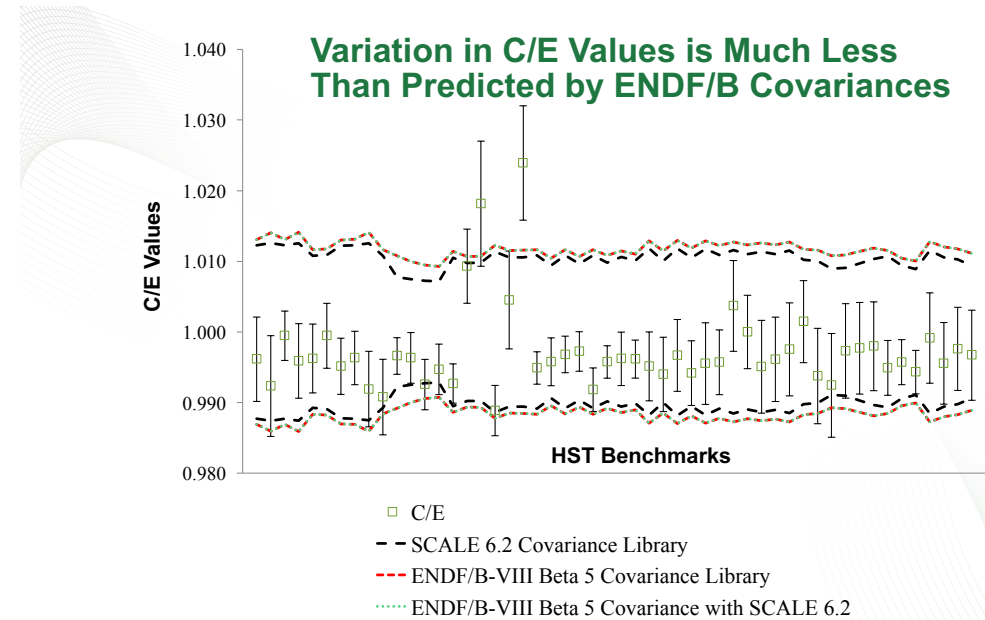
Nuclear data uncertainties are in danger of being smaller than what can be measured experimentally

(5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.



Slide from of D. Neudecker, WPEC 2018

Nuclear data uncertainties are too large to reflect how well we actually know critical systems



Slide from of M. Williams, CSEWG 2017

Have your cake and eat it too: solving the discrepancy with nuclear data correlations

We cannot experimentally measure nuclear data to precision below 1%,

$$\delta\bar{\nu} > 1\%, \quad \delta\sigma_f > 1\%$$

But, only 1% uncertainty in $\bar{\nu}$ results in 1% uncertainty in k_{eff} (more than \$1 of reactivity),

$$k_{\infty} = \frac{(\bar{\nu} \pm 1\%) \Sigma_f}{\Sigma_a} \rightarrow 1\% \text{ uncertainty in } k_{\infty}$$

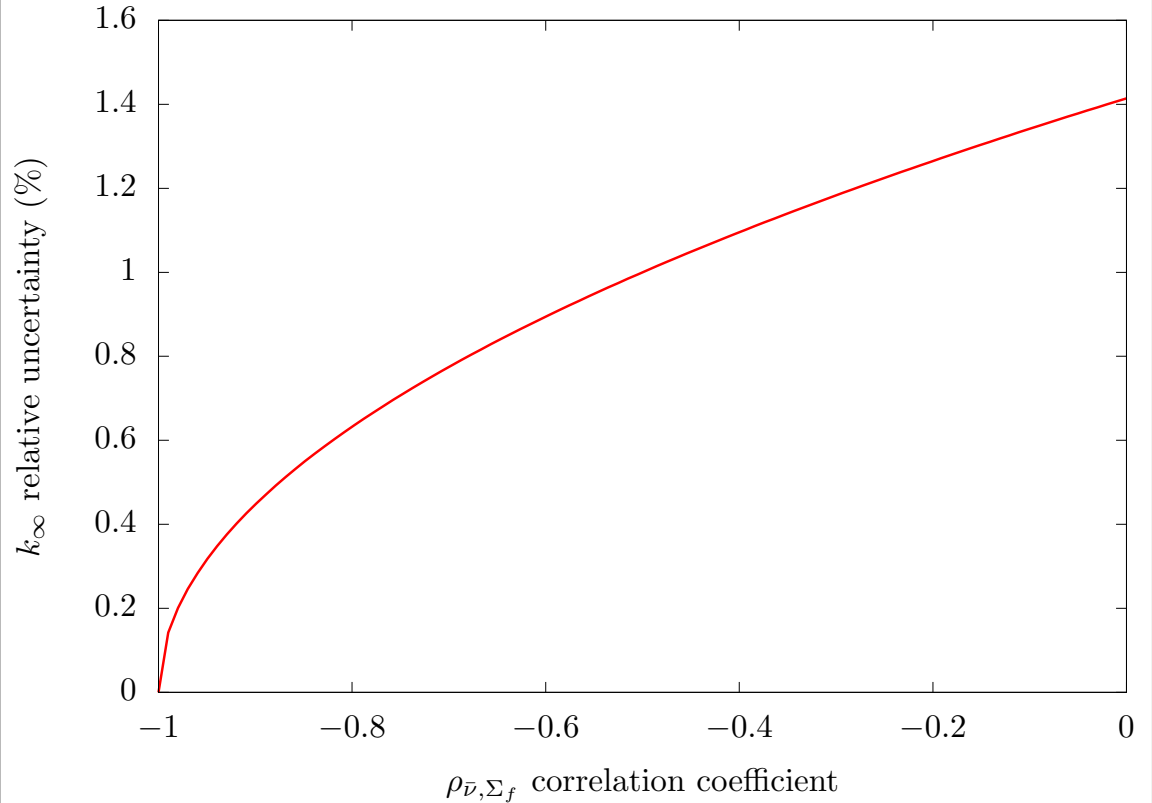
However, the ability to predict k_{eff} with better accuracy than 1% **does not imply** the knowledge of the cross sections to better than 1%.

It only says that we know the integral of the cross sections (in the appropriate spectra) to better than 1%.

Have your cake and eat it too: solving the discrepancy with nuclear data correlations

- A negative correlation coefficient between multiplicative terms allows you to keep realistic uncertainties for differential nuclear data which will propagate to realistic uncertainties on integral applications.
- Example:

$$k_{\infty} = \frac{\bar{\nu} \Sigma_f}{\Sigma_a}, \quad \frac{\delta \bar{\nu}}{\bar{\nu}} = 1\%, \quad \frac{\delta \Sigma_f}{\Sigma_f} = 1\%$$



$$\frac{\delta k_{\infty}}{k_{\infty}} = \sqrt{\left(\frac{\delta \bar{\nu}}{\bar{\nu}}\right)^2 + \left(\frac{\delta \Sigma_f}{\Sigma_f}\right)^2 - 2\rho_{\bar{\nu}, \Sigma_f} \left(\frac{\delta \bar{\nu}}{\bar{\nu}}\right) \left(\frac{\delta \Sigma_f}{\Sigma_f}\right)}$$

- The discrepancy comes from non-systematic treatment
- The solution will be non-systematic, (no one mathematical equation)
- However, **I promise** to
 1. Document exactly what is done, therefore, everything will be reproducible
 2. Test and iterate with the nuclear data community and users



Philosophy

1. 20/80 rule, start with only on the most impactful cross-correlations
2. Augment the ENDF/B-VIII.0 covariance matrix (not adjust)
3. Estimate the bulk correlation coefficient (coarse group structure)

Realization

1. $^{239}\text{Pu}, ^{235}\text{U}, ^{238}\text{U} \sigma_{fis} - \bar{\nu}$
2. Only add new cross-correlations, do not adjust variances or existing correlations
3.

Fast group	20 MeV - 50 keV*
Inter. group	50 keV - 0.625 eV
Thermal group	0.625 eV - 10^{-5} eV

The goal of the first iteration was not to “solve” the problem outright, but to show conservative progress in the right direction

*Selected to match the boundary of the SCALE 56-group structure

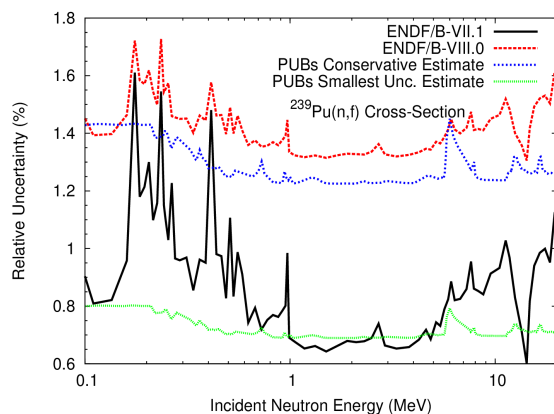
1. Use GLLS TSURFER to do global nuclear data adjustment to ICSBEP in VALID
2. Extract posterior cross-correlations, ignore posterior variance
3. Show that bulk cross-correlations are only weakly dependent on choice of integral system



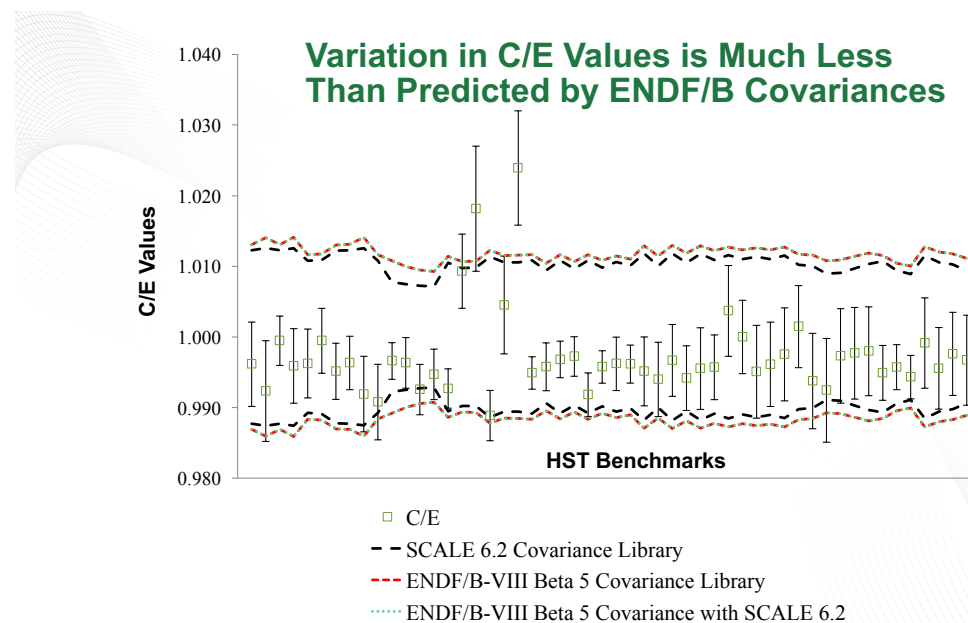
The problem of too small uncertainties on differential data and too large uncertainties on integral data

TSURFER GLLS forces the propagated posterior uncertainty to equal the spread in C/E data through a reduction of the variances and all posterior cross-correlations. We only take the reduction in variance due to a small subset of cross-correlations.

(5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.



Slide from of D. Neudecker, WPEC 2018



Slide from of M. Williams, CSEWG 2017

Philosophy

1. 20/80 rule
2. Do not change uncertainty on differential data
3. Include benchmarks beyond ICSBEP (e.g. shielding and transmission)
4. Iterate with testing community frequently. Increase the number of cross-correlations and fidelity in energy domain.
5. Do not aspire to reduce propagated uncertainty to level of C/E discrepancy in integral data

Realization

1. Prioritize work on only the most impactful cross-correlations. The vision is not to have a full covariance matrix for the library
2. Only add cross-correlations, do not adjust variances
3. Collaboration with community
4. Test that uncertainty on “unstudied” integral systems is not significantly reduced
5. Reduce uncertainty as possible by realistic estimation of “generic” cross-correlations independent of integral system

$^{239}\text{Pu } \sigma_{fis} - \bar{\nu}$

PU-SOL-THERM (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-1	-2	-2
fission thermal	-7	-10	-10
PU-SOL-THERM (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-2	-3	-3
fission thermal	-9	-15	-16
MIX-COMP-FAST			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-4	-5	-5
fission thermal	N/A	N/A	N/A
MIX-SOL-THERM (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-2	-3	-3
fission thermal	-8	-13	-14
MIX-SOL-THERM (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-3	-4	-4
fission thermal	-11	-17	-18
MIX-COMP-THERM (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-3	-5	-5
fission thermal	-4	-7	-7
MIX-COMP-THERM (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-4	-5	-5
fission thermal	-6	-10	-11
All cases in VALID containing plutonium			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission intermediate	-3	-3	-3
fission thermal	-7	-10	-10

$$^{235}\text{U } \sigma_{fis} - \bar{\nu}$$

INTER-MET-FAST (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-33	-37
fission intermediate	-28	-20	-23
fission thermal	-38	-26	-30
INTER-MET-FAST (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-34	-38
fission intermediate	-28	-20	-23
fission thermal	-39	-27	-31
LEU-COMP-THERM (single experiment from each benchmark series)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-10	-8	-13
fission intermediate	-24	-17	-32
fission thermal	-23	-13	-36
LEU-COMP-THERM (all experiments)			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-9	-9	-11
fission intermediate	-23	-18	-30
fission thermal	-23	-13	-36

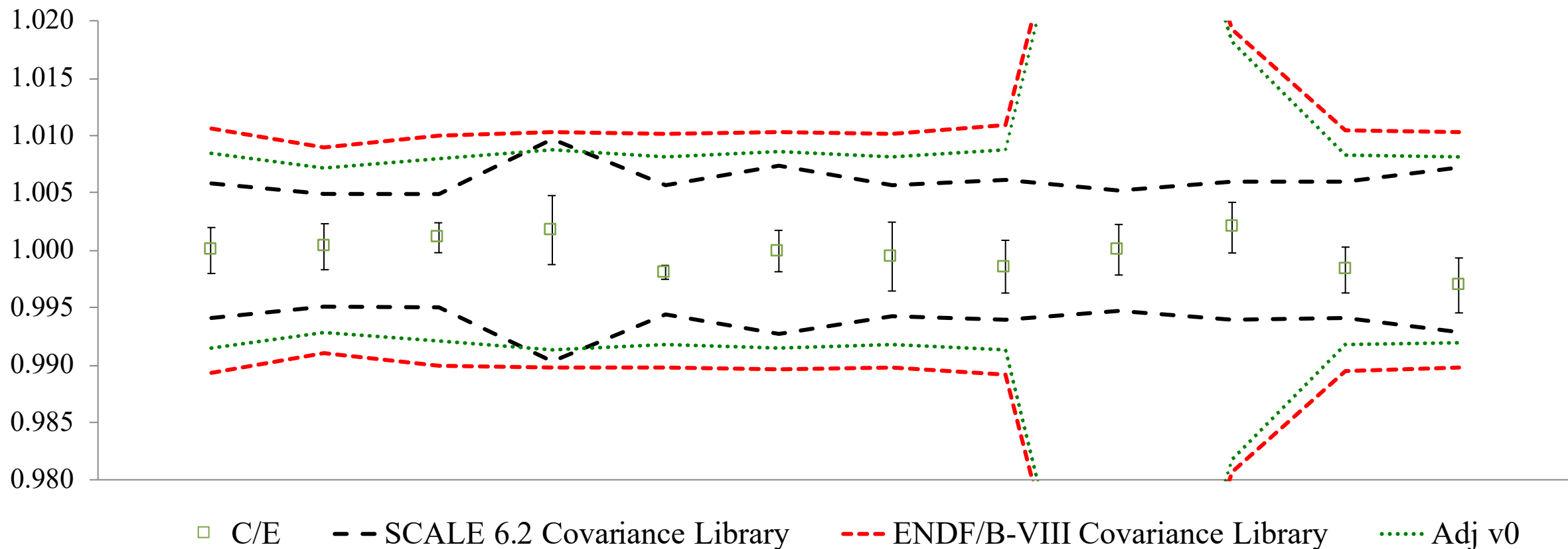
$$^{238}\text{U} \sigma_{fis} - \bar{\nu}$$

HEU-MET-FAST: single experiment from each benchmark series	-5
HEU-MET-FAST: all experiments	-5
INTER-MET-FAST: single experiment from each benchmark series	-5
INTER-MET-FAST: all experiments	-5
LEU-COMP-THERM: single experiment from each benchmark series	-4
LEU-COMP-THERM: all experiments	-12
MIX-COMP-FAST	-3
All uranium-containing cases	-6

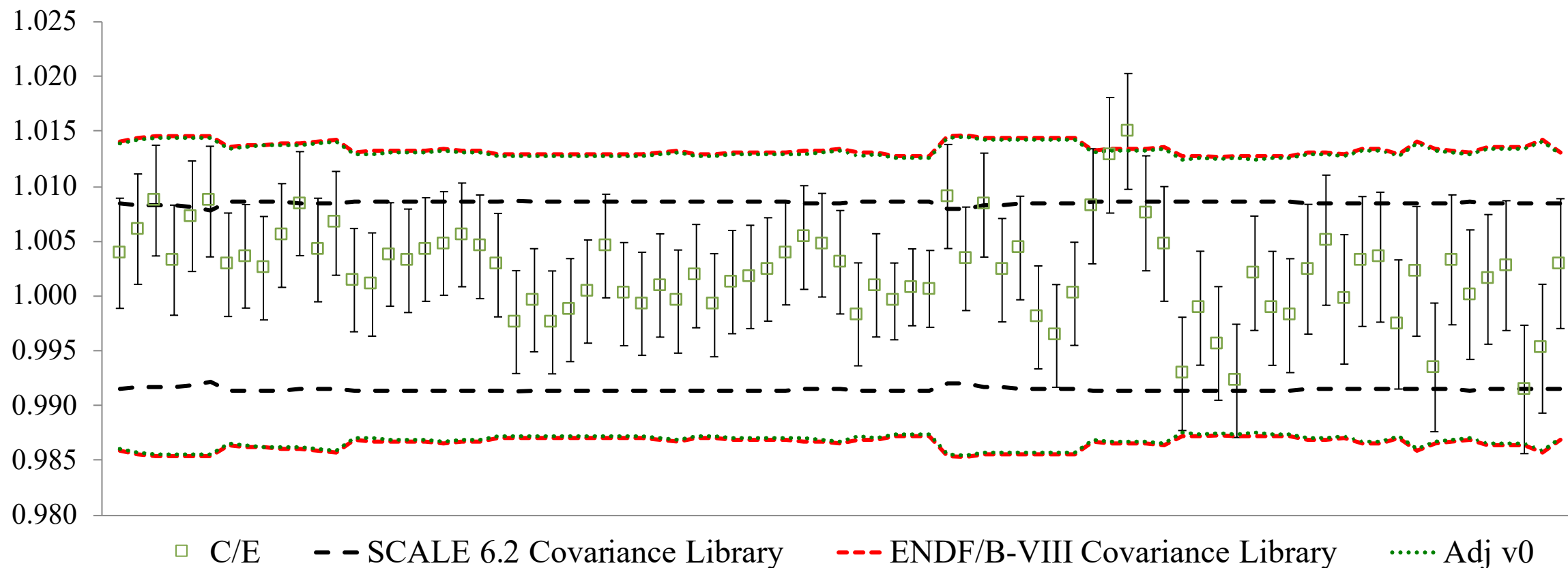
First iteration: estimated cross-correlations

²³⁹ Pu			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-53	-33	
fission intermediate	-1	-2	-2
fission thermal	-7	-10	-11
²³⁵ U			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-46	-33	-13
fission intermediate	-28	-20	-32
fission thermal	-38	-26	-33
²³⁸ U			
	nu-bar fast	nu-bar intermediate	nu-bar thermal
fission fast	-5		
fission intermediate			
fission thermal			

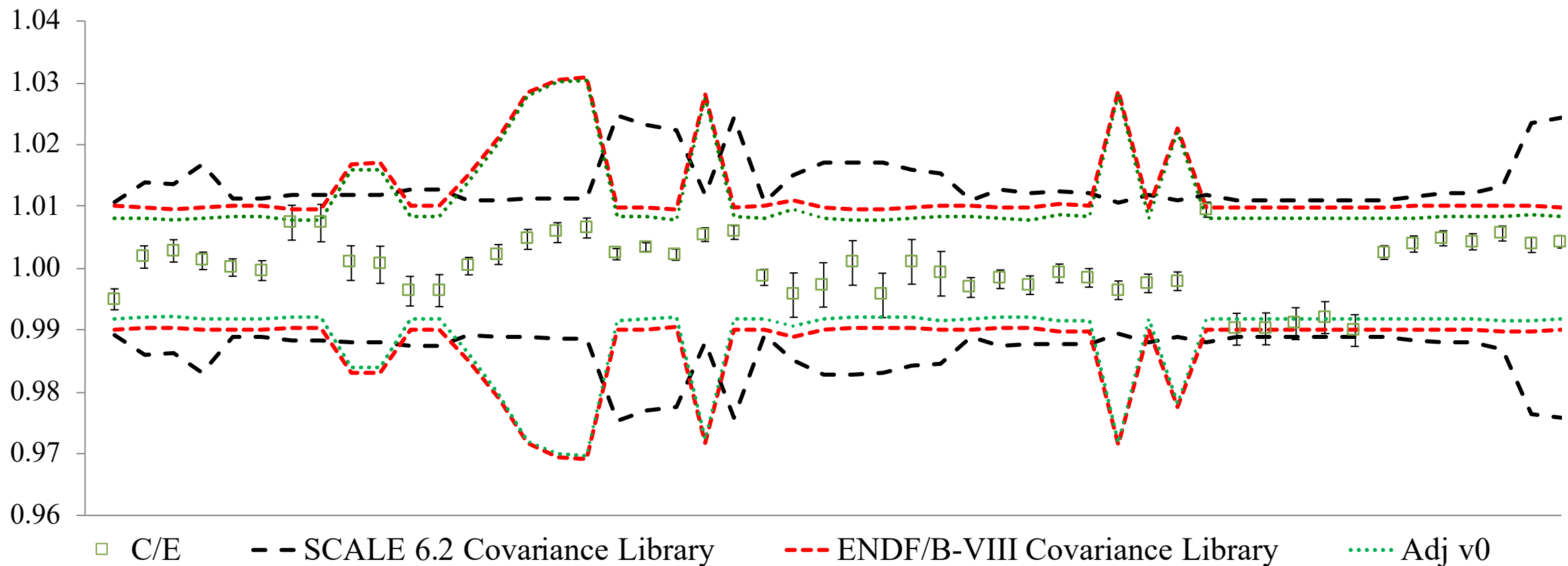
Results for PU-MET-FAST systems



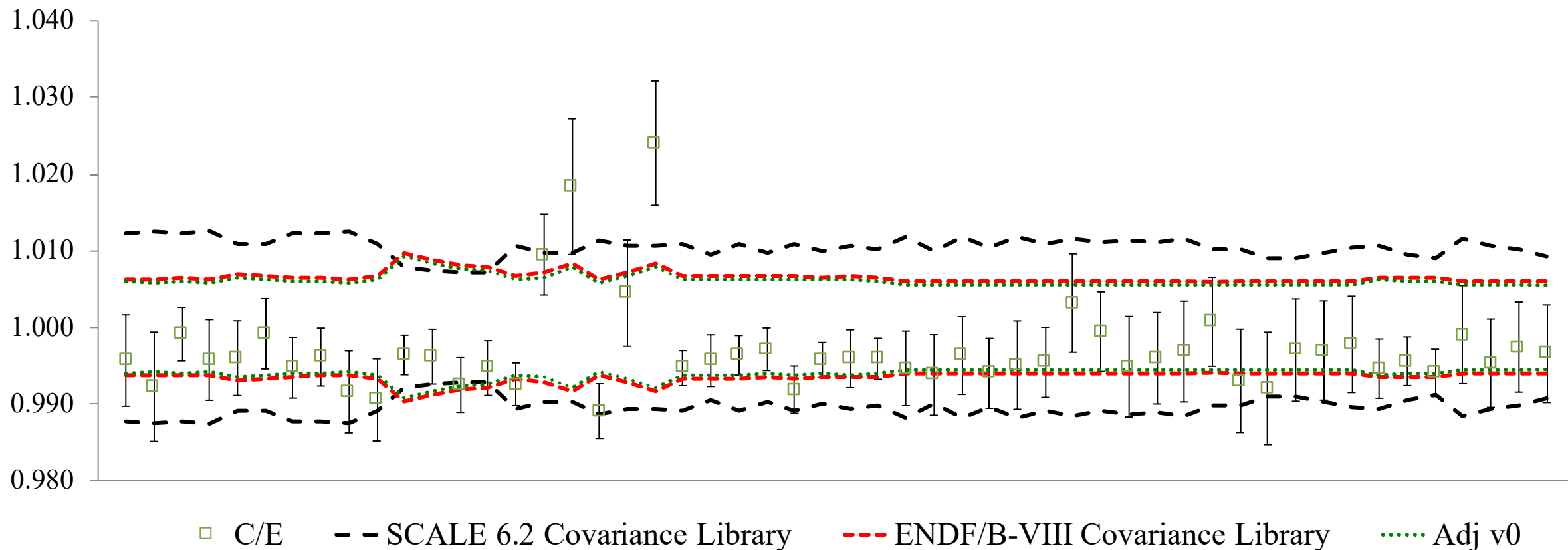
Results for PU-SOL-THERM systems



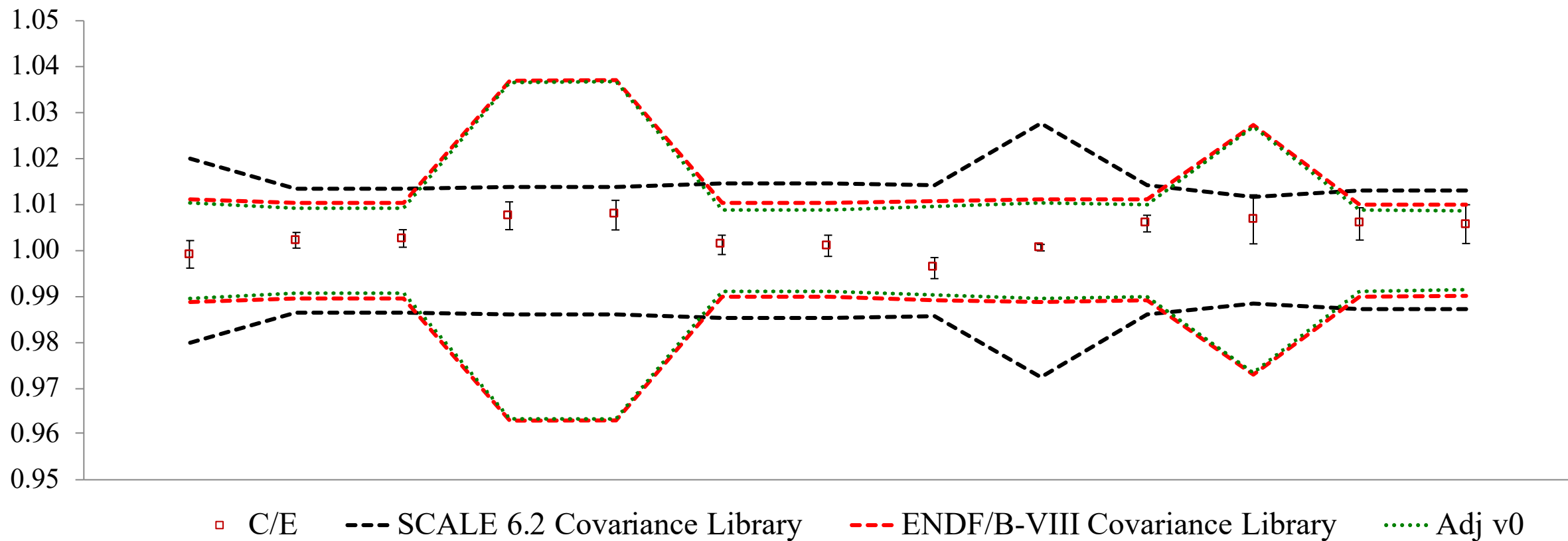
Results for HEU-MET-FAST systems



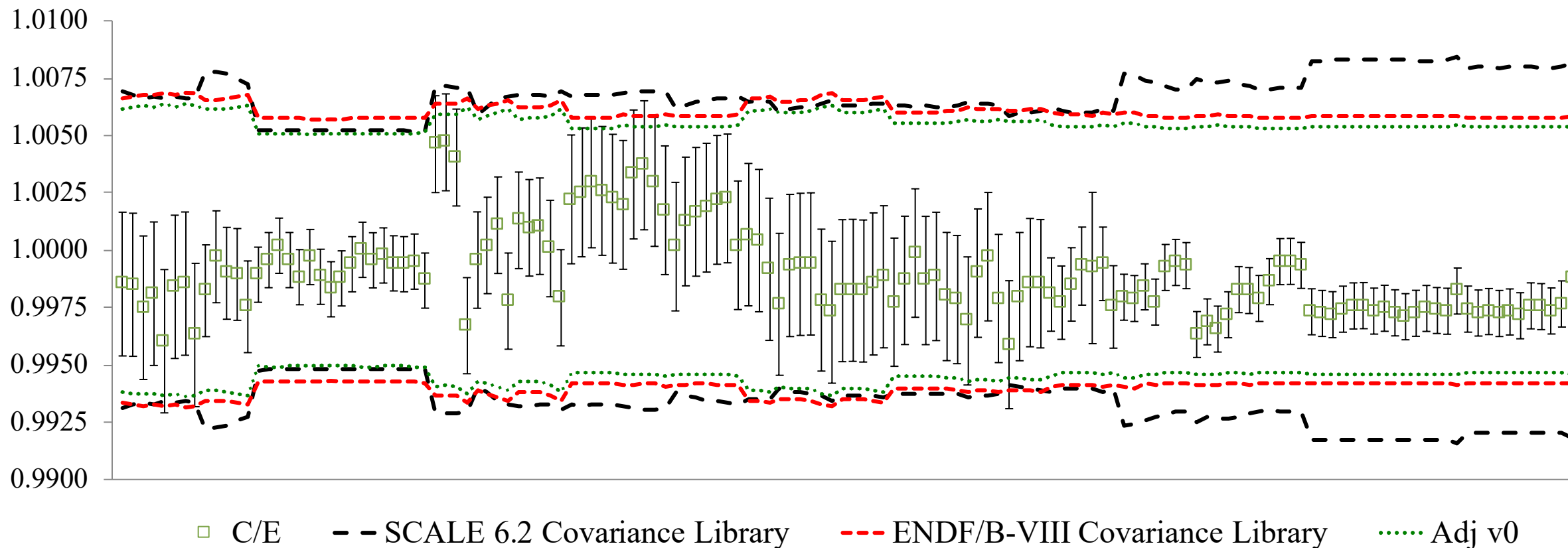
Results for HEU-SOL-THERM systems



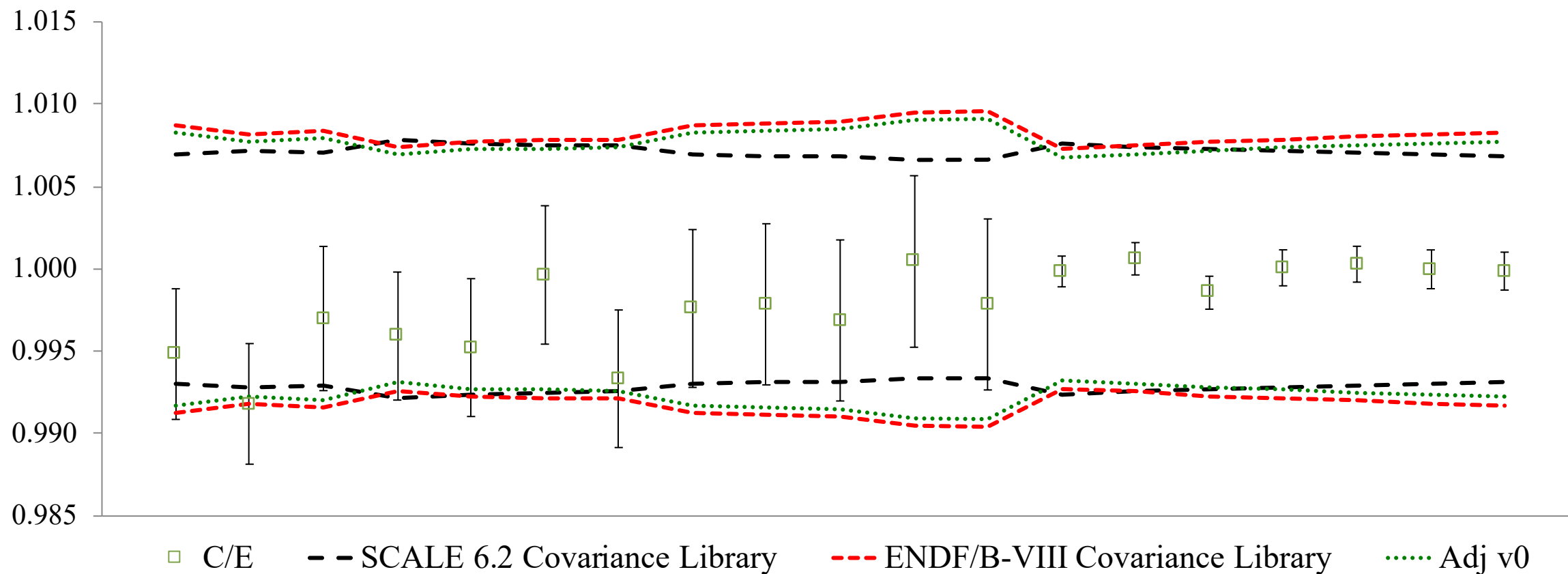
Results for IEU-MET-FAST systems



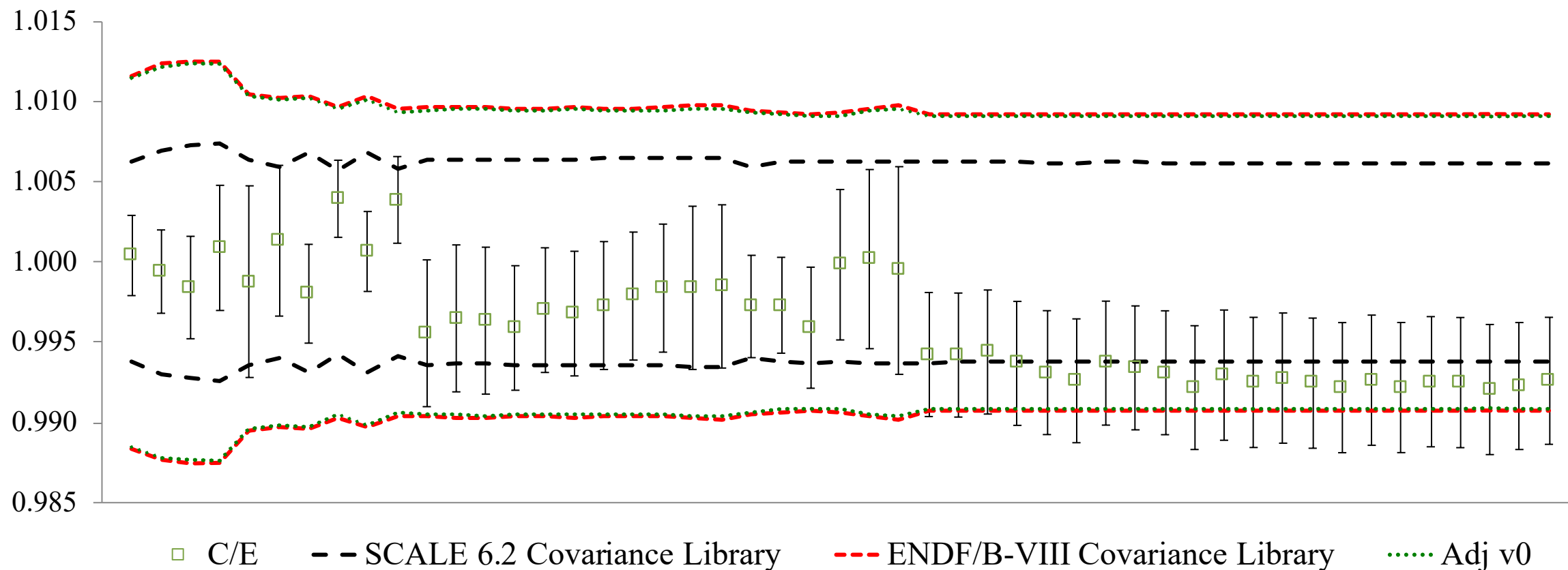
Results for LEU-COMP-THERM systems



Results for LEU-SOL-THERM systems



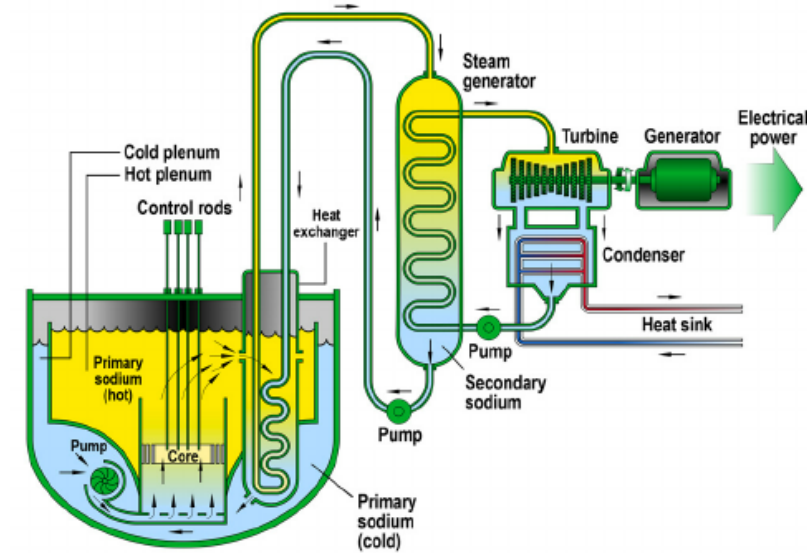
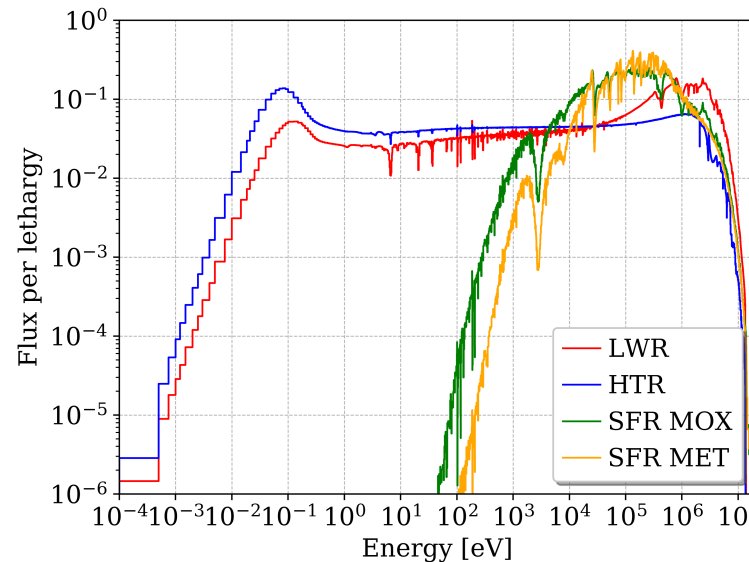
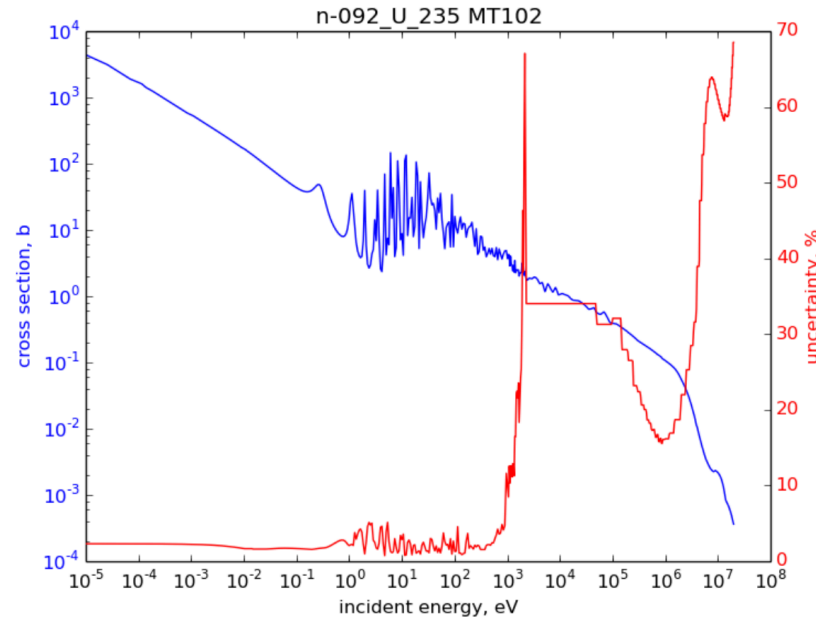
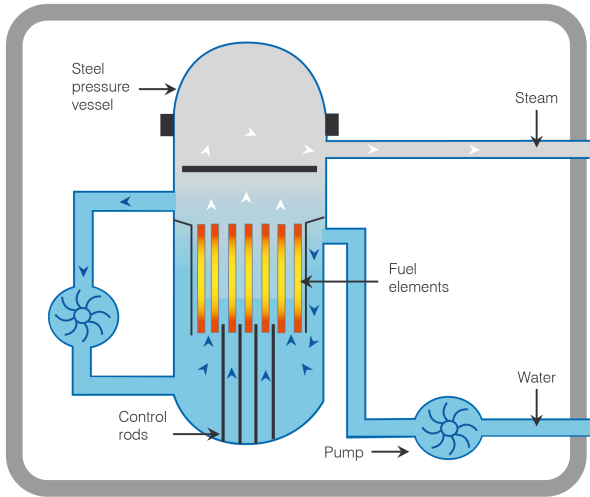
Results for MIX-COMP-THERM systems



Through a careful examination of nuclear data correlations (energy, reaction, isotope), propagated uncertainties on well known systems can be small and large for systems without vast validation data

WORLD NUCLEAR ASSOCIATION

A Boiling Water Reactor (BWR)



ENDF/B-VIII.0 Augmented Covariance Data

The first iteration

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