

**NCSP  
Technical  
Program  
Review**

**2019-03-26**

# **Impact of Outliers and ENDF/B-VIII.0 on NCS Validation and USLs**

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# Comparison of Benchmarks and Applications

## • Goals

- Determine the impact of rejection of benchmark outliers on NCS validation
- Compare ENDF/B-VIII.0 for criticality safety calculations relative to previous, mostly ENDF/B-VII.1, criticality validation suites and some applications.
  - Benchmarks from ICSBEP handbook Pu, HEU, LEU, IEU, MIX, <sup>233</sup>U
  - Thermal, intermediate, fast and mixed spectrum
  - Computational results compared with ICSBEP results for benchmarks

## • ENDF/B-VIII.0

### • N sub library

- CIELO evaluations, light elements, structural materials, <sup>236m</sup>Np, <sup>240</sup>Pu, <sup>241,243</sup>Am  $\bar{\nu}$

### • Thermal Scattering Library

- |                    |            |   |                                    |
|--------------------|------------|---|------------------------------------|
| – H in light water | lwtr       | → | h-h2o                              |
| – Ice              | --         | → | h-ice, o-ice                       |
| – D in heavy water | hwtr       | → | d-d2o, o-d2o                       |
| – Polyethylene     | poly       | → | h-poly                             |
| – Beryllium metal  | be         | → | be-met                             |
| – Beryllium oxide  | be-o,o-be  | → | be-beo, o-beo                      |
| – Zirc hydride     | h-zr, zr-h | → | h-zrh, zr-zrh                      |
| – Lucite           | --         | → | h-luci                             |
| – Graphite         | grph       | → | grph (crystalline), grph10, grph30 |
| – ...others...     |            |   |                                    |

# Benchmark Outlier Rejection

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- **Whisper Identification of Outliers**

- **Generalized Linear Least Squares (GLLS)**

- $\chi_{min}^2$  by GLLS adjustment – degree to which linear regression can fit benchmark experimental data within nuclear covariance data
- Value of  $\chi_{min}^2$ /number of benchmarks should be unity for perfect regression model
- Rejected using iterative diagonal chi-squared method until  $\chi_{min}^2 < 1.2$
- 10% of Whisper-1.1 library identified as outliers
- Whisper computed USL can include or exclude identified outliers

- **Rejection of Outliers**

- **ANSI/ANS-8.24-2007:**

- *“Rejection of data outliers shall be based on the inconsistency of the data with known physical behavior or on established statistical rejection methods.”*

- **ANSI/ANS-8.24-2017:**

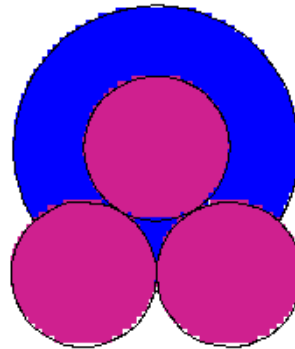
- *“Identification of data outliers may be based on established statistical rejection methods; rejection of outliers shall be based on the inconsistency of the data with known physical behavior in the experimental data.”*

# Impact of Rejected Benchmarks on Validation

- Application parameter study models for use with MCNP6.2/Whisper-1.1
- Pu and HEU: metal, oxide, solution

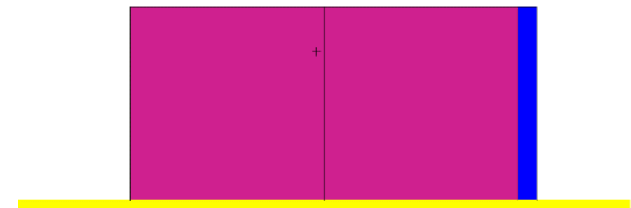
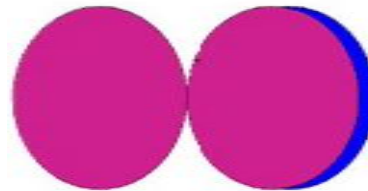
- **Metal and Oxide**

- Metal- or oxide- water mixture
- 3 cylinders
- Water, steel reflection
- H/D variation



- **Solution**

- Metal-water mixture
- 2 cylinders
- Water, steel reflection
- H/D variation

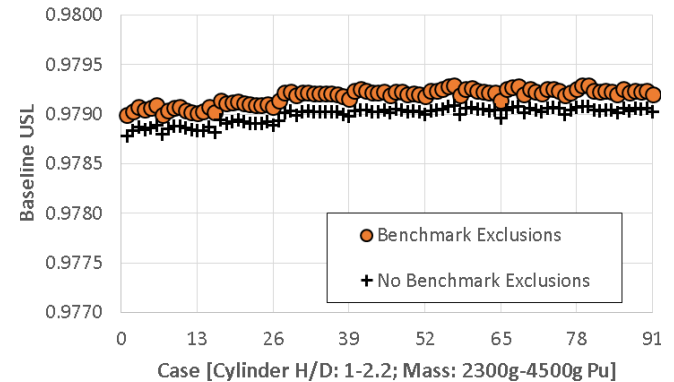
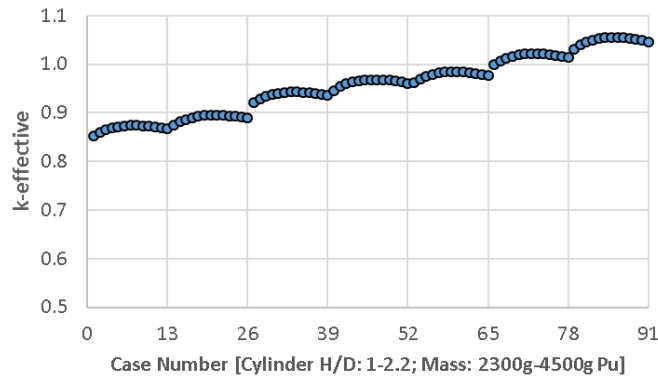


- MCNP6.2 calculations using 1,000,000 neutrons
- Whisper-1.1 calculation of Bias, Bias Uncertainty, MOS → USL at 99% confidence level

# Results of Benchmark Rejection Study

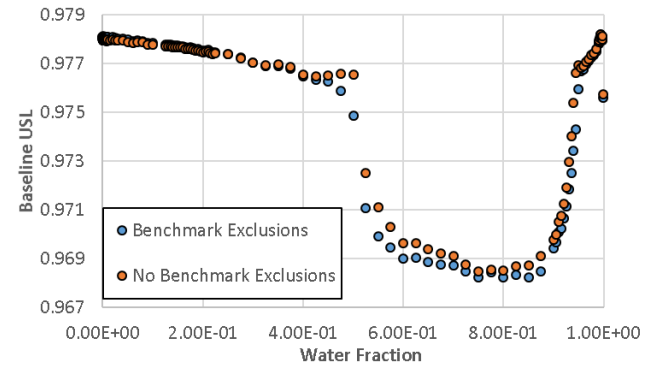
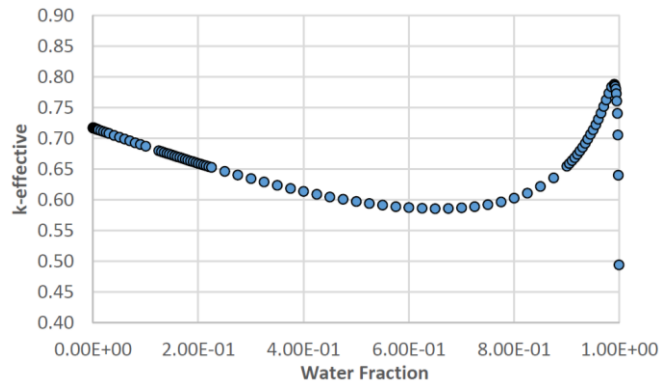
## Pu Metal

$$\text{USL}_{\text{exclusions}} - \text{USL}_{\text{all}} = 0.00021$$



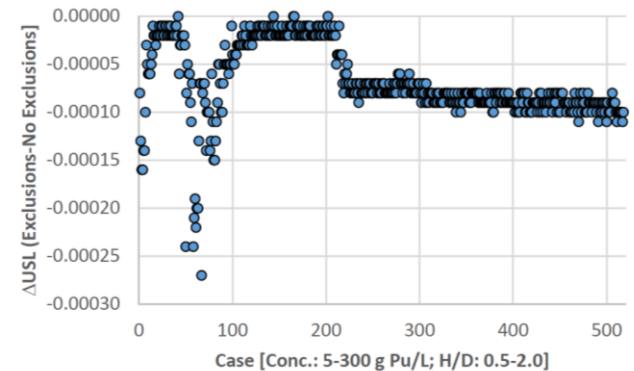
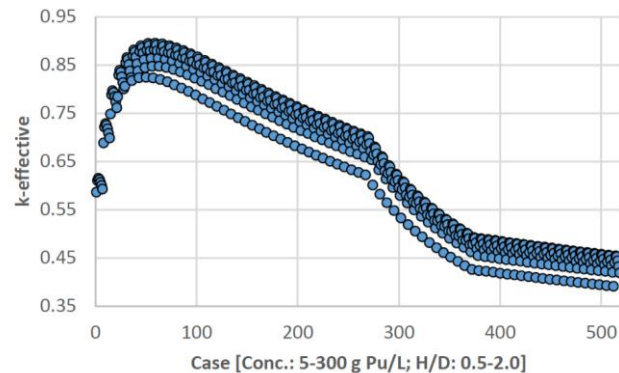
## Pu Oxide

$$\text{USL}_{\text{exclusions}} - \text{USL}_{\text{all}} = -0.00234$$



## Pu Solution

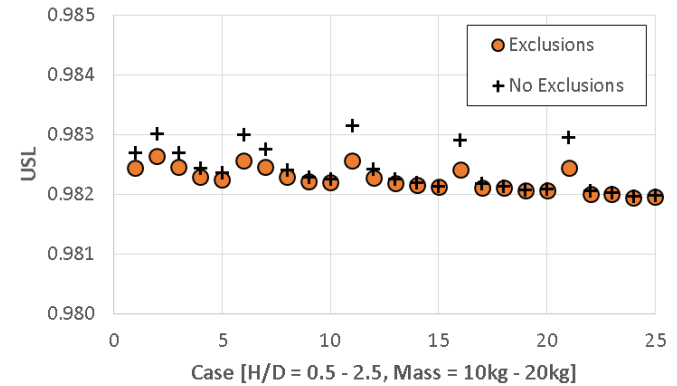
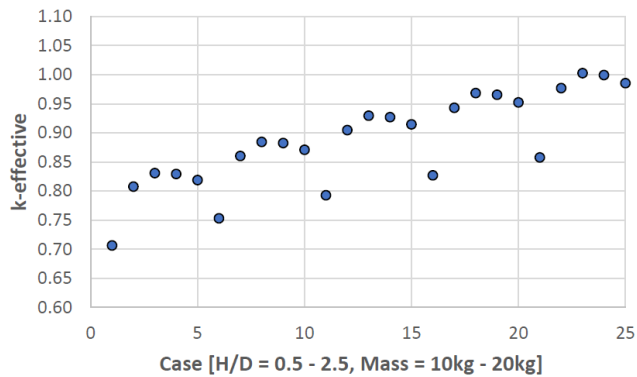
$$\text{USL}_{\text{exclusions}} - \text{USL}_{\text{all}} = -0.00026$$



# Results of Benchmark Rejection Study

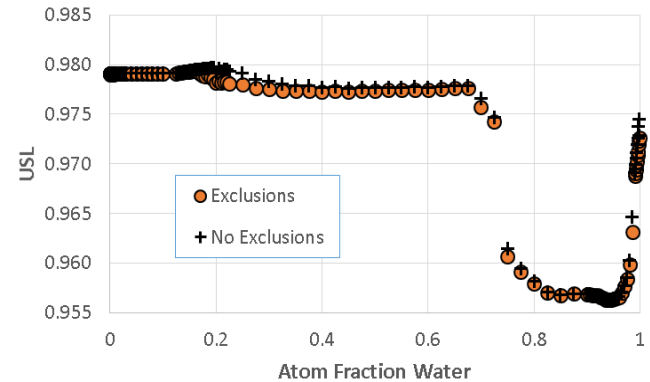
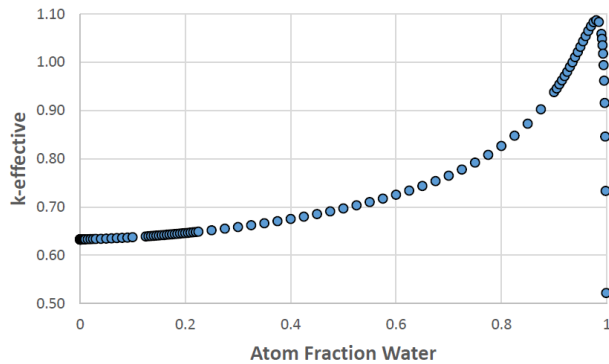
## HEU Metal

$$\text{USL}_{\text{exclusions}} - \text{USL}_{\text{all}} = -0.00050$$



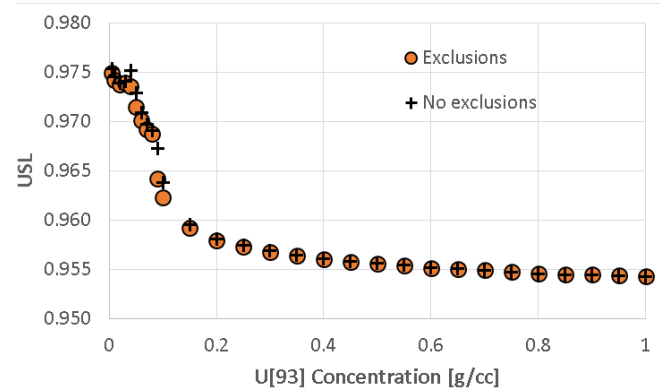
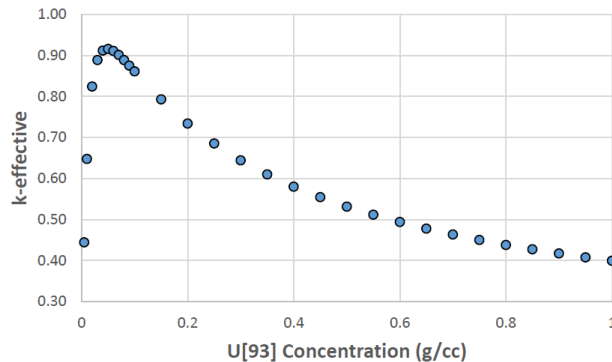
## HEU Oxide

$$\text{USL}_{\text{exclusions}} - \text{USL}_{\text{all}} = -0.00208$$



## HEU Solution

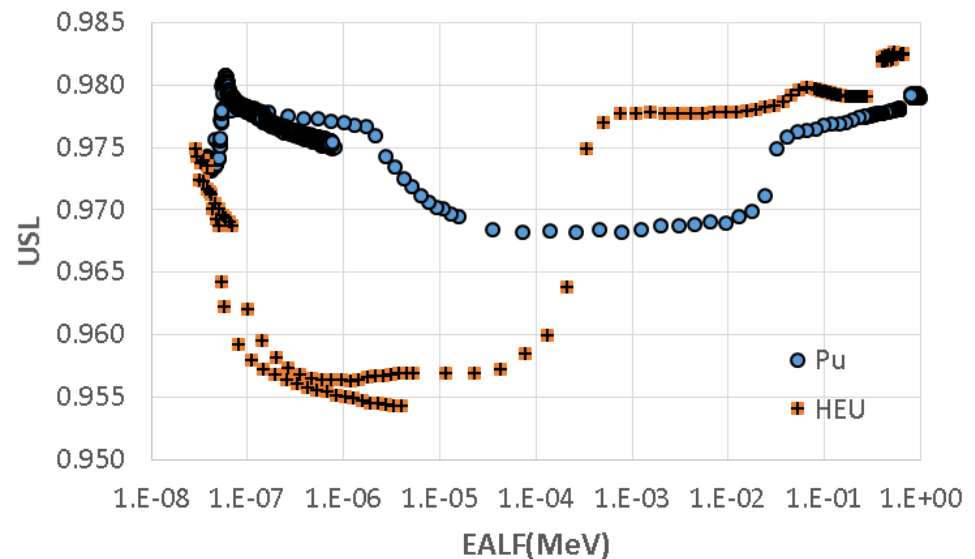
$$\text{USL}_{\text{exclusions}} - \text{USL}_{\text{all}} = -0.00307$$



# Results of Benchmark Rejection & ENDF/B-VIII.0 Study

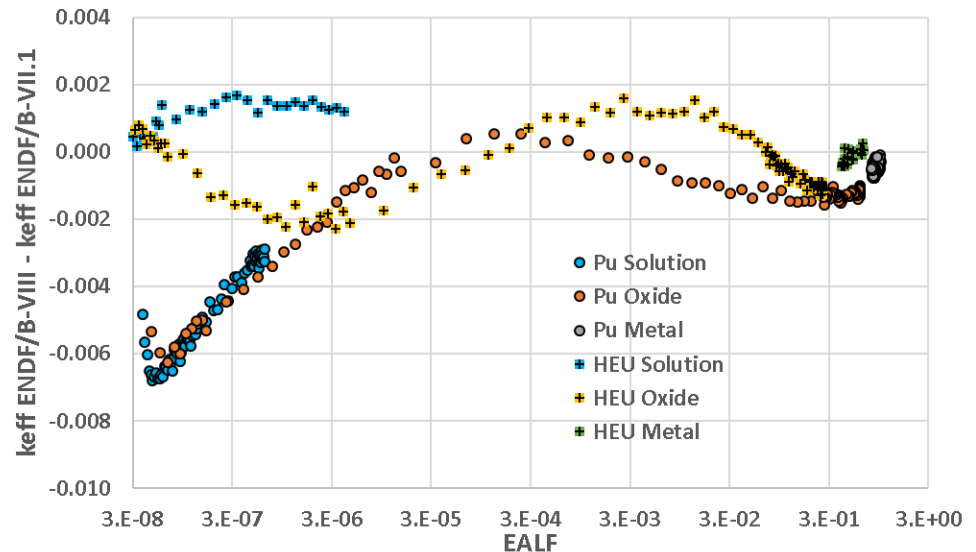
## Rejection Study USL Differences

USL Difference: $ \text{USL}_{\text{exclusions}} - \text{USL}_{\text{all benchmarks}} $	
Pu metals	0.00021
Pu oxides	0.00234
Pu solutions	0.00026
HEU metals	0.00050
HEU oxides	0.00208
HEU solutions	0.00307



## ENDF/B-VII.1 vs. ENDF-B/VIII.0 K-effective Differences

- Applications from benchmark rejection study
- $\Delta k$ -effective –VIII.0 & –VII.1 as function of lethargy
- Lower  $k$ -effective in thermal Pu for ENDF/B-VII: correcting over prediction



# Results of Validation\_Criticality 31 problems

## • Results

- Good agreement with both ENDF-B-VII.1 and ENDF/B-VIII.0 nuclear data libraries

Suite	# OF CASE S	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
<b>VAL_CRIT</b>	<b>31</b>	<b>0.56</b>	<b>0.9999</b>	<b>0.0057</b>	<b>0.59</b>	<b>0.9989</b>	<b>0.0059</b>
<sup>233</sup> U	7	0.66	0.9962	0.0058	0.74	0.9956	0.0065
HEU	7	0.22	0.9994	0.0023	0.19	0.9987	0.0014
IEU	6	0.76	1.0029	0.0083	0.87	1.0027	0.0099
LEU	2	0.47	0.9975	0.0055	0.47	0.9970	0.0050
Pu	9	0.50	1.0018	0.0046	0.33	1.0004	0.0032

Benchmark	k-eff ex.	k-eff ENDF/B-VII.1	k-eff ENDF/B-VIII.0	ENDF/B-VII.1 C/E	ENDF/B-VIII.0 C/E		
<sup>233</sup> U	FLAT23	1.0000	0.9974	0.9978	0.9974	0.9978	
	FLSTF1	1.0000	0.9845	0.9819	0.9845	0.9819	
	JEZ233	1.0000	1.0000	1.0007	1.0000	1.0007	
	ORNL11	1.0006	1.0018	0.9994	1.0012	0.9988	
	SB25	1.0000	1.0007	1.0000	1.0007	1.0000	
	UMF5C2	1.0000	0.9960	0.9969	0.9960	0.9969	
HEU	SB5RN3	1.0015	0.9954	0.9949	0.9939	0.9934	
	FLAT25	1.0000	1.0034	0.9999	1.0034	0.9999	
	GODIVA	1.0000	0.9988	0.9990	0.9988	0.9990	
	GODIVR	0.9985	0.9989	0.9979	1.0004	0.9994	
	ORNL10	1.0015	1.0001	0.9981	0.9986	0.9966	
	TT2C11	1.0000	1.0009	0.9988	1.0009	0.9988	
	UH3C6	1.0000	0.9965	0.9969	0.9965	0.9969	
	ZEUS2	1.0001	0.9976	1.0006	0.9975	1.0004	
	IEU	BIGTEN	1.0045	0.9952	0.9948	0.9908	0.9904
		ICT2C3	1.0017	1.0035	1.0036	1.0018	1.0019
		IMF03	1.0000	1.0019	0.9988	1.0019	0.9988
		IMF04	1.0000	1.0082	1.0052	1.0082	1.0052
	LEU	STACY36	0.9988	0.9981	0.9987	0.9993	0.9999
		ZEBR8H	1.0030	1.0185	1.0232	1.0155	1.0201
Pu	BAWXI2	1.0007	1.0021	1.0012	1.0013	1.0005	
	LST2C2	1.0024	0.9960	0.9958	0.9936	0.9935	
Pu	FLATPU	1.0000	1.0004	0.9981	1.0004	0.9981	
	HISHPG	1.0000	1.0121	1.0078	1.0121	1.0078	
	JEZ240	1.0000	0.9999	1.0014	0.9999	1.0014	
	JEZPU	1.0000	0.9990	0.9996	0.9990	0.9996	
	PNL2	1.0000	1.0050	0.9990	1.0050	0.9990	
	PNL33	1.0024	1.0068	1.0047	1.0043	1.0023	
	PUBTNS	1.0000	0.9980	0.9979	0.9980	0.9979	
	PUSH2O	1.0000	0.9998	1.0001	0.9998	1.0001	
	THOR	1.0000	0.9976	0.9973	0.9976	0.9973	



# Results of Various Benchmark Suites

- **Results ENDF/B-VIII.0 improved for:**

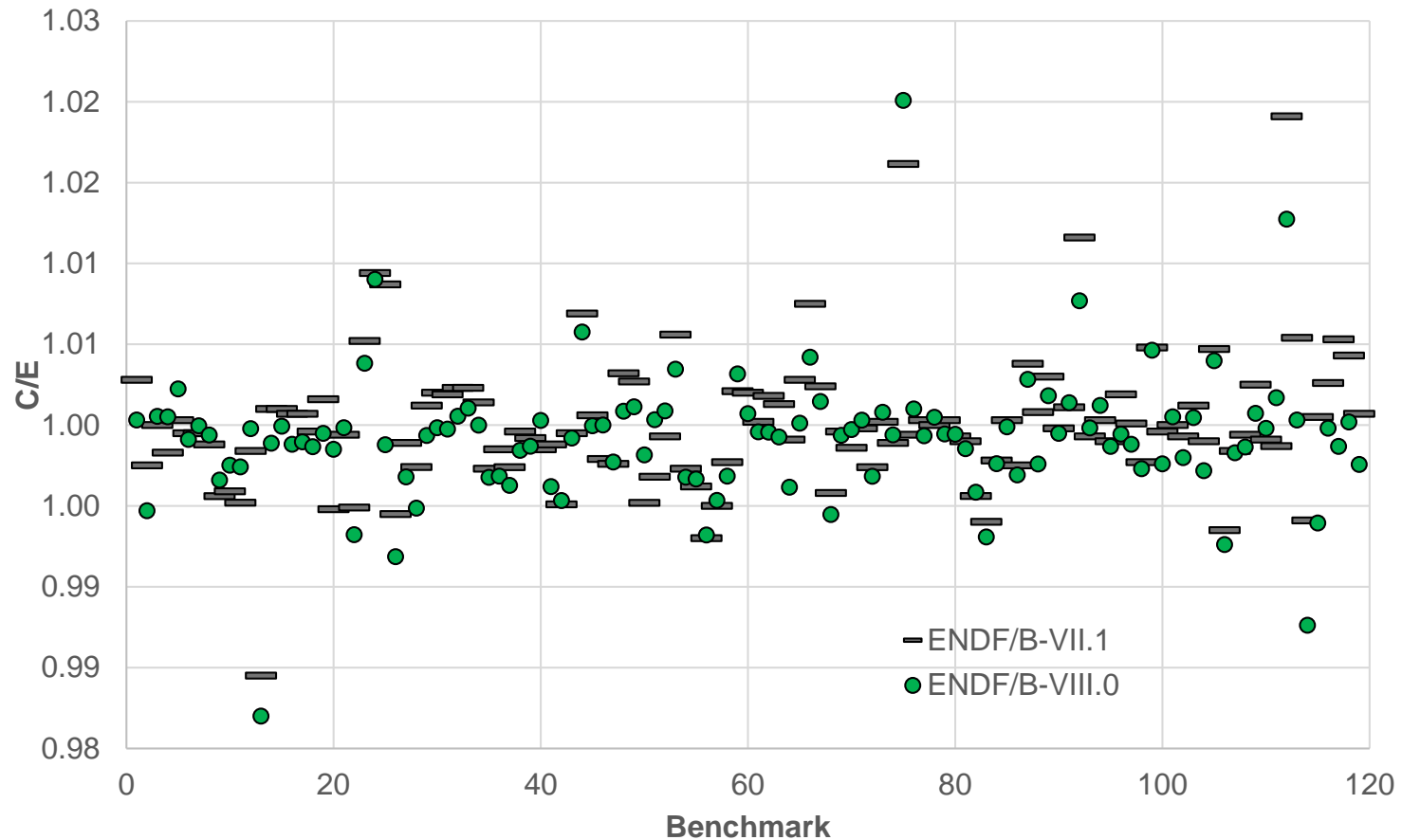
- Pu overall  
  **PU-SOL**
- HEU overall  
  **HEU-MET**
- MIX
- IEU
- <sup>233</sup>U-MET-FAST

- **Preliminary results for other series appear to be acceptable**

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
VALIDATION_CRIT_EXTENDED	119	0.42	0.9994	0.0039	0.41	0.9986	0.0038
WHISPER	1101	0.74	1.0017	0.0072	0.76	1.0003	0.0076
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
WHISPER: PU-COMP	36	2.06	1.0177	0.0106	2.14	1.0186	0.0108
WHISPER: PU-MET	68	0.66	1.0040	0.0054	0.73	1.0039	0.0063
WHISPER: PU-SOL	158	0.64	1.0045	0.0045	0.47	0.9999	0.0047
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
WHISPER: HEU-COMP	26	1.50	1.0143	0.0046	1.57	1.0151	0.0044
WHISPER: HEU-MET	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041
WHISPER: HEU-SOL	93	0.47	1.0000	0.0047	0.49	0.9998	0.0049
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027
WHISPER: <sup>233</sup> U	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102
WHISPER: <sup>233</sup> U: COMP-THERM	9	0.20	0.9995	0.0020	0.33	0.9971	0.0016
WHISPER: <sup>233</sup> U: MET-FAST	10	0.25	0.9982	0.0019	0.17	0.9993	0.0017
WHISPER: <sup>233</sup> U: SOL-INTER	33	1.72	0.9837	0.0056	1.99	0.9809	0.0056
WHISPER: <sup>233</sup> U: SOL-THERM	106	0.87	0.9999	0.0087	0.92	0.9971	0.0088

# Results of Validation\_Crit\_Extended, 119 cases

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
VALIDATION_CRIT_EXTENDED	119	0.42	0.9994	0.0039	0.41	0.9986	0.0038



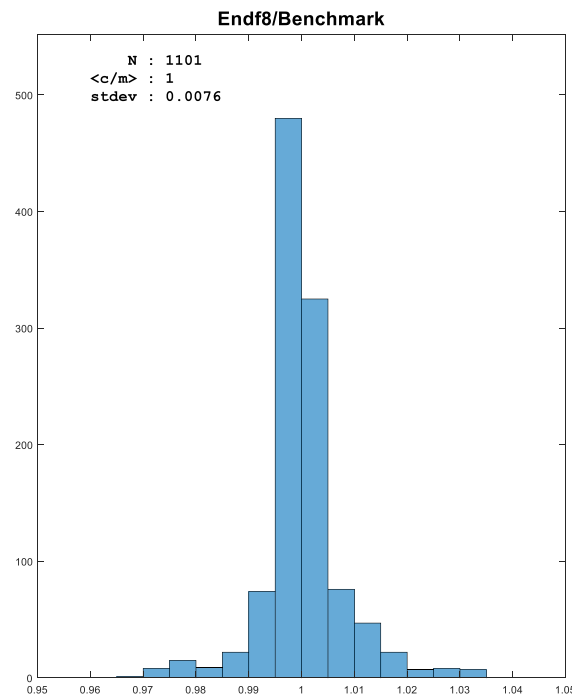
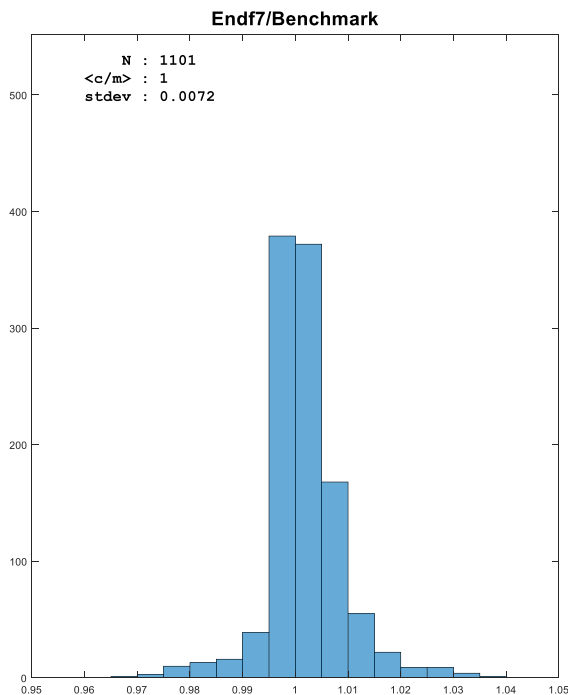
# Results of Whisper Library, 1101 cases

## • ENDF/B-VIII.0

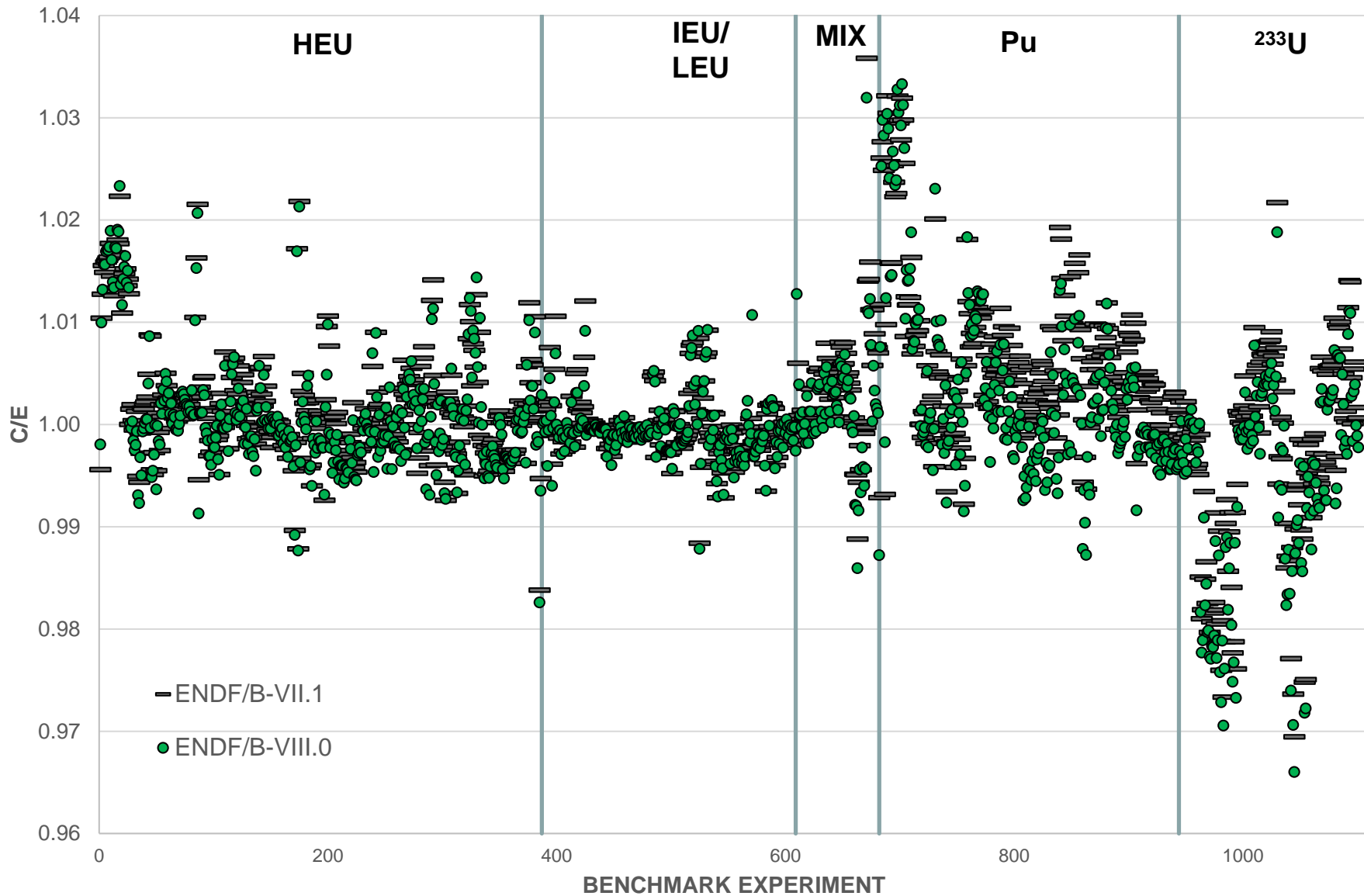
- Large benchmark set
- Good performance, higher std.
- Agreement with results in Nuclear Data Sheets<sup>1</sup>

D. A. Brown, et. al, "ENDF/B-VIII.0: The 8<sup>th</sup> Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data", Nuclear Data Sheets 148 (2018) 1-142

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER	1101	0.74	1.0017	0.0072	0.76	1.0003	0.0076
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027
WHISPER: <sup>233</sup> U	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102



# Results of Whisper Library, 1101 cases

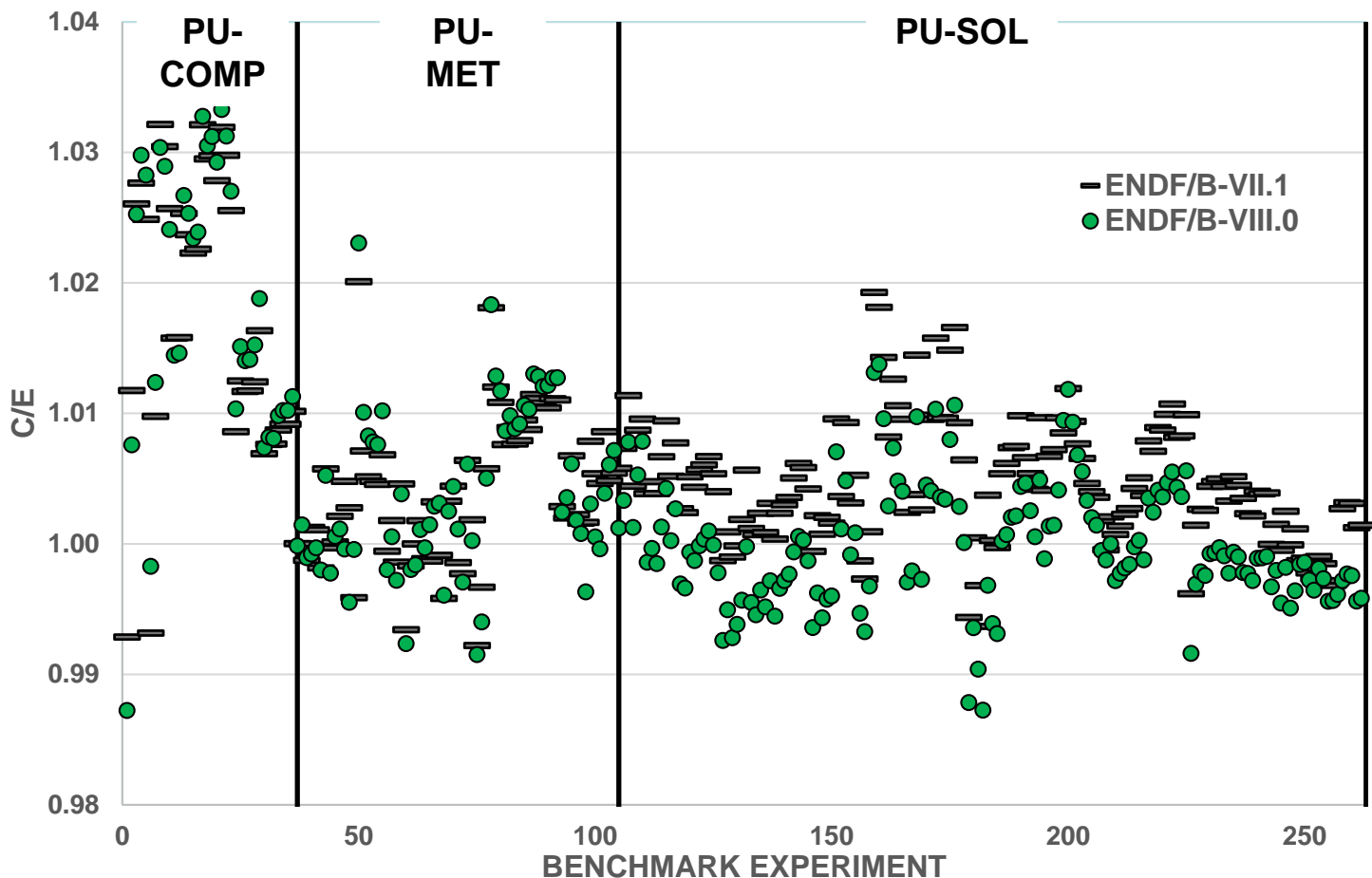


# Results of Whisper Library, 262 Pu cases

## • Pu results

- Improved ENDF/B-VIII.0 for Pu overall and specifically Pu solution
- Pu metal about the same
- Pu compounds not great for –VII.1 or –VIII.0, mixed spectrum

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
WHISPER: PU-COMP	36	2.06	1.0177	0.0106	2.14	1.0186	0.0108
WHISPER: PU-MET	68	0.66	1.0040	0.0054	0.73	1.0039	0.0063
WHISPER: PU-SOL	158	0.64	1.0045	0.0045	0.47	0.9999	0.0047

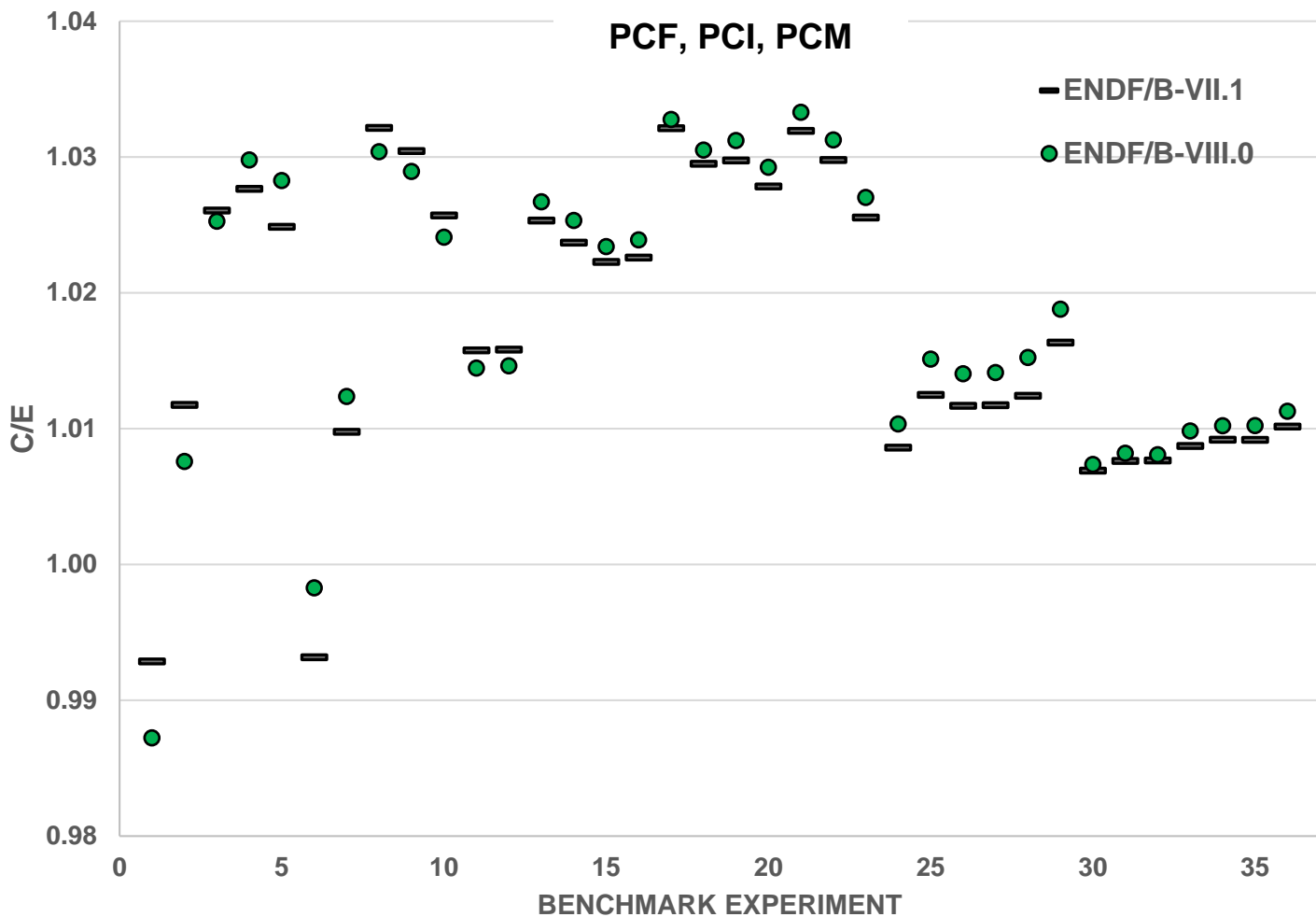


# Results of Whisper Library, 36 PU-COMP cases

## Pu results

- PU-COMP highest standard deviation and RMS of Whisper suite
- Mixed and intermediate spectrum

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
WHISPER: PU-COMP	36	2.06	1.0177	0.0106	2.14	1.0186	0.0108

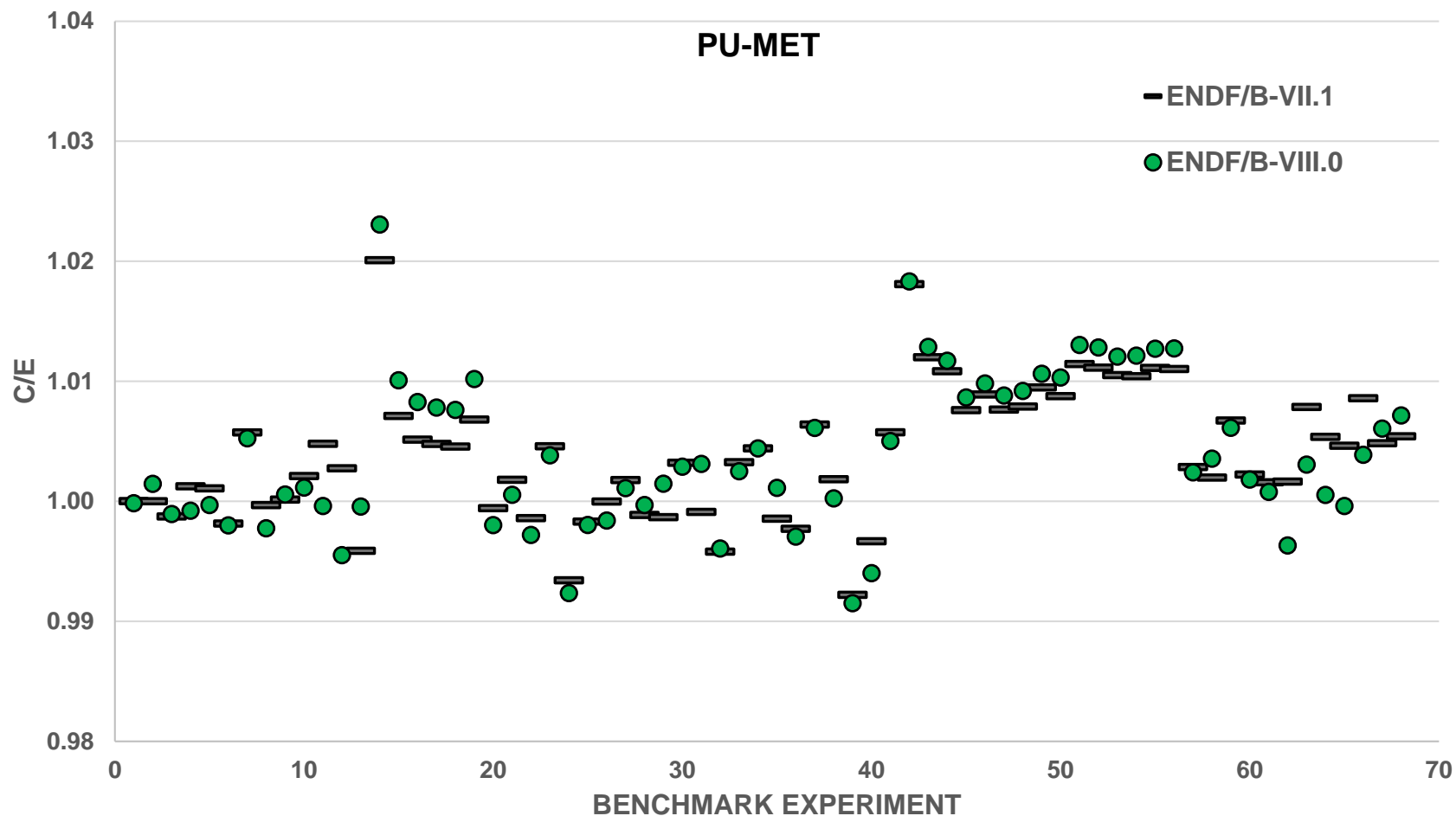


# Results of Whisper Library, 68 PMF cases

## •Pu results

- Pu metal slightly better
- PMF19,21,38,44: BeO
- PMF42: steel

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
<i>WHISPER: PU-MET</i>	68	0.66	1.0040	0.0054	0.73	1.0039	0.0063

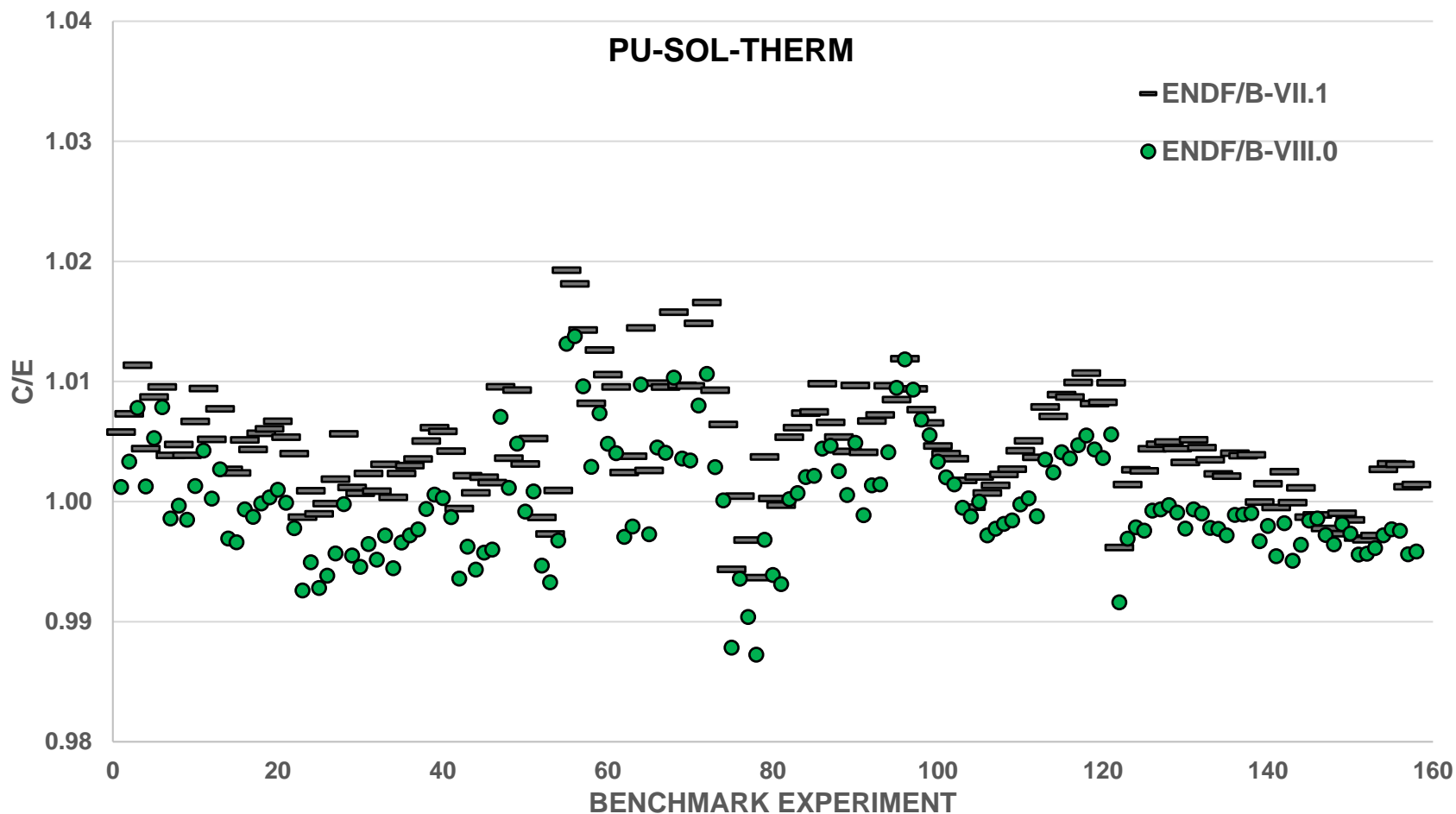


# Results of Whisper Library, 158 PST cases

## • PU-SOL

- previously over predicted ~500 pcm
- High experimental uncertainty

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: Pu	262	0.97	1.0062	0.0075	0.95	1.0035	0.0088
<i>WHISPER: PU-SOL</i>	158	0.64	1.0045	0.0045	0.47	0.9999	0.0047



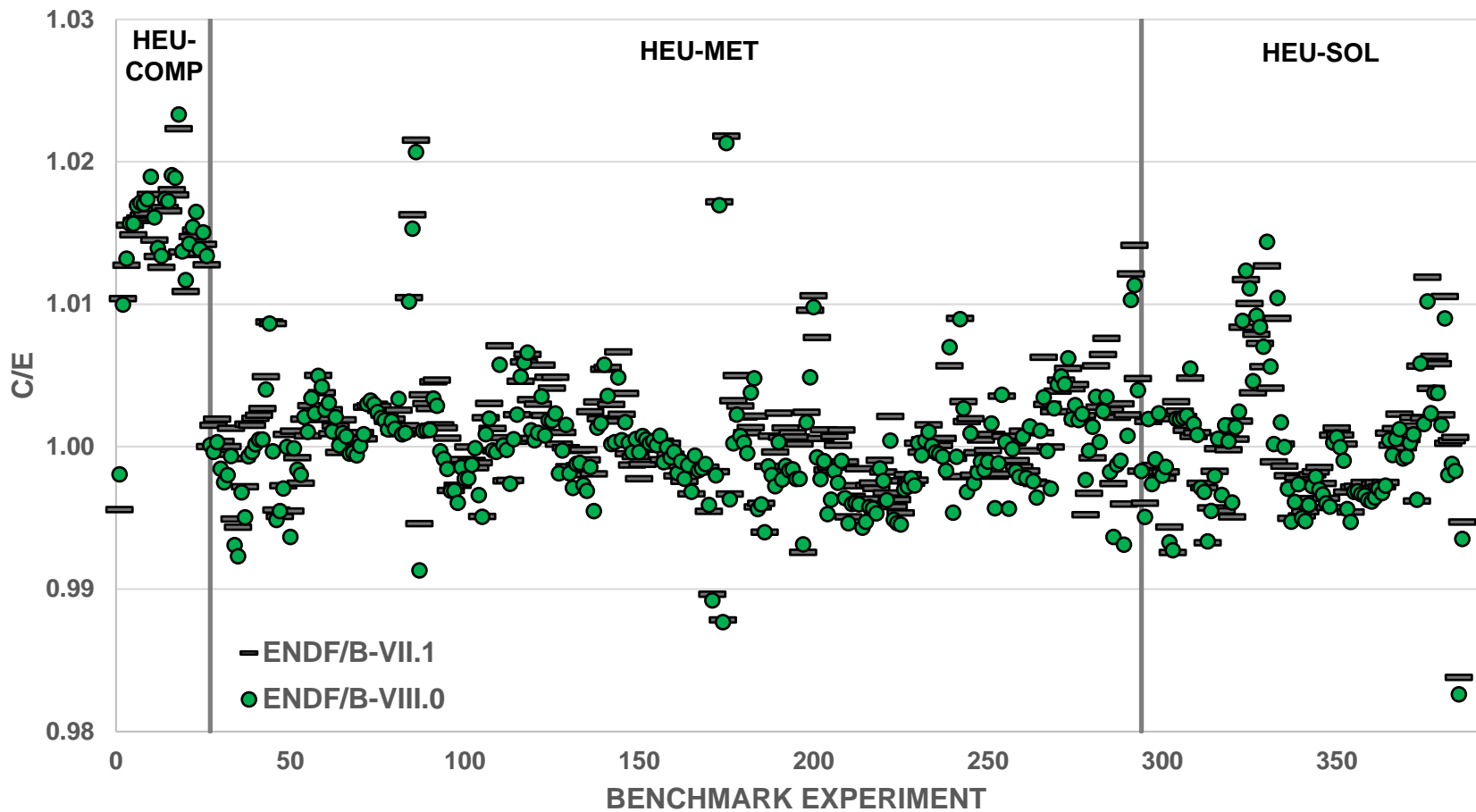


# Results of Whisper Library, 386 HEU cases

## HEU results

- Improved ENDF/B-VIII.0 for HEU, overall, HEU-MET specifically

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
WHISPER: HEU-COMP	26	1.50	1.0143	0.0046	1.57	1.0151	0.0044
WHISPER: HEU-MET	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041
WHISPER: HEU-SOL	93	0.47	1.0000	0.0047	0.49	0.9998	0.0049

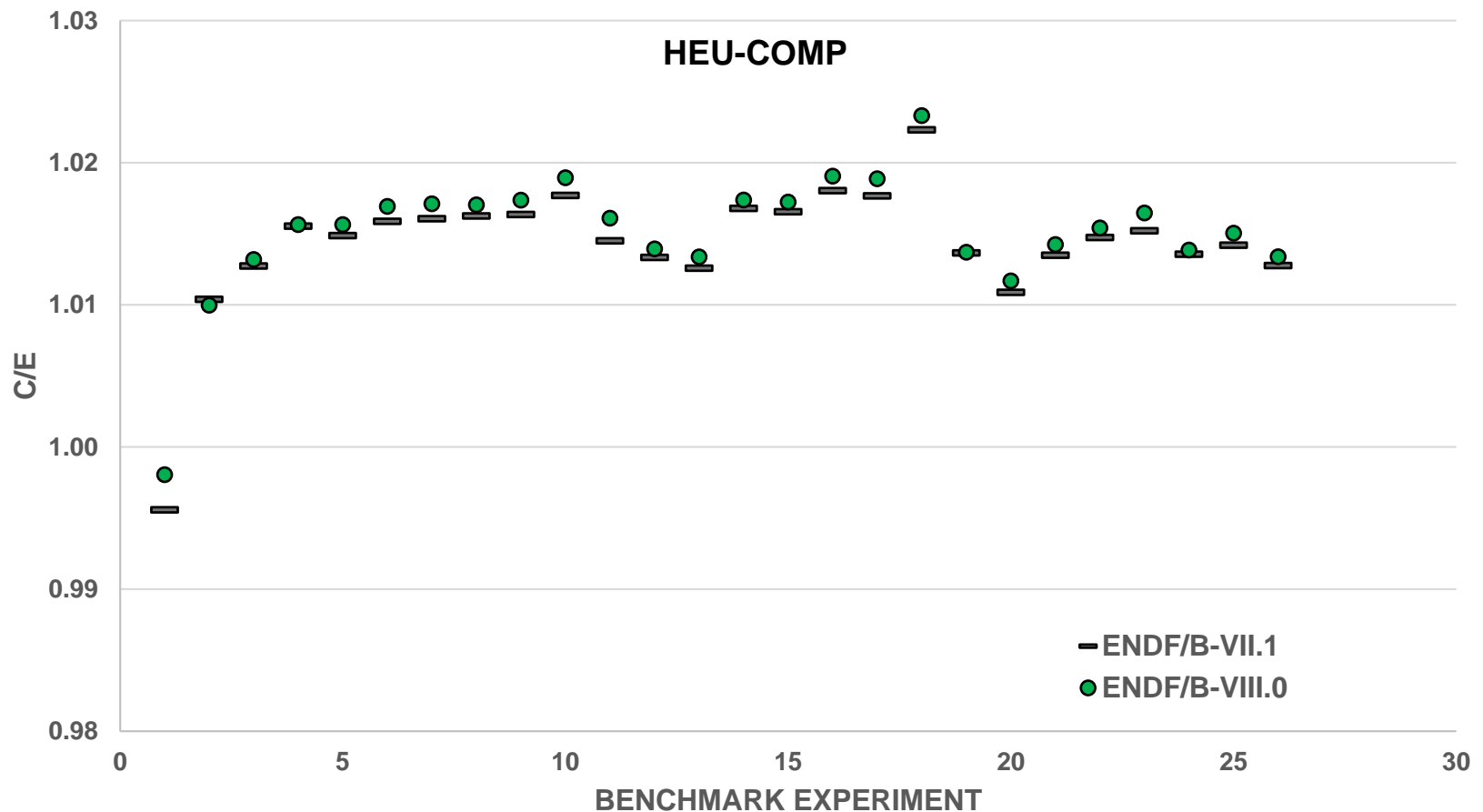


# Results of Whisper Library, 26 HEU-COMP cases

## • HEU-COMP

- Still over predicted

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
WHISPER: HEU-COMP	26	1.50	1.0143	0.0046	1.57	1.0151	0.0044

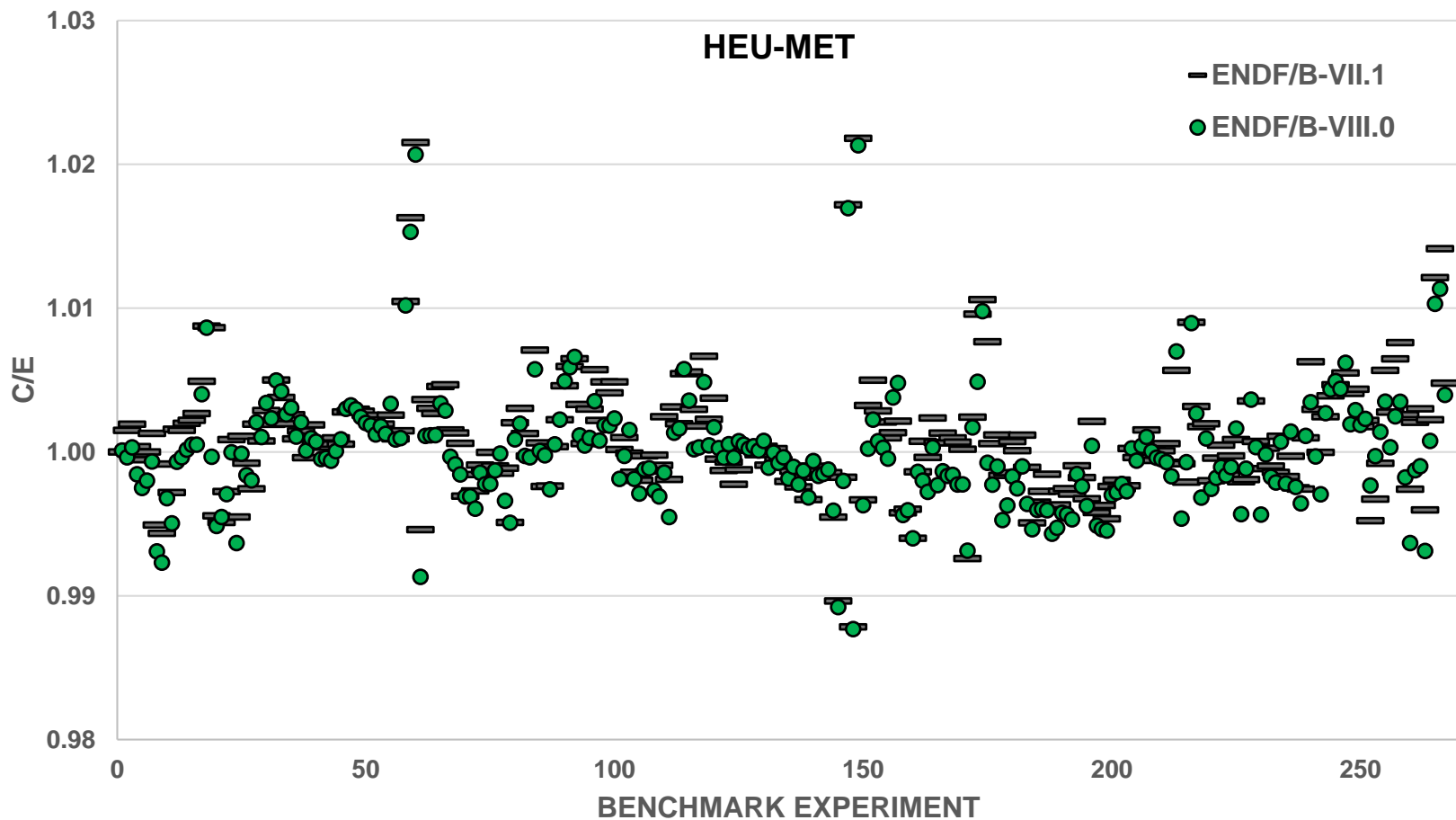


# Results of Whisper Library, 267 HEU-MET cases

## HEU results

- Improved ENDF/B-VIII.0 for HEU-MET
- Improved HMF w/ BeO

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
<i>WHISPER: HEU-MET</i>	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041

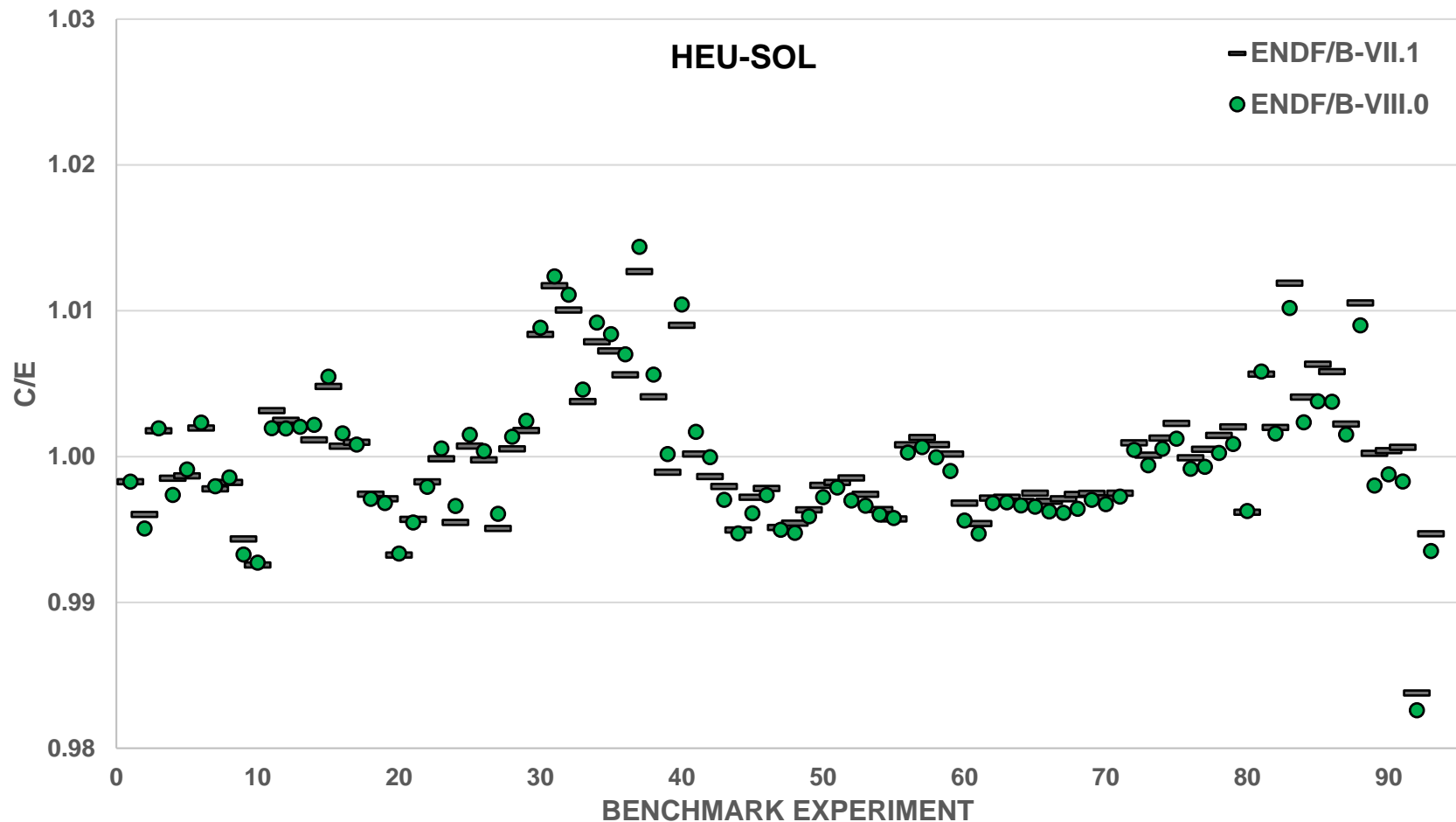


# Results of Whisper Library, 93 HEU-SOL cases

## HST results

- Artificially shifted thermal  $^{235}\text{U}$  v, capture, fission data eliminated in -VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: HEU	386	0.57	1.0016	0.0055	0.63	1.0009	0.0057
WHISPER: HEU-SOL	93	0.47	1.0000	0.0047	0.49	0.9998	0.0049



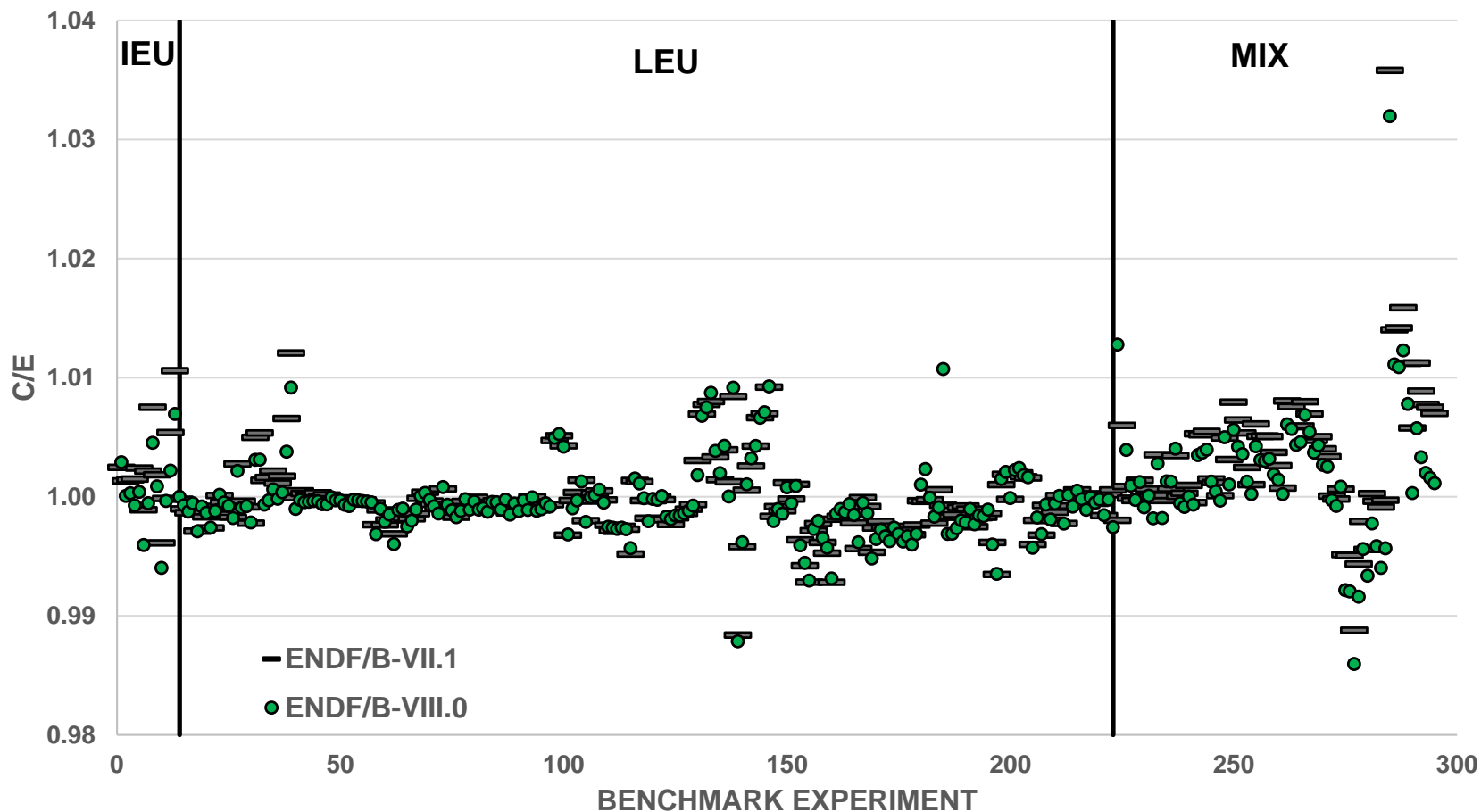
# Results of Whisper Library, 295 IEU,LEU,MIX cases

## • IEU, LEU, MIX results

– Improved ENDF/B-VIII.0 for MIX & IEU

– LCT ~same, but good

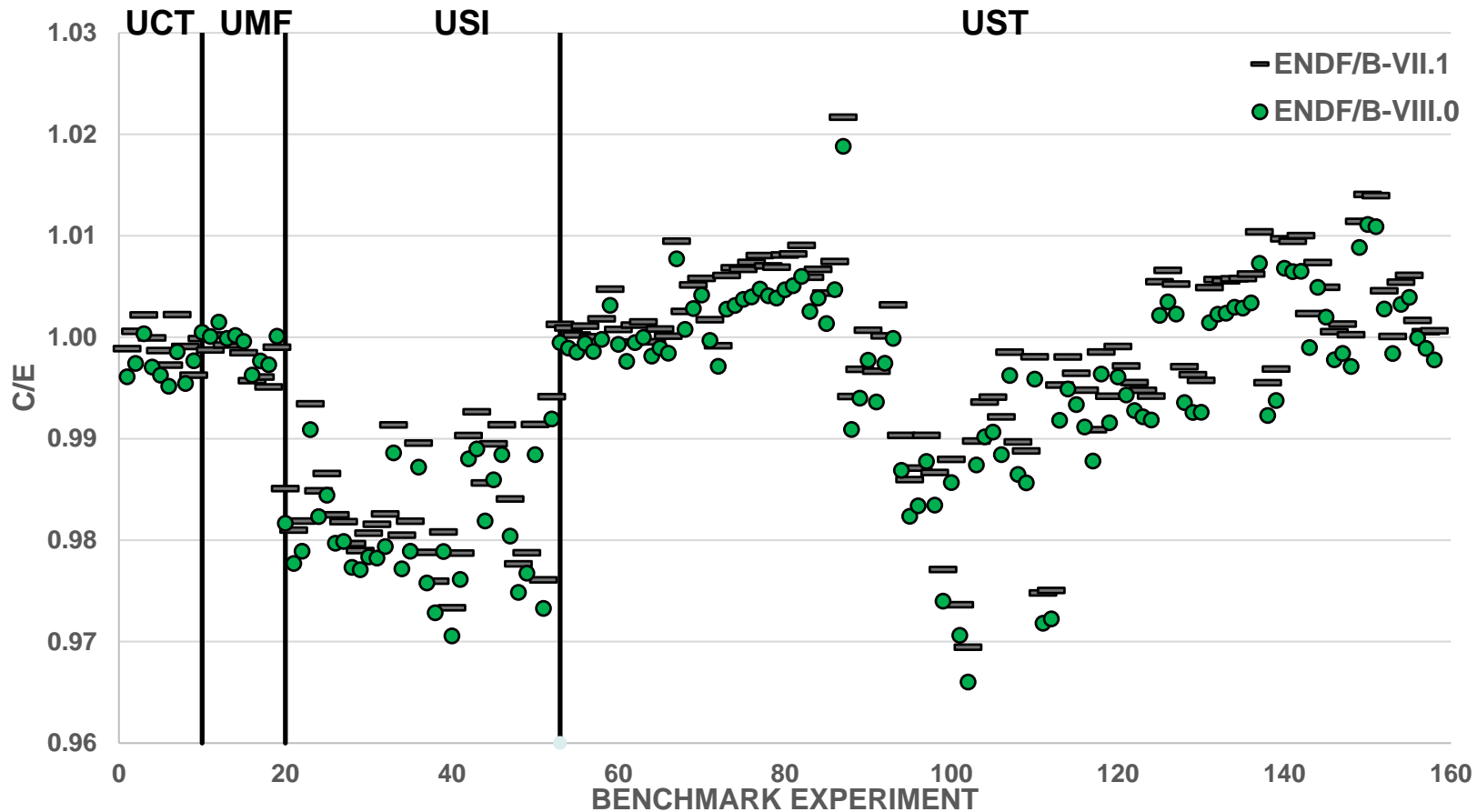
Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027



# Results of Whisper Library, 158 $^{233}\text{U}$ cases

- **ENDF/B-VIII.0**
- Better UMF
- Poor performance in intermediate & thermal energy for –VII.1 & –VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: $^{233}\text{U}$	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102
WHISPER: $^{233}\text{U}$ : COMP-THERM	9	0.20	0.9995	0.0020	0.33	0.9971	0.0016
WHISPER: $^{233}\text{U}$ : MET-FAST	10	0.25	0.9982	0.0019	0.17	0.9993	0.0017
WHISPER: $^{233}\text{U}$ : SOL-INTER	33	1.72	0.9837	0.0056	1.99	0.9809	0.0056
WHISPER: $^{233}\text{U}$ : SOL-THERM	106	0.87	0.9999	0.0087	0.92	0.9971	0.0088



# Conclusions

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- **Benchmark Rejection Study**

- Differences in USL are small whether excluding outliers or including all benchmarks in Whisper library
- Neither inclusion nor exclusion is consistently conservative

- **ENDF/B-VIII.0 Testing**

- Results thus far are promising
- More comparisons with new TSL treatment

- **Future Work**

- Incorporate new covariance data into Whisper
- Run benchmark rejection with new nuclear data
- Compare USLs for applications
- Incorporate feedback on Whisper-1.1 library
- Adopt ENDF/B-VIII.0 into validation suites

- **Questions?**

# Extra Slides

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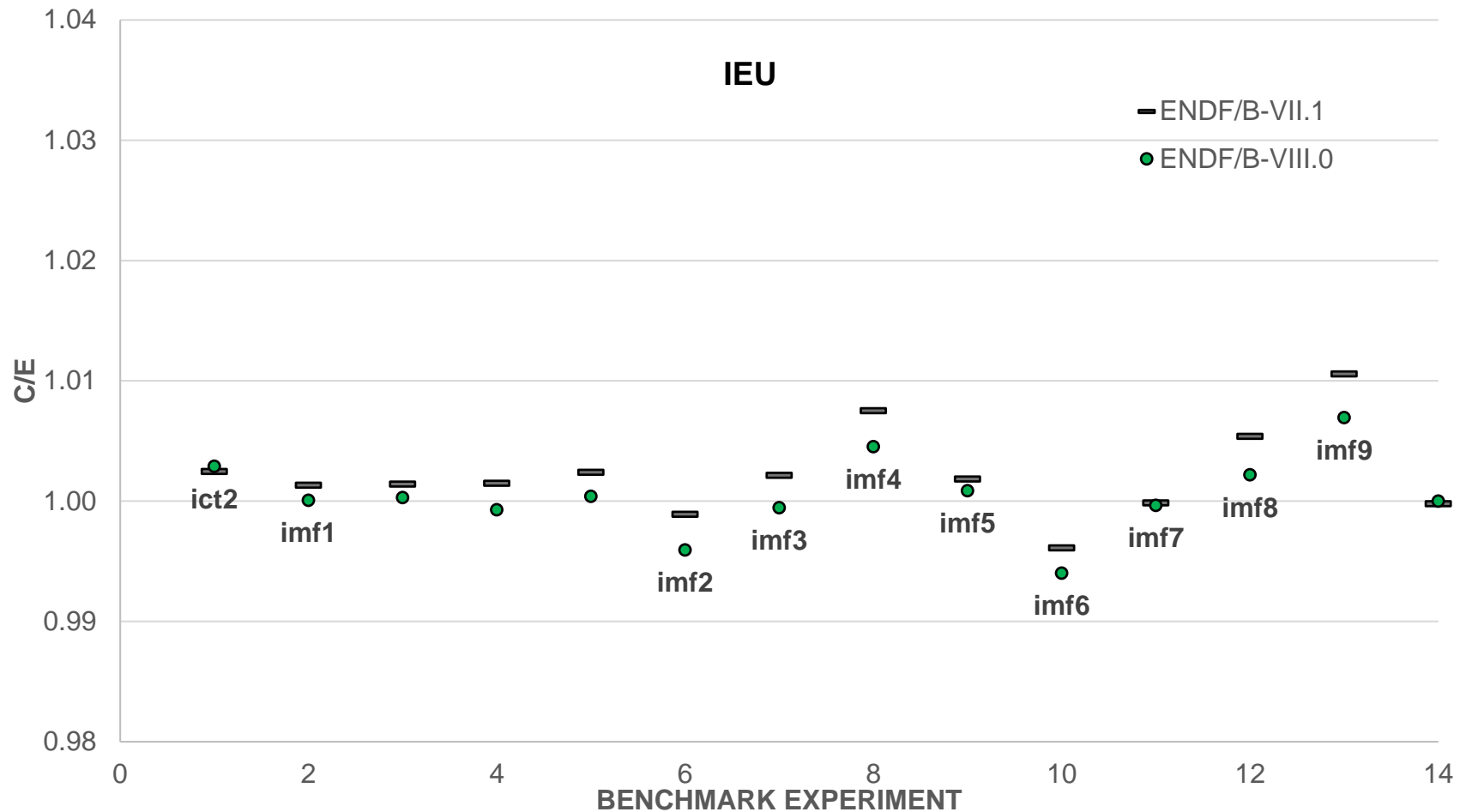


# Results of Whisper Library, 14 IEU cases

## • ENDF/B-VIII.0 results

– Improved for IEU

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: IEU	13	0.43	1.0024	0.0038	0.32	1.0005	0.0033

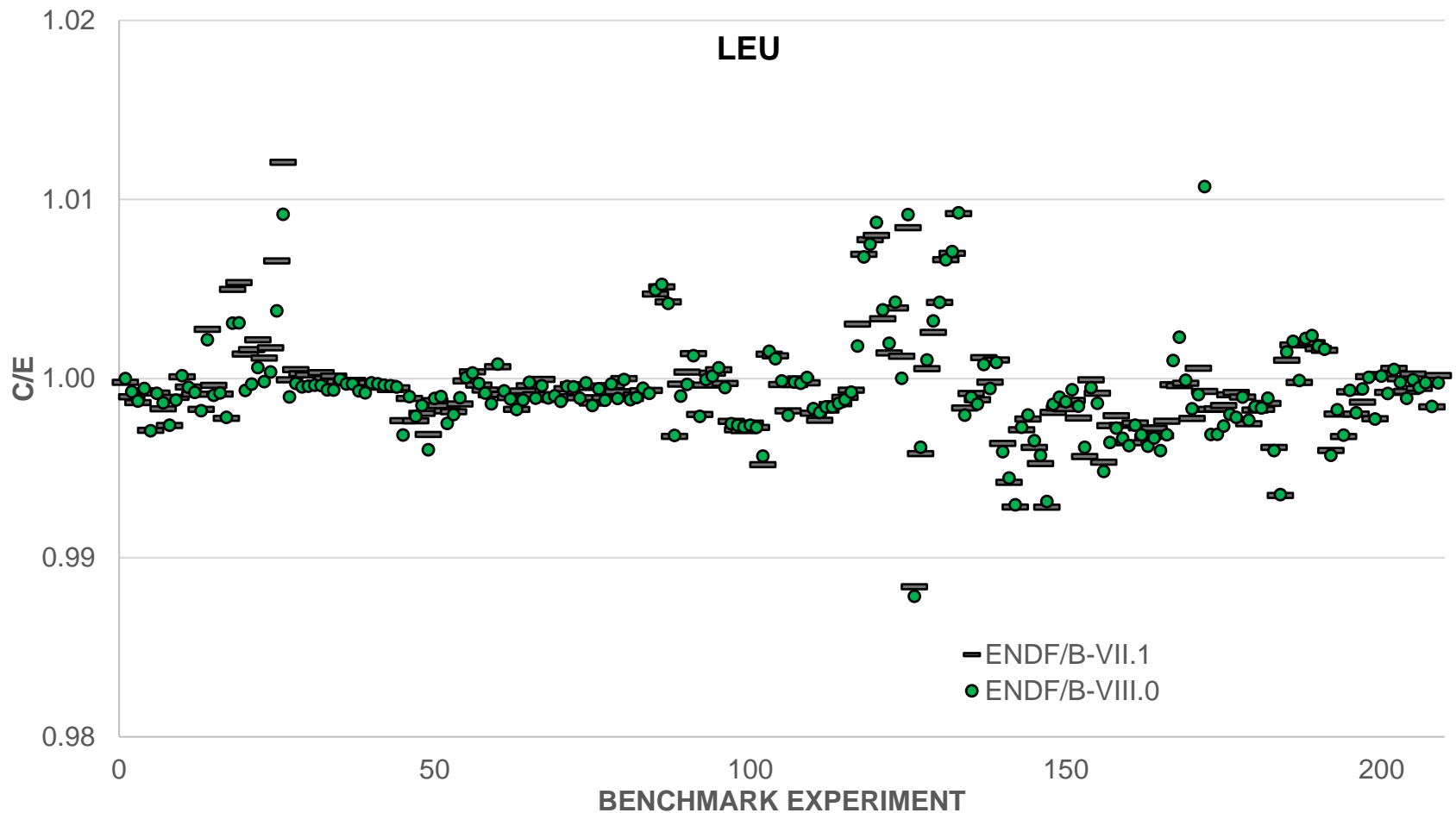


# Results of Whisper Library, 209 LEU cases

- ENDF/B-VIII.0 results**

– Same for LEU

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: LEU	209	0.28	0.9995	0.0028	0.28	0.9994	0.0027



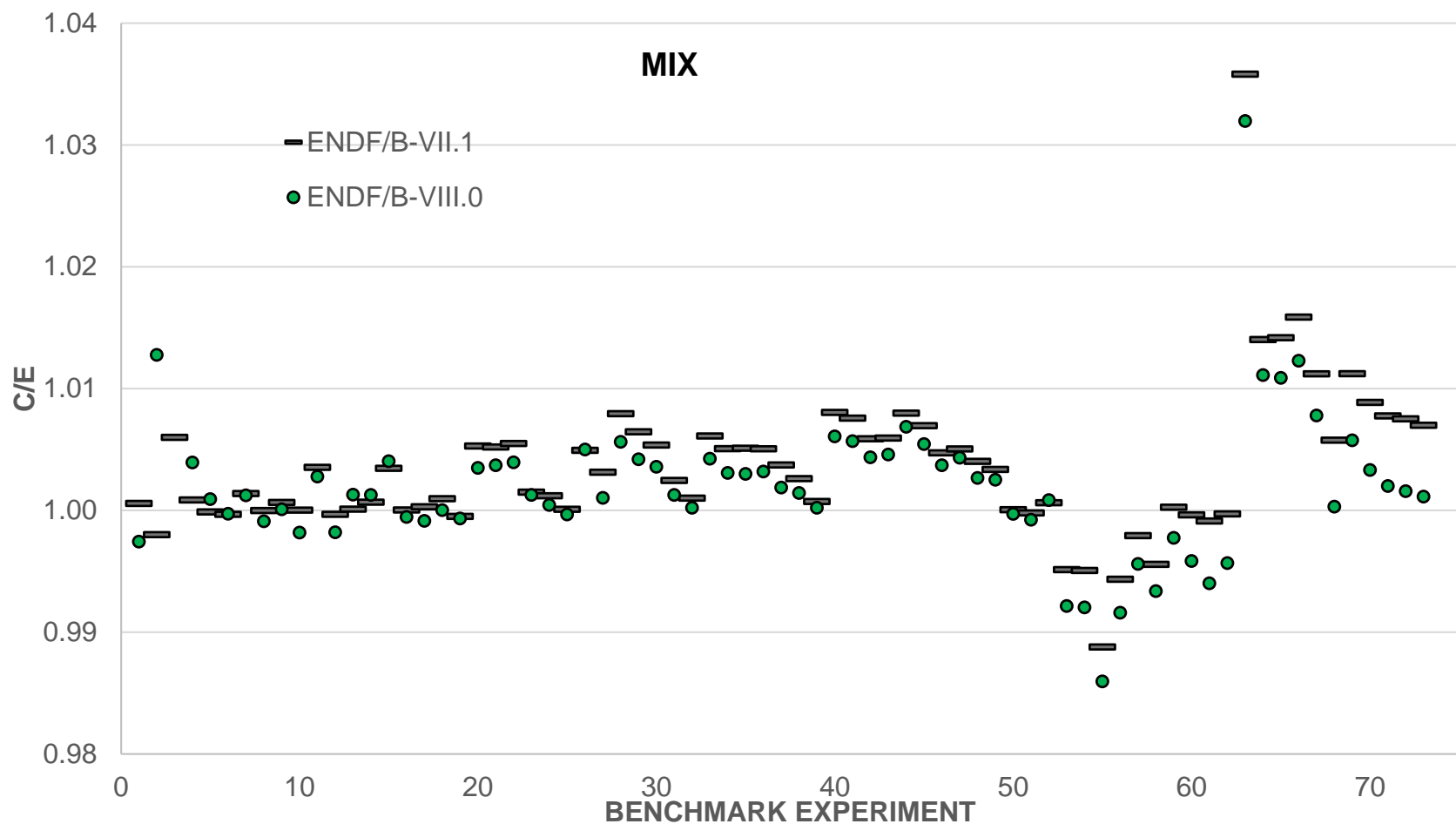
# Results of Whisper Library, 73 MIX cases

- ENDF/B-VIII.0 results**

- Improved for MIX

- MMF4,7 improved be-met

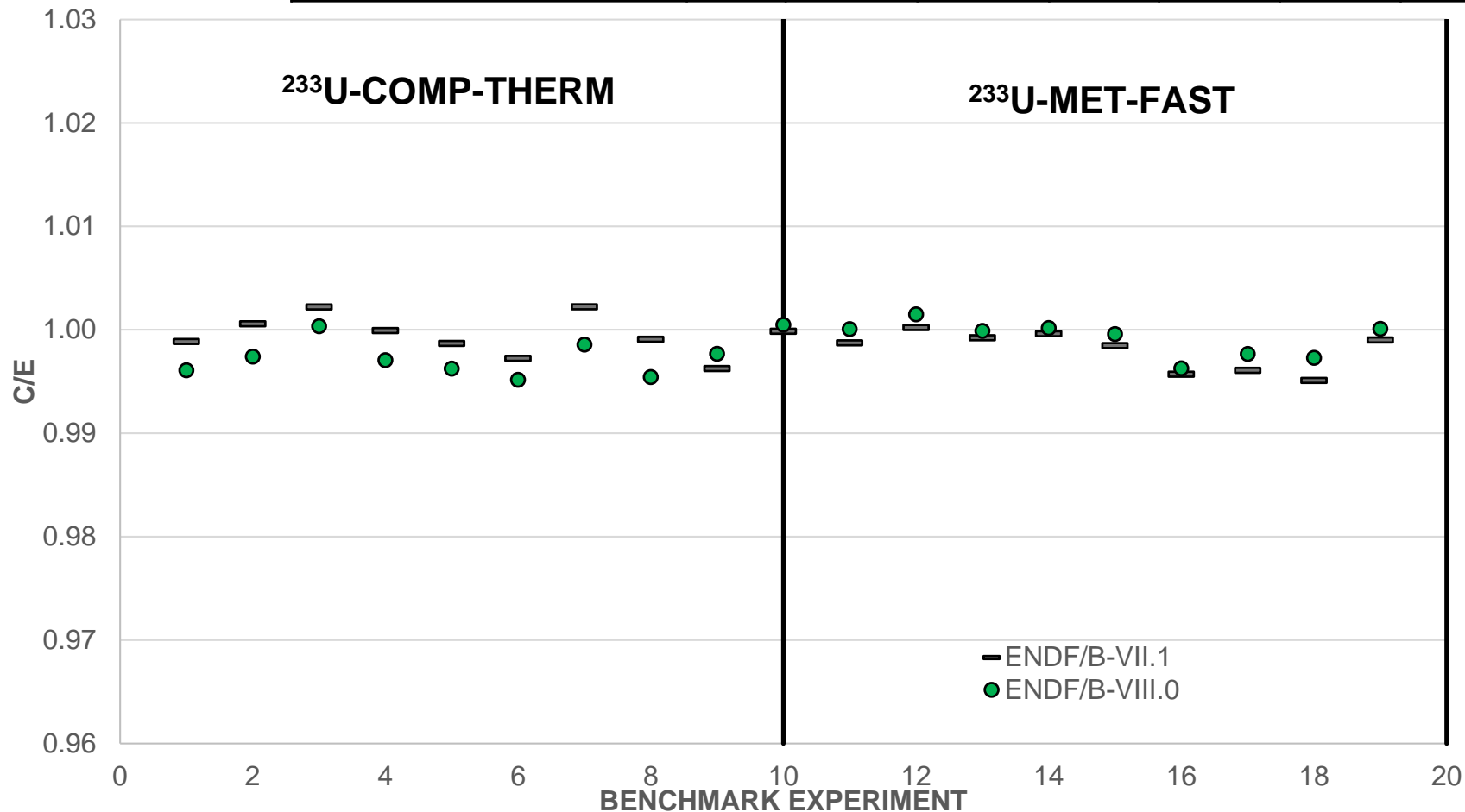
Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: MIX	73	0.70	1.0035	0.0060	0.61	1.0018	0.0058



# Results of Whisper Library, 19 $^{233}\text{U}$ CT,MF cases

- **ENDF/B-VIII.0**
- Improved UCT004 w/ d-d2o, improved UMF

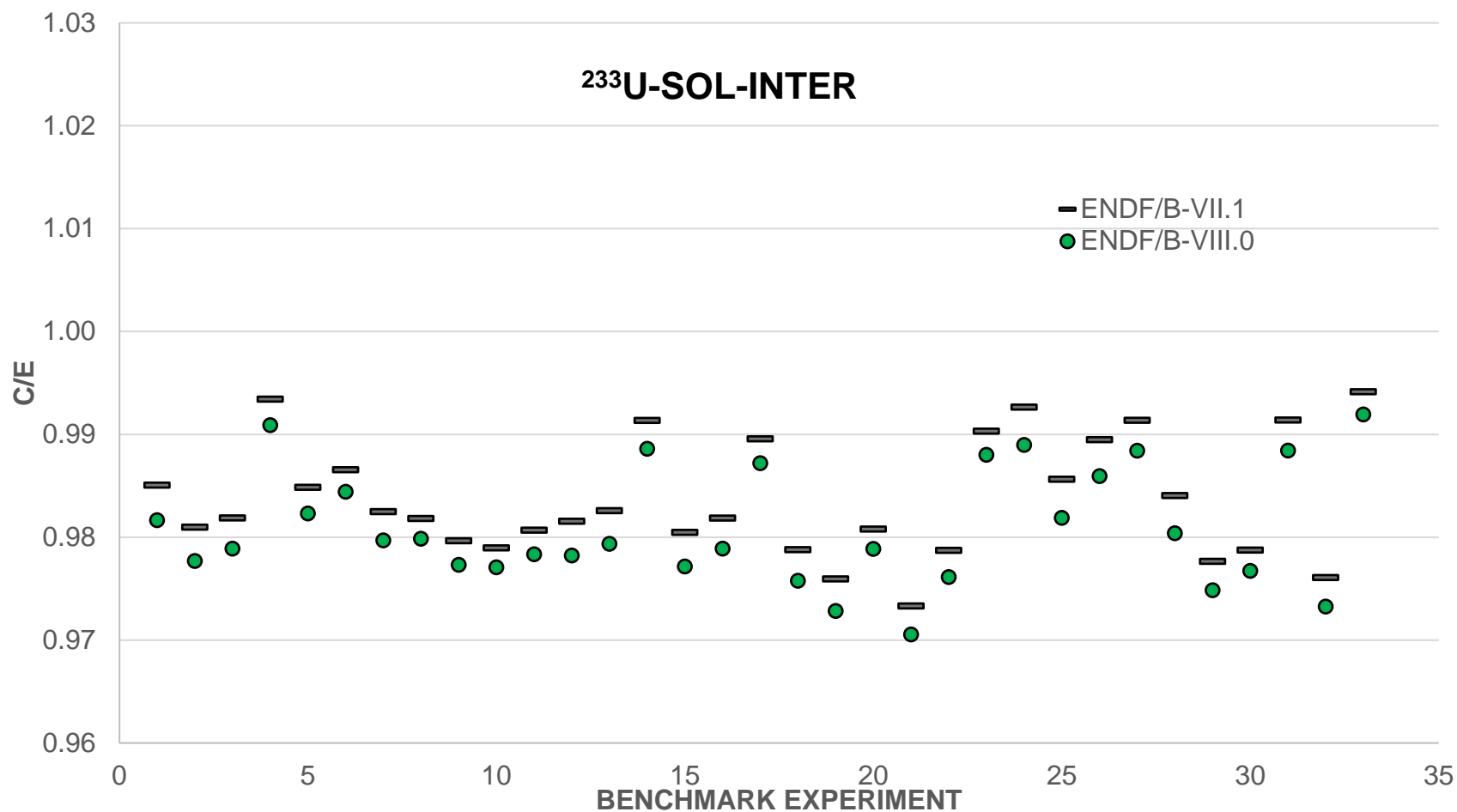
Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: $^{233}\text{U}$	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102
WHISPER: $^{233}\text{U}$ : COMP-THERM	9	0.20	0.9995	0.0020	0.33	0.9971	0.0016
WHISPER: $^{233}\text{U}$ : MET-FAST	10	0.25	0.9982	0.0019	0.17	0.9993	0.0017



# Results of Whisper Library, 33 $^{233}\text{U}$ cases

- **ENDF/B-VIII.0**
- Poor performance in USI for –VII.1 & VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: $^{233}\text{U}$	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102
WHISPER: $^{233}\text{U}$ : SOL-INTER	33	1.72	0.9837	0.0056	1.99	0.9809	0.0056



# Results of Whisper Library, 106 $^{233}\text{U}$ cases

- **ENDF/B-VIII.0**
- Poor performance in UST thermal energy for –VII.1 & VIII.0

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
WHISPER: $^{233}\text{U}$	158	1.06	0.9964	0.0100	1.18	0.9939	0.0102
WHISPER: $^{233}\text{U}$ : SOL-THERM	106	0.87	0.9999	0.0087	0.92	0.9971	0.0088

