Updated: Fast Benchmarking of ENDF/B-VIII beta Files

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Background

- “First, do no harm”. (Chadwick Nov 2012, LA-UR-12-26066)
- An update to my 2016 talk in the validation session
- This work aims to ensure that the good fit to Fast Benchmark k-effectives, seen in VII.0 and VII.1 is maintained in VIII.
- Will also highlight any issues associated with group-wise processing.

The Benchmark Suite

- A suite of simple spherically symmetric systems taken from the ICSBEP.
  - U5/Pu/U3/MIXed cores.
  - Fast systems.
  - Metal systems.

ICSBEP BENCHMARK SYSTEMS	
HEU-MET-FAST-001	PU-MET-FAST-026
HEU-MET-FAST-018	PU-MET-FAST-027
HEU-MET-FAST-027	PU-MET-FAST-028
HEU-MET-FAST-028	PU-MET-FAST-029
HEU-MET-FAST-002	PU-MET-FAST-002
HEU-MET-FAST-032	PU-MET-FAST-030
HEU-MET-FAST-003	PU-MET-FAST-031
HEU-MET-FAST-057	PU-MET-FAST-032
MIX-MET-FAST-001	PU-MET-FAST-005
MIX-MET-FAST-002	PU-MET-FAST-006
MIX-MET-FAST-007	PU-MET-FAST-008
PU-MET-FAST-010	PU-MET-FAST-009
PU-MET-FAST-011	U233-MET-FAST-001
PU-MET-FAST-018	U233-MET-FAST-002
PU-MET-FAST-001	U233-MET-FAST-003
PU-MET-FAST-022	U233-MET-FAST-004
PU-MET-FAST-023	U233-MET-FAST-005
PU-MET-FAST-024	U233-MET-FAST-006
PU-MET-FAST-025	

Data and Processing

- Existing data from VII.0 and VII.1 compared to newly processed data from NNDC Gforge tagged as beta4.1 and beta5.

- ENDFB-VIII betas were processed into group-wise format using NJOY 2012 and NJOY2016.

- Data were further processed into for use in a proprietary deterministic transport code.

Processing Errors

- NJOY2012.64 processes all but U235 and Pu239 in beta 5 with no errors.
- U235 and Pu239 from beta5 required NJOY2016 commit aa2ada4.

- Ho166m1 fails during local checking
  - Energy range partial matrices and cross sections don’t agree.
- Sub-Actinide fission, TENDL data have MT18 in MF8/10.

Comparisons

- Calculations were performed on a 460 group energy grid ranging from 1e-9 to 20 MeV.
- Results were compared to the benchmark k-effectives (C-E). These C-Es were then compared for each beta library.
- The results were also compared as an ensemble using 2 goodness of fit metrics.

“Goodness of fit” metrics

“Chi Squared”

$$\text{“}\chi^2\text{“} = \Sigma \frac{((k_{calc} - k_{exp})/\delta k_{exp})^2}{n}$$

- Traditional Chi squared test but accounts for the uncertainty in the experimental value.
- If χ<1 then, on average calculations match benchmarks to within experimental error.

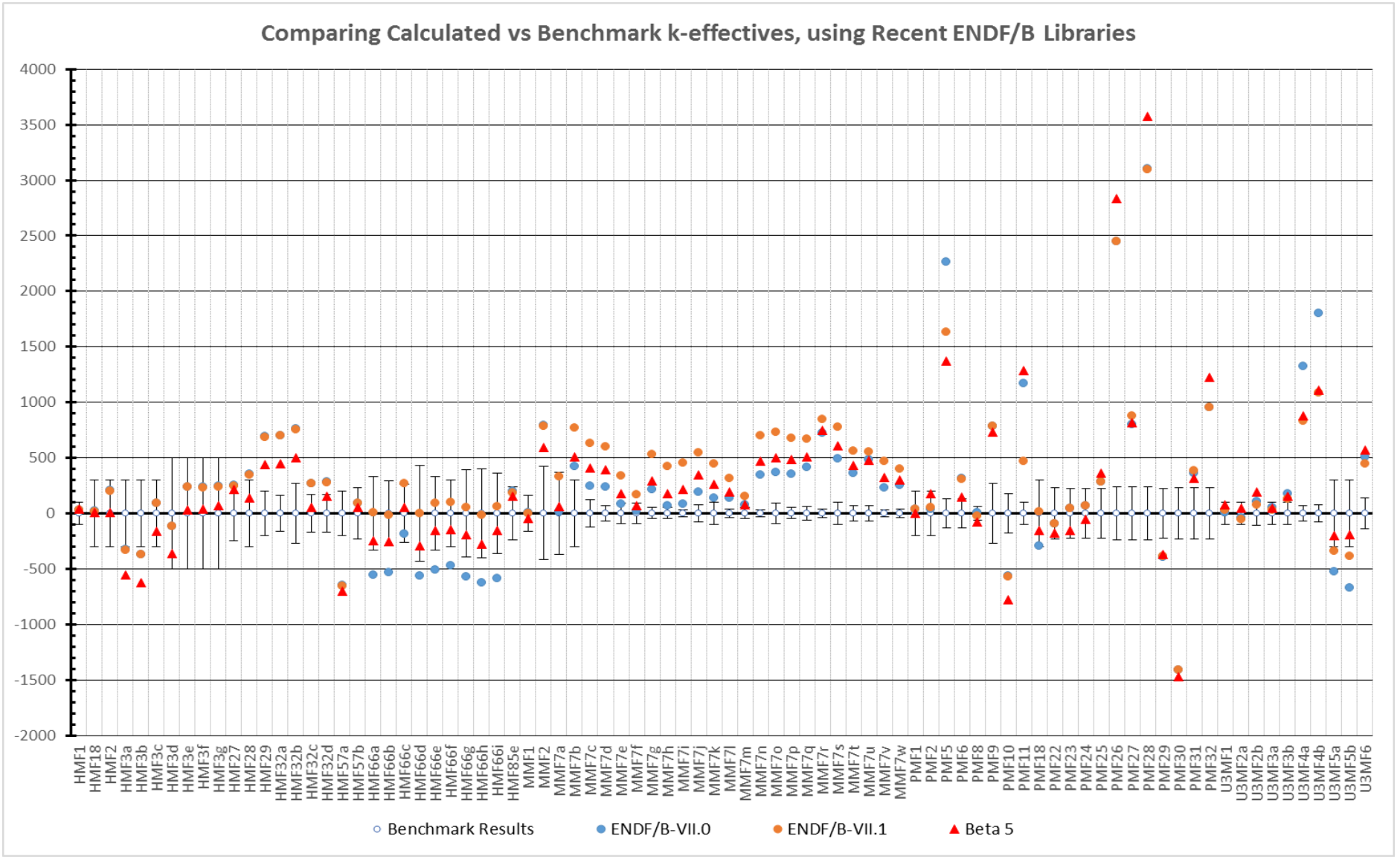
Average Difference

$$\langle|\Delta|\rangle = \Sigma \frac{|k_{calc} - k_{exp}|}{n}$$

- Magnitude of the average difference between Calculation and Benchmark k-effective.
- In pcm, smaller values show better fit to benchmarks

- May not be statistically correct, however both metrics give reliable indications of how well data reproduce benchmark calculations.

The Full Suite of Results



Goodness of Fit Metrics

	ENDF/B-VII.0		ENDF/B-VII.1		Beta 1		Beta 2		Beta 3		Beta 4.1		Beta 5	
	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq
ALL	454.53	31.33	439.89	42.00	457.97	44.50	434.20	40.97	445.62	48.79	413.00	29.22	412.93	29.21
HEU	370.22	2.86	230.92	2.17	245.62	1.62	181.38	1.35	181.33	1.35	223.613	1.4617	223.8	1.4623
MIX	271.86	33.82	515.32	102.96	527.12	108.89	475.67	93.49	543.19	121.75	346.12	51.26	346.00	51.25
PU	771.67	40.58	697.63	27.54	758.25	36.09	817.34	41.17	778.07	37.86	804.36	37.94	803.92	37.91
Bare	79.34	0.44	81.83	0.44	103.28	0.60	81.29	0.47	80.77	0.46	110.63	0.62	110.63	0.62
U	338.55	3.94	330.14	3.69	272.26	2.59	252.03	2.37	252.97	2.33	277.02	3.19	277.02	3.19
Be	345.05	24.90	384.62	73.56	430.39	77.91	361.64	66.83	410.88	87.01	294.92	36.68	295.00	36.66
All-Be	545.51	37.96	479.15	19.51	495.82	24.07	503.82	25.83	490.58	25.43	513.17	26.74	513.00	26.73

Overall Performance

	ENDF/B-VII.0		ENDF/B-VII.1		Beta 1		Beta 2		Beta 3		Beta 4.1		Beta 5	
	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq
ALL	454.53	31.33	439.89	42.00	457.97	44.50	434.20	40.97	445.62	48.79	413.00	29.22	412.93	29.21

- K-effectives similar to 7.0/7.1/previous betas
- Overall b5 performs better than both 7 and 7.

Different Core Materials

	ENDF/B-VII.0		ENDF/B-VII.1		Beta 1		Beta 2		Beta 3		Beta 4.1		Beta 5	
	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq
ALL	454.53	31.33	439.89	42.00	457.97	44.50	434.20	40.97	445.62	48.79	413.00	29.22	412.93	29.21
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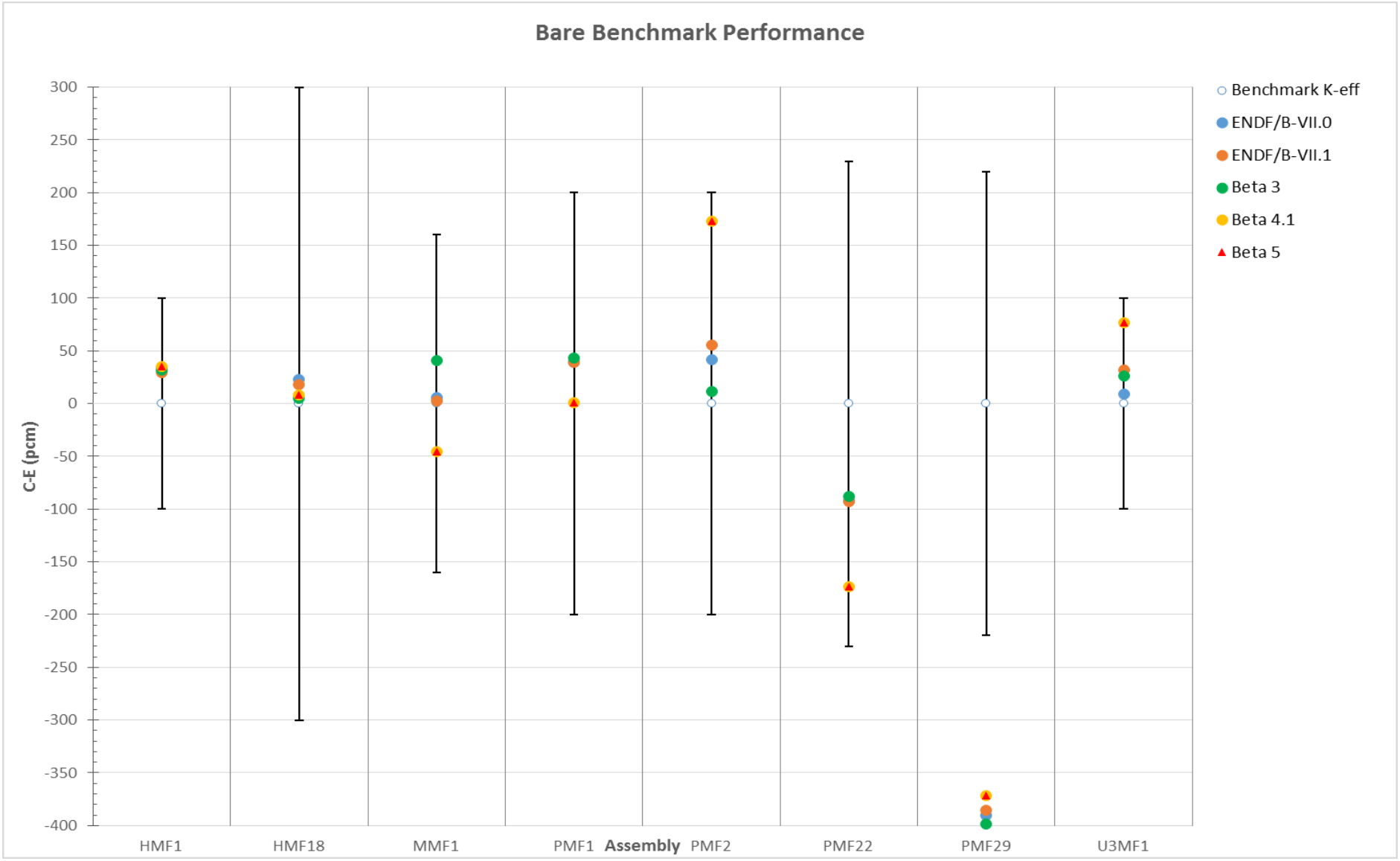
- Performance gains caused mainly by large improvement in Mixed Metal Systems since 7.1. “Chi squared” is halved.
- Pu systems worse than 7.1 better than 7.0
  - Different for “Chi squared” and average difference.

Bare Benchmarks

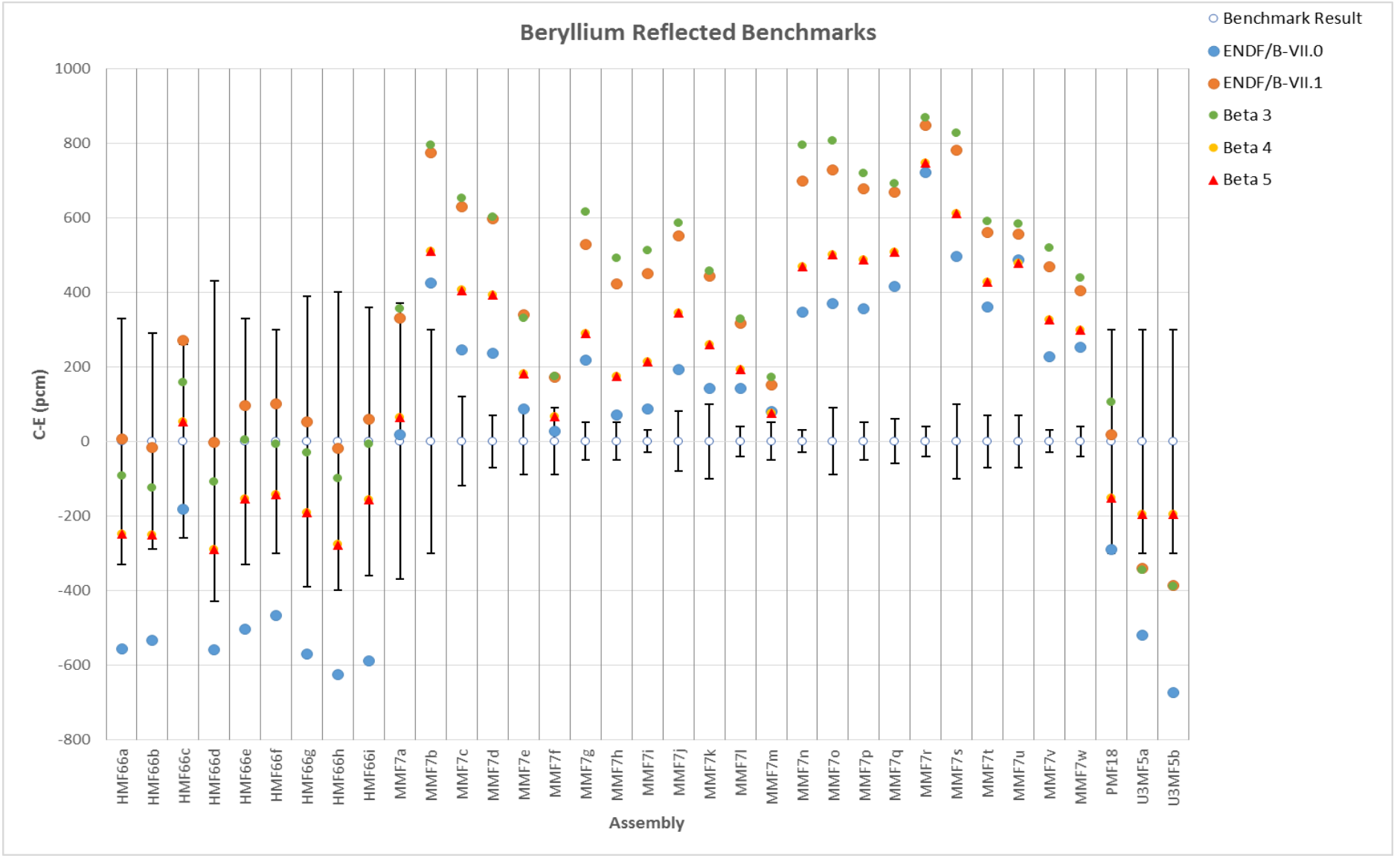


Reflectors

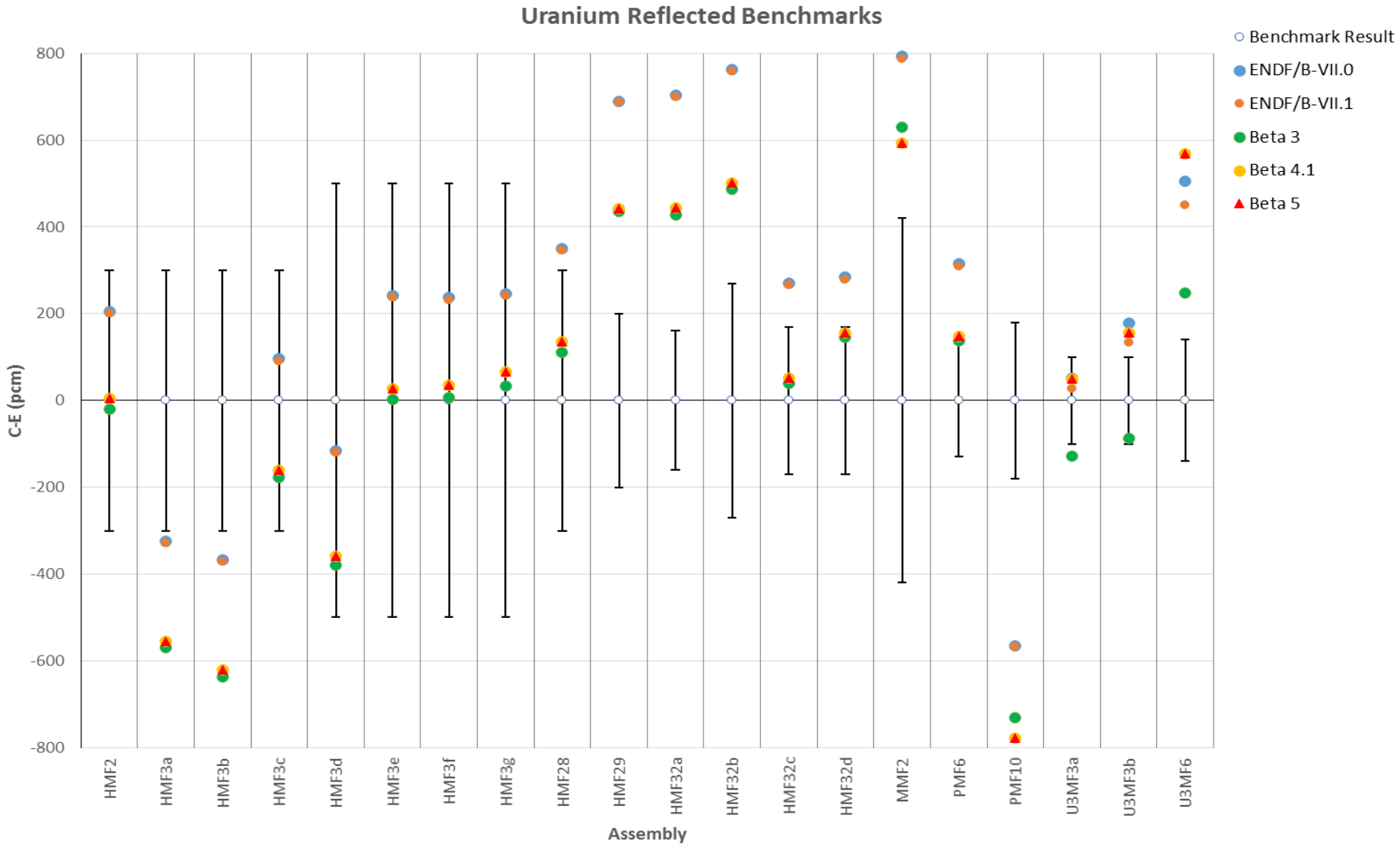
	ENDF/B-VII.0		ENDF/B-VII.1		Beta 1		Beta 2		Beta 3		Beta 4.1		Beta 5	
	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq	Ave Diff	Chi Sq
Bare	79.34	0.44	81.83	0.44	103.28	0.60	81.29	0.47	80.77	0.46	110.63	0.62	110.63	0.62
U	338.55	3.94	330.14	3.69	272.26	2.59	252.03	2.37	252.97	2.33	277.02	3.19	277.02	3.19
Be	345.05	24.90	384.62	73.56	430.39	77.91	361.64	66.83	410.88	87.01	294.92	36.68	295.00	36.66

- Be still “interesting”
  - Ave Diff better than both 7 and 7.1
  - “Chi squared” sits between that for 7 and 7.1
    - Perhaps extreme values have improved more than those close to the error bar.
  - Calculations that were high with 7.0 are reduced without taking those calculated low outside the error bars.

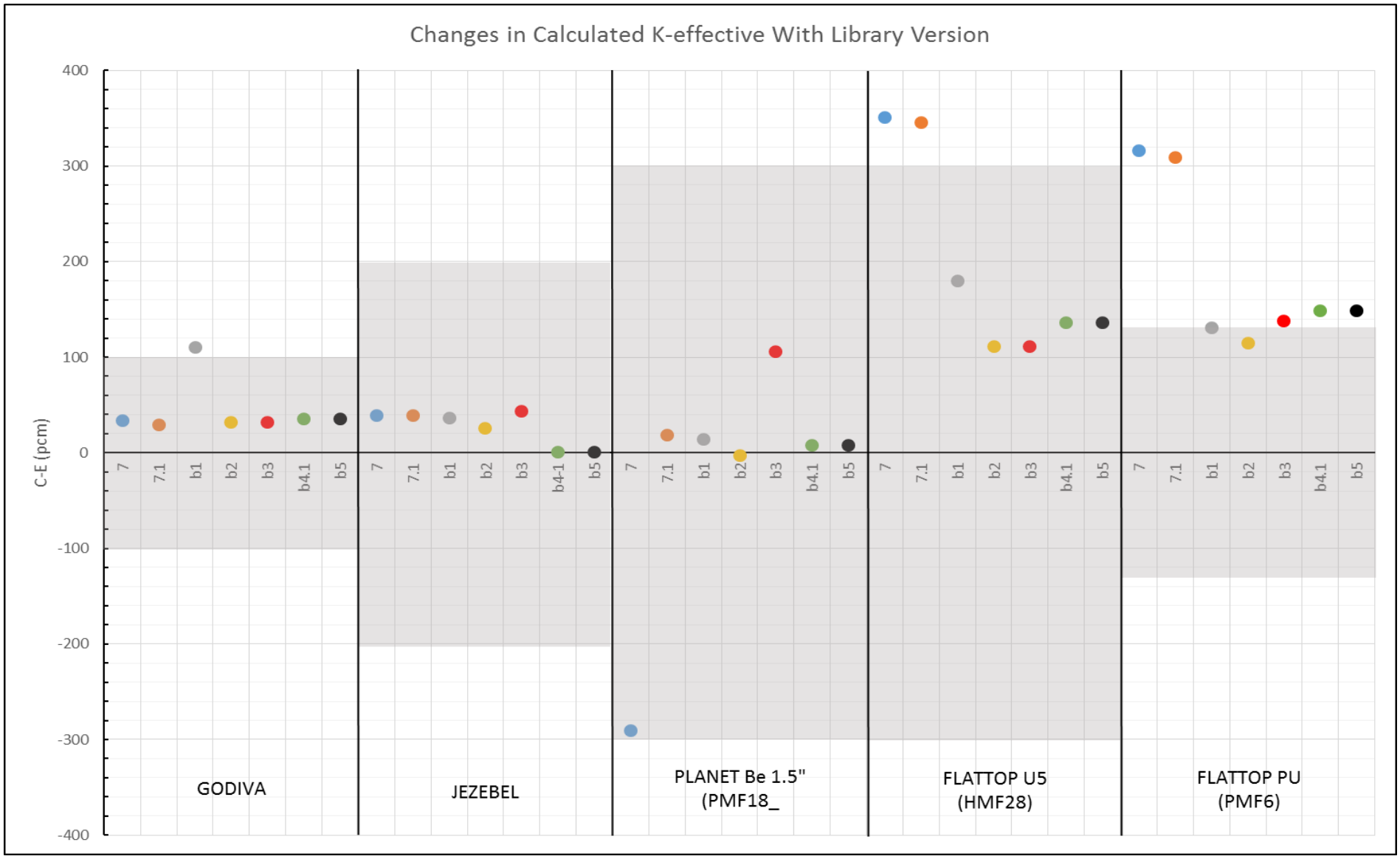
Beryllium Reflected Benchmarks



Uranium Reflected Benchmarks



Fit to Benchmark vs Library Version



Summary

- Libraries successfully processed for group-wise purposes with no major issues.
- “First, do no harm”.

- Many physics improvements to data, though good match to fast assemblies is maintained.