Fast Benchmarking of ENDF/B-VIII beta Files

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Background

- "First, do no harm". (Chadwick Nov 2012, LA-UR-12-26066)

- Since 2012, significant $ and hrs have been spent updating ENDF/B-VII.1.

- Many significant changes to benchmark calculations.

- 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 beta1, beta2 and beta3.

- ENDFB-VIII betas were processed into group-wise format using NJOY 2012.64 (Thanks Skip).

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

Processing Errors

- C^{12} no MF1 MT451.

- As^{73} error in Iunion, ill behaved threshold (fixed for Beta 3).

- Es^{254m1} and Es^{255} no MF1 MT451.

- Fe^{56} in Beta 3, issue in MF1

- Also Ho^{166m1} fails during local checking due to error in matrix data.

  - Yet to determine if this is a code or evaluation problem.

Comparisons

- Calculations were performed on a 460 group energy 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 $\chi < 1$ 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

Comparing Calculated vs Benchmark k-effectives, using Recent ENDF/B Libraries
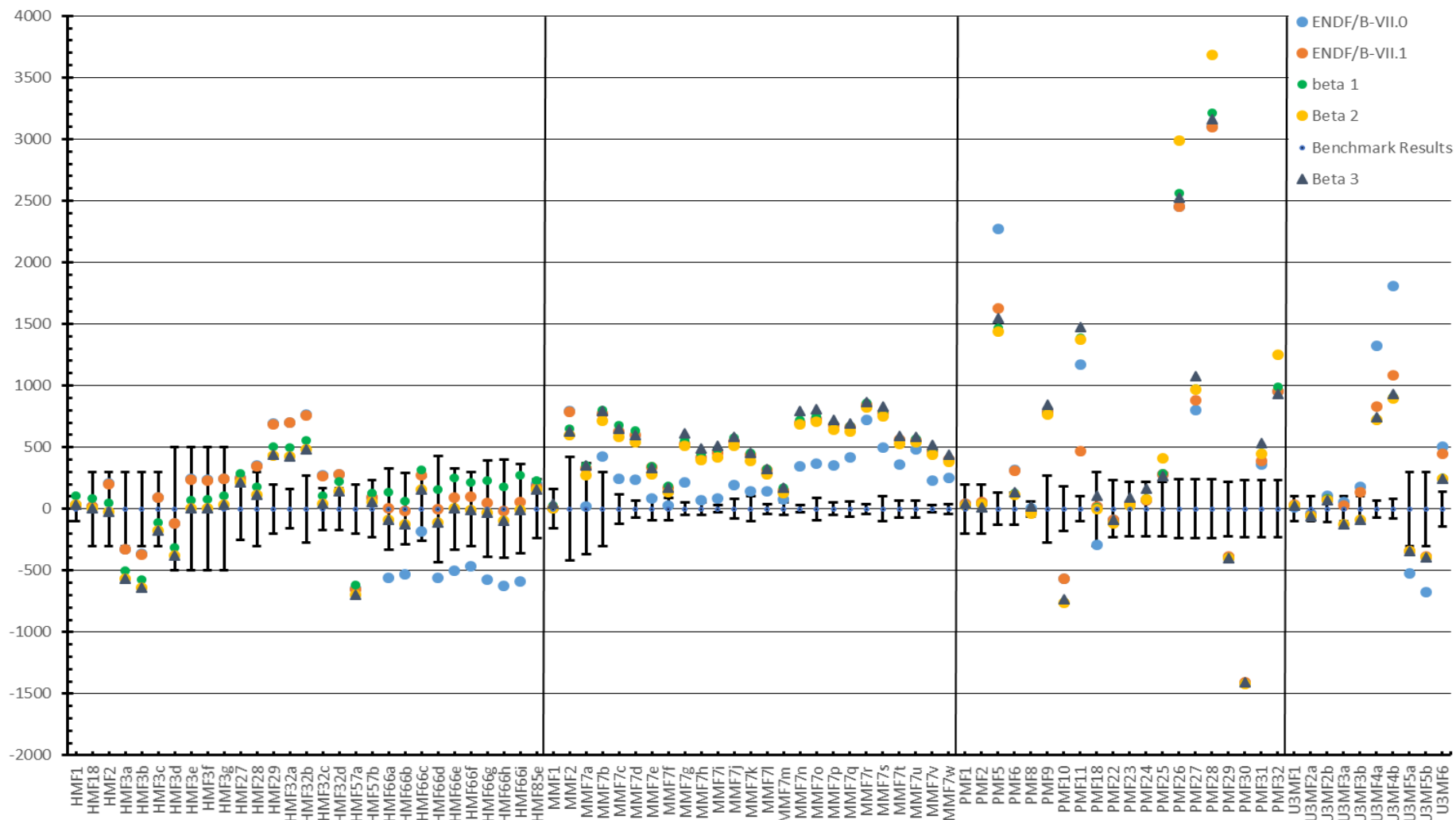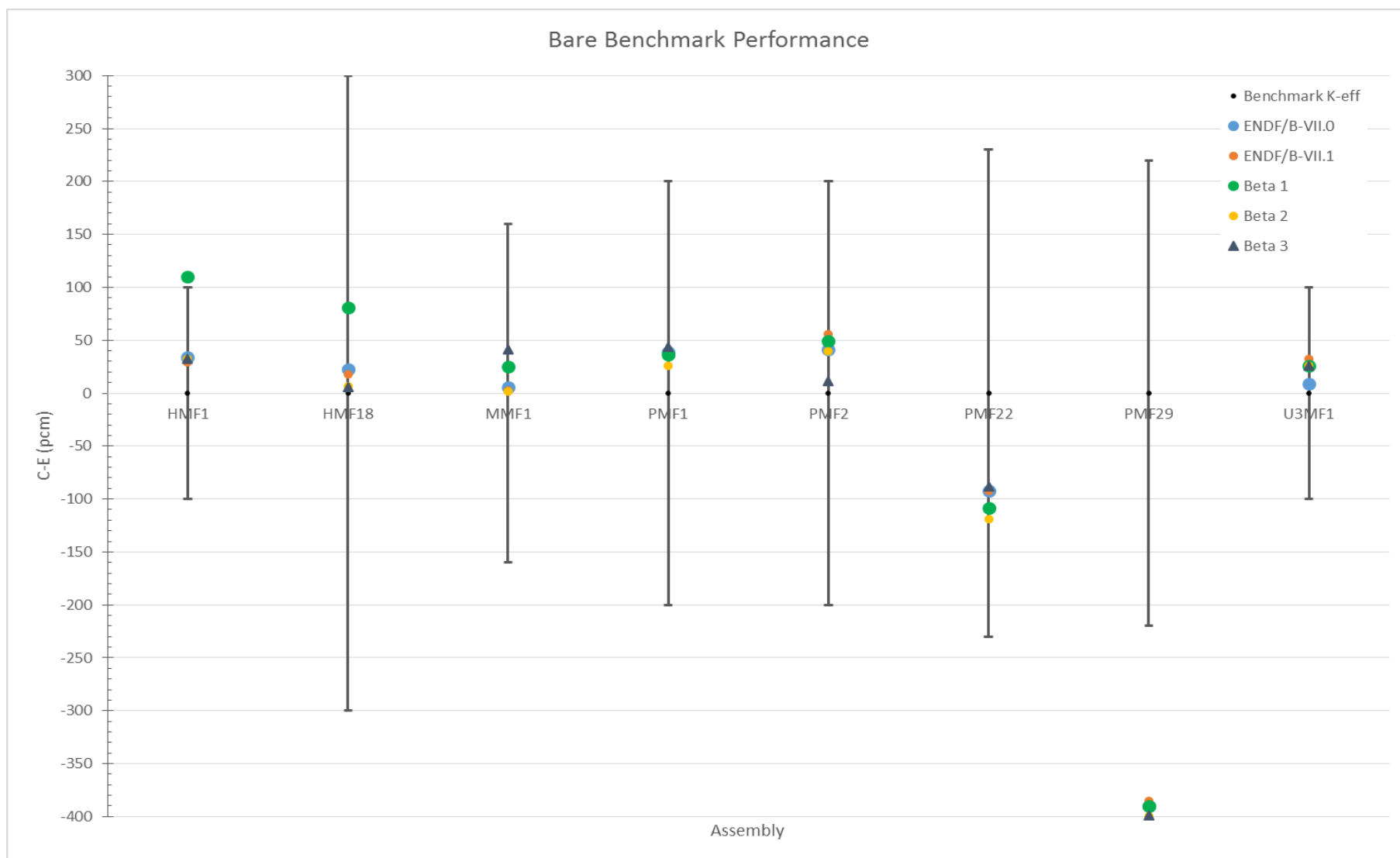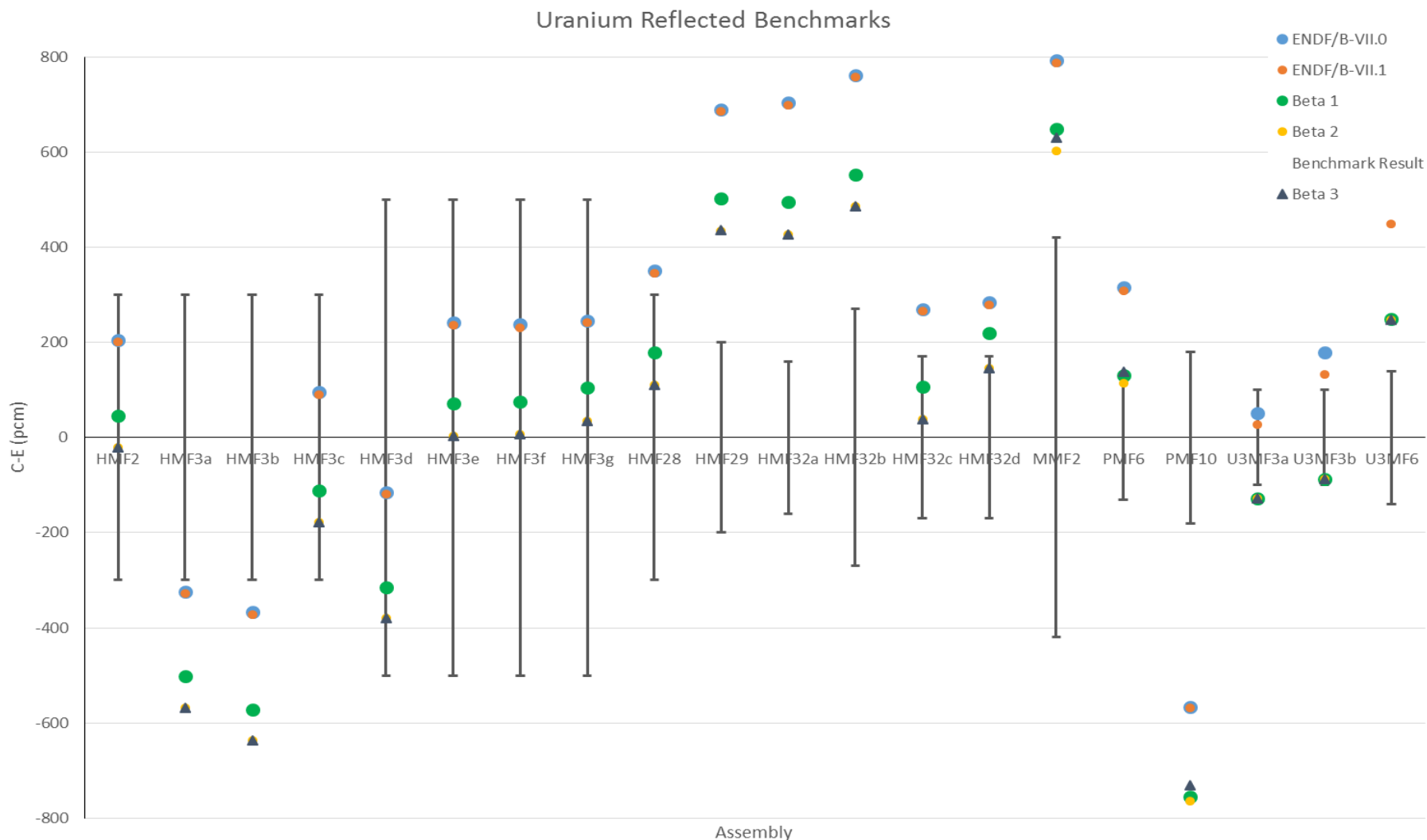
Goodness of Fit Metrics

	ENDF/B-VII.0		ENDF/B-VII.1		Beta 1		Beta 2		Beta 3	
	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
HEU	370.22	2.86	230.92	2.17	245.62	1.62	181.38	1.35	181.33	1.35
MIX	271.86	33.82	515.32	102.96	527.12	108.89	475.67	93.49	543.19	121.75
PU	771.67	40.58	697.63	27.54	758.25	36.09	817.34	41.17	778.07	37.86
Bare	79.34	0.44	81.83	0.44	103.28	0.60	81.29	0.47	80.77	0.46
U	338.55	3.94	330.14	3.69	272.26	2.59	252.03	2.37	252.97	2.33
Be	345.05	24.90	384.62	73.56	430.39	77.91	361.64	66.83	410.88	87.01
All-Be	545.51	37.96	479.15	19.51	495.82	24.07	503.82	25.83	490.58	25.43

Bare Benchmarks

Bare Benchmark Performance

Legend:
- Benchmark K-eff
- ENDF/B-VII.0
- ENDF/B-VII.1
- Beta 1
- Beta 2
- Beta 3

C-E (pcm)

Assembly: HMF1, HMF18, MMF1, PMF1, PMF2, PMF22, PMF29, U3MF1

Uranium Reflected Benchmarks

Uranium Reflected Benchmarks

Beryllium Reflected Benchmarks
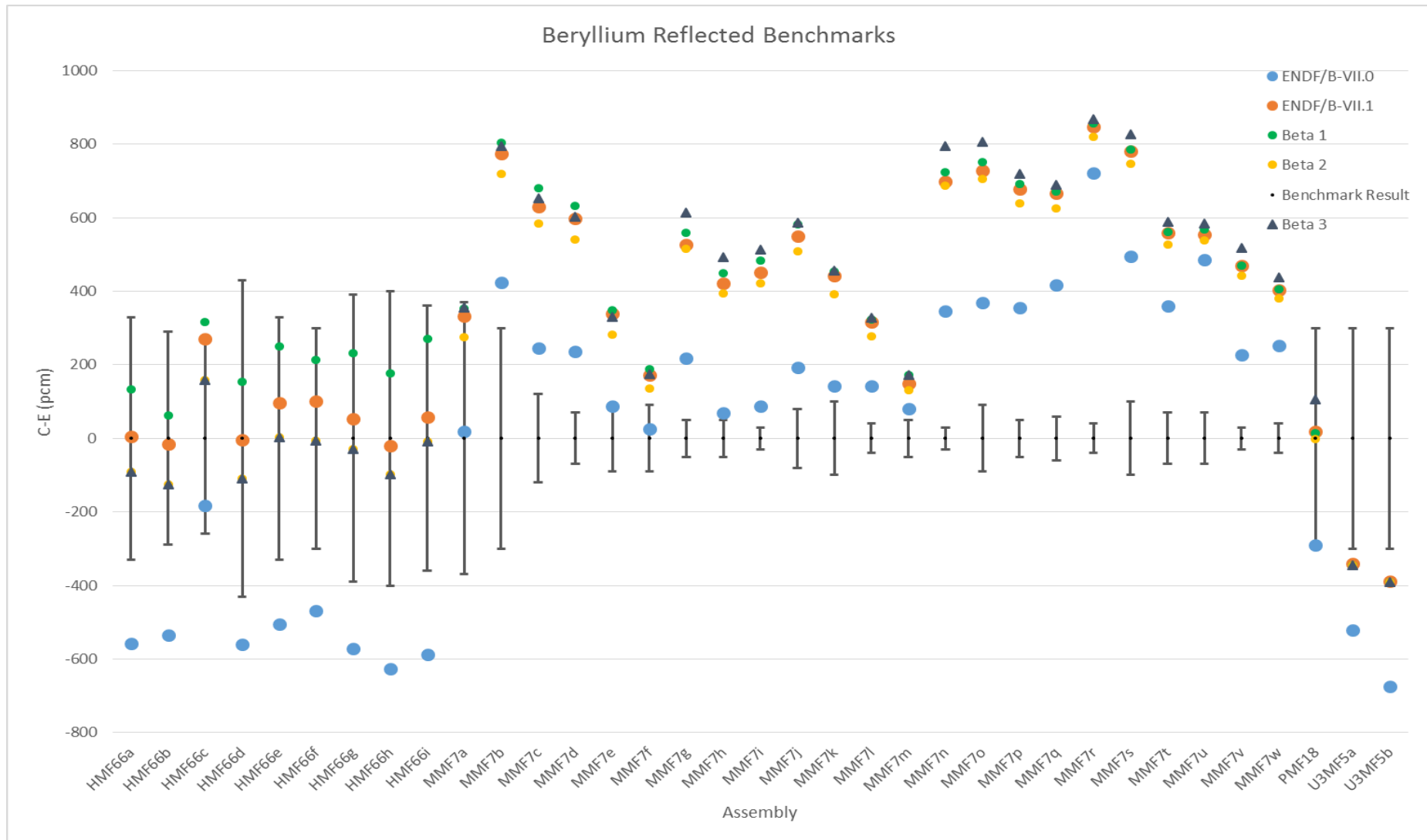
Fit to Benchmark vs Library Version

Changes in Calculated K-effective With Library Version
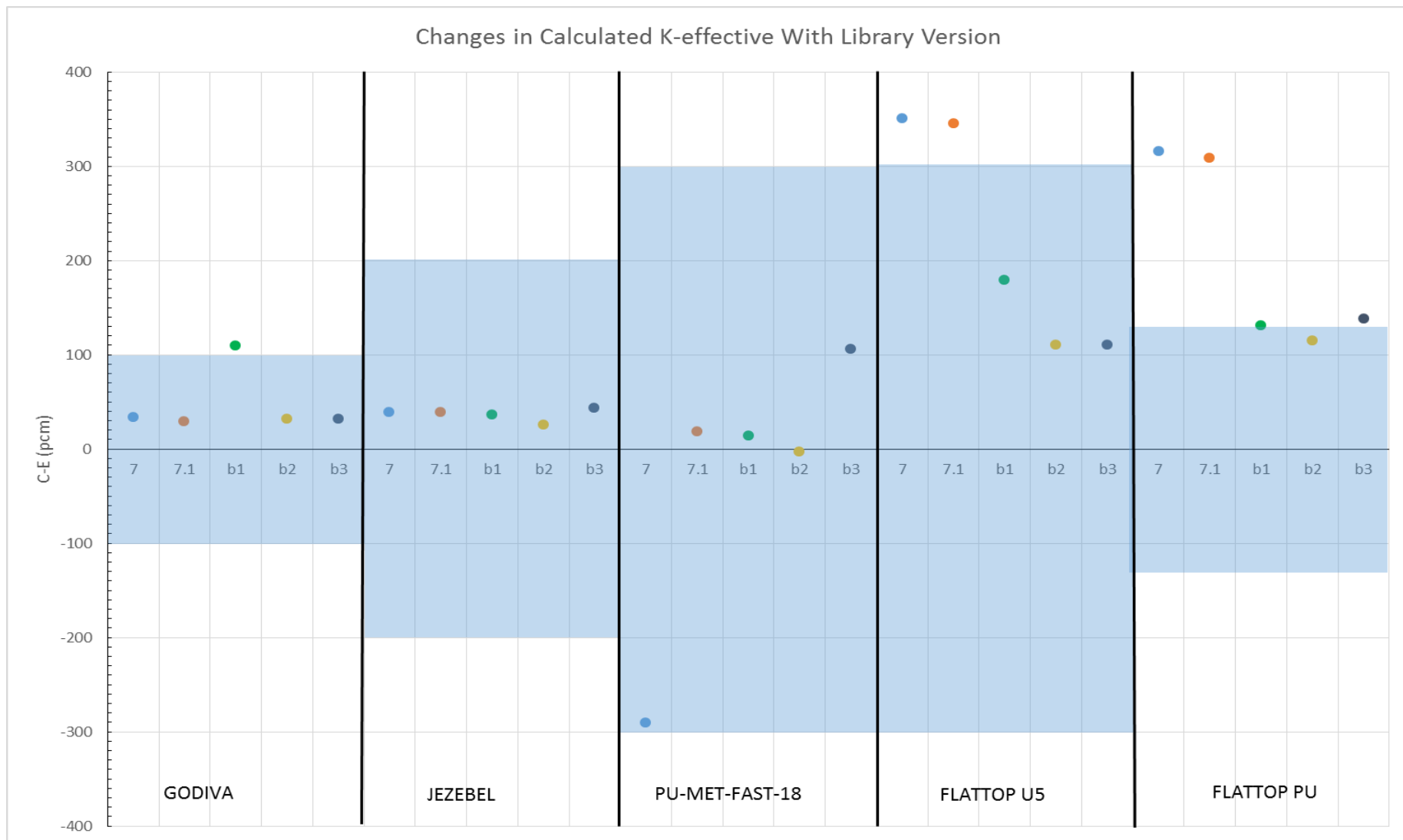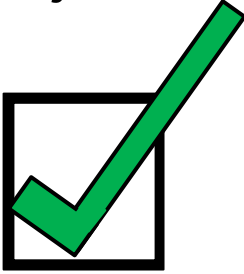
Summary

- Libraries successfully processed for group-wise purposes with no major issues.

- "First, do no harm".

- Good Match to Fast Assemblies is maintained.
  - Slight improvement for HEU.
  - Slightly worse for Pu, but beta 3 starting to bring it back to VII.1.
  - Be reflectors improvement seen in b2 undone in b3 (Pu?) marked change in PMF18.