Multi-Application Validation of ENDF/B-VIII.1

Jesse Brown, Kang Seog Kim, Rike Bostelmann, Germina Ilas

Oak Ridge National Laboratory

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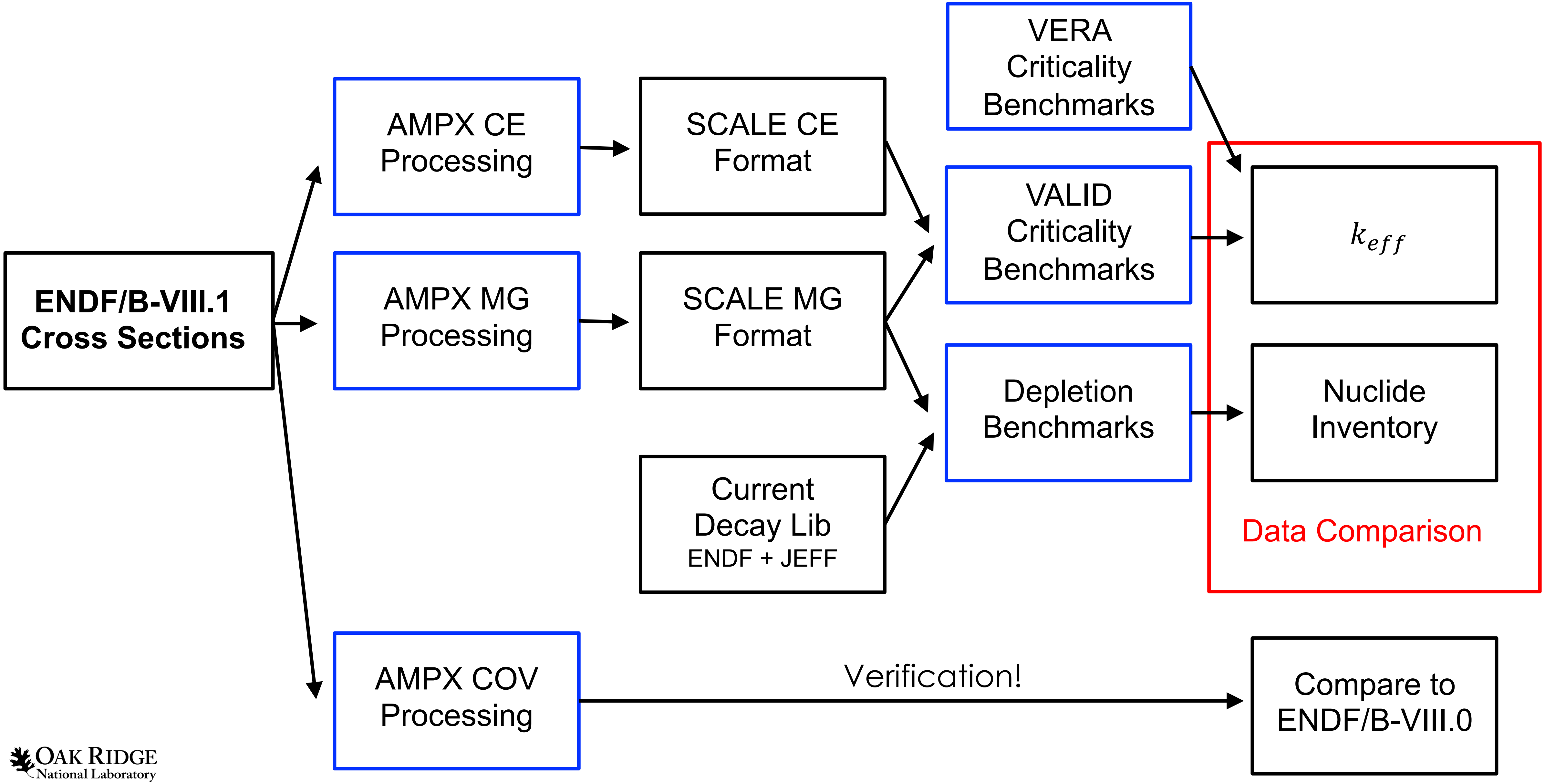
ENDF-8.1 Validation Methods Supporting NRC



ORNL Definition of 8.1-beta2 for testing

- neutrons : commit b8fdd619, tag = version.VIII.1-Beta2 ***(but!)***:
  - Also tested ^{239}Pu $\bar{\nu}$ update from Capote
- photoat : commit e26c3d25, <no tags>, phase1
- thermal_scatt : e7c477bd5, tag = version.VIII.1-Beta2, ***(but!)***:
  - For conflicting files we use ORNL evaluations and new H_2O:
    - CH_2
    - $C_5O_2H_8$
    - H_2O (new low temp.)
  - We do not process:
    - Uranium/Plutonium TSLs (see Chris' talk)
    - Mixed-elastic TSLs
      - ZrH_2, ZrH_x, ZrC, N-UN, ^{7}LiH, ^{7}LiD
    - Too many Bragg edges
      - BeO, CF_2, ZrH_2
    - How to use?:
      - CaH_2

ENDF/B-VIII.1-beta2
(as of Oct. 1st, 2023)

Nuclear + Atomic physics issues

SCALE will be changed in the future to recognize new MT

AMPX memory issues when Bragg edges > 7000

AMPX processing

- SCALE-data size is becoming a problem **(due to TSLs)**
  - ENDF-7.1 = 19 GB
  - ENDF-8.0 = 28 GB (63 GB XML)
  - ENDF-8.1 = 96 GB (230 GB XML)
  - This is partially an “us” problem (SCALE XS sampling and Bragg edges)
  - Sometimes requires more memory than available in RAM for SCALE jobs

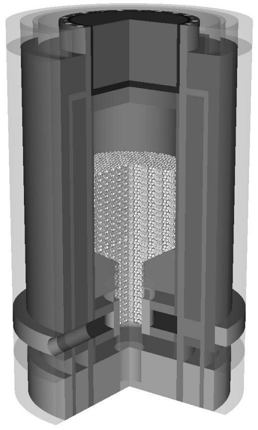
Validation & Verification

Use many different application spaces

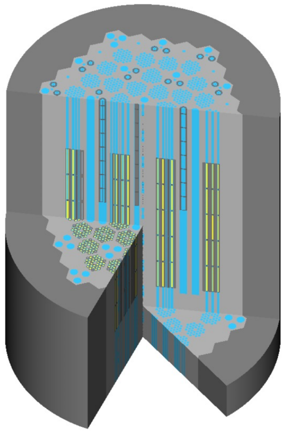
- Criticality benchmarks (VALID, *see Marshall & Greene talk*)
- Reactor Criticality (BWR, PWR, Advanced Reactors)
- Depletion RCA
- Depleted Fuel Reactivity (VERA Suite)

Validation: Advanced Reactor Criticality

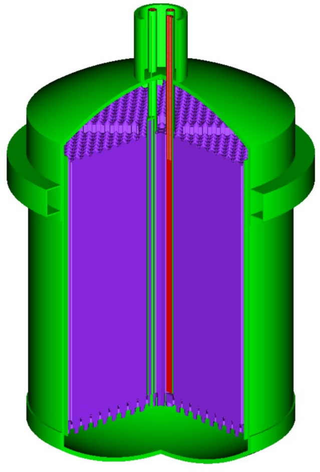
HTR-10	k_{eff}	Δk [pcm]
Benchmark	1.00000 +/- 0.00370	(ref)
ENDF/B-VII.1	1.00301 +/- 0.00019	301 +/- 370
ENDF/B-VIII.0	1.00650 +/- 0.00019	650 +/- 370
ENDF/B-VIII.1	1.00587 +/- 0.00019	587 +/- 370
HTTR		
Benchmark	1.00250 +/- 0.00710	(ref)
ENDF/B-VII.1	1.00725 +/- 0.00019	475 +/- 710
ENDF/B-VIII.0	1.01062 +/- 0.00019	812 +/- 710
ENDF/B-VIII.1	1.01013 +/- 0.00019	763 +/- 710
MSRE*		
Benchmark	0.99978 +/- 0.00420	(ref)
ENDF/B-VII.1	1.01917 +/- 0.00019	1939 +/- 420
ENDF/B-VIII.0	1.02168 +/- 0.00019	2190 +/- 420
ENDF/B-VIII.1	1.01776 +/- 0.00019	1798 +/- 420
EBR-II		
Benchmark	1.00927 +/- 0.00618	(ref)
ENDF/B-VII.1	1.00738 +/- 0.00019	-189 +/- 618
ENDF/B-VIII.0	1.00713 +/- 0.00019	-214 +/- 618
ENDF/B-VIII.1	1.00450 +/- 0.00019	-477 +/- 618



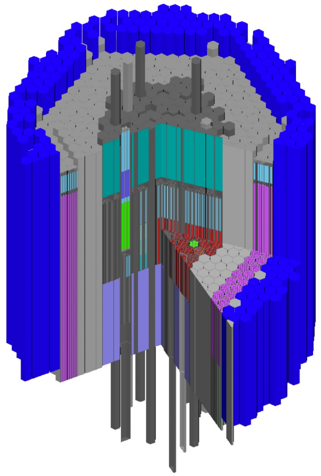
HTR-10* (pebble-bed HTGR)



HTTR* (prismatic HTGR)



MSRE* (graphite moderated MSR)



EBR-II* (SFR)

- Fresh fueled HTGR: similar performance of 8.1 vs. 8.0, but ~300 pcm difference to 7.1 because of ^{235}U and ^{238}U updates
- **Fresh fueled MSRE: almost 400 pcm difference between 8.1 and 8.0 almost exclusively because of ^{19}F updates**
- **SFR with HEU fuel at various levels of burnup: 260 pcm difference between 8.1 and 8.0, almost exclusively because of ^{52}Cr and ^{53}Cr updates**

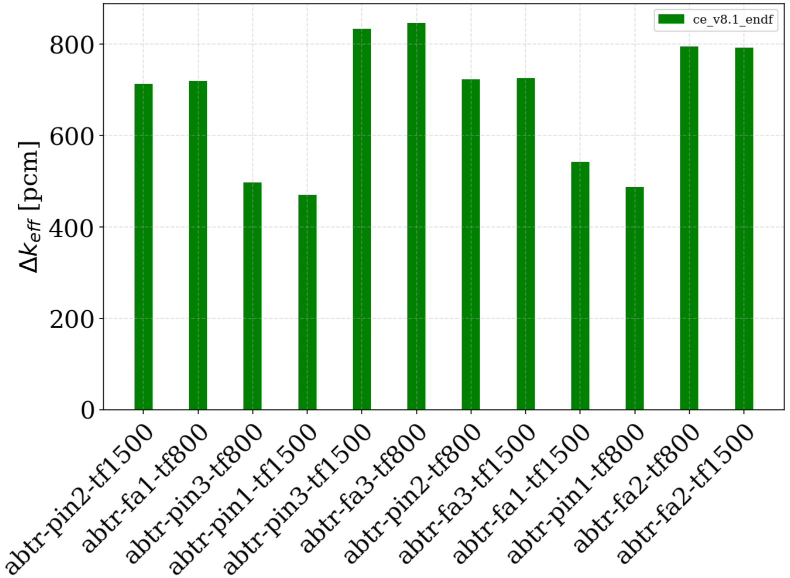
**Known discrepancy between MSRE calculation and experiment, update to specifications expected*

*Benchmarks specified in the IRPhE Handbook

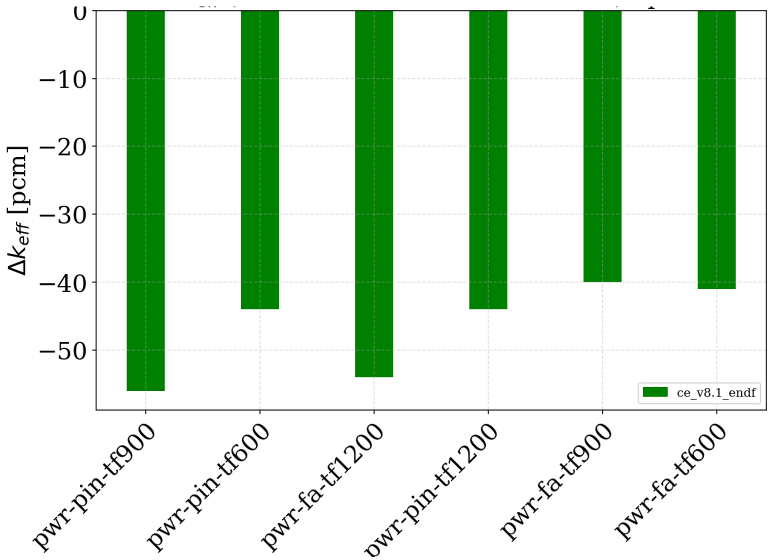
Verification: MADRE Suite

- Suite of simple unit cell and assembly based on various reactor concepts developed for SCALE library testing: LWR, HTGR, SFR, MSR
- k_{eff} results with ENDF/B-VIII.1 compared to ENDF/B-VIII.0

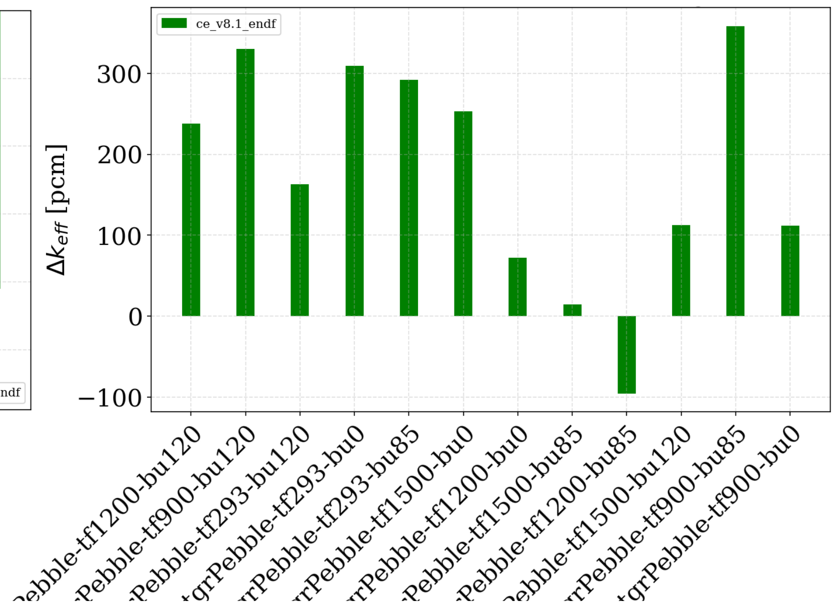
ABTR pin cells and assemblies



PWR pin cells and assemblies



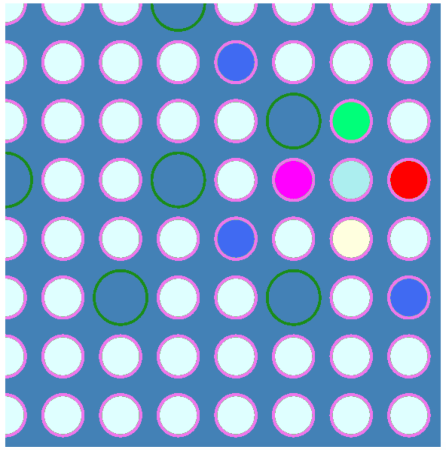
HTGR pebble



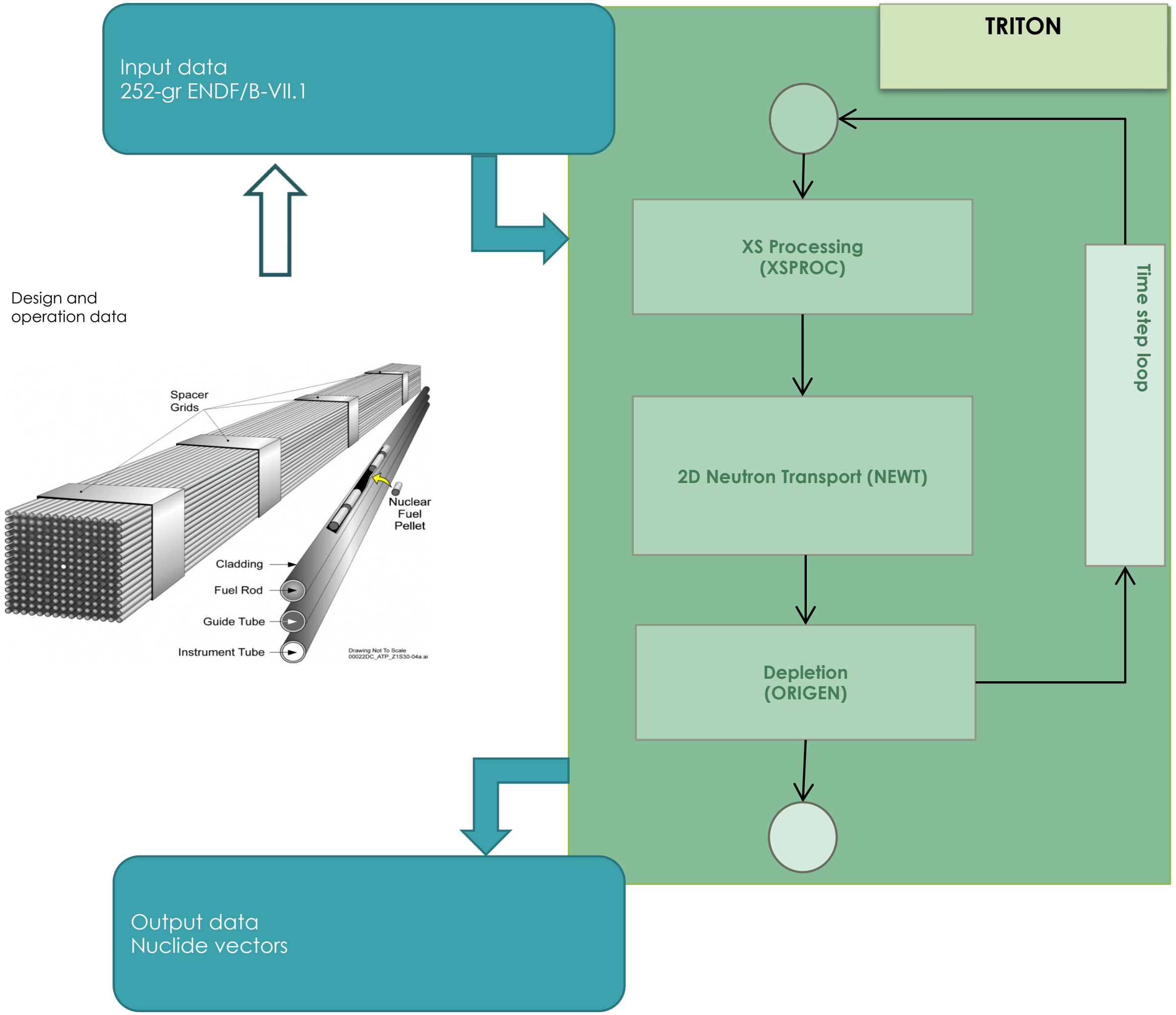
- Fresh fueled **LWR**: small k_{eff} differences of less than 150 pcm
- U/TRU fueled **SFR**: k_{eff} larger by up to 800 pcm
- **HTGR** models: k_{eff} differences between -220 and 800 pcm depending on temperature and burnup
- **MSR** models: k_{eff} differences between -220 and 300 pcm depending on burnup, temperature, spectrum (moderation)

Validation: Depletion RCA (Ilas)

- Goesgen/MALIBU
- GKN
- Radiochemical Analysis (RCA)
- ENDF-7.0/7.1 Decay Data

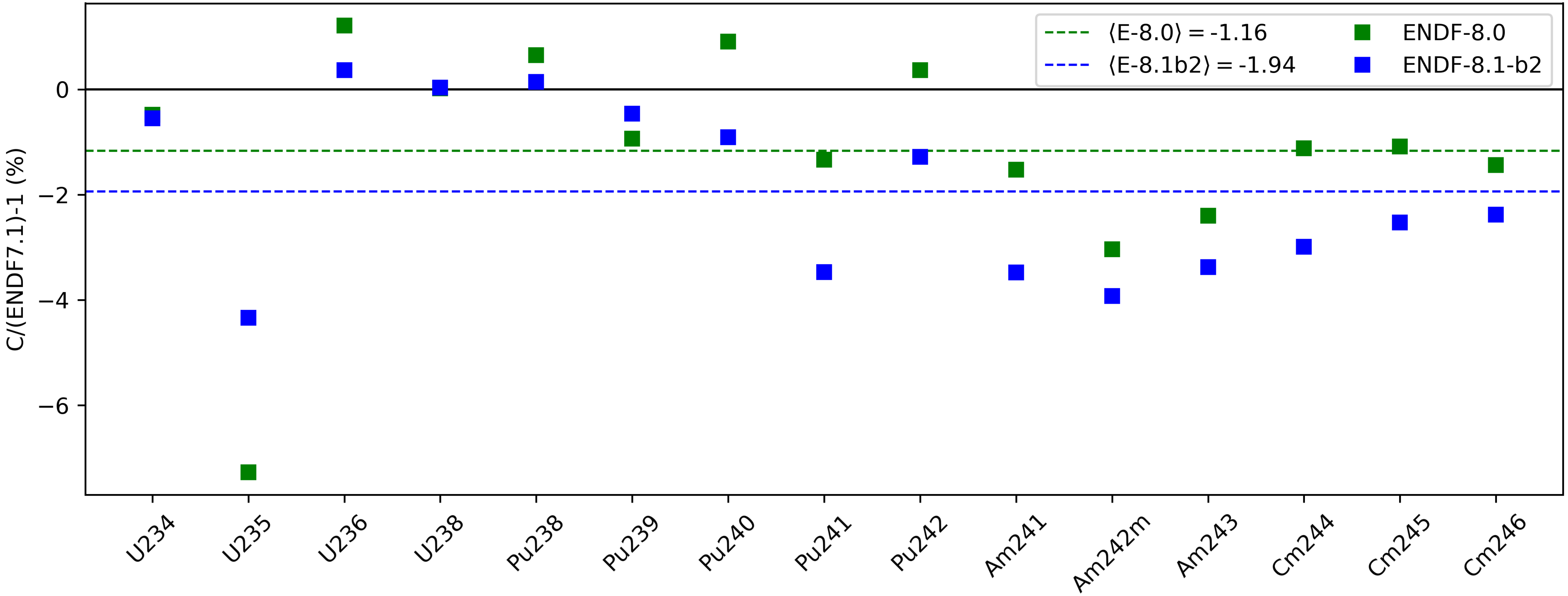


¼ assembly model for Gosgen GU3 sample



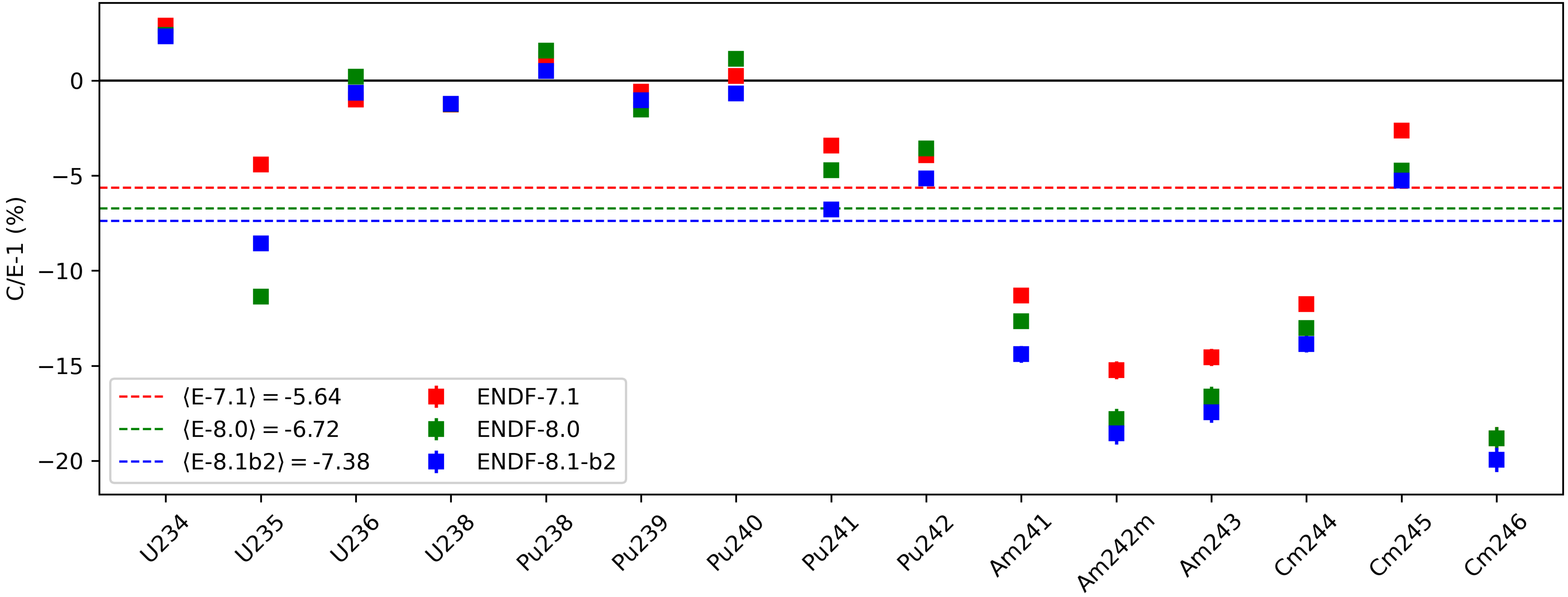
Validation: Depletion RCA vs ENDF-7.1

- Goesgen Reactor, GGU1 sample
- Actinides
- ~70 GWd/t
- UO_2 fuel



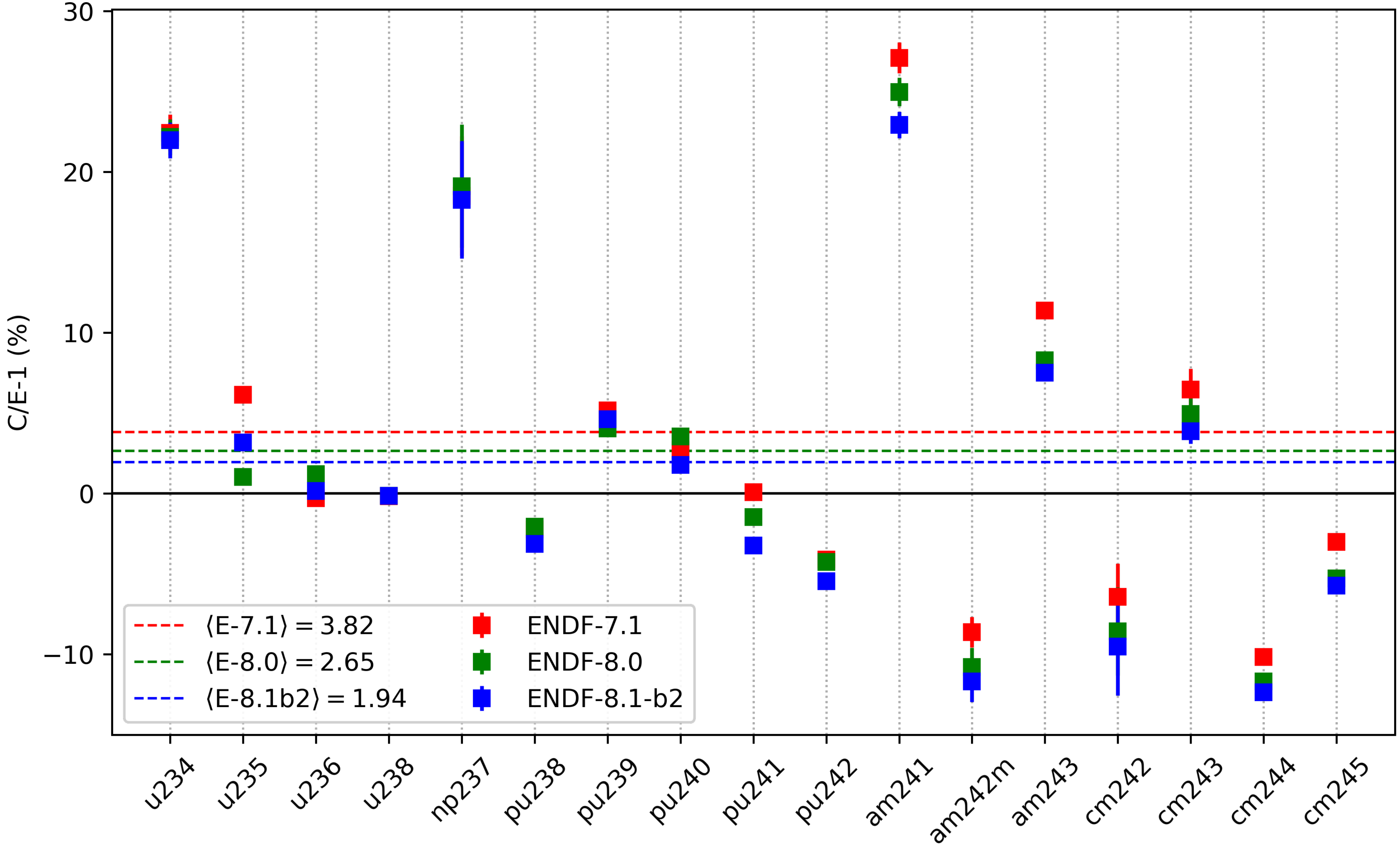
Validation: Depletion RCA vs. Experiment

- Goesgen Reactor, GGU1 sample
- Actinides
- ~70 GWd/t
- UO_2 fuel



Validation: Depletion RCA vs. Experiment

- GKN Reactor
- Actinides
- ~54 GWd/t
- UO_2 fuel

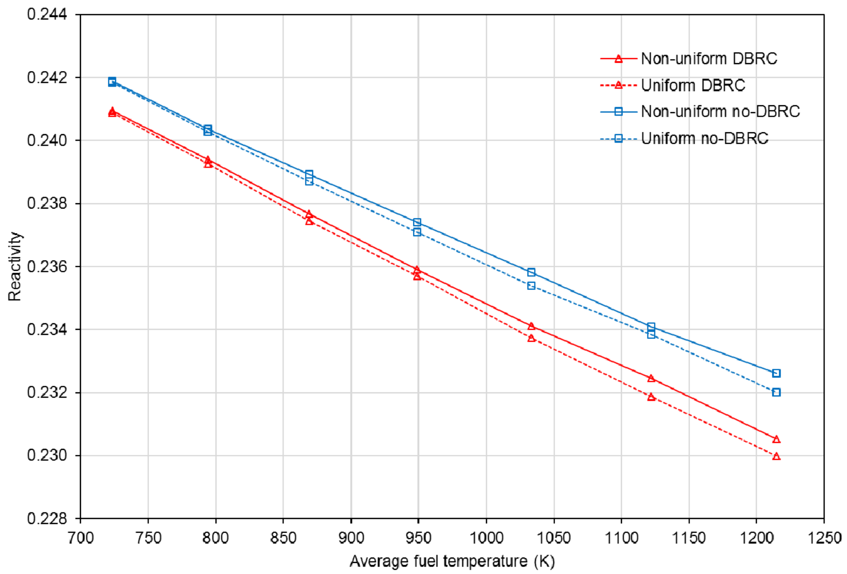


Verification: Depleted Fuel Reactivity(Kim)

- **Previous investigation on depletion computational benchmarks**
  - SERPENT 2.1: ENDF/B-VII.1 and VIII.0 ACE format libraries
  - ENDF/B-VIII.0
    - Underestimate reactivities by ~600 pcm at high burnup (60 MWd/kgU)
    - Dominant nuclides: ^{239}Pu, ^{235}U, ^{16}O, ^{238}U, ^{242}Pu, ^{240}Pu (in order)

- **Additional investigation**
  - ENDF/B-VII.1 vs VIII.0 vs VIII.1 beta2
    - Replace cross sections of VIII.0 for 6 nuclides with ENDF/B-VIII.1 beta2
    - ^{239}Pu, ^{235}U, ^{16}O, ^{238}U, ^{242}Pu, ^{240}Pu and Capote's ^{239}Pu
  - Benchmark calculations
    - Program
      - SERPENT 2.1
    - Typical PWR single fuel pin (1C) and fuel assembly (2C)
      - 3.1 w/o ^{235}U
      - 900 K for fuel, 600 K for cladding and moderator
    - Depletion
      - Same fission kappa values and power density

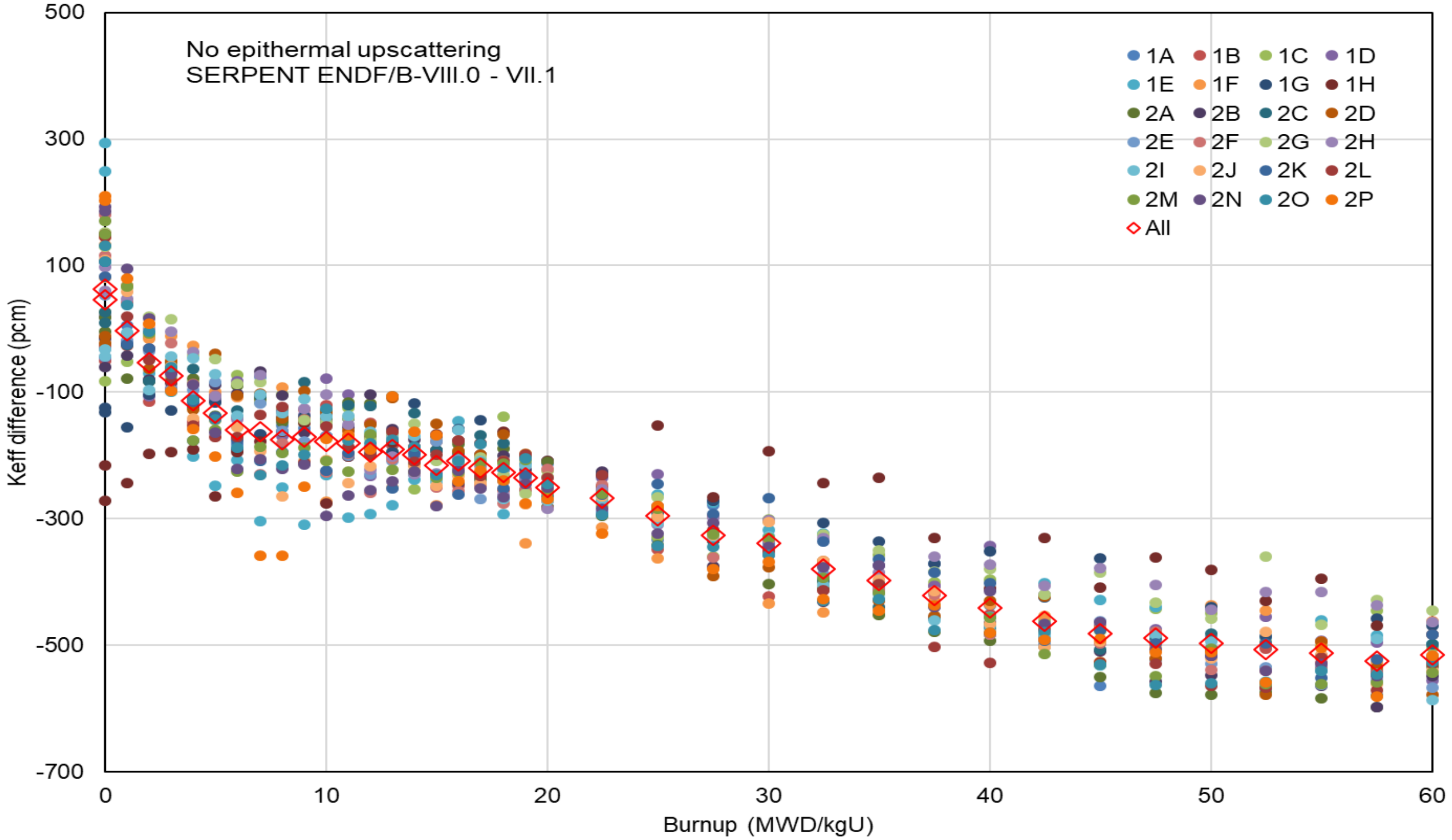
Reminders from CSEWG 2019
- ENDF/B-VII.1 has ***low*** reactivity at high burnup
- DBRC ***lowers*** reactivity! (not used)



https://indico.bnl.gov/event/6642/contributions/32059/attachments/25350/37909/CSEWG2019_11042019_r1.pdf

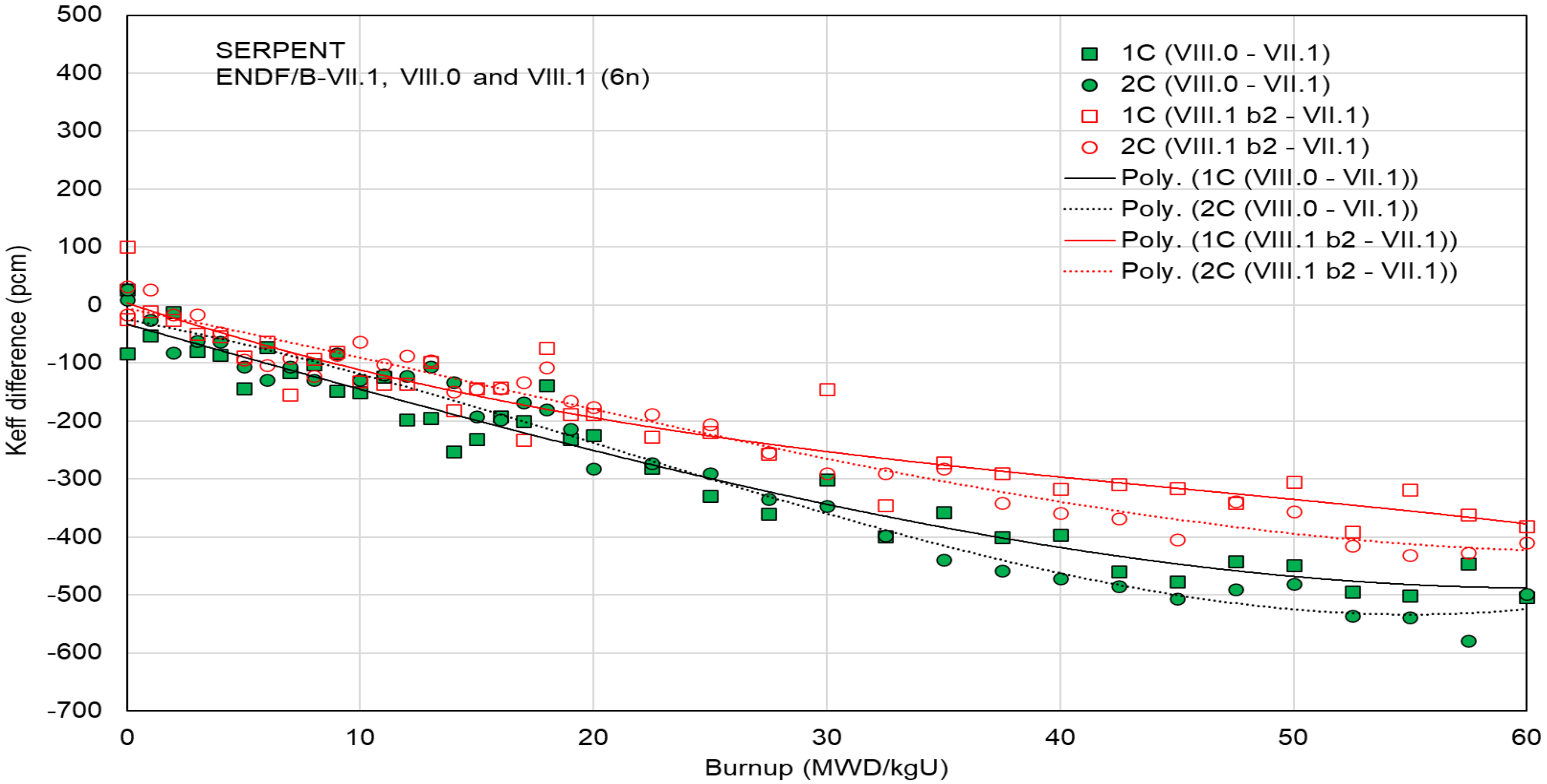
Verification : **ENDF/B-VII.1 vs. ENDF/B-VIII.0**

- **Reactivity underestimation**
  - VERA Depletion Benchmark Problems
    - PWR single pins and assemblies: SERPENT2 Monte Carlo
  - ENDF/B-VIII.0 reactivities are much lower
    - Influencing nuclides: ^{239}Pu, ^{235}U, ^{16}O, ^{238}U, ^{242}Pu, ^{240}Pu (in order)



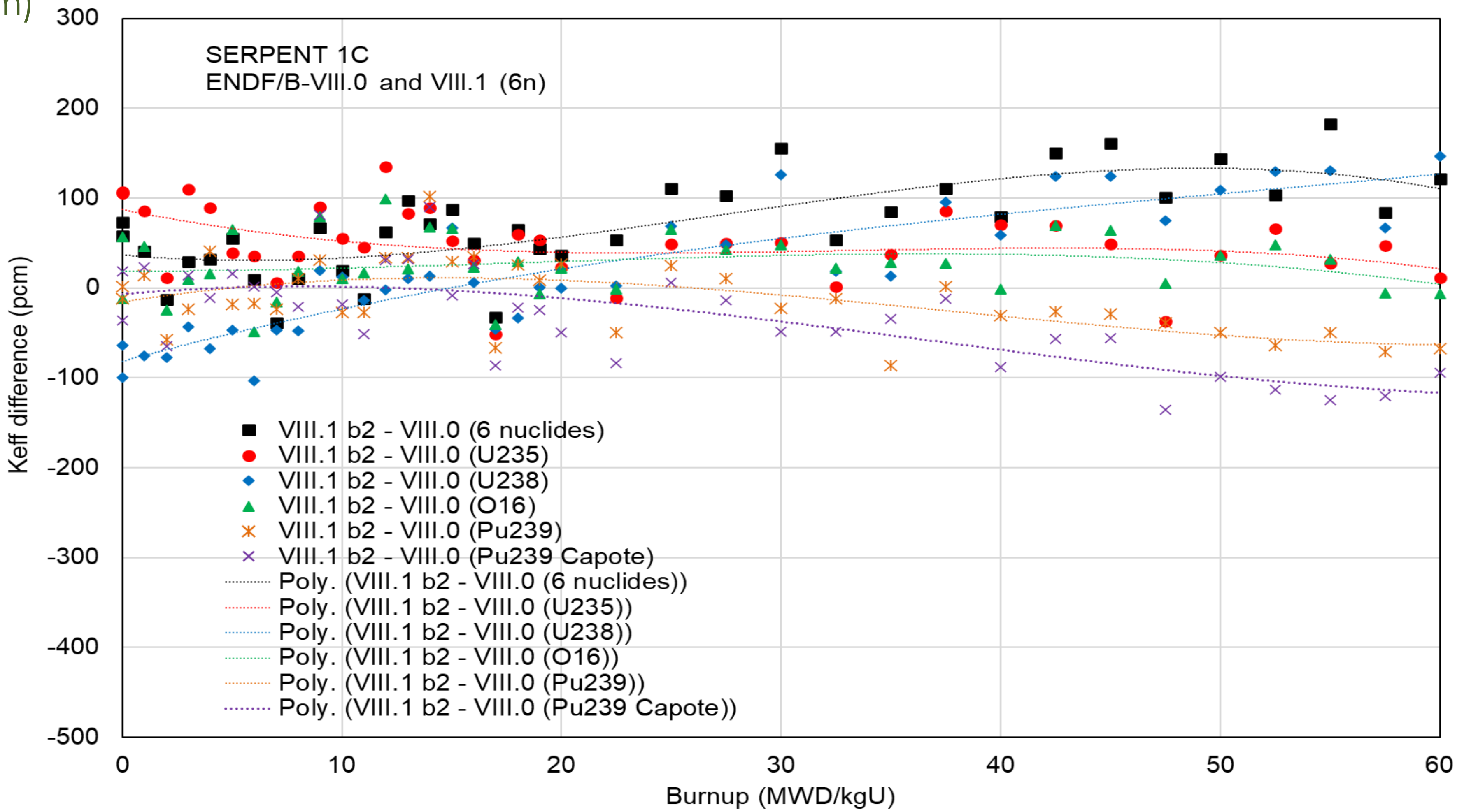
Verification: **ENDF/B-VII.1 vs. VIII.0 vs. VIII.1 beta2**

- **Reactivity underestimation**
  - VERA Depletion Benchmark Problems
    - PWR single pins and assemblies: SERPENT2 Monte Carlo
  - ENDF/B-VIII.0 reactivities are much lower
    - Influencing nuclides: ^{239}Pu, ^{235}U, ^{16}O, ^{238}U, ^{242}Pu, ^{240}Pu (in order)



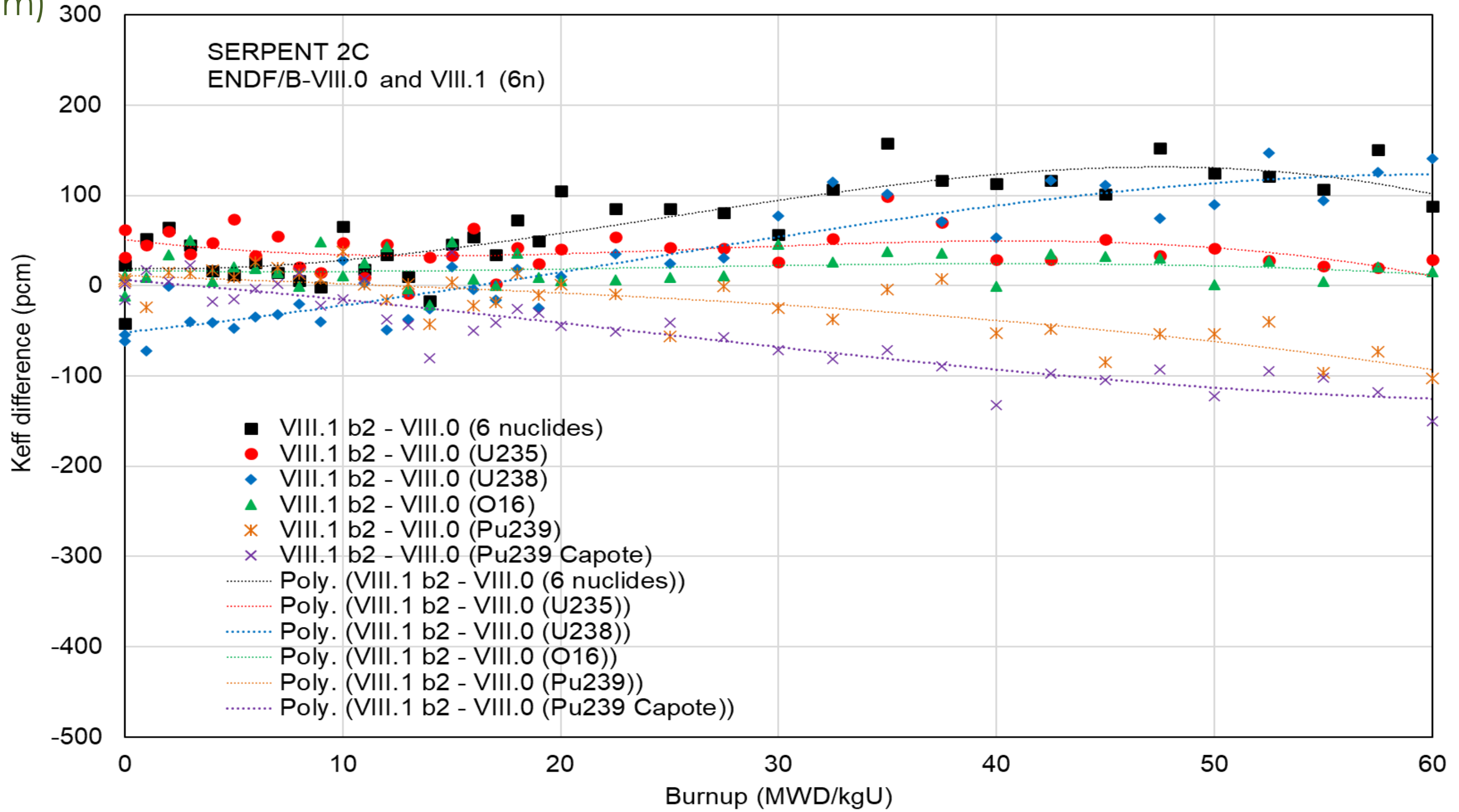
Verification: **ENDF/B-VIII.0 vs. VIII.1 beta2 (I)**

- **VERA 1C problem (PWR single fuel pin)**
  - ENDF/B-VIII.0 library + 6 nuclides with ENDF/B-VIII.1 beta2 data
    - ^{239}Pu, ^{235}U, ^{16}O, ^{238}U, ^{242}Pu, ^{240}Pu
    - Overall (+100 pcm), ^{239}Pu (-50 pcm), ^{239}Pu (Capote, -100 pcm), ^{235}U (0 pcm), ^{16}O (0 pcm), ^{238}U (+100 pcm)



Verification: **ENDF/B-VIII.0 vs. VIII.1 beta2 (II)**

- **VERA 2C problem (PWR single fuel assembly)**
  - ENDF/B-VIII.0 library + 6 nuclides with ENDF/B-VIII.1 beta2 data
    - ^{239}Pu, ^{235}U, ^{16}O, ^{238}U, ^{242}Pu, ^{240}Pu
    - Overall (+100 pcm), ^{239}Pu (-50 pcm), ^{239}Pu (Capote, -100 pcm), ^{235}U (0 pcm), ^{16}O (0 pcm), ^{238}U (+100 pcm)



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Depleted Fuel Reactivity Discussion

- **ENDF/B-VII.1 vs. ENDF/B-VIII.0 vs. ENDF/B-VIII.1 beta 2**
  - Most influencing nuclides between VII.1 and VIII.0
    - U-238, Pu-239, O-16 and U-235
    - U-238: +300 pcm at 0 burnup & getting decreased at high burnup
    - O-16: -150 pcm at all burnup steps
    - U-235: -150 pcm at all burnup steps
    - Pu-239: -200 pcm at high burnups
  - VIII.0 vs. VIII.1 beta 2
    - Overall (6 nuclides): +100 pcm
    - ^{239}Pu: -50 pcm
    - ^{239}Pu (Capote): -100 pcm
    - ^{235}U: 0 pcm
    - ^{16}O: 0 pcm
    - ^{238}U: +100 pcm
  - VIII.1 beta 2 is slightly better, but there is a similar concern for low reactivity at high burnup points

Conclusions

- We need ***many applications*** to rigorously test library
- TSLs motivating changes to SCALE XS sampling
- Advanced reactors:
  - Decreasing reactivity for 8.1b2 compared to 8.0, some unexpected nuclides causing major differences (F-19, Cr), no clear performance difference when compared to experiment
- Depletion RCA:
  - High impact isotopes closer to 7.1
  - Small improvement on average (U-5, Pu-9, BC FPs), worse for Am and Cm
- Fuel reactivity:
  - 8.1b2 is higher reactivity at high burnups than 8.0, but likely under-predicting k_{eff} for PWRs at high burnups

Acknowledgements

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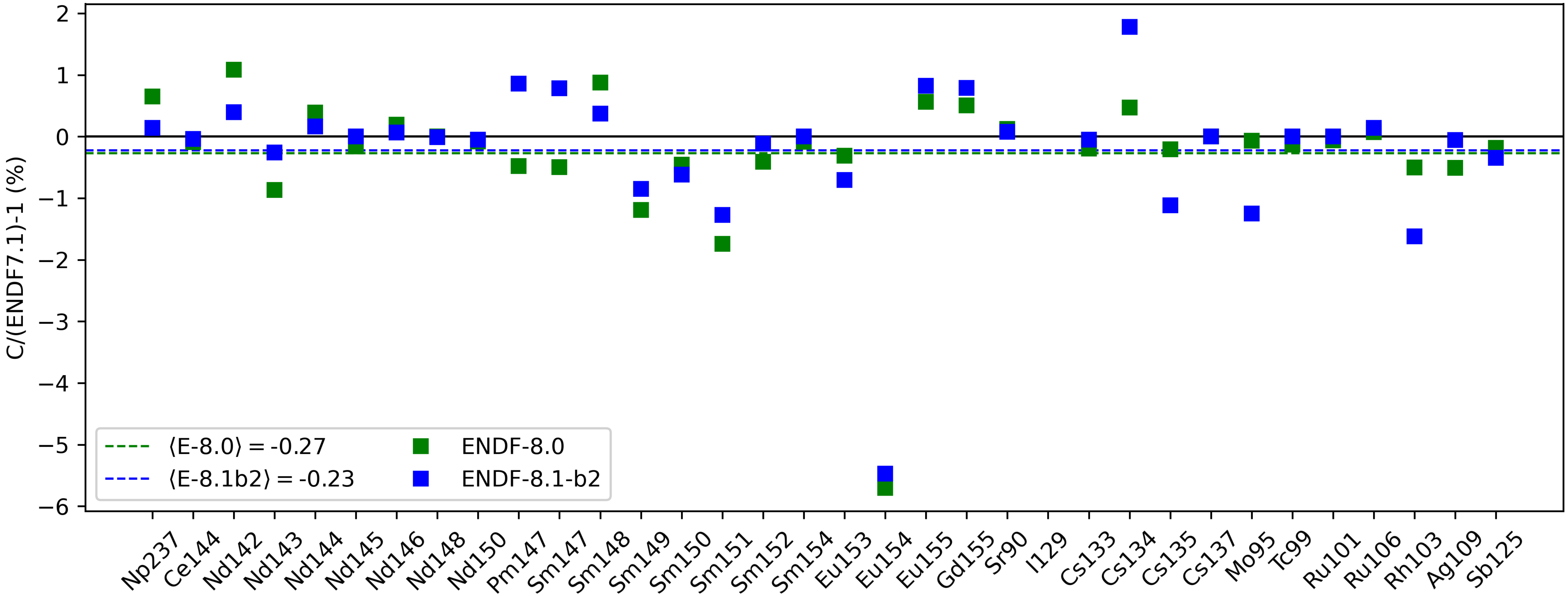
- The entire Nuclear Energy and Fuel Cycle Division at ORNL

Backup Slides

Validation: Depletion RCA

- Goesgen Reactor
- Fission Products



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Validation: Depletion RCA

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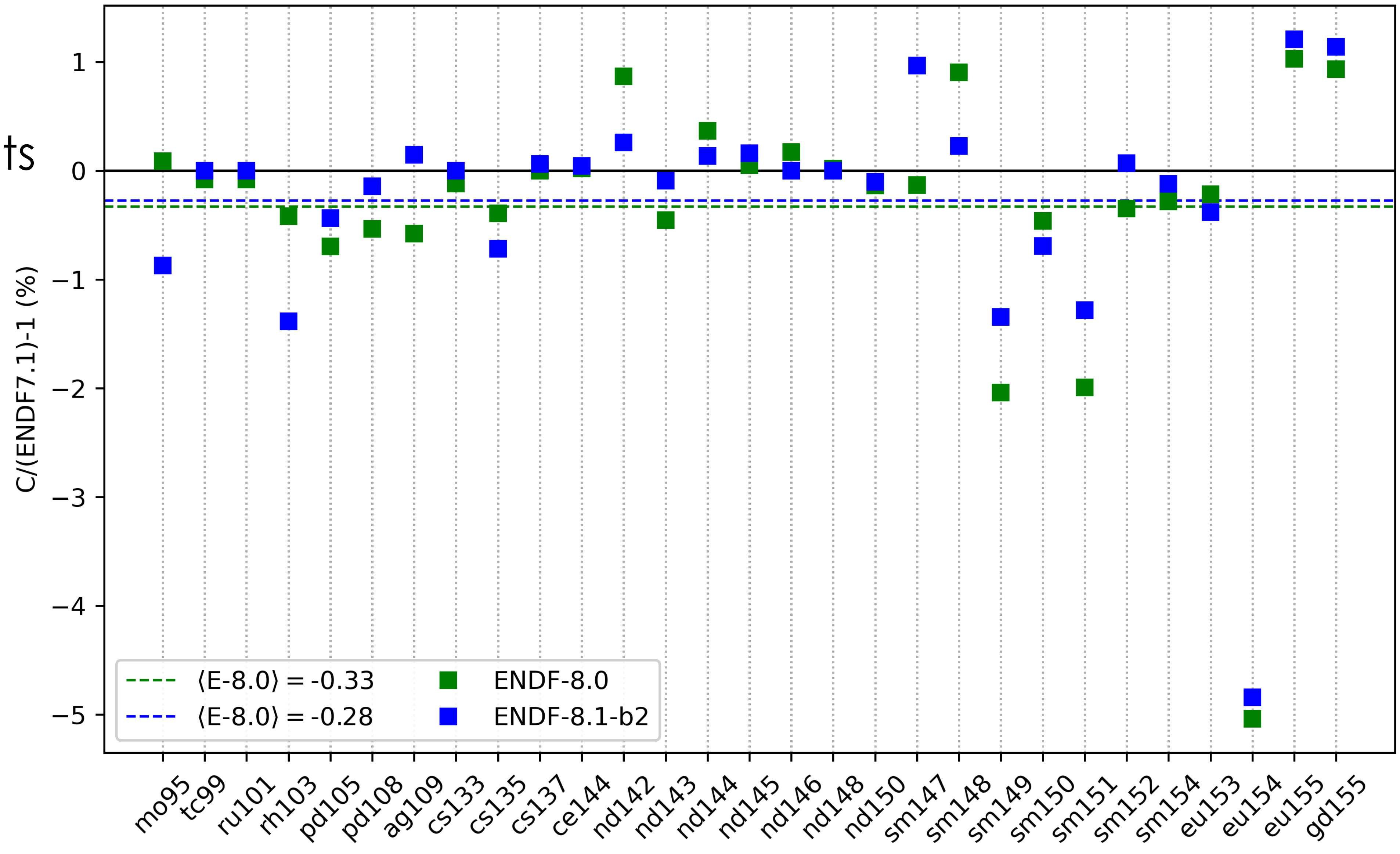
- Fission Products



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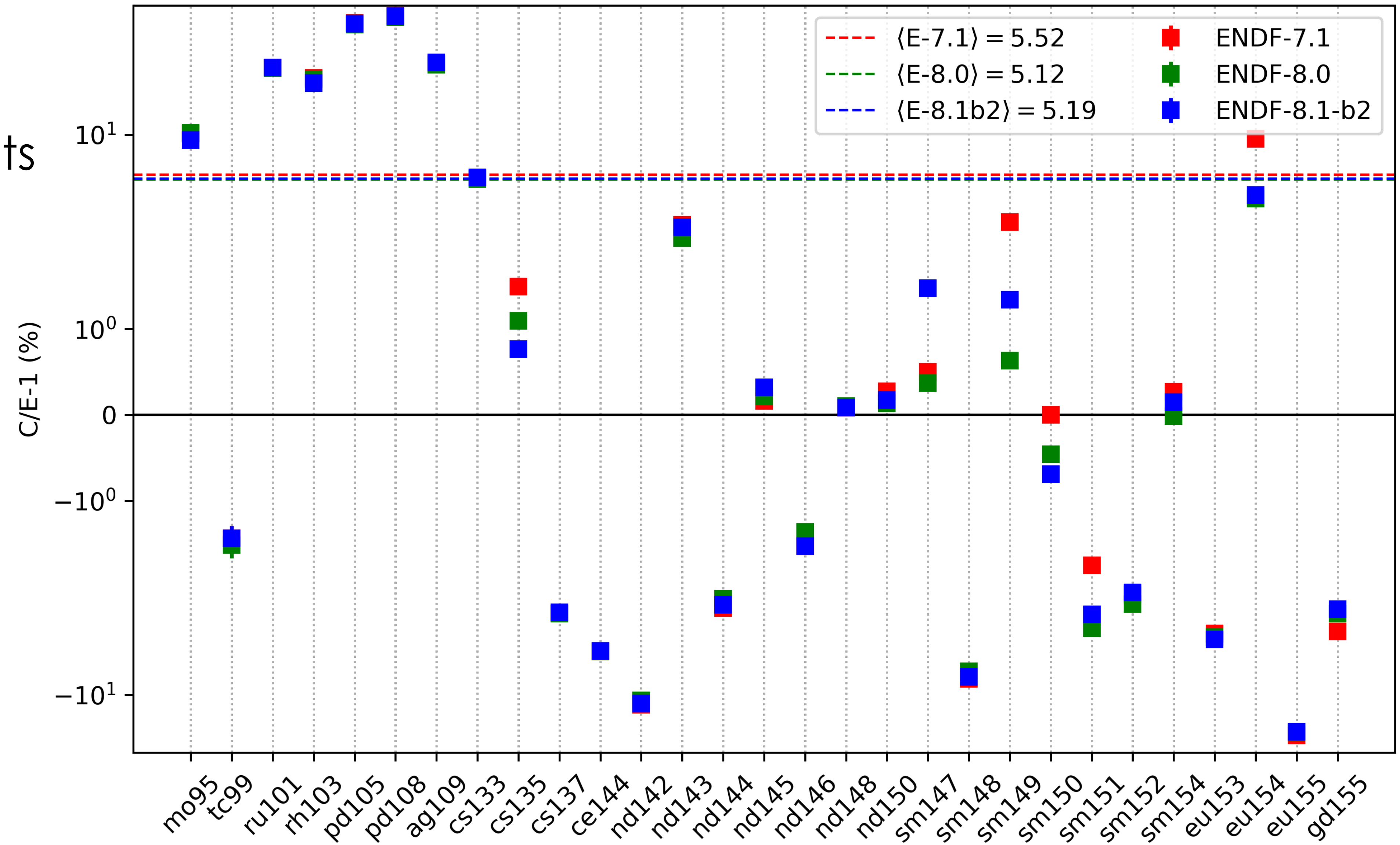

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Validation: Depletion RCA

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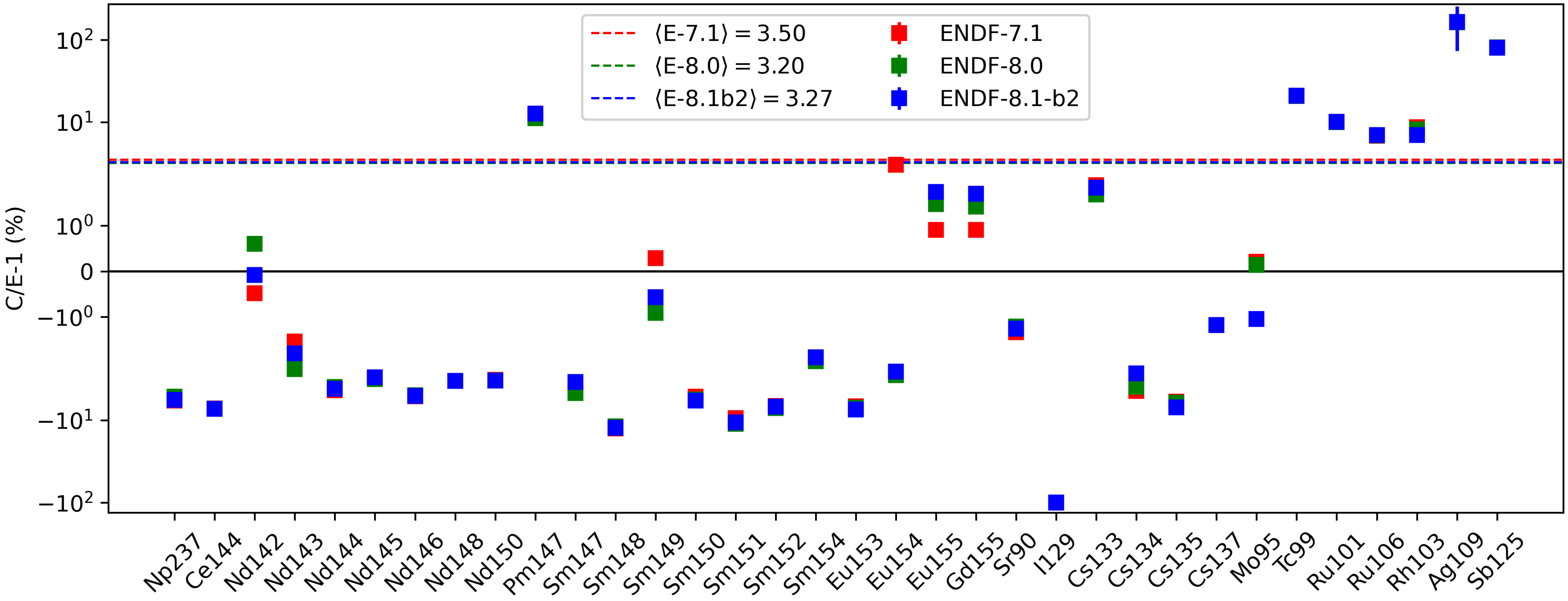

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