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Title: Questionable Benchmarks

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Questionable Benchmarks

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Questionable Benchmarks

- Effort at LANL to identify benchmarks with questionable keff results or uncertainties
- Selection of benchmark classes were investigated (ie HMF, PMF, etc)
- Multiple methods used
- Brief review of some benchmarks were done, with subjective comments of quality of benchmark and uncertainty analysis
- Results are being written as a journal paper, LANL report is >80 pages so not all results can be presented here

Some caveats

- Not official work of the ICSBEP subgroup or SG-8
- Questionable doesn't mean "bad", it means it should be investigated further
- Meant at input for those groups to help triage which benchmarks to look at first
- This wasn't the most thorough review and should not be seen as a final judgement
- Original intent of these benchmarks may have been very different than how they are used today – some benchmarks may be very useful, but may not be useful in a validation suite
- Any statements should not be viewed as negative towards the benchmark authors – standards have changed over time

List of Methods

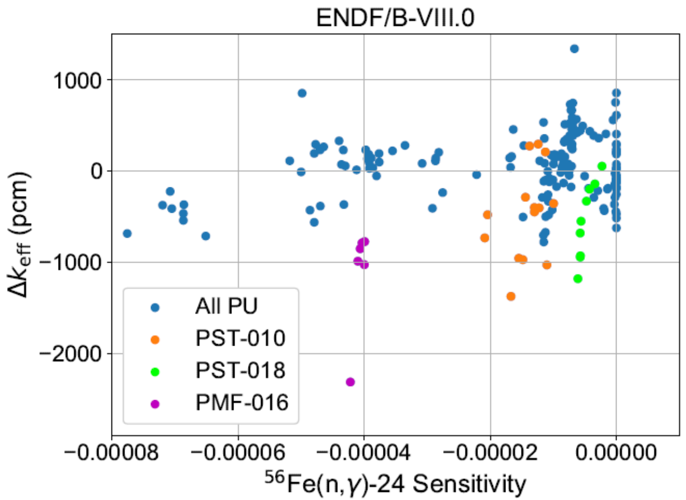
- Random Forest/SHAP
- Whisper
- Simulation/Experiment (C/E) keff >1.02 or <0.98
- 50 pcm uncertainty cutoff
- Histograms
- Similarity coefficients
- Related benchmarks

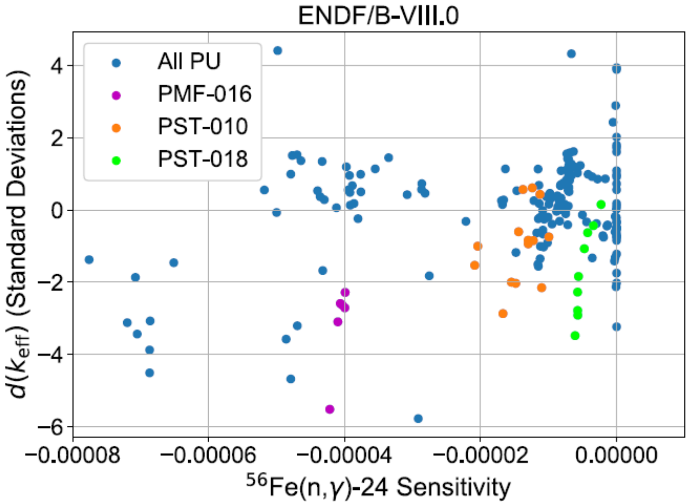
Methods: Random Forest and SHAP

- Random Forest and SHAP are machine learning techniques
- Random Forest models the bias in Δkeff between experimental and simulated keff values (ENDF/B-VIII.0, MCNP-6.2) as a function of keff sensitivity.
- SHAP (SHapley Additive exPlanations) is used to assess the importance of each ‘feature’ (Sensitivity values and measurement attributes for each energy group)

Methods: Random Forest and SHAP

- Some examples of results
- PMF-016 has most of it's results ~1000 pcm for Δkeff (experiment – simulation) but one results is >2000 pcm different.

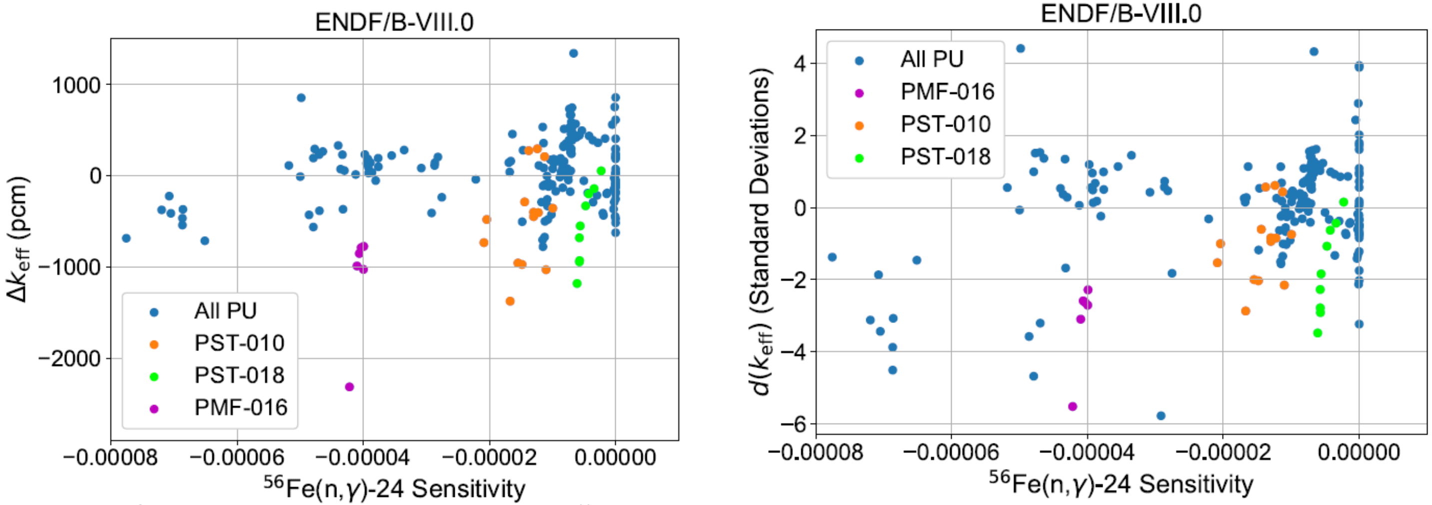




Plots from D. Neudecker et al., "Enchancing Nuclear Data Validation Analysis by Using Machine Learning," Nuclear Data Sheets 167:36-60 (2020).

Methods: Random Forest and SHAP

- Some examples of results
- PMF-010 and PST-018 have large spreads in Δkeff
- Could be a nuclear data issue, could be a model/benchmark issue



Plots from D. Neudecker et al., “Enchancing Nuclear Data Validation Analysis by Using Machine Learning,” Nuclear Data Sheets 167:36-60 (2020).

Methods: Whisper

- Whisper computes a χ^2_{min} related to the degree to which the linear regression can fit the benchmark experimental data within the nuclear data covariances.
- The benchmark with the largest $\chi^2_{diag,i}$ is removed until a certain threshold χ^2_{min} value is reached, removed benchmarks are classified as questionable, remaining are accepted.

Methods: Simulation/Experiment keff <0.98 or >1.02

- These limits are somewhat arbitrary, but any benchmark with large differences between experimental and simulation keff values should be investigated.
- This relates to +/- 2000 pcm difference between experiment and simulation
- Could be nuclear data issues, could be issues with the benchmark or benchmark model

Methods: Cut-off of 50 pcm keff uncertainty

- All benchmarks with keff uncertainties below 50 pcm were listed as questionable
- Very likely uncertainty analysis is lacking for these benchmarks
- These low uncertainties may be justified, but a more thorough review is needed to determine that

Methods: Histograms of Classes

- For each benchmark “class” (ie PST, PMF, HMF…) a histogram of keff uncertainties for those benchmarks were generated.
- The benchmarks with the lowest uncertainties for each “class” were identified as questionable

Methods: Similarity Coefficients

- Similarity coefficients (based on sensitivities) for all pairs of benchmarks were generated.
- For those benchmarks which are extremely similar to each other (similarity coefficient of >0.99), keff uncertainties were compared.
- If keff uncertainties differed by >50%, the pair of benchmarks were listed as questionable
- Again, this doesn’t mean that one of those benchmarks is “wrong” or “bad”, but is a method for triaging benchmarks to investigate further

Methods: Related Benchmarks

- If a questionable benchmark is found by another method, and it was part of a series of experiments undertaken by the same group with the same or very similar equipment in the same time period, those other benchmarks are included as questionable.
- Likely the same issues exist in both sets

Results: Benchmarks with questionable keff values

Method	Benchmarks
ML	PST: 004, 006, 007, 010, 018, 028; PMF: 014, 016; HST: 001, 025, 050; HMF: 003, 005, 025, 051, 057, 072, 084, 092, 093; MMF: 007; UST: 013, 015; LCT: 005, 022, 024, 025, 028;
Related Benchmarks	PMF: 012, 013, 015 (related to PMF014); PST: 001 (related to PST007), 005 (related to PST004);
C/E	PCF: 001, 002; PCI: 001; PCM: 002; PCT: 002; PMF: 008, 015, 018, 026, 028, 035, 045; PMI: 002; PST: 001, 002, 007, 008, 009, 010, 011, 013, 015, 017, 019, 020, 024, 025, 031, 040; HCF: 003; HCI: 003, 004, 005, 006; HCM: 002; HCT: 002, 006; HMF: 003, 007, 021, 041, 052, 053, 057, 060, 064, 067, 070, 073; HMI: 001, 005; HMM: 005; HMT: 001, 003, 006, 011, 012, 026, 027; HSI: 001, 002; HST: 001, 003, 004, 006, 014, 015, 016, 017, 018, 019, 020, 021, 025, 026, 037, 038, 039, 044, 047, 048, 050; ICF: 002; ICI: 003, 004, 005; ICM: 001, 002, 003; ICT: 001, 005, 011; IMF: 005, 009, 013; IST: 001; LCT: 003, 004, 010, 012, 015, 017, 028, 033, 045, 066, 068, 069; MCF: 001; MCI: 006; MCT: 012, 013, 014; MMF: 007, 008; MMI: 001; MMT: 001; MST: 001, 002; SMF: 004, 011, 014; UCT: 001; UMF: 001, 002, 003, 006; USI: 001; USM: 002; UST: 002, 003, 004, 012, 013, 014, 015, 016, 017;

Results: Benchmarks with questionable keff values

Whisper	HCT: 002-015–017, 002-021–022; HMF: 007-006, 007-032–034, 007-036–037, 007-039–040, 025-005, 038-001, 040-001, 051-001, 051-003, 051-009, 051-014–018, 057-001, 057-003, 057-005, 064-001, 064-003, 090-001–002, 092-003, 093-001, 094-002; HMI: 006-001, 006-004; HMT: 012-001, 014-001; HST 001-009—010; LCT: 007-003, 027-002–004; LST: 007-001, 007-003; MMF: 007-002; MST: 001-003–004, 001-011, 003-001–004; 003-006–007; PCM: 001-001–003, 002-001–006, 002-010–016; PMF: 016-001, 039-001, 041-001; PST: 009-003, 010-001, 010-013, 012-006–007, 018-002, 028-001–009; UMF: 004-002; UST: 001-008, 001-010–011, 001-016, 001-018, 001-020–022, 001-030, 001-032, 012-003, 012-006, 015-008–009, 015-018–019, 016-016, 016-021, 016-023, 016-031–033;

Results: Benchmarks with underestimated keff uncertainties

Method	Benchmarks
ML	PST: 022, 028, 032; PMF: 005, 008, 011, 020, 035, 041, 044; HST: 011; HMF: 007, 038, 051, 088, 090, 091, 092, 093, 100; IMF: 001, 002; MMF: 004, 005,010; UMF: 002, 004; UST: 012, 016; LCT: 027; LST: 04;
Related Benchmarks	PMF: 010, 018; UMF: 003, 005; MMF: 001 (related to PMF005, UMF002, UMF004); PMF: 022, 023, 025, 029, 030, 036; MMF: 009 (related to PMF: 035, 41 and MMF: 010); PST: 012, 029, 030, 031 (related to PST: 022, 028, 032); UST: 017 (related to UST: 012, 016); HCT: 009, (related to HCM003); LCT: 043, 044, 046, 054, 058, 067, 077, 082, 083, 084, 088, 089, 090, 091, 092;
Cut-off of 50 pcm	LMT: 005; HCT: 009; HCM: 003, 004; HMF: 047, 051, 059, 069, 071, 074, 076, 099; IMF: 001; LCT: 046, 054, 058, 067, 088, 092; HMT: 011; HMM: 014, 020;

Results: Benchmarks with underestimated keff uncertainties

Histograms	PMF: 001, 008, 011; HMF: 047, 051, 059, 071, 076; IMF: 001; MMF: 009, 010; HMT: 011; LMT: 005, 007; HMM: 014, 020; ICI: 004; HCT: 009, 021; ICT: 011, 013, 014, 015; LCT: 046, 054, 058, 067, 088, 092; MCT: 017; HCM: 003; ICM: 002; USI: 001; PST: 012, 027, 028, 030, 033; HST: 011, 022, 024, 025, 028, 034, 049; IST: 002, 003; LST: 004; UST: 012, 013, 015, 016, 017; MST: 006;
Similarity Coefficients	HMF: 051-009-d, 051-014-d, 051-015-d, 051-016-d, 051-017-d, 051-018-d, 069-001-s; HMT: 031-001-s: IMF: 001-003-ideal, 001-004-ideal; LCT: 007-002, 007-003, 007-004, 007-006, 007-007, 007-009, 007-010, 027-002, 027-003, 027-004, 079-006, 079-007, 079-008, 079-009, 079-010; PST: 028-001-d, 028-002-d, 028-003-d, 028-004-d, 028-005-d, 028-007-d, 028-008-d, 28-009-d, 032-001-d, 032-002-d, 032-003-d, 032-013-d;

Brief review of ‘questionable’ benchmarks

- One hour reviewing each benchmark identified as ‘questionable’
- Looked for obvious problems in description, uncertainty analysis, modeling
- Not a recommendation to the ICSBEP – more in-depth analysis is needed
  - Can be a starting point
- Examples on the next two slides of the review that was performed

Identifier	# of Cases	Year	$\delta k^e_{\rm eff}$ (pcm)	Related Benchmarks	Subjective Opinion on $k_{\rm eff}$ ^{e}	Comments	w
PST004 (4.1.1)	13	1994	350–470	PST: 005	Poor–Average	Performed early 1950s (limited information)	0.75
PST006 (4.1.2)	3	1996	350	-	Poor–Average	Performed early 1950s (limited information)	0.75
PST007 (4.1.3)	11	2004	470	PST: 001	Poor–Average	Performed early 1950s (limited information); study hydrogen content	0.33
PST010 (4.1.4)	14	2004	350–480	-	Poor–Average	Study hydrogen content	0.5
PST018 (4.1.5)	9	2006	300–340	PST: 001, 007, 020, 021	Average–Good (4–9), Suspect (1–3)	Study extrapolation of solution volume to criticality	0.33 (1–3), 1 (4–9)
PST028 (4.1.6)	18 (15 acceptable)	2004	120	PST: 022, 029–032	Average–Good	Study UQ of alloy materials, Mn-unc likely overstated	0.5
PMF012 (5.1.1)	1	1996	210	PMF: 013–015	Below average	Model highly homogenized, $k^e_{\rm eff}$ not based fully on experiment	0.33

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8.1.9 HEU-MET-FAST-072

HMF072 describes three critical configurations containing cylindrical HEU discs with interleaved carbon steel (iron), with and without polyethylene, surrounded by a thick copper reflector. The experiment was conducted at the Los Alamos Critical Experiment Facility (LACEF) in 2002. Irrespective of any interstitual material, these HEU/copper reflected configurations are commonly referred to as "Zeus" criticals.

The evaluation was performed by D.K. Hayes of Los Alamos National Laboratory in 2004. Revision 1 is dated September 30, 2006. The revision history states that this was a "technical" revision without further detail. The MCNP models for these critical configurations are derived from the Revision 1 description.

The uncertainty analysis is reasonably complete, consistent with modern expectations, although we note one omission below and so could benefit from a re-review. In particular Section 2.0 notes that the MCNP sensitivity calculations performed at the time of evaluation are for a total of 6,000,000 active neutron histories. The stochastic uncertainty from those jobs is likely near 200 pcm, resulting in a near 300 pcm combined uncertainty when attempting to evaluate the impact of calculations with and without a specific perturbation. These calculations should be rerun for a much greater neutron history number. It also seems that the uncertainty due to polyethylene attributes needs a second look. The Case 1 uncertainty is ~240 pcm while for Case 3 it is ~690 pcm, with poly-ethylene related uncertainty being the sole difference. The polyethylene mass uncertainty provided in Table 22, which translates

Summary

- Investigation and initial review of ‘questionable benchmarks’ was performed at LANL
- Used multiple methods including machine learning techniques to identify ‘questionable benchmarks’ and/or benchmarks with low uncertainties
- Those benchmarks were then reviewed for obvious errors
- Not a recommendation to ICSBEP, but can be used as a starting point for a more comprehensive review
- Journal paper being written on this work.

Questions?

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