

ENDF/B-VIII.0 CROSS SECTION TESTING FOR COPPER NUCLEAR CRITICALITY SAFETY APPLICATIONS

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ABSTRACT

In the update from ENDF/B-VII.1 to ENDF/B-VIII.0, copper cross sections were significantly altered in the intermediate and fast spectrum of the ENDF-VIII.0 library. Performance of this ENDF data requires validation to determine whether recent evaluation has proven beneficial. To examine the performance of the new library, particularly new copper data, critical benchmarks from the ICSBEP handbook were chosen for their sensitivity to copper cross section changes and modeled using SCALE continuous energy Monte Carlo simulations. Selected benchmarks were modeled in ENDF-VII.1 and ENDF-VIII.0 to compute k_{eff} within a statistical uncertainty of 10 pcm and compared in reference to the benchmark experimental criticality. Due to spectrum choices in selection based on the changes to cross section data, the set of benchmarks consist of intermediately enriched uranium, highly enriched uranium, or plutonium systems. 11 separate benchmark evaluations containing 32 individual configurations highly sensitive to copper were selected, modelled, and compared to benchmark experimental criticality. This work demonstrates a significant decrease in the deviation between calculated and experimental criticality as a result of the ENDF-VIII.0 library; a decrease in absolute mean deviation from 522.5 ± 39.3 to 249.6 ± 39.3 , and a decrease in root mean square deviation from 630.8 ± 46.1 to 338.1 ± 74.9 . Additionally, the role of recently evaluated copper data in this improved agreement is presented, confirming the benefit of reaffirming cross section data.

KEYWORDS: Copper Cross Sections, Criticality Safety

1. INTRODUCTION

Having long been recognized in criticality safety applications as a source of discrepancies between calculated and experimental k_{eff} , copper (^{63}Cu and ^{65}Cu) was identified as an isotope of interest by the US Department of Energy's Nuclear Criticality Safety Program (NCSP) and re-evaluated, being recently incorporated into the ENDF-VIII.0 cross section library. As was expected, there were significant alterations to the ENDF-VII.1 library, particularly in the elastic scattering and neutron capture cross sections.

For a comprehensive understanding of the changes in the cross sections, Brookhaven National Laboratory's (BNL) National Nuclear Data Center (NNDC) was used to plot and determine ENDF-VIII.0 relative to ENDF-VII.1, as opposed to the select energy ranges mentioned in the release [1]. Doing so illustrated the energies which had undergone the greatest changes: the intermediate, resonant, and fast energy regimes.

In order to validate ENDF-VIII.0 and demonstrate the effects of the new copper cross sections, the International Criticality Safety Benchmark Evaluation Project (ICSBEP) and International Reactor Physics Experiment Evaluation (IRPhE) Handbooks were inspected for benchmarked experiments containing significant amounts of copper. The IRPhE Database and Analysis Tool (IDAT) and Database for the International Handbook of Evaluated Criticality Safety Benchmark Experiments (DICE) databases were utilized to search the handbooks, as well as provide a rudimentary quantitative method for determination of copper significance. These programs contained cross section sensitivity data for most benchmarks. The sensitivity of a benchmark to an isotope or reaction indicates the dependence of the problem's criticality on said isotope's or reaction's change; such as occurs from a change in the cross section library or density. Using an arbitrary yet significant cutoff of .01 % $\Delta k/\Sigma$ for filtering experiments, experiments highly sensitive to copper cross sections (^{63}Cu and ^{65}Cu scattering and capture cross sections) could be found. Using the list of selected benchmarks, as well as additional expert opinion on benchmark quality and spectrum suitability, a final list of 11 benchmark evaluations containing 32 configurations was compiled. This paper presents the selected benchmarks and their corresponding criticalities in ENDF-VII.1 and ENDF-VIII.0 and studies the impacts copper cross section changes have made in the agreement between calculated and experimental data, as well as overall changes from the ENDF-VIII.0 library.

2. BENCHMARK SELECTION AND MODELING

At the root of the selection process was the use of sensitivity data to determine benchmarks which would appropriately contain copper. As stated, this selection was done through use of the DICE database included with the ICSBEP handbook. Sensitivity data is a quantitative measure of the importance of macroscopic cross sections on criticality. Therefore, copper sensitive benchmarks will contain more copper, with copper having a larger impact on k_{eff} than benchmarks with less copper or with more important materials (i.e. a core surrounded by copper will be more copper sensitive than the same core surrounded by water with a similar volume of copper surrounding that). Benchmarks that contain significant volumes of copper with no significant sensitivity provide no use for testing the impacts of copper cross section changes; with the wrong spectrum or low sensitivity, changes cannot be attributable to copper, and cannot be measured. Values tabulated and presented by DICE are reaction independent energy integrated cross section sensitivities, which for summed total reactions is equivalent to density perturbations [2]. As shown by Rearden et al. (2010), the sensitivity coefficient for a reaction can be expressed thusly for a perturbation α in the reaction's macroscopic cross section.

$$S_{k,\alpha} = \frac{\alpha}{k} \times \frac{dk}{d\alpha} \cong \frac{\alpha}{k} \times \frac{k_{\alpha^+} - k_{\alpha^-}}{\alpha^+ - \alpha^-} \quad (1)$$

Using DICE, the sensitivity energy profile can be plotted as well to see overlap between the sensitivity profile and energies of interest from cross section changes. For benchmarks that have significant copper sensitivity in the intermediate and fast spectrum, Equation 1 demonstrates how such a change in cross sections can impact these sensitive benchmarks. Using this selection process, and the cutoff of .01 % $\Delta k/\Sigma$, a final list of 11 benchmark evaluations was compiled. Included evaluations are as follow: PMF-013 [3]; PMF-014 [4]; PMF-040 [5]; HMF-072 [6]; HMF-073 [7]; HMF-084 [8]; HMF-085 [9]; HMI-006 [10]; IMF-020 [11]; IMF-022 [12]; IMI-001 [13]. In evaluation HMF-084 only the 6th and 18th configurations were used, and in HMF-085 only the 1st 2nd and 4th.

After selection of benchmarks, the SCALE code system and control module CSAS were used to model the configurations in continuous energy Monte Carlo simulations, following dimensional material and

temperature specifications found in Section 3 of the ICSBEP evaluation. Simulations were performed to produce a statistical uncertainty in criticality of 10 pcm for all calculated data presented. In the occasions where simplified benchmark specifications were provided, they were ignored in favor of detailed models for accuracy.

3. ENDF/B-VII.1 AND ENDF/B-VIII.0 k_{eff} AND EXPERIMENTAL DEVIATION

Using models of the benchmark, the CSAS module was used to run criticality calculations on the inputs. For ENDF-VII.1 data, the “ce_v7.1_endf” identifier was used in the SCALE 6.2.3 release. As ENDF-VIII.0 data is not yet publicly available with SCALE releases, ENDF-VIII.0 simulations were done on the Romulus Linux cluster at Oak Ridge National Laboratory, using SCALE 6.2.3. ENDF-VIII.0 data was linked from SCALE 6.3 beta cross section data using a bash shell and called by the arbitrary identifier “ce_v8.0_endf”. Criticality values calculated in ENDF-VII.1 and VIII.0 are tabulated in Table I, as well as the associated benchmark experimental criticality (experimentally determined criticality value, adjusted by simplification bias detailed in ICSBEP Section 2) and uncertainty. Experimental benchmark criticalities are subtracted from calculated criticalities in ENDF-VII.1 and VIII, producing the C-E (pcm) data tabulated in Table 1. Since the Monte Carlo uncertainty is small, C-E values have uncertainty effectively the same as the experimental criticalities as error propagation results in a change in uncertainty of <1 pcm, and therefore are not displayed. Figure 1 incorporates Table 1 data into a plot, displaying the range of effects ENDF-VIII.0 has on C-E. Uncertainty in experimental criticality is shown to 2σ , with 95% containment easier to visualize than 68%. Regardless of choice of σ , it is notable the improvement ENDF-VIII.0 data results in, with 41% of benchmarks in ENDF-VII.1 bounded by 2σ , as opposed to 94% of ENDF-VIII. Expressing deviation in terms of σ results in an average deviation of 3.49σ for ENDF-VII.1 and 1.24σ for ENDF-VIII. A summary of the deviations comparing ENDF-VII.1 and VIII.0 is included in Table II.

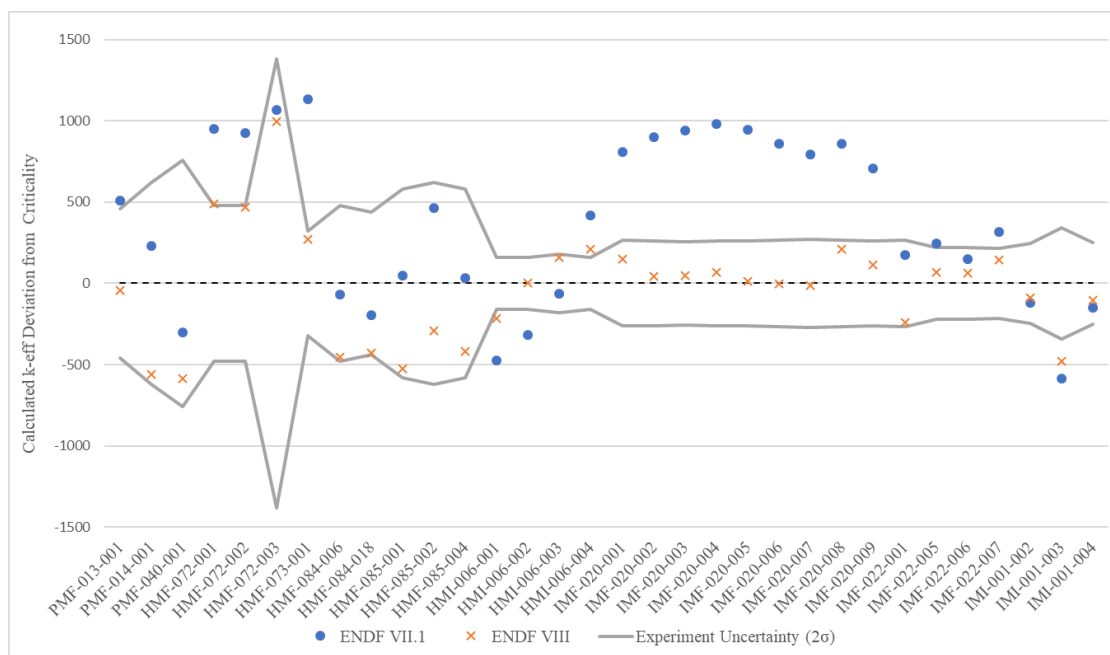


Figure 1. Change in C-E from ENDF-VII.1 to ENDF-VIII

Table I. ENDF-VII.1 and ENDF-VIII: Evaluations listed with their SCALE calculated criticality and deviation from experimental benchmarked criticality, in ENDF-VII.1 and VIII.

Evaluation	Benchmark Experimental Criticality	ENDF-VII.1 Calculated Criticality	ENDF-VIII.0 Calculated Criticality	ENDF-VII.1 C-E	ENDF-VIII.0 C-E
PMF-013-001	1.0034±0.0023	1.008478	1.002945	507.8	-45.5
PMF-014-001	1.0037±0.0031	1.005991	0.998093	229.1	-560.7
PMF-040-001	1.0000±0.0038	0.996986	0.994139	-301.4	-586.1
HMF-072-001	0.9991±0.0024	1.008625	1.00400	952.5	490
HMF-072-002	1.0002±0.0024	1.009461	1.004903	926.1	470.3
HMF-072-003	1.0016±0.0069	1.012248	1.011543	1064.8	994.3
HMF-073-001	1.0004±0.0016	1.011725	1.003111	1132.5	271.1
HMF-084-006	0.9994±0.0024	0.998733	0.994852	-66.7	-454.8
HMF-084-018	0.9995±0.0022	0.997567	0.995215	-193.3	-428.5
HMF-085-001	0.9998±0.0029	1.000285	0.994529	48.5	-527.1
HMF-085-002	0.9997±0.0031	1.004361	0.996792	466.1	-290.8
HMF-085-004	0.9996±0.0029	0.999946	0.995422	34.6	-417.8
HMI-006-001	0.9977±0.0008	0.992957	0.99554	-474.3	-216
HMI-006-002	1.0001±0.0008	0.996944	1.000122	-315.6	2.2
HMI-006-003	1.0015±0.0009	1.000844	1.00311	-65.6	161
HMI-006-004	1.0016±0.0008	1.005763	1.003725	416.3	212.5
IMF-020-001	1.0006±0.00132	1.008681	1.002075	808.1	147.5
IMF-020-002	1.0015±0.0013	1.010477	1.001935	897.7	43.5
IMF-020-003	1.0004±0.00129	1.009798	1.000899	939.8	49.9
IMF-020-004	1.0008±0.0013	1.010595	1.001484	979.5	68.4
IMF-020-005	1.0014±0.0013	1.010837	1.001528	943.7	12.8
IMF-020-006	1.0012±0.00133	1.009771	1.001177	857.1	-2.3
IMF-020-007	1.0011±0.00136	1.009041	1.00097	794.1	-13
IMF-020-008	1.0003±0.00133	1.008878	1.00241	857.8	211
IMF-020-009	1.0007±0.00131	1.007758	1.001857	705.8	115.7
IMF-022-001	1.0057±0.00134	1.00744	1.003272	174	-242.8
IMF-022-005	1.00022±0.0011	1.002669	1.000908	244.9	68.8
IMF-022-006	1.00564±0.0011	1.007132	1.006273	149.2	63.3
IMF-022-007	1.00147±0.00107	1.004649	1.002924	317.9	145.4
IMI-001-002	1.00042±0.00123	0.999204	0.999531	-121.6	-88.9
IMI-001-003	1.00131±0.00172	0.995446	0.996491	-586.4	-481.9
IMI-001-004	1.0010±0.00126	1.008478	1.002945	-148.4	-102.6

Beyond expression of deviation in relative terms of σ , absolute deviations were calculated as the absolute mean and root mean square (RMS) of C-E values. The standard derivations of both were used, and error propagated accordingly. For absolute mean, error propagation is elementary, but RMS error propagation is slightly more detailed and is expressed in Equation 2 with x_n and δx_n representing individual configuration C-E values and associated uncertainties.

$$\delta_{RMS} = \sqrt{\sum_{n=1}^N \left(\frac{x_n}{\sqrt{N} \sqrt{\sum_{n=1}^N x_n^2}} \right)^2} \delta x_n^2 = \sqrt{\frac{1}{N \sum_{n=1}^N x_n^2}} \sqrt{\sum_{n=1}^N x_n^2 \delta x_n^2} \quad (2)$$

These determinations of average deviation and associated uncertainty result in absolute and RMS means of 523 ± 39 and 631 ± 46 for ENDF-VII.1, and 250 ± 39 and 338 ± 75 for ENDF-VIII. A summary of deviations comparing ENDF-VII.1 and VIII.0 are included in Table II.

Table II. Average Deviations from Experimental Criticality: Comparison of ENDF-VII.1 and VIII.

Average:	ENDF-VII.1	ENDF-VIII
Relative Deviation	3.49 σ	1.24 σ
Absolute Mean Deviation	522.5 $\pm$ 39.3	249.6 $\pm$ 39.3
Root Mean Square Deviation	630.8 $\pm$ 46.1	338.1 $\pm$ 74.9

4. EFFECT OF ENDF/B-VIII.0 COPPER ON k_{eff} AND EXPERIMENTAL DEVIATION

With the system criticalities changing from the full adaptation of ENDF-VIII.0 data as shown, further study was conducted to determine the role of copper cross section changes on criticality. Rather than model benchmarks entirely in ENDF-VII.1 and ENDF-VIII, the base library of the benchmark was taken to mean all other isotopes present, apart from copper. The base library was constructed by disassembling the ENDF-VII.1 and ENDF-VIII.0 xml files that direct SCALE cross section library determinations and using a shell bash command to link the ENDF-VIII.0 designations for Cu-63 and Cu-65 into the ENDF-VII.1 base library. All isotopes apart from Cu-63 and Cu-65 are now ENDF-VII.1, while Cu-63 and Cu-65 use ENDF-VIII.0 data; the only new ENDF-VIII.0 data in the model is that of copper. This allows the effect of the copper data update to be determined, as the effect of only ENDF-VIII.0 copper data can be compared to the already produced ENDF-VII.1 systems. The results of this isotope swapping can be seen in Table III.

Of interest is the rightmost column, the deviations from experimental criticality where the copper cross sections are replaced with ENDF-VIII. As expected for the sensitivity profile and known cross section changes, in every case the C-E value decreases. Of course, whether this results in improved agreement with experimental results is not a given. In the same manner as in the comparison between VII.1 and VIII, the relative deviation, absolute mean, and root mean square were calculated to determine the change in overall deviation between calculated and experimental criticalities. In the same method as above, the absolute mean decreased from an average of 522.5 ± 39.3 pcm to an average of 295.5 ± 39.3 pcm, with the RMS decreasing from 630.8 ± 46.1 pcm to 363.8 ± 39.7 pcm, and relative deviation decreasing from 3.49σ to 2.10σ . When presented alongside data for full library comparison in Table IV and Figure 2, the effect of the copper data changes is shown to be a significant factor in the entire change from the library update.

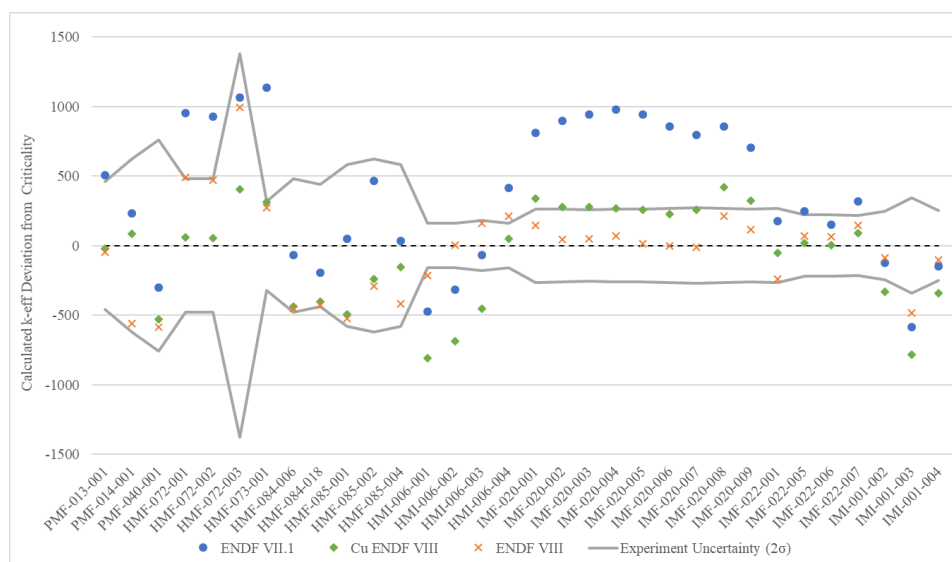
Table III. Cu ENDF-VIII.0 Replacement: Evaluations listed with their SCALE calculated criticality and deviation from experimental benchmarked criticality, in ENDF-VII.1 and with Copper ENDF-VIII.0 Cross Sections.

Evaluation	Benchmark Experimental Criticality	ENDF-VII.1 Calculated Criticality	Cu ENDF-VIII.0 Calculated Criticality	ENDF-VII.1 C-E	Cu ENDF- VIII.0 C-E
PMF-013-001	1.0034±0.0023	1.008478	1.003178	507.8	-22.2
PMF-014-001	1.0037±0.0031	1.005991	1.004551	229.1	85.1
PMF-040-001	1.0000±0.0038	0.996986	0.994714	-301.4	-528.6
HMF-072-001	0.9991±0.0024	1.008625	0.999689	952.5	58.9
HMF-072-002	1.0002±0.0024	1.009461	1.000754	926.1	55.4
HMF-072-003	1.0016±0.0069	1.012248	1.005623	1064.8	402.3
HMF-073-001	1.0004±0.0016	1.011725	1.003542	1132.5	314.2
HMF-084-006	0.9994±0.0024	0.998733	0.99503	-66.7	-437
HMF-084-018	0.9995±0.0022	0.997567	0.995449	-193.3	-405.1
HMF-085-001	0.9998±0.0029	1.000285	0.994861	48.5	-493.9
HMF-085-002	0.9997±0.0031	1.004361	0.997314	466.1	-238.6
HMF-085-004	0.9996±0.0029	0.999946	0.998041	34.6	-155.9
HMI-006-001	0.9977±0.0008	0.992957	0.989594	-474.3	-810.6
HMI-006-002	1.0001±0.0008	0.996944	0.993239	-315.6	-686.1
HMI-006-003	1.0015±0.0009	1.000844	0.996964	-65.6	-453.6
HMI-006-004	1.0016±0.0008	1.005763	1.002088	416.3	48.8
IMF-020-001	1.0006±0.00132	1.008681	1.003985	808.1	338.5
IMF-020-002	1.0015±0.0013	1.010477	1.004271	897.7	277.1
IMF-020-003	1.0004±0.00129	1.009798	1.003161	939.8	276.1
IMF-020-004	1.0008±0.0013	1.010595	1.00346	979.5	266
IMF-020-005	1.0014±0.0013	1.010837	1.003944	943.7	254.4
IMF-020-006	1.0012±0.00133	1.009771	1.003457	857.1	225.7
IMF-020-007	1.0011±0.00136	1.009041	1.00367	794.1	257
IMF-020-008	1.0003±0.00133	1.008878	1.004476	857.8	417.6
IMF-020-009	1.0007±0.00131	1.007758	1.003937	705.8	323.7
IMF-022-001	1.0057±0.00134	1.00744	1.005152	174	-54.8
IMF-022-005	1.00022±0.0011	1.002669	1.00042	244.9	20
IMF-022-006	1.00564±0.0011	1.007132	1.005676	149.2	3.6
IMF-022-007	1.00147±0.00107	1.004649	1.002355	317.9	88.5
IMI-001-002	1.00042±0.00123	0.999204	0.997124	-121.6	-329.6
IMI-001-003	1.00131±0.00172	0.995446	0.99347	-586.4	-784
IMI-001-004	1.0010±0.00126	1.008478	0.997565	-148.4	-343.5

Table IV. Average Deviations from Experimental Criticality: Comparison of ENDF-VII.1 and VIII.

Average:	ENDF-VII.1	Cu ENDF-VIII	ENDF-VIII
Relative Deviation	3.49 σ	2.10 σ	1.24 σ
Absolute Mean Deviation	522.5 $\pm$ 39.3	295.5 $\pm$ 39.3	249.6 $\pm$ 39.3
Root Mean Square Deviation	630.8 $\pm$ 46.1	363.2 $\pm$ 39.7	338.1 $\pm$ 74.9

Whereas 24 of the 32 benchmarks improve with a full library update, 21 of them improve from the copper cross section data alone. With ENDF-VIII.0 copper cross sections, the percentage of uncertainty-bounded experiments rises from 42% to 72%, accounting for more than half of the full library change to 94%.

**Figure 2. Result of ENDF-VIII.0 Copper Cross Section Insertion**

5. CONCLUSIONS

In this selection of copper sensitive benchmarks, substantial improvement in the agreement between calculated and experimental criticality was observed as a result of updating ENDF-VII.1 to ENDF-VIII. The average deviation between the two decreased a full 2σ relative to experimental uncertainty. In absolute terms, the RMS and absolute mean deviations decreased nearly 300 and over 250 pcm respectively. As expected, there was a substantial decrease in criticality due to the introduction of ENDF-VIII.0 copper cross section data alone. This decrease countered the significant supercriticality observed in many ENDF-VII.1 simulations of the selected benchmarks. As a result, copper cross sections accounted for a significant portion of the noted overall improvement between the C-E values of ENDF-VII.1 and ENDF-VIII. Considering the improvement in absolute deviation (absolute mean and RMS) and statistical agreement (calculations falling within experimental uncertainty) over multiple independent experimental assemblies, there is a substantial basis for arguing that these improvements are a result of genuine improvements in copper cross section data.

NOMENCLATURE

pcm: **per cent milli**, 1E-5 change in k

PMF: **PU-MET-FAST** ICSBEP evaluation identifier; a **Plutonium Metal Fast** energy system

HMF: **HEU-MET-FAST** ICSBEP evaluation identifier; a **Highly enriched uranium Metal Fast** energy system

HMI: **HEU-MET-INTER** ICSBEP evaluation identifier; a **Highly enriched uranium Metal Intermediate** energy system

IMF: **IEU-MET-FAST** ICSBEP evaluation identifier; an **Intermediately enriched uranium Metal Fast** energy system

IMI: **IEU-MET-INTER** ICSBEP evaluation identifier; an **Intermediately enriched uranium Metal Intermediate** energy system

C-E: Calculated criticality minus benchmark **E**xperimental criticality

ACKNOWLEDGMENTS

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