# Identifying Gaps in Critical Benchmarks

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## INTRODUCTION

The International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook[1] is a well documented collection of data of over 4000 high quality nuclear measurements, known as benchmarks. These benchmarks are used for many applications, including validation of nuclear data, testing of nuclear codes, and as a tool in the design process of nuclear systems. In fact, nuclear data are often adjusted so that simulation codes more accurately simulate nuclear benchmarks. The vast majority of these measurements are critical measurements of reactors and other critical systems. Those thousands of measurements include many different materials, fuels, and compositions. However, it's rather hard to identify gaps in integral benchmarks. For example, the question "Which energy regions, materials, and interactions are not covered by the existing benchmarks?" is not easy to answer. This paper aims to answer that question, and gives some insight into how well simulations of benchmarks agree with experimental data. This is done through a systematic analysis of sensitivity files of the ICSBEP benchmarks.

Sensitivities are the relative change in reactivity for a relative change in cross section, $(\delta k/k)/(\delta\sigma/\sigma)$. The ICSBEP Handbook contains sensitivity data files (SDFs) for 4180 unique benchmarks, generated by NEA, ORNL, and IPPE, using the MCNP®[2] and SCALE[3] codes. The vast majority of these files were created with ENDF/B-VII.0[4] using 238 energy groups. Although this is not the most recent version of ENDF, sensitivities are relative quantities, and should be stable between different libraries. These SDFs contain sensitivities for every isotope/material and neutron interaction, for the entire simulation, all as a function of neutron energy.

## HEATMAPS OF NUMBER OF BENCHMARKS

These SDF files were processed with a custom built python script which created a separate file for each isotope/material and interaction (for example, $^{235}$U capture or $^{200}$Hg inelastic scattering). Each of these separated files contains the name of each benchmark which contains that isotope/material and the sensitivity as a function of energy. With these files generated, another script was written to tally the number of benchmarks that were sensitive to that isotope/material, where a benchmark was defined as "sensitive" if the absolute value of the sensitivity was greater than $10^{-3}$. The absolute sensitivity threshold of $10^{-3}$ is slightly arbitrary, but was selected to filter out insensitive benchmarks. Choosing a higher sensitivity threshold would ensure that only the most sensitive benchmarks are analyzed, however, in many cases, this significantly reduces the number of benchmarks, and may result in missing trends or perceiving there is a deficiency when none exists. However, choosing a sensitivity value that is too low results in many benchmarks that are not very sensitive being plotted, and information may be missed in the noise. To visually represent this data, it was plotted as a function of energy, for a specific interaction.

Figure 1 is an example of one such plot for total cross section, where the color on the heatmap represents the number of benchmarks that are sensitive to that interaction, at that specific energy. On the right axis, the total number of unique benchmarks sensitive to that isotope/material is also listed (benchmarks can and often are sensitive to multiple energy bins, particularly in the regions where cross sections are smooth).

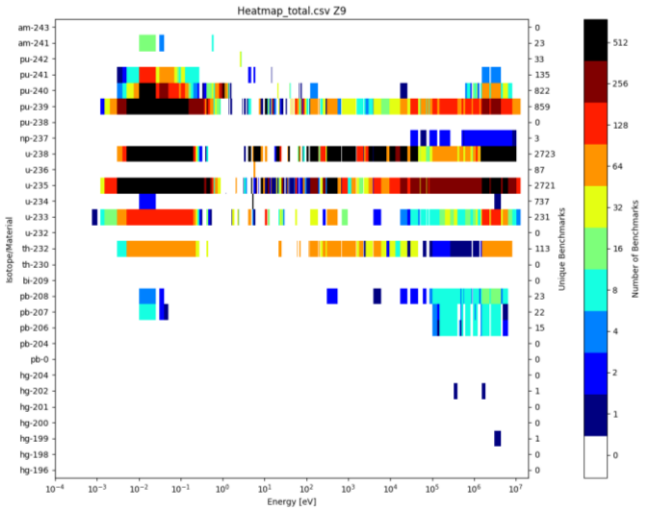


Fig. 1: Total Cross Section Heatmap, Hg-Am

Unsurprisingly, $^{235}$U, $^{238}$U, and $^{239}$Pu all have many benchmarks that are sensitive to changes in total cross section, especially in the fast and thermal energy spectra. However, there are still spaces where no benchmarks are sensitive, even for $^{235}$U. This is mainly due to two effects, flux and cross section. Most benchmarks are either fast or thermal systems, with a small minority having a mixed spectra or intermediate energy spectra. Because of this, the intermediate energy region is undersampled compared to the other energy regions. The second effect is cross section, and this is most clearly seen in $^{234}$U. There are over 700 unique

benchmarks that are sensitive to $^{234}$U, but only one energy bin where more than three benchmarks are sensitive to $^{234}$U, the energy bin from 5.0 eV to 5.4 eV. Even though the flux in many of the benchmarks that contain $^{234}$U is low at this energy, these benchmarks are sensitive to $^{234}$U at that energy because $^{234}$U has a nearly 23,000 barn resonance in the capture cross section at 5.16 eV.

With these heatmaps, it is easier to answer the question, "Which energy regions, materials, and interactions are not covered by the existing benchmarks?" However, these heatmaps give no indication of the quality of the benchmarks or underlying nuclear data.

## AVERAGE C/E HEATMAPS

Steven van der Marck has simulated a large number of the ICSBEP benchmarks (roughly 2000), and these results were included in the 2016 ICSBEP Handbook. He simulated the benchmarks using the JENDL-4.0[5], JEFF-3.1.1[6], and ENDF/B-VII.1[7] cross section libraries. If there was a bias in a cross section of a particular isotope, then it might be possible to find this bias by looking at the average C/E ($k_{eff}$ for the computation divided by $k_{eff}$ for the experiment) for the benchmarks that are sensitive to that isotope and interaction. With van der Marck's results and the files created previously, another script was written to calculate the average C/E for the benchmarks sensitive to each isotope/material and interaction, as a function of energy. These results were then plotted; Figure 2 is an example of one such plot. An average C/E value of 1.0 would indicate that on average, the simulations of $k_{eff}$ agreed with the experimental $k_{eff}$. If the average C/E was much greater than or much less than 1.0, that might indicate that there is a problem with the cross sections of that material used in that simulation. For example, if the average C/E for $^{235}$U was greater than 1.0, that could indicate that the fission cross section is too high or that the capture cross section is too low. It should be noted that while sensitivity values are relative, and therefore do not vary greatly between libraries, changes in nuclear data between libraries will impact $k_{eff}$ values, and therefore C/E values. Figure 2 represents the C/E values when simulated with the ENDF/B-VII.1 cross section library.

One result from Figure 2 is $^{239}$Pu from 100 ev – 100 keV, the average C/E seems to be much higher than 1.0, indicating that there may be an issue with $^{239}$Pu cross sections in the intermediate energy region. One way to probe this question is to take a look at simulation and experiment values for all of the benchmarks of an individual isotope.

## INDIVIDUAL (C-E)/E HEATMAPS

Instead of plotting the average C/E for all the benchmarks sensitive to that particular interaction, each individual C/E value can also be plotted for a specific isotope. To make it easier to see differences, this data was plotted in Figure 3, except as (C-E)/E. Figure 3 is a plot of the (C-E)/E values as a function of energy for the benchmarks sensitive to $^{239}$Pu total cross section, colored by the type of fuel (metal, solution, or compound). This data can also be colored by fuel (LEU, IEU, HEU, MIX, PU, $^{233}$U, etc.), by energy spectra (fast, intermediate, thermal, or mixed), or by sensitivity (so that higher sensitivity data points stand out). A few interesting things to note – when there is a horizontal string of data points with the same (C-E)/E value, those are usually from the same benchmark (the same benchmark is sensitive to that interaction/isotope at multiple energies). There are also vertical lines that appear, for example, in the region of 10 – 100 eV, which correspond to resonances.

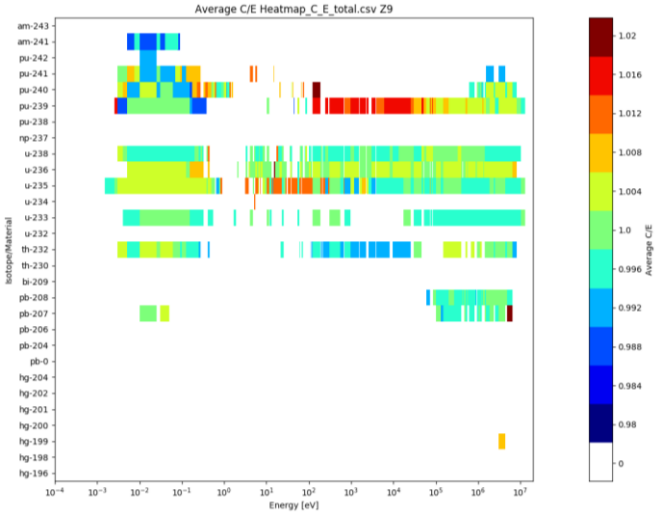


Fig. 2: Average C/E Heatmap, Hg-Am, ENDF/B-VII.1 Library

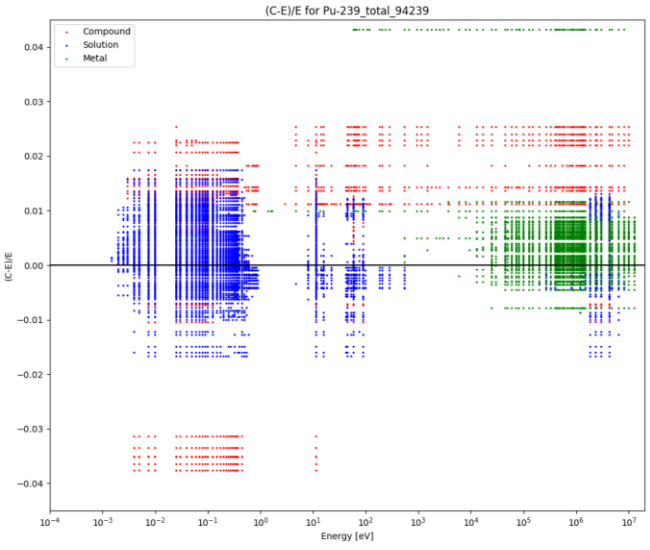


Fig. 3: Individual (C-E)/E Heatmap for $^{239}$Pu, ENDF/B-VII.1 Library

As was noted previously, the benchmarks sensitive to $^{239}$Pu in the intermediate energy region tend to all be high (have a (C-E)/E above 0, or a C/E above 1) and this can be seen in Figure 3. However, Figure 3 also reveals something else – most of these outliers were also compound systems. In fact, most of the compound systems for $^{239}$Pu are either very high or very low; this could also be caused by low quality benchmarks.

Even in the thermal and fast regions, there is a slight bias for $^{239}$Pu, which could suggest the fission cross section (or nu-bar) for $^{239}$Pu is too high in these regions. Without digging into these individual benchmarks in depth, it would be hard to come to a definitive conclusion that cross sections in one region or another are too high or too low, but this method gives a new way of identifying where issues with nuclear data may exist.

Additionally, reviewing existing experiments in this way is a useful tool for determining what new experiments would be valuable. In the $^{239}$Pu example, many of the benchmarks sensitive to $^{239}$Pu in the 1 keV - 10 keV region all have a (C-E)/E well above 0. This might suggest that a new measurement, designed to be sensitive to $^{239}$Pu cross sections in the 1 keV – 10 keV region would be a useful addition and would be able to validate nuclear data in this energy region.

One important note: this data is not complete, as not all benchmarks have sensitivity files or $k_{eff}$ values. Of the 4913 benchmarks, 4180 of them have sensitivity data, and S. van der Marck simulated $k_{eff}$ values for 1977 of those benchmarks.

Another interesting note about sensitivities is that the sensitivity of any particular isotope/material is inherently tied to the overall system. For example, $^{16}$O has a smooth cross section, however, if you look at Figure 4, it's easy to see there are a few energies (near 10 eV) where many benchmarks are sensitive to oxygen cross sections.

The reason for this is due to large capture resonances in $^{238}$U, oxygen scattering near a resonance can scatter neutrons into or out of that resonance, making the system sensitive to oxygen scattering at those specific energies. Interestingly, because scattering can scatter neutrons into or out of a resonance, the sensitivity varies wildly; at energies just above a large capture resonance, the oxygen scattering sensitivity is highly negative, since a neutron scattered at that energy may scatter into the $^{238}$U resonance. However, for neutrons at the energy of the $^{238}$U resonance, scattering with oxygen will lower the neutron energy enough to escape the resonance, making the sensitivity very high and positive.

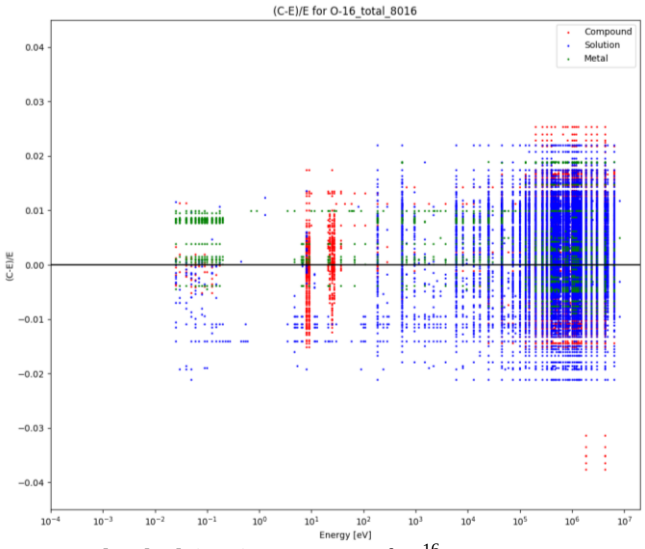


Fig. 4: Individual (C-E)/E Heatmap for $^{16}$O, ENDF/B-VII.1 Library

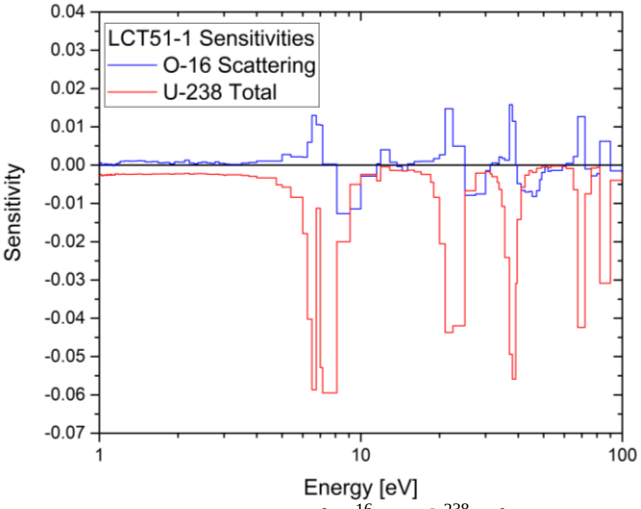


Fig. 5: LCT51-1 Sensitivities for $^{16}$O and $^{238}$U from DICE

This can be seen in Figure 5, a comparison between the $^{16}$O scattering sensitivity and $^{238}$U total sensitivity for LCT51-1, a benchmark with $UO_2$ pin fuel and $H_2O$ moderator (sensitivity data was plotted from DICE[8]). Additionally, this effect seems to occur mostly in compound fueled systems with $UO_2$ fuel, suggesting that the benchmark is specifically sensitive to scattering interactions taking place in the oxygen in the fuel, as opposed to oxygen in the $H_2O$ moderator (which is dominated by hydrogen scattering).

## CONCLUSION

Results shown here represent a small fraction of the results produced in this work; plots were generated for all isotopes which have a benchmark sensitive to it. Additional work is

also ongoing to evaluate ENDF/B-VIII.0[9]. While still not complete (some benchmarks are missing sensitivity files) this work will help to answer questions about what isotopes, energies, and interactions are covered well by existing benchmarks, which benchmarks are missing, and which additional integral measurements might be needed.

## ACKNOWLEDGMENTS

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