Data Assimilation for Fission Neutron Multiplicity Data

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Outline

Data uncertainties are becoming more important.

- The combination of simulation and experimental data to understand or constrain nuclear data is an important task.
- Data assimilation or calibration exercises run the risk of getting the right answer for the wrong reasons.
- For example, the calibrated data could produce simulations that match eigenvalues for particular experiments but fail on other integral experiments.
- The more experimental data we use the better we can calibrate the data.

- In this work, we tackle the problem of calibrating the mean number of fission neutrons per induced fission in ^{239}Pu, as a function of incident neutron energy.
- Similar work has been performed recently with a focus on calibration of energy-independent parameters of fission spectra based on MCNP simulations of sub-critical experiments (Arthur et al. 2019).
    - This work utilized a genetic algorithm to optimize the width of induced and spontaneous fission number distributions, as well as the mean number of neutrons produced per spontaneous fission for ^{240}Pu.
    - The optimization space of each parameter was limited by the variance of each parameter, and new values of multiplicity moments were predicted using finite difference estimated sensitivities.
    - The simulations were able to demonstrate positive matches to moments of multiplicity distributions, with the greatest effect from the ^{240}Pu fission rate.

Our work is a different approach than existing methods.

- Previous work in (Siefman et al. 2018) measured the effects of perturbing data from ENDF/B-VII.1 and how well two stochastic methods, Monte Carlo Bayesian Analysis (MOCABA) and Bayesian Monte Carlo (BMC), compared to the commonly used Generalized Linear Least Squares (GLLS).
- It was demonstrated that both these stochastic methods performed as well as GLLS; however, they both needed more data to reduce the uncertainty, with MOCABA needing less data than BMC.
- The novelty of this paper is that it includes a penalty in the calibration that is not present in GLLS.
- In addition, while (Siefman et al. 2018) focused on critical systems, the experimental data used for this paper are from both critical and subcritical systems.

The potential calibration space that we investigate is large.

- The work described herein adds complementary results to prior work by analyzing the energy-*dependent* effects of for subcritical experiments and criticality benchmarks, where the space is large enough that computing sensitivities via finite-difference would be computationally prohibitive.
- This work attempts to utilize a set of pre-existing MCNP (C.J. Werner (editor) 2017) simulations of experiments to build a statistical model that can be used for nuclear data evaluation.
- These simulations were generated previously using random samples of the energy-dependent space (Bolding 2013).
- Computationally, using this pre-existing data to build a statistical model introduces minimal cost, relative to the original simulations, whereas the use of global optimization methods directly would require many additional, expensive MCNP simulations.
- Ideally, this approach will lead to a proposed adjustment to the nuclear data, but it should at least provide insight for data evaluators on where in energy for ^{239}Pu has been artificially altered.

- Experimentally generated multiplicity distributions are important because they indirectly provide passive information about neutron sources and multiplication in a subcritical system of interest (Reilly et al. 1991).
- High-quality experimental measurements of a sphere of plutonium referred to as the BeRP ball were used to generate neutron multiplicity distributions.
- Multiplicity distributions were generated for five different moderator thicknesses. Previous work has investigated the cause of a known overbias between multiplicity distributions generated by MCNP simulations and the experimental data Miller, Mattingly, et al. n.d.
- A simulated multiplicity distribution is generated by post-processing time-dependent tallies of analog neutron histories reaching the detector, using an assumed detector dead time approximation.
- The cause of the overbias is believed to be inaccuracies in the nuclear data because equivalent simulations of ^{252}Cf experiments did not demonstrate this overbias (Miller, Mattingly, et al. n.d.). Additionally, increased moderator thickness lead to higher differences, indicating the potential need for energy-dependent corrections.

We use a suite of MCNP simulations with perturbed for ^{239}Pu.

- In this work, we will utilize pre-existing MCNP simulated data of these simulations from Bolding 2013, consisting of multiplicity distributions and criticality benchmarks.
- The MCNP simulations were performed using energy-dependent perturbations of for ^{239}Pu to demonstrate the need to include simulations of subcritical experiments in the evaluation of nuclear data.
- The perturbations were generated by producing random samples of the covariance matrix provided by ENDF/B-VII.1 for of ^{239}Pu. The covariance contains average uncertainty values across 50 energy groups, with the slowest energy group containing no data.
- Of interest to this work, is that the cross-correlation terms between groups are negligible (Bolding 2013), which does not preserve the smoothness of sampled data between energy groups.

- Samples were generated assuming a multi-variate Gaussian distribution for the uncertainty of in each group.
- We call the vector of the adjustments Δ.
- Five hundred (500) realizations of the nuclear data were generated, and then MCNP simulations were performed to calculate the simulated multiplicity distributions.
- The Jezebel criticality benchmark was also simulated for each realization of the nuclear data to demonstrate the effect on k_{eff}.
- This benchmark was chosen because it is a bare critical sphere of Pu and it is known that for ^{239}Pu was artificially increased in the epithermal range to match this benchmark.

- Neutron Multiplicity Distributions
  - Provide multiplication information
  - Passive assay of sub-critical, fissionable systems
- Multiplicity Counting
  - Array of large detectors
  - Time-dependent detection information

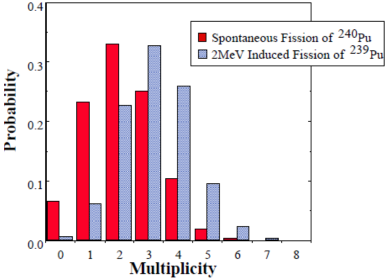
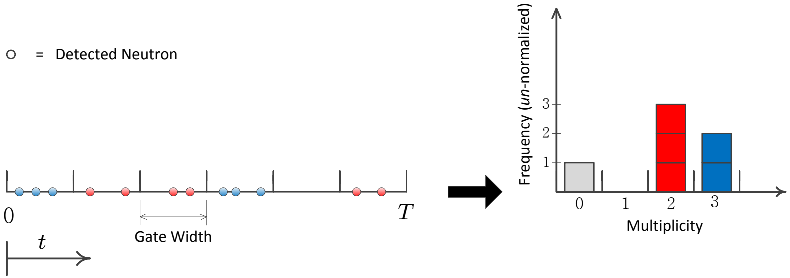
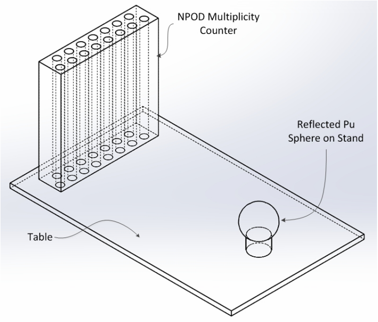


Figure: Multiplicity distributions [PANDA Manual, 1991]

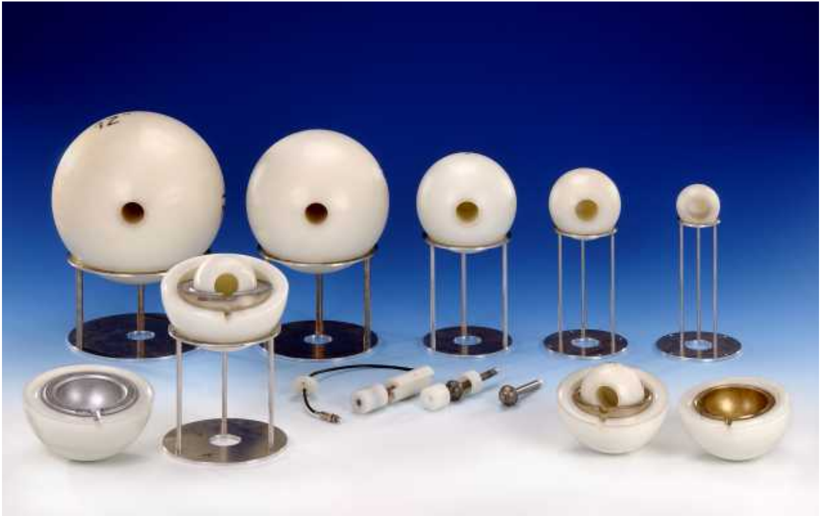


- Normalize to form a PDF
- Typically use factorial moments

Multiplicity experiments record how the distribution changed with differing moderators.



- Performed at LANL for verifying subcritical simulations
- Experimental Parameters
  - 94% ^{239}Pu sphere
  - NPOD multiplicity counter
  - 5 experiments
    - HDPE shells: None, 0.5 cm, 1.0 cm, 1.5 cm, 3.0 cm
- Recorded multiplicity distributions are well verified
- Repeated with ^{252}Cf



A χ^2 metric is used to compare simulation and experiment.

- The sets of resulting data were compared using a χ^2 statistic as a metric of the reduction in bias in multiplicity distributions, without sacrificing the accuracy of k_{eff} in criticality experiments.
- The χ^2 statistic for each Δ, is defined as

$$\chi^2(\Delta) = \frac{(k_{\text{sim}} - 1)^2}{\sigma^2(k_{\text{sim}}) + \sigma^2(k_{\text{exp}})} + \sum_{\text{exp}} \frac{1}{N_{b,\text{exp}}} \sum_i \frac{(S_i - E_{i,\text{exp}})^2}{\sigma^2(S_i) + \sigma^2(E_i)}, \tag{1}$$

  where

  - the sum over i represents each bin in the multiplicity distribution (i.e., a multiplet),
  - the sum over experiments represents each of the 5 moderator thicknesses,
  - S_i and E_i are the MCNP simulated and experimental value of multiplicity for bin i, respectively,
  - the N_b values are the number of bins that have a non-zero value;
  - the uncertainties in the denominator include counting statistics of the simulated multiplicity distribution via MCNP, as well as the experimentally estimated uncertainties.
- Equation (1) also includes a contribution from the computed value of k_{eff} relative to the Jezebel benchmark.
- A lower value of χ^2 indicates a better match for a particular Δ.
- Note that because all simulations are weighted equally, the terms in the statistic are weighted such that improved accuracy in multiplicity distributions produces a greater effect than improved accuracy in k_{eff}.

We build a Gaussian Process model to estimate $\chi^2(\Delta\nu)$.

- In our study, we use Gaussian process regression (GPR) (McClarren 2018) to build a statistical model of $\chi^2(\Delta\bar{\nu})$ from the 500 sets of MCNP simulations.
- Using this model we then seek to minimize the discrepancies between the simulations and the experimental measurements.
- However, we also desire to penalize the calibration problem to reduce the chance of large deviations from the evaluated data.
- Philosophically, we take this approach because we do not want all of the discrepancy between simulation and experiment to be removed via calibrating $\bar{\nu}$.

Our calibration metric contains a total variation penalty term.

- Our calibration problem is ill-posed because there could be many adjustments to $\Delta\bar{\nu}$ that could yield a small value for χ^2.
- Additionally, because of the negligible cross-correlation terms in the covariance matrix the randomly sampled date has many non-physical, opposite adjustments between adjacent energy groups in smooth regions of .
- Therefore, we seek to add constraints. We borrow from compressed sensing (Candes, Romberg, and Tao 2005; Vaquer, McClarren, and Ayzman 2016) by adding a regularization term to the minimization problem to avoid oscillatory corrections such as adding a large positive addition in one group and a large negative addition in the next unless such an adjustment gives a large improvement in χ^2.
- To quantify the oscillatory nature of an adjustment we use the total variation (TV) norm:

$$\mathrm{TV}(x) = \sum_{i=1}^{N-1} |x_i - x_{i+1}|, \tag{2}$$

where N is the length of the vector.

We calibrate to a minimize χ^2, total variation, and the divergence from the original data.

- Given the considerations of desiring small adjustments and non-oscillatory adjustments, we look to minimize the metric

$$L = \frac{\chi^2(\Delta\bar{\nu})}{100} + \mathrm{TV}(\Delta\bar{\nu}) + \|\Delta\bar{\nu}\|_2, \tag{3}$$

  over all possible perturbations $\Delta\bar{\nu}$ to the data.
- The metric weights χ^2 to give it the same order of magnitude as the total variation and the magnitude of the perturbation.
  - For the MCNP simulations the value of $\chi^2(\Delta\bar{\nu})$ was about 200 or greater, and our weighting makes it several times as important as the other two components of the metric.
- To minimize L we use a Markov chain Monte Carlo procedure where new values of $\Delta\nu$ where sampled from independent normal distributions centered at the current chain state.
  - Sampled values of Δ we accepted as the new chain state if they decreased the value of L or if they increase the value of L by a percentage smaller than a random number in 0 to 1.
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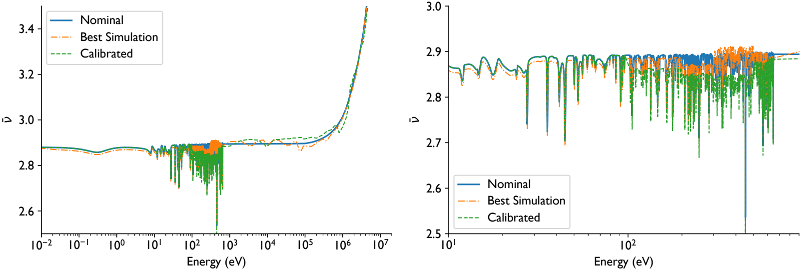
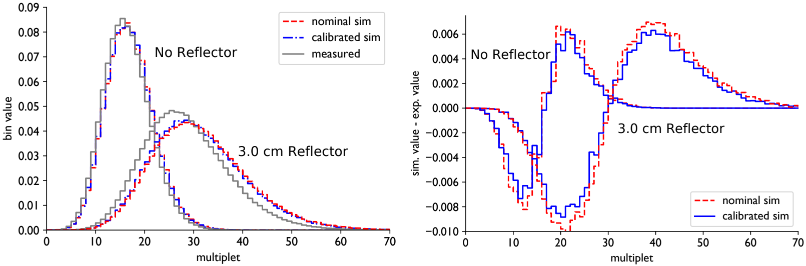
The best values of the calibrated data show a lowering of the multiplicity in the resonance range.



The calibrated data shifts the peak of the multiplicity distribution of the 3 cm reflector toward the experiment.



The error in the multiplicities is reduced by a factor between 10 and 15%.

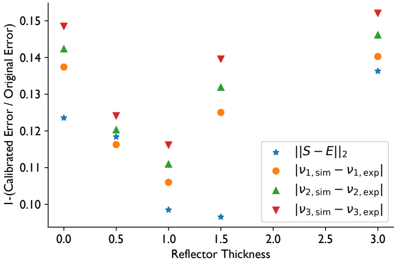
- To quantify the improvement we computed the difference between the multiplicities in a simulation and the experimentally measured multiplicities and take the 2 norm, $\|S - E\|_2$, where S is the vector of simulated responses at each multiplet, and E is the experimentally measured values.
- We also compute the first 3 factorial moments for the simulations and the measured data; a factorial moment is computed as

$$\nu_1 = \sum_{\ell=1}^{\max} \ell S_\ell,$$

$$\nu_2 = \sum_{\ell=2}^{\max} \ell(\ell-1) S_\ell,$$

$$\nu_3 = \sum_{\ell=3}^{\max} \ell(\ell-1)(\ell-2) S_\ell.$$

- Though not shown, we have found that higher moments demonstrate a larger improvement as the moment order is increased.



The performance on Jezebel does degrade.

- The value for k_{eff} using the calibrated data on Jezebel were $k_{\mathrm{eff}} = 0.9984$ ± 0.00032.
- This compares with the nominal data where $= 0.99995 \pm 0.00010$.
- The nominal data is within 1 standard deviation of the benchmark value of 1 ± 0.0020, whereas the calibrated data is 5 standard deviations from 1 but still within the one standard deviation uncertainty in the experiment.
- This is an undesirable result, despite the fact that the multiplicity distributions were improved.
- We believe that this is the result of the large uncertainties in the $\mathrm{k_{eff}}$ simulations used in the calibration procedure. These values for $\mathrm{k_{eff}}$ were computed only to an uncertainty of ± 0.001, and, as a result, 53% of the simulations in the data set where within one standard deviation of 1. This large uncertainty could cause the calibration procedure to discount how perturbations in to (E) will affect $\mathrm{k_{eff}}$.

The use of total variation in a calibration procedure has benefits.

- We have introduced a new approach to adjusting nuclear data using the total-variation norm to avoid oscillatory adjustments.
- We used an MCMC sampling procedure and a Gaussian process regression emulator to perform the calibration.
  - The MCMC sampler was used to minimize the a loss function that was a combination of the χ^2 value for a perturbation, the total variation of the perturbation, and the magnitude of the perturbation.
- We believe that this approach can produce nuclear data adjustments that avoid unnecessary oscillations in the adjustment.
- For the adjustment for (E) for ^{239}Pu we find that our calibration improved agreement with experimental multiplicity measurements. The covariances for the simulations are likely under-predicted, as the calibration based on samples of the covariance data were not able to strongly correct the distributions while preserving smoothness.
- We should generate more samples to test this hypothesis in future work.
- Future work should investigate this type of adjustment procedure on other nuclear data types. We believe the physical ideas encoded in the TV norm make it potentially useful for a variety of problems.

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