Med-Fi Covariances: caveats, with Optical Potentials as an example

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Distribution of data with select covariances: do not stray far from the line of stability

Evaluations that include (n,el), (n,n'), (n,2n), and (n,γ) covariances:



"the goal is completeness, not high fidelity. [...] Neither would the existence of this body of data remove at all the necessity for a more methodical and accurate evaluation of important covariance data, such as is underway at several Laboratories."

"In order to accomplish this large task, there was minimal utilization of experimental data."

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Image credit to Robert Casperson

What does it mean in practice? In regions where theory works well data can be used to gauge parameters and uncertainties

- Fit optical model potential to reproduce data.
- Reproduce ENDF result (obtained using generalized least squares)
- Post-fit, use various methods (Kalman Filter/Backward-Forward Monte Carlo) to obtain covariances by mixing theory with data.



In a perfect world, with data statistically distributed, both methods seem to work

- BFMC mean is closer to the true value post-data introduction.
- Multiple realizations, each get assigned a different weight according to agreement to data.
- But how do pathogenies in the data manifest/propagate to the evaluation?



Most codes can handle inputs that are correlated across small mass ranges.

- Example: optical potential parameters: Linear with mass/isospin asymmetry
- Hauser-Feshbach calculations: Same level density/strength function/(fission) parameters for a given nucleus regardless if it is reached by neutron absorption, (γ,n), (n,2n) etc.



Result is a more robust fit, that also extends across multiple nuclei. Can we extend data to discern mass dependence ?



Need: correlated data sets are highly valuable.

If data is abundant, we can try to ignore theory

- ²³⁹Pu(n,tot) cross section has multiple measurements across various energy ranges.
- Clear normalization disagreements between various experiments.
- ENDF evaluation is smooth in this case, not necessarily the case for other actinides.



By binning the data in small energy increments we can discern driving parts

- Make small (10 keV) bins in energy and fit a straight line.
- The uncertainties **are** plotted here.
- Line can be evaluated at mid-bin as a reference.
- Clearly, while the data could follow the linear model, statistically speaking, they don't agree with it (>3σ discrepancies).



We can re-do the fit excluding each data point and see how they compare

- Single data point dominates the fit (difference of ~1%).
- Uncertainty of prediction almost doubles.
- Looking back, it corresponds to a single point that has ~1 order of magnitude less uncertainty than the rest (from Harvey, 1988, σ_{tot} =12.2 b at 0.075 MeV).
- The rest of the measurements are a perturbation of 0.4% of the mean.



Bootstrapping also points to the same conclusions.

- Take a subset of data points, replicate them to have the same total number of data, repeat.
- Hover between the two values, but now the rest of the experiments have a larger weight.



Iterative outlier rejection can be automated



Images credit to Cole Pruitt

Conclusions

- We use what data exists to constrain the model(s).
- Moving to regions of the chart vs specific nuclei represents new challenges.
- Should test data sets for consistency with one another: could be automated?
- Inflating error bars could also work (used by PDG).
- Is automatic exclusion a weapon of math destruction?
- Cases where data is sparse require further attention (for example, ²³⁹Pu(n,2n))
- As is, only applies to fast region (>100 keV). Connect regions?