Title: Using MCNP-calculated sensitivities and machine learning to identify unconstrained physics spaces in nuclear data

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Design Similarity to PF -4 Casting
Using MCNP-calculated sensitivities and machine learning to identify unconstrained physics spaces in nuclear data

Presenter: D. Neudecker


2021 MCNP User Symposium, July 14, 2021
MCNP simulations rely on nuclear data.

Prompt Fission Neutron
Spectrum = Energy distribution
of outgoing neutrons

Fission cross-section = probability of fission

Average Prompt Neutron Multiplicity = Av. Number of outgoing neutrons

Prompts 239Pu

Average Prompt Neutron Multiplicity

ENDF/B-VIII.0

ENDF/B-VII.0

Experimental Data

Neutron Energy (MeV)

Outgoing Neutron Energy (MeV)

Cross Section (b)

Fission cross-section obtained in the cross section evaluation on the 2006 standards and the tables are direct output from EDA as point-wise and C(n,n) cross sections had been evaluated using EDA code as GMAP. For the element standards, the tabular output is directly from EDA and the tables are made available at https://www-nds.iaea.org/standards/ together with the evaluated reference Cross Sections for should be smooth. For all the tabular data, the values in the node at 0.1 keV both for the evaluation. 0.1 keV both for the evaluation. For all the evaluations other than those for the light elements standards, the tabular output is directly from EDA, and the additional cross sections obtained in the cross section evaluation process are given in the Tables by “xx”. Smoothing has been applied for regions where are marked by “x” and one corrected point is labelled.
Nuclear data are validated, in turn, often by using MCNP and with respect to criticality.


Av. Prompt Neutr. Multiplicity

Fission Cross-section

Ω \cdot \nabla \psi(r, E, \Omega) + \Sigma_t(r, E, \Omega)\psi(r, E, \Omega)

= \int \int_0^{4\pi} \Sigma_s(r, E' \rightarrow E, \Omega' \rightarrow \Omega)\psi(r, E', \Omega')d\Omega'dE'

+ \frac{1}{k} \int_0^{4\pi} \frac{\chi_f(E')}{4\pi} \int_0^{4\pi} \tilde{\nu}_t(r, E')\Sigma_f(r, E', \Omega')b(r, E', \Omega')d\Omega'dE'
Validation with many $k_{\text{eff}}$ values is a highly under-determined problem, where thousands of nuclear data yield one $k_{\text{eff}}$ value!

**Problem:** which nuclear data values (out of 20,000!) are those that lead to bias in simulating 1000s of validation experiment??

Highly under-determined and complexly intertwined problem leading to unconstrained spaces in nuclear data!

Traditional methods: human brain cannot assess all this complex data at once -> targeted comparison of data with and without an isotope or looking at bare spheres for the actinides -> one could miss issues you are not looking for.

Perfect problem for ML!!!
Unconstrained physics spaces: We can change nuclear data widely within differential constrains and still get the same \( k_{\text{eff}} \)!

Differences in ENDF/B-VIII.0 and JEFF3.3 nuclear data represent uncertainty in the differential information.

Both ENDF/B-VIII.0 and JEFF3.3 compute Jezebel \( k_{\text{eff}} \) equally well using MCNP6 but contributions per reaction differ drastically (Thanks to Mike Rising)
Here, we want to tease out these unconstrained physics spaces using ML and various integral responses.

1. Integral experiments provide vital, non-unique input.
2. Random forest highlights potential issues in nuclear data.
3. Differential experiments and theory further inform nuclear physics.
4. Results:
   - Better nuclear physics understanding of studied observables, or
   - Teasing out unconstrained physics spaces in nuclear data.

See D. Neudecker et al., NDS 167, 36 (2020).
D. Neudecker et al., LA-UR-21-22465, submitted.
We use as ML algorithms random forest and SHAP metric.

• Random forests: Build a prediction model for the bias as non-linear function of potentially informative features:
  \[ \Delta = E - C = f(X_1, \ldots, X_{21000}) + \epsilon \]

• Importance of features assessed with SHAP metric

Step 1 (validation input): simulating 3 integral responses and calculating sensitivities to nuclear data.

1100 crits
40 pulsed spheres

Sensitivities to nuclear data

DN et al., NDS 167, 36, 2020; DN et al., ANE 159, 108345 2021. (thanks to Jen Alwin)

Jezebel (PU-MET-FAST-001)

ENDF/B-VIII.0

14 reaction rates in crits

(Brown et al., NDS 148, 1, 2018)
Steps 2 & 3: ML highlights issue in nuclear data that are explored with differential data and theory -> "a success story"

$^{241}\text{Pu}(n,f)$ cross section among 10 most important reactions related to bias in simulations of validation experiments.

Potential issue in nuclear data given differential experimental data, but where should curve go?

Nuclear theory does not constrain enough to solve the issue.

DN et al., LA-UR-21-22465, submitted.
Feedback loop with ML and validation experiments indicates that lower $^{241}$Pu(n,f) cross section leads to reduced bias.

Using FAUST tool (Wim Haeck), we see that Dirty Jezebel $k_{eff}$ bias reduces from 143 pcm to 4 pcm while average of bias in $k_{eff}$ sensitive to $^{241}$Pu(n,f) improves slightly.

DN et al., LA-UR-21-22465, submitted.
Now an example of finding an unconstrained physics space. ML finds issue in several, inter-twined nuclear data.

This plot illustrates what $^{235}$U nuclear data were highlighted as potentially leading to bias in various integral responses.
There is considerable space in differential data, cannot pin down what nuclear data is wrong -> unconstrained space!

We need better experiments or improved nuclear theory to better constrain these nuclear data that are critical input of MCNP simulations!
Summary

• We are using ML methods and various integral responses to pin down potential issues in nuclear data underlying MCNP and highlight unconstrained physics spaces in nuclear data.

• Identifying unconstrained physics spaces in nuclear data could potentially motivate future measurements or theory developments which in turn leads to better nuclear data for MCNP. These experiments are often designed with the help of MCNP.

• MCNP is also heavily used to simulate various integral responses and to get sensitivities that feed into the ML algorithm.
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