Using Machine Learning Algorithms for Large-scale Nuclear-data Validation.

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Seminar at Universidad Politecnica de Madrid, shortened for SG-46, Nov. 11, 2020

Thanks to: M. Grosskopf, M. Herman, W. Haeck, S. Vander Wiel, M. Rising, O. Cabellos, A. Clark, S. Kahler, T. Kawano, P. Talou.

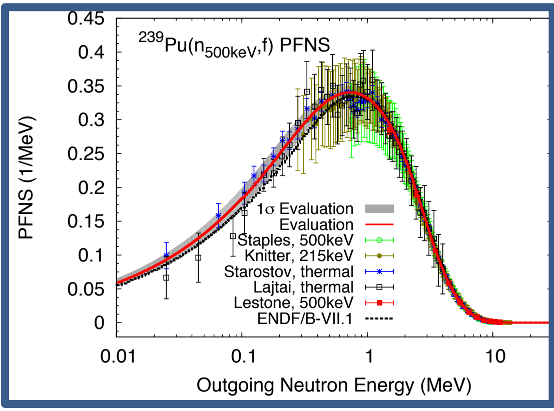
Based on: D. Neudecker et al., Nucl. Data Sheets 167, 36-60 (2020) and continuing work for the LDRD-DR project EUCLID.

LA-UR-20-28240

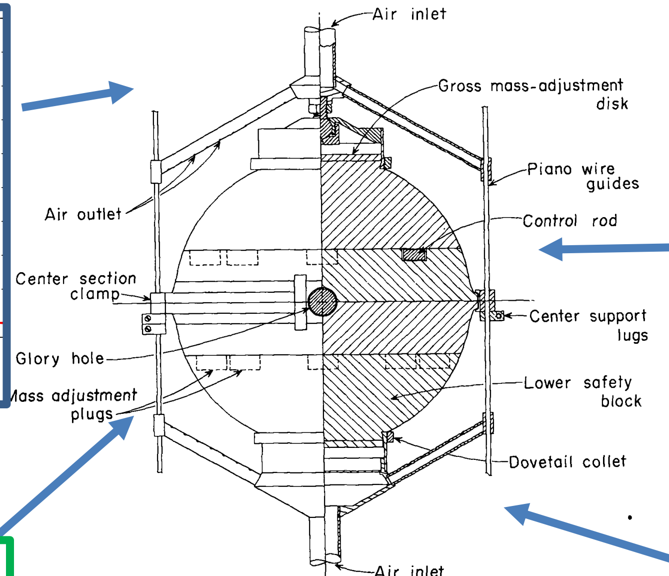
Why should we use machine learning for nuclear-data validation??

A *set of nuclear data* are validated by simulating and comparing to integral experiments.

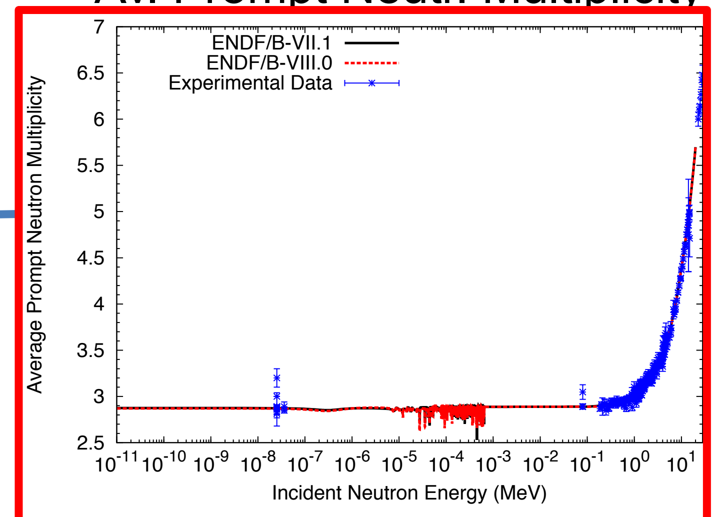
Prompt Fiss. Neutr. Spectr.



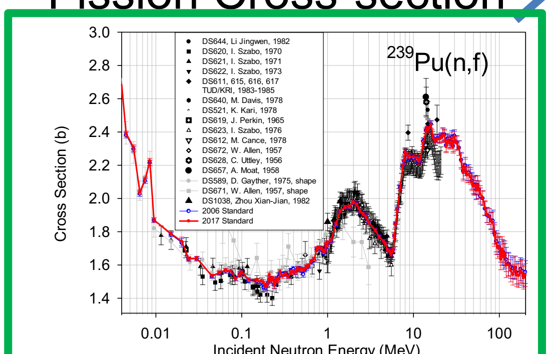
Jezebel critical assembly



Av. Prompt Neutr. Multiplicity



Fission Cross-section



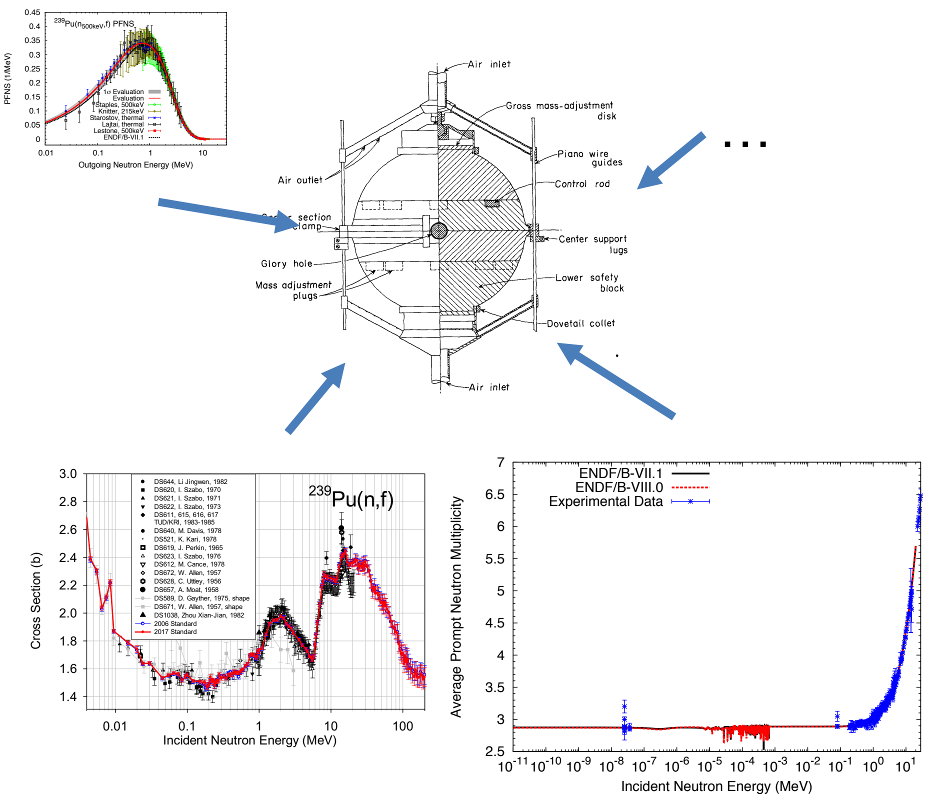
$$\Omega\cdot\nabla\psi(\boldsymbol{r},E,\Omega)+\Sigma_t(\boldsymbol{r},E,\Omega)\psi(\boldsymbol{r},E,\Omega)$$

$$=\int_0^\infty\int_{4\pi}\Sigma_s(\boldsymbol{r},E'\to E,\Omega'\to\Omega)\psi(\boldsymbol{r},E',\Omega')d\Omega'dE'$$

$$+\frac{1}{k}\frac{\boxed{\chi_f(E)}}{4\pi}\int_0^\infty\int_{4\pi}\boxed{\bar{\nu}_t(\boldsymbol{r},E')}\boxed{\Sigma_f(\boldsymbol{r},E',\Omega')}\psi(\boldsymbol{r},E',\Omega')d\Omega'dE'$$

1 k_{eff} value simulated by 20,000 nuclear data values. Which nuclear data causes difference to exp. k_{eff}?

Simulating the Jezebel critical assembly



Problem: human brain cannot assess which of 20,000 nuclear data are related to imperfect simulation of integral exp.

Gap: need systematic method to identify imperfect nuclear data via integral experiments

Impact of solving problem:

- more targeted (cost-effective) nuclear data research
- Identify need for integral and differential experiments
- Better data for application calc.

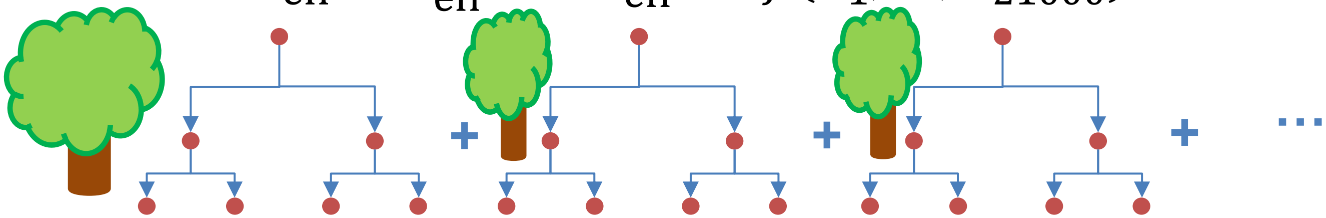
Machine learning algorithms used for nuclear-data validation

We address this problem by augmenting nuclear data validation by using machine learning methods.

<u>Machine learning methods used</u>:

- Random forests: Build a prediction model for the bias as a non-linear function of the large set of potentially informative features:

$$\Delta k_{\mathrm{eff}} = \mathrm{k}_{\mathrm{eff}}^{\mathrm{expt}} - \mathrm{k}_{\mathrm{eff}}^{\mathrm{sim}} = f(X_1, \ldots, X_{21000}) + \epsilon$$



- Importance of features assessed with SHAP metric

<u>Data</u>:

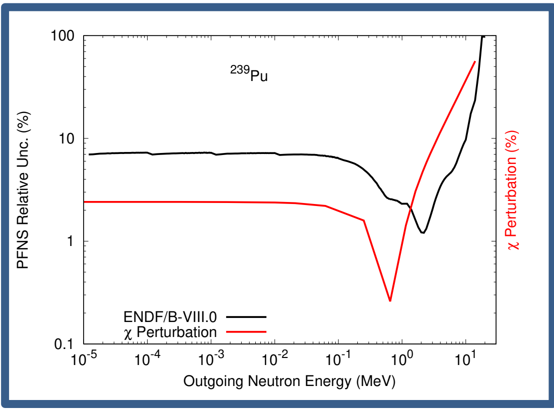
- Input: 875 Δk_{eff} values using ENDF/B-VII.1 and ENDF/B-VIII.0
- Features: for each experiment:
  - ~21000 sensitivity coefficients of nuclear data related to $k_{\mathrm{eff}}^{\mathrm{sim}}$
  - ~ 50 measurement features (e.g., reflector material, spectrum)

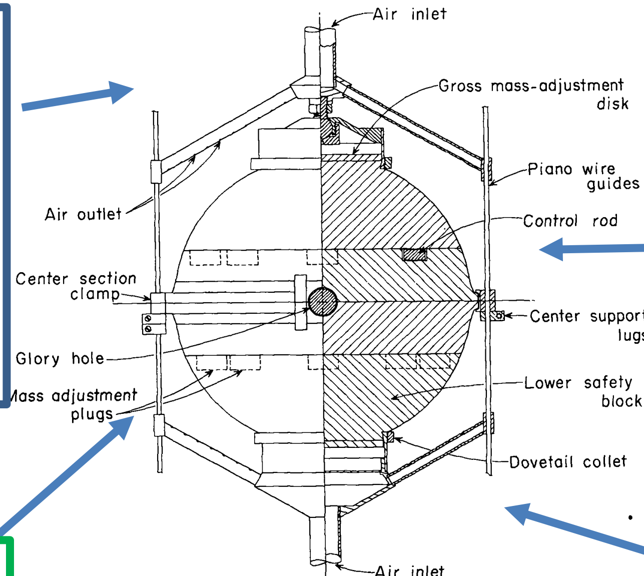
BUT DOES IT WORK??

INVESTIGATING FABRICATED BIASES IN NUCLEAR DATA PERTURBED TO SIMULATIONS OF ICSBEP CRITICAL ASSEMBLIES

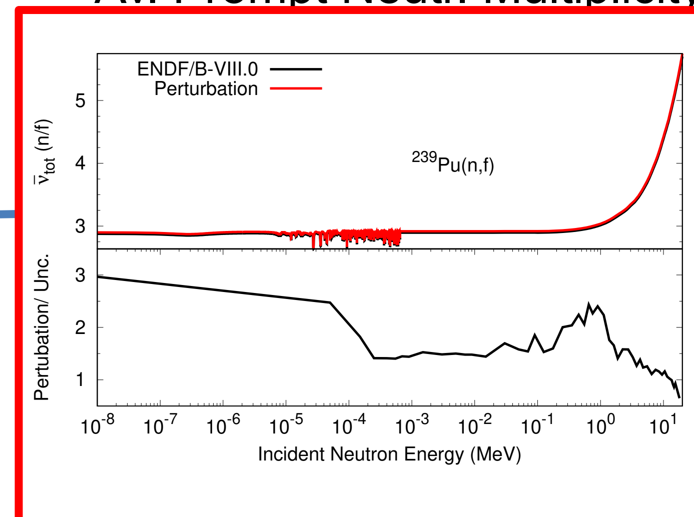
ML algorithms is tested by perturbing changes in total ^{239}Pu fission source term data to k^{sim}_{eff} values.

Total Fiss. Neutr. Spectr.

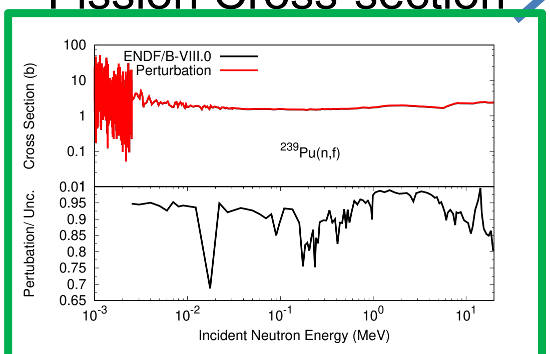




Av. Prompt Neutr. Multiplicity



Fission Cross-section

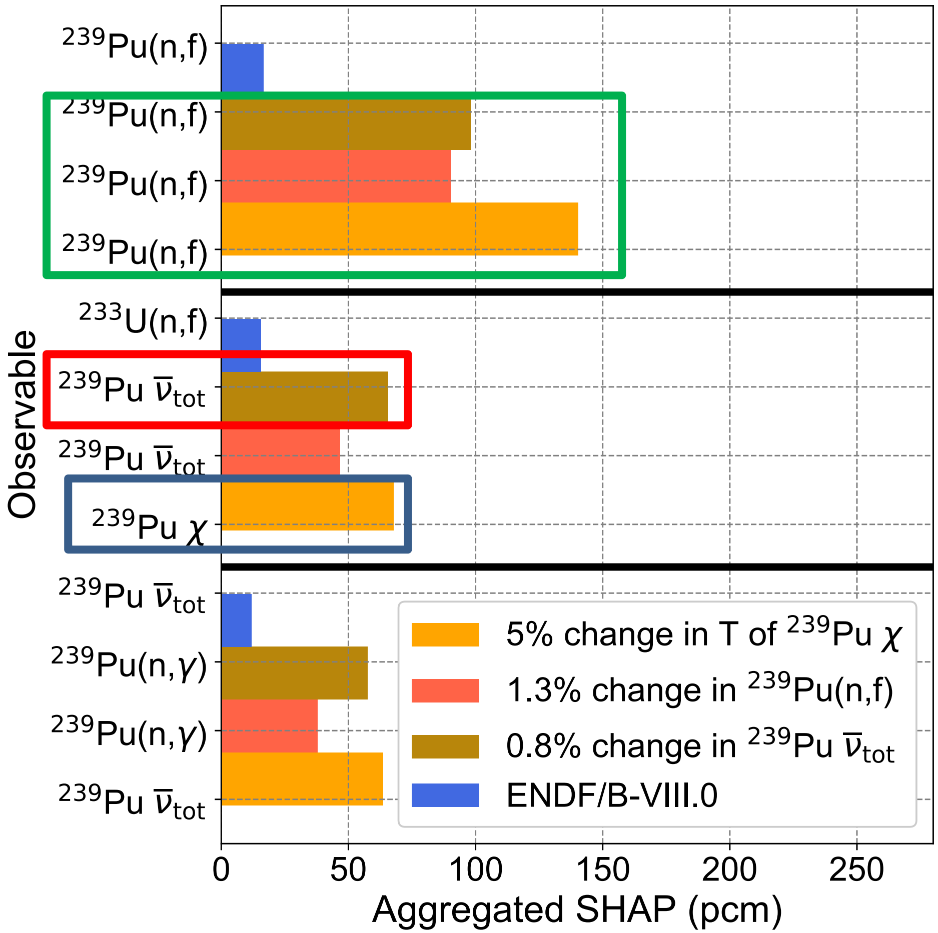


$$\Omega \cdot \nabla\psi(\boldsymbol{r},E,\Omega) + \Sigma_t(\boldsymbol{r},E,\Omega)\psi(\boldsymbol{r},E,\Omega)$$

$$= \int_0^\infty \int_{4\pi} \Sigma_s(\boldsymbol{r},E' \to E,\Omega' \to \Omega)\psi(\boldsymbol{r},E',\Omega')d\Omega' dE'$$

$$+ \frac{1}{k}\frac{\boxed{\chi_f(E)}}{4\pi}\int_0^\infty \int_{4\pi} \boxed{\bar{\nu}_t(\boldsymbol{r},E')}\boxed{\Sigma_f(\boldsymbol{r},E',\Omega')}\psi(\boldsymbol{r},E',\Omega')d\Omega' dE'$$

Yes, ML correctly finds fabricated nuclear data biases impacting simulation of ICSBEP crits.



BUT:

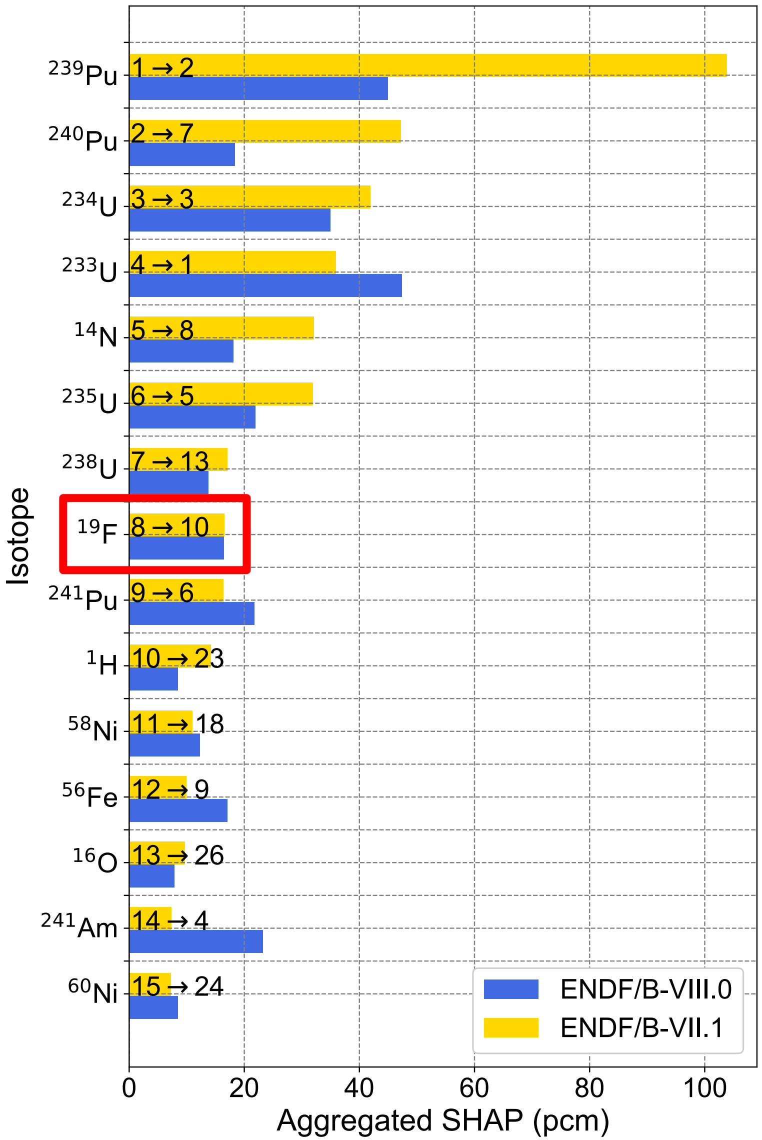
Physics correlations between nuclear data arising from how k_{eff} is simulated have to be considered for the correct interpretation of ML results.

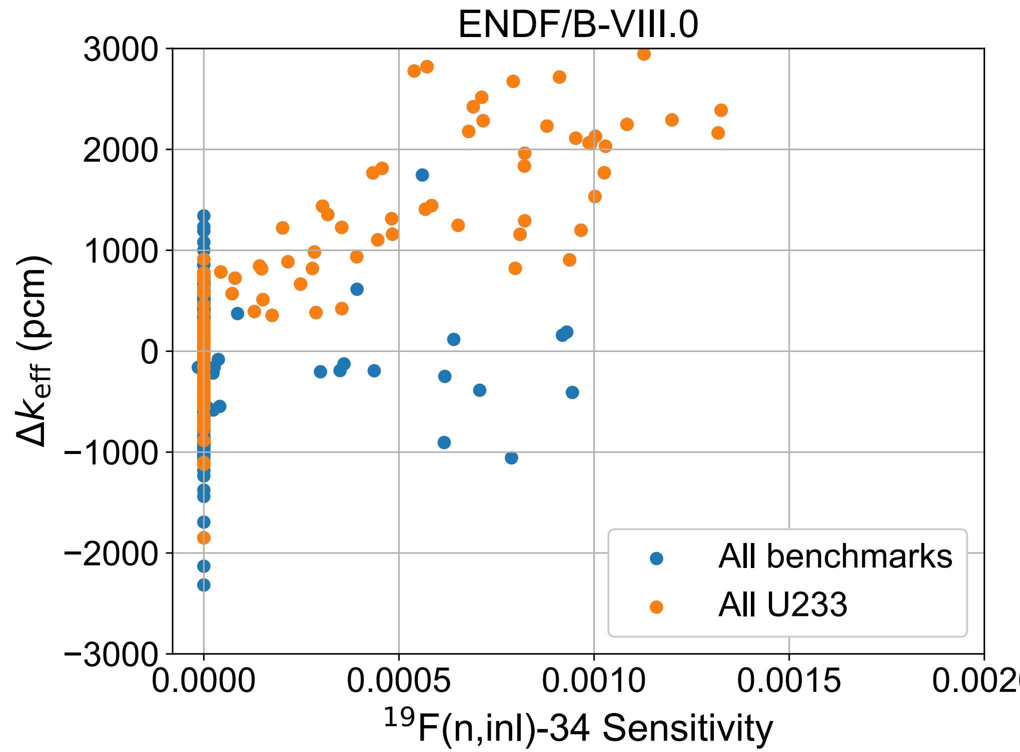
$$+\frac{1}{k}\boxed{\frac{\chi_f(E)}{4\pi}}\int_0 \int_{4\pi} \boxed{\bar{\nu}_t(\boldsymbol{r},E')}\boxed{\Sigma_f(\boldsymbol{r},E',\Omega')}\psi(\boldsymbol{r},E',\Omega')d\Omega' dE'$$

BUT DOES IT WORK FOR REAL CASES??

INVESTIGATING WHETHER ML FINDS *UNKNOWN* SHORTCOMINGS IN CURRENT LIBRARIES

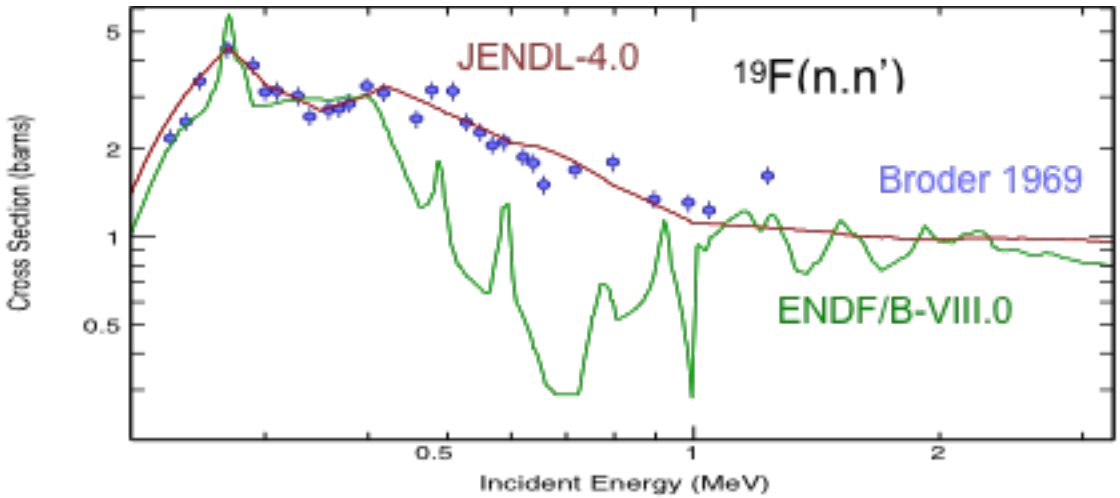
ML points towards potential issue in ^{19}F ENDF/B-VII.1=VIII.0 nuclear data relevant for small-scale exp.





Several ^{19}F nuclear data observables, over a broad energy range, were highlighted as important to predict bias.

Yes, ML correctly identifies unknown issues in current nuclear data libraries.



Issue in ^{19}F(n,inl) nuclear data was hiding in plain sight due to:

- **sheer amount of nuclear data to look through.**
- **expert judgment validation overlooked it because lesser importance for simulating k_{eff}.**

ML caught it given the strong trend but suffers from correlation effect.

ML AUGMENTS EXPERT JUDGMENT NUCLEAR DATA VALIDATION RATHER THAN REPLACES IT.

Validation of ^{241}Pu nuclear data: this is a challenge for ML due to compensating errors

Energy ranges and observables highlighted as problematic by ML.

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
7e-8-1e-5						
1-5.5e^{-4}						
5.5e^{-4}-2.5e^{-2}						
2.5e^{-2}-2.479						
2.479-4.8						
4.8-8.187						

No Diff. Exp.

Exp. Agree with evaluation but freedom to move

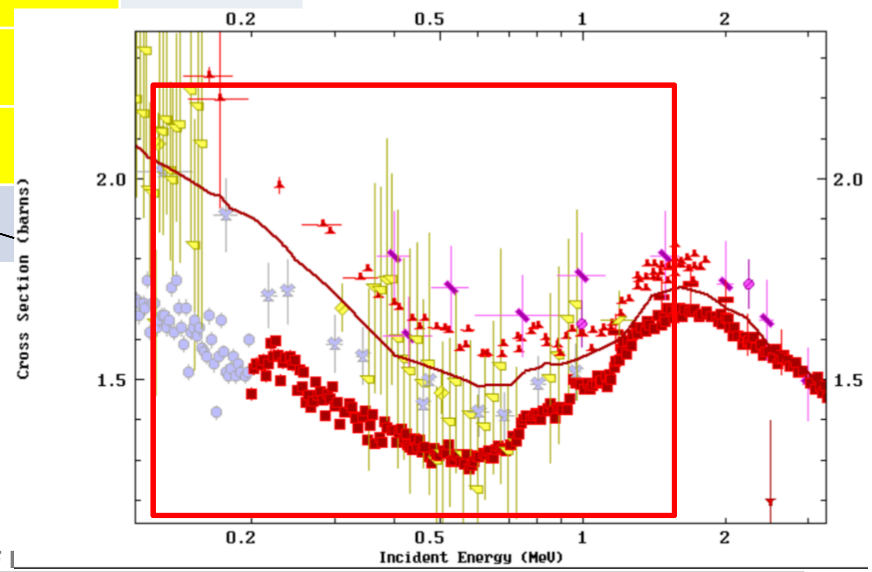
Diff. Exp. Disagree with evaluation

Validation of ^{241}Pu nuclear data: multiple option of wrong data …

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
7e-8-1e-5						
1-5.5e^{-4}						
5.5e^{-4}-2.5e^{-2}						
2.5e^{-2}-2.479						
2.479-4.8						
4.8-8.187						

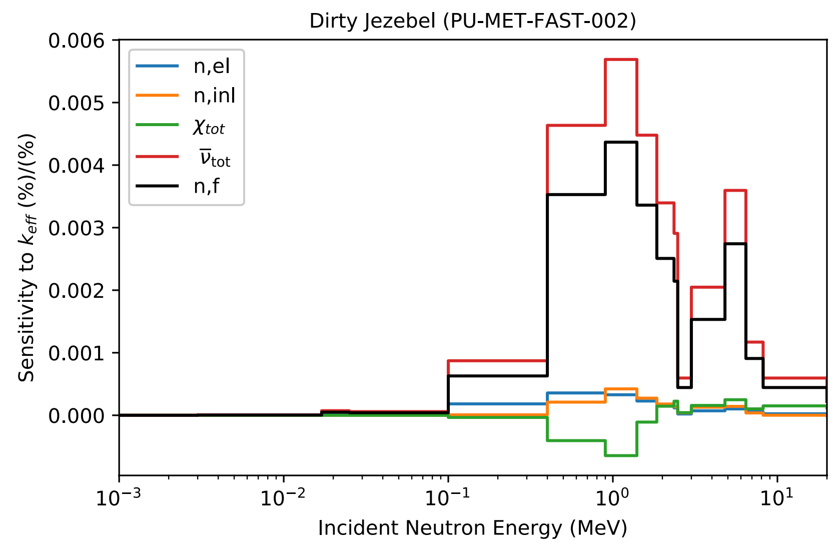
Some questions on the functional form.

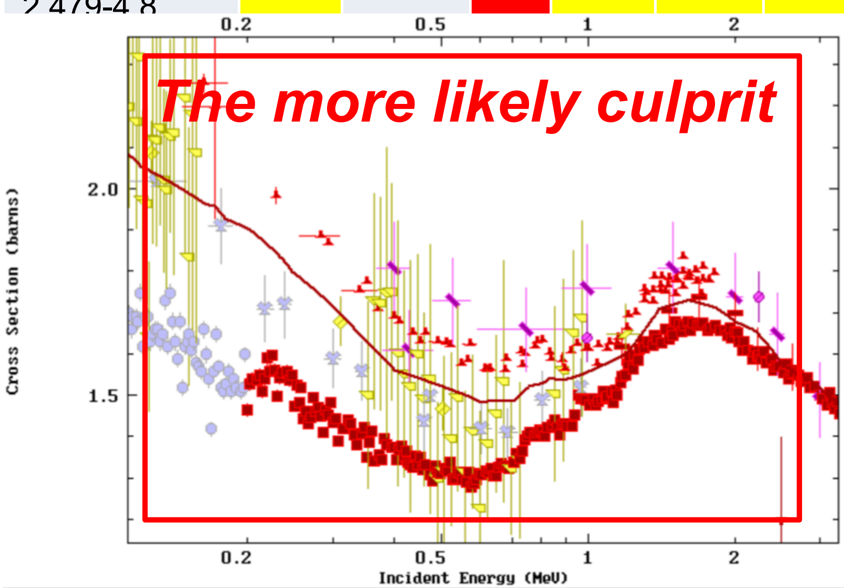
Unphysical functional form!!!



Validation of ^{241}Pu nuclear data: multiple option of wrong data … *experts & differential data can help!*

Energy (MeV)	PFNS	Nu-bar	(n,f)	(n,g)	(n,el)	(n,inl)
Thermal						
7e-8-1e-5						
1-5.5e^{-4}						
5.5e^{-4}-2.5e^{-2}						
2.5e^{-2}-2.479						
2.479-4.8						





The changes required to correct nuclear data according to differential data are not large enough (see sensitivities) to solve issues in simulating critical assemblies.

Take-home message:

- We can use exciting new statistics techniques, such as ML, to further nuclear-data science.
- But do not underestimate the value of expert judgment!

Thank you for your attention!

Acknowledgements

Research reported in this publication was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory.

We gratefully acknowledge the support of the Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory.

This work was supported in part by the DOE Nuclear Criticality Safety Program, funded and managed by the NNSA for the Department of Energy.