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Validating Nuclear Data by Means of Machine Learning Methods

CSEWG, Validation Session 11/4/19

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Authors on related paper: D. Neudecker, M. Grosskopf, M. Herman, W. Haeck, P. Grechanuk, S. Vander Wiel, M. Rising, A.C. Kahler, N. Sly, P. Talou

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Addressing doubts of last CSEWG whether machine learning can be used for nuclear data validation:

We answer the following questions:

- Can **machine learning methods** help us **identify potential shortcomings in nuclear data that significantly impact simulations of nuclear data benchmarks** (e.g., ICSBEP critical assemblies)?

- Can machine learning methods help us identify shortcomings in nuclear data that ***traditional nuclear data validation methods are unlikely to pin-point***?

Addressing doubts of last CSEWG whether machine learning can be used for nuclear data validation :

- Can machine learning methods help us identify potential shortcomings in nuclear data that significantly impact simulations of nuclear data benchmarks?
- Can machine learning methods help us identify shortcomings in nuclear data that traditional nuclear data validation methods are unlikely to pin-point?

<u>We investigate that by testing whether ML finds</u>:

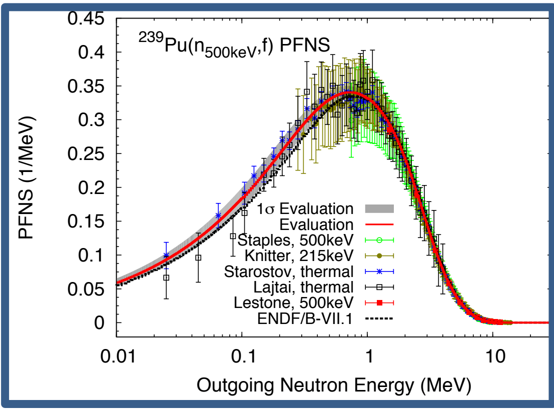
- ✓ fabricated shortcomings in nuclear data perturbed to simulations of ICSBEP crits.
- ✓ Known actual shortcomings in previous and current libraries
- ✓ Unknown actual shortcomings in current nuclear data libraries

WHY SHOULD WE USE MACHINE LEARNING FOR NUCLEAR DATA VALIDATION??

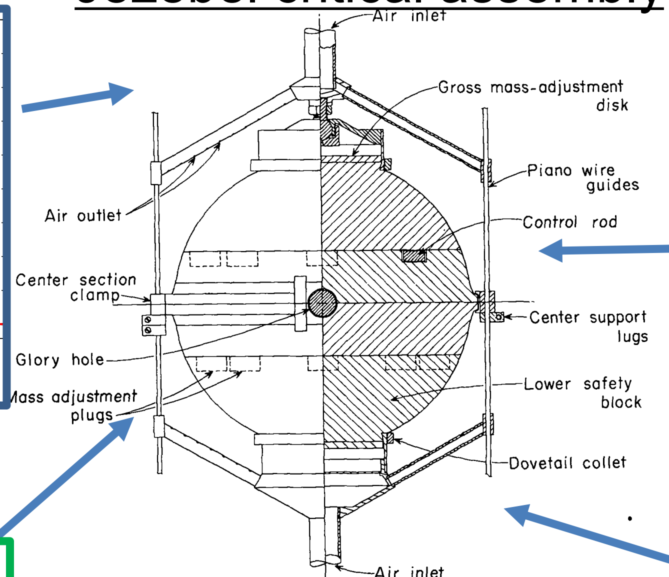
Nuclear data validation is really a big data problem:

<u>*1*</u> k_{eff} value simulated by ~thousand nuclear data. Which nuclear data causes difference to exp. k_{eff}?

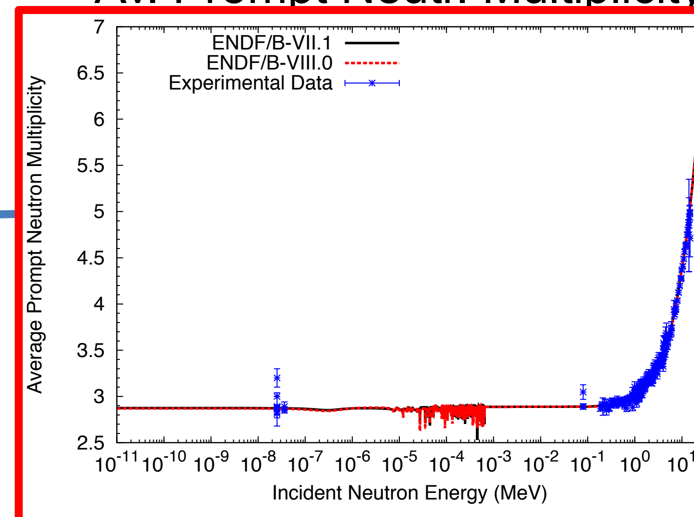
Prompt Fiss. Neutr. Spectr.



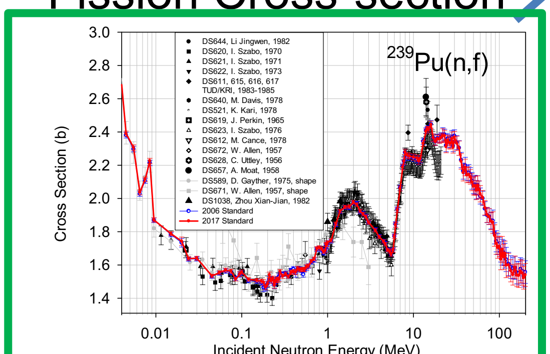
<u>Jezebel critical assembly</u>



Av. Prompt Neutr. Multiplicity



Fission Cross-section



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

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

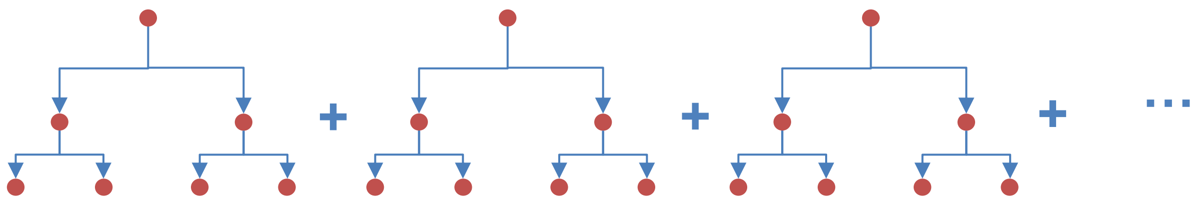
$$+\frac{1}{k}\frac{\boxed{\chi_f(E)}}{4\pi}\int_0^\infty\int_{4\pi}\boxed{\bar{\nu}_t(\boldsymbol{r},E')}\boxed{\Sigma_f(\boldsymbol{r},E',\Omega')}\psi(\boldsymbol{r},E',\Omega')d\Omega'dE'$$

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:

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



- Importance of features assessed with SHAP metric

<u>Data</u>:

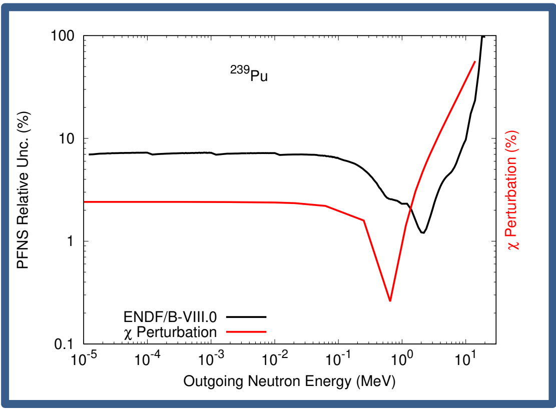
- Input: 875 $\Delta \mathrm{k}_{\mathrm{eff}}$ values using ENDF/B-VII.1 and ENDF/B-VIII.0
- Features: for each experiment:
  - ~21000 sensitivity coefficients of nuclear data related to $\mathrm{k}_{\mathrm{eff}}^{\mathrm{sim}}$
  - ~ 50 measurement features (e.g., reflector material, spectrum)

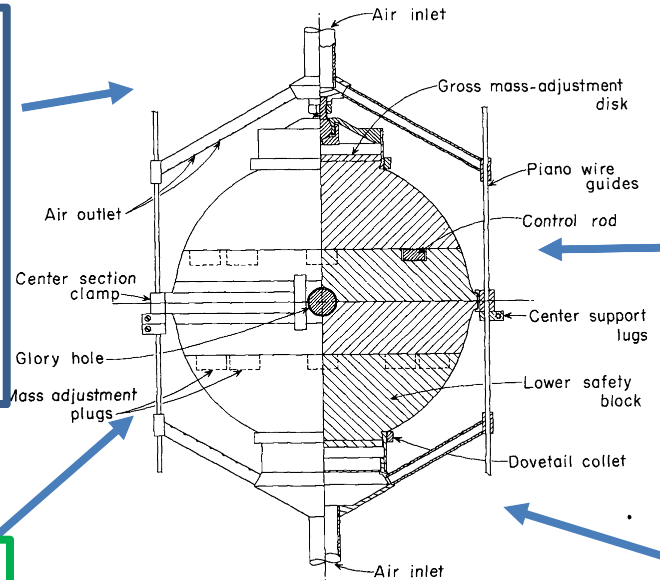
BUT DOES IT WORK??

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

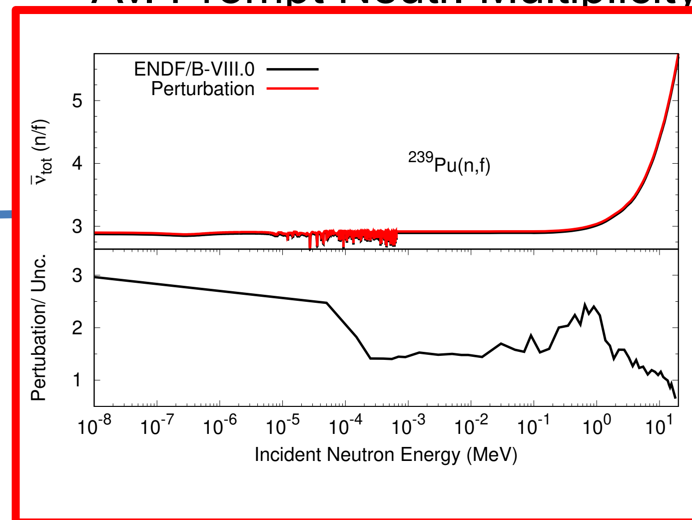
ML algorithms is tested by perturbing changes in total ^{239}Pu fission source term data to k^{sim}_{eff} values.

Total Fiss. Neutr. Spectr.

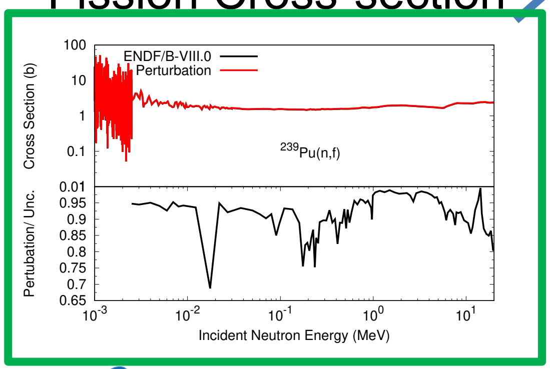




Av. Prompt Neutr. Multiplicity



Fission Cross-section

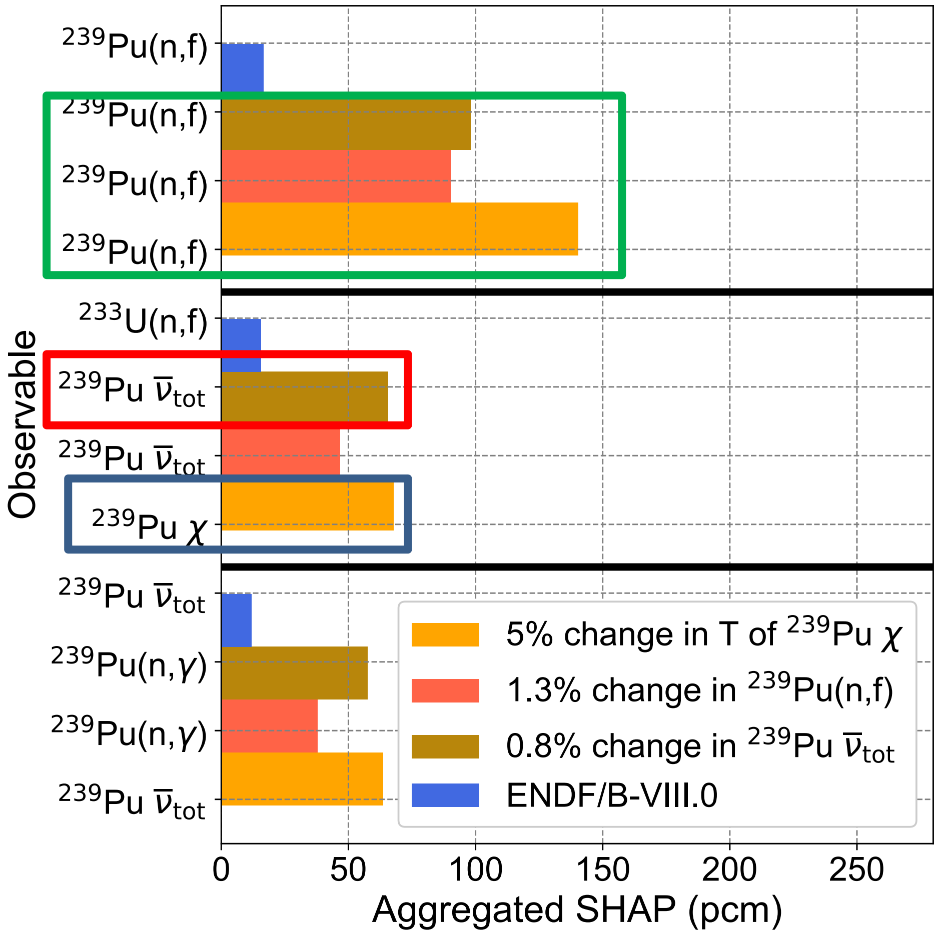


$$\Omega\cdot\nabla\psi(\boldsymbol{r},E,\Omega)+\Sigma_t(\boldsymbol{r},E,\Omega)\psi(\boldsymbol{r},E,\Omega)$$

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

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

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



BUT:

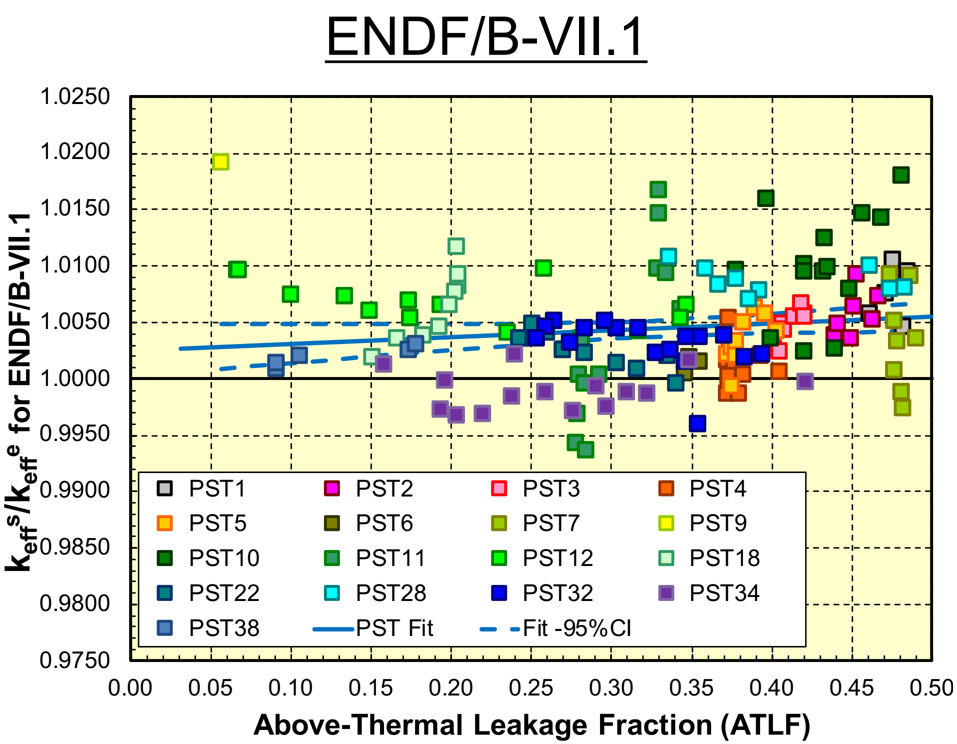
Physics correlations between nuclear data arising from how k_{eff} is simulated have to be considered for the correct interpretation of ML results.

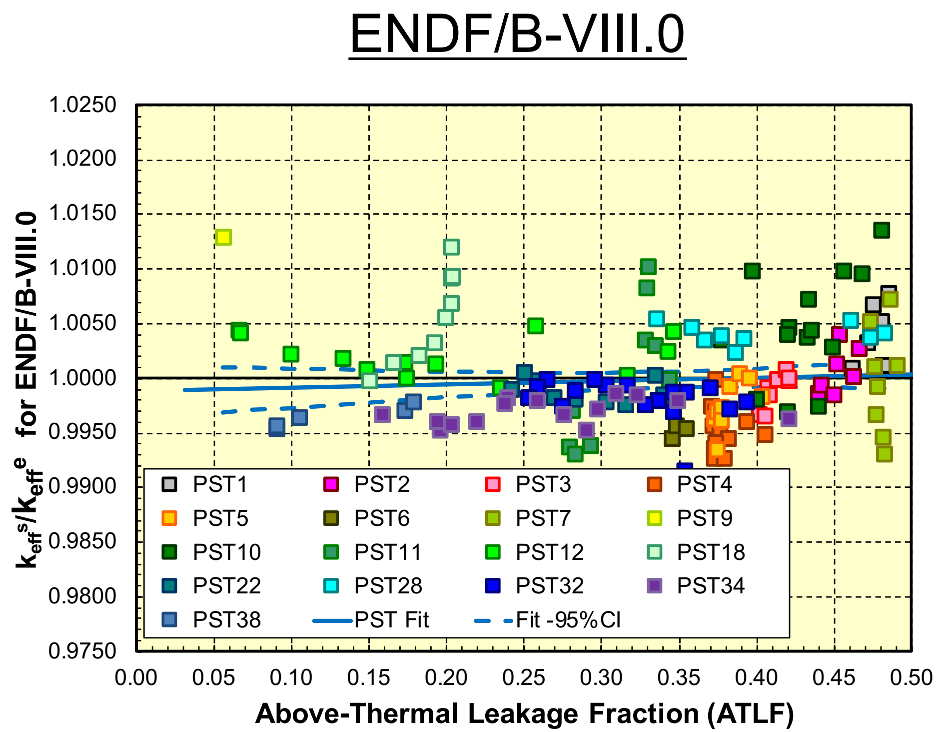
$$+\frac{1}{k}\boxed{\frac{\chi_f(E)}{4\pi}}\int_0\int_{4\pi}\boxed{\bar{\nu}_t(\boldsymbol{r},E')}\boxed{\Sigma_f(\boldsymbol{r},E',\Omega')}\psi(\boldsymbol{r},E',\Omega')d\Omega' dE'$$

BUT DOES IT WORK FOR REAL CASES??

INVESTIGATING WHETHER ML FINDS *KNOWN* SHORTCOMINGS IN PREVIOUS LIBRARIES

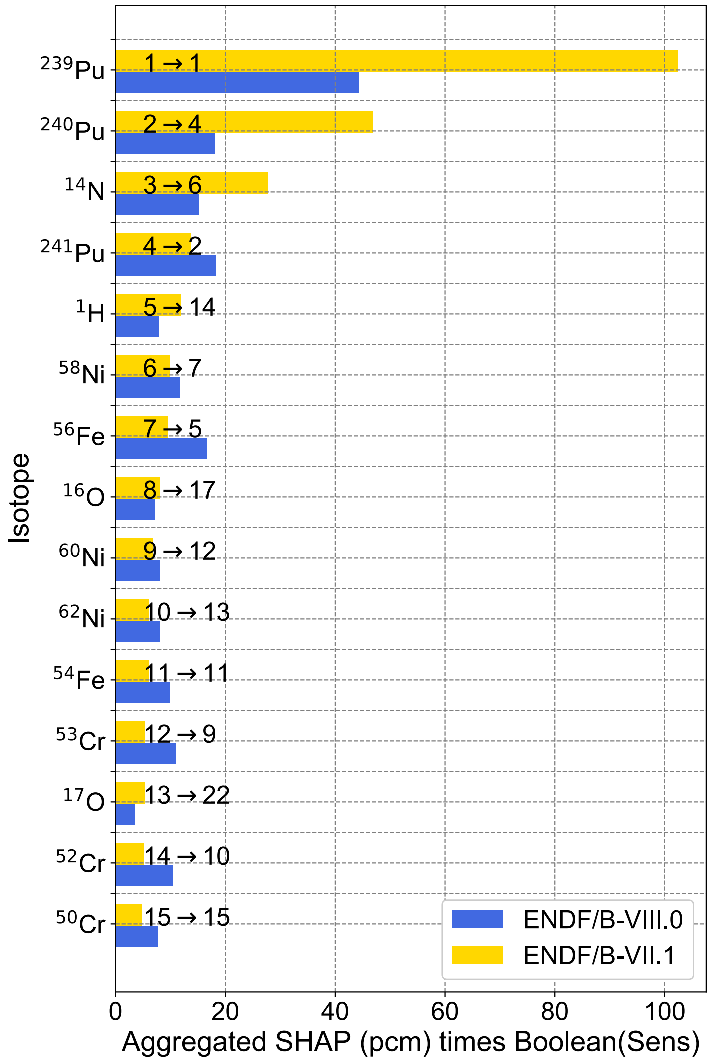
Significant biases in ENDF/B-VII.1 ^{239}Pu resonance and thermal data were removed in ENDF/B-VIII.0.

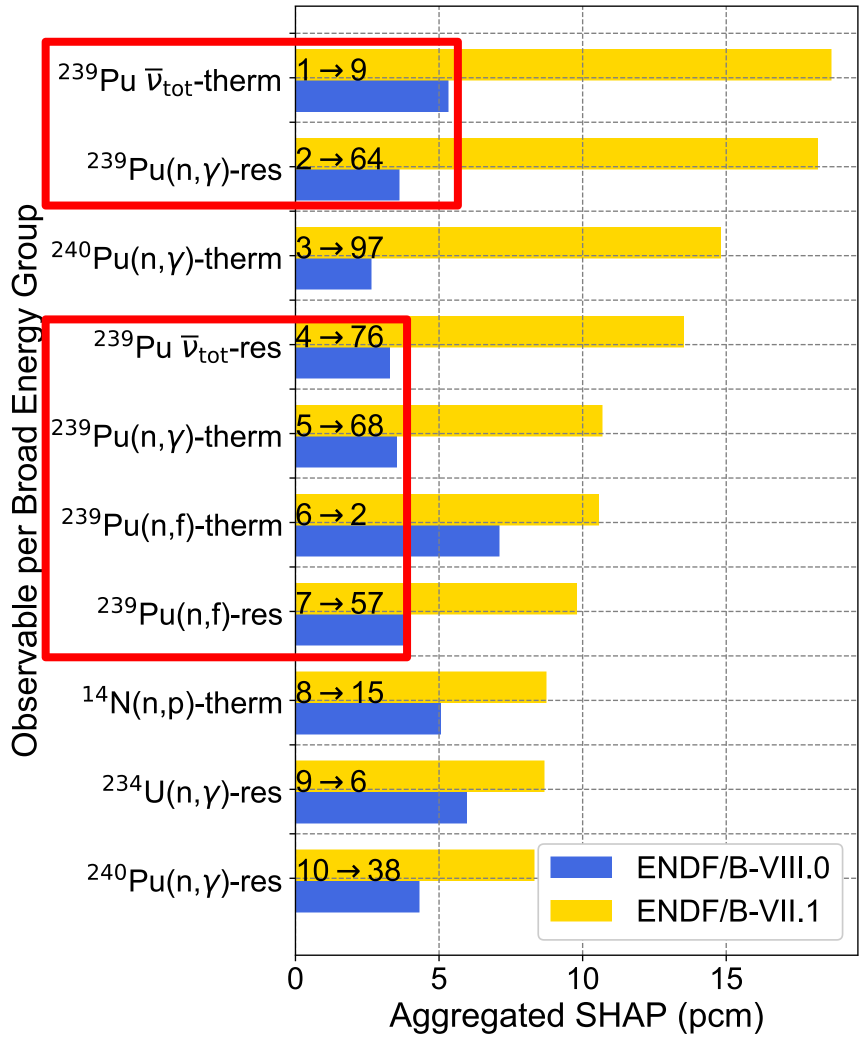




The PST assemblies strongly depend on thermal and resonance ^{239}Pu nuclear data.

Yes, ML correctly identifies actual, known, issues in ENDF/B-VII.1 compared to ENDF/B-VIII.0.

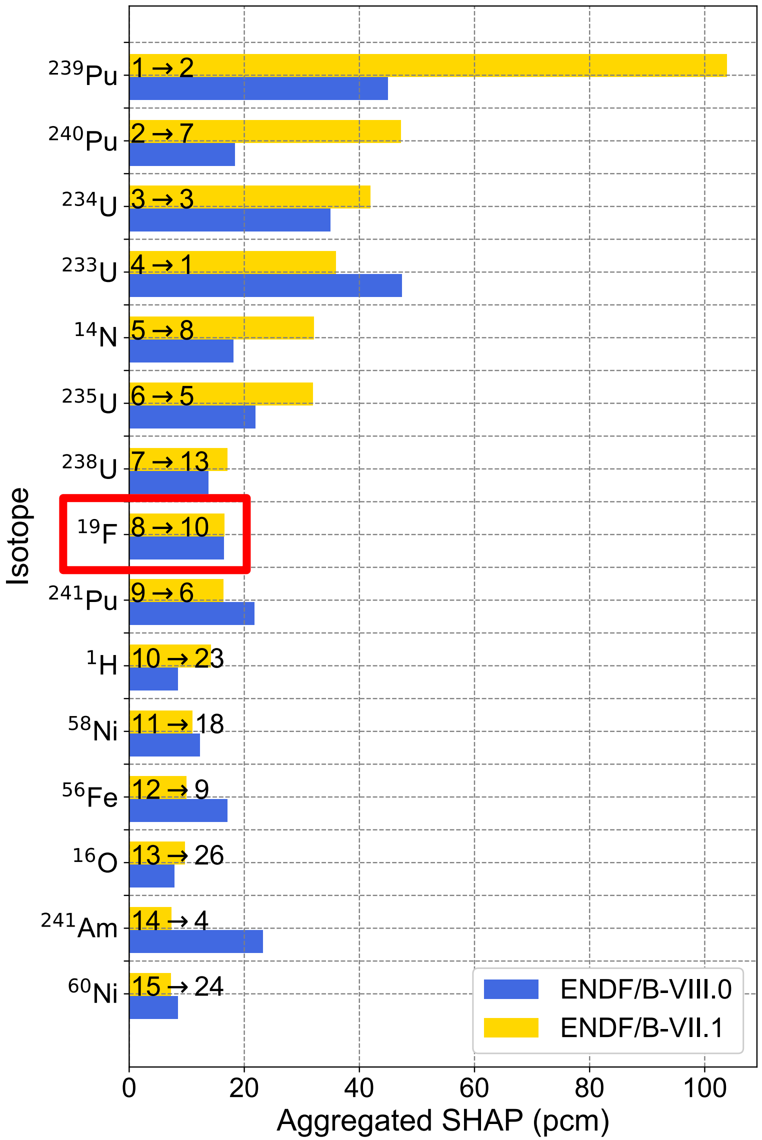


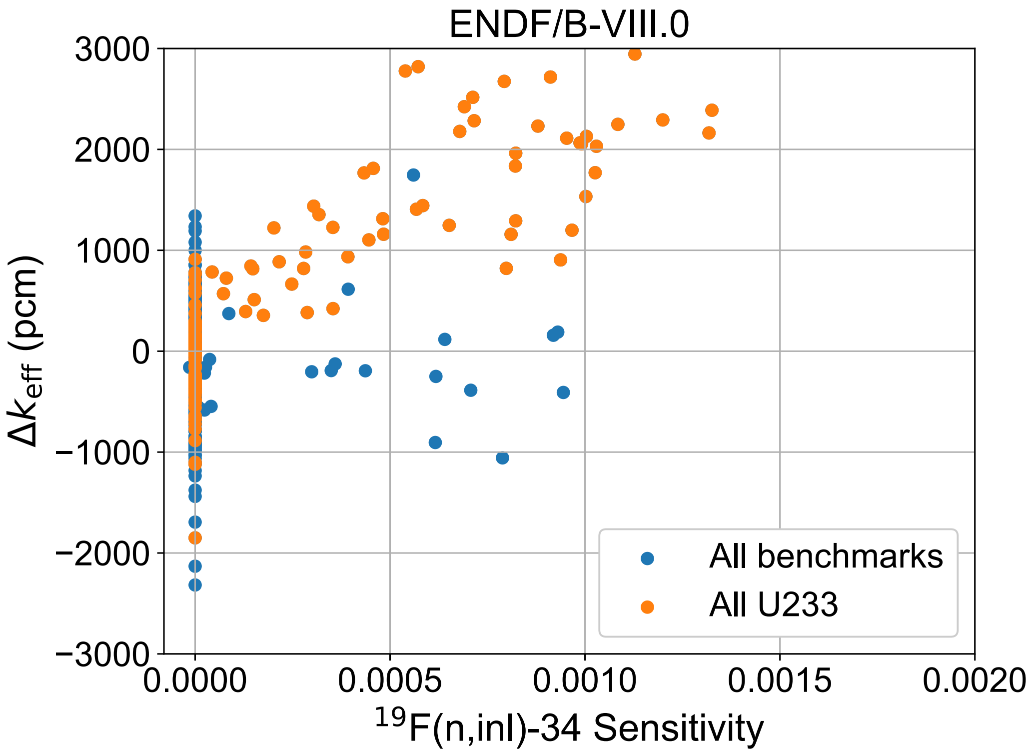


BUT DOES IT WORK FOR REAL CASES??

INVESTIGATING WHETHER ML FINDS *UNKNOWN* SHORTCOMINGS IN CURRENT LIBRARIES

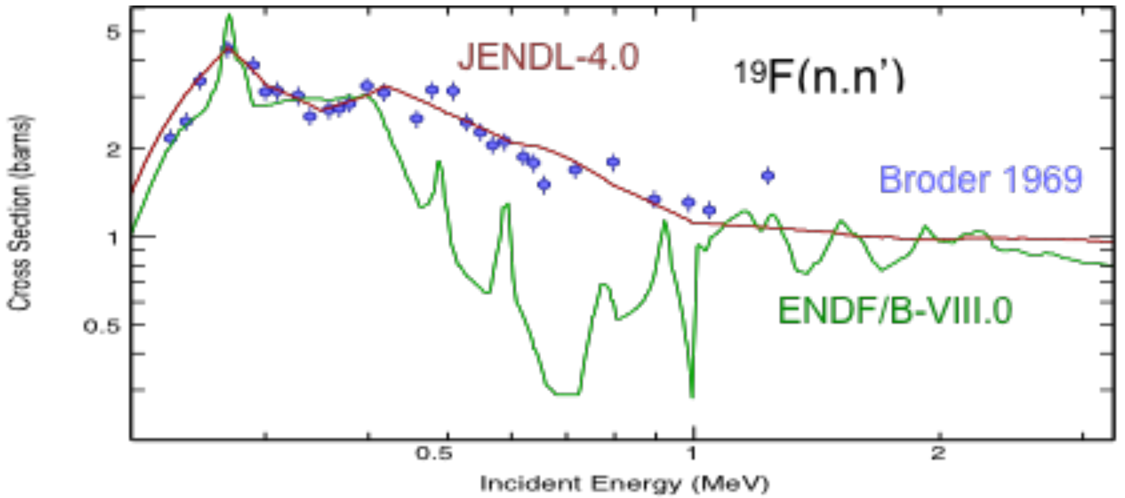
ML points towards potential issue in ^{19}F ENDF/B-VII.1=VIII.0 nuclear data relevant for small-scale exp.





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.

Also, ML pointed us towards doubtful benchmark values, underestimated unc. or *both*:

Benchmark Series	Uncertainties (pcm)	Unc. range (pcm)
PST: **4, 6, 7, 10, 18,** 22, ***28,*** 32; PMF: 5, **8,** 11, **14, 16,** 20, 35, 41, 44	**470,350,470, 480, 320-340,** 150-240,***120***, 193 (strong trends, maybe nuclear data?); 130, **60**, 100, **310**, **300-420**, 170, 160, 160, 210-260	70-620; 60-500
HST: **1**, 11, **25**, **50**; HMF: **3**,**5**,7,**25**,**38**,***51***,**57**,**72**, **84**, **88, 90, 91**,***92***, ***93***, **100** HMM: 15, 16, 17	**350-600**, 230, **250-1110**, **790-900;** **300-500**,**360**,120-560,**140-160**,**70-90**,***10-50***,**190-400**,**240-690**,**190-450**,**80,70,90**, ***110-130***, ***120***, **70;** 80, 70-80, 80	230-900; 10-690 70-380
IMF: **1, 2;** MMF: 4, 5,**7**,10	**30, 90;** 130, 170, **230-450**, 90	30-530, 90-480
U233MF: **2,4;** U233ST: **12**, **13**, **15**, 16	**100, 70-80;** **100-710**, **200-890**, **290-750**, 260-470	70-300; 100-890
LCT: **5, 22, 24, 25, 27**, **28;** LST: **4**	**210-660, 350-460, 400-540, 410-520, 120-150**, **432-540**; **80-110**	70-660; 90-120

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Main take-aways of this work:

- Can ML help us identify potential shortcomings in nuclear data (ND) that significantly impact benchmark simulations?

Yes, ML can find nuclear data shortcomings but is affected by correlation effects.

- Can ML help us identify shortcomings in ND that traditional ND validation methods are unlikely to pin-point?

Yes, because we investigate all data simultaneously by looking for trends in data versus biases in benchmark simulations.

ML is a tool that can augment (rather than replace) the expert's ability to validate nuclear data.

- Outlook: validate whole ENDF/B-VIII.0 library with that machinery.