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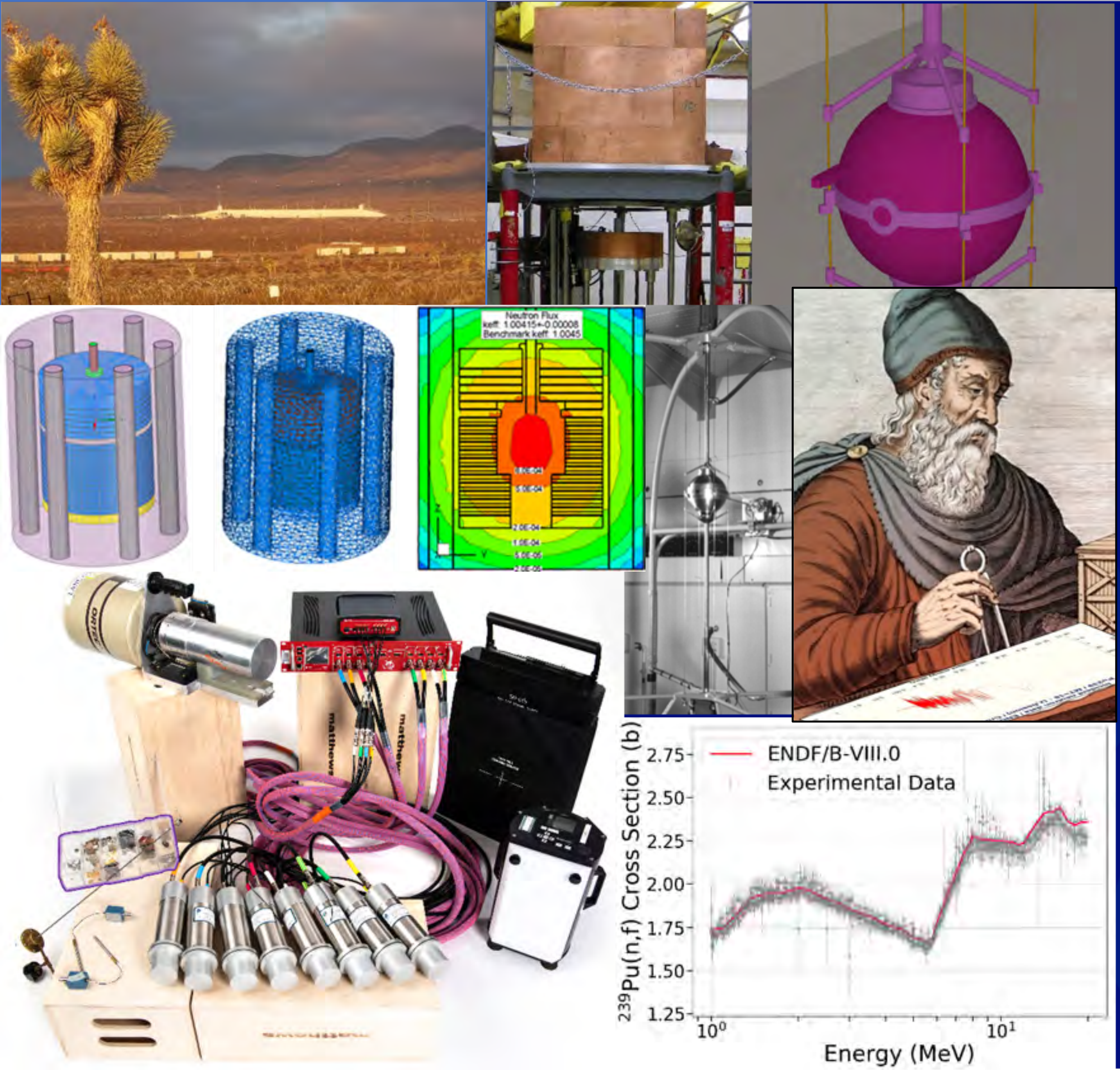

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Using Machine Learning Algorithms for Large-scale Nuclear-data Validation

D. Neudecker (presenter)

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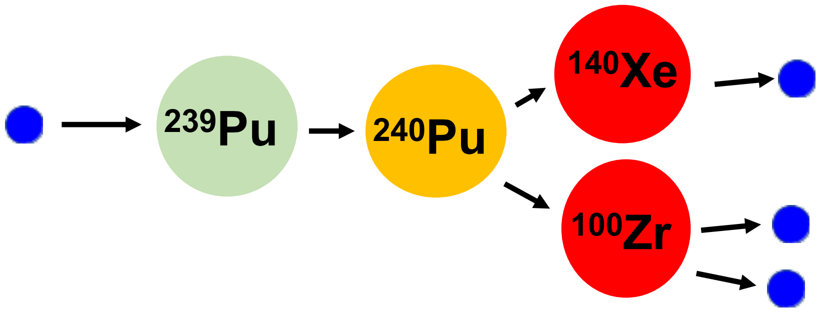
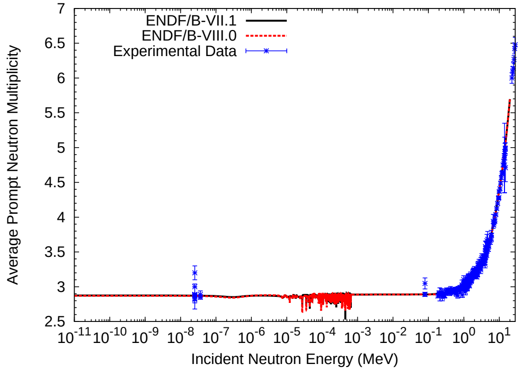
3rd Workshop of Spanish Users on Nuclear Data on
“Machine Learning in Nuclear Science and Technology Applications”

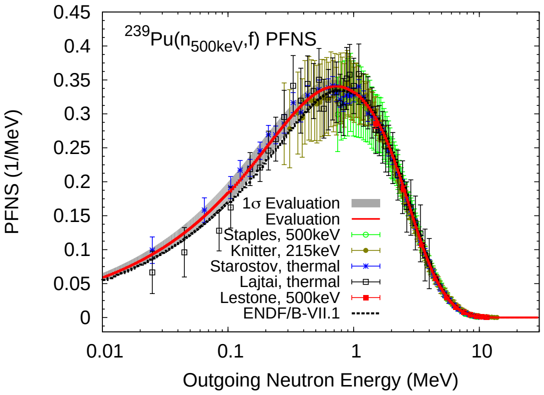
Nuclear data tabulate physics reactions of the nucleus for many isotopes/ materials for use in application simulations.



Average Prompt Neutron Multiplicity= Av. Number of outgoing neutrons



Prompt Fission Neutron Spectrum= Energy distribution of outgoing neutrons



Fission cross-section=probability that fission happens

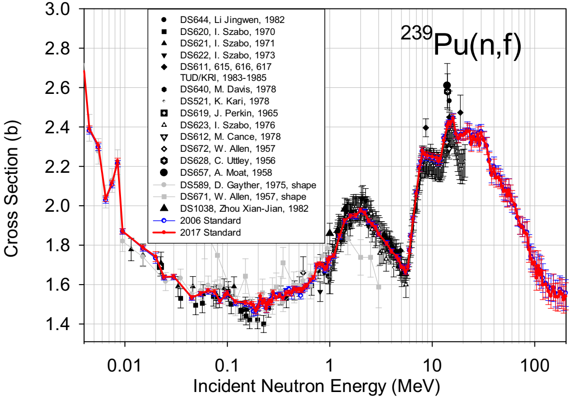
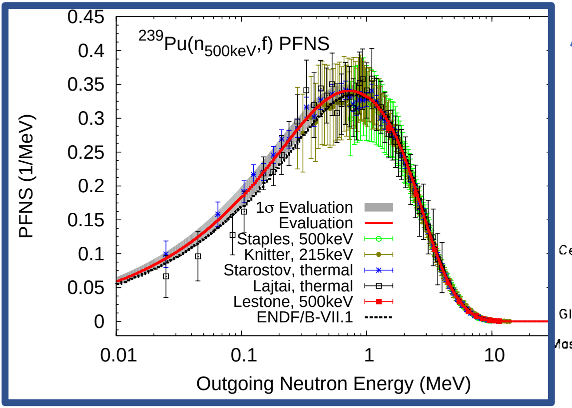


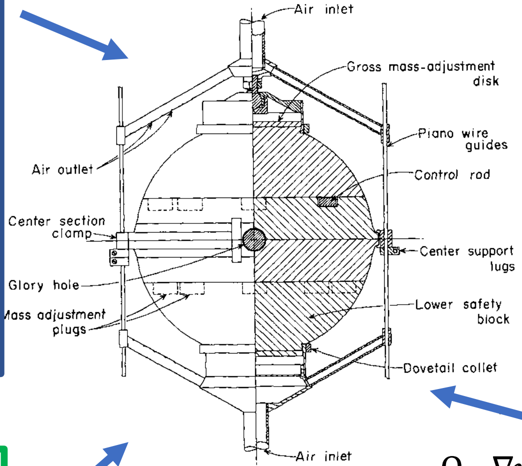
Fig. from Carlson et al., NDS 148, 143 (2018).

Before nuclear data are released, they are validated with experiments representing applications on a small scale.

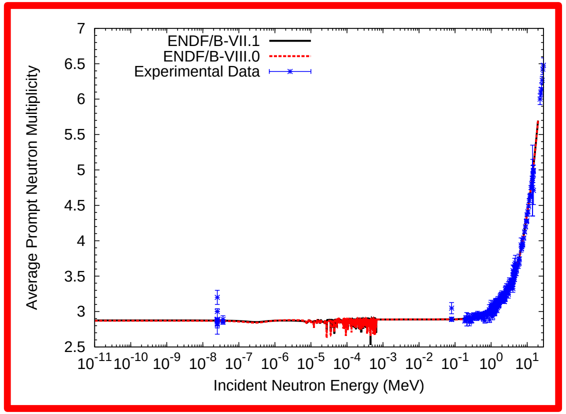
Prompt Fiss. Neutr. Spectr.



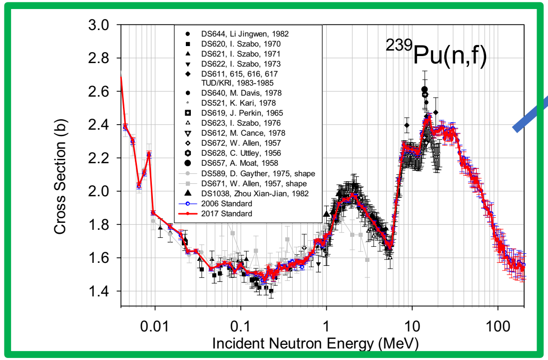
Jezebel critical assembly



Av. Prompt Neutr. Multiplicity



Fission Cross-section



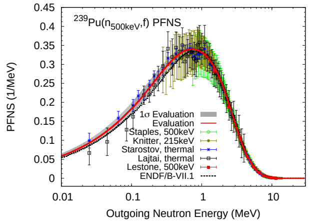
$$\Omega\cdot\nabla\psi(\boldsymbol{r},E,\Omega)+\Sigma_t(\boldsymbol{r},E,\Omega)\psi(\boldsymbol{r},E,\Omega)$$

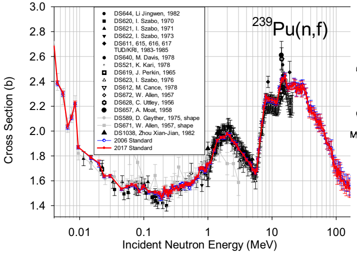
$$=\int_0^\infty\int_{4\pi}\Sigma_s(\boldsymbol{r},E'\to E,\Omega'\to\Omega)\psi(\boldsymbol{r},E',\Omega')d\Omega'dE'$$

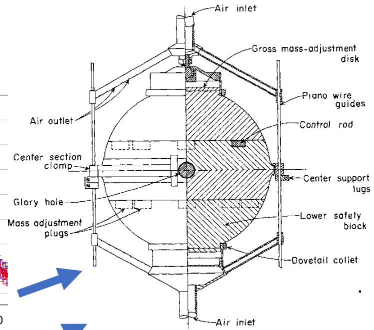
$$\dots$$

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

Question: what nuclear data lead to bias when comparing simulated and exp. values of >1000 validation exp?







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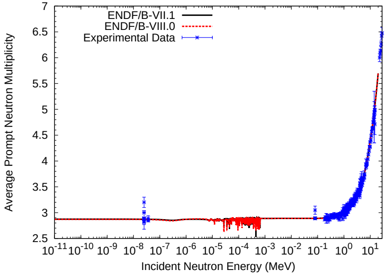
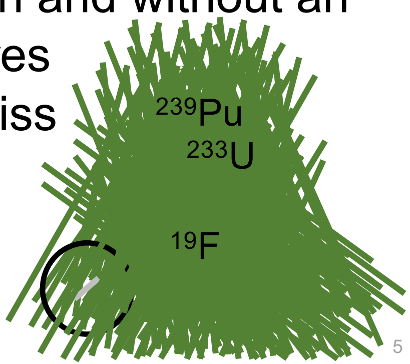


Problem: which nuclear data values (out of 20,000!) are those that lead to bias in simulating 1000s of validation experiment??

Highly under-determined and complexly intertwined problem!

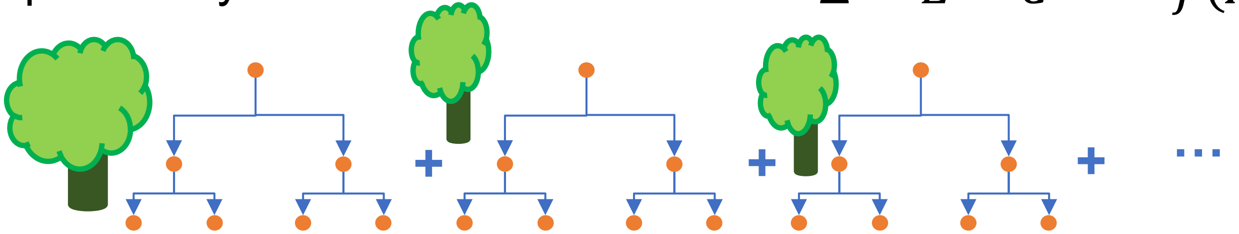
Traditional methods: human brain cannot assess all this complex data at once -> targeted comparison of data with and without an isotope or looking at bare spheres for the actinides -> one could miss issues you are not looking for.



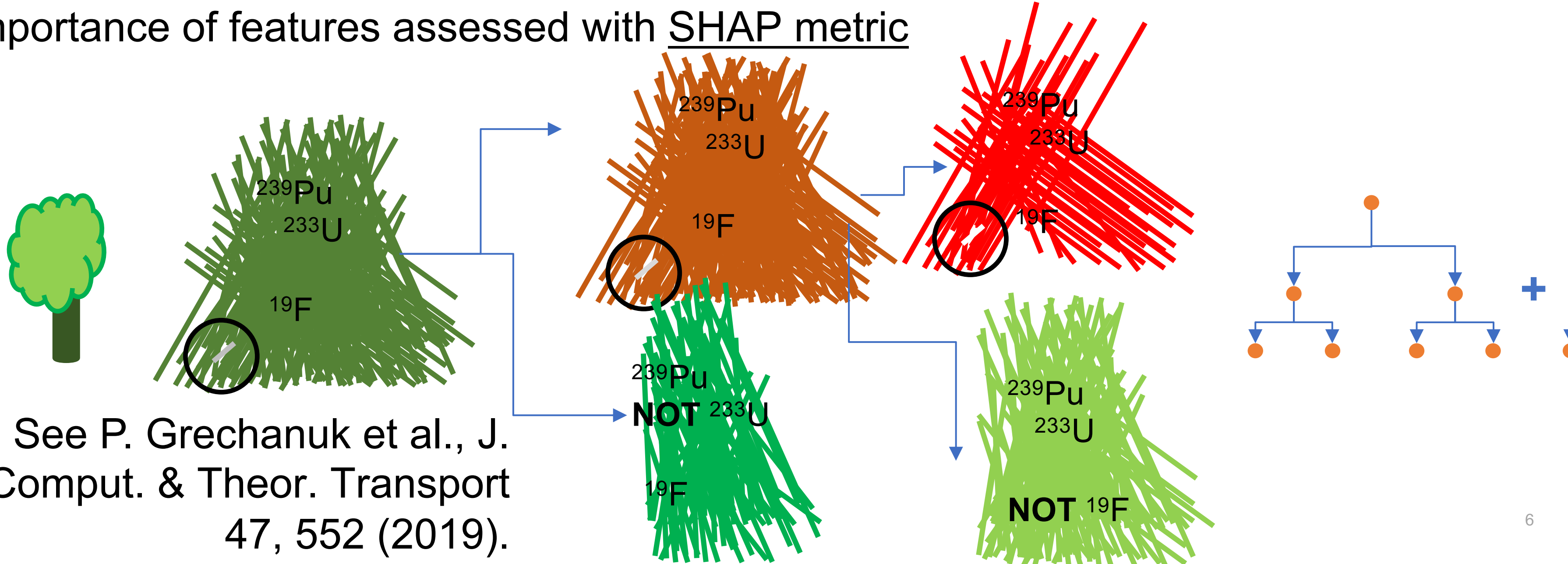
Perfect problem for ML!!!

We solve this question with random forest and SHAP metric.

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

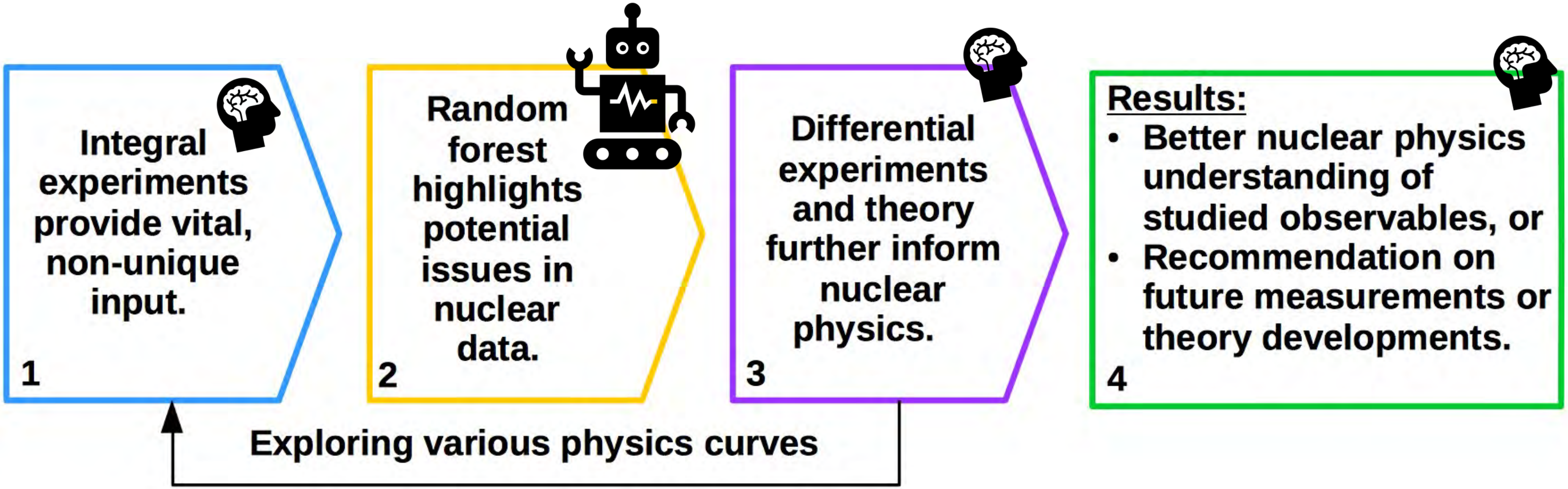


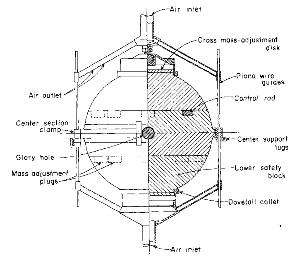
- Importance of features assessed with SHAP metric

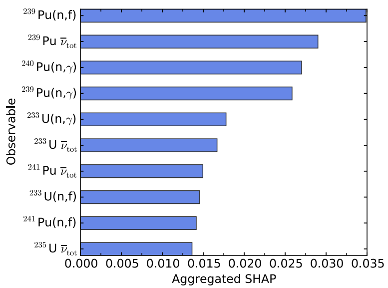


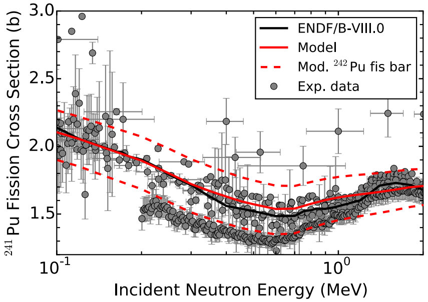
See P. Grechanuk et al., J. Comput. & Theor. Transport 47, 552 (2019).

Comment: ML algorithm is only one step in the algorithm. The human is needed to provide input and analyze results!







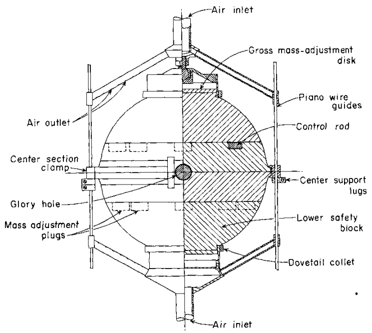


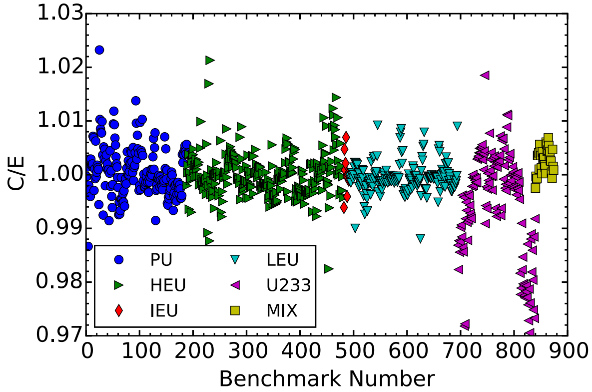
See D. Neudecker et al., NDS 167, 36 (2020).
D. Neudecker et al., LA-UR-21-22465, submitted.

Step 1: validation input is 2 types of validation experiments, nuclear-data sensitivities, and measurement features.

<u>Validation experiments used:</u>

- 875 criticality experiments
- 15 LLNL pulsed-sphere neutron-leakage spectra





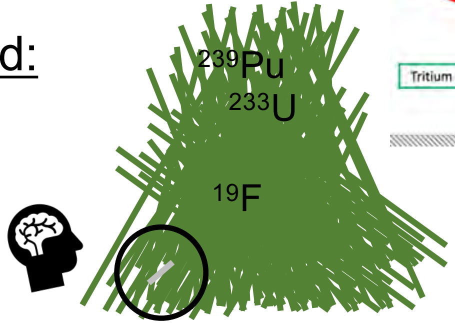
See D. Neudecker et al., NDS 167, 36 (2020).

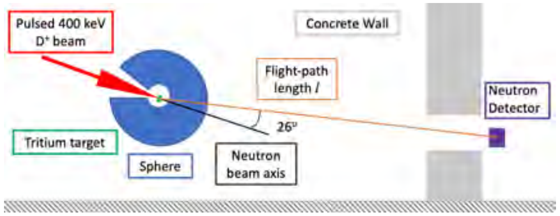
<u>Features:</u> for each experiment:

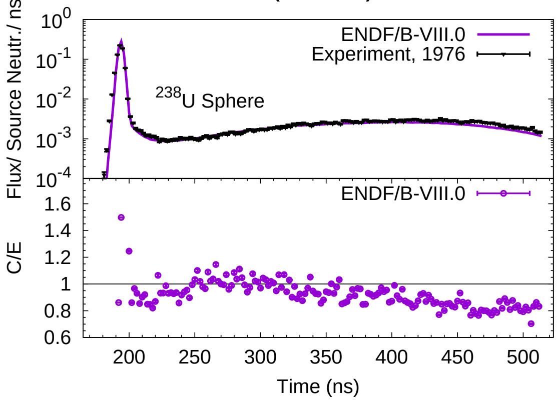
- ~21000 sensitivities of nuclear data to simulated quantity
- ~ 50 measurement features

<u>Nuclear data used:</u>

- ENDF/B-VII.1
- ENDF/B-VIII.0

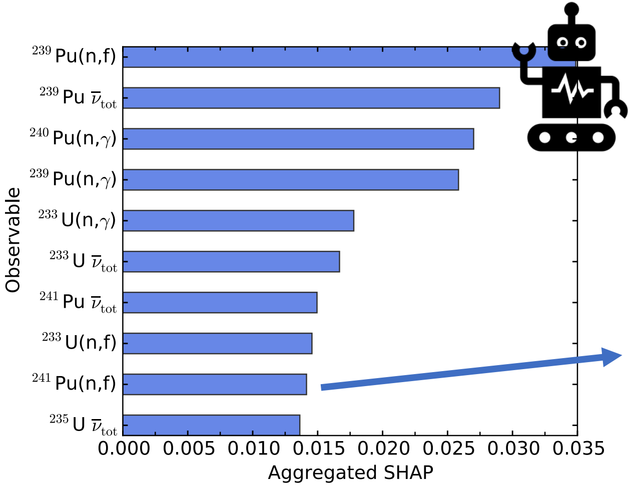


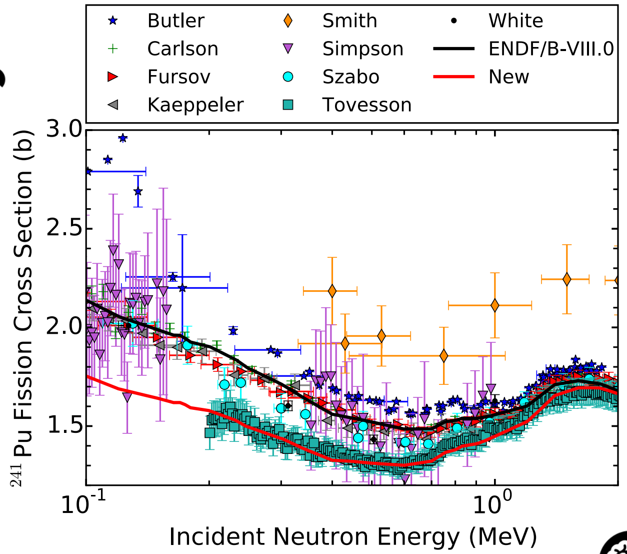


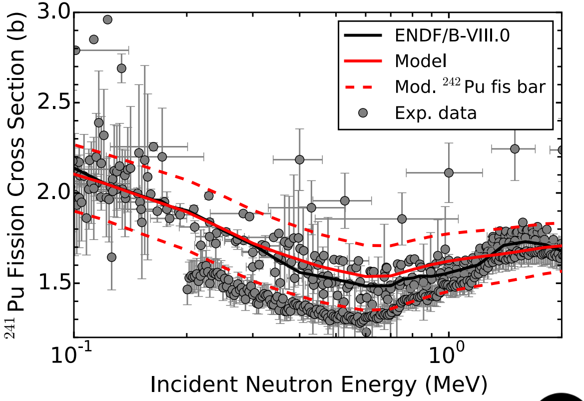


See D. Neudecker et al., ANE 159, 108345 (2021).

Steps 2 and 3: ML algorithm highlights issue in nuclear data that are explored with differential data and theory.







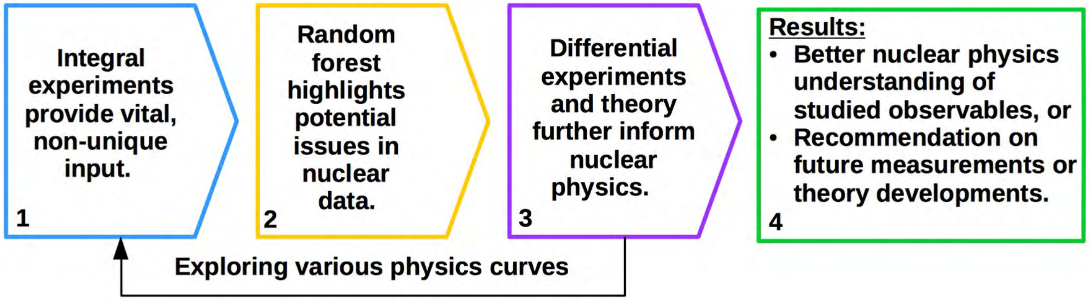
^{241}Pu(n,f) cross section among 10 most important reactions related to bias in simulations of validation experiments.

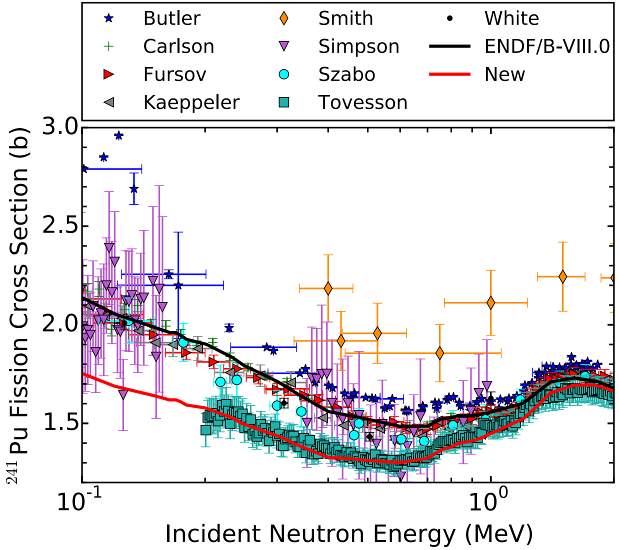
Potential issue in nuclear data given differential experimental data, but where should curve go?

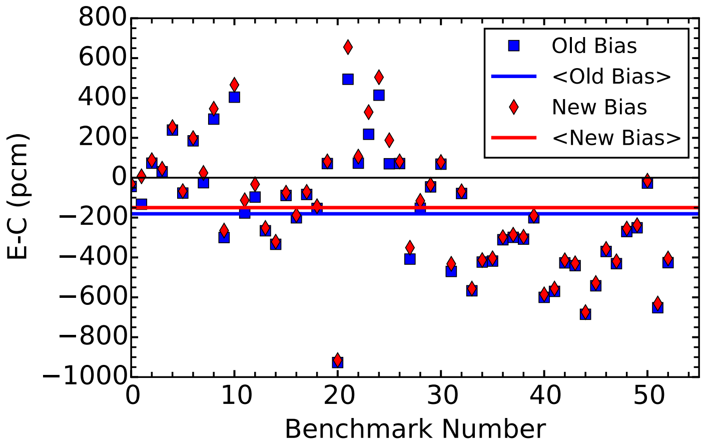
Nuclear theory does not constrain enough to solve the issue.

D. Neudecker 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.



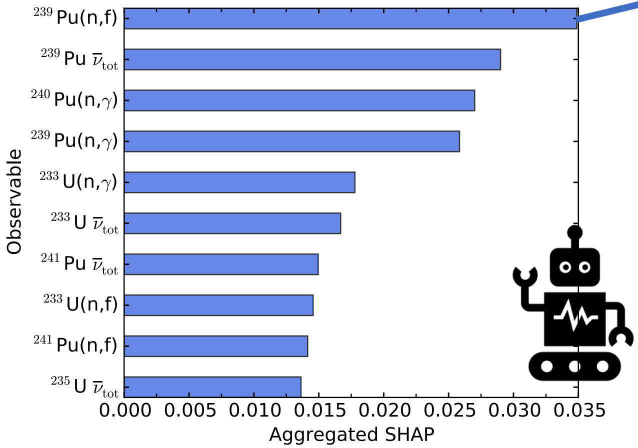


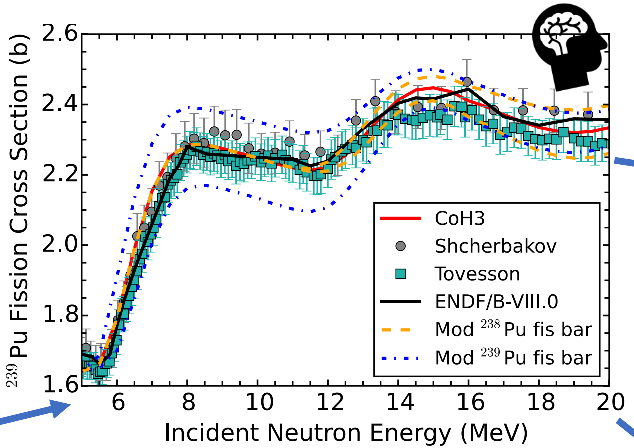


D. Neudecker et al., LA-UR-21-22465, submitted.

If no clear understanding can be reached, how nuclear data should be corrected -> needs for new exp./ theory

ML indicates issues in ^{239}Pu(n,f) cross section above 6 MeV.





Large discrepancies between differential exp. and freedom in theory -> unclear where nuclear data should go.

Validation experiments also cannot inform us where nuclear data should go.

New exp. and theory developments needed.

Observable	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
PFNS	*all*	th	*all*	*all*	*all*
(n,f) cs		> 6 MeV	t; f	f	
(n,f) $\bar{\nu}$	*f*	*0.3–100 keV*	f	all	r, f
(n,γ) cs			< 1 MeV	< 1 MeV	t
(n,inl) cs		*f*	*f*	*f*	*f*
(n,2n) cs			*f*		
(n,tot) cs	all	r, f	f	*f*	f

D. Neudecker et al., LA-UR-21-22465, submitted.

Conclusions

- **ML can** helps us find trends between nuclear-data sensitivities and bias in simulating validation experiments that **point towards potential shortcomings in nuclear data.**
- This **can help scientists to resolve issues in nuclear data, or at least suggest future experiments and theory developments to resolve these issues.**
- Humans may miss such trends without ML due to large amount of complex and inter-dependent data that pose a highly underdetermined problem.
- **Human is needed:**
  - To interpret and analyze results,
  - Provide meaningful input from physics point of view.

Thank you for your attention!

Acknowledgements

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