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

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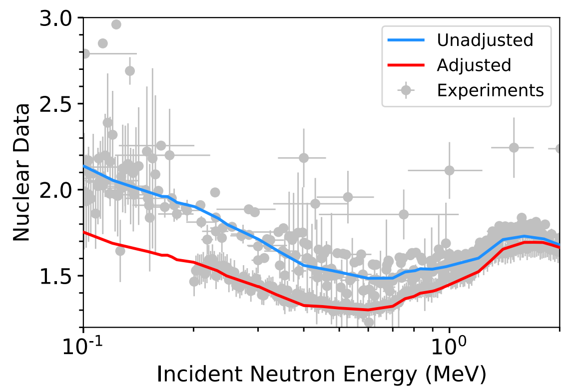

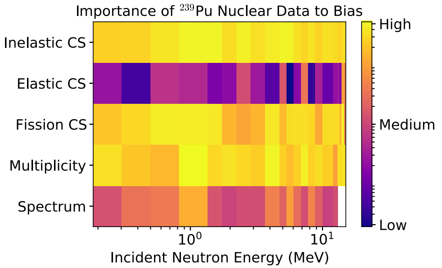

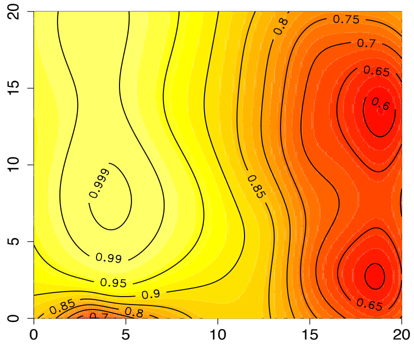

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Using MCNP-calculated sensitivities and machine learning to identify unconstrained physics spaces in nuclear data

Presenter: D. Neudecker

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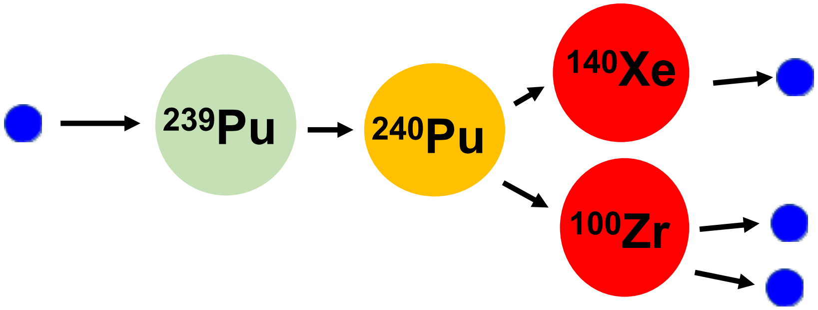
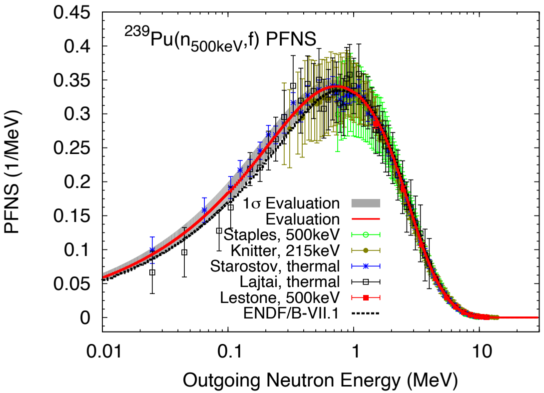
2021 MCNP User Symposium, July 14, 2021

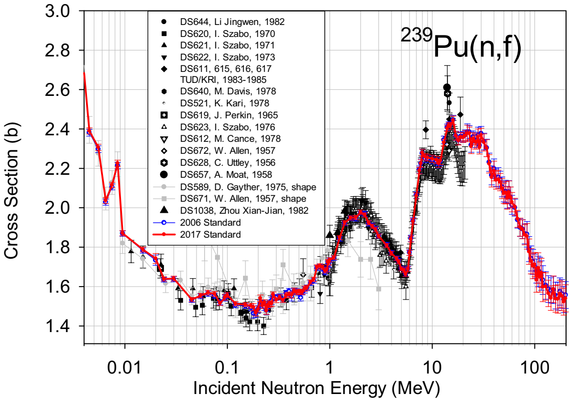
MCNP simulations rely on nuclear data.



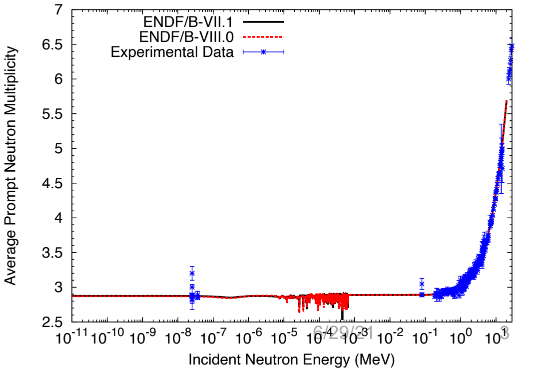
Prompt Fission Neutron Spectrum= Energy distribution of outgoing neutrons



Fission cross-section = probability of fission

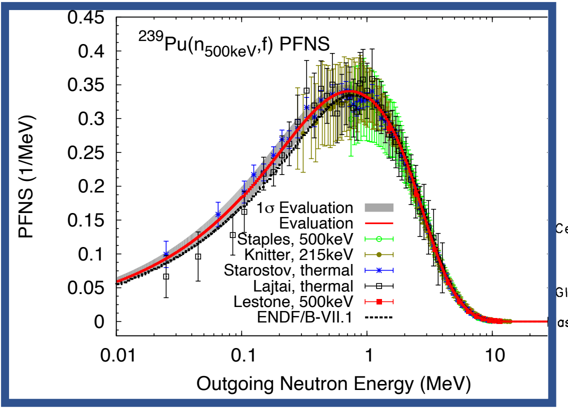


Average Prompt Neutron Multiplicity= Av. Number of outgoing neutrons

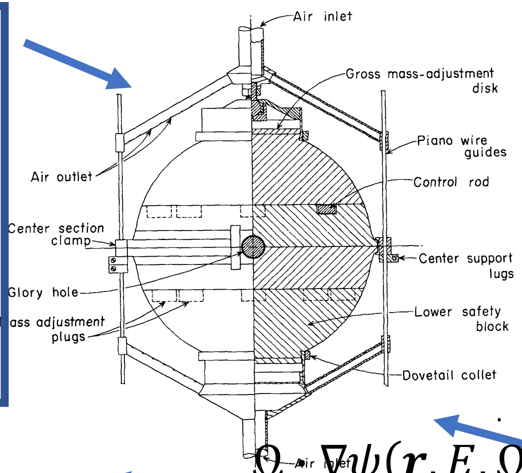


Nuclear data are validated, in turn, often by using MCNP and with respect to criticality.

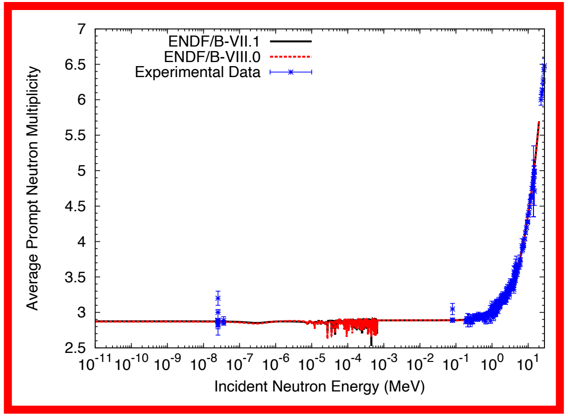
Prompt Fiss. Neutr. Spectr.



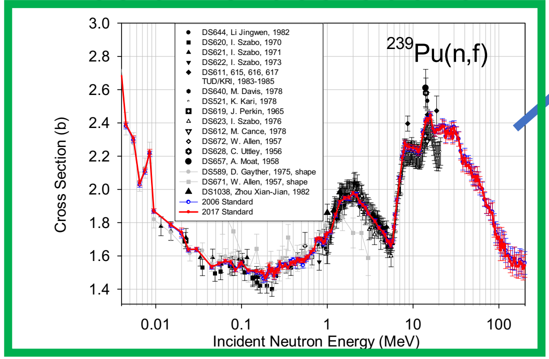
Jezebel critical assembly



Av. Prompt Neutr. Multiplicity



Fission Cross-section



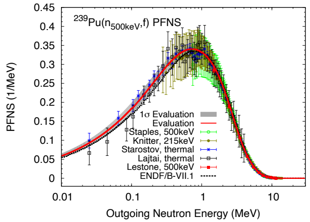
$$\Omega\cdot\nabla\psi(\boldsymbol{r},E,\Omega)+\Sigma_t(\boldsymbol{r},E,\Omega)\psi(\boldsymbol{r},E,\Omega)$$

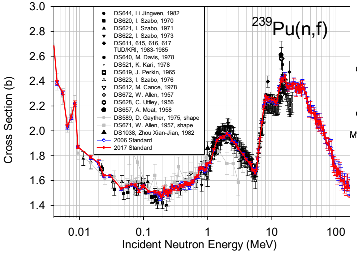
$$=\int_0^\infty\int_{4\pi}\Sigma_s(\boldsymbol{r},E'\rightarrow E,\Omega'\rightarrow\Omega)\psi(\boldsymbol{r},E',\Omega')d\Omega'dE'$$

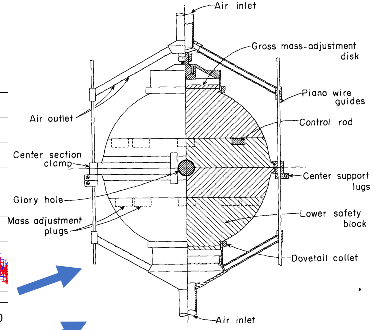
$$\cdots$$

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

Validation with many k_{eff} values is a highly under-determined problem, where thousands of nuclear data yield one k_{eff} value!







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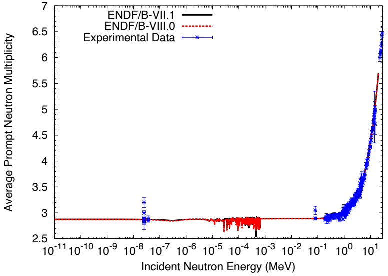


Problem: which nuclear data values (out of 20,000!) are those that lead to bias in simulating 1000s of validation experiment??

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

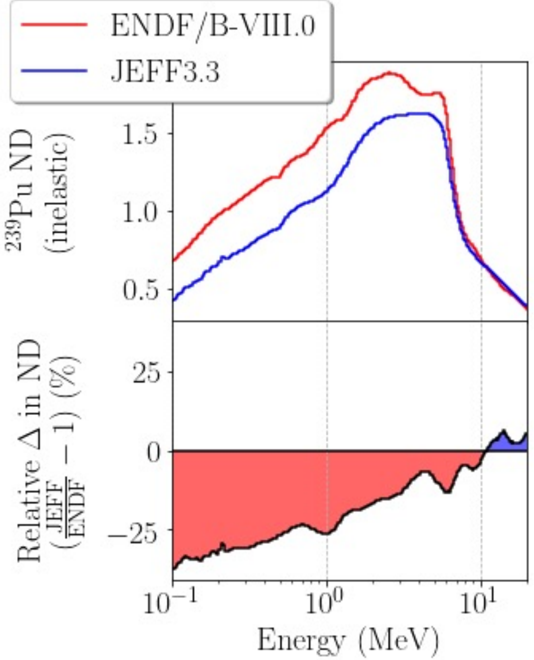
Traditional methods: human brain cannot assess all this complex data at once -> targeted comparison of data with and without an isotope or looking at bare spheres for the actinides -> one could miss issues you are not looking for.

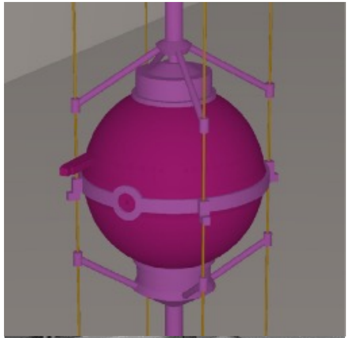
Perfect problem for ML!!!

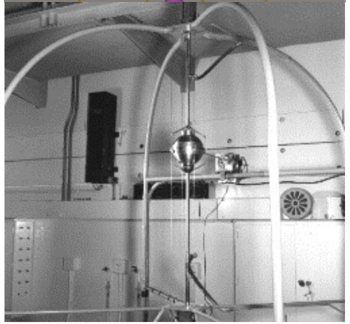
Unconstrained physics spaces: We can change nuclear data widely within differential constrains and still get the same k_{eff}!

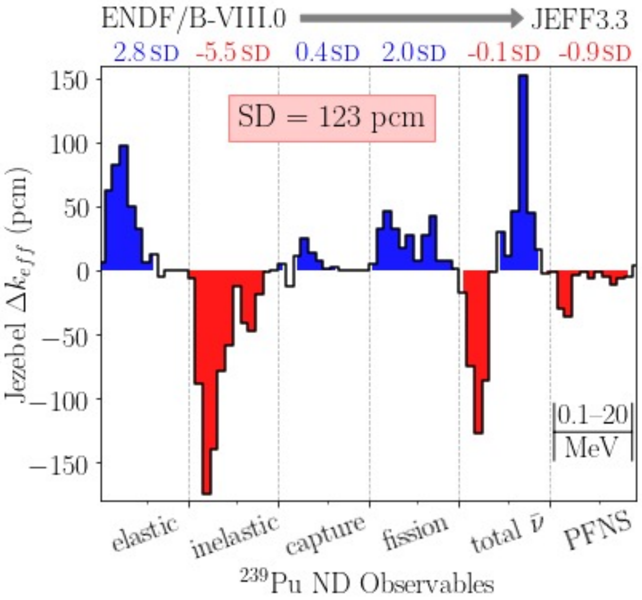
Differences in ENDF/B-VIII.0 and JEFF3.3 nuclear data represent uncertainty in the differential information.

Both ENDF/B-VIII.0 and JEFF3.3 compute Jezebel k_{eff} equally well using MCNP6 but contributions per reaction differ drastically







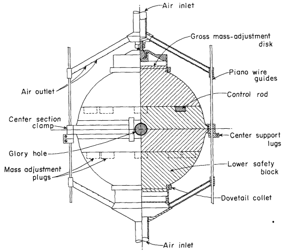


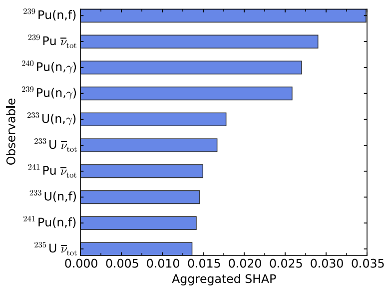
(Thanks to Mike Rising)

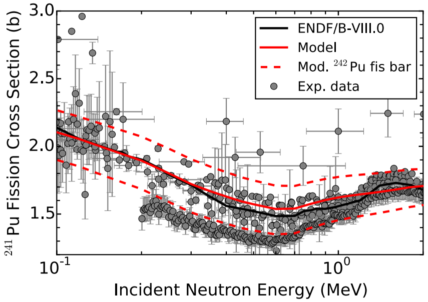
Here, we want to tease out these unconstrained physics spaces using ML and various integral responses.

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.

Exploring various physics curves



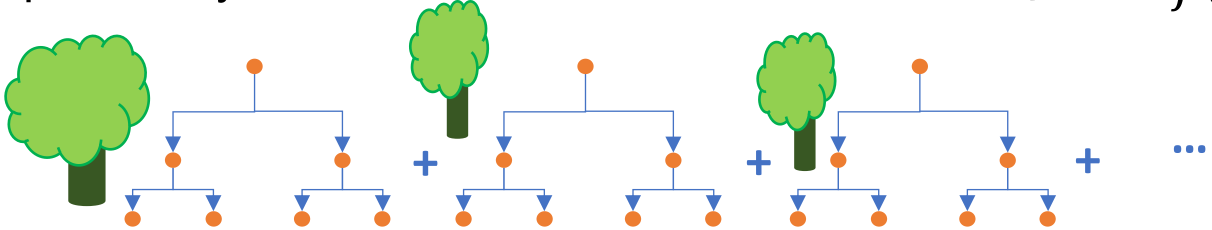




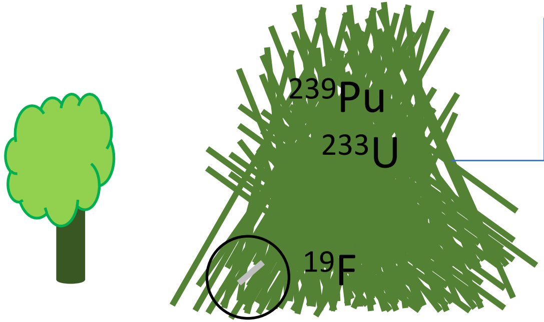
See D. Neudecker et al., NDS 167, 36 (2020). D. Neudecker et al., LA-UR-21-22465, submitted.

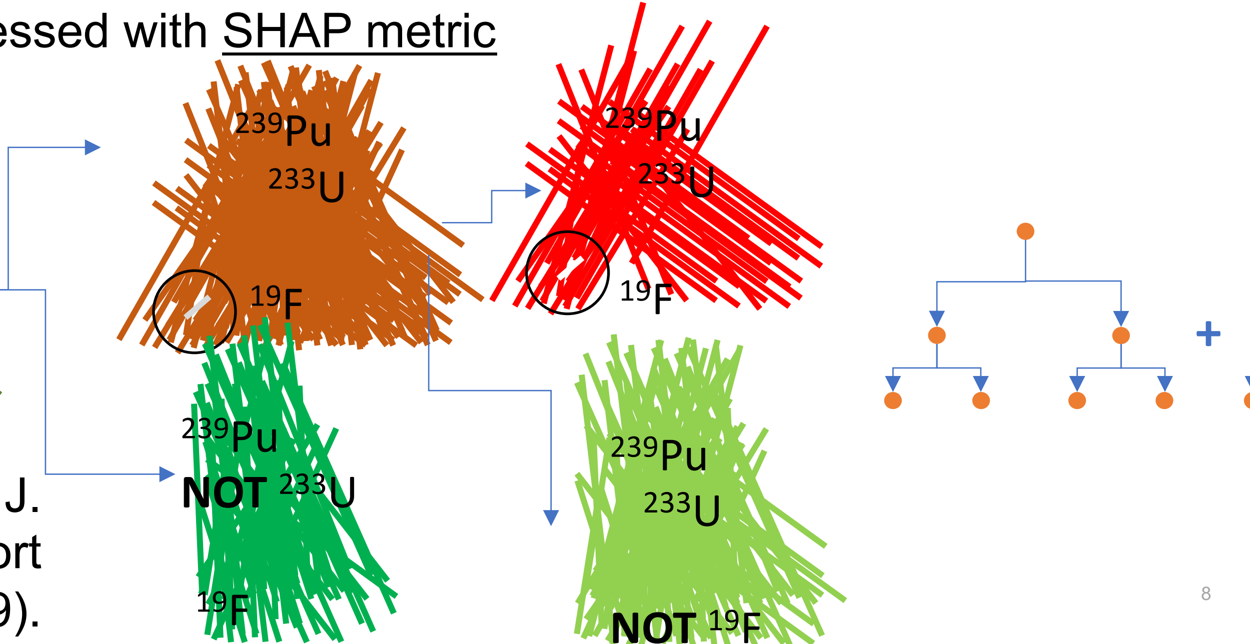
We use as ML algorithms random forest and SHAP metric.

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



- Importance of features assessed with SHAP metric

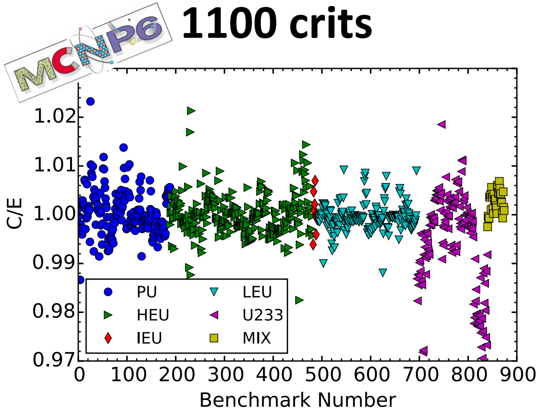




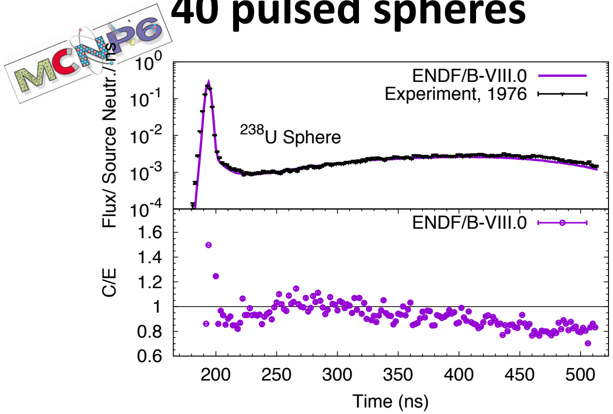
See P. Grechanuk et al., J. Comput. & Theor. Transport 47, 552 (2019).

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

1100 crits



40 pulsed spheres

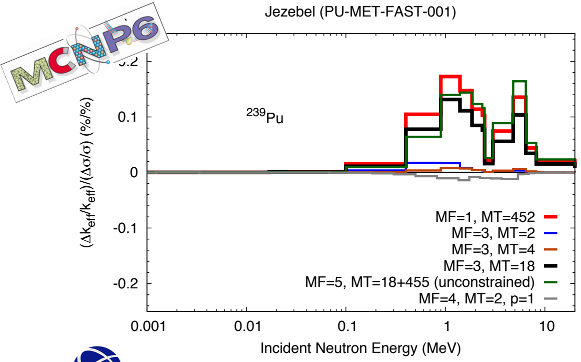


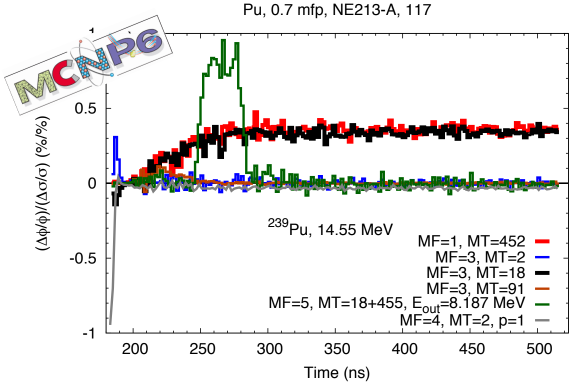
14 reaction rates in crits

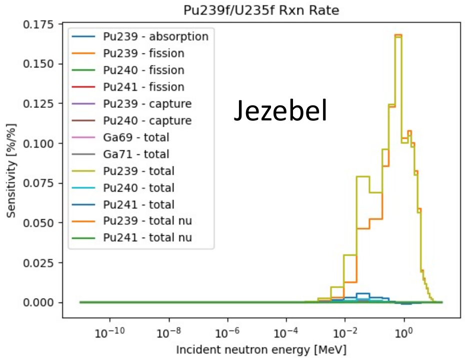
Assembly	Quantity	$U238f/U235f$	$Np237f/U235f$	$U233f/U235f$	$Pu239f/U235f$
Godiva	Calc	0.1583	0.8318	1.5793	1.3846
(HMF001)	Exp-B	0.1643 ±0.0018	0.8516±0.012		1.4152 ± 0.014
	Exp-A	0.1642 ±0.0018	0.837 ±0.013	1.59±0.03	1.402±0.025
	Calc/Exp	C/E=0.9636	C/E=0.9767	C/E=0.9933	C/E=0.9784
Jezebel	Calc	0.2121	0.9770	1.5560	1.4273
(PMF001)	Exp-B	0.2133 ±0.0023	0.9835 ±0.014		1.4609 ± 0.013
	Exp-A	0.2137 ±0.0023	0.962 ±0.016	1.578 ±0.027	1.448 ±0.029
	Calc/Exp	C/E=0.9943	C/E=0.9934	C/E=0.9924	C/E=0.9770
Flattop-Pu	Calc	0.1801	0.8593		
(PMF006)	Exp-B	0.1799 ±0.002	0.8561 ±0.012		
	Exp-A	0.180 ±0.003	0.84 ±0.01		
	Calc/Exp	C/E=1.0011	C/E=1.0037		

(Brown et al., NDS 148, 1, 2018)

Sensitivities to nuclear data



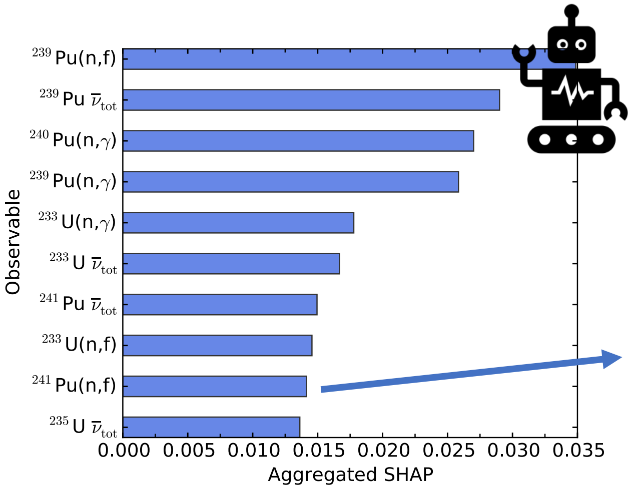


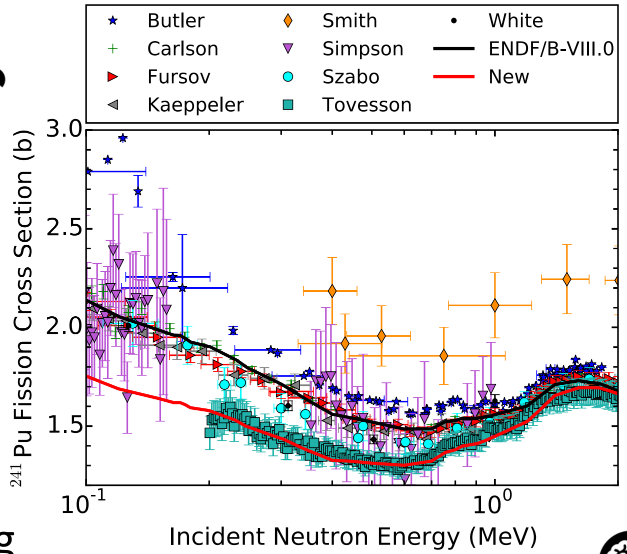


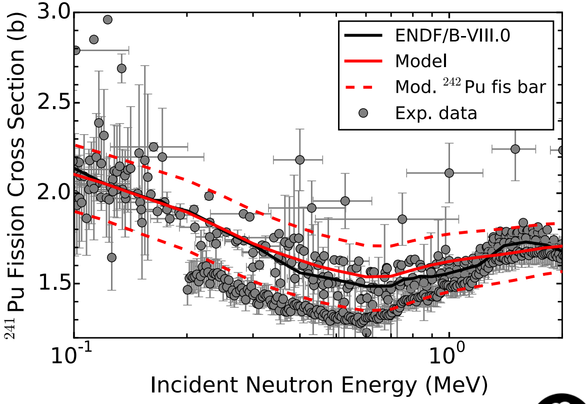
DN et al., NDS 167, 36, 2020; DN et al., ANE 159, 108345 2021.

(thanks to Jen Alwin)

Steps 2 & 3: ML highlights issue in nuclear data that are explored with differential data and theory -> "a success story"







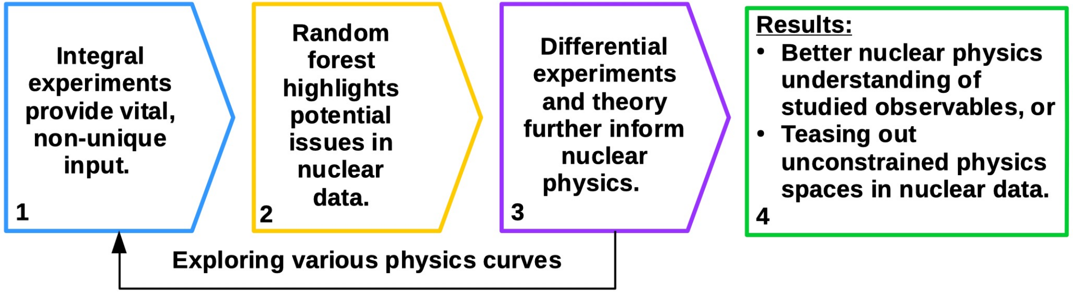
^{241}Pu(n,f) cross section among 10 most important reactions related to bias in simulations of validation experiments.

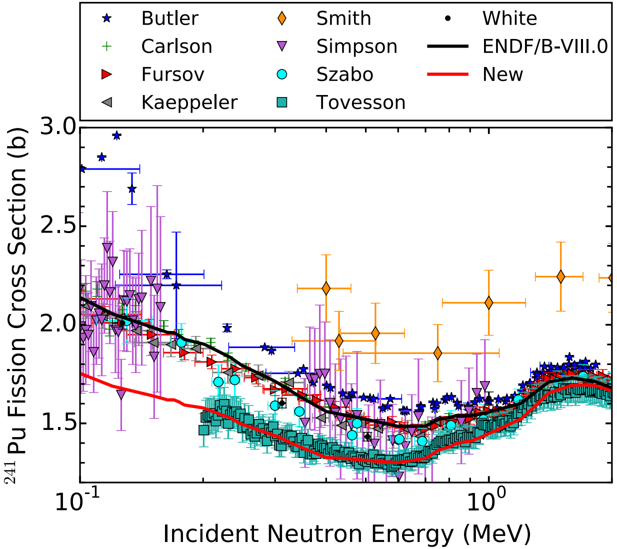
Potential issue in nuclear data given differential experimental data, but where should curve go?

Nuclear theory does not constrain enough to solve the issue.

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.



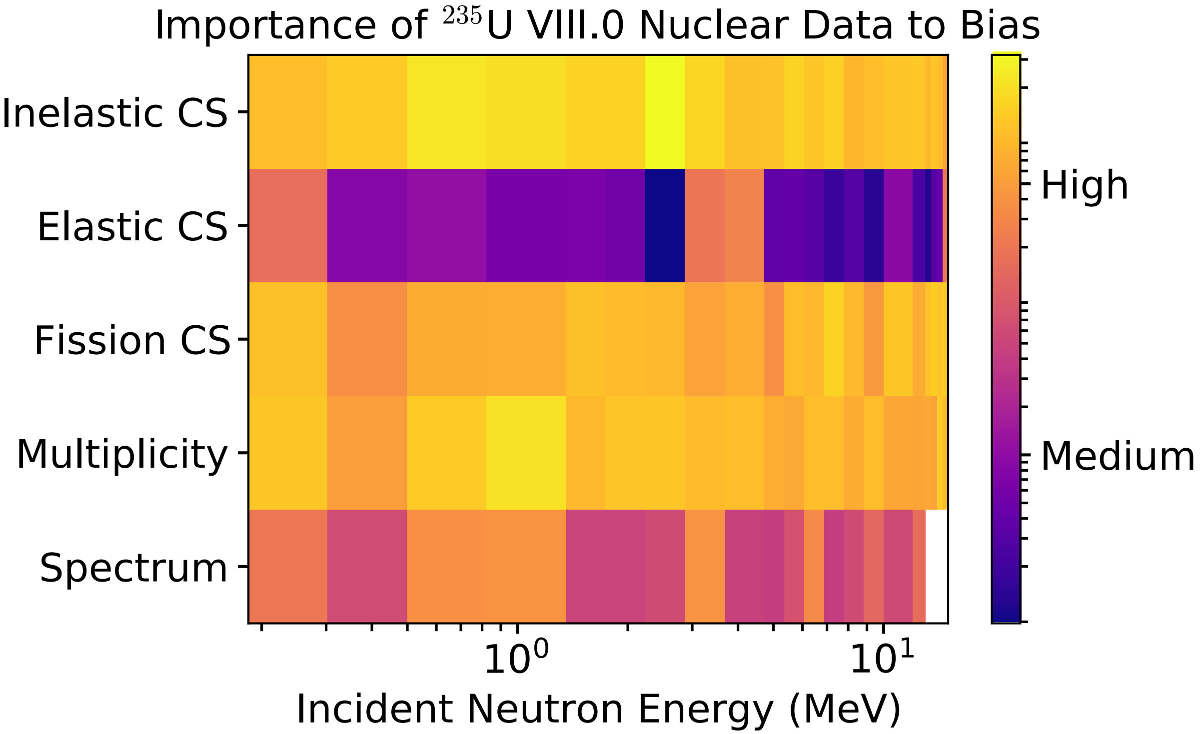


Using FAUST tool (Wim Haeck), we see that Dirty Jezebel k_{eff} bias reduces from 143 pcm to 4 pcm while average of bias in k_{eff} sensitive to ^{241}Pu(n,f) improves slightly.

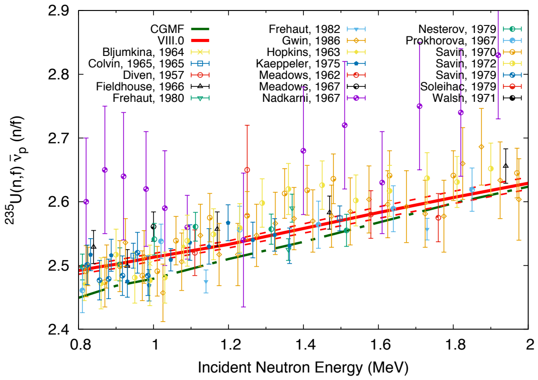
DN et al., LA-UR-21-22465, submitted.

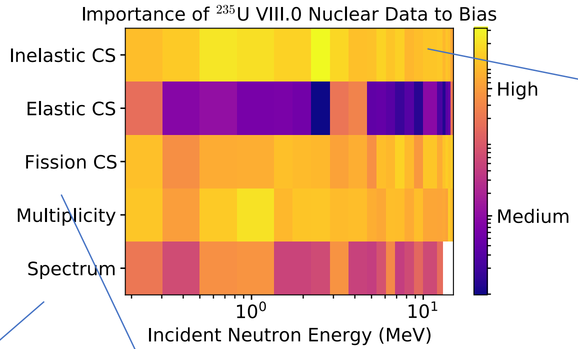
Now an example of finding an unconstrained physics space. ML finds issue in several, inter-twined nuclear data.

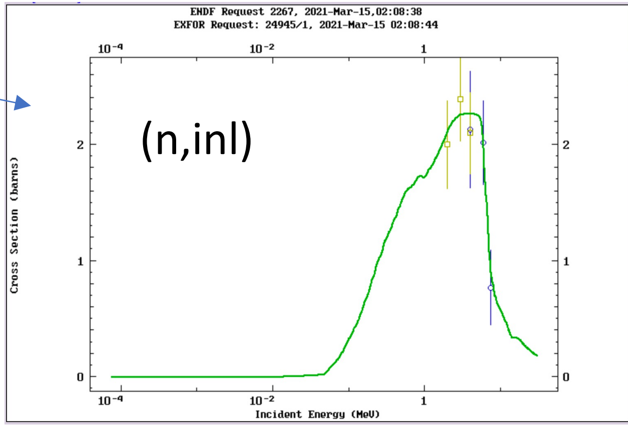
This plot illustrates what ^{235}U nuclear data were highlighted as potentially leading to bias in various integral responses.

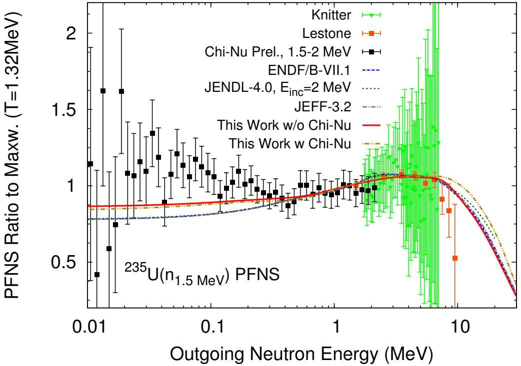


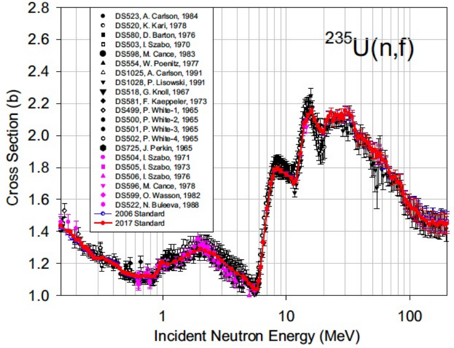
There is considerable space in differential data, cannot pin down what nuclear data is wrong -> unconstrained space!











From A.D. Carlson, NDS 148, 143 2018.

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.

Acknowledgements

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