Using Machine Learning Algorithms in Nuclear Data Evaluations

uncovering hidden patterns in sensitivity profiles

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Unraveling the nuclear data problem

- Accurate nuclear data are key to the success of criticality-safety simulations

- Some basic questions:

  - How do we produce accurate nuclear data?
  - How do we know they are accurate or deficient?
  - Can we identify specific deficiencies?
  - Can we eliminate compensating errors?

This Talk:

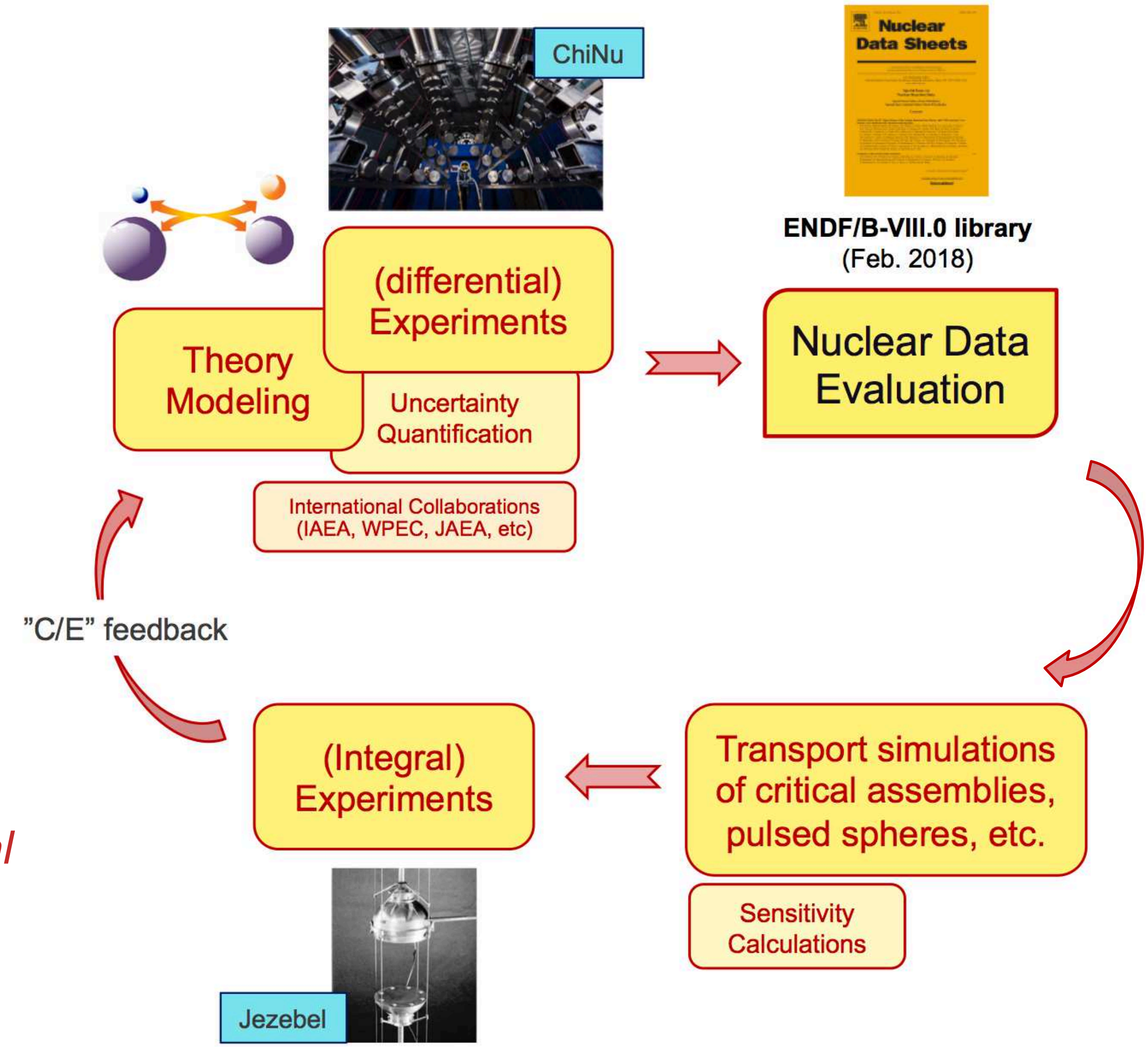
- A very brief tour of the nuclear data evaluation process
- How machine learning algorithms can help in the inverse problem?
- Scoping studies of machine learning in nuclear data
- Perspectives

The nuclear data evaluation process

- Experimental *differential* data, e.g., (n,2n) cross section
- Physics model calc. to describe **all** reactions
- Bayesian statistical techniques, model parameter fitting, etc.

➔ Final product: tabulated data files (mean values + covariance)

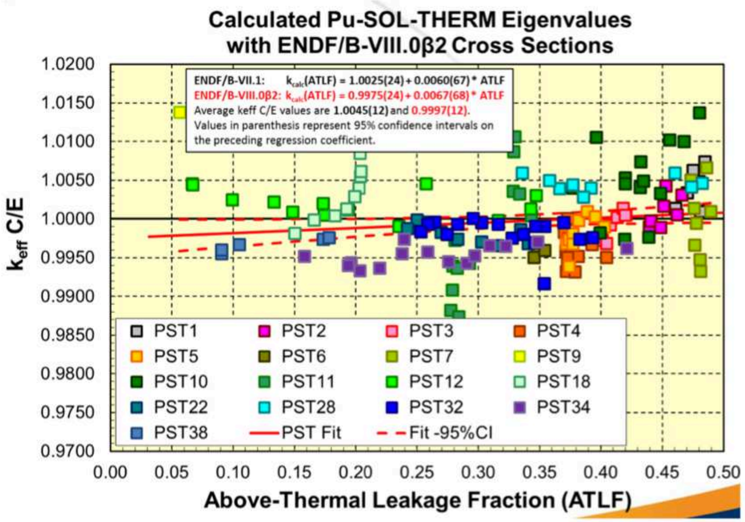
- Feedback loop from *integral* data ("C/E" results)

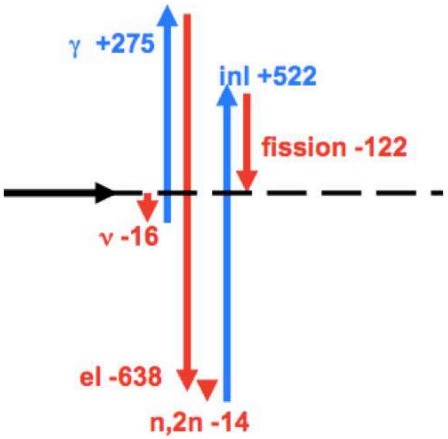


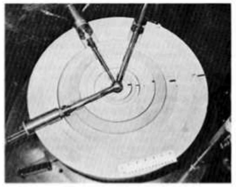
The validation of nuclear data uses simulations of integral data to check C/E values

- Many integral benchmarks are used, but their interpretation is difficult (**inverse problem**)
- We often get the right answers for the wrong reasons
- Lots of room for **compensating errors!**
- The use of integral benchmarks is not reflected in the ENDF covariances

Jezebel critical assembly







Pulsed spheres

Trends/biases along meaningful axes can provide useful feedback on underlying nuclear data

Compensating errors between nuclear reaction channels in the simulation of the Jezebel assembly (ENDF/B-VII.1 vs JEFF-3.2)

Many configurations with reflected materials

Moving beyond the current situation

- Large-scale use of **sensitivity profiles**
  - How does a change in the cross section σ impact the integral *k* value?
  - More generally, how does a change in a feature f impact an integral quantity Q?

$$S_{k,\sigma} = \frac{\Delta k/k}{\Delta\sigma/\sigma}$$

$$S_{Q,f} = \frac{\Delta Q/Q}{\Delta f/f}$$

- Importance of **metadata** in integral benchmarks
  - Geometry, composition, experimental technique, etc.
  - Going beyond (x,y,dy); X_i=experimental features

$$(y, dy) = f(x|X_i)$$

- More **realistic UQ studies** of differential and integral experiments
  - Wrong estimates of uncertainties and correlations can significantly bias statistical results

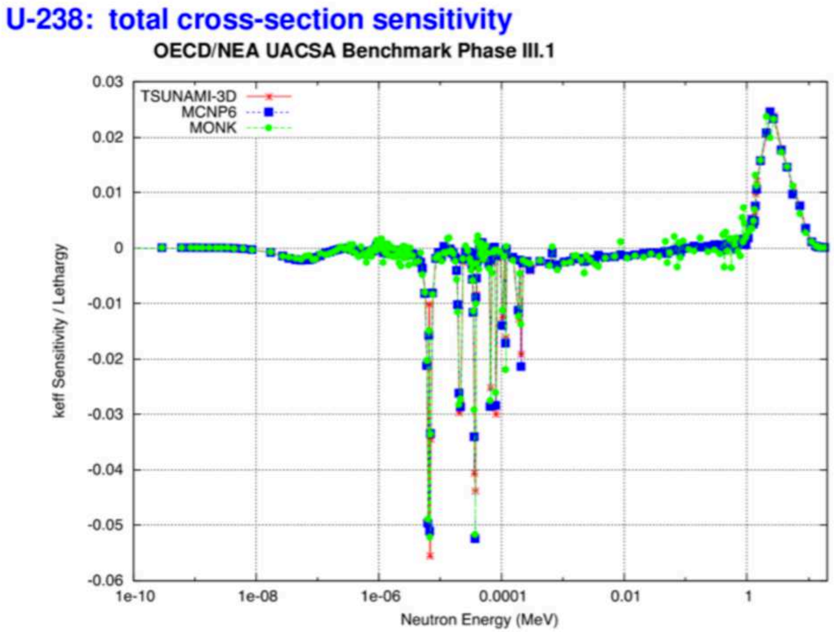
- Use of **machine learning** algorithms to identify hidden patterns and correlations in zoology of integral data

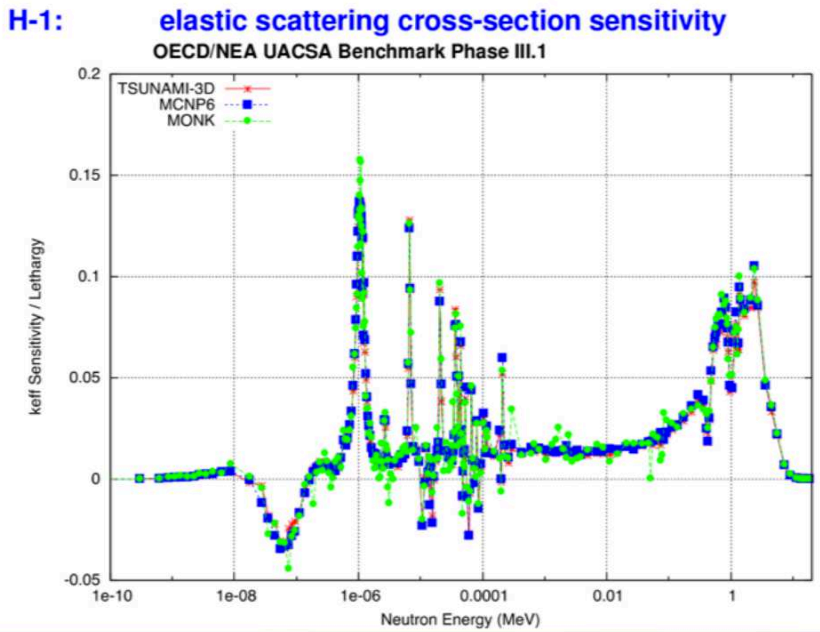
Develop a database/catalog of sensitivity profiles using MCNP6 and Whisper

- Use MCNP6 perturbation/sensitivity features
  - Can compute profiles of k_{eff} – nuclear data sensitivity profiles
  - How does a relative change in the cross section impact k_{eff} of the system?

$$S_{k,\sigma} = \frac{\Delta k/k}{\Delta\sigma/\sigma}$$

  - For a single system, these (energy-dependent) profiles are unique





Recent R&D work on applying machine learning algorithms to Whisper benchmark catalogue

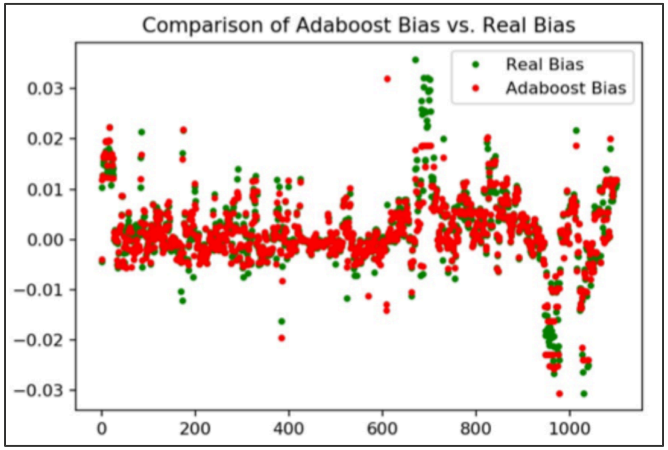
- Oregon State University PhD student, Pavel Grechanuk
  - Began ML research in summer of FY17
    - Explored ML algorithms to predict k_{eff} bias using only sensitivity profiles

$$B_i \approx f(S^i_{k,\sigma})$$

  - Continued ML research in summer of FY18
    - Using the SHAP metric to understand feature importance in predicting bias
    - Explored ML algorithms to cluster benchmarks together
    - Explored the genetic algorithm to perform nuclear data assimilation for the most important nuclear data quantities found in the bias prediction and clustering steps
  - Future work under an established subcontract between XCP-3 and OSU supported through both NCSP and ASC/PEM-NP
- This R&D work has led to a larger LANL team effort, spanning several groups (XCP, T, CCS), to develop robust ML tools for nuclear data evaluation

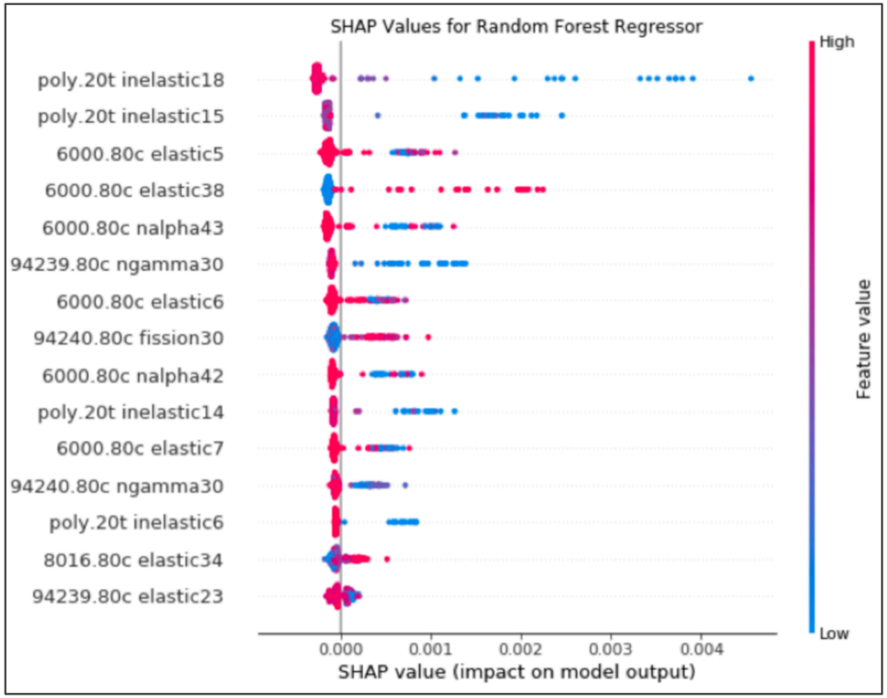
Bias prediction and feature importance

- With the bias known for all Whisper-1.1 catalogue cases, the generalized model predictions are promising



- What are the underlying hidden patterns in the nuclear data that are most related to the bias predictions?

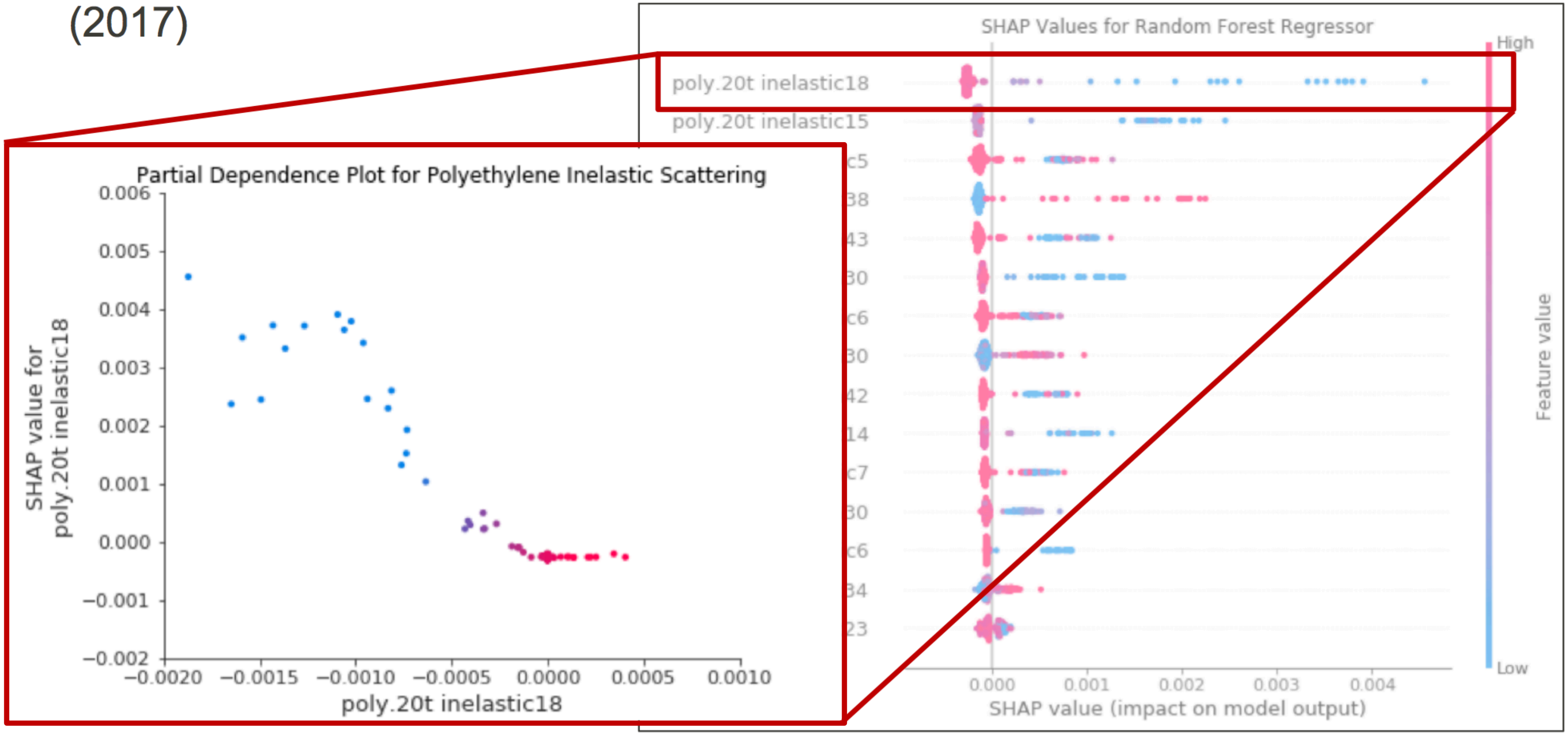
- From the machine learning methods, **feature importance** can be used to identify what nuclear data has a high likelihood to be related to the bias predictions



- Pu benchmarks used in this study

SHAP feature importance

- Shapley Additive exPlanation (SHAP) metric for feature importance
  - For each benchmark, estimate the additive contribution to the predicted bias for each feature
  - "A Unified Approach to Interpreting Model Predictions" Lundberg, Lee (2017)



Clustering benchmarks based on sensitivity profiles

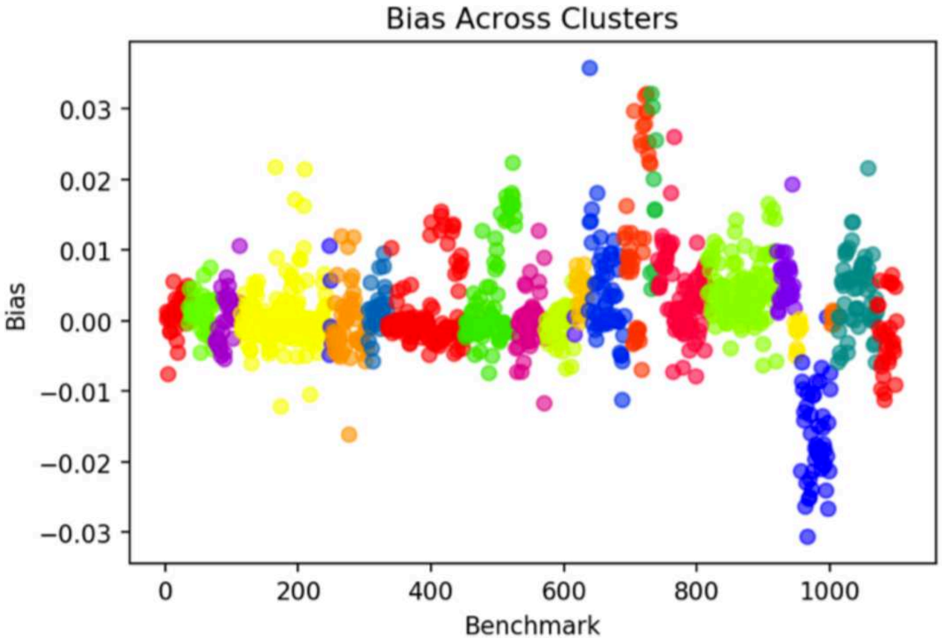
- Clustering is used to find inherent relationships in the data
  - Objects in the same cluster are more similar to each other than those in other clusters
  - Used to find groups of benchmarks that have similar sensitivity profiles, $S^i_{k,\sigma}$

- Can train and test on a few clusters at a time
  - Well populated classes of benchmarks skew the overall model
  - Training and testing on a subset of the data leads to a more specialized and accurate model
  - More accurate model $\leftrightarrow$ More accurate feature importance

- Can use clustering to find similar benchmarks for:
  - Benchmark selection for statistical analysis in Whisper
  - Finding regions in sensitivity space that are sparse (more benchmarks needed, see cluster #11 with mix-comp-fast on next slide)

Clustering Whisper benchmarks

- Finds 24 clusters ranging in population from 2 to 133
  - Segregated mainly based on materials present and spectrum



Cluster	Number of Cases	Benchmark Types
0	33	heu-met-fast
1	41	heu-met-fast, heu-met-mixed
2	38	heu-met-fast
3	133	heu-met-fast
4	5	heu-met-inter
5	54	heu-sol-therm, leu-comp-therm, u233-comp-therm
6	29	heu-met-fast, ieu-met-fast
7	117	leu-comp-therm, heu-comp-therm, heu-met-therm
8	77	heu-comp-therm, leu-comp-therm, heu-sol-therm
9	44	leu-comp-therm, heu-sol-therm
10	43	heu-sol-therm, leu-sol-therm
11	2	mix-comp-fast
12	20	mix-met-fast
13	54	pu-sol-therm, mix-sol-therm, mix-comp-therm
14	39	pu-comp-mixed, pu-sol-therm
15	11	pu-comp-mixed, pu-met-fast
16	75	pu-met-fast, mix-met-fast
17	105	pu-sol-therm, mix-sol-therm, mix-comp-therm
18	26	pu-sol-therm, mix-sol-therm,
19	10	u233-met-fast
20	45	u233-sol-therm, u233-sol-inter
21	10	u233-sol-therm
22	60	u233-sol-therm
23	29	u233-sol-therm, u233-comp-therm

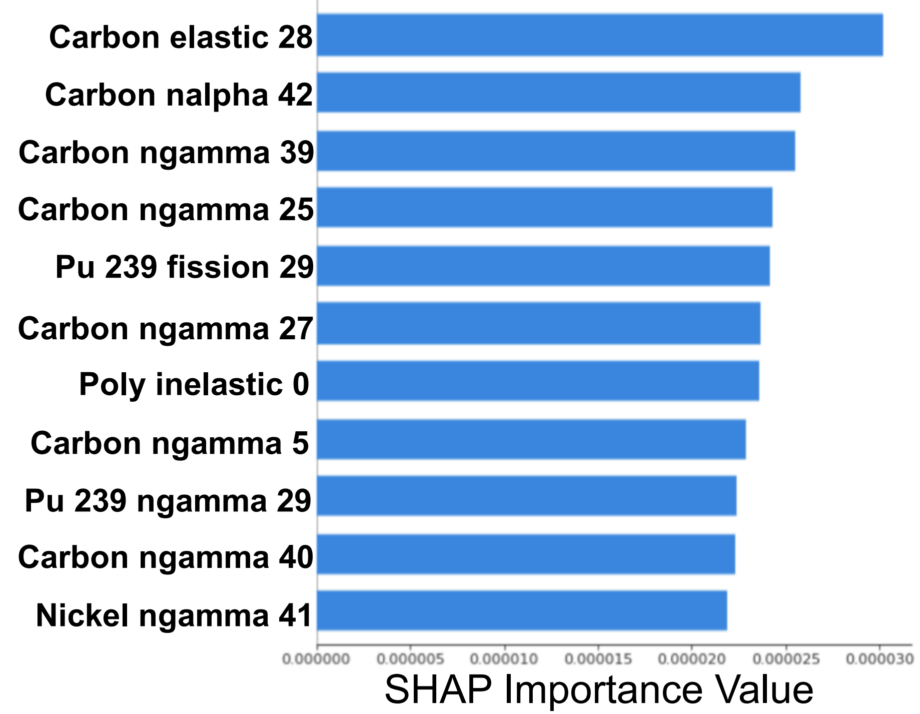
Benchmark clustering, bias predictions, feature importance and nuclear data assimilation

- In FY18, we took a preliminary look at combining several machine learning algorithms together in order to understand where they can be applied within the nuclear data evaluation process
  - Identify a cluster of benchmarks to study, e.g. PMF systems
  - Build a random forest model to predict the k_{eff} bias within this cluster
  - Select the most important features to predicting the bias
  - Apply genetic algorithm to optimize perturbations of the most important features
- We will continue scoping out these methods to find robust methodologies to support nuclear data evaluations

SHAP analysis points to potential deficiencies in ENDF/B-VII.0

- Recent results from Mike G. using Random Forest & SHAP analysis
- This work focuses on finding known and unknown issues in ENDF/B-VII.0 to test ML algorithms capabilities. Once that is successful, we will do production runs validating ENDF/B-VIII.0
- Used all Pu benchmarks
- Carbon: known issue because of questionable benchmarks
- $^{239}Pu(n,\gamma)$ in energy-bin 29 fixed in ENDF8

PRELIMINARY: Questionable nuclear data related to small-scale exp.



Using integral experiment metadata as feature importance

- If only sensitivity profiles are used, only nuclear data observables will be highlighted as related to bias between simulated and experimental benchmark value

- Experiments can be characterized by their MCNP input deck (metadata): geometry, material composition, source definition, analysis method, etc.

- The final result, e.g., difference between simulated and measured k_{eff}, is a function of nuclear data **and** experimental metadata

Conclusions & Future Work

- Using the Whisper-1.1 catalogue of 1100+ criticality safety benchmarks, several machine learning methods were applied to predict k_{eff} bias, cluster similar benchmarks together, find highly important features in the nuclear data and optimize perturbations to important cross sections.

- Need to examine all of the machine learning results more closely, especially the *initial* nuclear data adjustment results
  - Comparison to GLLSM is needed (already underway)
  - Inclusion of the nuclear data covariance is essential
    - The accuracy of the nuclear data covariance data could be problematic

- Using more features of the benchmarks (metadata) is being explored to see if they can help in clustering benchmarks or finding systematic outliers

Acknowledgements

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Questions ?