PAUL SCHERRER INSTITUT

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Predicting the Bias in Calculations of Spent Nuclear Fuel Characteristics

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Workshop on ML in Nuclear Science and Technology Applications

Background and Motivation

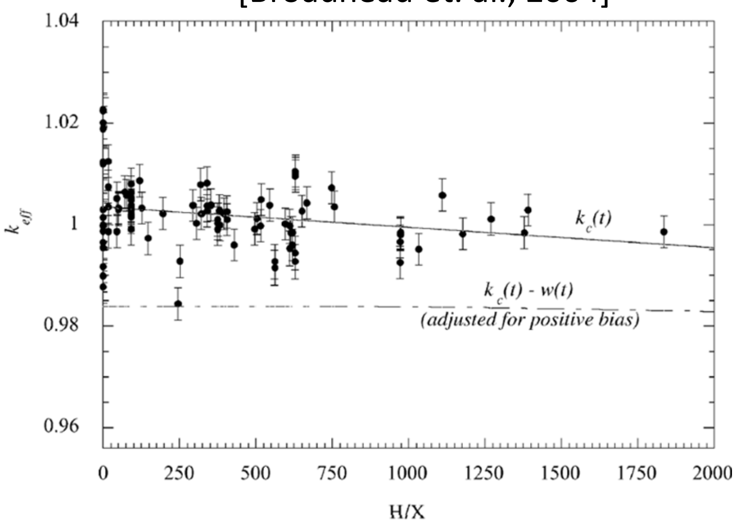
- SNF characterization relies on calculations (measurements are extremely expensive, difficult)
- A question arises: How can we be sure about these calculations?
- Validation is required *a priori,* modelling benchmarks which have their characteristics measured, and comparing calculations to measurements (e.g., $C-E$ or C/E)
  - Limited measurements (e.g., ~300 SNF decay heat measurement worldwide) and actual SNF are ~13,000 SNF in Switzerland alone
  - Benchmarks cover ranges of SNF properties, area-of-applicability (AOA), and realistic SNF calculations usually have different properties
- We need to predict the bias (i.e., predictive modeling), by comparison with validation benchmarks

In criticality safety, methods are established

ANS-8.17: Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors

ANS-8.24: Validation of neutron transport methods for nuclear criticality safety calculations

[Broadhead et. al., 2004]



Overview of this work

Research Questions:

- Could the bias be predicted for SNF properties (decay heat and nuclide concentration) given a set of validation benchmarks?
- What properties would be informative into these predictions?
- What are the assumptions of these predictions?

$$C - E = f(X) + \varepsilon$$

Hypotheses:

- Bias prediction is based on neutronically similar benchmarks → Neighborhood-based schemes
- Integral SNF properties, such as spectral index, burnup, and correlations could be informative toward the bias prediction

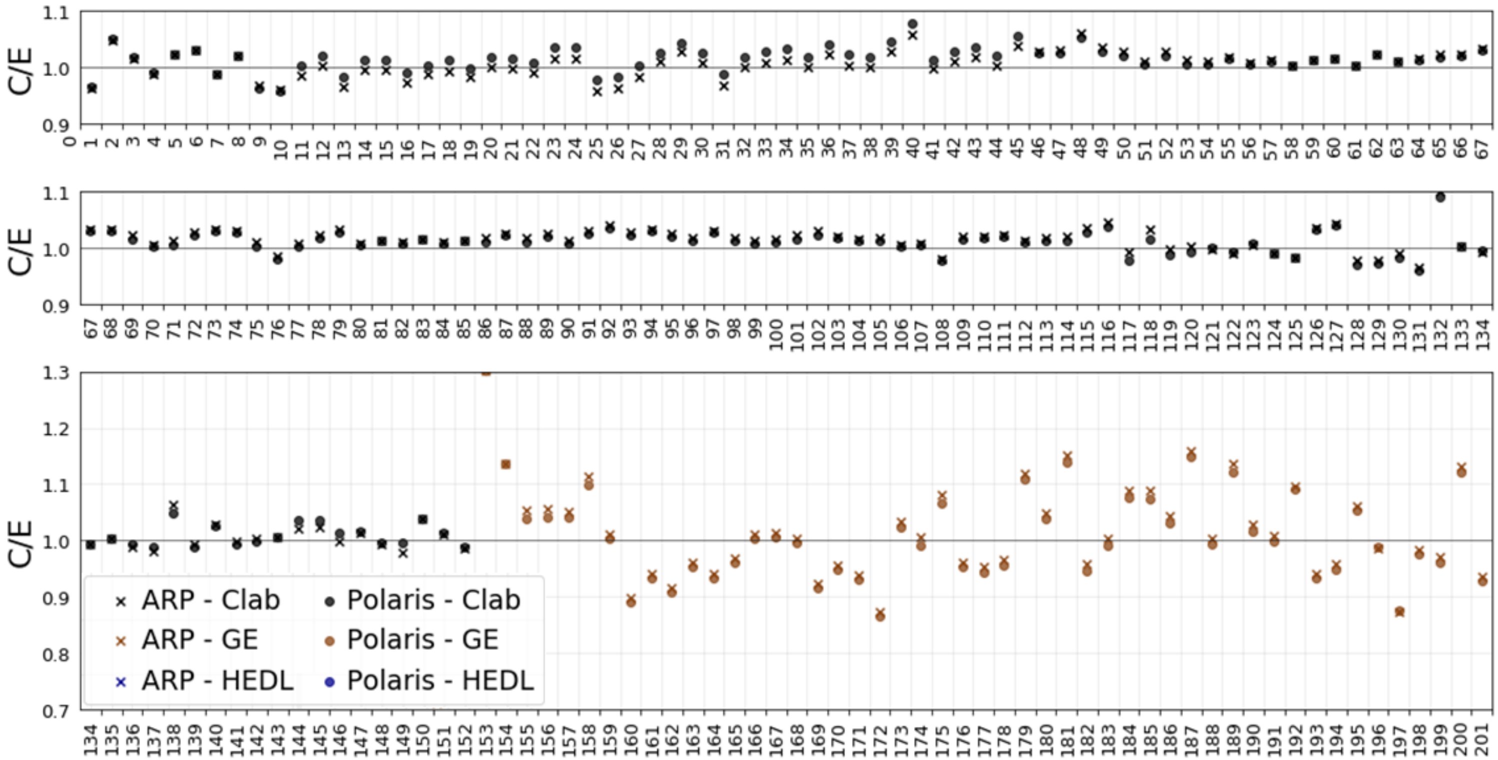
Research Steps

1. **Collecting data:** SNF validation benchmarks (calculations and measurements)
2. **Extracting features:** sensitivity analysis and uncertainty propagation
3. **Application of data-driven techniques (novelty of this work):** Machine Learning models and algorithms

Research Steps

1. **Collecting data:** SNF validation benchmarks (calculations and measurements)

Decay heat labelled-data

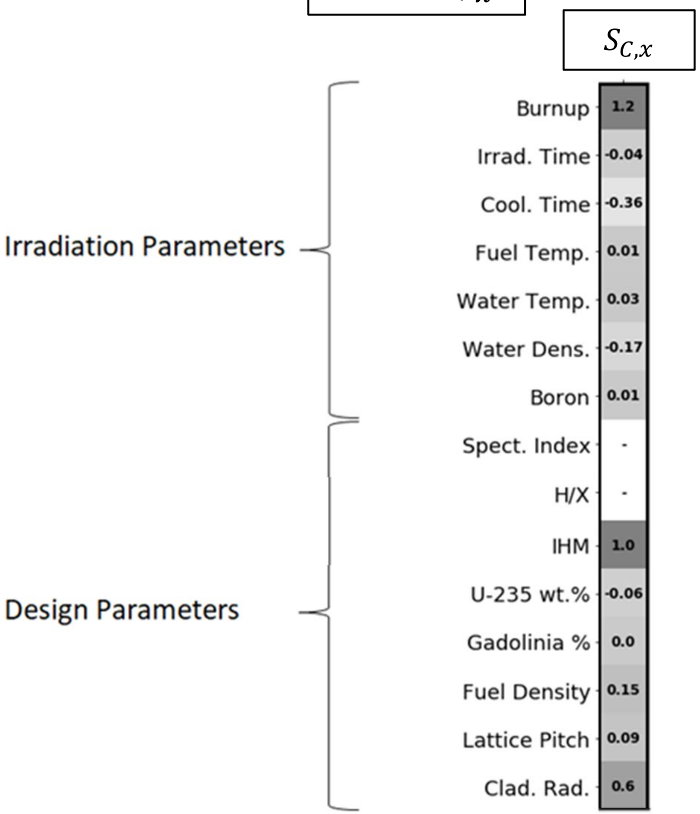


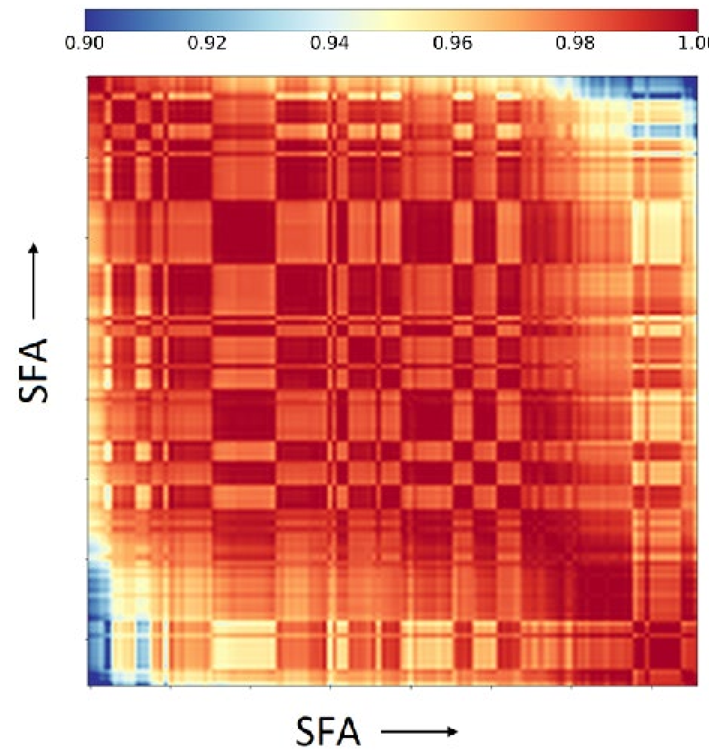
Research Steps

1. **Collecting data:** SNF validation benchmarks (calculations and measurements)
2. **Extracting features:** sensitivity analysis and uncertainty propagation

$$S_{C,x} = \frac{\partial C / C}{\partial x / x}$$

$$\rho_{ij} = \frac{1}{N-1} \sum_{k=1}^{N} \frac{\left(DH^{i}{}_{k} - \overline{DH}_{i}\right)\left(DH^{j}{}_{k} - \overline{DH}_{j}\right)}{\sigma_i\, \sigma_j}$$





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Research Steps

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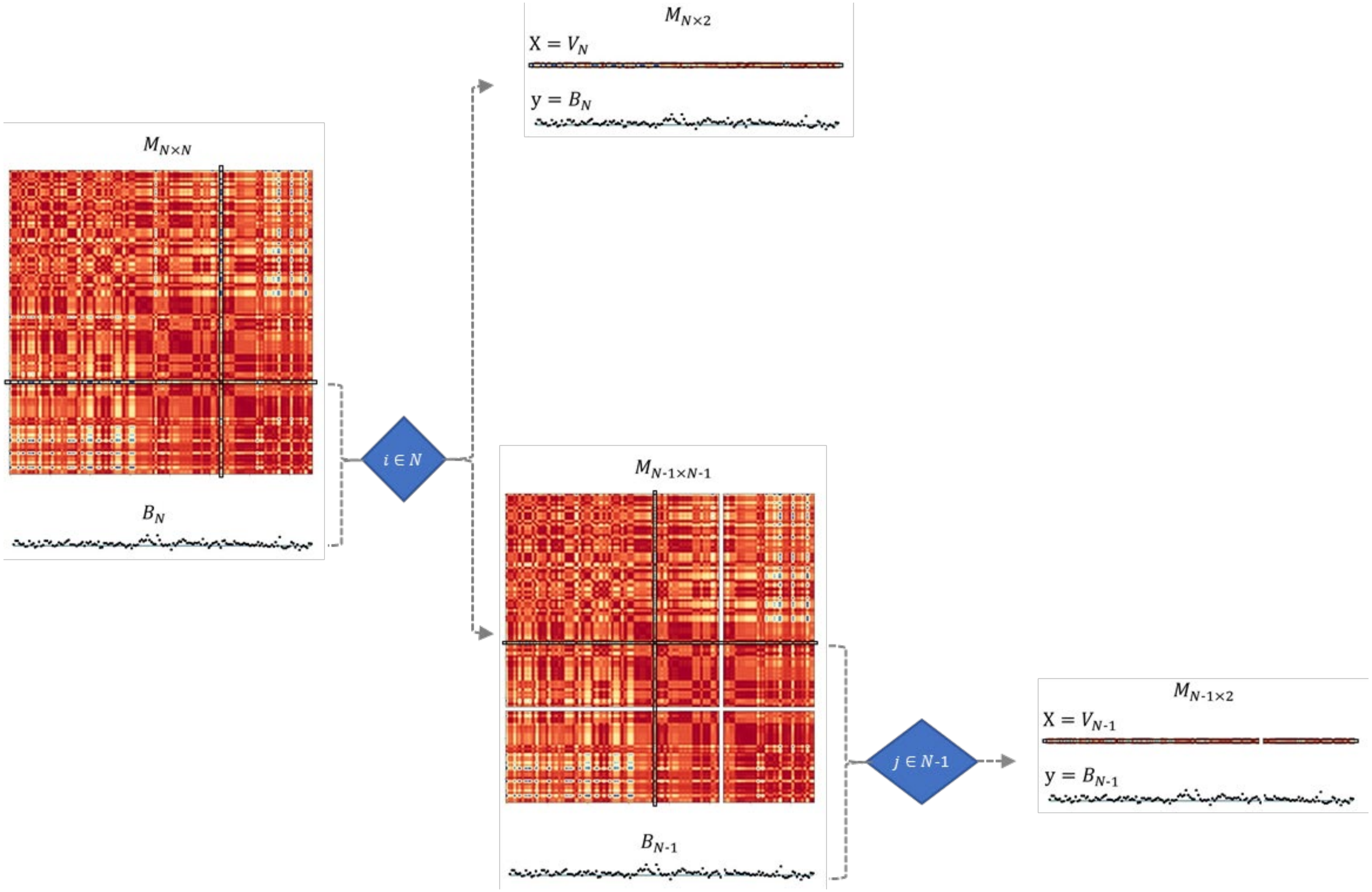


Research Steps

1. **Collecting data:** SNF validation benchmarks (calculations and measurements)
2. **Extracting features:** sensitivity analysis and uncertainty propagation
3. **Application of data-driven techniques (novelty of this work):** Machine Learning models and algorithms

$$C - E = f(X) + \varepsilon$$

Hypotheses

– Bias prediction is based on neutronically similar benchmarks

– Integral SNF properties, such as spectral index (*SI*) correlations between benchmarks, could be informative toward the bias predictions

Linear Model (~ criticality safety)

$LM\ with\ cutoffs$: $B_{(\rho=1)} = I_{\rho > co}(\rho)\beta\rho$

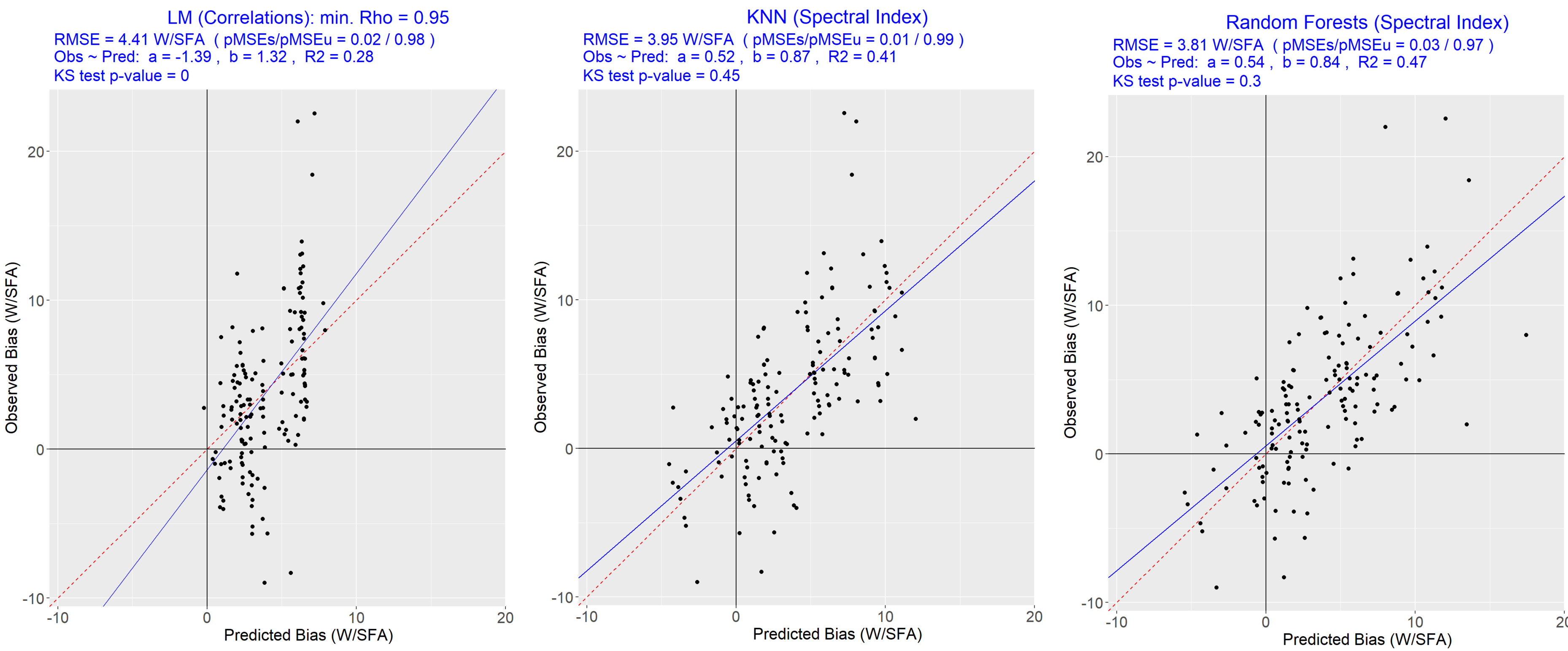
Neighborhood-based Schemes

$KKNN$: $B_{(\rho=1)} = \sum_{k=1}^{K} w_k B_k$

RF: $B_{(\rho=1)} = \frac{1}{N}\sum_{n=1}^{N}\left(\sum_{\rho\,\in\,[C/O,\,1]} w_n B_\rho\right)$

Results : Decay Heat

- Comparing predictions to observations (Features: SI or Correlations)
- Statistical testing, Kolmogorov–Smirnov test, testing whether model-predicted biases originate from the same distribution as observed ones at p-value = 0.05

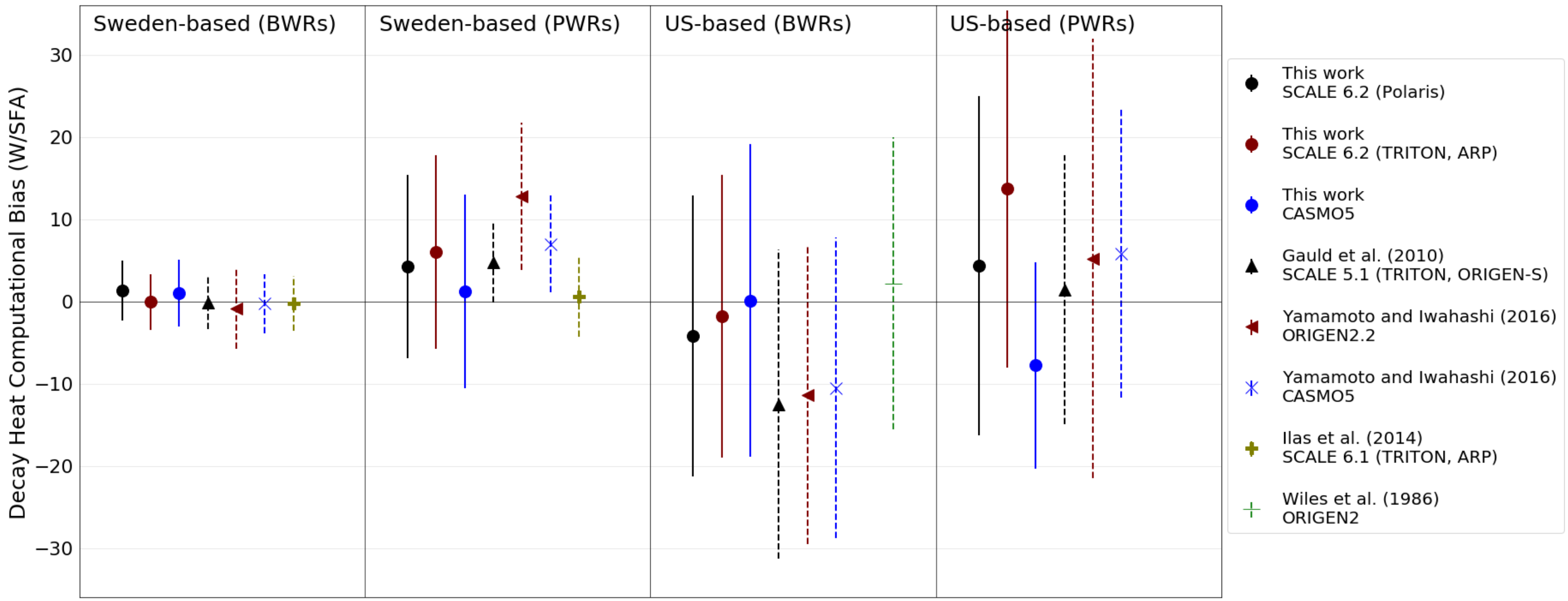


Summary

- SNF calculations are being validated (i.e., decay heat and nuclide concentration)
- Machine Learning models are being analyzed for their predictive performance, comparing bias model predictions to observed ones
- We have shown that the bias could be predicted from validation data (benchmarks), meaning we could support activities such as license applications, and decisions on safety margins
- Neighborhood based schemes (neutronically similar benchmarks) predict biases statistically similar to observed ones
- The models rely only on few SNF features, namely:
  - Spectral index (neutron flux)
  - Correlation between benchmarks
- **Ongoing work:** bias prediction for other quantities, i.e., actinides conc. (U-235 and Pu-239) and a fission product (Cs-137), using also neighborhood-based schemes and SNF features measuring similarities

Thanks everyone – do you have questions?

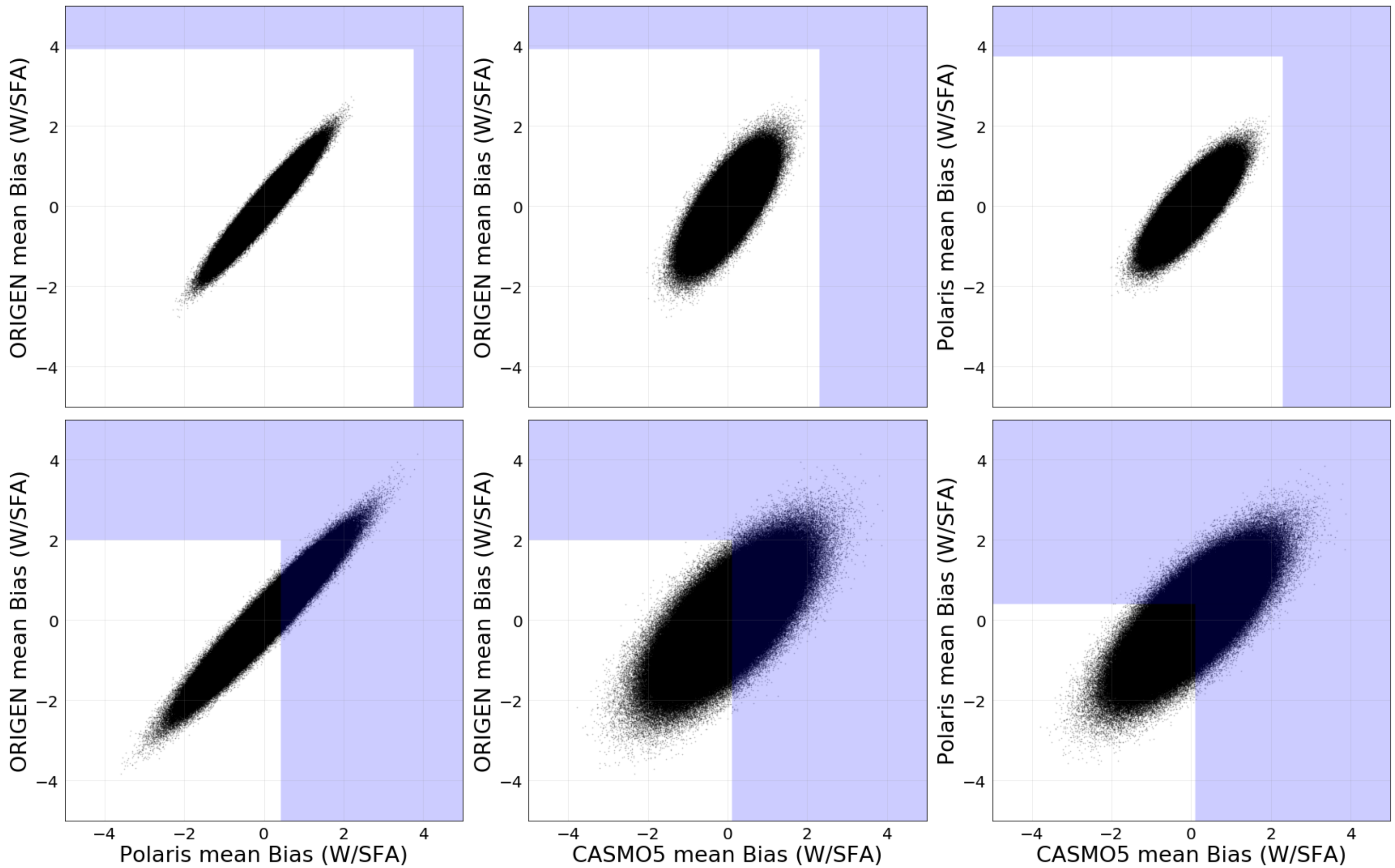
Appendix : Validation



Appendix : Selecting Benchmarks

$$H_0\!: C_P \text{ or } C_O \text{ or } C_C = E$$

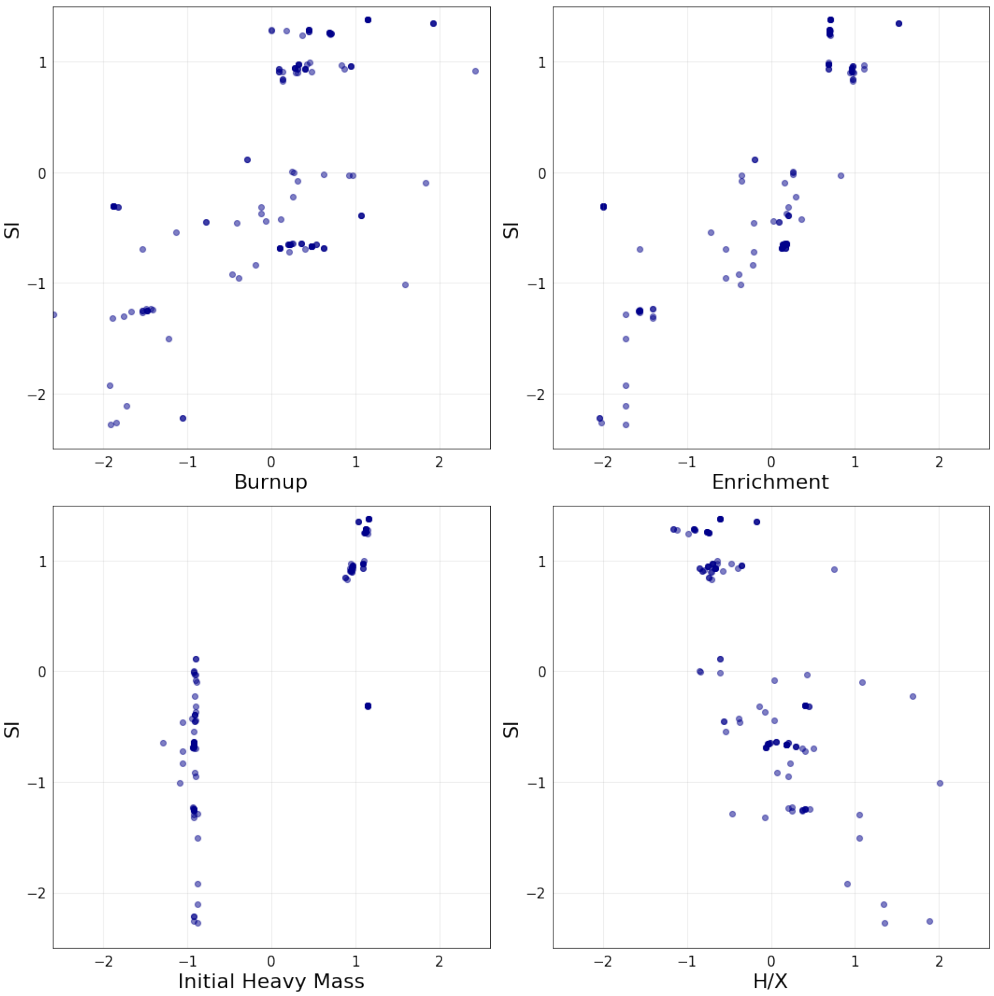
$$H_a\!: C_P \text{ and } C_O \text{ and } C_C \neq E$$



Appendix : Spectral Index

$$SI_i = \frac{\emptyset_{E>0.625\ eV}}{\emptyset_{total}}$$

$$SI = \frac{\sum_1^n (BU_i \times SI_i)}{\sum_1^n (BU_i)}$$



Appendix : Final Models

Table. Test errors of the applied models along with fractions of the explained variances.

Design Matrix	Model	MAE ± 1σ (W/SFA)	R^2
Spectral Index	RF	2.94 ± 2.42	0.47
	KNN	3.01 ± 2.56	0.41
	KKNN	2.97 ± 2.40	0.46
Correlation	RF	2.99 ± 2.67	0.44
	KNN	3.35 ± 2.69	0.32
	KKNN	3.49 ± 2.60	0.30

Appendix : Ongoing Activities

Bias prediction for other quantities, i.e., concentration of actinides (U-235 and Pu-239) and a fission product (Cs-137), using neighborhood-based schemes and SNF features measuring similarities