Predicting the Bias of SNF Depletion Calculations: Application of Polaris, Sampler, and Machine Learning

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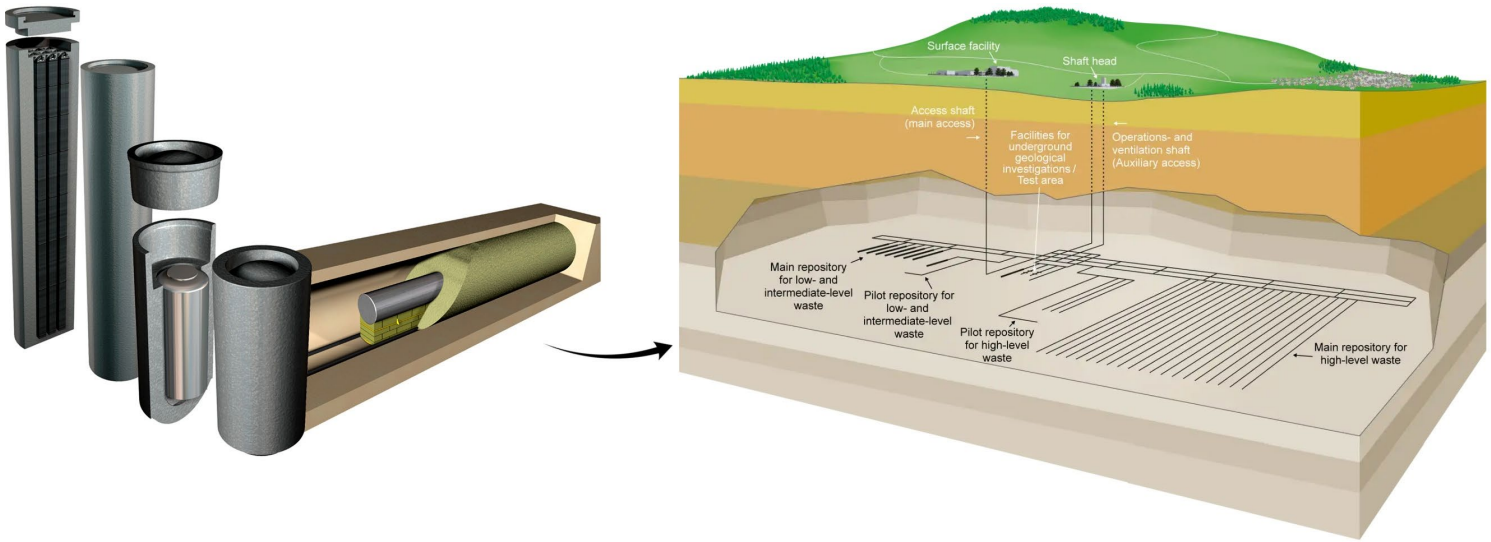
Background

- Nagra, the WMO in Switzerland, plans for nuclear waste disposal in deep geological repository



- General licence application is in preparation, to be submitted around 2024
- SNF is high-level waste, ~13k FA by the end-of-life of the Swiss NPPs
- SNF characteristics, *e.g.*, decay heat, are calculated using codes (*e.g.*, Polaris) and data (*e.g.*, fuel irradiation data)

 WMO: Waste Management Organization SNF: Spent Nuclear Fuel FA: Fuel Assembly

Background

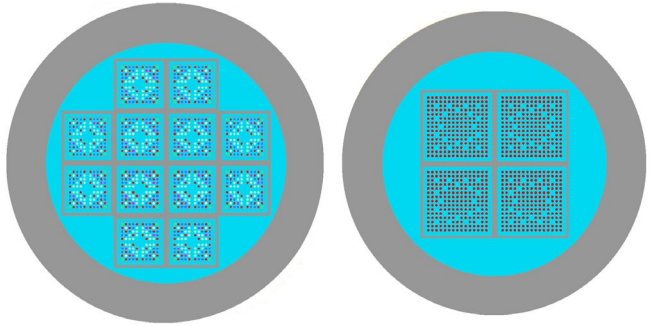
Downstream Applications

Requiring accuracy and precision of the bias

Economics

Reducing DH uncertainty could lead to reduction in the no. of disposal canisters

$$\sum DH \leq 1500\ W$$

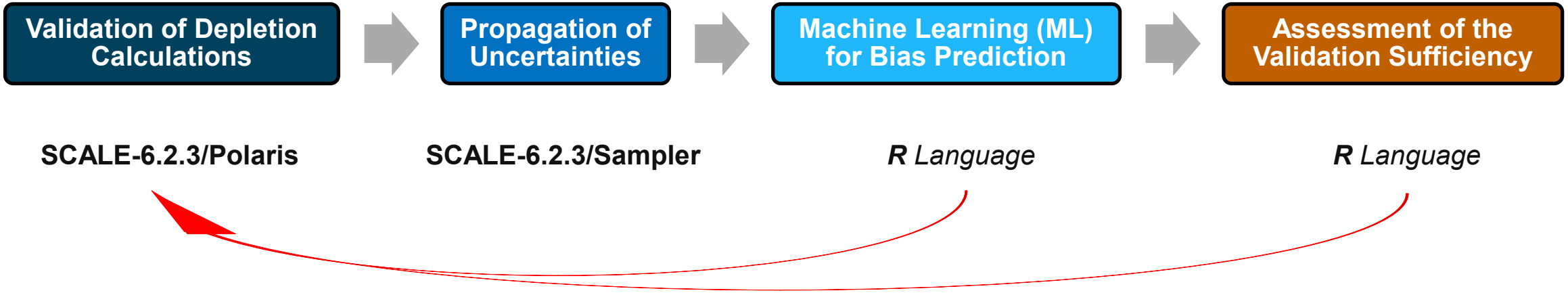


Safety

Ensure subcriticality, *e.g.*, burnup credit CSA penalizes k_{eff} with bias and uncertainty (*e.g.*, nuclide concentrations (Gauld and Mertyurek, 2019))

DH: Decay Heat CSA: Criticality Safety Analysis

Main topics



$$Bias \rightarrow B = C - E$$

– **Few measurements, with limited range of properties**

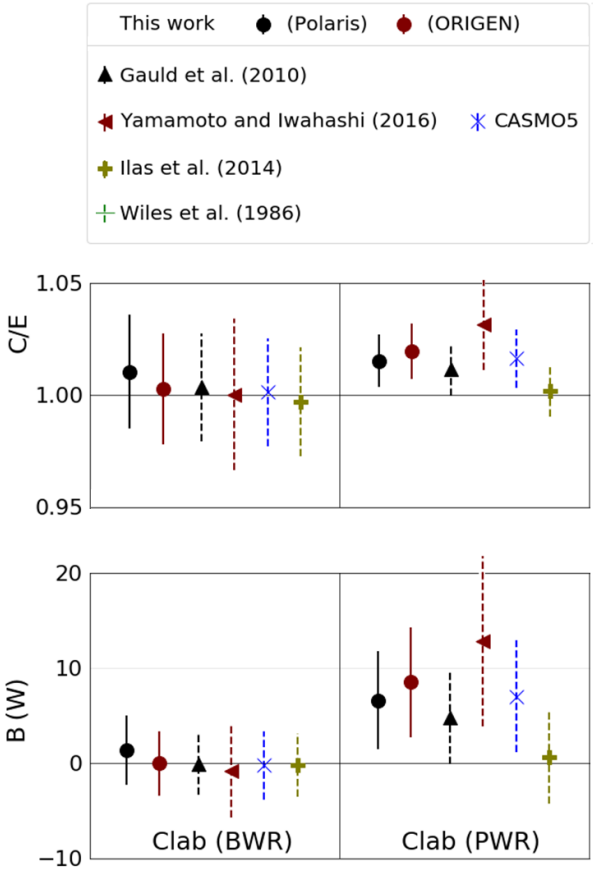
~ hundreds of PIE, SFCOMPO (F. Michel-Sendis et al., 2017)

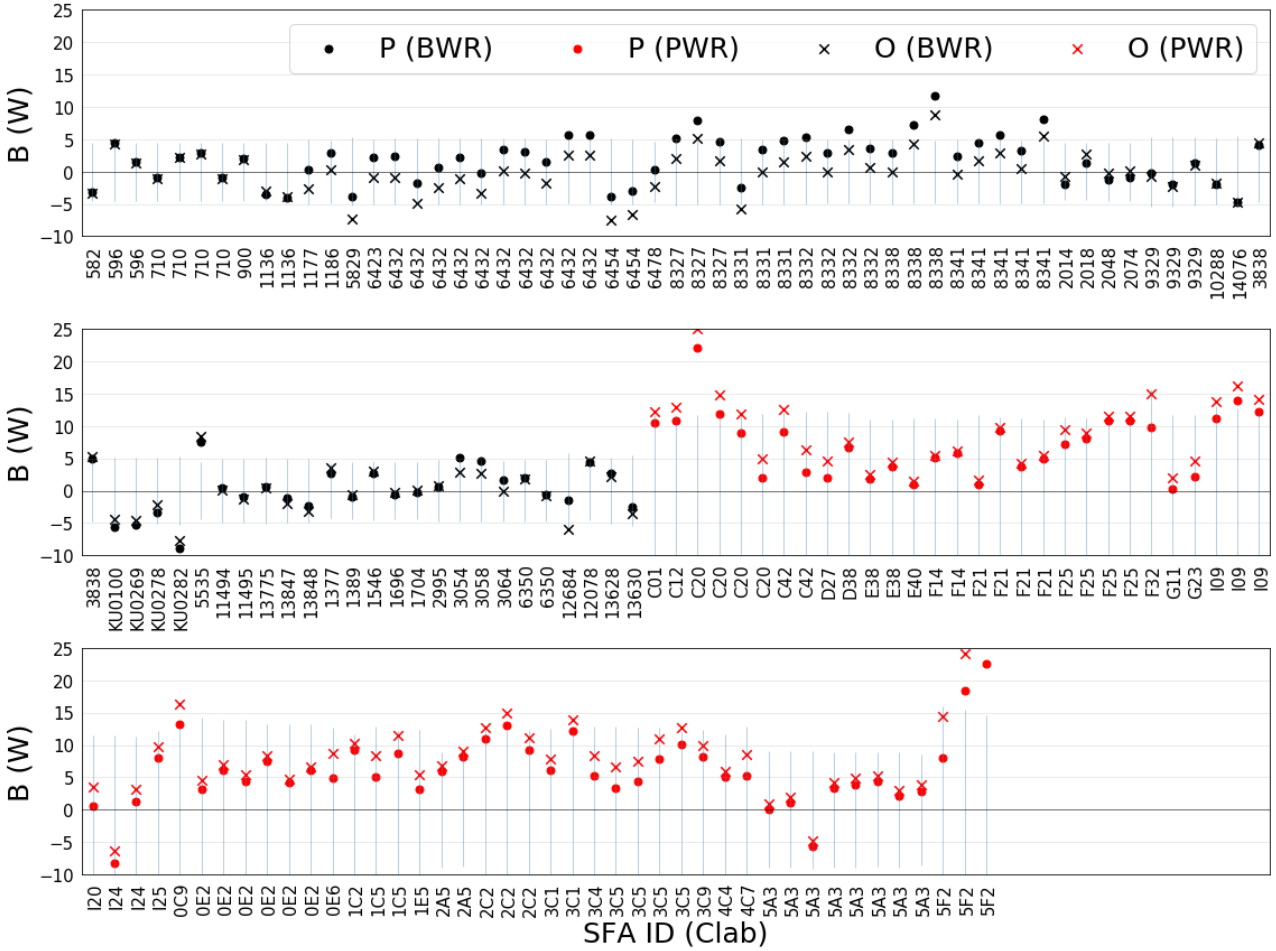
~ 133 DH FA at Clab <51 GWd/tU (SKB, 2006) & <55 GWd/tU (EPRI, 2020)

 ML: Machine Learning DH: Decay Heat PIE: Post Irradiation Examination

Topic 1: Validation of the depletion calculations

Calculations using **SCALE-6.2.3 Polaris** and **ORIGEN** applied on the **152** DH measurements at **Clab** (SKB, 2006)





– On average, calc. DH are within 5% of the measured ones

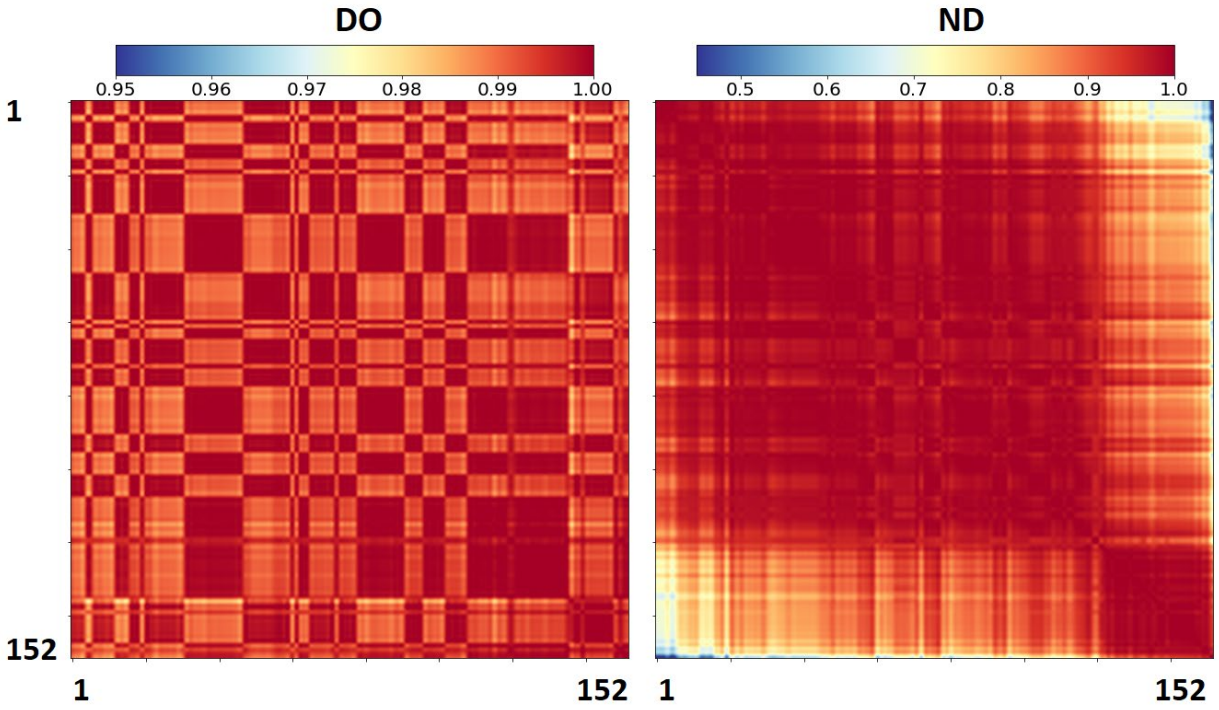
– Large variances (potential improvements)

Topic 2: Uncertainty propagation of ND and DO uncertainties (also SA)

Calculations using **SCALE-6.2.3 Sampler/Polaris** applied on the **152** DH measurements at **Clab** (SKB, 2006)

Bias informative features (Spectral index $SI_i = \frac{\emptyset_{Fast}}{\emptyset_{Total}}, SI = \frac{\sum_1^n (BU_i \times SI_i)}{\sum_1^n (BU_i)}$, Calc. value $\boldsymbol{C}$, Correlation coeff. $\boldsymbol{\rho_{ij}} = \frac{1}{N-1} \sum_{k=1}^{N} \frac{(C^i{}_k - \bar{C}_i)(C^j{}_k - \bar{C}_j)}{\sigma_i \, \sigma_j}$)

$\boldsymbol{\rho}$ between calc. DH, ordered by BU (top to bottom, left to right)



 SA: Sensitivity Analysis DH: Decay Heat ND: Nuclear Data DO: Design & Operation BU: Burnup

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Topic 3: Application of Machine Learning (**ML**) for the bias prediction

$$\boldsymbol{C - E = f(X) + \epsilon}$$

$f(X)$ predictable part (systematic bias)

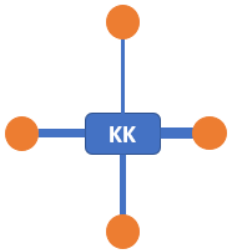
ϵ unpredictable part (random bias)

f model (e.g., similar benchmarks)

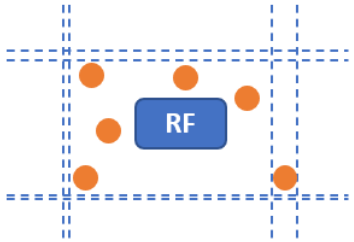
X bias informative features,

- assumptions: correlations ρ
- many features/selection (RFE): SI, C, ρ

Weighted k-Nearest Neighbors **KKNN**: $B_{(\rho=1)} = \sum_{k=1}^{K} w_k B_k$, $w_k \propto f(\Delta\rho)$



Random Forest **RF**: $B_{(\rho=1)} = \frac{1}{N}\sum_{n=1}^{N} w_n B_n$, $I_{\rho > co}$



 ML: Machine Learning RFE: Recursive Feature Elimination

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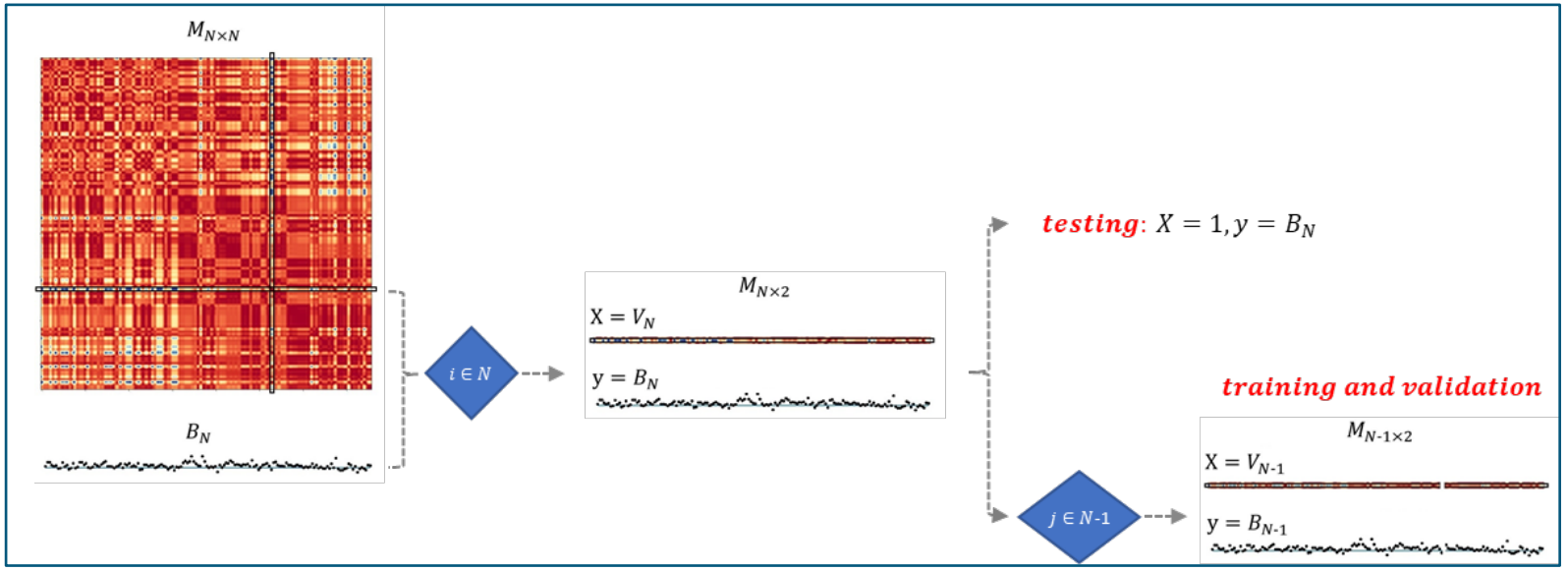

Application in ML algorithm	Method
Resampling technique	LOOCV
Test metrics	R^2, KS-test, Regression
Treatment of outliers	Z-score, Cook's distance (3σ and distance, apply AND)
Multiple measurements (same FA)	Random sampling

RFE: Recursive Feature Elimination LOOCV: Leave-one-out Cross-validation FA: Fuel Assembly

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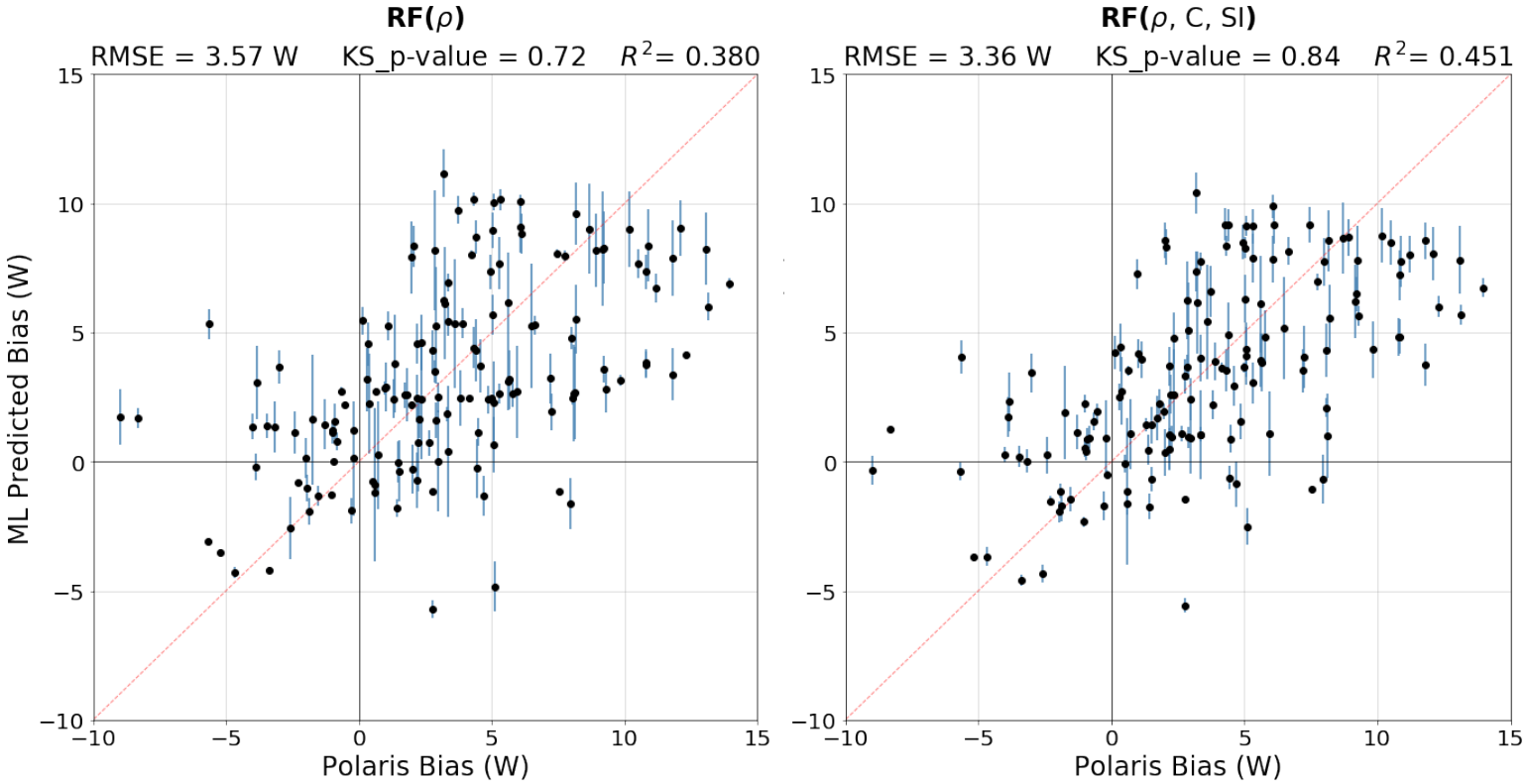
Topic 3: Application of Machine Learning (**ML**) for the bias prediction

RF model predicted bias of the DH benchmarks of Clab-2006, using **LOOCV**:

- 149 measurements on 83 FA
- 3 outliers (of multiple measurements on C20 and 5F2 FA), 2% of the data

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



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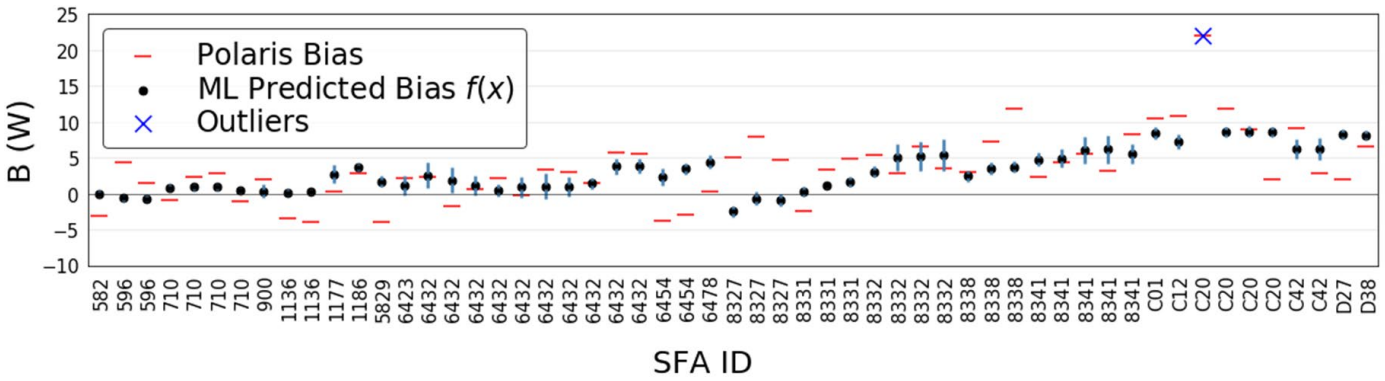
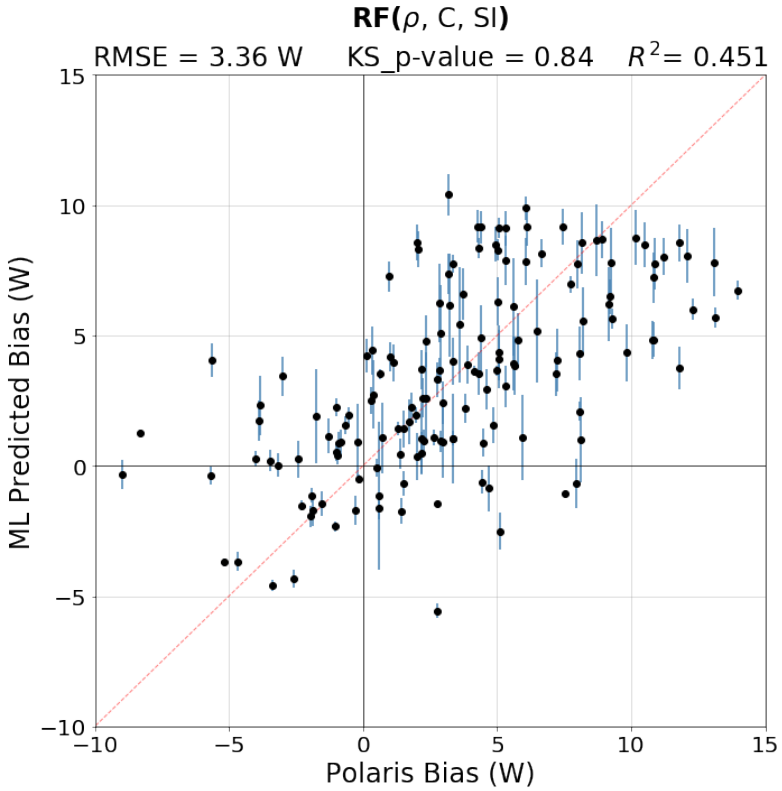
$$\bar{B} \pm \sigma \rightarrow f(\rho, C, SI) \pm \epsilon$$





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Topic 4: Assessment of the sufficiency of the measurements

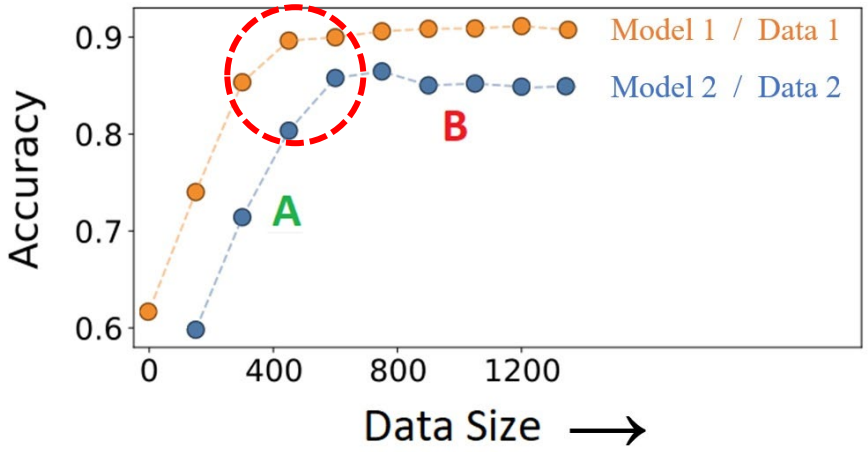
Sufficiency of the measurements/experimental gaps, range of applicability?

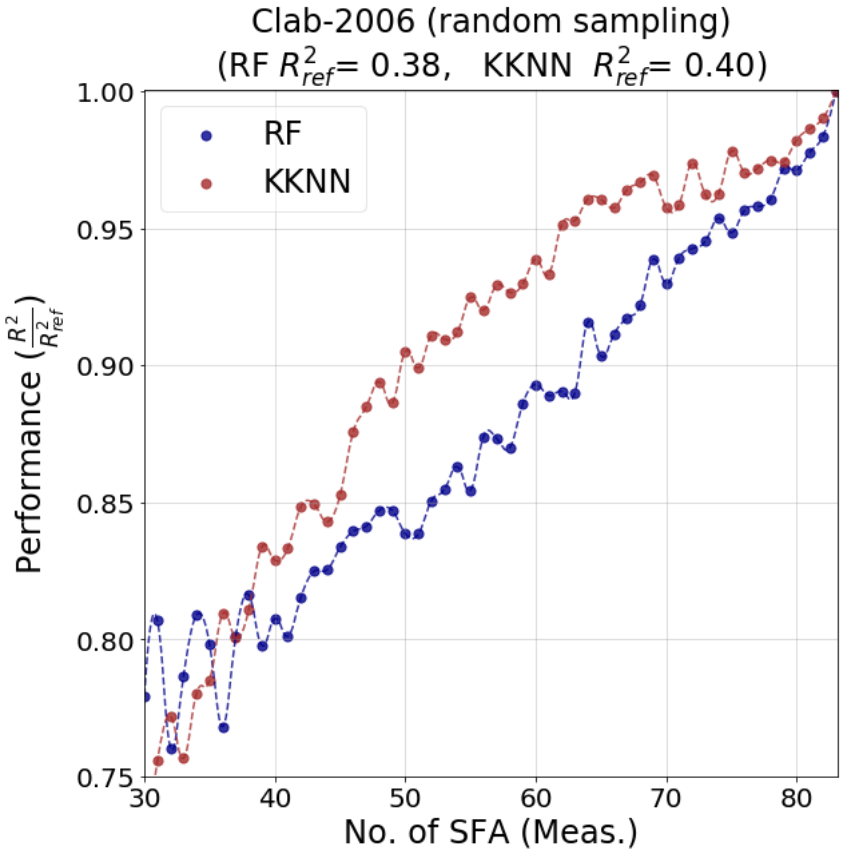
83 FA DH measurements at Clab: <51 GWd/tU 11-27 yrs of cooling (SKB, 2006)

1. No MOX
2. No high burnup

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

$f(X)$, ϵ predictable/unpredictable





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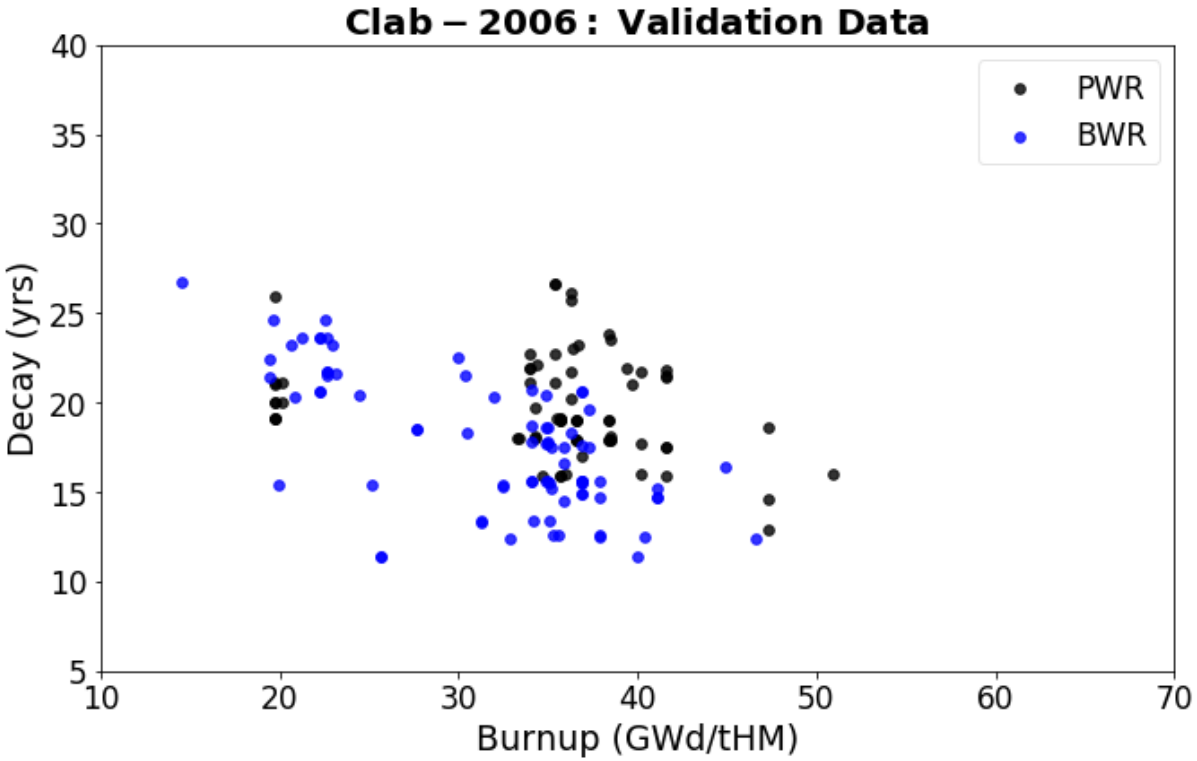
1. 3 pin-cells having the same H/X ratio as the full lattice: W15x15 UO_2 and MOX, GE14 UO_2
2. Sampler perturbations (625 ND and 625 DO)
3. ML on the application side

Validation →



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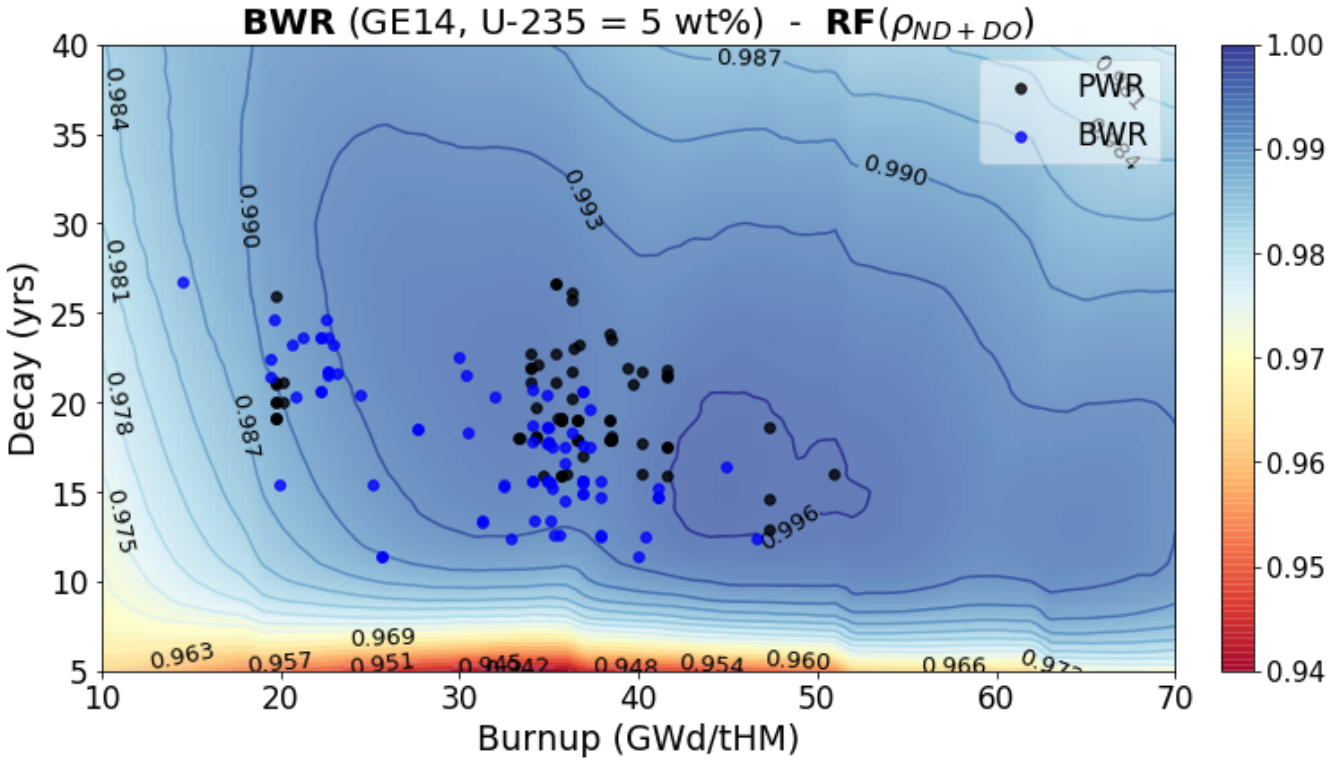

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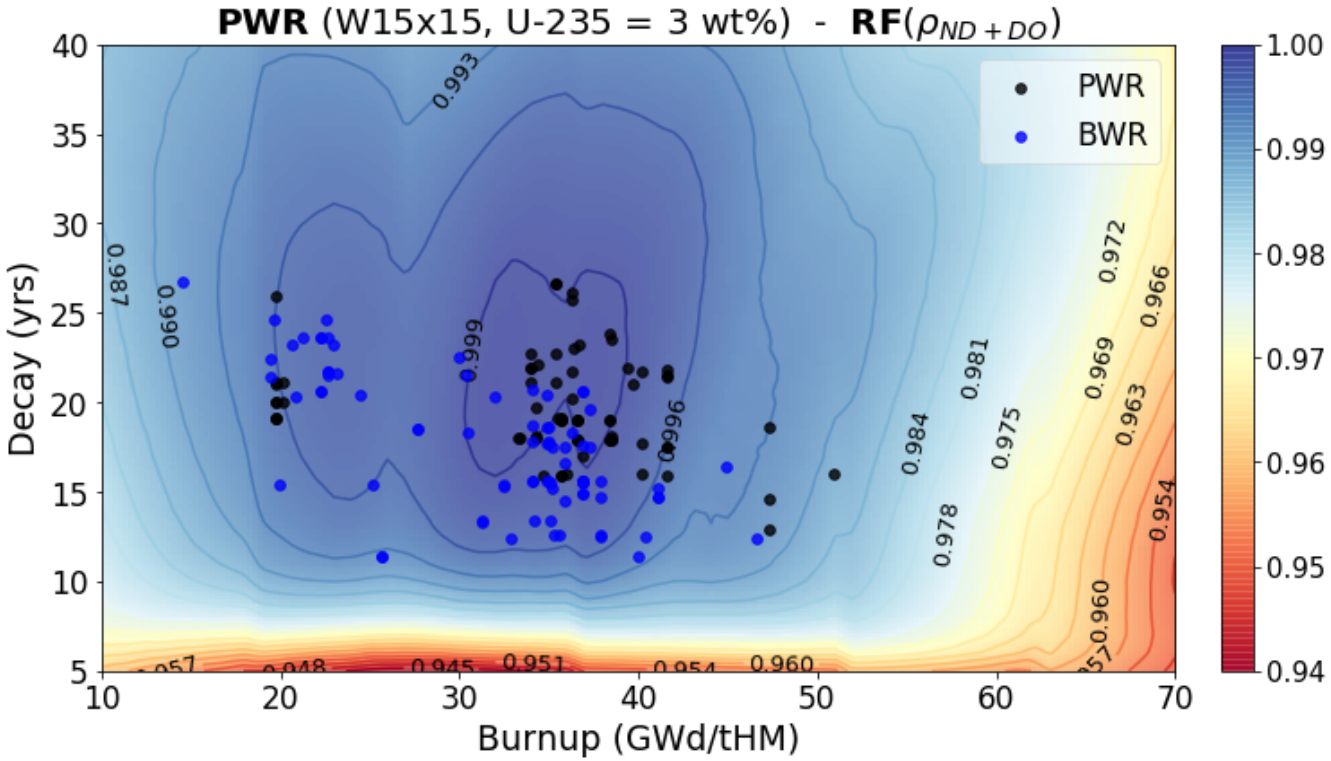

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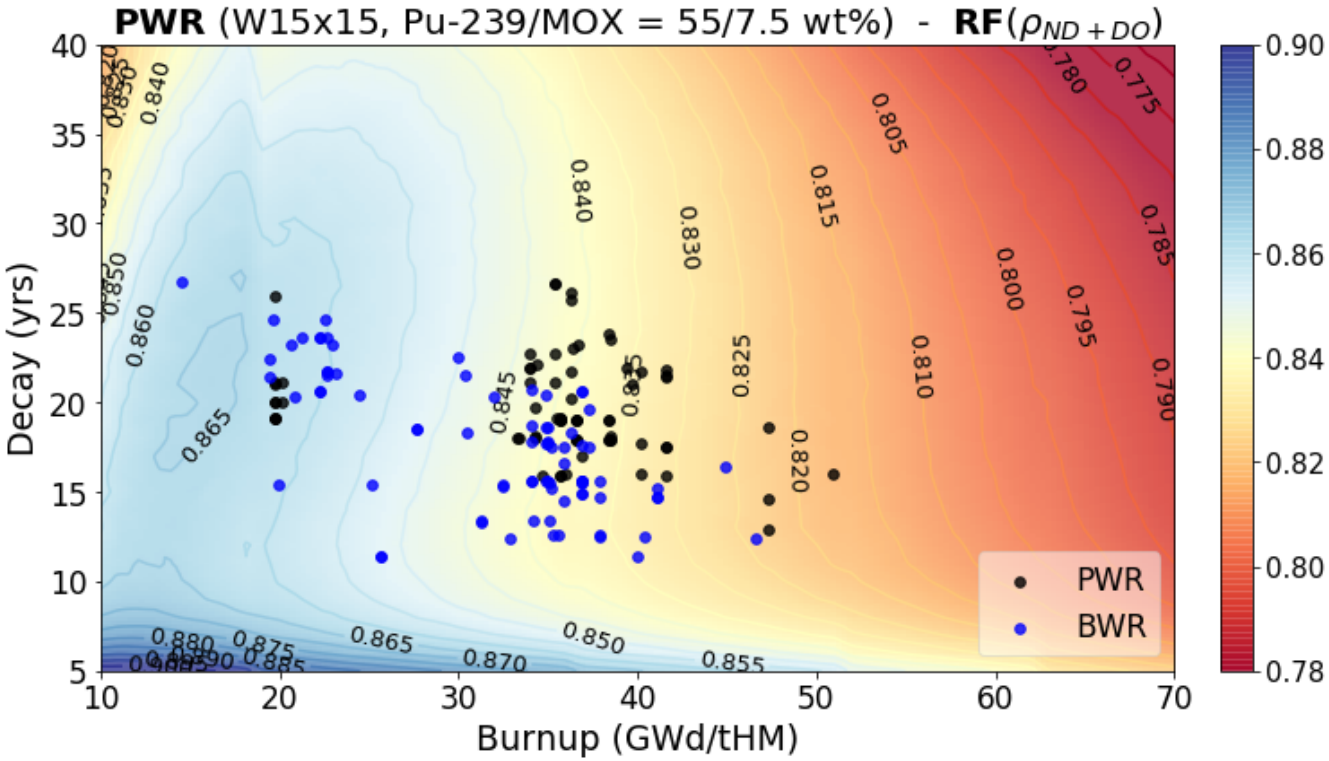

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Summary

SCALE in our organization

- Support SNF characterization and downstream applications
- Polaris & ORIGEN calculate fuel assembly wise decay heat and nuclide inventory (large-scale verification)
- Sampler is used for uncertainty propagation

+ Machine Learning

- Bias prediction in applications (*e.g.*, potentially for decay heat and nuclide inventory for burnup credit)
- Assessment of the validation data, highlight the parameters of potential future measurements

+ Participation in international projects using SCALE (Polaris, ORIGEN, KENO, Sampler)

- EJP-EURAD (decay heat and PIE analysis, activated cladding samples)
- NEA WPNCS subgroups (decay heat and PIE analysis)

thank you

for your attention

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