PAUL SCHERRER INSTITUT

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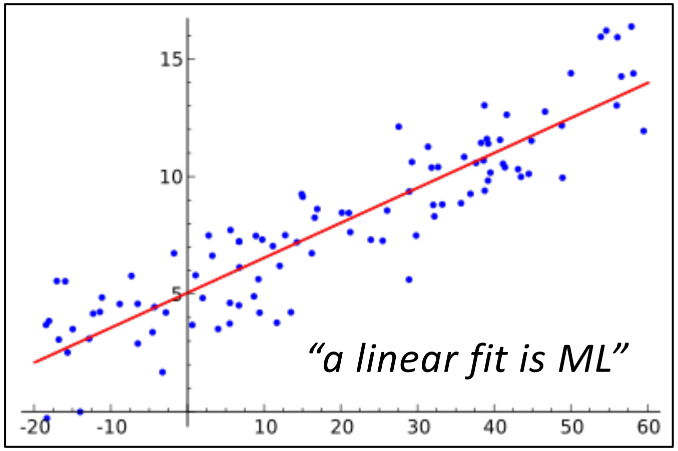
Combining ML and reactor physics for characterization and safety analysis of Used Nuclear Fuel

ETSON AI workshop, PSI, 20-21 October 2022

Summary

- Background and goal

- ML for understanding decay heat biases
  - *Weighted k-Nearest Neighbors*
  - *Random Forest*



- ML for simulating canister criticality
  - *Neural Network*

- ML for optimizing canister loadings
  - *Genetic Algorithm*

- ML for criticality uncertainty due to nuclear data
  - *Lasso Monte Carlo*

- ML for nuclear data and nuclear data uncertainties
  - *Bayesian Monte Carlo*

Background and goal

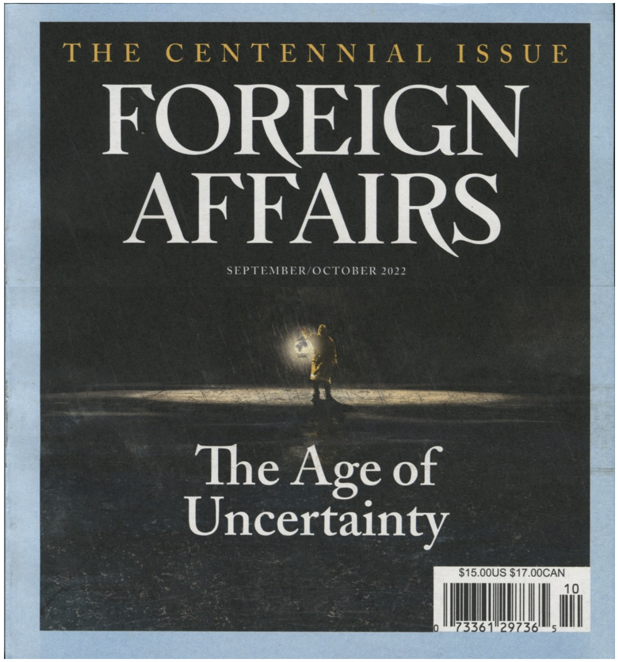
- **Machine learning** (**ML**) is a field of inquiry devoted to understanding and building methods that 'learn', (*i.e.* methods that leverage data to improve performance on some set of tasks).

- ML is used here in applied physics to complement Human Learning (HL).

- Based on "*command and control*": needs automation, integration (one-stop shop) and code control, from cradle to grave.

- Very computer intensive.

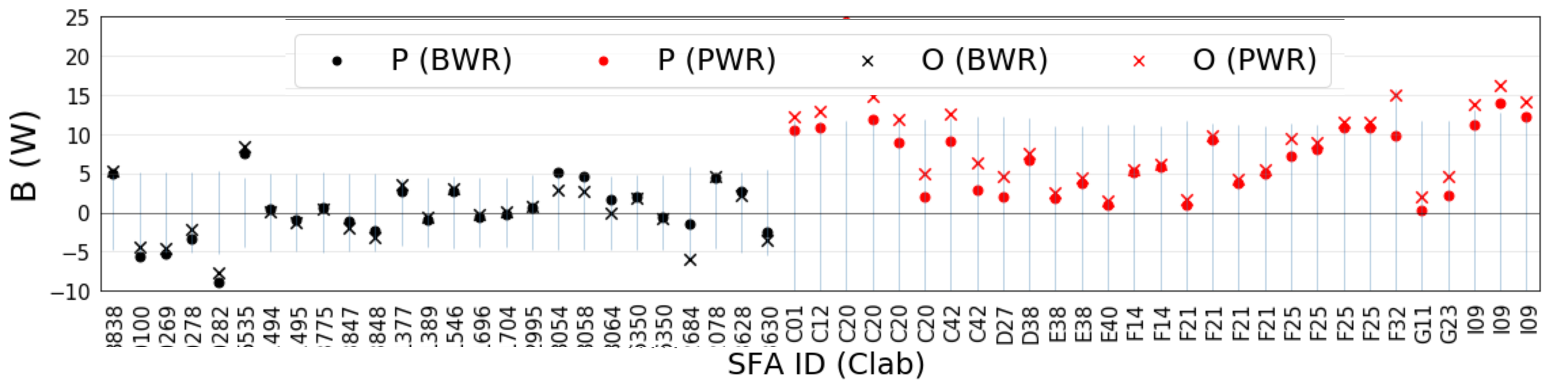
- Goals pursued in this work:
  – Supplement measured data
  – Perform optimization
  – Reduce biases
  – Estimate uncertainties (uncertainty is in the air)



ML for understanding decay heat bias (1/2)

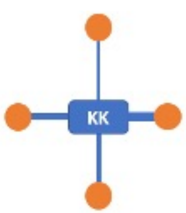
- Work performed between PSI, Nagra & EPFL (A. Shama)

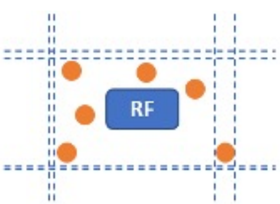
- Goal: Reduce the decay heat bias for B = C – E
- Why: Safety and economy of disposal canisters



- Methods:

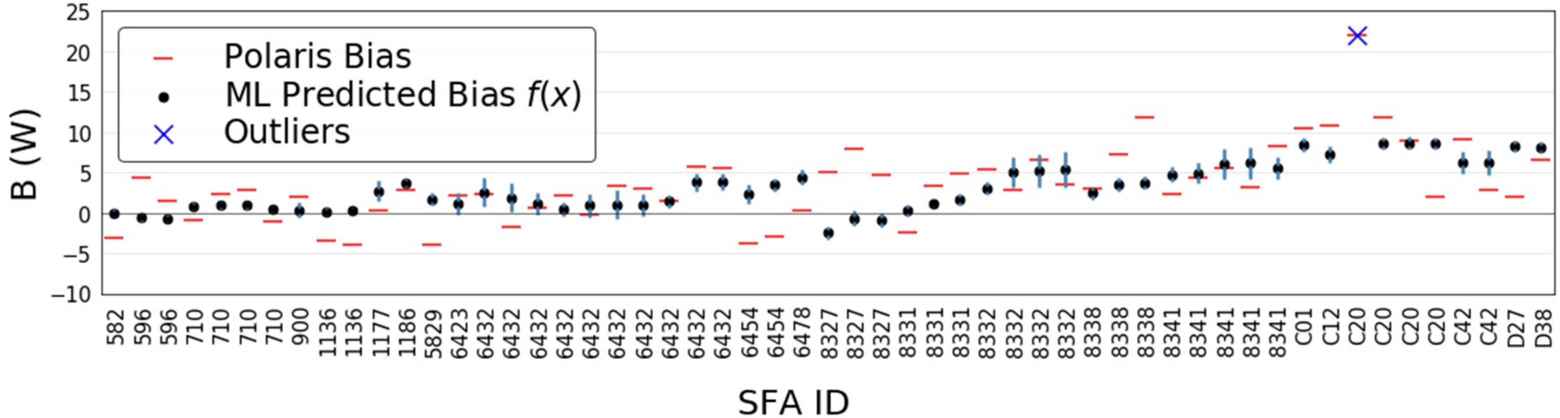
- **Weighted k-Nearest Neighbors WkNN** $B_{(\rho=1)} = \sum_{k=1}^{K} w_k \, B_k \,, \quad w_k \propto f(\rho)$
- **Random Forest RF** $B_{(\rho=1)} = \sum_{n=1}^{N} w_n \, B_n \,, \quad I_{\rho > co}$



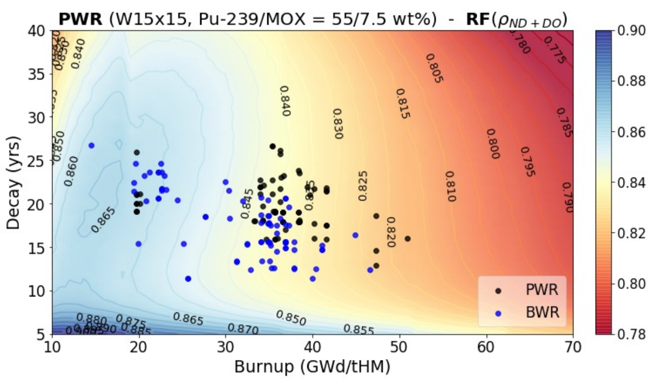


ML for understanding decay heat bias (2/2)

- Outcome:
  - Decay heat bias explained (reduced) by ≃ 50 %
  - Finding of outliers



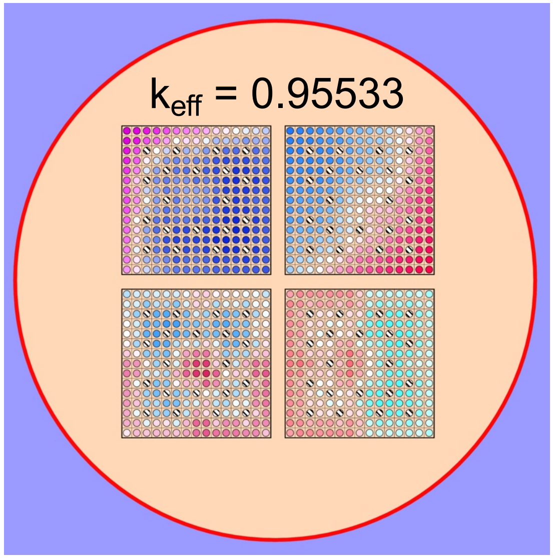
  - Finding of “where new measurements should be performed” to efficiently improve our knowledge

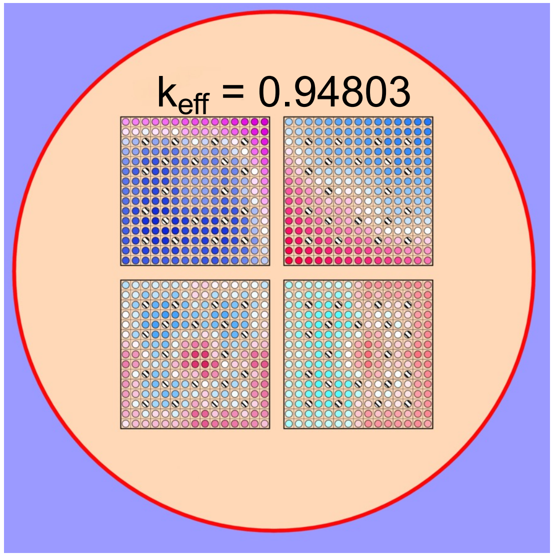


ML for simulating canister criticality (1/2)

- Work performed between PSI, EPFL & Uppsala University (V. Solans)

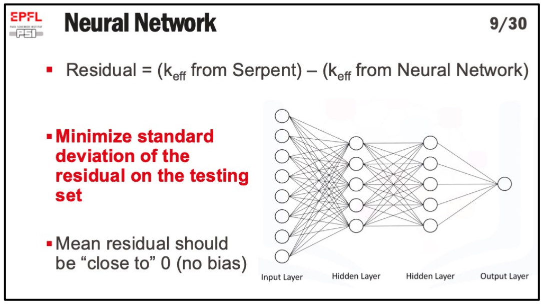
- Goal: optimize canister loading while minimizing criticality
- Why: Safety and economy of disposal canisters



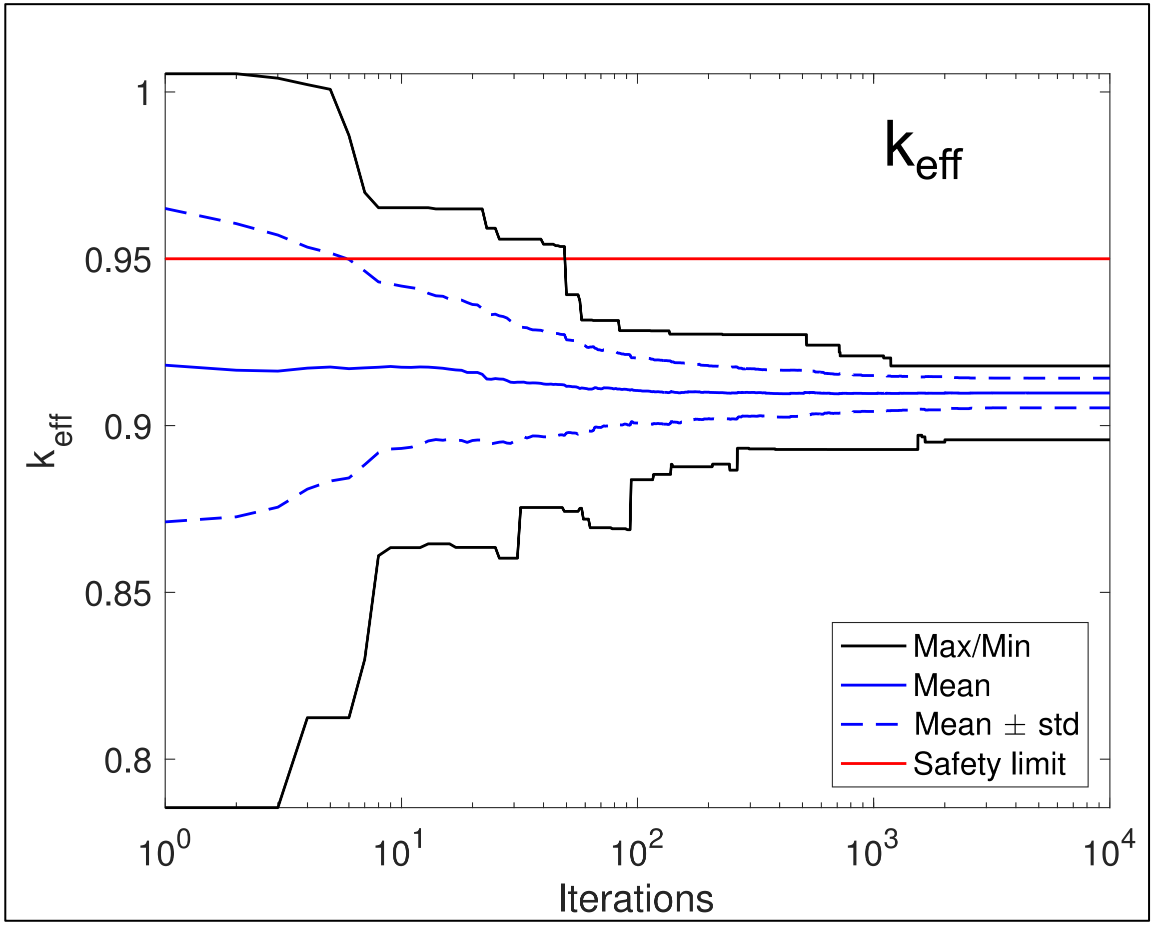


- Methods:
  – Considering orientations and assemblies: “enormous” filling possibilities
  – Replace Monte Carlo transport (very long) with a surrogate model
  – Realistic assembly filling
  – Train a neural network

ML for simulating canister criticality (2/2)



- Outcome:
  - – minimization of canister k_{eff},
  - – maximize homogeneity,
  - – and finally minimize canister number



ML for canister loading optimization (1/2)

- Work performed between PSI, Nagra, EPFL & Uppsala University (V. Solans)

- Goal: optimize canister loading while minimizing decay heat
- Why: Safety and economy of disposal canisters

N	Possible arrangements (3D/2D)
4	12 288 / 1 536
8	10^9 / 10^7
212	10^{476} / 10^{428}
12 000	10^{42738} / 10^{40029}

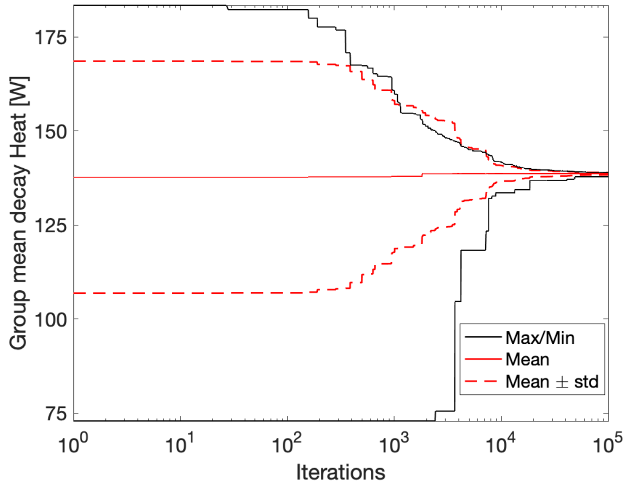
N: number of assemblies

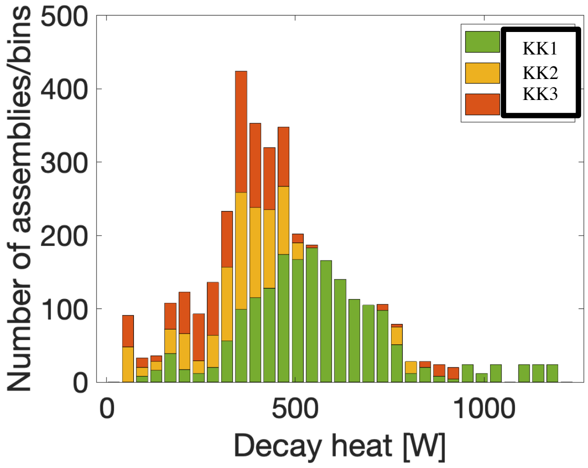
- Methods:
  – Considering 12 000 assemblies: “enormous” filling possibilities
  – Benchmark different codes
  – Use of genetic algorithm (GA)

ML for canister loading optimization (2/2)

- Outcome:
  – minimization of number of canister,
  – maximize decay heat homogeneity,
  – Benchmark different GA algorithms in different institutes (LAB-1 & LAB-2)

	Canisters			Duration
	Total	BWR	PWR	(days)
LAB-1	1873	867	1006	3375
LAB-2	1910	917	993	3486





ML for criticality uncertainty due to nuclear data (1/2)

- Work performed between PSI & ETH (A. Alba)

- Goal: obtain uncertainties on decay heat due to nuclear data
- Why: Safety and economy of disposal canisters

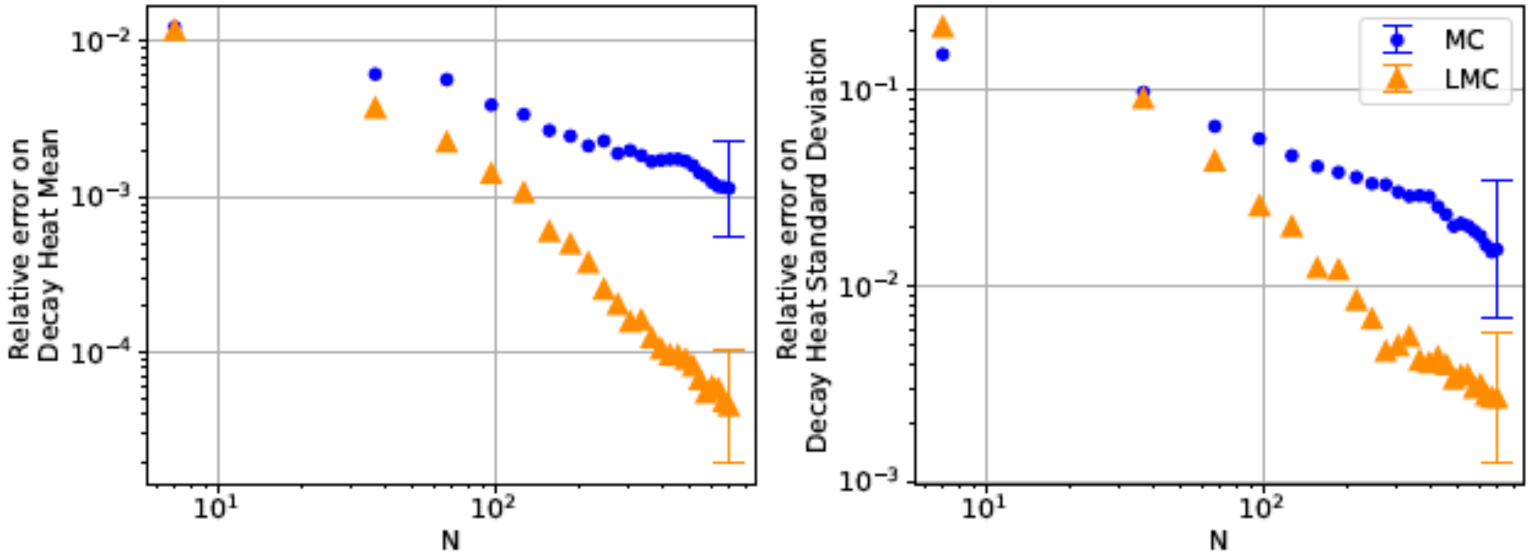
$$\texttt{CASMO5}: \underbrace{\begin{pmatrix}\text{Fresh fuel parameters}\\ \text{Irradiation history}\\ \text{Reactor parameters}\\ \text{Nuclear Data}\end{pmatrix}}_{\text{Uncertain Input}} \rightarrow \begin{pmatrix}\text{Decay Heat}\\ \text{Isotopic Content}\\ \text{etc...}\end{pmatrix}$$

$$\begin{array}{llll} f: & \mathbb{R}^{15\,557} & \rightarrow & \mathbb{R} \\ & (\textit{nuclear data}) & \mapsto & f\,(\textit{nuclear data}) = \text{Decay Heat} \end{array}$$

- Methods:
  - Realistic irradiation history
  - Deterministic calculations (CASMO5)
  - Use of Lasso Monte Carlo: Multi-level Monte Carlo + Lasso

ML for criticality uncertainty due to nuclear data (2/2)

- Outcome: Uncertainties obtained with a reduce calculation time by a factor 5



ML for for nuclear data and nuclear data uncertainties (1/2)

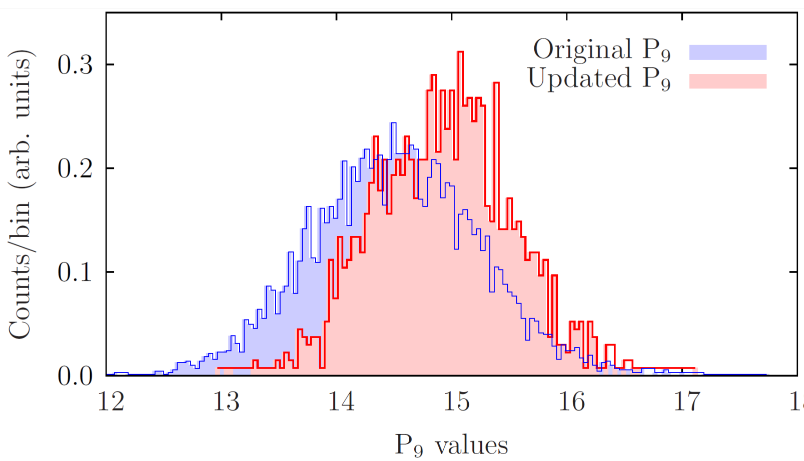
- Work performed between PSI, IAEA, CEA and Brussels Free University
- Goal: assess uncertainties on nuclear data (e.g. cross sections)

- Why: Nuclear data are used everywhere. They are not constants, they are uncertain

- Methods:
  - Neutron interaction modelling (TALYS)
  - Vary model parameters (TMC) and models
  - Use of Bayesian Monte Carlo

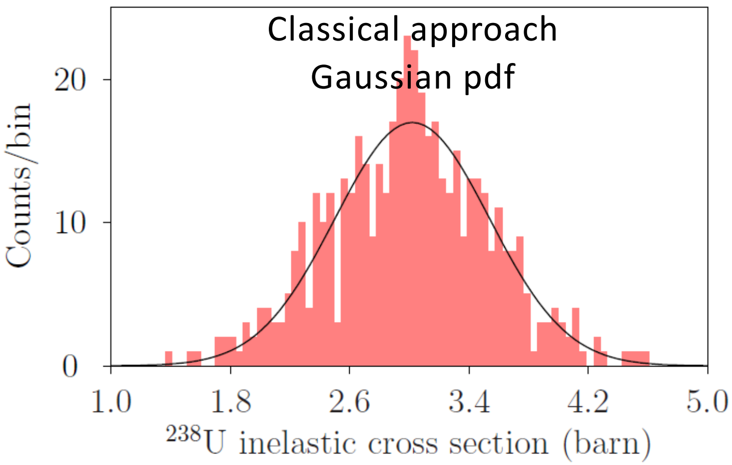
$$\chi_i^2 = \sum_{j=1}^{\mathrm{FY}} \left(\frac{C_j^{(i)} - E_j}{\Delta E_j} \right)^2$$

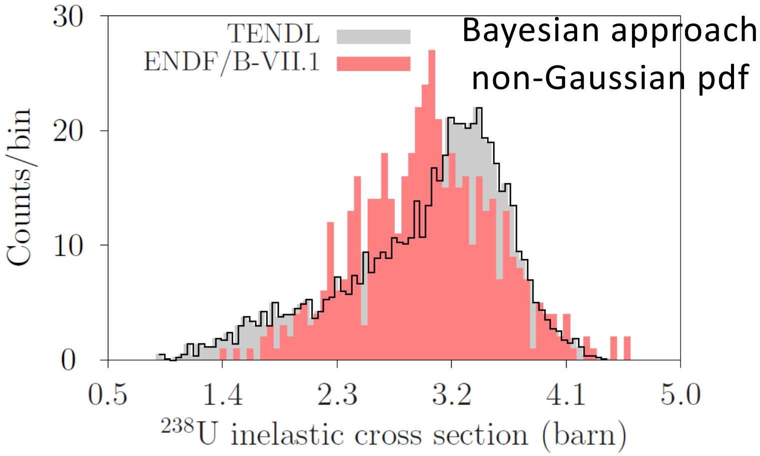
$$\omega_i = \frac{e^{-\chi_i^2/2}}{e^{-\chi_{\min}^2/2}}$$



ML for for nuclear data and nuclear data uncertainties (1/2)

- Outcome:
  - uncertainty (or pdf) based on mathematically-sound approach
  - No Gaussian distributions
  - Automated (ML) library (TENDL) which complement JEFF and ENDF/B





  - Extension to short-lived isotopes (for dosimetry, transients, decay heat, astrophysics…)

Conclusion

- “One of the things you learn as president is you’re always dealing with probabilities” (Obama)

  $\longrightarrow$ same for nuclear physicists
- Safer and more optimized nuclear environment: ML can help

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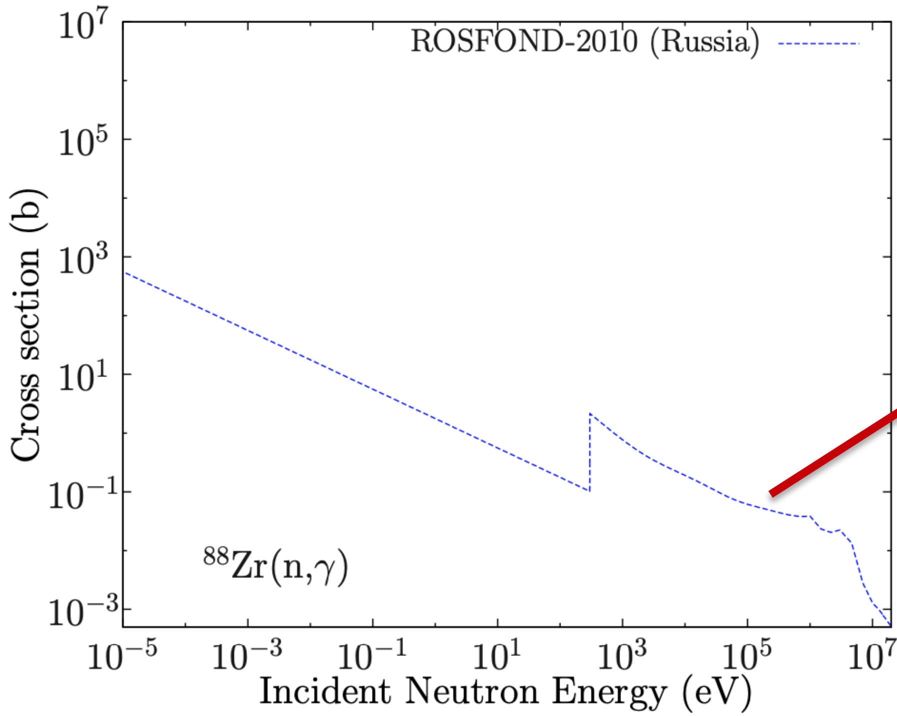

Human knowledge (simple assumption)

Conclusion

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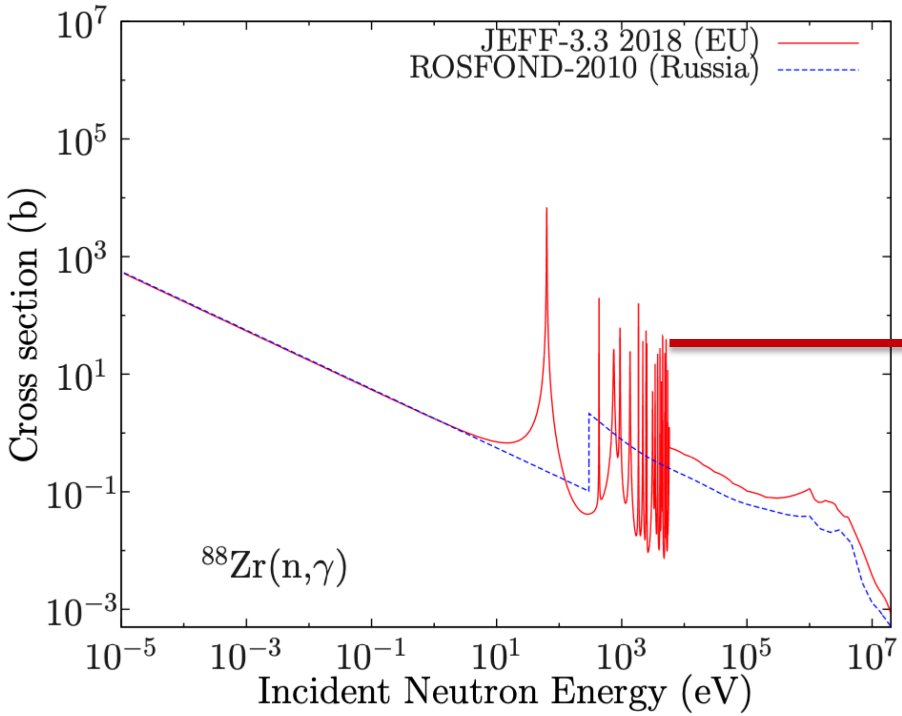

Human Learning
(simple assumption)
+
Machine Learning

Conclusion

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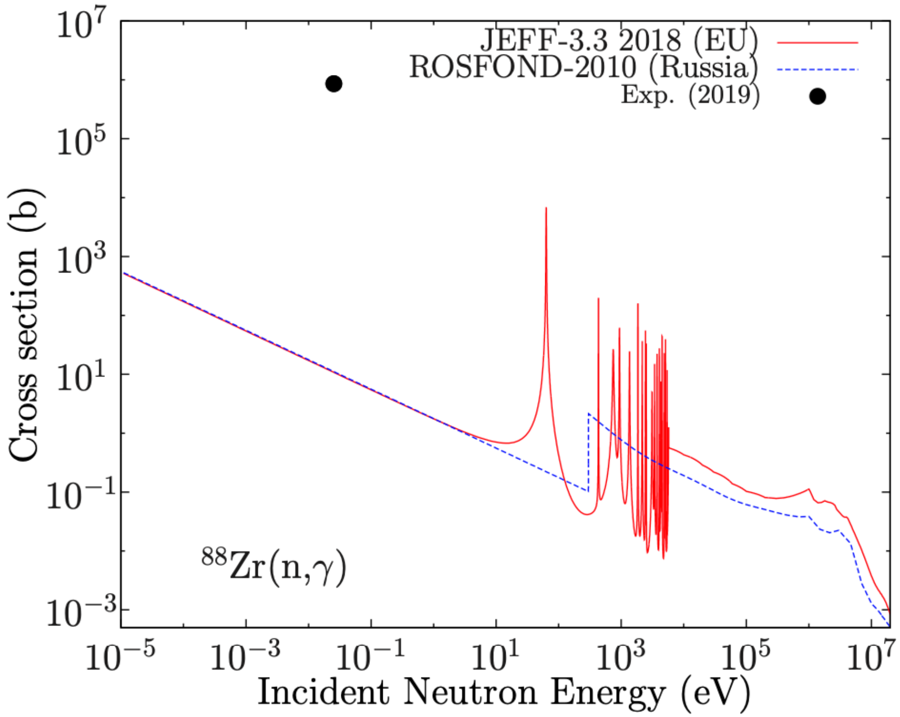

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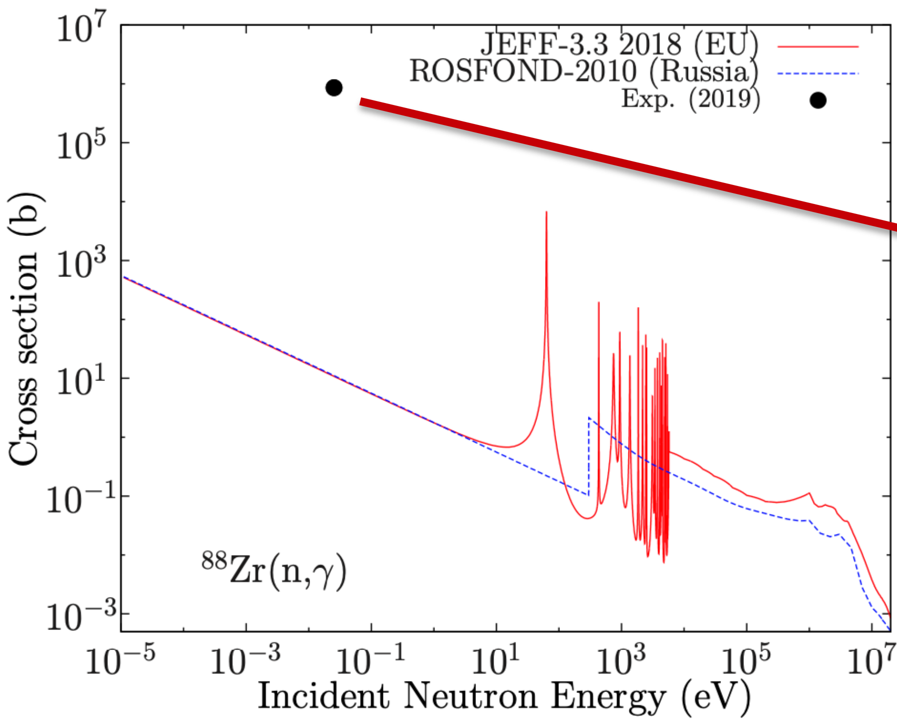

Human Learning
(simple assumption)
+
Machine Learning
+
Reality check
=
Improved knowledge

Publications

- Decay heat bias:
  [1] Validation of spent nuclear fuel decay heat calculations using Polaris, ORIGEN and CASMO5, https://www.sciencedirect.com/science/article/pii/S0306454921006344

- Canister criticality
  [2] Optimisation of used nuclear fuel canister loading using a neural network and genetic algorithm, https://link.springer.com/article/10.1007/s00521-021-06258-2

- Canister loading optimization
  [3] Loading optimization for Swiss used nuclear fuel assemblies into final disposal canisters, https://www.sciencedirect.com/science/article/pii/S0029549320303915

- Criticality uncertainty
  [4] Lasso Monte Carlo, a Novel Method for High Dimensional Uncertainty Quantification, A. Alba, http://arxiv.org/abs/2210.03634

- Nuclear data
  – Many (authors: A. Koning, D. Rochman, S. Goriely, E. Alhassan…)

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Wir schaffen Wissen – heute für morgen