Arnau Albà, PhD student :: Supervisors: A. Adelmann, D. Rochman

Surrogate Models for Uncertainties on Decay Heat and Nuclide Inventory in Nuclear Depletion Calculations

CEIDEN Workshop, May 27th 2021

Contact: arnau.albajacas@psi.ch

Spent Nuclear Fuel (SNF) remains a safety hazard up to a million years due to:

- Radiation

- Decay heat

- Criticality

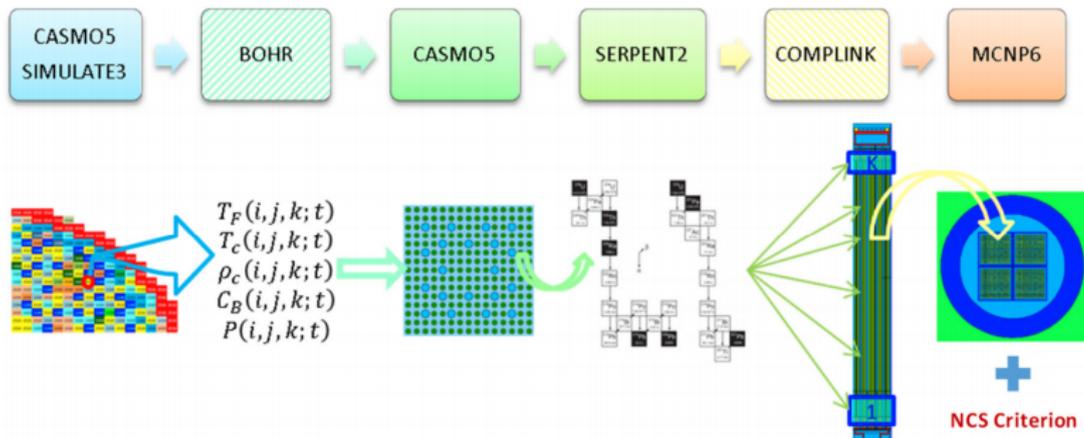It is thus crtical to **quantify the risks** to ensure safe handling, storage, and long-term disposal.

PAUL SCHERRER INSTITUT
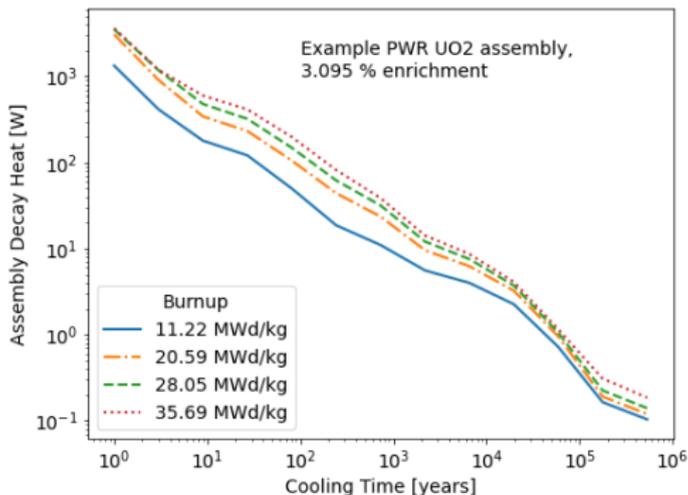
SNF is characterised by:

- Isotopic inventory $[cm^{-3}]$

- Decay heat $[W/t]$

- Criticality k_{eff}

Risk assessment is computationally expensive, and is carried out for:

- Between 12 and 13 thousand FAs expected in Switzerland

- Many time steps into the future

- Quantities of interest need to include **uncertainties**

Procedure developed at PSI [1] to compute quantities of interest:

$$T_F(i,j,k;t)$$
$$T_c(i,j,k;t)$$
$$\rho_c(i,j,k;t)$$
$$C_B(i,j,k;t)$$
$$P(i,j,k;t)$$

CASMO5 SIMULATE3 → BOHR → CASMO5 → SERPENT2 → COMPLINK → MCNP6

NCS Criterion

Nominal values of decay heat, isotopic content, and k_{eff} are not enough.

We require **Best Estimate Plus Uncertainty (BEPU)** to:

- better assess risks
- reduce exposure
- minimise costs

Uncertainty in deterministic codes? Yes! Through uncertainty propagation from input uncertainties in:

- FA characteristics (e.g. pin radius, enrichment)
- Operating history (e.g. burn-up, cooling cycles)
- Nuclear data
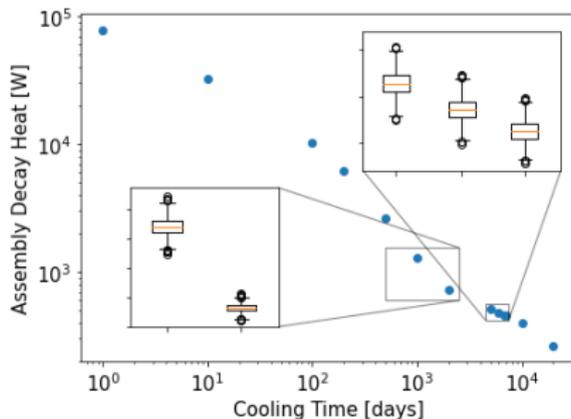
CASMO5 is a reactor lattice code, here used to simulate depletion in the reactor:

$$f : \underbrace{\begin{pmatrix} \text{Fresh fuel parameters} \\ \text{Irradiation history} \\ \text{Reactor parameters} \\ \text{Nuclear Data} \end{pmatrix}}_{\textit{Uncertain input parameters}} \rightarrow \begin{pmatrix} \text{DH w.r.t. cooling time} \\ \text{Isotopic inventory at discharge time} \end{pmatrix}$$

Propagation of Nuclear Data uncertainty to CASMO5 output:

(1) Sample Nuclear Data points from a covariance perturbation matrix [2]

(2) Perform hundreds of CASMO5 simulations with random sampling of the Nuclear Data

(3) Reconstruct histogram from output [3]

Decay heat 500 days after dicharge

$DH = (5.24 \pm 0.19) kW/t$
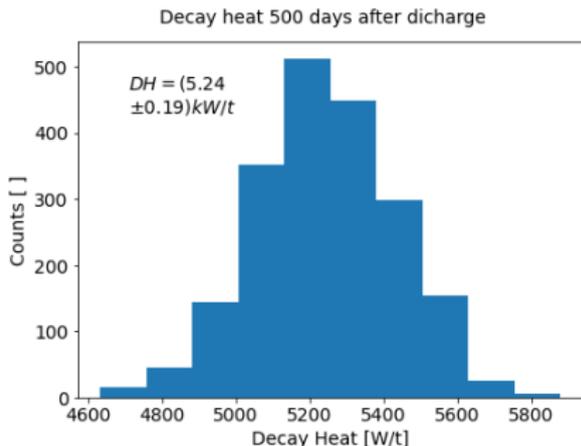
However,

- Stochastic sampling is computationally expensive

- Unfeasible for the over 12 thousand SNFs [4] expected in Switzerland (~ 900 years of computational time!)

- Impractical for optimisation tasks

Solution: train fast surrogate models that can replace CASMO5 calculations

Surrogate Model for Nuclear Data Uncertainties

Training data:

- CASMO5 simulations of one FA with a specific irradiation history with **different nuclear data** sampled from a covariance matrix [2].
- Training set is **deterministic** and without uncertainty.

Output:

- Decay heat $DH(t_j)$, at t_j timesteps during cooling time
- Isotope densities ρ_i

$$f' : \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{15557} \end{pmatrix}}_{\text{nuclear data}} \rightarrow \begin{pmatrix} \{DH(t_j)\}_{j=1,2,\ldots} \\ \{\rho_i\}_{i=1,2,\ldots} \end{pmatrix} \tag{1}$$

Trained model is used it for stochastic sampling in a fraction of the time

Challenges:

- Large input might require dimensionality reduction e.g. PCA [5], encoder-decoder [6]
- Only applicable to a specific FA. Transfer learning as an option.

Thank you to PSI and Swiss-Nuclear for co-sponsoring this project.

Thank you for your attention. Questions?

References

Alexander Vasiliev, Jose Herrero, Marco Pecchia, Dimitri Rochman, Hakim Ferroukhi, and Stefano Caruso.

Preliminary Assessment of Criticality Safety Constraints for Swiss Spent Nuclear Fuel Loading in Disposal Canisters.

Materials, 12(3):494, January 2019.

Number: 3 Publisher: Multidisciplinary Digital Publishing Institute.

O. Leray, H. Ferroukhi, M. Hursin, A. Vasiliev, and D. Rochman.

Methodology for core analyses with nuclear data uncertainty quantification and application to Swiss PWR operated cycles.

Annals of Nuclear Energy, 110:547–559, December 2017.

J.J. Herrero, D. Rochman, O. Leray, A. Vasiliev, M. Pecchia, H. Ferroukhi, and S. Caruso.

Impact of nuclear data uncertainty on safety calculations for spent nuclear fuel geological disposal.

EPJ Web of Conferences, 146:09028, 2017.

Stefano Caruso and Manuel Pantelias Garcés.

Spent Nuclear Fuel Management in Switzerland: Perspective for Final Disposal.

page 18, IAEA headquarters, Vienna, Austria, June 2015.

Tom Howley, Michael G. Madden, Marie-Louise O'Connell, and Alan G. Ryder.

The Effect of Principal Component Analysis on Machine Learning Accuracy with High Dimensional Spectral Data.

In Ann Macintosh, Richard Ellis, and Tony Allen, editors, *Applications and Innovations in Intelligent Systems XIII*, pages 209–222, London, 2006. Springer.

Alexander Scheinker, Frederick Cropp, Sergio Paiagua, and Daniele Filippetto.

Adaptive Latent Space Tuning for Non-Stationary Distributions.

arXiv:2105.03584 [physics, stat], May 2021.

arXiv: 2105.03584.