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Solving the Nuclear Decay Equation with Physics Informed Neural Networks

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PSI FoKo Poster Event
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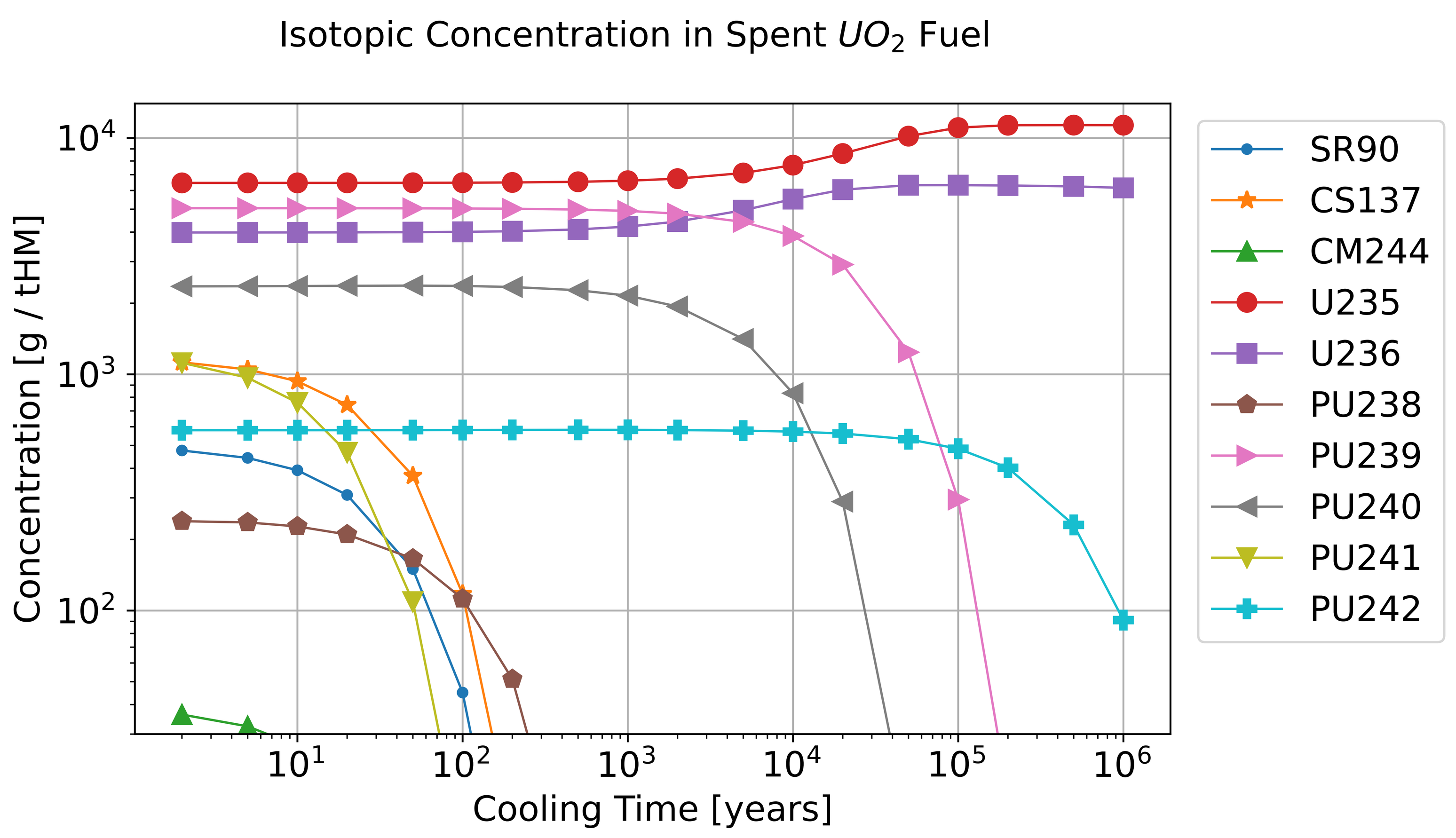
Background and Motivation



Burn-up calculation of Ringhals-2 PWR [1].

Radioactive decay and transmutation in nuclear fuel is governed by the **decay equation**:

$$\frac{d\boldsymbol{N}(t)}{dt} = A\boldsymbol{N}(t)\,, \quad \text{with} \quad \boldsymbol{N}(t=0) = \boldsymbol{N}_0\,,$$

where

- $\boldsymbol{N}(t) \in \mathbb{R}^n$ isotopic concentrations.
- $A \in \mathbb{R}^{n\times n}$ **stiff** matrix containing **uncertain nuclear data** (e.g. decay rates, cross-sections,...).
- Number of isotopes up to $n = 4000$.

Computationally demanding to solve [2] due to stiffness $||A|| = \frac{|\lambda_{max}|}{|\lambda_{min}|} \sim 10^{20}$.

Decay equation is used for

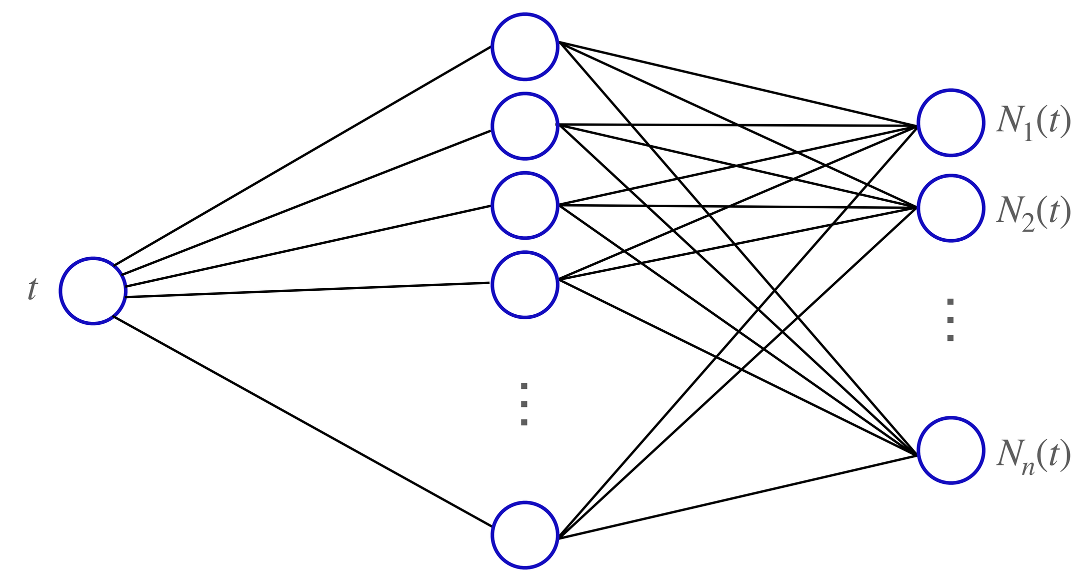
- Reactor core simulations
- Calculation of isotopic concentration in spent fuel
- Criticality safety of spent fuel repository [3]

Physics Informed Neural Networks (PINNs) [4]

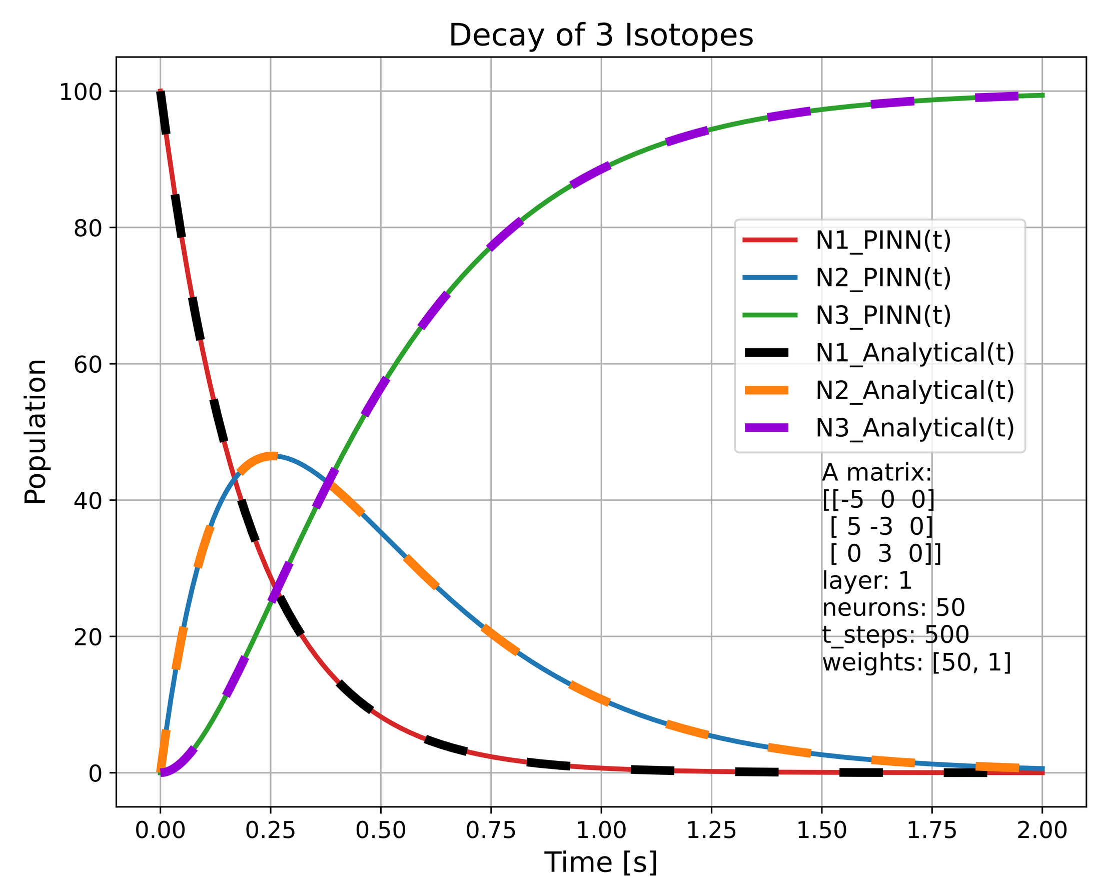
- Neural networks can approximate any continuous function (Universal Approximation Theorem)
- PINNs are neural networks, that take into account underlying physics described by differential equations
- PINN is used to solve the decay equation by approximating the solution $\boldsymbol{N}(t)$
- Loss function for training the neural network:

$$\mathcal{L} = w_{ODE}\left|\left|\sum_{i=1}^{T}\frac{d\tilde{\boldsymbol{N}}(t_i)}{dt} - A\tilde{\boldsymbol{N}}(t_i)\right|\right|_2^2 + w_{IC}||\tilde{\boldsymbol{N}}(t_0) - \boldsymbol{N}_0||_2^2\,,$$

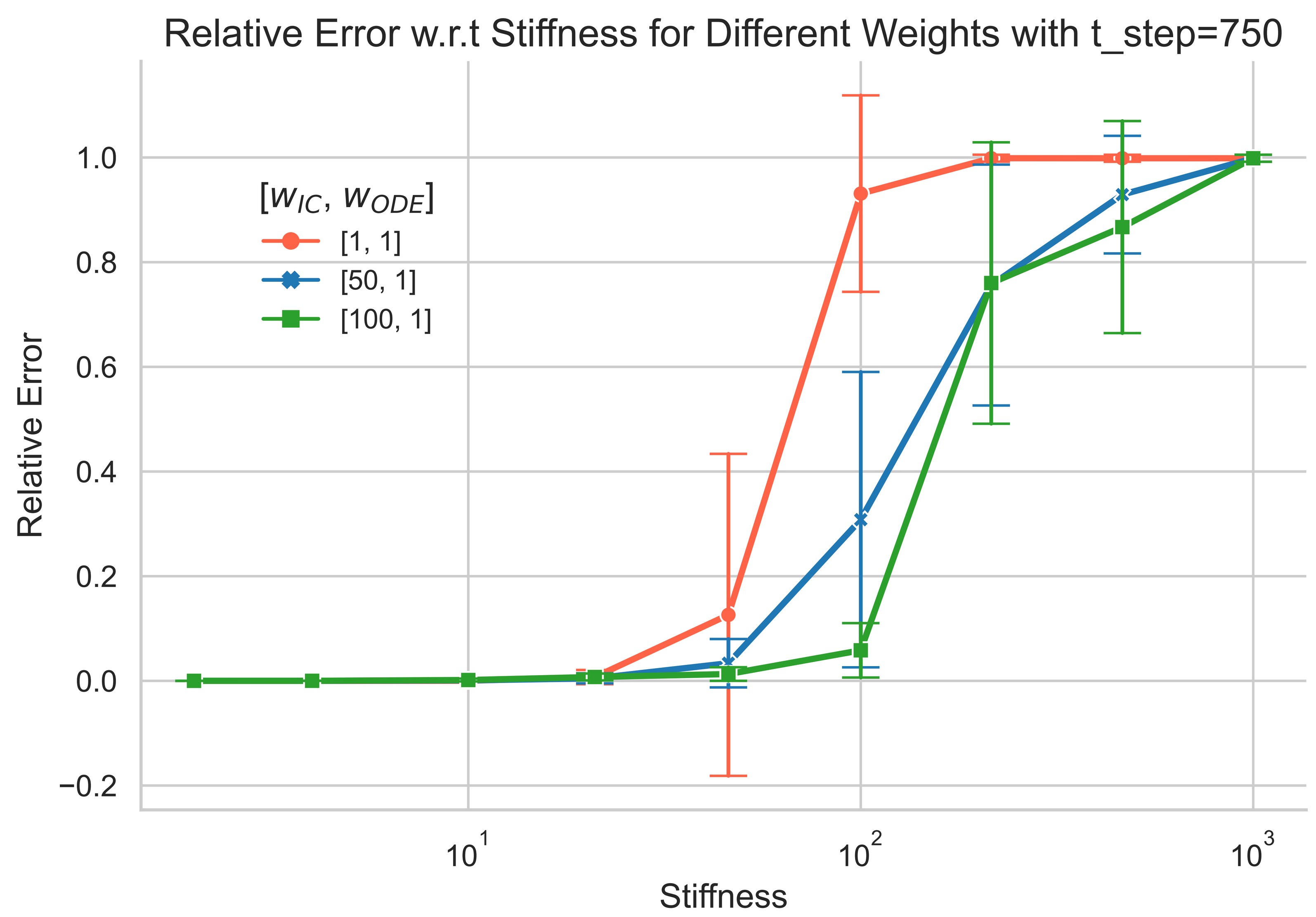
where $\tilde{\boldsymbol{N}}$ is a neural network, w_{ODE}, $w_{IC} \in \mathbb{R}$ are weights and T the time steps.



Preliminary Results: 3-Isotope Problem



Preliminary Results: Increasing Problem Stiffness



Ongoing and Future Work

- Adaptive weight w_{IC}
- Solve large systems, $A \in \mathbb{R}^{4000\times 4000}$
- Include transmutation matrix
- Compare to state-of-the-art methods
- Uncertainty quantification $A \pm \Delta A$ (e.g. with **transfer learning**)
- Publication

Conclusions

Correct choice of weights and number of time steps is important for solving stiff problems.

Acknowledgements

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[1] F. Sturek, L. Agrenius, and O. Osifo. Measurements of decay heat in spent nuclear fuel at the Swedish interim storage facility, Clab. Technical Report R-05-62, Svensk Kärnbränslehantering AB, December 2006.

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[3] Geologische Tiefenlager - ENSI, December 2020. `https://www.ensi.ch/de/dokumente/richtlinie-ensi-g03-deutsch/`.

[4] M. Raissi, P. Perdikaris, and G. E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378:686–707, February 2019.