Surrogate Modelling for Core Degradation in pressurized Water Reactors

Helmholtz AI Conference 2024 - Session S-05b - Applications of AI: AI in Science Experiments

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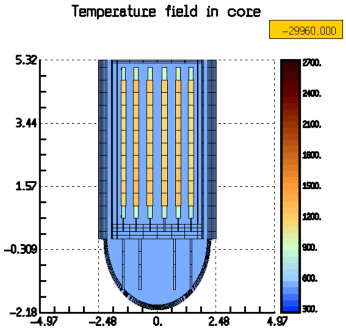
Motivation

Challenges of classical numerical simulation models:

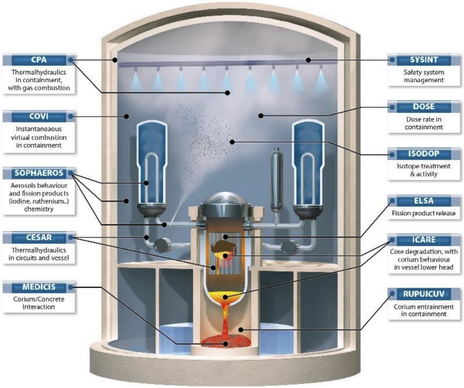
- Based on finite element and finite difference methods (FEM/FDM)
- Solving partial differential equation (PDE) systems may require high computing resources
- Can be challenging if resources are limited

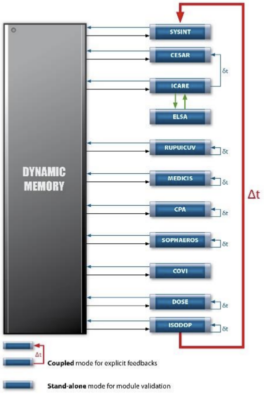
Example: ASTEC

- **A**ccident **S**ource **T**erm **E**valuation **C**ode
- Simulation code for severe accidents in nuclear facilities with **pressurized water reactors** (**PWRs**) used for operator training
- Modular numerical simulation code, based on FEM and FDM methods



ASTEC - Overview





- Modelling of physical processes (thermal-hydraulics, core degradation, fission product (FP) transport), ...
- Simulation in either **coupled** or **stand-alone** mode

ASTEC - Data flow

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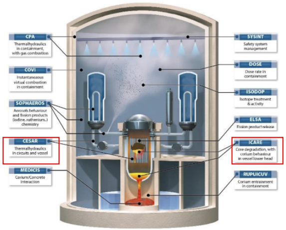
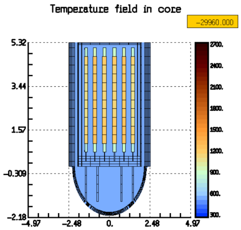
- (Thermodynamic) variables (core temperature, pressure, ...)
- Output data dimension is $(C \times M \times T)$ per variable $(C : \textit{channel}, M : \textit{meshes}, T : \textit{time})$

Input deck → ASTEC → Output

Input
geometry
physical model
scenario ...



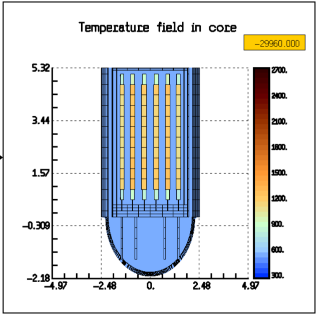


Problem: actual runtime of simulation exceeds simulated time
$\rightarrow$ Improvement of ASTEC needed for more useful operator training

Surrogate modelling - Problem setting

Input | Model | Output

Input deck parameters P_{In} → **ASTEC** (Modules) →



Surrogate modelling - Problem setting

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Input

Model

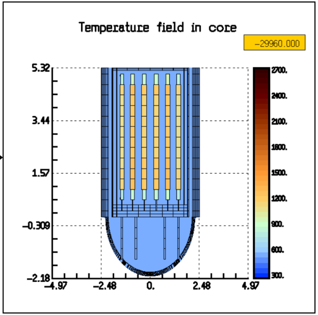
Output

$V(t) \in \mathbb{R}^{(C \times M \times T)}$

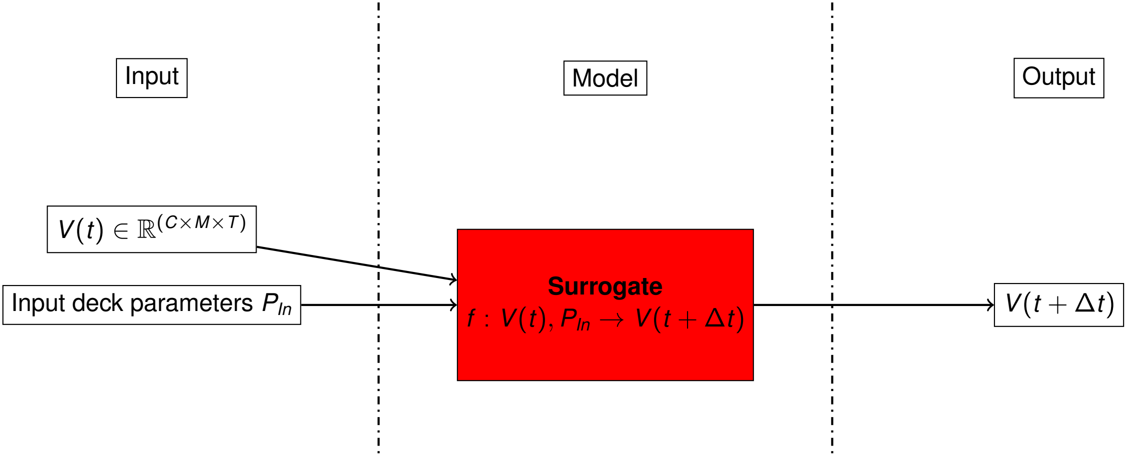
Input deck parameters P_{In}

Surrogate

$f : V(t), P_{In} \rightarrow V(t + \Delta t)$



Surrogate modelling - Problem setting



Surrogate modelling - Considerations and assumptions

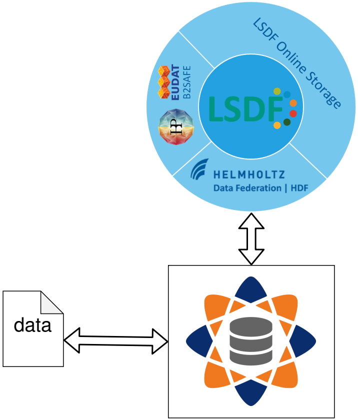
1. Data-driven surrogate models require a lot of data

$\rightarrow$ Build comprehensive training database

ASSAS Database for Training Data

Training database

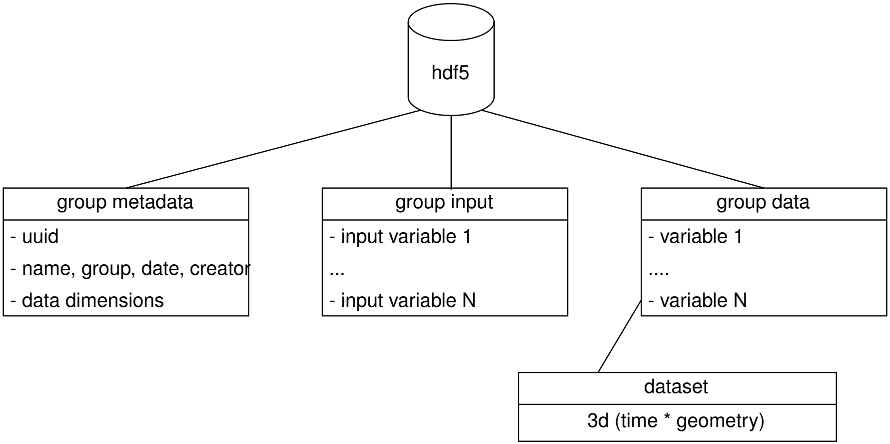
- Pre-processing of training data
- Reproducibility ⇒ **FAIR** principles [4]
- Use of Large Scale Data Facility (**LSDF**) to handle large amounts of data
  - **F**indable: additional NoSql database to handles uuids for each dataset
  - **A**ccessible: LSDF ensures storage for training data on long-term scope
  - **I**nteroperable: use of common standards (hdf5, netCDF)
  - **R**eusable: general and meaningful meta data



ASSAS Data Hub:

- Store and handle training data on **LSDF**
- Available on
  `https://github.com/Helmholtz-AI-Energy/assas-data-hub`
- Generic template for other applications (in progress)

Hdf5 Data Structure



$$3d(time * geometry) \rightarrow (C \times M \times T)$$

Surrogate modelling - Considerations and assumptions

1. **Data-driven surrogate models require a lot of data**

   → Build comprehensive training database

2. **Choice of Model**

   - **Long Short-Term Memory Network** (**LSTM**) for sequenced time series data

LSTM Reference Model

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- Training window $\Rightarrow$ number of previous samples as input
- Prediction window $\Rightarrow$ number of samples to predict
- $(C \times M)$ input features of LSTM for each ASTEC variable
- Train and validation split of 0.8

Training on exemplary dataset

- Variables=5, channels=4, meshes=15, samples=589
- Applied resampling to 710 samples (frequency $f = \frac{1}{100s}$)
- $(V \times C \times M) = 300$ input features of LSTM per ASTEC scenario

$[Sequence] \Rightarrow Target$

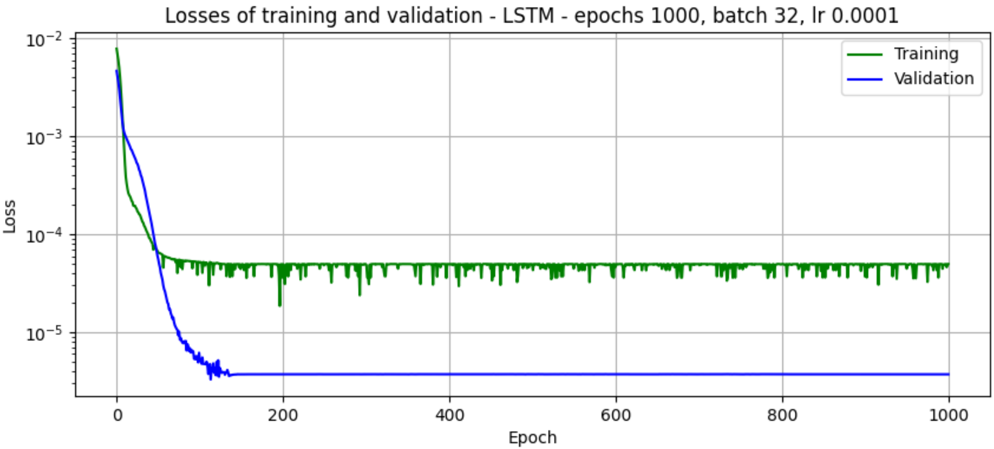
$[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]$

Sequencing $\Rightarrow$

$[0, 1, 2, 3] \Rightarrow [4, 5]$

$[1, 2, 3, 4] \Rightarrow [5, 6]$ ...

LSTM Reference Model



Surrogate modelling - Considerations and assumptions

1. **Data-driven surrogate models require a lot of data**

$\rightarrow$ Build comprehensive training database

2. **Choice of Model**

- **Long Short-Term Memory Network** (**LSTM**) for sequenced time series data

- Modelling of a simulation described by PDEs

$\rightarrow$ **Fourier Neural Operator** (**FNO**)
  - Fast and mesh-invariant solution for PDE systems [1]

- **Adaptive Fourier Neural Operators (AFNO)** [2]
  - Combination of FNO and vision transformer (ViT) technique
  - **Fourier Forecasting Neural Network** (**FourCastNet**) as similar approach in the field of **numerical weather prediction** [3]

Fourier Neural Operator

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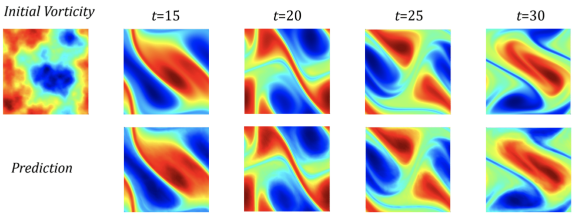
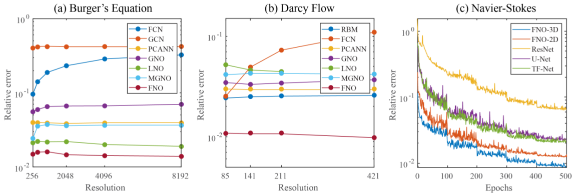
- Data-driven approach to solve time-dependent PDE systems (Navier-Stokes, Darcy flow, ...)
- FNO show the best performance against other models (Ideal point-wise Feedforward Neural Network (FNN), Fully Convolution Network (FCN) [1]

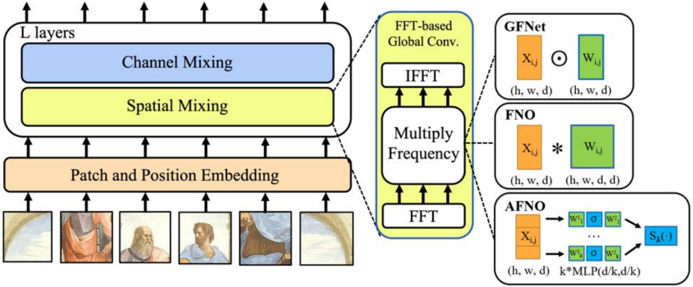




Adaptive Fourier Neural Operator

$$v_{t+1}(x) := \sigma \cdot (W \cdot v_t(x) + (K(a;\phi))(x))$$

- Mapping between function spaces
- Iterative updates $v_t(x) \rightarrow v_{t+1}(x)$
- Learning of matrix W in Fourier space
- Performs block-wise channel mixing of weights



AFNO as a Surrogate Model for ASTEC

- Data of one ASTEC variable $\Rightarrow$ AFNO channel
- Autoregressive training to predict next time step
- Train and validation split of 0.8
- Accumulate the data for each scenario

$[Sequence] \Rightarrow Target$

$[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]$

Sequencing $\Rightarrow$

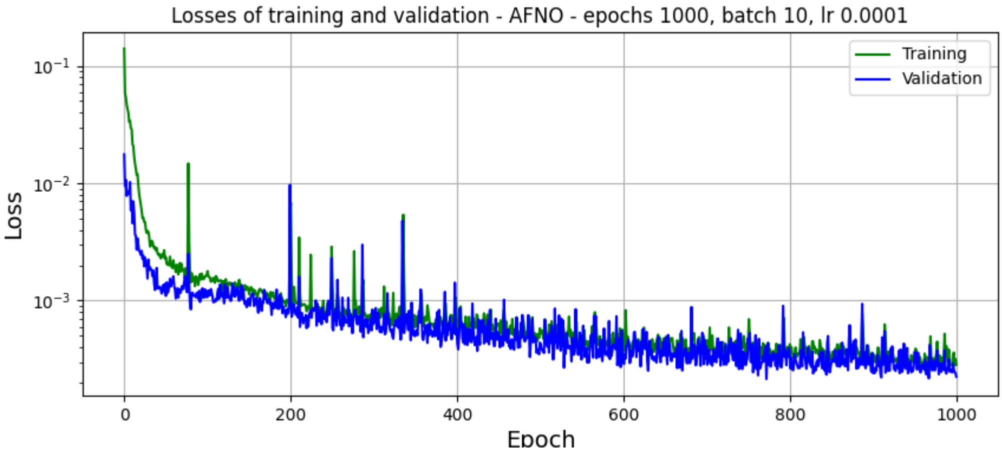
$[0, 1, 2, 3] \Rightarrow [4]$

$[1, 2, 3, 4] \Rightarrow [5]$

Training on exemplary dataset

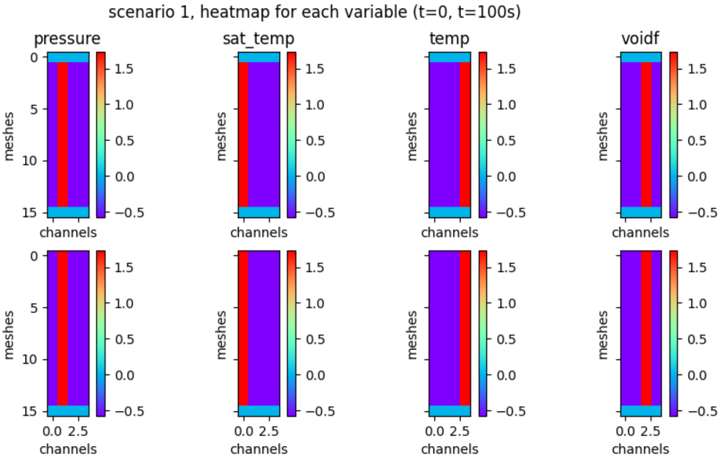
- Variables=5, channels=4, meshes=15, samples=589
- No resampling applied

AFNO Model - Exemplary Training



AFNO Model - First Results

Ground truth for $t = 0s$ and $t = 100s$



Outlook and Future Work

Next steps:

1. Train both models on simulation data for Station Blackout (**SBO**) and Loss of Coolant Accident (**LOCA**) ASTEC scenarios with each 100 different cases
2. Consider other operator learning techniques
3. Train on other ASTEC scenarios

References

[1] Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart **and** Anima Anandkumar. *Fourier Neural Operator for Parametric Partial Differential Equations*. 2021. arXiv: `2010.08895 [cs.LG]`.

[2] John Guibas, Morteza Mardani, Zongyi Li, Andrew Tao, Anima Anandkumar **and** Bryan Catanzaro. *Adaptive Fourier Neural Operators: Efficient Token Mixers for Transformers*. 2022. arXiv: `2111.13587 [cs.CV]`.

[3] Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, Zongyi Li, Kamyar Azizzadenesheli, Pedram Hassanzadeh, Karthik Kashinath **and** Animashree Anandkumar. *FourCastNet: A Global Data-driven High-resolution Weather Model using Adaptive Fourier Neural Operators*. 2022. arXiv: `2202.11214 [physics.ao-ph]`.

[4] Mark Wilkinson, Michel Dumontier, IJsbrand Jan Aalbersberg, Gaby Appleton, Myles Axton, Arie Baak, Niklas Blomberg, Jan-Willem Boiten, Luiz Olavo Bonino da Silva Santos, Philip Bourne, Jildau Bouwman, Anthony Brookes, Tim Clark, Merce Crosas, Ingrid Dillo, Olivier Dumon, Scott Edmunds, Chris Evelo, Richard Finkers **and** Barend Mons. *The FAIR Guiding Principles for scientific data management and stewardship*. **march** 2016. DOI: `10.1038/sdata.2016.18`.