

Beyond Numerical Solvers: AI-Driven Surrogate Models for Reactor Simulation Codes at UNIST CORE Laboratory

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1. Introduction of AI-Driven Models at UNIST CORE

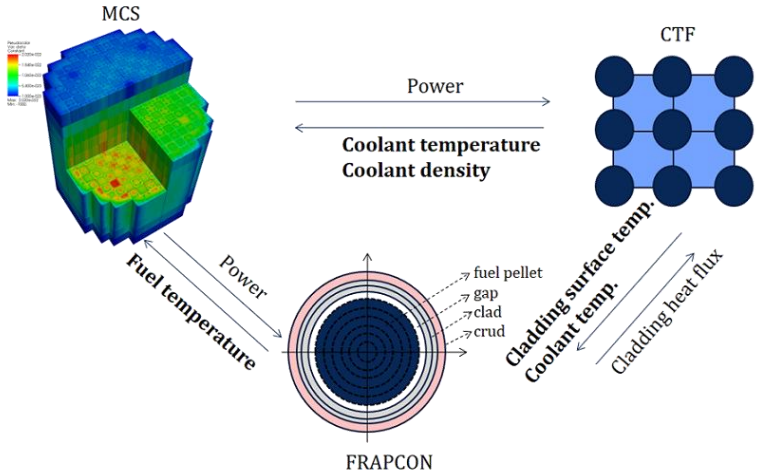
Reactor simulation software at UNIST CORE

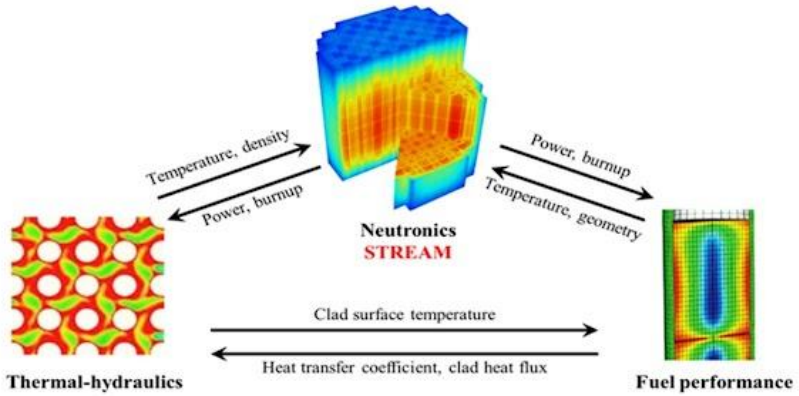
- **UNIST CORE Lab is specialized in developing reactor simulation software for high-fidelity steady-state and transient analysis.**

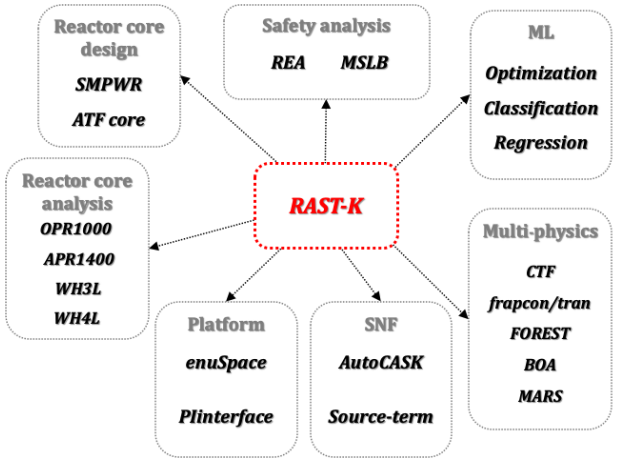
MCS is a general-purpose **Monte-Carlo** code with TH feedback and capability to run steady state-depletion and time-dependent problems.

STREAM is a **deterministic neutron transport** code for high-fidelity steady-state depletion and transient reactor analysis based on **MOC** solver.

RAST-K is a **nodal diffusion** code with fast solving schemes for thermal and fast reactors.







AI applications at UNIST CORE

- **UNIST CORE develop a plethora of AI models covering a variety of use-cases and tasks:**
  - **Practical models for grid power supply and demand forecast.**
    - Multivariate energy sources with account for weather and lunar calendar.
  - **AI surrogate models of STREAM and RAST-K.**
    - XSNET – replacement of STREAM.
    - RAST-K QS surrogate model for load follow simulation.
    - Barcode CNN model.
    - RAST-K surrogate model for forecasting global and local parameters for loading pattern optimization.
    - Visual transformer-based RAST-K surrogates.
  - **Loading pattern optimization.**
    - Simulated annealing, genetic algorithms, reinforced learning.
  - **Time-series forecasts and operator assistance tools.**
    - Anomaly detection, control rod adjustment, time-dependent core status report, etc.
    - Load follow strategy optimization.

Key literature references

[1] A.B.A. Ferreira et al., "Power substation load forecasting using interpretable transformer-based temporal fusion neural networks", ***Electric Power Systems Research*** 238 (2025) 111169

[2] **S. Dzianisau**, H. Kim, C. Kong, D. Yun, D. Lee, "Development of Barcode Model for Prediction of PWR Core Design Parameters Using Convolutional Neural Network," Transactions of the Korean Nuclear Society Autumn Meeting, Goyang, Republic of Korea, October 24-25, 2019.

[3] S. Jeong and H. C. Lee, Effect of Surrogate Model on Screening-based Simulated Annealing for OPR-1000 Loading Pattern Optimization, Transactions of the Korean Nuclear Society Spring Meeting 2026, Jeju, Korea, May 7 – 8, 2026.

[4] **S. Dzianisau**, K. Saeju, H. C. Lee, D. Lee, "Development of an Artificial Neural Network Model for Generating Macroscopic Cross-Sections for RAST-AI," **Ann. Nucl. Energy**, 186:109777, 2023.

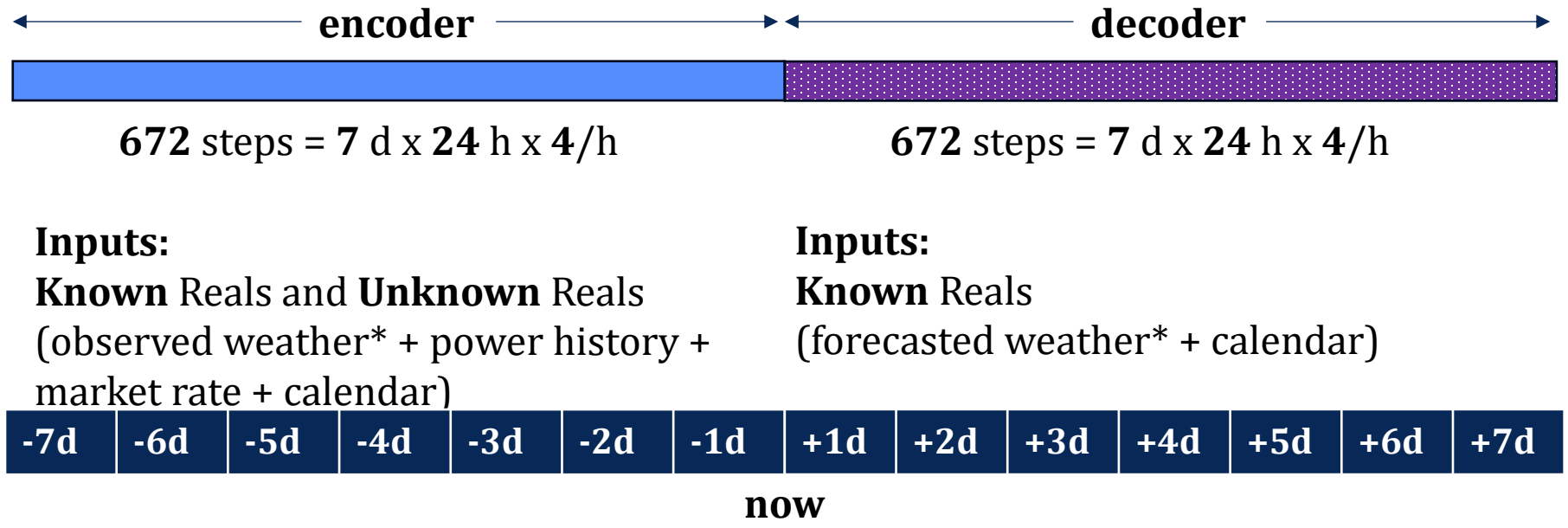
[5] **S. Dzianisau**, D. Lee, "Application of Artificial Neural Network for Assembly Homogenized Equivalence Parameter Generation," **Prog. Nucl. Energy**, 2024.

[6] H. Yu, H. Hong and J. Yoon, "Analysis of the APR1400 Benchmark Using High-Fidelity Pin-Wise Core Calculation Codes", **Energies**, 17, 3498, 2024

2. Time series forecasts

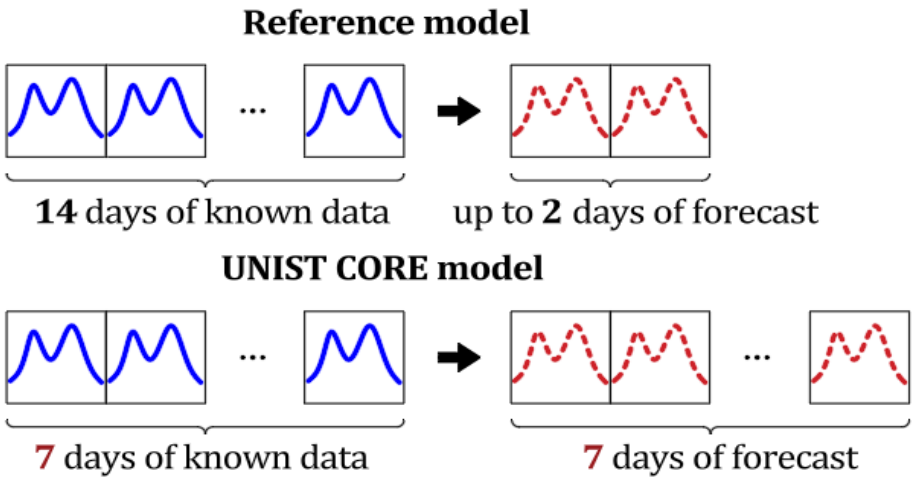
Power supply and demand forecast

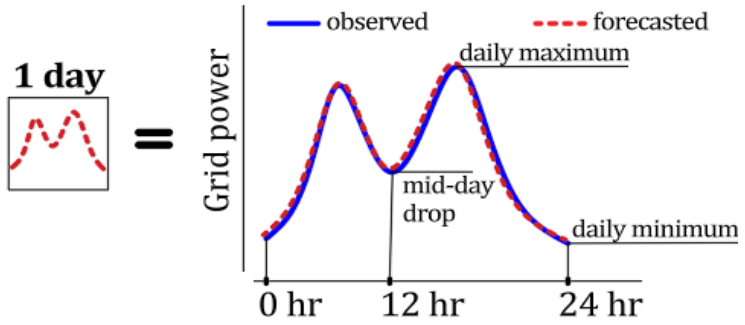
- **Temporal Fusion Transformer (TFT)[1] model for multivariate time series forecast with 15-minute time-step.**



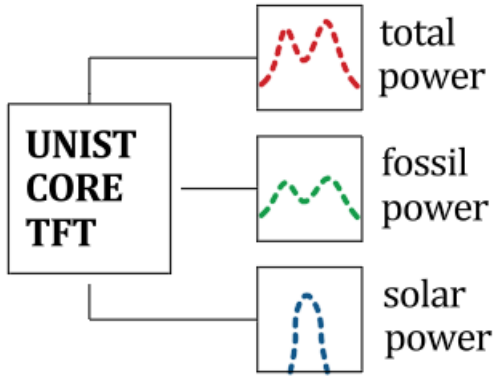
Power supply and demand forecast

▪ UNIST CORE TFT model – results:





Multivariate output



	Reference model [1]		UNIST CORE model	
Metric	**MAPE,%**	**MAE, MW**	**MAPE,%**	**MAE, MW**
Mean	-	-	2.911	1,887*
Best	**1.470**	**3,522**	**1.311**	**784**
Worst	-	-	5.867	4,017

Median window mean percent error (MAPE)

UNIST CORE TFT	total power - 2.46% fossil power - 2.65% solar power - 0.33%

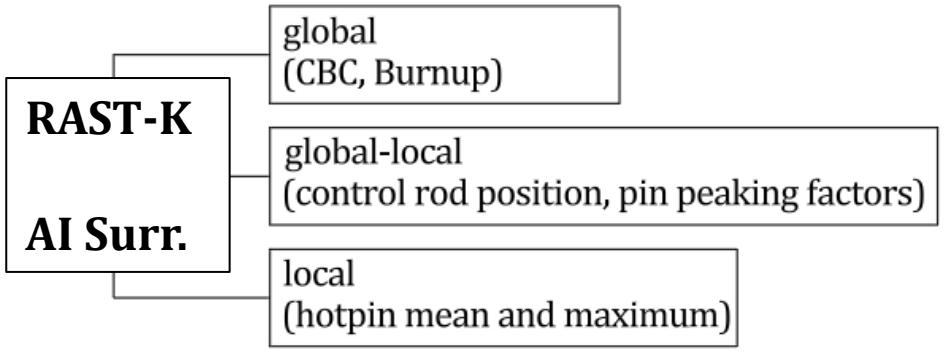
Maximum window mean percent error (MAPE)

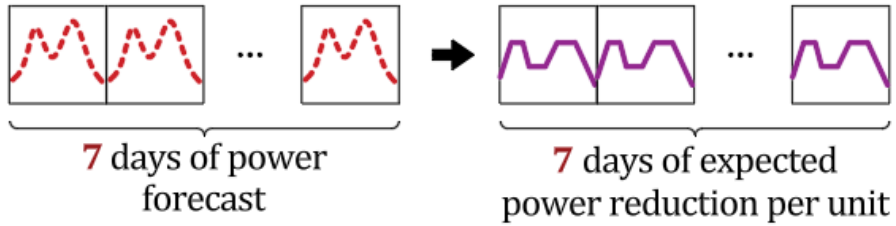
UNIST CORE TFT	total power - 5.13% fossil power - 5.87% solar power - 0.53%

* 7-day long year-long average with 15-minute time step and overlapping days across the entire year.

RAST-K surrogate for load follow operation

- **TFT model as a RAST-K surrogate for time-series multivariate local parameter forecast based on the TFT model for power supply and demand.**





Inputs	Outputs
7-day history: power, pin peaking factors, CBC, hot pin, control rod movements, burnup, N_I35, N_Sm49, N_Xe35, D_1, D_2, a_1, a_2 **7-day known (forecast):** power ('from Model_A')	**7-day forecast:** pin peaking factors, CBC, hot pin, control rod movements

RAST-K surrogate for load follow operation

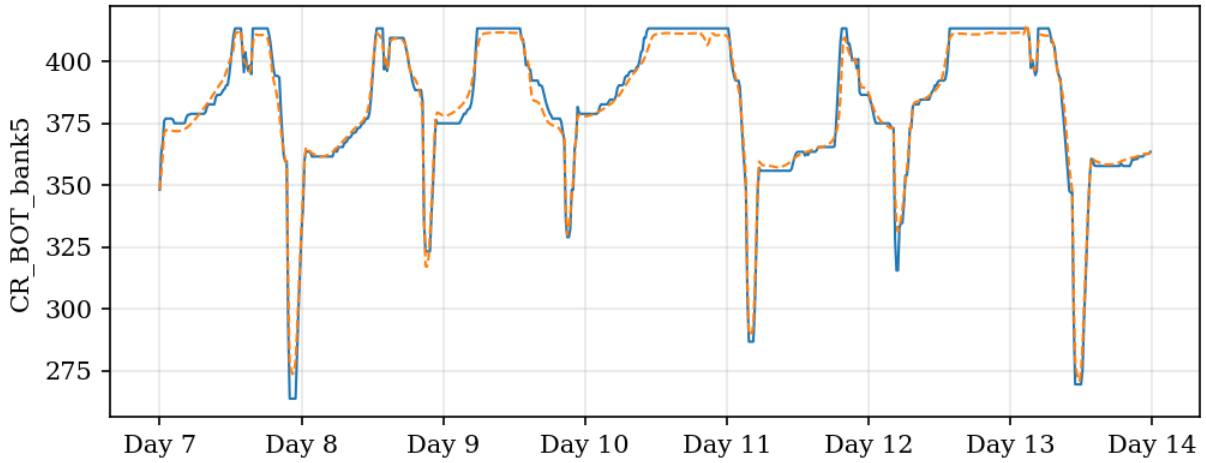
- **UNIST CORE RAST-K TFT surrogate results:**

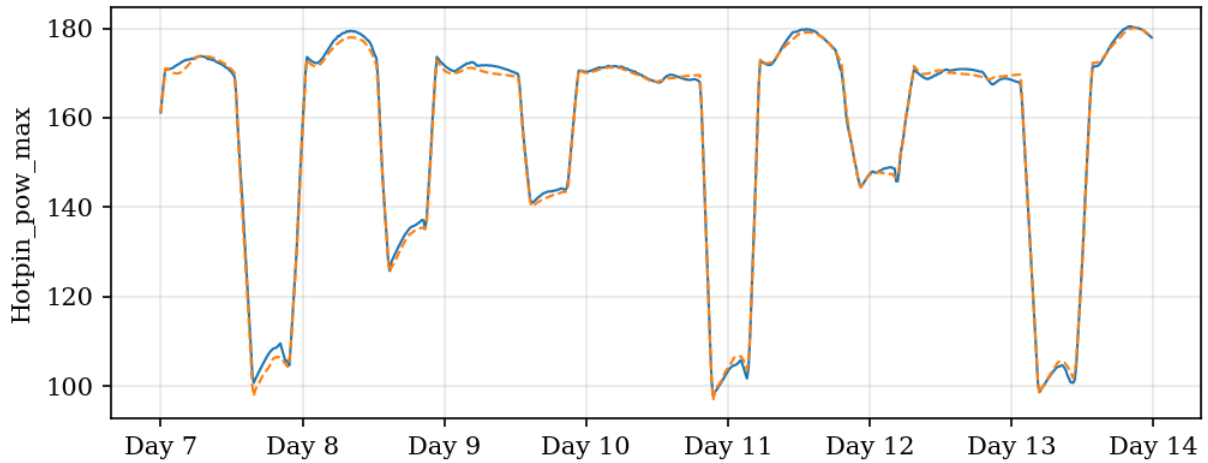
Metric	MAPE	MAE
CBC	1.02 %	8.29 ppm
Hotpin_pow_max	1.21 %	1.865 W/cm^3

Metric	MAPE	MAE
F_q	1.24 %	0.0230
F_{dH}	0.33 %	0.0047

Metric	MAPE	MAE
CR_BOT_bank 5	1.06 %	3.58 cm
CR_BOT_bank 8	0.48 %	1.76 cm

Metric	MAPE	MAE
F_z	1.24 %	0.0155
F_{xy}	0.34 %	0.0051



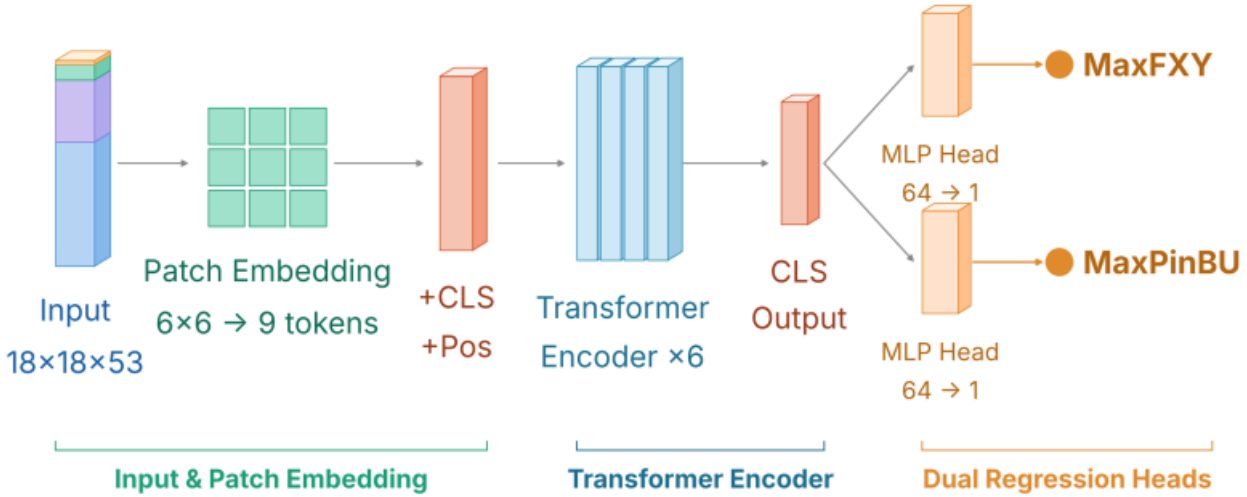


3. Loading pattern optimizations

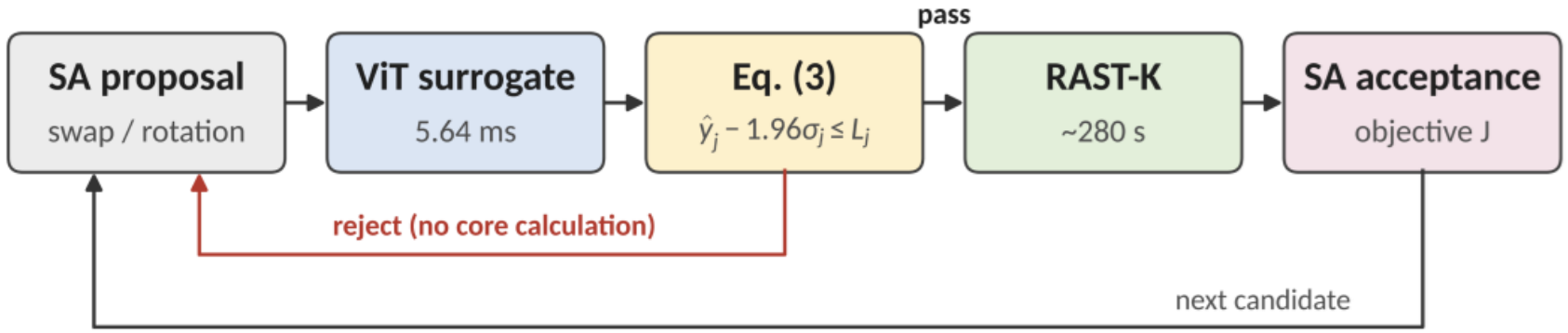
ANN model selection for SA algorithm

- **Two model types were considered: CNN (our previous Barcode CNN work)[2] and Vision Transformer (ViT)[3].**
  - **Two regression heads predict MaxFxy and MaxPinBU;**
  - **894,600 samples were split into 740,000 / 100,000 / 54,600 samples.**

Metric	CNN	ViT
MaxFXY MRE (%)	1.81	0.63
MaxPinBU MRE (%)	0.45	0.17
MaxFXY MAE	0.0374	0.0131
MaxPinBU MAE (GWd/MTU)	0.2848	0.1053
Parameters	43.0 M	3.7 M

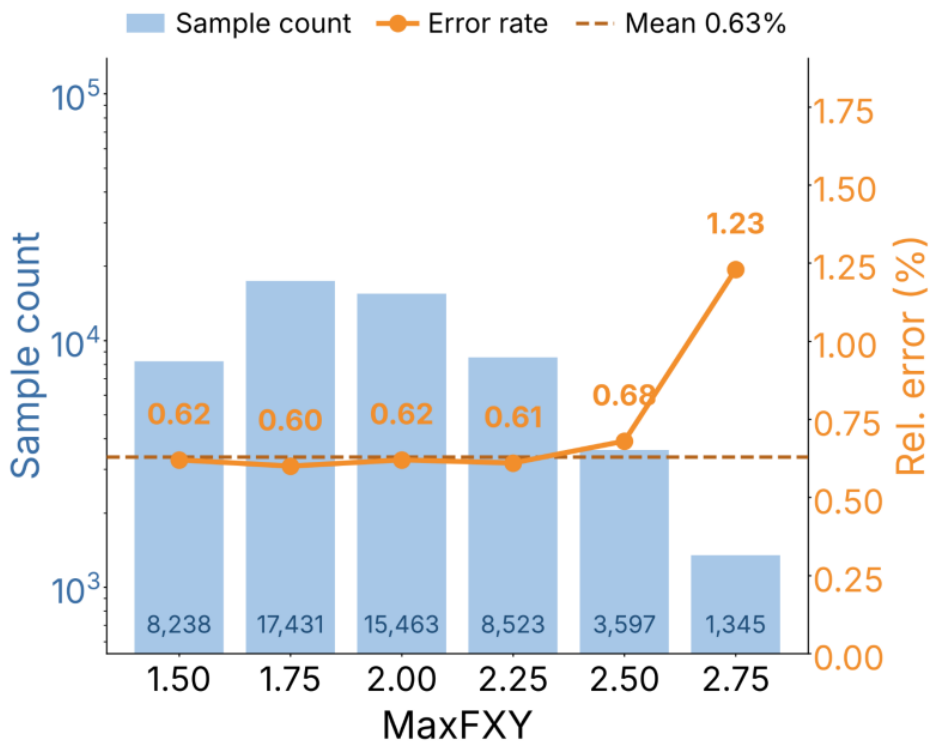


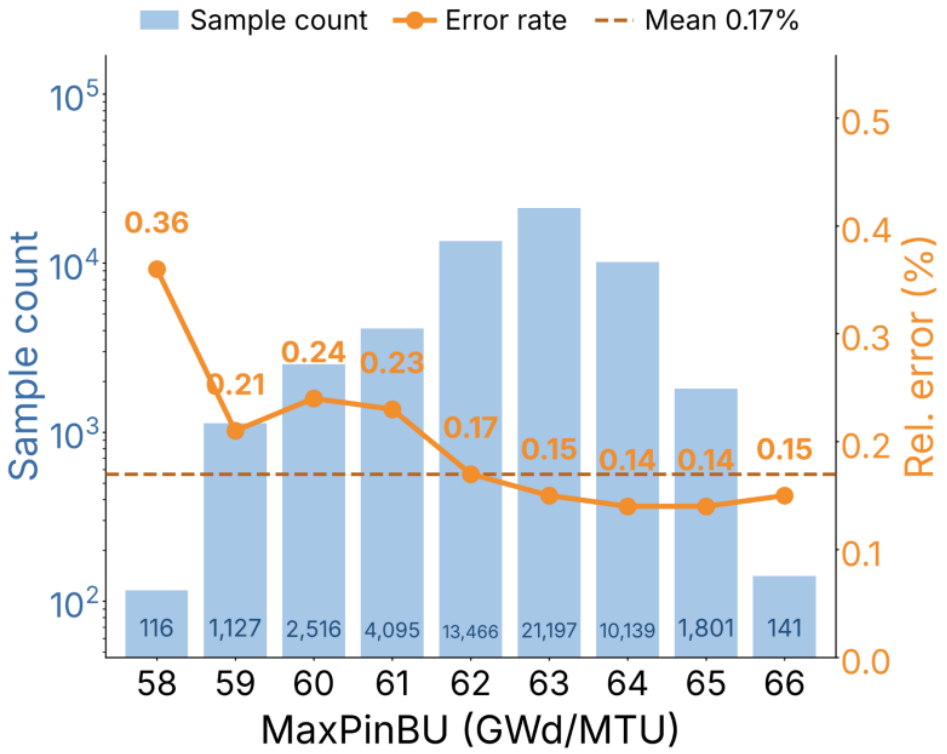
LP optimization algorithm



ViT performance for the target parameters

- **Performance per bracket is reported below.**
  - **MaxFXY error stays within 0.60–0.68% up to 2.75 and rises to 1.23% in the 2.75–3.00 range (1,345 samples).**
  - **MaxPinBU error is highest (0.36%) in the 58–59 GWd/MTU range (116 samples) and below 0.25% elsewhere.**
  - **The MaxFXY screening limit of 1.8 lies in a well-populated range with about 0.6% error**



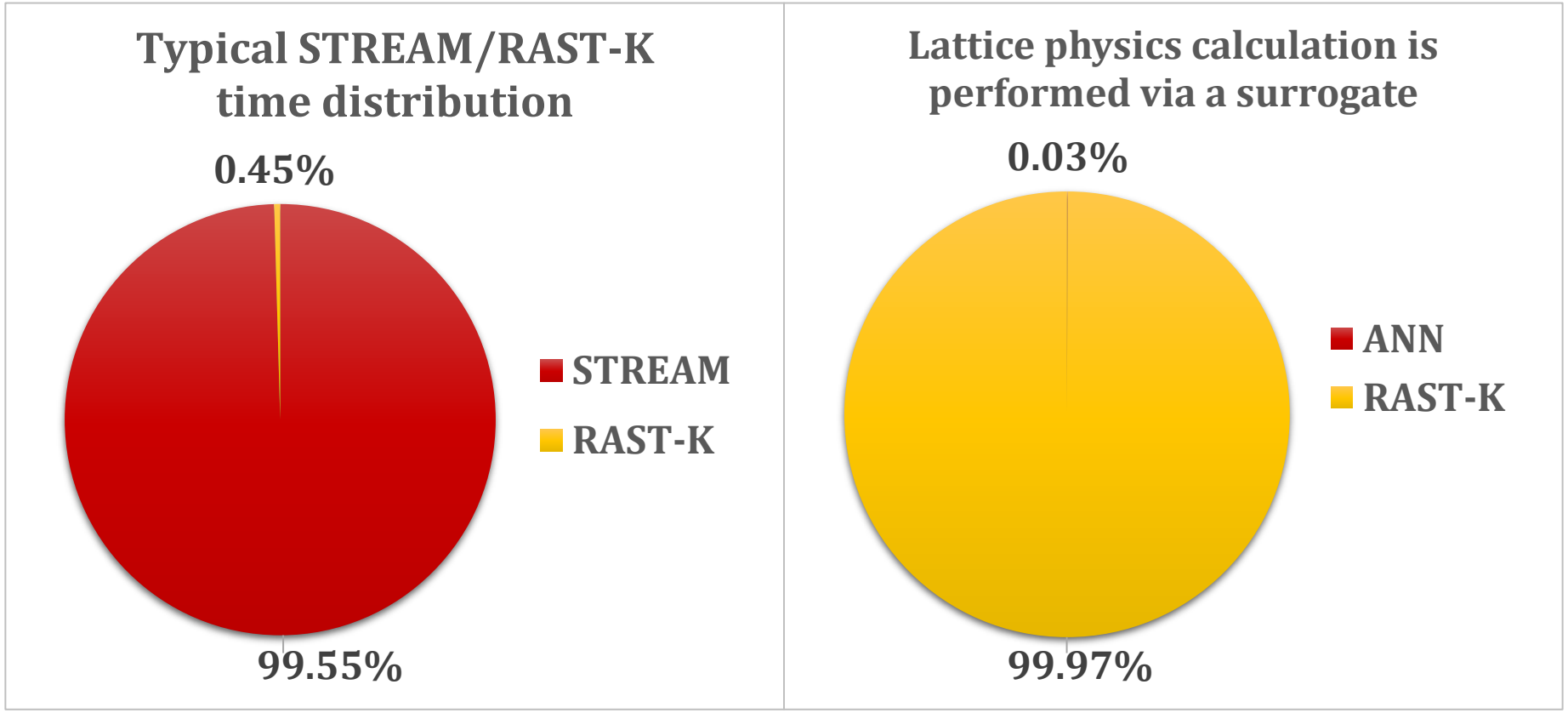


4. AI Surrogates of STREAM

Our motivation

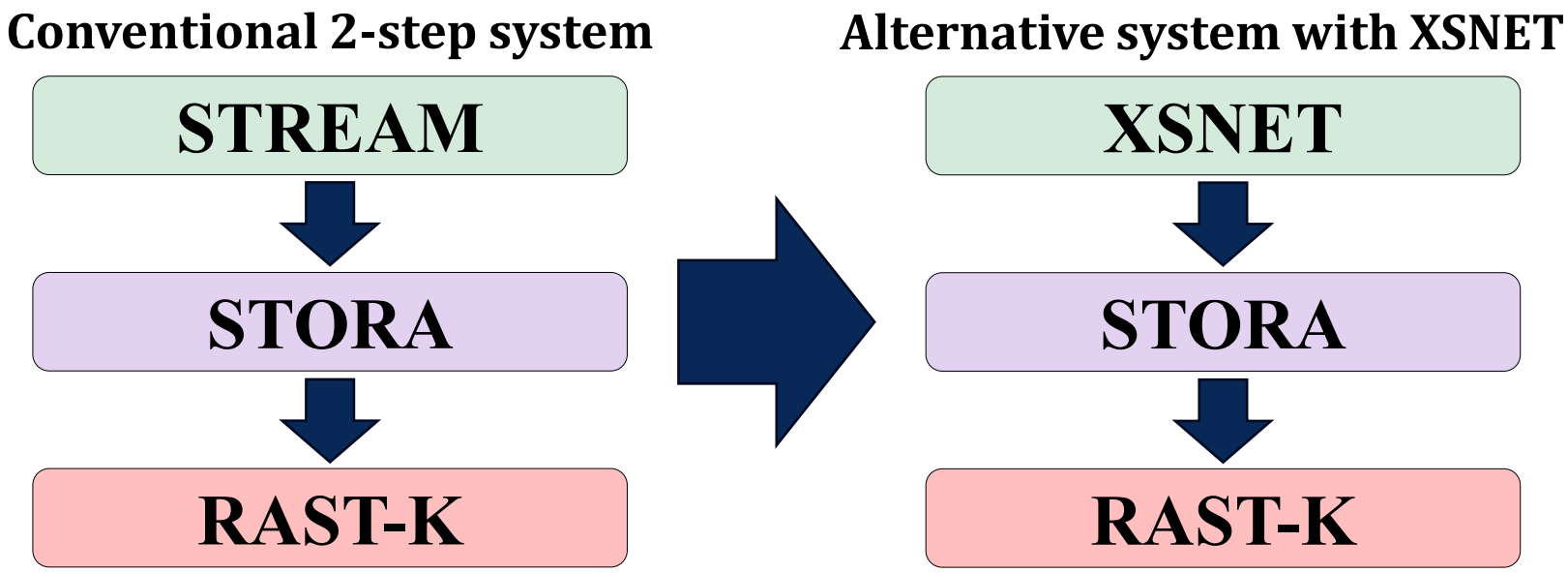
- **Lattice physics calculation is the most time-consuming part of the 2-step approximation method.**

20-step full-core OPR-1000 depletion with 10 FA types via STREAM/RAST-K



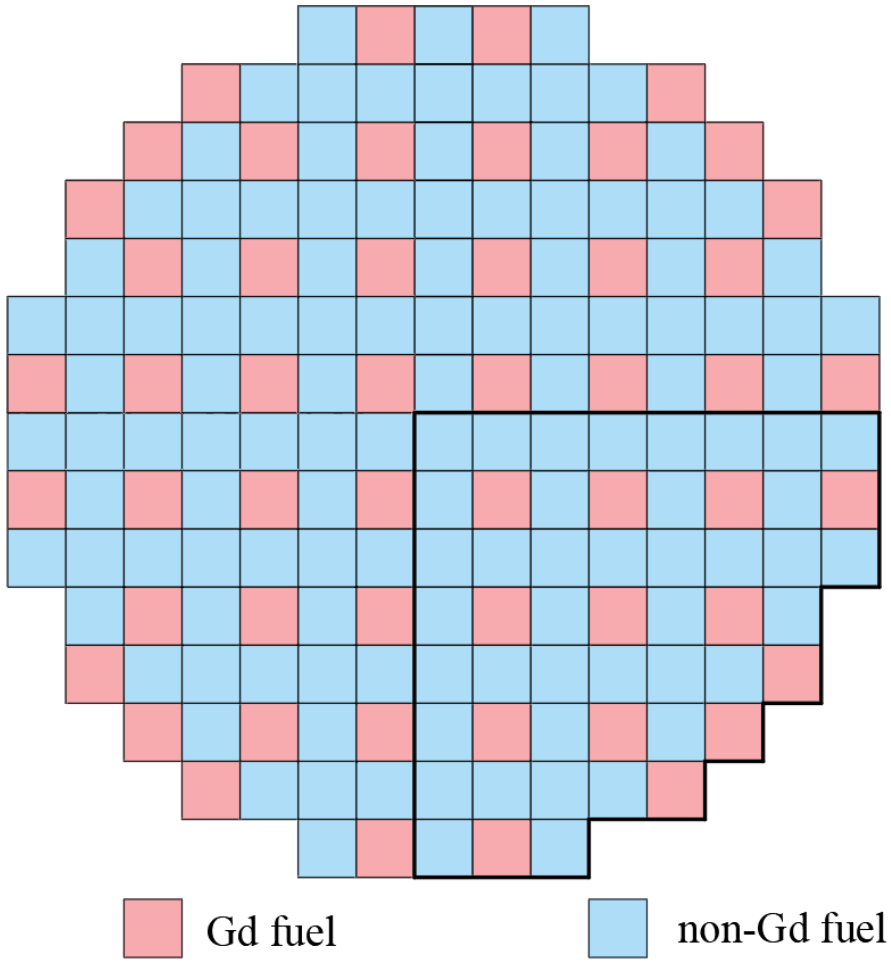
How XSNET is used

- The code capabilities progressed from a basic few-geometry fresh fuel forecast[4] with a handful of global FA parameters to the ultimate form of XSNET[5].
- XSNET[5] acts as a full replacement of STREAM in a 2-step code system.
  - It generates the same .STN file as STREAM.
  - The .STN file unlocks full functionality of RAST-K.

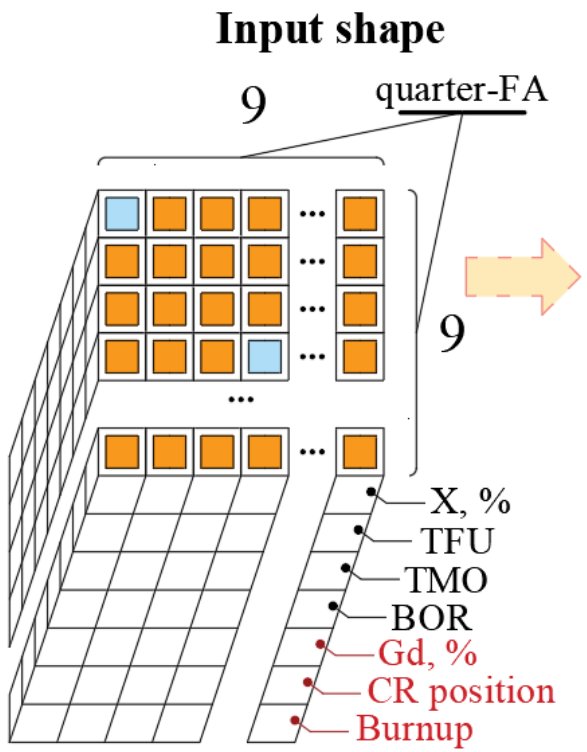


Neural Network Model and Reactor Design

OPR-1000 3D quarter-core model



ANN design and input structure



ANN Model

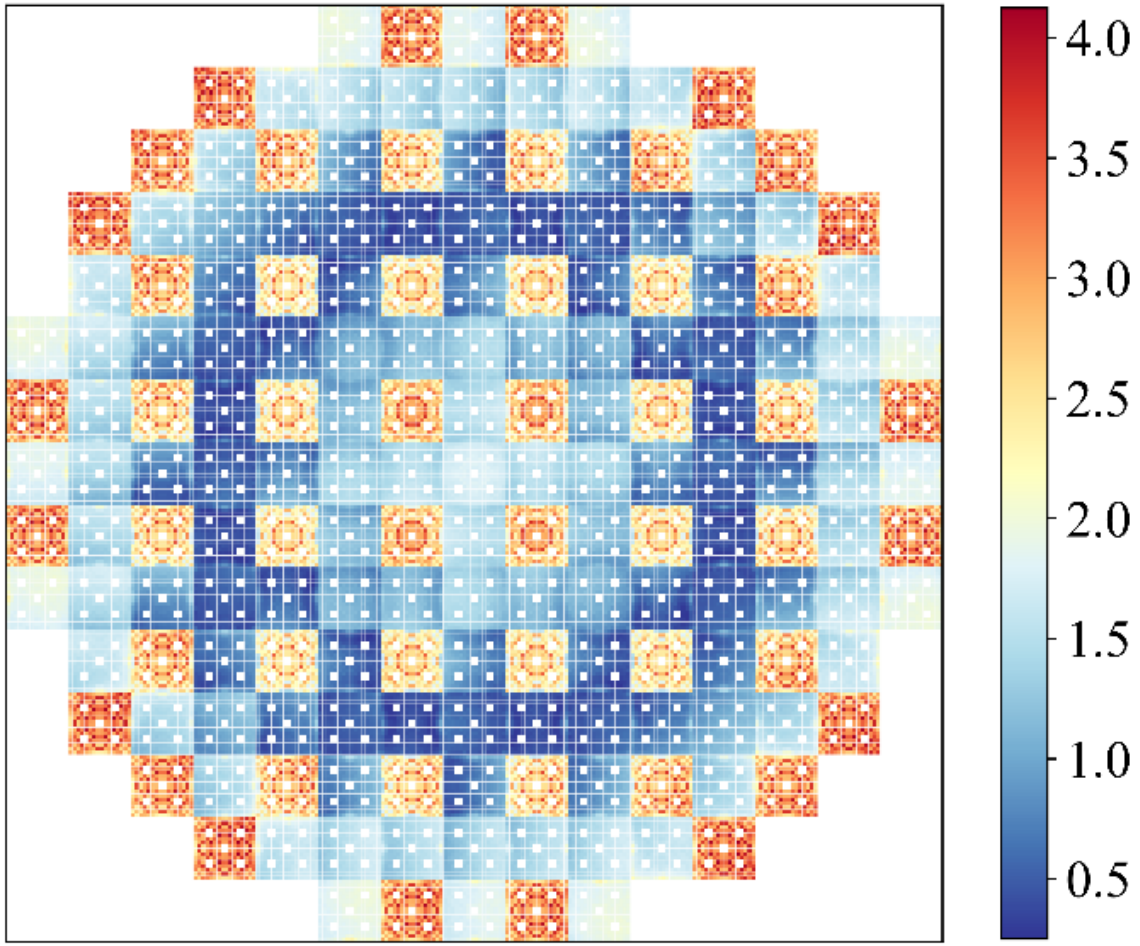
- Convolution layer 2D, ReLU, 128 filters
- Convolution layer 2D, ReLU, 128 filters
- Flattening Layer
- Dense Layer #1, eLU, 6296* neurons
- Dense Layer #2, eLU, 6296 neurons
- Dense Layer #3, eLU, 6296 neurons
- Dense Layer #4, eLU, 6296 neurons
- **Dense Layer #5, ReLU, 1574 neurons**

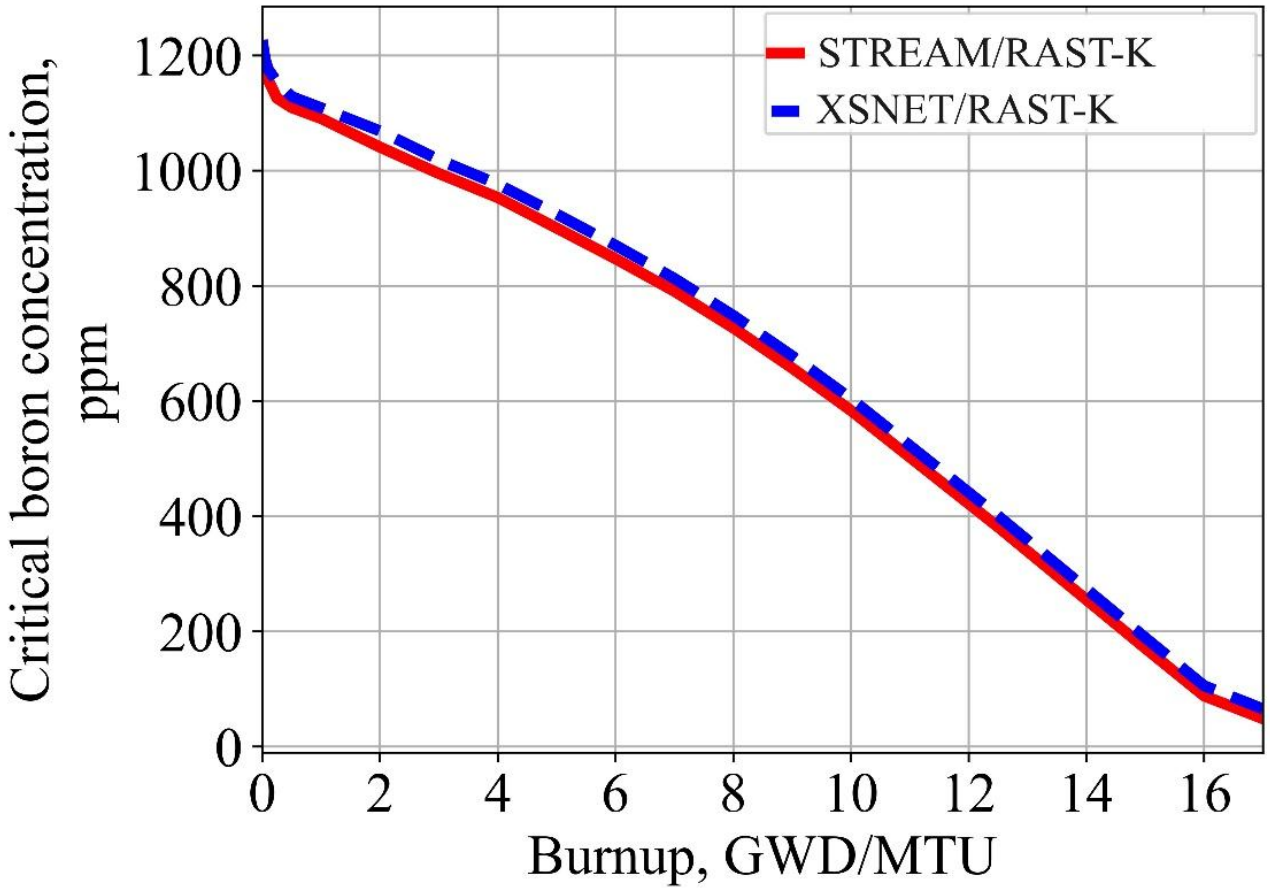
* 6,296 neurons per layer is 1,574 neurons in the output layer multiplied by 4

Core-wise stats – critical boron concentration

- **Averaged across all tested samples.**

Distribution of LP-averaged pin power RD, %



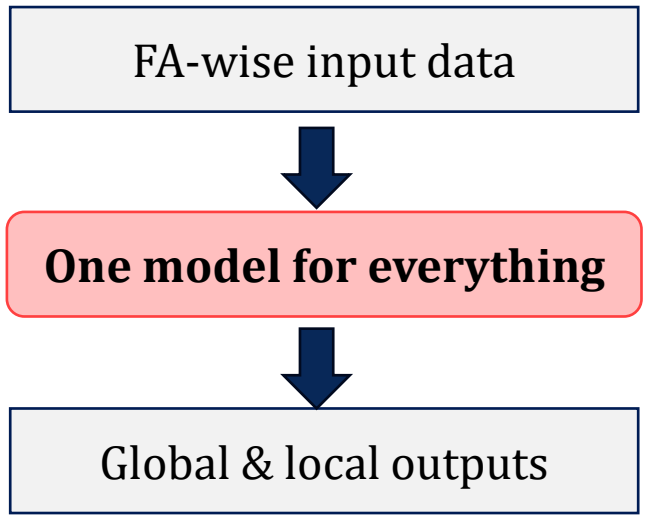


5. AI Surrogates of RAST-K

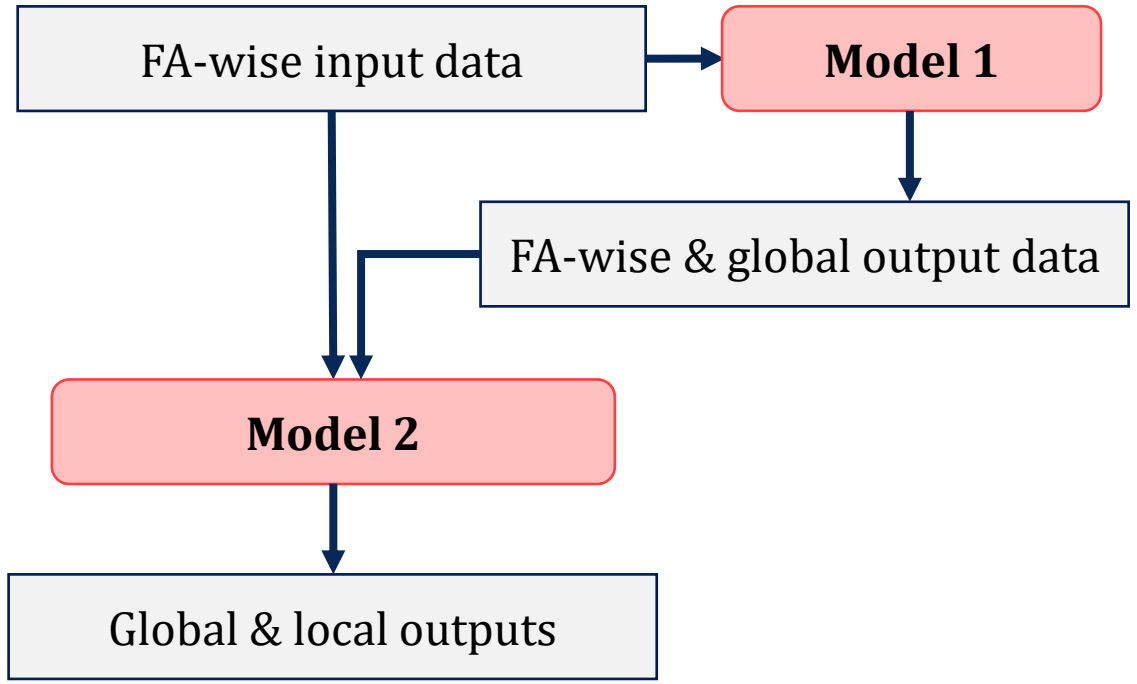
AI surrogate of RAST-K

- **Usually, either homogenized macroscopic XS or other FA-averaged material-related data is provided as inputs.**

Industry approach – direct model:
one model forecasts everything



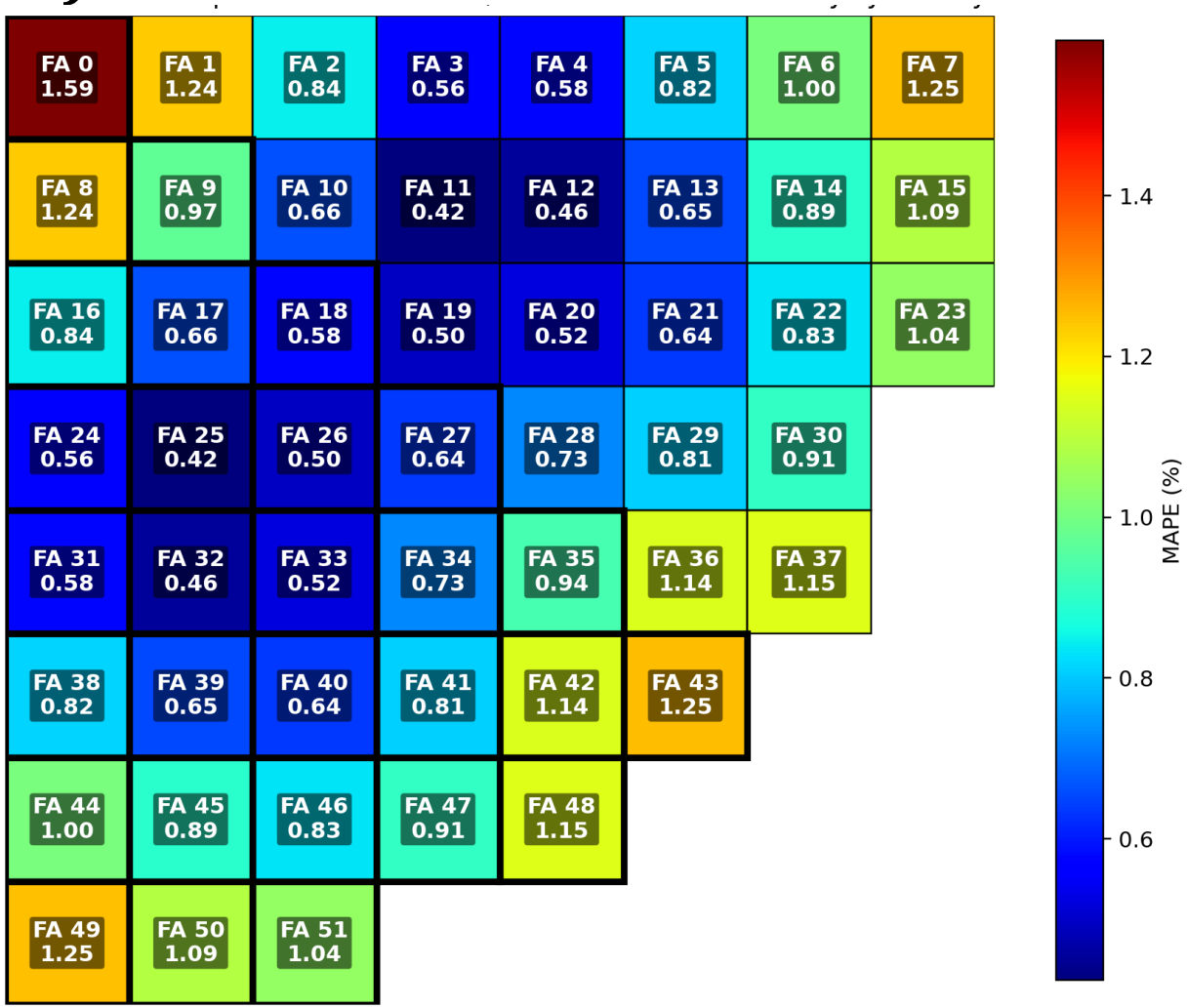
Tandem model (UNIST CORE) approach:
each model forecasts what it is designed for



Tandem model – Model 1

- **Global results and FA power plots (MAPE, %):**

Target	MAE	MAPE (%)	RMSE (%)	Max AE	Max APE (%)
Burnup	**43.5**	0.3	56.3	208.9	1.8
CBC	**4.8**	0.4	6.2	20.6	2.2
EFPD	**1.4**	0.3	1.8	6.7	1.8



Tandem model – Model 2

- **Global results and pin peaking factors:**
  - **Direct forecast - macroscopic XS only:**

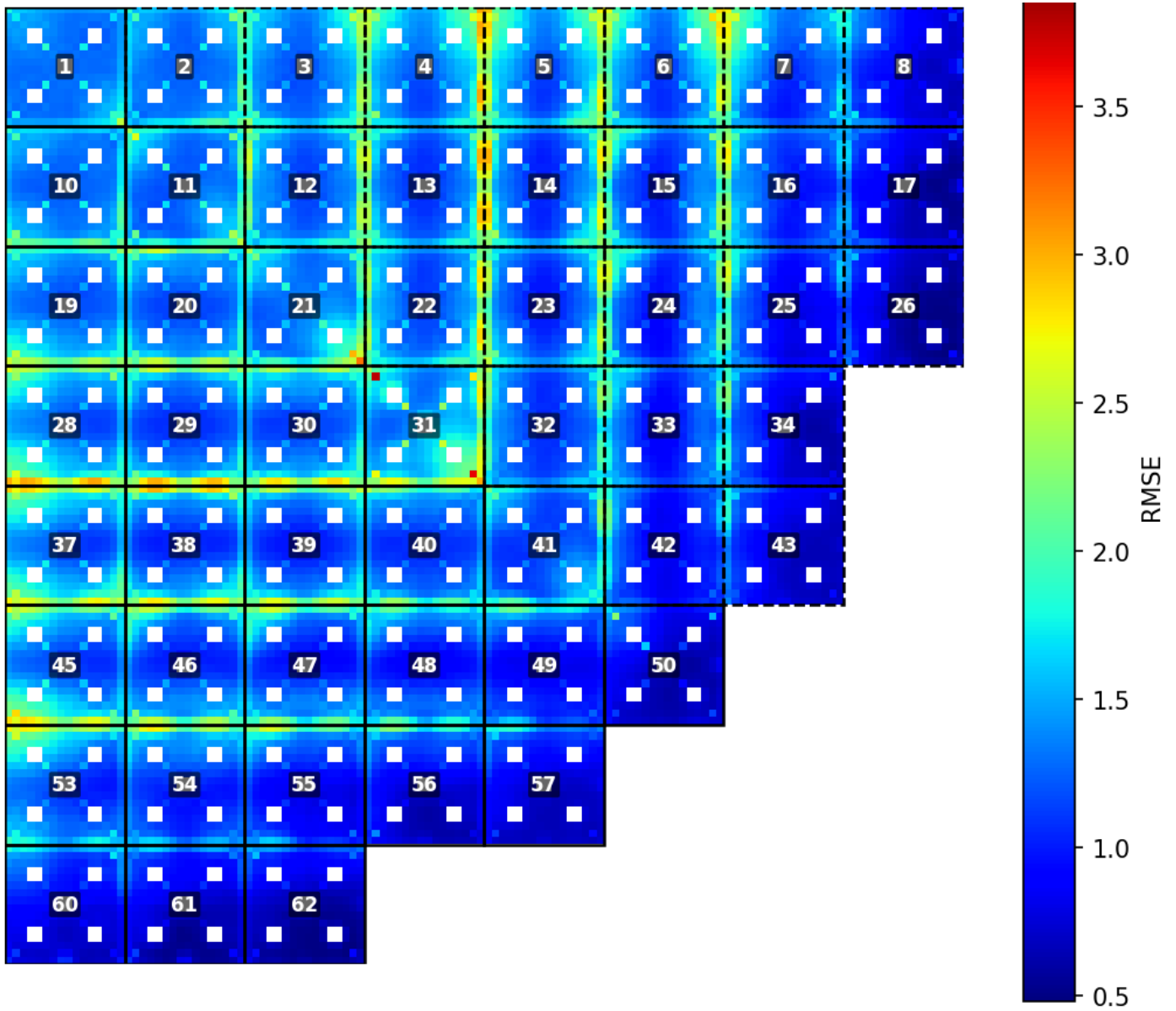
Target	MAE	MAPE (%)	RMSE (%)	Max AE	Max APE (%)
Burnup	67.5	0.4	85.2	363.6	3.0
CBC	8.5	0.7	11.0	35.7	4.8
EFPD	2.1	0.4	2.7	11.8	3.0
F_Q	0.082	2.585	0.110	0.585	19.122
F_{dH}	0.056	2.344	0.075	0.422	15.739
F_Z	0.002	0.169	0.004	0.033	2.564

  - **Macroscopic XS and reference FA powers:**

Target	MAE	MAPE (%)	RMSE (%)	Max AE	Max APE (%)
Burnup	**53.1**	0.3	68.0	275.5	2.1
CBC	**6.6**	0.5	8.4	37.0	4.9
EFPD	**1.7**	0.3	2.2	8.8	2.1
F_Q	0.036	**1.191**	0.052	0.576	19.323
F_{dH}	0.026	**1.131**	0.035	0.175	8.175
F_Z	0.001	**0.104**	0.002	0.017	1.219

Tandem model – Model 2

- **RMSE pin power results:**
  - **Typical whole-core PWR RMSE[6] (via KARMA/ASTRA against KARMA reference):**
    - average core-wise < 1%
    - max < 4%
  - **Model 2 Observed RMSE:**
    - average core-wise – 1.4%
    - max < 4%



Tandem model – Model 1 & Model 2

- **Global results and pin peaking factors:**
  - **Reference FA powers:**

Target	MAE	MAPE (%)	RMSE (%)	Max AE	Max APE (%)
Burnup	53.1	0.3	68.0	275.5	2.1
CBC	**6.6**	0.5	8.4	37.0	4.9
EFPD	**1.7**	0.3	2.2	8.8	2.1
F_Q	0.036	**1.191**	0.052	0.576	19.323
F_{dH}	0.026	**1.131**	0.035	0.175	8.175
F_Z	0.001	**0.104**	0.002	0.017	1.219

  - **Tandem (Model 1 FA powers):**

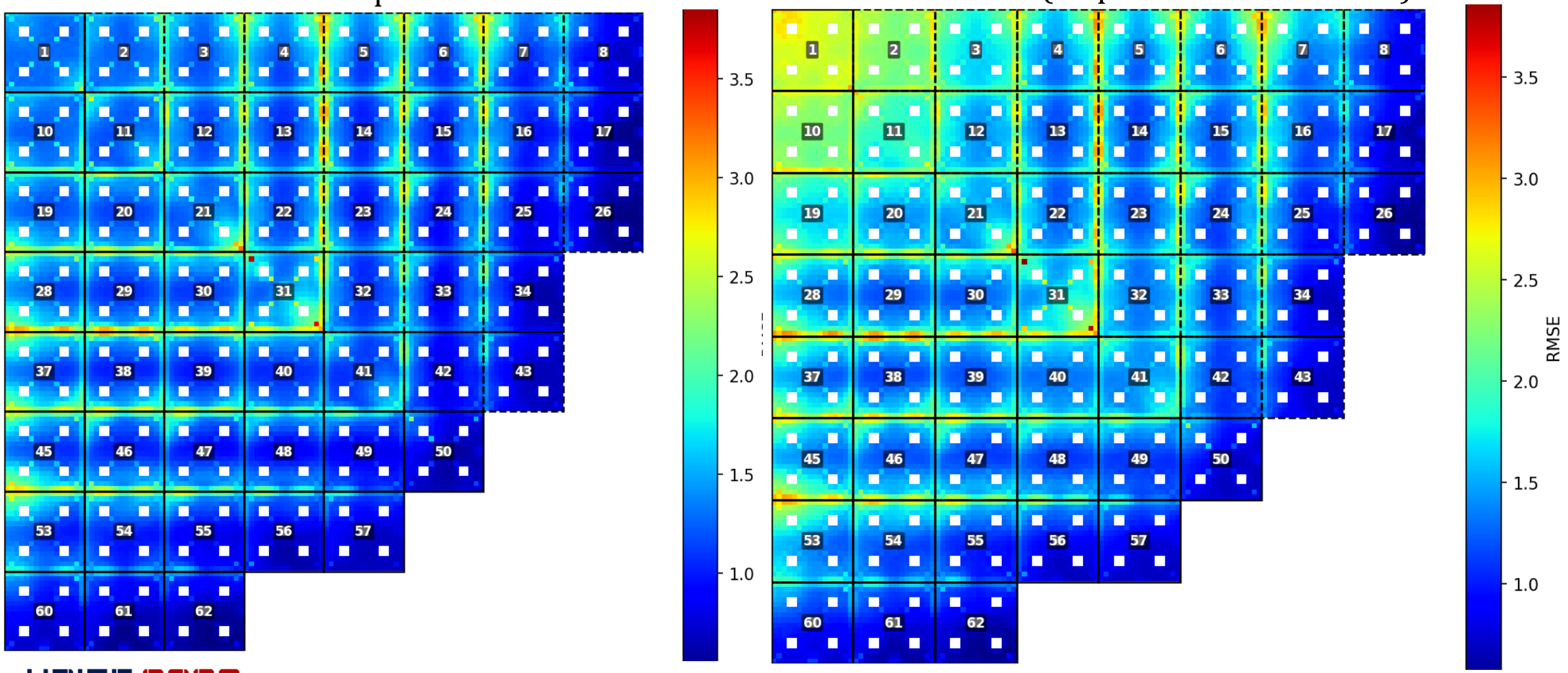
Target	MAE	MAPE (%)	RMSE (%)	Max AE	Max APE (%)
Burnup	**52.5**	0.3	67.4	267.6	2.0
CBC	6.7	0.6	8.5	33.6	4.6
EFPD	**1.7**	0.3	2.1	8.6	2.1
F_Q	0.044	**1.392**	0.062	0.578	19.380
F_{dH}	0.032	**1.345**	0.044	0.233	7.779
F_Z	0.001	**0.107**	0.002	0.016	1.259

Tandem model – Model 1 & Model 2

- **Impact of Model 1's FA power forecast accuracy on pin power:**

Reference FA powers

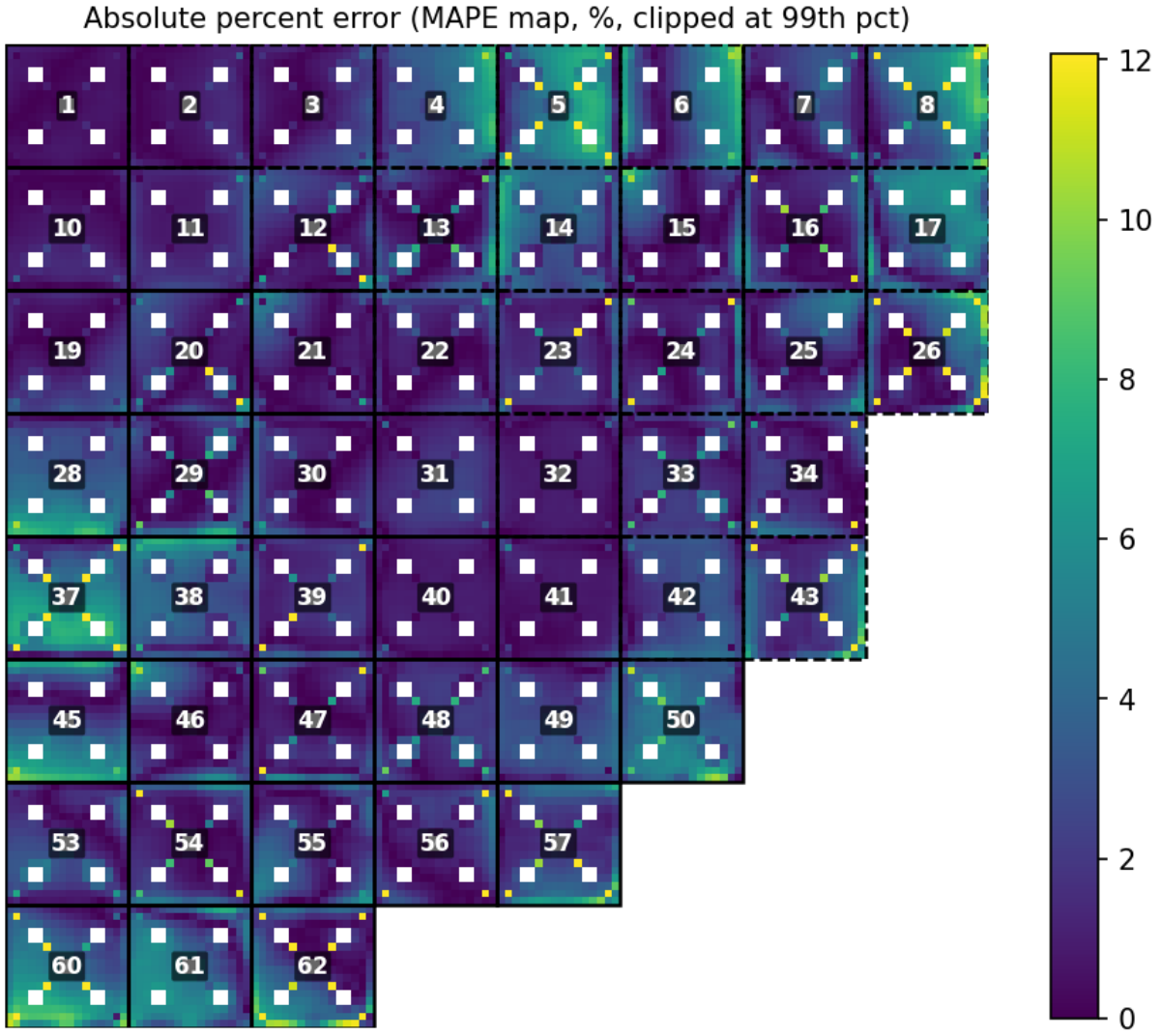
Tandem model (FA powers from Model 1)



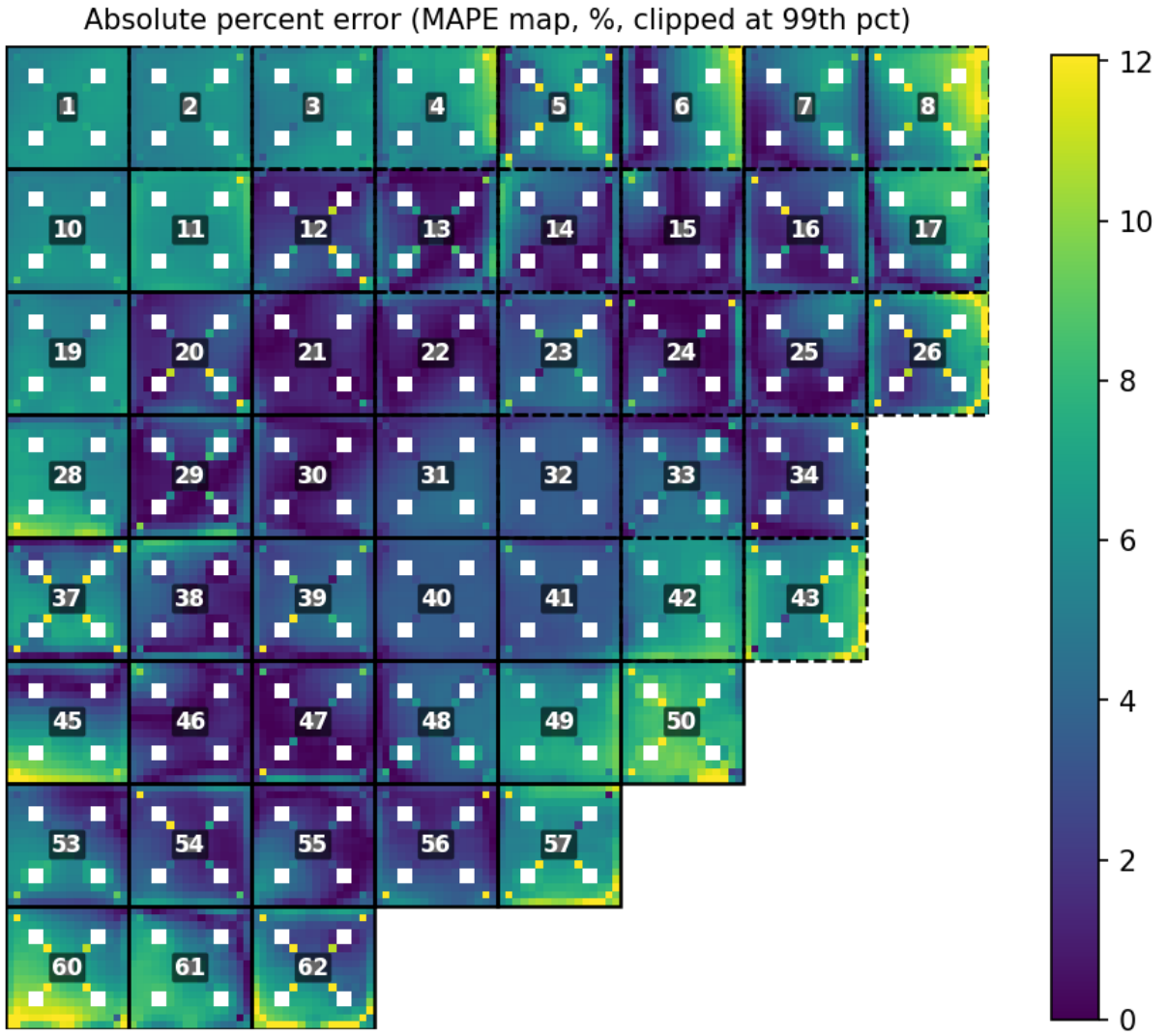
Tandem model – Model 1 & Model 2

- **Worst test LP pin power results:**

Reference FA powers



Tandem (Model 1 FA powers)



6. Conclusions and closing remarks

Next steps in UNIST CORE

- **Presented works include:**
  - **Practical models for grid power supply and demand forecast.**
  - **AI surrogate models of STREAM and RAST-K.**
  - **Loading pattern optimization tools.**
  - **Time-series forecasts and operator assistance tools.**
- **The goal of UNIST CORE laboratory is to develop practical AI-powered models that can be of use for the industry.**
  - **Some of the works are still ongoing and were not reported in this presentation.**
  - **See one of our latest studies as a poster during the conference*.**

* **Poster Session PO2E07**
Hyungjoon Baek, Dongmin Yun, and Deokjung Lee (UNIST), “Performance of a Vision Transformer Surrogate in SA-Based APR-1400 Loading Pattern Search”

Contacts

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