

Advances in the multi-scale bridging within NEAMS for TH applications: leveraging high-fidelity data

Dillon Shaver¹

With contributions from
Elia Merzari^{1,2}, Luiz Aldeia², Guilherme Gottens², and Ricardo Balin¹

¹Argonne National Laboratory

²Pennsylvania State University



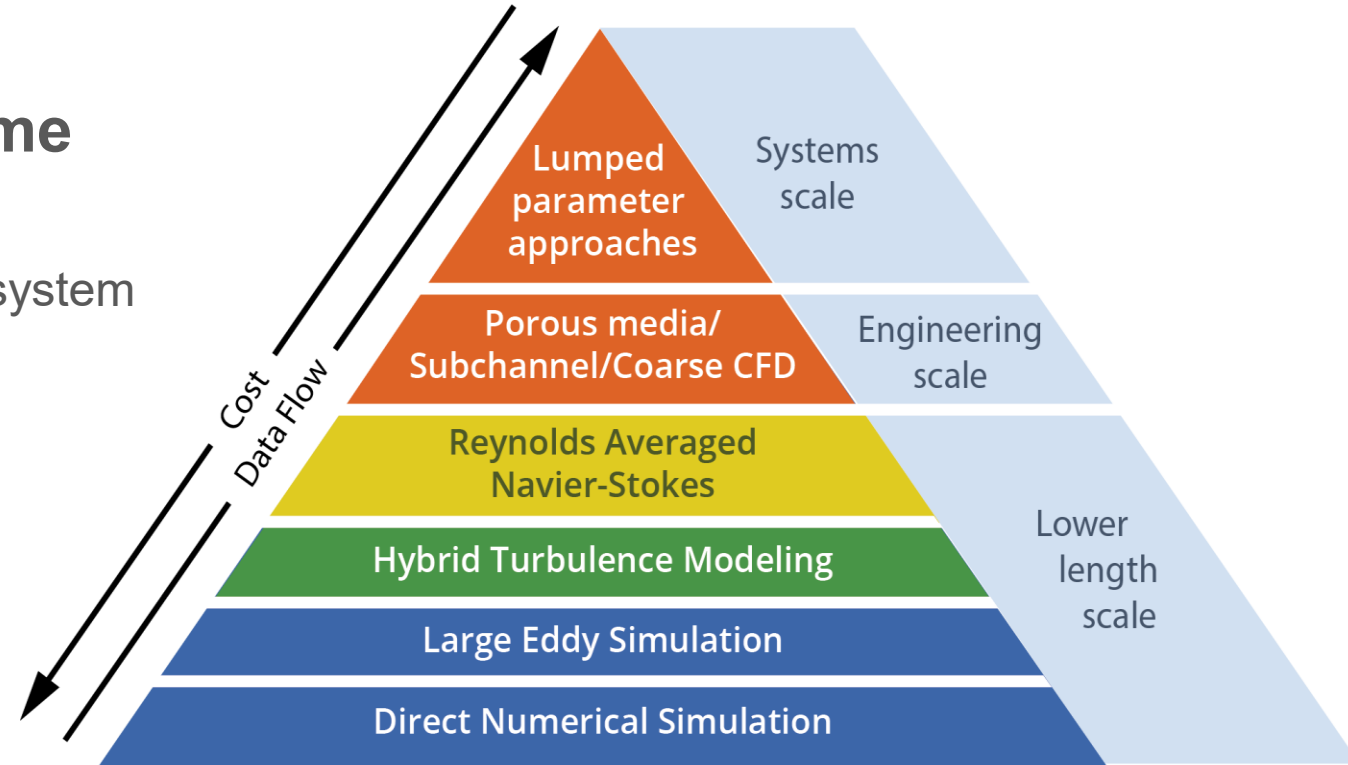
U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy

Multiscale Approach

Thermal and Fluid Flow phenomena involve a wide range of length and time scales

- Resolving all scales for a realistic engineering system of interest is often computationally not feasible.
- On the other hand, if scales are not resolved, closures need to be provided to ensure reasonable accuracy, as all scales contribute to the dynamics.
- Multiscale/multi-resolution simulation hierarchy



Plant Scales

System Codes Reduced-order models Sub-channel
System Analysis Module (SAM)

Engineering Scales

Porous media modeling Momentum Sources (Coarse CFD)

Fine Scales

RANS CFD Hybrid CFD LES/DNS

Pronghorn

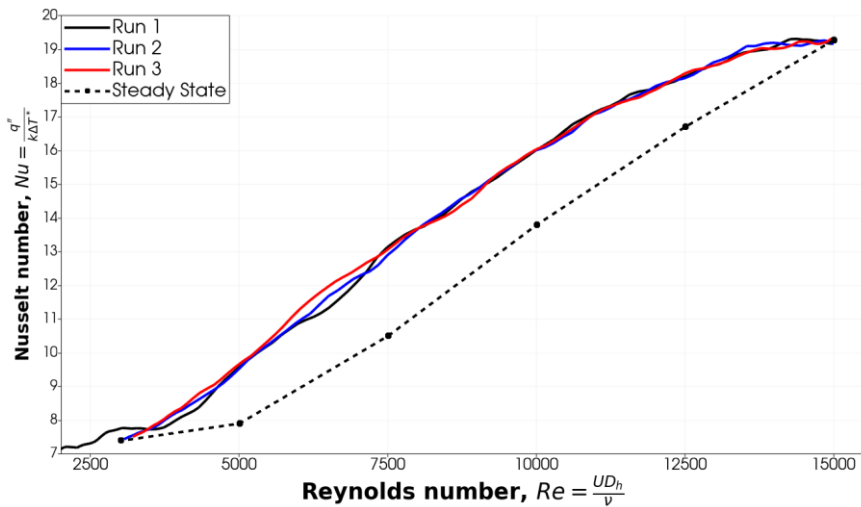
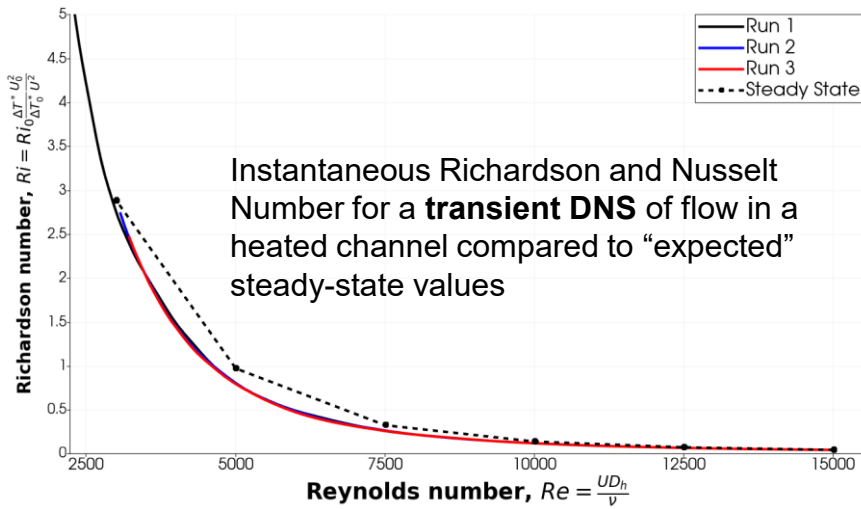
Nek5000/NekRS

Leveraging AI/ML Methods

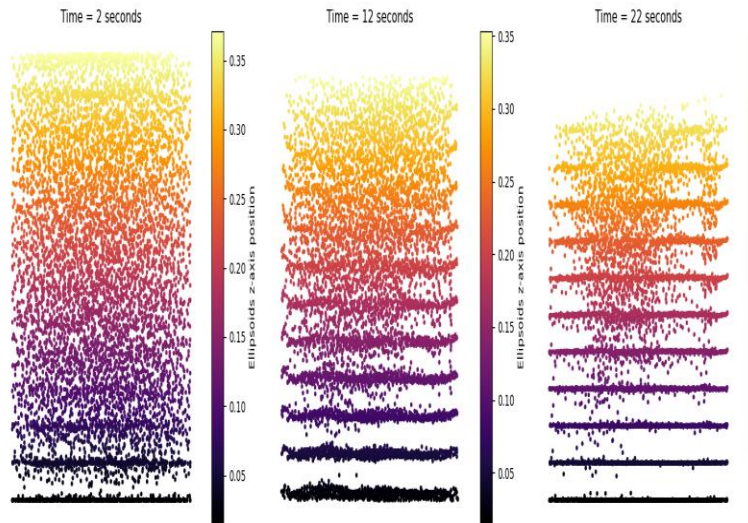
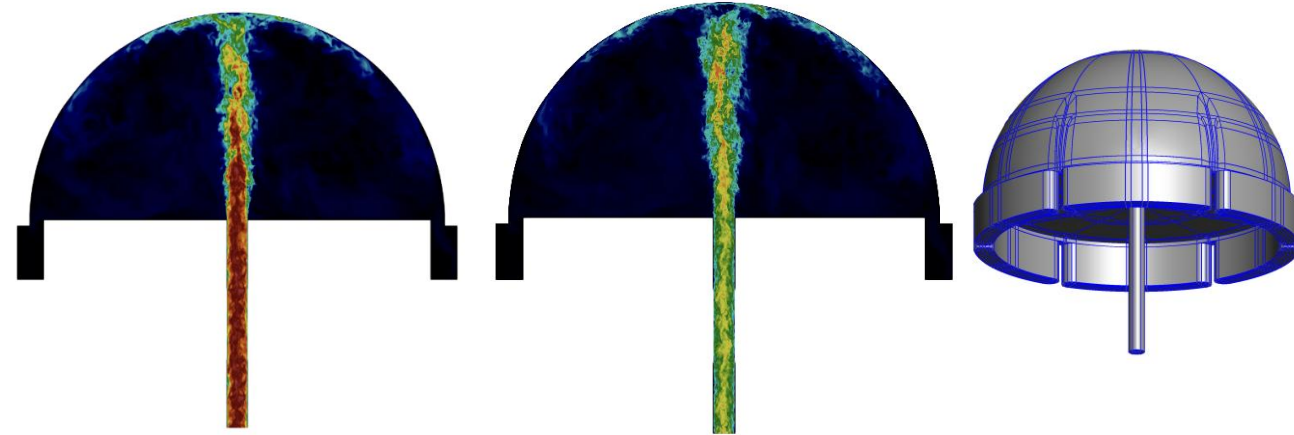
- Making the most of the high-fidelity simulations that are performed
 - Using data-rich results to generate lower-fidelity models
- Decreasing *time to solution* for high-fidelity analysis
 - Making the tools easier to use (agentic AI)
 - Replacing costly steps in the solution process with AI surrogates



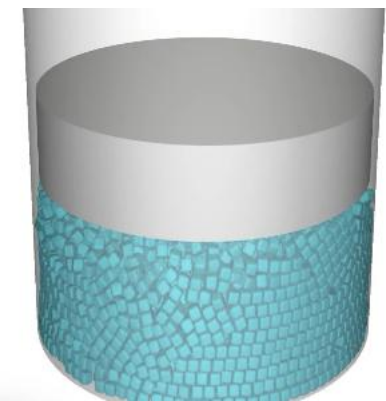
Early Highlight: Transient simulations



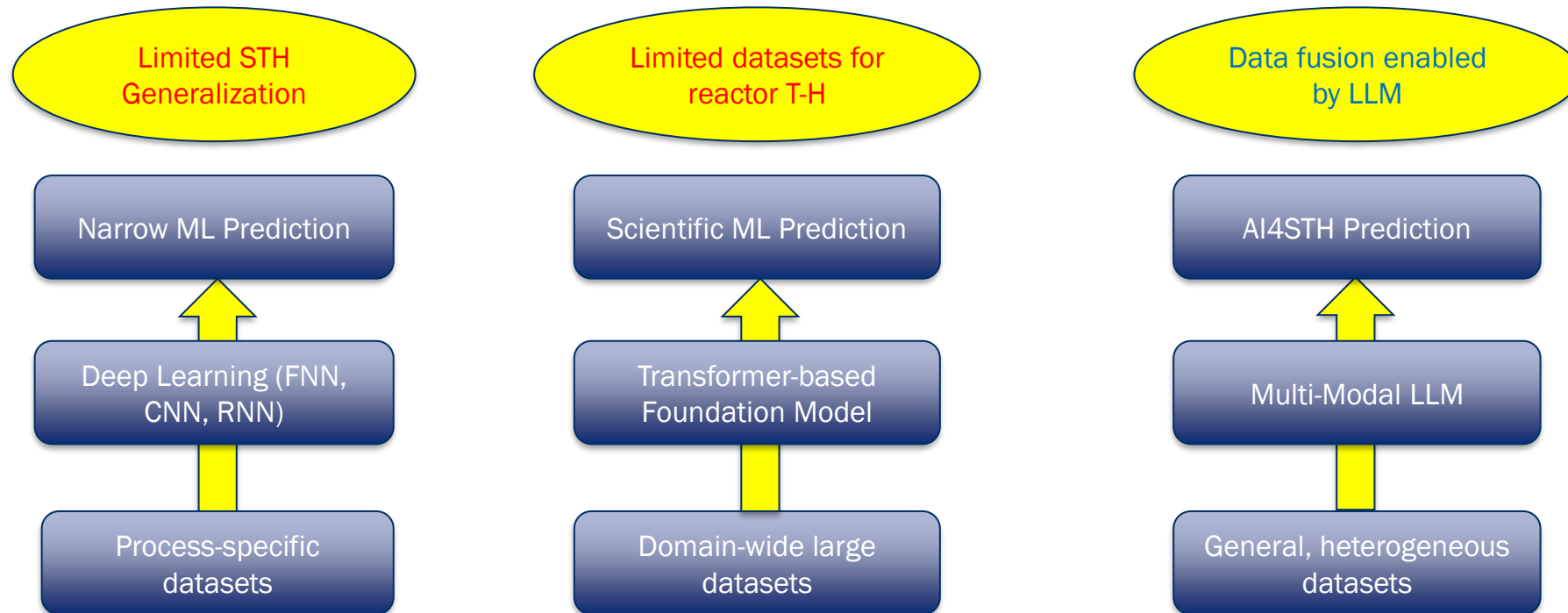
Right: transient simulation of a jet entering a large enclosure



Below and Left: settling of ellipsoid "pebbles" in an annular bed



Data-Driven ML-aided Multiscale Integration



Including a wide range of Hybrid Physics-Informed NN (studied in the NEAMS IRP Phase I)

Special-purpose Generative Pre-trained Transformer (GPT) e.g., ClimaX Foundation Model for Weather Forecast

Leverage LLM transfer learning for system TH multiscale integration (studied in NEAMS IRP Phase II)

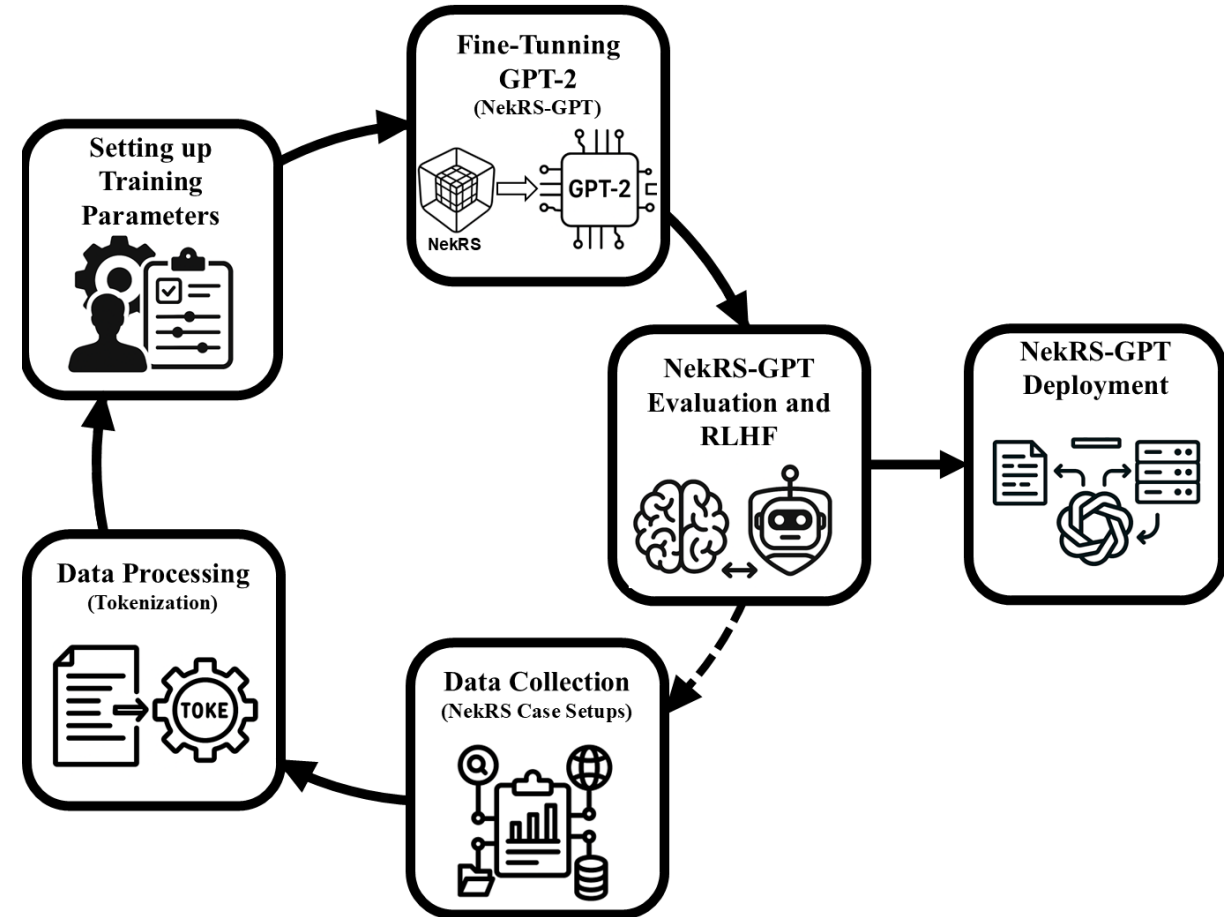


U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy

NekRS-GPT

- Integration of GPT-based tools with NekRS high-fidelity CFD solver
- Aimed at accelerating simulation workflows and model development
- Enables AI-assisted diagnostics, parameter tuning, and result interpretation
- Potential to reduce expert workload and streamline multiscale simulation pipelines
- Currently in early-stage development and testing with promising results
- **More details available in a recent paper published at NURETH-21 (Nguyen et al.)**



NekRS-GPT

- **NekRS-GPT**: fine-tuned GPT-2 model to automate NekRS CFD case setup
- Generates **executable, error-free input files in seconds**, reducing manual effort
- Accuracy: **100% (simple)**, **70% (intermediate)**, **50% (complex)**; improved to 100% with RLHF on benchmark cases
- Major gains in **efficiency and error reduction**, but generalization remains challenging
- Future work: expand training, integrate debugging/post-processing workflows
- High-performance computing (e.g., **Aurora**, **Frontier**) essential for next-phase development

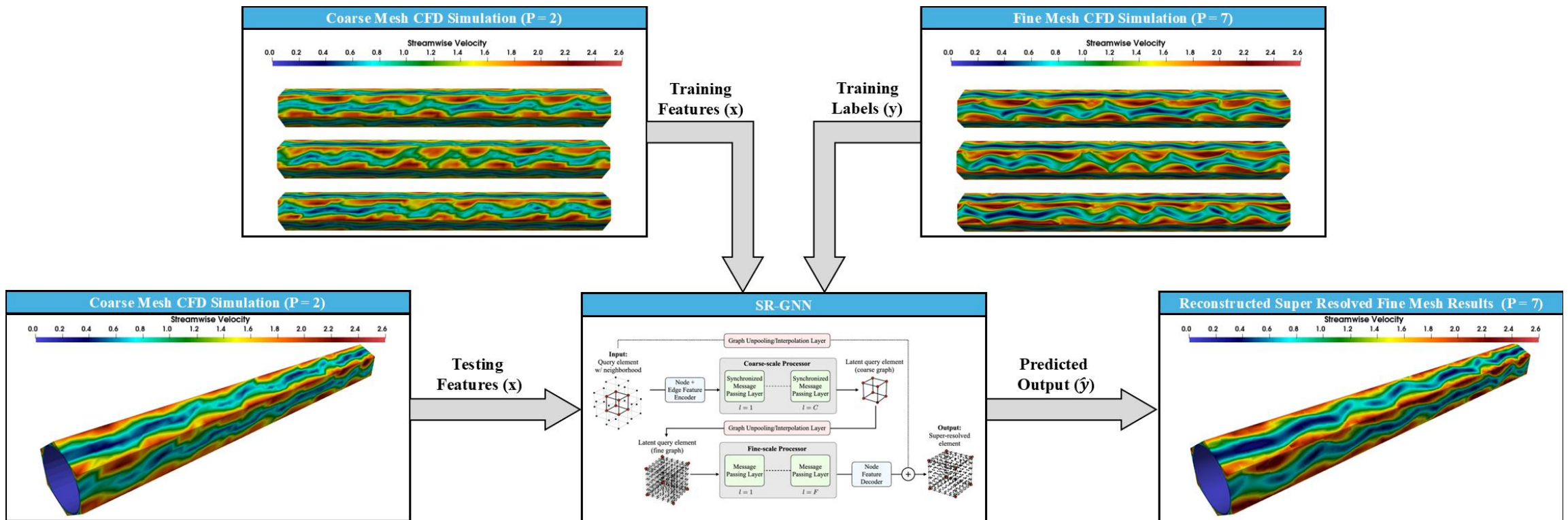
Case Type	Number of Cases	User Accuracy (%)	NekRS-GPT Accuracy (%)	NekRS-GPT Accuracy (%) after RLHF
Simple	8	100	100	100%
Intermediate	10	100	70	100%
Complex	10	100	50	100%

Case Type	Averaged manual Setup Time (min)	Averaged NekRS-assisted setup time (min)	Time reduction (%)
Simple	20	5	75
Intermediate	40	15	62.5
Complex	90	50	44.4



NekML: Machine Learning for NekRS

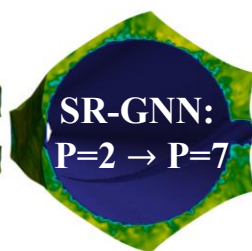
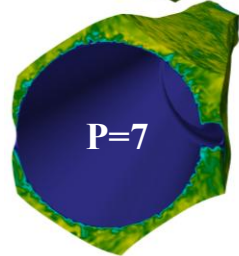
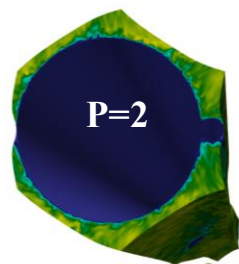
- Running high-fidelity simulations from non-physical initial conditions to steady state is costly and tedious. Can we replace this process with an AI surrogate?



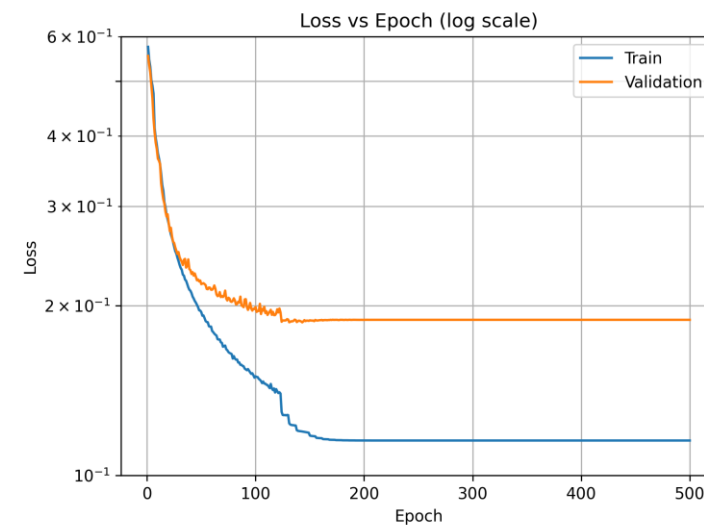
NekML: Machine Learning for NekRS

Demonstration for flow around an interior wire-wrapped fuel pin

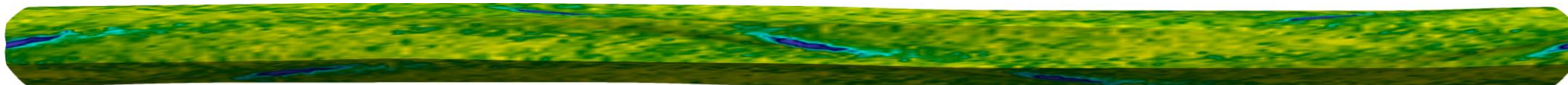
$Re=10,000$



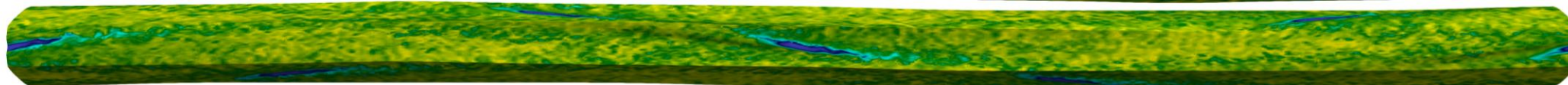
Inference:
Rel. L^2 RMS = $7.557e-2$



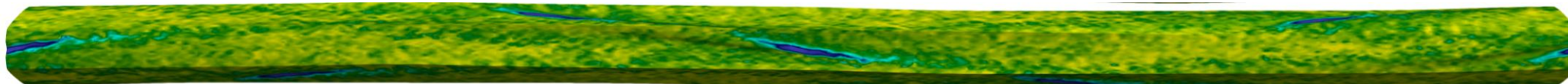
$P=2$



SR-GNN: $P=2 \rightarrow P=7$



$P=7$



U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy



U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy