

Use of ML in Surrogate Models to Efficiently Bridge Between Mesoscale and Continuum Scale

L. Capolungo (LANL)



U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy

Opinion on prospect of AI/ML as an engine for nuclear engineering

Prospects

- ❑ AI/ML enables physics-based simulations at previously inaccessible scales (homogenization, surrogate modeling, code-development)
- ❑ Could reduce time-to-decision from decades to years
- ❑ Direct relevance to MSR, LWR, and advanced reactor programs (i.e. we are already practitioners and have had successes)

Current use cases (non-exhaustive)

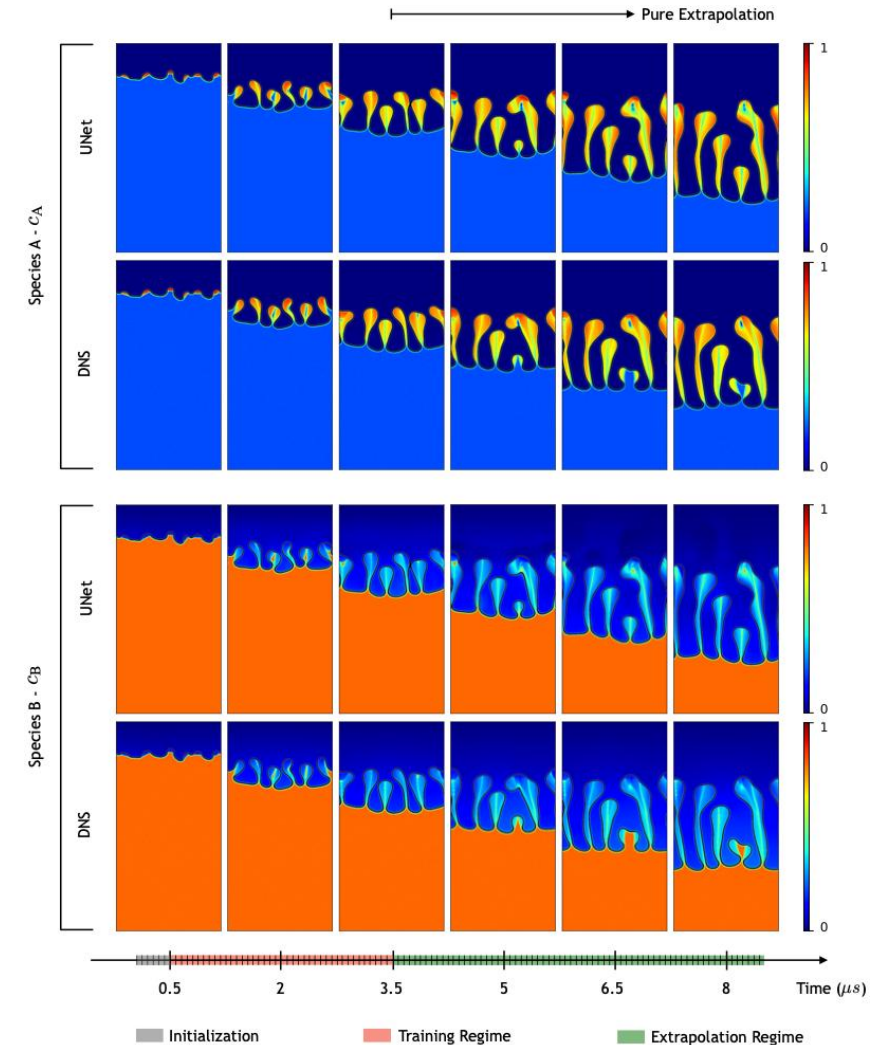
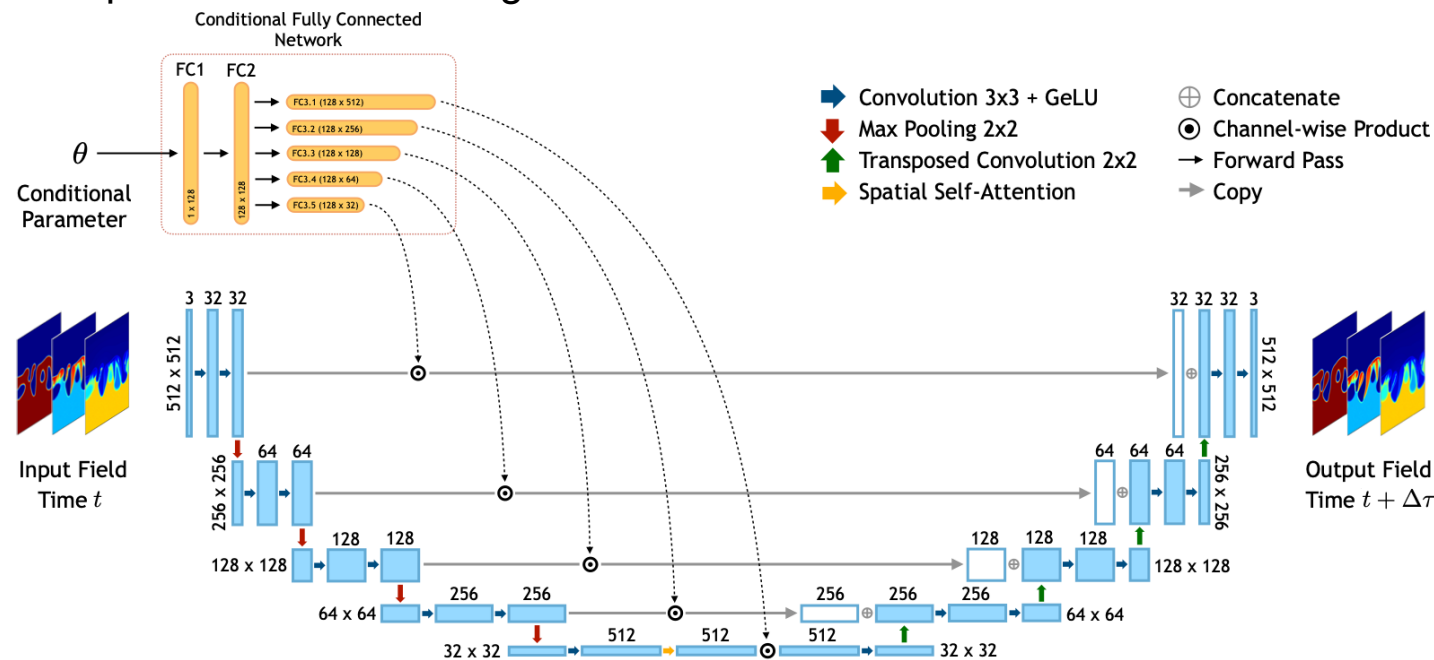
- ❑ AI-accelerated corrosion, creep, fracture, and irradiation models, surrogate constitutive models embedded in reactor-scale solvers, uncertainty-aware predictions for risk-informed decisions

ML driven accelerated molten salt corrosion simulations

Credit: C. Bonneville, N. Bieberdorf, M.Asta, L. Capolungo, C. Safta, H. Najm

The problem:

- Molten salt corrosion of structural metals is largely driven by diffusion transports at the salt metal interface.
- Linking the salt composition to the corrosion kinetics and modes requires simulations with extremely fine resolution (i.e $<1\text{nm}$).
- Current phase field simulations are too costly to perform simulations over representative time/length scales.



Advance made: We introduced a U-NET ML based algorithm and trained it on using a phase field model. The new U-NET is found to lead to a 56000 times gain in numerical performance.

High accuracy surrogate constitutive models

Credit: P. Robbe, A. Hedge, C. Bonneville, C. Safta, A. Ruybalid, H. Najm, L. Capolungo

The problem:

- Advanced microstructure informed constitutive models broadly applicable to arbitrary loading scenarios (tensile loading, creep loading, fatigue) under extreme environments (high temperatures) are necessary to both perform structural level simulations of component performance and to design new materials.
- However, the numerical cost of these models can be prohibitive.
- Surrogate models could address these challenges

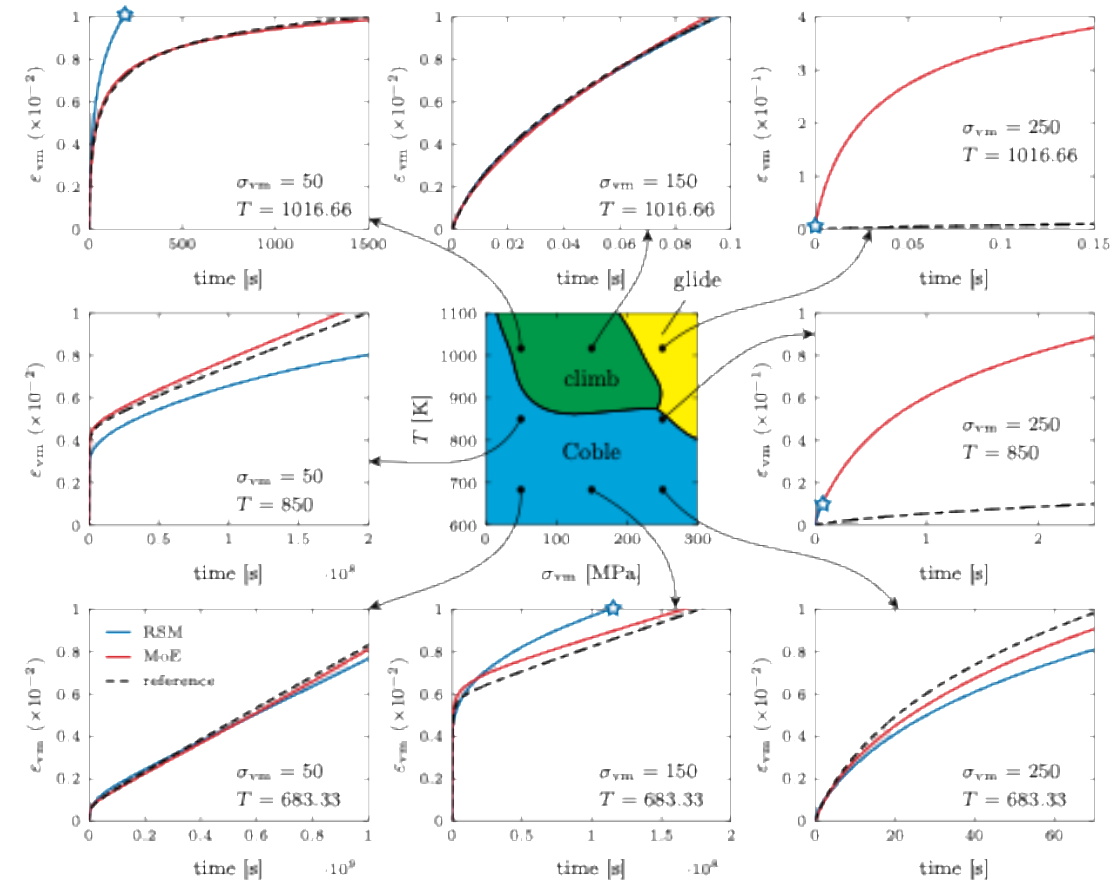
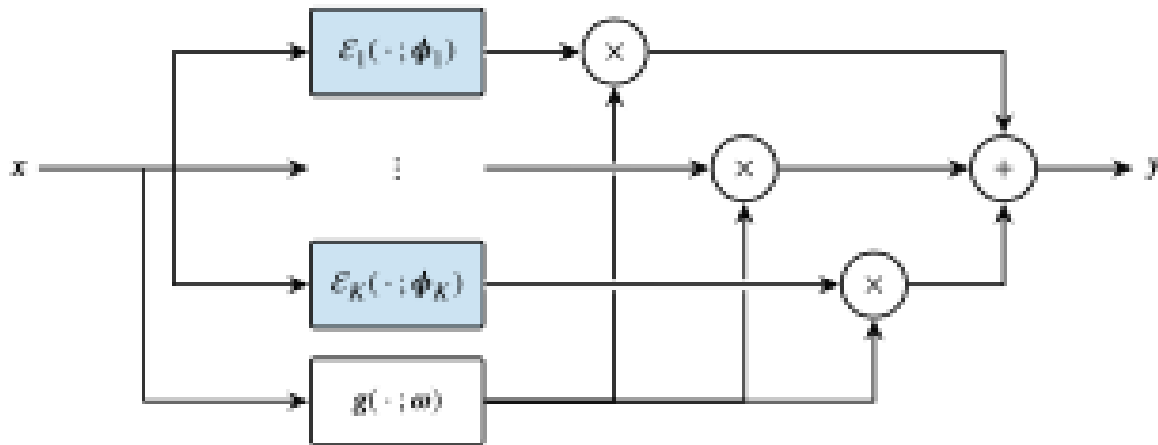


Figure 7: A comparison between the RSM (—) and MoE (—) surrogate constitutive models and the validation data when predicting the strain ϵ_{vm} for a dose rate $\dot{\phi} = 1 \times 10^{-8}$ dpa/s. We also indicate the different creep mechanisms from Figure 1: glide (■), climb (■) and Coble (■). A ★ indicates the last value that can be predicted with the RSM surrogate, which is restricted to the support of the training data.

Advance made: A new generation of surrogate constitutive models was derived using a ML based mixture of experts approach. The MoE model is highly accurate in most loading regimes



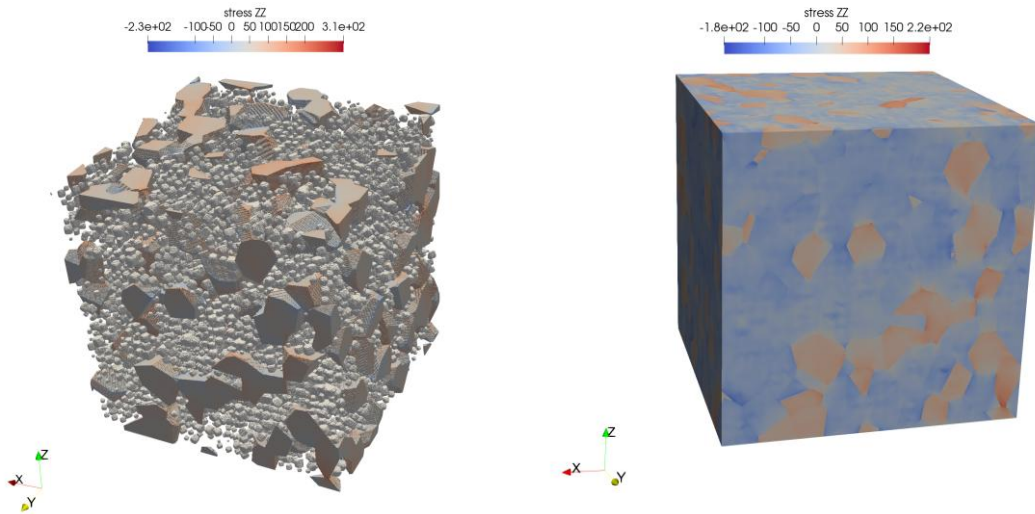
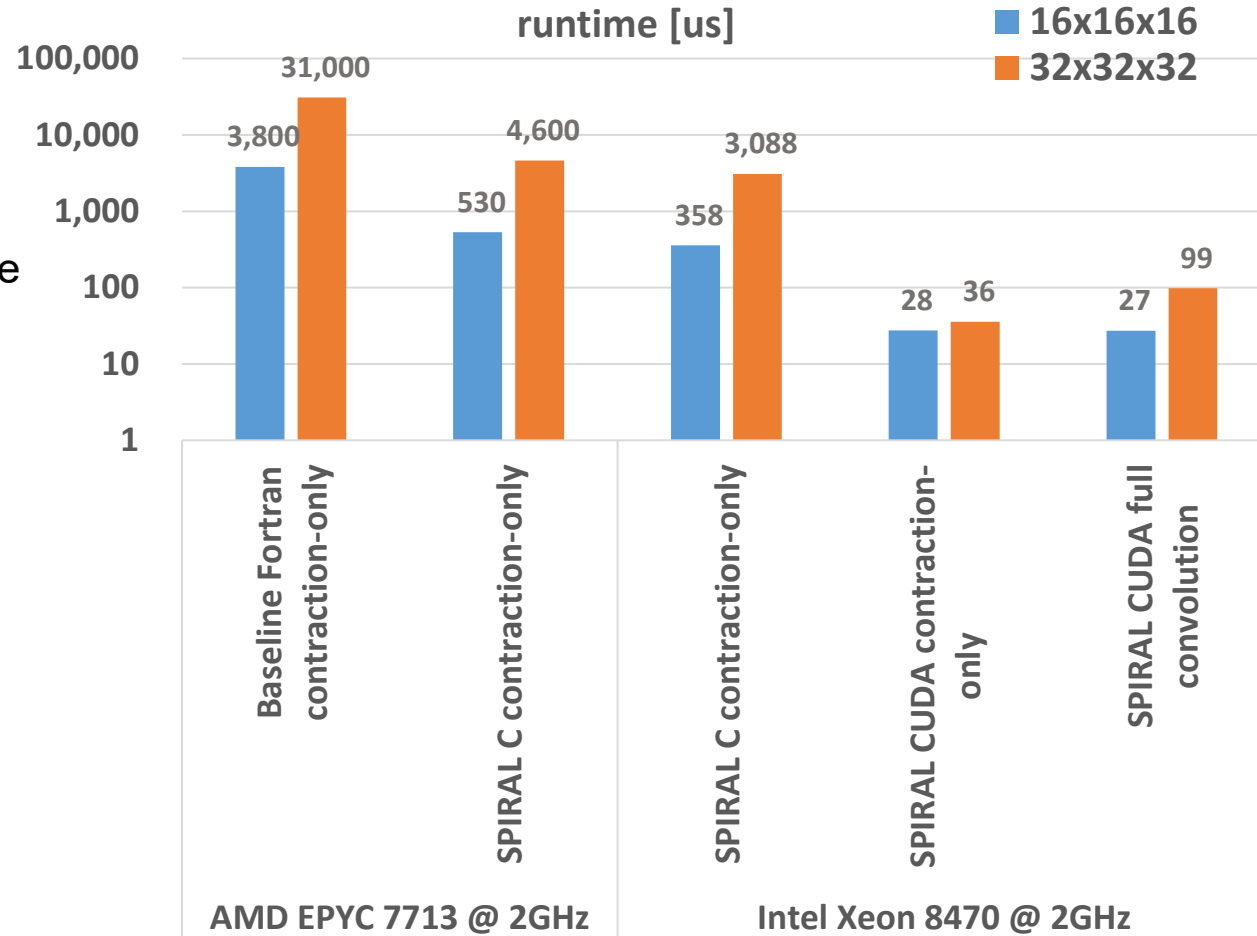
U.S. DEPARTMENT
of ENERGY | Office of
Nuclear Energy

AI/ML to optimize code performance and portability

Credit: P. Robbe, A. Hedge, C. Bonneville, C. Safta, A. Ruybalid, H. Najm, L. Capolungo

The problem:

- Most legacy numerical codes for predicting the mechanical performance and microstructure evolution of materials were primarily developed by scientists with primary expertise in computational materials science.
- Modernizing and evolving the structure of these tools to leverage new computational architectures and improve performance is a typical bottleneck due to lack of expertise and support.



512x512x512 Voxel simulations of mechanical fields in a Ni based superalloy at 400C.

Advance made: We extended and used an AI/ML based code-development framework (SPIRAL FTX) to improve the performance of LAPX and facilitate its portability onto GPU architectures.



U.S. DEPARTMENT
of **ENERGY** | Office of
Nuclear Energy

The future? Agentic AI

Agentic AI is an AI system that can: **autonomously plan, decide, and act** to achieve a goal, rather than just responding once to a prompt.

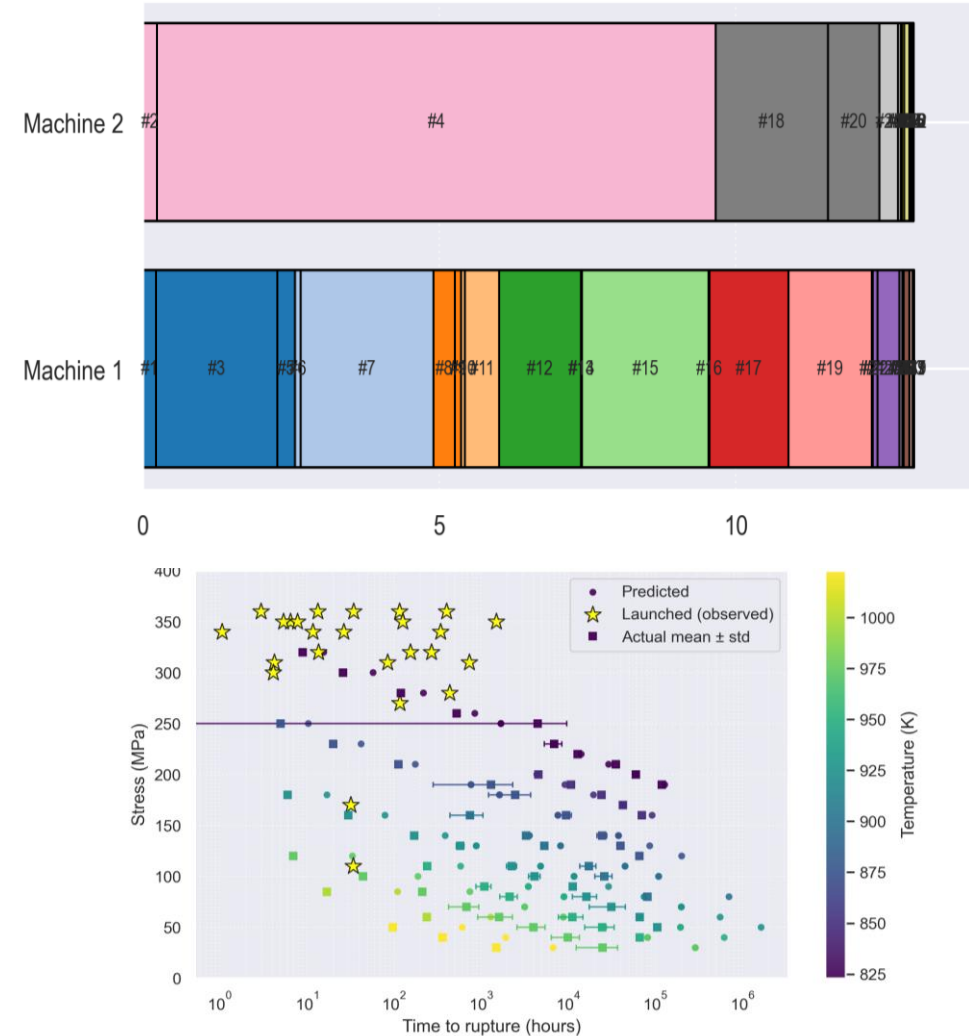
The problem: Assessing the creep rupture life of metals typically requires many tests, including some that typically last more than 10 years.

Tools are needed to rapidly screen the likely long term creep performance of metals whilst accounting for constraints (e.g. time, risk acceptance, equipment cost)

A proposed solution: Develop an agentic AI which proposes a design of experiments (which tests, how many tests) and indicates the net benefit of each test.

Approach: Given prior knowledge of the response of materials with similar features as the material to be tested, using a high accuracy predictive creep rupture life model, Bayesian inference and Machine learning to generate surrogate models, one can design a scheduler.

Advance made: In this proof-of-concept example, the AI proposes which creep tests should be performed (yellow stars) given a 13-week timeline and availability of only two creep frames



U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy



U.S. DEPARTMENT
of **ENERGY**

Office of
Nuclear Energy