



# HPC4MDF

*Providing US Manufacturers with a Simulation Framework for Directed Energy Deposition (DED) Additive Manufacturing*

PRESENTED BY

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Computational Sciences and Engineering Division

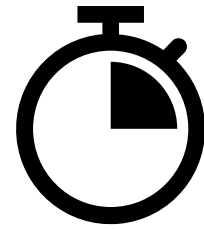


U.S. DEPARTMENT  
of **ENERGY**

ORNL IS MANAGED BY UT-BATTELLE LLC  
FOR THE US DEPARTMENT OF ENERGY



# US manufacturers need resilient supply chains for large-scale metal components

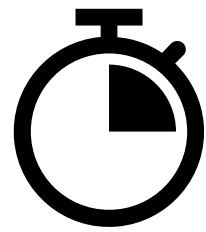
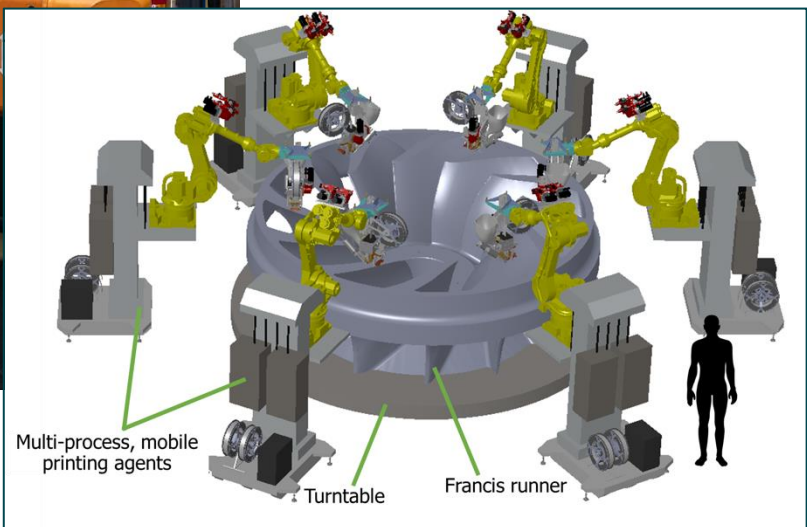
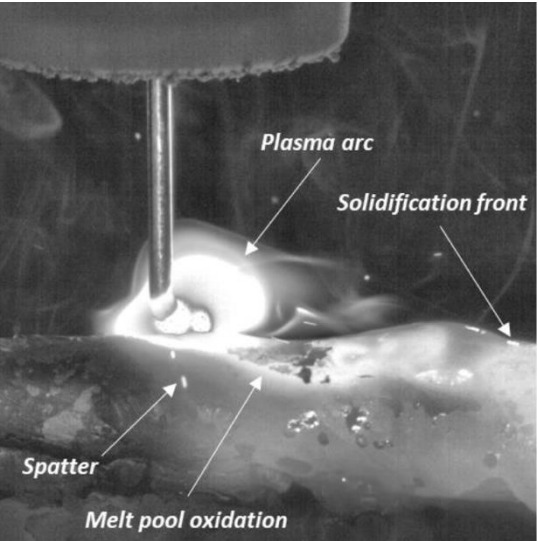


**Lead times are too long for large castings (years)**

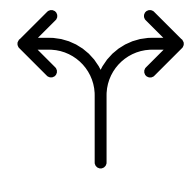


**Most large-scale foundries are outside the US**

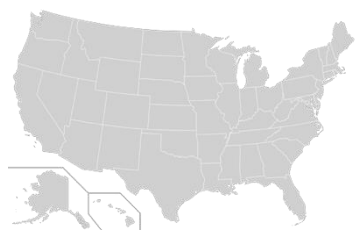
# Wire-arc additive manufacturing (WAAM) is a promising alternative to casting for large-scale metal components



**Shorter lead times**



**Agile production**



**Domestic suppliers**



**Path to qualification via welding standards**

# US manufacturers need an improved simulation toolchain for large-scale WAAM to predict location-specific properties

**Bigger parts mean longer prints and more costly iteration on process parameters**

**Existing commercial simulation tools lack the computational performance needed for these workflows**

# AMMTO funded HPC4MDF to tackle this challenge, integrating unique capabilities at LLNL and ORNL into the Manufacturing Demonstration Facility ecosystem



## ORNL MDF Team

Matt Rolchigo, John Coleman, Ashley Gannon, Bruno Turcksin, Daniel Arndt, Gerry Knapp, Bhagya Prabhune, Yousub Lee, Shramana Ghosh, Alex Plotkowski

## LLNL Team

Tim Dunn, Jerome Solberg, Saad Khairallah

## Funding

This project is funded by the US Department of Energy, Office of Critical Minerals and Energy Innovation, Advanced Materials and Manufacturing Technologies Office.

## Facilities

This project used resources from the Manufacturing Demonstration Facility at ORNL, the Oak Ridge Leadership Computing Facility at ORNL, the CADES computing environment at ORNL, and the Livermore Computing Complex at LLNL.

# In HPC4MDF we are developing a smart framework for large-scale DED and demonstrating its use



## **Develop a DED smart manufacturing framework**

- *Spatial variability of thermal conditions and microstructure*
- *Cloud-deployable*



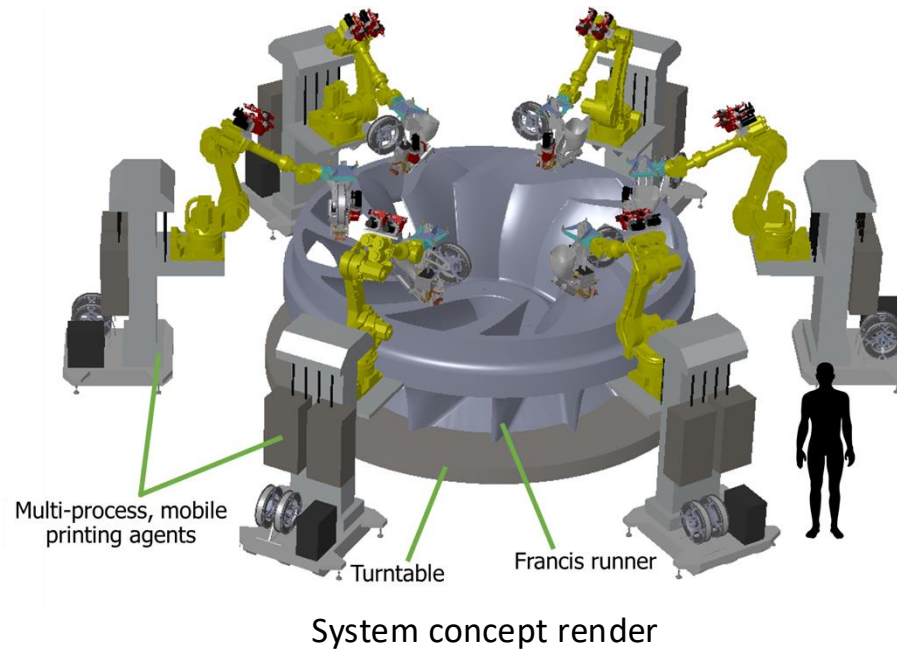
## **Demonstrate the framework for a DOE-relevant problem**

- *AMMTO/WPTO Rapid RUNNERS hydrorunner*

*Framework can both be used directly and to derisk commercial code development*

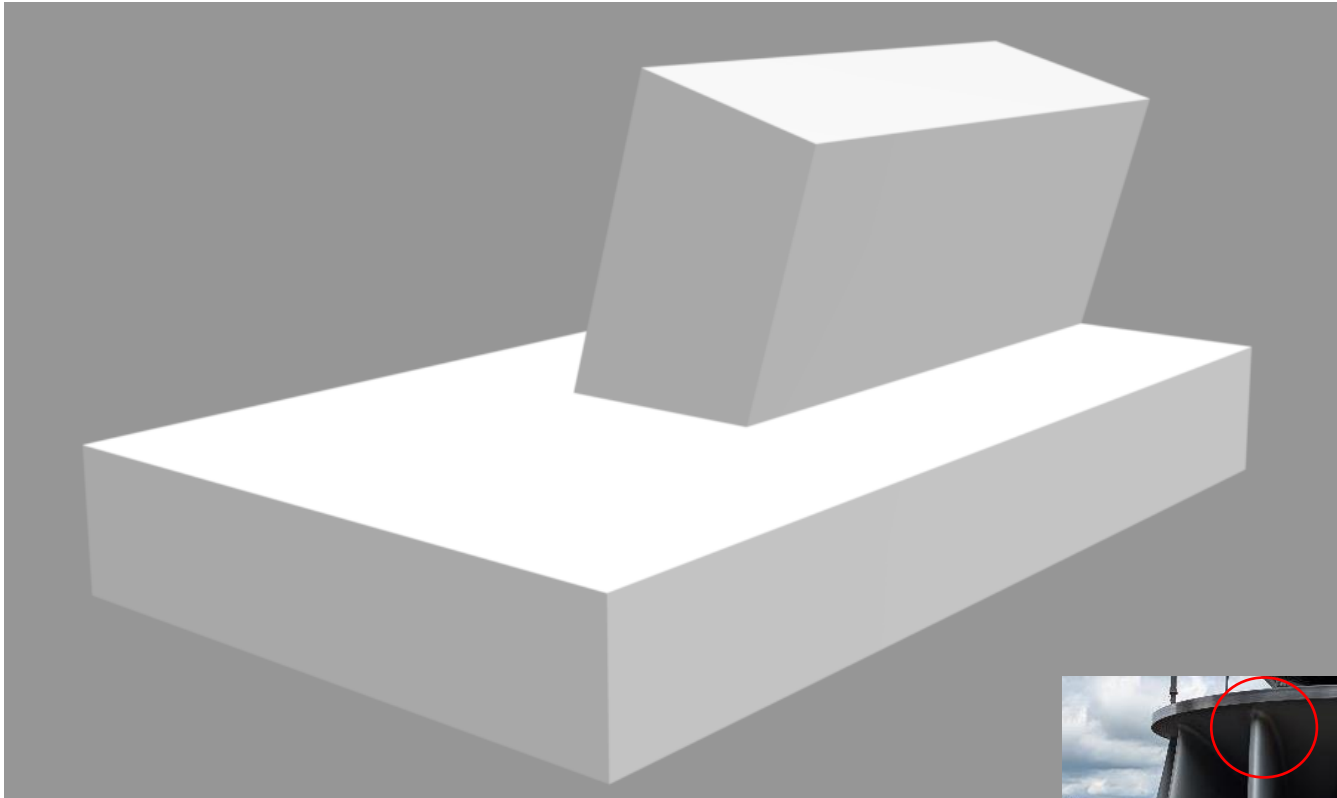


# Rapid RUNNERS is a FY26-28 DOE project to demonstrate the viability of additive manufacturing for hydroelectric turbine runners



*Target Wilson runner*  
**4.3 m diameter**  
**32 tons**

**One of the FY26 deliverables for Rapid RUNNERS is a WAAM print of a representative T-joint between the blade and band**



This is our initial demonstration component for the HPC4MDF framework



# Rapid RUNNERS has several simulation-relevant challenges

## The prints are huge

*Large meshes, long simulated times, high stakes*

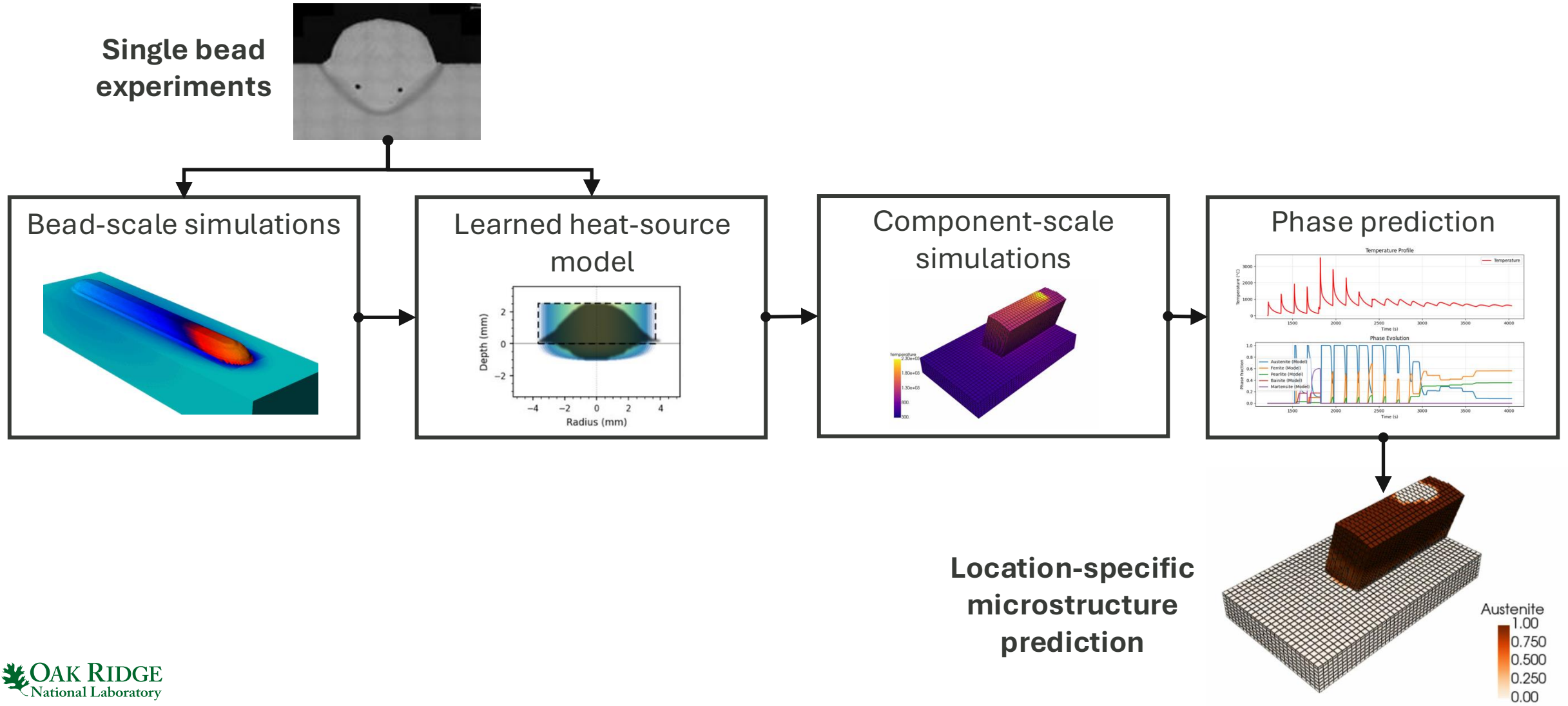
## Multiple robots are printing the part

*Simulations must support multiple heat sources and 5-axis toolpaths*

## Solid-state phase transitions matter for 410 stainless steel

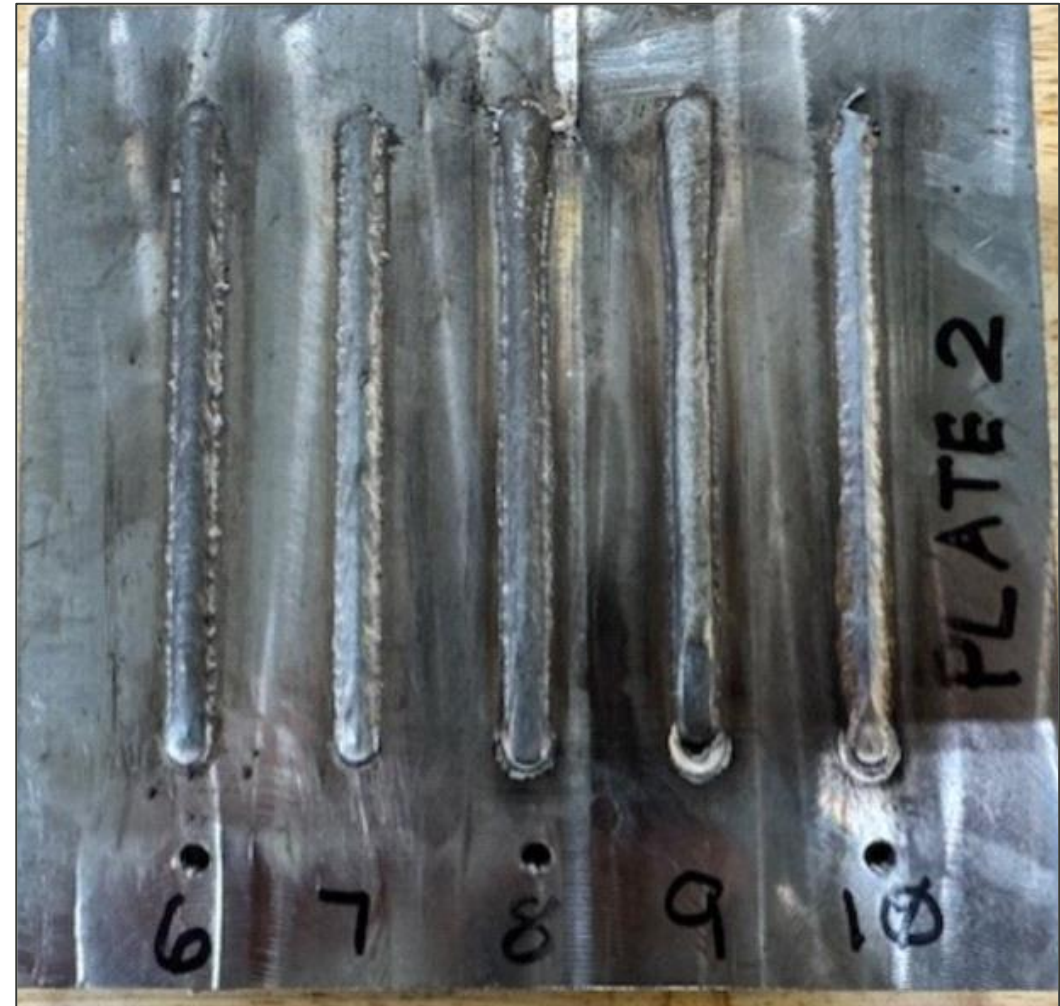
*Retained  $\delta$ -ferrite, hydrogen embrittlement in martensite, transformation strains*

# The HPC4MDF framework turns single-bead experiments into microstructure predictions across a part

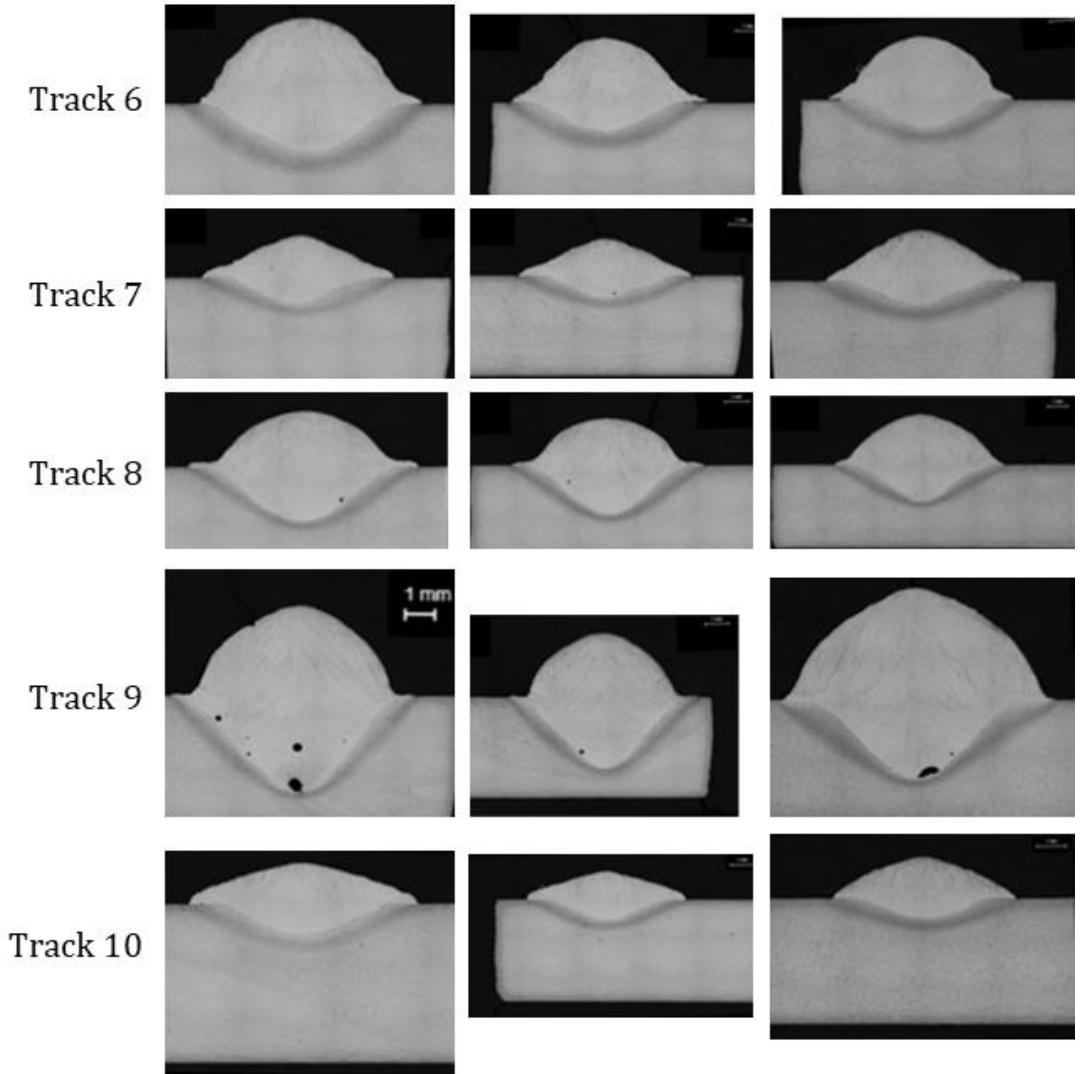
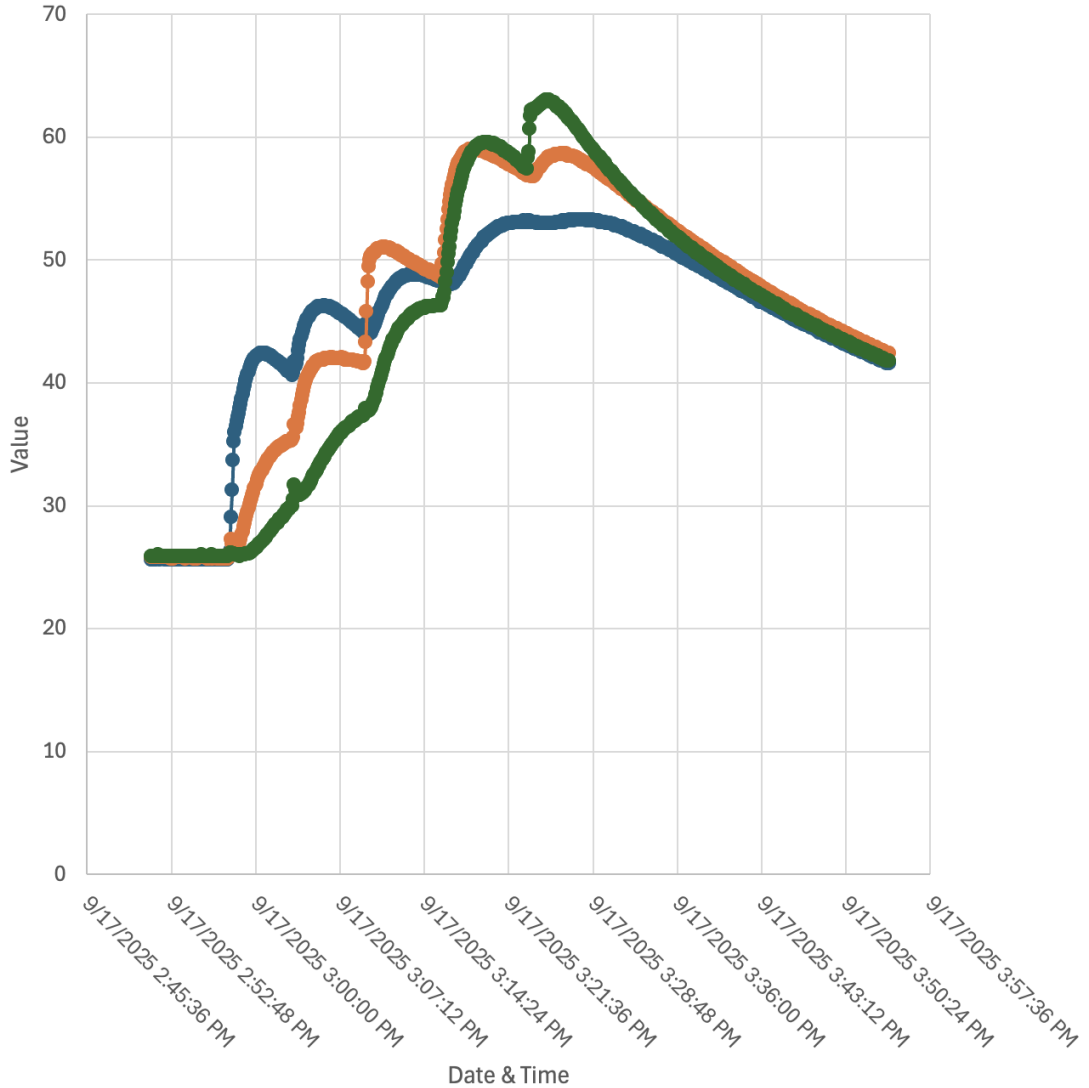


**Let's take a look at how the HPC4MDF smart manufacturing framework makes this prediction**

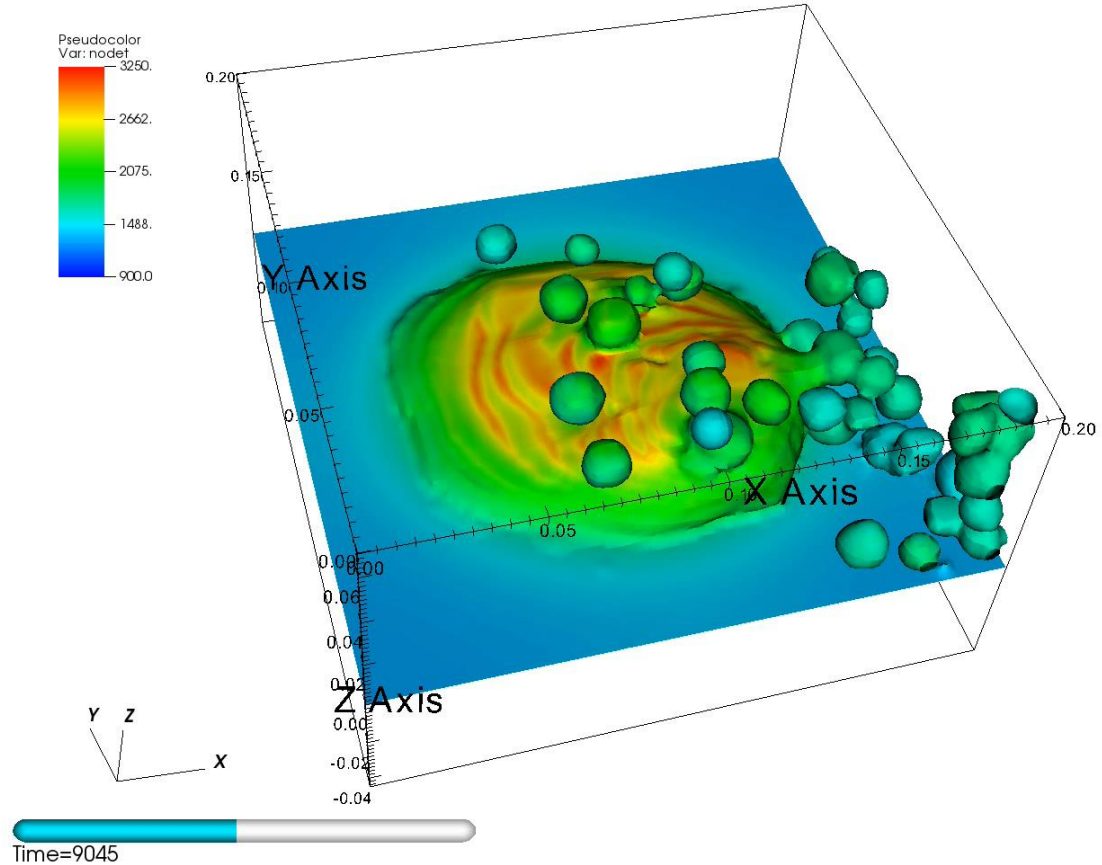
First, we performed 10 quick single-bead experiments at the MDF for a variety of travel speeds and wire feed rates



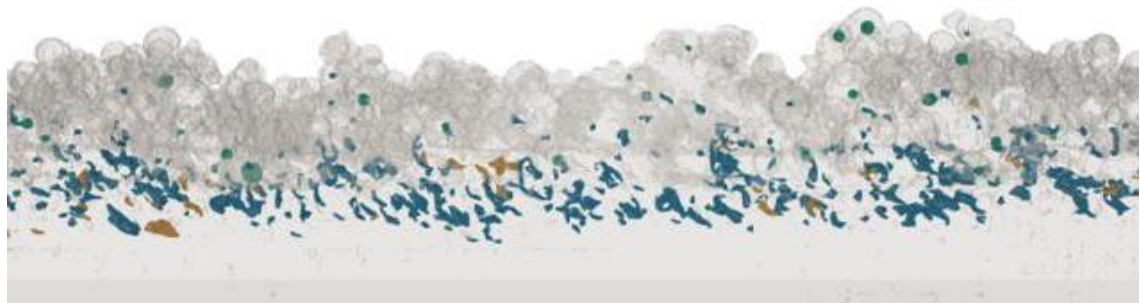
# We extracted temperature data from three thermocouples and did ex-situ bead geometry characterization






# We use LLNL's highly utilized ALE3D code to study the detailed bead geometry, leveraging past success for laser-powder DED



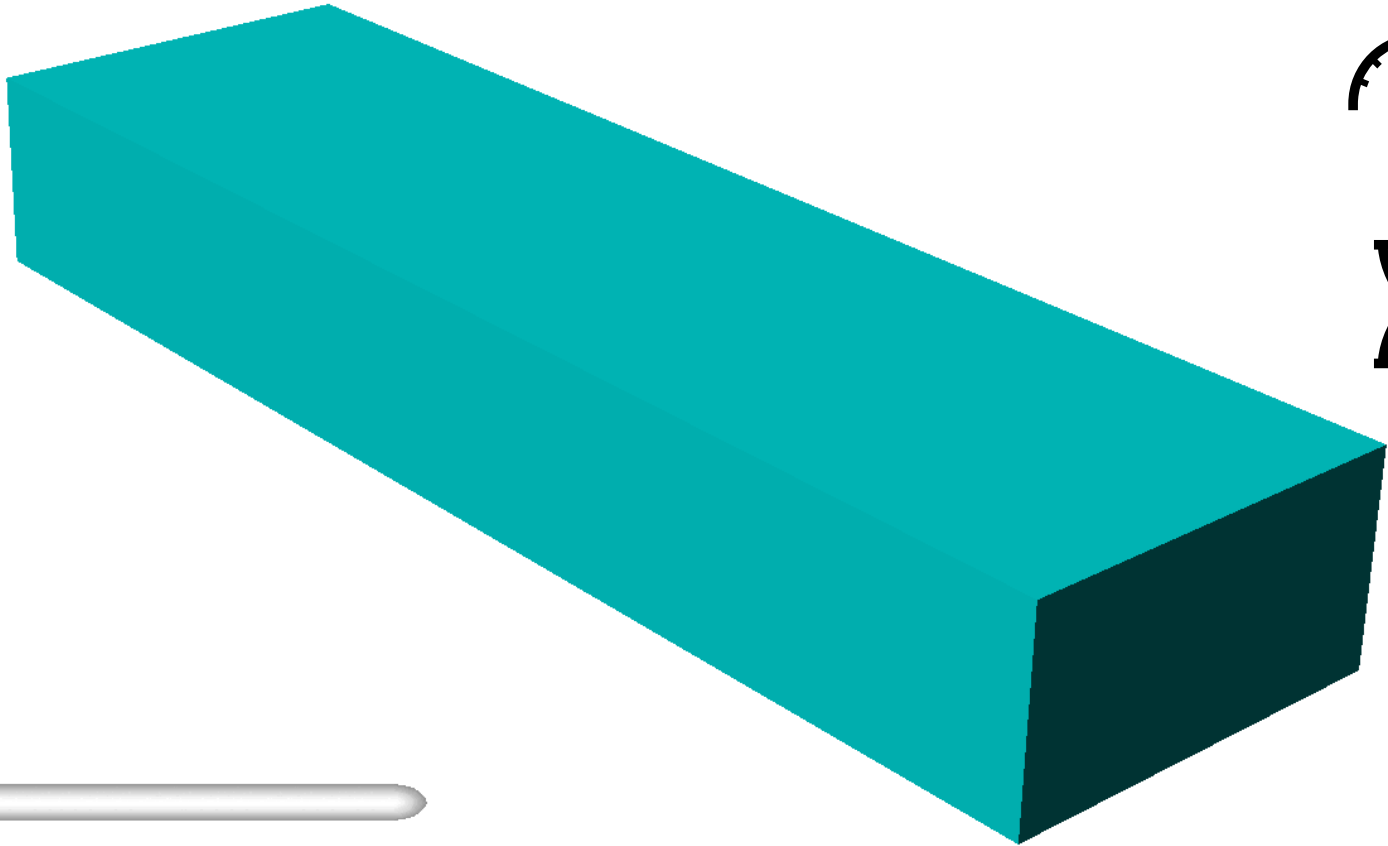
Weber et al, PNAS Vol 2, 1-9 (2023)



-  spherical pore, SnS (pores from powder)
-  non-spherical, NS (lack of fusion)
-  vapor pore, VP (air-cushioning)

# We calibrate ALE3D to reproduce the WAAM bead geometry in the experiments

Pseudocolor  
Var: tkelv  
3100.  
2400.  
1700.  
1000.  
300.0  
Max: 310.5  
Min: 298.2



Melt pool depth



Arc penetration  
New material temperature



36-108 minutes per simulation

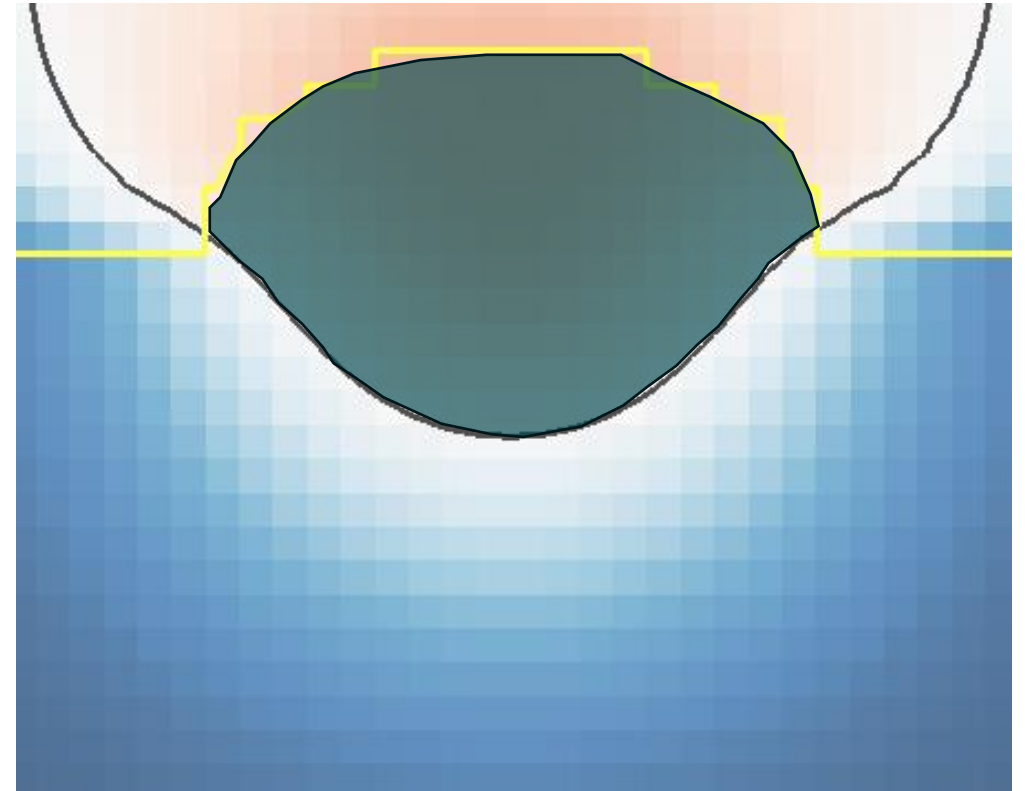


Time=1000

# Calibrating each print condition separately, simulations matched experiments within measurement uncertainty



2.61 mm



2.61 mm

# Transitioning to the component scale, we use ORNL's open-source Adamantine code



Built on **scalable, GPU-capable** libraries: deal.II, Kokkos, Trilinos, ArborX



Up to **10x faster than real-time** for thermal simulations



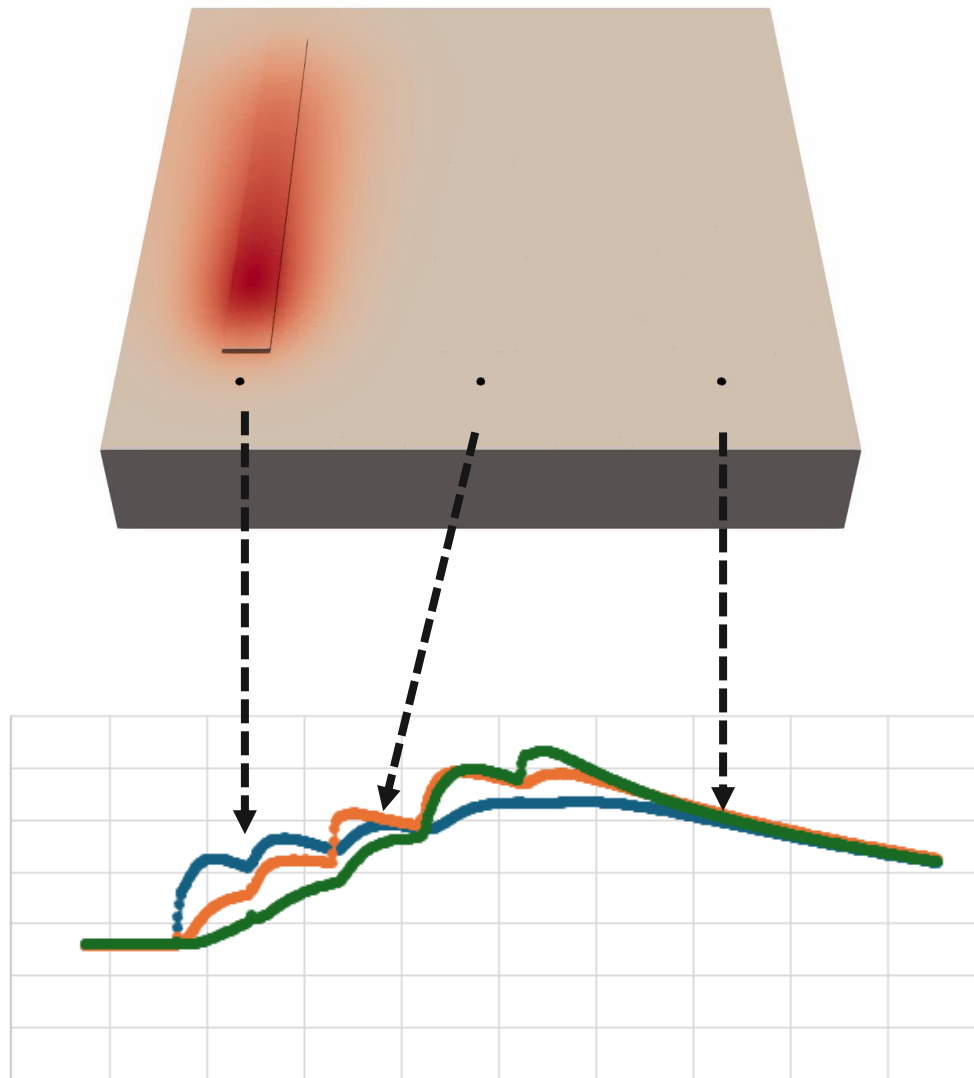
Adamantine *and its key dependencies* developed at ORNL, **we can modify and integrate at-will**



**Integrated into the MDF** digital ecosystem



# We use a two-stage process to calibrate Adamantine, starting with macroscale heat input/output from the thermocouples



Thermocouple time series

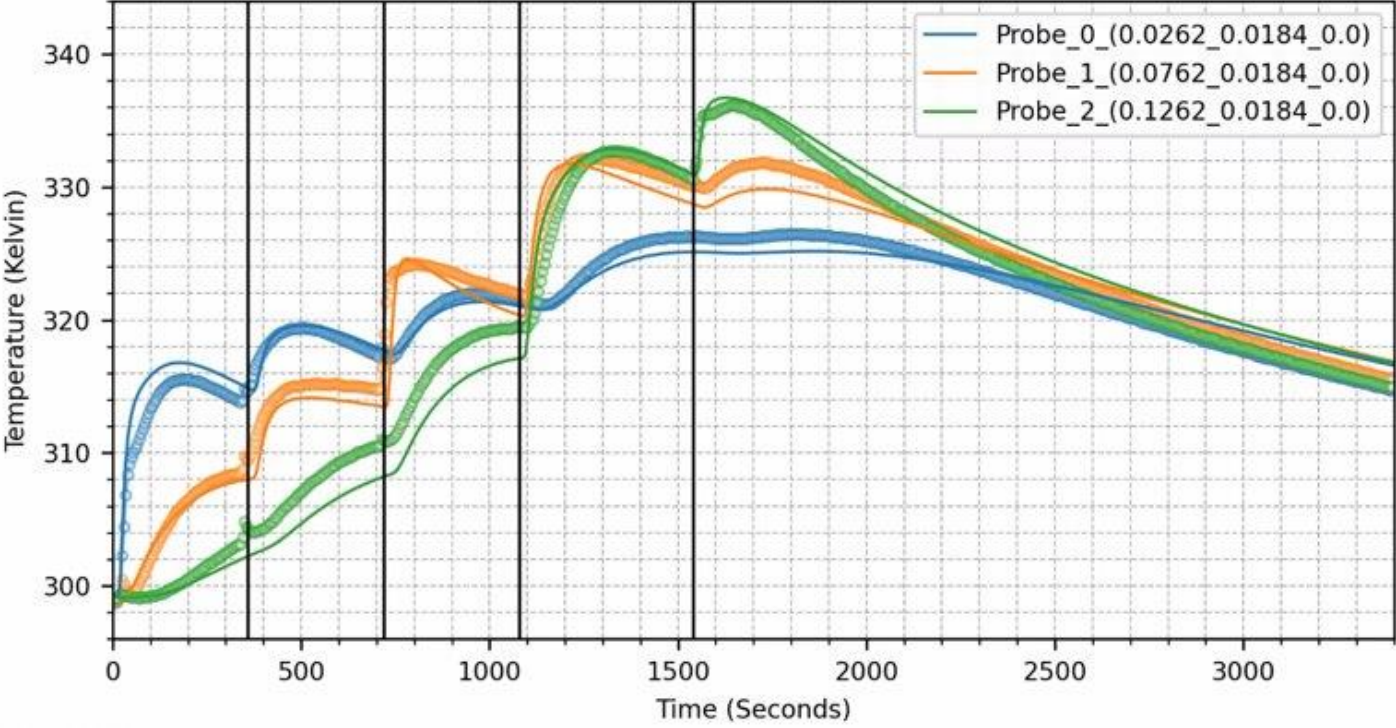
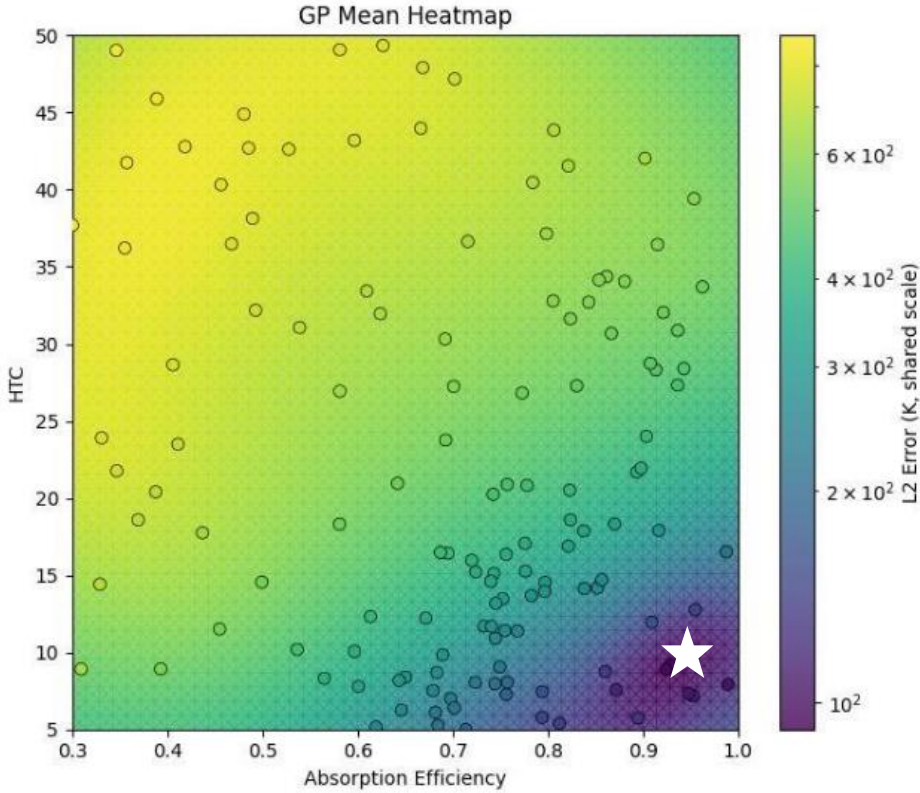


Heat source efficiency  
Convective cooling

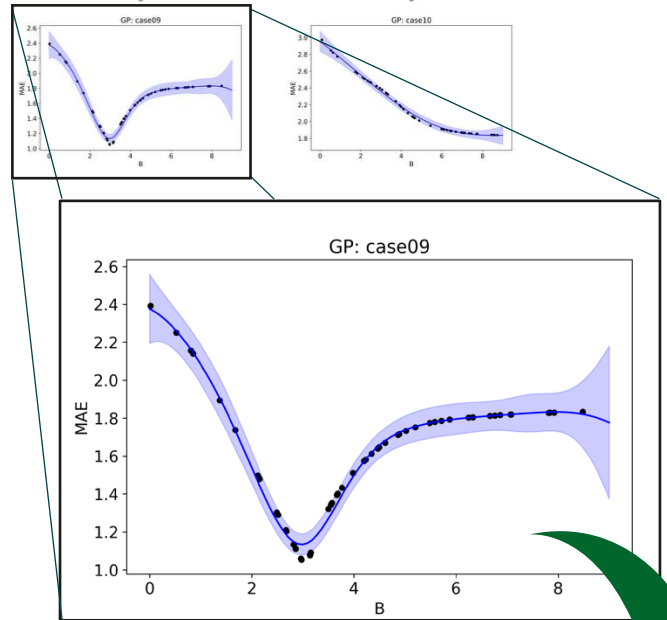
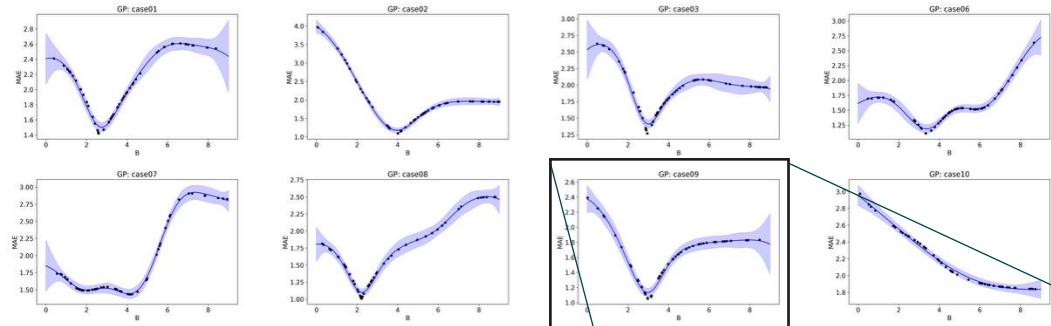


< 2 hours per simulation  
on 8 CPU cores

# We found a consistent calibration across the beads despite the coarse simulation geometry



# In the second calibration stage, we calibrate the heat source shape for each printing condition



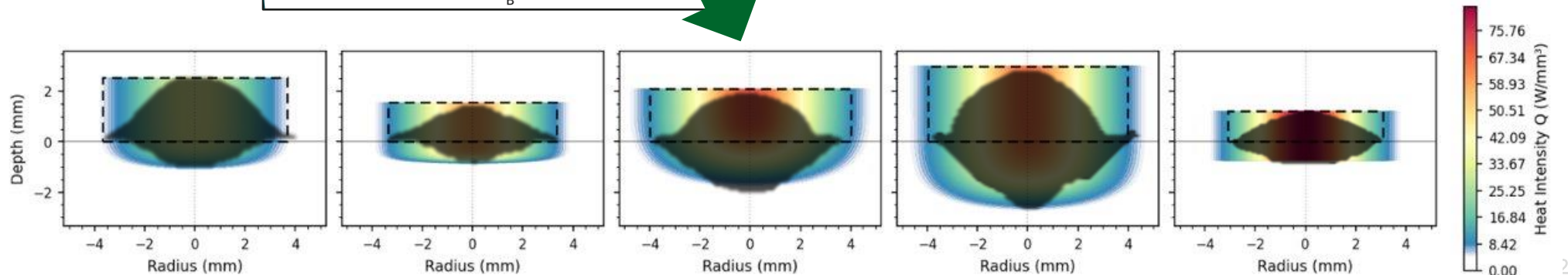
ALE3D temperature  
Experimental depth



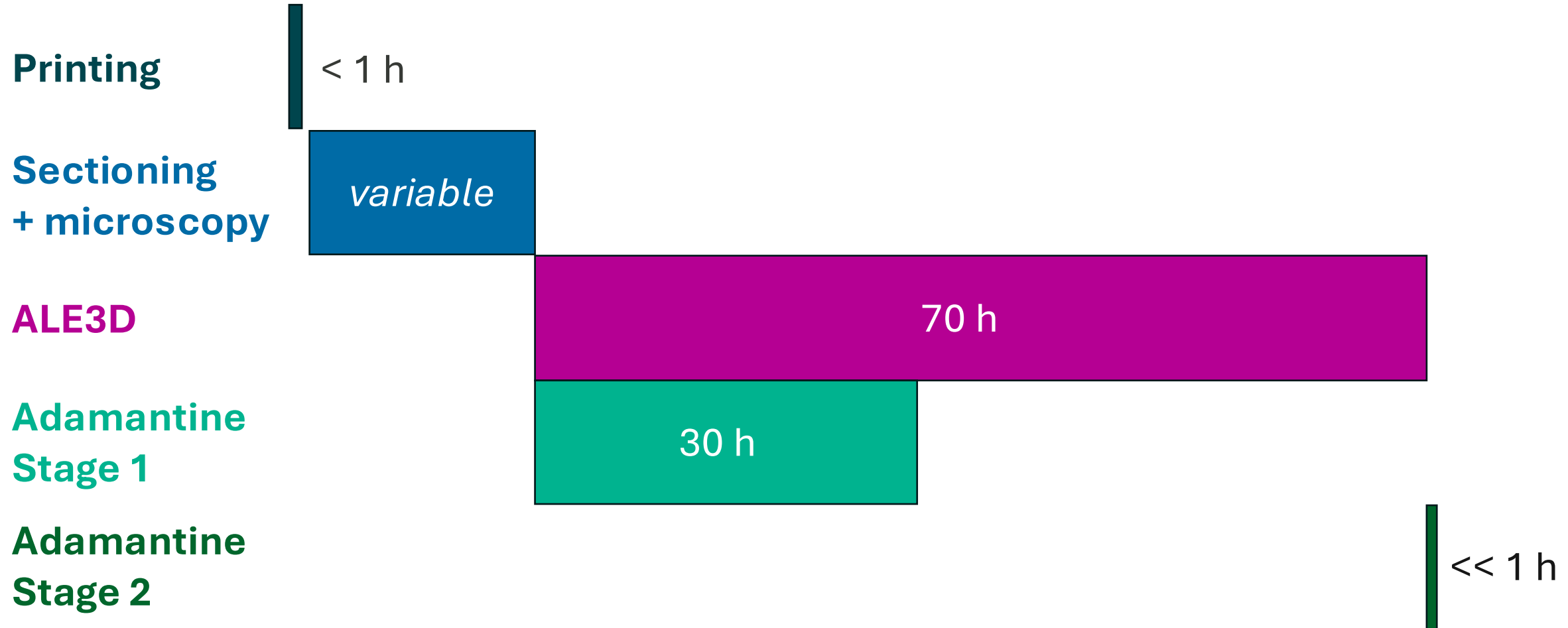
Heat source shape  
parameter



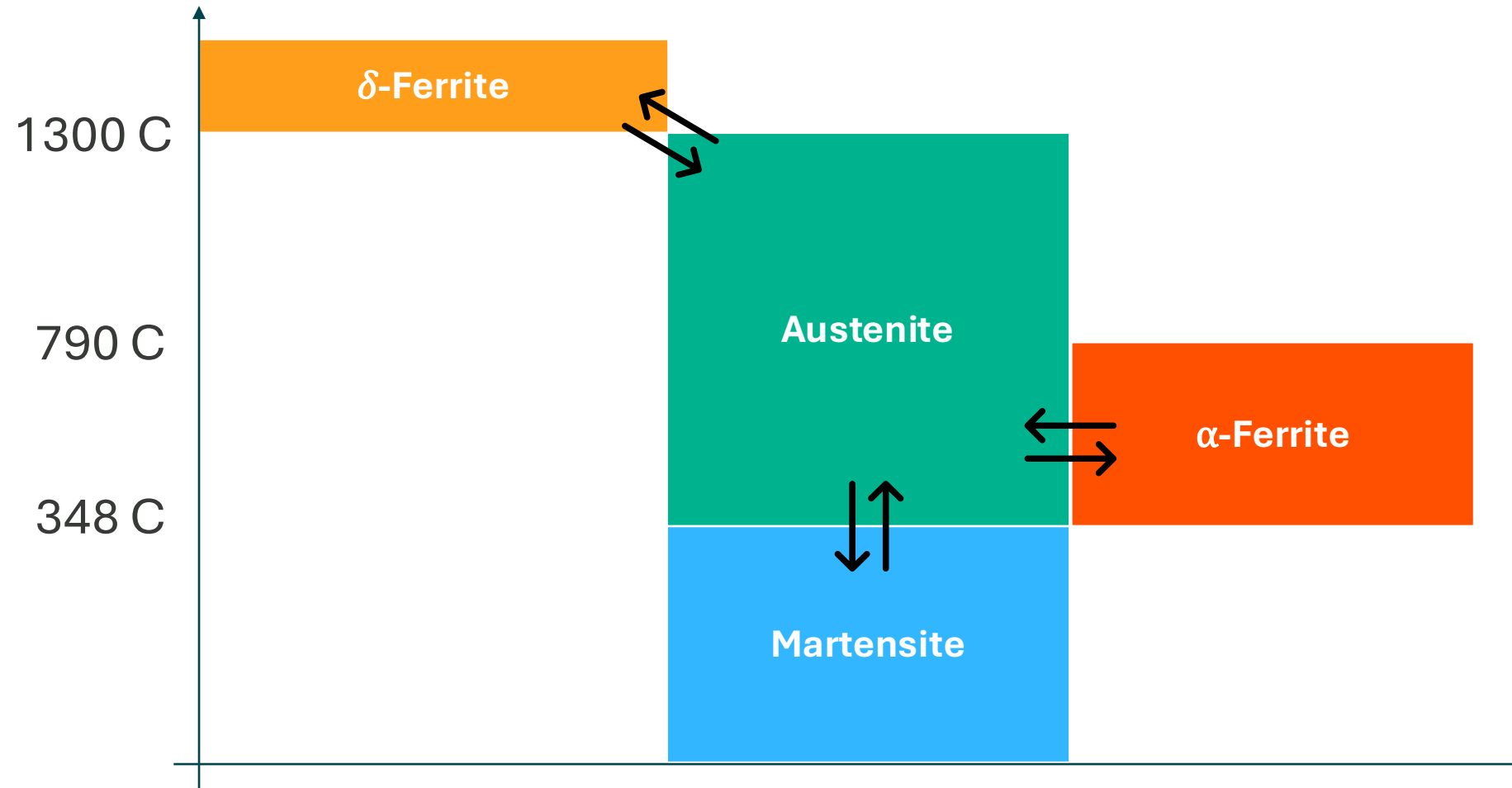
<1 second per  
simulation



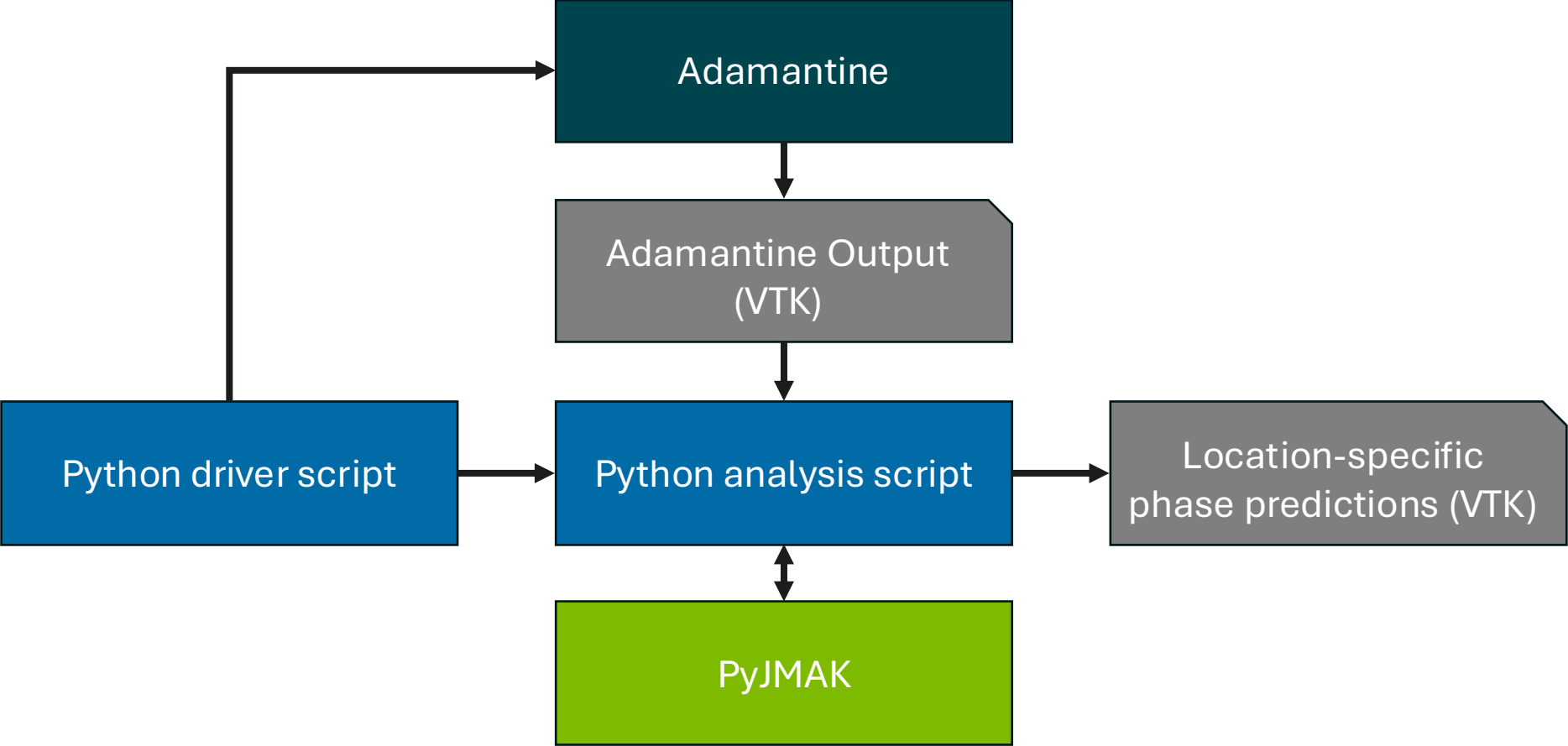
Overall, this calibration pipeline takes about 3 days of mostly passive time (neglecting sectioning and microscopy)



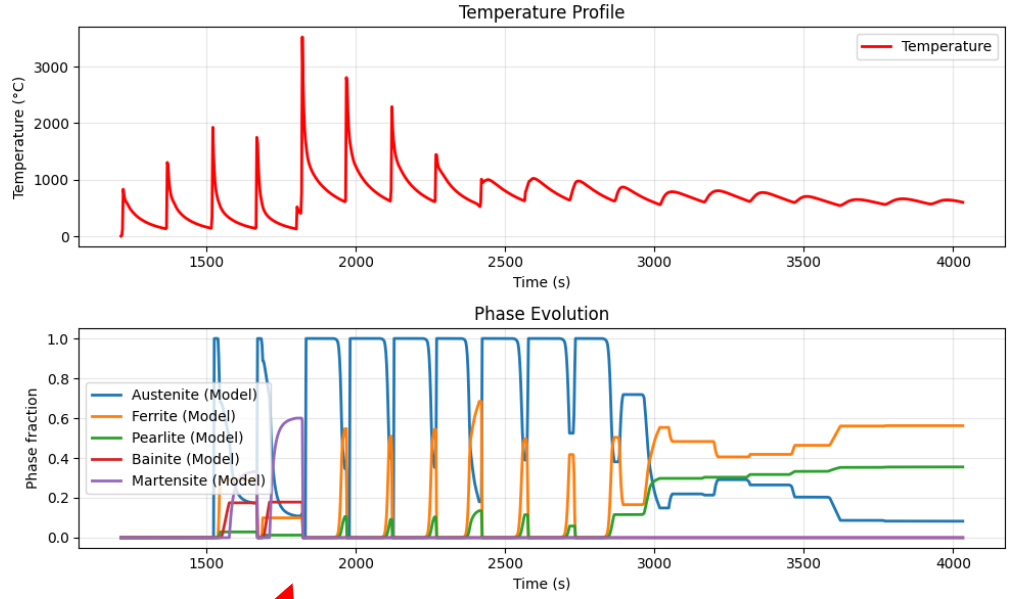
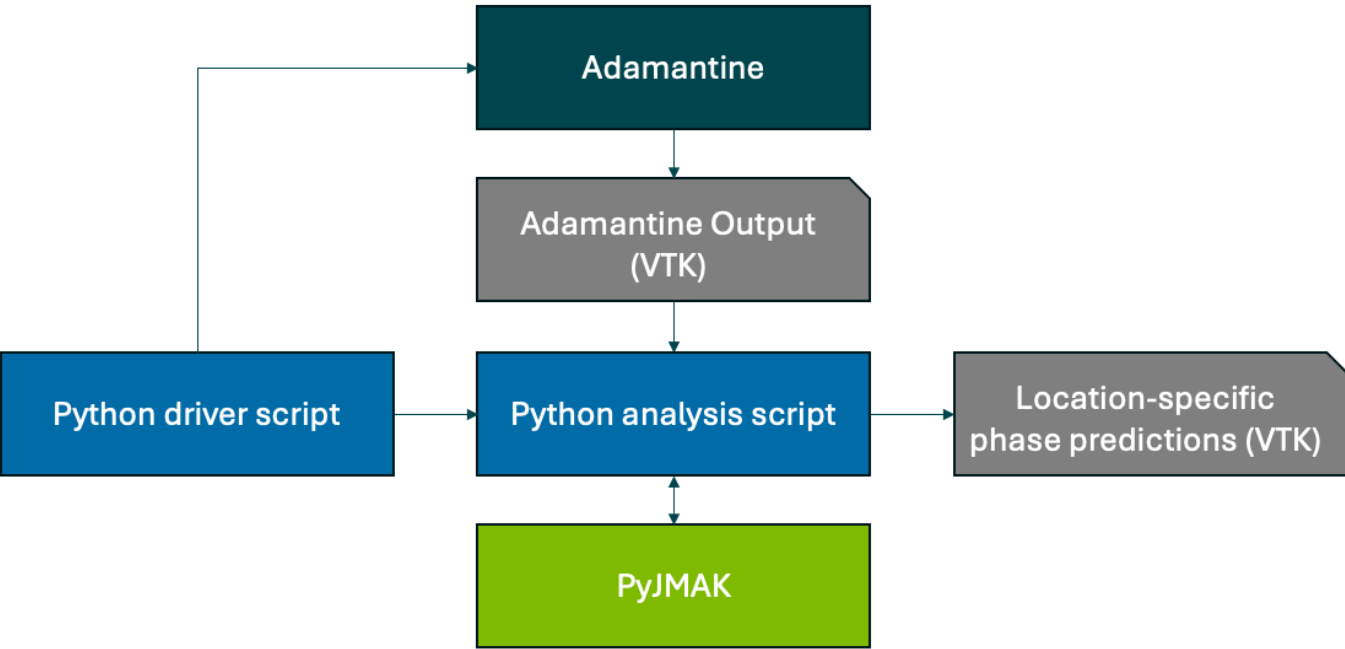
# With Adamantine calibrated, next we predict the complex phase transformations in 410NiMo stainless steel



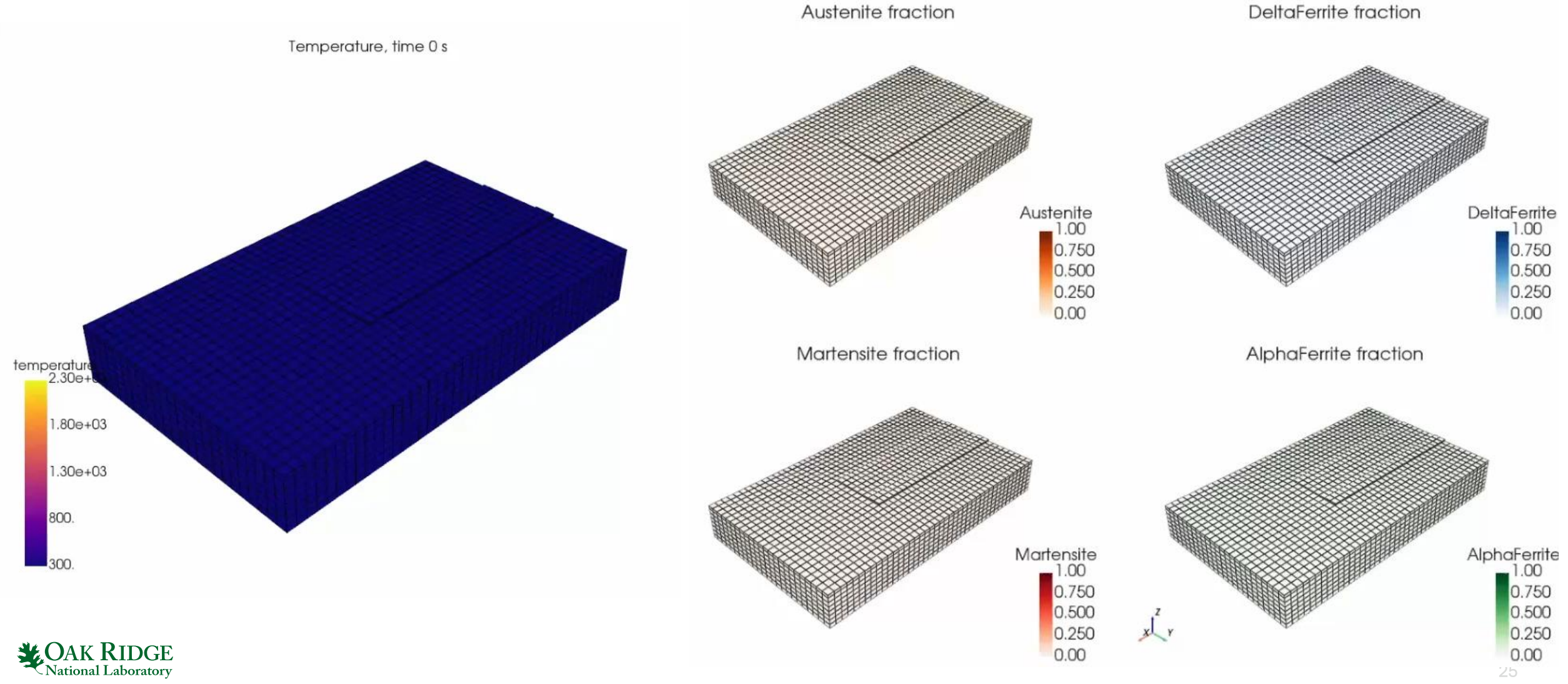
# To predict this phase evolution, we use ORNL's PyJMAK code with file-based coupling to Adamantine



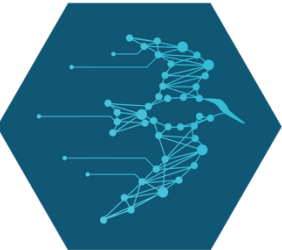
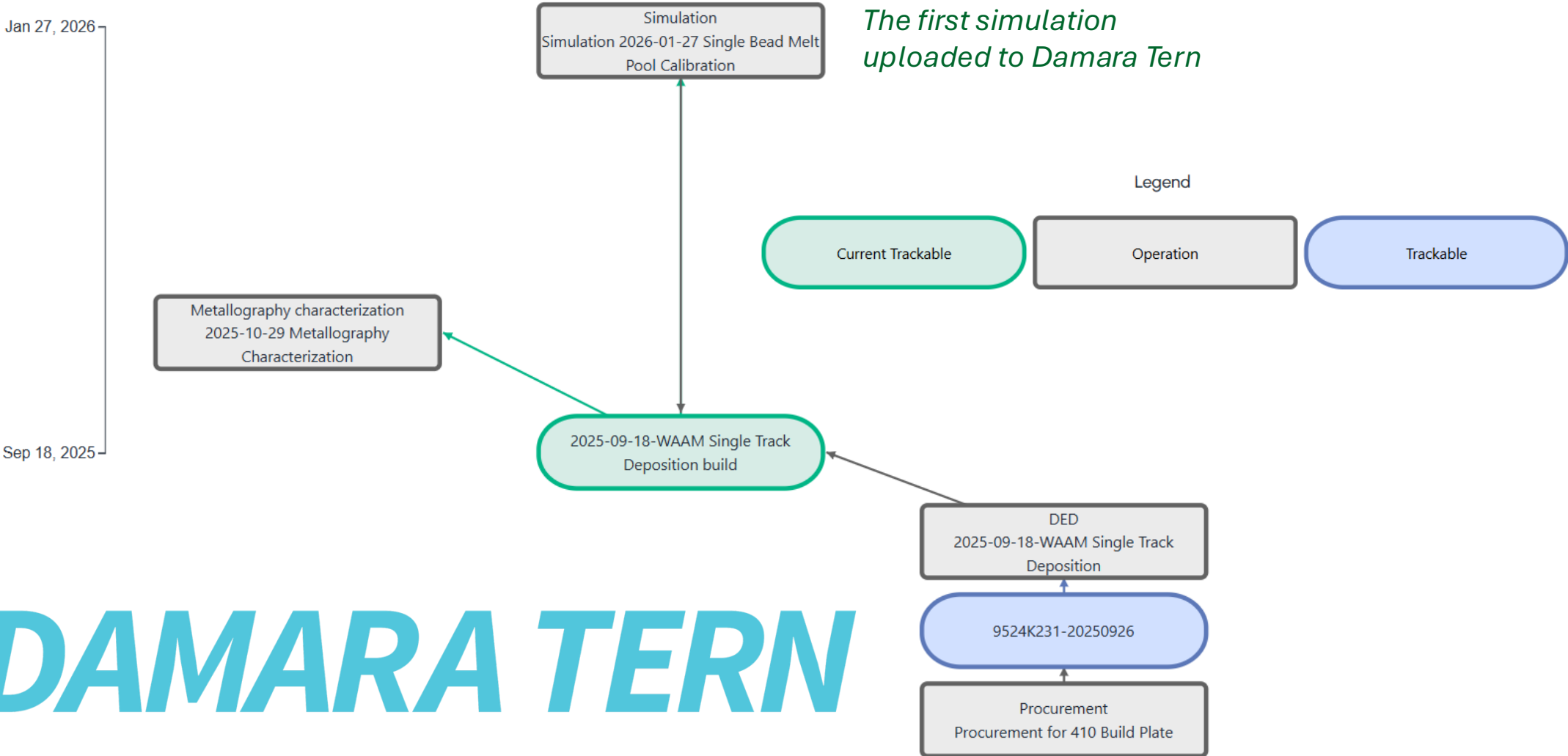
# To predict this phase evolution, we use ORNL's PyJMAK code with file-based coupling to Adamantine



# With the HPC4MDF framework, we can predict the phase fractions for the RUNNERS T-joint, with validation underway



# Throughout this workflow, we track the steps and data using the Damara Tern, the MDF's federated data platform

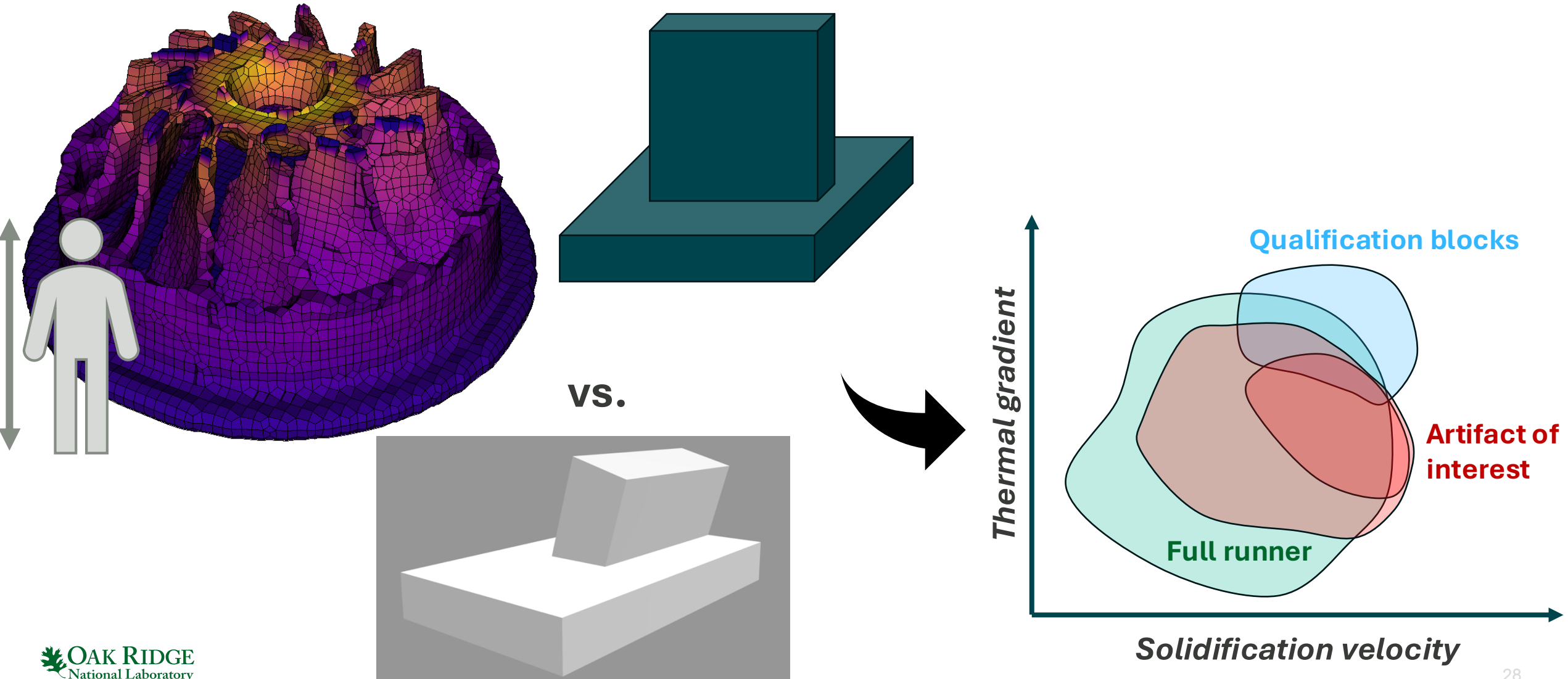


# DAMARA TERN

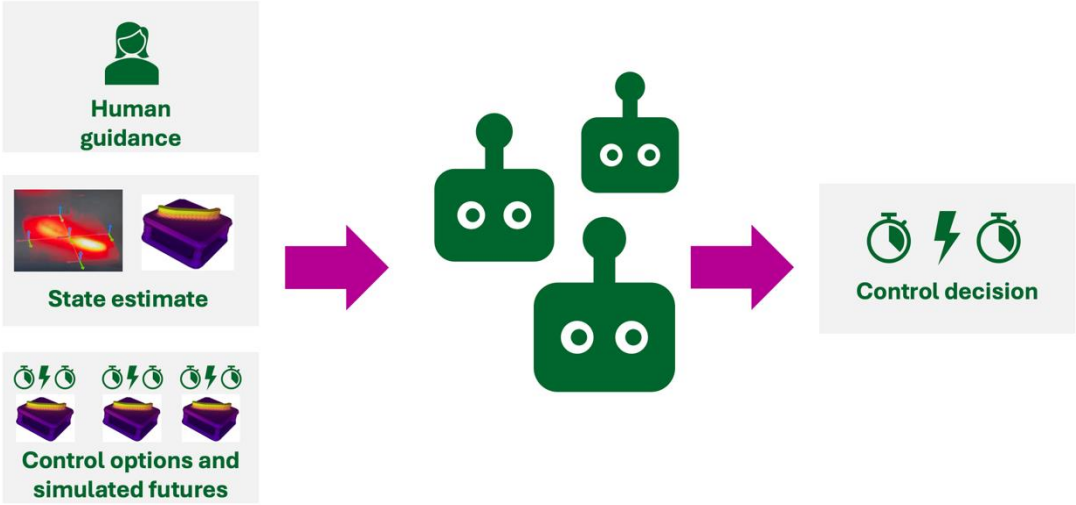
**With this new capability in place, we're  
ready to apply it and extend it further**



# We are currently using the framework to evaluate how representative qualification artifacts are of a full-size runner




# The HPC4MDF framework can be integrated into agentic workflows at the MDF, where Adamantine plays a central role



*LOOP: Agent-in-the-loop adaptive control of additive manufacturing*

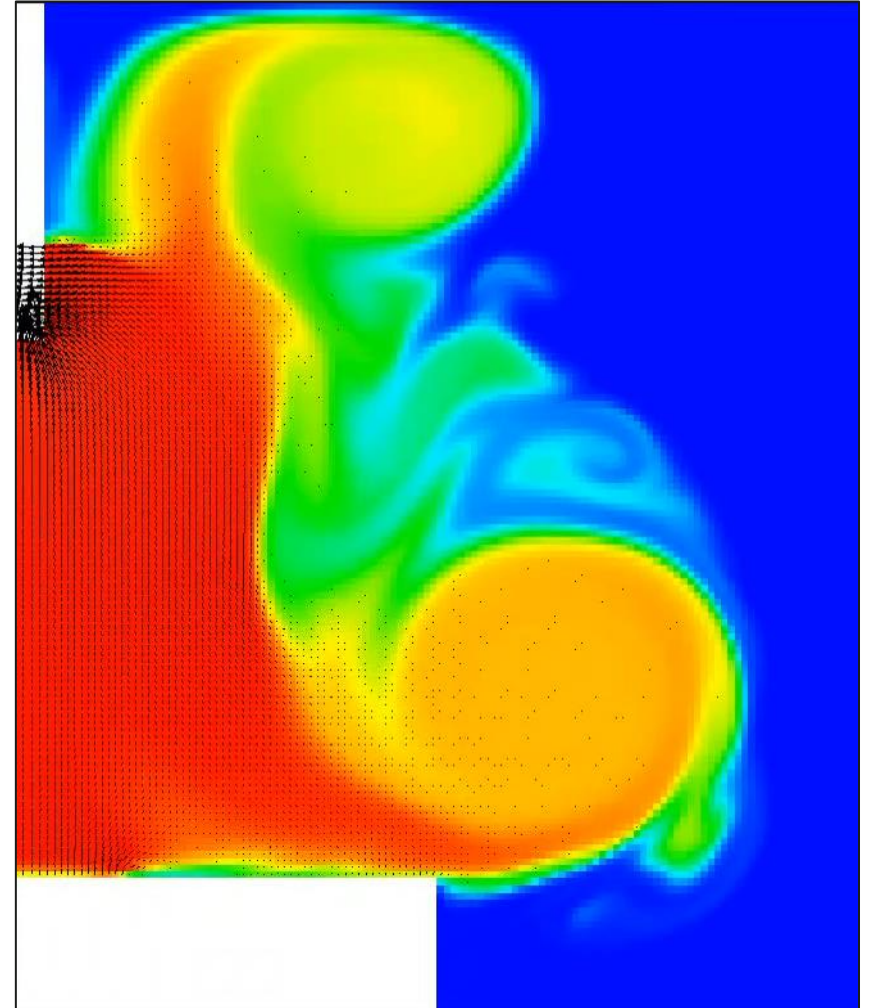
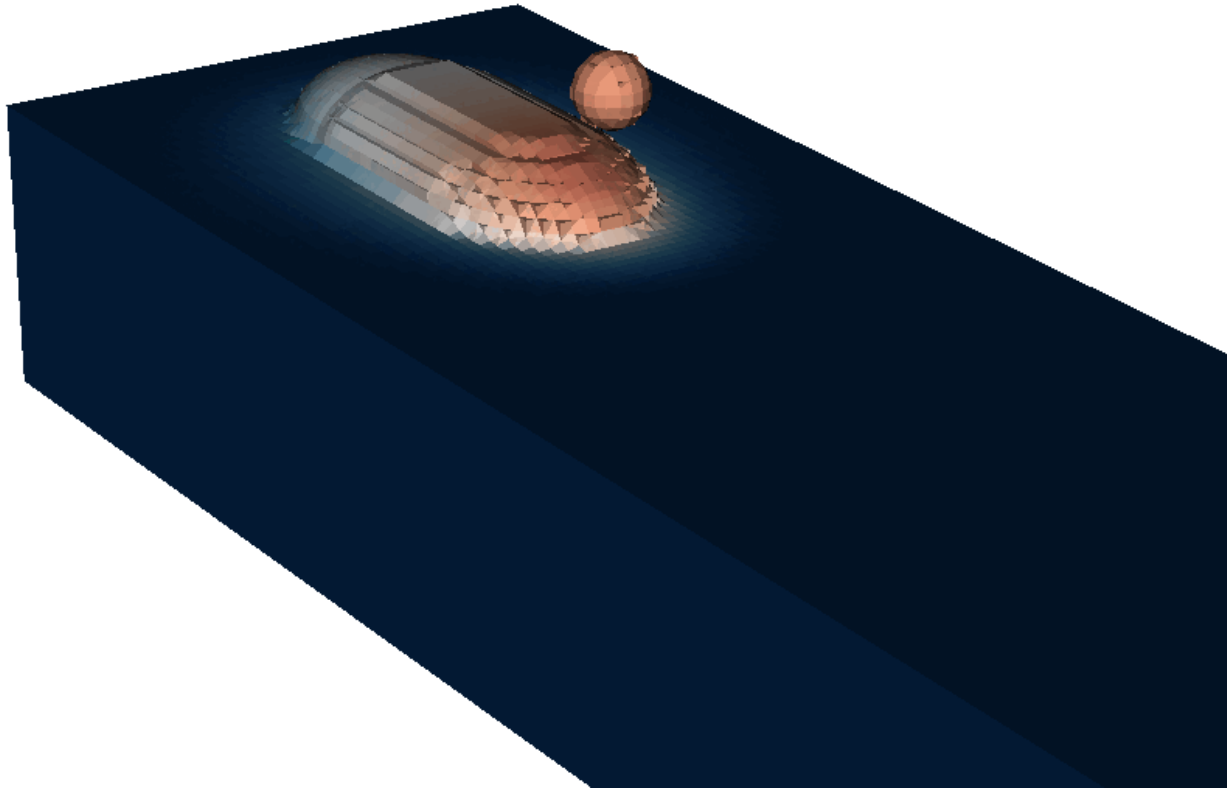
## Genesis Mission



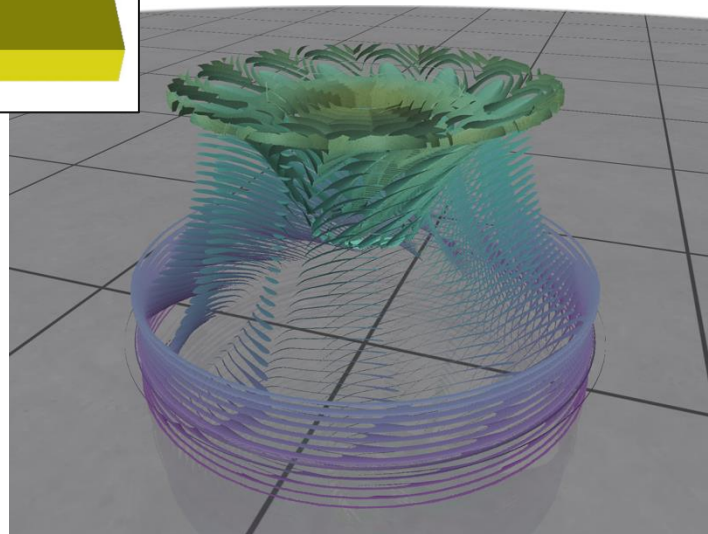
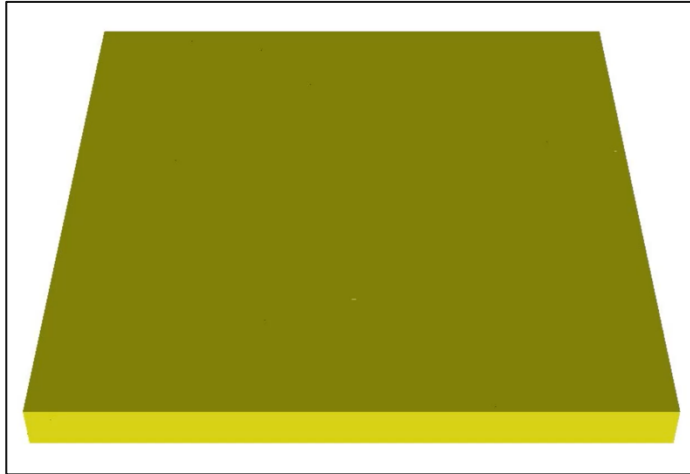
- Autonomously Designed
- Autonomously Manufactured and Constructed
- Autonomously Generated Regulatory Documents
- Autonomously Operated

*PROMETHEUS: Delivering nuclear energy that is faster, safer, cheaper*

# Moving beyond thermal simulations, the team is investigating hydrodynamics and plasma simulations with ALE3D



# In HPC4MDF we are adding initial support for 5-axis in Adamantine, but toolpath generation remains a research topic



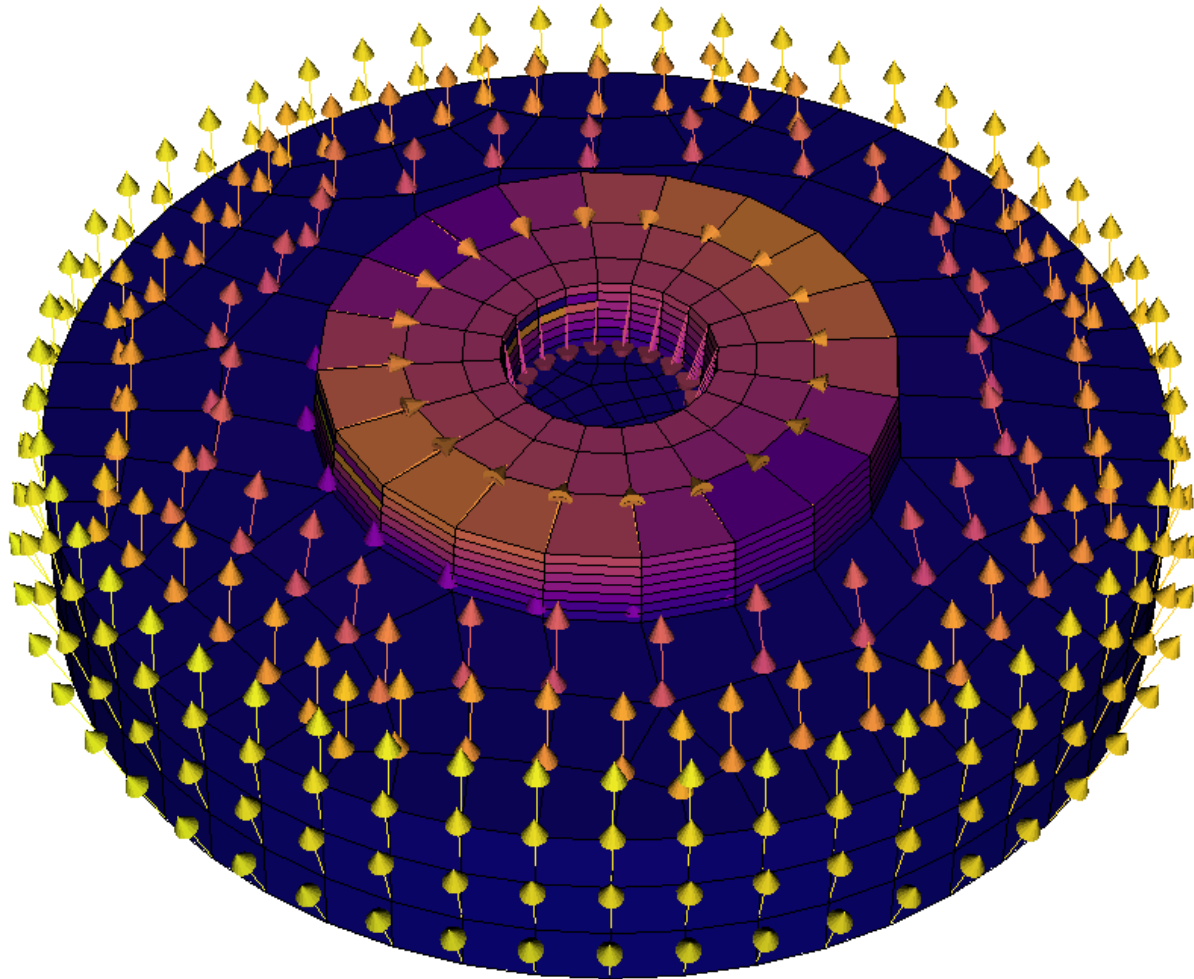
*Courtesy of Liam White (ORNL)*

Quaternion-based heat source added to Adamantine

Currently limited to rotations while the welder is off

Level-set-based methods are a promising path forward for generating toolpaths

# In HPC4MDF we are adding initial support for GPU thermoplasticity in Adamantine for distortion/residual stress

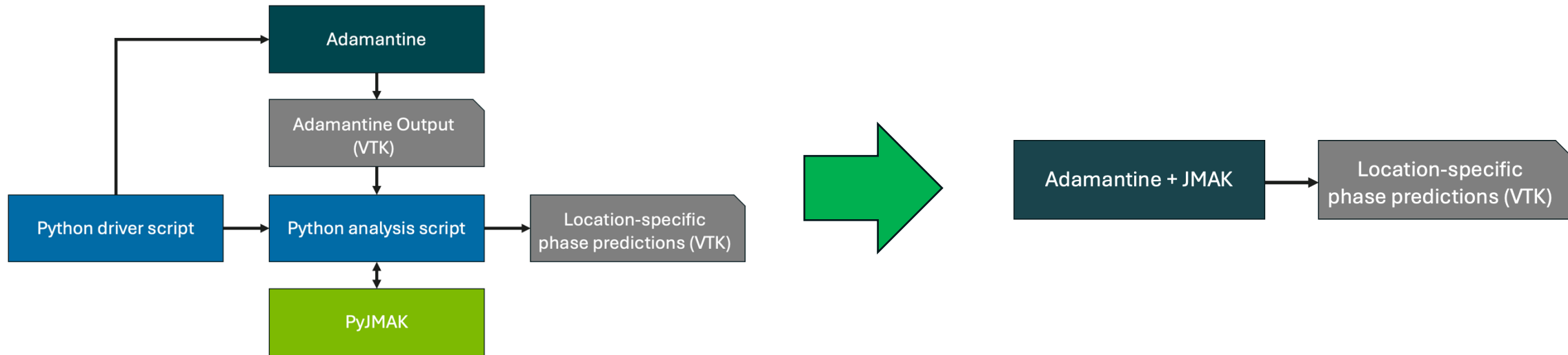


GPU-accelerated simulations running on OLCF Frontier

Currently infinitesimal strain and simple constitutive laws

Need finite strain and more complex constitutive laws

# The downsides for file-based coupling of Adamantine and PyJMAK motivate tighter integration in the future



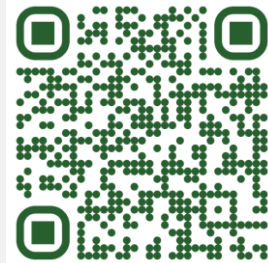
*Non-intrusive, but slow with extra bookkeeping*  
*Microstructure effects on mechanics impossible*

*Intrusive, but fast*  
*Microstructure effects on mechanics possible*

# To move US industry forward, we want to make these capabilities available to the broader community

## Component-level simulations: Adamantine

Open Source: <https://github.com/adamantine-sim/adamantine>



## Bead-level simulations: ALE3D

**Export controlled**

*Cloud version being investigated (ALE3D4I)*

## Calibration framework: Dial

Open source: <https://github.com/INTERSECT-DIAL/dial>



Distributed  
INTERSECT Active  
Learning



## Phase prediction: PyJMAK

*Open-source release in progress*

## Additional resources

<https://github.com/adamantine-sim/adamantine-tutorials>

<https://github.com/adamantine-sim/adamantine-utils>

<https://github.com/adamantine-sim/workflow-scripts>



# INNOVATION DAYS SERIES:

## *SimCamp 2025/6*

- Summer 2026
- Expanding to a 3-day event
- Covering tools for:
  - Laser processing
  - Large-scale AM
  - Microstructure evolution
  - Coupled workflows
  - ...and more!



Join the mailing list

# In summary, the new HPC4MDF smart manufacturing platform:

- 1) Provides critical capabilities for US industry, integrated into the MDF ecosystem
- 2) Serves as an insertion point to test new computational approaches going forward
- 3) Derisks development for commercial codes

