OAK RIDGE National Laboratory | MANUFACTURING DEMONSTRATION FACILITY

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Adamantine Overview

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Computational Science and Engineering

U.S. DEPARTMENT of ENERGY

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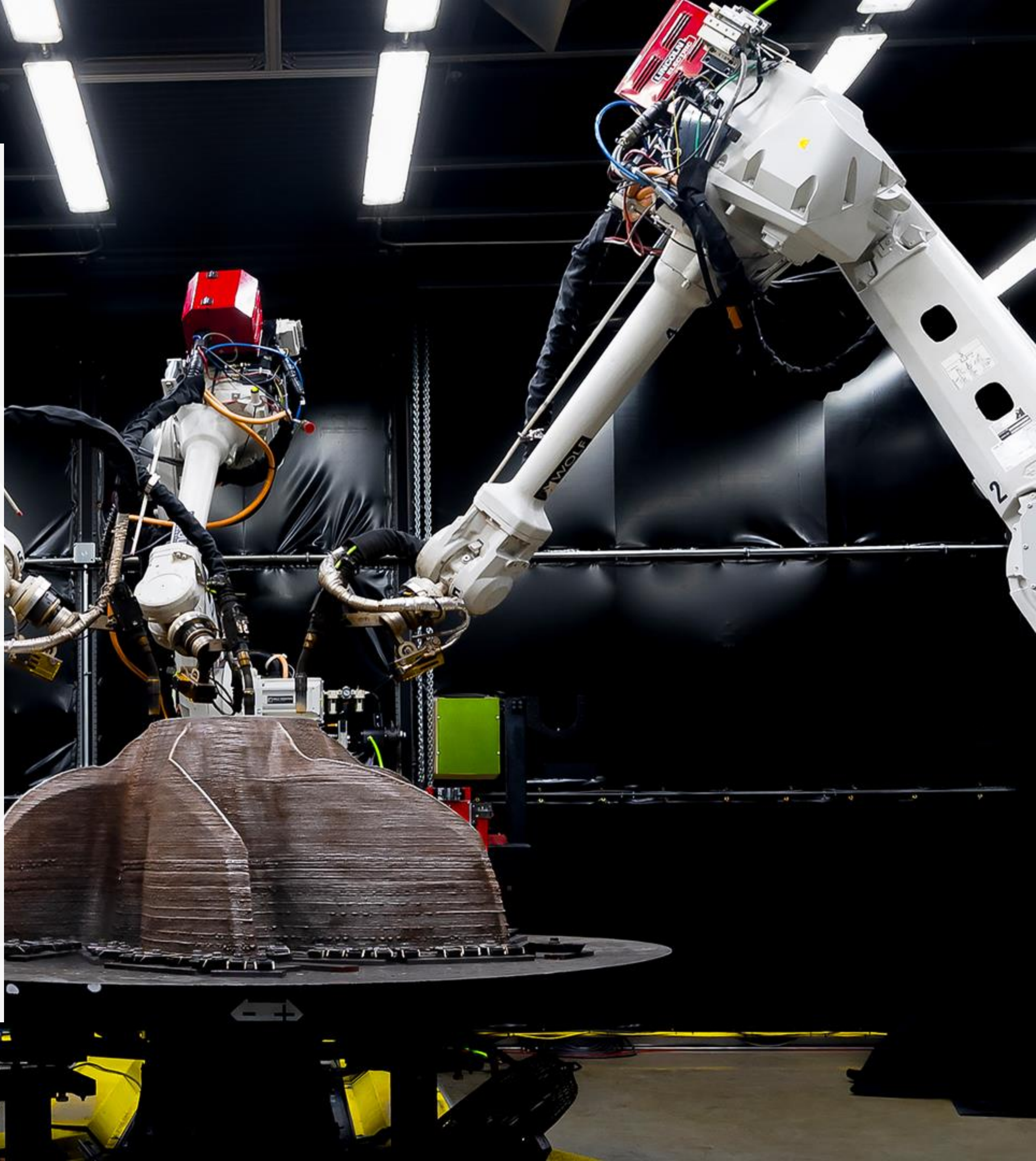
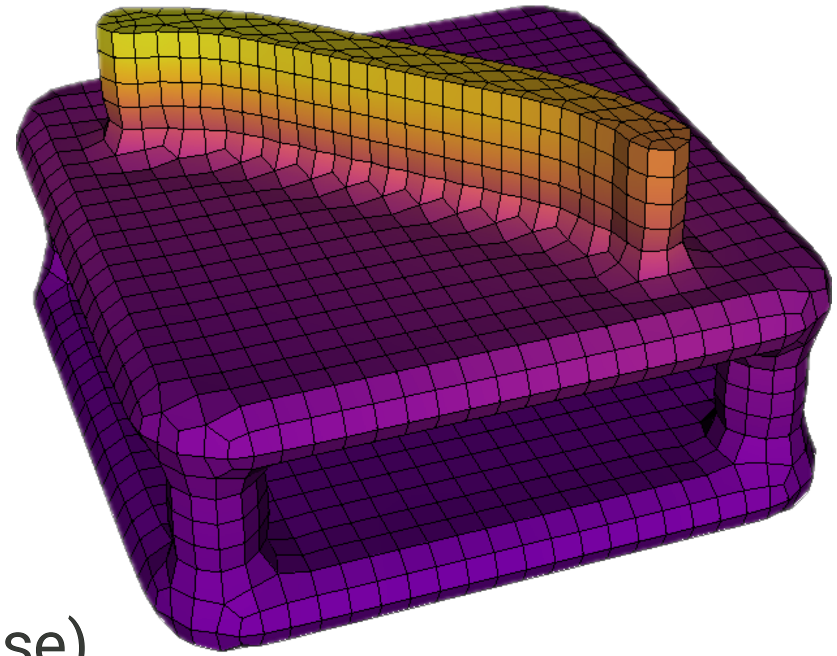


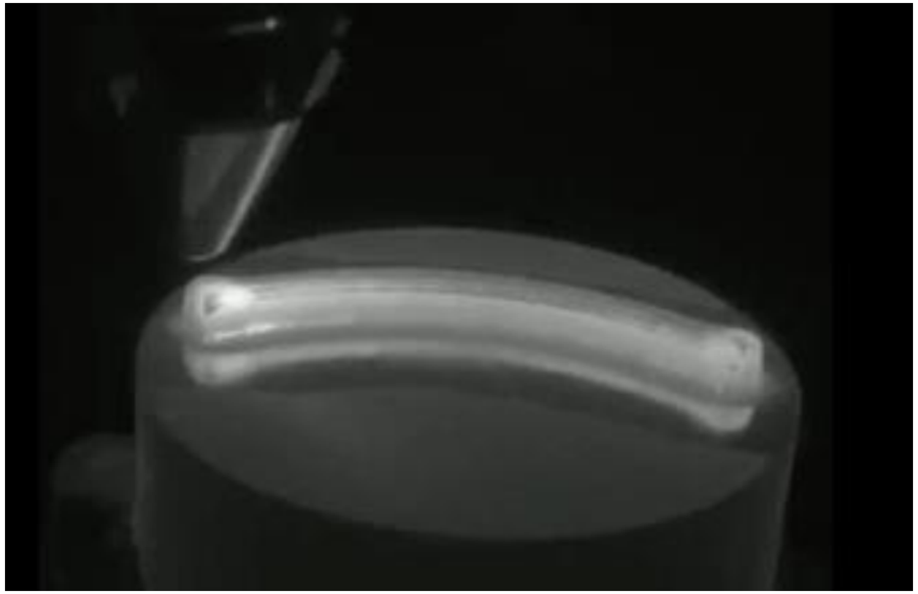
What is adamantine?

- Finite element thermomechanical code for part-scale AM
- Use temperature-dependent material properties with phase change
- Explicit in time
- Use adaptive mesh refinement
- Integrates with SCOPS
- Experimental GPU support
- License: Apache 2.0 with LLVM exception (LLVM license)
- GitHub: https://github.com/adamantine-sim/adamantine
- Website: https://adamantine-sim.github.io/adamantine



Our goal: Monitoring printing with a real-time digital twin

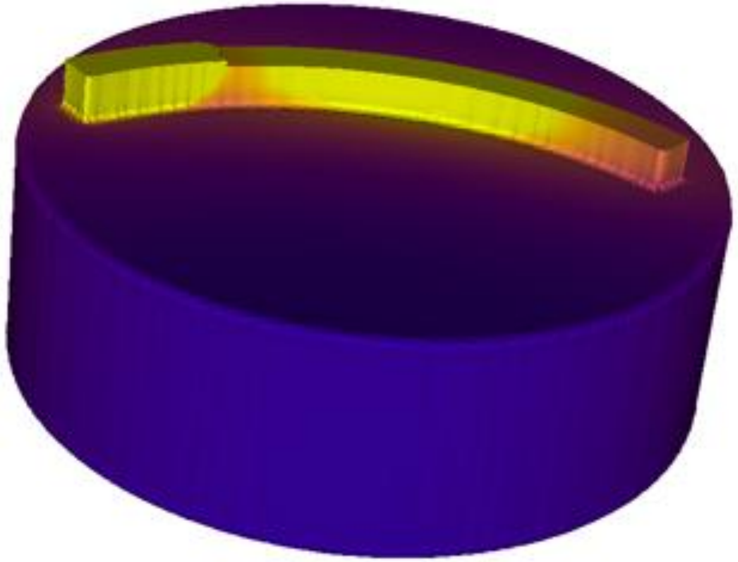
In-situ observations



Tied to reality
Only part of the outer surface

+

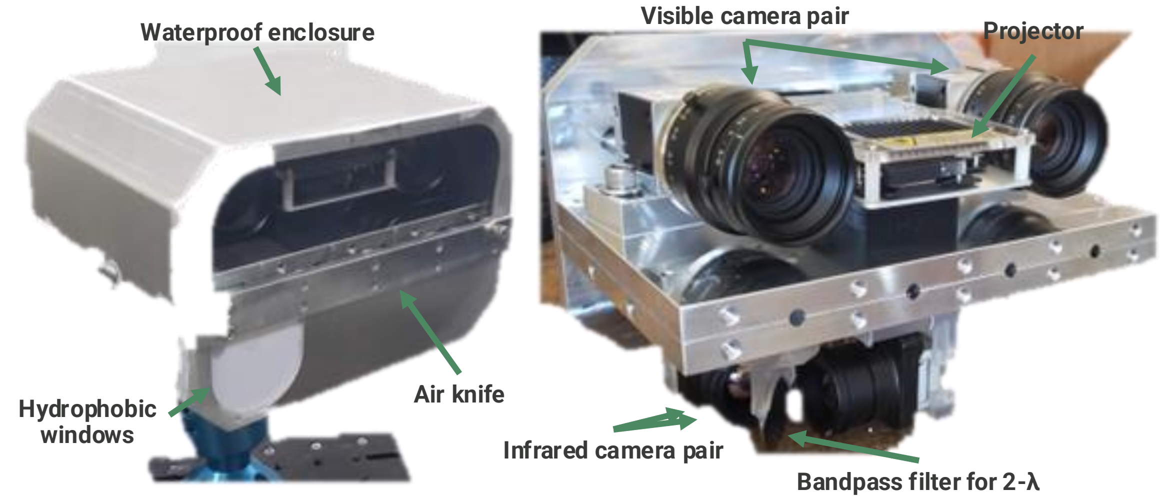
Simulations

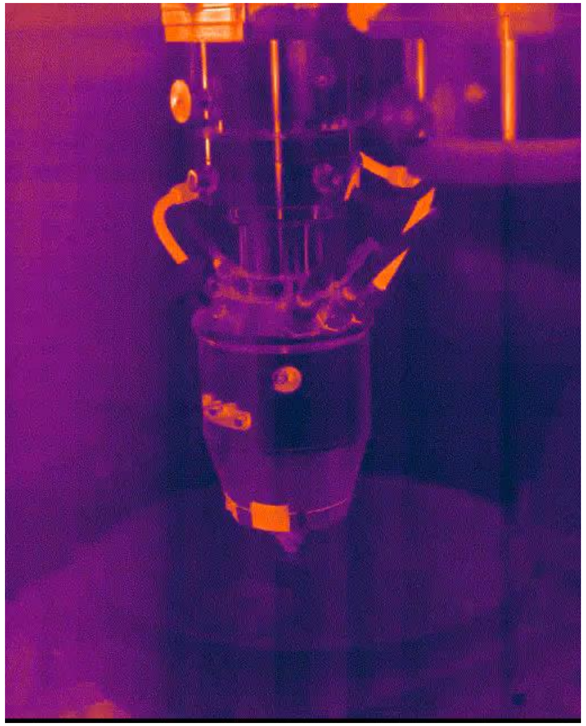


Not tied to reality
Full 3D volume

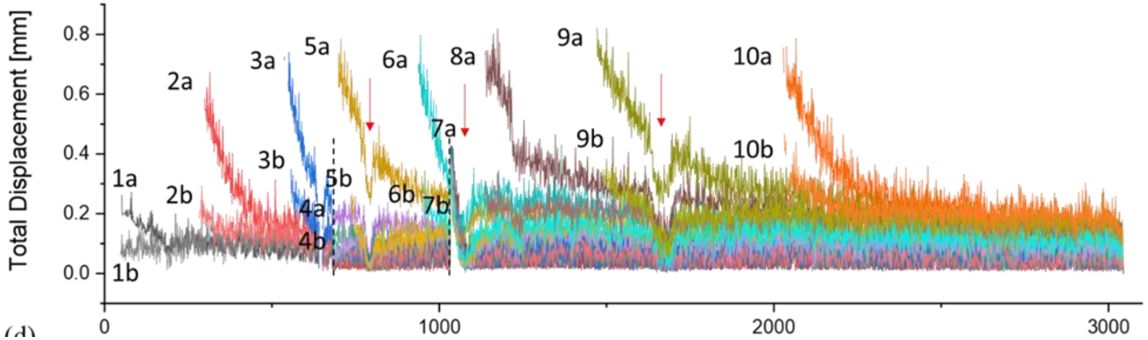
Together, estimate tied to reality for the full 3D volume

SCOPS: Stereo Correlated Optical and Pyrometric Sensing



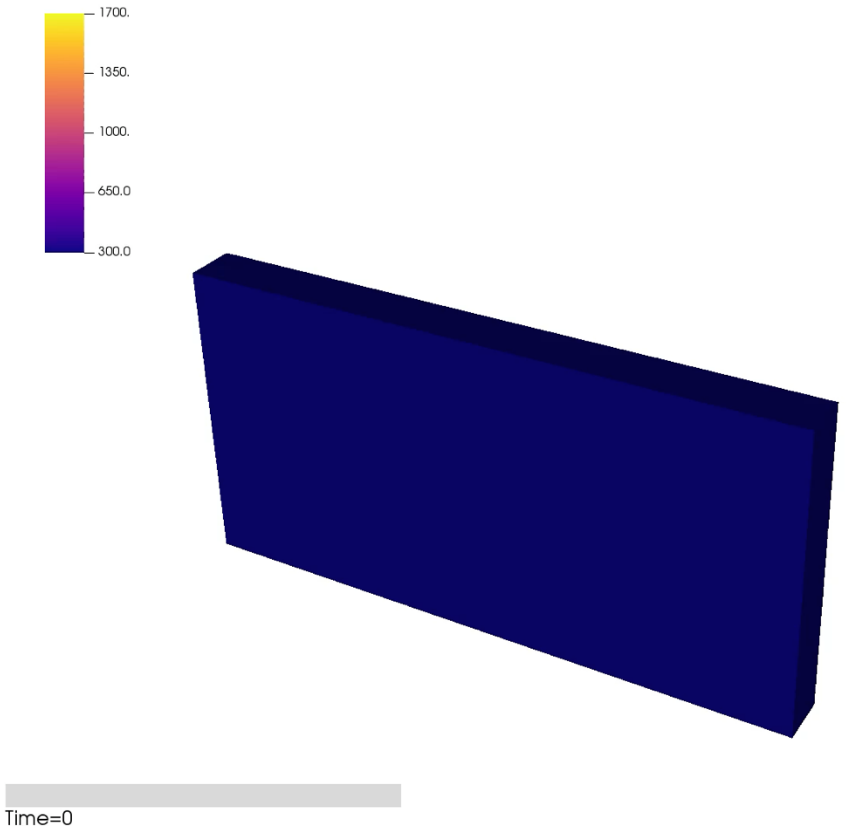


- Directed Energy Deposition welding induces distortion.
  Control requires measurement.
  - DIC tracks surface roughness features in 3D, IR tracks temperature over time
  - *Thermoplastic* history observed
- Imaging enhances simulation.
  - Validation, or *assimilation*
- Works for all DED classes



Faster than real time simulation

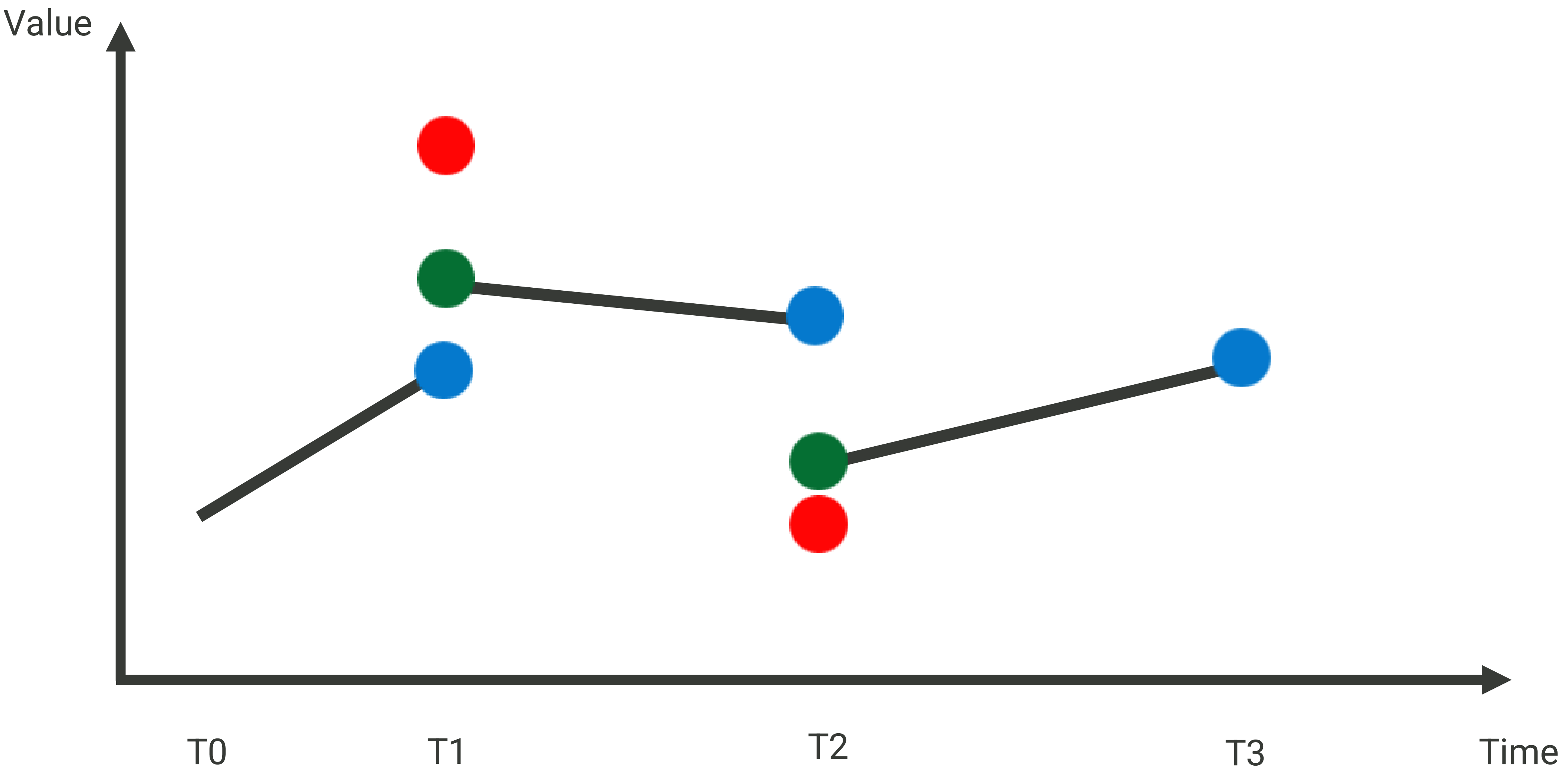
- Fast simulations are necessary to
  - Assimilate data in real-time
  - Close the loop and have simulations guide the printing process
- Simulation must be at least 3X faster than real time
- Extensive use of matrix-free algorithms and vectorization



Combining experimental data and simulation with data assimilation

- "Data assimilation is the approximation of the true state of some physical system at a given time by combining time-distributed observations with a dynamical model in an optimal way" (Data Assimilation Methods, Algorithms, and Applications by Marc Asch, Marc Bocquet, and Maelle Nodet)
- First developed for weather forecast
- Two main classes of methods: statistical methods and variational methods

Combining experimental data and simulation with data assimilation



Stochastic Ensemble Kalman Filter

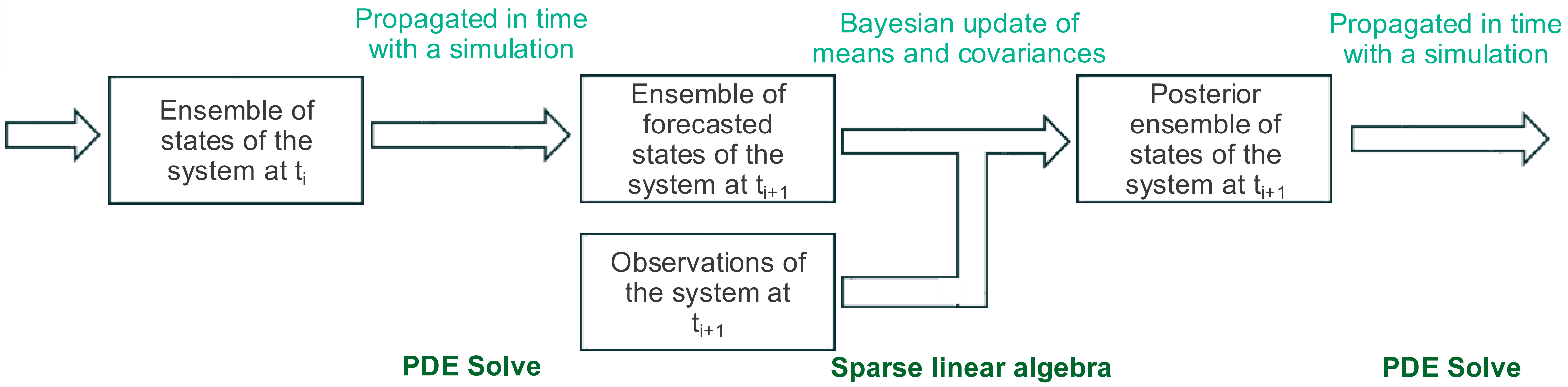
- Covariance approximated by sample covariance from an ensemble of simulations
- Random perturbations added to simulated and observed states
- Assimilation yields an updated ensemble of states consistent with both simulations and observations

$$x_i^a = x_i^f + K[y - Hx_i^f]$$
$$K = P^f H^T \left(HP^f H^T + R\right)^{-1}$$

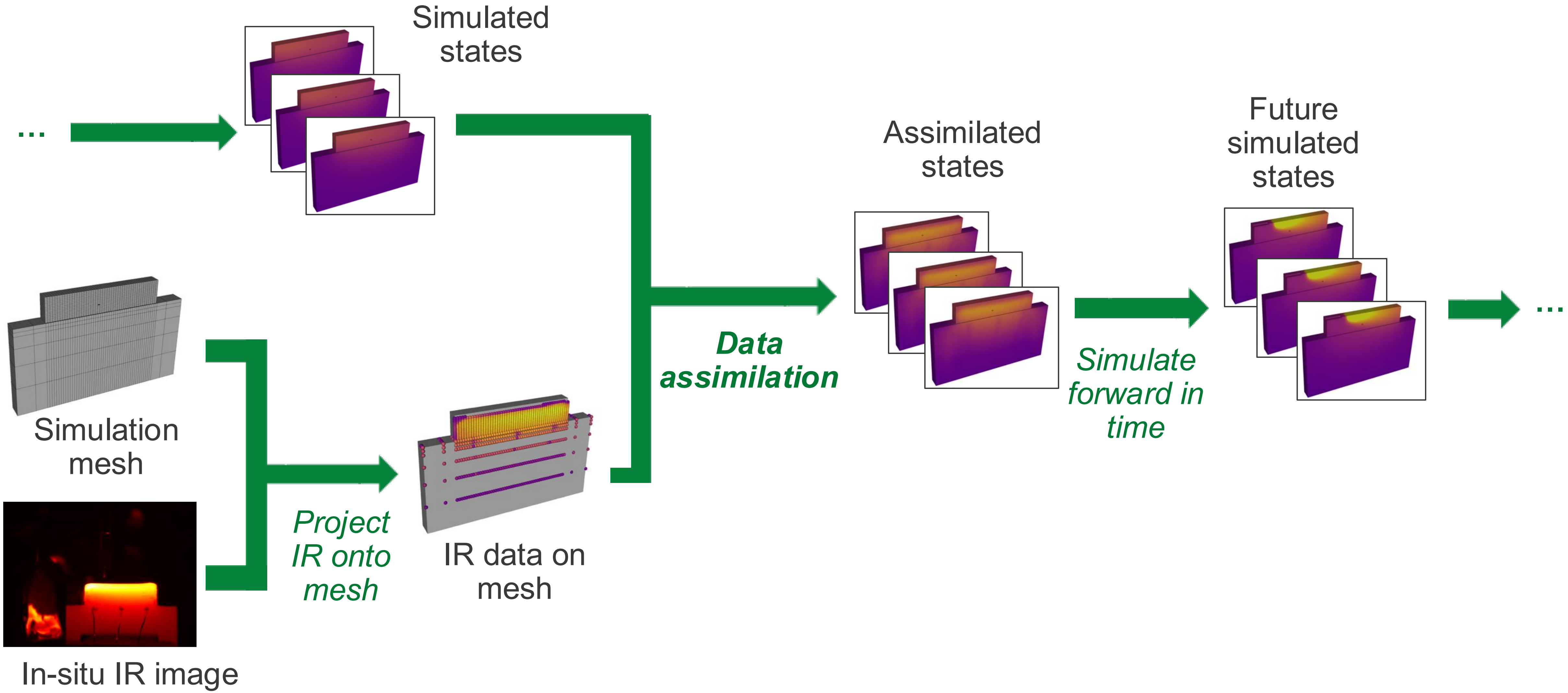
x_i^a: Updated states K: Kalman gain P: Simulation error covariance H: Observation matrix

x_i^f: Simulated states y: Observations R: Observation error covariance

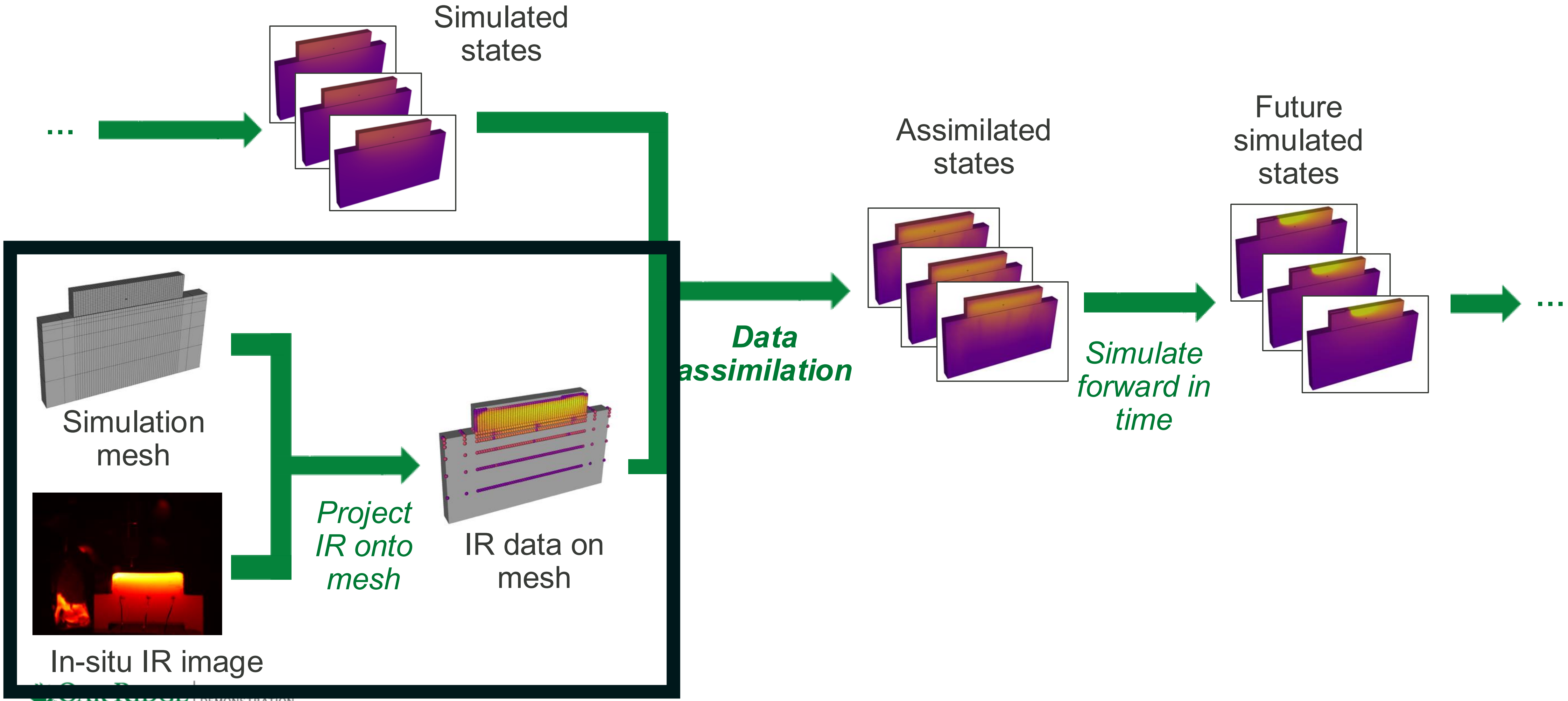
Data assimilation workflow



Data assimilation workflow



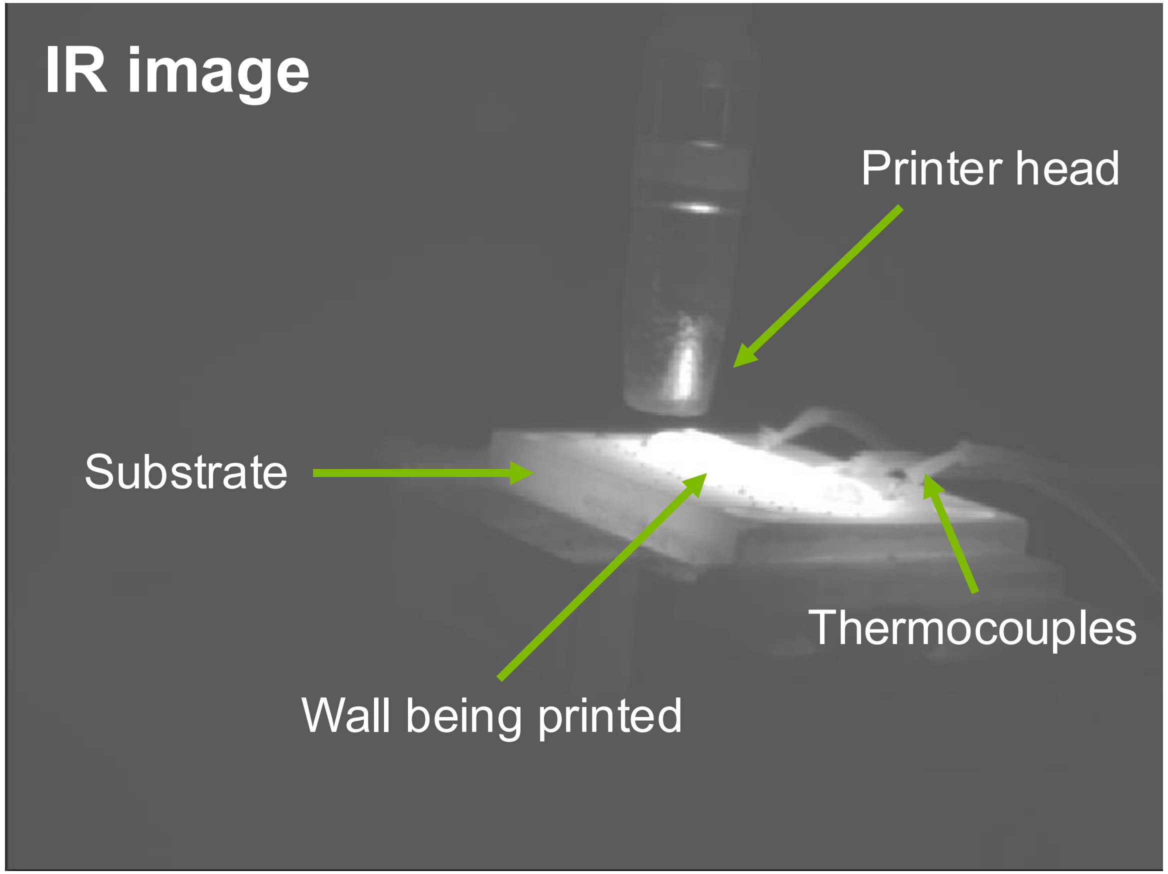
Projecting the IR data onto the simulation mesh

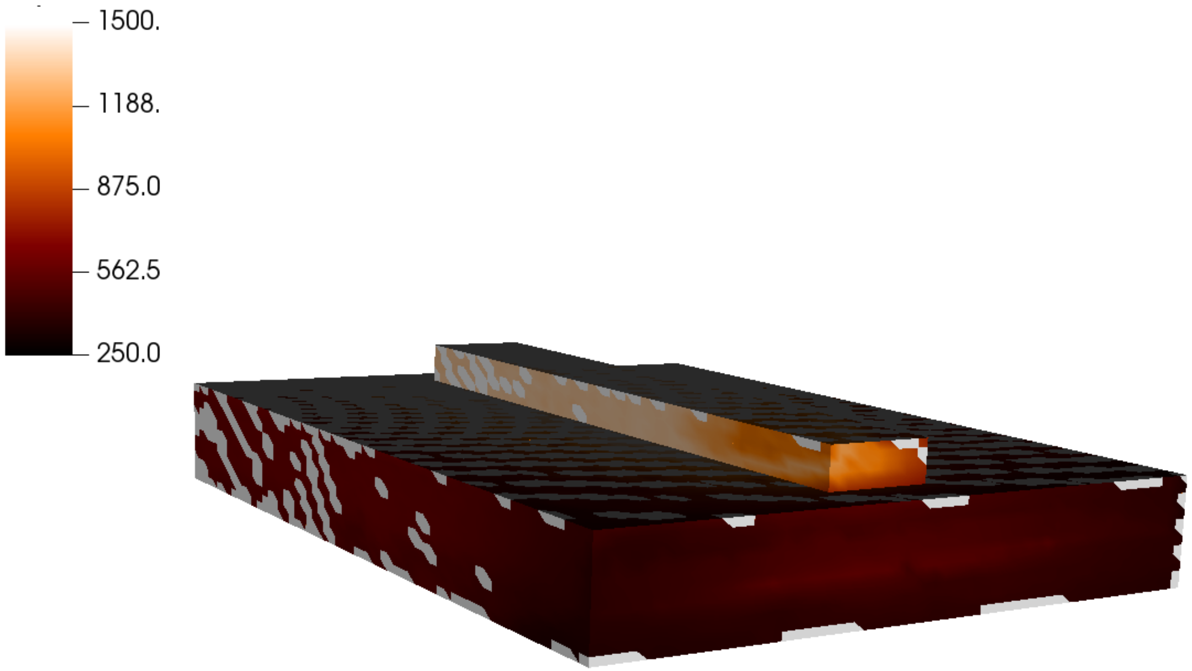


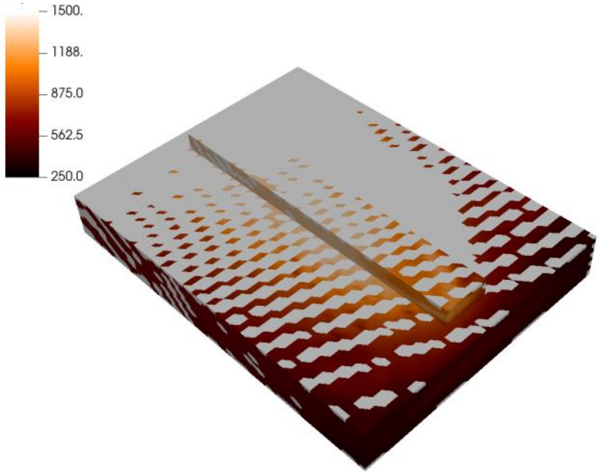
Projecting the IR data onto the simulation mesh

- Useful for data assimilation, calibration, and error estimation
- Need to calibrate the different coordinate systems
- SCOPS provides ray files and associated temperatures
- Use **distributed** ray-tracing capabilities to project the temperature onto the mesh
- Set the temperature to the closest quadrature point

Projecting the IR data onto the simulation mesh







Coordinate transformations nominally handled in ROS
Camera coordinates -> Substrate coordinates

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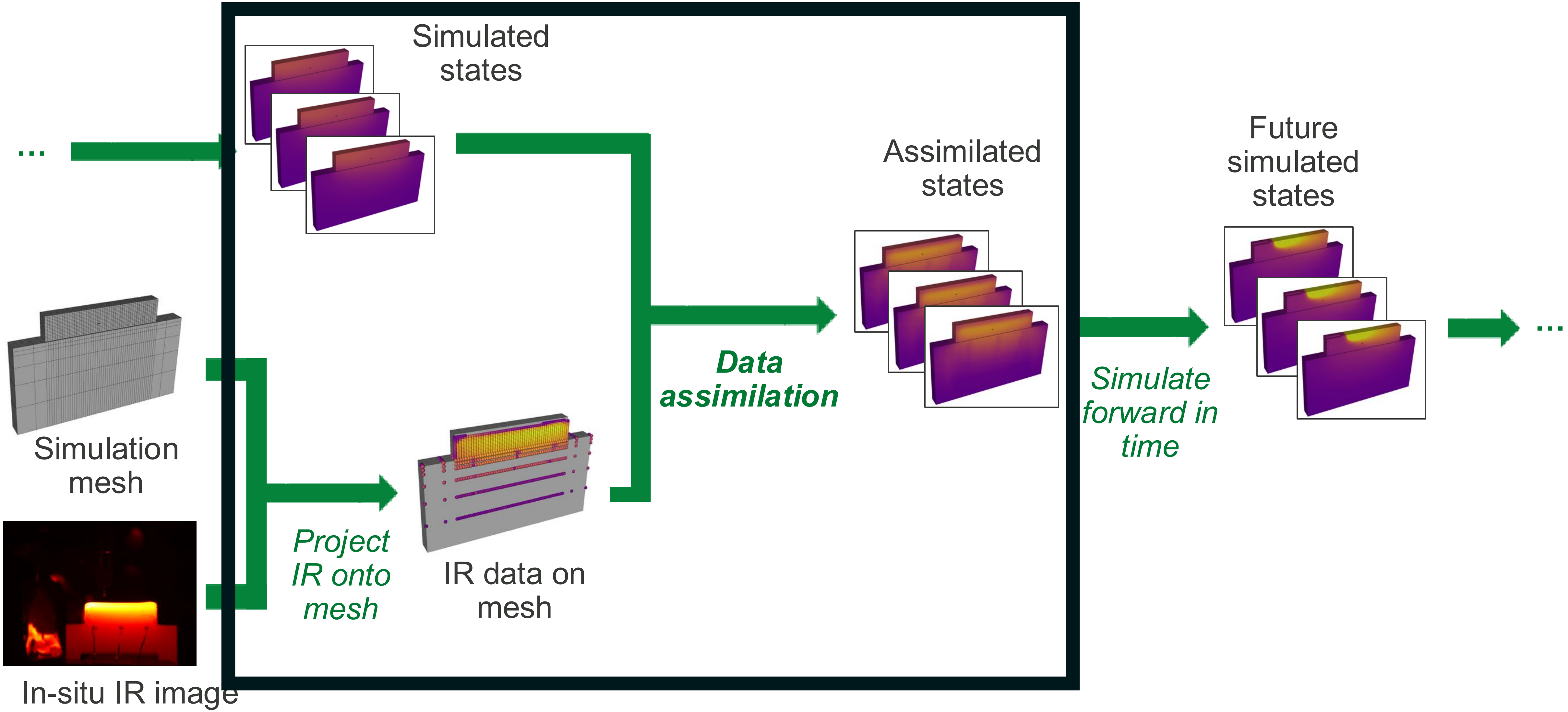
Ensemble simulations for data assimilation



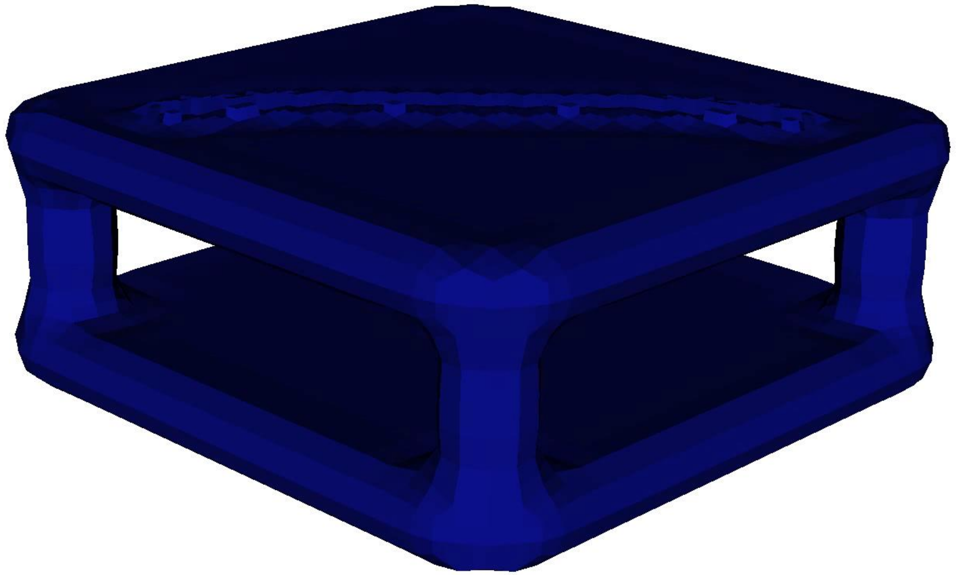
Ensemble simulations for data assimilation

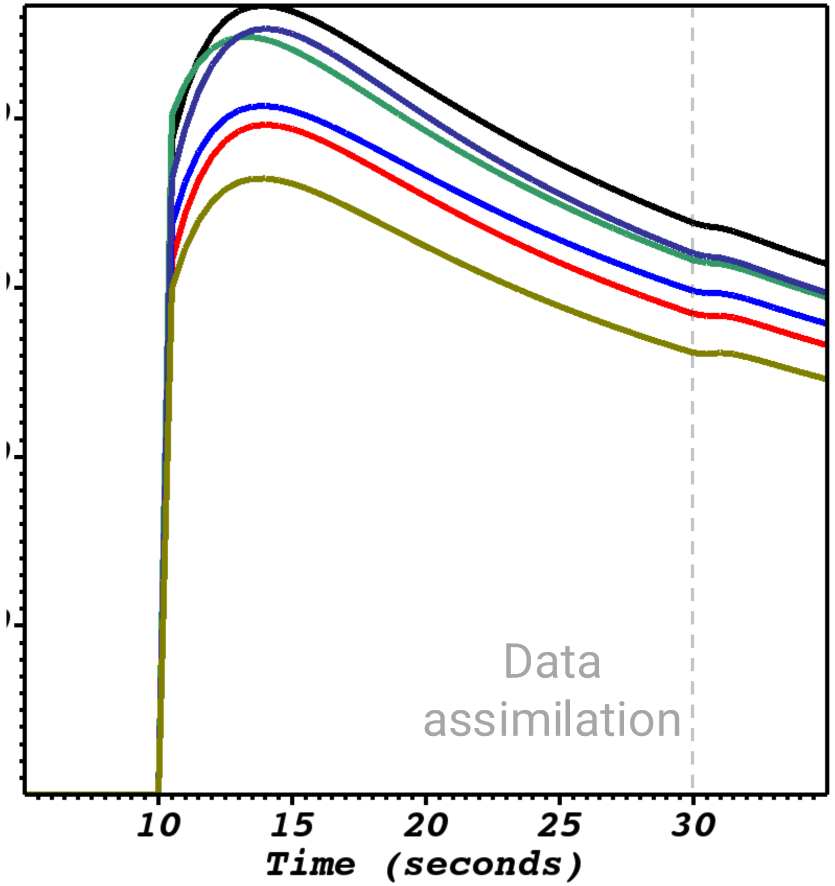
- Our EnKF requires multiple (< 10) simulations with slightly different parameters
- All the simulations use identical meshes with the same partition
- In parallel:
    - If $\text{Nproc} \leq \text{N}$, distributes the simulations evenly across the processors. First processor might take a larger workload.
    - If $\text{Nproc} > \text{N}$, Nproc needs to be a multiple of N. This ensures that all the simulations are partitioned in the same way.

Ensemble simulations for data assimilation

- Simulations are synchronized when experimental data is available
- Ensemble states are gather on rank 0
- Kalman gain and the assimilated states computed on rank 0
- Assimilated states are scattered back to the original ranks
- Current implementation cannot handle large amounts of data -> SCOPS filters the IR data

Ensemble simulations for data assimilation



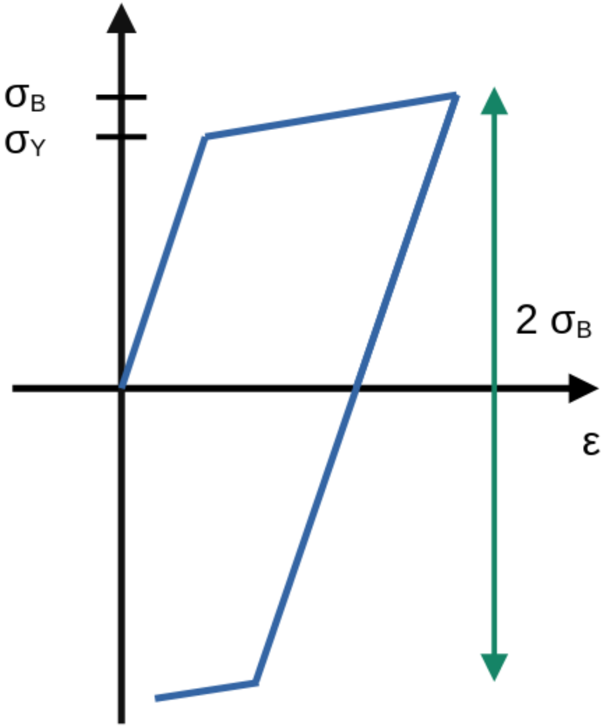


Thermomechanical simulation

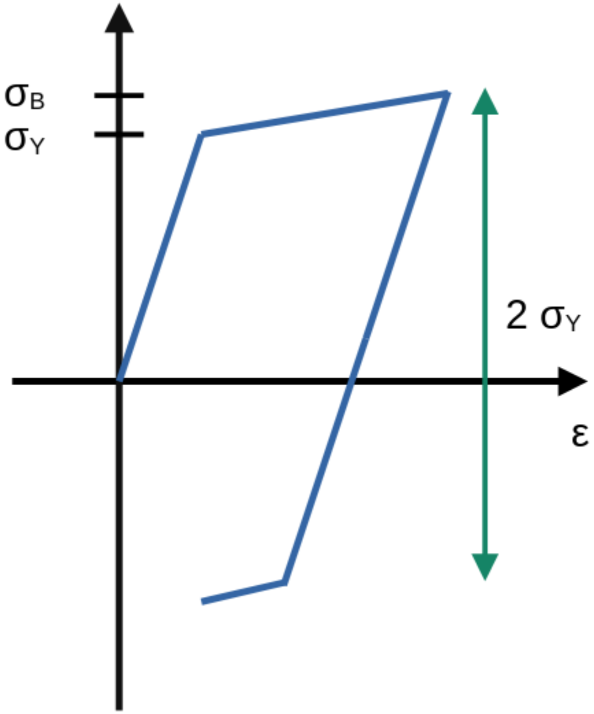
- Material properties must be isotropic → this is not true for thermal simulation
- Infinitesimal displacement → we do not support large deformations
- One-way coupling from the temperature evolution to the mechanical evolution → neglect the effect of deformation on the thermal simulation
- Plasticity constitutive laws supported: isotropic and kinematic hardening
- Currently comparing results with Abaqus

Plasticity constitutive laws

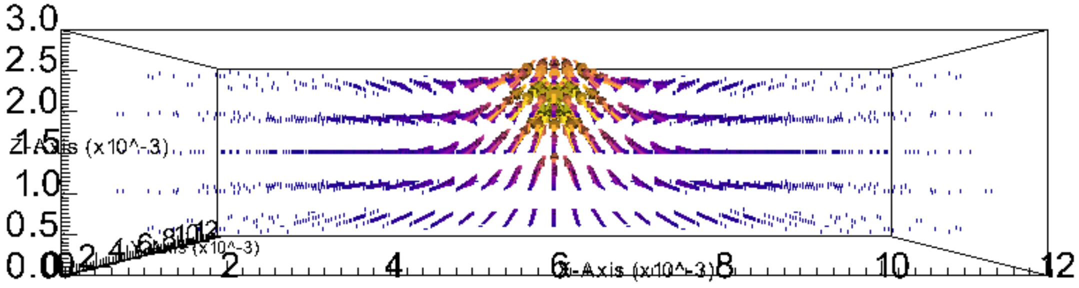
Isotropic hardening: uniform expansion of the material's yield surface in stress space

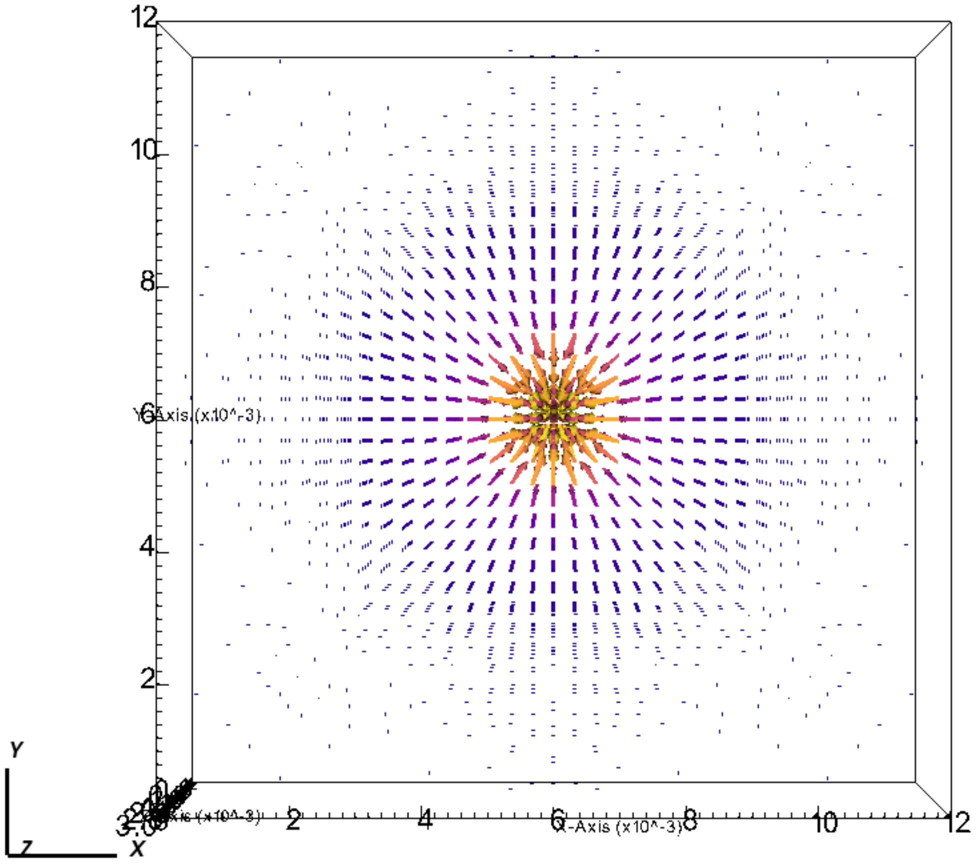


Kinematic hardening: yield surface in stress space moves without any change in its shape or size



Thermoelastic simulation: displacement field





Thank you for your attention!

Any questions?