Adamantine, a thermomechanical code for additive manufacturing

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What is adamantine?

- Open-source thermomechanical code for AM
- Uses matrix-free finite element method
- Explicit time stepping
- Extensive use of AMR
- Thermal capability is mature, thermoplasticity is experimental
- Experimental GPU support

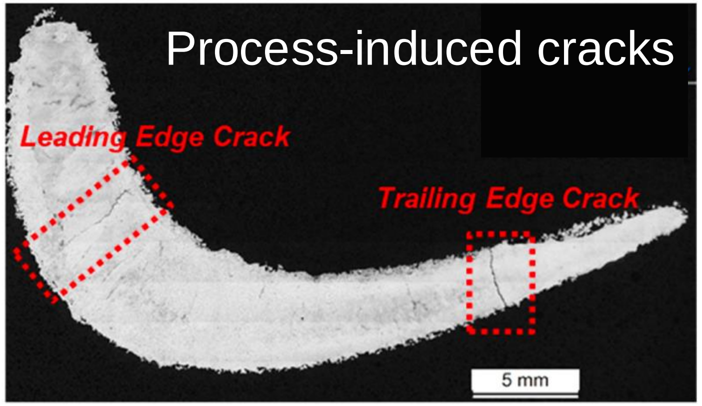
Requirement for adamantine: perform thermomechanical simulations faster than real-time

https://github.com/adamantine-sim/adamantine

Motivation

Part quality is sensitive to process conditions

- Any change in machine, geometry, composition can require nonintuitive process changes
- Short range: Microstructure, porosity
- Long range: Residual stress
- Process design for a new alloy can take 100s of builds and over a year
- Need consistent quality, robust to stochastic effects



Lee, et al, Additive Manufacturing, 2020.

Process monitoring: Want to know if the part is good enough to use (nondestructively)

Process control: Adaptively change the process so that the part is good enough to use

Why do we need adamantine?

- Grand challenge for additive manufacturing: print part that are born qualified
- What do need to get there?

Process Planni

adamantine

rocess parameters that
we expect to give us the
properties we want

Process Monitori

adamantine

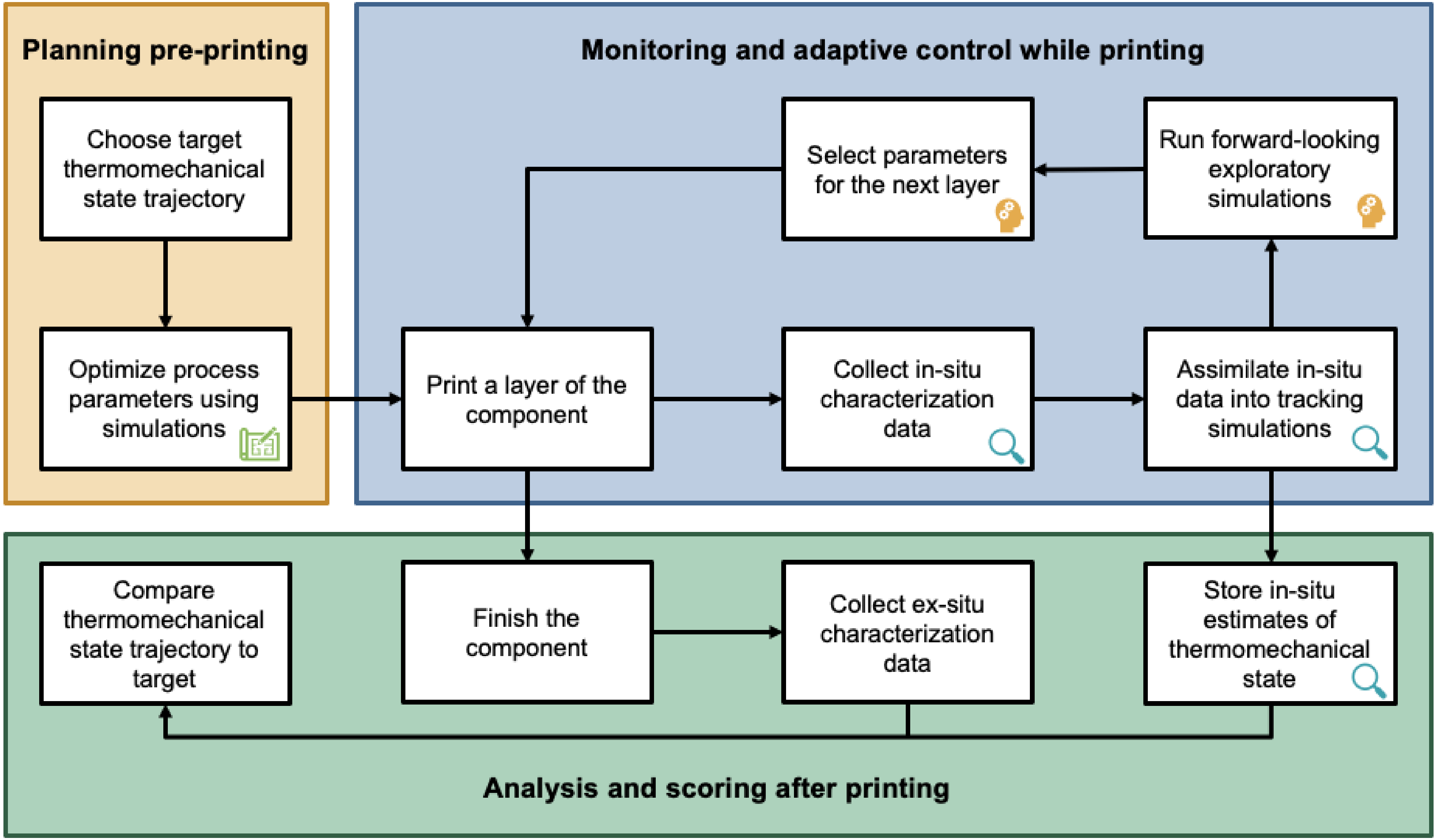
termine whether the
process is happening as
planned

Adaptive Control

adamantine

the process if it gets off
track

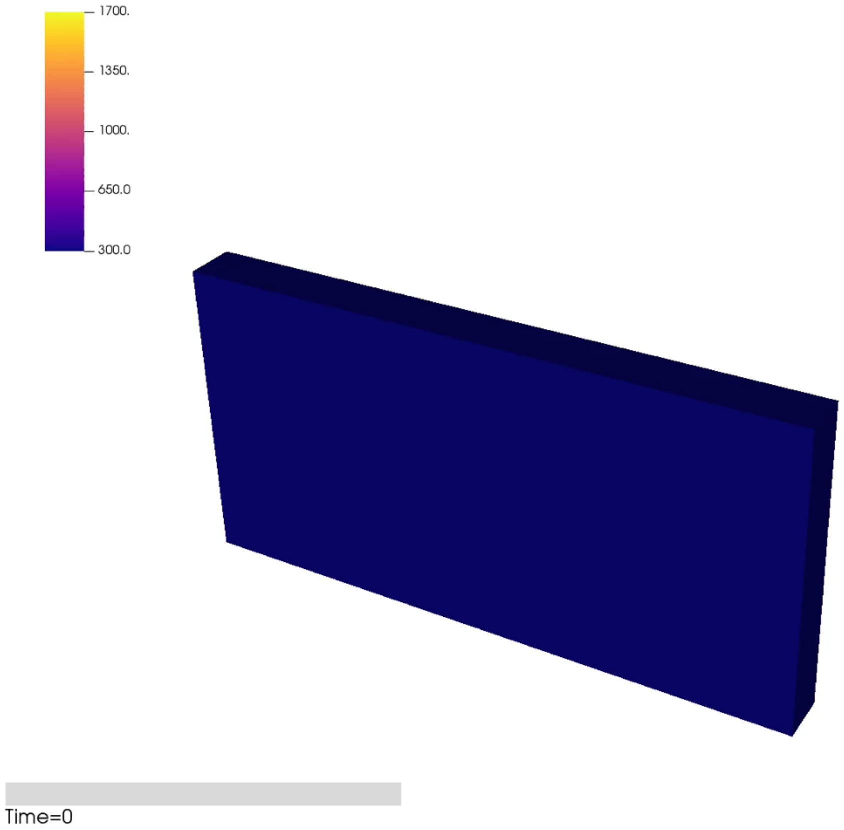
A workflow for automated planning, monitoring and control



Planning phase: Fast predictive model

Role: Used throughout workflow to estimate system response to process parameters

Approach: adamantine – open-source ORNL finite element code for thermomechanics



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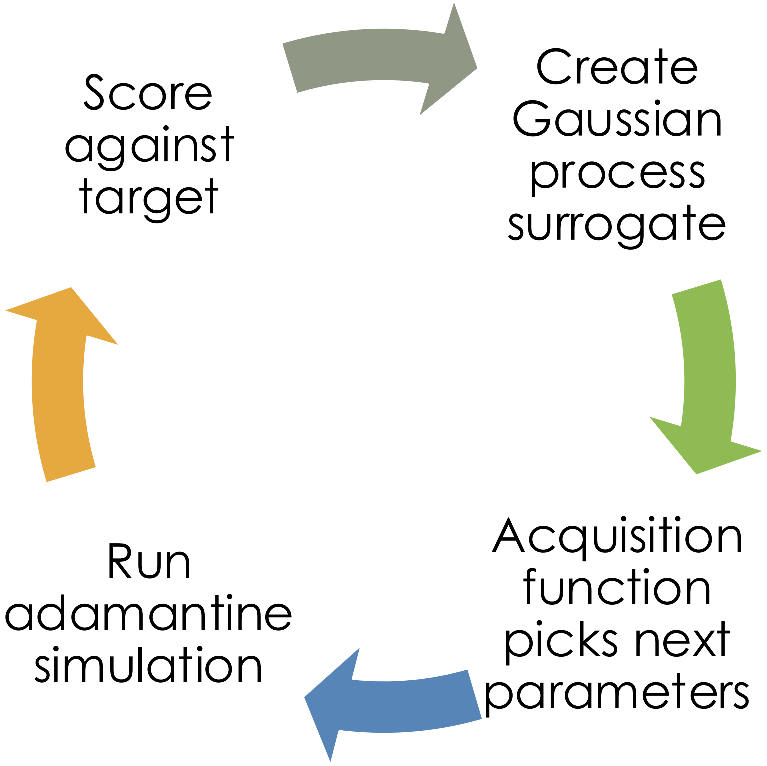
Planning phase: Model-based process optimization

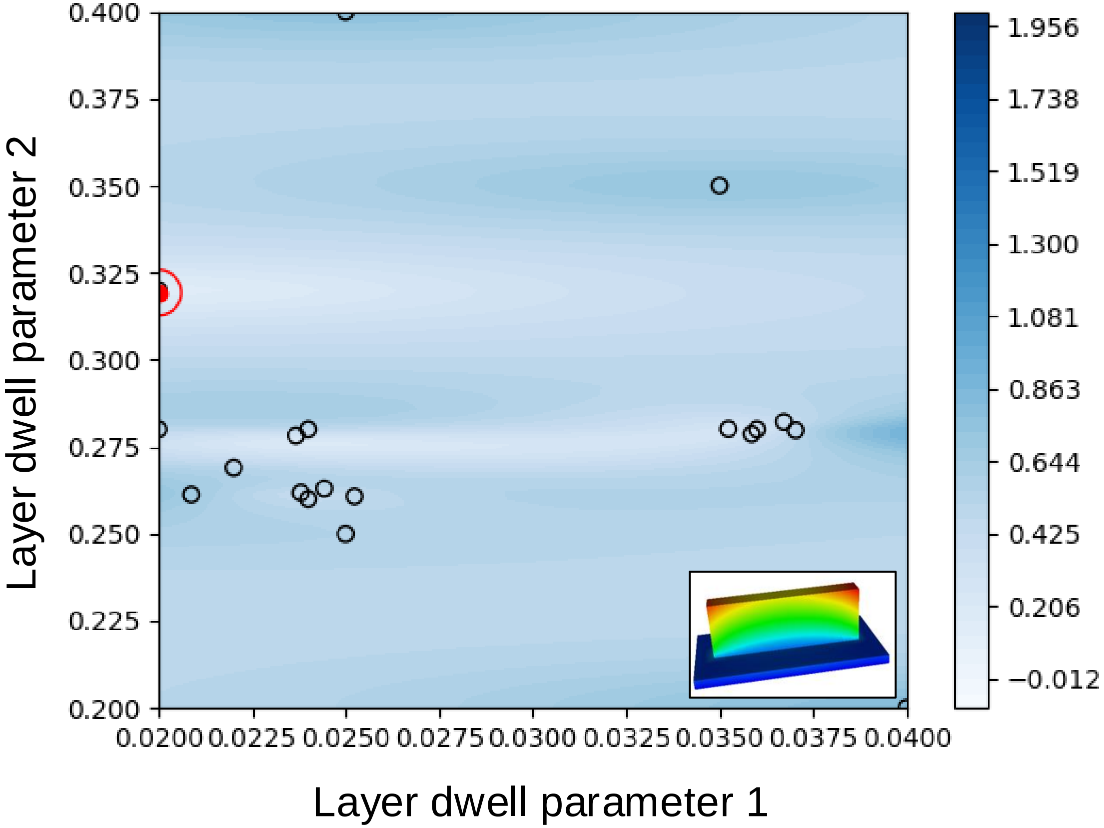
Role: Determine printer parameters expected to give the target thermomechanical path

Approach: PDE-constrained Bayesian optimization deployed in a cloud service

Active learning loop



Example:
Targeted displacement along wall

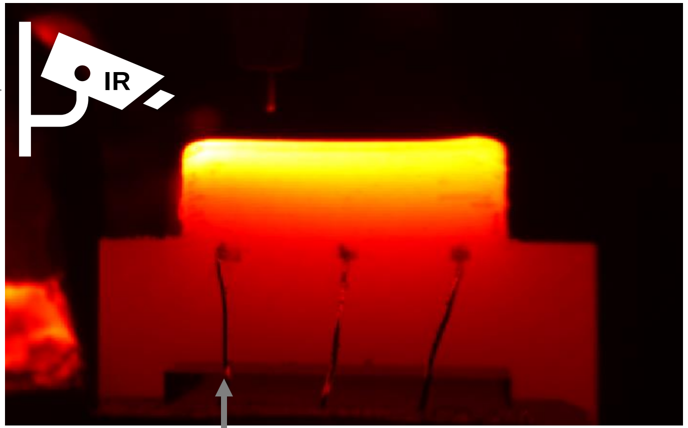


Monitoring phase: In-situ characterization

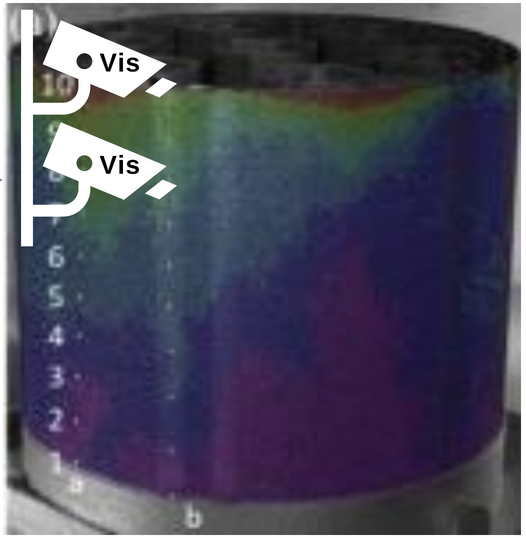
Purpose: Obtain in-situ temperature and strain information

Approach: Infrared camera, stereo-pair visible-wavelength cameras, and thermocouples coordinated by SCOPS software

IR imaging (surface temperature)



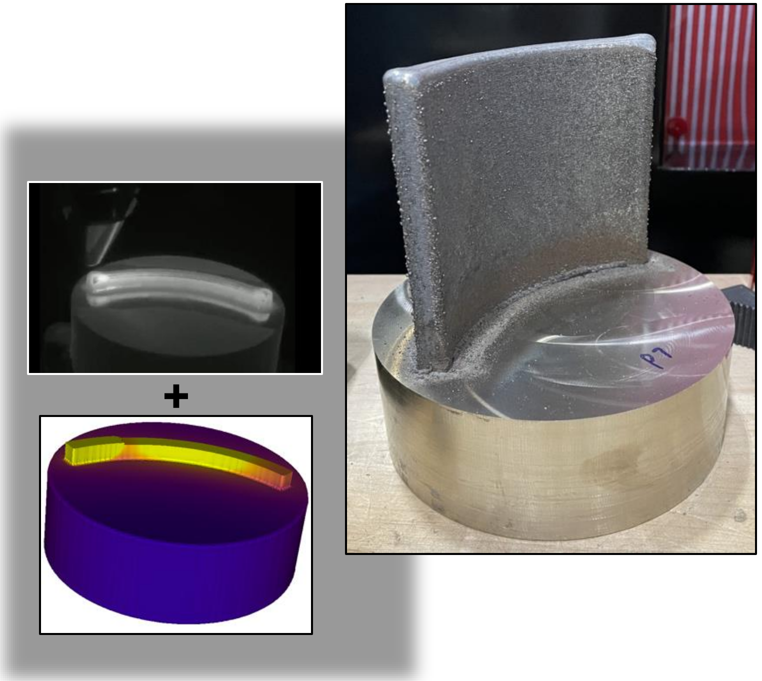
Stereo visible imaging (surface strain with DIC)



Dashboard for monitoring the print

ROS

Monitoring printing with a digital shadow



Data to accelerate qualification

Digital shadow provides part-specific process data with quantified uncertainty

Use Bayesian methods to *assimilate* observations into simulations for the best estimate of the thermomechanical evolution

Observations are tied to reality, but not for the whole 3D volume

Simulations are not tied to reality, but available for the whole 3D volume

→ Estimate tied to reality for the whole 3D volume

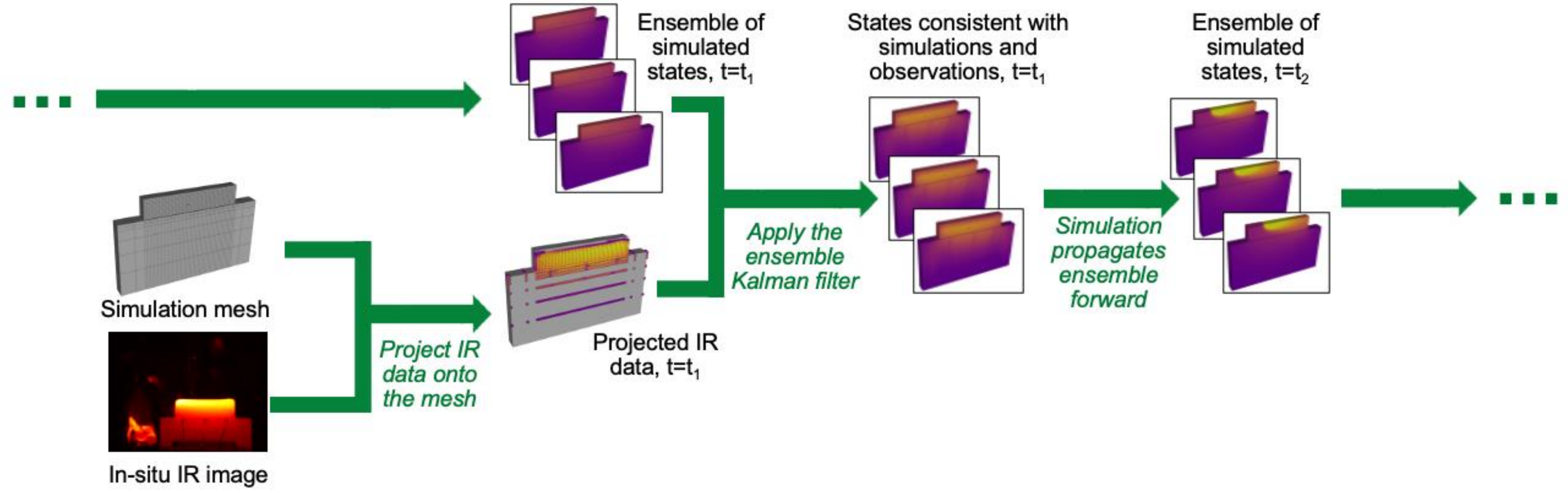
Monitoring phase: Real-time data assimilation

Purpose: Obtain an estimate of the full 3D temperature distribution for a *specific print*

Approach: An ensemble Kalman filter (Bayesian method to incorporate observations into simulations)

Note

This workflow is only possible with faster-than-real-time simulations

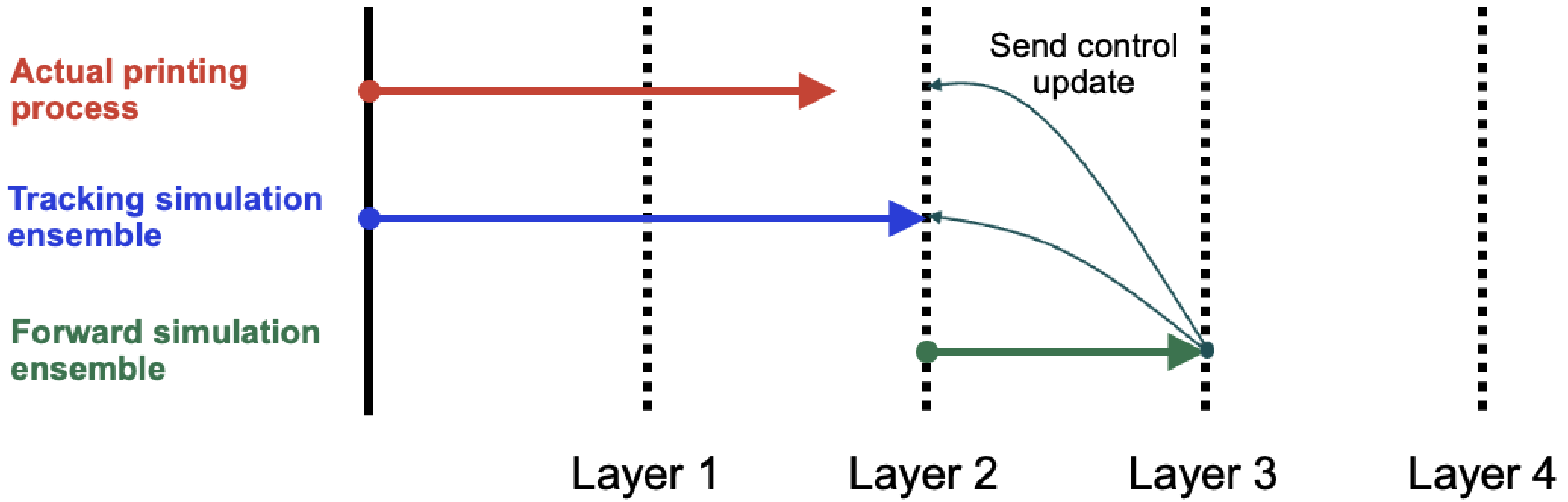


Control phase: Simulation-based adaptive control

Role: Adjust process parameters on-the-fly to stay on the target thermomechanical path

Approach: One-shot optimization using forward looking simulations to determine best parameters for upcoming layers

Timeline of the adaptive control loop



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Putting it together: Simulation-based adaptive control

Role: Adjust process parameters on-the-fly to stay on the target thermomechanical path

Approach: One-shot optimization using forward looking simulations to determine best parameters for upcoming layers

Set the target (Plan):

Want the thermomechanical evolution for the real print to match the evolution from an optimized simulation result

Estimate deviation from the target (Monitor):

Assimilate in-situ imaging data into tracking simulations to form a digital shadow, using INTERSECT for low-latency data transfers

Adjust the parameters to best match the target (Control):

Use INTERSECT to launch ensembles of simulations to explore the impact of varied process parameters on the upcoming layer and send the best to the printer

Putting it together: Simulation-based adaptive control

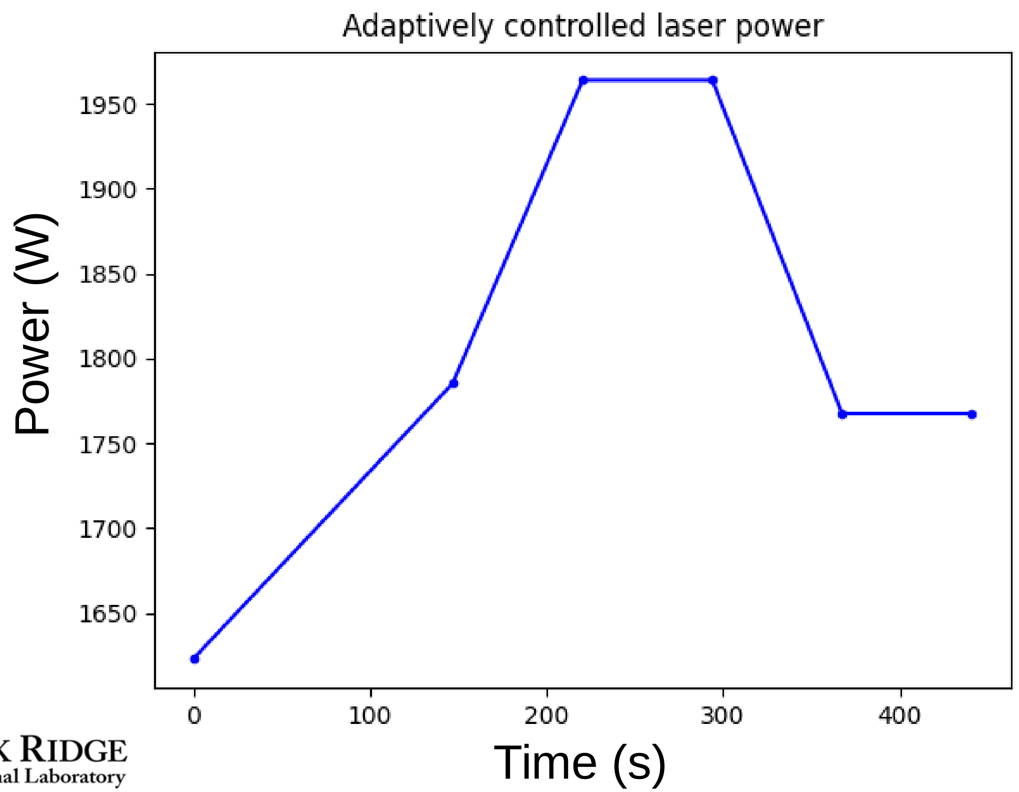
Role: Adjust process parameters on-the-fly to stay on the target thermomechanical path

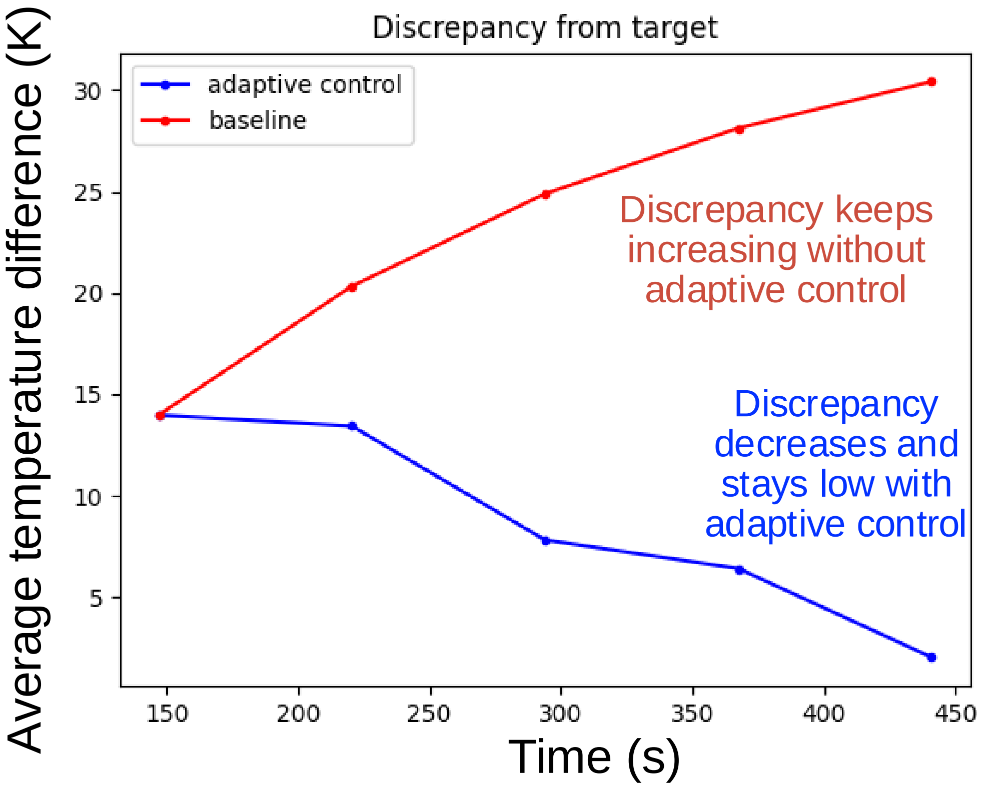
Approach: One-shot optimization using forward looking simulations to determine best parameters for upcoming layers

Runs 3x faster than the experiment!

Results for a *virtual* test

Adjusting electric arc power to match a target temperature evolution





What is special about adamantine?

- Designed for additive manufacturing: heat sources, material states, material deposition, …
- Designed with existing ORNL workflow/need in minds
- Tight collaboration with experimentalists
- Faster than real-time requirement
- Data assimilation
- Open-source

ArborX

- Open-source library for (distributed) geometric search
- Based on Kokkos
- Capabilites:
  - k-nearest-neighbors (k-NN)
  - Range search (radius search, intersections)
  - Ray tracing
  - Clustering algorithms (minimum spanning tree, density-based clustering)
  - Interpolation: moving least square

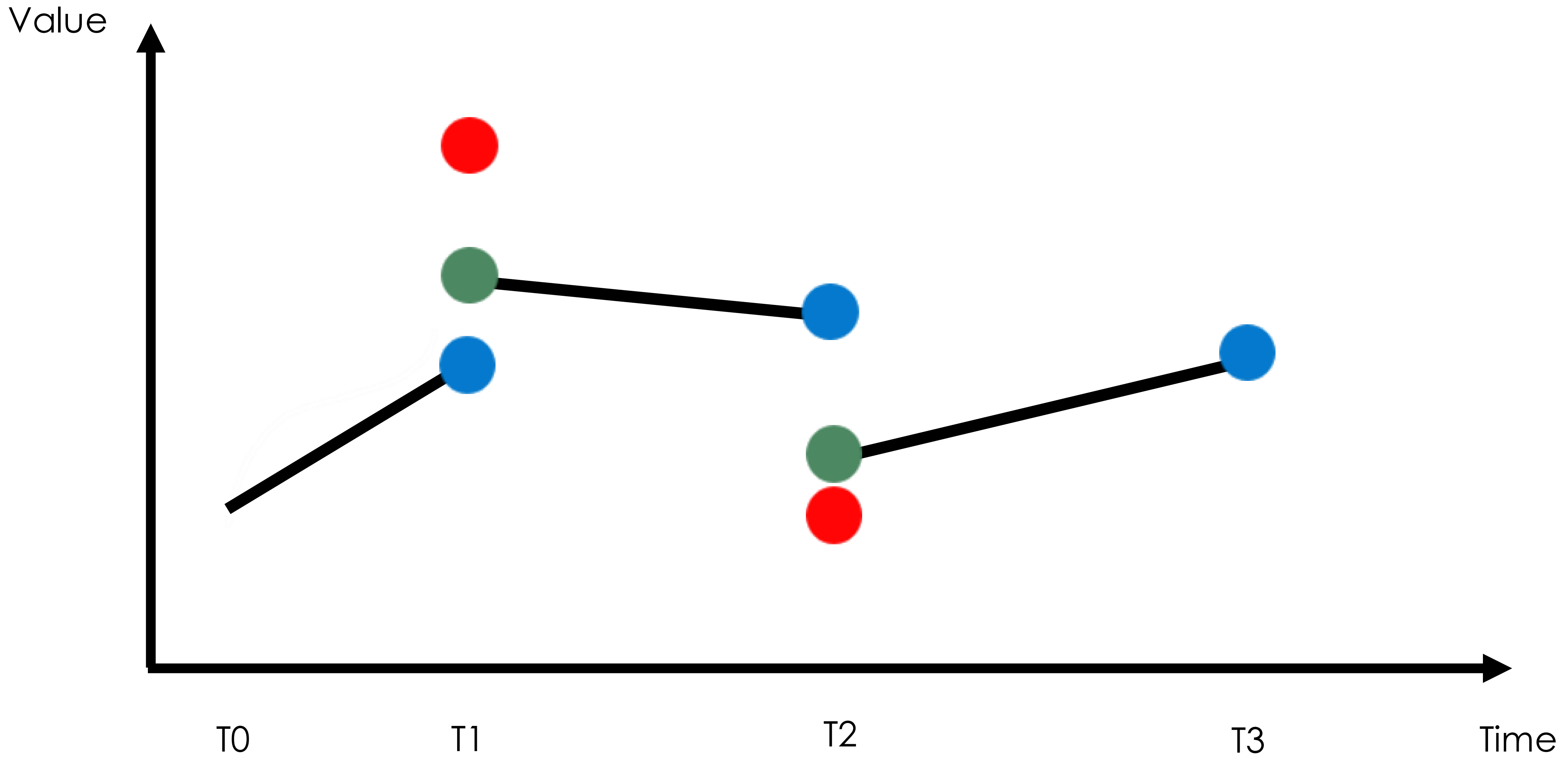
Material deposition

- Use hp capabilities to model material deposition: FE_Nothing → FE_Q
- Use ArborX to get cells to activate
- Need to extend SolutionTransfer to set values to newly activated cells: not trivial when dealing with hanging nodes in parallel → parallel::distributed::experimental::FieldTransfer

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

Data assimilation



Ensemble Kalman filter

Stochastic EnKF

- 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

x_i^f: Simulated states

y: Observations

H: Observation matrix

K: Kalman gain

P: Simulation error covariance

R: Observation error covariance

Ensemble Kalman filter

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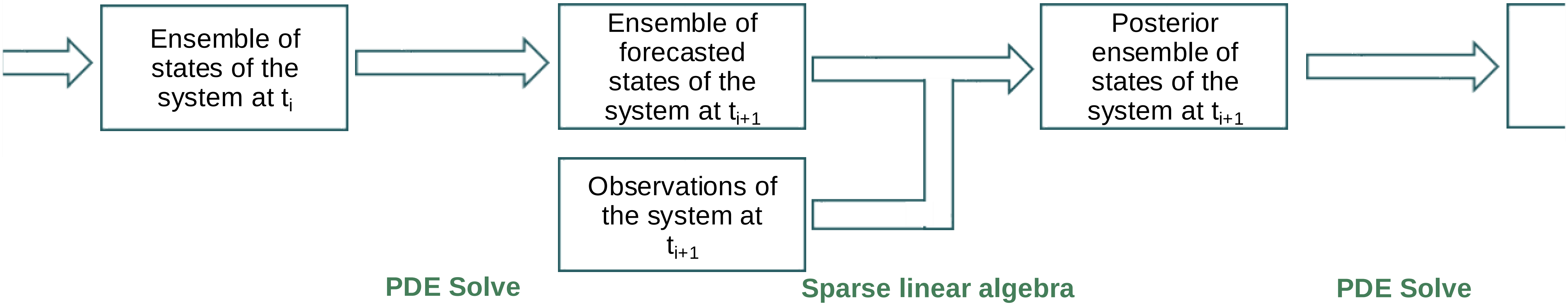

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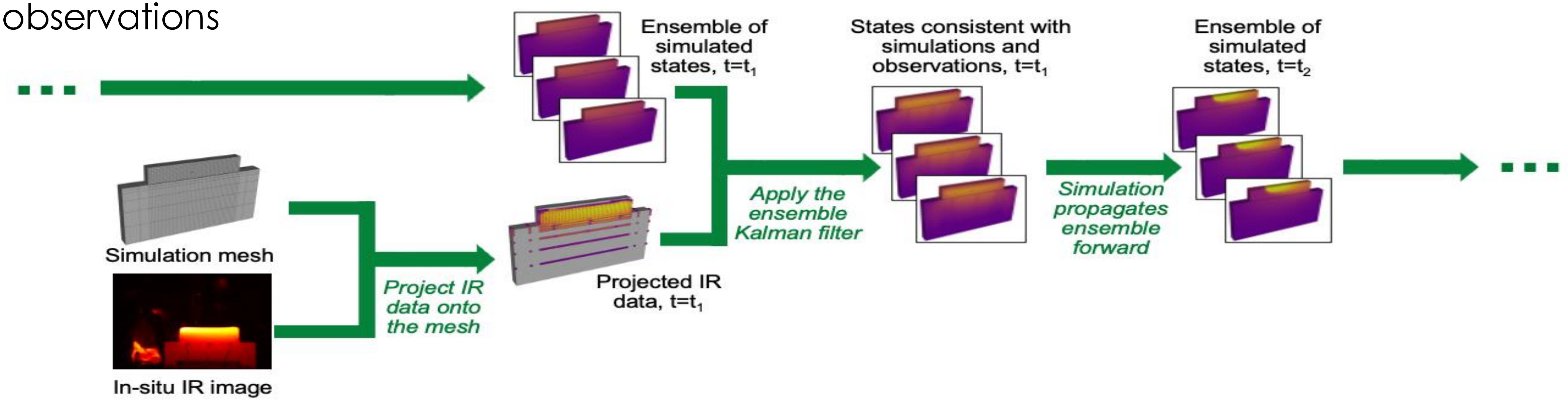
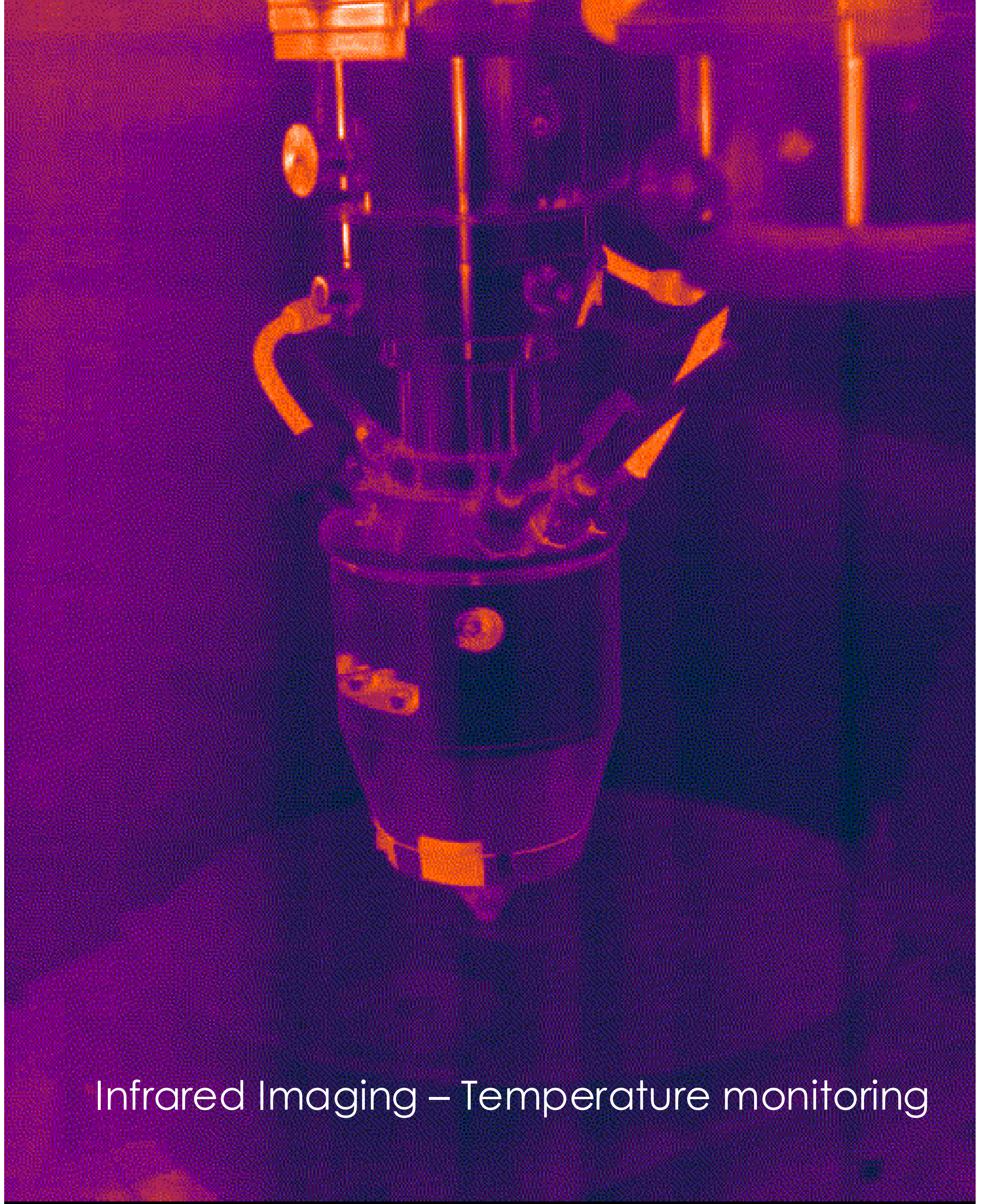


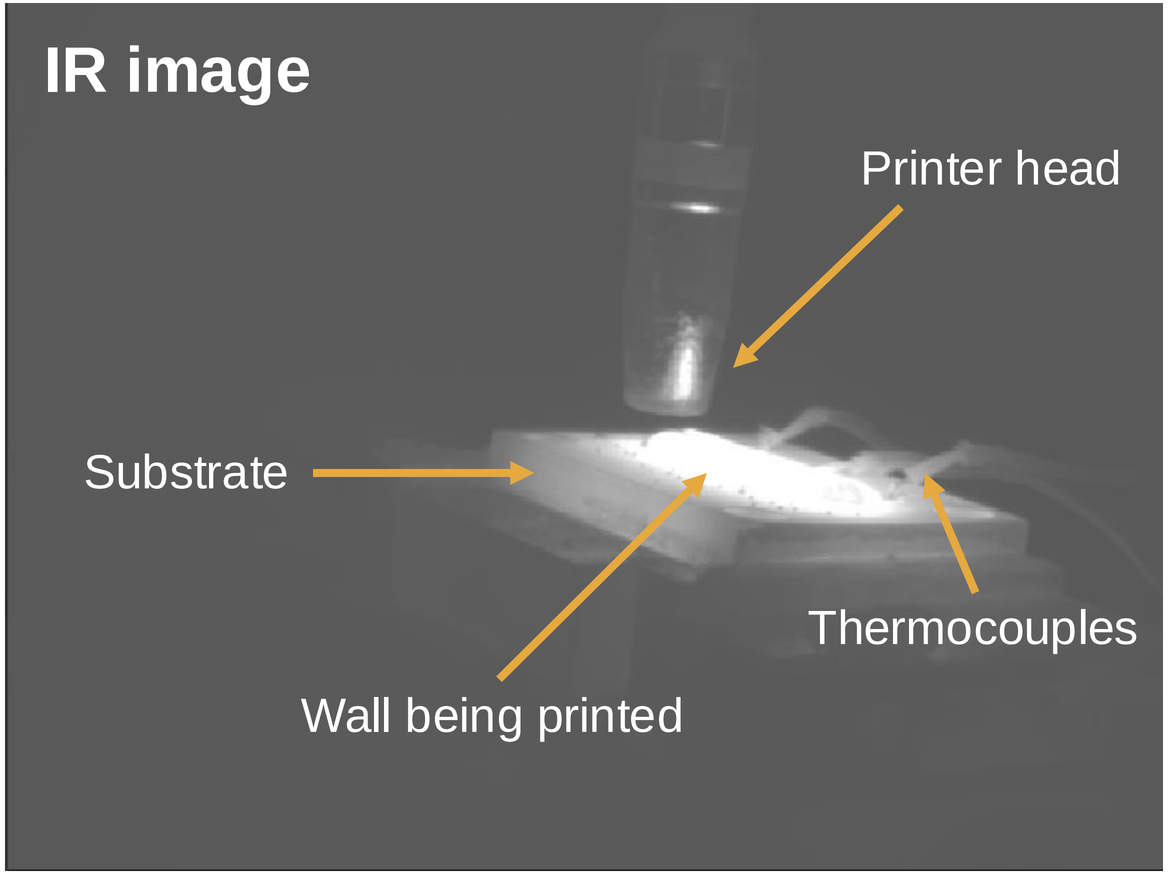
Experimental Data

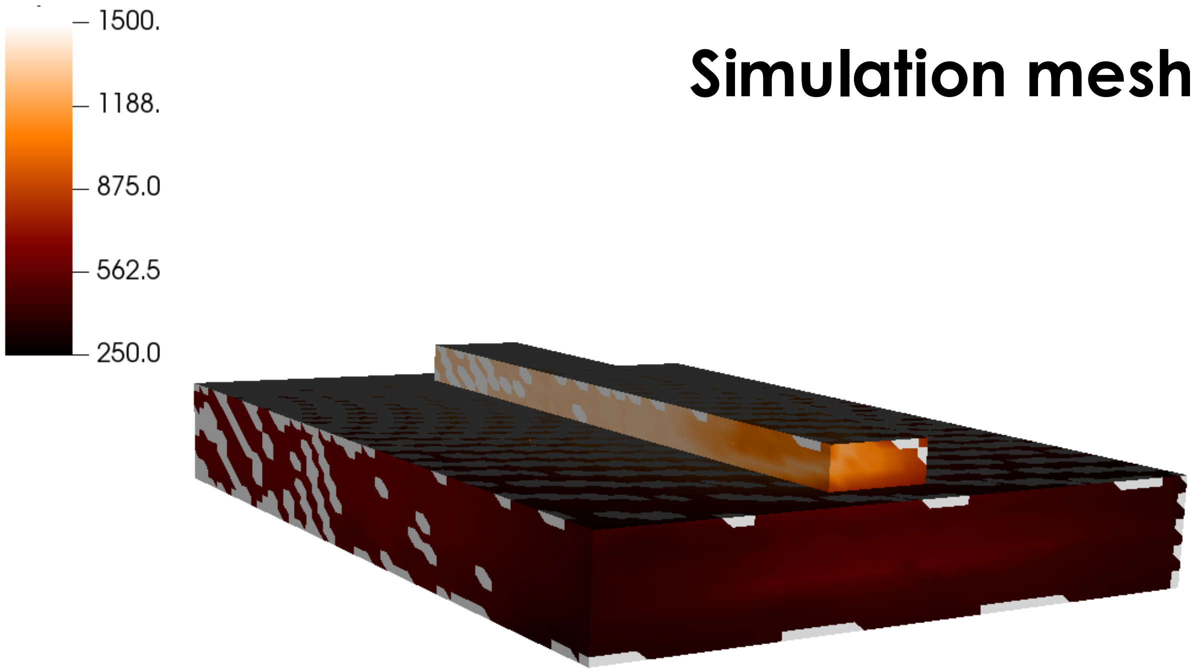


Project the experimental data

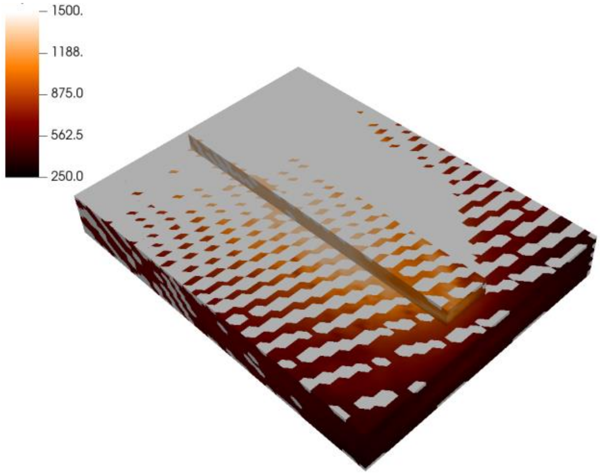
- Coordinate system needs to be calibrated otherwise the camera data and the simulation won't match
- Camera cannot see everything (complex geometry, room to put cameras)
- Use ArborX **distributed** ray-tracing capabilities
- Project the temperature to the closest quadrature point

Projecting the IR data onto the simulation mesh





Simulation mesh

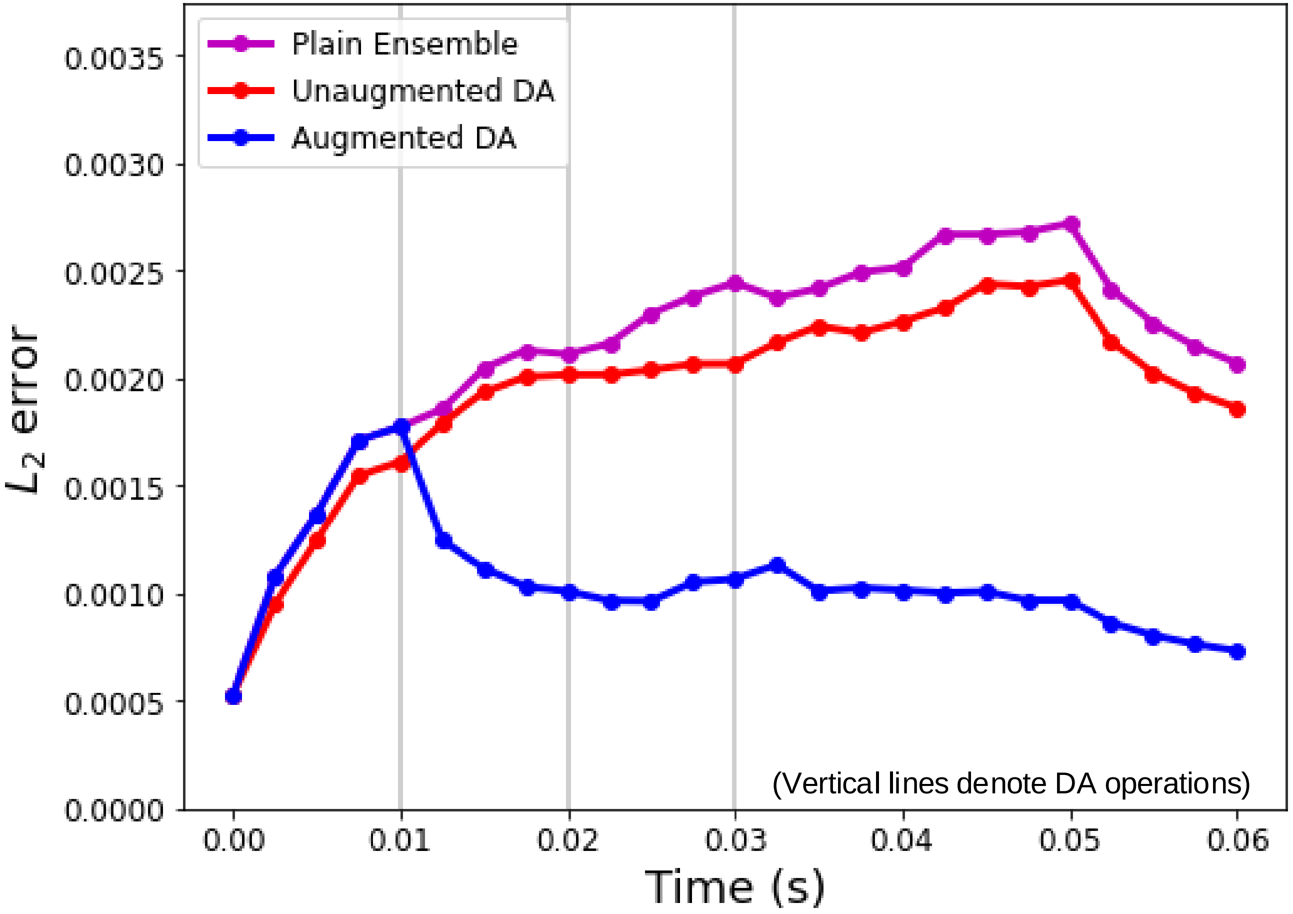


Coordinate transformations nominally handled in ROS
Camera coordinates -> Substrate coordinates
Automated calibration still underway

Ensemble simulations

- Our EnKF requires multiple (< 10) simulations with different parameters
- To simplify computations: use the same mesh for all simulations
- In parallel:
  - If Nproc ≤ N, distributes the simulations evenly across the processors. First processor might take a larger workload.
  - If Nproc > N, Nproc needs to be a multiple of N. This ensures that all the simulations are partitioned in the same way.
- Kalman filter is computed on proc 0

Data assimilation results: Global error



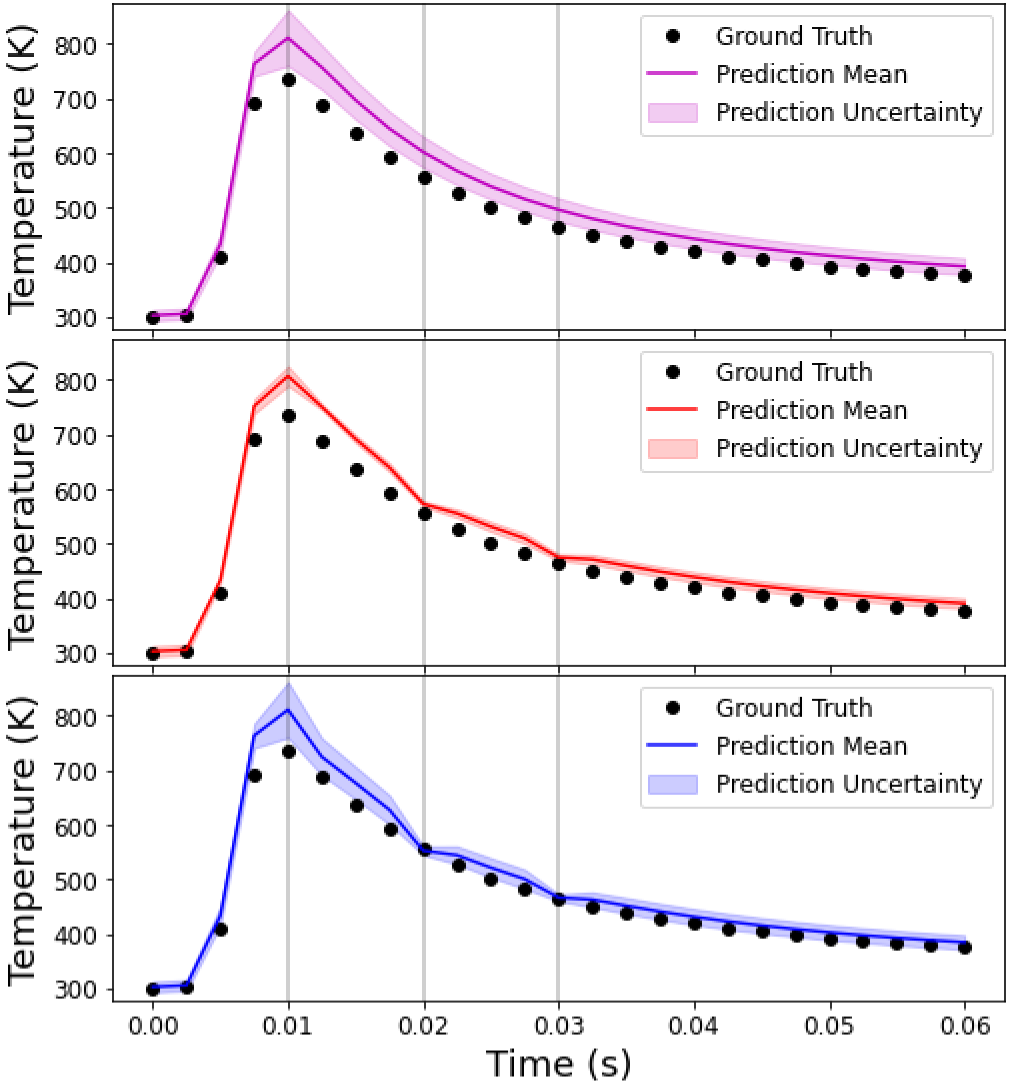
- **Unaugmented DA:** slight improvement over plain ensemble
  - Changes *local* to the region near the thermocouple
  - Changes limited to the three DA operations
- **Augmented DA:** significant improvement
  - "Learns" the correct absorptivity at first DA operation
  - Improves the results *globally* for the rest of the simulation

Data assimilation results: Local error

Plain ensemble

Unaugmented DA

Augmented DA



- Comparing predictions to the reference *at the thermocouple location*
- Small but clear effects at DA operations
  - Mean deflects toward reference
  - Uncertainty decreases
- Augmented DA only slightly better than unaugmented DA
  - Improved absorptivity estimate has limited effect since the laser has passed
- Uncertainty in unaugmented DA lower than others due to no variation in absorptivity across the ensemble

Future work

- Distributed (thermo)mechanical simulations
- Add data assimilation for neutron data
- Improve physical models (heat sources, plasticity)
- Output more postprocessed quantities
- Support more manufacturing processes (hybrid, 5-axis, …)
- Improve GPU support

Thank you for your attention

Any questions?