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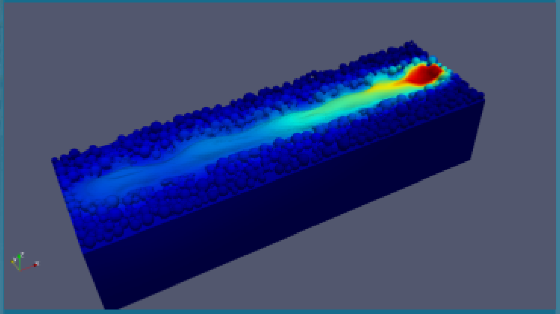
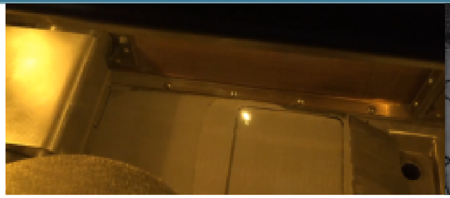
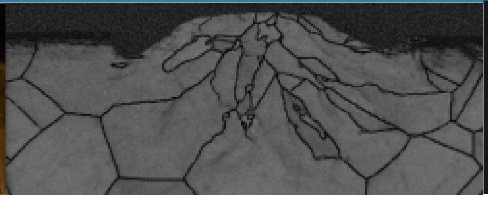
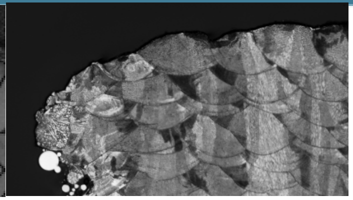
Uncertainty quantification for quantitative validation of laser powder bed fusion process outcomes









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Sandia National Laboratories

17th U. S. National Congress on Computational Mechanics

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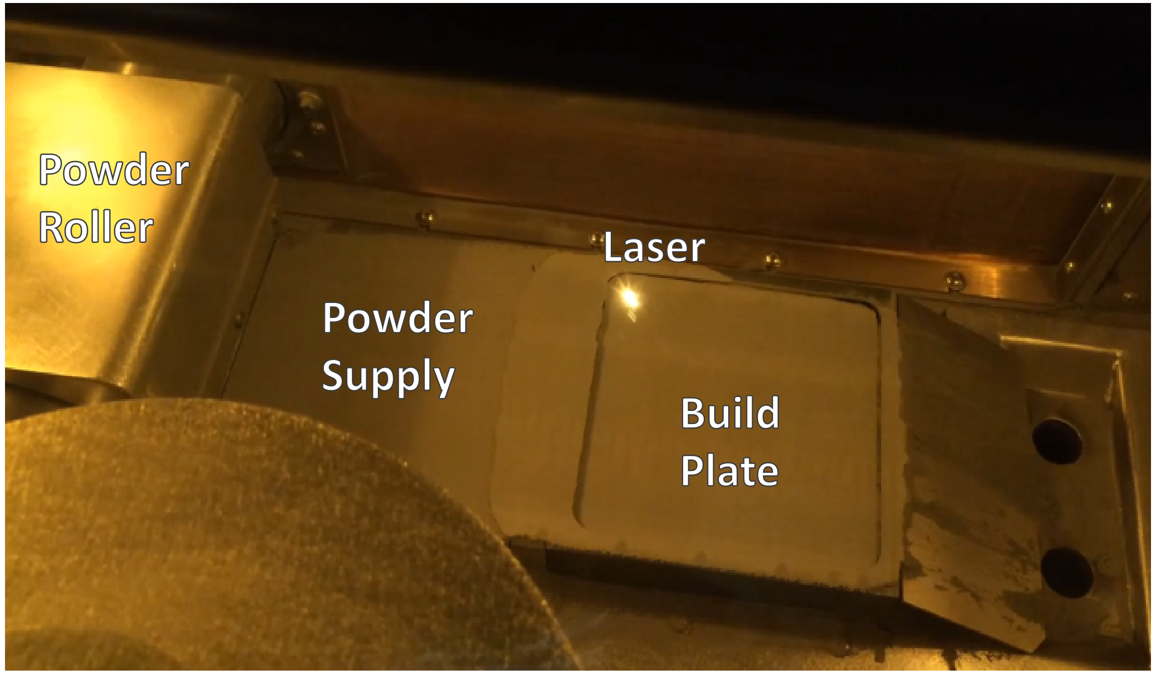
Laser Powder Bed Fusion Qualification Challenges

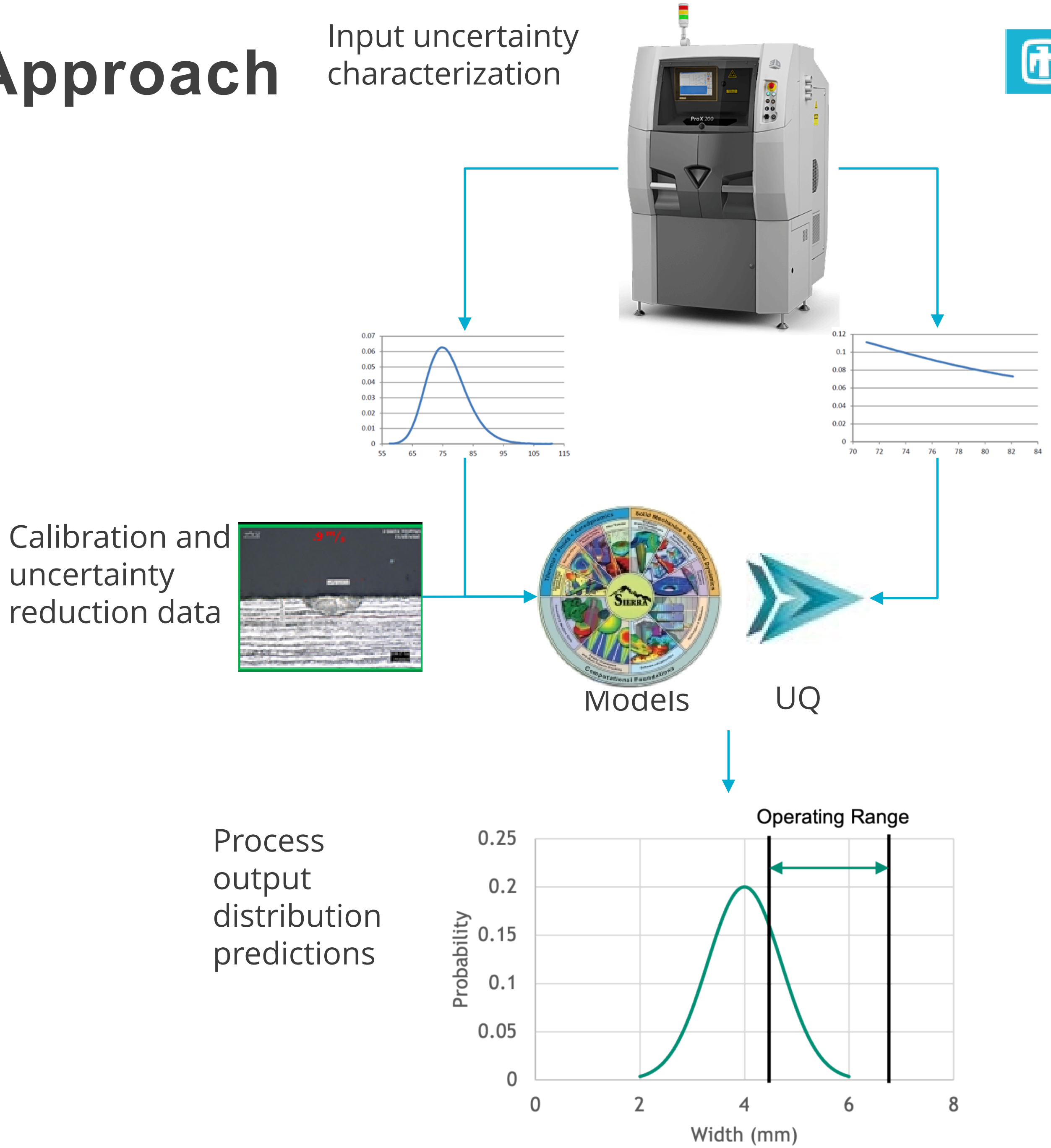
- Laser Powder Bed Fusion (LPBF) is a leading additive technology for producing functional metal parts for critical applications
- Part qualification remains an expensive, time-consuming, often ill-defined process
- Process physics of laser-induced melting and re-solidification produces difficult to predict, often unrepeatable outcomes
  - Anisotropic microstructures
  - Thermally-induced residual stresses and distortions
- Mod-Sim and UQ possible path forward to reduce cost of part qualification
- Model-based evidence to support process qualification



Optical image of LPBF machine in operation

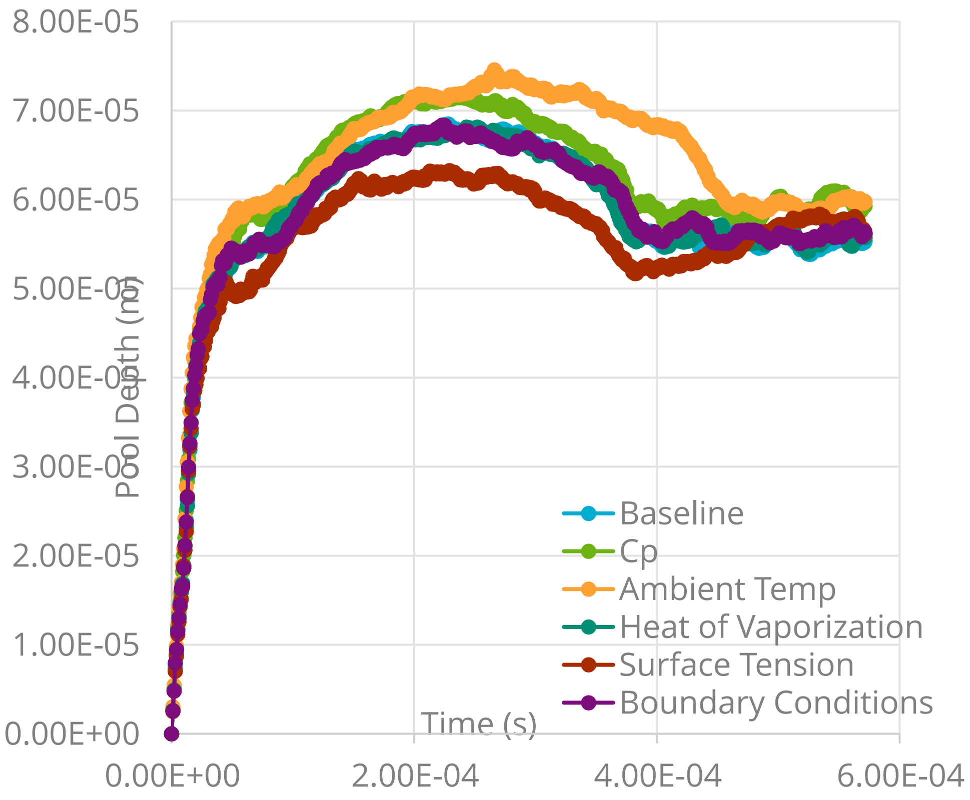
Uncertainty Quantification Approach

- Uncertainty quantification techniques allow uncertainties in model inputs to be propagated to model predictions
- Allows prediction of probability distributions for quantities of interest
- Goal is to take what we know about the uncertainties in machine operation and propagate them through physics models to predict distributions of as-built:
  - Dimensional accuracy
  - Microstructural features

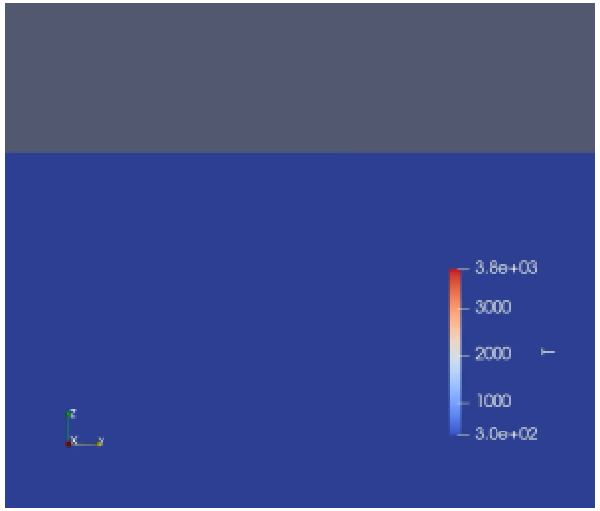


Input Uncertainties

- Huge number of parameters governing process physics
  - Laser power
  - Laser size/shape
  - Laser path
  - Build plate stepping
  - Gas flow
  - Ambient chamber temperature
  - Laser attenuation
  - Oxygen content
  - Feedstock
  - Chemical composition
  - Thermophysical properties
- Measurements, physical intuition, sensitivity analysis used to reduce dimensionality



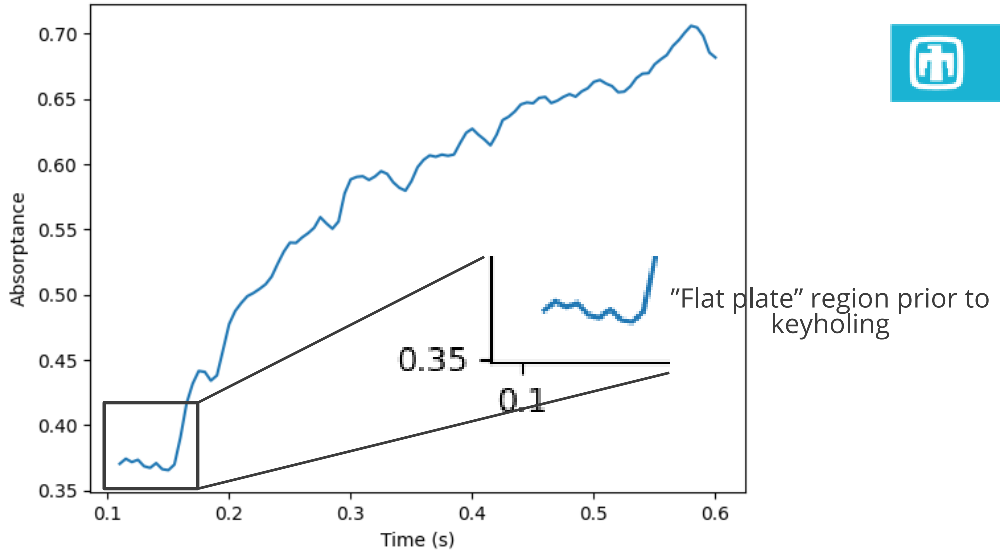
Sensitivity study results for selected parameters



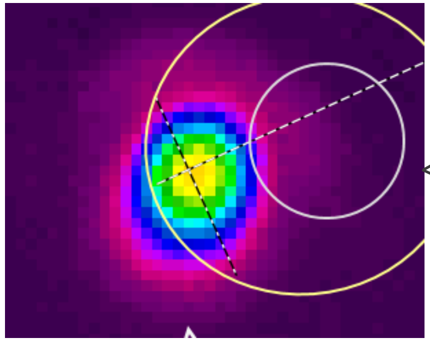
Example of high fidelity model used to predict spot weld behavior

Estimating Uncertain Distributions

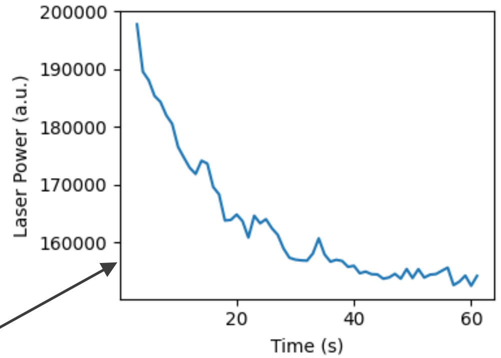
- Five uncertain parameters identified as inputs to high fidelity model
  - Index of refraction [0.1682 - 0.2632]
    - Calibration to ”flat plate” region of NIST integrating sphere absorptance data for spot weld
  - Material sulfur content (controls surface tension) [0.0005 - 0.0030 %wt]
    - Material specification
  - Ambient chamber temperature [300 – 700 K]
    - Literature review for thermocouple measurements in LPBF build chambers
  - Laser power [87 – 139 W]
    - Beam characterization study
  - Laser radius [26.8 – 36.5 um]
    - Beam characterization study
- All probability distributions uniform
- Feedstock (powder) uncertainties not needed for initial bead-on-plate simulations

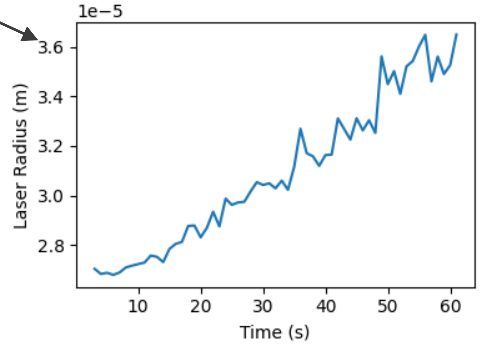


Time resolved absorptance data for spot weld



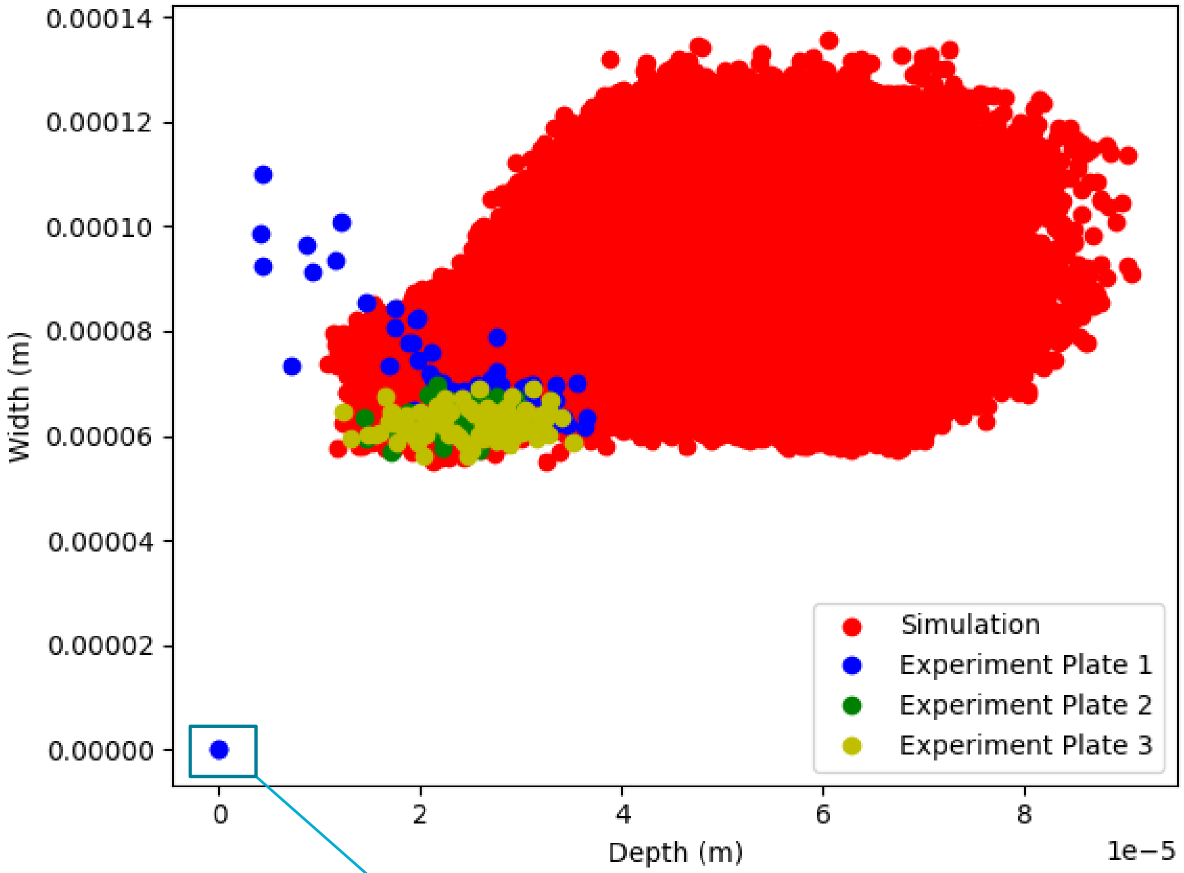
Beam characterization results



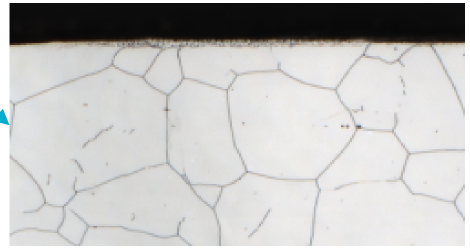


Validation of Bead on Plate Dimensions

- Uncertain parameters propagated through high fidelity model using gaussian process surrogates
- Compared to bead-on-plate cross section metallography measurements
- Predicted distribution bounds the observed results for 91/100 samples in first case
  - Contains a number of laser misfires, attributed to using non-standard baseplate
- Repeating using standard baseplate in two experiments, all samples bounded by predicted distribution
- At this point, **model has seen no calibration data**, just estimates of uncertain inputs



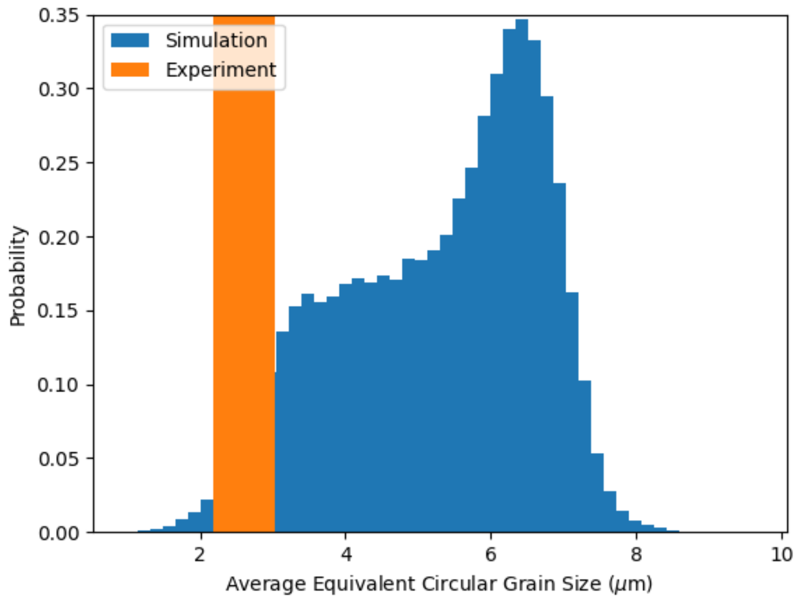
Distributions of predicted and measured melt pool widths and depths

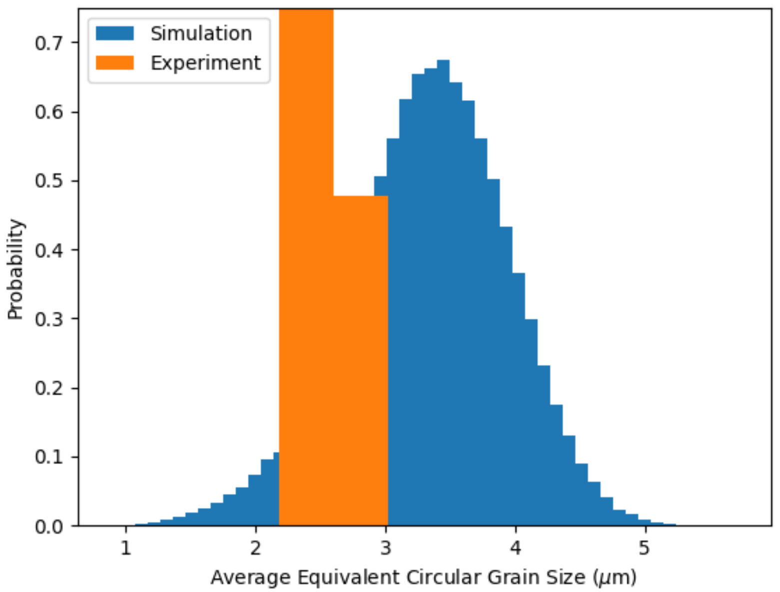


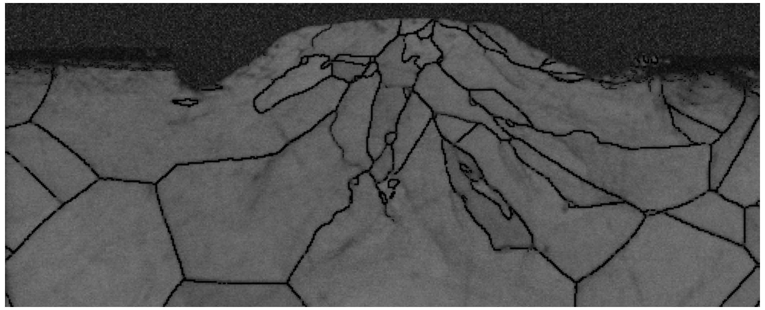
Validation of Bead on Plate Microstructure

- Thermal results combined with undercooling-based microstructure prediction code (SPPARKS) to calculate average grain size
  - Additional uncertain parameter: nucleation site density [1e12 – 1.25e17]
  - Runs gambit of possible values (no sites in simulation volume to each pixel is a site)

- Compared to 5 EBSD cross section images from bead-on-plate builds
  - Predictions bound results, but window is large
  - Nucleation site density needs to be calibrated
  - Calibration on 1 EBSD result gives tighter prediction interval



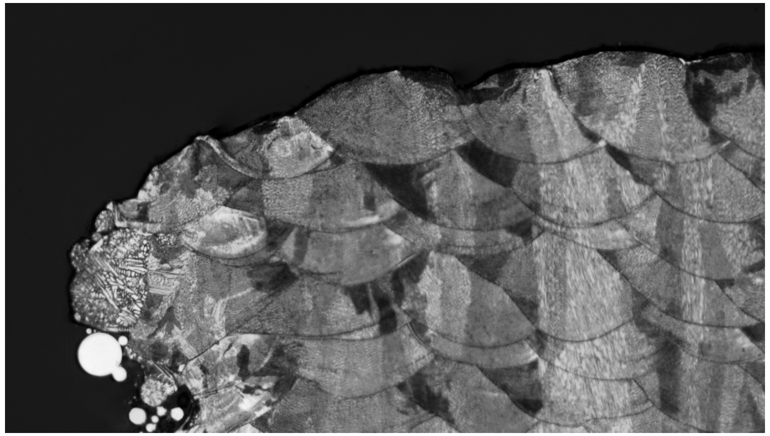




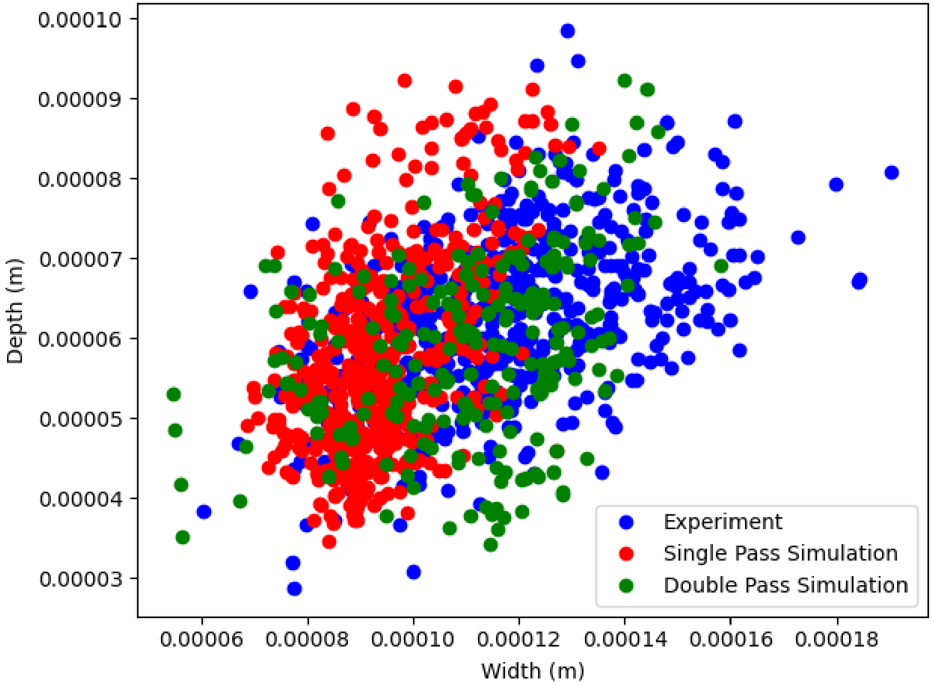
Melt Pool EBSD image with grain boundaries

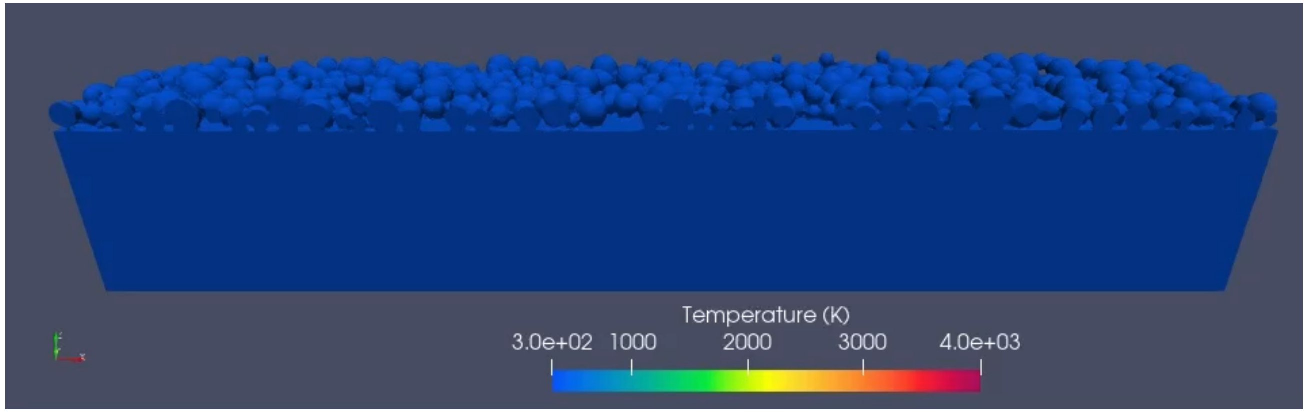
Melt bead shapes with powder

- High fidelity model run including powder particles
- Compared to metallography images of 2cm cubes. Melt pool shapes of top layer measured
- Measurements span larger area than predictions
- Real process is many laser passes – expanding to two pass simulations extends prediction window
- 3+ passes needed?
- Multiple powder bed realizations?



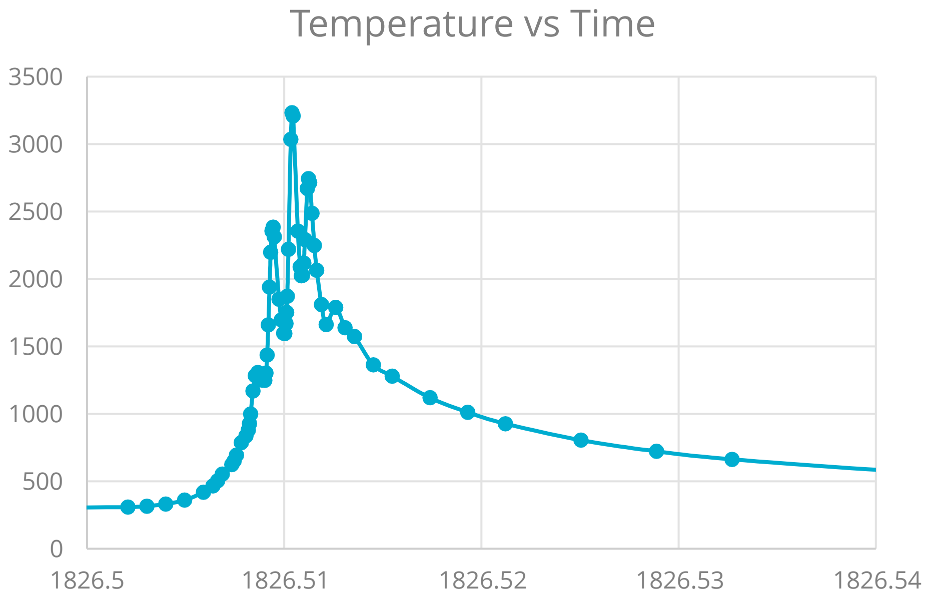
Metallography image of built cube showing overlapping melt pools



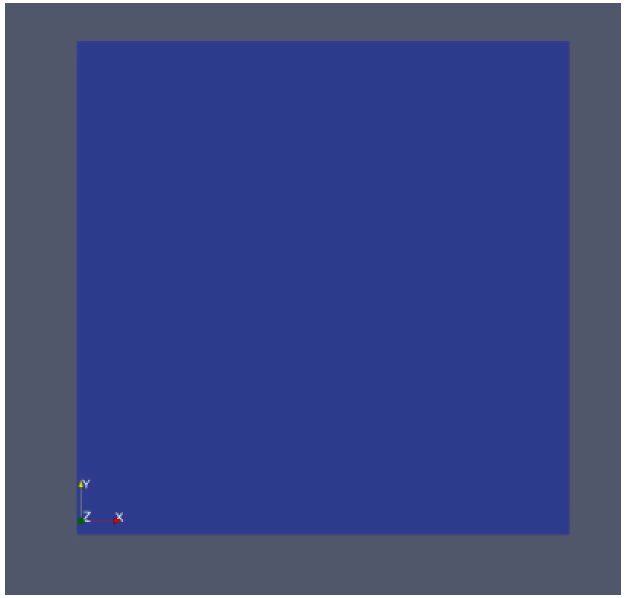


Part Scale Predictions

- Gaining confidence that uncertainties in thermal-fluid model account for observed variations in melt pool shape
- Most real QoIs are at part scale. Thermal-fluid model only provides 3D melt pool shapes
- Model simplifications are needed for tractable performance
  - Thermal only
  - Continuum powder representation
  - Volumetric laser source
  - Linear physics (allows analytical solution)
- Mechanical: rapid computation of pointwise thermal histories
- Microstructure: compute temperatures only in solidification region with time stepping



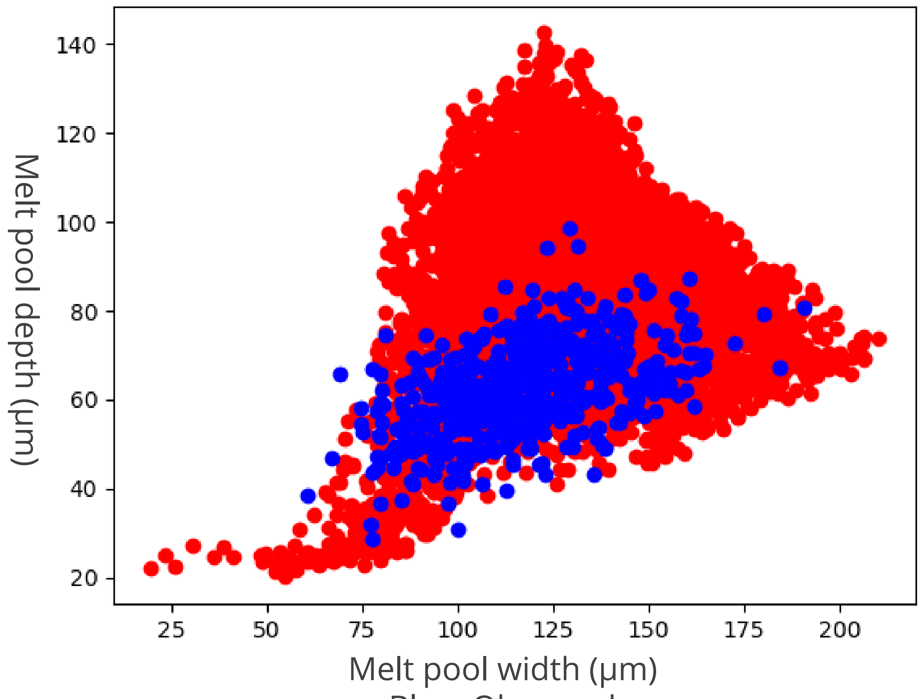
Example time-temperature trace for point in part build simulation



Full layer thermal history computed with analytical model

Part Scale UQ

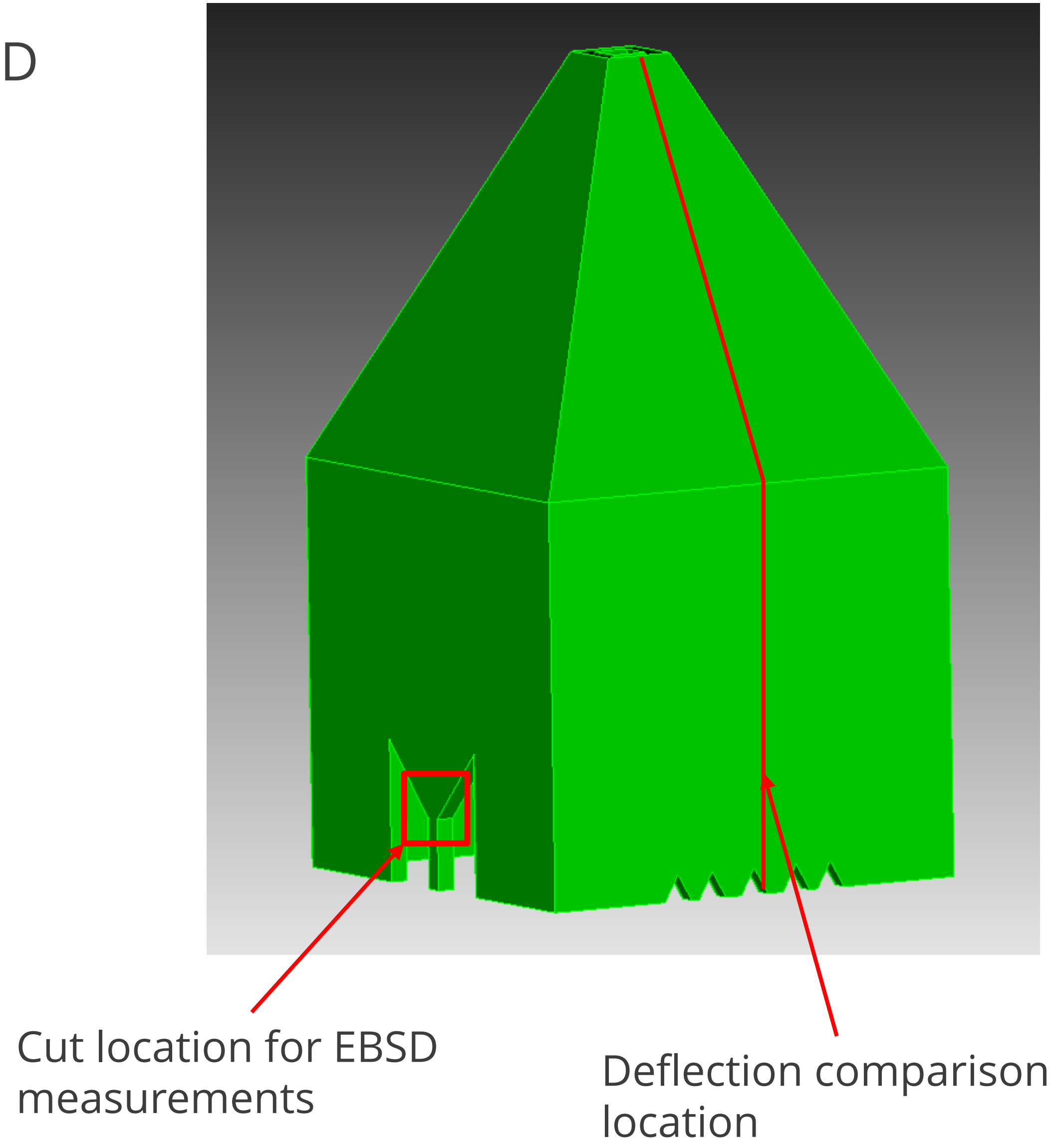
- How to account for model form uncertainties in simplified part-scale model?
- Analytical model has only 7 constant parameters [k, c_p, ρ, P, σ_x, σ_y, σ_z]
- Approach
  - Attempt to account for model form uncertainty through parametric uncertainty
  - Generate distributions for heat source parameters (P, σ_x, σ_y, σ_z) that bounds range of melt pool shapes
  - Uniform distributions for k and c_p that span range of temperature-dependent properties (including latent heat effects)
- Use thermal results as inputs to microstructure and mechanical models



Blue: Observed
Red: Reduced fidelity model

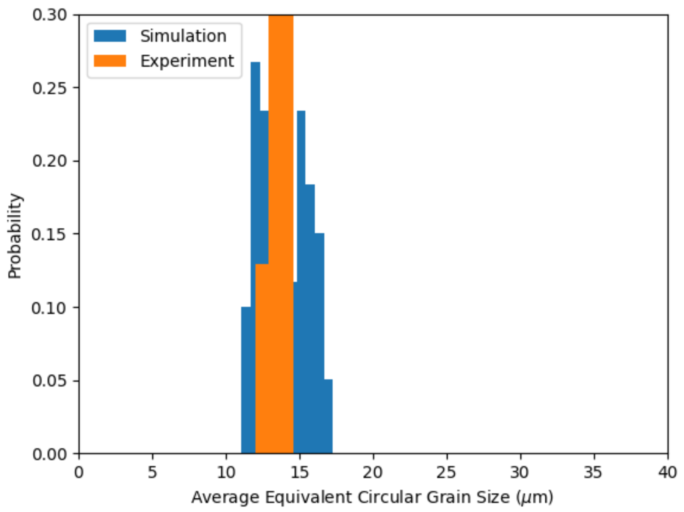
Part Scale Measurements

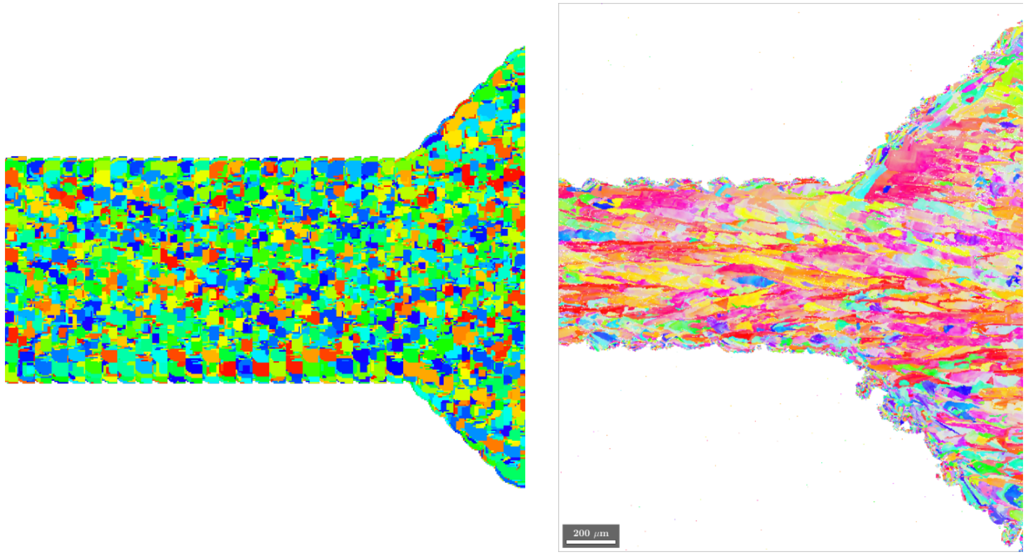
- 2cm ‘house’ geometry builds performed. EBSD and blue light coordinate measurements collected
- Various features added to create areas of microstructural/mechanical interest
- Cut for EBSD in “arch” section of geometry
- Deflections compared along outer wall in the middle



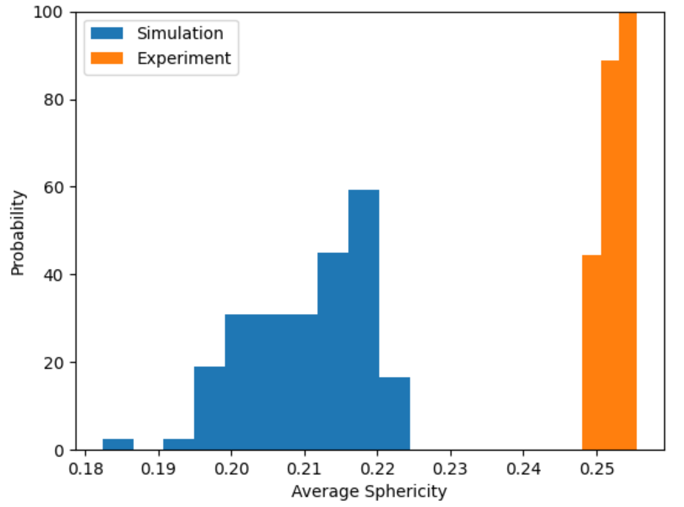
Part Scale Microstructure

- Using SPPARKS undercooling based microstructure model
- Simulating small "window" of the part matching to EBSD cut
- Agreement for grain size, not shape. Metrics admittedly coarse
- Low sensitivity to thermal model uncertainties – explore sensitivity to nucleation parameters
- Need better methods to quantify microstructure



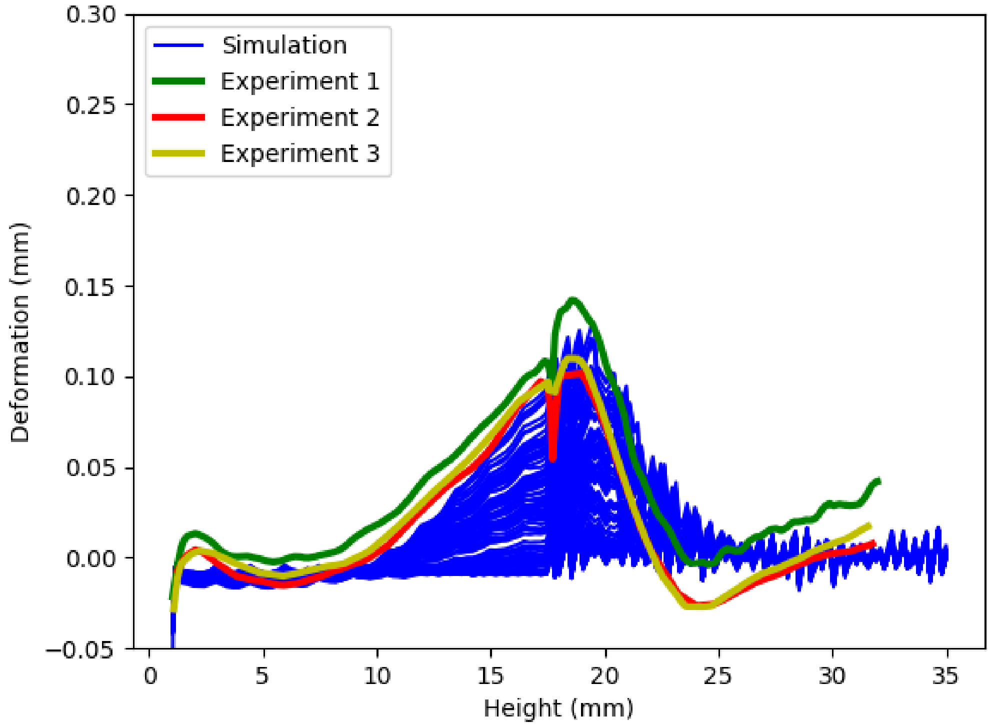


EBSD image vs SPPARKS simulation of "arch" region of small house



Part Scale Deflection

- Make use of analytical pointwise temperature histories
- Impose pointwise stress source that's a function of max thermal gradient magnitude
- Currently underestimating distortion observations
- Likely missing some uncertainties
  - Where to compute maximum gradient?
  - $\boldsymbol{\sigma}(\max(|\nabla T|))$
  - Mechanical model parameters
- Exploring other approaches
  - Calibration of $\boldsymbol{\sigma}(\max(|\nabla T|))$ from small-scale models
  - Coarse time stepping



Conclusions and future work

- Uncertainty quantification techniques have shown promise in bounding laser powder bed fusion build outcomes, particularly at bead scale
- Work is planned to fully propagate uncertainties from process physics to part distortion, residual stress, and material properties
- Model form uncertainty quantification is an outstanding challenge in reduced fidelity conduction models and rapid solid mechanics models
- Final goal is to predict outcome distributions for part performance that can be used to assist with process qualification