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Uncertainty Quantification and Bayesian Calibration of a Powder-Scale Model for Selective Laser Melting

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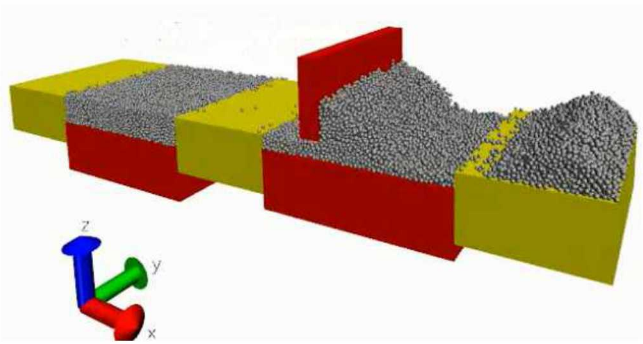
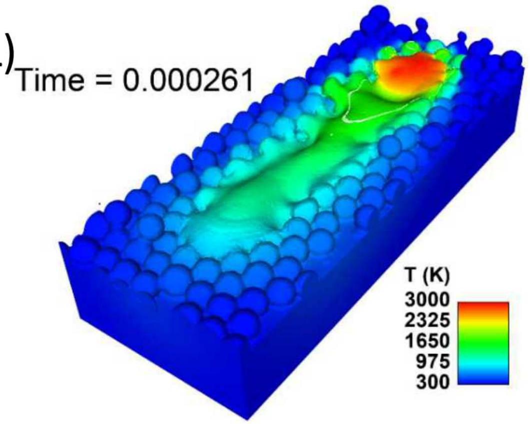
SLM Model Scales

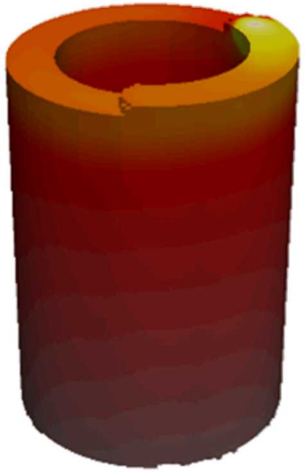
- Powder scale/Mesoscale
  - Powder packing and spreading
  - Microstructure
  - Melt pool dynamics
  - Surface characterization
  - Pore formation
- Part scale/Macroscale
  - Residual stresses
  - Mechanical properties
  - Distortion



Powder Spreading
(Dan Bolintineanu, SNL)



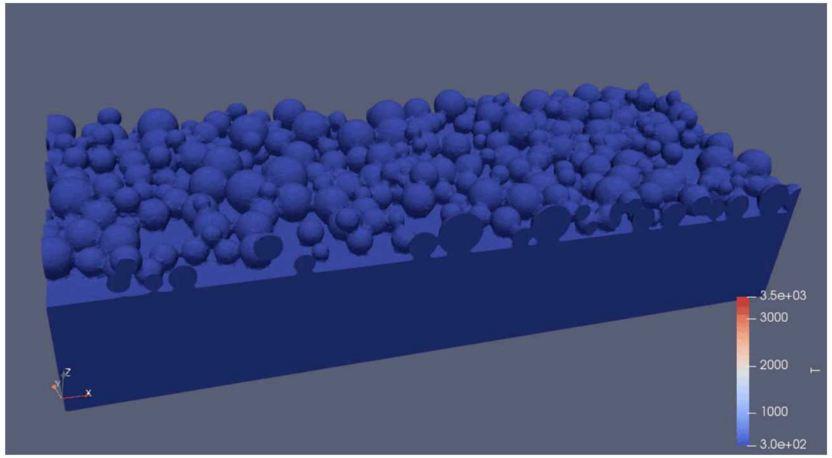
Melt Flow
(Mario Martinez, SNL)



Part scale model
(Kyle Johnson, SNL)

Mesoscale Model Details

- Resolves individual powder particles and detailed melt physics
- Melting/solidification
  - Temperature-dependent viscosity fixes metal in place until melt temperature is reached
- Melt flow
  - 2 Phase liquid-gas flow
  - Interface tracked using level set advection
  - Interface-conforming mesh generated on the fly – allows discontinuous physics across interface
- Surface tension
  - Discontinuous stress across interface
  - Temperature dependent
- Vapor recoil pressure
  - Temperature dependent momentum flux along interface

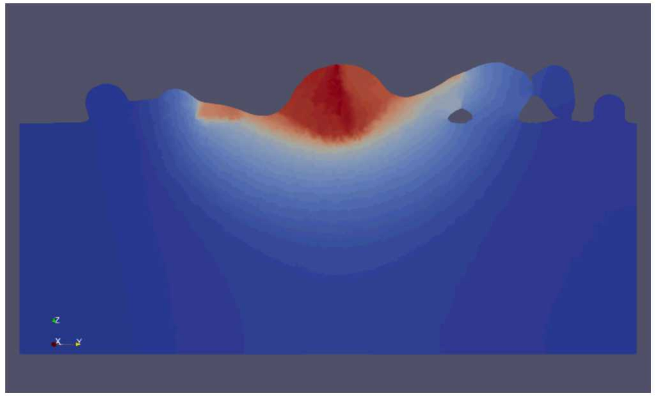


SLM Melt Flow

Why Mesoscale Model UQ?

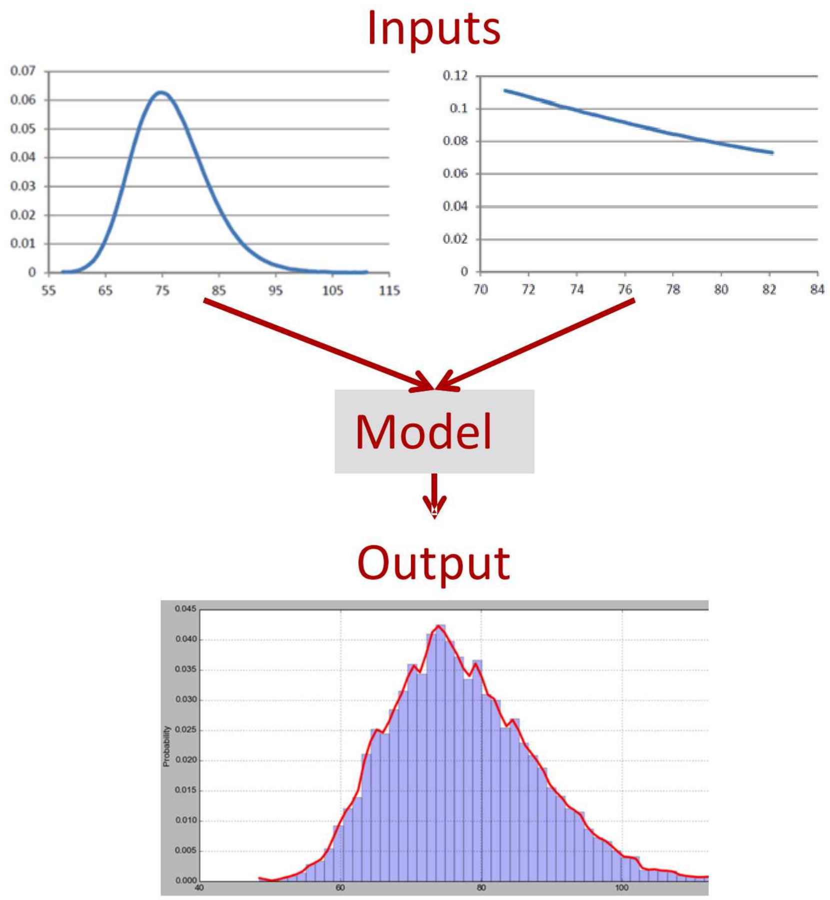
- Allows model input uncertainty to be propagated to model outputs
- Defines how “close” model predictions need to be to agree with experimental data
- Used to identify model deficiencies and needed improvements
- If mesoscale models used as inputs or to inform other models:
  - Need to know predictive capability
  - Need estimate of output uncertainties
- Mesoscale experimental data is (relatively) easy to obtain

=?



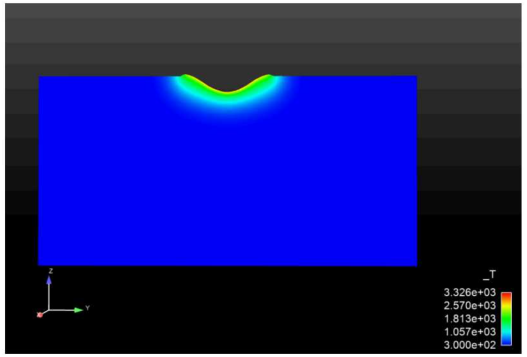
UQ Methodology

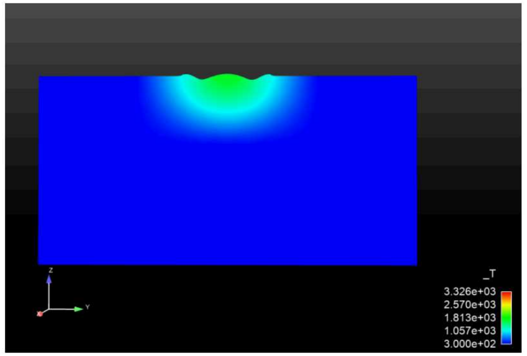
- Goal of UQ is to construct probability distribution of model outputs given distributions of inputs
- Sampling:
  - Draw samples from input distributions
  - Run through model
  - Construct output distributions from set of results
- Requires many model evaluations to accurately calculate statistics
- Impractical for expensive mesoscale models
- Surrogate model is needed to make UQ tractable
- Once agreement with experiment is obtained, can also be used for calibration



Getting Started: Flat Plate Line Scans

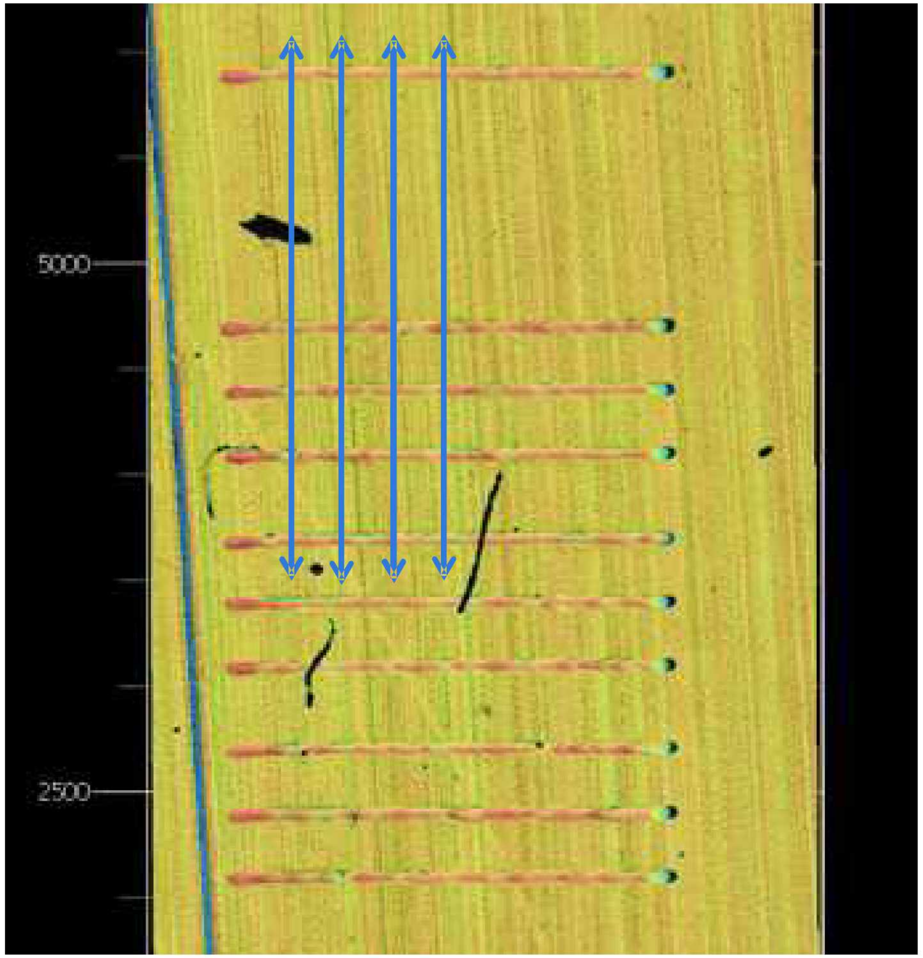
- Model applied to laser scan on flat SS316 plate with no powder
- Assumed dominant uncertainties are laser absorption coefficient, laser diameter, and surface tension coefficient
  - Laser absorption: Uniform random 0.1-0.6
  - Laser diameter: Uniform random 100um-200um
  - Surface tension @ 3100K: Uniform random 0-1 N/m
- Model predictions compared to experimental data for:
  - Melt track shape: surface profilometry
  - Melt track depth: metallography



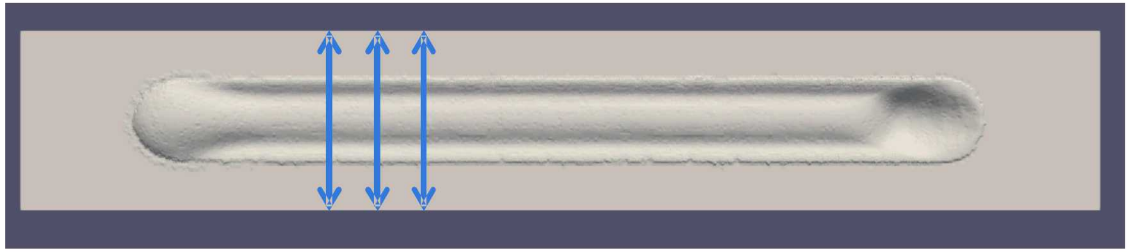


Flat Plate Scan Cross Sections

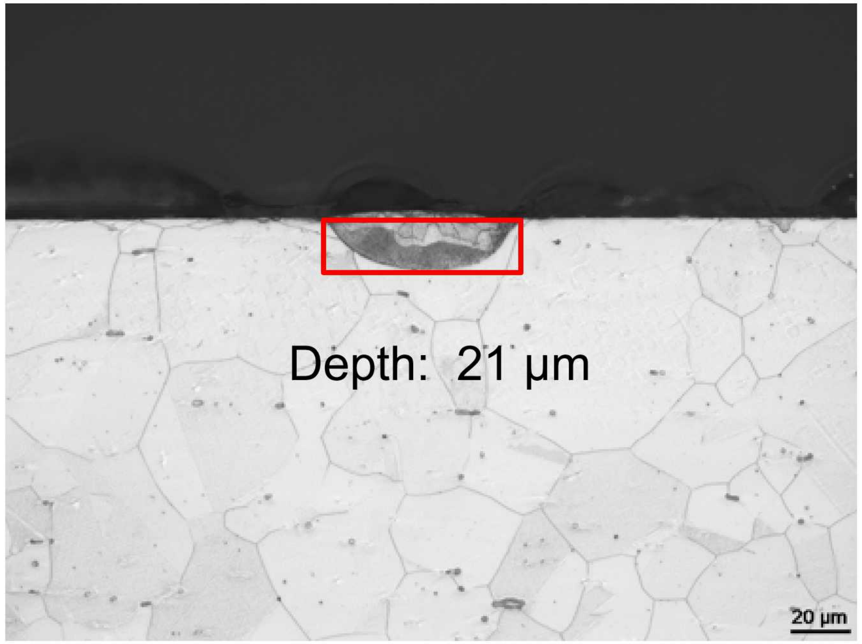
Flat Plate Results 103W 1.4m/s: Track Shape



Profilometry Results
(Bradley Jared, SNL)

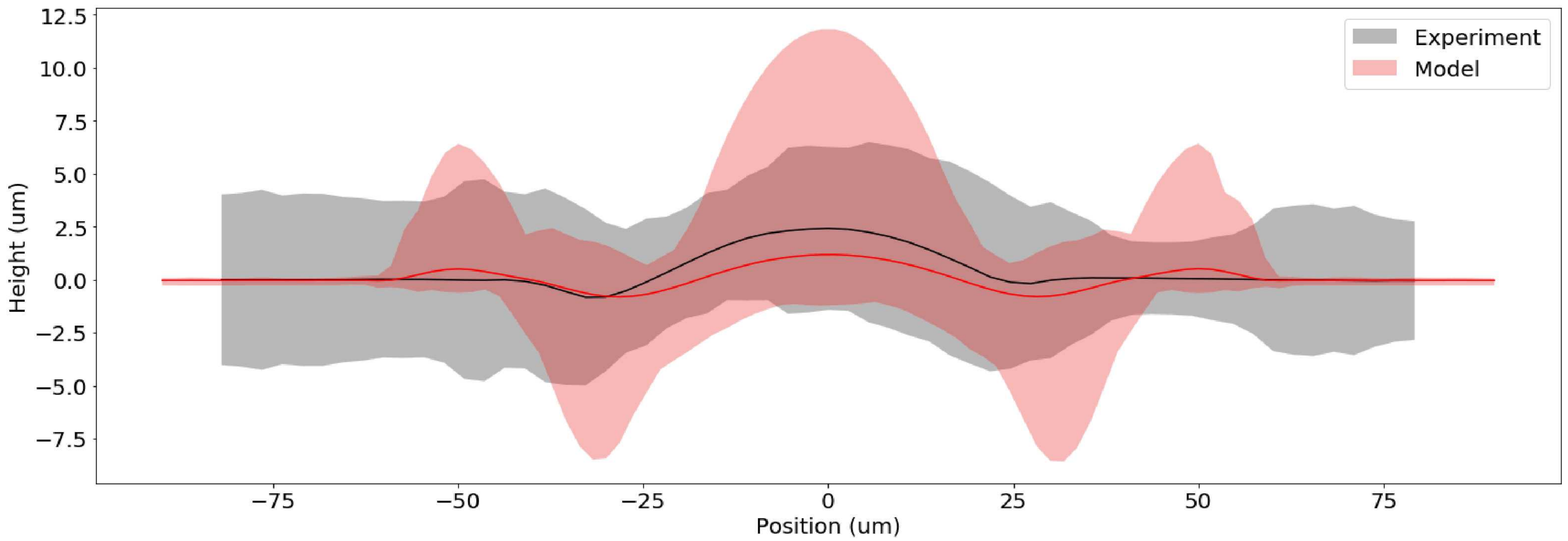


Simulated Melt Track



Metallography Cross Section
(Bradley Jared, SNL)

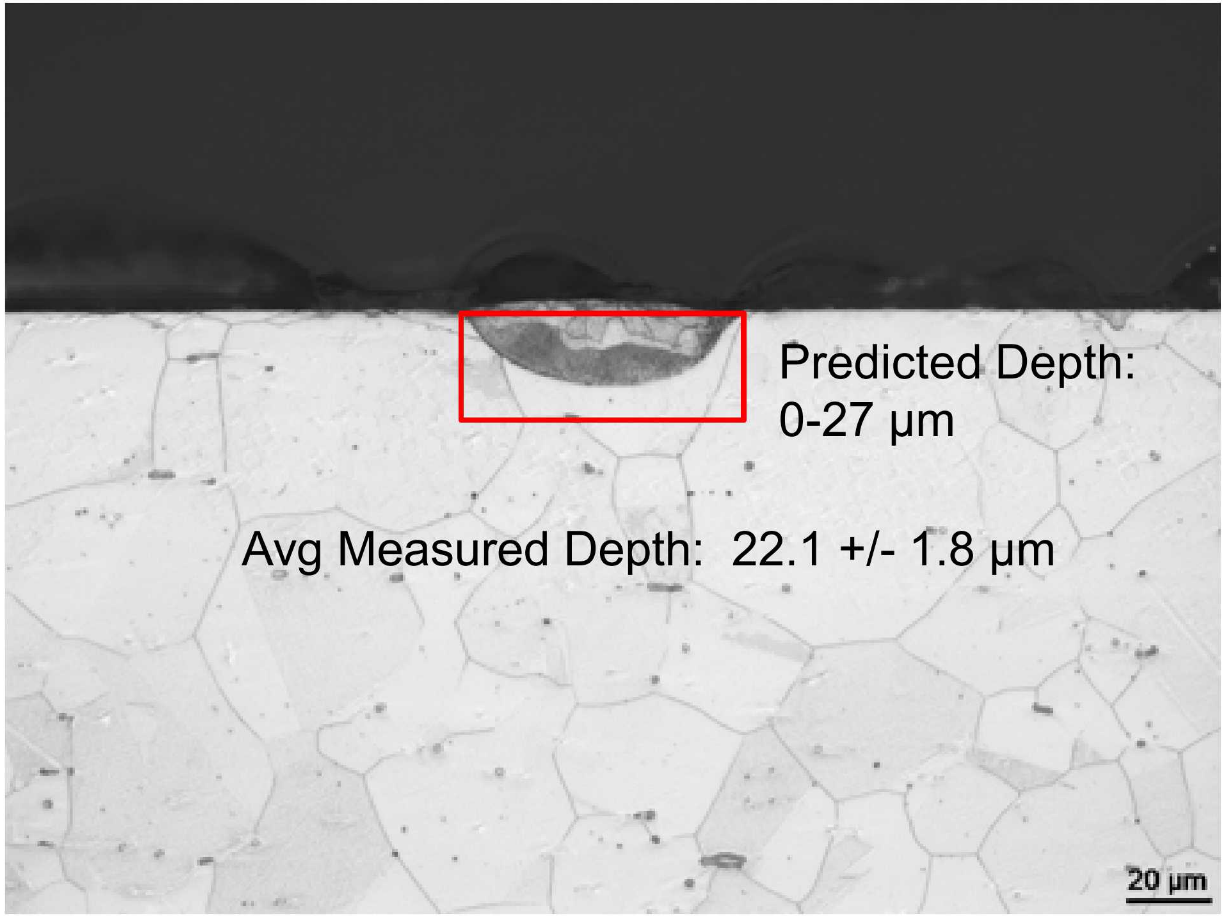
Flat Plate UQ 103W 1.4m/s: Track Shape



Comparison of Predicted and Experimental Results for Track Shape
Bands represent 2 standard deviations

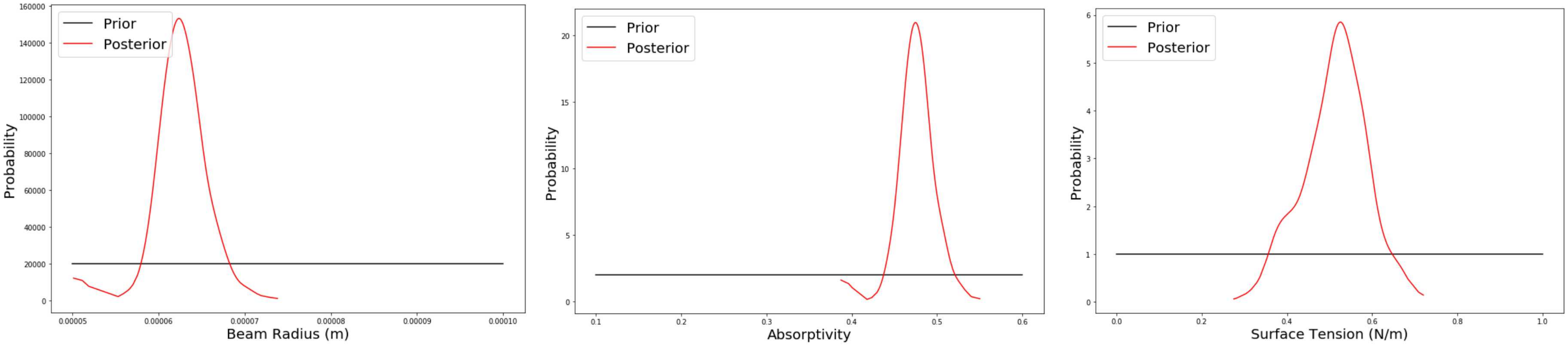
- Model and experimental predictions overlap for calculated uncertainties
- Calculated model uncertainties are large due to large uncertainties in inputs

Flat Plate UQ 103W 1.4m/s: Track Depth



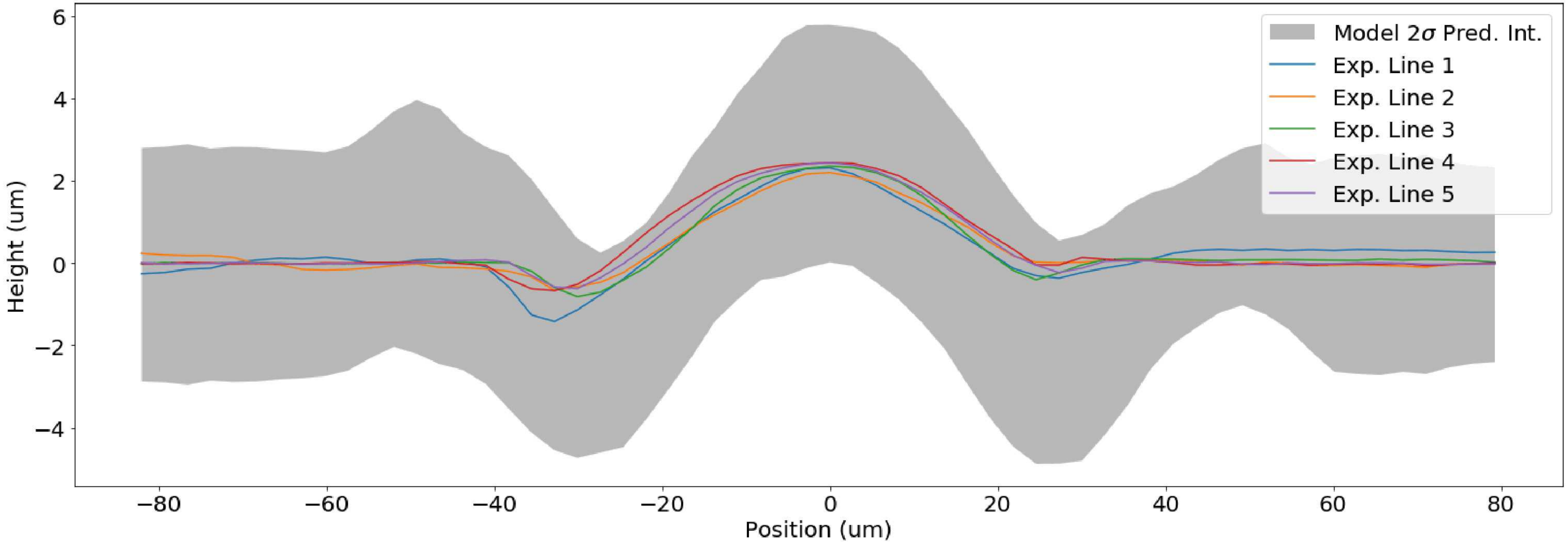
- Model and experimental predictions overlap for calculated uncertainties
- Calculated model range represented 2 standard deviations

Model Parameter Calibration



- Posterior probability distribution given observed experimental data calculated for all uncertain inputs
- Monte Carlo Markov Chains used to sample from posterior distribution
- Posterior distributions represent knowledge gained about the input parameters by observing the experimental results

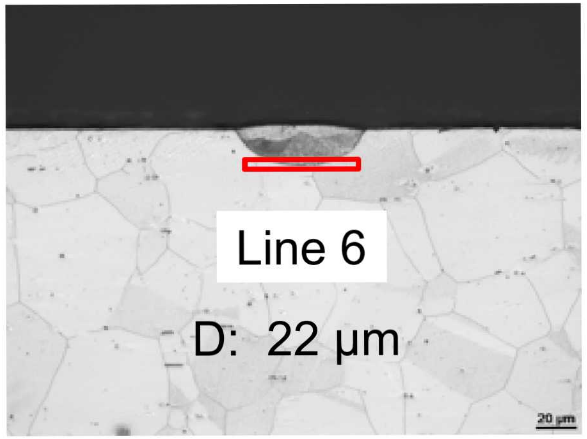
Testing on Unused 1.4m/s Data: Track Shape

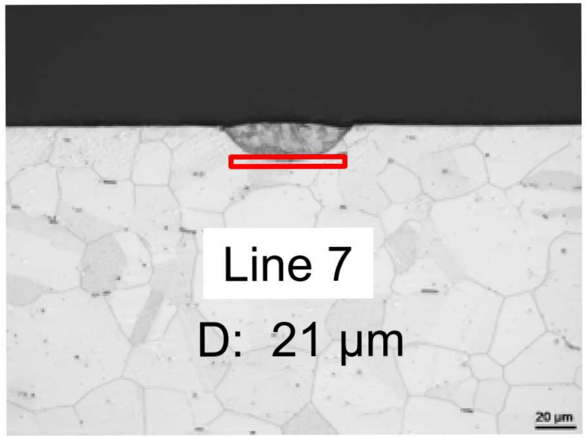


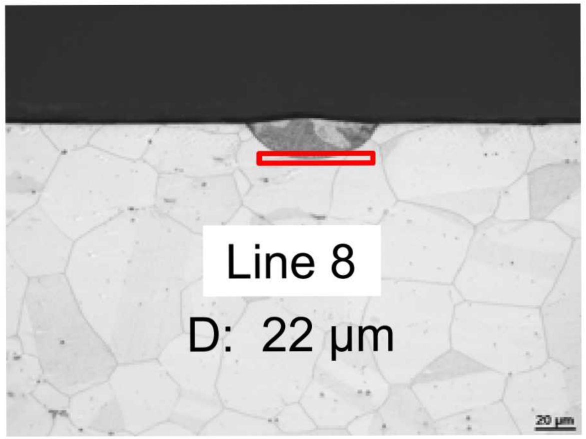
Comparison of Predicted and Experimental Results for Track Shape
Band represents 2 sigma prediction interval

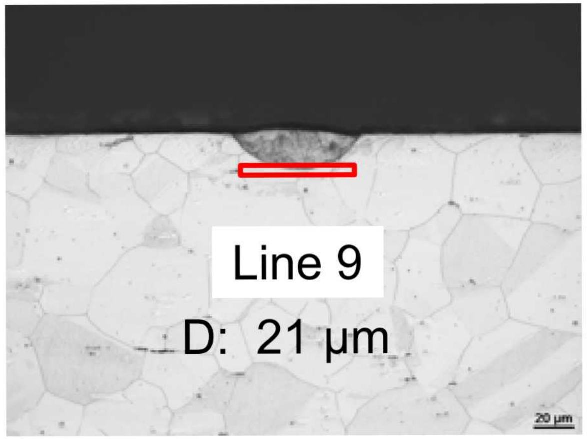
- Results with calibrated parameters match up well with unused data and model uncertainties are reduced

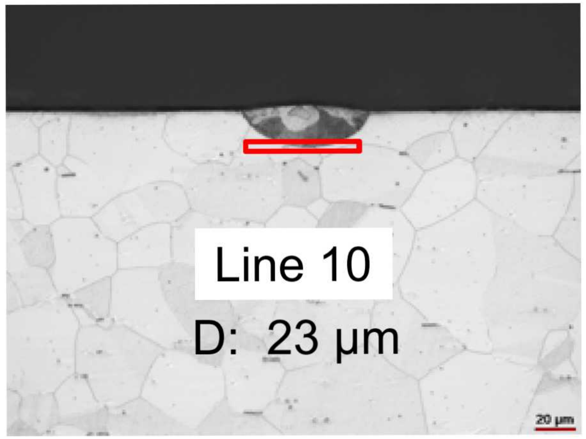
Testing on Unused 1.4m/s Data: Track Depth









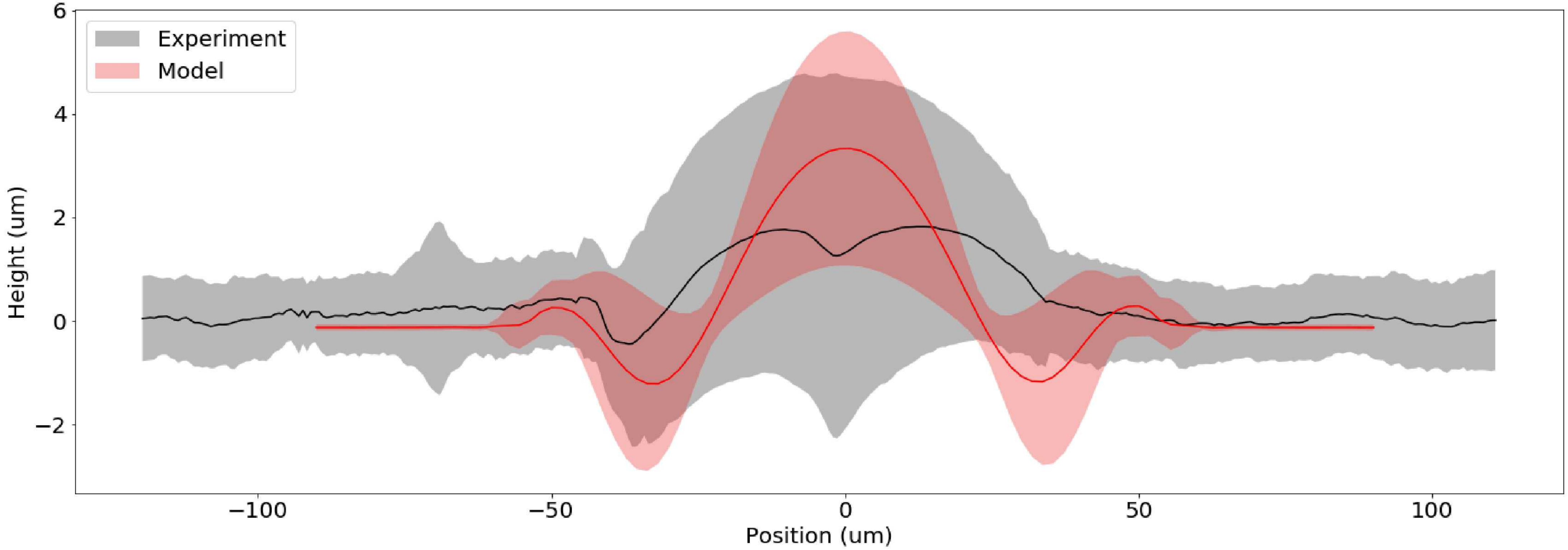


2-Sigma Prediction Interval is 20-24 µm

Red Boxes indicate prediction interval

- Results with calibrated parameters match up well with unused data and model uncertainties are reduced

103W 1.2m/s Prediction: Track Shape

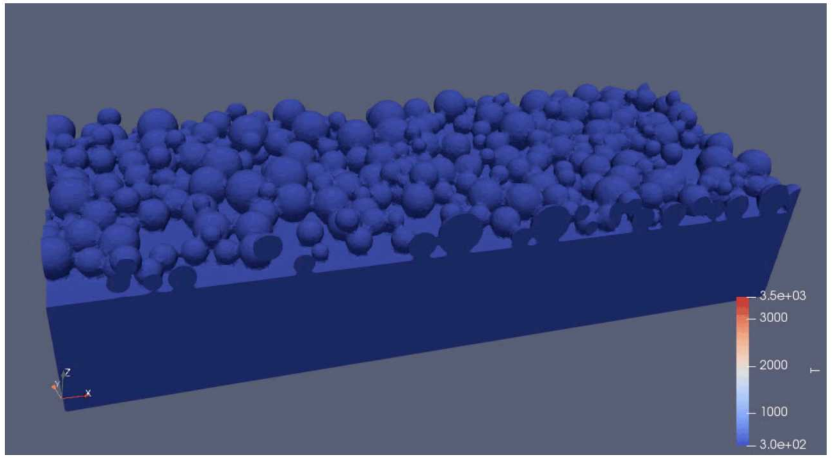


Comparison of Predicted and Experimental Results for Track Shape
Bands represent 2 standard deviations

- Model predictions line up with experiment to within uncertainties:
  - Only 1 experimental result available for these conditions: may not represent true variability
  - Experimental average seems to give a shorter, broader, peak
  - Some calibrated parameters (ie. absorptivity) are likely dependent on processing conditions

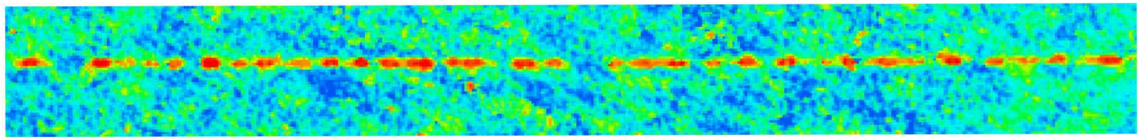
Powder Line Scans

- Model applied to laser scan on 30um layer of SS316 powder on top of plate
- Input uncertainties:
  - Laser absorptivity: Uniform 0.3-06
  - Beam diameter: Normal (avg=100um std=10um)
  - Heat of Vaporization: Normal (avg=7.4e6 J/kg std=1.5e6 J/kg)
- Model predictions compared to experimental data for:
  - Melt track shape: surface profilometry
  - Cross section metallography



Powder Scan

Powder Results 103W 1.4m/s: Track Shape



Profilometry Results
(Bradley Jared, SNL)

Metallography Cross Section
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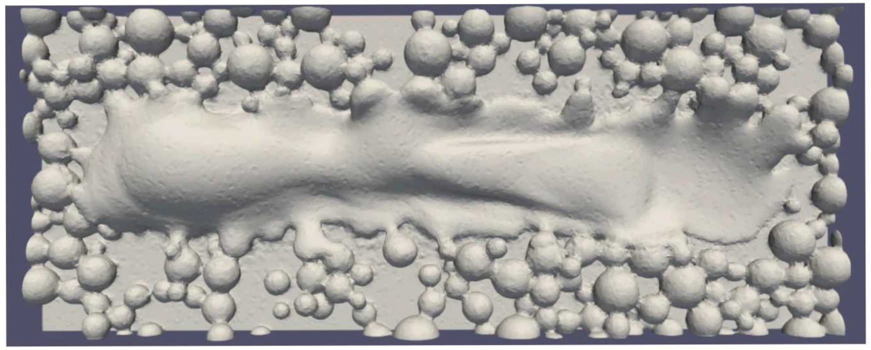
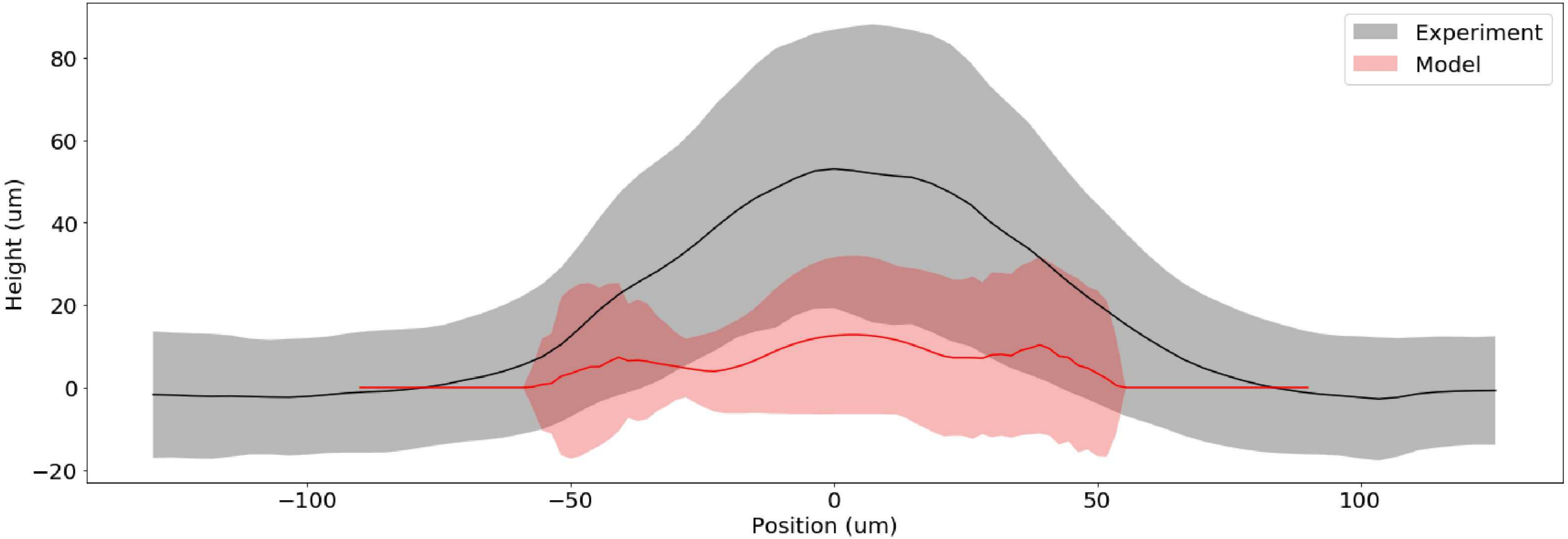


Simulated Melt Track a=0.45

Powder UQ 103W 1.4m/s: Track Shape



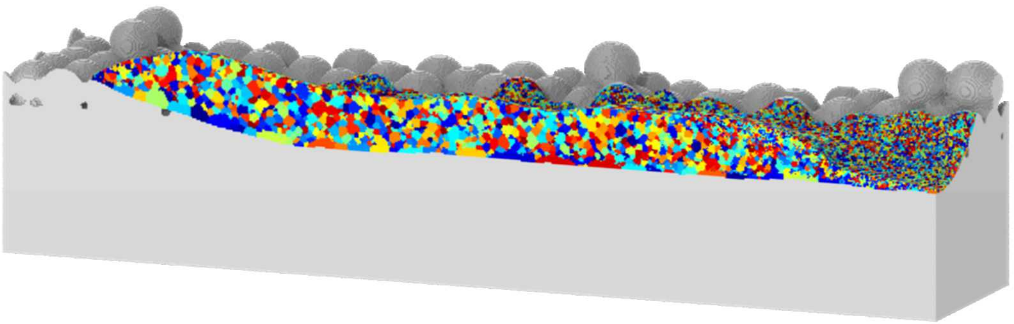
Comparison of Predicted and Experimental Results for Track Shape
Bands represent 1 standard deviation

- Lots of experimental variation: track breakup, build surface roughness, particle locations/packing fraction
- Need to select laser parameters that don't give a broken track
  - Model also unable to predict track break-up – unmodeled physics or track too short

Conclusions and Next Steps

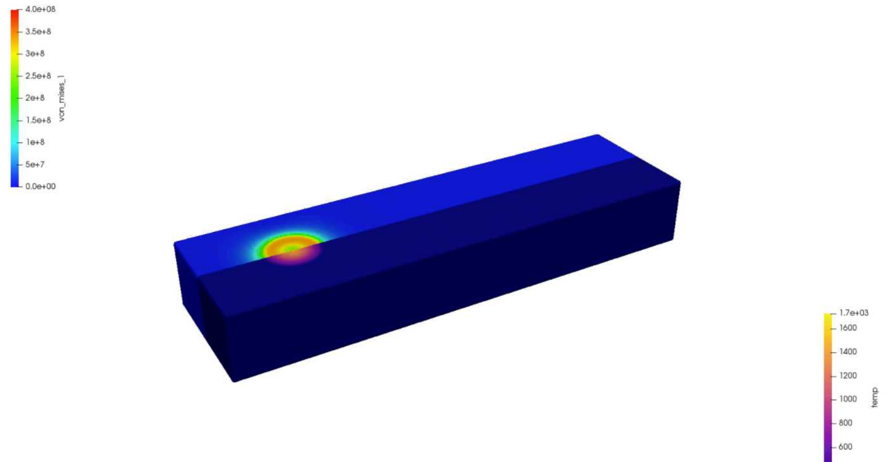
- Model calibration for flat plate scans predicts results for same processing conditions
- Results for different processing conditions still agree, but not as well
  - Investigate including processing condition dependence on material absorptivity
  - Model improvements to remove dependence
- Large uncertainty in powder data due to track breakup
  - Need to repeat using better processing conditions
  - Model doesn’t predict track break-up – track too short?
  - Other neglected physics in model (ie powder motion) may also play a role

Mesoscale Model-Based Work



Microstructure Predicted from Mesoscale Model Results (Theron Rodgers, SNL)

- Model calculated temperature field and track shape mapped onto regular grid
- KMC algorithm performs microstructure prediction driven by temperature



Residual Stress Predicted from Mesoscale Model Results (Lauren Beghini, Michael Stender, Kurtis Ford, Michael Veilleux, SNL)

- Model calculated temperature field and track shape mapped onto conformal hex mesh
- Elastoviscoplastic temperature and rate dependent material model used to calculate deformation and residual stress