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INTERNATIONAL DESIGN ENGINEERING TECHNICAL CONFERENCES & COMPUTERS AND INFORMATION IN ENGINEERING CONFERENCE

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SURFACE ROUGHNESS SURROGATE MODELING IN METAL 3D PRINTING USING KRIGING AND BATCH EXPERIMENTAL DESIGN

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  - Surface roughness surrogate modeling approaches
- Methodology
  - Design of experiment
  - Kriging
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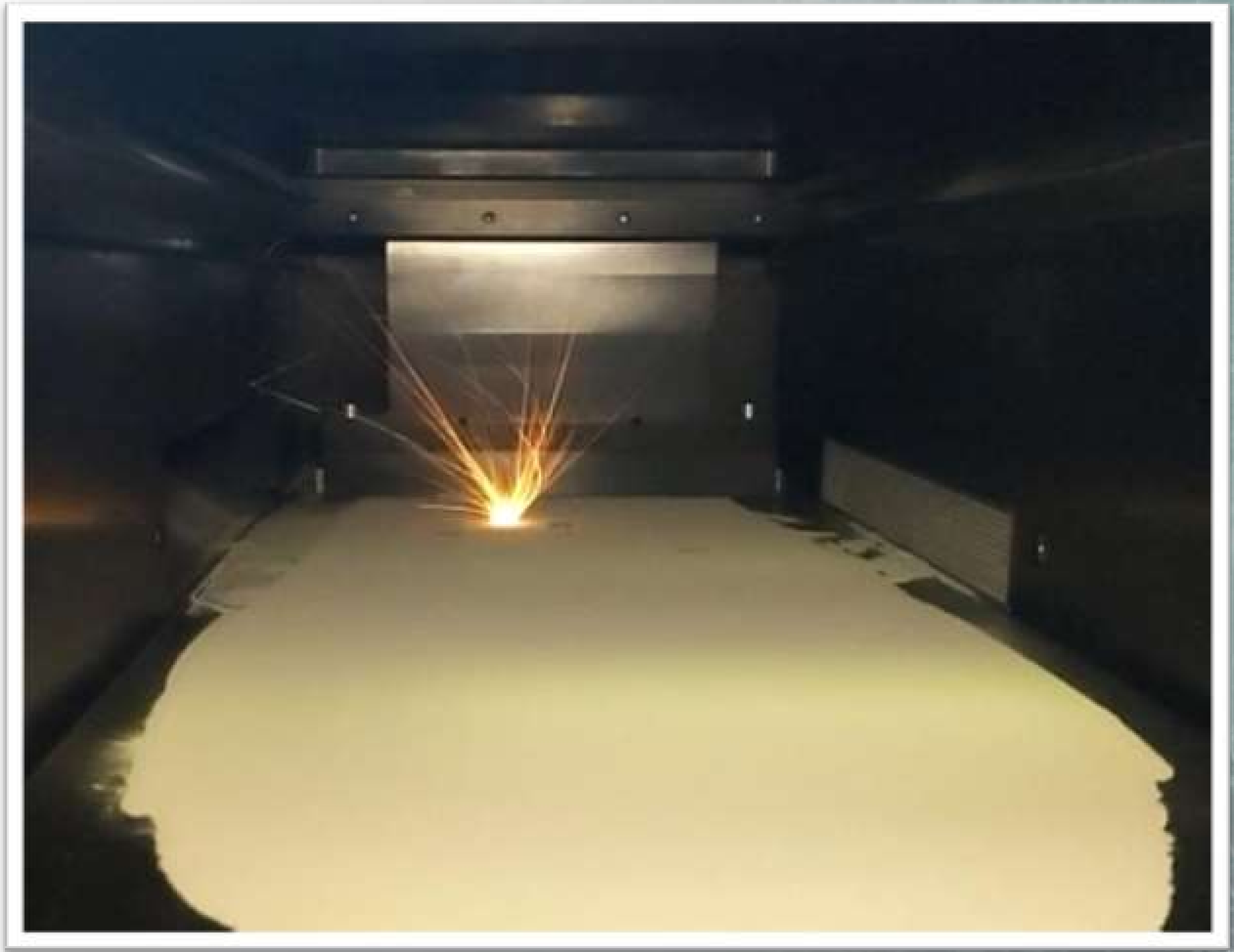
- Experimentation & results
  - Experimental data collection
  - Uncertainty-aware surrogate model
  - Final model
- Conclusion and future work

Image: Aconity3D GmbH. Fair Use

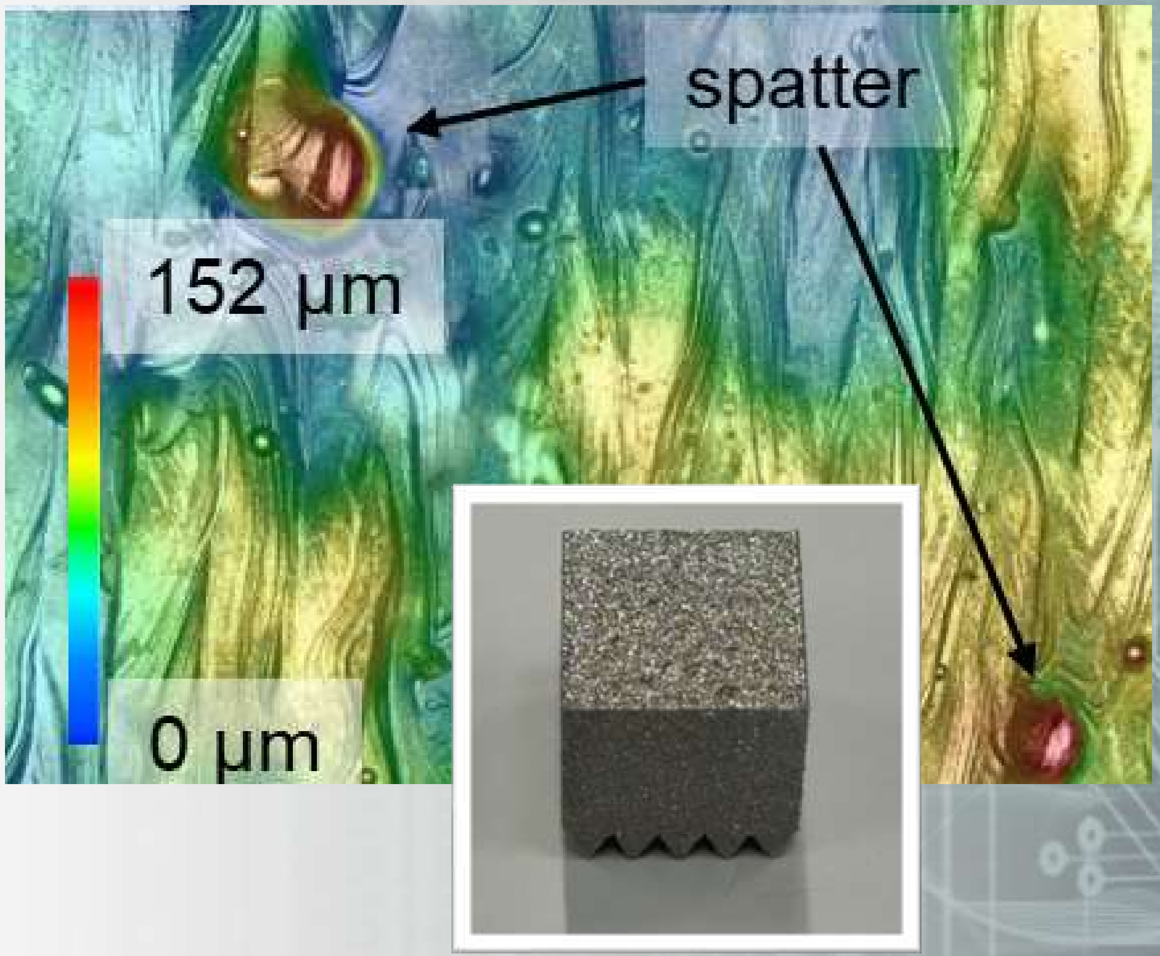
Background LPBF AM

- Laser Powder Bed Fusion (LPBF) builds components layer by layer by fusing metal powder with a laser.
- Enables production of highly complex geometries not achievable with traditional subtractive methods.
- Particularly valuable in fields such as aerospace (lightweight structures) and biomedical (custom implants) applications.



Background Surface Roughness

- A persistent challenge in LPBF is variable surface roughness caused by the fusion process.
  - Aerospace systems for example require smooth surfaces to reduce friction, wear, and drag.
  - Biomedical applications like on the other hand implants benefit from rough surfaces improves osseointegration and implant bonding.
- Controlling roughness is challenging but critical for large-scale adoption of LPBF.

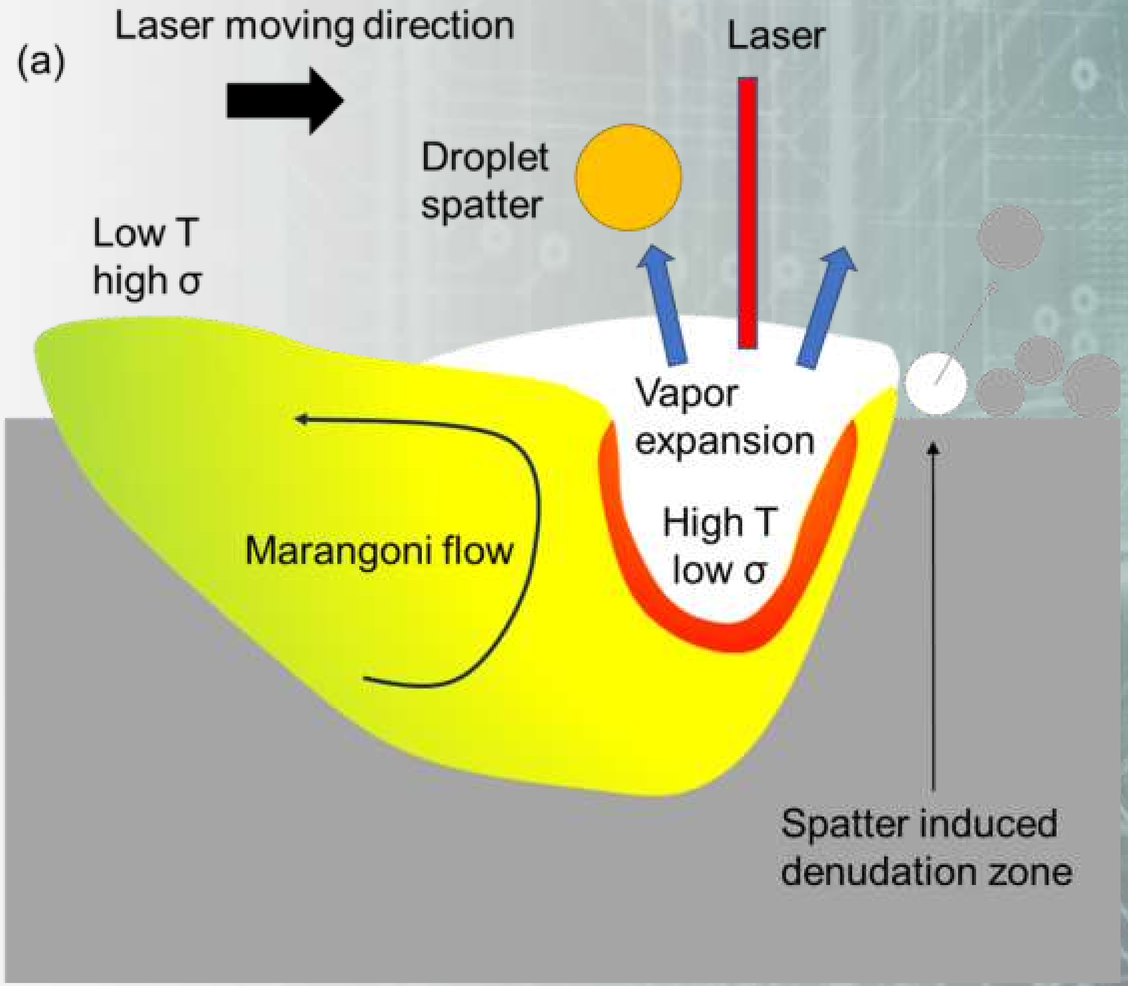


Welding is a Chaotic Process

- In LPBF we can easily control:
  - Laser power
  - Laser speed
  - Laser spot size
  - Hatch spacing
  - Layer thickness: 30 µm
- Other parameters can be adjusted:
  - Powder size
  - Powder packing
- In general, LPBF has a fair amount of uncertainty in the process

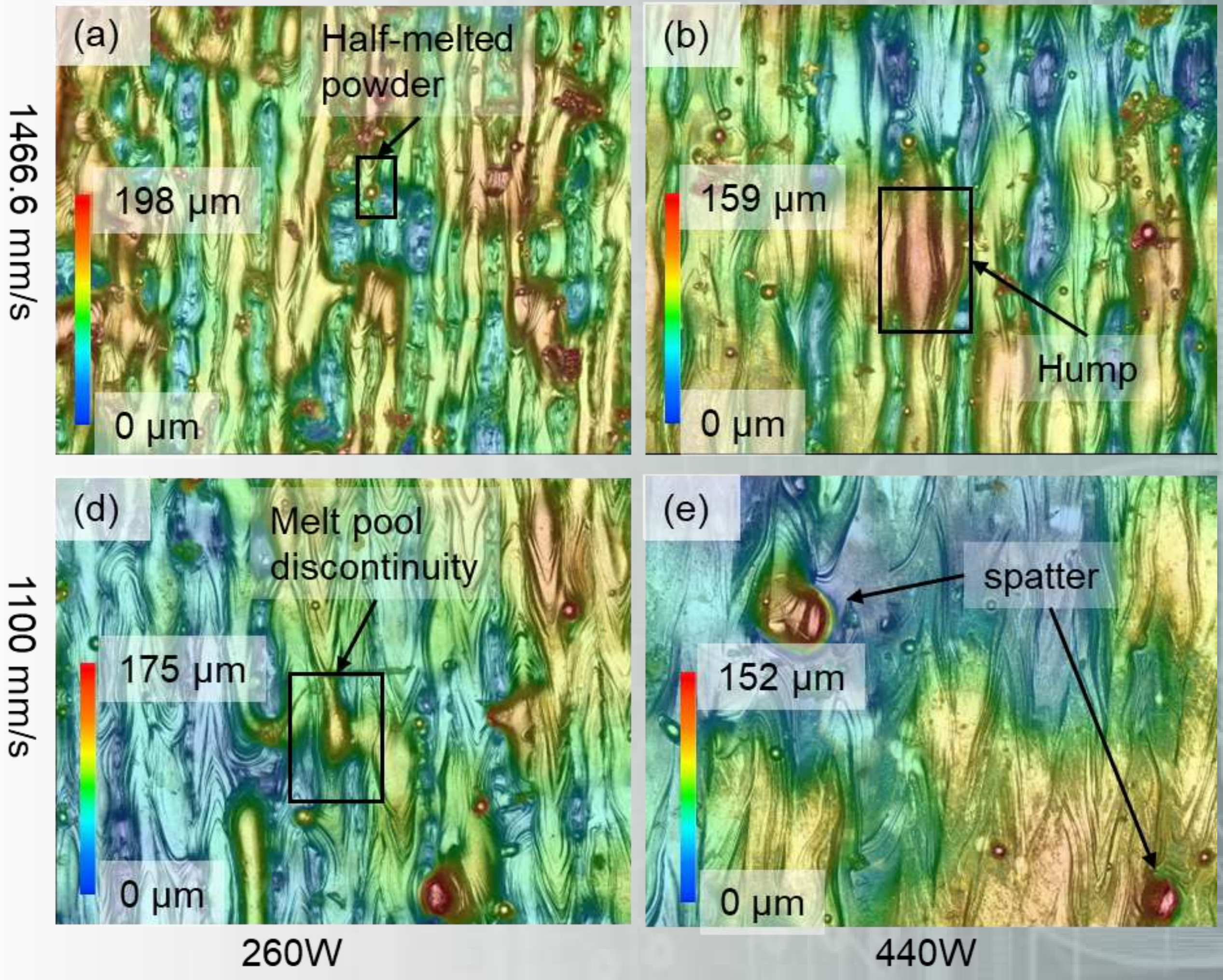
Melt pool physics

- Surface quality is strongly linked to melt pool behavior :
  - Spatter formation: higher laser power ejects particles that solidify as defects.
  - Denudation: gas expansion pushes powder away, destabilizing the melt pool.
  - Hump formation: repeated spatter buildup creates uneven ridges.



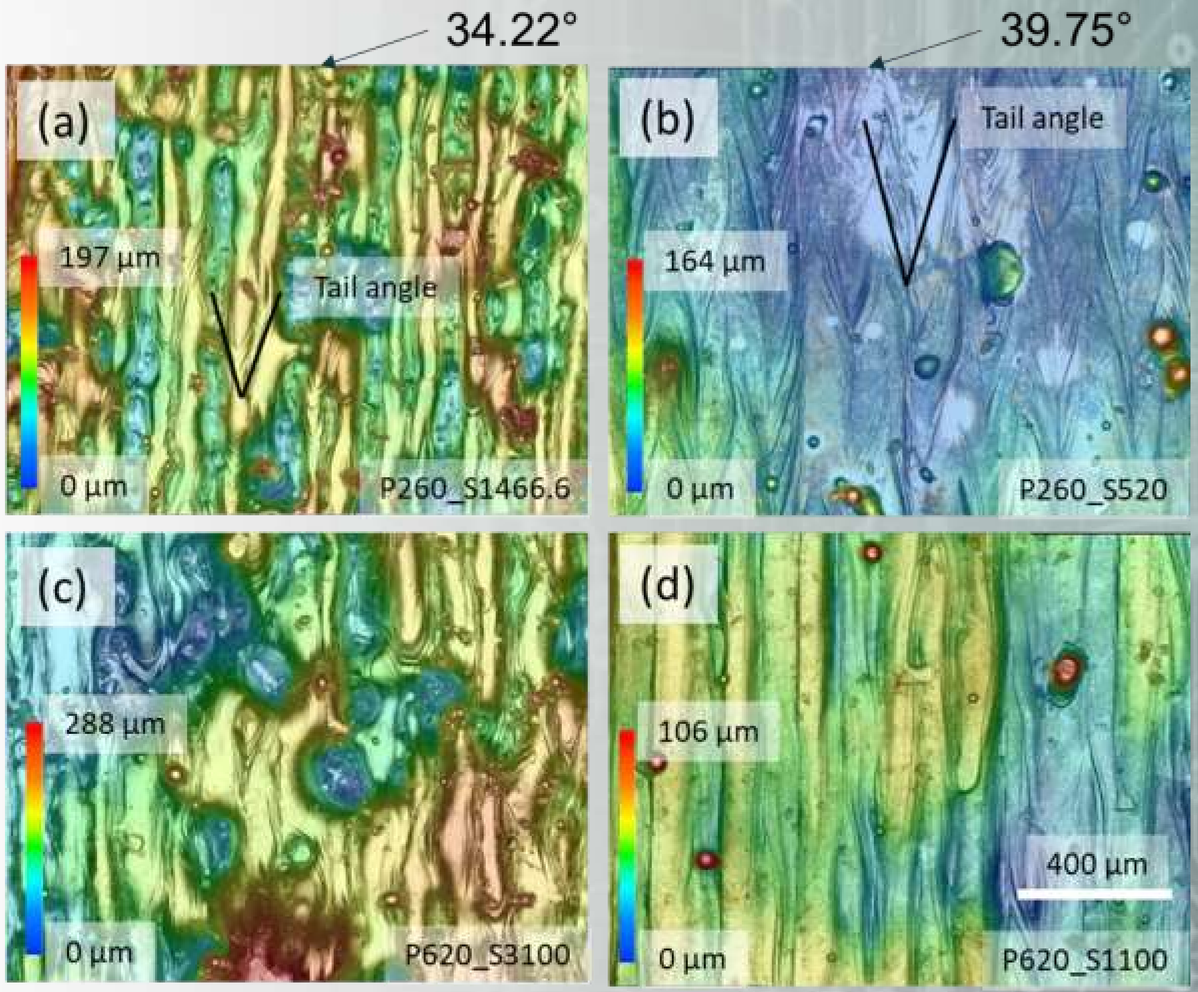
Effect of Power on Top Surface

- Increasing laser power generally increases surface roughness.
- High power creates more spatter, which settles on the surface and forms irregularities.
- Results show rougher top and vertical surfaces that require costly post-processing.



Effect of Scanning Speed on Top Surface

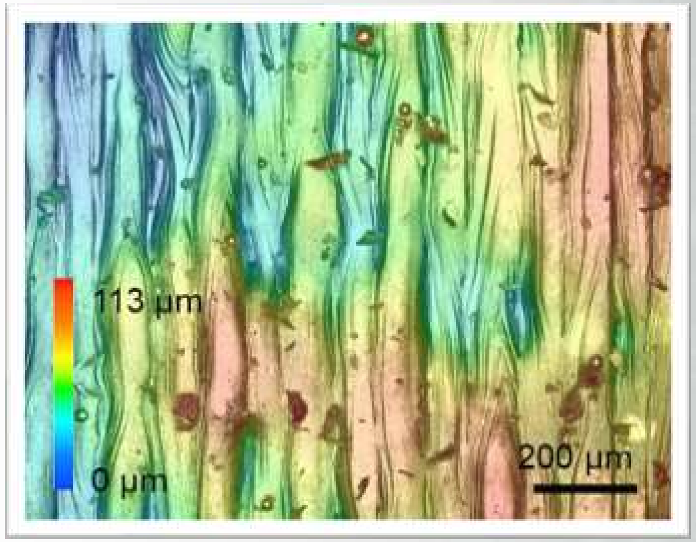
- Higher scan speeds stretch the melt pool, making it more unstable.
- Leads to Plateau–Rayleigh instability:
  - Surface tension breaks the melt pool into droplets when perturbed.
  - Causes uneven deposition and droplet solidification on the surface.
- Faster scans generally promote rougher surfaces with increased irregularity.

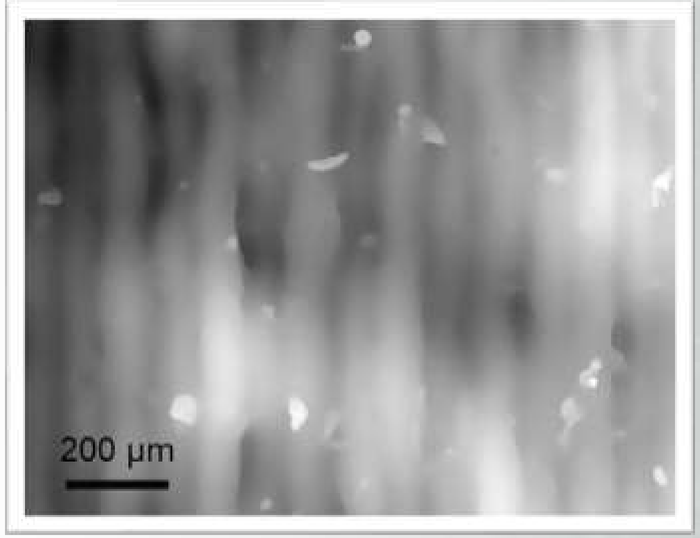


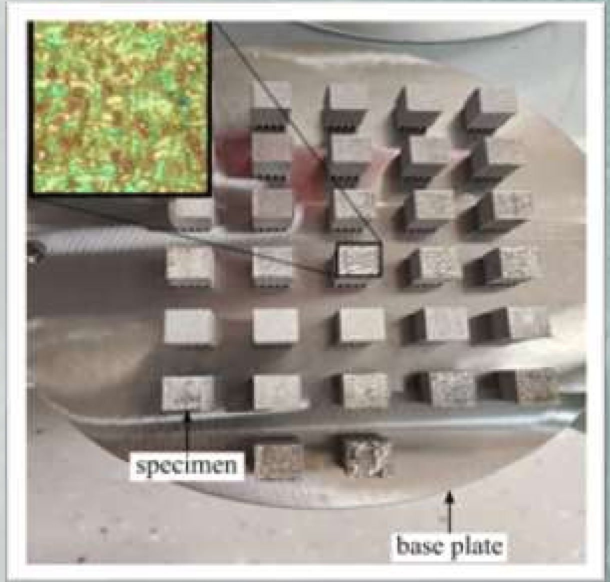
The Characterization Method

- Printed test cubes were removed from the build plate for analysis.
- Optical profilometry was used to acquire depth maps.
- Depth maps converted into surface roughness metric (Sa).

$$S_a = \frac{1}{A}\iint_A |z(x,y)|dxdy$$





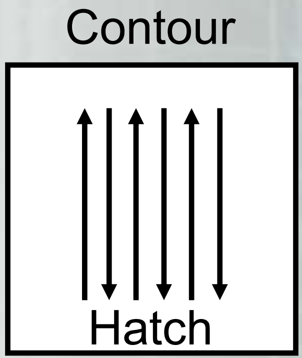


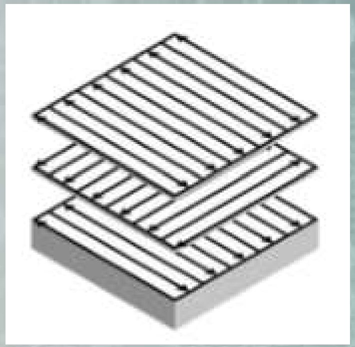
The Design of experiment

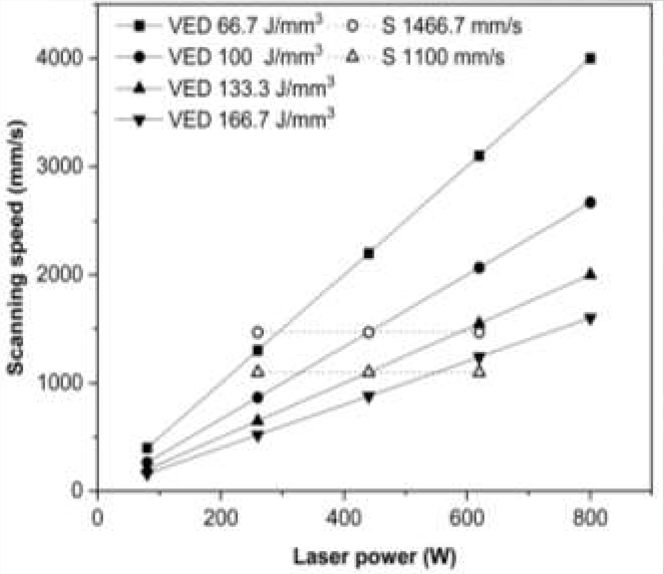
- Initial dataset: 26 points sampled across the process domain.
- Only laser power and scan speed were varied; other parameters held constant.
- Laser powder bed fusion AM
- Machine: Aconity3D MIDI
- Materials: 316L stainless steel
- Conditions:
  - Simple hatch with 100 μm spacing
  - Laser spot size: 100 μm
  - Layer thickness: 30 μm

$$VED = \frac{P}{S * H * T}$$

P: Power
S: Scanning speed
H: Hatching space
T: Layer thickness



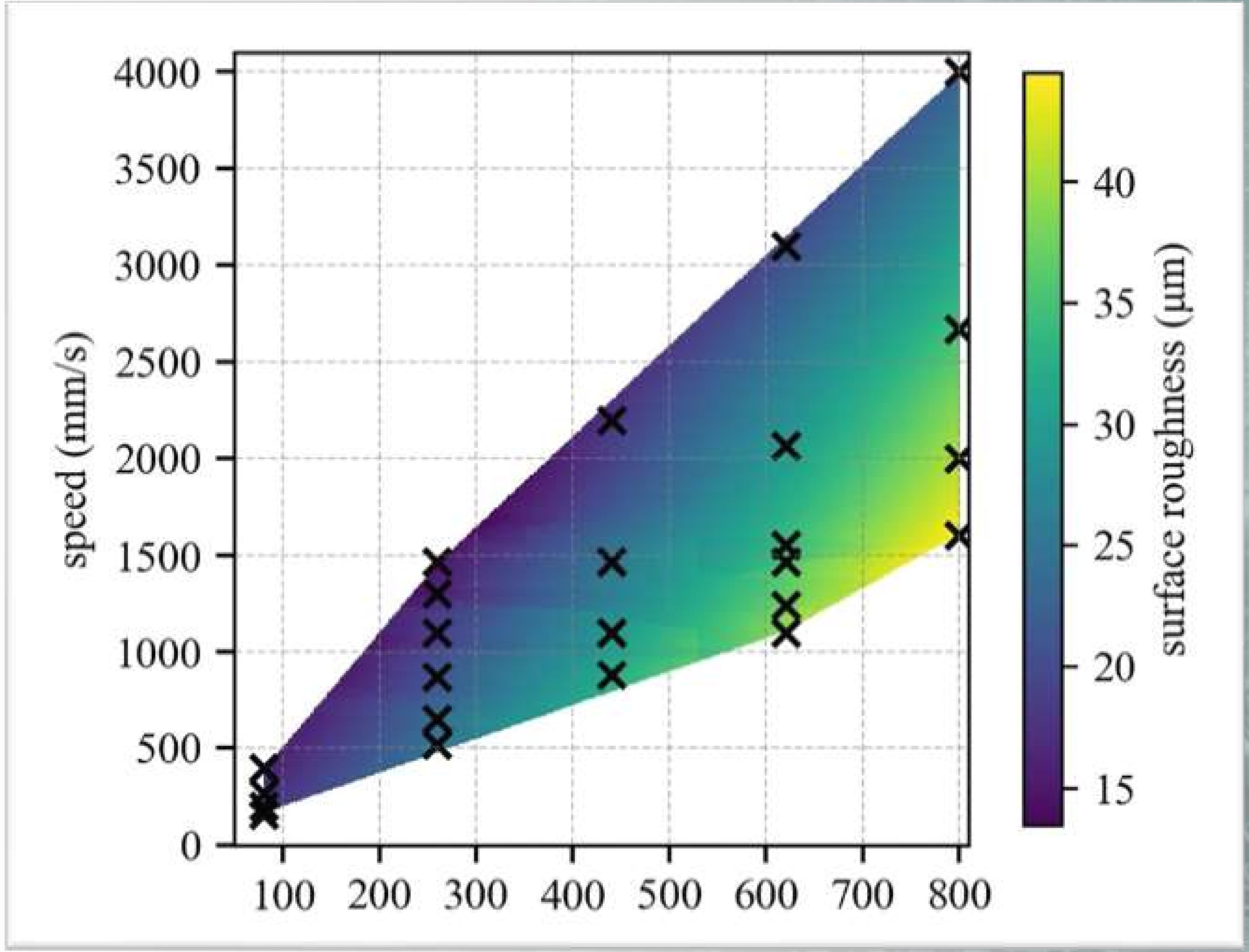




https://aconity3d.com/products/aconity-midi

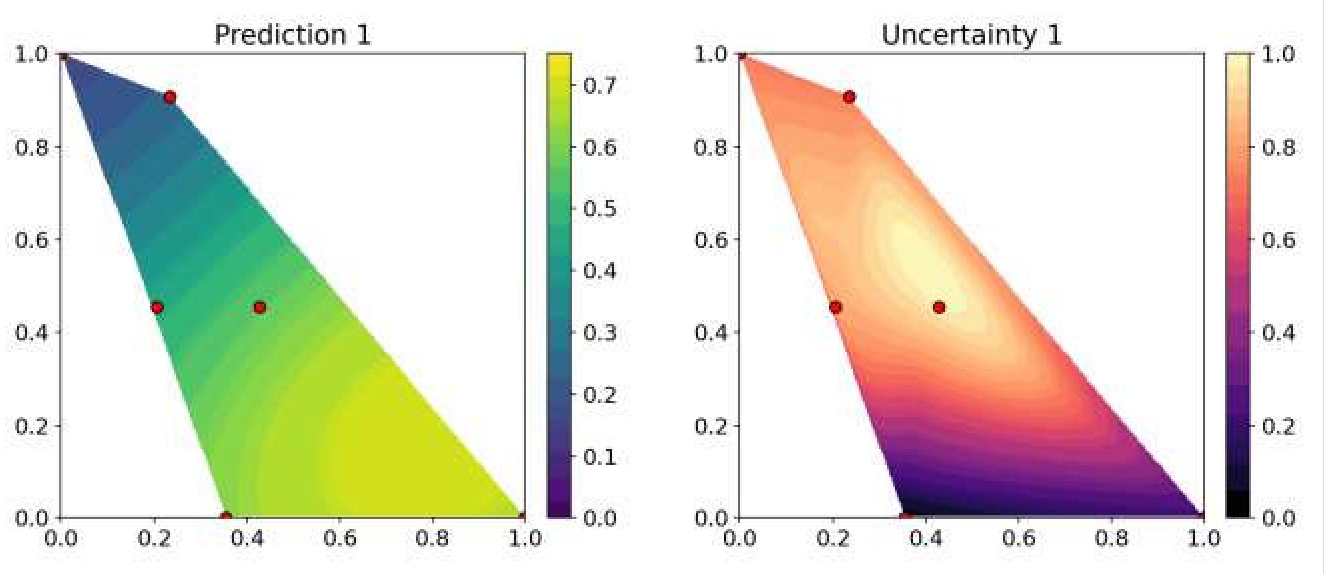
Surrogate Modeling Approach

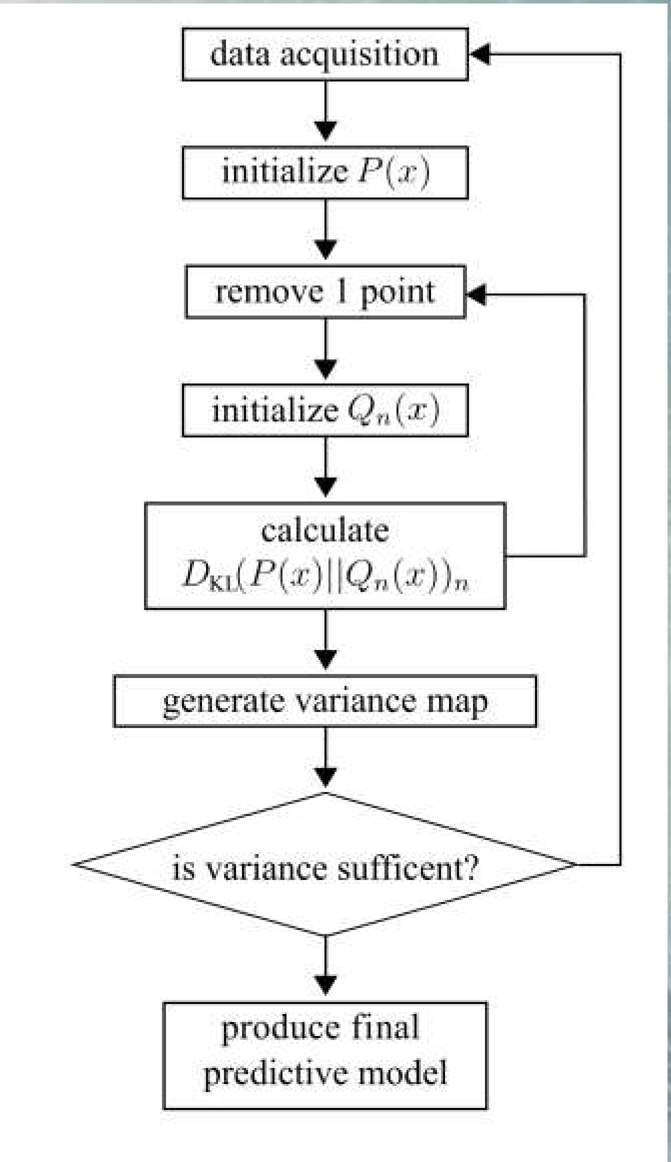
- Exact relationship between parameters and roughness depends on printer hardware and material properties.
- Brute force sampling of design space is expensive and time-intensive.
- Uncertainty-aware surrogate modeling can characterize design space with minimal samples.
- Enables rapid optimization of new materials/processes.
- Allows prediction of desired roughness with far fewer tests.



Proposed Design of Experiments Algorithm

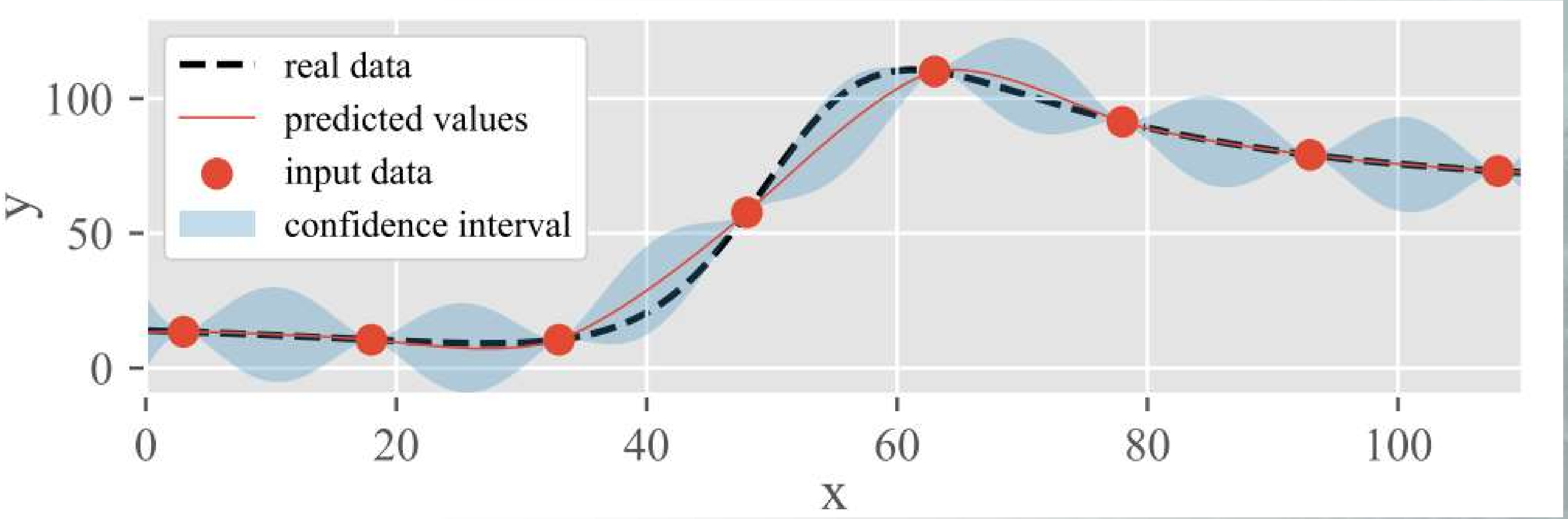
- Kriging with Iterative Spatial Prediction of Uncertainty (KRISP-U).
- Combines Universal Kriging with cross-validation.
- Identifies regions of high model uncertainty.
- Guides new sampling in those regions for more efficient model refinement.
- Produces a robust surrogate model with fewer experimental points.





Kriging

- Kriging: geostatistical interpolation method widely used in mining & environmental sciences.
- Based on regionalized variable theory:
  - Closer data points are more correlated than distant ones.
  - Variance structure captured by a variogram.



Universal Kriging

- Accounts for global trends (e.g., roughness increases with laser power).
- Captures both broad effects and local variability.
- A spatially continuous process Z at a location x represented as:

$$z(x) = \mu(x) + \epsilon(x)$$

- In matrix notation, the estimated value $\hat{z}(x_0)$ can be solved for as:

$$\hat{z}(x_0) = q_0^{\mathrm{T}} \cdot \hat{\beta} + \lambda_0^{\mathrm{T}} \cdot \epsilon$$

where

- q_0 is a vector of the predictors at x_0.
- $\hat{\beta}$ is a vector that contains the estimated drift term coefficients.
- λ_0 is a vector of n kriging weights determined by the covariance function.
- ϵ is a vector that contains all the regression residuals (solved iteratively).

Regression Coefficient Vector

- $\hat{\beta}$, can be solved for by generalized least squares:

$$\hat{\beta} = (q^T \cdot C^{-1} \cdot q)^{-1} \cdot q^T \cdot C^{-1} \cdot z$$

where

- **z** is the sampled observations
- q is the matrix of the predictors at all observed locations.
- C is the covariance matrix of residuals.

$$C = \begin{bmatrix} C(x_1, x_2) & \cdots & C(x_1, x_n) \\ \vdots & \ddots & \vdots \\ C(x_n, x_1) & \cdots & C(x_n, x_n) \end{bmatrix}$$

Variogram Model

- The power variogram model, $s \cdot d^{\alpha} + n$, forms the piecewise semivariance function $\gamma(d)$:

$$\gamma(d) = \begin{cases} 0 & d = 0 \\ s \cdot d^{\alpha} + n & 0 \leq d \end{cases}$$

where

- *s* is a scaling factor
- *d* is the distance between point covariance pairs $C(x_i, x_j)$
- α is the exponent (between 1 and 1.99)
- *n* is the nugget term

when $\gamma(d) = n - C(x_i, x_j)$. Given:

$$\mathbf{e} = \mathbf{z} - \mathbf{q} \cdot \widehat{\boldsymbol{\beta}}$$

$\hat{z}(x_0)$ can be iteratively solved for.

Predicted Mean and Variance

- After solving for the residuals, the predicted value can be obtained:

$$\hat{z}(x_0) = q_0^{\mathrm{T}} \cdot \hat{\beta} + \lambda_0^{\mathrm{T}} \cdot \left(z - q \cdot \hat{\beta}\right)$$

- As can the variance of the predicted value:

$$\sigma^2(x_0) = n - c_0^{\mathrm{T}} \cdot C^{-1} \cdot c_0 + \left(q_0 - q^{\mathrm{T}} \cdot C^{-1} \cdot c_0\right)^{\mathrm{T}} . \left(q^{\mathrm{T}} \cdot C^{-1} \cdot q\right)^{-1} \cdot \left(q_o - q^{\mathrm{T}} \cdot C^{-1} \cdot c_o\right)$$

- A more compact way of expressing universal kriging (UK) is:

$$[\hat{z}(x_0), \sigma^2(x_0)] = UK((x_0)|D = \{(x, z)\})$$

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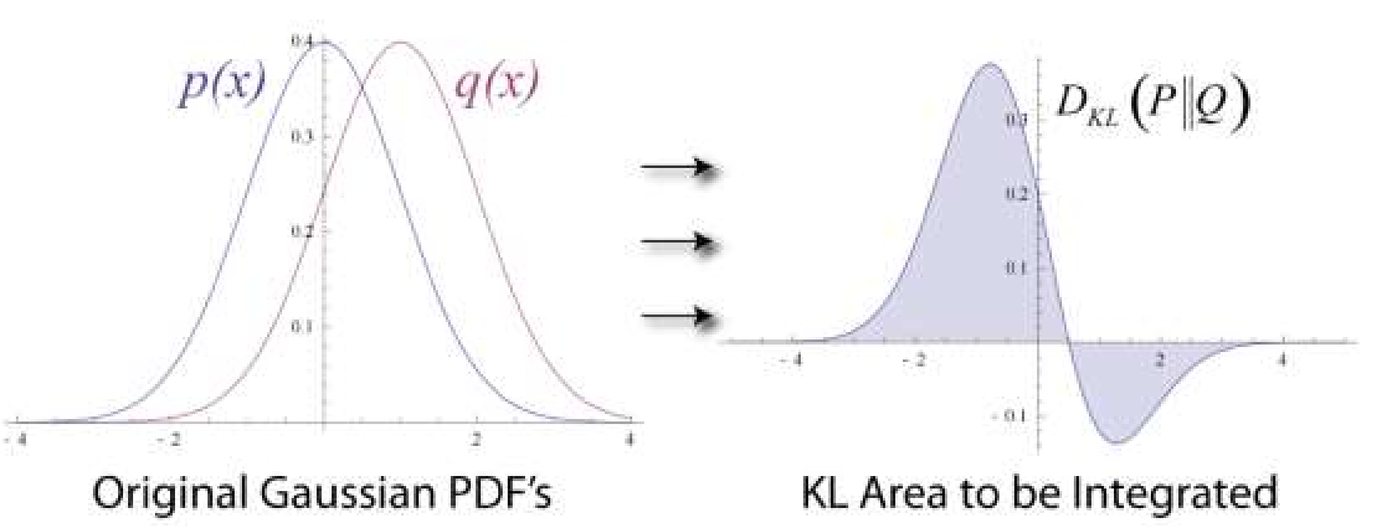
Relative Entropy

- Tracking changes in changes in probability distributions.



- Kullback-Leibler Divergence (KLD):

$$D_{\mathrm{KL}}(P||Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx$$

- allows for a computationally simple measure of dissimilarity between two probabilities.

Image: Z Pei, Fair Use, reproduced from
https://blogs.cuit.columbia.edu/zp2130/kl_divergence/

Merging Kriging and Relative Entropy

- Recall that kriging provides:

$$\hat{z}(x_0) = q_0^{\mathrm{T}} \cdot \hat{\beta} + \lambda_0^{\mathrm{T}} \cdot \left(z - q \cdot \hat{\beta}\right)$$

- and:

$$\sigma^2(x_0) = n - c_0^{\mathrm{T}} \cdot C^{-1} \cdot c_0 + \left(q_0 - q^{\mathrm{T}} \cdot C^{-1} \cdot c_0\right)^{\mathrm{T}} . \left(q^{\mathrm{T}} \cdot C^{-1} \cdot q\right)^{-1} \cdot \left(q_o - q^{\mathrm{T}} \cdot C^{-1} \cdot c_o\right)$$

- KLD is simplified for distribution represented by mean (μ) and variance (σ).

$$D_{\mathrm{KL}}(P||Q) = \log\left(\frac{\sigma_q}{\sigma_p} + \frac{\sigma_p^2 + (\mu_p - \mu_q)^2}{2\sigma_q^2} - 1/2\right)$$

- Which gives us a way to monitor changes in probability distributions an any given point *x*.

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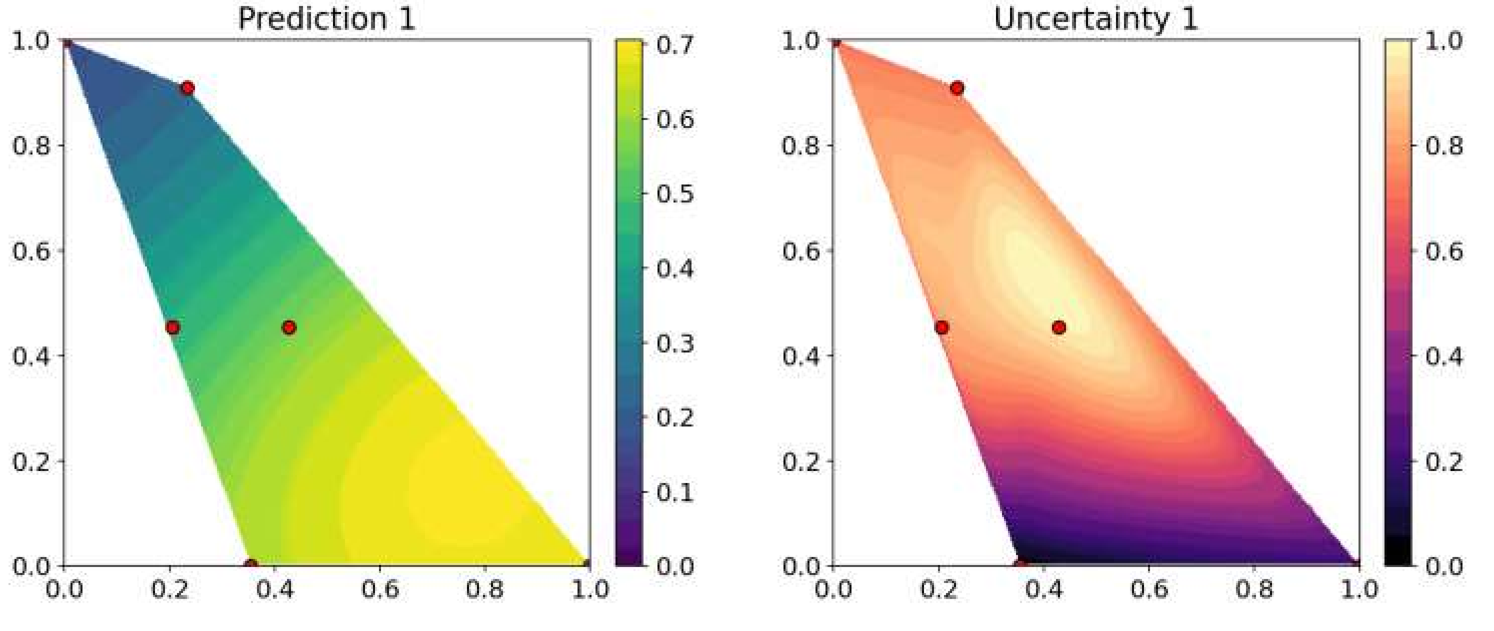
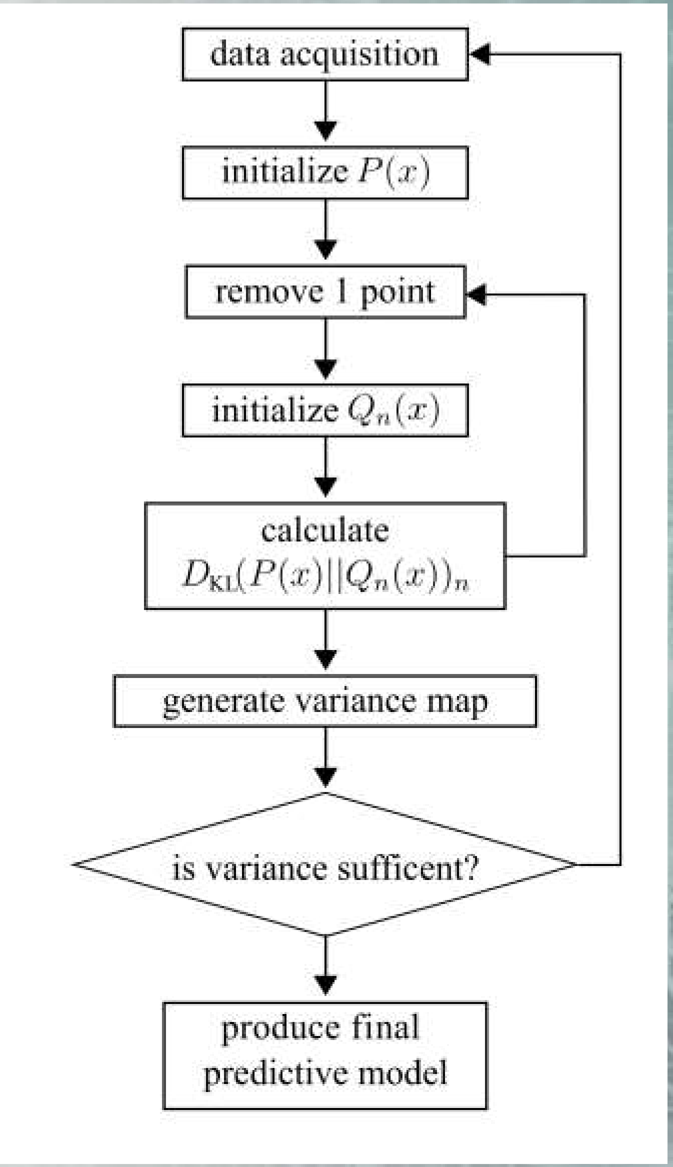
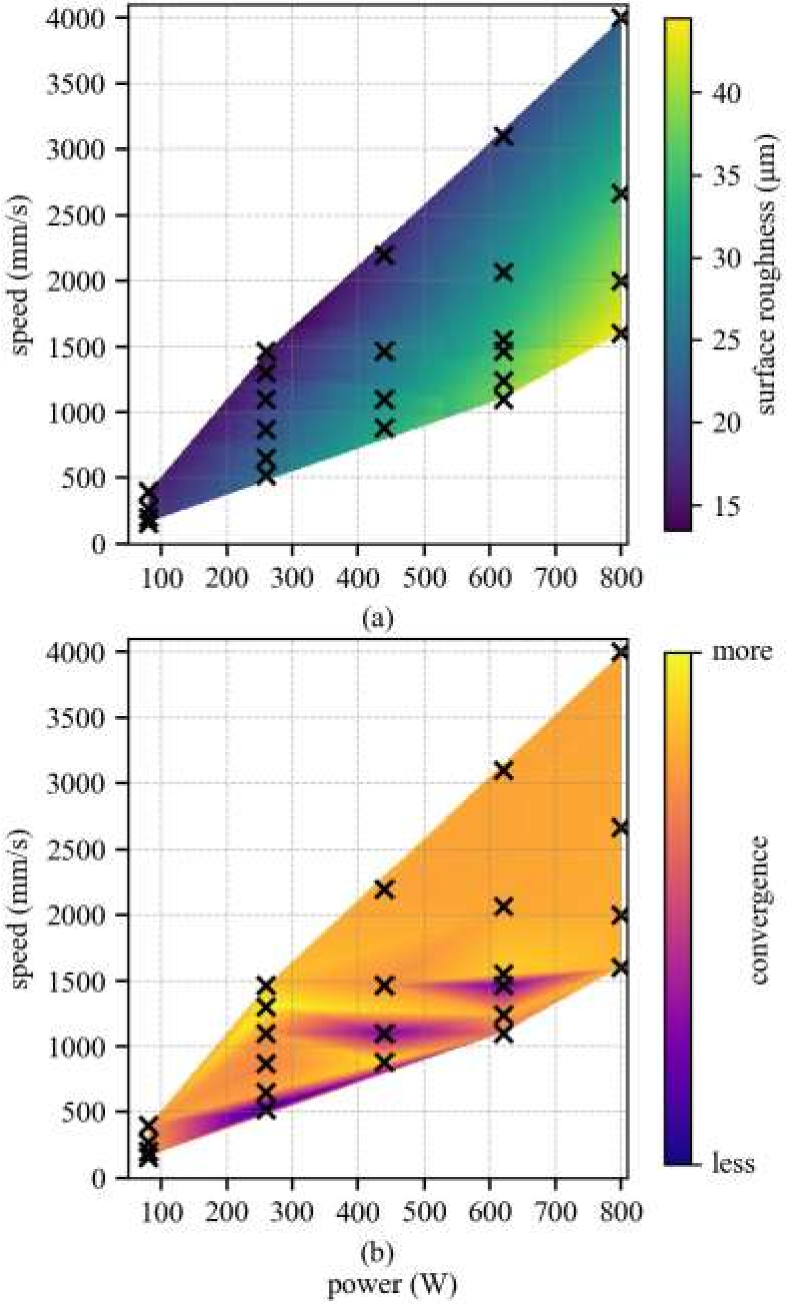




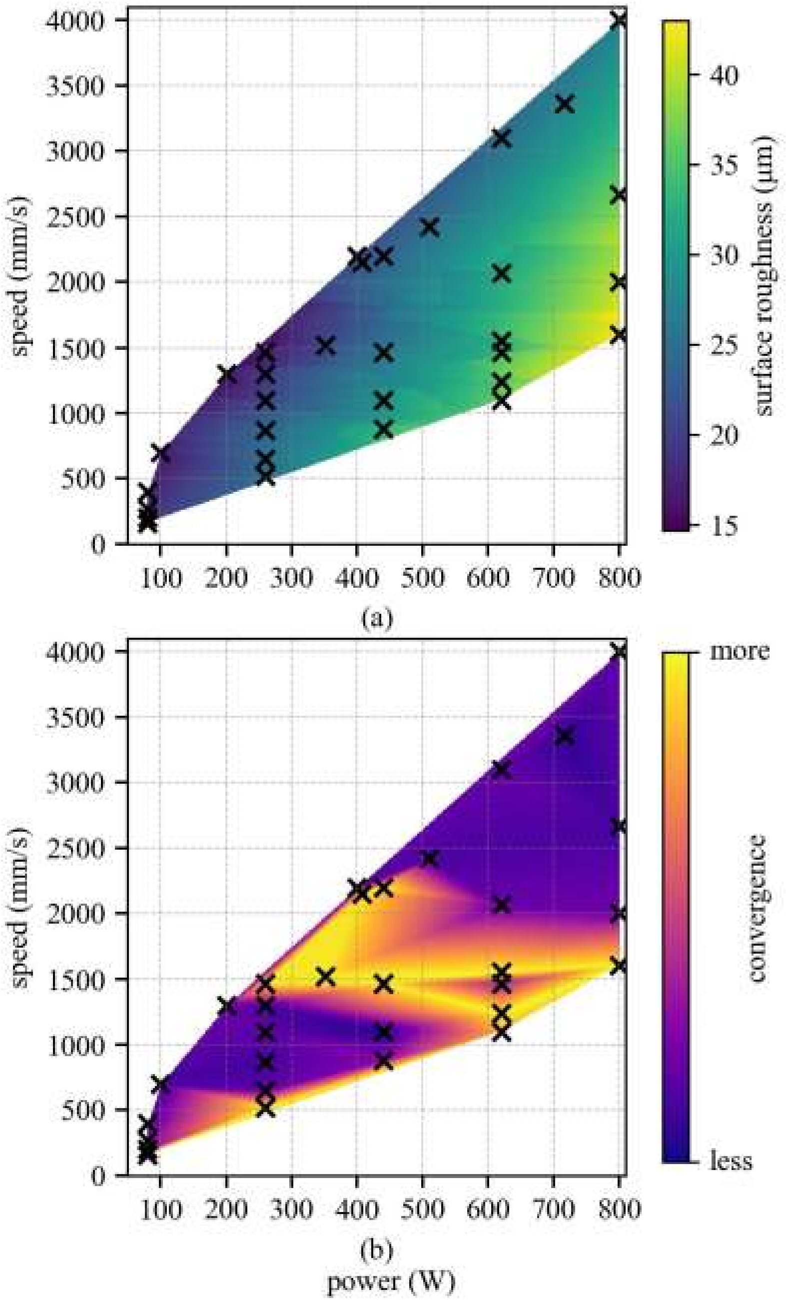
Initial model

- Experimental data used to tune Kriging hyperparameters.
- Initial run identified regions of high uncertainty within the domain.



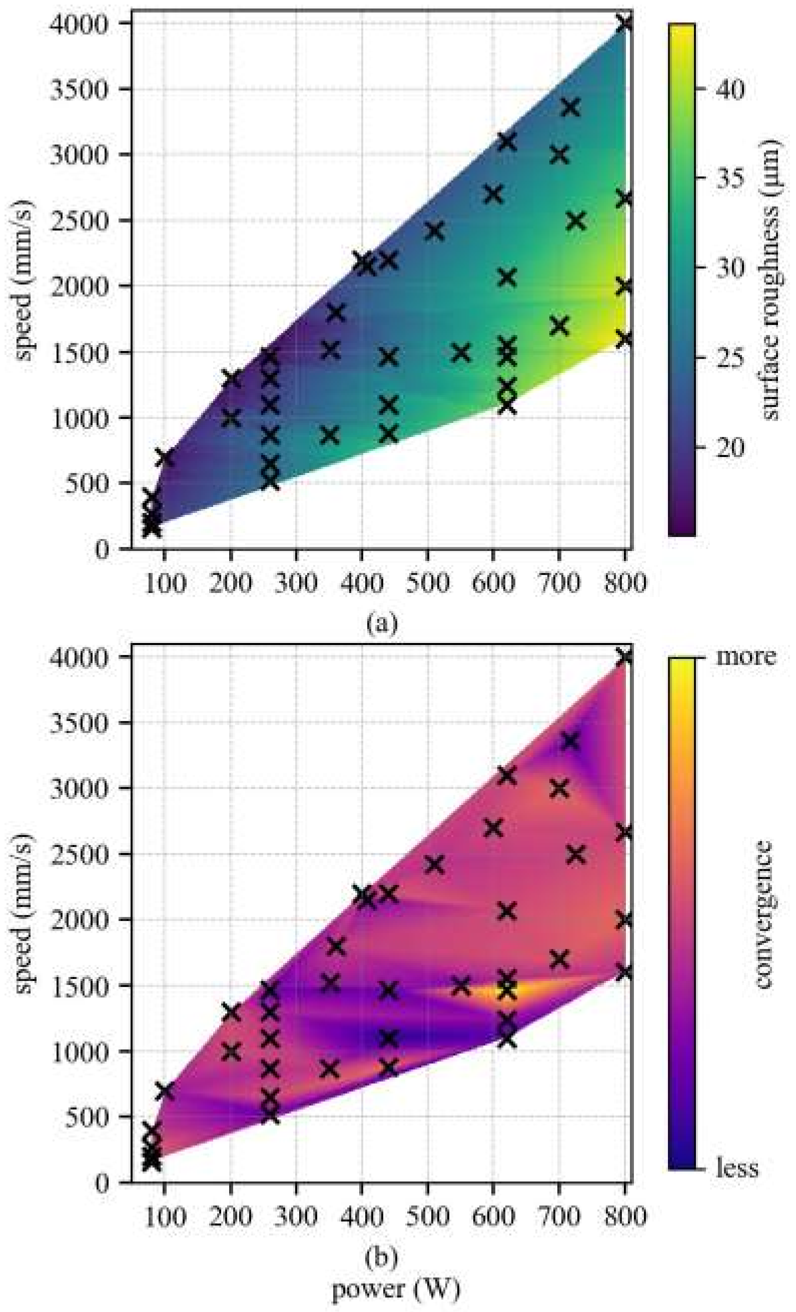
Iterative Refinement

- 7 additional samples taken in the previously observed high uncertainty regions
- New dataset used to retrain and refine the surrogate model.



Final model

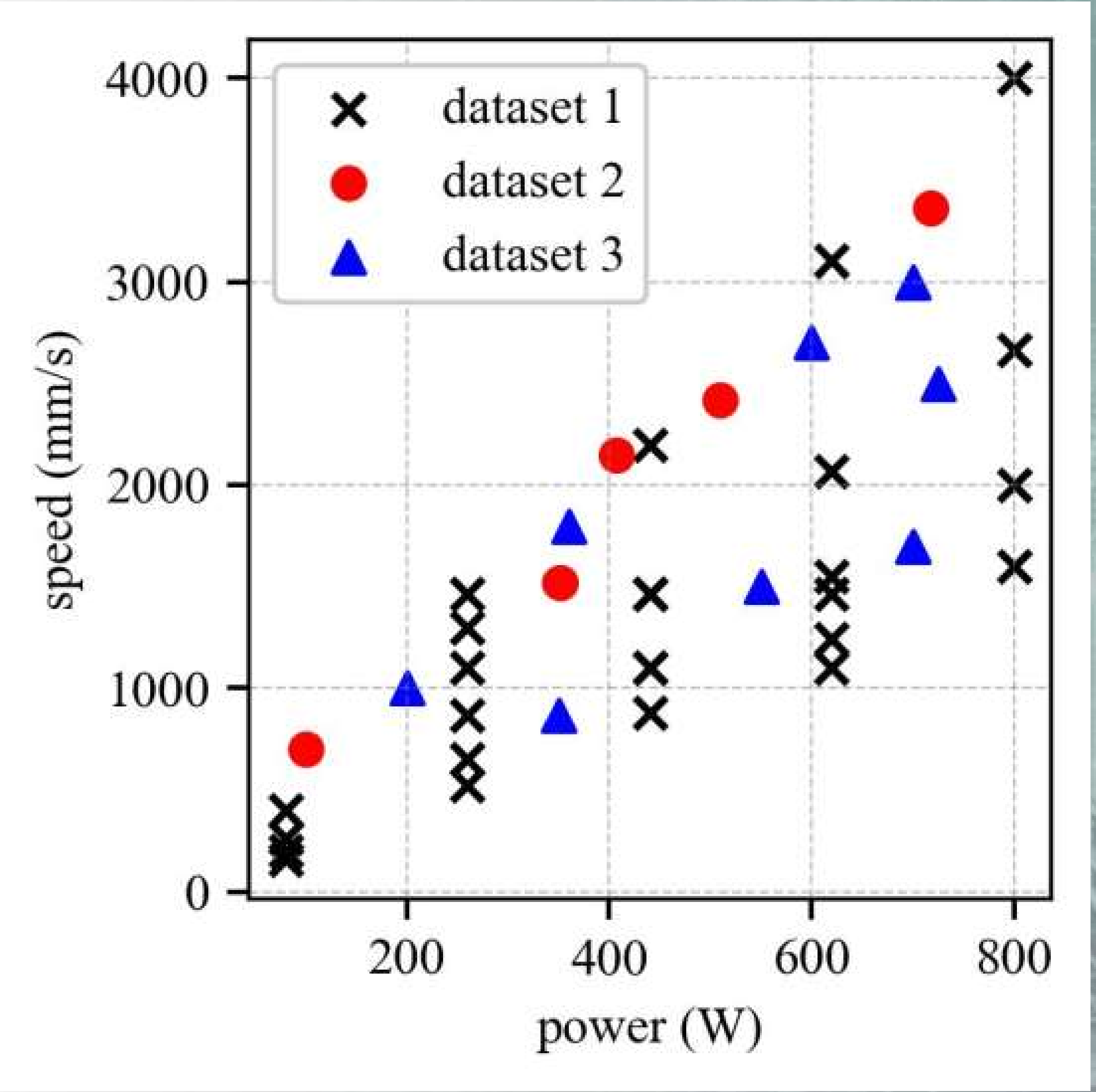
- Additional sampling performed in updated high-uncertainty regions.
- Final model shows uniform uncertainty distribution which indicates convergence.
- This final dataset treated as “ground truth” for comparison.



Conclusion

- Adding only 7 new samples reduced model error dramatically:
  - Average error reduced by 68.3% from Dataset 1 to Dataset 2.
- Iterative sampling efficiently targets regions of maximum impact.
- Confirms algorithm's ability to rapidly reduce uncertainty in experimental domains.

	MSE	MAE	MAPE	number of samples
Dataset 1	1.52	1.01	2.35%	26
Dataset 2	0.68	0.69	1.72%	33



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Thank You for Your Time

GitHub Repository

https://github.com/ARTS-Laboratory/KRISP-U

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