

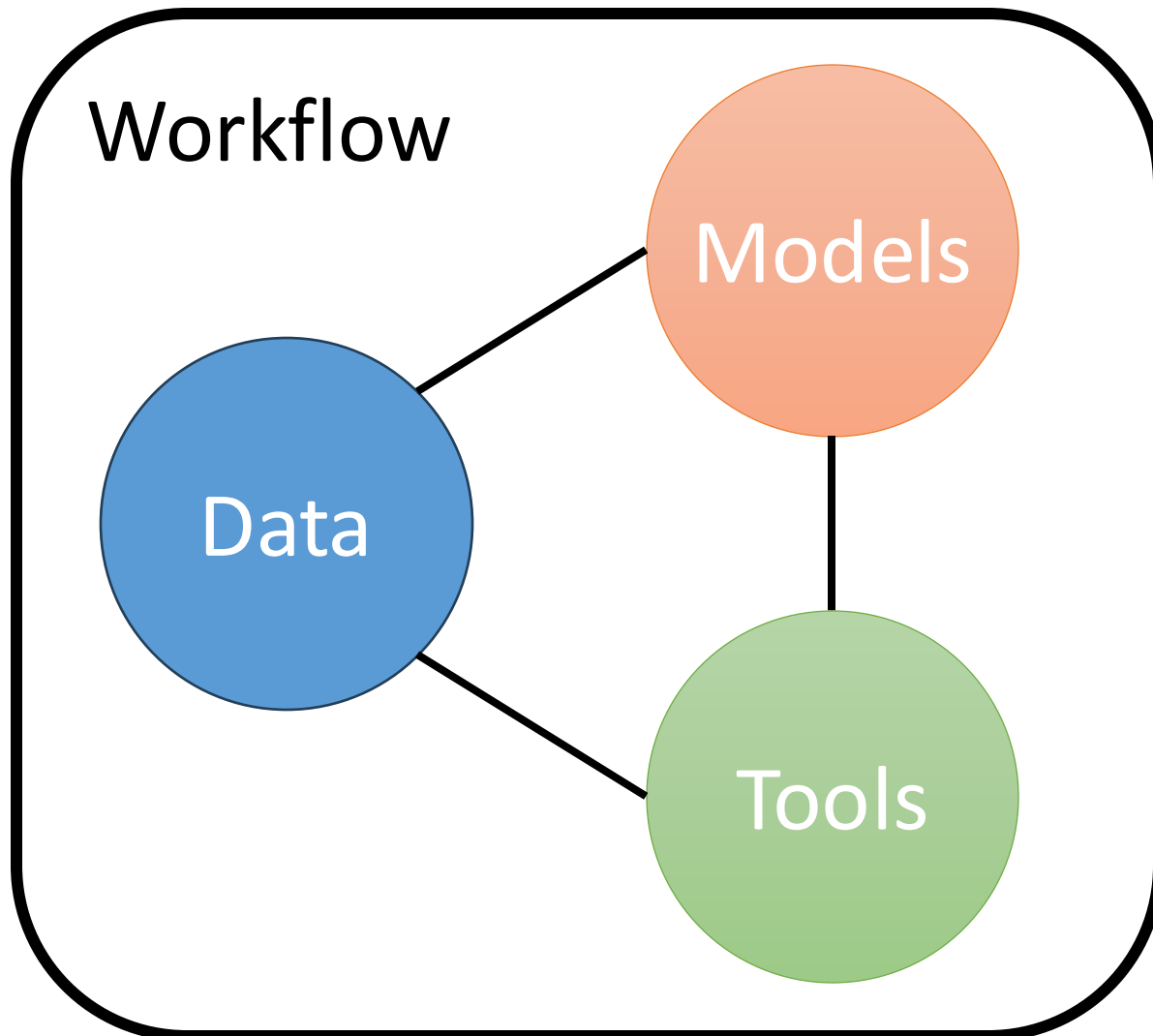
# Toward the Verification, Validation, and Uncertainty Quantification Strategy for Digital Twins

Shengyen Li

Engineering Laboratory, NIST

Integrated Computational Materials Engineering for Material Design

# Trouble with Integration



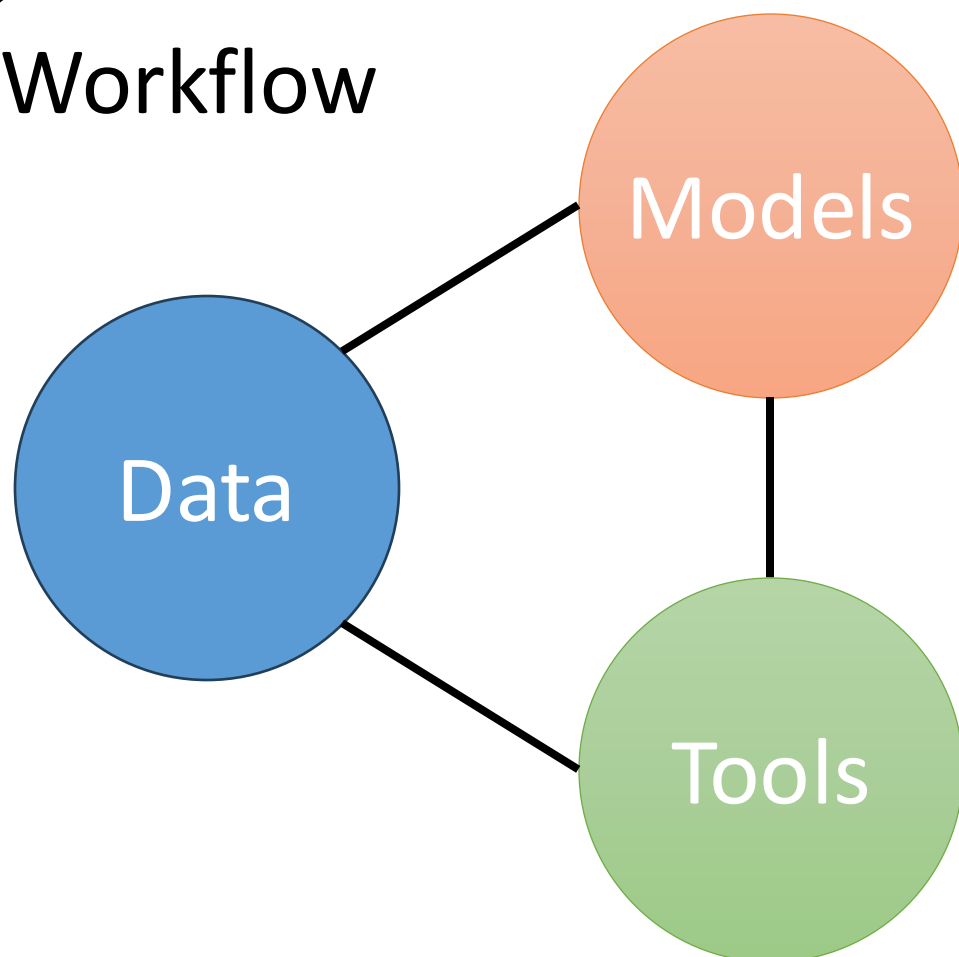
Engineering  
Application

## Data sources

- <https://www.nist.gov/programs-projects/configurable-data-curation-system-cdcs>
- <https://ambench2022.nist.gov>
- <https://ambench.nist.gov>

# Trouble with Modeling

## Workflow



## Sample Models

Physics-based  
model

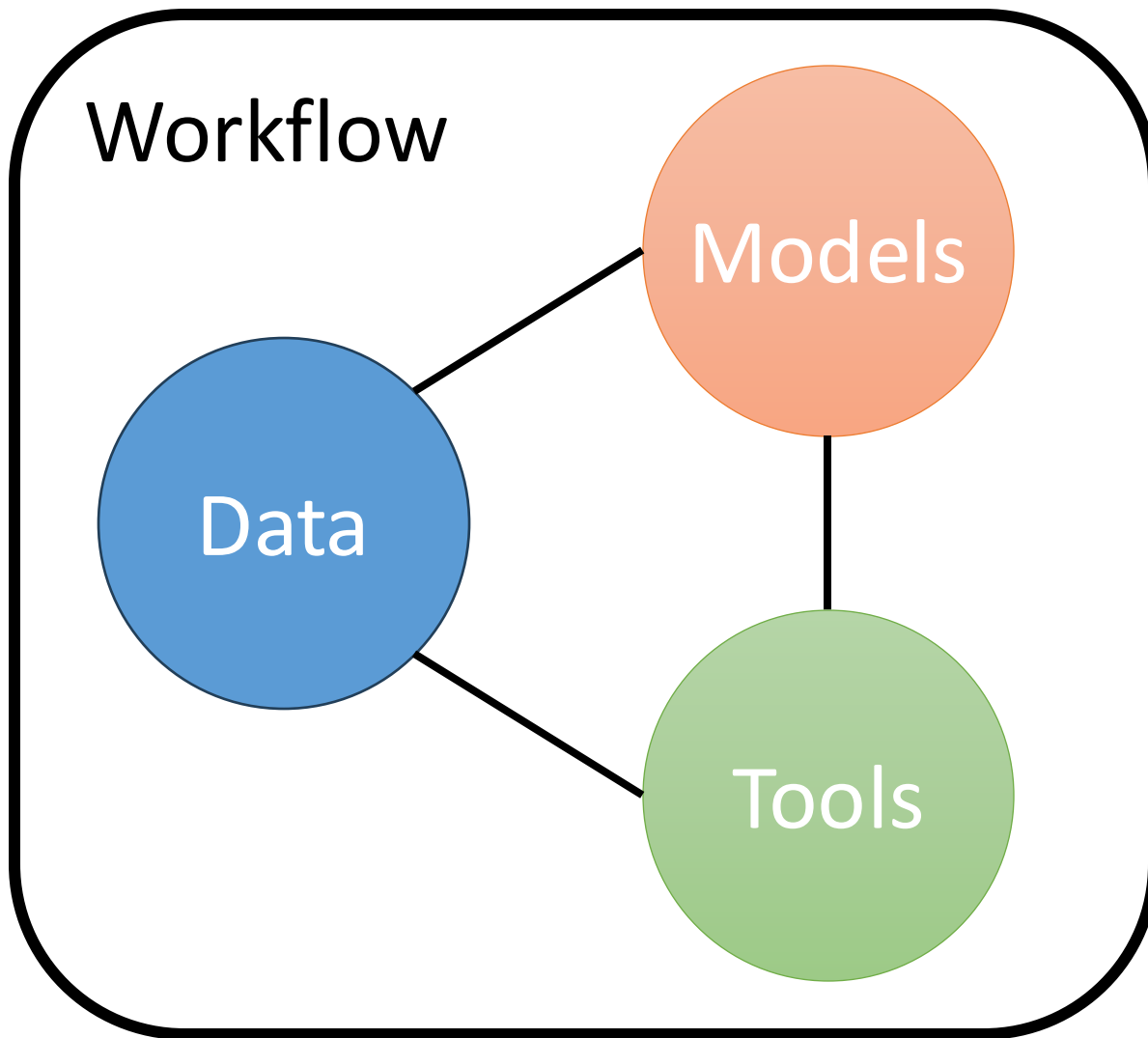
$$\dot{N}(t) = Z\beta N_0 \exp\left(\frac{-\Delta G^*}{K_B T}\right) \exp\left(\frac{-\tau}{t}\right)$$

Polynomial regression  $y = f(x_1, x_2, x_3 \dots)$

Neural network

$$y = \dots f_2(f_1(x_1, x_2, f_2(x_3) \dots))$$

# Trouble with Workflow



## Homogeneous NON-Steady-State Nucleation

Russell, 1978; Wagner et al., 2001

$$\dot{N}(t)$$

## Growth/Coarsening

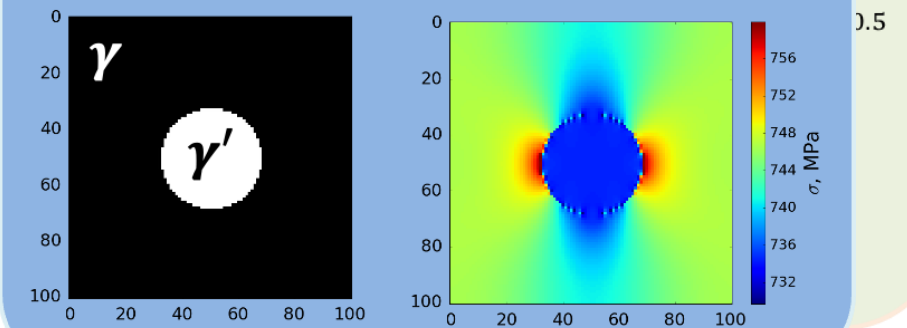
Rougier et al., 2013; Perez et al., 2008

$$\frac{dR}{dt} = \frac{D_i^\gamma}{C_i^\gamma - \bar{C}_i^\gamma}$$

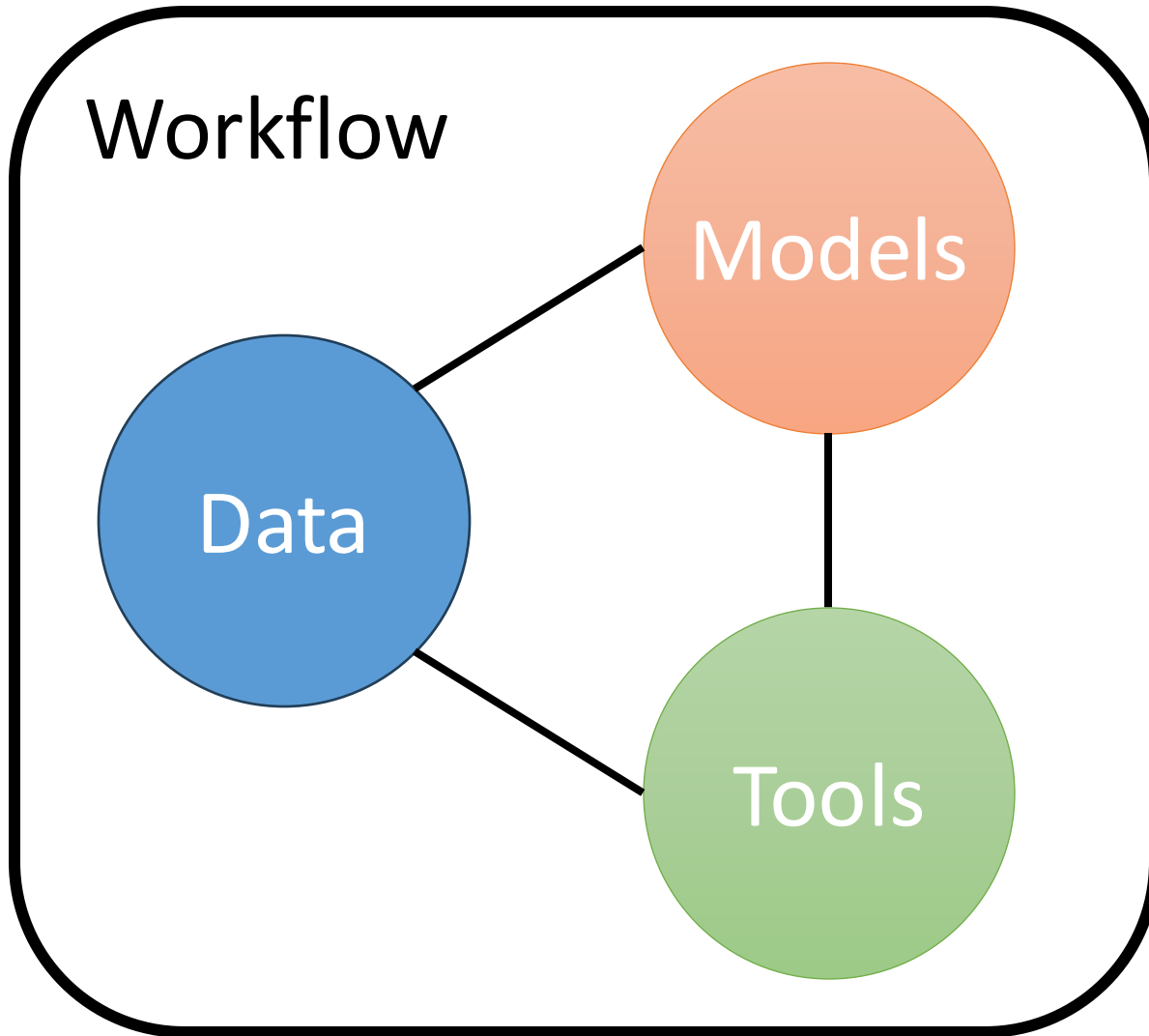
$$\sigma_{YS} = \sigma_0 + \sigma_{SS} + \sigma_{H-P} + \sqrt{\sigma_{\rho,0}^2 + \sigma_p^2}$$

$$F_{\text{eff}} = \left[ (6\bar{R}\gamma' E_{\text{eff}} V^{\gamma'})^{0.5} \right]$$

## Elastic Deformation: PyMKS



# Trouble with ~~Workflow~~ Trust



## Homogeneous NON-Steady-State Nucleation

Russell, 1978; Wagner et al., 2001

$$\dot{N}(t)$$

## Growth/Coarsening

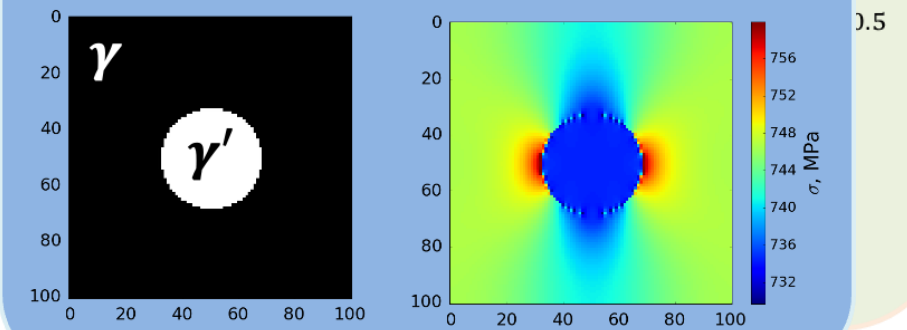
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## Elastic Deformation: PyMKS



# Trustworthiness of Workflow

- Trustworthiness of simulations, hardware, integration and beyond
- A checklist to assess the trustworthiness of simulations in the 4 phases of the development lifecycle

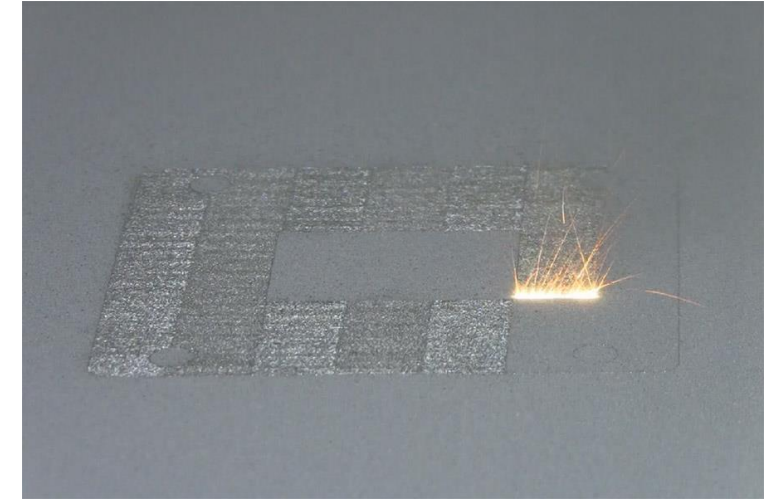
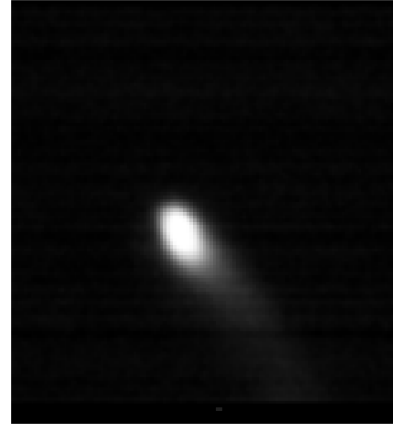
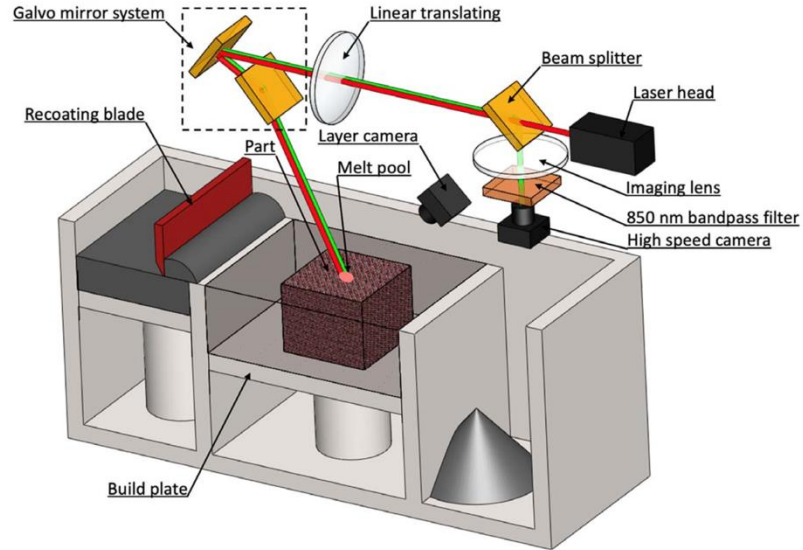
Definition	Development	Deployment	Maintenance
Context of Use	Problem Space	Hardware Integration	Hardware maintenance
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Resources	Data Variability	Uncertainty Propagation	
Constraints	Uncertainty Quantification	Workflow Refinement & Validation	
	Computational Detail	Scalability	

# Trustworthiness of Simulations

- Trustworthiness of simulations, hardware, integration and beyond
- A checklist to assess the trustworthiness of simulations in the 4 phases of the development lifecycle

Definition	Development	Deployment	Maintenance
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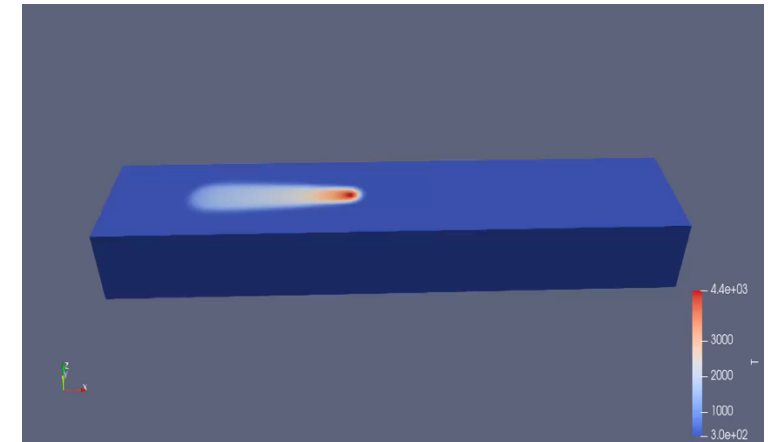
# Use case for Additive Manufacturing



```
N0001 G01 X57.5000 Y-9.4974 Z-3.4790 F1000 L0 D1.00
N0002 G01 X57.4989 Y-9.5000 L285
N0003 G01 X57.3794 Y-9.5000 L0
N0004 G01 X57.5000 Y-9.2160 L285
N0005 G01 Y-8.9345 L0
N0006 G01 X57.2600 Y-9.5000 L285
N0007 G01 X57.1405 Y-9.5000 L0
N0008 G01 X57.5000 Y-8.6530 L285
N0009 G01 Y-8.3715 L0
```

G-code

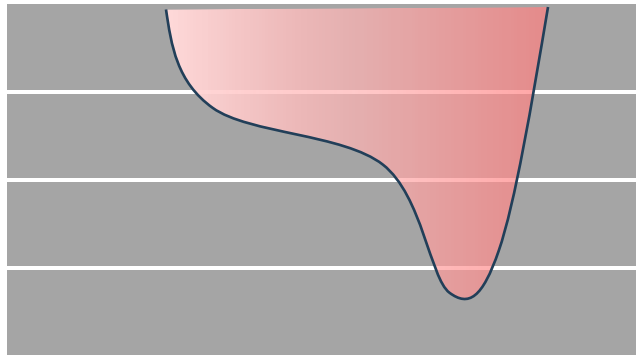
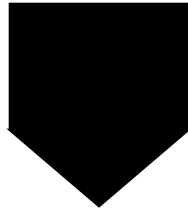
Model





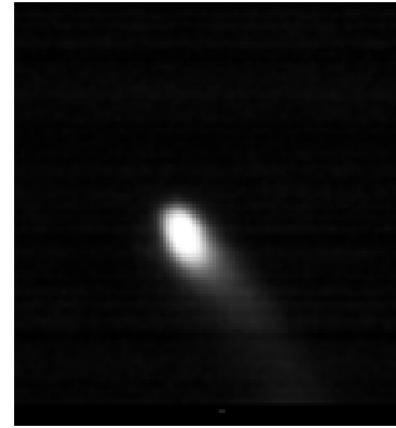
# Challenges

- Laser Power
- Scanning Speed



- Location: X, Y, Z
- Laminar Gas Flow

- Material
- Layer Thickness
- Substrate Temperature



4,770,436 images

Melt pool feature

Length

Width & Depth

Microstructure

Texture

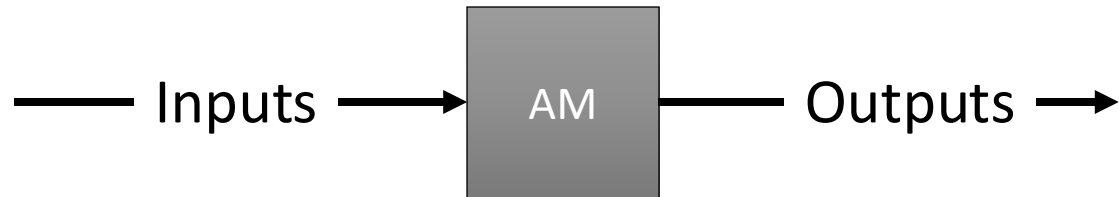
Defects

Properties

Lane2020Process  
Yang2022Investigating

“... there are over 100 of such processing parameters...”  
Oliveira 2020 Processing

# Problem Space



## Command file

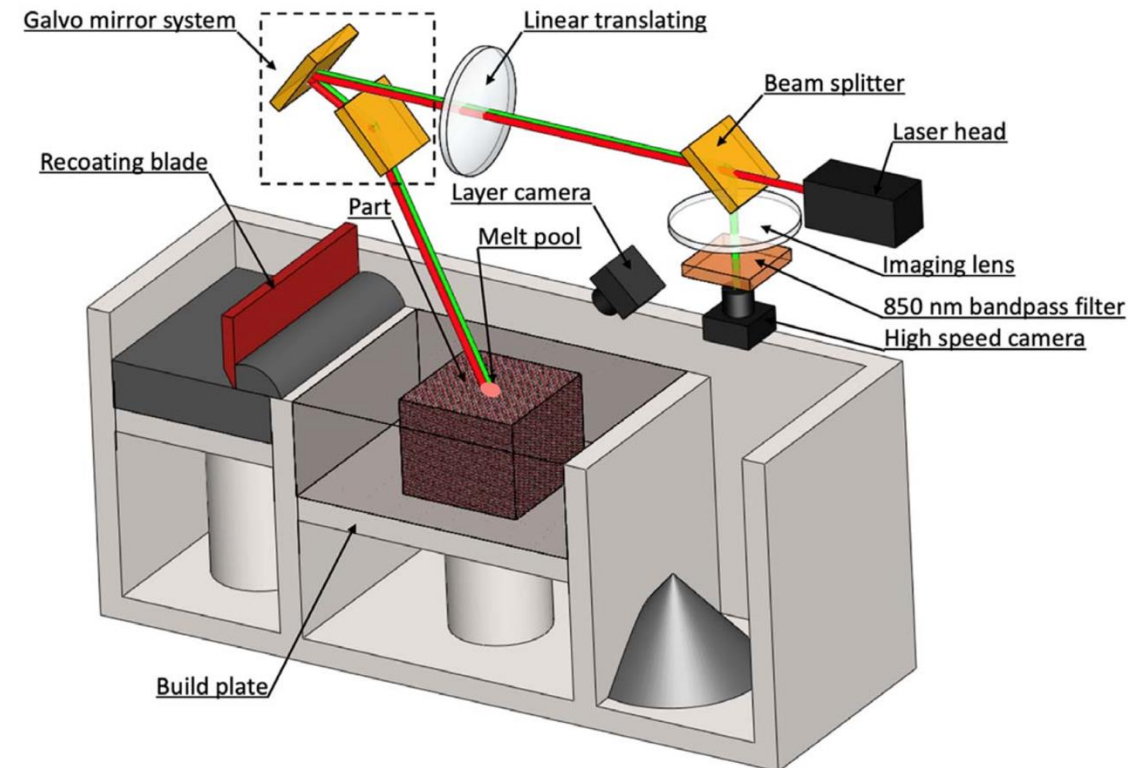
- Laser location
- Laser power
- Time

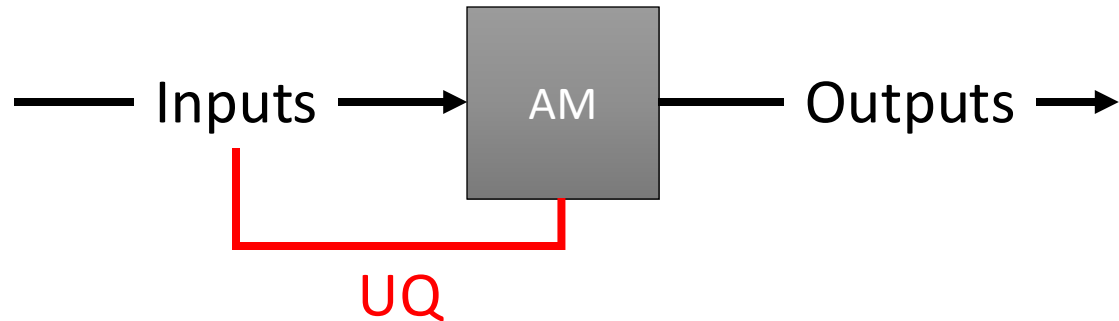
## Data acquisition file

- Laser location
- Laser power
- Time

## Melt pool images

- ~4770 image/layer
- 250 layers





## Command file

- Laser location
- Laser power
- Time

## Data acquisition file

- Laser location
- Laser power
- Time

## Melt pool images

- ~4770 image/layer
- 250 layers

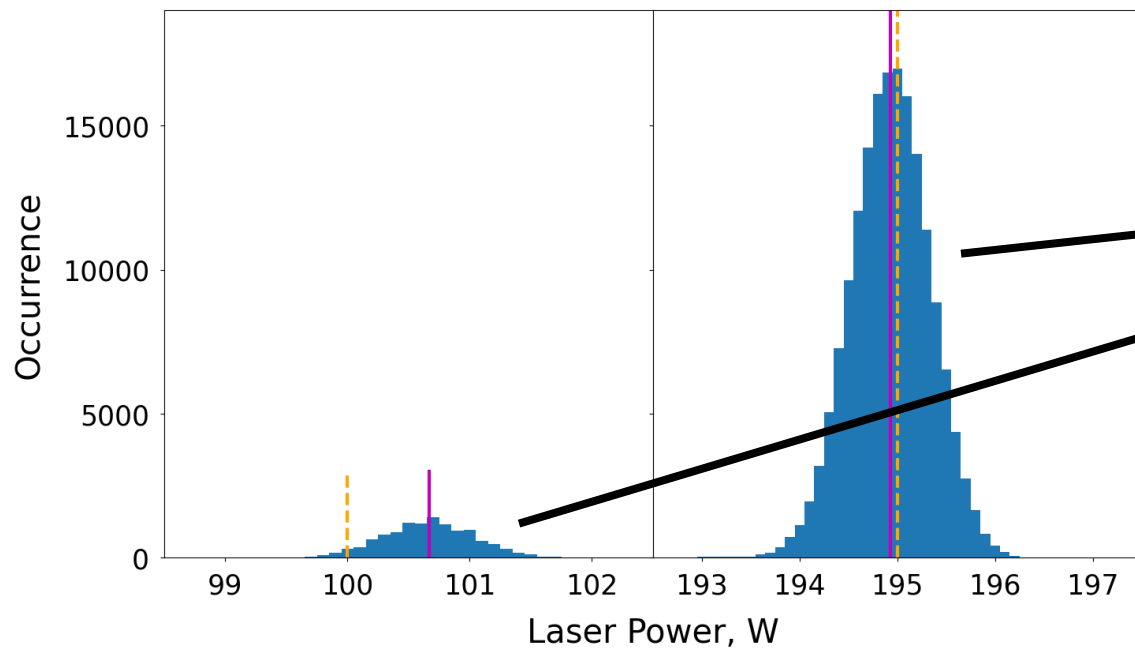
## VVUQ to evaluate data quality

UQ: Uncertainty Quantification

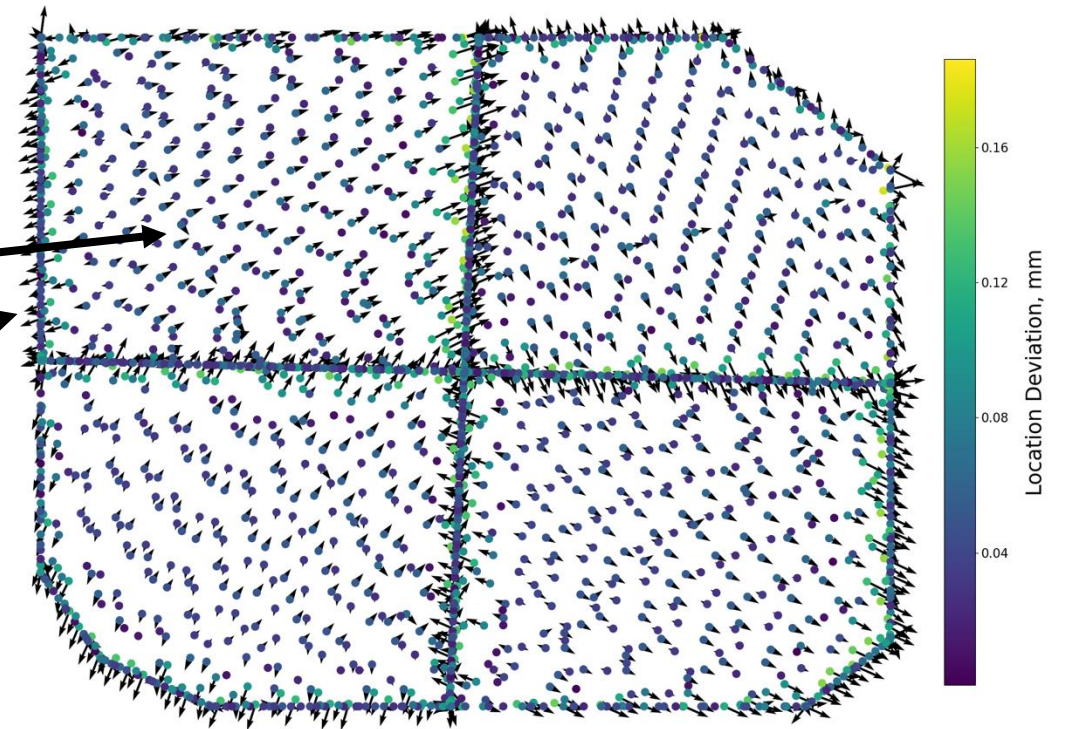
SA: Sensitivity Analysis

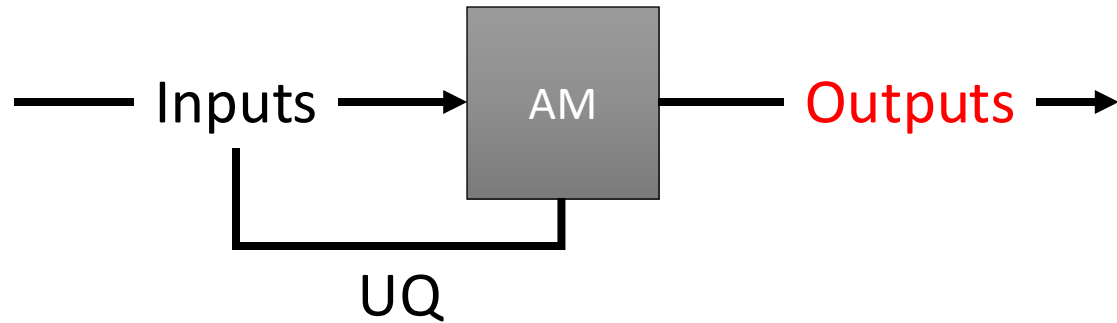
# Variability of the control

Laser power



Laser location





## Command file

- Laser location
- Laser power
- Time

## Data acquisition file

- Laser location
- Laser power
- Time

## Melt pool images

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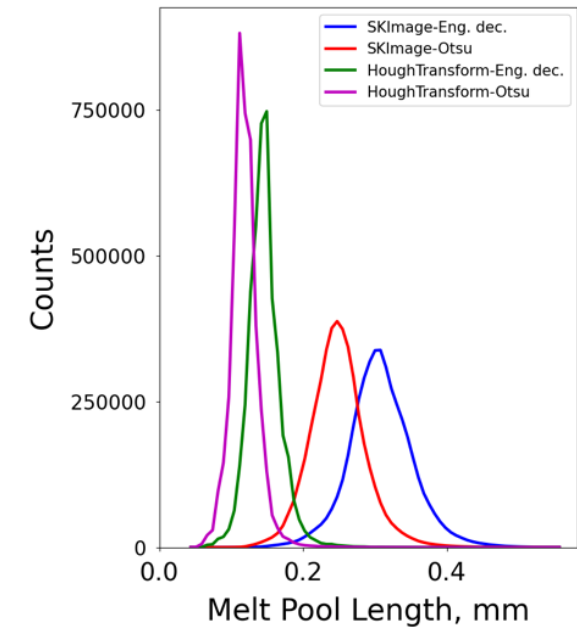
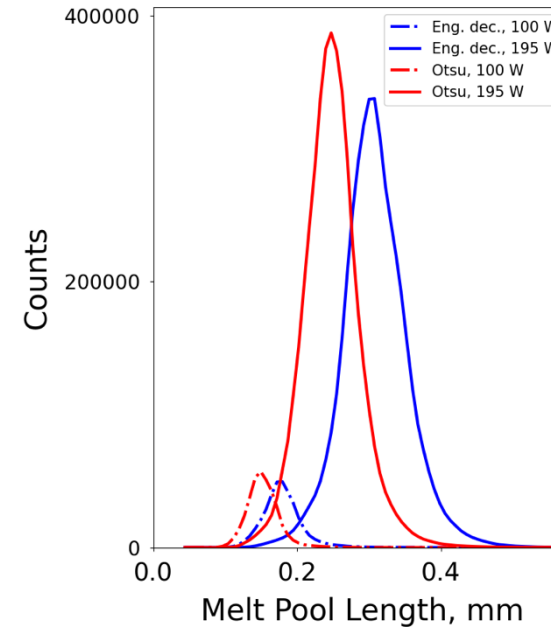
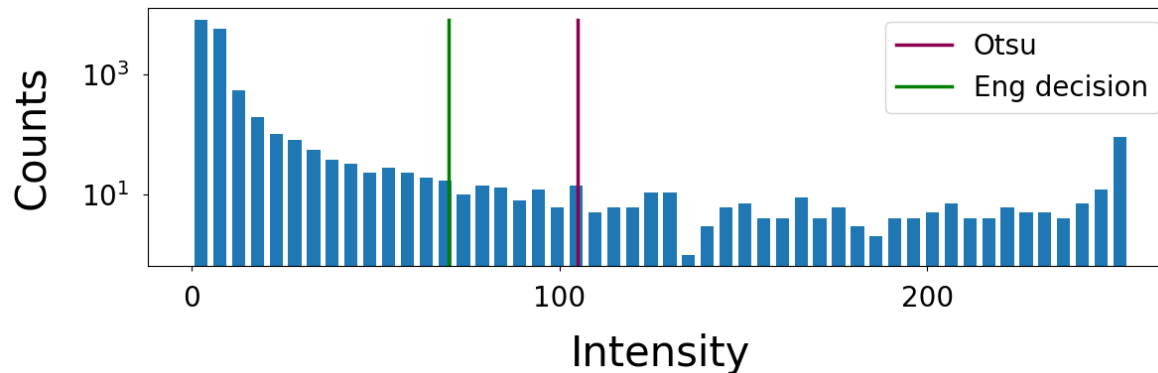
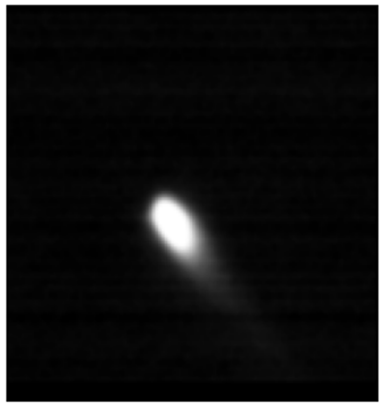
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UQ: Uncertainty Quantification

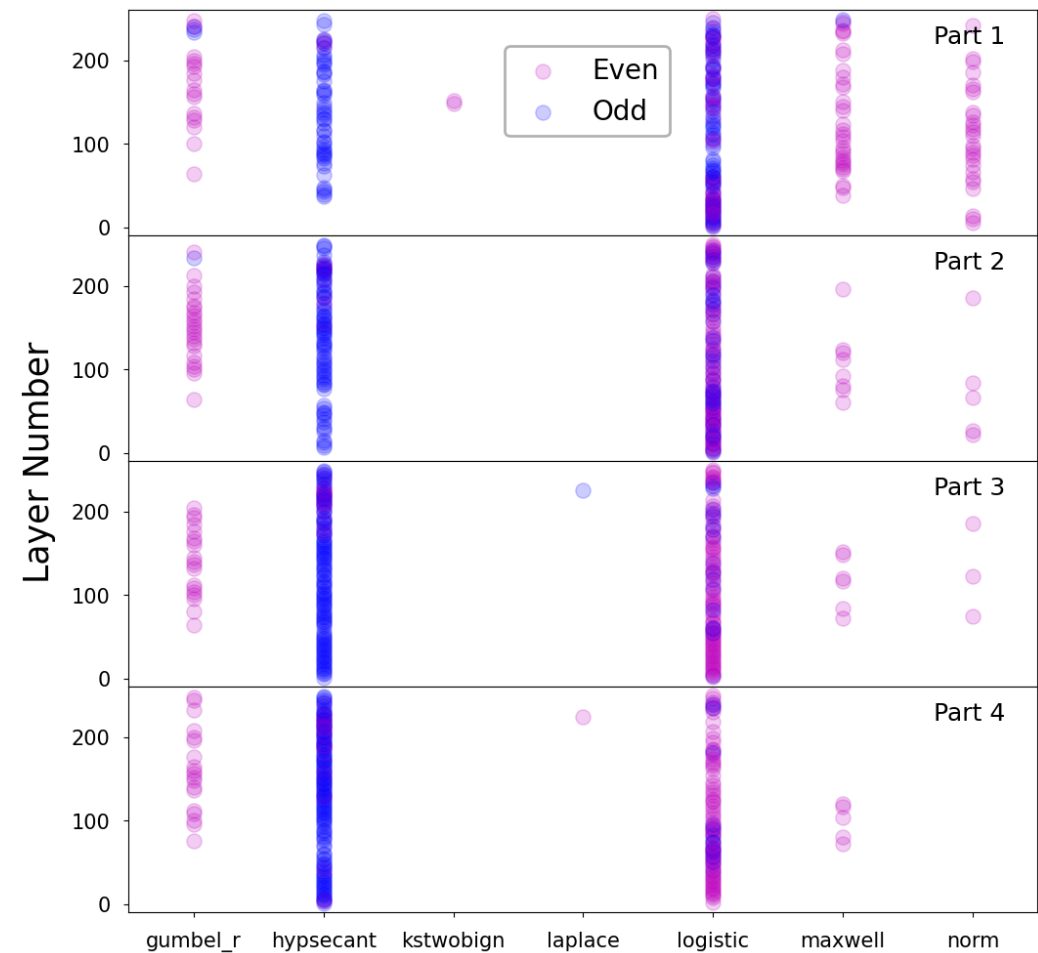
SA: Sensitivity Analysis

# Statistical Analysis & Feature Selection

Make images usable & define problem space

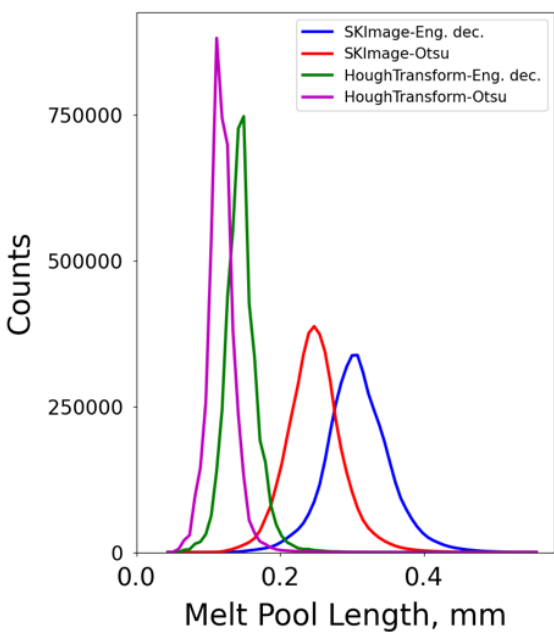
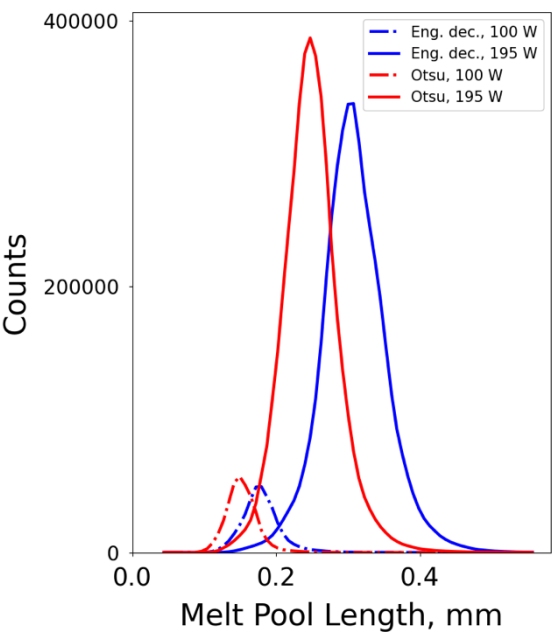


# Statistical Analysis & Feature Selection

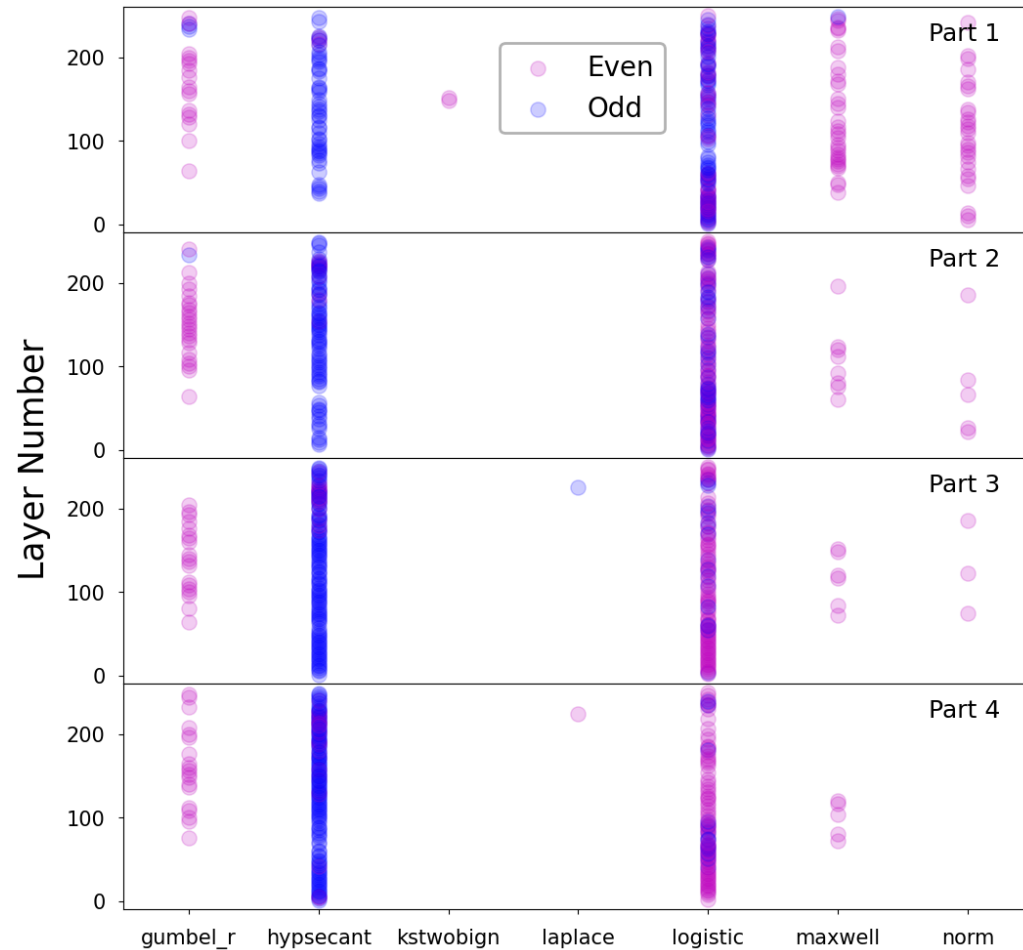


Probability Distribution Function

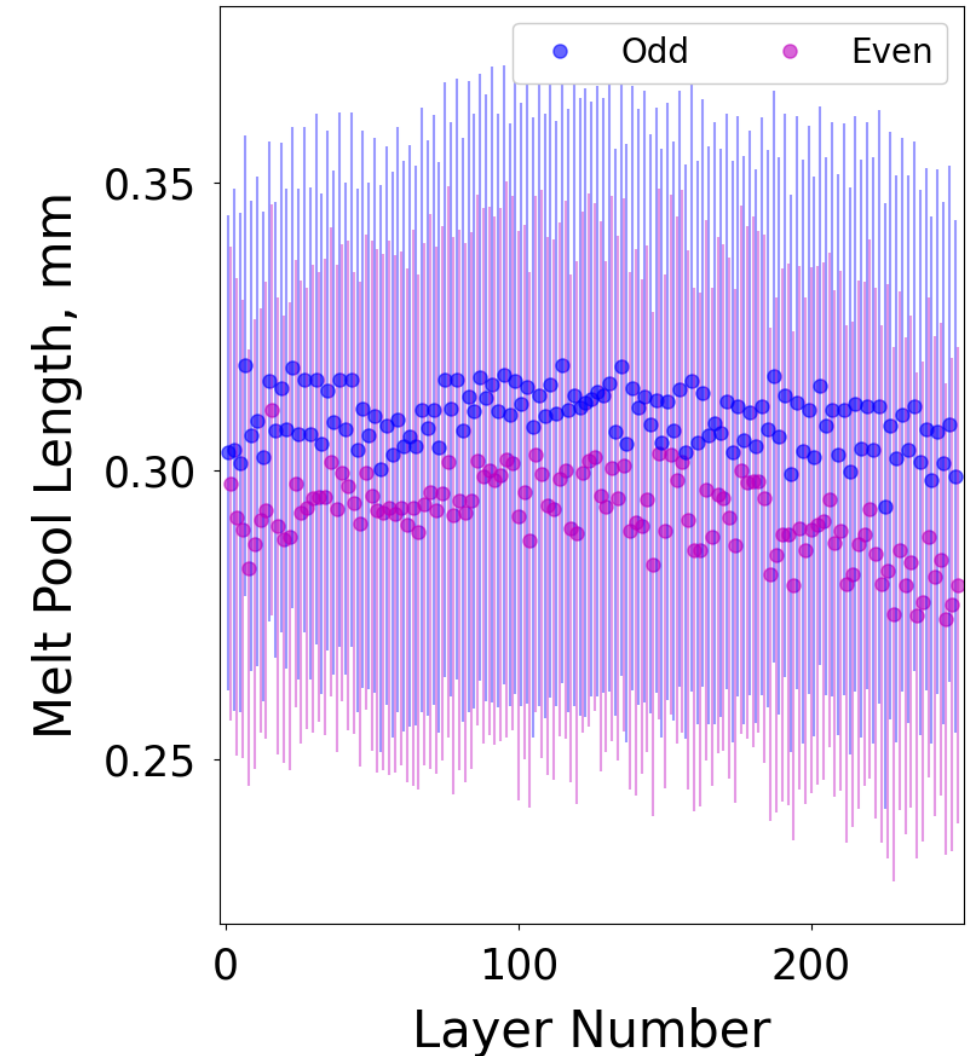
Make images usable & define problem space



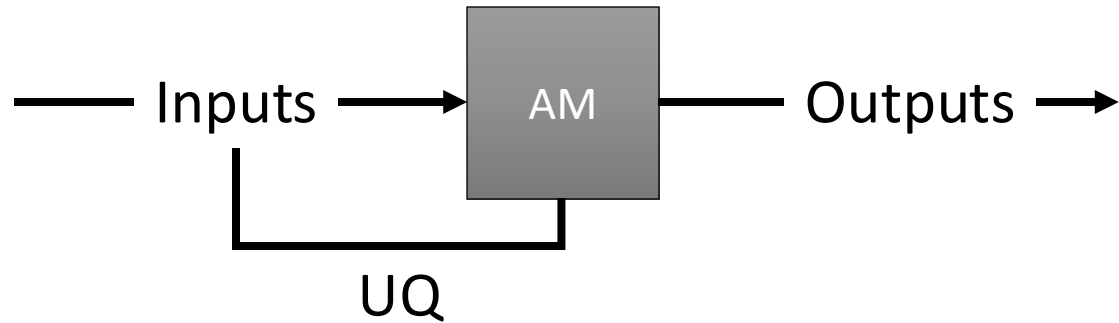
# Statistical Analysis & Feature Selection



Probability Distribution Function







Command file

- Laser location
- Laser power
- Time

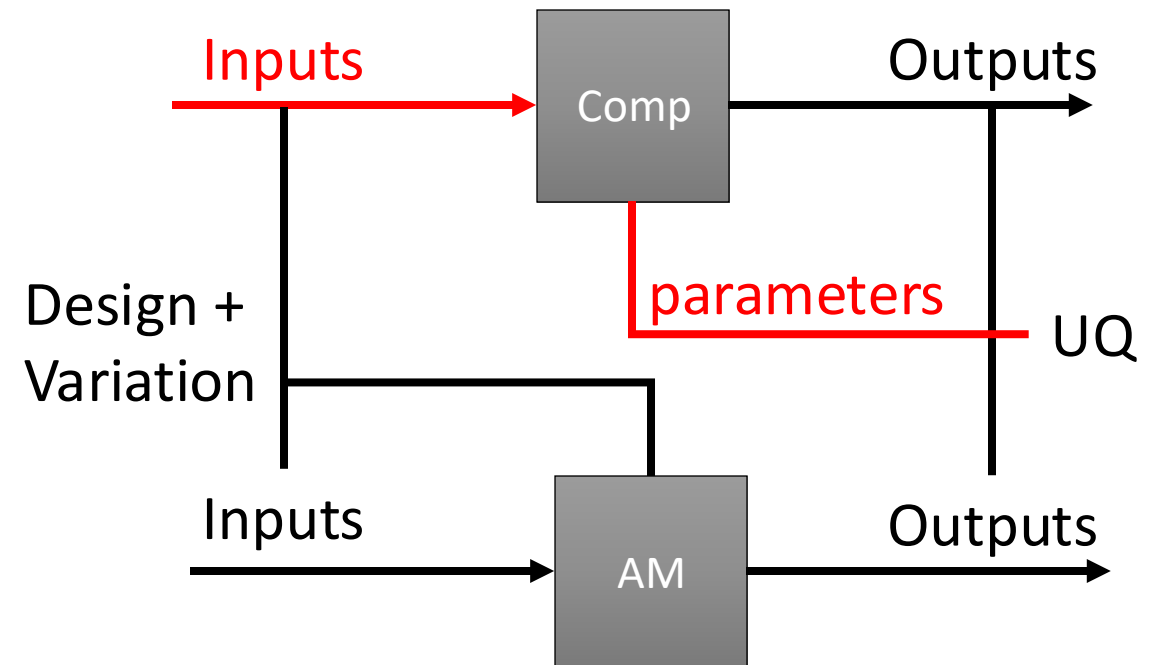
Data acquisition file

- Laser location
- Laser power
- Time

Melt pool images

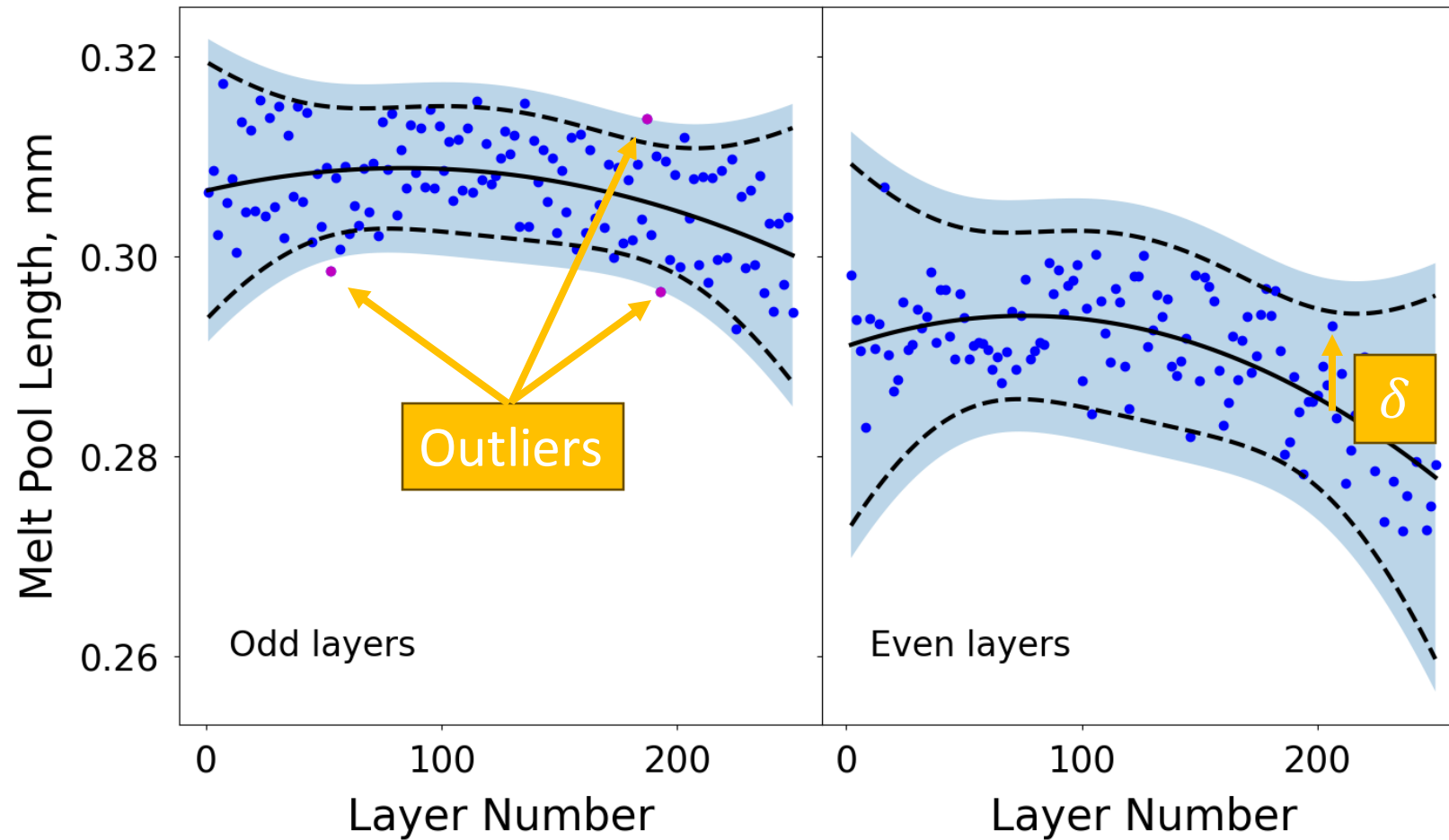
- ~4770 image/layer
- 250 layers

**VVUQ to evaluate data quality**



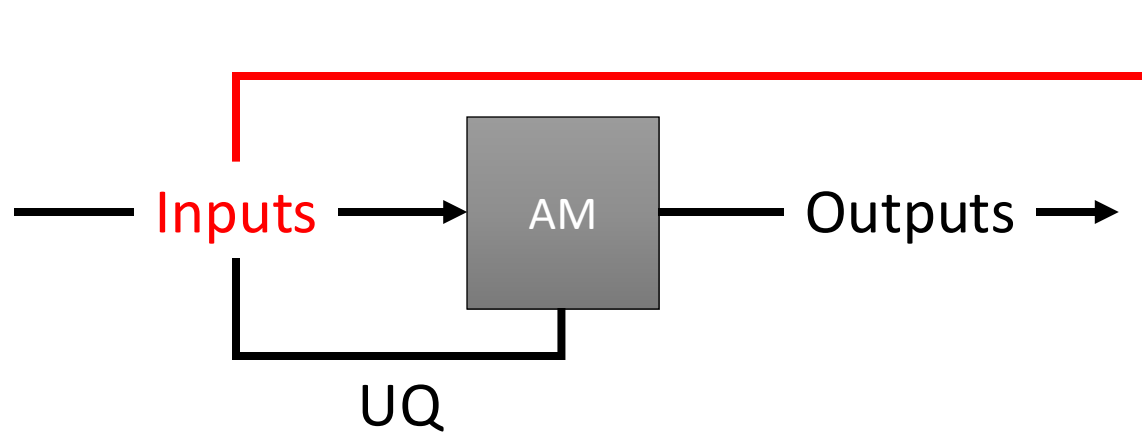
**VVUQ to assess model quality**

# Melt Pool Length Prediction



$$MPL = f_{2P}(\text{layer height}) + \delta$$

Bayesian regression, PyMC3



Command file

- Laser location
- Laser power
- Time

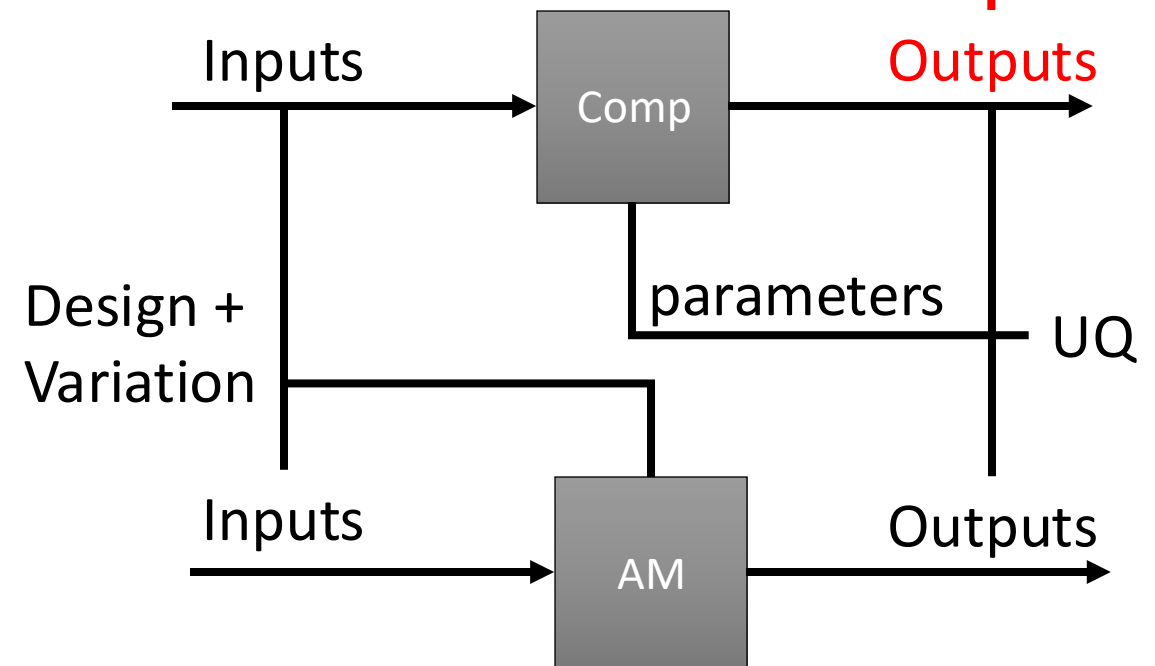
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Melt pool images

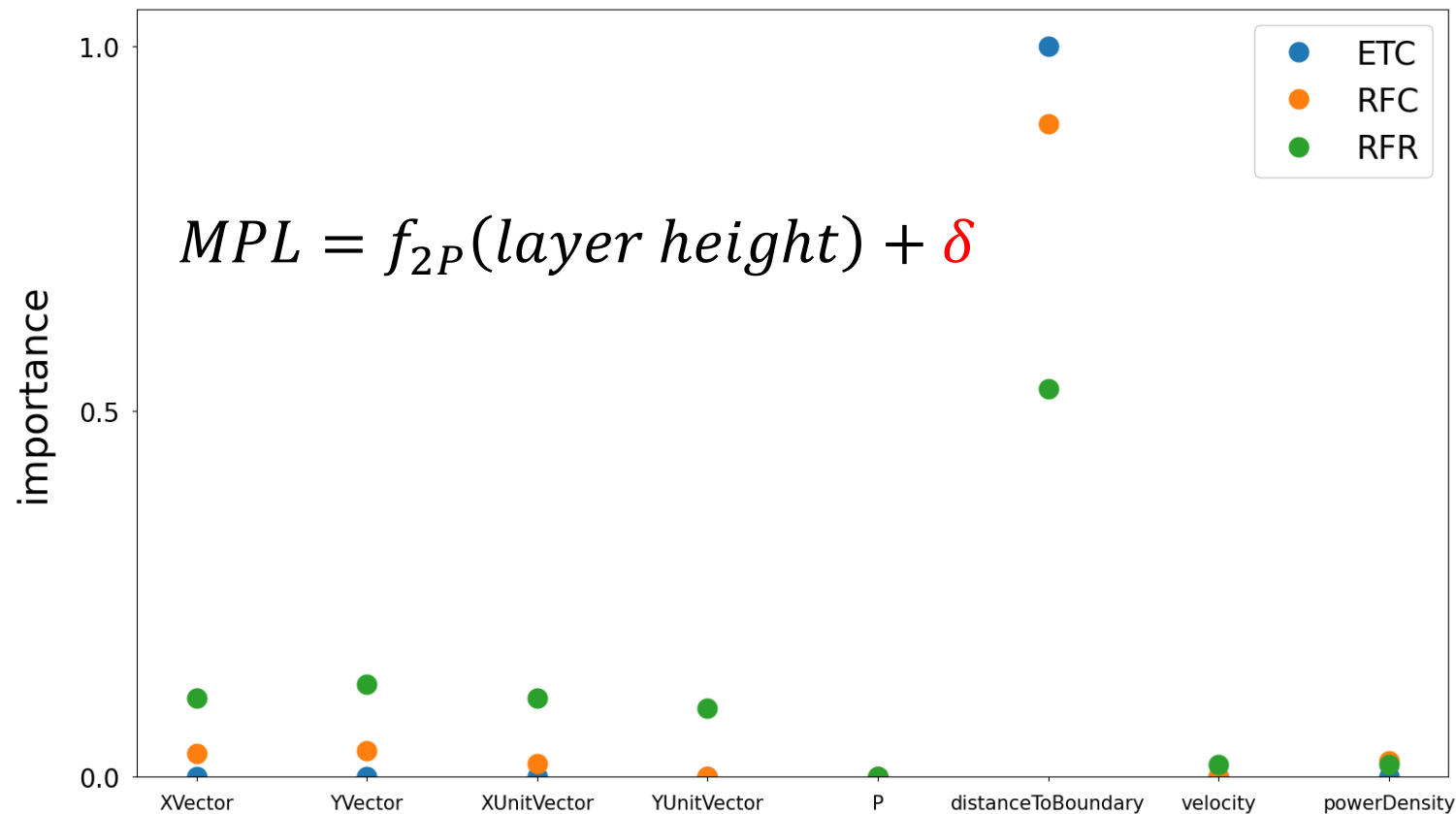
- ~4770 image/layer
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**VVUQ to evaluate data quality**



**VVUQ to assess model quality**

# Feature Selection



ETC: Extra-trees classifier

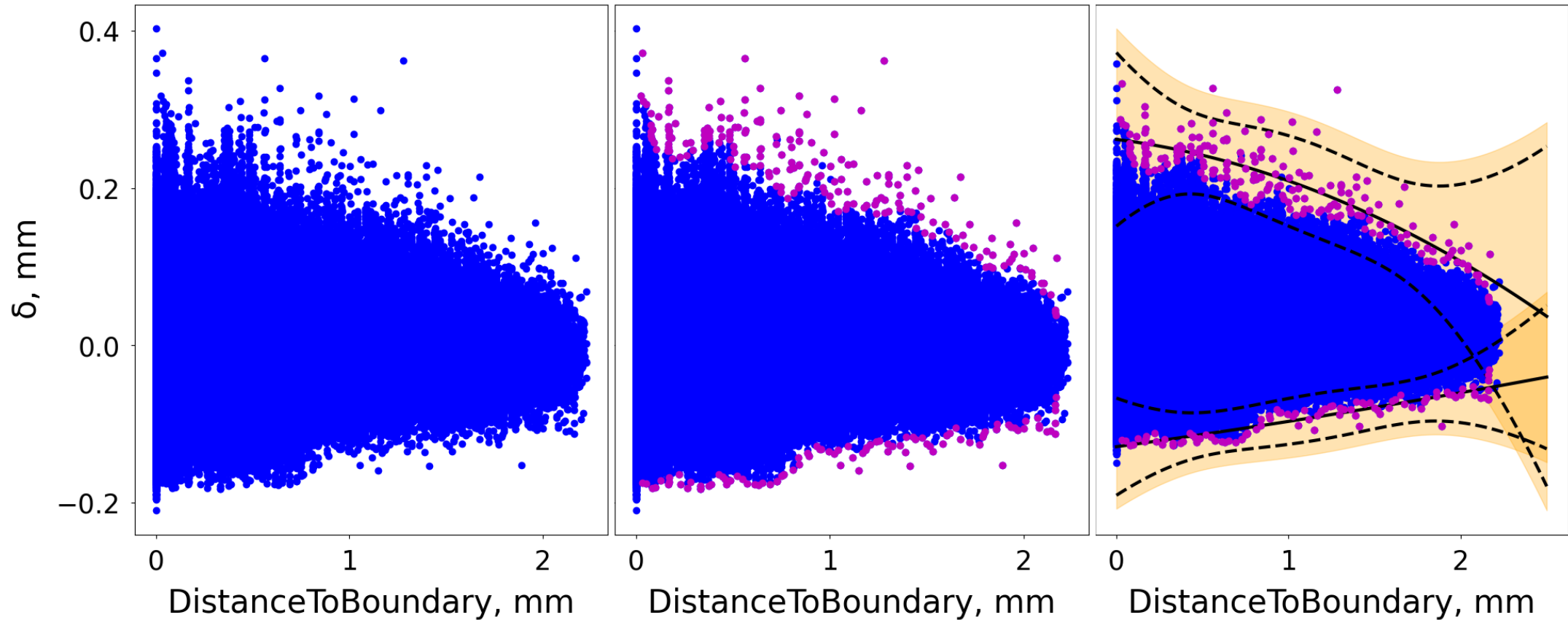
RFC: Random forest classifier

RFR: Random forest regression

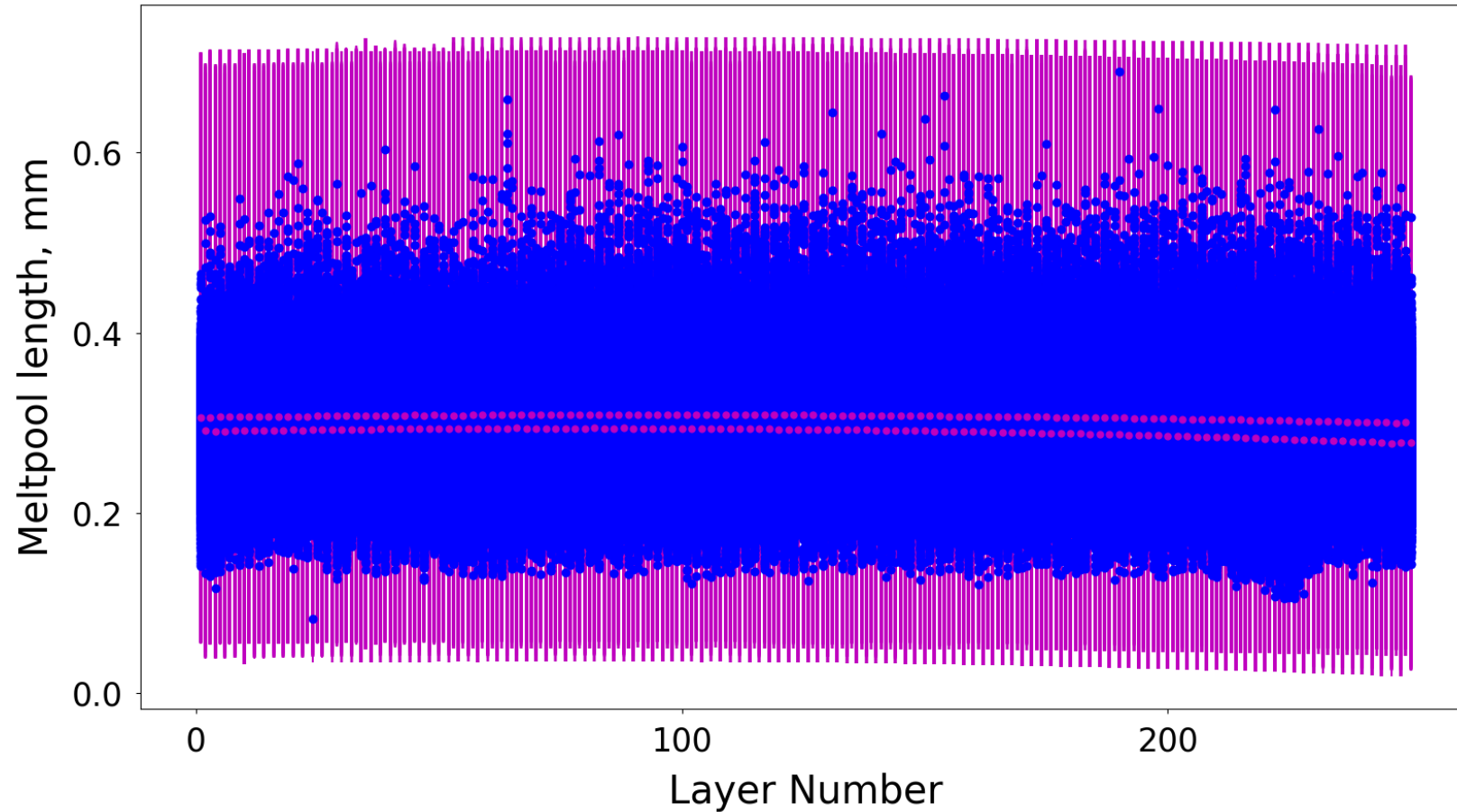
# Uncertainty Quantification

Alpha shape

PyMC3

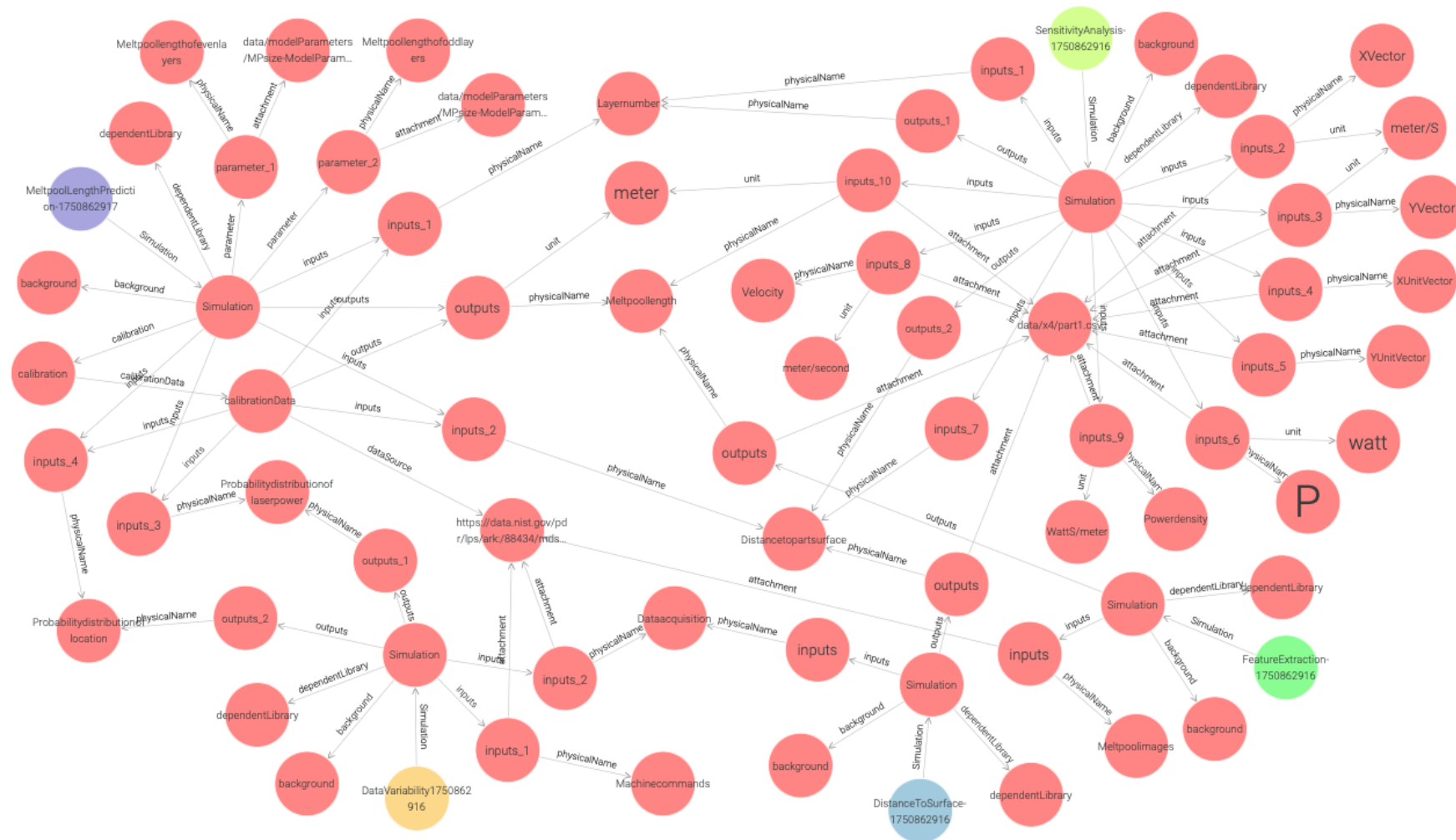


# Melt Pool Length Prediction



$$MPL = f_{2P}(\text{layer height}) + \sum_{i=1}^2 f_i(DtB) + \delta$$

# Modeling Workflow



# Modeling Workflow – Reusable & Scalable

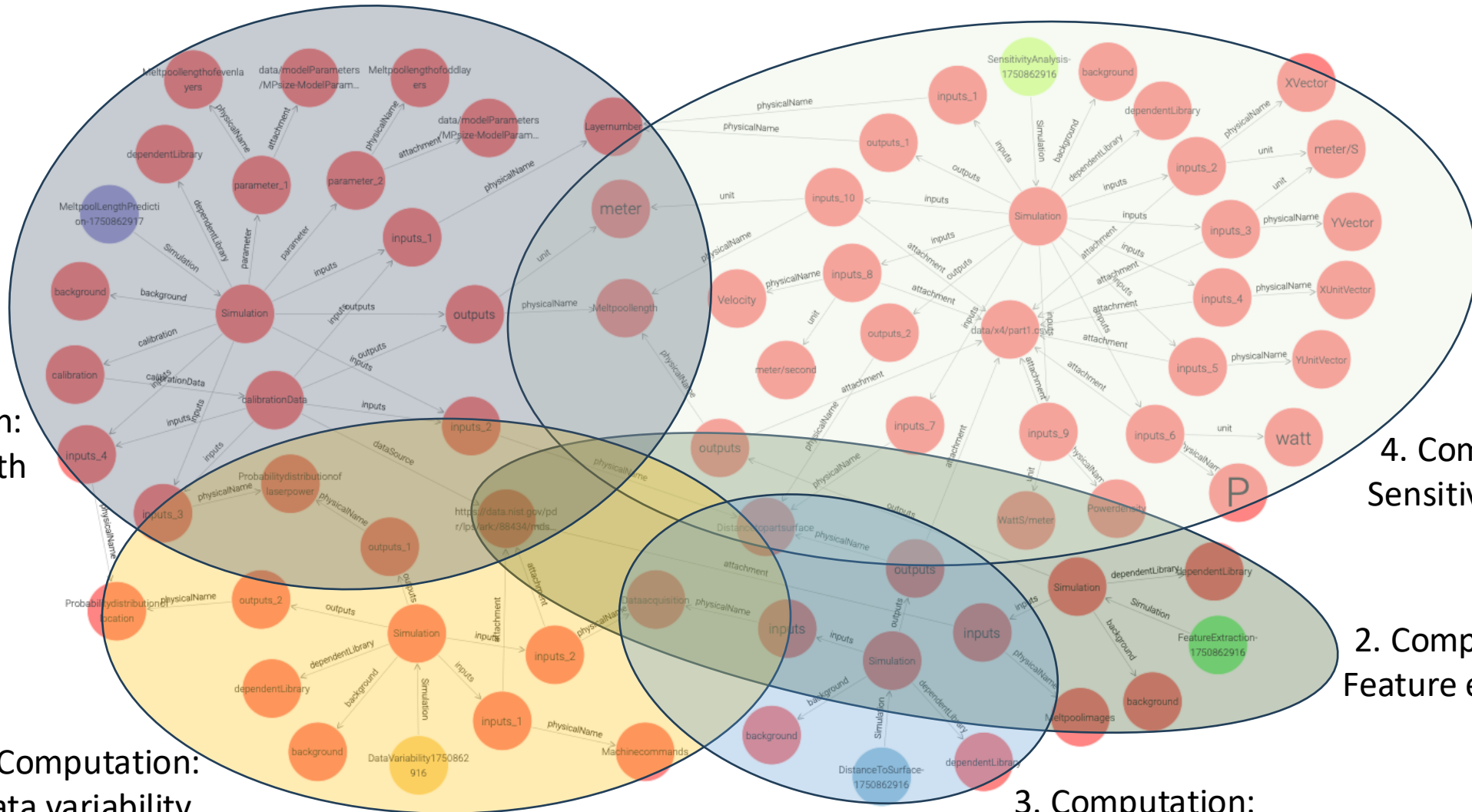
5. Computation:  
Melt pool length  
prediction

1. Computation:  
Data variability

4. Computation:  
Sensitivity analysis

2. Computation:  
Feature extraction

3. Computation:  
Distance to surface



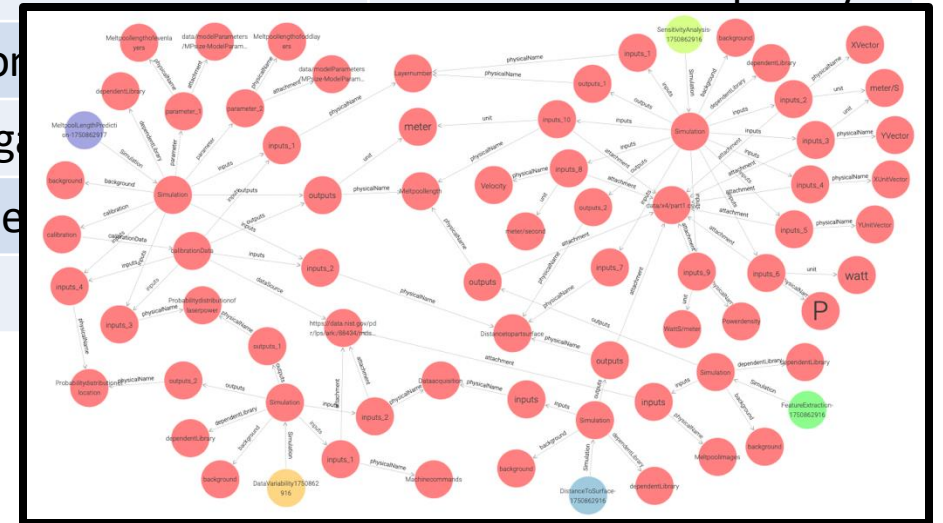


# Summary: Trustworthiness of Workflow

- A checklist is proposed to assess the trustworthiness of computational models at different phases of the lifecycle
- It enables the **Reusability, Scalability, Transparency**, and **(Interoperability)** of simulations

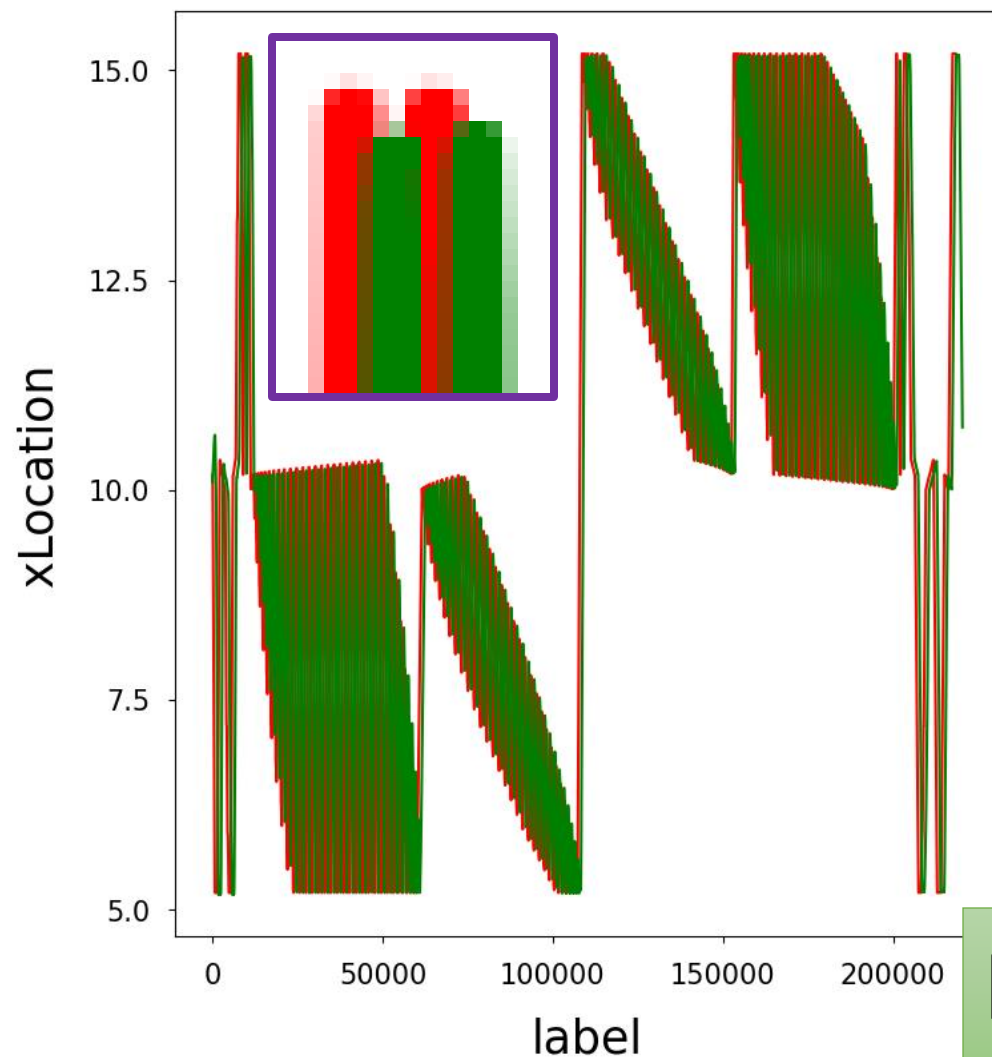
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shengyen.li@nist.gov

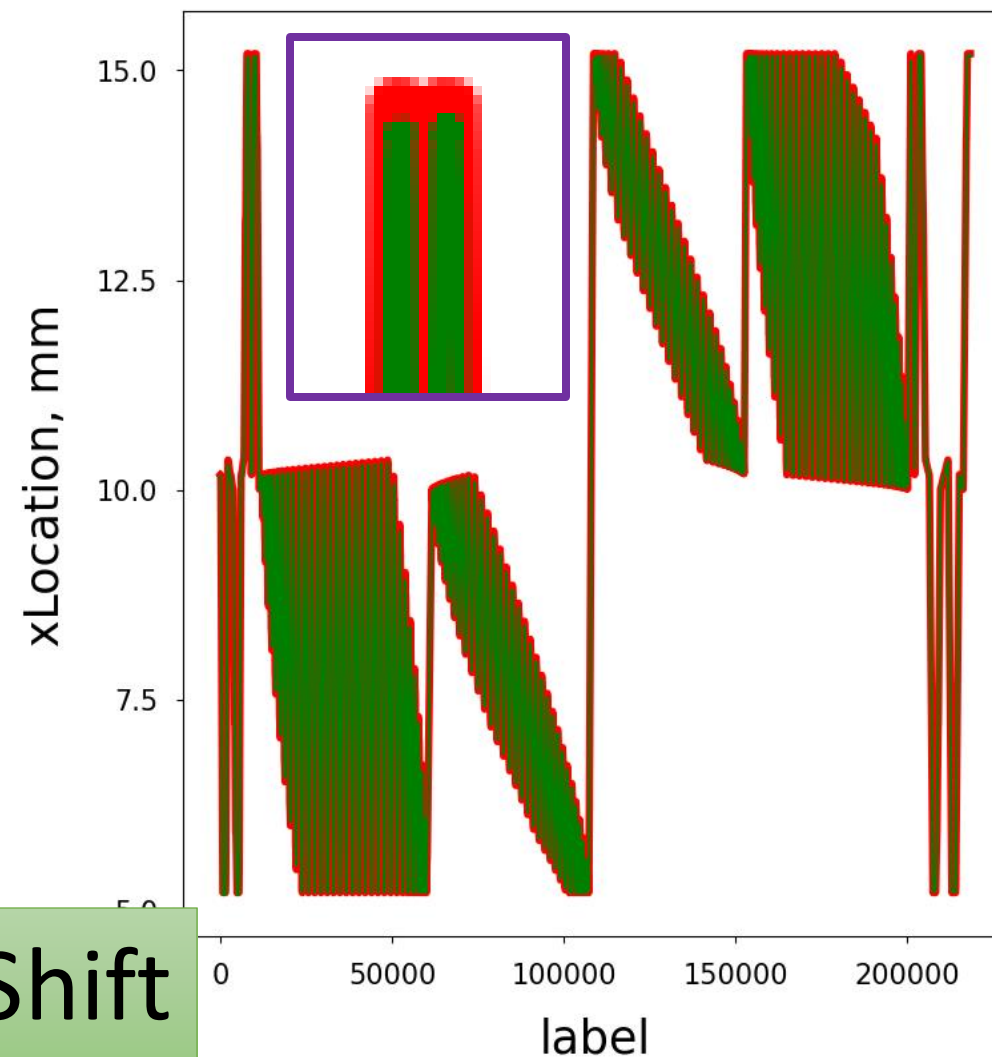




# Data Preparation



Phase Shift

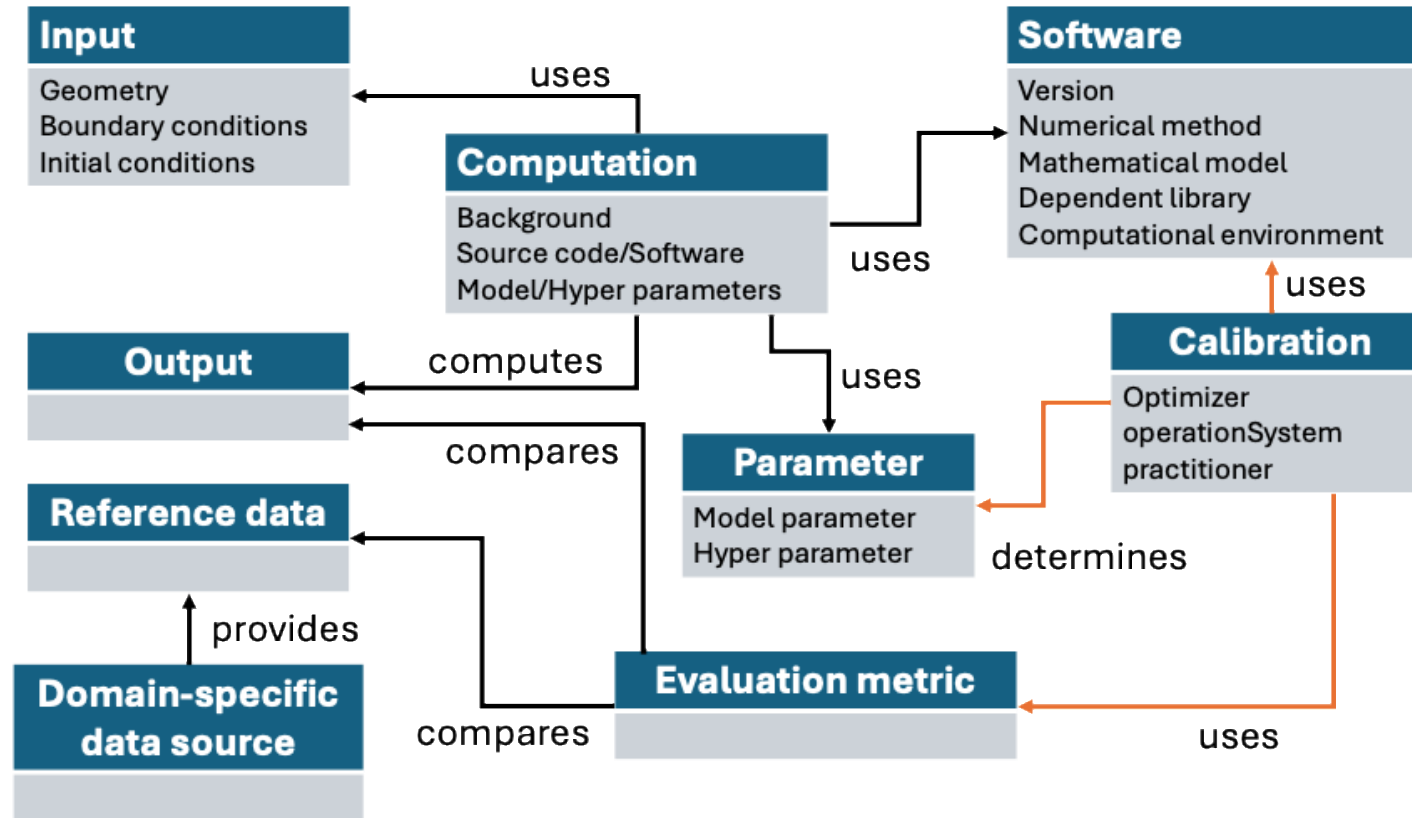


# Trustworthiness of Simulations

- Trustworthiness of simulations, hardware, integration and beyond
- A checklist to assess the trustworthiness of simulations in the 4 phases of the development lifecycle
- More specific information from ASME, ANS, IEEE, ISO, FDA, ...

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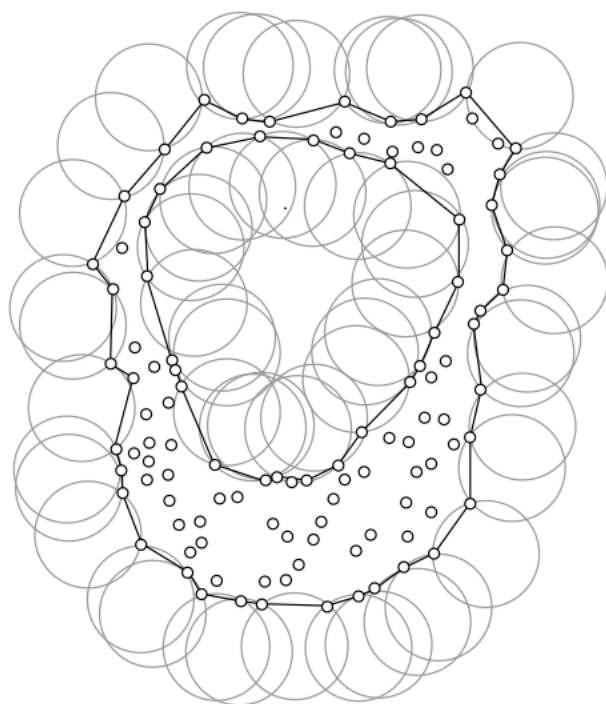
# Data Model for Computation



- A conceptual model has been implemented to address **interoperability**, **reusability**, and **scalability**.
- A Python library has been developed to translate the formats among XML schema, JSON, and JSON-LD.

## Alpha shape

Introduction to Alpha Shapes, Kaspar Fischer



## NIST



6 sigma:

Goal: 3.4 defects per million opportunities

For Creation/Improvement

1. Define: Identify the problem and project goals.
2. Measure: Collect data to understand current performance.
3. Analyze: Identify root causes of defects.
4. Design/Improve: Implement and test solutions.
5. Verify/Control: Maintain improvements using monitoring and controls.



# Next steps

- Review and define vocabulary for computation
- Stress test this model using a material digital twin for additive manufacturing
- Iteratively validate this metadata model to improve the maturity level
- Work with DT groups for other examples

