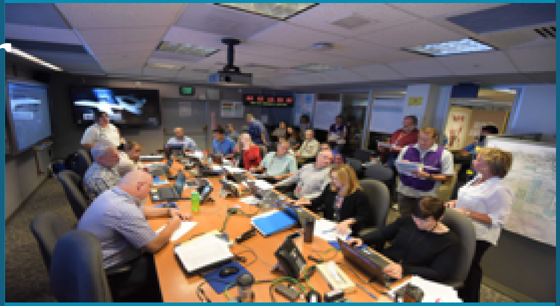
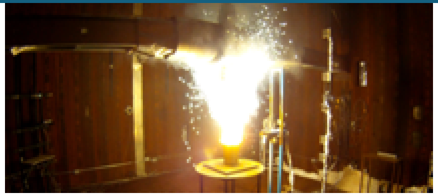
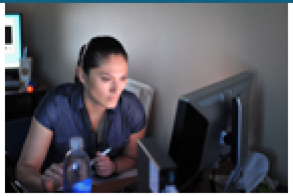
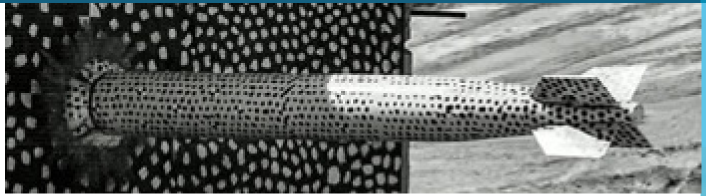
SAND2023-00939C

Development of structure-property linkages for damage in crystalline microstructures using Bayesian inference and unsupervised learning





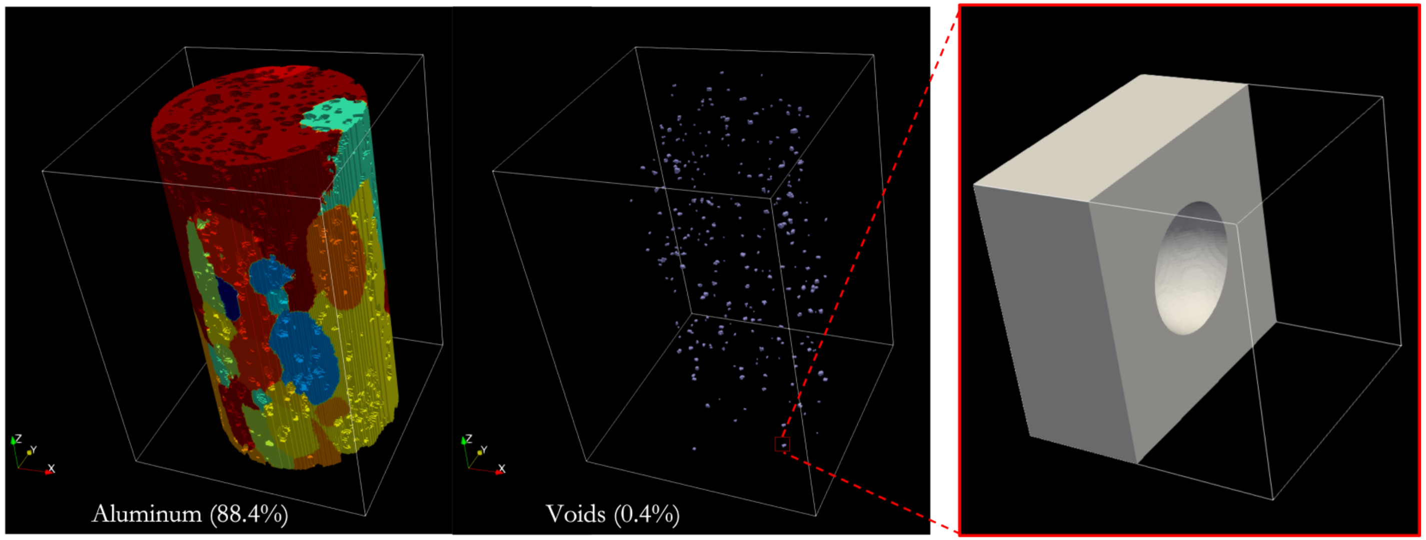


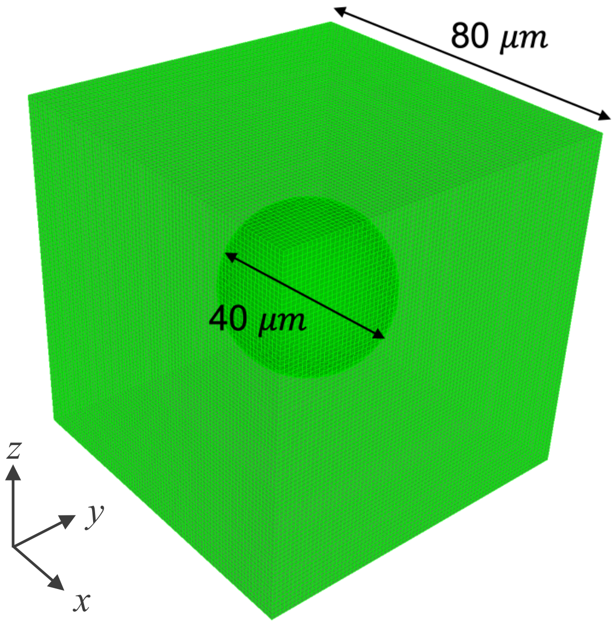


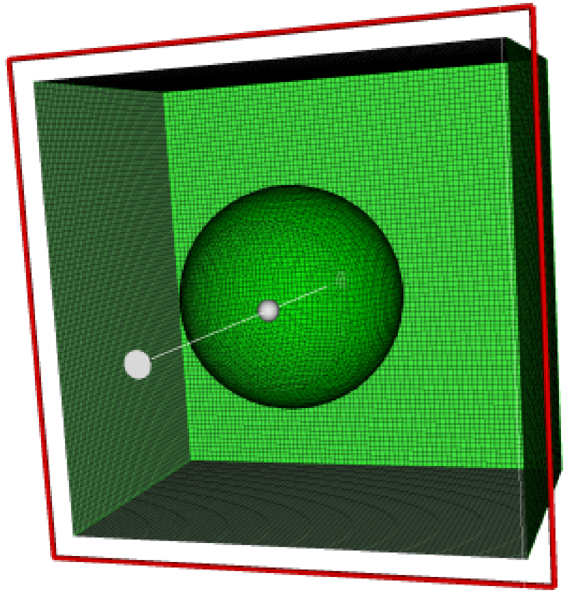
David Montes de Oca Zapiain[1], Anh Tran[1], Hojun Lim[1]

[1]Sandia National Laboratories, Albuquerque, NM 87185, USA

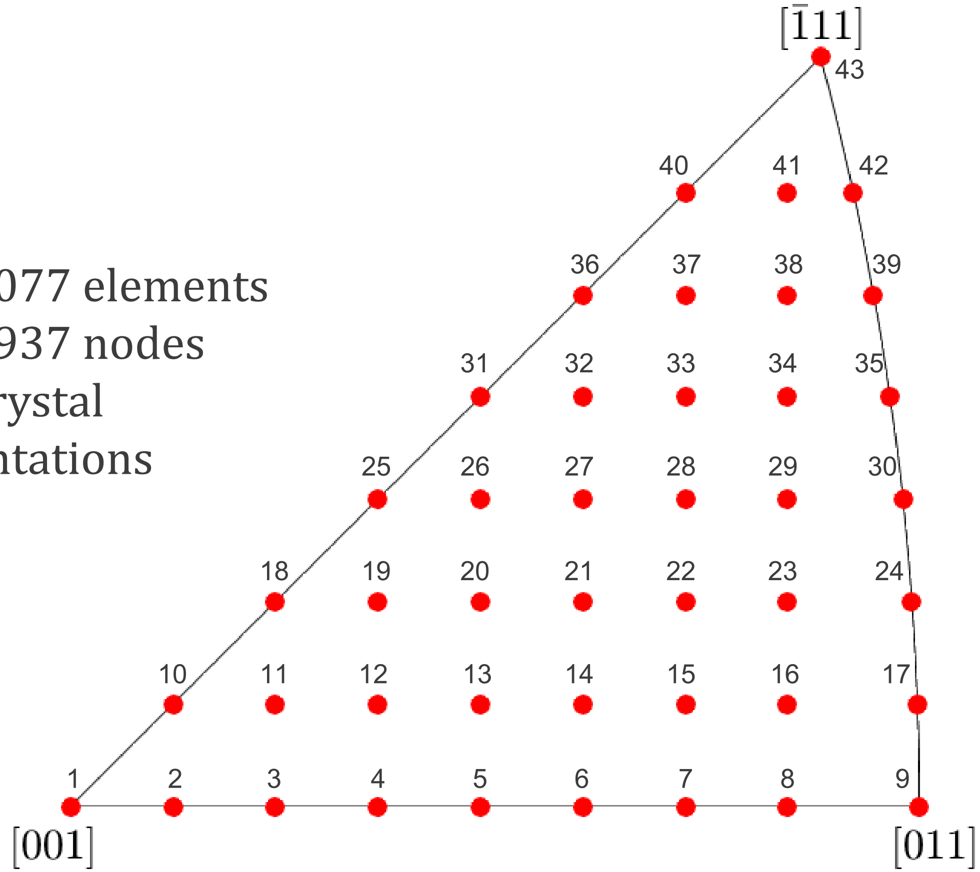
Quantifying the effects of voids and particles in polycrystalline deformation using CPFEM





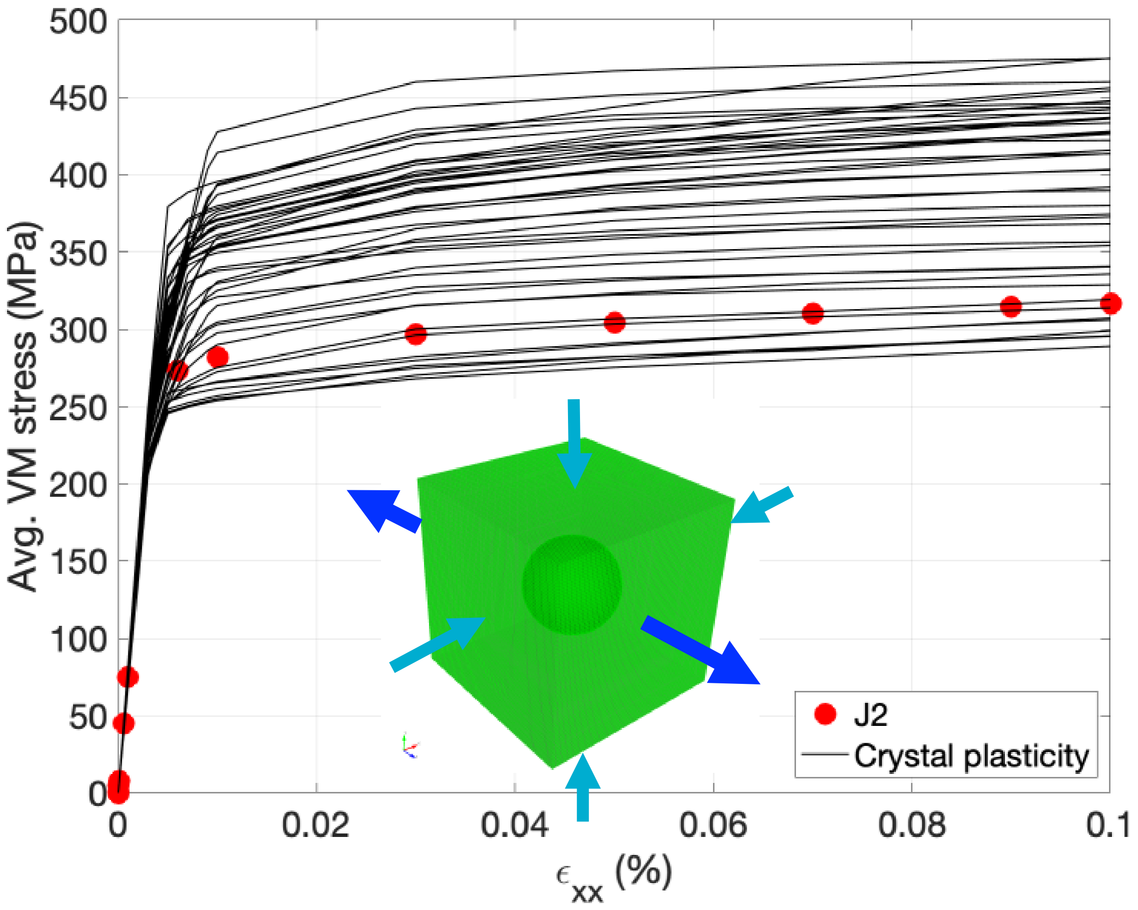


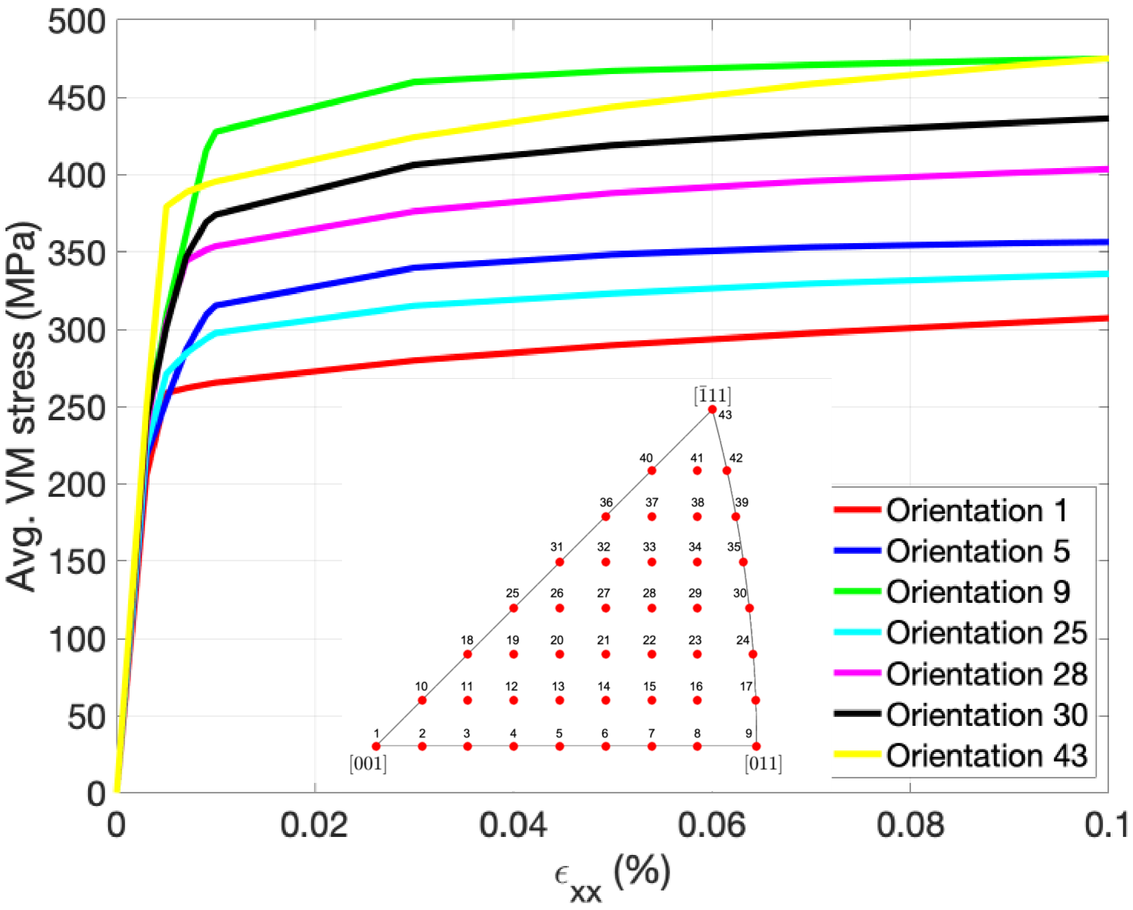
496,077 elements
518,937 nodes
43 crystal orientations



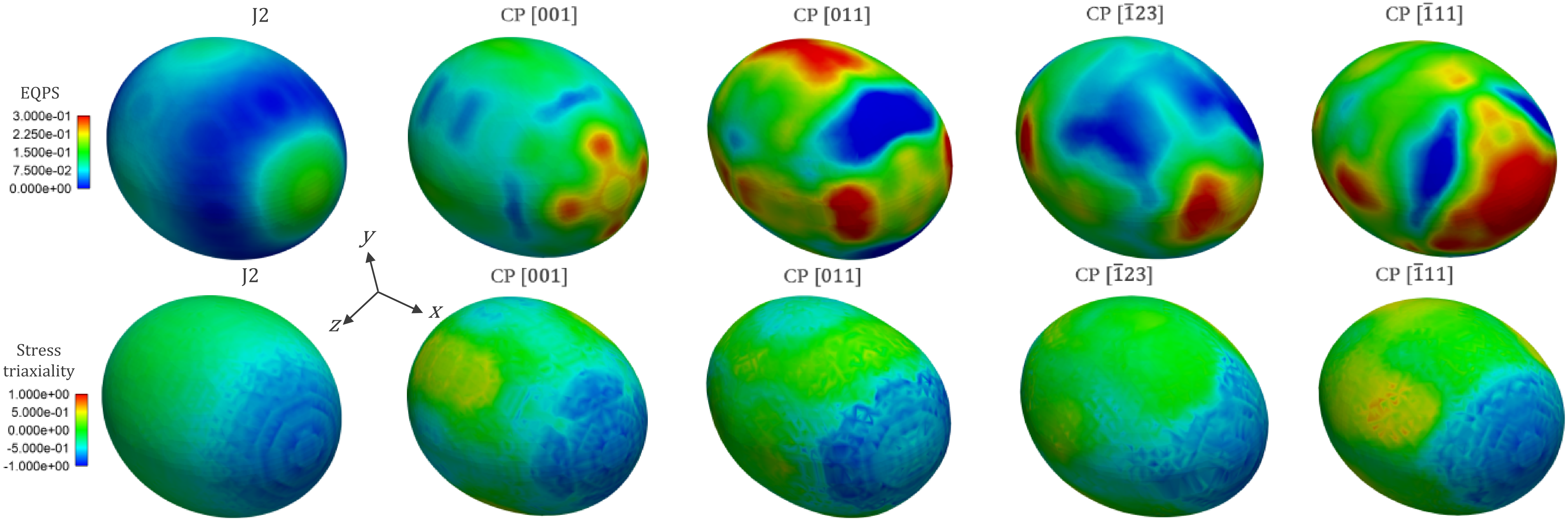
A spherical void in a single crystal cube – CP-FEM simulations

- Isochoric BC: $\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon & 0 & 0 \\ 0 & -0.5\varepsilon & 0 \\ 0 & 0 & -0.5\varepsilon \end{bmatrix}$
- CP parameters for Al6061



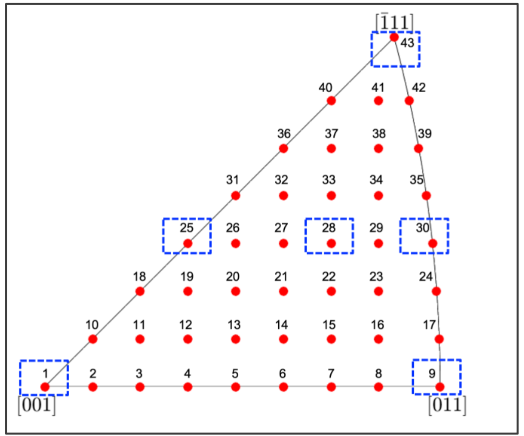


Relating Void Growth to Damage



- Experimental analysis showed that void growth was the main failure mode under high stress triaxiality.
- Under low stress triaxiality, the crack developed in the way of combined shear and void growth modes.
- In negative stress triaxiality, the fracture was controlled by shear only.

- Fields of EQPS and stress triaxiality at 10% deformation.
- Fields show great dependence on orientation.

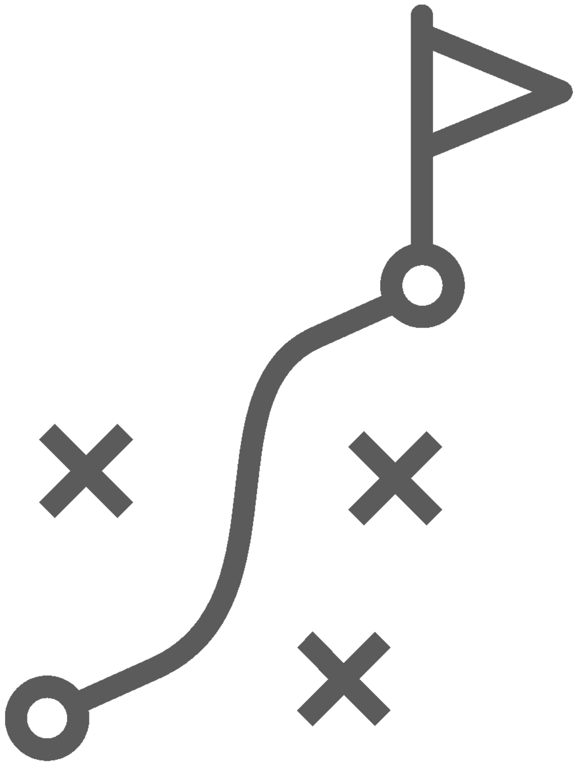


Full-field analysis is expensive and not scalable

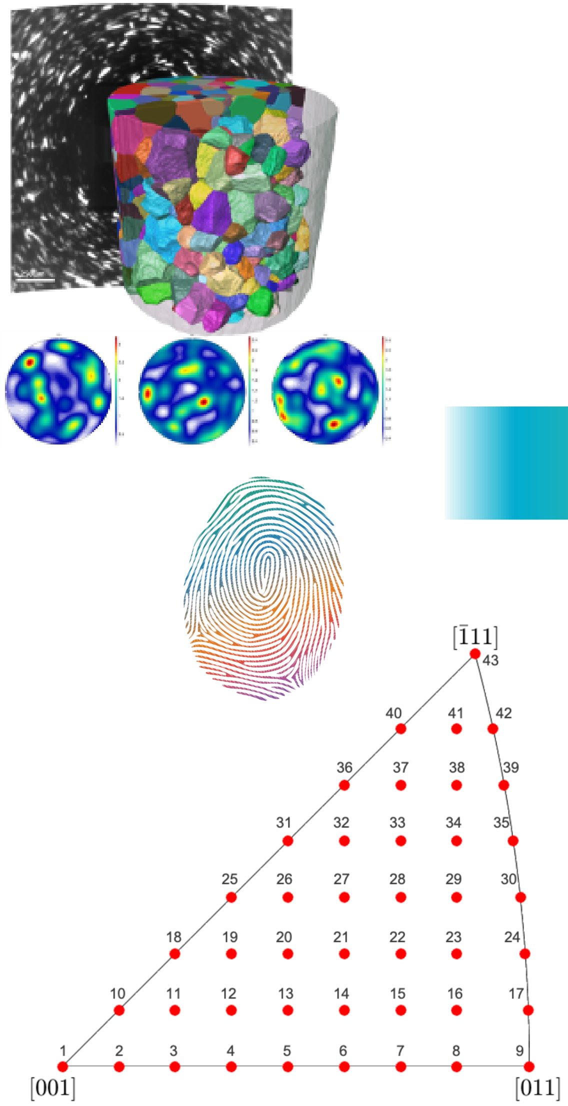
- Full-field CPFEM analysis enabled us to draw some general conclusions and validate the effect texture has.

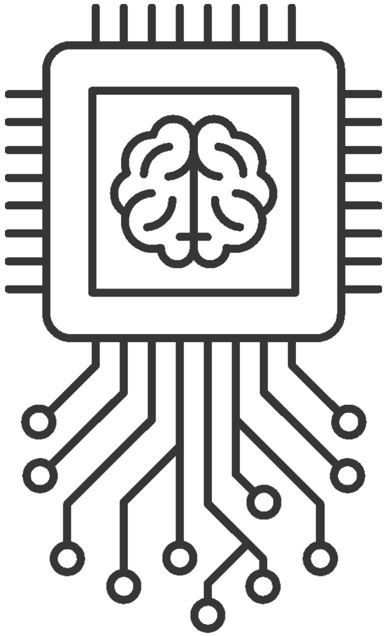
- Nevertheless, these insights needed significant computational expense, given that each simulation required ~10 hours with ~300 CPUs.

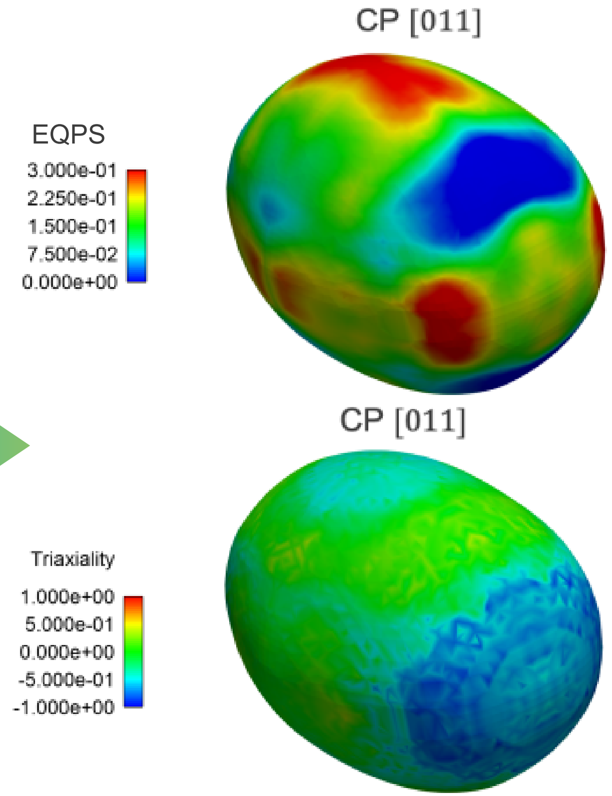
- Therefore, there is a critical need for a more efficient linkage between the structure and the property.



Leverage data-driven approaches to establish an accurate model

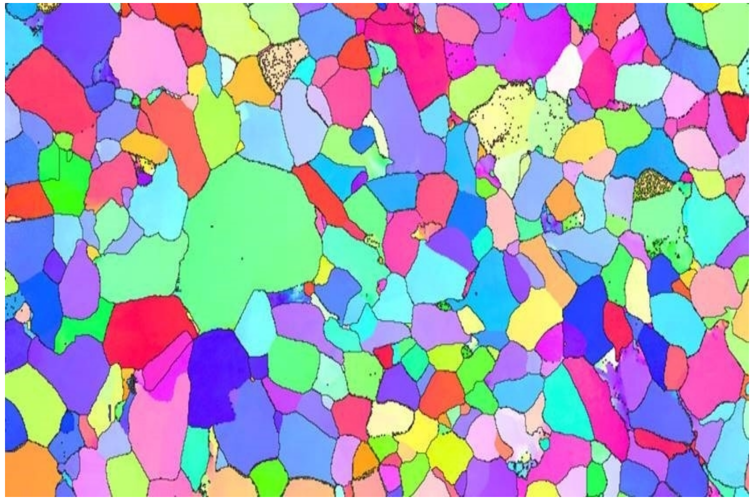




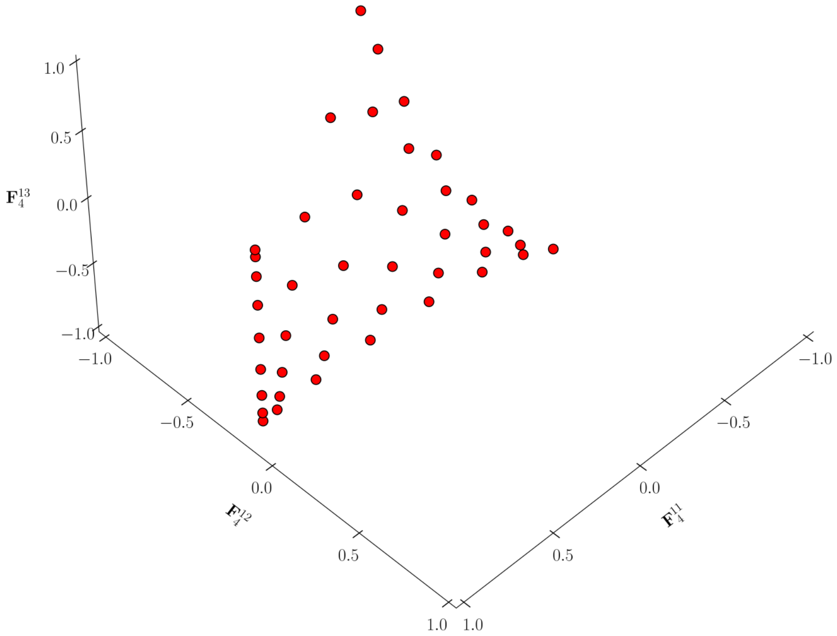


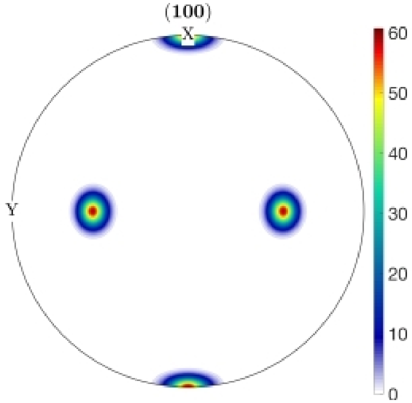
Establishing a fingerprint of the data (Input)

Colors denote the crystal lattice orientation



- GSH representation of 43 different orientations





$f_s(g)$ is the probability distribution of the orientation of the crystal lattice

Fourier series representation

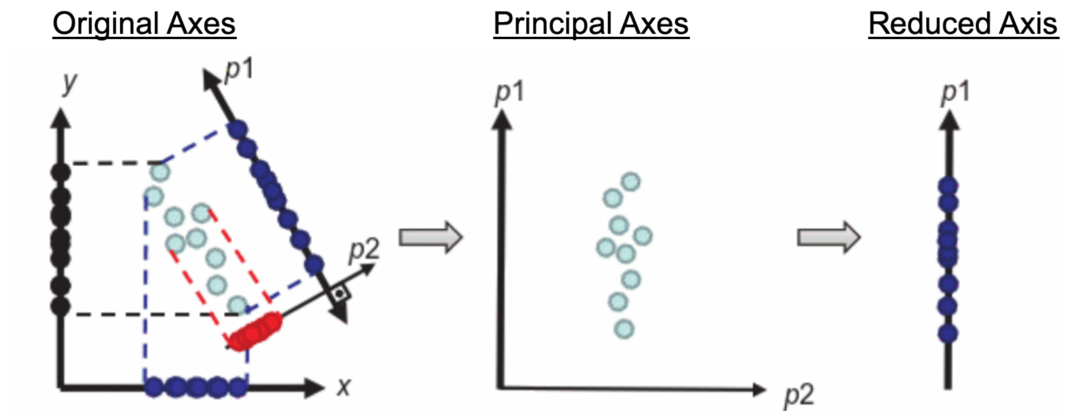
$$T_l^{mn}(g) = T_l^{mn}(\varphi_1, \Phi, \varphi_2) = e^{im\varphi_1} P_l^{mn}(\Phi) e^{im\varphi_2}$$

$$f_s(g) = \sum_{\mu,n,l} F_{ls}^{\mu n} T_l^{\mu n}(g),$$

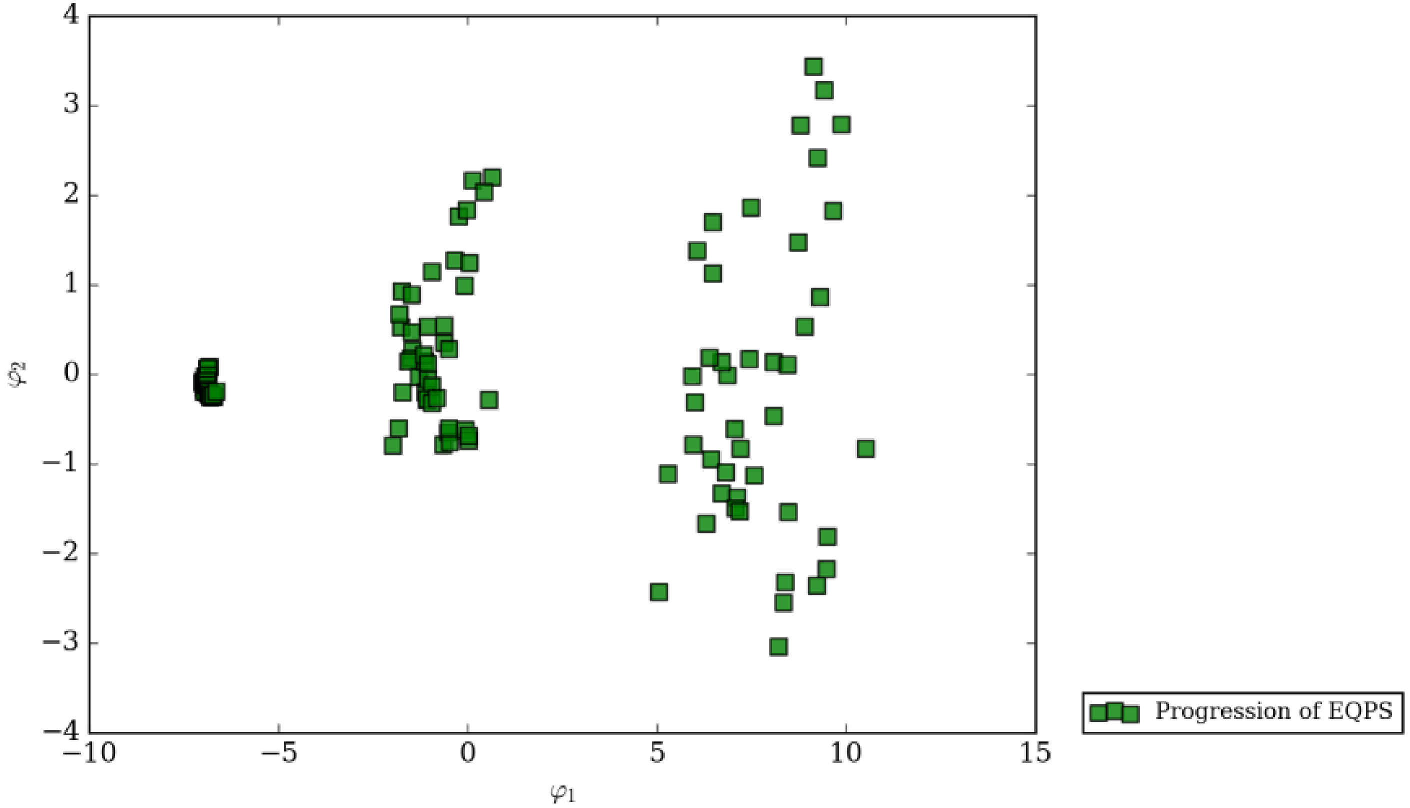
$$F_{ls}^{\mu n} = (2l+1) \int_{FZ} f_s(g) T_l^{\mu n*}(g) dg$$

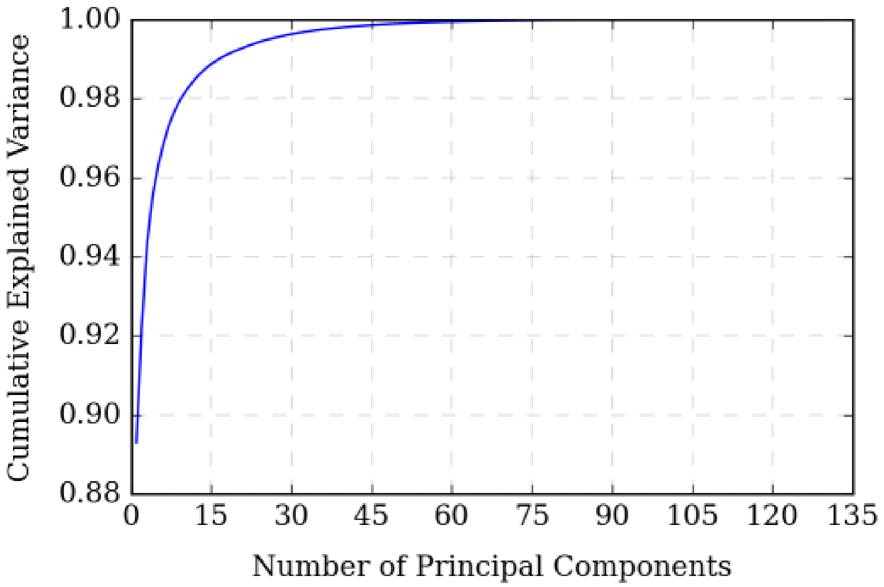
- Orthogonal Basis functions.
- Customized to account for symmetry.

Establishing a fingerprint of the data (Output)



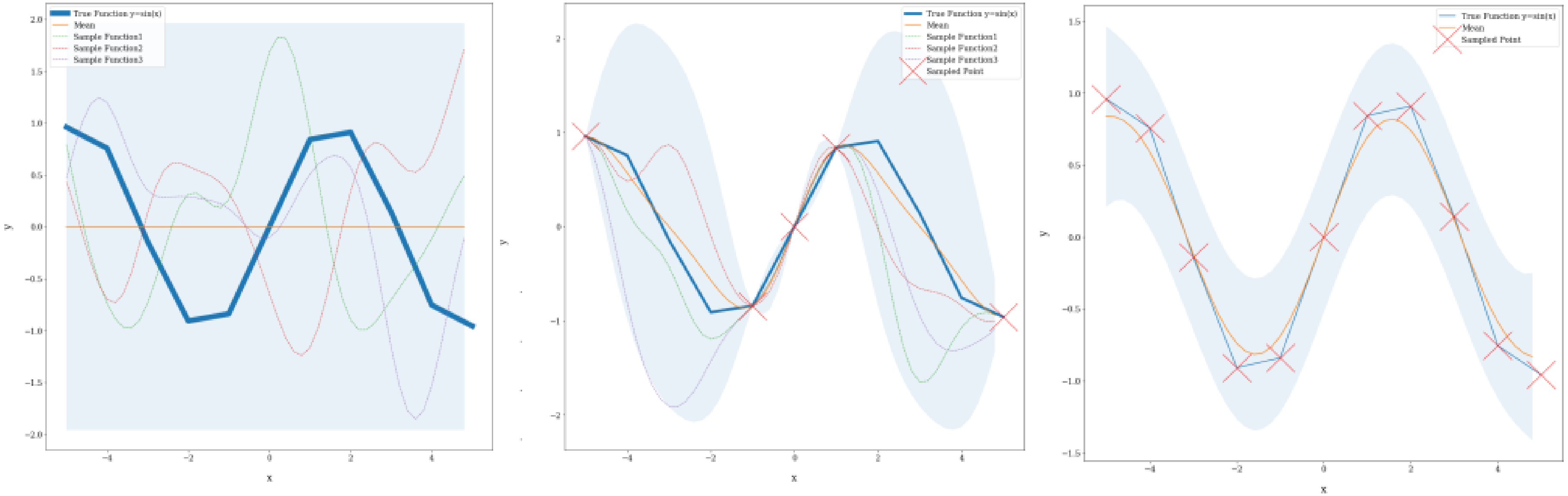
- Represent the values of each variable of interest (EQPS and Triaxiality) with 129 PC components.
- Reconstruct the values using the fitted PC transformation.





Establishing Structure-Property Linkage with GPR

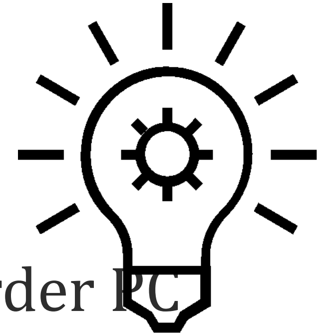
- Connect the GSH coefficients to the PC components for EQPS and Triaxiality using Gaussian Processes Regression (GPR).
  - 43 orientations (6 snapshots between 0 and 10% deformation).
- GPR is non-parametric model building approach, which employs kernel-based interpolation on a training dataset to make predictions for new (test) inputs.
- A Gaussian Process is a distribution over functions that follows a multivariate Gaussian fully specified by a mean function and a covariance function.
- Sampling points (i.e., training data) within the specified domain constrains the distribution from which the functions are drawn.
- Sampling more points eventually enables us to learn the underlying function.



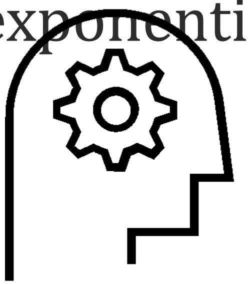
[Rasmussen(2003)]

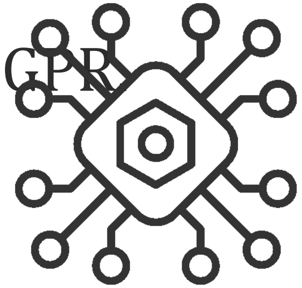
Structure-Property Linkage: GPR Details

- Connect the GSH coefficients to the PC components for EQPS and Triaxiality using Gaussian Processes Regression (GPR).
  - 43 orientations (6 snapshots between 0 and 10% deformation).



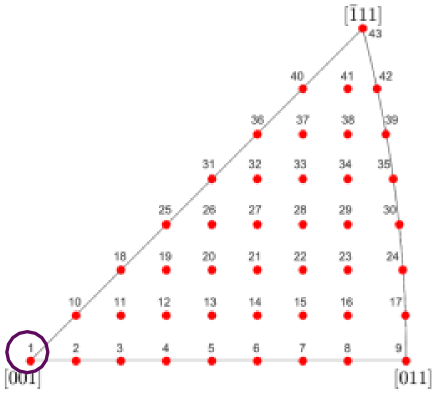
- Normalize the output to [-1,1] in order to be able to better predict higher order PC Components.
- We will fit an individual GP for each individual QoI (i.e., the PCA of EQPS and triaxiality) .
- A squared exponential kernel with constant noise was used for each GPR

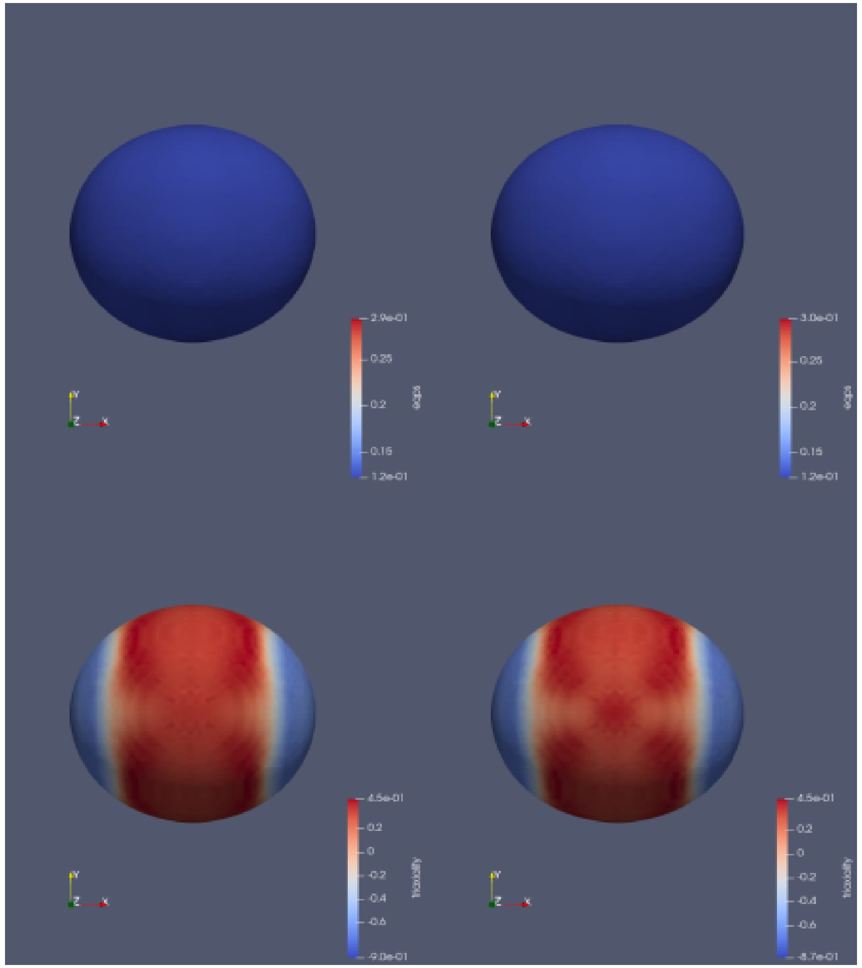


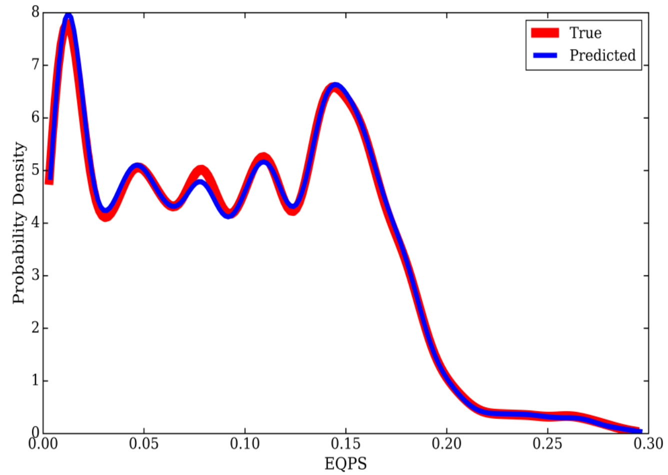


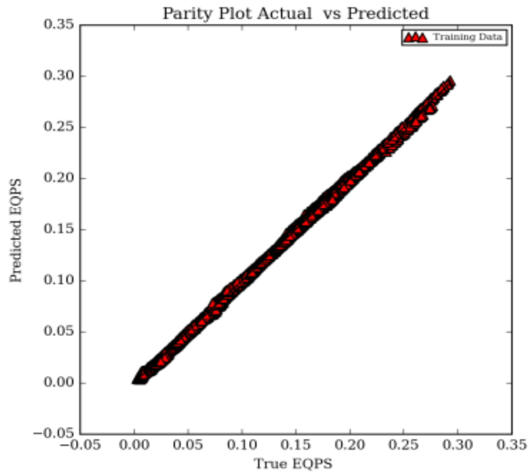
Results: Interpolating in Time

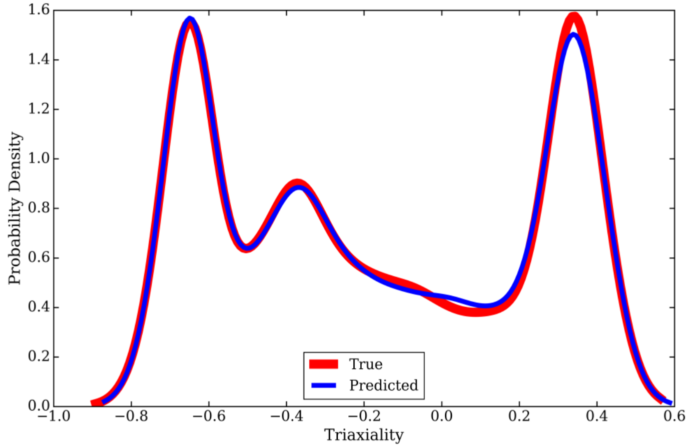
- Orientation 1:
  - Evolution EQPS (top) and triaxiality (bottom).
  - Comparing true (left) vs. predicted (right).

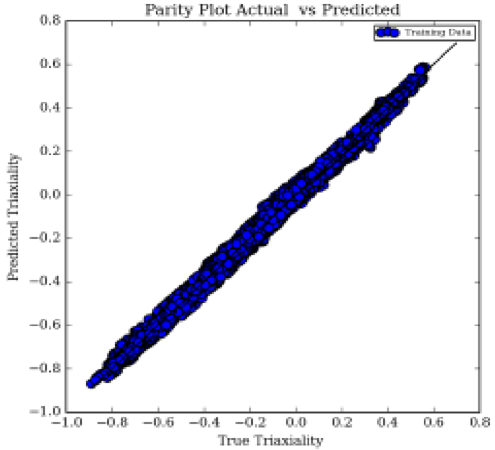




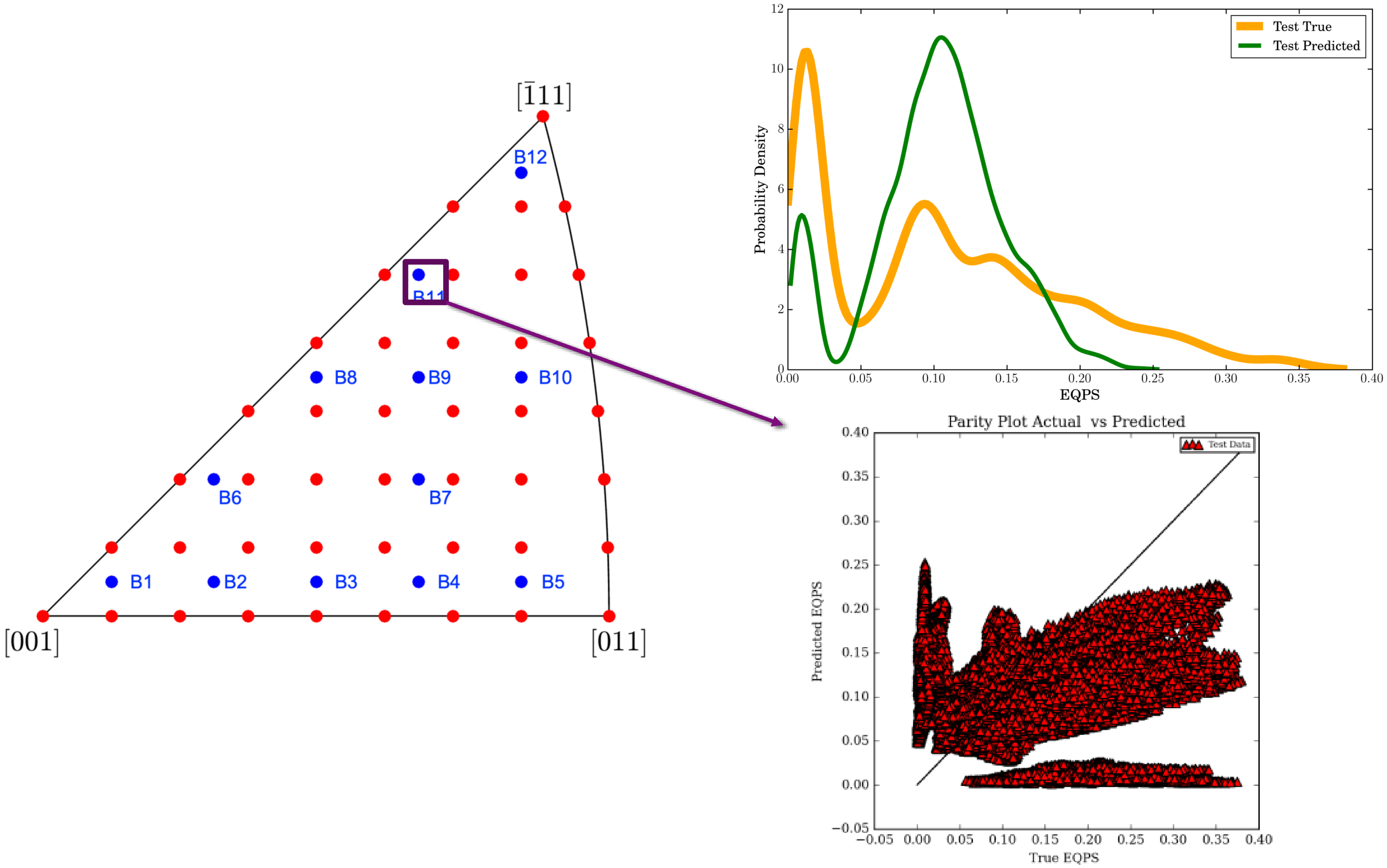




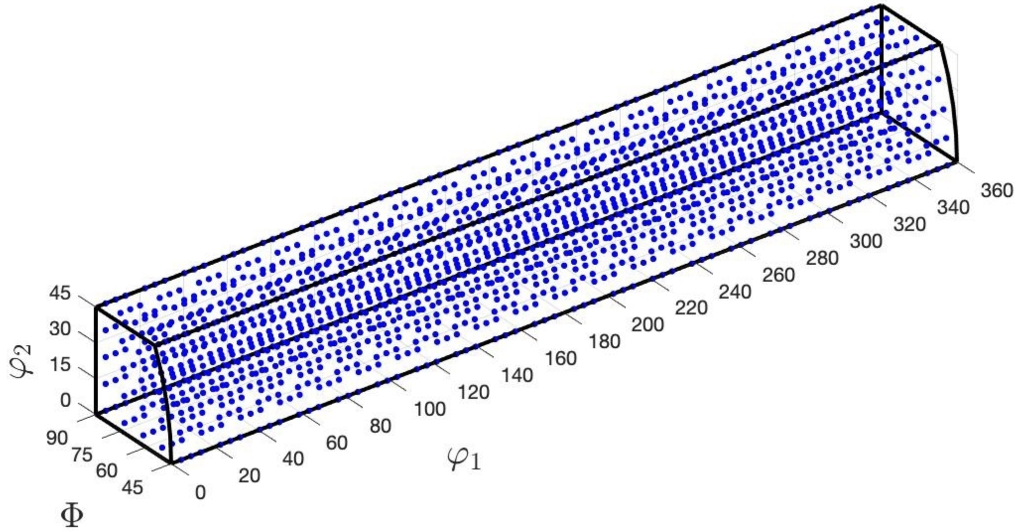




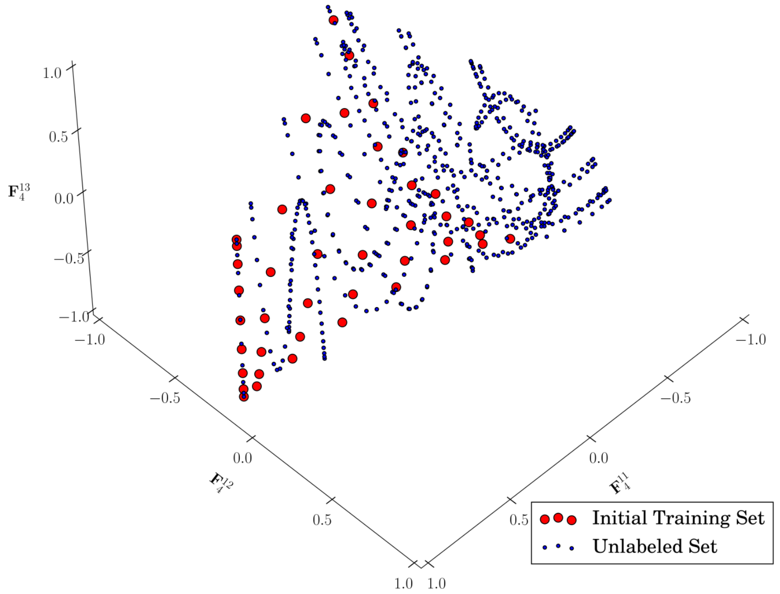
Results: Interpolating in Time and Texture

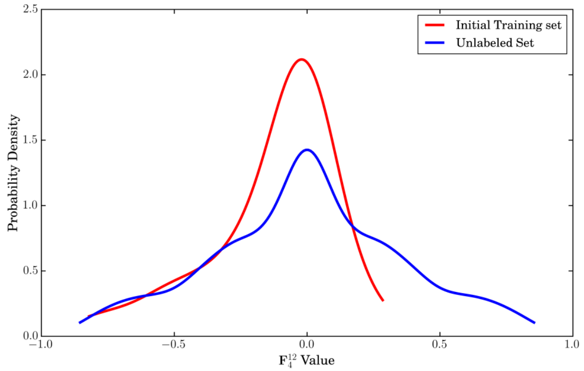


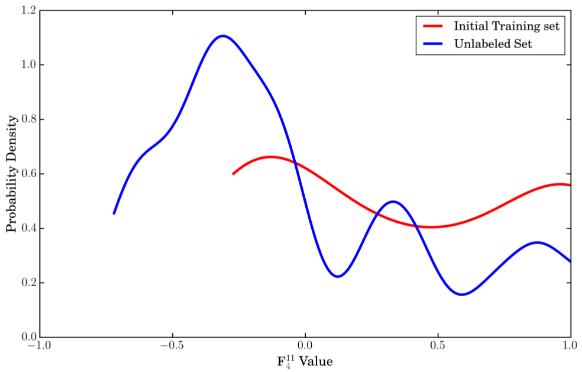
Expanding model to interpolate in texture space

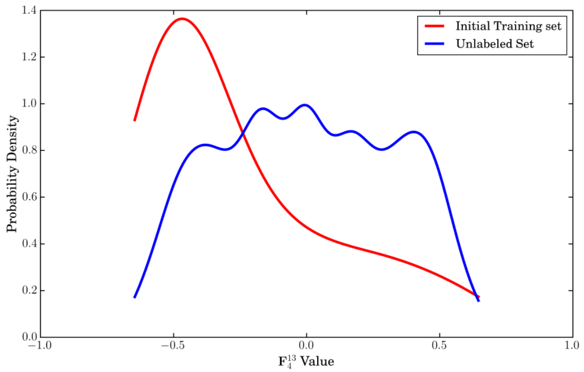


- Sample the Fundamental Zone of Cubic Crystals with 2770 orientations.





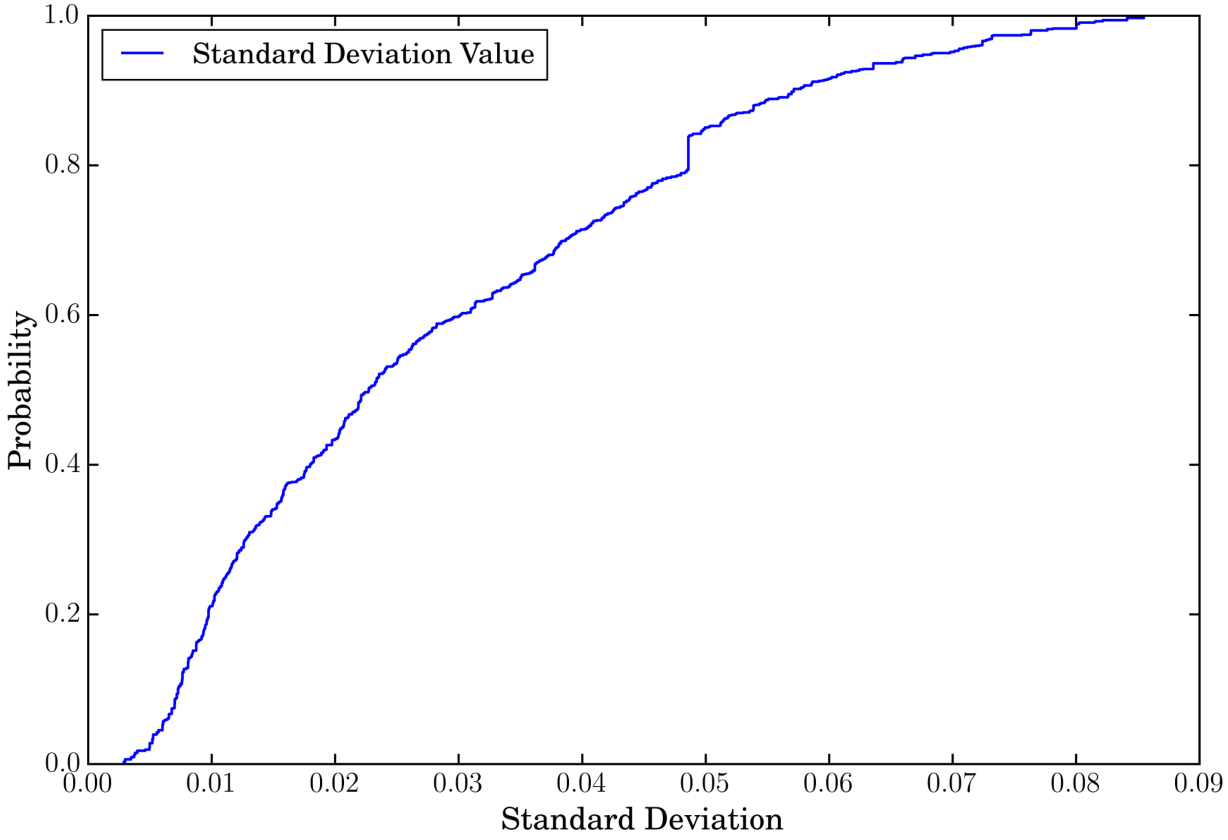




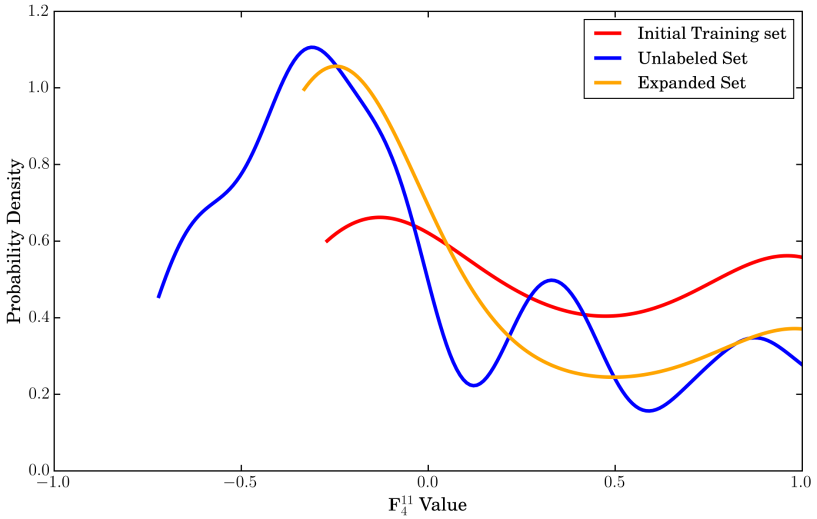
Identify most uncertain points using GPR-based model

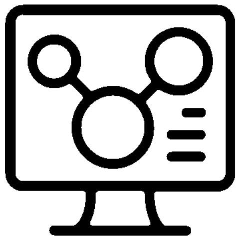
- Use existing model to predict the value of PC scores for the unlabeled set.
- Quantify uncertainty using average standard deviation across PC scores.

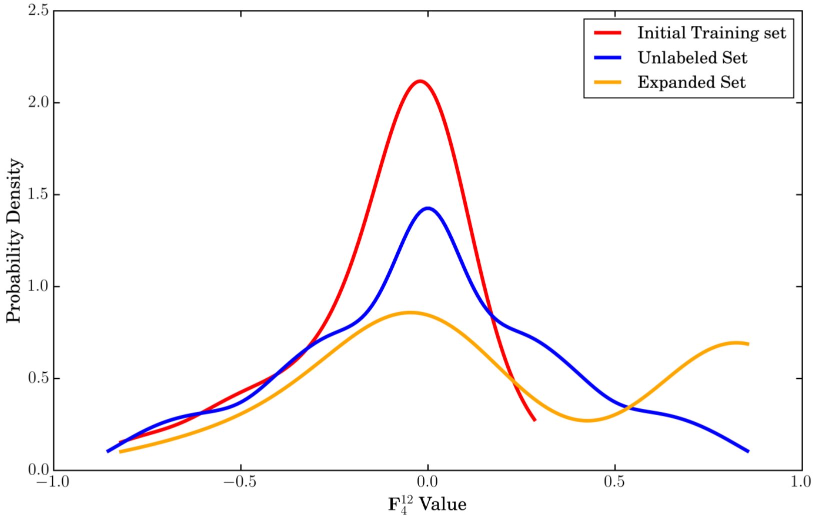
- Select top 1% uncertain (26 points).

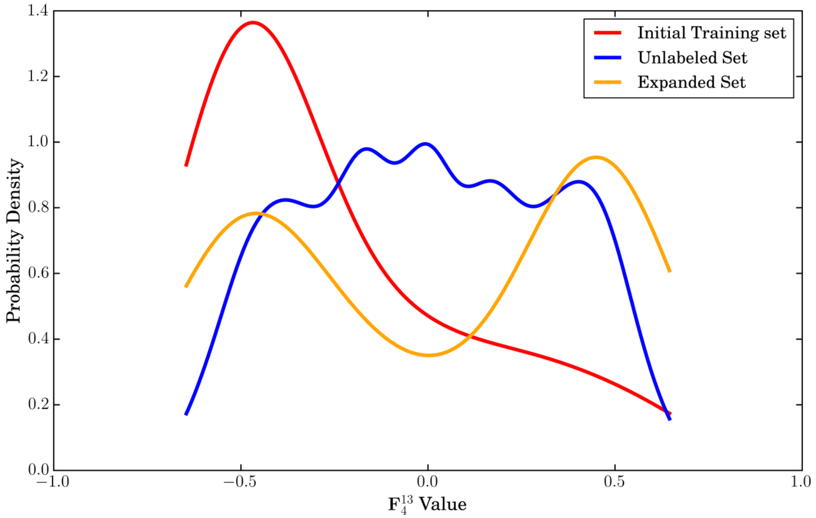


Incorporating Most Uncertain Points (In progress)



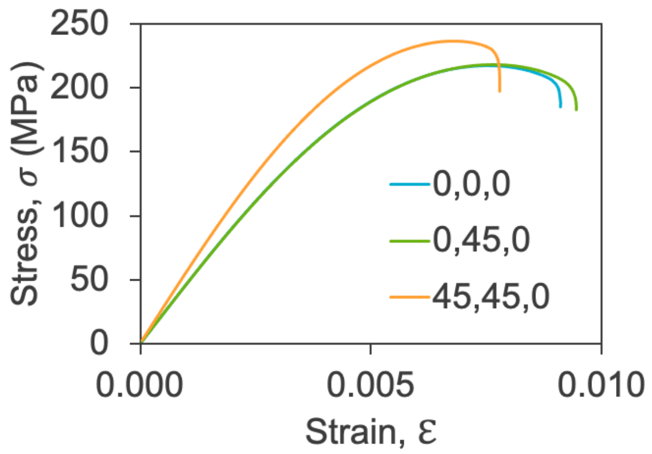


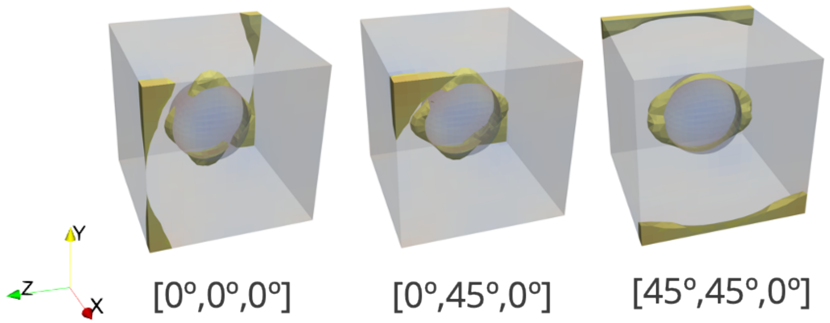




Future Work: Incorporating Efficient Model Building to more complex models

- A coupled crystal plasticity (CP) and phase-field fracture (PFF) model, solved within FEM MOOSE framework



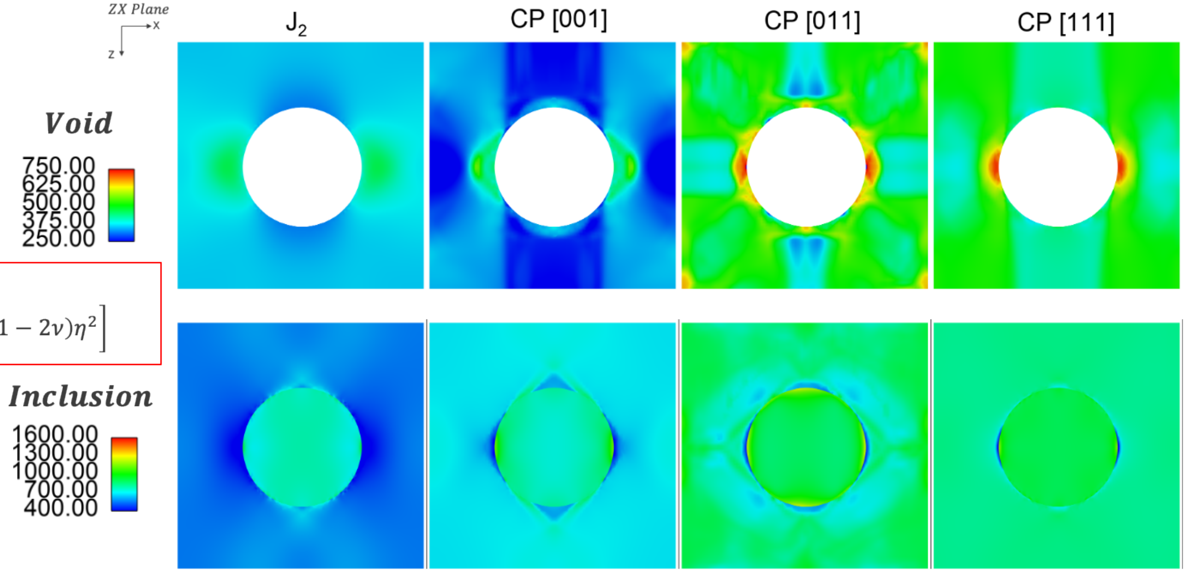


- Fracture propagation also exhibit dependencies on the orientations

- Incorporating a failure criteria into CP simulations.

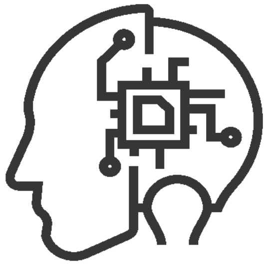
Failure criteria:

$$\sigma^* = \sigma_{mises}\left[\frac{2}{3}(1+\nu) + 3(1-2\nu)\eta^2\right]$$

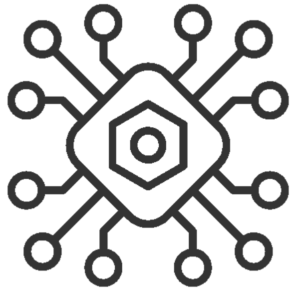


- Void simulations predict ductile failure of the matrix.
- Single crystals with hard inclusions predict matrix decohesion and particle cracking.
  - In both cases, [011] and [111] are anticipated to be the weakest crystallographic orientations compared to [001]

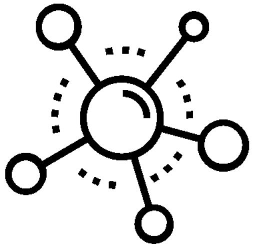
Conclusions



- CPFEM is a robust tool that enables us to obtain fundamental understanding of experimentally observed behavior.

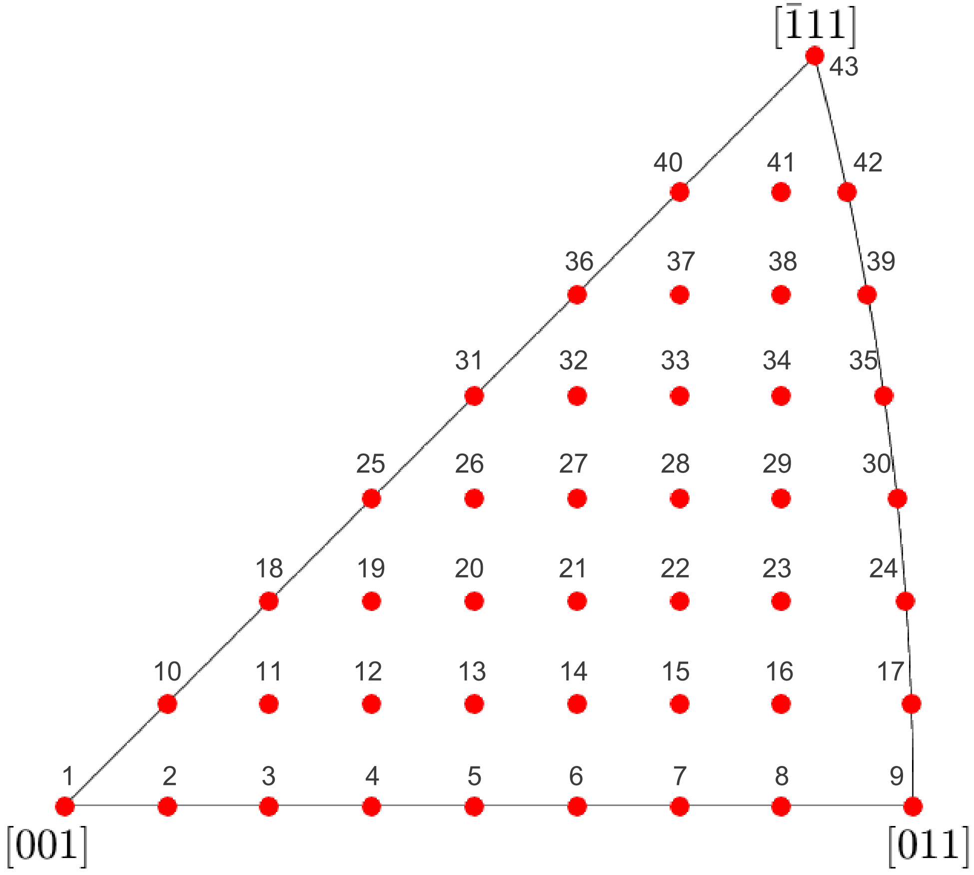


- Data-driven representations allow for the identification of fingerprints that can be then used to build accurate models.



- The capability to perform UQ on obtained results allows one to identify areas in the input space worth exploring.

Appendix



[$\bar{1}$11]
43
40
41
42
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30
18
19
20
21
22
23
24
10
11
12
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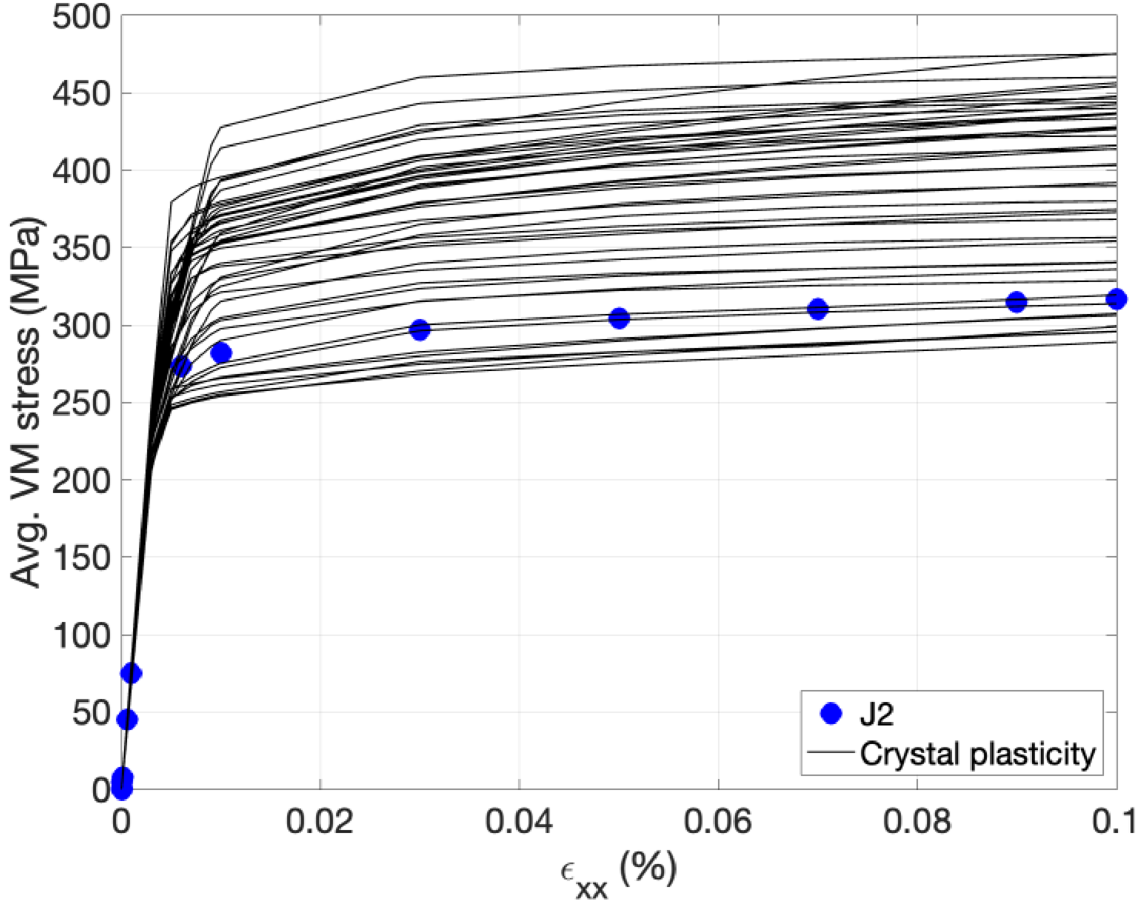
16
17
1
2
3
4
5
6
7
8
9
[001]
[011]

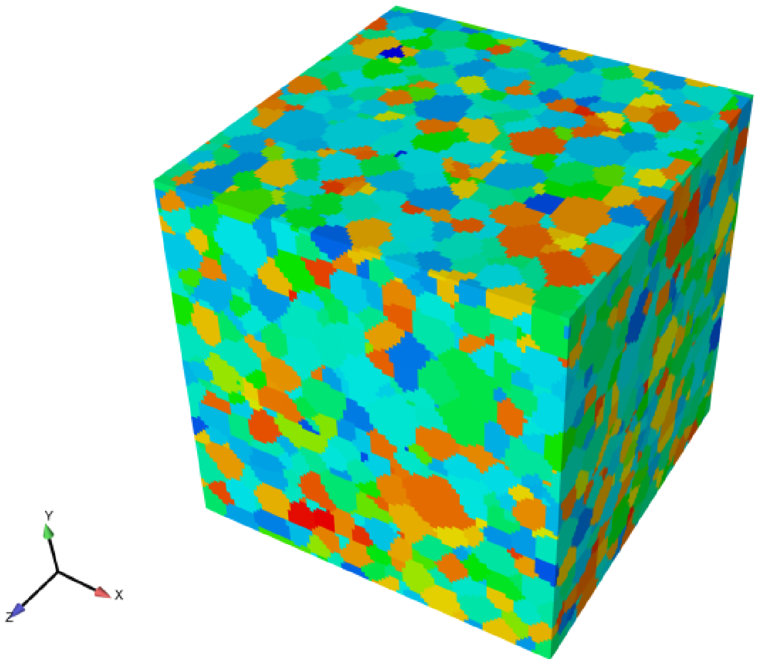
(a)

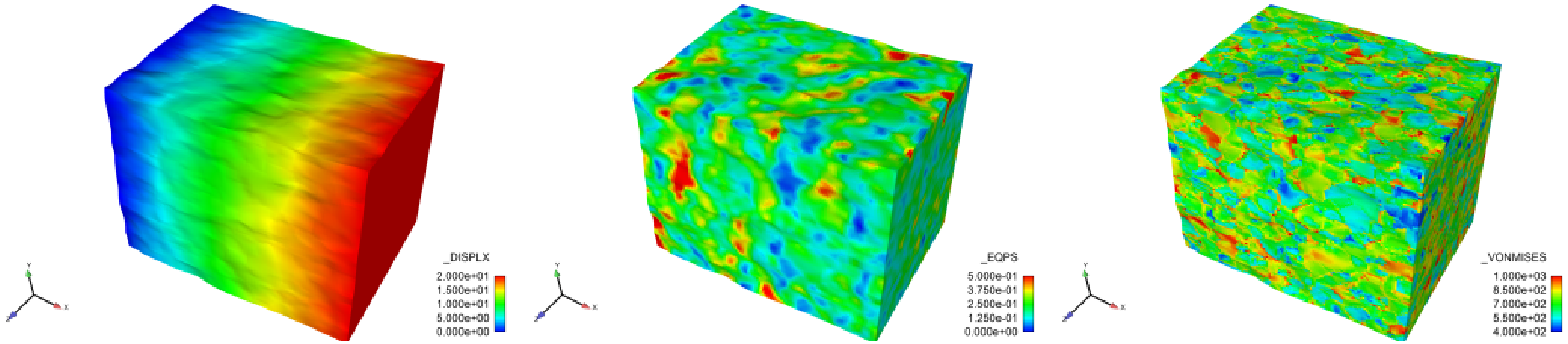


Avg. VM stress (MPa)
500
450
400
350
300
250
200
150
100
50
0
0
0.02
0.04
0.06
0.08
0.1
ϵ_{xx} (%)
J2
Crystal plasticity

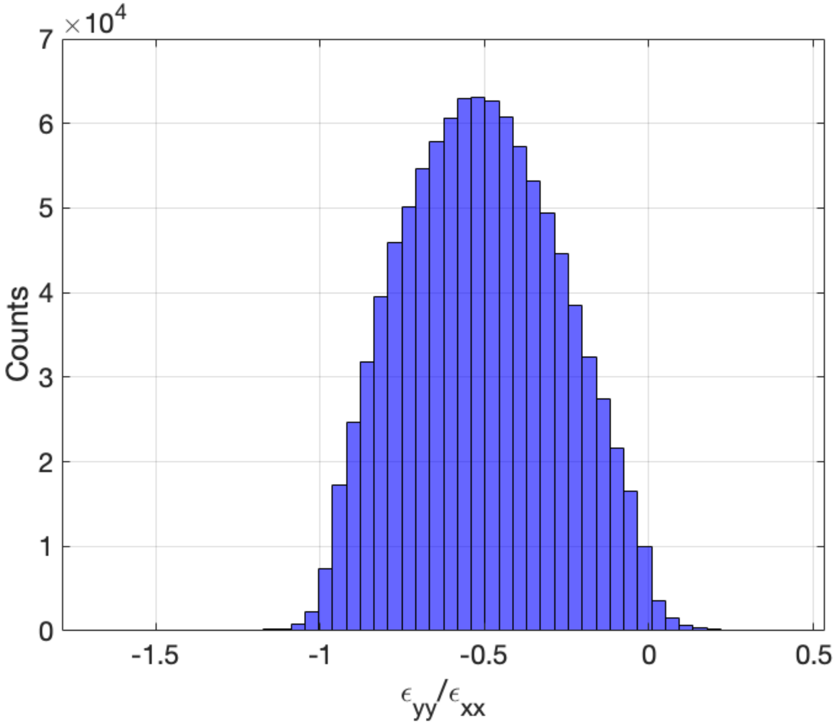
(b)

Check boundary conditions for polycrystalline deformation

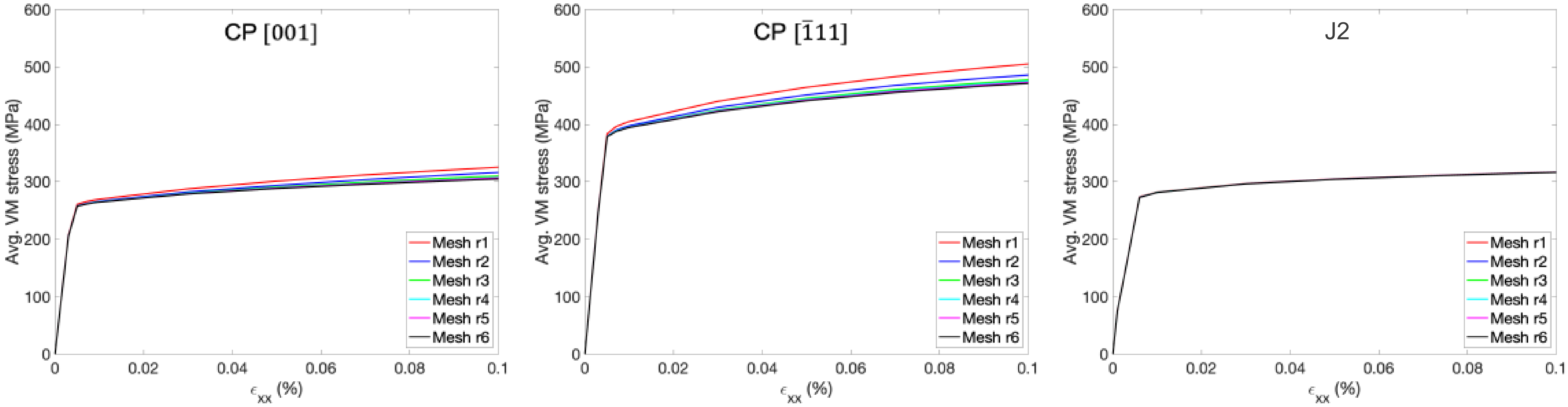




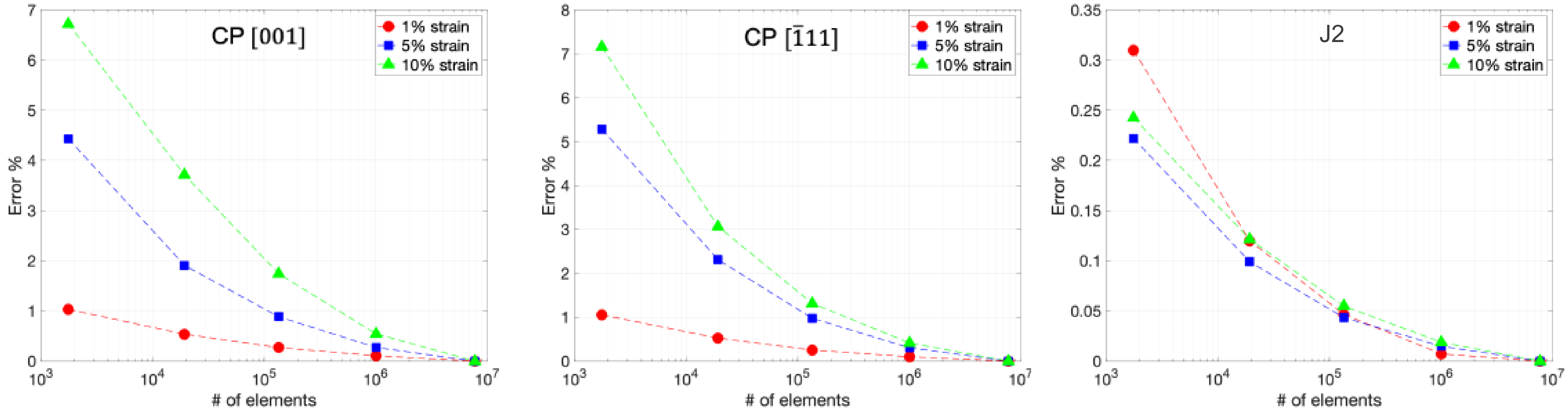
$$\varepsilon_{avg.} = \begin{bmatrix} 0.0953 & -0.0002 & -0.0002 \\ -0.0002 & -0.0486 & 0.0011 \\ -0.0002 & 0.0011 & -0.0447 \end{bmatrix}$$



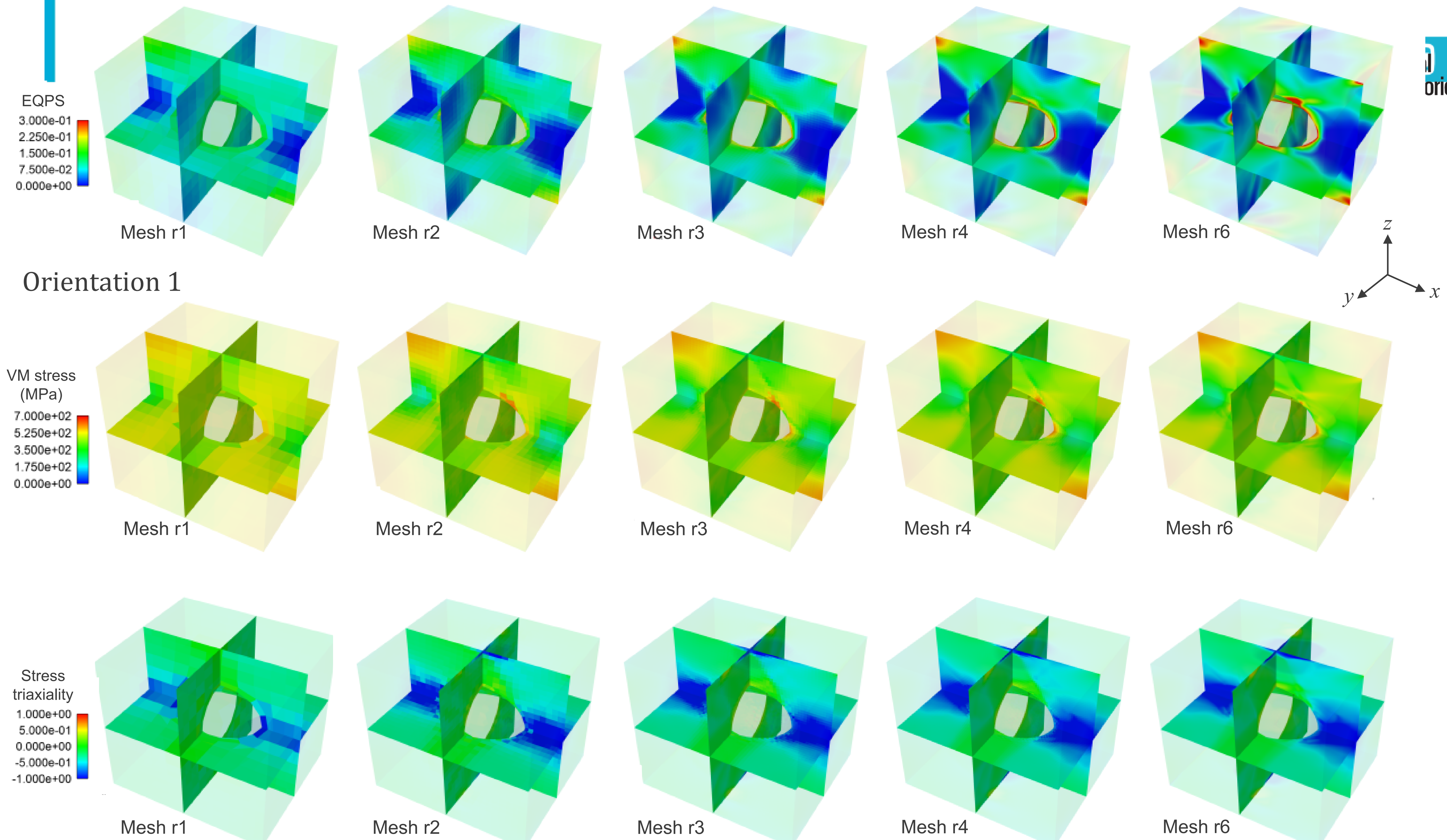
Mesh sensitivity



(a)



(b)


EQPS
3.000e-01
2.250e-01
1.500e-01
7.500e-02
0.000e+00
Mesh r1
Mesh r2
Mesh r3
Mesh r4
Mesh r6
Orientation 1
VM stress (MPa)
7.000e+02
5.250e+02
3.500e+02
1.750e+02
0.000e+00
Mesh r1
Mesh r2
Mesh r3
Mesh r4
Mesh r6
Stress triaxiality
1.000e+00
5.000e-01
0.000e+00
-5.000e-01
-1.000e+00
Mesh r1
Mesh r2
Mesh r3
Mesh r4
Mesh r6
z
y
x

GP fundamentals

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Let $\mathcal{D}_n = \{\mathbf{x}_i, y_i\}_{i=1}^n$ denote the set of observations and $\mathbf{x}$ denote an arbitrary test points

$$\mu_n(\mathbf{x}) = \mu_0(\mathbf{x}) + \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}(\mathbf{y} - \mathbf{m}) \quad (1)$$

$$\sigma_n^2(\mathbf{x}) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{k}(\mathbf{x}) \quad (2)$$

where $\mathbf{k}(\mathbf{x})$ is a vector of covariance terms between $\mathbf{x}$ and $\mathbf{x}_{1:n}$, $\mathbf{K}$ is the *covariance matrix*.

GP fundamentals

- assuming stationary kernel $\rightarrow k(\mathbf{x}, \mathbf{x}')$ only depends on $r = ||\mathbf{x} - \mathbf{x}'||$
- the covariance matrix: symmetric positive semidefinite matrix made up of pairwise inner products

$$\mathbf{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i) = \mathbf{K}_{ji} \tag{3}$$

- kernel choice: smoothness assumption, e.g. $\mathcal{C}^\infty$

Matérn kernels:

$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j) = \theta_0^2 \frac{2^{1-\nu}}{\Gamma(\nu)} (\sqrt{2\nu} r)^\nu K_\nu(\sqrt{2\nu} r), \tag{4}$$

K_ν is a modified Bessel fuction of the second kind and order ν.

Common kernels:

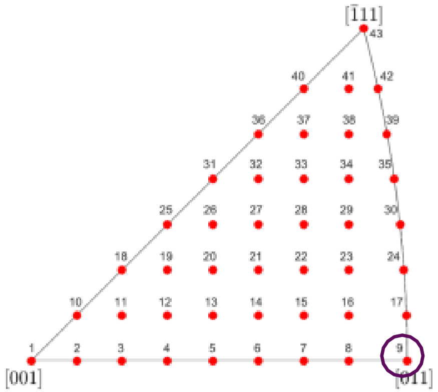
- $\nu = 1/2$ (very rough): $k_{\text{Matérn}1/2}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp(-r)$
- $\nu = 3/2$: $k_{\text{Matérn}3/2}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp(-\sqrt{3} r)(1 + \sqrt{3} r)$,
- $\nu = 5/2$: $k_{\text{Matérn}5/2}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp(-\sqrt{5} r)\left(1 + \sqrt{5} r + \frac{5}{3} r^2\right)$,
- $\nu \rightarrow \infty$ (very smooth): $k_{\text{sq-exp}}(\mathbf{x}, \mathbf{x}') = \theta_0^2 \exp\left(-\frac{r^2}{2}\right)$

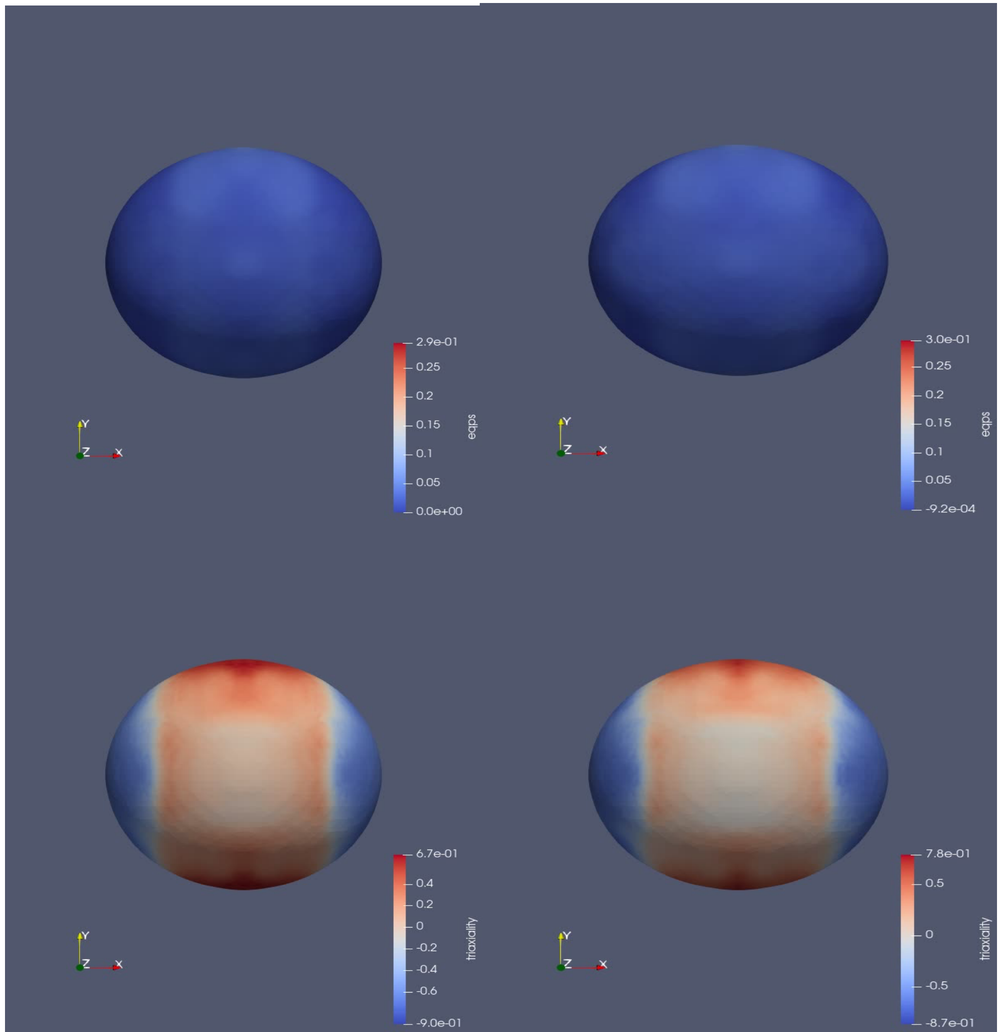
Log (marginal) likelihood function:

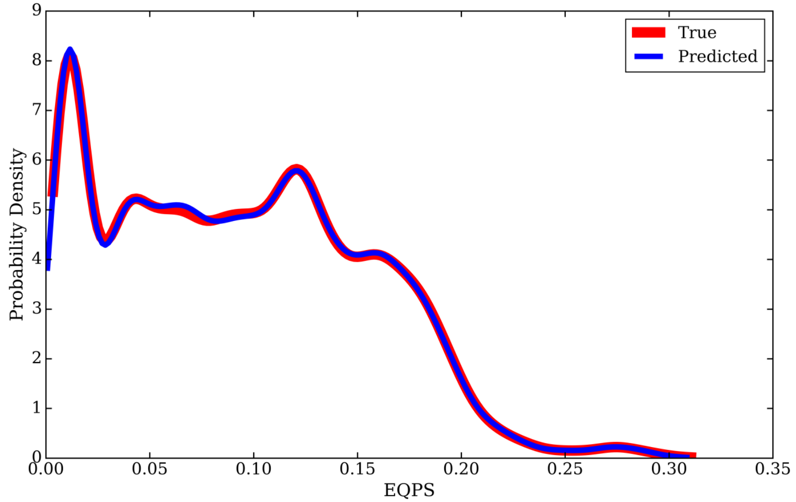
$$\log p(\mathbf{y}|\mathbf{x}_{1:n}, \theta) = -\underbrace{\frac{n}{2}\log(2\pi)}_{\text{data likelihood } \downarrow \text{ as } n\uparrow} - \underbrace{\frac{1}{2}\log|\mathbf{K}^\theta + \sigma^2 \mathbf{I}|}_{\substack{\text{“complexity” term} \\ \text{smoother covariance matrix}}} - \underbrace{\frac{1}{2}(\mathbf{y} - \mathbf{m}_\theta)^T (\mathbf{K}^\theta + \sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \mathbf{m}_\theta)}_{\substack{\text{“data-fit” term} \\ \text{how well model fits data}}} \tag{5}$$

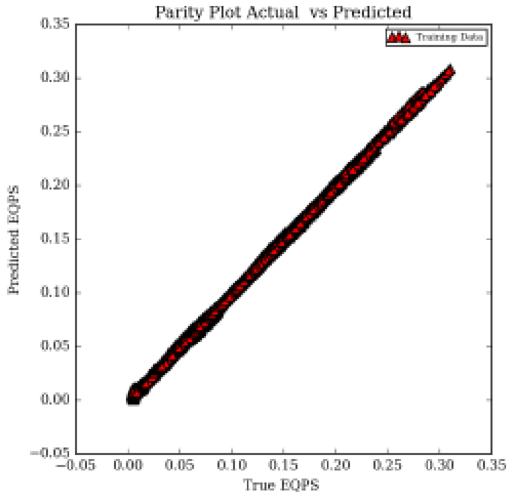
Results: Interpolating in Time

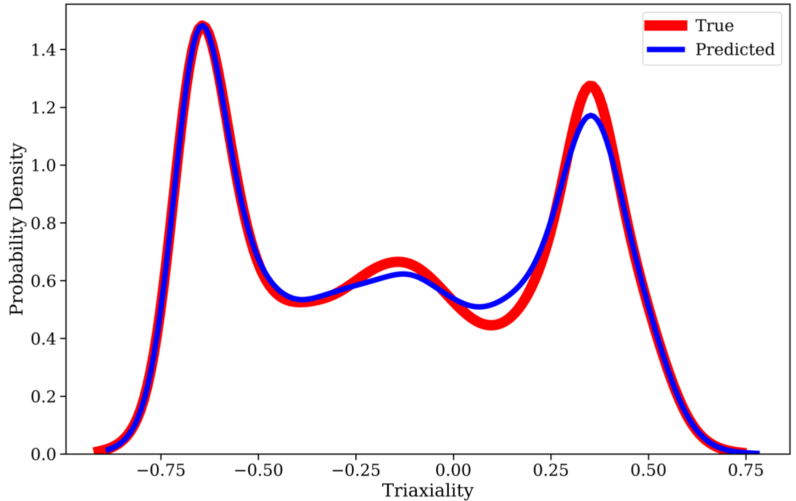
- Orientation 9:
  - Evolution EQPS (top) and triaxiality (bottom).
  - Comparing true (left) vs. predicted (right).

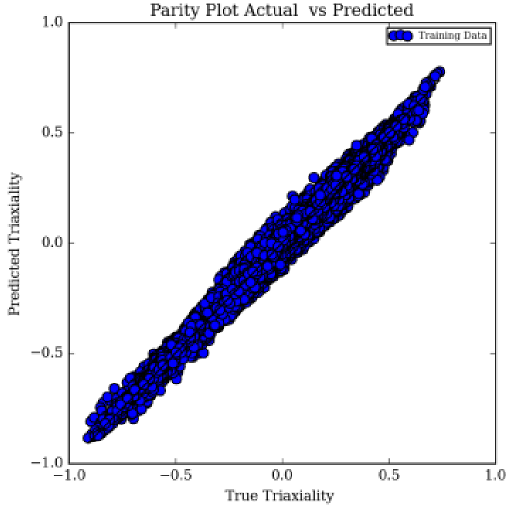












Results with 43 orientations.

$$f(\varphi 1, phi, phi2, t) = eqps, vm, triaxility$$

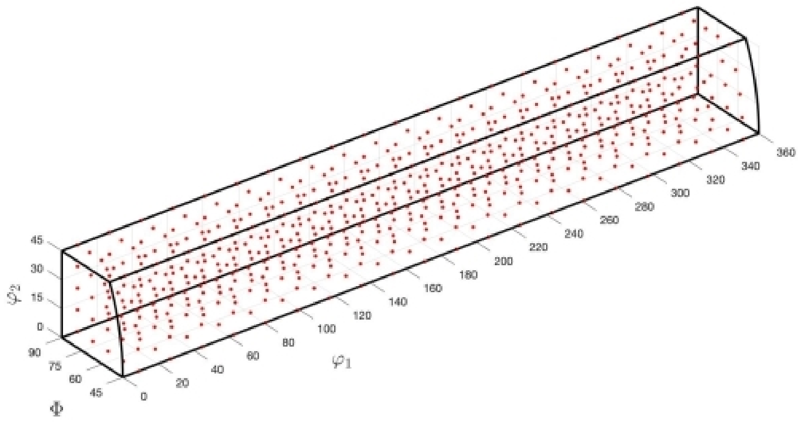
Training on ~600 and testing on ~500

$f(phi1, phi, phi2, t) = eqps, vm, triaxility$ in training (results next week)

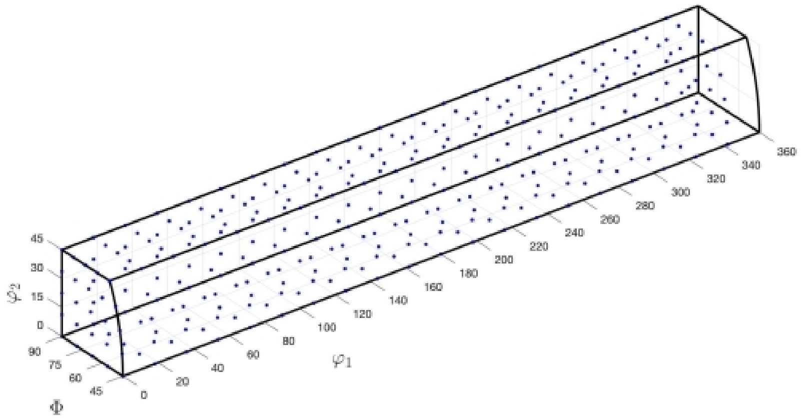
$f(GSH\_2, GSH\_3, GSH\_4, t) = eqps, vm, triaxility$ (will start running now) plus to present

Generate 1000 new orientations (with their GSH)
Run them on the trained model and just identify the 95^{th} percentile of most uncertain.

Expanding model to interpolate in texture space

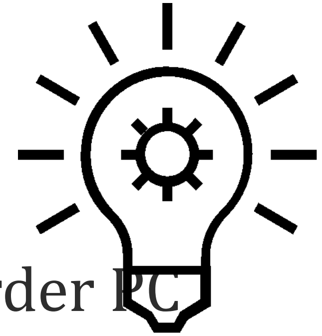


- Sample the Fundamental Zone of Cubic Crystals with 1100 orientations.
  - 650 within the FZ
  - 450 at the Bounding Surfaces



Structure-Property Linkage: GPR Details

- Connect the GSH coefficients to the PC components for EQPS and Triaxiality using Gaussian Processes Regression (GPR).
    - 1100 orientations (10 snapshots between 0 and 10% deformation).



- Normalize the output to [-1,1] in order to be able to better predict higher order PC Components.
- We will fit an individual GP for each individual QoI (i.e., the PCA of EQPS and triaxiality) .
- A squared exponential kernel with constant noise was used for each GPR