Reduced Order Representation of Crystallographic Texture for Surrogate Modelling and Uncertainty Quantification

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Motivation

Process

Process parameters

From welding, forming, additive manufacturing etc.

CFD
Finite Volume

Structure

Material microstructure

Texture, grain size and morphology, phase composition etc.

Crystal plasticity
Phase field
Finite element analysis

Property

Macroscopic quantities of interest

Monotonic/cyclic stress strain behaviour, yield surface, fatigue indicators etc.

Finite element analysis
Assessment codes

- Fatigue damage
- Creep damage
- Weld residual stress modelling
- Etc.

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Process

Process parameters

From welding, forming, additive manufacturing etc.

Structure

Grainsize

Crystallographic texture

Morphology

Property

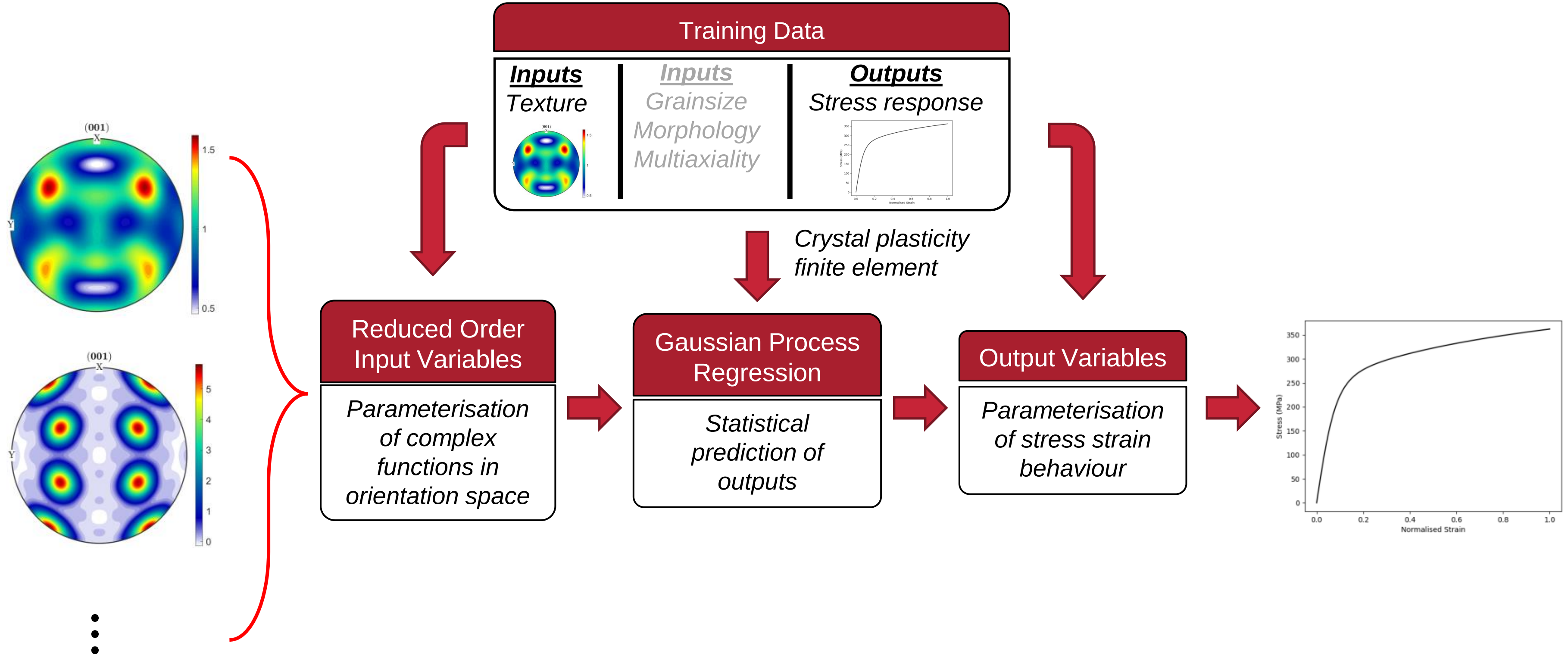
Crystal plasticity finite element analysis

Macroscopic quantities of interest

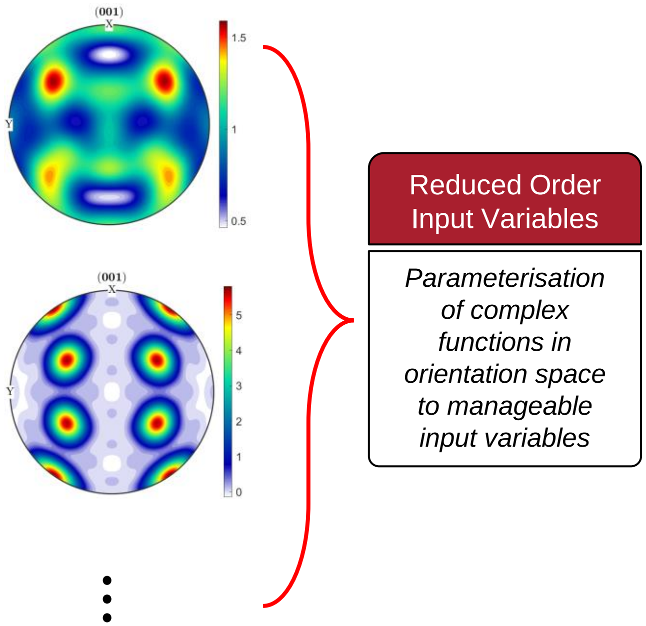
Monotonic/cyclic stress strain behaviour, yield surface, fatigue indicators etc.

- Fatigue damage
- Creep damage
- Weld residual stress modelling
- Etc.

Summary of Modelling Approach



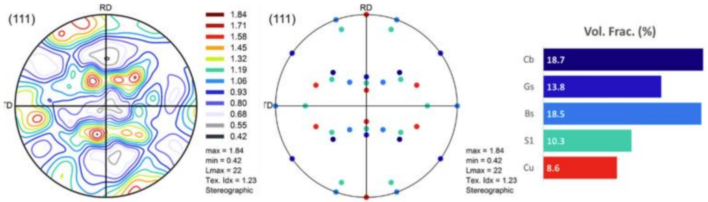
Parameterisation of Crystallographic Texture



- Objective is to reduce the **orientation distribution function** to a **small number of input parameters** for the surrogate model.
- Options include **generalised spherical harmonics (GSH), Rodrigues parameterisation**, binning orientations in **Euler angle** space etc.
- To appropriately capture variance in texture these require far too many input variables.
- The problem is they **over generalise** densities in the orientation distribution function they can represent.

Parameterisation of Crystallographic Texture

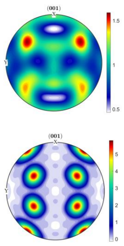
Actually only interested in narrow subset of **physically possible** orientation distribution functions.[1]



<u>Principal component analysis (PCA) linear transformation</u>

$$\mathbf{S} = \mathrm{Cov}(x_i, x_j) = \mathbb{E}[(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j])]$$

$$\mathbf{S}\mathbf{a} = \lambda \mathbf{a}$$



Texture observations

Generalised Spherical Harmonics (GSH)

GSH components (>10000)

$$\begin{pmatrix} & \cdots & \\ \vdots & \ddots & \vdots \\ & \cdots & \end{pmatrix}$$

Texture observations

Principal Component Analysis (PCA)

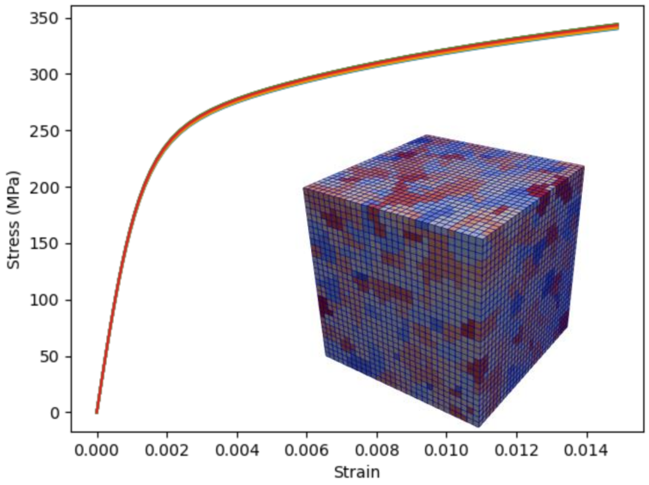
Most influential PCA components (~10)

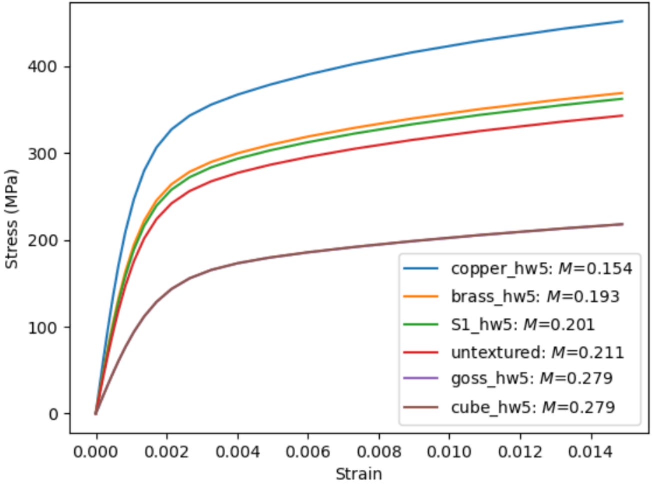
$$\begin{pmatrix} & \cdots & \\ \vdots & \ddots & \vdots \\ & \cdots & \end{pmatrix}$$

1. Mokhtarishirazabad, M., McMillan, M., Vijayanand, V.D., Simpson, C., Agius, D., Truman, C., Knowles, D. and Mostafavi, M., 2023. Predicting residual stress in a 316L electron beam weld joint incorporating plastic properties derived from a crystal plasticity finite element model. *International Journal of Pressure Vessels and Piping*, *201*, p.104868.

Creating the Training Dataset

- Sufficiently large RVE shows **limited spread** in resulting stress strain curves.
- Morphology kept consistent and only **texture is changed** by sampling new orientations for each grain.
- Curves shown here all for an untextured, equiaxed RVE.

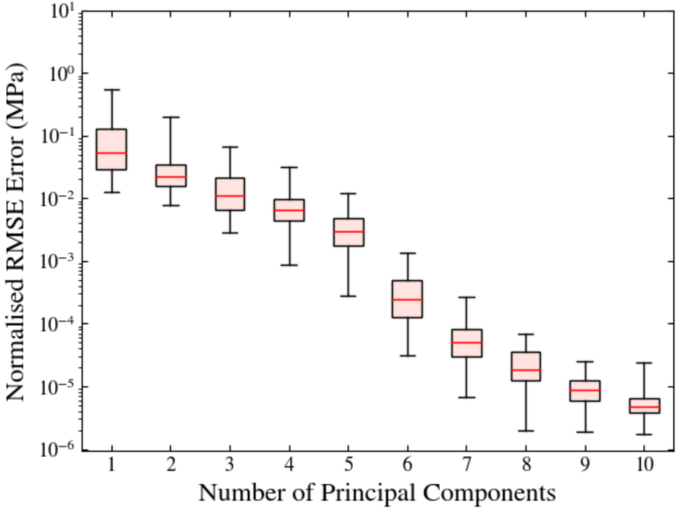


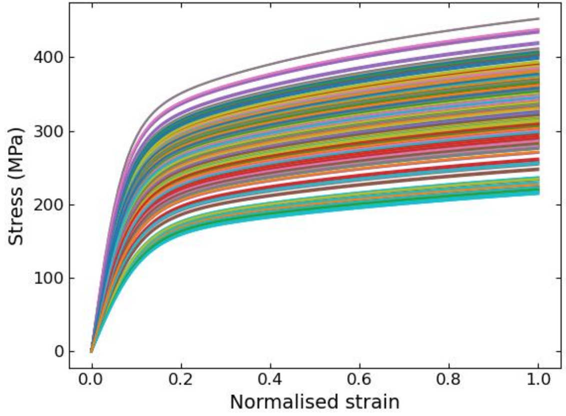


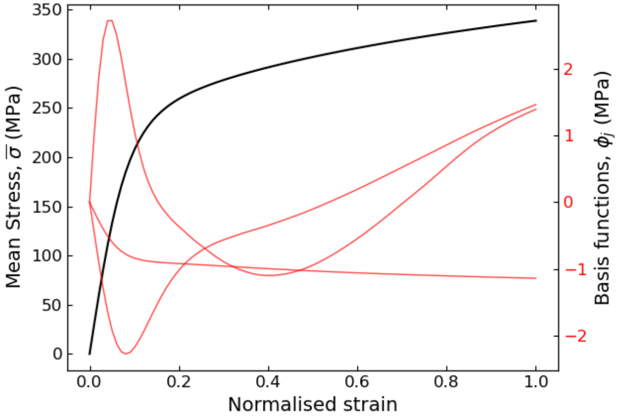
Gaussian Process Model Outputs (Functional Principal Component Analysis

Functional principal component analysis (fPCA) allows parameterisation of the stress-strain curve by scalar fPCA scores:

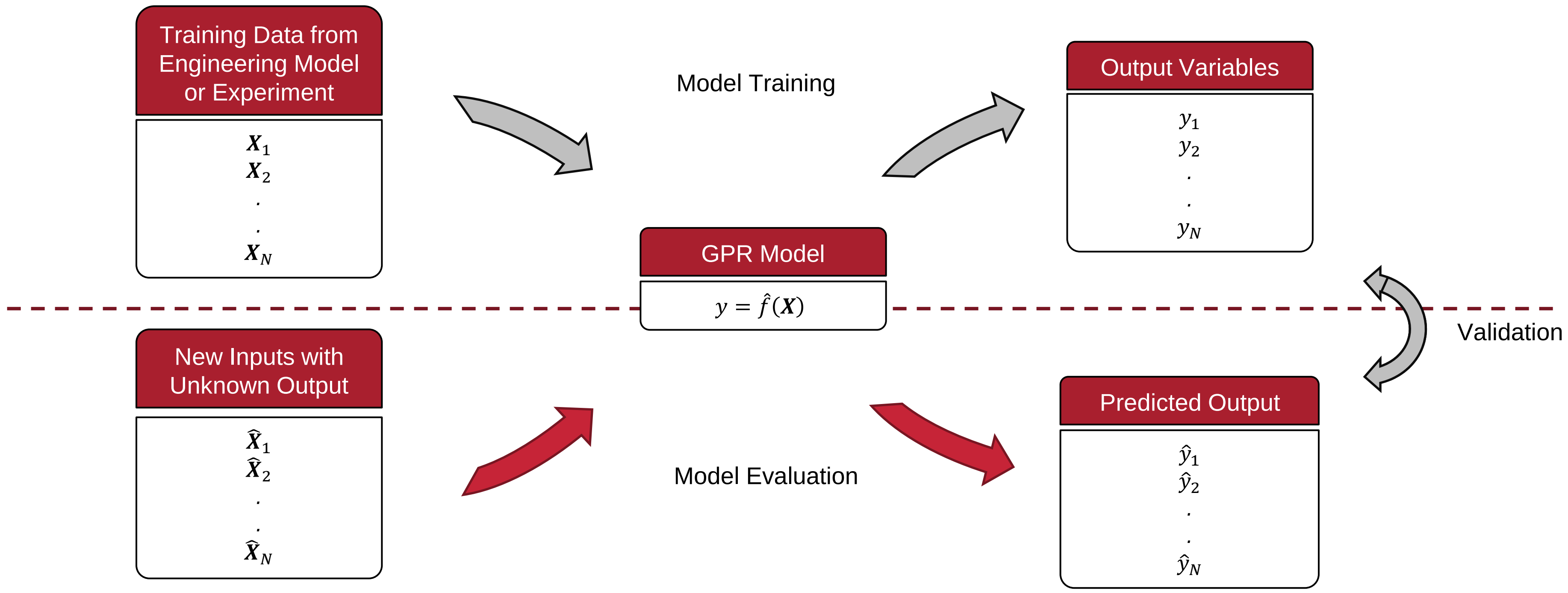
$$\sigma_i(\varepsilon') \approx \overline{\sigma}(\varepsilon') + \sum_{j=1}^{J} c_{ij}\phi_j(\varepsilon')$$







Gaussian Process Regression



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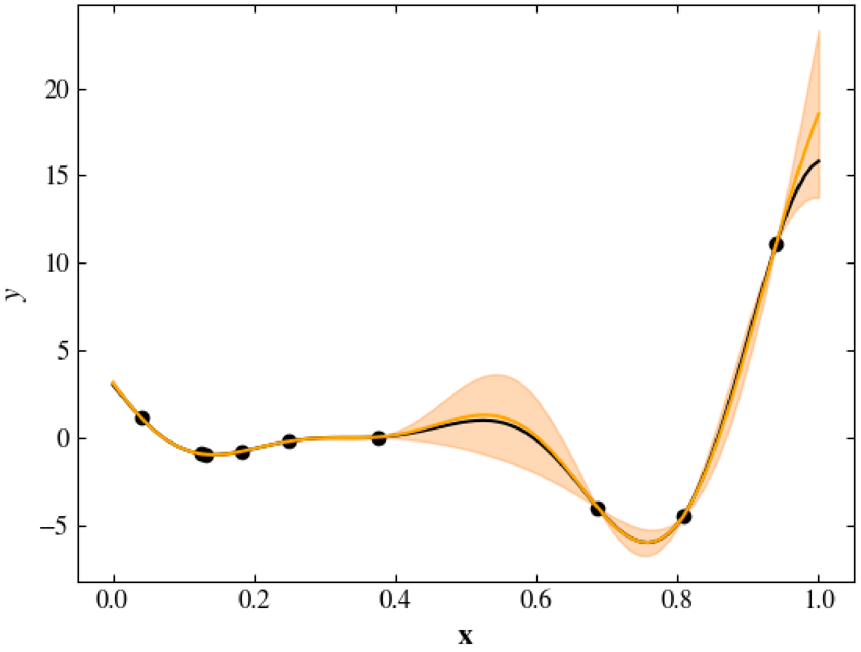
Gaussian Process Regression

Predicts a **conditional probability** at each point giving an estimate for the output value and **a variance**.

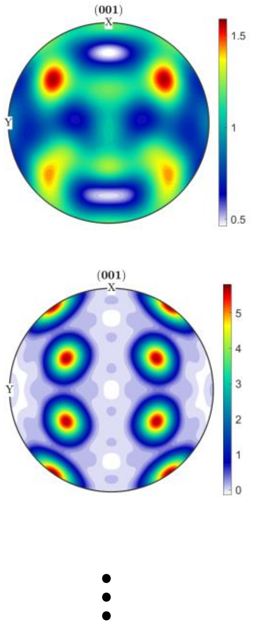
Relationship between points described by a **kernel function**:

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{1}{2\ell}|\mathbf{x} - \mathbf{x}'|^2\right)$$

This determines the effect of any two points on each other.



Summary of Modelling Approach



Training Data

Inputs	***Inputs***	***Outputs***
Texture	*Grainsize*	*Stress response*
	Morphology	
	Multiaxiality	

Crystal plasticity finite element

Reduced Order Input Variables

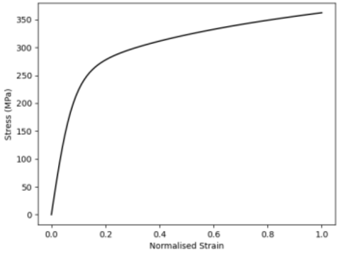
Parameterisation of complex functions in orientation space

Gaussian Process Regression

Statistical prediction of outputs

Output Variables

Parameterisation of stress strain behaviour



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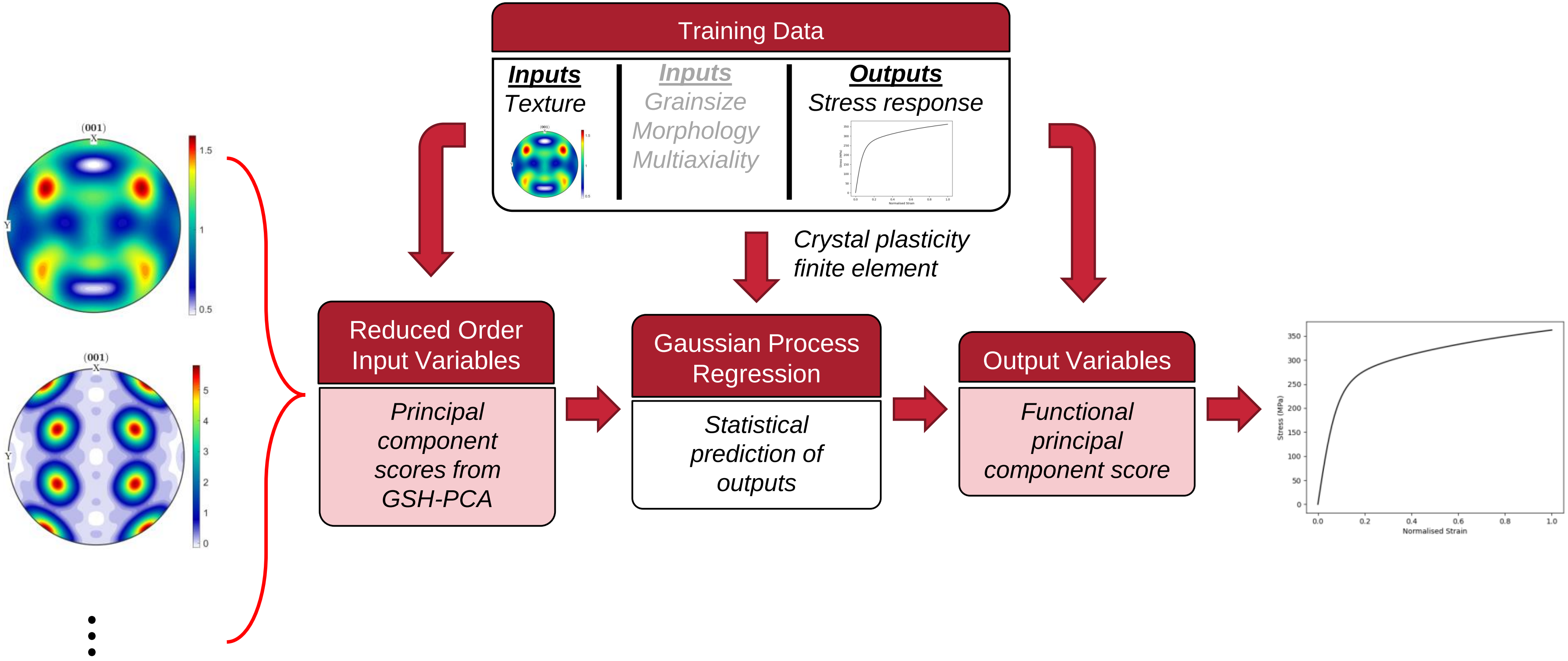
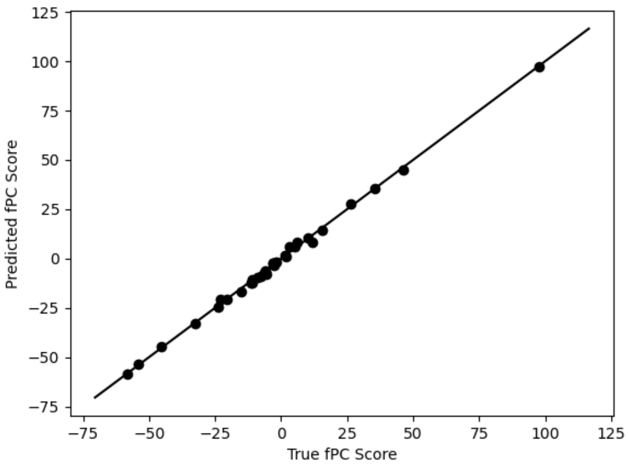
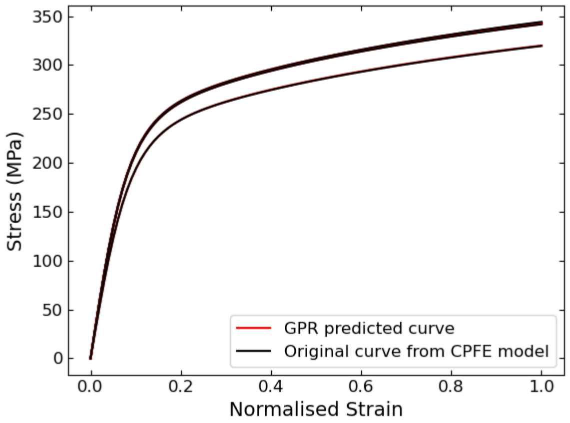


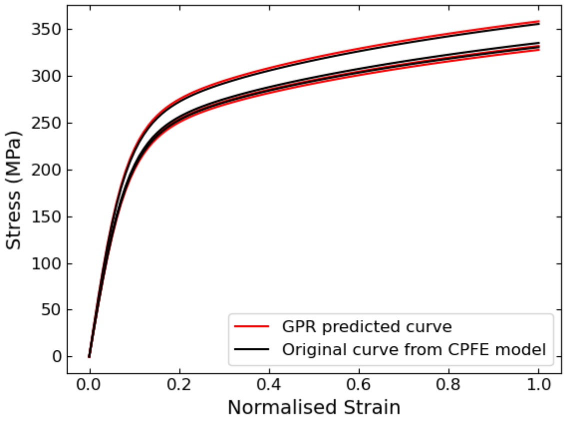
Results from Gaussian Process Prediction

- 750 different textures are used to train the GPR model.
- 32 textures are kept aside at random to validate the GPR model:





Best performing predictions



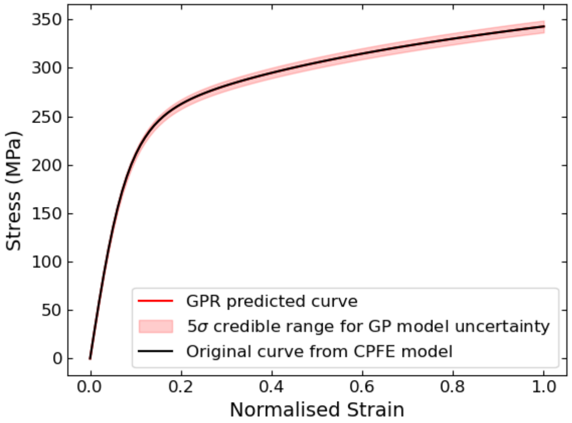
Worst performing predictions

Results including Model Uncertainty

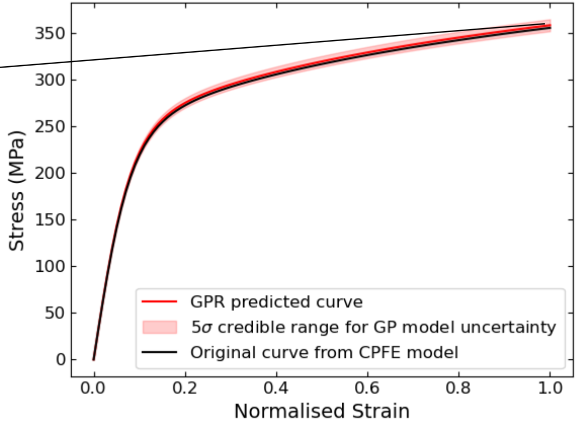
- Uncertainties can be propagated through the fPCA representation of the stress strain curve to visualise variance across the domain.

$$\sigma^2(\varepsilon') = \hat{\sigma}_\mu^2(\varepsilon') + \sum_{j=1}^{J} \sigma_j^2 \phi_j^2(\varepsilon') + \hat{\sigma}_\epsilon^2$$

- Model uncertainty for 5σ credible range equivalent to ± 6.1 MPa at maximum.



Best performing prediction



Worst performing prediction

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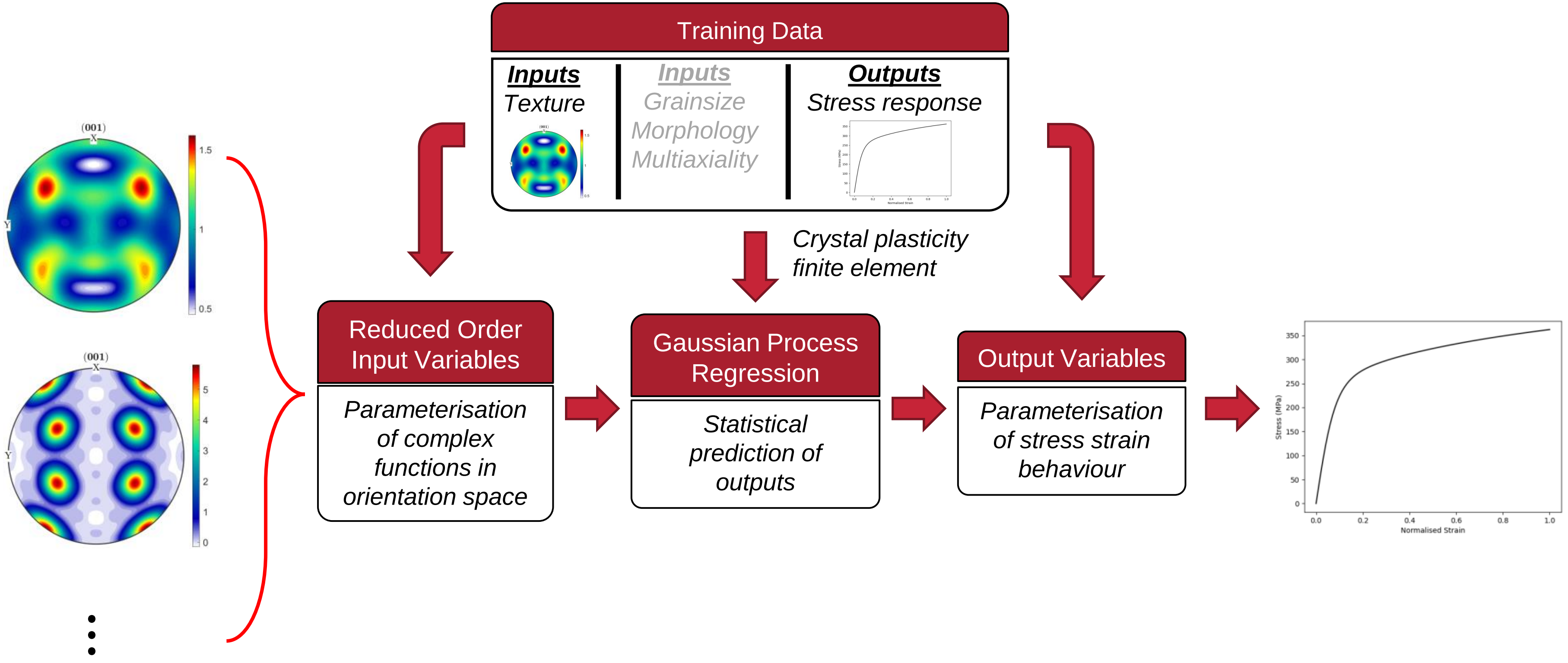

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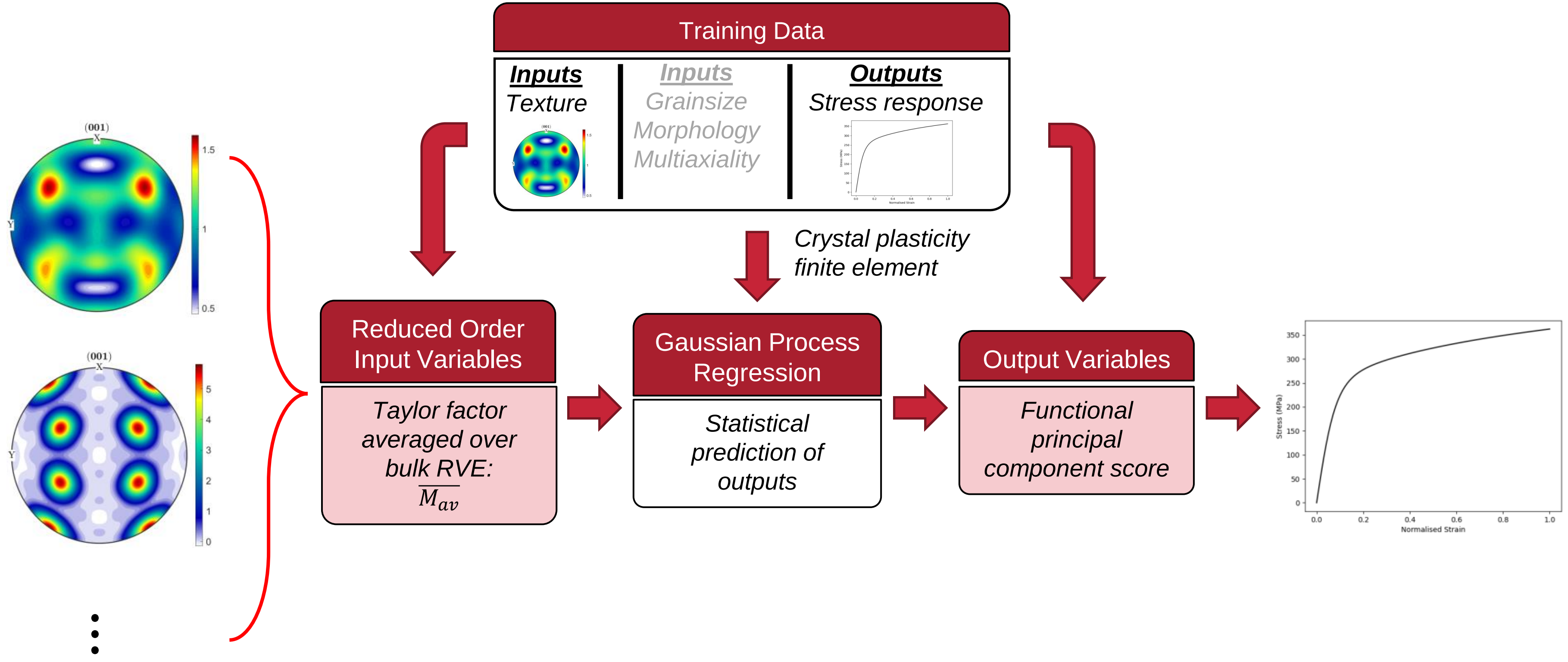
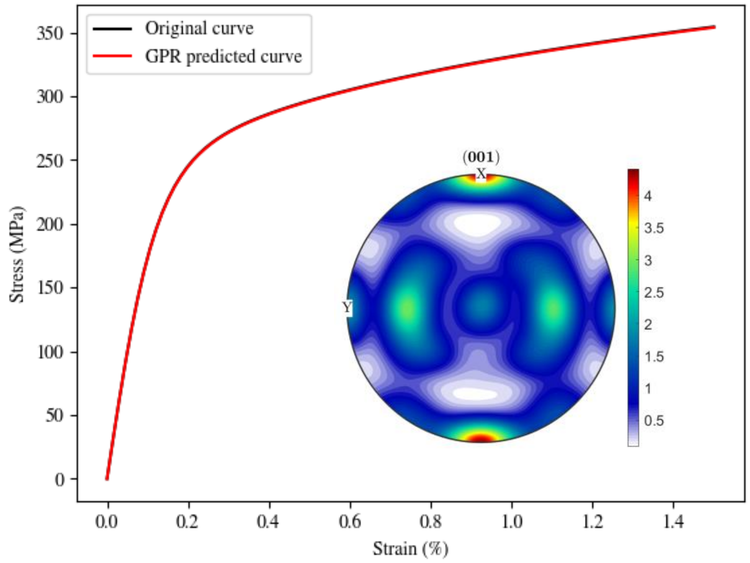
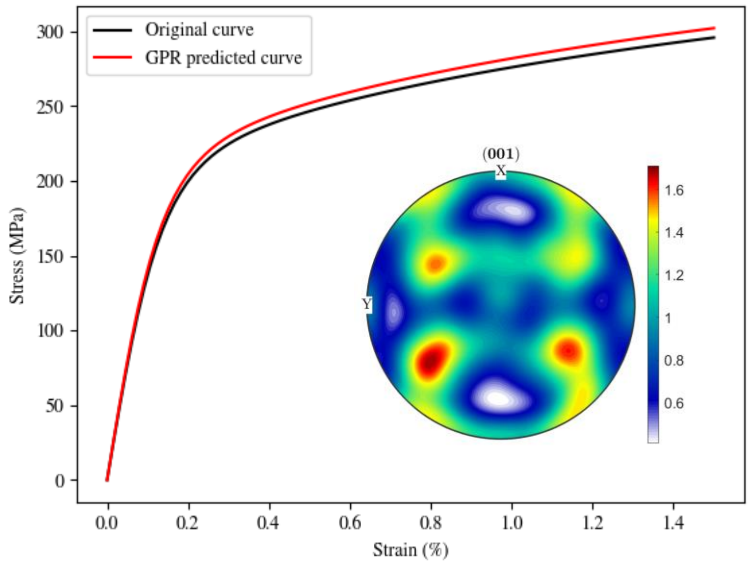


Results from Gaussian Process Prediction from Taylor Factor



Best performing prediction



Worst performing prediction

Summary

- This framework demonstrates an example of surrogate modelling for **process-structure-property** linkages.

- Can act **alongside physical models** to provide **uncertainty quantification**.

- These methods (PCA, fPCA, GP) **generalisable** to other physical models and processes.

- Requires consideration of important **engineering parameters** rather than using hidden latent parameters.

Future Work

- Comparison of Taylor factor and GSH-PCA parameterisations.
- Quantification and propagation of uncertainties related to variation in texture across a feature, experimental uncertainty, omitted variables (such as grain misorientation).
- Application to microstructures indicative of welded features to feed into macroscopic weld FE models.
- Inclusion of grainsize and morphology into the model inputs.

Thank you for your attention

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Gaussian Process Regression

Gaussian process regression predicts a conditional probability at each testing datapoint therefore giving an **estimate for the output value and a variance** at each point:

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{y}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X,X) & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{bmatrix}\right)$$

The relationship between points in the input variable space can be described by a **kernel function**:

$$k(\mathbf{x},\mathbf{x}') = \sigma_f^2 \exp\left(-\frac{1}{2\ell}|\mathbf{x}-\mathbf{x}'|^2\right)$$

Model evaluation is done by considering the conditional probability of the multivariate Gaussian:

$$\mathbf{y}_*|X_*,X,\mathbf{y} \sim \mathcal{N}(K(X_*,X)K(X,X)^{-1}\mathbf{y},$$
$$K(X_*,X_*) - K(X_*,X)K(X,X)^{-1}K(X,X_*))$$