Uncertainty Quantification in Multiscale Deformation Processes

Nicholas Zabaras
Materials Process Design and Control Laboratory
Sibley School of Mechanical and Aerospace Engineering
101 Rhodes Hall
Cornell University
Ithaca, NY 14853-3801
Email: zabaras@cornell.edu
URL: http://mpdc.mae.cornell.edu/
Outline

- Introduction

- Uncertainty Quantification at a Material Point
  - Microstructure Model Reduction Strategies
  - Constructing a Reduced Surrogate Microstructure Space
  - Stochastic PDE Solver – Computing Properties
  - Applications

- Multiscale Microstructure Model Reduction and Uncertainty Quantification of Multiscale Problems

- Summary
Goal: quantifying property variability of materials due to microstructure uncertainty.
- (Initial) Microstructures of engineering materials are random.
- Properties of the material/product are microstructure dependent.
- Uncertainty quantification is important.

Challenge:
- High dimensional stochastic input.
- Time consuming stochastic/deterministic simulation.

Strategy:
- Model reduction techniques.
- Efficient SPDE solver.
- Robust physical solver.
Uncertainty Sources

**Macroscale uncertainties**
- Initial and boundary conditions (e.g. Die shape)
- Dual microstructures
- Process parameters:
  - Temperature
  - Strain rate
  - etc.

**Mesoscale uncertainties**
- Topology
- Two-phase features
- Orientation
- Model Parameters: CRSS, etc.

**Microscale uncertainties**
- Particle size/volume fraction
- Particle shape
- Dislocation configuration
- Parameters: APB energy, etc.

Uncertainty propagation
Uncertainty Quantification at a Material Point
Problem Definition

Problem definition

Given:
- Microstructure samples

Goal:
- Distributions of microstructure properties.
- Convex hull of microstructure properties.

Methodologies

- Model reduction to reduce the dimensionality of stochastic input.
- Evaluate the probability density of the reduced microstructure representation variables,
- PCE or Maximum Entropy to map reduced coordinates to a known distribution.
- Monte Carlo, Adaptive sparse grids and Bayesian regression to solve the underlying stochastic partial differential equations.
Overview

Microstructure space

START: Extract microstructural features

Low-dimensional space

Low-D points

Model reduction

Feature reconstruction

Low-D representation reconstruction

Sample from hypercube

Low-D space Map to hypercube

Unit hypercube

Property variability

Property convex hull

Property distribution

END

Database

Reconstruct microstructures

Solve SPEDs

Obtain Properties

Property convex hull

END

Property distribution

Solve SPEDs

Obtain Properties

Database

Reconstruct microstructures
Model Reduction at One Material Point

KLE, KPCA, Manifold Learning
A probability space \((\Omega, F, P)\) with sample space \(\Omega\), corresponding to all microstructures resulted from certain random process, \(F \subset 2^\Omega\), being the \(\sigma\)-algebra of subsets in \(\Omega\), and \(P : F \rightarrow [0,1]\), as the probability measure.

Each sample \(\omega \in \Omega\) is a random microstructure which can be described by a discretized representation \(y(\omega) = (y_1, \ldots, y_M)^T : \Omega \rightarrow Y \in \mathbb{R}^M\).

The input space information is only given as a set of samples \(y_i, i = 1, \ldots, N\).

The variability of a microstructure sensitive property \(A = A(y)\) of the given input space is of interest.

It is necessary to construct the input space that has the same statistical properties with the given samples. Since the input space is high-dimensional, model reduction is needed: construct a low-dimensional surrogate microstructure space.
Karhunen-Loeve Expansion

- Microstructure (feature) samples:

- Construct covariance matrix of these samples

\[
\tilde{C} = \frac{1}{N-1} \sum_{i=1}^{N} (y_i - \bar{y})^T (y_i - \bar{y}), \quad \bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i
\]

- The truncated Karhunen-Loeve Expansion of a random vector \( y \) is

\[
y(\omega) = \bar{y}(\omega) + \sum_{i=1}^{d} \sqrt{\lambda_i} \phi_i(\omega) \xi_i(\omega)
\]

where \( \phi_i, \lambda_i \) are the \( i \)th eigenvector and eigenvalue of \( \tilde{C} \), respectively. \( \{\xi_i(\omega)\} \) are a set of uncorrelated random variables satisfying

\[
E(\xi_i(\omega)) = 0, \quad E(\xi_i(\omega)\xi_j(\omega)) = \delta_{ij}, \quad i, j = 1, \ldots, d
\]

Random field is thus transformed to a low-dimensional space \( \xi \in \mathbb{R}^d \)
In general, the components of the stochastic input $y \in \mathbb{R}^M$ are not linearly related.

PCA/KLE attempt to approximate the data with a linear surface (plane) such that reconstruction error is minimized. This in general is not very appropriate – non linear model reduction is needed.

Solution: nonlinearly map the given samples to a feature space $F$, where PCA performs better.

For PCA, $\Phi(y) = y$
Covariance matrix in the feature space:

\[
C\Phi \frac{1}{N} \sum_{i=1}^{N} \tilde{y}(i) \sim (i)^T = \tilde{\Phi} = \Phi(y) - \Phi
\]

Eigenvalue problem:

\[
CV = \lambda V
\]

KL expansion:

\[
\Phi(y) = \sum_{i=1}^{M_F} \sqrt{\lambda_i} V_i \eta_i + \bar{\Phi} = \sum_{i=1}^{M_F} z_i V_i + \bar{\Phi}
\]

Reformulate the eigenvalue problem using the ``kernel trick’’:

\[
\tilde{K}U \tilde{A} \tilde{U} \quad \text{where} \quad \tilde{K} \Phi \tilde{K}_j = \left(\tilde{\Phi}(y_i) \cdot \tilde{\Phi}(y_j)\right)
\]

\[
U \alpha = [\alpha_1, \alpha_\alpha, \ldots, \alpha_N]
\]

\[
\tilde{\Lambda} = \text{diag} \left(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_N\right)
\]

The eigenbasis of the covariance matrix \( C \) is projected to the given samples by

\[
V_i \Phi = \sum_{j=1}^{N} \tilde{\alpha}_{ij} \sim (j) = \Phi \sum_{j=1}^{N} \frac{\alpha_{ij}}{\sqrt{\tilde{\lambda}_i}} \sim (j)
\]
PCA/KPCA Formulation

Any sample in F: \[ \Phi(y) = \sum_{i=1}^{N} z_i \mathbf{V}_i + \Phi \approx \sum_{i=1}^{r} z_i \mathbf{V}_i + \Phi = \sum_{i=1}^{N} \beta_i \Phi(y_i) \]

where \[ \beta = AZ + \frac{1}{N} \quad A = \mathbf{H} \mathbf{U}_r \alpha = \left( \mathbf{I} - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right) \left[ \tilde{\alpha}_1, \ldots, \tilde{\alpha}_r \right] \quad Z = [z_1, \ldots, z_r]^T \]

Reduced representation:

\[ z_i = V_i \Phi \tilde{y}(\cdot) = \sum_{j=1}^{N} \tilde{\alpha}_{ij} \Phi \tilde{y}(\cdot) \Phi \tilde{y}(\cdot) = \sum_{j=1}^{N} \tilde{\alpha}_{ij} \tilde{K}(y, \cdot) \mathbf{k}^{T} \mathbf{H} \mathbf{k} y - \frac{1}{N} \mathbf{H} \mathbf{k} 1 \]

Gaussian Kernel: \[ K_{ij} = k(y_i, y_j) = \exp \left( -\frac{\|y_i - y_j\|^2}{2\sigma^2} \right) \]

In PCA \[ k(y_i, y_j) = y_i \cdot y_j \]

Construct reduced-order space by initial samples \( z_i \)

For each random sample \( \xi \) in the reduced space, we can obtain its corresponding high-dimensional counterpart (pre-image problem)
Pre-Image Problem

- Sample $\xi$, and find/approximate the input realization $y$

  Draw random sample $\xi$
  \[
  \text{PCA/KPCA}
  \]
  Construct high-D representation $\Phi(y)$
  \[
  \text{Pre-imaging}
  \]
  Recover microstructure feature $y$

K-nearest neighbor: $y \approx \hat{y} = \frac{\sum_{i=1}^{K} \frac{1}{d_i} y_i}{\sum_{i=1}^{K} \frac{1}{d_i}}$

Gauss kernel:
\[
d_i^2(\hat{y}, y_i) \Phi \| \hat{y} - \Phi y_i \|^2 = -2\sigma^2 \ln \left(1 - 0.5\tilde{d}_i^2 (\Phi(y), \Phi(y_i)) \right)
\approx -2\sigma^2 \ln \left(1 - 0.5\tilde{d}_i^2 (\Phi(y), \Phi(y_i)) \right)
\]

X. Ma and N. Zabaras, 2011
Given some experimental correlation that the microstructure/property variation satisfies.

Construct several plausible ‘images’ of the microstructure/property.

Each of these ‘images’ consists of, say, $n$ pixels.

Each image is a point in $\mathbb{R}^n$-dimensional space.

But each and every ‘image’ is related.

That is, all these images lie on a unique curve (manifold) in $\mathbb{R}^n$.

Can a low-dimensional parameterization of this curve be computed?

**Strategy:** based on a variant of the ‘manifold learning’ problem.
An Intuitive Picture of The Strategy

Given a set of $N$ unordered points belonging to a manifold $\mathcal{M}$ embedded in a high-dimensional space $\mathbb{R}^n$, find a low-dimensional region $\mathcal{A} \subset \mathbb{R}^d$ that parameterizes $\mathcal{M}$, where $d << n$.

Ensure that nearby points on the manifold map to nearby points in the low-dimensional space and faraway points map to faraway points in the low-dimensional space.

Linear approach

Non-linear approach: unraveling the curve
Key Concept

1) Geometry can be preserved if the distances between the points are preserved – Isometric mapping.

2) The geometry of the manifold is reflected in the geodesic distance between points.

3) First step towards reduced representation is to construct the geodesic distances between all the sample points.

Euclidian dist

Geodesic dist

Pt A

Pt B
Algorithm:

1) Compute the low-dimensional representation of a set of N unordered sample points belonging to a high-dimensional space.

Given N unordered samples → Compute pairwise geodesic distance → Perform MDS on this distance matrix → N points in a low dimensional space

2) For an arbitrary point \( \xi \in A \) must find the corresponding point \( y \in M \). Compute the mapping from \( A \rightarrow M \) based on k-nearest neighbors.

B. Ganapathysubramanian and N. Zabaras, 2008
Construction of Reduced Surrogate Space

Probability Density of the Reduced Order Microstructure Variables
Motivation

- After model reduction, a set of reduced representations/variables are obtained.

- The probability distribution of the reduced representation needs to be computed using the known data/realizations.

- Methodologies that map arbitrary distribution to a well-shaped distribution is needed.

- Strategies:
  - Polynomial Chaos expansion (PCE).
  - Maximum Entropy (MaxEnt).
Polynomial Chaos Expansion (PCE)

Map the reduced space to a known distribution.

\[ \xi_i = \sum_{j=0}^{p} \gamma_{ij} \psi_j(\eta_i), \quad i = 1, \ldots, r \]

Uniform-Legendre PCs

\[ \gamma_{ij} = \frac{E\left[ \xi_i \psi_j(\eta_i) \right]}{E\left[ (\psi_j(\eta_i))^2 \right]} = \frac{2j + 1}{2} \int_{-1}^{1} \xi_i \psi_j(\eta_i) d\eta_i, \quad i = 1, \ldots, r, \quad j = 0, \ldots, p \]

To compute the integral, a map between \( \xi_i \) and \( \eta_i \) is needed.

Mapping through CDF

\[ \xi_i = \Gamma_i(\eta_i), \quad \Gamma_i \equiv F_{\xi_i}^{-1} \circ F_{\eta_i} \]

where \( F_{\xi_i} \) and \( F_{\eta_i} \) are the CDFs of the two random variables, respectively.
Another way to construct the distribution of $\xi$ is Maximum Entropy Estimation.

**Maximum Entropy Estimation (MaxEnt):** amongst the probability distributions that satisfy our incomplete information about the system, the probability distribution that maximizes entropy is the least-biased estimate that can be made. It agrees with everything that is known but carefully avoids anything that is unknown.

The form of MaxEnt distribution is

$$p^*(x) = \frac{e^{-\sum_{n=1}^{N} \lambda_n f(x)}}{Z}, \quad Z = \int e^{-\sum_{n=1}^{N} \lambda_n f(x)} \, dx$$

which maximize the entropy

$$H(p) = -\sum_{i=1}^{M} p(x_i) \log(p(x_i))$$

and satisfies constraints

$$E(f_n(x)) = M_n, \quad n = 1, 2, ...$$

When the uncorrelated constraints are satisfied, the MaxEnt distribution is a standard Gaussian distribution

$$\xi \sim N(0, I)$$
Inverse CDF Transformation

Uncorrelated Gaussian random variables are independent in current case. To employ Sparse Grid Collocation method, Gaussian distribution needs to be transformed to a uniform hypercube \([0,1]^d\).

The cumulative distribution function (CDF) for standard Gaussian is

\[
\Phi_{\xi_i}(\xi_i) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\xi_i}{\sqrt{2}} \right) \right]
\]

which is uniformly distributed in \([0,1]\).

Given a point in the hypercube \(\zeta \in [0,1]^d\), we can also find a corresponding point in the original distribution by

\[
\xi_i = \Phi^{-1}(\xi_i), \quad i = 1, \ldots, d
\]

This process transforms a node in sparse grid back to a point in Gaussian distribution, and it can be further recovered to a texture realization.
Stochastic Partial Differential Equation Solver

Adaptive Sparse Grid Collocation
Sparse grid collocation is an effective method to solve SPDEs. It approximates the multi-dimensional stochastic space using interpolating functions on a set of collocation points. The collocation method collapses the multi-dimensional problem to solving $M$ ($M$ is the number of collocation points) deterministic problems.

Denote the one dimensional interpolation form: $U^i(f) = \sum_{j=1}^{m_i} f(Y^i_j) \cdot a^i_j$

In high dimensions, a simple case is the tensor product formula

$$
(U^i \otimes \cdots \otimes U^i_N)(f) = \sum_{j_1=1}^{m_1} \cdots \sum_{j_N=1}^{m_N} f(Y^i_{j_1}, \ldots Y^i_{j_N}) \cdot (a^i_{j_1} \otimes \cdots \otimes a^i_{j_N})
$$

Using Smolyak algorithm:

$$
A_{q,N} = \sum_{|\mathbf{i}|=q} \left( \Delta^i \otimes \cdots \otimes \Delta^i_N \right)(f) = A_{q-1,N}(f) + \sum_{|\mathbf{i}|=q} \left( \Delta^i \otimes \cdots \otimes \Delta^i_N \right)(f)
$$

where $U^0 = 0, \Delta^i = U^i - U^{i-1}, |i| = i_1 + \cdots i_N$

Hierarchical surplus:

$$
\omega^i_j = f(Y^i_{j_1}, \ldots, Y^i_{j_N}) - A_{q-1,N}(f)(Y^i_{j_1}, \ldots, Y^i_{j_N})
$$

Hierarchical basis

$$
f = f(Y^3)a_1^5 + f(Y^2)a_2^3 + f(Y^3)a_3^3 + f(Y^3)a_4^3 + f(Y^3)a_5^3$$

Nodal basis

$$
f = w_1 a_1^1 + w_2 a_2^2 + w_3 a_3^3$$
The interested function can be approximated by

\[
u(x, \xi(\omega)) = \sum_{i \leq q} \sum_j \alpha_j^i(x) \omega_j^i(\xi(\omega))
\]

Stochastic process Hierarchical surplus Interpolating function

The mean of the random solution is evaluated as

\[
E(u(t)) = \sum_{i \leq q} \sum_j \alpha_j^i(x) \cdot \int_L \omega_j^i(\xi) \, d\xi
\]

The variance of the solution can be computed as:

\[
\text{Var}[u(x)] = E\left[u^2(x)\right] - \left(E[u(x)]\right)^2 = \sum_{i \leq q} \sum_{j \in B_i} \nu_j^i(x) \cdot I_j^i - \left(\sum_{i \leq q} \sum_{j \in B_i} \omega_j^i(x) \cdot I_j^i\right)^2
\]

In the context of adaptivity, new support nodes are added to the hypercube only if the error indicator is larger than a threshold \(\varepsilon\):

\[
\gamma_j^i = \frac{\|\alpha_j^i(x) \cdot \int_L \omega_j^i(\xi) \, d\xi\|_{L_2}}{\|E_{\|\|d-1}\|_{L_2}} > \varepsilon
\]

Equal spaced Newton-Cotes grid:

\[
\gamma_j^i = \frac{j-1}{m_i-1}, \text{ for } j = 1, \ldots, m_i, \text{ if } m_i > 1; \ 0.5, \text{ for } j = 1, \text{ if } m_i = 1
\]
Investigating Property Variability Due to Microstructure Uncertainties

Microstructure space

START: Extract microstructural features

Low-dimensional space

Model reduction

Feature reconstruction

PCE

Low-D points

Low-D space

Unit hypercube

Property variability

Property convex hull

END

Property distribution

Solve SPEDs

Obtain Properties

Database

Reconstruct microstructures

Property convex hull

Property distribution

Sample from hypercube

Map to hypercube

Unit hypercube

Solve SPEDs

Obtain Properties

Database

Reconstruct microstructures

Property convex hull

Property distribution

Sample from hypercube

Map to hypercube

Unit hypercube
Applications
Example: Mechanical Response Variability

Problem definition

Given:
- Grain size snapshots constrained by moments (mean size, standard deviation, higher-order moments) of single phase polycrystals.
- Texture snapshots from random process.

Goal:
- The variability in material properties and response

Methodologies

- Model reduction to reduce the complexity of stochastic input
  - Nonlinear Model Reduction (manifold learning) to reduce grain size space
  - Karhunen-Loeve Expansion to reduce texture space
- Adaptive sparse grid collocation to solve stochastic partial differential equations

Microstructures obtained from certain process satisfy some specific experimentally determined statistics of grain size distribution.

Each microstructure that satisfies the given statistics of the grain size distribution is a point that lies on a manifold embedded in a high-dimensional space.

For microstructures having the same mean grain size, a “sorted grain size vector”, whose dimension is invariant, can be used to carry the grain size information.

The difference between two microstructures is conveniently measured by Euclidean distance.

\[
D(A, B) = \left( \sum_{i=1}^{n} (GS_i^A - GS_i^B)^2 \right)^{1/2}
\]
The properties of a polycrystalline microstructure are highly dependent on its texture: orientation distribution of grains.

**Orientation representation:** Rodrigues parameters

\[ r_1 = w_1 \tan \frac{\phi}{2}, \quad r_2 = w_2 \tan \frac{\phi}{2}, \quad r_3 = w_3 \tan \frac{\phi}{2} \]

**Texture representation:** Orientation Distribution Function (ODF)

A discrete form: \( \tau(r) = \{r_1^1, r_2^1, r_3^1, \ldots, r_1^n, r_2^n, r_3^n\} \)

Orientation dependence of slip system (anisotropy in crystalline materials)

\[
\mathbf{m}^{j,\alpha} = R^j \mathbf{m}^{\alpha}_{local} \\
\mathbf{n}^{j,\alpha} = R^j \mathbf{n}^{\alpha}_{local}
\]

where 
\[
R^j = \frac{1}{1 + \mathbf{r}^j \cdot \mathbf{r}^j} \left( \mathbf{I} - \frac{\mathbf{r}^j \mathbf{r}^j}{\mathbf{r}^j \cdot \mathbf{r}^j} \right) + 2 \left( \mathbf{r}^j \otimes \mathbf{r}^j - \mathbf{r}^j \times \mathbf{r}^j \right)
\]
Generation of Initial Texture Samples

Initial texture samples can be obtained by a sequence of random processing simulations with various deformation rate

\[ L = \omega_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_4 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} + \omega_5 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} + \omega_6 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_7 \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} + \omega_8 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \]

\( \omega_1, \omega_2, \ldots, \omega_8 \) are random coefficients corresponding to tension/compression, plain strain compression, shear and rotation.

The slip systems are updated during deformation as

\[ m_\alpha^t = F^e(t)m_0^\alpha \]

\[ n_\alpha^t = F^{e-T}(t)n_0^\alpha \]

Therefore the new orientations can be recovered from the rotation part of the elastic deformation gradient.

\[ F^e(t) = R^e(t)U^e(t) \]
Material: FCC nickel
Deterministic solver: Crystal plasticity with Taylor homogenization.
Hardening law (Taylor strain hardening law):

$$\hat{\tau} - \hat{\tau}_0 = \alpha \mu b \sqrt{\rho}$$

with dislocation density rate

$$\dot{\rho} = \sum_{\kappa} \left\{ \frac{1}{L_s b} + k_1 \sqrt{\rho} - k_2 \rho \right\} |\dot{\gamma}_\kappa|$$

Upon calculating the incremental shear strain, elastic and plastic deformation gradient can be updated and Cauchy stress is computed as

$$\mathbf{T} = \mathbf{C}^e \mathbf{E}^e$$

Homogenized effective stress and strain

$$\overline{\sigma}_{\text{eff}} = \sqrt{\frac{3}{2}} \mathbf{T}' \cdot \mathbf{T}'$$

where

$$\mathbf{T} = \langle \mathbf{T} \rangle = \frac{1}{V} \int_V \mathbf{T} dV$$

$$\overline{\mathbf{D}} = \langle \mathbf{D}^p \rangle = \frac{1}{V} \int_V \mathbf{D}^p dV$$
Simulation Procedure

Get grain size and texture snapshots

- Grain size
  - Nonlinear Model reduction
- Texture
  - Karhunen-Loeve Expansion

Reduced features

Adaptive sparse grid collocation

reconstruct

Deterministic solver

Construct property distributions

Microstructure domain: 1mm x 1mm x 1mm cube containing 54 grains.

Examine the effective stress variability of polycrystalline microstructures satisfying different constraints subjected to homogeneous compression.

\[ L = 0.002 \text{ sec}^{-1} \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 1.5 & 0 \\ 0 & 0 & -1 \end{bmatrix} \]

Grain size sample constraints:
(1) Mean volume 0.0185 mm³
(2) 2nd moment 3.704x10⁻⁴mm⁶
(3) 3rd moment 8.637x10⁻⁶mm⁹

Texture generation:
(a) \[ L = \omega_1 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]
(b) \[ L = \omega_1 \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

with \( \omega_1, \omega_2 \sim [-0.002, 0.002] \text{ sec}^{-1} \)

Run the simulation for 500 seconds.
Numerical Examples

Grain size effect

Effective stress distribution at strain 0.2
Numerical Examples

\[ L = \omega_1 \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]
Elastic Properties

An example take orientation distribution function (ODF) in the Rodrigues space as the stochastic input.

**Approach**
- Karhunen-Loeve expansion
- Maximum Entropy Principle

\[
A_0(s, \omega) = \bar{A}_0(s) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}f_i(s,t)Y_i(\omega)
\]

**Continuum representation of texture in Rodrigues space**

**Variation of stress-strain response**

**FCC copper**

**Property convex hull**

Cornell University
Materials Process Design and Control Laboratory
Fatigue of Superalloys

- The superalloy microstructure is modeled by homogenized single crystal with effective properties.

- Taylor model: all grains have the same deformation. No realistic microstructure is required. Computationally efficient.

- Finite element model: the boundary nodes have the same deformation while heterogeneous deformation is allowed within the microstructure. Realistic microstructure. More accurate but less efficient.
Fatigue Indicator Parameters (FIPs)

- Strain-based FIPs are employed to measure the fatigue properties of nickel-based superalloy microstructures.
- The FIPs are evaluated throughout the third loop of cyclic deformation.
- Cumulative plastic strain per cycle

\[ P_{cyc} = \int_{cyc} \sqrt{\frac{2}{3}} \dot{p} dt = \int_{cyc} \sqrt{\frac{2}{3}} D^p : D^p dt \]

- Maximum range of cyclic plastic shear strain

\[ \Delta \gamma^p_{\text{max}} = \max_\theta \left( \max_{\text{cyc}} \left( \gamma^p_\theta \right) - \min_{\text{cyc}} \left( \gamma^p_\theta \right) \right) \]

- Cumulative net plastic shear strain

\[ P_r = \max \left( \int_{cyc} \dot{\gamma}^p_{ij} n_i t_j dt \right) \]

- The Fatemi-Socie parameter

\[ P_{FS} = \frac{\Delta \gamma^p_{\text{max}}}{2} \left[ 1 + k^* \frac{\sigma_{n,\text{max}}}{\sigma_y} \right] \]

- Maximum range of cyclic plastic shear strain

\[ P_{mps} = \frac{\Delta \gamma^p_{\text{max}}}{2} \]

- Maximum range of cyclic plastic shear strain
Testing Case

- Polycrystalline microstructures with homogenized grains implemented in the Taylor model.
- Initial input samples: 1000 randomly generated microstructures composed of 54 grains represented by grain size and texture features.

- Model Reduction: PCA/KPCA on microstructure features.
$f_{p_1} = 0, f_{p_2} = 0.42, f_{p_3} = 0.11 \quad \varepsilon = -0.70\% \sim 0.70\% \quad \dot{\varepsilon} = 0.001s^{-1}$

**Taylor**

$max P_{cyc} = 1.51 \times 10^{-2}, max P_r = 1.12 \times 10^{-4}, max P_{FS} = 6.50 \times 10^{-3}, max P_{mps} = 5.98 \times 10^{-3}$

**FEM**

$max P_{cyc} = 1.99 \times 10^{-2}, max P_r = 8.16 \times 10^{-4}, max P_{FS} = 7.90 \times 10^{-3}, max P_{mps} = 6.76 \times 10^{-3}$
Generation of Initial Samples

- Initial texture: obtained by a sequence of random processing simulations with various deformation rate

\[
L = \omega_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
\]

\(\omega_1, \omega_2, \omega_3\) are random coefficients corresponding to tension/compression, rotation, and shear, respectively.

The slip systems are updated during deformation as

\[
m^\alpha_t = F^e(t)m^\alpha_0
\]

\[
n^\alpha_t = F^{e^T}(t)n^\alpha_0
\]

- Initial grain sizes: obtained by sampling in a lognormal distribution. The mean grain size is fixed at 0.0328mm.

- The above process is only for generating data having inherent correlation. After that, the only accessible information of the input is the data. No knowledge of how they are generated is assumed.
$f_{p1} = 0, f_{p2} = 0.42, f_{p3} = 0.11 \quad \varepsilon = -0.7\% \sim 0.7\% \quad \dot{\varepsilon} = 0.001s^{-1}$

The texture dominate the FIPs variability
**FIPs (PCA)**

![Graphs of max Pcyc, max Pr, max PFS, and max Pmmps](graph_images)

- Max Pcyc
- Max Pr
- Max PFS
- Max Pmmps

**Init**

- PCA-4dim
- PCA-5dim
- PCA-6dim
ASGC: level 8, converge to err=0.0001

PDF

max $P_{FS}$

max $P_{PS}$

max $P_{cyc}$

max $P_{mps}$

ASGC-PCA-4dim
ASGC-PCA-5dim
ASGC-PCA-6dim
MC-PCA-6dim
ASGC (KPCA)
Convex Hull

MC-PCA

MC-KPCA

ASGC-PCA

ASGC-KPCA
Some of the tails predicted by ASGC are not captured by MC.
Combined Volume Fraction and Texture Variation

\[ f_{p_1} = 0, f_{p_2} \sim N(0.3, 0.5), f_{p_3} \sim N(0.11, 0.14) \]
\[ \varepsilon = -0.7\% \sim 0.7\% \]
\[ \dot{\varepsilon} = 0.001 s^{-1} \]
Uncertainty Quantification in Multiscale Deformation Processes

Bi-orthogonal Decomposition
Motivation: Microstructure features are location specific. Traditional construction of reduced-order stochastic models for one point cannot see the microstructure correlation between points in the macroscale. The location dependence causes the “curse of dimensionality” in stochastic multiscale simulations.

Goal: Consider the correlation of microstructures between different points. Separate random variables from coordinates. Dramatically reduce the dimensionality of the stochastic multiscale input.

Grain structures of a nickel-base superalloy turbine disk having dual-microstructures.
Bi-orthogonal Decomposition

- Start from realizations of the microstructure random field ($A$) varying in both micro ($s$) and macro-scale ($x$): $A(x, s, \omega) : X \times S \times \Omega \rightarrow \mathbb{R}$
- Project $A$ to a set of bi-orthogonal bases

$$A(x, s, \omega) = \overline{A}(x, s) + \hat{A}(x, s, \omega)$$

$$= \overline{A}(x, \Phi) + \sum_{i=1}^{\infty} \sqrt{\rho_i} \psi_i(s) \hat{(}, \omega)$$

$$\approx \overline{A}(x, \Phi) + \sum_{i=1}^{d} \sqrt{\rho_i} \psi_i(s) \hat{(}, \omega)$$

- The inner product in the microstructure domain is denoted as

$$\langle \psi_i, \psi_j \rangle := \int_{S} \psi_i(s) \psi_j(s) ds$$

- The inner product in the spatial domain is defined as

$$\{ \Phi_i, \Phi_j \} := \int_{X} \left< \Phi_i(x, \omega) \cdot \Phi_j(x, \omega) \right> dx$$

- The orthogonality conditions:

$$\langle \psi_i, \psi_j \rangle = \delta_{ij} \quad \{ \Phi_i, \Phi_j \} = \delta_{ij}$$
By minimizing the distance between the Karhunen-Loeve expansion and the random field, the microscale basis can be computed by

\[ \psi_i(s) = \Phi \frac{1}{\sqrt{\rho_i}} \{ \hat{A}, \}_{i} \]

The macroscale basis is obtained through orthogonality condition

\[ \Phi_i(x, \omega) = \frac{1}{\sqrt{\rho_i}} \int_S \hat{A}(x, s, \omega) \psi_i(s) ds \]

The eigenvalue problem in K-L expansion can be defined as

\[ \rho_i \psi_i(s) = \int_S C(s, s') \psi_i(s') ds' \]

The covariance matrix is

\[ C(s, s') = \{ \hat{A}(x, s, \omega), \hat{A}(x, s', \omega) \} \]

Or in discrete form:

\[ C(s, s') = \frac{1}{n_r} \sum_{j=1}^{n_r} \sum_{i_n=1}^{n_{el}} \sum_{i_m=1}^{n_{int}} \hat{A}_j(x_{i_m}, s, \xi_j) \hat{A}_j^T(x_{i_m}, s', \xi_j) \hat{W}_{i_n} | J_{i_n} | \]

if realizations of the random field are given as \( A_i(x, s, \omega_i), \) where \( i = 1, \ldots, n_r \)
The random field $\mathbf{A}(\mathbf{x}, \mathbf{s}, \omega)$ is decomposed into a set of microscale modes $\psi_i(\mathbf{s})$ and spatial-random coupled modes $\Phi_i(\mathbf{x}, \omega)$.

$\Phi_i(\mathbf{x}, \omega)$ is still high-dimensional. By assuming independence of these macromodes, the random variable can be further separated from spatial modes via a second level KLE

$$\Phi_i(\mathbf{x}, \omega) \approx \tilde{\Phi}_i(\mathbf{x}) + \sum_{j=1}^{r_i} \sqrt{\lambda^i_j} \psi^i_j(\mathbf{x}) \phi^i_j(\omega) \quad i = 1, \ldots, d$$

$\lambda^i_j$ and $\psi^i_j$ are eigenvalues and eigenvectors, respectively, of the covariance matrix

$$\tilde{\mathbf{C}}_i = \frac{1}{N-1} \sum_{k=1}^{N} (\Phi^k_i - \bar{\Phi}_i)^T (\Phi^k_i - \bar{\Phi}_i)$$

The dimensionality of the reduced representation of the $i$th macromode $\Phi_i$ is $r_i$. The total dimensionality $r$ of the reduced space of feature $\mathbf{A}(\mathbf{x}, \mathbf{s}, \omega)$ is then the sum of all $r_i$.

$$r = \sum_{i=1}^{d} r_i$$
Polynomial Chaos Expansion

- After performing the second level KLE on macro modes $\Phi_i(x, \omega)$, we separated the randomness from spatial coordinates. The random term $\phi^j_i(\omega)$ can be mapped to well-shaped distribution by polynomial chaos expansion (PCE):

$$
\phi^j_i(\omega) = \sum_k \gamma^j_k \gamma^k_i \left( \zeta^j_i(\omega) \right)
$$

The choice of polynomial $\gamma^k_i$ of random variable $\zeta^j_i$ that follows well-shaped distribution (e.g. Gaussian or Uniform) depends on the specific distribution of $\zeta^j_i$.

- In the current work, we choose $\zeta^j_i$ to be uniformly distributed between -1 and 1. Therefore, $\gamma^k_i$ are Legendre polynomials. The coefficients of the PCE can be computed by

$$
\gamma^j_k = \frac{\left\langle \phi^j_i \left( \zeta^j_i \right) \gamma^k_i \left( \zeta^j_i \right) \right\rangle}{\left\langle \left( \gamma^k_i \left( \zeta^j_i \right) \right)^2 \right\rangle} = \frac{2k+1}{2} \int_{-1}^{1} \phi^j_i \left( \zeta^j_i \right) \gamma^k_i \left( \zeta^j_i \right) d\zeta^j_i
$$

where $i = 1, \ldots, d; \ j = 1, \ldots, r_i; \ k = 0, \ldots, p$.
Procedure

- Training: establish the mapping between microstructure space and reduced-order space.
- Testing: sample in the low-D space and reconstruct real microstructures

(a) Multiscale microstructure sample
(b) Macro-random coupled modes
(c) Reduced surrogate space
(d) Uniform distribution
(e) Properties distribution

Forging
\[ \nabla_n \cdot \langle P_r \rangle_h + f_r = 0 \]
\[ \tau - \tau_0 = \alpha \mu b \sqrt{\rho} \]

Bi-orthogonal KLE
\[ A(x,s,\omega)\Phi(x,s) + \sum_{i=1}^{d} \rho_i \Psi_i(s) \approx (x,\omega) \]

Stochastic Multiscale Simulation

Second-level KLE
\[ \Phi_i(x,\omega) = \hat{\Phi}_i(x) \]
\[ + \sum_{j=1}^{r} \sqrt{\lambda_j} \psi_j(x\mathbf{\Phi} / \psi / \omega) \]

PCE
\[ \phi_i(\omega_i) = \sum \gamma_i^{jk}(x) \Gamma_i^{jk}(\xi_j) \]
The input to the stochastic simulation is a set of ingot samples whose microstructures at different points are random but correlated. The input ingots are resulted from pre-processes. To obtain the random input ingots having correlated microstructures, we generate them through a random deformation process.

- A set of workpieces whose surfaces are randomly curved are pushed against a flat die.
- The microstructures at all points of all the initial ingots are assumed to be identical.
- The resulted microstructures at different point of different ingot are distinct due to the random shape of the initial ingots.
Initial Surface

- The surface of initial workpieces are described by a degree 6 Bezier curve

\[ R_\beta (a, \omega) = 0.5 \left( 1 + \sum_{i=0}^{6} \beta_i (\omega) \varphi_i (a) \right) \]

\[ \varphi_0 (a) = (1 - a)^6 \quad \varphi_4 (a) = 15a^4 (1-a)^2 \]

\[ \varphi_1 (a) = 6a(1-a)^5 \quad \varphi_5 (a) = 6a^5 (1-a) \]

\[ \varphi_2 (a) = 15a^2 (1-a)^4 \quad \varphi_6 (a) = a^6 \]

\[ \varphi_3 (a) = 20a^3 (1-a)^3 \quad a = x / L \]

- \( \beta_i \) are selected to be uniformly distributed in \((-0.1, 0.1)\).

- 1000 initial samples are generated. The resulted microstructures (or more precisely, texture) are the input to the stochastic simulation.
Mesh of the macroscale workpiece: 10x6 quadrilateral elements.
Microstructure representation: grain sizes and orientations of 20 grains.
Uncertainty source $A$: random textures

The total dimensionality of the stochastic input: $10 \times 6 \times 4 \times 20 \times 3 = 14400$.
The first 3 macro modes are preserved which captures around 98% of the total energy.

The expectation of macro modes energy is identical to the corresponding eigenvalue.
The macro modes are further decomposed by the second level KLE. Each decomposition preserves more than 95% of the total energy of the macro mode. The dimensionality of reduced macro modes are $r_1 = 2$, $r_2 = 3$, $r_3 = 3$, respectively. The dimensionality of the reduced space of the microstructure feature is therefore $r = r_1 + r_2 + r_3 = 8$.

$$P_{eigen}(r_i) = \frac{\sum_{k=1}^{r_i} \lambda_k}{\sum_{k=1}^{X} \lambda_k}$$
\[ A(x, s, \omega) \Phi \bar{A}(x, s) + \sum_{i=1}^{d} \sqrt{\rho_i} \psi_i(s) \ i(\ , \omega) \]

Reconstructed vs. Original Texture

\[ e = \frac{1}{\dim} \sum_{i=1}^{\dim} \left| \frac{R_{\text{Original}}^i - R_{\text{Restored}}^i}{R_{\text{Original}}^i} \right| = 0.0426 \]
Reconstructed Mean

Initial samples

4032 MC reconstructed samples
Initial samples

4032 MC reconstructed samples
Statistics of One Point

(a)

(b)

(c)

(d)
A More Realistic Modeling of Microstructures

Microstructure image representation with a FFT-based physical solver
Motivation

- Microstructures are better represented by images than statistical features.
- Full-field simulators directly interrogate realistic microstructures provide more reliable estimation to effective and local mechanical response/properties than mean-field methods (Taylor model, self-consistent model, etc.).
- Full-field simulators, e.g. finite element method, are usually time consuming. An efficient method with high accuracy is of great interest.
- An alternative strategy: FFT-based simulator based on Greens function method in combination with fast Fourier transform solving equilibrium equations.
- Merit: no complex meshing, no inversion of huge matrix, consider both intergranular and intragranular interactions, take image as input.
The governing equations are equilibrium equations + boundary conditions.

Elasto-plastic problem:

Equilibrium (stress rate divergence): \( \dot{\sigma}_{ij,j} = 0 \) + Periodic boundary conditions.

Solution strategy:

- Represent a local quantity by a mean plus fluctuation.
  \( \dot{\sigma}(x) = L_0 : \dot{\varepsilon}(x) + \phi(x) \)
  \( \dot{\sigma}_{ij,j} = L_{0ijkl} \dot{\varepsilon}_{kl,j} + \phi_{ij,j} = L_{0ijkl} \nu_{k,ij} + \phi_{ij,j} = 0 \)

- Reformulate the equilibrium equation using Greens function method.
  \(-L_{0ijkl} G_{km,ij} (x - x') + \delta_{im} \delta(x - x') = 0\)

- Transform reformulated equations to Fourier space through FFT.
  \( \hat{\xi}_i \hat{\xi}_j L_{0ijkl} \hat{G}_{km} (\hat{\xi}) = -\delta_{im} \)

- Solve for \( \hat{G}_{km}(\hat{\xi}) \): \( \hat{G}_{ij}(\hat{\xi}) = -\left( A^{r-1} \right)_{ij} \)
  \( A'_{ik} = \hat{\xi}_i \hat{\xi}_j L_{0ijkl} \)

- Update strain related quantities in Fourier space then transform them back to real space.
  \( \hat{\varepsilon}_{ij}(\hat{\xi}) = \hat{\Gamma}^{sym}_{ijkl}(\hat{\xi}) \hat{\phi}_{kl}(\hat{\xi}) \)
  \( \hat{\omega}_{ij}(\hat{\xi}) = \hat{\Gamma}^{antisym}_{ijkl}(\hat{\xi}) \hat{\phi}_{kl}(\hat{\xi}) \)
  \( \hat{\Gamma}_{ijkl}(\hat{\xi}) = -\hat{\xi}_j \hat{\xi}_l \hat{G}_{ik}(\hat{\xi}) \)
  \( \forall \hat{\xi} \neq 0 \text{ and } \hat{\varepsilon}_{ij}(0) = \hat{E} \)
  \( \forall \hat{\xi} \neq 0 \text{ and } \hat{\omega}_{ij}(0) = \hat{\Omega} \)

- Update stress related quantities in real space following constitutive laws.
Elasto-plastic Constitutive Equations

- The strain rate is additively decomposed into elastic and plastic parts:
  \[ \dot{\varepsilon}(x) = \dot{\varepsilon}^e(x) + \dot{\varepsilon}^p(x) \]
  \[ \dot{\varepsilon}^p(x) = \sum_{\alpha} m^{(\alpha)}(x) \dot{\gamma}^{(\alpha)}(x) \quad \text{trace}\left(\dot{\varepsilon}^p(x)\right) = 0 \]

- Constitutive relations:
  \[ \dot{\sigma}(x) = L^e(x) : \dot{\varepsilon}^e(x) \]
  \[ \sigma(x) = L^p(\dot{\varepsilon}^p(x)) \]
  \[ \sigma(x) = \sigma^n(x) + \dot{\sigma}(x) dt \]

  - \( L^e \): linear elastic stiffness tensor (C11, C12, C44).
  - \( L^p \): nonlinear plastic stiffness relation (e.g. inversion of \( M_s \)).

- The strain rate is related to both stress and stress rate by the constitutive model. The nonlinear connection can be explored iteratively using Newton-Raphson scheme:
  \[ F(\dot{\varepsilon}^e(x)) = \varepsilon^e(x) - \varepsilon^p(x) - \dot{\varepsilon}(x) = 0 \]
  \[ \dot{\varepsilon}_{i+1}^e(x) = \dot{\varepsilon}_i^e(x) - \alpha \left[ \frac{dF}{d\dot{\varepsilon}^e} \right]^{-1} F_i\left(\dot{\varepsilon}_i^e(x)\right) \]

\[ \frac{dF}{d\dot{\varepsilon}^e} = \frac{d\varepsilon^e}{d\dot{\varepsilon}^e} + \frac{d\varepsilon^p}{d\dot{\varepsilon}^e} = I_4 + \frac{d\varepsilon^p}{d\sigma} \frac{d\sigma}{d\dot{\varepsilon}^e} = I_4 + M^p \cdot d\varepsilon^e : L^e \]
Algorithm: Basic Formulation

- Basic formulation: based on the exact expression of Greens function for linear elastic, homogeneous reference material.
- CEP: crystal elasto-plasticity; CVP: crystal visco-plasticity.

For each time step, the iterative algorithm can be:

1. At the beginning of the 1st iteration, give an initial guess to the strain rate: \( \frac{\partial \varepsilon}{\partial t}^0(x) = \hat{\varepsilon}(x) \). Then compute initial stress (or CVP), \( \frac{\partial \sigma}{\partial t}^0(x) \), or stress rate (for CEP), \( \frac{\partial \sigma}{\partial t}^0(x) \), using local constitutive relations.
2. Compute the polarization field, \( \varphi(x) \), for the ith iteration.
3. Transform the polarization to field Fourier space via FFT: \( \hat{i \varphi} = \text{FFT} \left( \varphi(x) \right) \)
4. Compute strain rate in the Fourier space at the (i+1)th iteration:
   \[
   \frac{\partial \varepsilon}{\partial t}^{i+1}(\xi) = \text{sym} \left( \hat{\Gamma}(\xi) \cdot \hat{i \varphi}(\xi) \right); \quad \forall \xi \neq 0, \quad \text{and} \quad \hat{i \varepsilon}^{n+1}(0) = \hat{\varepsilon} \]
5. Transform strain rate back to the real space through inverse FFT: \( \frac{\partial \varepsilon}{\partial t}^{i+1}(x) = \text{FFT}^{-1} \left( \frac{\partial \varepsilon}{\partial t}^{i+1}(\xi) \right) \)
6. Compute stress (or stress rate) field using updated strain rate according to constitutive model.
7. Check the convergence
   \[
   \delta = \left| \frac{i+1 \varepsilon - i \varepsilon}{i+1 \varepsilon} \right|
   \quad \text{and} \quad \epsilon = \left( \frac{\| \text{div} \left( \frac{i+1 \sigma}{\partial t} \right) \|^2}{\| \frac{i+1 \sigma}{\partial t} \|^2} \right)^{1/2} = \left( \frac{\| \xi \cdot \frac{i+1 \sigma}{\partial t} \|^2}{\| \frac{i+1 \sigma}{\partial t} \|^2} \right)^{1/2}
   \]

Equilibrium error
Example: Plane Strain

- Example: An elasto-plastic FCC aluminum microstructure containing 64 grains (with random orientation) discretized by 16x16x16 voxels.

- Applied strain rate: plane strain.

\[
\dot{\mathbf{E}} = 10^{-3} \begin{bmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1
\end{bmatrix}
\]

Deformed microstructure
Example: Plane Strain

- Strain, plastic strain, and stress fields:

  CVPFFT

  CEPFFT

  CPFEM

  **Strain**

  **Plastic strain**

  **Stress**
Effective Mechanical response

- Effective stress – strain curve of the microstructure.

\[ \dot{E} = 10^{-3} \times \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \]
Texture

- Pole figures of deformed microstructures:

  ![Pole figures of deformed microstructures](image)

  - CEPFFT
  - CPFEM
  - CVPFFT

Deformed frequency grid in Fourier space
The comparison of computation time of CEPFFT and CPFEM is plotted in seconds.
Graphical Model for Multiscale Disk Forging Problems

Problem Definition:

- **Input Microstructure Reduction (PCA)**
- **Multiscale Forging Solver**
- **Macro properties**

Main results:

- **True**
- **Gaussian Model**
- **Nonparametric Model**

For any new input microstructure
Conclusions

- Model reduction is needed in reducing complexity of stochastic microstructure input.
- Different (linear/nonlinear) model reduction techniques can be employed for different problems.
- The low-dimensional surrogate space needs to be constructed so new samples can be generated.
- The model reduction strategy can be applied to a variety of problems regarding uncertainty quantification of polycrystalline materials (thermal, deformation, flow problems, …)
- The bi-orthogonal decomposition can effectively reduce the dimensionality of multiscale stochastic input.
- More realistic representation of microstructures is currently of interest (using image based model reduction techniques – probabilistic PCA/mixture PCA, GTM, …)
- FFT-based full-field physical solver provides an efficient way of solving stochastic problems taking realistic microstructure samples as the input.