DATA DRIVEN MODEL REDUCTION OF STOCHASTIC INPUT MODELS WITH APPLICATIONS TO MULTISCALE MATERIALS MODELING

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- Thermal and fluid transport in heterogeneous media are ubiquitous

- Range from large scale systems (geothermal systems) to the small scale

- Most critical devices/applications utilize heterogeneous/polycrystalline/functionally graded materials

- Properties depend on the distribution of material/microstructure

- But only possess limited information about the microstructure/property distribution (e.g. 2D images)

Incorporate limited information into stochastic analysis:
- worst case scenarios
- variations on physical properties

Thermal transport through polycrystalline materials

Hydrodynamic transport through heterogeneous permeable media
FRAMEWORK FOR ANALYSIS OF HETEROGENEOUS MEDIA

1. Property extraction
Extract properties P1, P2, .. Pn, that the structure satisfies.
These properties are usually statistical: Volume fraction, 2 Point correlation, auto correlation

2. Microstructure/property reconstruction
Reconstruct realizations of the structure satisfying the correlations.

3. Reduced model
Construct a reduced stochastic model of property variations from the data. This model must be able to approximate the class of structures.

4. Stochastic analysis
Solve the heterogeneous property problem in the reduced stochastic space for computing property variations.

**INPUT STOCHASTIC MODELS: LINEAR APPROACH**

**Methodology for creating linear models from data**

- Given some limited information (either in terms of statistical correlation functions or sample microstructure/property variations)

- Utilize some reconstruction methodology to create a finite set of realizations of the property/microstructure.

- Utilize this data set to construct a model of this variability

Use Proper Orthogonal Decomposition (POD), Principal Component Analysis (PCA) to construct a reduced order model of the data.

\[ \begin{align*}
    &= a_1 + a_2 + \ldots + a_n
\end{align*} \]

Convert variability of property/microstructure to variability of coefficients.

Not all combinations allowed. Developed subspace reducing methodology\(^1\) to find the space of allowable coefficients that reconstruct plausible microstructures

LINEAR APPROACH TO MODEL GENERATION

Successfully applied to investigate effect of heterogeneous media in diffusion phenomena in two-phase microstructures.

PCA based methods are easy to implement and are well understood.

But PCA based methods are linear projection methods

*Only guaranteed to discover the true structure of data lying on a linear subspace of the high dimensional input space*

PCA works very well when the input space is linear

What about when the input space is curved/non-linear?

PCA based techniques tend to overestimate the dimensionality of the model

Further related issues:
- How to generalize it to other properties/structures?
  Can PCA be applied to other classes of microstructures, say, polycrystals?
- How does convergence change as the amount of information increases? Computationally?
- Find structure of data lying on a possibly non-linear subspace of the high-dimensional input data.

- PCA finds a low-dimensional embedding of the data points that best preserves their variance as measured in the high-dimensional input space. Variance is measured based on Euclidian distance. This results in a linear subspace approximation of the data.

- But what if the data lie on nonlinear curve in high-dimensional space?

- Have to unfold/unravel the curve

- Need non-linear approaches
NONLINEAR REDUCTION: THE KEY IDEA

Set of images. Each image = 64x64 = 4096 pixels
Each image is a point in 4096 dimensional space.
But each and every image is related (they are pictures of the same object). *Same object but different poses.*
That is, all these images lie on a unique curve (manifold) in $\mathbb{R}^{4096}$.
Can we get a parametric representation of this curve?

**Problem:** Can the parameters that define this manifold be extracted, ONLY given these images (points in $\mathbb{R}^{4096}$)

**Solution:** Each image can be uniquely represented as a point in 2D space (UD, LR).

**Strategy:** based on the ‘manifold learning’ problem

Different images of the same object: changes in up-down (UD) and left-right (LR) poses

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[Images of a 3D object in different poses]
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Based on principles from psychology and cognitive sciences.

How does the brain interpret/store/recall high-resolution images at different poses, locations?

A low-dimensional parameterization of this very high-dimensional space

**Effectively constructs a surrogate space of the actual space.**

Performs all operations on this surrogate low-dimensional parametric space and maps back to the input space

These ideas are being increasingly used in problems in vision enhancement, speech and motor control, data compression

Different images of the same object: changes in up-down (UD) and left-right (LR) poses
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.
A FORMAL DEFINITION OF THE PROBLEM

State the problem as a parameterization problem (also called the manifold learning problem)

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 $d << n$

Classical methods in manifold learning have been methods like the Principle Component Analysis (PCA) and multidimensional scaling (MDS).

These methods have been shown to extract optimal mappings when the manifold is embedded linearly or almost linearly in the input space.

In most cases of interest, the manifold is non-linearly embedded in the input space, making the classical methods of dimension reduction highly approximate.

Two approaches developed that can extract non-linear structures while maintaining the computational advantage offered by PCA$^{1,2}$.

AN INTUITIVE PICTURE OF THE STRATEGY

- Attempt to reduce dimensionality while preserving the geometry at all scales.

- 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
MATHEMATICAL DETAILS: AN OVERVIEW

Start from N samples lying on a curve that is embedded in a high-dimensional space.

What are the properties of this curve $\mathcal{M}$?

Generate an isometric transformation (parameterization) from this curve to a low-dimensional region. **Proof of existence of this mapping**

Next step is to extract some knowledge of the geometry of this curve. Utilize the concept of geodesic distance to encode this knowledge of the geometry.

How is this geodesic distance defined and computed?

How is this information used in numerically constructing the required mapping?
Given a set of N sample points \{x_i\} lying on \( \mathcal{M} \) Must have a notion of distance between these sample points. Define an appropriate function

\[
D: \mathcal{M} \times \mathcal{M} \rightarrow [0, \infty)
\]

that determines the difference between any two points

Ensure that it satisfies the properties of positive-definiteness, symmetry and the triangle inequality.

Lemma 1: \((\mathcal{M}, D)\) is a metric space

Lemma 2a: \((\mathcal{M}, D)\) is a bounded metric space

Lemma 2b: \((\mathcal{M}, D)\) is dense

Lemma 2c: \((\mathcal{M}, D)\) is complete

Theorem: \((\mathcal{M}, D)\) is compact

A compact manifold embedded in a high-dimensional space can be isometrically mapped to a region in a low-dimensional space.


A compact manifold embedded in a high-dimensional space can be isometrically mapped to a region in a low-dimensional space.

Isometry encoded into the geodesic distances

Have no notion of the geometry of the manifold to start with. Hence cannot construct true geodesic distances!

\[ D_M(i, j) = \inf_{\gamma} \{\text{length}(\gamma)\} \]

Approximate the geodesic distance using the concept of graph distance \( D_G(i,j) \): the distance of points far away is computed as a sequence of small hops.

This approximation, \( D_G \), asymptotically matches the actual geodesic distance \( D_M \). In the limit of large number of samples\(^1,2\). (Theorem 4.5 in Ref. 1)

\[ (1 - \lambda_1)D_M(i, j) \leq D_G(i, j) \leq (1 + \lambda_2)D_M(i, j) \]

2. M.Bernstein, V. deSilva, J.C.Langford, J.B.Tenenbaum, Graph approximations to geodesics on embedded manifolds, Dec 2000
Proof of theorem is based on ideas from geometry, differential algebra and simple probability arguments

Theorem 4.5: Let $\mathcal{M}_{S_2}$ be a compact manifold of $\mathbb{R}^n$ isometrically equivalent to a convex domain $\mathcal{A} \subset \mathbb{R}^d$. Let $\lambda_1$, $\lambda_2$ and $0 < \mu < 1$ be given, and let $\epsilon > 0$ be chosen such that $\epsilon < s_\circ$ and $\epsilon \leq \frac{2}{\pi} r_\circ \sqrt{24\lambda_1}$. A finite sample set \{x_i\}, $i = 1, \ldots, N$ is chosen randomly from $\mathcal{M}_{S_2}$ with a density $\alpha$, with $\alpha > \frac{\log(\frac{V}{\mu \eta_d(\lambda_2 \epsilon/16)^d})}{\eta_d(\lambda_2 \epsilon/8)^d}$, where $V$ is the volume of $\mathcal{M}_{S_2}$ and $\eta_d$ is the volume of the unit ball in $\mathbb{R}^d$. The neighborhood graph $G$ is constructed on \{x_i\}. Then, with probability at least $1 - \mu$, the following inequalities hold for all $x, y$ in $\mathcal{M}_{S_2}$:

$$(1 - \lambda_1)D_M(x, y) \leq D_G(x, y) \leq (1 + \lambda_2)D_M(x, y)$$

Using this approximation – can compute the pair wise geodesic distance matrix, $M$, between all the $N$ sample points
FROM THE MATRIX, M, TO A LOW-DIMENSIONAL MAP

Have N objects, the preceding developments provided a means of computing the pair wise distances between them.

Convert this set of pair wise distances into points in a low-dimensional space

Given a matrix, M, of pairwise distances between N objects, find a configuration of points in a low-dimensional space such that the coordinates of these N points yield a Euclidean distance matrix whose elements are identical to the elements of the given distance matrix M.

This is a straightforward problem in multivariate statistical analysis¹.

Can easily solve the problem using the concept of Multi Dimensional Scaling² (MDS)

2. T. F. Cox, M. A. A. Cox, Multidimensional scaling, 1994, Chapman and Hall
MULTI DIMENSIONAL SCALING

Given the N x N matrix of the geodesic distances, M, with elements d_{ij}.

Compute the symmetric N x N matrix, A, with elements a_{ij} = -1/2 d_{ij}^2.

Suppose that the N low-dimensional points that we are interested in finding (the parameters of the N objects in high-dimensional space) are \( \{y_i\} \)

Denote the N x N matrix of the scalar product of these N low-dimensional points as B,

\[
b_{ij} = \sum_{k=1}^{d} y_{ik} y_{jk} = y_i^T y_j \quad \text{B} = YY^T
\]

Can show that A, and B, are related as \( \text{B} = \text{HAH} \)

where H is the centering matrix, \( h_{ij} = \delta_{ij} - 1/N \)
MULTI DIMENSIONAL SCALING (contd.)

\( \mathbf{B} \) is a positive definite matrix and can be written in terms of its eigen values and eigen vectors as:

\[
\mathbf{B} = \mathbf{\Gamma} \Lambda \mathbf{\Gamma}
\]

Where \( \Lambda \) is the diagonal matrix of the eigenvalues and \( \mathbf{\Gamma} \) is the corresponding matrix of eigenvectors. \( \mathbf{B} \) will have a decaying eigen-spectrum. From \( \mathbf{B} = \mathbf{YY}^T \) and \( \mathbf{B} = \mathbf{\Gamma} \Lambda \mathbf{\Gamma} \) we get:

\[
\mathbf{Y} = \mathbf{\Gamma}_d \Lambda_d^{1/2}
\]

The above equation is an estimate of \( \mathbf{Y} \) in terms of the largest \( d \) eigenvalues of the eigenvalue decomposition of the squared geodesic distance matrix

From N points in a high-dimensional space to N points in a low-dimensional space
THE NONLINEAR MODEL REDUCTION ALGORITHM

Given a set of N sample points \( \{x_i\} \) lying on \( \mathcal{M} \)

The complete algorithm consists of three simple steps

**Step 1:**
- Construct the neighborhood graph: Determine which points are neighbors, Construct the weighted graph with edges given weights corresponding to the distances, \( \mathcal{D} \), between the points

**Step 2:**
- Estimate the shortest intrinsic path- the geodesic lengths: Compute the shortest path length, \( \mathcal{M} \), between the points in the weighted graph, using, say, Floyd’s algorithm

**Step 3:**
- Construct the d-dimensional embedding: Perform classical Multi Dimensional Scaling on the geodesic distance matrix, \( \mathcal{M} \), to extract a set of N points in a low-dimensional space
CHOOSING THE OPTIMAL DIMENSIONALITY, $d$

The MDS procedure in the dimension reduction methodology constructs the eigen-value decomposition of a matrix. The low-dimensional representation correspond to the largest $d$ eigenvalues of this matrix.

How is the value of $d$ chosen?

Given a set of $N$ unordered samples $\{x_i\} \in M_{S_2} \subset \mathbb{R}^n$ and a dimension reduction strategy that parameterizes $M_{S_2}$ in a low-dimensional region $A \subset \mathbb{R}^d$, find the optimal dimensionality, $d$ of the region $A$.

Use ideas from recent development on estimating the intrinsic dimensionality of manifolds (Costa and Hero$^1$)

Elegant ideas from differential geometry and graph theory.

Connect dimensionality to the rate of convergence of a graph theoretic quantity

CHOOSING THE OPTIMAL DIMENSIONALITY, $d$

Based on very elegant ideas linking graph theory with differential geometry.

Based on the theorem of Beardwood-Halton-Hammersley$^{1,2}$.

Based on concepts in geometric probability, the theorem relates the structure/geometry of embedded manifolds to the graph structure of a finite set of points on these embedded manifolds.

The theorem states that the length functional of the minimal spanning graph is related to the entropy of density of distribution of a finite set of points in an embedded manifold (with some specific properties).

Costa and Hero$^1$ extended/applied this theorem to general embedded manifolds.

Ganapathysubramanian and Zabaras$^3$ applied it to the model reduction problem.

The length functional of the minimal spanning tree of the geodesic matrix, $M$, is related to the intrinsic dimensionality of the low-dimensional representation of the manifold $1,2$.

**Theorem 4.6:** Let $M_{S_2}$ be a smooth $d$ dimensional manifold embedded in $\mathbb{R}^n$ through a conformal map $\varphi : \mathbb{R}^d \rightarrow M_{S_2}$. Let $2 \leq d \leq n$. Suppose that $\{x_i\}$, $i = 1, \ldots, N$ are random vectors in $M_{S_2}$. Assume that each of the edge lengths $|e_{ij}|_M$ in the edge matrix (or the matrix of manifold distances) $M$ converge to $|\varphi^{-1}(x_i) - \varphi^{-1}(x_j)|_2$ as $N \rightarrow \infty$ (i.e the graph distance converges to the true manifold distance). This is guaranteed by Theorem 4.5. Then the length functional, $L(\{x\})$ of the GMST satisfies:

$$
\lim_{N \rightarrow \infty} \frac{L(\{x\})/N^{(d'-1)/d'}}{N^{(d'-1)/d'}} = \begin{cases} 
\infty & \text{if } d' < d; \\
\beta_m C & \text{if } d' = d; \\
0 & \text{if } d' > d. 
\end{cases}
$$

From the above theorem, can easily extract the dimensionality.

Taking the logarithm of the main result of the algorithm,

\[ \log(L) = a \log(N) + \varepsilon \quad \text{with} \quad a = \frac{d - 1}{d} \]

where \( L \) is the length functional of the minimal spanning tree of the geodesic matrix, \( N \) is the number of samples and \( d \) is the optimal dimensionality.

Use readily available algorithms (Kruskal’s algorithm or Prim’s algorithm) to compute \( L \) for different sample sizes

Perform a least squares fit for the value of \( a \)
THE NONLINEAR MODEL REDUCTION FRAMEWORK

Given N unordered samples

N points in a low dimensional space

The procedure results in N points in a low-dimensional space. The geodesic distance + MDS step (Isomap algorithm\(^1\)) results in a low-dimensional convex, connected space\(^2\), \( \mathcal{A} \subset \mathbb{R}^d \).

Using the N samples, the reduced space is given as:

\[ \mathcal{A} = \text{convex hull}(\{x_i\}) \]

\( \mathcal{A} \) serves as the surrogate space for \( \mathcal{M} \).

Access variability in \( \mathcal{M} \) by sampling over \( \mathcal{A} \).

BUT have only come up with \( \mathcal{M} \rightarrow \mathcal{A} \) map .... Need \( \mathcal{A} \rightarrow \mathcal{M} \) map too

The Reduced Order Stochastic Model

Only have N pairs to construct $\mathcal{A} \rightarrow \mathcal{M}$ map. Various possibilities based on specific problem at hand. But have to be conscious about computational effort and efficiency.

Illustrate 3 such possibilities below. Error bounds can be computed\(^1\).

1. Nearest neighbor map

2. Local linear interpolation

3. Local linear interpolation with projection

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THE LOW DIMENSIONAL STOCHASTIC MODEL

Algorithm consists of two parts.

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

For using this model in a stochastic collocation framework, must sample points in $\mathcal{A} \rightarrow \mathcal{M}$

2) For an arbitrary point $\xi \in \mathcal{A}$ must find the corresponding point $x \in \mathcal{M}$. Compute the mapping from $\mathcal{A} \rightarrow \mathcal{M}$

\[ \mathcal{A} \subset \mathbb{R}^d \quad \mathcal{M} \subset \mathbb{R}^n. \]
NUMERICAL EXAMPLE

Given an experimental image of a two-phase metal-metal composite (Silver-Tungsten composite).

Find the variability in temperature arising due to the uncertainty in the knowledge of the exact 3D material distribution of the specified microstructure.

**Problem strategy:**

- Extract pertinent statistical information from the experimental image
- Reconstruct dataset of plausible 3D microstructures
- Construct a low-dimensional parametrization of this space of microstructures
- Solve the SPDE for temperature evolution using this input model in a stochastic collocation framework

TWO PHASE MATERIAL

Experimental image

Realizations of 3D microstructure

Experimental statistics

GRF statistics
The developments detailed before are applied to find a low-dimensional representation of these 1000 microstructure samples.

The optimal representation of these points was a 9-dimensional region

Able to theoretically show that these points in 9D space form a convex region in $\mathbb{R}^9$.

This convex region now represents the low-dimensional stochastic input space

Use sparse grid collocation strategies to sample this space.
The construction of the stochastic solution: through sparse grid collocation level 5 interpolation scheme used

Number of deterministic problems solved: 26017

Computational domain of each deterministic problem: 65x65x65 pixels

Total number of DOF: $65^3 \times 26017 \approx 7 \times 10^9$

Computational platform: 50 nodes on local Linux cluster (x2 3.2 GHz)

Total time: 210 minutes
Seamlessly couple stochastic analysis with multiscale analysis.

Multiscale framework (large deformation/thermal evolution) + Adaptive stochastic collocation framework

Provides roadmap to efficiently link any validated multiscale framework

Coupled with a data-driven input model strategy to analyze realistic stochastic multiscale problems.
OTHER APPLICATIONS OF THIS FRAMEWORK

From unordered samples in high-dimensional space to a convex space representing the parameterization

- This methodology has significant applications to problems where working in high-dimensional spaces is computationally intractable.
- Can pose the problem in a low-dimensional space

visualizing
property evolution, process-property maps, searching and contouring, representing input uncertainty, data mining …
Stochastic design/optimization framework

Most critical components in many applications/devices are usually fabricated from polycrystalline/ functionally graded/ heterogeneous materials.

The properties at the device-scale (thermal and electrical conductivity, elastic moduli and failure mechanisms) depend on the microstructure and material distribution at the meso-scale.

Have to design the operating conditions/parameters taking into account this limited information about the microstructure.

Robust design in the presence of topological uncertainty

Given limited topological information about the microstructure, design the optimal (stochastic) heat flux to be applied on one end of the device such that a required (stochastic) temperature is maintained at the other end.

Design criterion:
- Maintain a specified thermal profile on the right wall
- This thermal profile is given in terms of a pdf, usually specified in terms of moments

Additional uncertainties:
- Do not know the exact microstructure that the device is made up of.
- Only know certain statistical correlations that the microstructure satisfies.
- Consider the microstructure to be a random field \( \Omega \).

Design variables:
- Must design the pdf of the optimal heat flux
Some input parameters, boundary conditions, initial conditions or operational sequences have a significant impact on the stochastic solution.

Improved input representation (i.e. lesser uncertainty) significantly reduces the uncertainty in the final solution.

The stochastic solution is **sensitive to which parameters or input terms?**

Need a robust, seamlessly interfacing methodology to estimate this.

- Which input parameters to consider as random?
- Quantify the effect of uncertainty on each parameter on system response
- Decide the length scale of experimentation and the needed fidelity of each measurement.
FEEDBACK TO EXPERIMENTS: STOCHASTIC SENSITIVITY

Completely non-intrusive. Validated wrapper software that interfaces with deterministic solver.

Based on adaptive sparse grid collocation techniques. Parallel, scalable framework.

Can be utilized in the design of experiments.

Applied in a design framework to estimate bounds on an input variable such that a given condition is satisfied in the presence of other sources of uncertainty.

Can be used to obtain estimates on which scale of modeling needs more information. This can be directly used to model experiments optimally.
Variability of Material Properties

➢ Problem definition

Given:
- Grain size snapshots constrained by moments (mean size, standard deviation, higher-order moments).
- 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

Zheng Li, Bin Wen and N. Zabaras, "Data-driven stochastic models for the representation of polycrystalline microstructures", Computational Materials Science, in press.
Microstructure Representation

Microstructures obtained from certain processes 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.

\[
D(A, B) = \left( \sum_{i=1}^{n} (GS_i^A - GS_i^B)^2 \right)^{1/2}
\]
**Generation of Random Microstructure Samples**

Given expected grain size statistical information such as mean size \( M_1 \), second order moment \( M_2 \), and/or higher order moments \( M_3 \), etc.,

\[
M_i = \frac{1}{n} \sum_{j=1}^{n} S_j^i
\]

samples can be generated by first randomly generating a set of grain size vectors having the same mean size \( M_1 \), and then following certain algorithm to satisfy higher order moments. To satisfy the first 3 moments:

**Step 1:** \( \hat{S}_i = S_i - M_1 \);
**Step 2:** \( \hat{S}'_i = \hat{S}_i \), and \( E_1 = \frac{1}{n} \sum_{i=1}^{n} S_i \);
**Step 3:** \( \hat{S}_i = \hat{S}_i - E_1 \);
**Step 4:** \( E_2 = \frac{1}{n} \sum_{i=1}^{n} S_i^2 \);
**Step 5:** \( \hat{S}_i = \hat{S}_i \sqrt{\frac{M_2}{E_2}} \);
**Step 6:** loop

\[
\hat{\delta}_i = \frac{3\hat{S}_i^2}{n};
\]
\[
d = \sum_{i=1}^{n} n\hat{\delta}_i^2, E_3 = \frac{1}{n} \hat{S}_i^3;
\]
\[
m = \hat{M}_3 - E_3;
\]

**Step 7:** error = norm(\( \hat{S}'_i - \hat{S}_i \));
**Step 8:** if error < cutoff, go to step 9, else go to step 1;
**Step 9:** \( S_i = M_1 + \hat{S}_i \).

where

\[
\hat{M}_1 = 0, \hat{M}_2 = M_2 - M_1^2, \quad \hat{M}_3 = M_3 - 3M_1M_2 + 2M_1^3
\]
Nonlinear Model Reduction on Grain Size Feature

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 $d << n$.

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: \( \tau(\mathbf{r}) = \left\{ r_1^n, r_2^n, r_3^n, \ldots, r_1^n, r_2^n, r_3^n \right\} \)

ODF in RF fundamental zone of FCC crystal

**Orientation dependence of slip system (anisotropy in crystalline materials)**

\[ \mathbf{m}_{local}^\alpha : \langle 111 \rangle \]
\[ \mathbf{n}_{local}^\alpha : [110] \]

\[ \mathbf{m}_{j,\alpha} = \mathbf{R}_j \mathbf{m}_{local}^\alpha \]
\[ \mathbf{n}_{j,\alpha} = \mathbf{R}_j \mathbf{n}_{local}^\alpha \quad \text{where} \quad \mathbf{R}_j = \frac{1}{1 + \mathbf{r}_j \cdot \mathbf{r}_j} \left( \mathbf{I} (1 - \mathbf{r}_j \cdot \mathbf{r}_j) + 2 (\mathbf{r}_j \otimes \mathbf{r}_j - \mathbf{I} \times \mathbf{r}_j) \right) \]
Generation of Initial Texture Samples

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

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

\[
\omega_5 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} + \omega_6 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_7 \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} + \omega_8 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}
\]

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

The slip systems are updated during deformation as

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

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

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

\[
\mathbf{F}^e(t) = \mathbf{R}^e(t)\mathbf{U}^e(t)
\]
Karhunen-Loeve Expansion on Texture Samples

Deterministic texture

Initial texture samples

Random process controlled by \( \{ \omega_1, \omega_2, \ldots, \omega_8 \} \)

Given \( N \) texture examples, construct covariance matrix of these samples

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

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

\[
\tau(r, \omega) = \bar{\tau}(r, \omega) + \sum_{i=1}^{d} \sqrt{\lambda_i} \phi_i(r) \eta_i(\omega)
\]

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

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

Texture random field thus transformed to low-dimensional space \( \eta \in \mathbb{R}^d \)
Maximum Entropy Estimation of the Distribution of $\eta$

To sample new texture, we can sample $\eta$ instead, and then transform it back to the texture space. The distribution of $\eta$ is needed.

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

$$\eta \sim N(0, I)$$
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

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

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

$$\eta_i = \Phi^{-1}(\zeta_i), \quad i = 1, ..., d$$

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.
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 interested function can be approximated by

\[ u(x, \xi(\omega)) = \sum_{|i| \leq q} \sum_{j} \alpha_i^j(x) \alpha_j^i(\xi(\omega)) \]

\[ \downarrow \quad \text{Stochastic process} \quad \downarrow \quad \text{Hierarchical surplus} \quad \downarrow \quad \text{Interpolating function} \]

The mean of the random solution is evaluated as

\[ E(u(t)) = \sum_{|i| \leq q} \sum_{j} \alpha_i^j(x) \cdot \int_L \alpha_j^i(\xi) d\xi \]

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

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

Material: FCC nickel
Deterministic solver: Crystal plasticity with Taylor homogenization.
Hardening law (Taylor strain hardening law):
\[ \hat{\tau} - \hat{\tau}_0 = \alpha \mu b \sqrt{\rho} \]
where dislocation density changing rate
\[ \dot{\rho} = \sum_k \left\{ \frac{1}{L_s b} + k_1 \sqrt{\rho} - k_2 \rho \right\} |\hat{\gamma}^k| \]
Upon calculating the incremental shear strain, elastic and plastic deformation gradient can be updated and Cauchy stress is computed
\[ T = C^e E^e \]
Homogenized effective stress and strain
\[ \bar{\sigma}_{eff} = \sqrt{\frac{3}{2} \bar{T} \cdot \bar{T}} \quad \text{where} \quad \bar{T} = \langle T \rangle = \frac{1}{V} \int_v T \, dV \]
\[ \bar{e}_{eff} = \int_0^t \sqrt{\frac{2}{3} \bar{D} \cdot \bar{D}} \, dt \quad \text{where} \quad \bar{D} = \langle D^p \rangle = \frac{1}{V} \int_v D^p \, dV \]
**Simulation procedure**

1. Get grain size and texture snapshots
2. Grain size: Nonlinear Model reduction
3. Texture: Karhunen-Loeve Expansion
4. Reduced features
5. Adaptive sparse grid collocation
6. Reconstruct
7. Deterministic solver
8. Construct property distributions

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Z. Li, B. Wen and N. Zabaras, Computational Materials Science (2010)
Numerical Examples

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.

Grain size sample constraints:

(1) Mean volume 0.0185 mm$^3$
(2) 2$^{nd}$ moment 3.704x10$^{-4}$mm$^6$
(3) 3$^{rd}$ moment 8.637x10$^{-6}$mm$^9$

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

Texture generation:

(a) $$L = \omega_1 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

(b) $$L = \omega_1 \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

with $$\omega_1 \sim [-0.002, 0.002] \text{sec}^{-1}$$

Run the simulation for 500 seconds.
Numerical Examples

1\textsuperscript{st} moment ((1)+(a))

1\textsuperscript{st} and 2\textsuperscript{nd} moments ((2)+(a))

1\textsuperscript{st}, 2\textsuperscript{nd}, and 3\textsuperscript{rd} moments ((3)+(a))

Grain size effect

Effective stress distribution at strain 0.2
### Texture effect

\[ L = \omega_1 \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]
Example 1: The effect of uncertainty in initial texture on macro-scale material properties for FCC copper

The initial texture samples are generated by a sequence of modes consisting of a simple compression mode and followed by a shear mode hence the velocity gradient is considered as:

\[
L = \alpha_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix}, \quad t < T_1
\]

\[
L = \alpha_2 \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad T_1 < t < T_2
\]

where \( \alpha_1 \) and \( \alpha_2 \) are uniformly distributed random variables between 0.2 and 0.6 (1/sec).

A simple compression mode examined. The random texture field is approximated by Karhunen-Loeve expansion and truncated after three terms. The correlation matrix has been obtained from 500 samples.

Find the distribution of the three random variables and construct a mapping between three dimensional hypercube and the distribution of these variables.
Use sparse grid collocation to obtain the stochastic characteristic of macroscale properties.

<table>
<thead>
<tr>
<th>Effective strain</th>
<th>Effective stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>0.004</td>
<td>0.004</td>
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<tr>
<td>0.006</td>
<td>0.006</td>
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<tr>
<td>0.008</td>
<td>0.008</td>
</tr>
<tr>
<td>0.010</td>
<td>0.010</td>
</tr>
</tbody>
</table>

Mean of A at the end of deformation process

Variance of A at the end of deformation process

<table>
<thead>
<tr>
<th>$\bar{E}$ (MPa)</th>
<th>$\text{Var}(E)$ (MPa)²</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.41e05</td>
<td>4.42e08</td>
</tr>
<tr>
<td>1.41e05</td>
<td>4.39e08</td>
</tr>
</tbody>
</table>

Adaptive Sparse grid (level 8)
MC 10,000 runs

FCC copper

B. Kouchmeshky and N. Zabaras, Computational Materials Science 47 (2009) 342--352,
Curse of Dimensionality

- In the one way coupling, the uncertainty is localized, i.e. the random microstructures are not the same (from the same distribution) at different locations.

- In this case, the random support space is the tensor product of all the support of the random variables. It will result in thousands of random variables on the macroscale.

- Most of the computational methods are intractable unless we can find the correlation between all the microstructures and construct a reduced order model.
At each macro scale point, due to the randomness of the microstructure, we will have a set of (microstructure) samples (realizations).

One can construct a reduced order stochastic model for each point (e.g. linear or non-linear POD). However, in this case, the reduced-order model cannot see the correlation between the set of random variables at different macropoints.

This will result in a huge dimension of the random space and thus the problem becomes computationally intractable.
Model Reduction on Both Scales

- Define a microstructure using its corresponding texture (ODF) as $A(x, s, \omega)$, which is a function of macroscopic coordinate $x$, microscopic coordinate $s$, and the random event $\omega$.

- We will use the bi-orthogonal decomposition to construct the reduced order model.

\[
\tilde{a}(x, s, \omega) = \log(A(x, s, \omega) - A_{\min})
\]

\[
\tilde{a}(x, s, \omega) = \bar{a}(x, s, \omega) + \hat{a}(x, s, \omega)
\]

where \( \hat{a}(x, s, \omega) = \sum_{i=1}^{\infty} \sqrt{\rho_i} \psi_i(s) \Phi_i(x, \omega) \) (1)

where $\psi_i(s)$ are modes strongly orthogonal in microscale space and $\Phi_i(x, \omega)$ are spatial random modes weakly orthogonal in macroscale space [1].

\[
(\psi_i, \psi_j) := \int_{\mathcal{R}} \psi_i(s) \psi_j(s) ds = \delta_{ij} \quad (2) \quad (\Phi_i, \Phi_j)^\# = \delta_{ij} \quad (3)
\]

where \( (f, g)^\# := \int_{D} <f, g> dx \quad <f, g> := \int_{\Omega} f(\omega) g(\omega) P(\omega) d\omega \)

$D$ macroscale domain, $\mathcal{R}$ microscale domain, $\Omega$ random sample space

B. Kouchmeshky and N. Zabaras, Computational Materials Science 48 (2010) 213--227
From (1) and (3) we can have

$$\sqrt{\rho_i \psi_i (s)} = (\hat{a}(x, s, \omega), \Phi_i (x, \omega))^\# = \int_D \langle \hat{a}(x, s, \omega), \Phi_i (x, \omega) \rangle dx$$

$$= \int_D \int_\Gamma \hat{a}(x, s, \omega) \Phi_i (x, \omega) dP(\omega) dx \tag{4}$$

From (1) and (2),

$$\sqrt{\rho_i \Phi_i (x, \omega)} = \int_{\mathbb{R}} \hat{a}(x, s, \omega) \psi_i (s) ds \tag{5}$$

Now From (4) and (5) we can derive

$$\rho_i \psi_i (s) = \int_{\mathbb{R}} \int_D \int_\Gamma \hat{a}(x, s, \omega) \hat{a}(x', s', \omega) dP(\omega) \psi_i (s') ds' dx$$

$$= \int_{\mathbb{R}} \int_D \int_\Gamma \frac{1}{n_r} \sum_{j=1}^{n_r} \hat{a}(x, s, \xi_j) \hat{a}(x', s', \xi_j) dx \psi_i (s') ds'$$

$$\Rightarrow \rho_i \psi_i (s) = \int_{\mathbb{R}} \left( \frac{1}{n_r} \sum_{j=1}^{n_r} \sum_{i_n=1}^{n_{el}} \sum_{i_m=1}^{n_{int}} \hat{a}(x_{i_m}, s, \xi_j) \hat{a}(x_{i_m}, s', \xi_j) \hat{\eta}_{i_m} \left| J_{i_n} \right| \psi_i (s') ds' \right)$$

$$\Rightarrow \rho_i \psi_i (s) = \int_{\mathbb{R}} C(s, s') \psi_i (s') ds' \quad \text{An eigenvalue problem in microscale space}$$
Construct the Reduced Order Representation of Texture

Step 1: Start from realizations of the texture

\[ A_i(x, s, \omega) \]

Step 2: Transform the realization using

\[ \tilde{a}_i(x, s, \omega) = \log(A_i(x, s, \omega) - A_{\text{min}}) \]

\[ \tilde{a}_i(x, s, \omega) = \bar{a}(x, s, \omega) + \hat{a}_i(x, s, \omega) \]

Step 3: Construct the Covariance using the snapshots

\[ C(s, s') = \frac{1}{n_r} \sum_{j=1}^{n_r} \sum_{i_m=1}^{n_e} \sum_{i_n=1}^{n_l} \hat{a}_j(x_{i_m}, s, \xi_j) \hat{a}_j^T(x_{i_m}, s', \xi_j) \hat{\eta}_{i_m} | J_{i_n} | \]

Step 4: Obtain the eigenvalues and eigenvectors: \( \rho_i, \psi_i(s) \)

Step 5: Obtain the spatial modes

\[ \Phi_i(x, \omega) = \frac{1}{\sqrt{\rho_i}} \int_{\mathbb{R}} \hat{a}(x, s, \omega) \psi_i(s) ds \]

Step 6: Decompose the spatial modes using the polynomial Chaos:

\[ \Phi_i(x, \omega) := \Phi_i(x, \zeta_1(\omega), \ldots, \zeta_{n_\text{d}}(\omega)) = \sum_j \phi_{ij}(x) \eta_j(\omega) \quad \phi_{ij}(x) = \frac{\langle \Phi_i(x, \zeta) \eta_j \rangle}{\langle \eta_j^2 \rangle} \]

\( \eta_i(\omega) \) are in a one to one correspondence to the Hermite polynomials.
Comparison between the original microstructure and the reduced order one

Original

Reconstructed

Mean(B) Mpa
Mean(G) Mpa
Mean(E) Mpa
Mean(B) Mpa
Mean(G) Mpa
Mean(E) Mpa
Comparison between the original microstructure and the reduced order one

Original

Reconstructed
Use Reduced Order Model to Reconstruct Texture

(a) Distribution of Bulk modulus;
(b) Distribution of Young’s modulus;
(c) Distribution of Shear modulus.

For one point on macro-scale. The bars represent the distribution obtained using the realizations of the texture and the solid line is the distribution obtained using the reduced order model for the texture.

\[ \tilde{E} := \left\| \frac{X^{p+1} - X^p}{X^{p+1}} \right\|_{L_2(\Omega)} \]

The relative error with respect to the order of polynomial chaos.

Bars: obtained using the realizations of the texture that were used in constructing the covariance.
Solid line: Obtained from the sampling the random variables and constructing the texture using the reduced order modeling.
Deterministic Solver: Multiscale forging FE simulation.

Macro

\[ \int_{B_n} \left( \mathbf{P}_r \cdot \nabla_n \tilde{\mathbf{u}} \right) dV_n = \int_{\Gamma_n} \mathbf{t} \cdot \tilde{\mathbf{u}} dA_n \]

formulation for macro scale
Update macro displacements

Macro-deformation gradient

Texture evolution update
Polycrystal averaging for macro-quantities
Integration of single crystal slip and twinning laws

\[ \tau^\alpha = \mathbf{T} \cdot \mathbf{S}^\alpha \]
After the interpolation in the stochastic space for the texture have been obtained one can use them to obtain the realizations of the texture. Using these realizations statistics of the macro-scale properties can be obtained.
Comparison of Mean and variance of the macro-scale properties with MC, Top left: Bulk modulus, Top right: Young modulus, Bottom: Shear modulus
Define a complete probability space \((\Omega, \mathcal{F}, \mathcal{P})\). We are interested to find stochastic functions \(u : \Omega \times D \to \mathbb{R}, p : \Omega \times D \to \mathbb{R}\) and \(S : \Omega \times [0, T] \times D \to \mathbb{R}\) such that for \(P\)-almost everywhere (a.e.) \(\omega \in \Omega\), the following holds:

\[
\nabla \cdot u(x, \omega) = 0, \quad u(x, \omega) = -K(x, \omega) \nabla p(x, \omega) \quad \forall x \in D
\]

\[
\frac{\partial S(x, t, \omega)}{\partial t} + u(x, t, \omega) \cdot \nabla S(x, t, \omega) = 0, \quad \forall x \in D, t \in [0, T]
\]

with the boundary condition

\[
p = \bar{p} \text{ on } \partial D_p, \quad u \cdot n = 0 \text{ on } \partial D_u.
\]

Length scale of the system,

Length scale of permeability variation,

**Multiscale paradigm**: Construct a strategy that solves for the coarse-scale features while accounting for the fine-scale features.

But exact permeability unknown. Some statistics or limited data.

Permeability is a realization from corresponding probability space \(K(\omega, .) \in \Omega\).
Solution Methodology: Stochastic Heterogeneous Multiscale Method

1. Generate collocation point
2. Generate the permeability sample given the collocation point, set coarse discretization
3. Compute the stiffness matrix for each coarse element
4. Compute the stochastic coarse-scale fluxes
5. Solve the subgrid problems for each basis function at quadrature points
6. Reconstruct the fine-scale velocity
7. Solve the transport problem
8. Solve the subgrid problems with coarse-scale flux
9. Return function value at collocation point
10. Solve stochastic multiscale problem with HDMR
11. POSTPROCESSING: Compute the statistics of the solution

Ma & Zabaras (2010)
Example

Fine-scale grid: 100×100
Coarse-scale scale grid: 20×20

\[ Y(\omega) = \log(K(\omega)) = \sum_{i=1}^{N} \sqrt{\lambda_i} \phi_i(x) Y_i \]

\[ \text{Cov}(x, y) = \sigma^2 \exp\left( -\frac{|x_1 - y_1|}{L} - \frac{|x_2 - y_2|}{L} \right) \]

where \( Y \) is a zero mean Gaussian random field with covariance function

\( L \) is the correlation length and \( \sigma \) is the standard deviation.
\[ L = 0.25, \quad \sigma = 0.2 \]

Therefore, we truncate the stochastic dimension after 50 terms.
Mean of the saturation at 0.4 PVI

MC method with deterministic problem solved on fine-scale grid directly

HDMR method with deterministic problem solved on coarse-scale grid and then solve the transport equation using reconstructed fine-scale velocity
MC method with fine scale solver

HDMR method with multiscale solver

➢ The saturation front has the largest variation occurred.