Representing Material Structure

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Hierarchical Material Structure

Kalidindi and DeGraef, ARMS, 2015
Well-Separated Length Scales and RVEs

Key Assumptions
- Homogenization length scales $L$ and $l$ exist (allows definition of material constitutive laws at these length scales)
- No major gradients occur at these length scales (fluctuations – even large ones – are allowed)
- $\omega_l$: length scale of a representative (structure) volume element (RVE)
- Well-separated length scales: $l < \omega_l \ll L$

Challenges: Interfaces, Atomistics
Local States and Local State Spaces

- **Local State**: a set of material structure attributes needed to completely specify all of the relevant material properties of interest at the selected length scale.

- **Local State Space**: the complete set of all theoretically possible local states one might expect to encounter in a given material system (including all the local states that may not even be present in a given sample of the selected material system)

Example: Multiphase Composites

\[
h = (\rho, c_i) \\
H = \{(\rho, c_i) | \rho \in \{\alpha, \beta, \gamma, \ldots\}, c_i \in C_i^\rho\}
\]
Polycrystalline Microstructures

\[
h = (\rho, c_i, g) \\
H = \{ (\rho, c_i, g) | \rho = (\alpha, \beta, \gamma, ...), c_i \in C_i^\rho, g \in FZ_\rho \}\]
Microstructure Function

\[ h(x, t) \]

- Deterministic
- Impractical to implement in practice due to the resolution limits and uncertainty inherent to the characterization techniques used
- Does not allow for the presence of mixed local states (e.g., grain/phase boundary region)
Microstructure Function

\[ m(h, x, t) \text{ or } m(h, x) \]

- Defined as the probability density associated with finding local state \( h \) at the spatial location \( x \) at time \( t \)

- Captures the probability of finding one of the local states that lie within a small interval \( dh \) centered around \( h \) at a selected \( x \); \( m(h, x)dhdx \) would represent the probability and \( m(h, x) \) the corresponding probability density

- Experiments typically produce only discretized information suitable to evaluating \( m(h, x) \)

Digital Representations

• Information is stored in discrete units
• Many examples in images, music, and videos; has completely transformed these domains
• Involves discretization (sampling) and quantization (rounding)
• Most experimental materials datasets are already digitized
• Much less in materials simulation datasets – but there are good reasons to pursue digital representations
• Digital representations allow us to exploit the tools of digital signal processing (DSP)
Discretized Microstructure Function

\[ m(h, x) \]

\[ \{ m_s^n | s = 0, 1, 2, ..., S - 1; n = 1, 2, ..., N \} \]

\[ m_s^n \] represents the total volume fraction of all local states from bin \( n \) in the spatial bin \( s \)

\[ \sum_{n=1}^{N} m_s^n = 1, \quad 0 \leq m_s^n \leq 1 \]
Discretized Microstructure Function

\[ s = (s_1, s_2) \]

\[ m_{(1,2)}^1 = 1, \quad m_{(1,2)}^2 = 0 \]

\[ m_{(2,1)}^1 = 0, \quad m_{(2,1)}^2 = 1 \]

Eigen microstructures
Discretized Microstructure Function

\[ m(h, x) \approx \sum_{\tilde{n}=1}^{N} \sum_{s=0}^{S-I} m_s^n \chi_n(h) \chi_s(x) \]

\[ m(h, x) = \sum_{n=1}^{N} \sum_{k=-\infty}^{\infty} M_k^n \frac{e^{i2\pi k \cdot x}}{L} \chi_n(h) \]

\[ m(g, x) = \sum_{s=0}^{S-I} \sum_{\mu, n, l} M_{ls}^{\mu n} \tilde{T}_l^{\mu n} (g) \chi_s(x) \]

\[ m(c, x) = \sum_{s=0}^{S-I} \sum_{n} M_s^n P^n (c) \chi_s(x) \]
Microstructure Ensemble

\[ \{(j)m^n_s; j = 1, 2, ..., J\} \]

a microstructure versus the microstructure

(SVE) (RVE)
Microstructure Statistics

\[ m(h, x) \approx \sum_{\tilde{n}=1}^{N} \sum_{s=0}^{S-I} m_s^n \chi_n(h) \chi_s(x) \]

\[ f_s^n = \frac{1}{J} \sum_{j=1}^{J} (j)m_s^n \quad j = 1, 2, \ldots, J \]

\[ f^n = \frac{1}{SJ} \sum_{j=1}^{J} \sum_{s} (j)m_s^n \]

1-point spatial correlations or 1-point statistics
Microstructure Statistics

2-point spatial correlations or 2-point statistics

\[
f_{rs}^{np} = \frac{1}{J} \sum_{j=1}^{J} (j)m_s^n (j)m_{s+r}^p
\]

\[
f_{r}^{np} = \frac{1}{S_r} \frac{1}{J} \sum_{s} \sum_{j=1}^{J} (j)m_s^n (j)m_{s+r}^p
\]

\(S_r\) is the number of spatial bins that allow the placement of both \(s\) and \(s+r\) with the microstructure volume being studied.

\(r\) indexes bins in vector space

Periodic Boundaries: \(S_r = S\)
**Microstructure Statistics**

**Non-periodic Boundaries**

\[ \mathbf{r} = r_1 \mathbf{i} + r_2 \mathbf{j} + r_3 \mathbf{k}, \quad S = S_1 S_2 S_3 \]

\[ S_r = (S_1 - |r_1|)(S_2 - |r_2|)(S_3 - |r_3|) \]

\[ f_{np}^r = \frac{\sum_s \Sigma_{j=1}^J (j) m_s^n (j) m_{s+r}^p}{S_r J} = \frac{\# \text{ Successes}}{\# \text{ Trials}} \]
Redundancies in 2-pt. Statistics

\[
f_r^{np} = \begin{pmatrix}
 f_r^{11} & \cdots & f_r^{1N} \\
 \vdots & \ddots & \vdots \\
 f_r^{N1} & \cdots & f_r^{NN}
\end{pmatrix}
\]

\[
f_r^{np} = f_r^{-pn} \quad \sum_{p=1}^{N} f_r^{np} = f^n
\]

For a two-phase material, if \(f_r^{11}\) is known then \(f_r^{12}, f_r^{21}\) and \(f_r^{22}\) can be calculated.

Niezgoda et al., Acta Materialia, 2008. 56(18), p. 5285-5292: Only (N-1) independent correlations (using DFTs)
Implicitly assume periodic boundaries

\[ f_{r}^{np} = \frac{1}{S_r} \sum_{s} m_s^n m_s^p \]

\[ M^n_k = \Im(m^n_s) = \sum_{s=0}^{S-1} m^n_s e^{2\pi i s \cdot k/S} \]

\[ F^{np}_k = \Im(f^{np}_r) = \frac{1}{S} M^n_k M^p_k \]

\[ f_{r}^{np} = f_{r}^{np*} \Rightarrow F^{np}_k = F^{np*}_{(S-1)-k} \]

Autocorrelations: \[ F^{nn}_k = F^{nn*}_k \]
Plotting 2-pt. Statistics Using DFTs

\[ M^n_k = \mathcal{S}(m^n_s) = \sum_{s=0}^{S-1} m^n_s e^{2\pi is \cdot k/S} \quad s = 0, 1, ..., S - 1 \]

\[ F^{np}_k = \mathcal{S}(f^{np}_r) = \frac{1}{S} M^{n^*}_k M^p_k \quad r = 0, 1, ..., S - 1 \]

Plotting: \( r = -(S - 1)/2, ..., -1, 0, 1, ..., (S - 1)/2 \)

\( (r = -S/2, ..., -1, 0, 1, ..., S/2 \text{ when } S \text{ is even}) \)

\[ f^{np}_r = f^{np}_{r+S} \]
Plotting 2-Point Correlations

- Image is converted into a smooth continuous pdf
- pdf allows easy statistical operations: mean, variance, ...
- Dominant features of the pdf can be connected to properties and tracked in manufacturing processes
Reconstruction from 2-pt Statistics

Original microstructure of 130x130x130 volume elements with orientation space binned into 512 distinct orientations. The far right shows bin 35 as blue and bin 5 as red in the original microstructure.

Bottom: Bins 35 and 5 are reconstructed exactly up to a linear shift!
Coherence Length

Coherence length (C) provides guidance on scan sizes

$$\lim_{|r| \to C} \frac{f_2(h, h'|r)}{f(h)f(h')} = 1$$

Example Digitally Created Microstructure:
Average Feature Size \(\sim 15\) pixels
Coherence Length for Auto-correlation \(\sim 125\) pixels
Features of Interest

Many local features of interest can be identified based on concepts of n-point statistics.
RVE

Elastic Modulus

RVE: 111 GPa
Sample: 111 GPa

Critically Stressed Volume Fraction

RVE: 0.0866
Sample: 0.0897
3% Error
Weighted SVE Sets

Critically Stressed Volume Fraction in Sample = 0.0897

0.0810
9.9% Error

0.0909
1.3% Error

0.0974
8.6% Error
Microstructure Representation

- Thinking of microstructure as a **digital signal** allows a generalized treatment at multiple hierarchical length/structure scales: $m^h_s$
- Intuitive measures of microstructure: average grain size, average spacing, ODF, MODF, ...
- Naturally organized extensible measures of microstructure: **n-point statistics**
- **Data Analytics**: seek objective low-dimensional representations for process-structure-property relationships
Dimensionality Reduction

Intuition and/or Known Physics and/or Data Driven

- Axes prioritized based on variance in the data
- Unsupervised (i.e., uninformed) and Independent
Hypothesis: PCA weights of $n$-point statistics provide objective measures of microstructure

$$f_r^{(j)} = \sum_{k=1}^{\min((J-1),R)} \alpha_k^{(j)} \varphi_{kr} + \bar{f}_r$$
Microstructure Databases

Data from H. Fraser’s group at OSU
Microstructure Databases

- Each point corresponds to a microstructure dataset.
- Datasets from the same heat treatment are shown as a hull.
- Volume of the hull can be related directly to the variance in structure between datasets.
- Euclidean distance is a metric of similarity or difference between samples.
- Quality control applications
Microstructure Databases

Figure 1(a)

Figure 2(a)

Figure 2(b)

Figure 2(c)

Figure 2(d)
Unsupervised Classification of Different Potentials Based on Atomic Structure

Collaboration with Becker and Trautt (NIST)
Visualization of 4-D Microstructure Datasets

Datasets from phase-field simulations of microstructure evolution (3-D space + time)
Overall Framework
Code Repositories

• **Spatial Statistics**

• **PyMKS**