Stochastic non-local lattice particle method for voxel level uncertainty quantification and material failure analysis

Yongming Liu*[1], Yi Gao[1], Haoyang Wei[1], Hailong Chen[2], Yang Jiao[1]

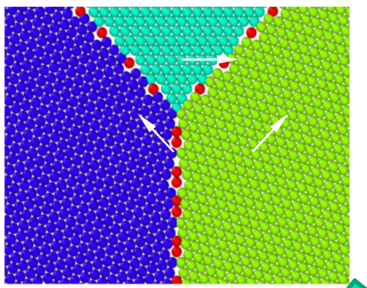
[1]*School for Engineering of Matter, Transport & Energy*
Arizona State University, Tempe, AZ, 85287

[2]*Mechanical Engineering Department*
University of Kentucky, Lexington, KY 40506

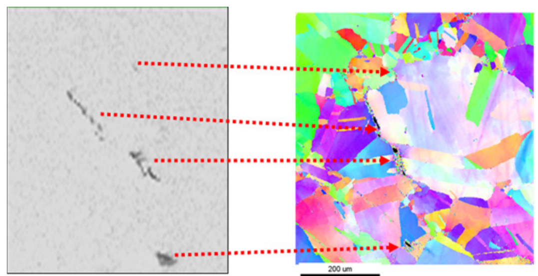
Outline

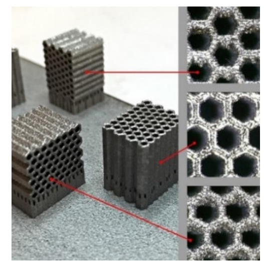
- Introduction and background
- *Extreme dimension* probabilistic computational material analysis
  - Pixel (Voxel) level deterministic mechanics model
  - Pixel (Voxel) level uncertainty quantification
  - Pixel (Voxel) level probabilistic solver
- Demonstration examples for Adjoint Lattice Particle Method (ALPM)
- Conclusions and future challenges

Introduction – extreme dimension in probabilistic computational materials

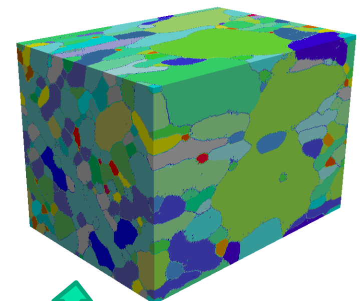


High fidelity computational model





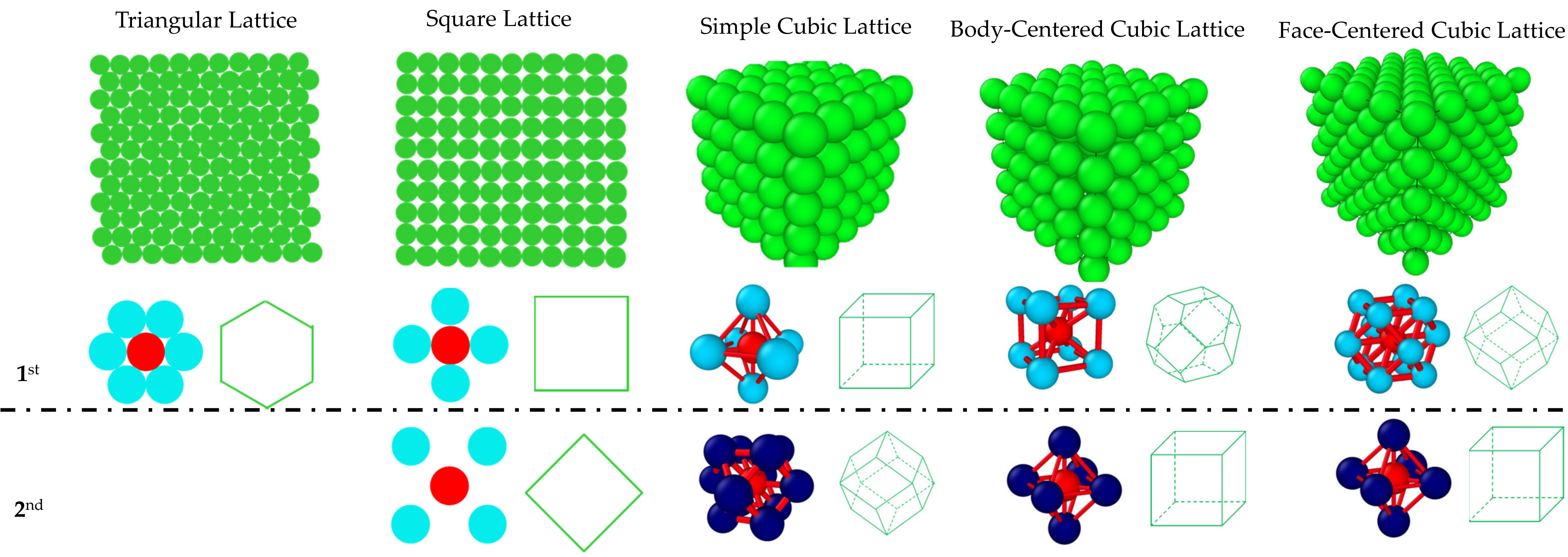
Observed randomness from multimodality imaging



High fidelity uncertainty quantification

- High fidelity model is preferred and sometime required
- The highest resolution is determined by image pixels/voxels
- Pixel/voxel level model for both mechanic model and UQ
- Issue: extreme dimension, especially for probabilistic analysis

Pixel/Voxel level computational mechanics model - nonlocal LPM 1



H. Chen, and Y. Liu. International Journal of Solids and Structures.

Pixel/Voxel level computational mechanics model - nonlocal LPM 2

The potential of a particle in terms of the spring elongation:

$$U_{particle} = \sum_{I=1}^{N_{cell}} U_{cell}^{I} = \sum_{I=1}^{N_{cell}} \left(\frac{1}{2} \sum_{J=1}^{N_I} k_{IJ} (\delta l_{IJ})^2 + \frac{1}{2} \left(\sum_{J=1}^{N_I} T_{IJ} \delta l_{IJ} \right) \left(\sum_{J=1}^{N_I} \delta l_{IJ} \right) \right)$$

The potential of a particle in terms of the strain components:

$$U_{continuum} = \sum_{I=1}^{N_{cell}} \frac{1}{2} (l_0^I)^2 \left(\sum_{b=1}^{N_I} k_{Ib} n_i^{Ib} \varepsilon_{ij} n_j^{Ib} n_k^{Ib} \varepsilon_{kl} n_l^{Ib} + \left(\sum_{b=1}^{N_I} T_{Ib} n_i^{Ib} \varepsilon_{ij} n_j^{Ib} \right) \left(\sum_{b=1}^{N_I} n_k^{Ib} \varepsilon_{kl} n_l^{Ib} \right) \right)$$

N_{cell} number of unit cells N_I number of neighbors for unit cell I l_0^I half length of a original spring of unit cell I

n_i^{Ib} the ith component of unit normal vector of unit cell I in the b direction ε_{ij} the strain matrix component

The potential is conservative, thus the material stiffness matrix can be obtained as :

$$U_{particle} = U_{continuum} \quad \Longrightarrow \quad C_{ijkl} = \frac{1}{V_1} \frac{\partial^2 U_{particle}}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

V_1 the volume of unit cell for the first nearest neighbors

H. Chen, and Y. Liu. International Journal of Solids and Structures.

Pixel/Voxel level computational mechanics model - nonlocal LPM 3

ARIZONA STATE UNIVERSITY

Analytical solution for model parameters

	2D Isotropic		3D Isotropic		
	TRI	SQR	SC	BCC	FCC
Plane strain	$k=\frac{4E}{\sqrt{3}(1+v)}$ $T=\frac{2\sqrt{3}}{9}\frac{E(4v-1)}{(1+v)(1-2v)}$	$k_1=\frac{2E}{1+v}$, $k_2=\frac{E}{1+v}$ $T=\frac{E(4v-1)}{6(1+v)(1-2v)}$	$k_1=\frac{2RE}{1+v}$, $k_2=\frac{2RE}{1+v}$ $T=\frac{RE(4v-1)}{9(1+v)(1-2v)}$	$k_1=\frac{2\sqrt{3}RE}{(1+v)}$, $k_2=\frac{4\sqrt{3}RE}{3(1+v)}$ $T=\frac{\sqrt{3}RE(4v-1)}{7(1+v)(1-2v)}$	$k_1=\frac{2\sqrt{2}RE}{1+v}$, $k_2=\frac{\sqrt{2}RE}{2(1+v)}$ $T=\frac{\sqrt{2}RE(4v-1)}{12(1+v)(1-2v)}$
Plane stress	$k=\frac{4E}{\sqrt{3}(1+v)}$ $T=\frac{2\sqrt{3}}{9}\frac{E(3v-1)}{(1+v)(1-v)}$	$k_1=\frac{2E}{1+v}$, $k_2=\frac{E}{1+v}$ $T=\frac{E(3v-1)}{6(1+v)(1-v)}$			

Pixel/Voxel level computational mechanics model - nonlocal LPM 4

Solution algorithm - atomic finite element method (AFEM)

The **total energy** of the particle system is a function of the particle positions

$$E_{total}(\mathbf{x}) = U_{total}(\mathbf{x}) - \sum_{I=1}^{N} \bar{\mathbf{f}}_{ext}^{I} \cdot \mathbf{x}_I \qquad \text{with} \qquad U_{total} = \sum U_{particle}(\mathbf{x})$$

Taylor expansion of the total energy gives

$$E_{total}(\mathbf{x}) \approx E_{total}\left(\mathbf{x}^{(0)}\right) + \left.\frac{\partial E_{total}}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{(0)}} \cdot \left(\mathbf{x} - \mathbf{x}^{(0)}\right) + \frac{1}{2}\left(\mathbf{x} - \mathbf{x}^{(0)}\right)^{T} \cdot \left.\frac{\partial^2 E_{total}}{\partial \mathbf{x} \partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{(0)}} \cdot \left(\mathbf{x} - \mathbf{x}^{(0)}\right)$$

$$\mathbf{K}_I = \begin{bmatrix} \frac{\partial^2 U_{total}}{\partial x_I \partial x_I} & \frac{\partial^2 U_{total}}{\partial x_I \partial y_I} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial x_1} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial y_1} & \cdots & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial x_{18}} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial y_{18}} \\ \frac{\partial^2 U_{total}}{\partial y_I \partial x_I} & \frac{\partial^2 U_{total}}{\partial y_I \partial y_I} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial x_1} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial y_1} & \cdots & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial x_{18}} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial y_{18}} \\ \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial x_1} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial y_1} & 0 & 0 & \cdots & 0 & 0 \\ \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial x_1} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial y_1} & 0 & 0 & & & 0 \\ \vdots & \vdots & \vdots & & \ddots & & \vdots \\ \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial x_{18}} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial x_I \partial x_{18}} & 0 & & & 0 & 0 \\ \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial x_{18}} & \frac{1}{2}\frac{\partial^2 U_{total}}{\partial y_I \partial y_{18}} & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

The state of minimal energy:

$$\frac{\partial E_{total}(\mathbf{x})}{\partial \mathbf{x}} = 0 \quad \Rightarrow$$

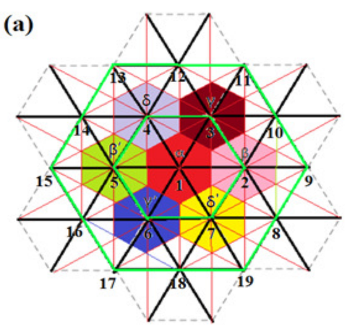
The Governing Equation:

$$\boldsymbol{Ku} = \boldsymbol{Q}$$

$$\mathbf{K} = \left.\frac{\partial^2 E_{total}(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{(0)}} = \left.\frac{\partial^2 U_{total}(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{(0)}}$$

$$\mathbf{Q} = -\left.\frac{\partial E_{total}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{(0)}} = \bar{\mathbf{f}}_{ext} - \left.\frac{\partial U_{total}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{(0)}}$$

(a)

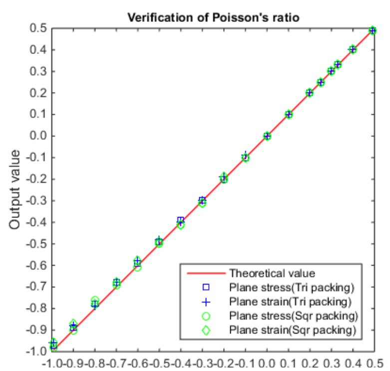


Lin, E., H. Chen and Y. Liu, Finite Elements in Analysis and Design.

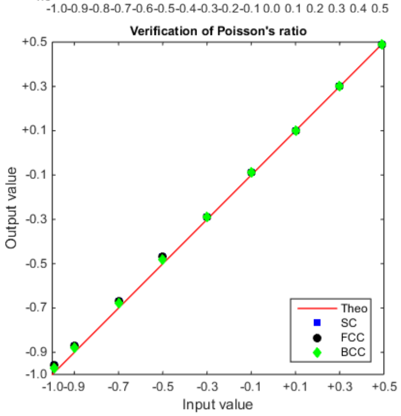
Pixel/Voxel level computational mechanics model - model verification

1. Poisson’s ratio verification

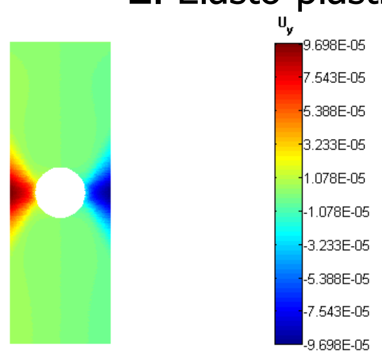
2D

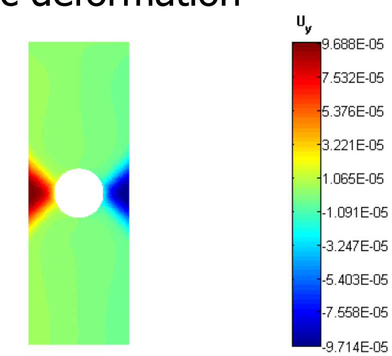


3D

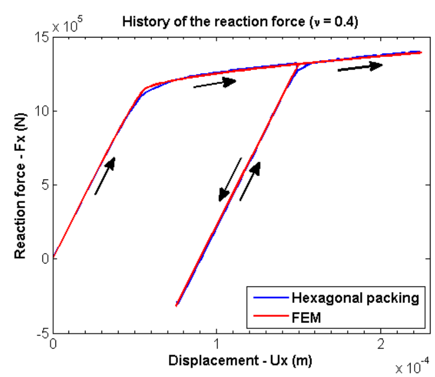


2. Elasto-plastic deformation

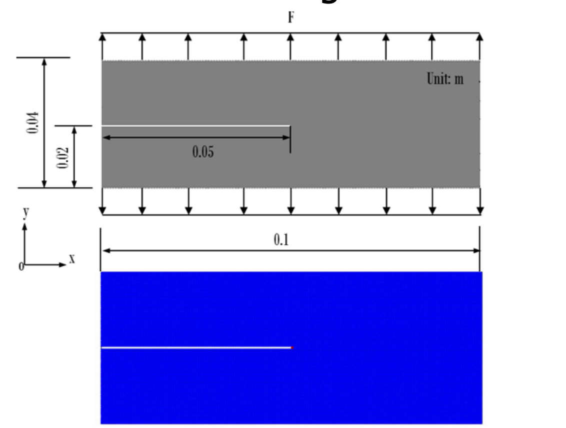


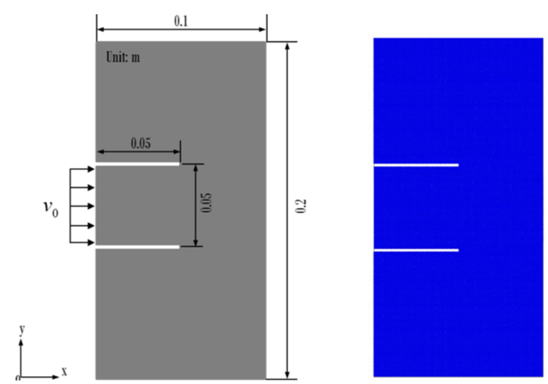


LPM **FEM**



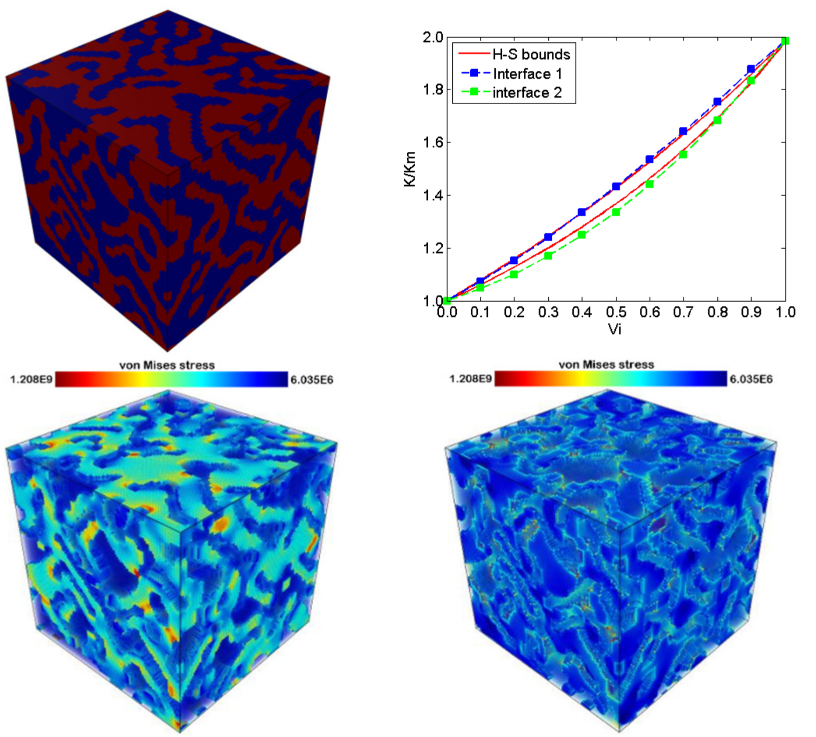
3. Crack branching under tension



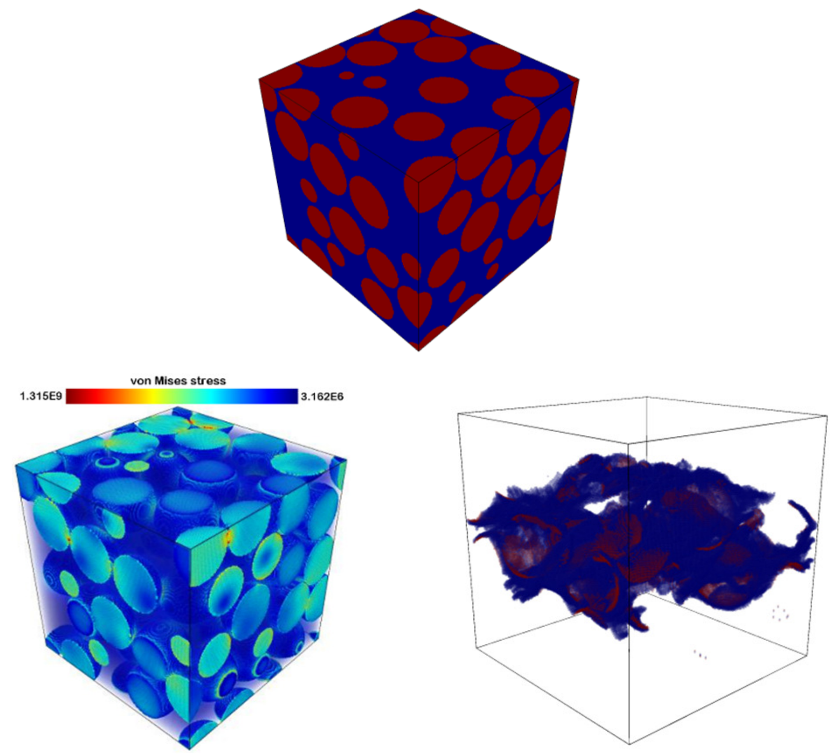


Pixel/Voxel level computational mechanics model - demonstration

1. Deformation (Bi-continuous case)

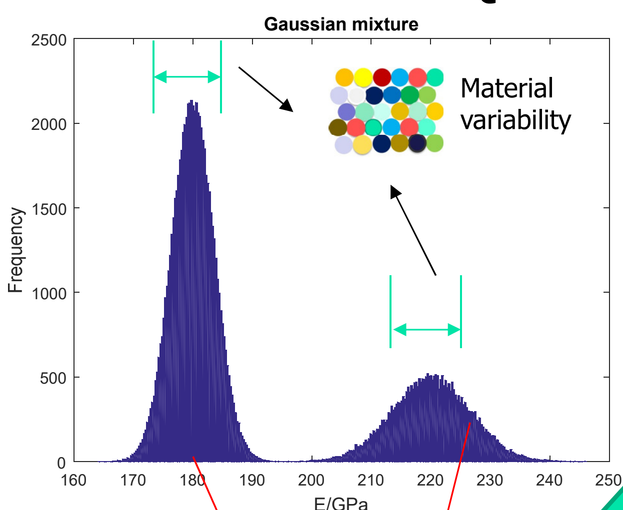


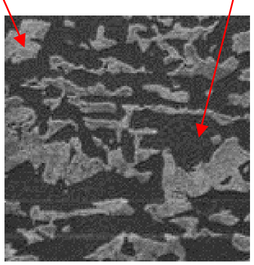
2. Fracture (Particulate reinforcement)

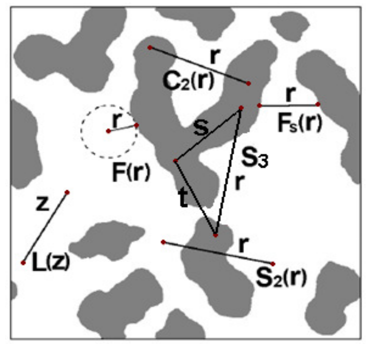


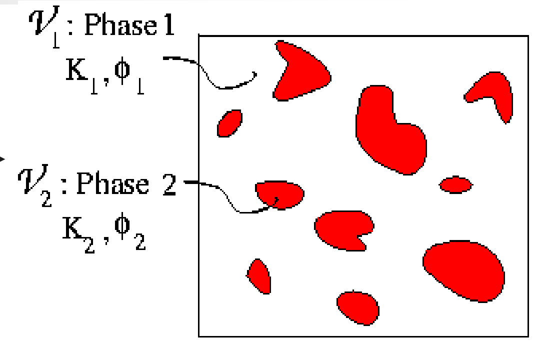
Pixel/Voxel level uncertainty quantification – UQ from two sources

Pixel level UQ







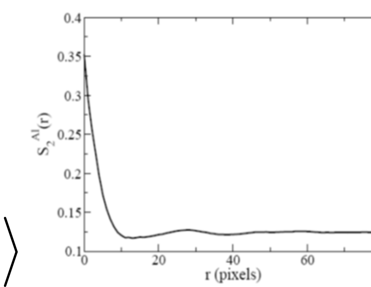


Phase Indictor Function

$$I^{(i)}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in V_i \\ 0 & \text{otherwise} \end{cases}$$

n-Point Correlation Function

$$S_n^{(i)}(\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_n) = \left\langle I^{(i)}(\mathbf{x}_1) I^{(i)}(\mathbf{x}_2) \ldots I^{(i)}(\mathbf{x}_n) \right\rangle$$



Correlation Function