Multiscale and Multidimensional Uncertainty Quantification in Integrated Computational Materials Engineering (ICME)

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Faculty Collaborators: Jian Cao, Wing Kam Liu

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ICME: Integrated Computational Materials Engineering

ICME Focus: Integrating data science, materials modeling, and manufacturing to design and deploy advanced materials systems

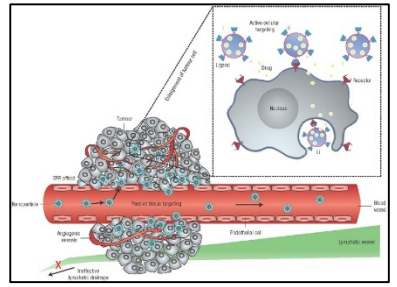
Wind & Solar Energies

Wang, C., et al. (2013). *Scientific reports, 3*.

Defense

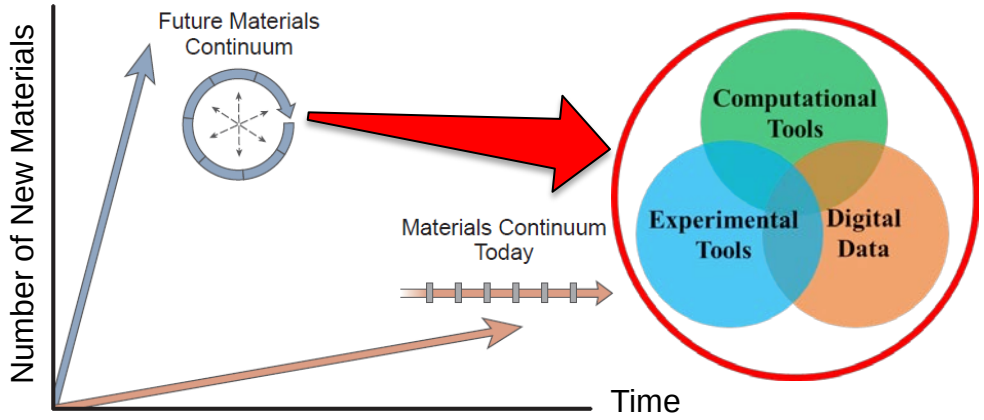
Chung, H.-S., et al. (2002). *AIAA, 317*, 14.

Drug Delivery

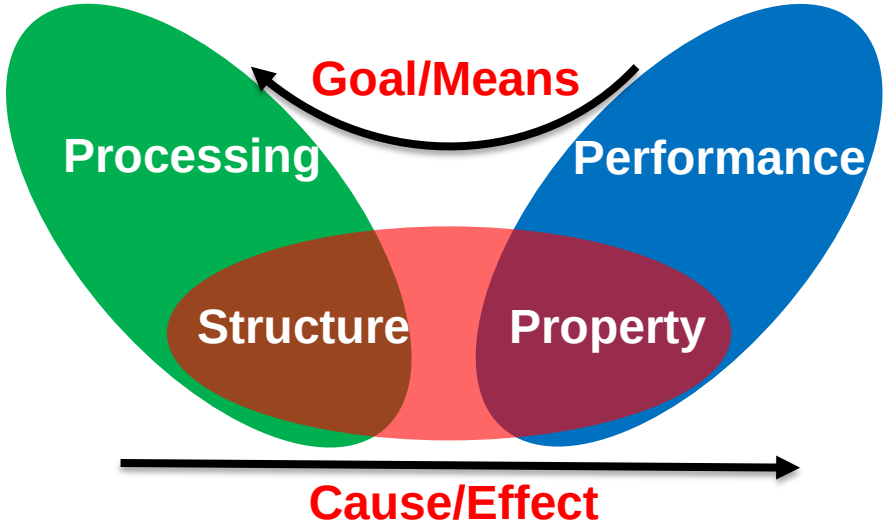


Peer, D., et al. (2007). *Nat Nano, 2*(12), 751.

Materials Genome Initiative (MGI)



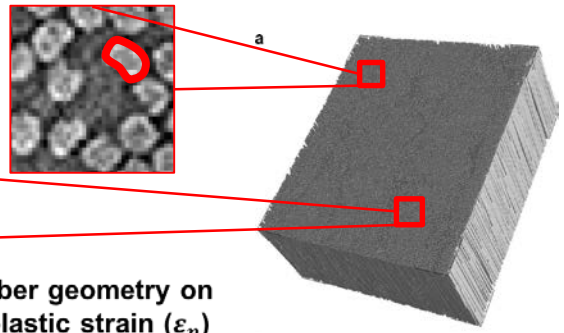
White, Ashley. *MRS Bulletin,* 37.08 (2012): 715-716.

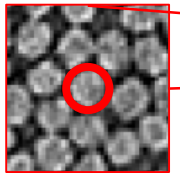


Olson, G. B. (1997). *Science, 277*(5330), 1237.

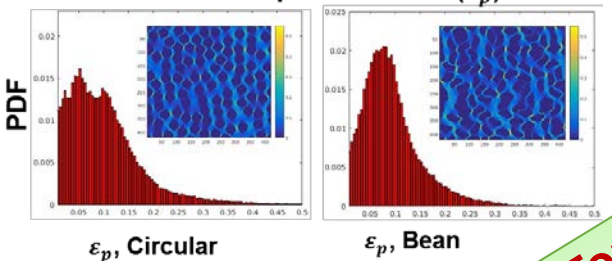
Microstructure Variations in Multiscale Carbon Fiber Reinforced Composites (CFRPs)

Spatial Variations:
- Fiber shape
- Fiber volume fraction

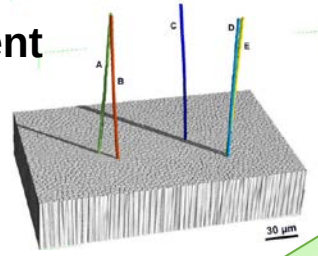




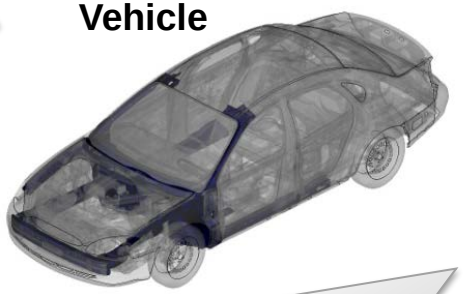
Effect of fiber geometry on effective plastic strain (ε_p)



Misalignment



Vehicle

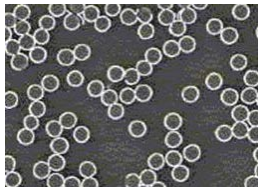


Sub-System

Component

Laminate

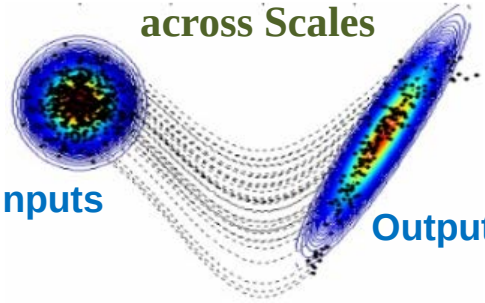
Microstructure: fiber & matrix



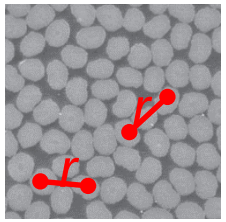
Top-down Goal-Driven Material Design

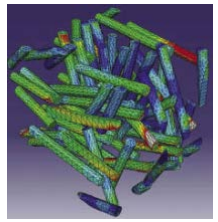
Bottom-up Stochastic Analysis & Modeling

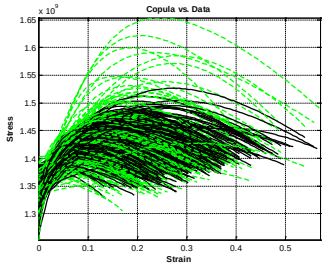
Uncertainty Propagation across Scales



Microstructure Modeling: Characterization & Reconstruction





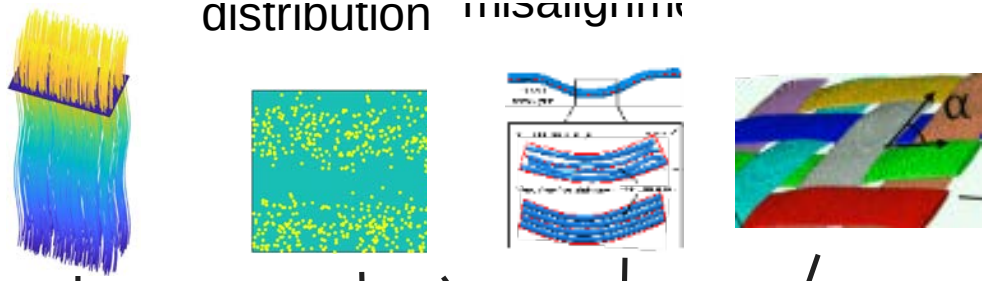


Stochastic Constitutive Relation

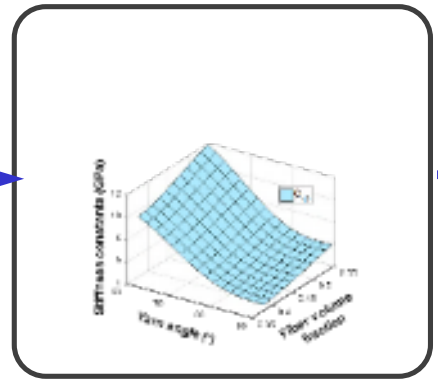
Reduce component weight (≥25%) and production cost (≤$4.27/lb)

Uncertainty Quantification in ICME of Light-Weight Composites

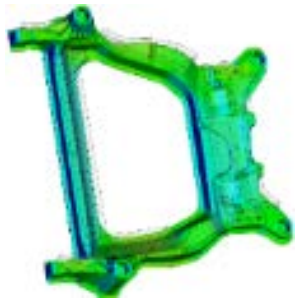
Source of Uncertainty



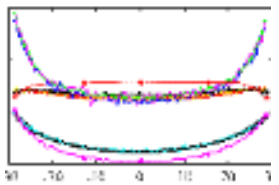
Parametric micro and meso RVE Library



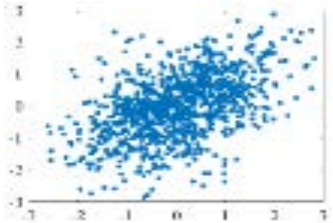
Maro model with spatial variations



Response Analysis



Gaussian Process Model



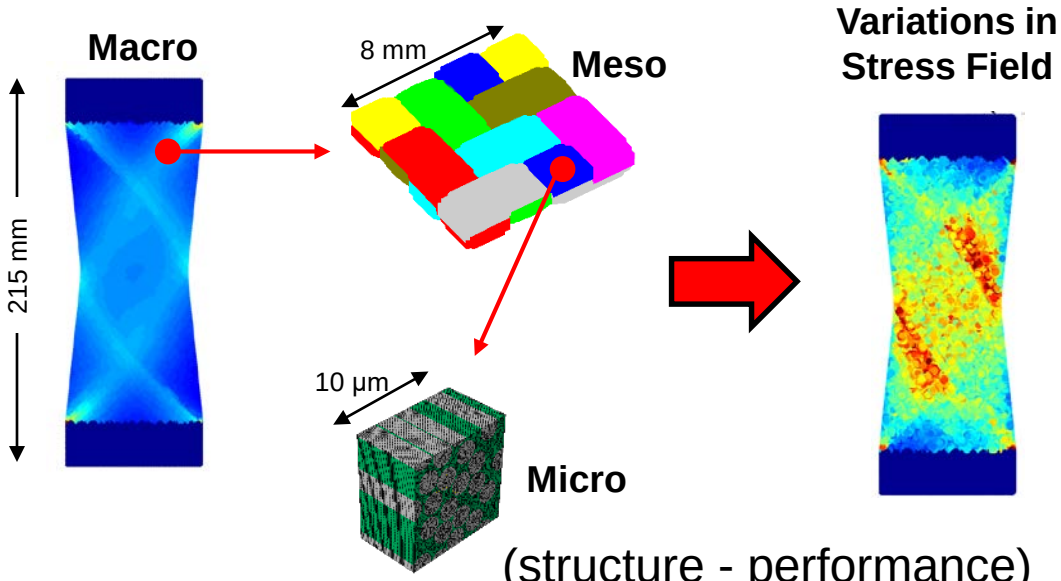
Developed to create spatial variations at different length scales

Uncertainty propagate from micro and meso scale level to macro scale level

Outline of Research Topics

1. Statistical Microstructure Characterization & Reconstruction

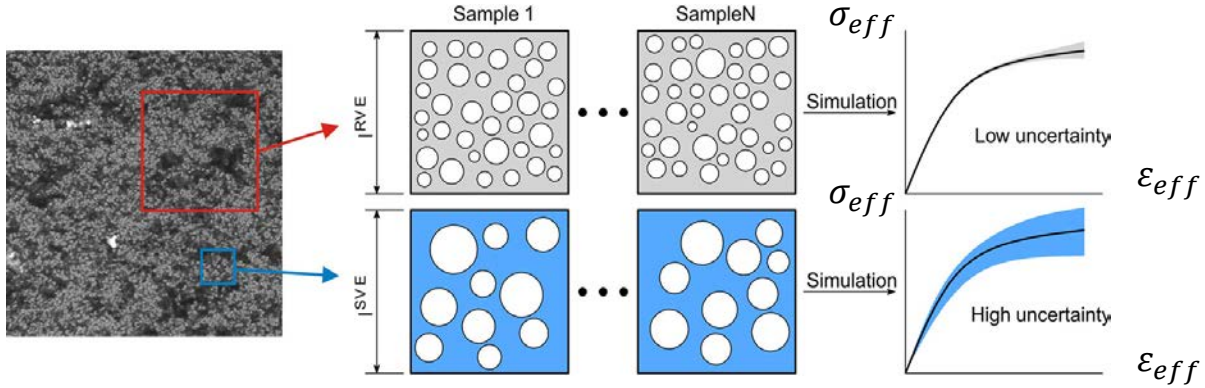
H. Xu, et al. *JMD* 135 (2013) 101010.
M.S. Green, et al. *CMAME* 254 (2013): 271-291.



(structure - performance)

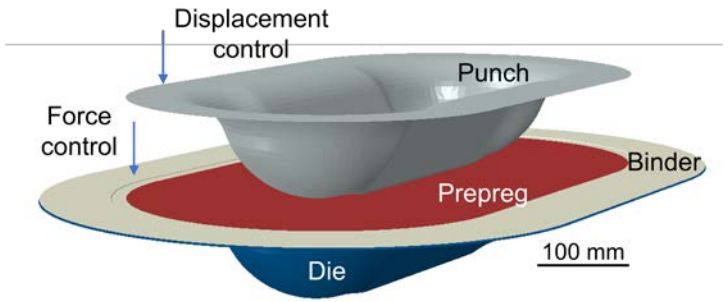
3. Bayesian Validation and Calibration of Multiscale Simulators

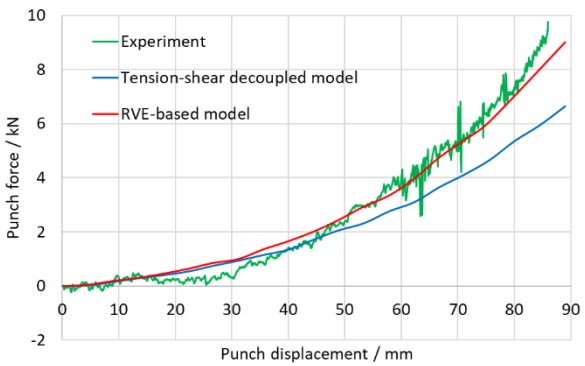
Zhang, et al., Composite Technology, 2018



2. Uncertainty Quantification and Propagation in Multiscale Materials

Bostanabad, R., et. al. (2018) *CMAME*, 338, 506-532.





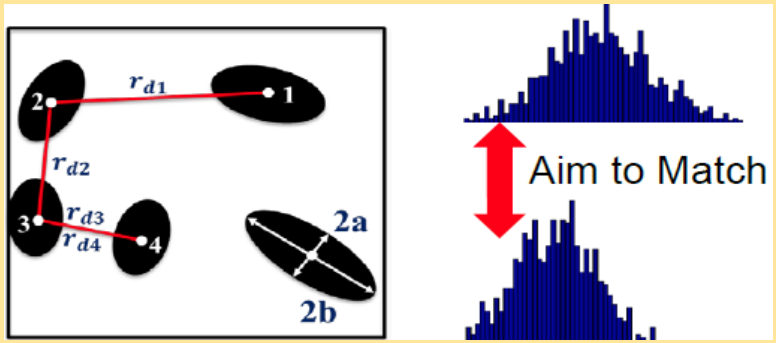
(processing – structure)

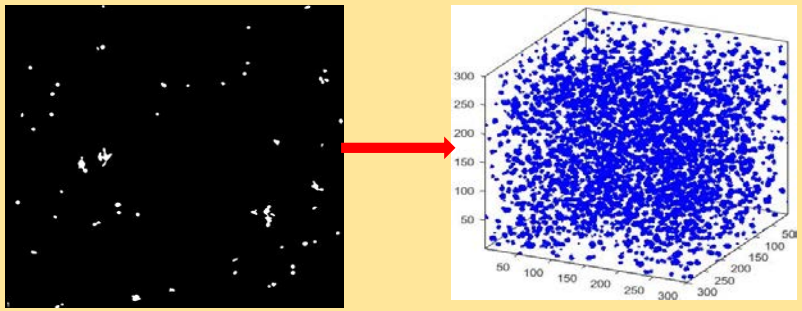
Microstructure Characterization and Reconstruction (MCR)

Objective: Stochastically characterize and subsequently reconstruct the microstructure to enable automation of material design

Physical Descriptors

- **Characterization via important structural parameters**
- **Reconstruction via hierarchical optimization**

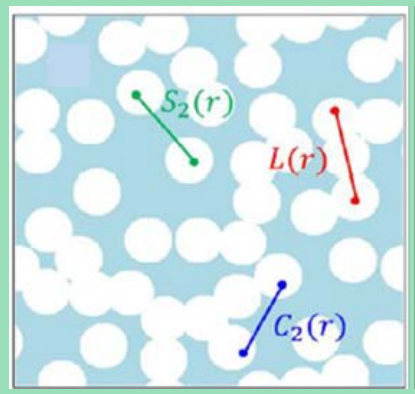


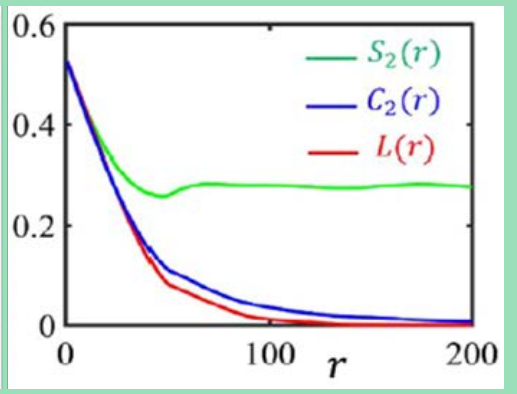


Xu, H. et. al. (2014) J Mech Design, 136, 051007.

Statistical Functions

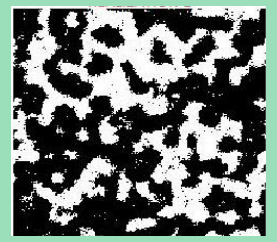
- **Spatial correlations characterized in a probabilistic sense:**

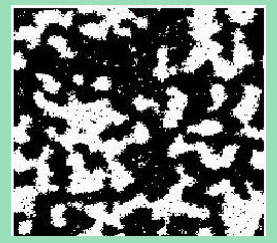


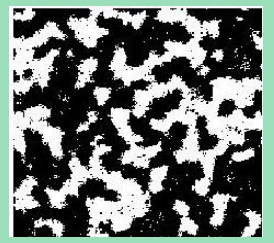


Target Image

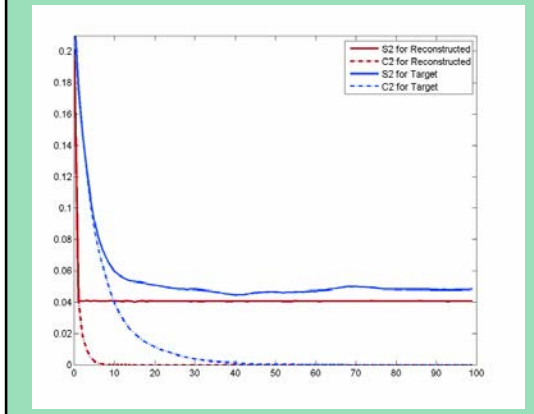
Statistically Equivalent Reconstructions

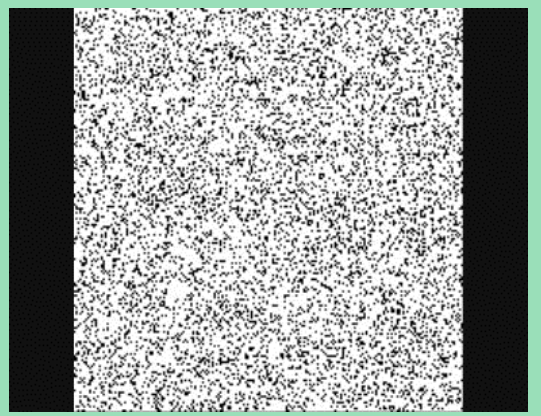






- **Reconstruction by optimization:**



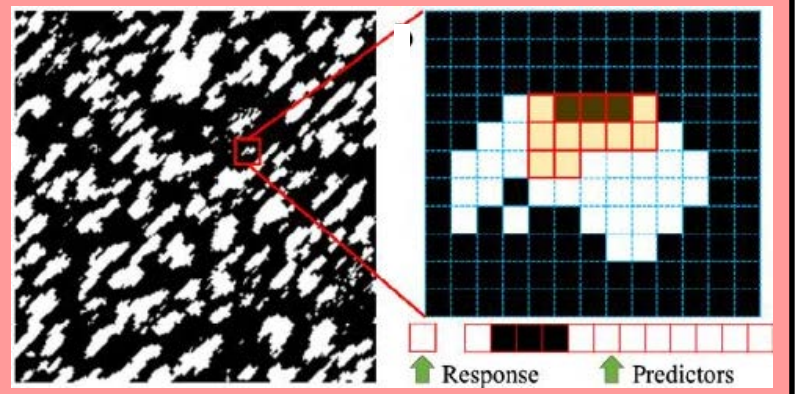


Torquato. S., et al. *J Chen Phys* 77 (1982) 2071-2077.

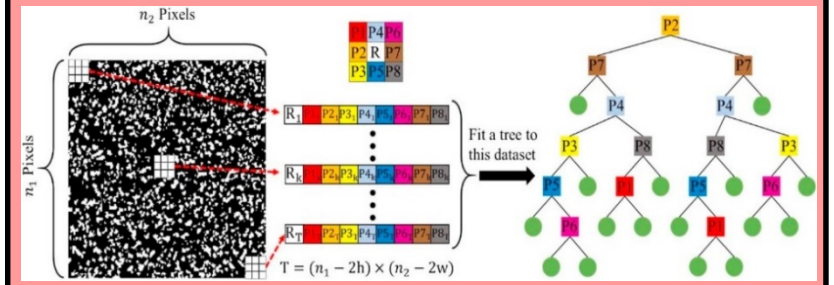
Model based MCR for Complex Morphology and Dimension Reduction

Supervised Learning

- Model phase values as functions of surrounding pixels



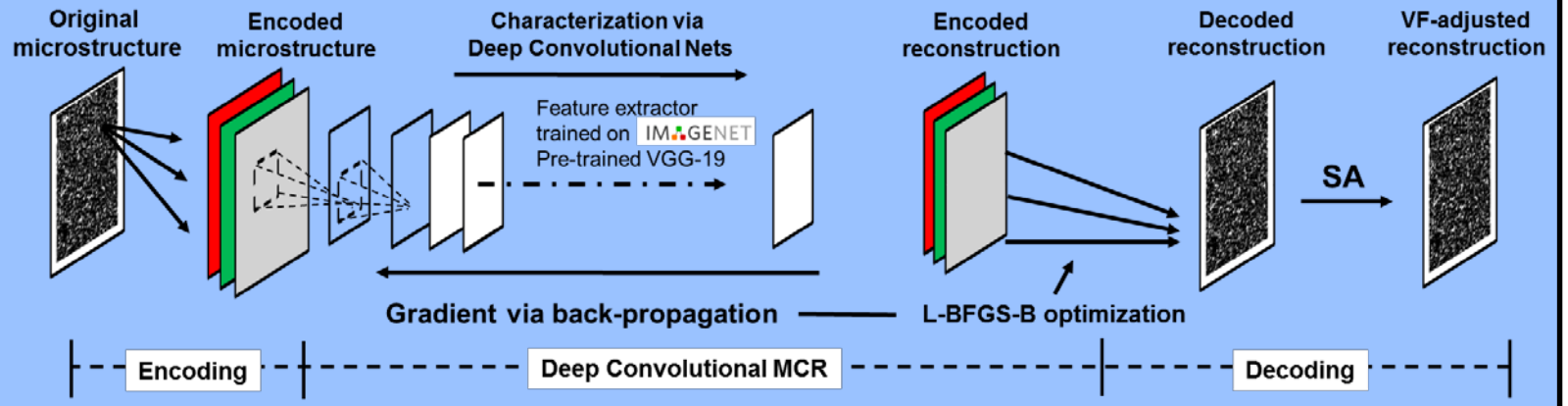
- Decision tree as the supervised learner



Bostanabad, R., et. al. (2016) *Acta Materialia*, 103, 89-102.

Deep Convolutional Network

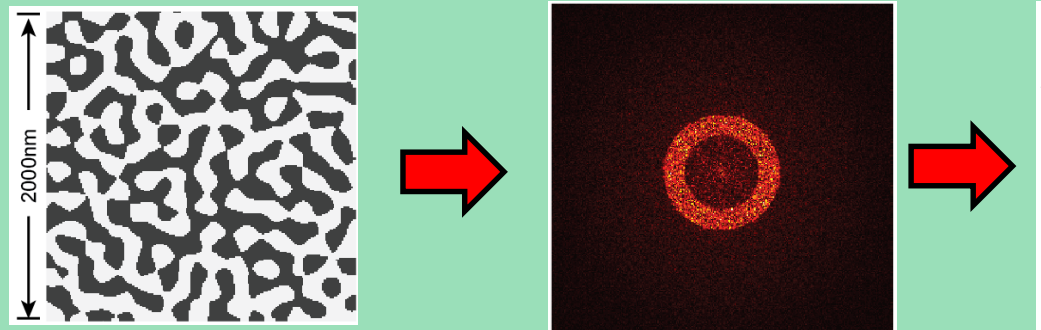
Li, X, et al. (2018) arXiv preprint arXiv:1805.02784; ASME JMD



Spectral Density Function

- Describes the structural spatial correlations in the frequency domain and enables *physics-aware dimension reduction*.

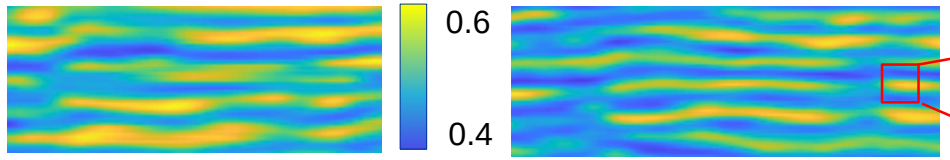
Structure $Z(\mathbf{r})$ → Fourier spectrum



Yu, S., et.al. (2017) Scientific reports, 7, 3752.

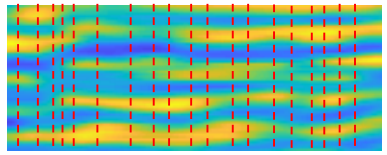
MCR for Unidimensional (UD) CFRP Composites

microstructure
(cross section)

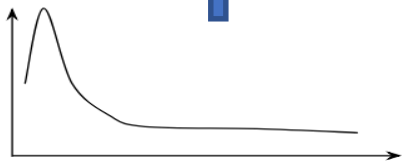


nonuniform fiber distribution

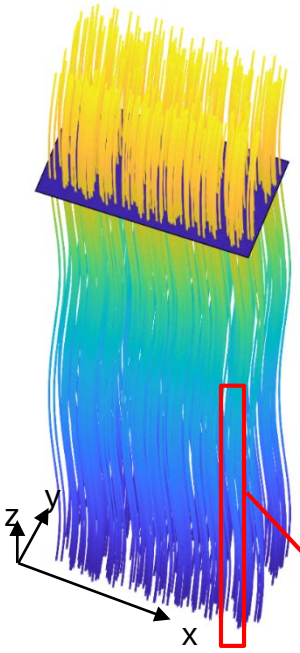
reconstruction



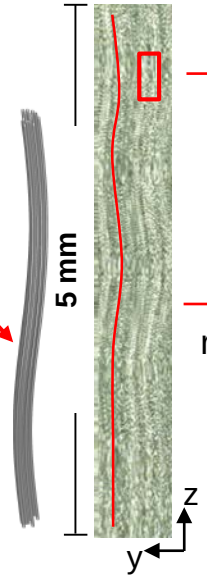
tree-structured nonhomogeneous Poisson point process



distribution of the distances between the separation lines



microstructure
(transverse)



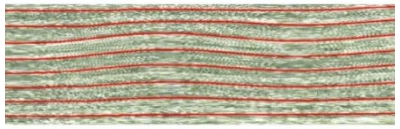
UD composites

fiber waviness

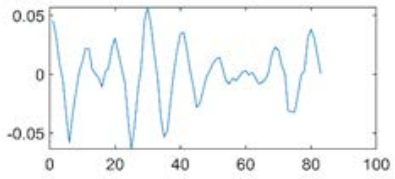
rotate 90°

angle characterization by
segmented linear regression

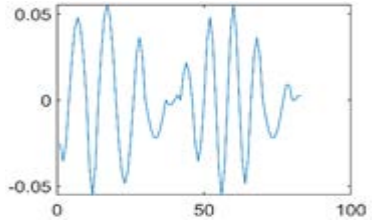
rotate 90°



local waviness angles

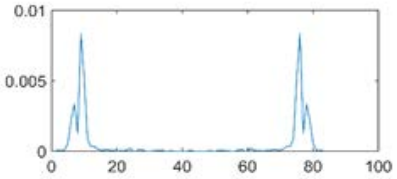


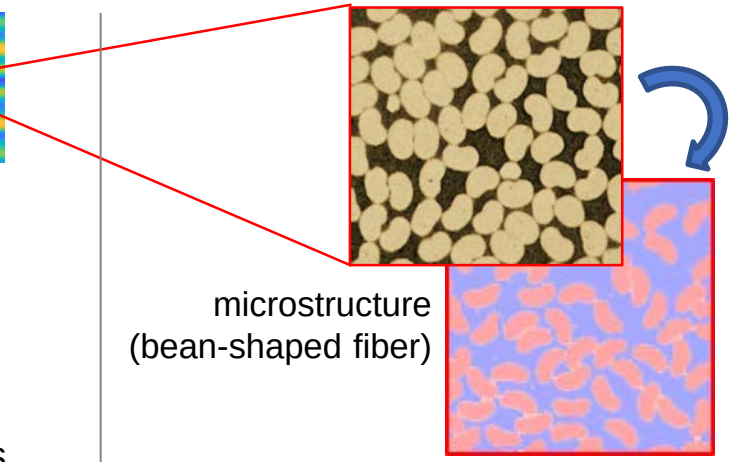
(averaged)



reconstruction

distribution of the angles in the frequency domain





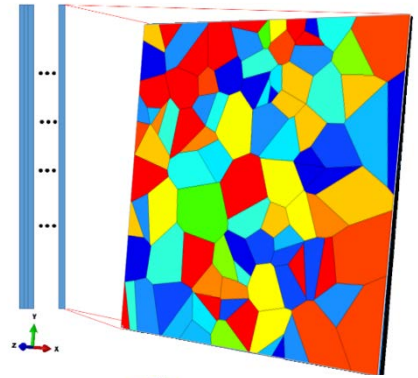
microstructure
(bean-shaped fiber)

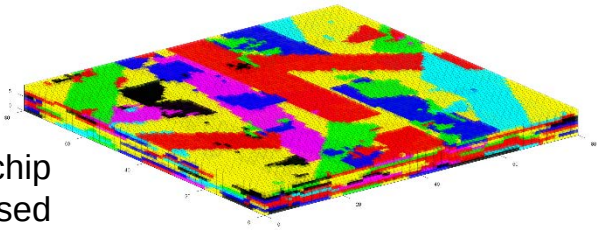
bean packing

RVE model

SMC
(sheet molding compound)
microstructure reconstruction

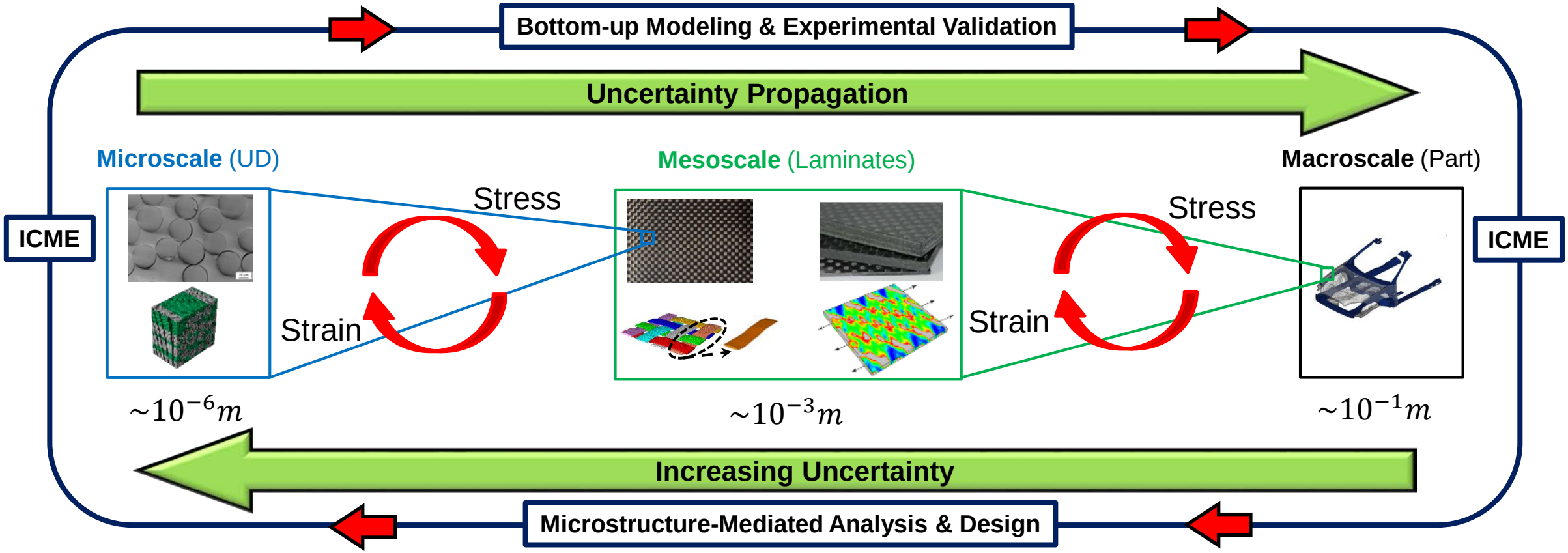
Method 1: Voronoi diagram based





Method 2: chip packing based

Integrating UQ & UP With ICME of Woven CRFP



Challenges:

- Computational expenses
- Existence of high dimensional, spatially correlated, multiscale coupled uncertainty sources with different characteristics.