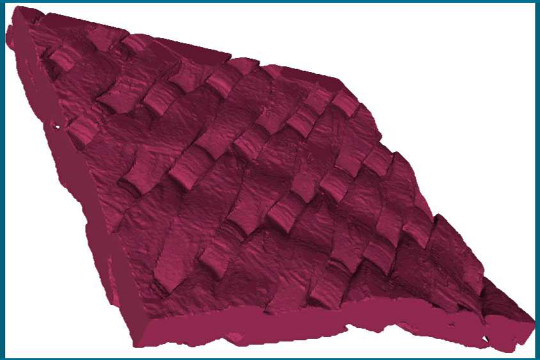
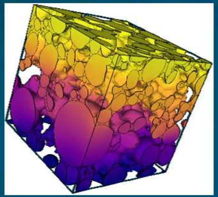
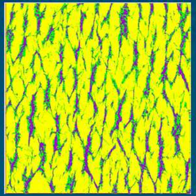
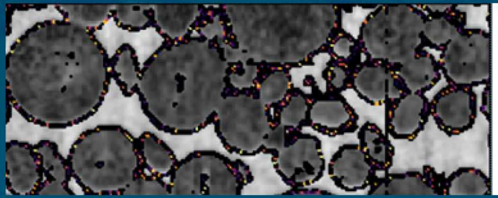
SAND2019-10880C

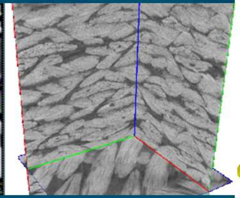
Image-based mesoscale ablation modeling

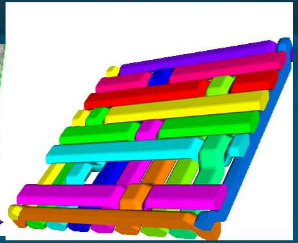












PRESENTED BY

Lincoln N. Collins, Cedric W. Williams, Scott A. Roberts

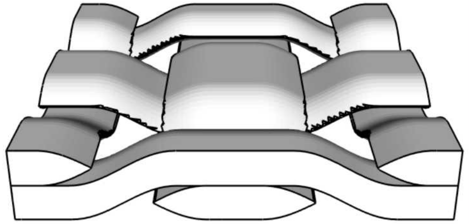
Thermal/Fluid Component Sciences
Engineering Sciences Center

UNCLASSIFIED UNLIMITED RELEASE
SAND2019-XXXX C

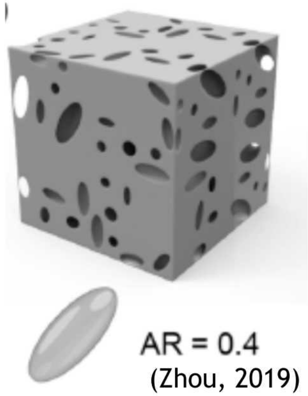
Motivation

Microscale properties

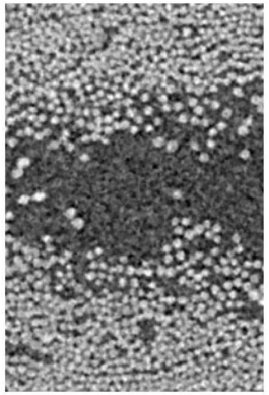
Geometry
-Analytical
-Image-based



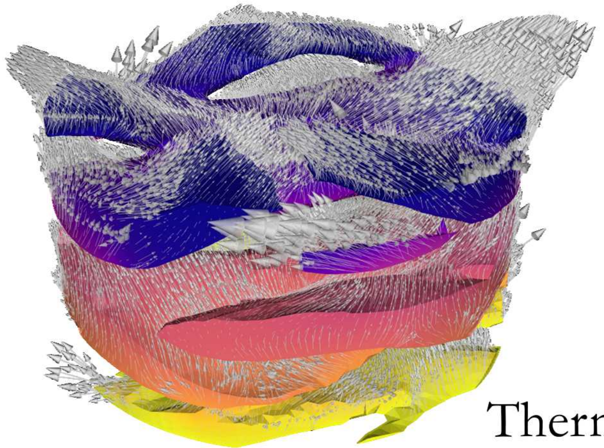
Constituent properties
(Fiber, fabric, resin, voids, filler)
Microscale parameters

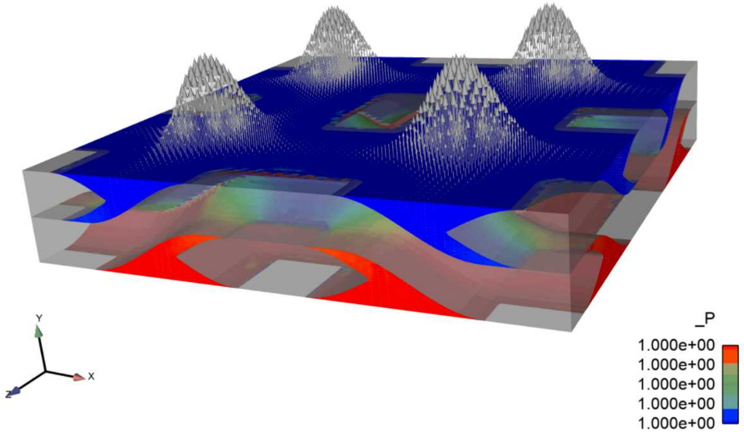


(Zhou, 2019)


(SNL, NASA)

Mesoscale simulations


Thermal



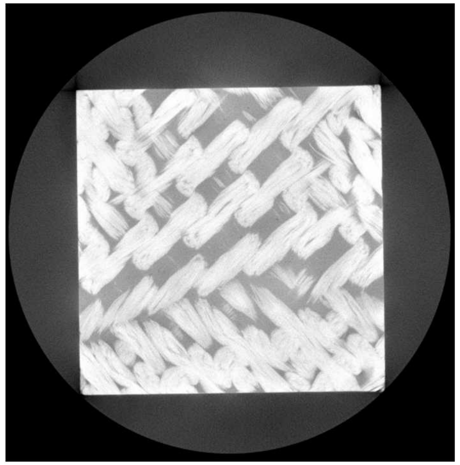
Permeability

Macroscale Performance


(NASA)

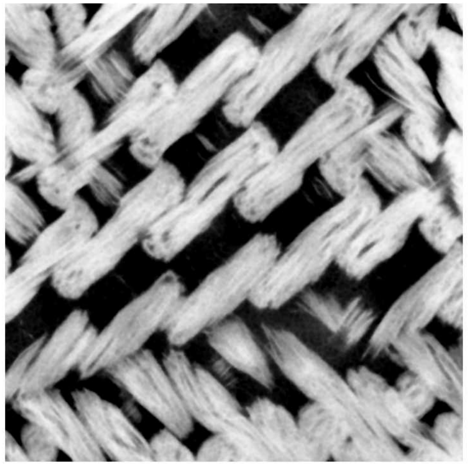
Geometry generation from image data

Raw image data (X-ray CT)

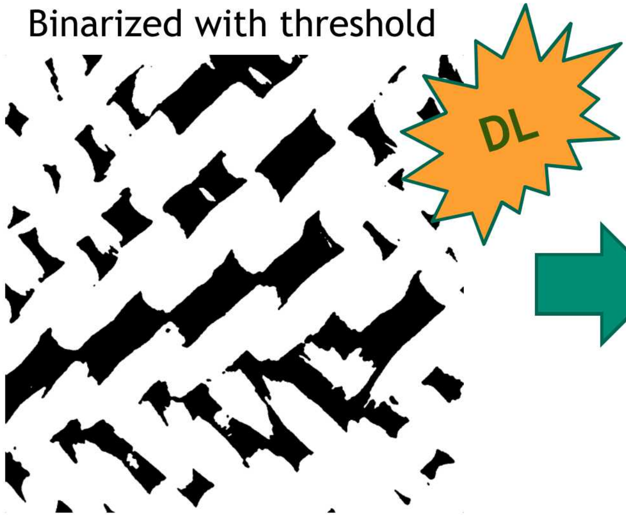


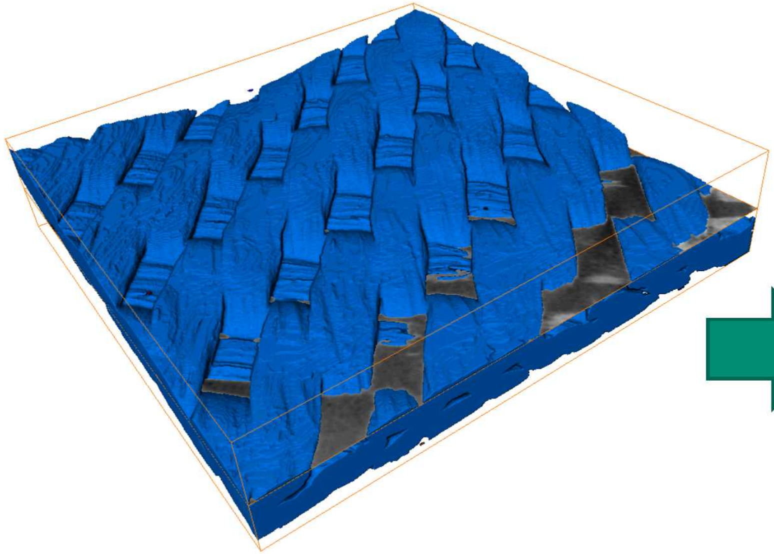
(SNL, NASA)

Filtered image data

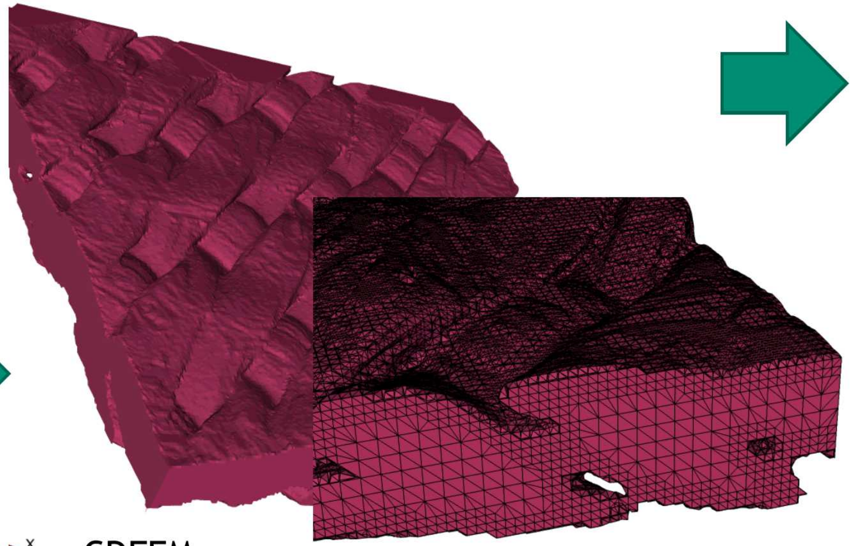


Binarized with threshold



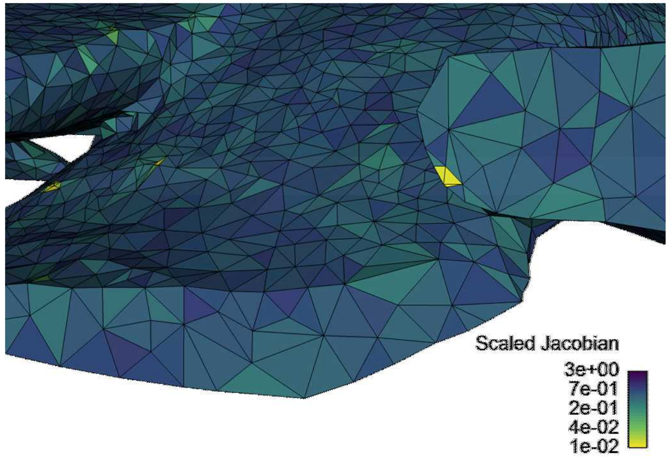


Reconstruct into faceted surface



CDFEM

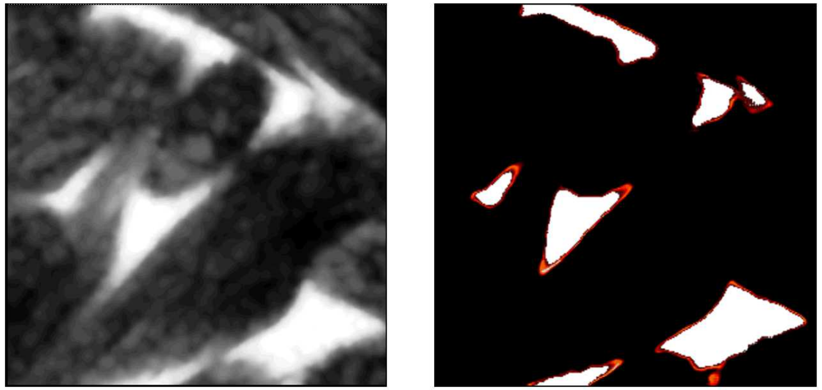
(Noble, 2010; Kramer, 2014; Roberts, 2016)



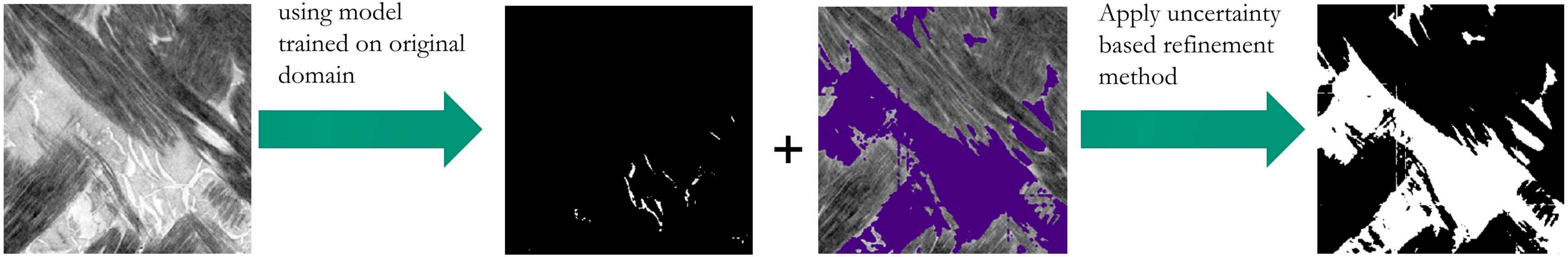
Emend to improve and coarsen mesh

Image segmentation using DL

- Train a 3D Convolutional Neural Network (CNN) to perform binary segmentation with labeled examples from one domain.
- Infer segmentations of domain-shifted CT scans.
- Obtain per-voxel epistemic uncertainty map by running inference multiple times with active dropout layers.
- Identify an appropriate uncertainty threshold.
- Flip the prediction for voxels with uncertainty over the threshold.



Accurate segmentations on held-out sub-volumes, with per-voxel UQ



(Martinez et al., 2019)

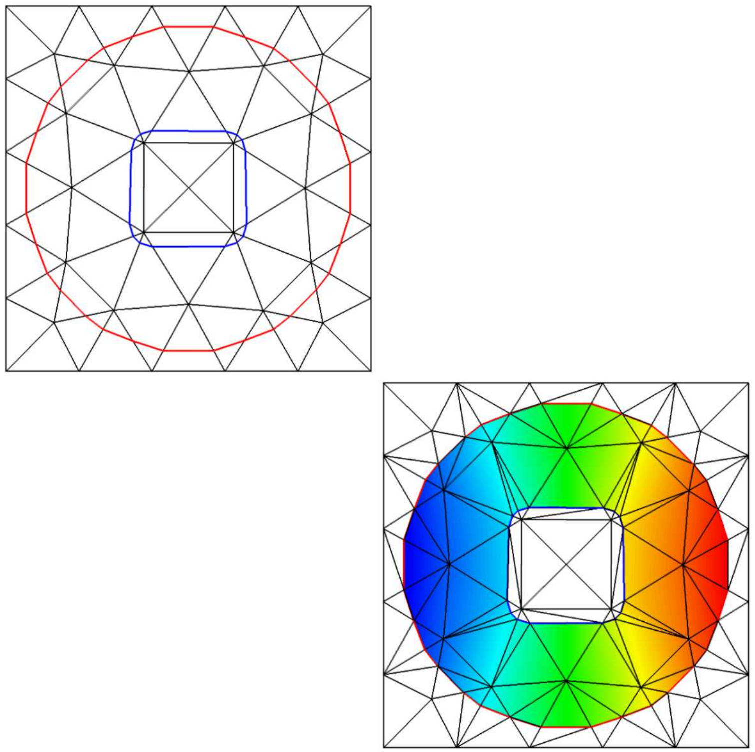
Conformal decomposition (CDFEM)

Concept

- Use level set fields to define phases
  - Solve for signed distance from interface

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0 \qquad \vec{n} = \nabla \phi, \kappa = \nabla \cdot \nabla \phi$$

- Decompose non-conformal elements into conformal ones

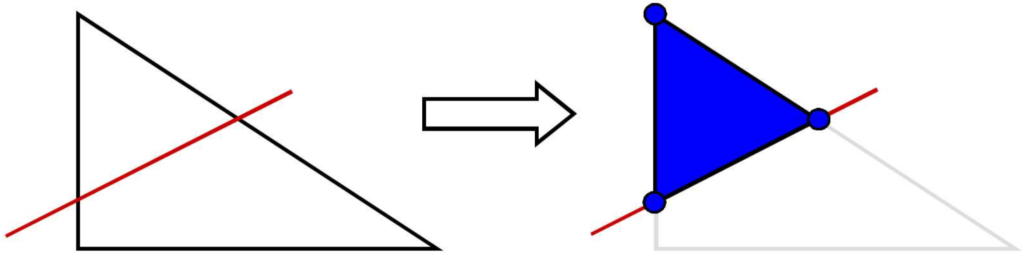


Properties

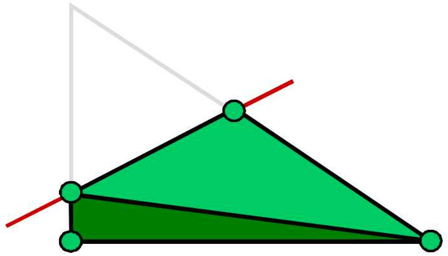
- Supports wide variety of interfacial conditions
- Avoids manual generation of boundary fitted mesh
- Supports general topological evolution

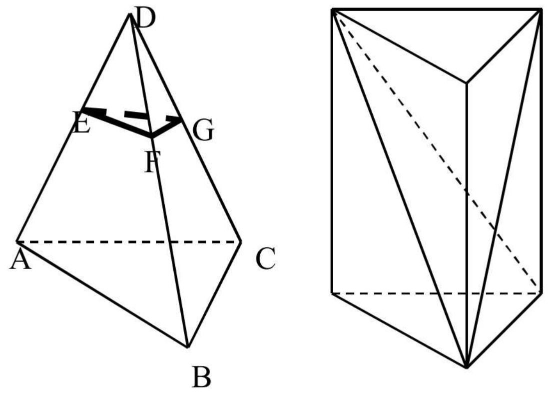
Similar to finite element adaptivity

- Uses standard finite element assembly including data structures, interpolation, quadrature. Affords discontinuous parameters.



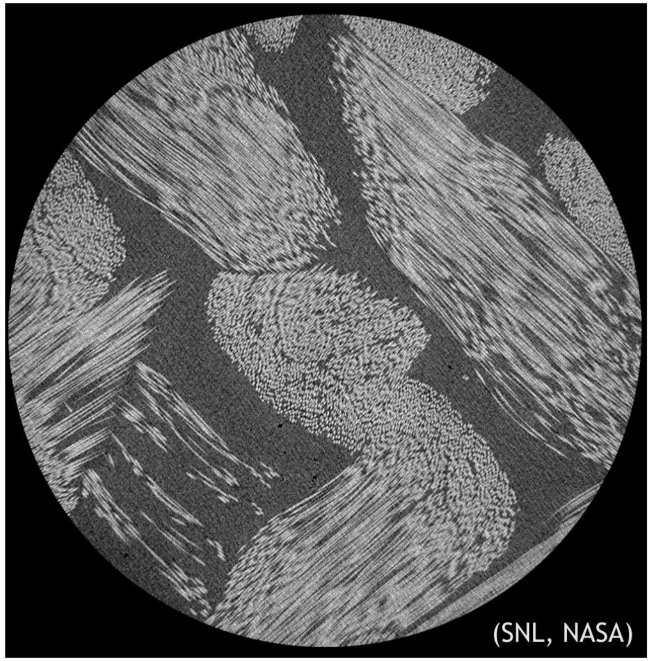
+

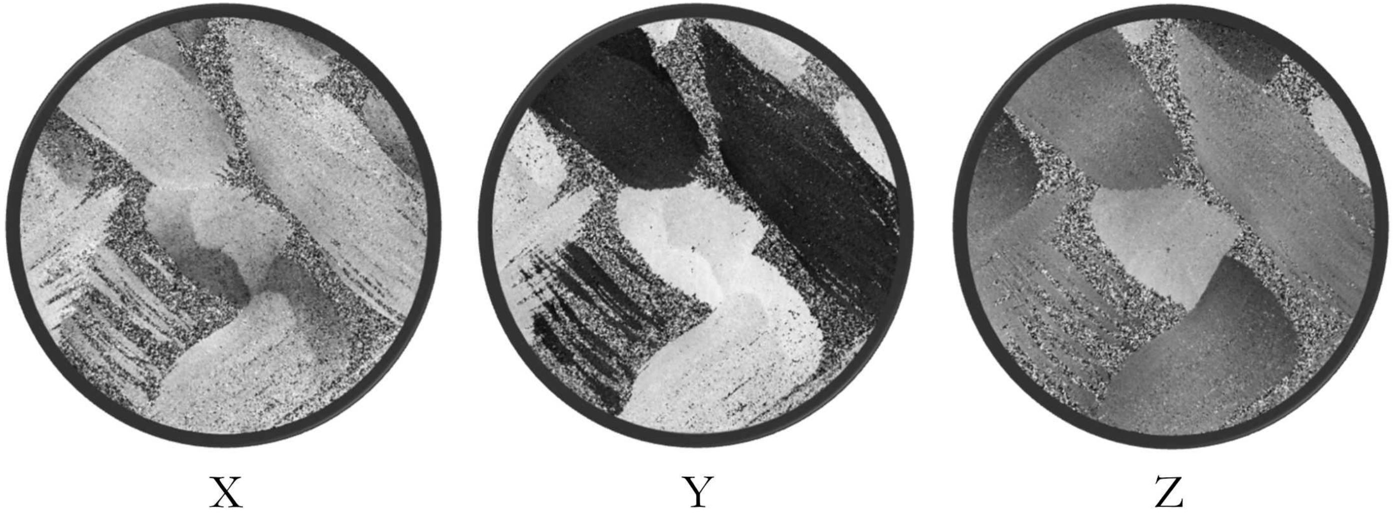




(Noble, 2010; Kramer, 2014; Roberts, 2018)

Image structure tensor





$$\nabla I_\sigma(x) = \nabla \left(G_\sigma * I\right)(x)$$

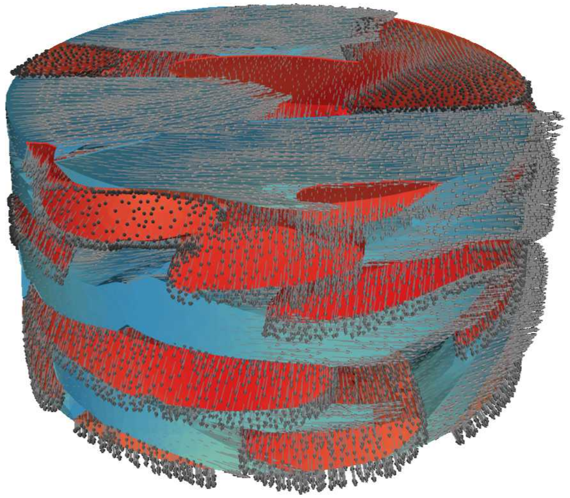
$$S_\sigma = \nabla I_\sigma \otimes \nabla I_\sigma = \begin{bmatrix} I^2_{\sigma,x} & I_{\sigma,x}I_{\sigma,y} & I_{\sigma,x}I_{\sigma,z} \\ I_{\sigma,x}I_{\sigma,y} & I^2_{\sigma,y} & I_{\sigma,y}I_{\sigma,z} \\ I_{\sigma,x}I_{\sigma,z} & I_{\sigma,y}I_{\sigma,z} & I^2_{\sigma,z} \end{bmatrix}$$

Structure tensor:

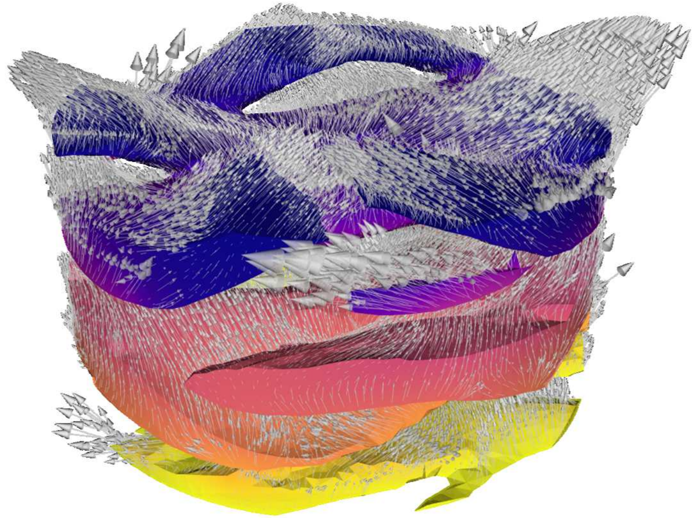
- Gradient tensor at each voxel
  - Uses Hessian of Gaussian-blurred intensity values
- Eigenvector associated with minimum eigenvalue denotes material direction
  - Lowest variation in image "texture"
- Requires rotation to common direction

Anisotropic segmentation and fiber orientation

θ



Material orientation



Heat flux

Separate fabric dimension:

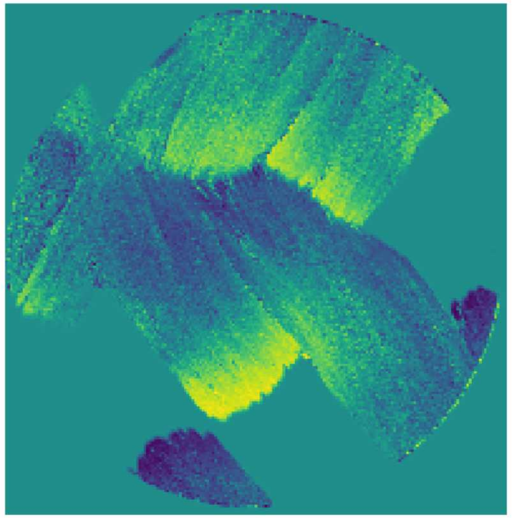
- Use in-plane orientation, θ, to label warp/weft yarns

Fiber orientation:

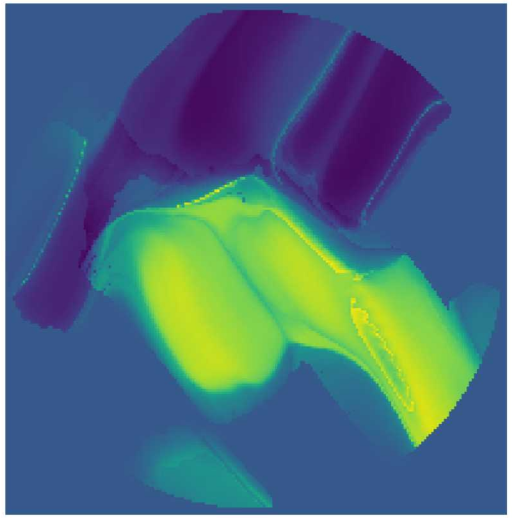
- 3-d orientation calculated per-voxel
  - Smoothed and embedded on finite element mesh

Thermal stress:

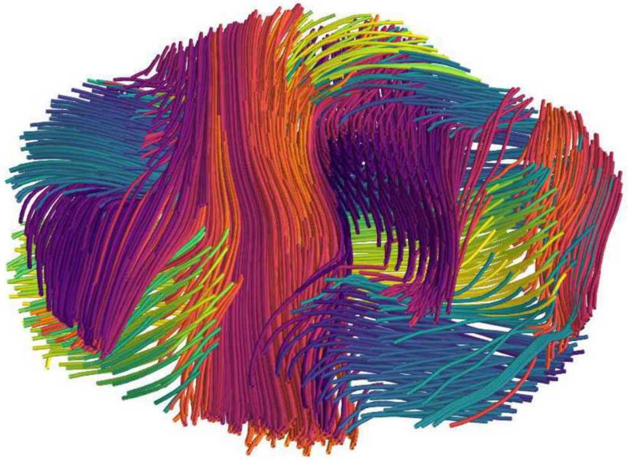
Fiber tractography

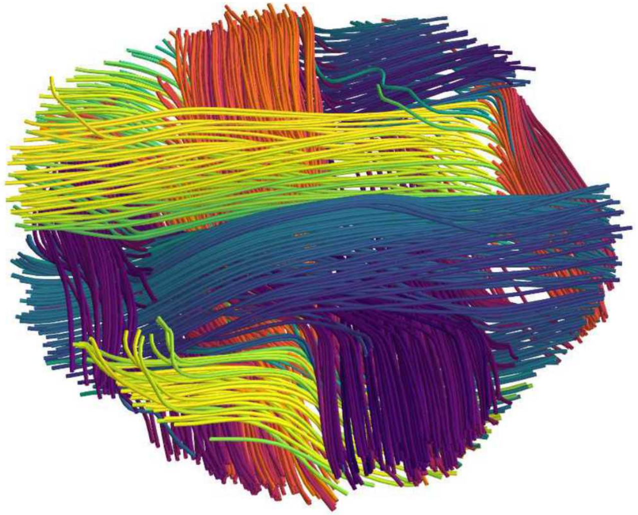


z-component



Path integral along streamline





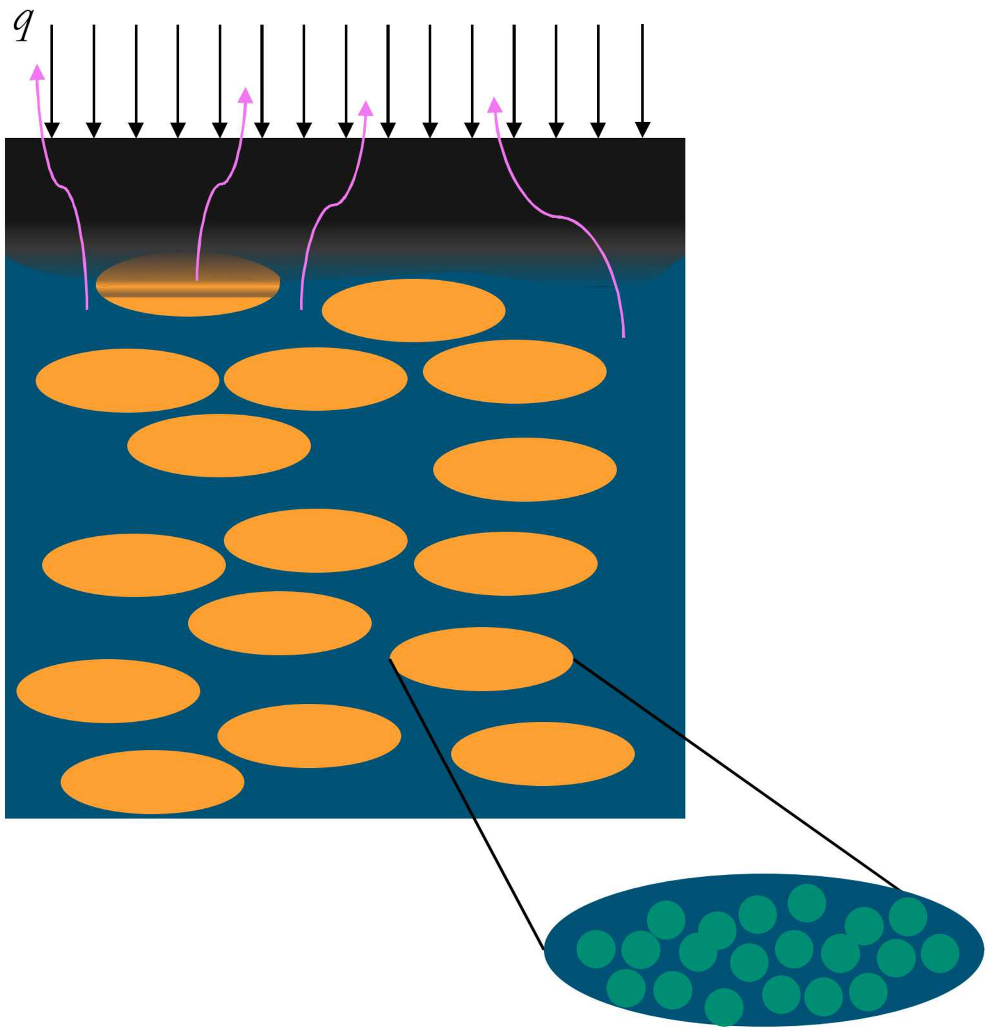
Separation of yarns:

- Requires choice of kernel to integrate along path
- Masking required to isolate directions

Fiber "reconstruction":

- Use orientation field and streamline to generate simulated fibers
- Export as .stl descriptions to CDFEM for simulations
- *Approximate* microscale behavior

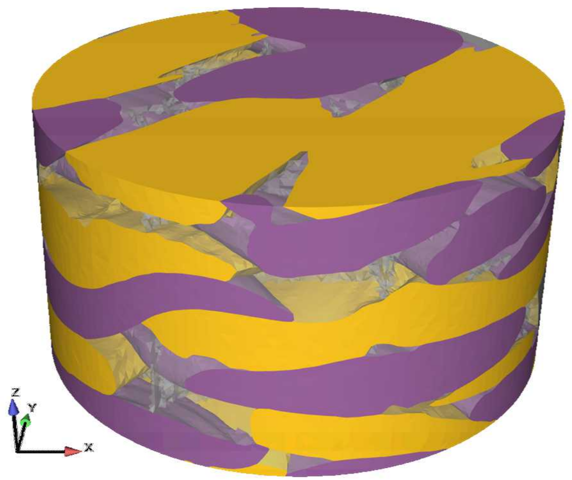
Mesoscale ablation modeling



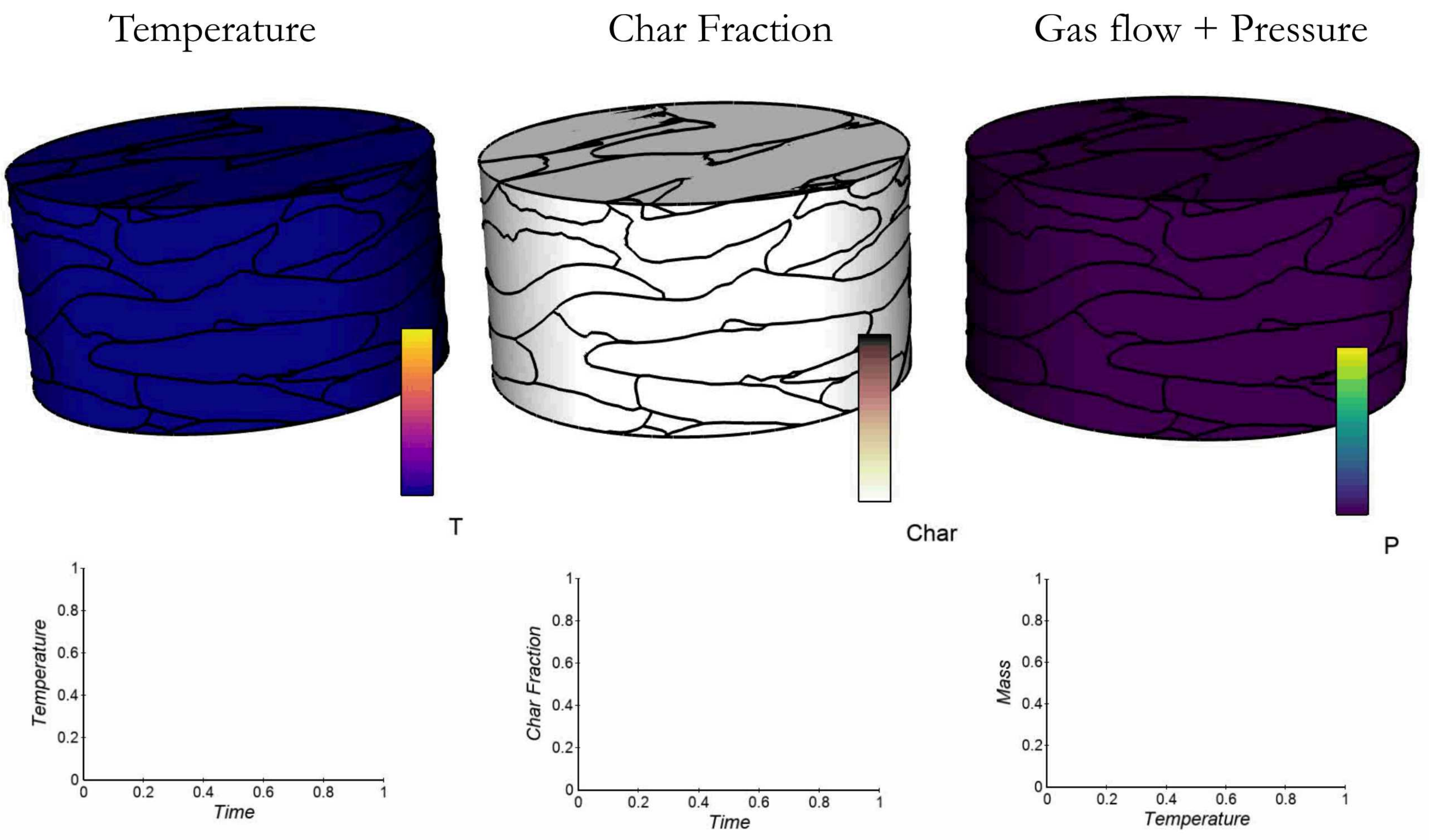
Mid-fidelity ablation model

- Mesoscale **porous** media
  - Two-phase:
    - Solid: 2 resin stages, fiber, char
    - Gas: single species
  - Matrix and yarn domains
- Porous **enthalpy** transport
  - Uptake from gas phase
- **Arrhenius** decomposition
  - Inert fibers
  - Volumetric
- Pyrolysis **gas transport**
  - Stokes flow with interpolated permeability
  - Generalized species transport
  - Gas-phase chemistry
  - Surface reaction with char
- **Dynamic** material properties
  - Mass fraction averaged
  - Temperature dependent

Results (work in progress…)

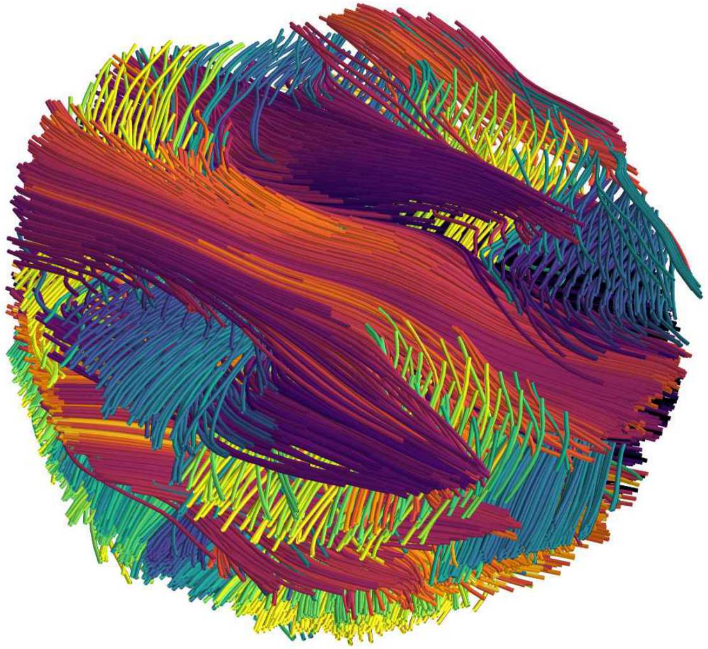


Warp
Weft
Matrix



Overview

- **Image-based simulations** are necessary for fully characterizing woven composites from the mesoscale
- **Machine learning and robust image analysis** can be adapted to various data sources, resolutions, and materials
- Image structure tensor allows for **material orientation**, object identification, and reconstruction of geometries
- Porous/volumetric ablation behavior allows for **multi-physics coupling**
  - Flexible kinetics formulation
  - Multiple species tracking/transport
  - Can be combined with sharp-interface treatment (oxidation)
  - Allows for integration with mechanics and expansion
  - **Can use image data as initial material conditions**



Thank you!

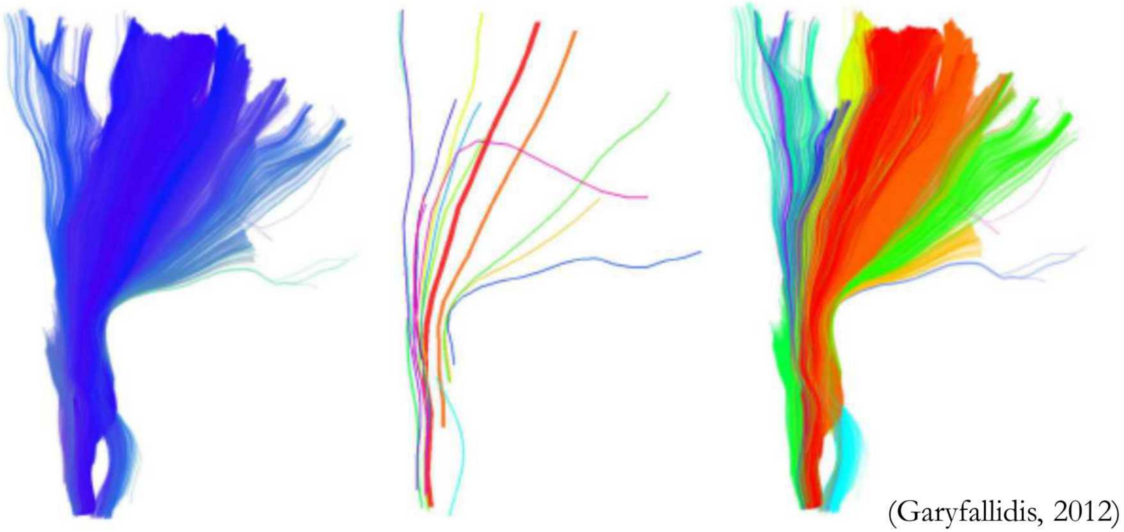
Supplementary: fabric analysis from reconstructed image data

Goal: separate individual yarns in image

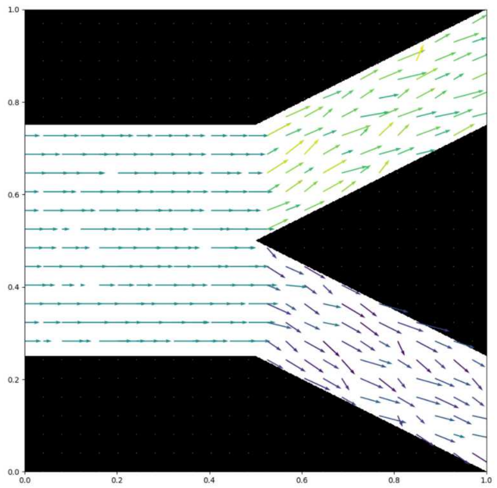
- Allows for path/cross section characterization, fabric analysis etc.
- Uses orientation from structure tensor

Elsewhere:

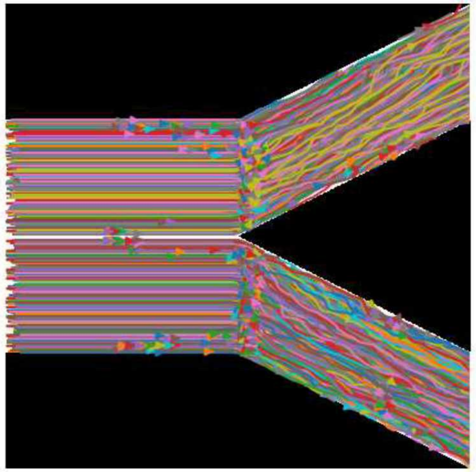
- Tractography of corticospinal tract using MRI
  - Indicates white matter orientation



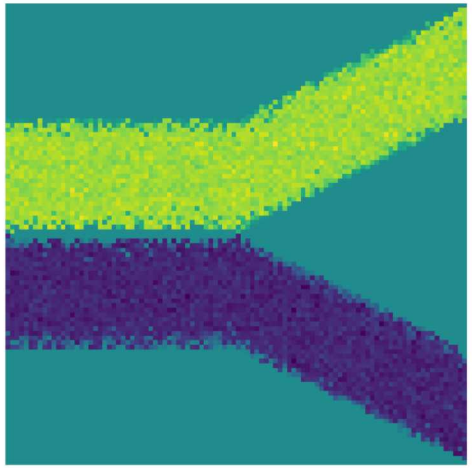
(Garyfallidis, 2012)



Data with orientation

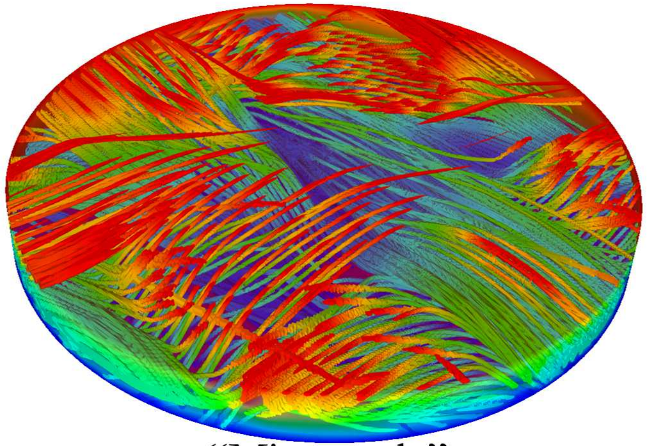


Generate streamlines using voxel locations as starting point (+/- direction)

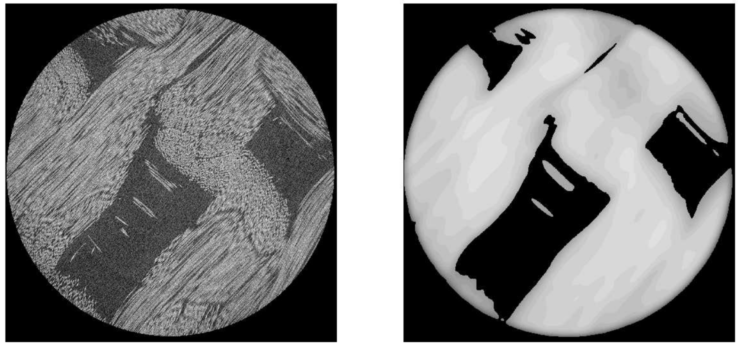


Assign pixel value based off line integral

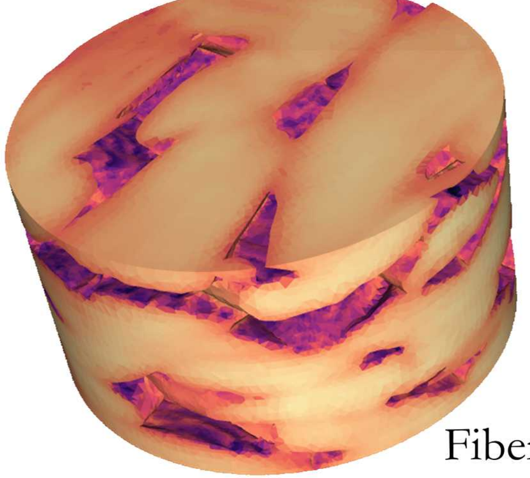
Supplementary: example results



"Microscale"



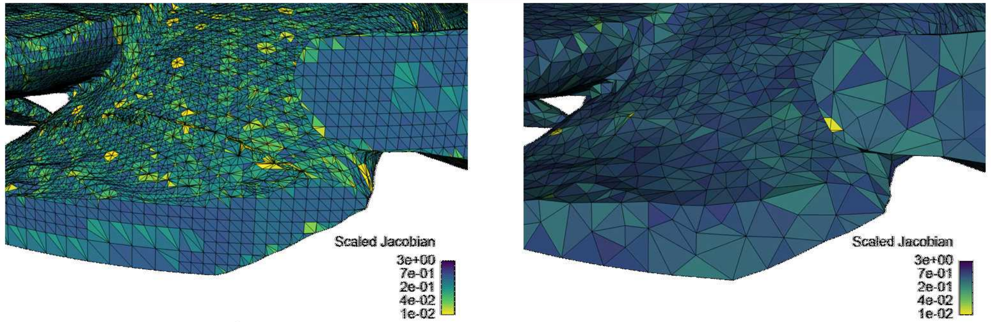
Smooth and rescale intensity to density approximation



Fiber density

	Fiber packing	Fiber Volume Fraction	Effective Conductivity
Isotropic (Inverse)	0.8	0.667	0.35205
Isotropic (Mixture)	0.8	0.667	3.84361
Anisotropic (Uniform)	0.8	0.667	0.46077
Anisotropic (Image)	0.779	0.649	0.43350
Microscale	-	0.209	0.32671

	Element Count	Average Scaled Jacobian	Min Scaled Jacobian	Effective Cond.*
CDFEM	4959942	0.4644	1.456e-9	4.706
Emend	478940	0.5464	1.235e-5	4.837



Emend improves minimum element quality 4 orders of magnitude, maintaining topology