PuMA and Multiscale Modeling

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Predictive Material Modeling (PMM) group

Entry System Modeling (ESM) project

Content of presentation

- Motivation

- Overview of PuMA
  - Functionalities
  - Advanced domain generation
  - Material response examples

- Effective properties for fibrous media
  - Fiber orientation
  - Thermal conductivity
  - Stress analysis

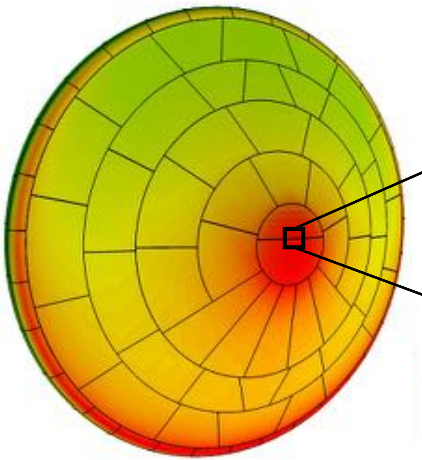
Modeling TPS

Macroscale

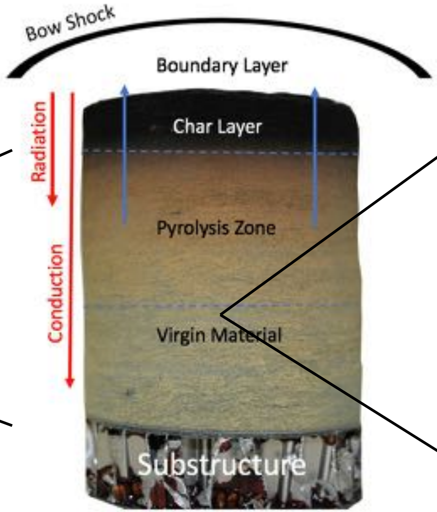
Full-scale material response solvers, using homogenized properties

Microscale

Homogenization of material properties to be used in macroscale models



Simulation of surface temperature for MSL heatshield



X-ray microtomography

Collect X-ray images of the sample as it rotates through 180°

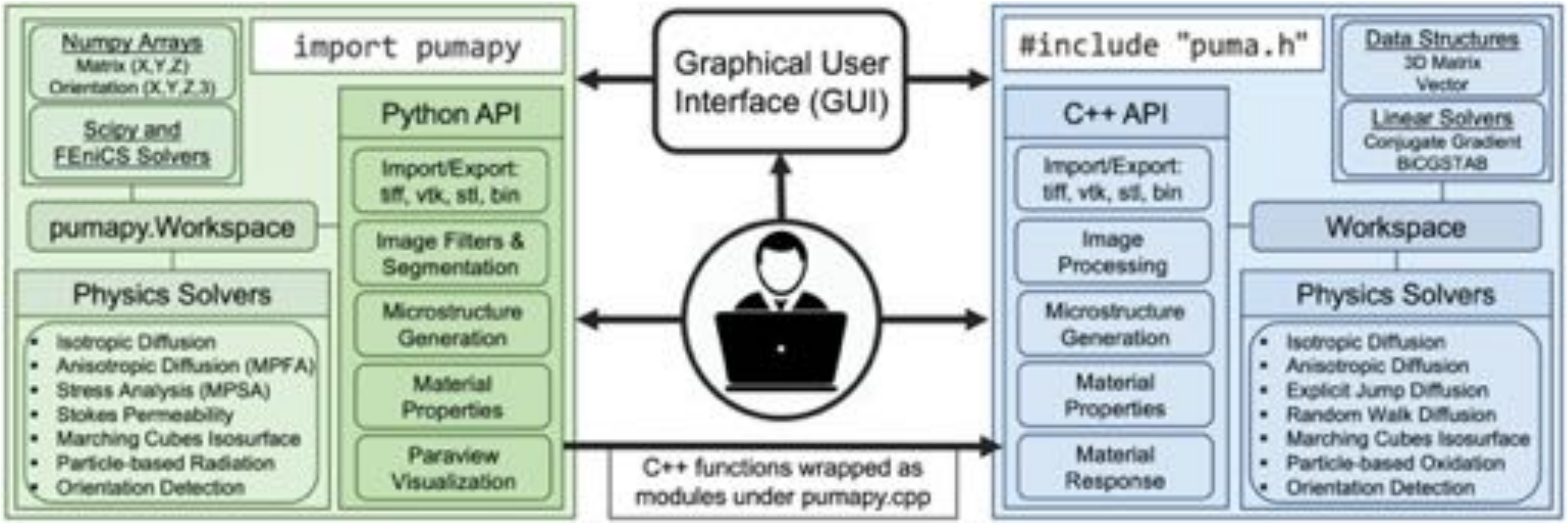
Use the series of images to reconstruct the 3D object

Courtesy of D. Parkinson
(ALS at Berkeley National Lab)

Porous Microstructure Analysis (PuMA)

Git repository: https://github.com/nasa/puma

Documentation and tutorials: https://puma-nasa.readthedocs.io



Improved processing of micro-CT weaves

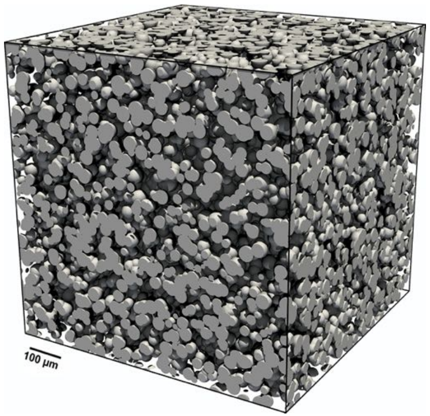
a) Adept 12 ply imported into PuMA GUI

b) 3D rendering of microstructure

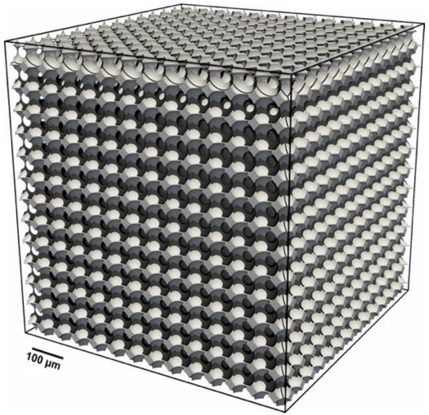
c) Post-processed weave after segmentation and orientation detection

Advanced domain generation

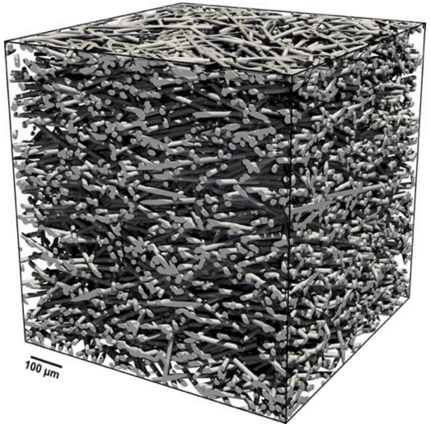
Packed Sphere Beds

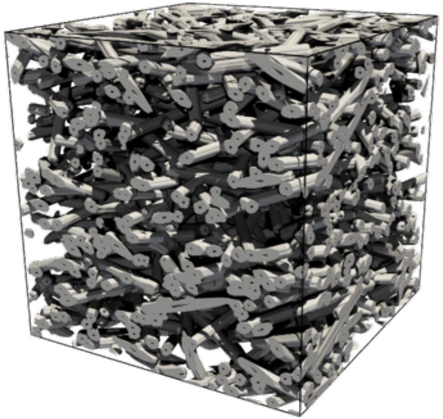


Periodic Foams



Fiber Structures

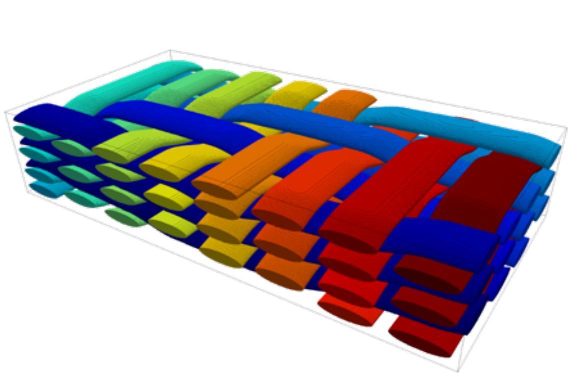




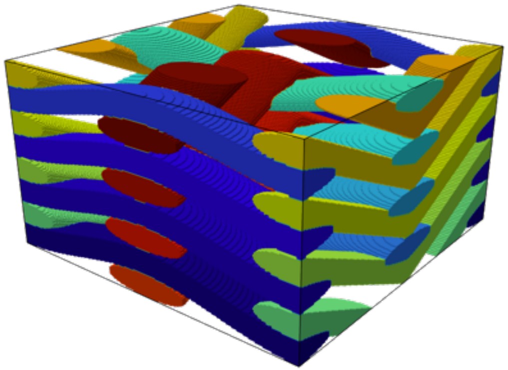
Artificial weave generator

Pumapy was coupled with TexGen's Python API to provide flexible synthetic weave generation.

Wrappers to convert from a TexGen geometry to a pumapy.Workspace were also implemented



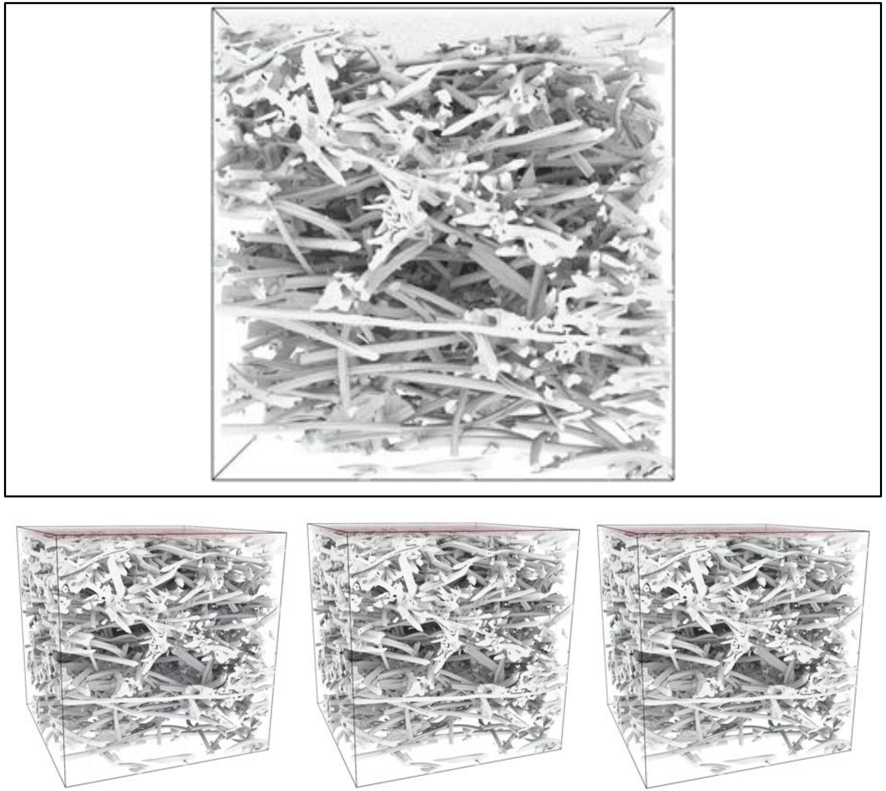
Layer-to-layer weave



3MDCP geometry

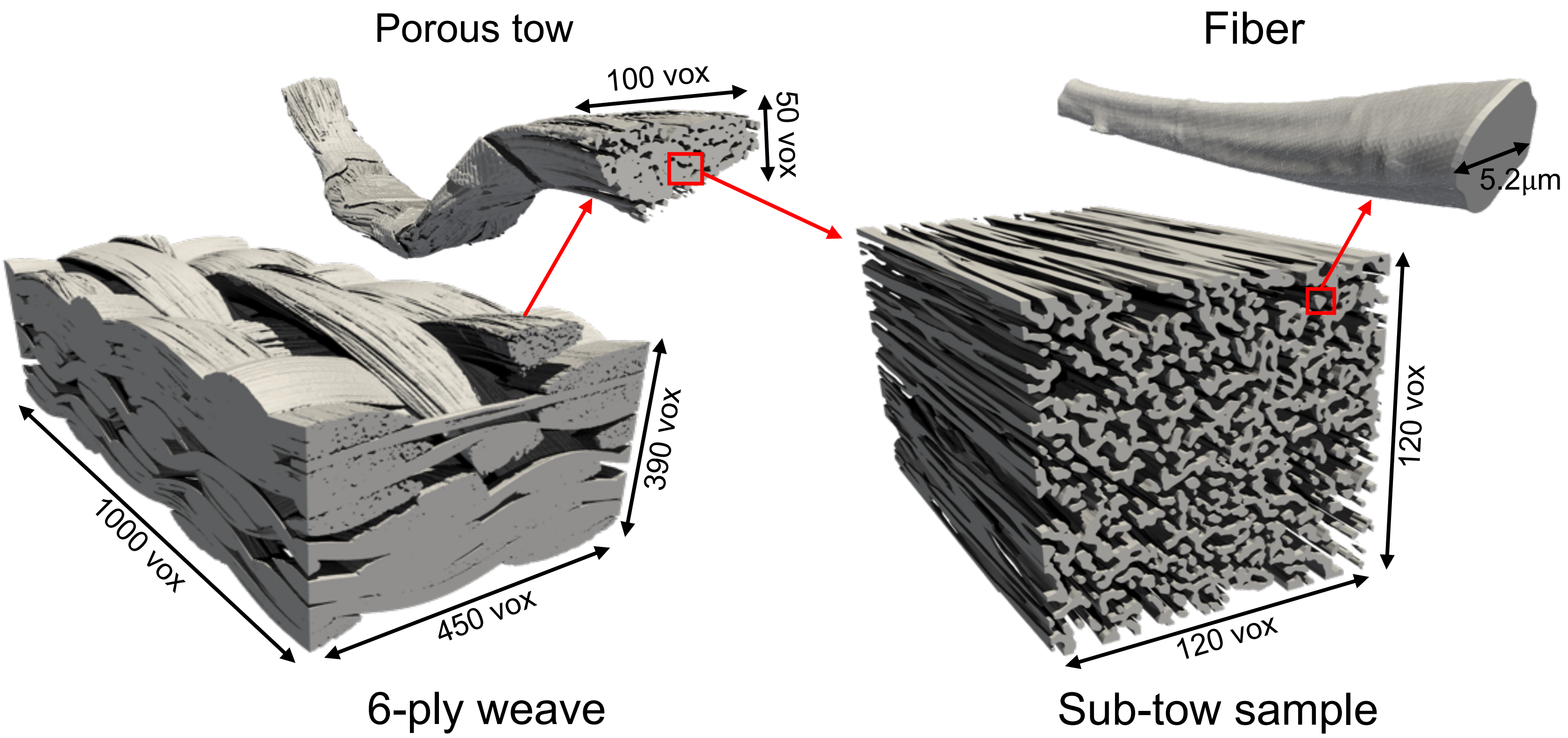
Material response examples

Oxidation simulation



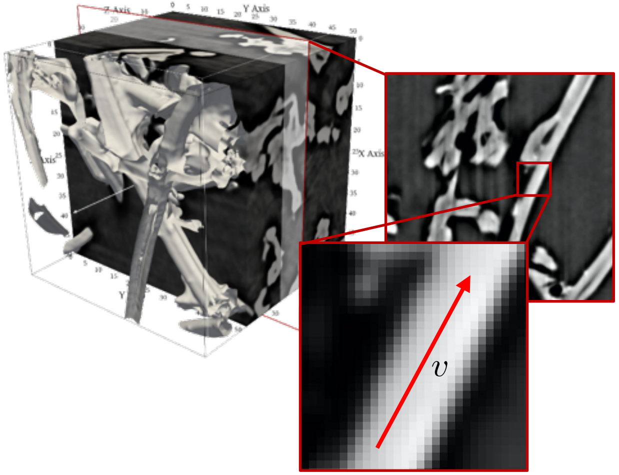
Hyperthermal beam

An anisotropic and multiscale problem



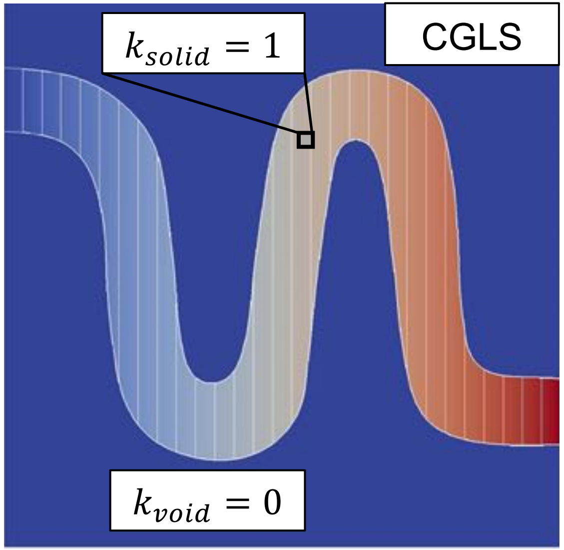
Fiber orientation methods

Structure tensor

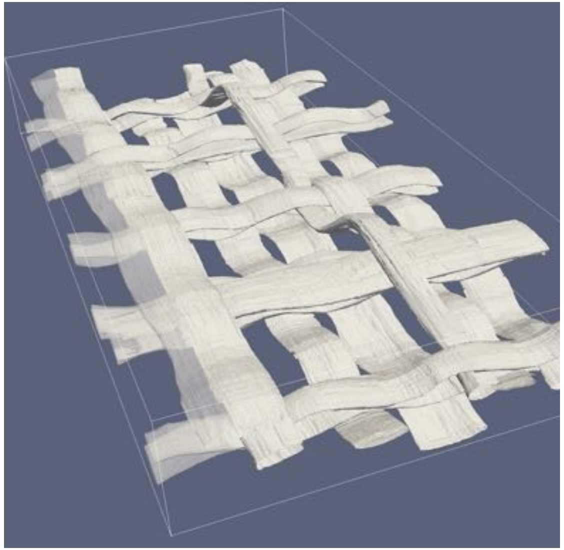


$$(I(x+v) - I(x))^2 \approx 0$$

Artificial flux

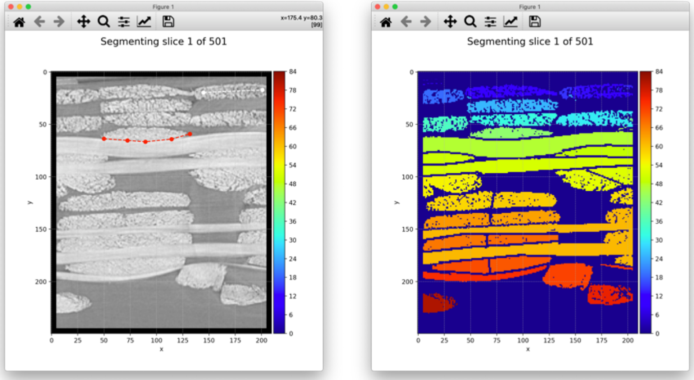


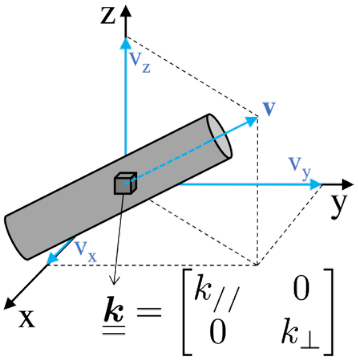
Ray casting

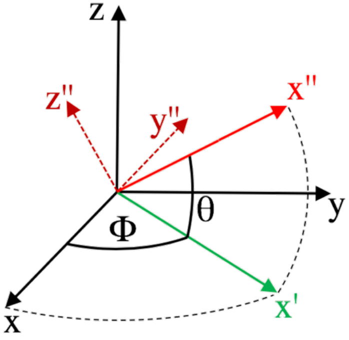


Micro-CT weave post-processing

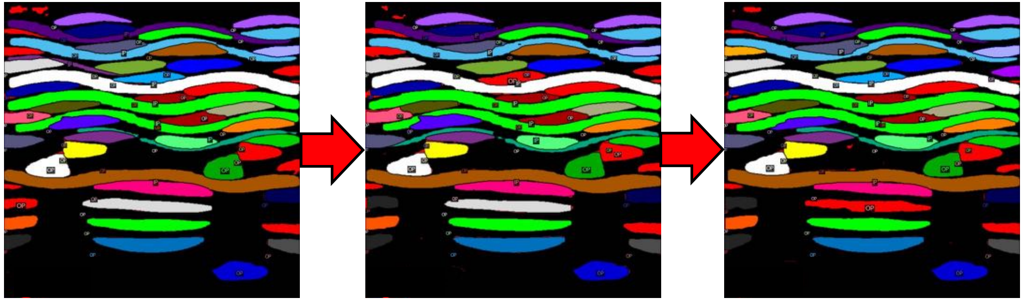
Individual fiber/tow panoptic segmentation and tracking







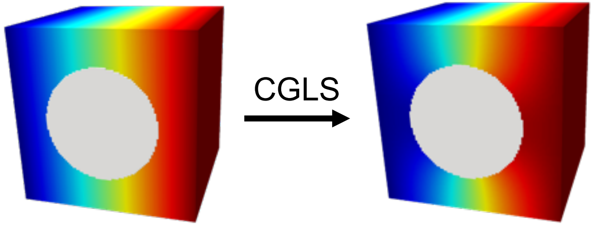
Detectron2



$$\boldsymbol{q} = \underbrace{\left[\boldsymbol{R}^{-1}\boldsymbol{k}''\boldsymbol{R}\right]}_{\boldsymbol{k}} \nabla T$$

$$\boldsymbol{R} = \begin{bmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Numerical method for solid conduction

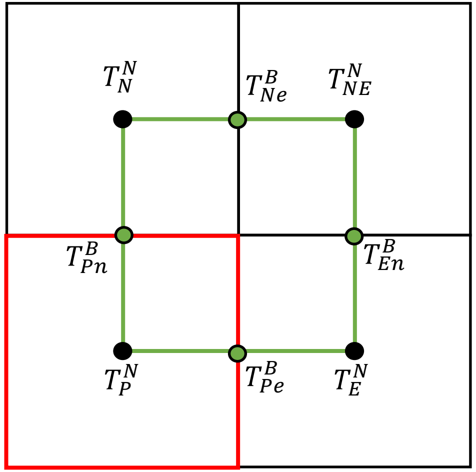


$$\rightarrow \boldsymbol{k}_{eff} = q^x \cdot L_x$$

$$\nabla \cdot \boldsymbol{q} = 0 \quad \longrightarrow \quad \boldsymbol{q}(x,t) = \boldsymbol{E}(x)\,\boldsymbol{T}^N(x,t)$$

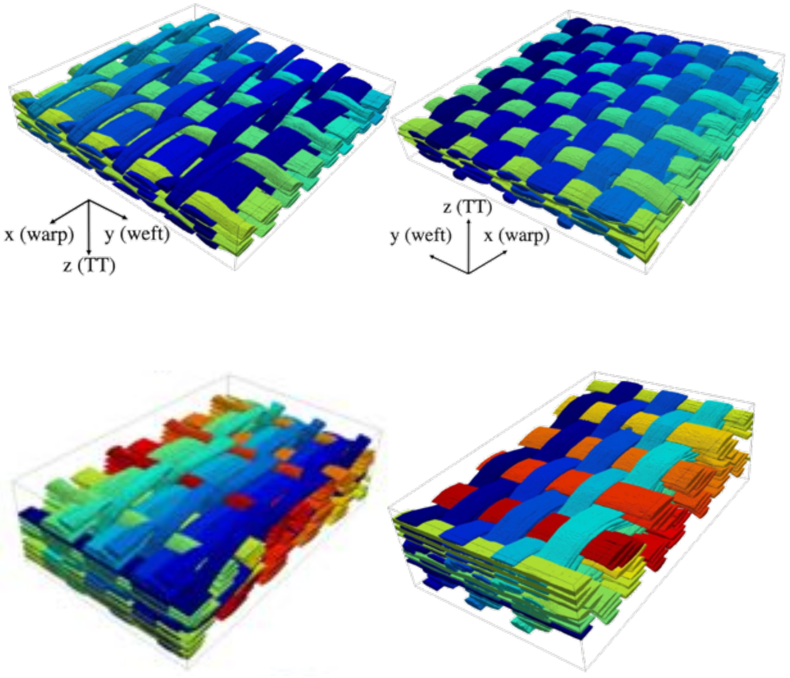
Multi-Point Flux Approximation (MPFA-O)*
i.e. continuity of fluxes and temperatures at Boundary points:

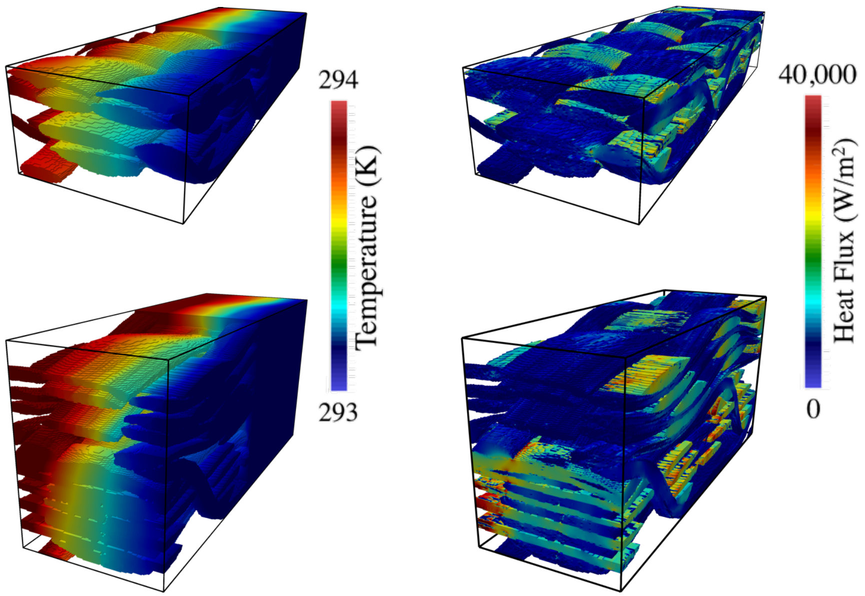
$$\boldsymbol{q}_P^{xx} = \boldsymbol{q}_E^{xx}$$
$$\boldsymbol{q}_P^{yy} = \boldsymbol{q}_N^{yy}$$
$$\vdots$$



*Ivar Aavatsmark. Multipoint flux approximation methods for quadrilateral grids. 9th *International forum on reservoir simulation 2007*, *Abu Dhabi*, pages 9–13.

Conductivity solver validation: ADEPT

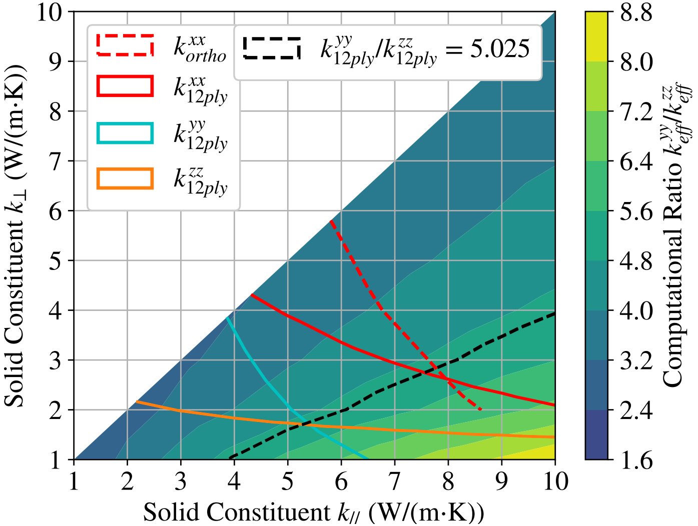


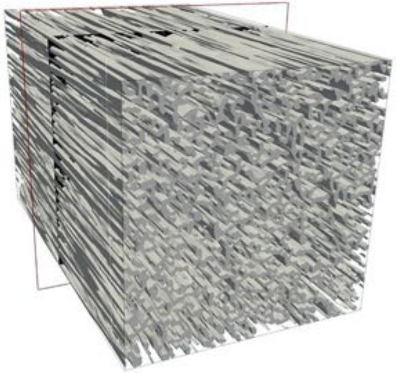


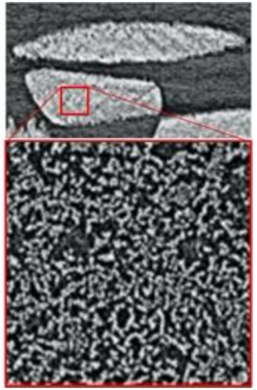
Single fiber conductivity estimation

Experimental value at room temperature:

$$\boldsymbol{k}_{exp}^{12ply} = \begin{bmatrix} 2.184 & - & - \\ - & 1.980 & - \\ - & - & 0.394 \end{bmatrix}$$





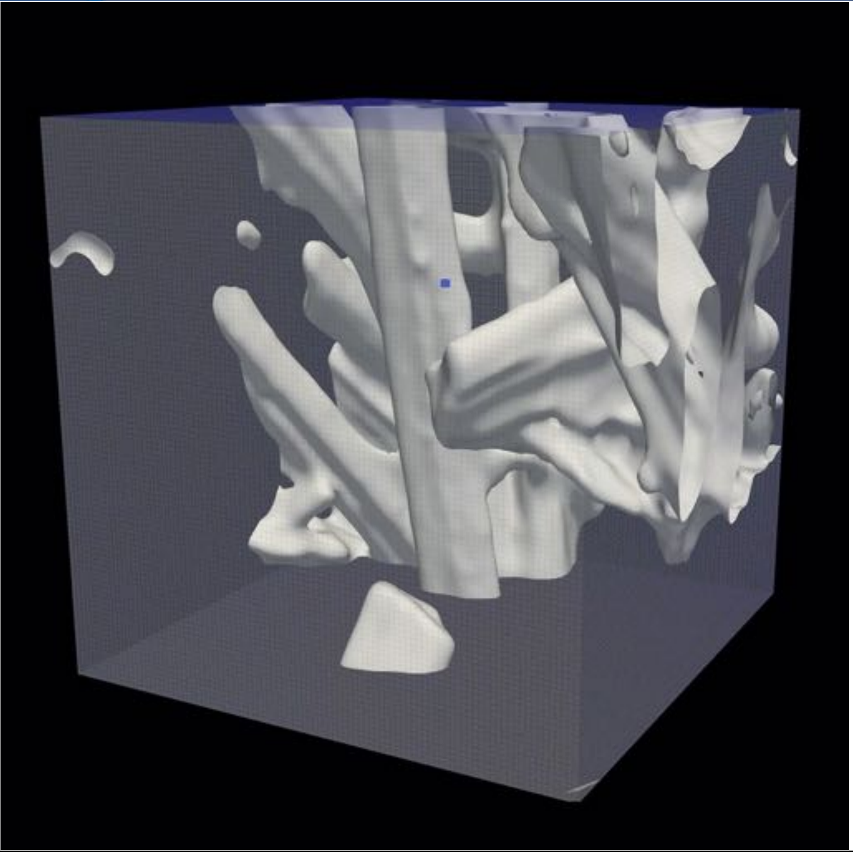


Single fiber thermal conductivity

$$[k_{//}, k_{\perp}] = [9.7, 5.5]\frac{\mathrm{W}}{\mathrm{mK}}$$

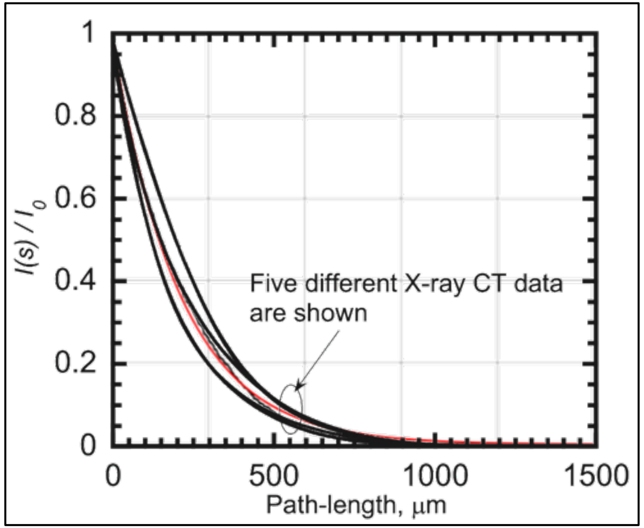
$$\boldsymbol{k}_{num}^{12ply} = \begin{bmatrix} 2.310 & -0.414 & 0.000 \\ -0.524 & 2.030 & 0.071 \\ 0.007 & 0.050 & 0.504 \end{bmatrix}$$

Radiative conduction



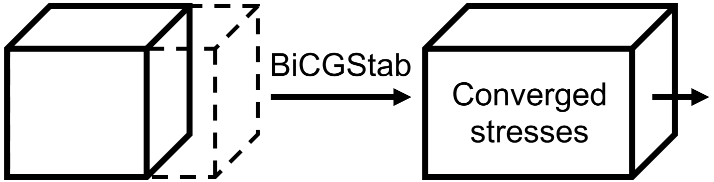
$$k_{\text{eff}} = k_{\text{sol}}(T) + k_{\text{rad}}(T) = k_{\text{sol}}(T) + \frac{16\sigma T^3}{3\beta}$$

$$\frac{I(s)}{I_0} = \exp(-\beta s) = 1 - \int_0^s F(s)ds.$$



Horiuchi, T. et al., 2018. Thermal Response Analysis of Porous Carbon-based Non-Ablative Heatshield in an Arcjet Flow Condition. *Transactions of the Japan Society for Aeronautical and Space Sciences*, *61*(5), pp.211-218.

Numerical method for stress analysis



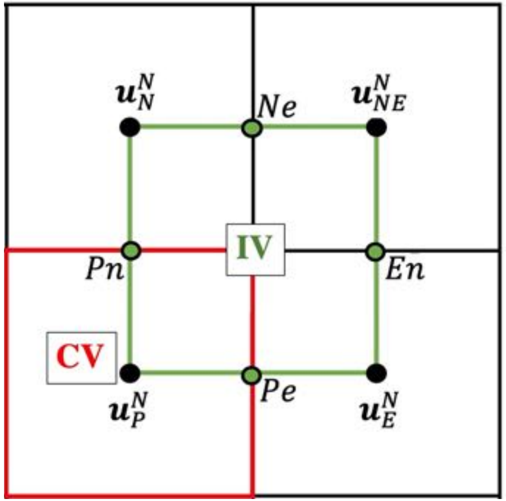
$$C_{eff} = \boldsymbol{\sigma}^x \cdot L_x$$

$$\nabla \cdot \boldsymbol{\sigma} = \nabla \cdot (\boldsymbol{C}\boldsymbol{\varepsilon}) = 0 \quad \longrightarrow \quad \boldsymbol{\sigma}(x,t) = \boldsymbol{E}(x)\boldsymbol{D}^N(x,t)$$

Multi-Point Stress Approximation (MPSA-W)*

Continuity of Stresses

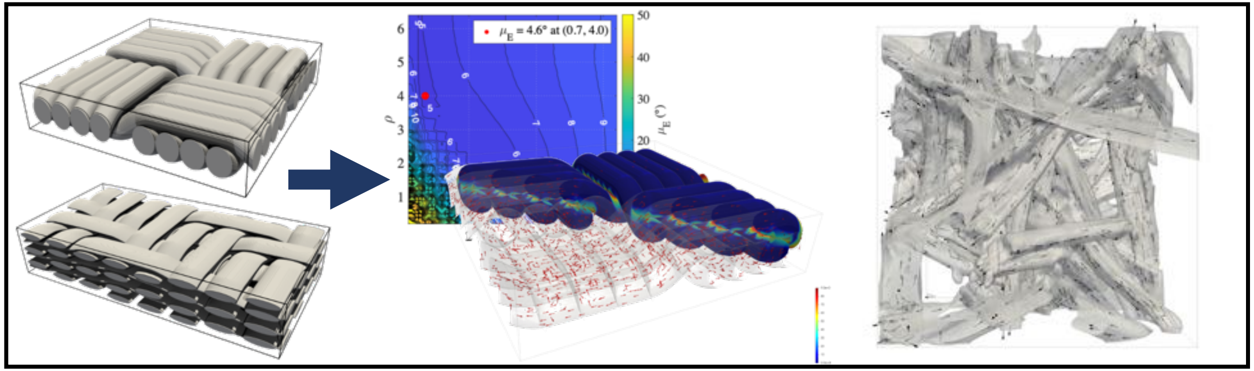
$$\boxed{\boldsymbol{\sigma}_P^{xx}} = \boldsymbol{\sigma}_E^{xx}$$
$$\boldsymbol{\sigma}_P^{yx} = \boldsymbol{\sigma}_E^{yx}$$
$$\vdots$$



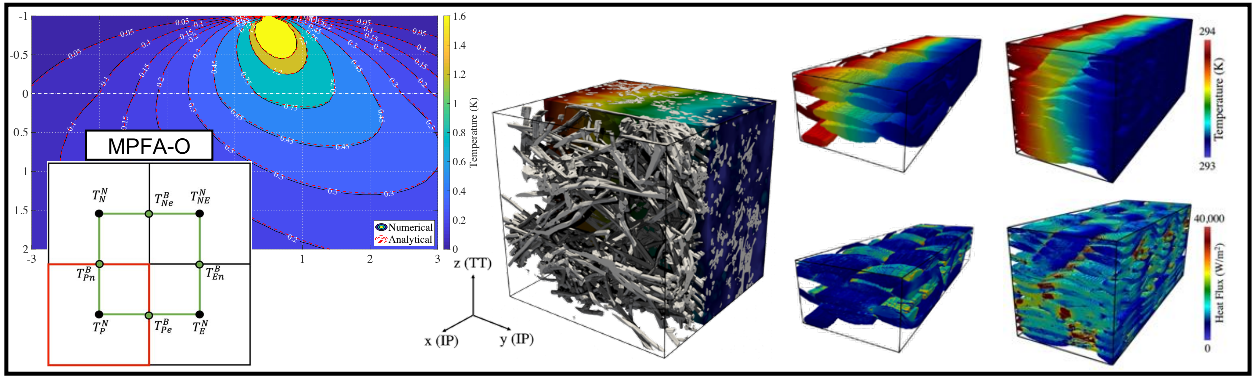
*Keilegavlen, E. and Nordbotten, J.M., 2017. Finite volume methods for elasticity with weak symmetry. Int. Journal for Numerical Methods in Engineering, 112(8), pp.939-962.

Conclusion

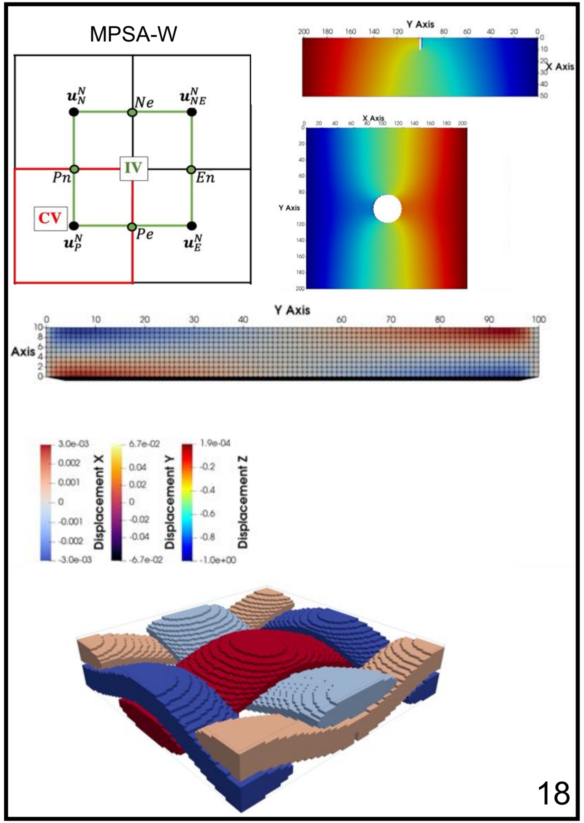
Part 1: Estimation of local orientation. *Computational Materials Science*, 178, p.109631. (2020)



Part 2: Computation of effective conductivity. *Computational Materials Science,* 186, p.109956. (2021)



Part 3: Computation of effective elasticity.
(work in progress)



Thank you. Questions?

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