PuMA and Multiscale Modeling

Presenter: Federico Semeraro

AMA at Thermal Protection Materials Branch (ARC-TSM)

January 11th, 2022

45th Annual Conference on Composites, Materials, and Structures

Predictive Material Modeling (PMM) group

Entry System Modeling (ESM) project

Content

- Motivation
- Overview of PuMA
  - Functionalities
  - Open-source release
  - Artificial generation
  - Micro-CT manipulation
- Effective properties for anisotropic porous media
  - Fiber orientation
  - Conductivity
  - Elasticity
  - Permeability

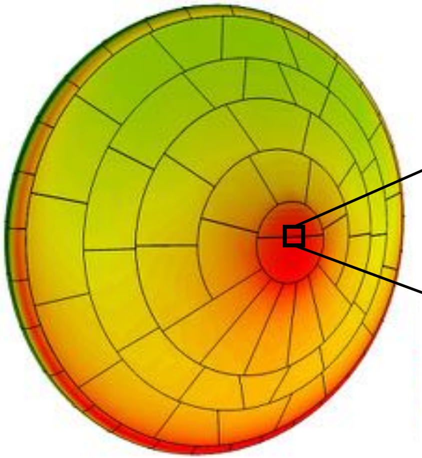
Modeling TPS

Macroscale

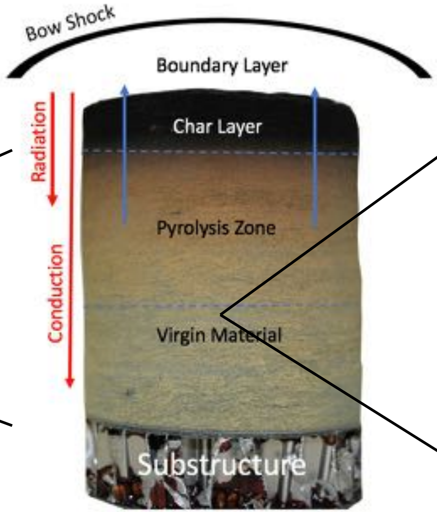
Full-scale material response solvers, using homogenized properties

Microscale

Homogenization of material properties to be used in macroscale models

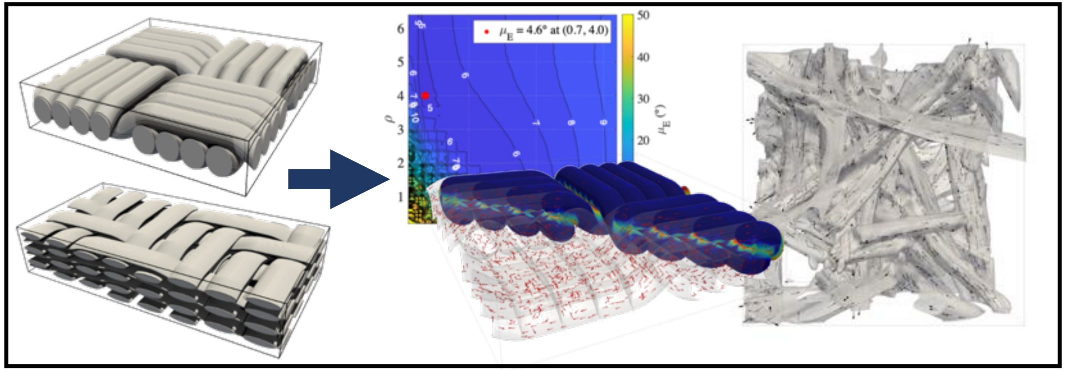


Simulation of surface temperature for MSL heatshield

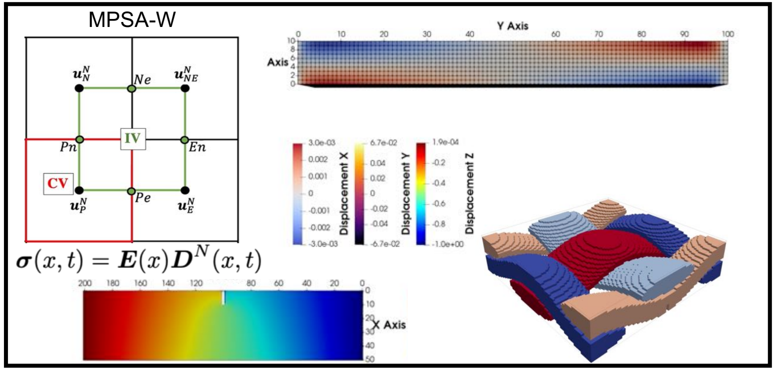


Overview of material properties computation

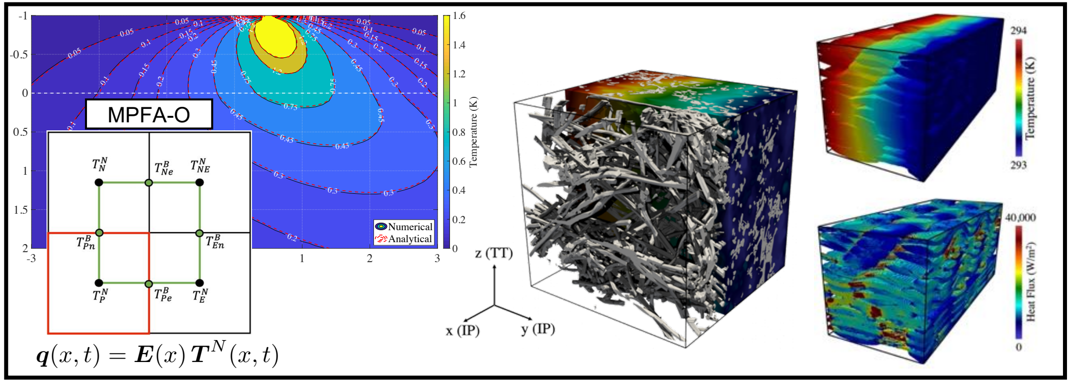
Part 1: Estimation of local orientation. *Computational Materials Science* (2020)



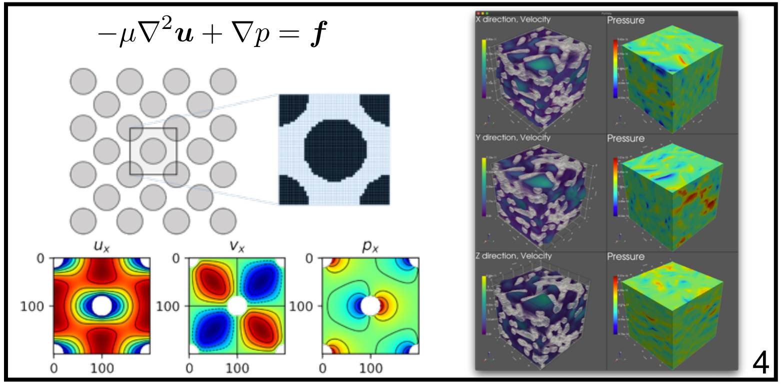
Computation of effective elasticity



Part 2: Computation of effective conductivity. *Computational Materials Science* (2021)



Computation of effective permeability



Porous Microstructure Analysis (PuMA) v3 release

Installation: conda install -c conda-forge puma

Open-source repository: https://github.com/nasa/puma

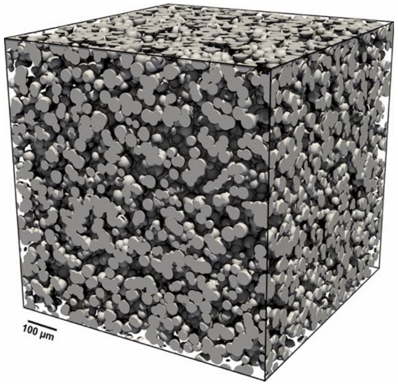
Documentation: https://puma-nasa.readthedocs.io

Video tutorials: PuMA YouTube channel

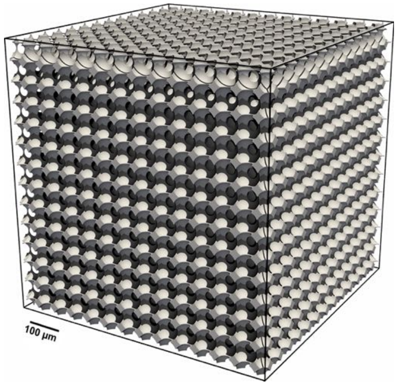
Ferguson, J.C., Semeraro, F., Thornton, J.M., Panerai, F., Borner, A., Mansour, N.N., 2021. Update 3.0 to “PuMA: The Porous Microstructure Analysis software”, *SoftwareX*

Artificial domain generation

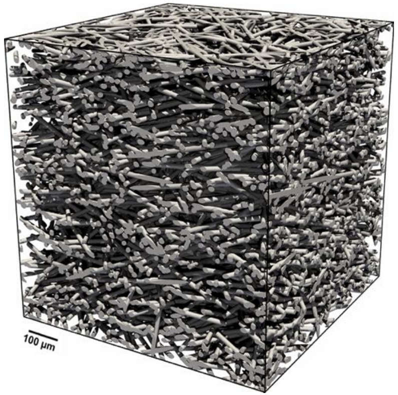
Packed Sphere Beds

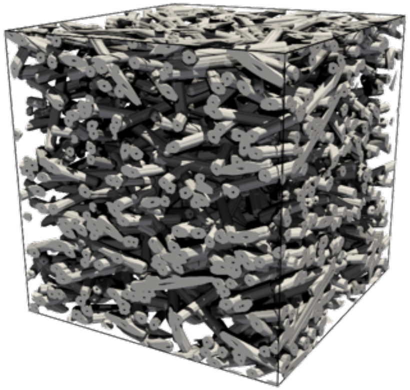


Periodic Foams

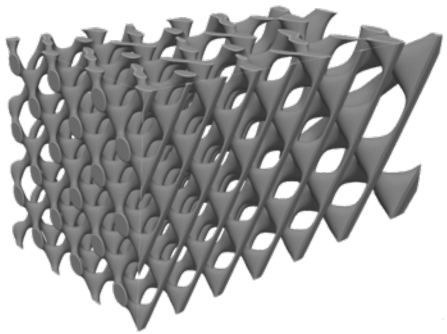


Fiber Structures



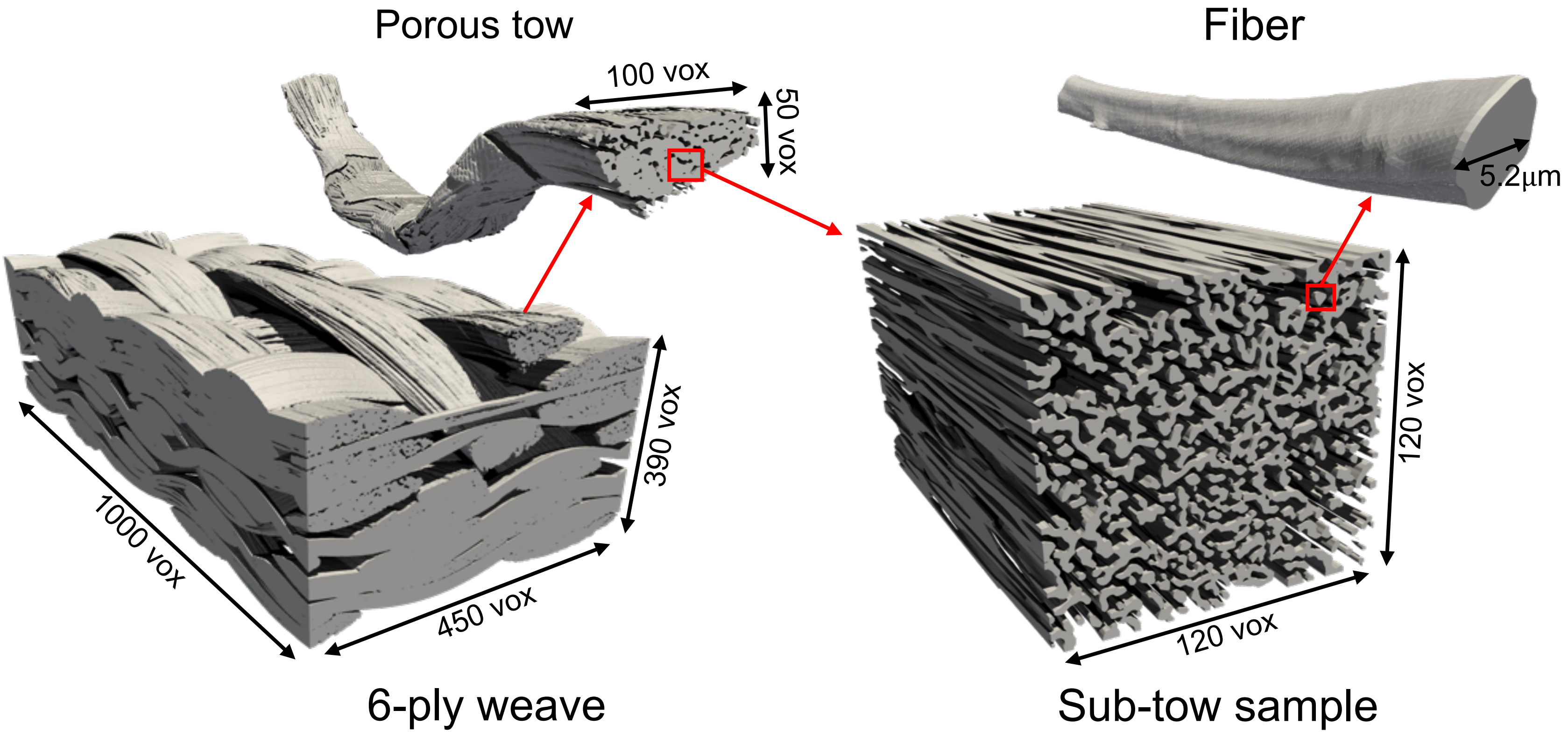


Triply Periodic Minimal Surface (TPMS)



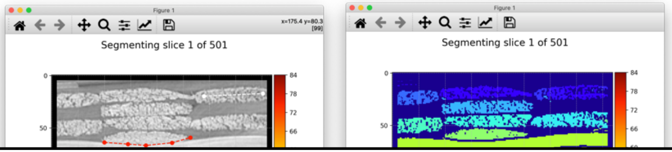
Woven geometries

Micro-CT weaves: anisotropic at multiple scales



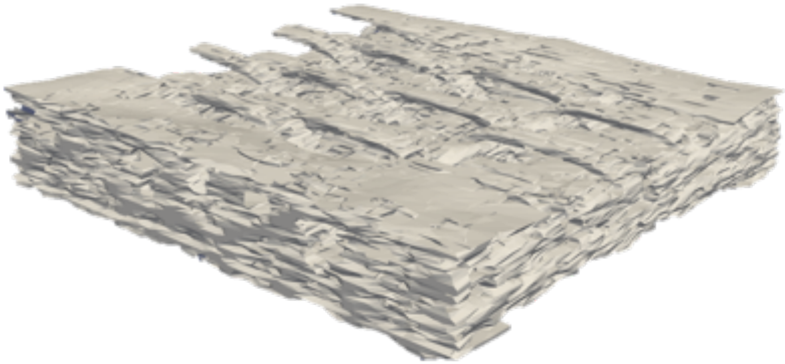
Weave segmentation and tow tracking

Manual labeling

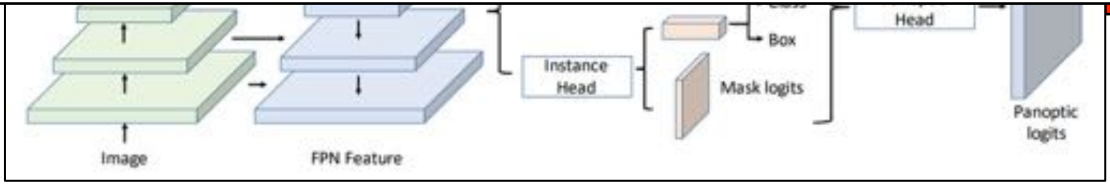


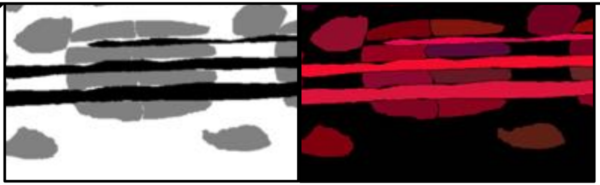
Tracking by IoU

Naïve threshold of original Micro-CT weave



Fully segmented weave



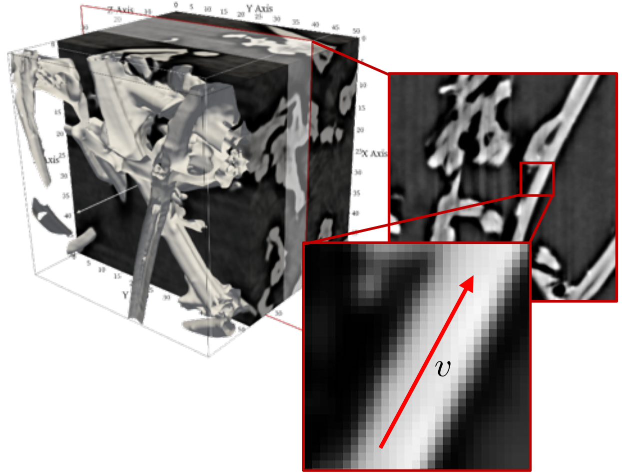


Semantic Classes Instances

Allred, A., Abbott, L.J., Doostan, A., Maute, K. Automated processing of x-ray computed tomography images via panoptic segmentation for modeling woven composite textiles, *Composite Structures (to appear)*

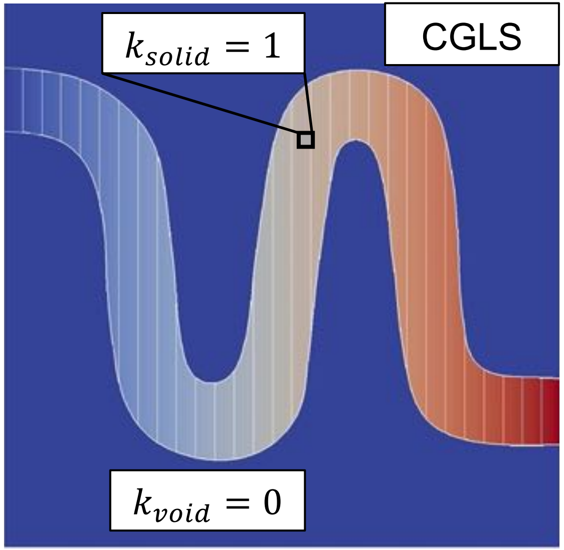
Orientation methods

Structure tensor

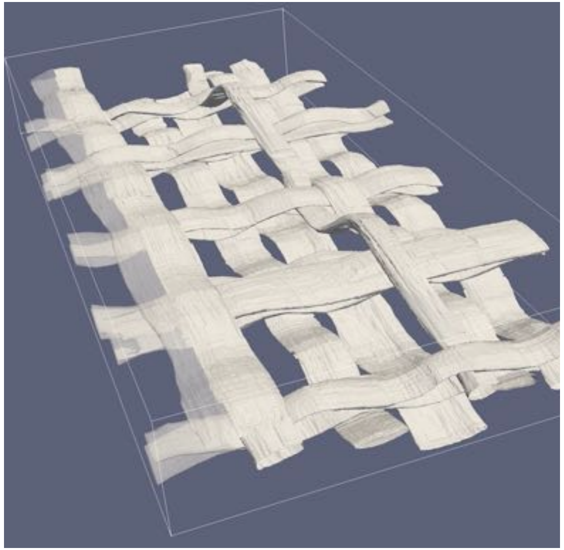


$$(I(x+v)-I(x))^2 \approx 0$$

Artificial flux

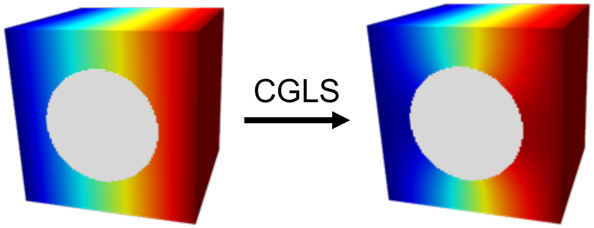


Ray casting



Semeraro, F., Ferguson, J.C., Panerai, F., King, R.J. and Mansour, N.N., 2020. Anisotropic analysis of fibrous and woven materials part 1: Estimation of local orientation. *Computational Materials Science*, *178*, p.109631.

Conductivity solver

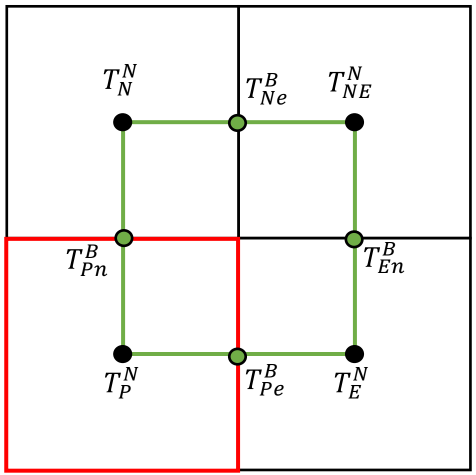


$$\rightarrow \boldsymbol{k}_{eff} = q^x \cdot L_x$$

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

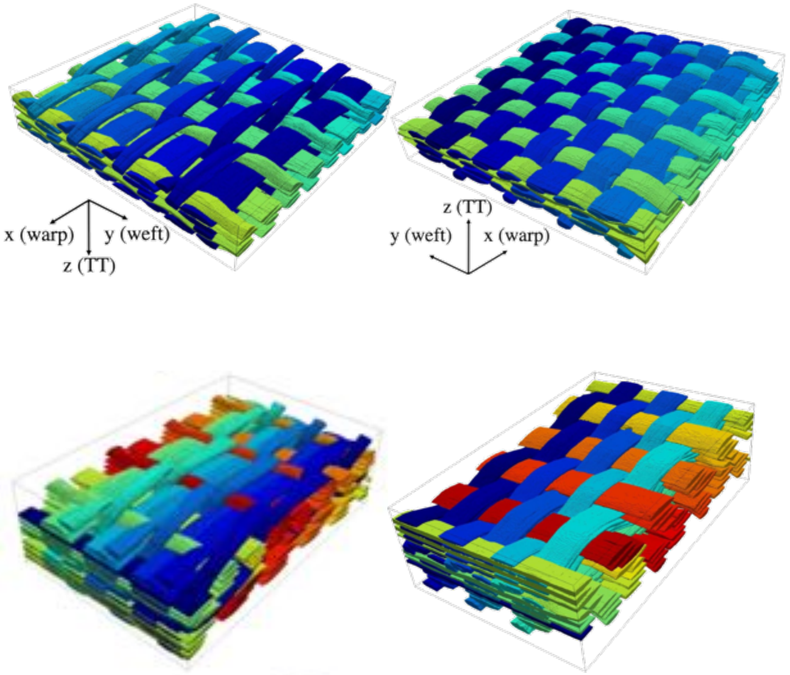
Multi-Point Flux Approximation (MPFA-O)*
i.e. continuity of fluxes and temperatures at Boundary points:

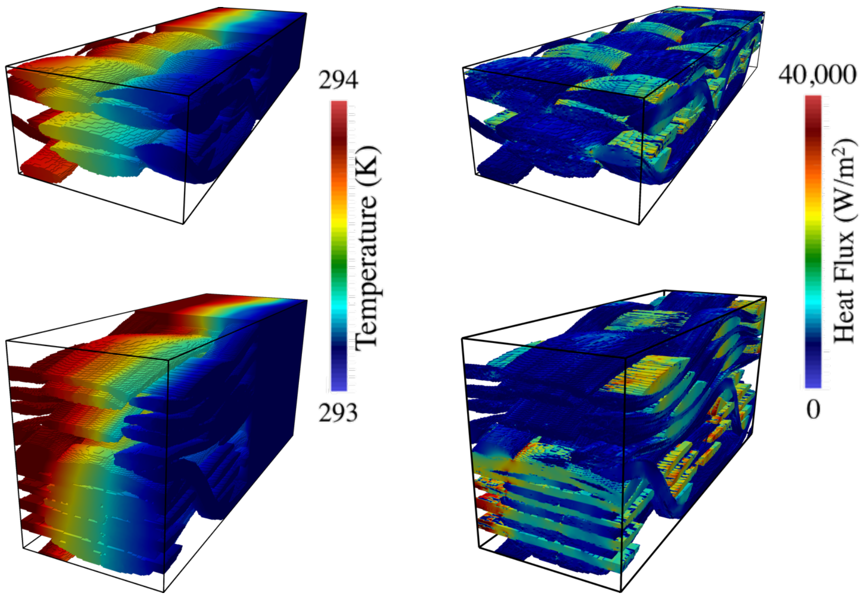
$$\boldsymbol{q}_P^{xx} = \boldsymbol{q}_E^{xx}$$
$$\boldsymbol{q}_P^{yy} = \boldsymbol{q}_N^{yy}$$
$$\vdots$$



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

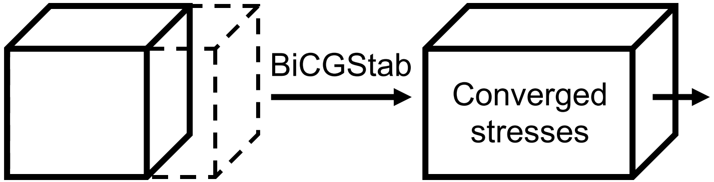
Conductivity solver validation: ADEPT





Semeraro, F., Ferguson, J.C., Acin, M., Panerai, F. and Mansour, N.N., 2021. Anisotropic analysis of fibrous and woven materials part 2: Computation of effective conductivity. Computational Materials Science, 186, p.109956.

Elasticity solver



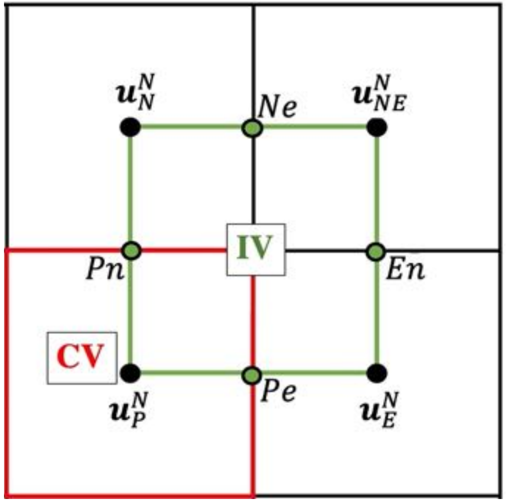
$$\boldsymbol{C}_{eff} = \boldsymbol{\sigma}^{x} \cdot L_x$$

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

Multi-Point Stress Approximation (MPSA-W)*

Continuity of Stresses

$$\begin{aligned} \boldsymbol{\sigma}_P^{xx} &= \boldsymbol{\sigma}_E^{xx} \\ \boldsymbol{\sigma}_P^{yx} &= \boldsymbol{\sigma}_E^{yx} \\ &\vdots \end{aligned}$$

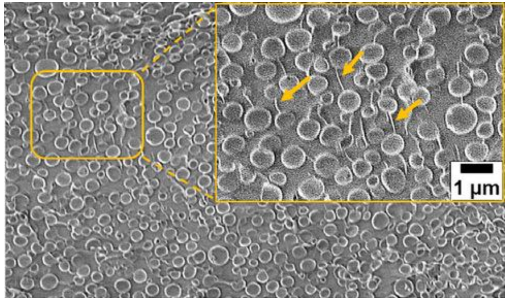


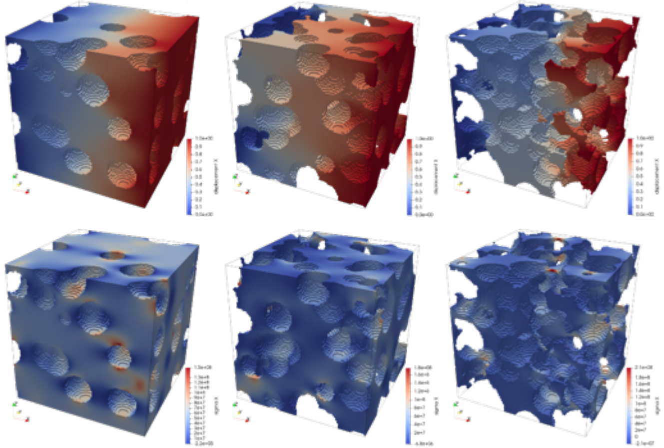
*Keilegavlen, E. and Nordbotten, J.M., 2017. Finite volume methods for elasticity with weak symmetry. Int. Journal for Numerical Methods in Engineering, 112(8), pp.939-962.

Elasticity solver validation: woven composite

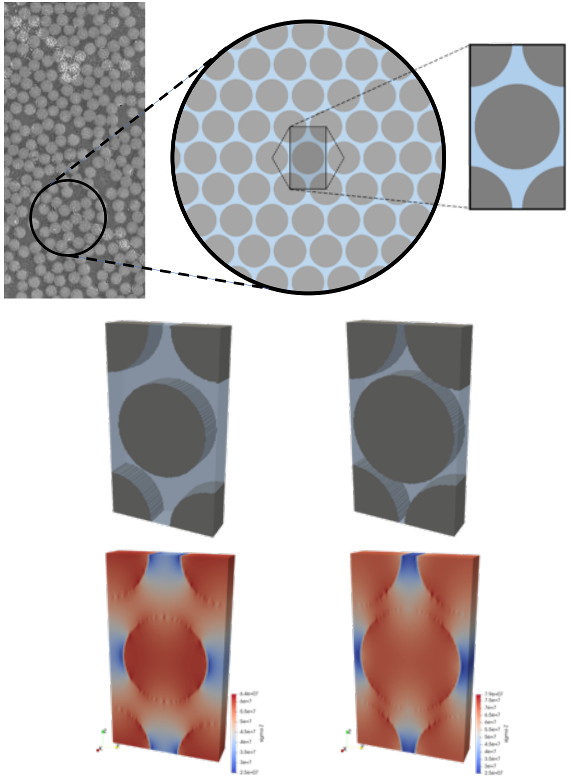
Fraile Izquierdo, S., Semeraro, F., Acin, M., 2022. Multi-Scale Analysis of Effective Mechanical Properties of Porous 3D Woven Composite Materials. *AIAA Scitech Forum*

Matrix: porous phenolic resin

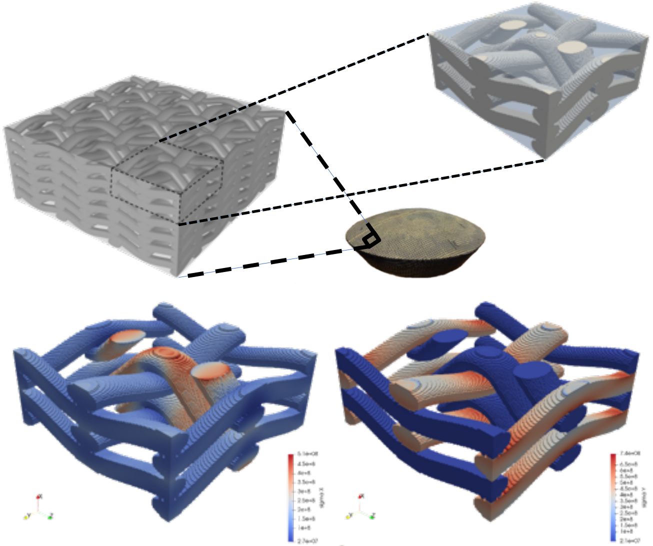


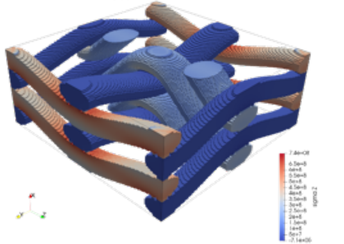


Intra-tow fiber packing



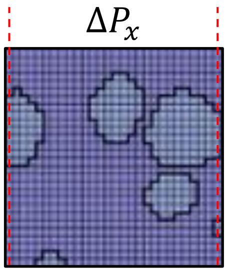
Woven unit cell



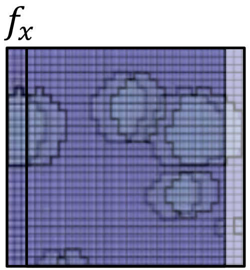


Permeability solver

- Governing equation for Stokes flow (valid for slow creeping regimes, $Re \approx 0$):



$$-\mu\nabla^2\boldsymbol{u} + \nabla p = \boldsymbol{f}$$



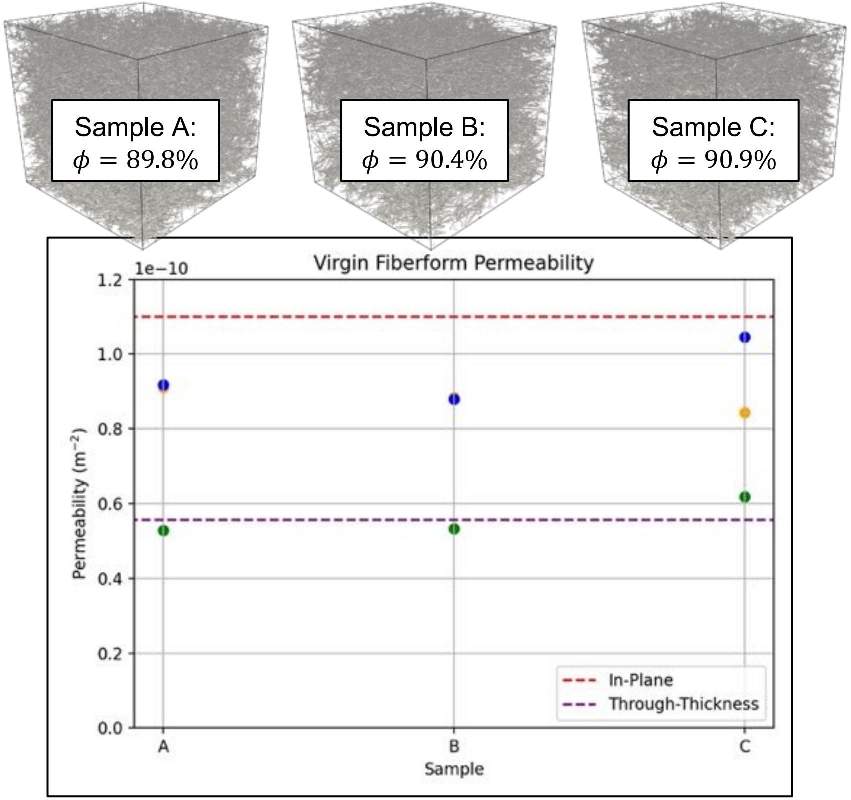
- Solved with FE scheme with Q1-Q1 discretization in velocity and pressure (plus pressure stabilization term)
- By imposing a unit body force f_i in the three Cartesian directions, we can homogenize the permeability as:

$$\begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{xy} & k_{yy} & k_{yz} \\ k_{xz} & k_{yz} & k_{zz} \end{bmatrix} = \frac{l^3}{|V|}\int_V u_i \, dV$$

Permeability validation: Fiberform

- Three 500^3 samples with voxel size = 2.6μm
- Run on V100 (32GB) with matrix-free PCG
- Experimental values* obtained from Fiberform samples with porosity $\phi = 87\%$

Sample	A	B	C	Exp*
K_{xx} (m^{-2} e-10)	0.910	0.884	0.845	1.100
K_{yy} (m^{-2} e-10)	0.918	0.879	1.046	1.100
K_{zz} (m^{-2} e-10)	0.529	0.533	0.619	0.557
Porosity ϕ (%)	89.8	90.4	90.9	87.0
Time (‘) (Avg its)	18.667 (1951)	13.383 (1355)	14.617 (1483)	-
DOFs (e6)	424.4	428.3	432.6	-

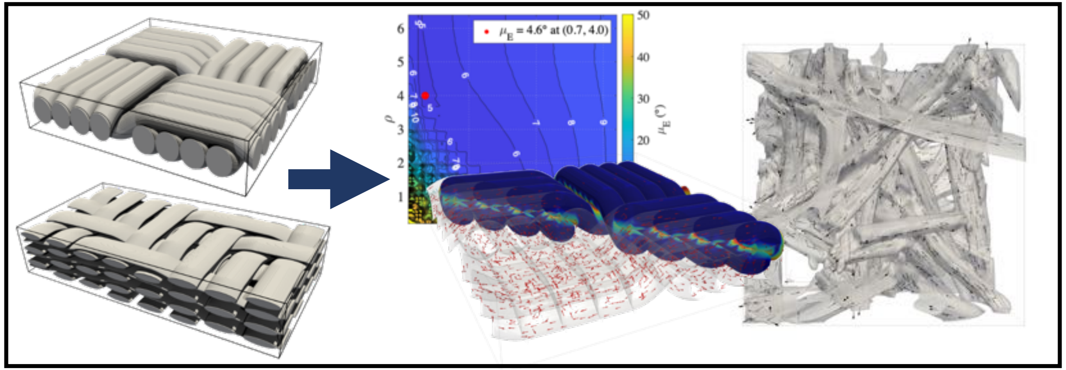


Lopes, P.C.F., Semeraro, F.

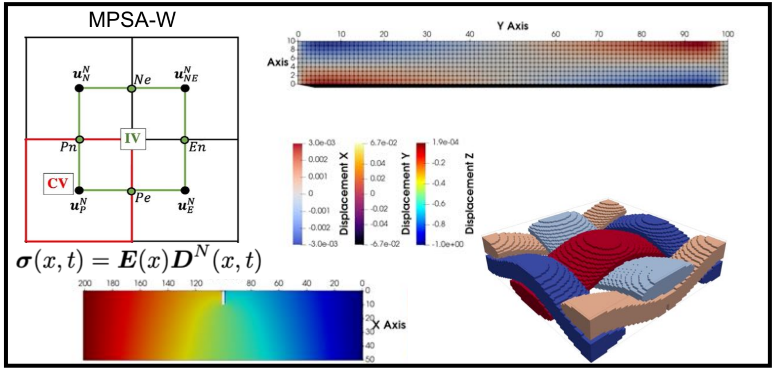
*Panerai, F., White, J.D., Cochell, T.J., Schroeder, O.M., Mansour, N.N., Wright, M.J., Martin, A., 2016. Experimental measurements of the permeability of fibrous carbon at high-temperature. *International Journal of Heat and Mass Transfer*, *101*, pp.267-273.

Questions?

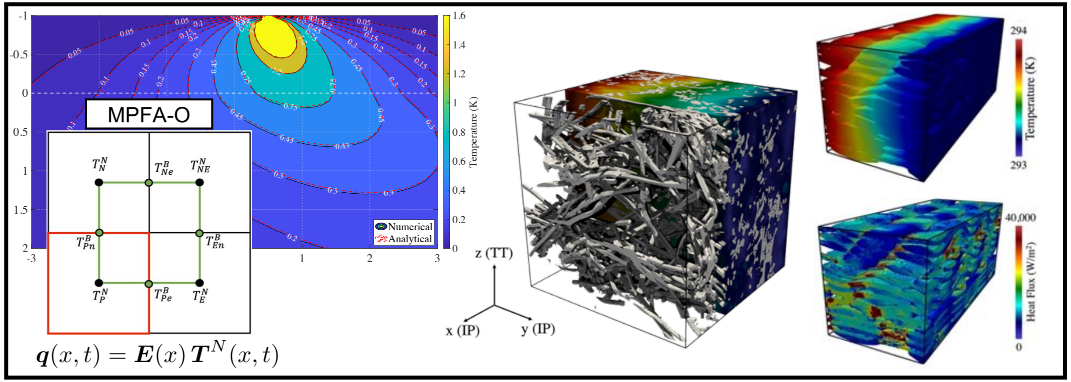
Part 1: Estimation of local orientation. *Computational Materials Science* (2020)



Computation of effective elasticity



Part 2: Computation of effective conductivity. *Computational Materials Science* (2021)



Computation of effective permeability