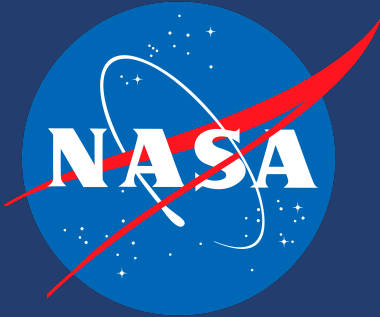


PuMA and Multiscale Modeling



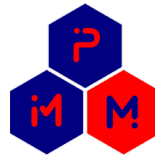
Presenter: Federico Semeraro

AMA at Thermal Protection Materials Branch (ARC-TSM)

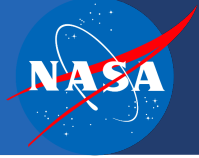
May 18th, 2022



Predictive Material Modeling (PMM) group



Entry System Modeling (ESM) project



Content

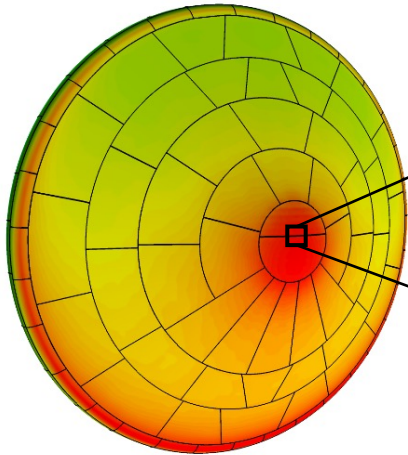
- Motivation
- Overview of PuMA
 - Functionalities
 - Open-source release
 - Artificial generation
 - Micro-CT manipulation
- Effective properties for anisotropic porous media
 - Fiber orientation
 - Conductivity
 - Elasticity
 - Permeability
 - Real-time micro-CT



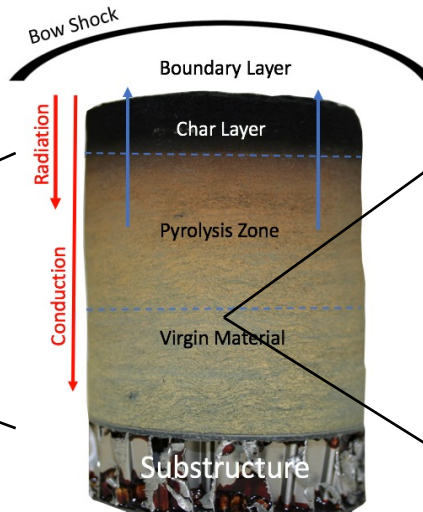
Modeling TPS

Macroscale

Full-scale material response solvers, using homogenized properties

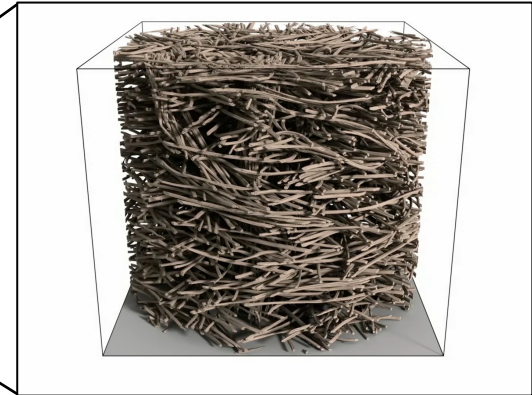


Simulation of surface temperature for MSL heatshield



Microscale

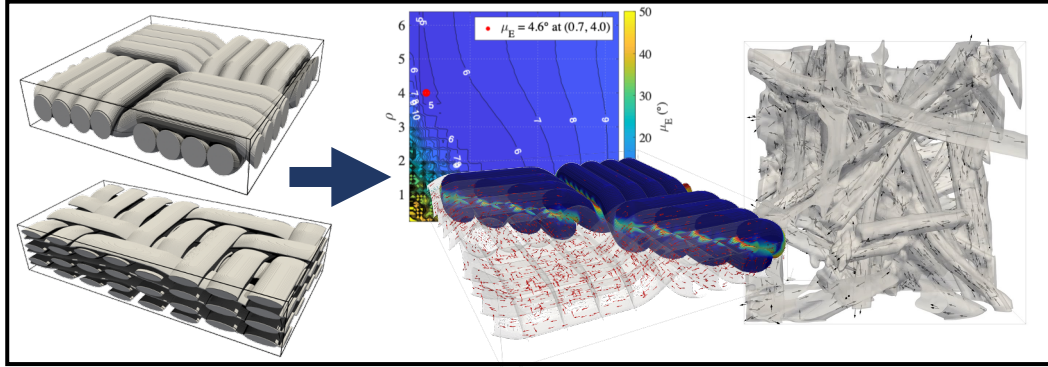
Homogenization of material properties to be used in macroscale models



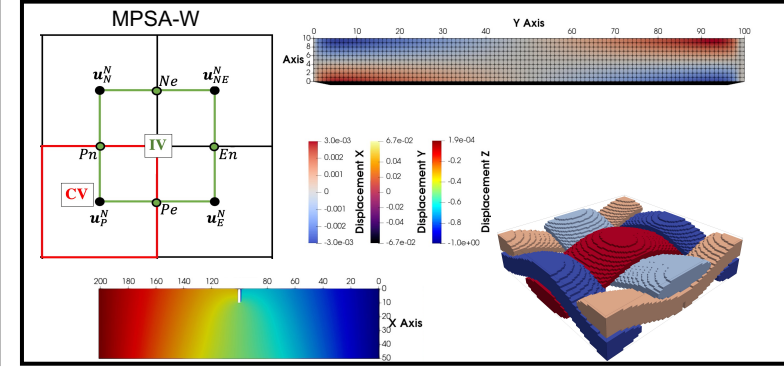


Overview of material properties computation

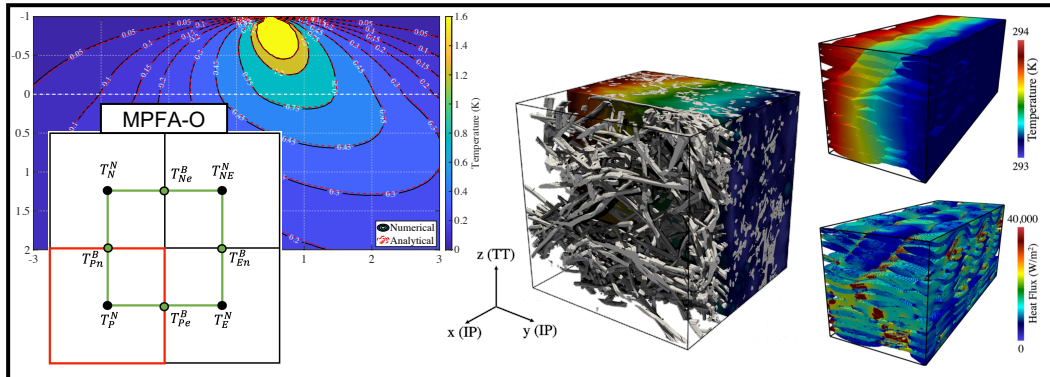
Part 1: Estimation of local orientation. *Computational Materials Science* (2020)



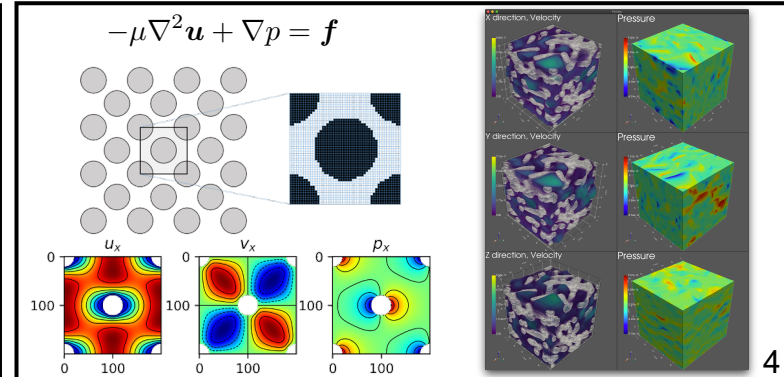
Computation of effective elasticity



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



Computation of effective permeability





Porous Microstructure Analysis (PuMA) v3 release



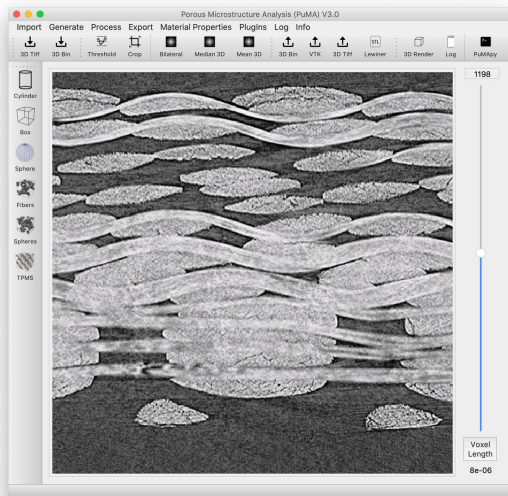
Installation: `conda install -c conda-forge puma`

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

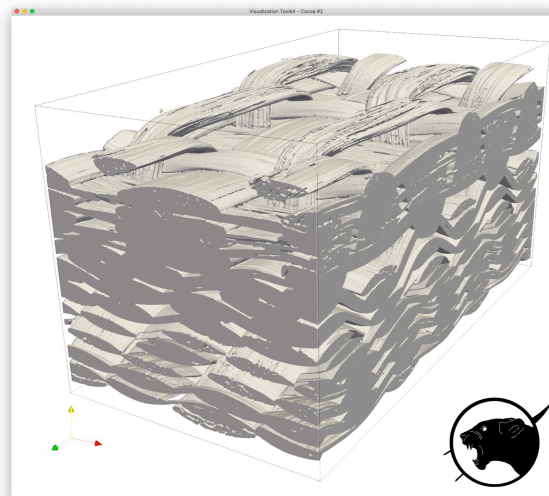
Documentation: <https://puma-nasa.readthedocs.io>

Video tutorials: [PuMA YouTube channel](#)

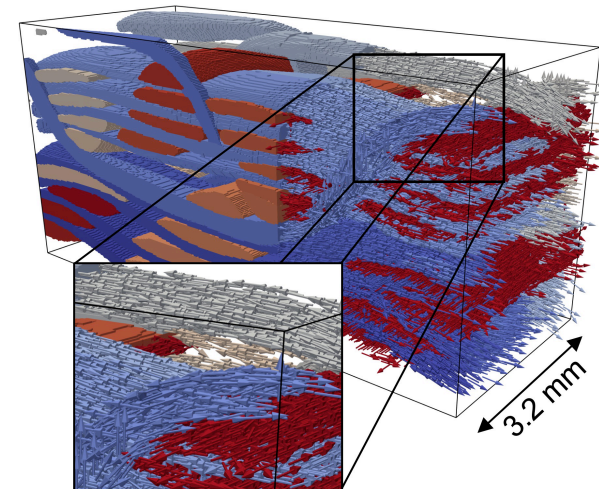
a)



b)



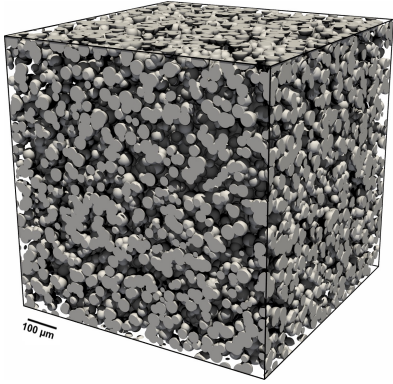
c)



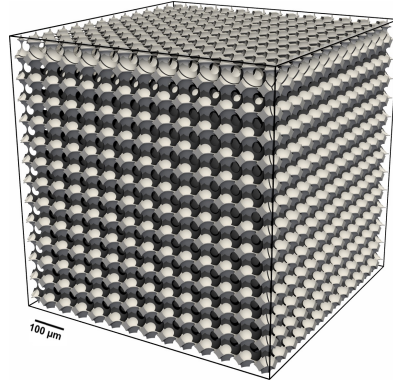


Artificial domain generation

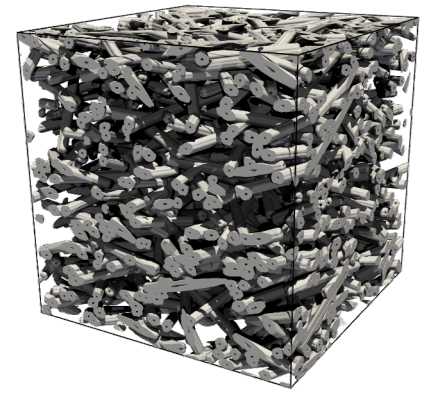
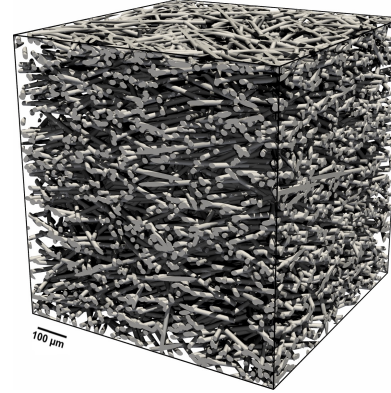
Packed Sphere Beds



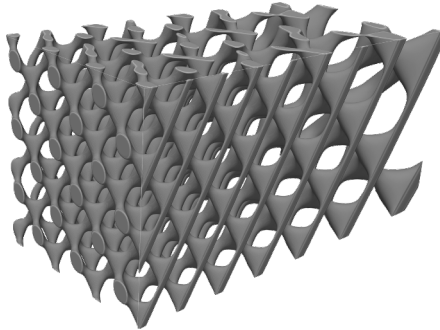
Periodic Foams



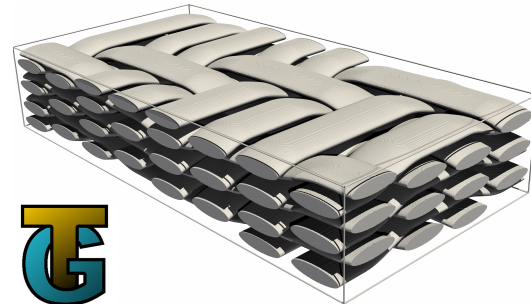
Fiber Structures



Triply Periodic Minimal Surface (TPMS)

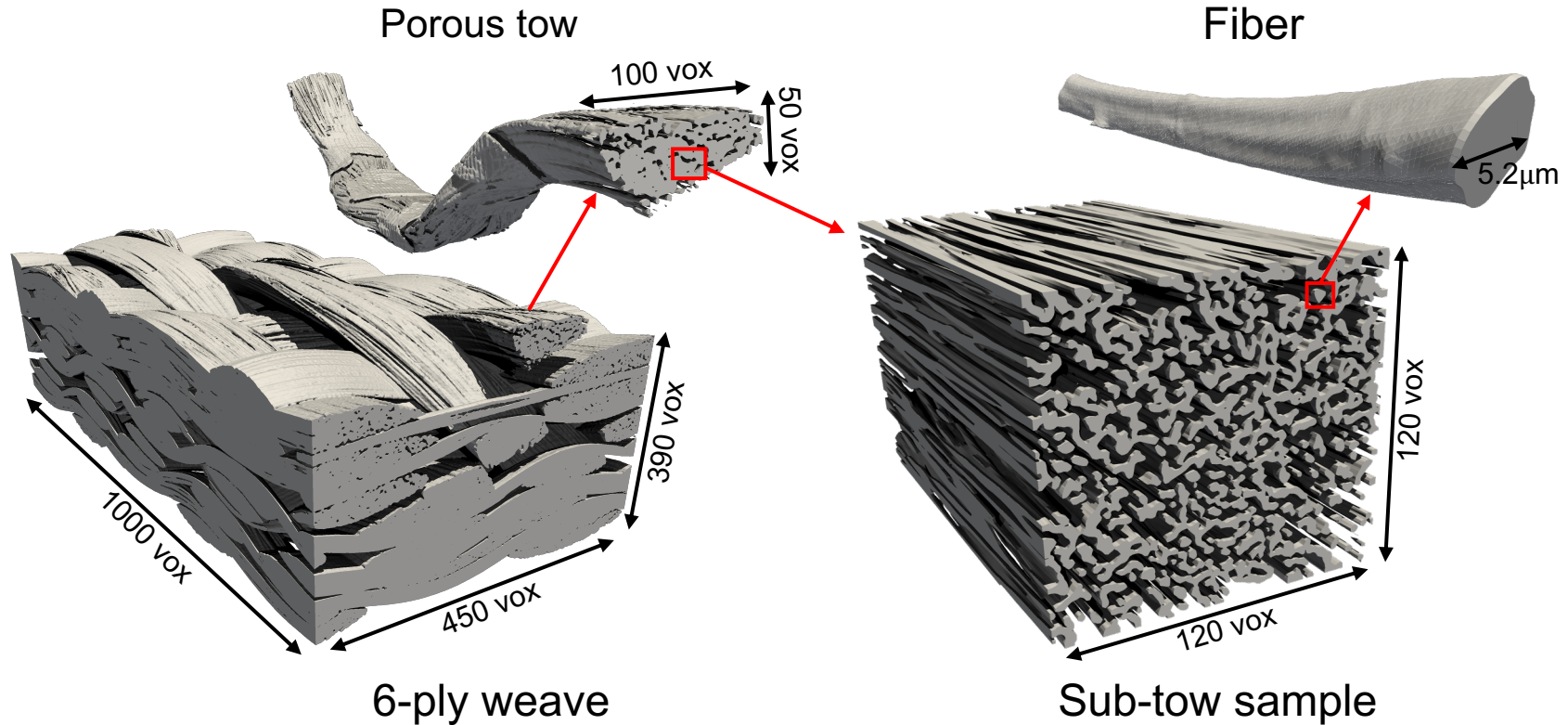


Woven geometries





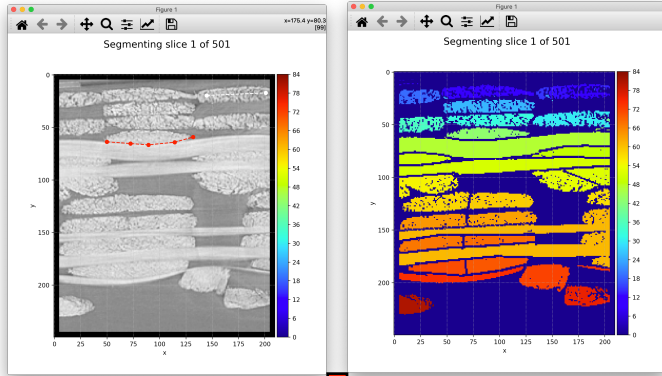
Micro-CT weaves: anisotropic at multiple scales



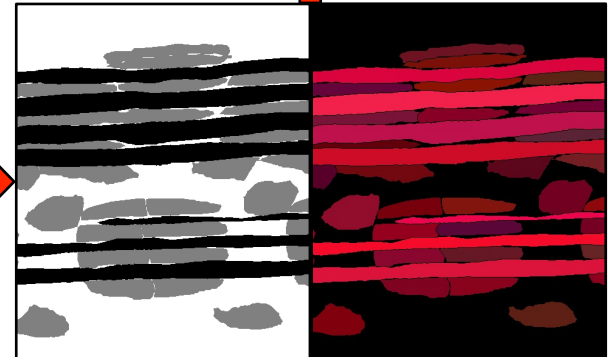
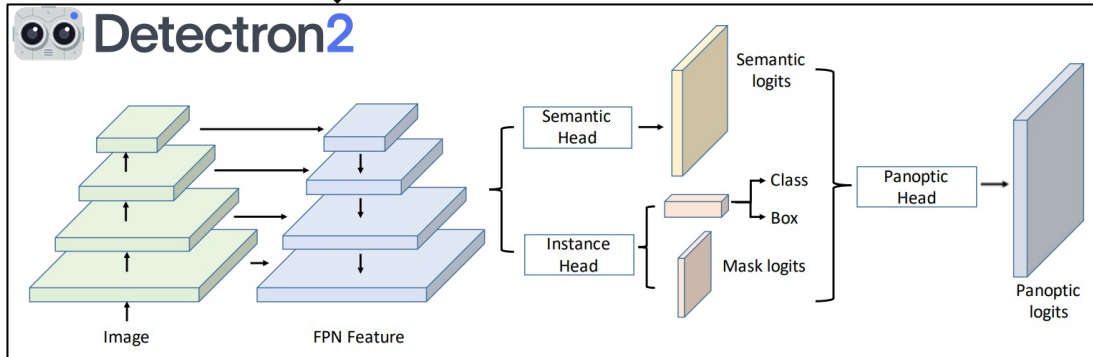
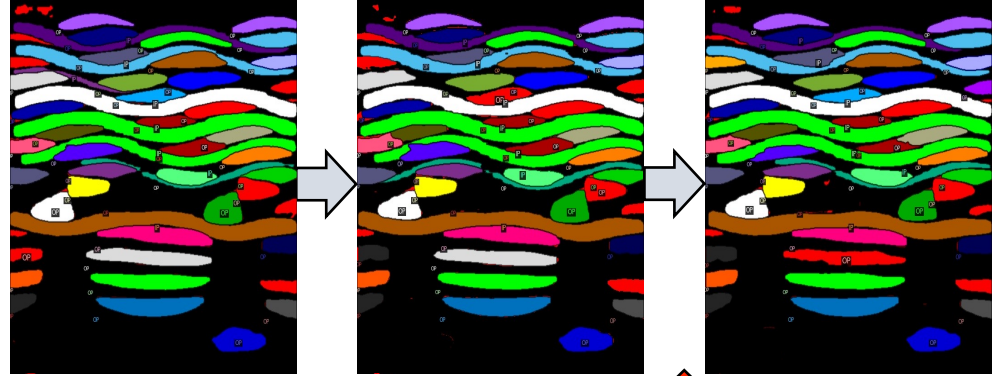


Weave segmentation and tow tracking

Manual labeling



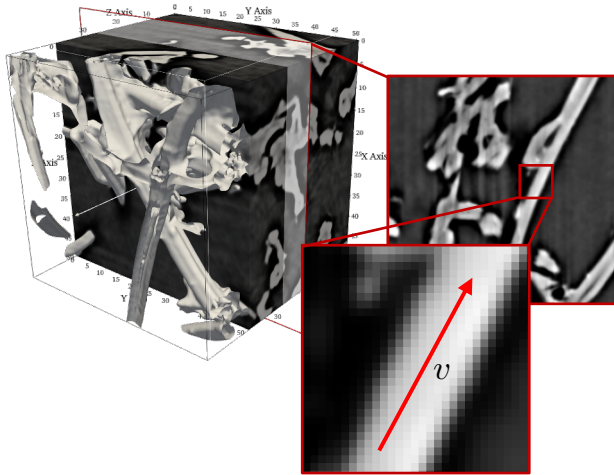
Tracking by IoU



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* (accepted)

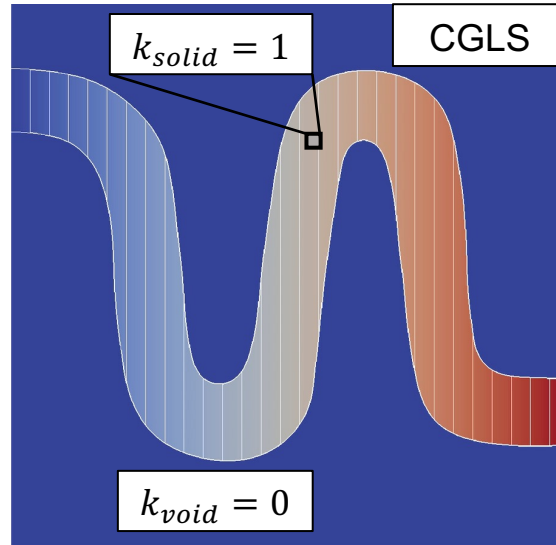
Orientation methods

Structure tensor

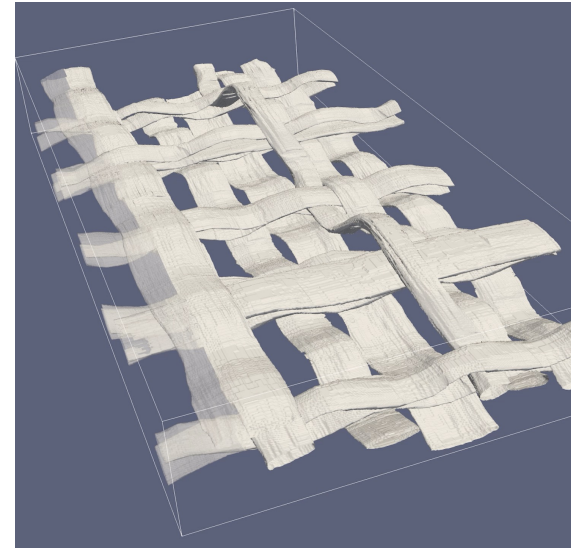


$$(I(x + v) - I(x))^2 \approx 0$$

Artificial flux



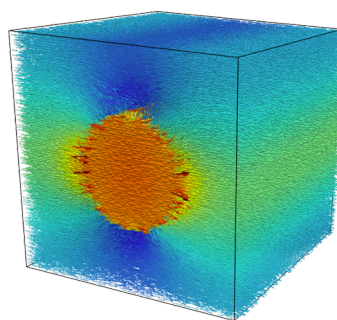
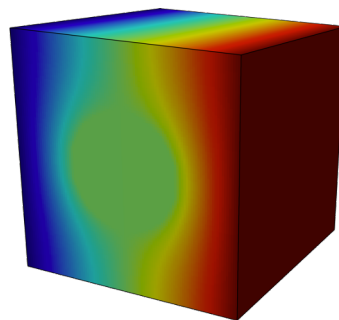
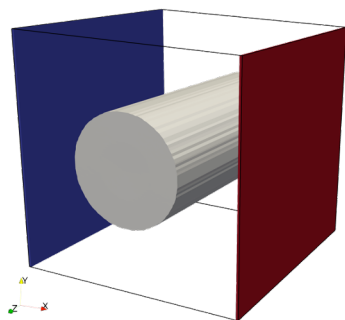
Ray casting



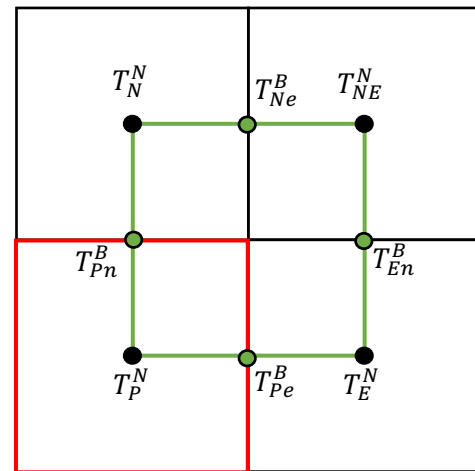


Conductivity solver

$$\nabla \cdot \mathbf{q} = 0 \quad \text{where} \quad \mathbf{q} = -\mathbf{k} \nabla T = - \begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{xy} & k^{yy} & k^{yz} \\ k^{xz} & k^{yz} & k^{zz} \end{bmatrix} \begin{pmatrix} \partial T / \partial x \\ \partial T / \partial y \\ \partial T / \partial z \end{pmatrix}$$



$$\mathbf{k}^x = -\mathbf{q} \cdot \mathbf{L}_x$$



Multi-Point Flux Approximation (MPFA-O)* local system (2D):

$$\mathbf{q} = \mathbf{E} \mathbf{T}^N$$

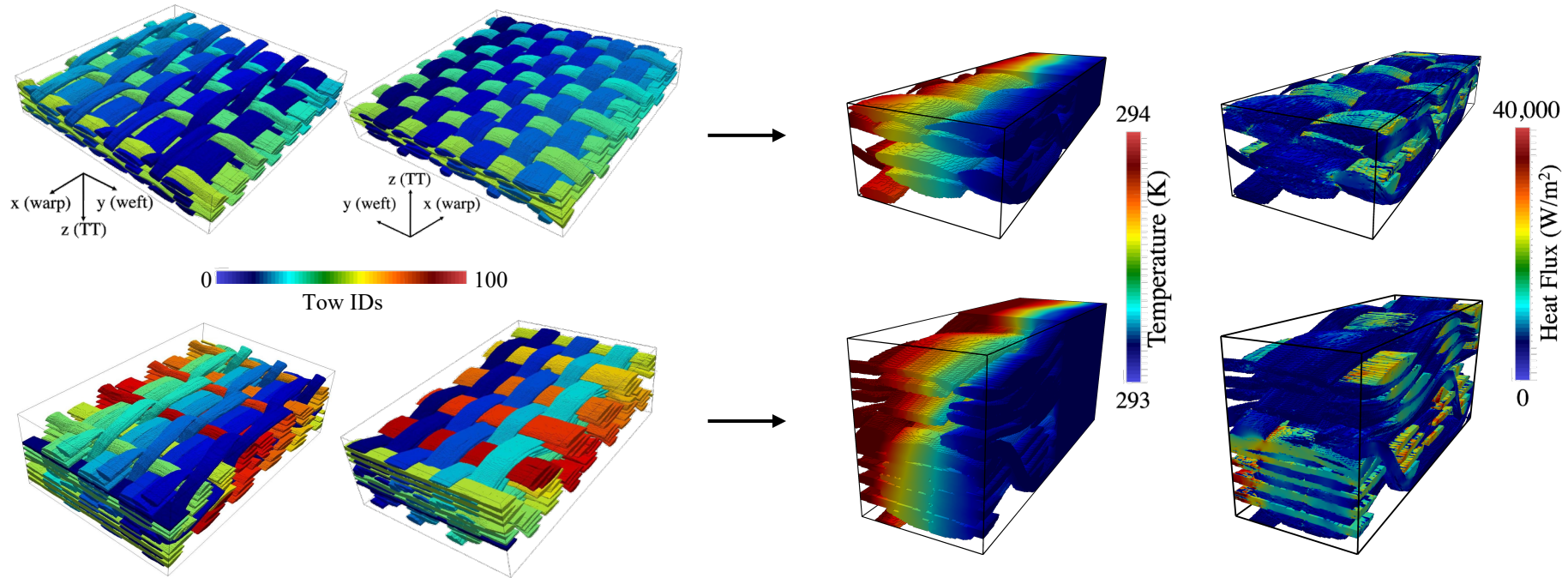
$$\boxed{q_P^x} = k_P^{xx} \frac{T_{Pe}^B - T_P^N}{h/2} + k_P^{xy} \frac{T_{Pn}^B - T_P^N}{h/2}$$

Unknowns: Continuity of fluxes:

$$\mathbf{T}^B = \begin{pmatrix} T_{Pe}^B \\ T_{Ne}^B \\ T_{Pn}^B \\ T_{En}^B \end{pmatrix} \quad \begin{aligned} \boxed{q_P^x} &= q_E^x \\ q_N^x &= q_{Ne}^x \\ q_P^y &= q_N^y \\ q_E^y &= q_{Ne}^y \end{aligned}$$



Conductivity solver validation: ADEPT

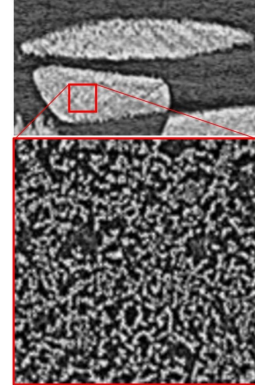
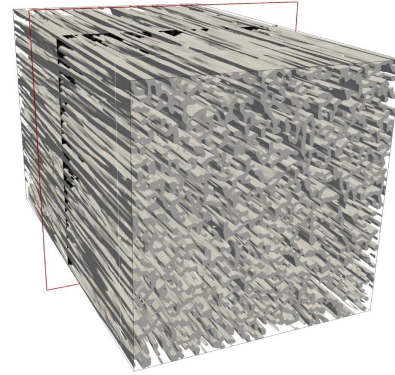
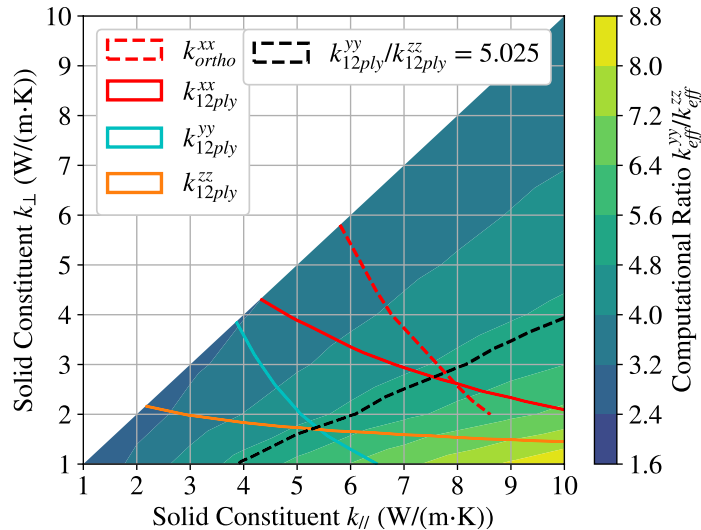


Semeraro, F., Ferguson, J.C., Acin, M., Panerai, F. and Mansour, N.N., 2021. Anisotropic analysis of fibrous and woven materials part 2: Computation of effective conductivity. Computational Materials Science, 186, p.109956.

Single fiber conductivity estimation

Experimental value at room temperature:

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



Single fiber thermal conductivity

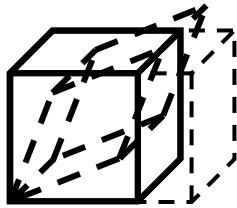
$$[k_{//}, k_{\perp}] = [9.7, 5.5] \frac{\text{W}}{\text{mK}}$$

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

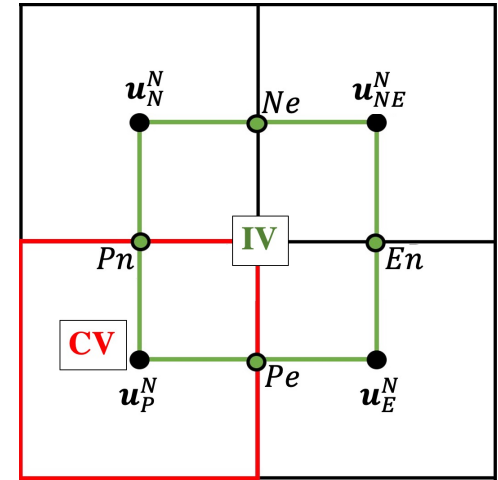
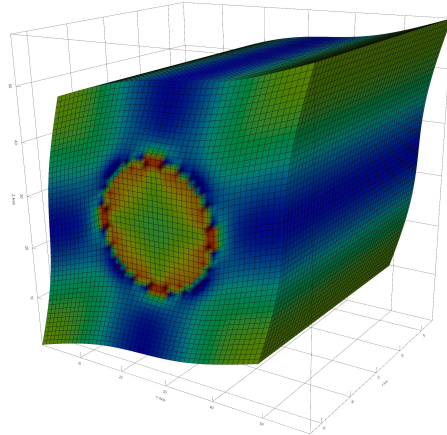


Elasticity solver

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad \text{where} \quad \boldsymbol{\sigma} = \mathbf{C} \boldsymbol{\varepsilon}$$



$$\mathbf{C}^4 = \frac{2L_x L_y}{L_x + L_y} \boldsymbol{\sigma}$$



Multi-Point Stress Approximation (MPSA-W)* local system enforcing displacement and stress continuity:

$$\boldsymbol{\sigma} = \mathbf{E} \mathbf{u}^N$$

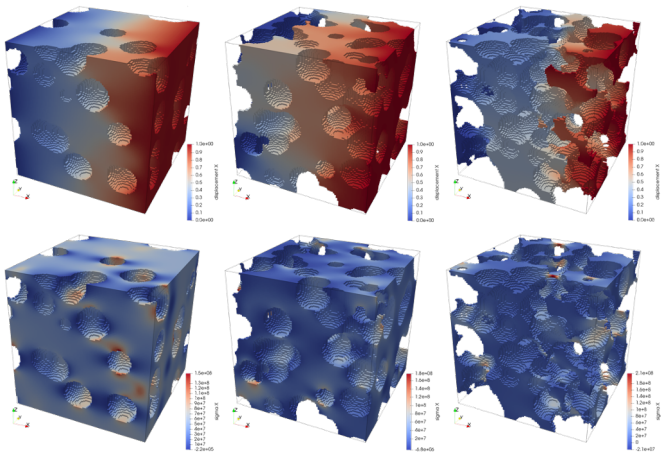
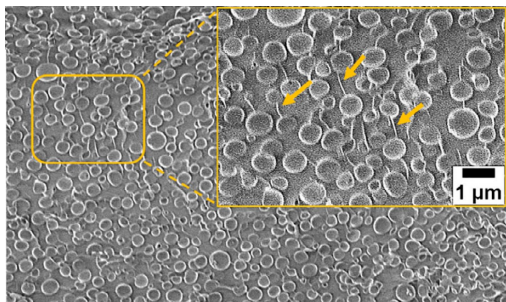
$$\boxed{\boldsymbol{\sigma}_P} = \mathbf{C}_P \mathbf{G}_P - \langle \mathbf{C} \tilde{\mathbf{Q}} \mathbf{G} \rangle_{IV} \quad \begin{pmatrix} \mathbf{S}_G \\ \mathbf{D}_G \end{pmatrix} \mathbf{G} = \begin{pmatrix} \mathbf{0} \\ \mathbf{D}_u \end{pmatrix} \mathbf{u}^N + \begin{pmatrix} \mathbf{F}_N \\ \mathbf{D}_d \end{pmatrix}$$



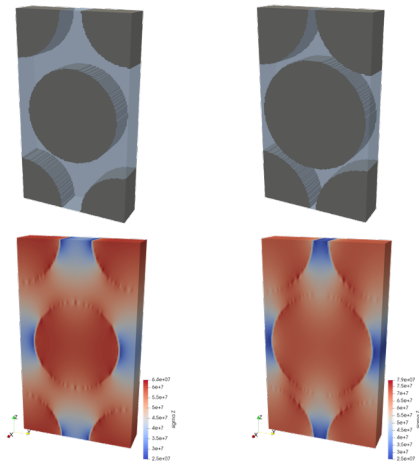
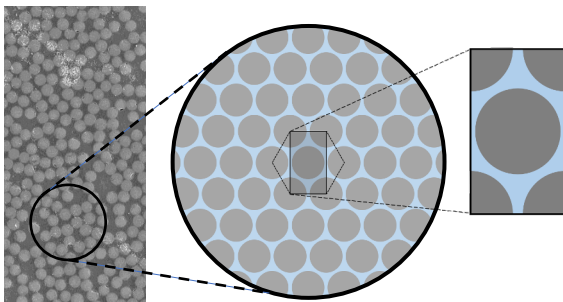
Elasticity solver validation: woven composite

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

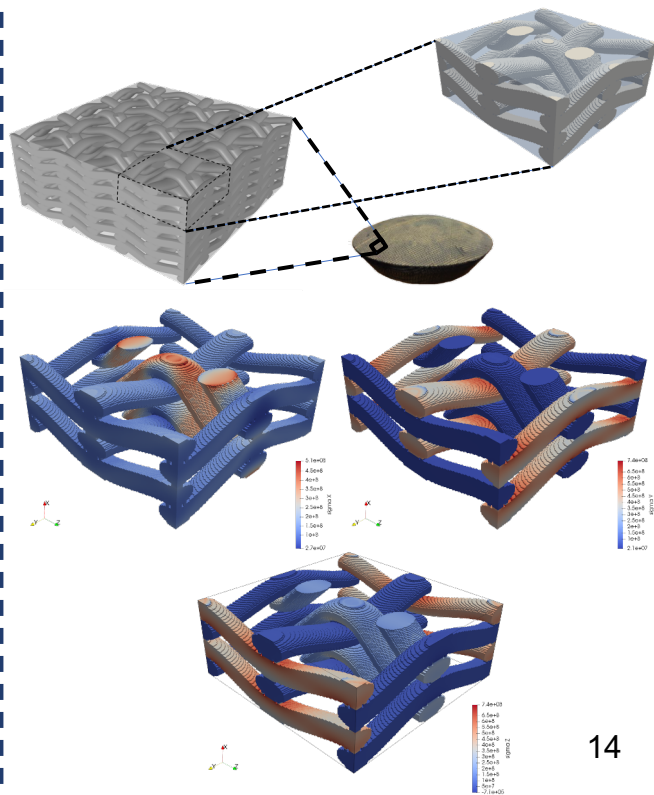
Matrix: porous phenolic resin



Intra-tow fiber packing

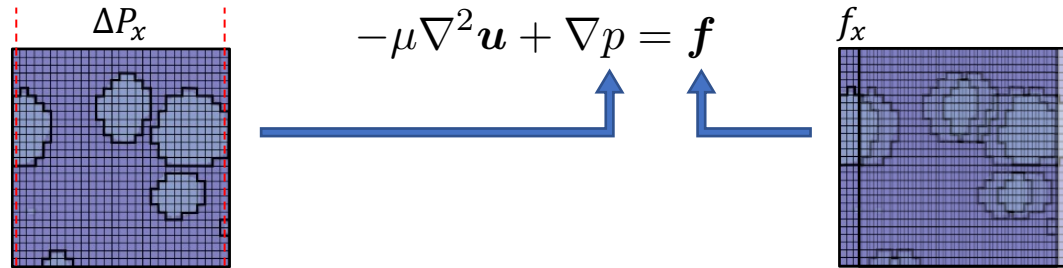


Woven unit cell



Permeability solver

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



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

- 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:

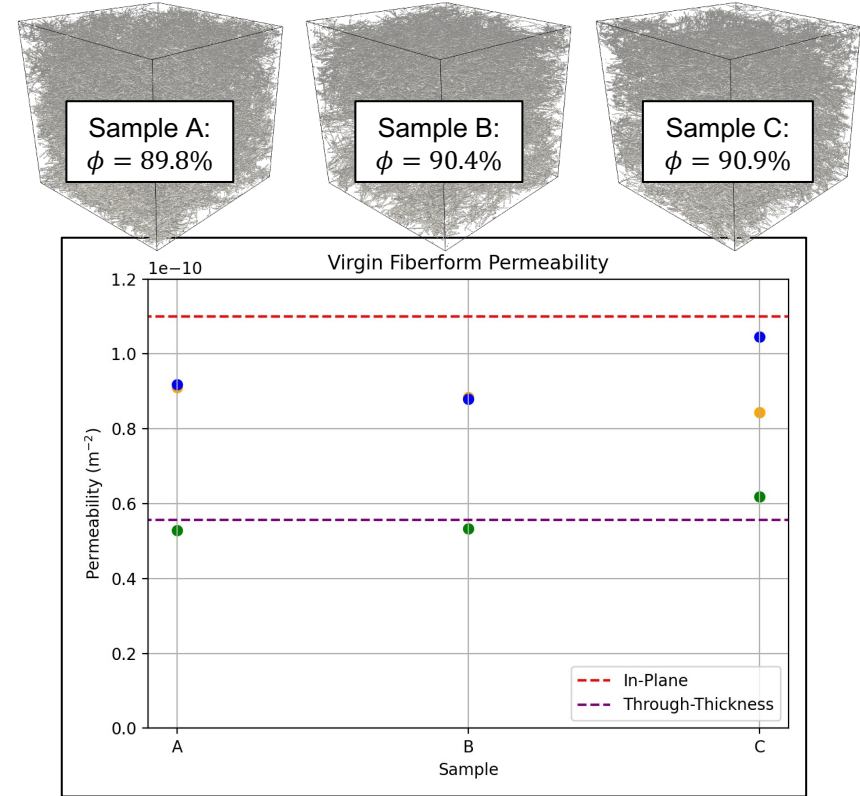
$$\begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{xy} & k^{yy} & k^{yz} \\ k^{xz} & k^{yz} & k^{zz} \end{bmatrix} = \frac{l^3}{|V|} \int^V u^i dV$$

Permeability validation: Fiberform

- Three 500³ 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	-

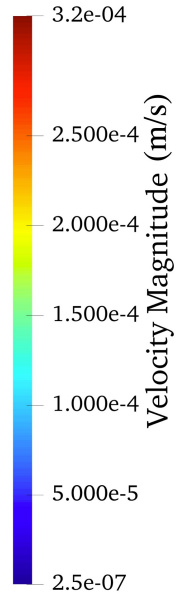
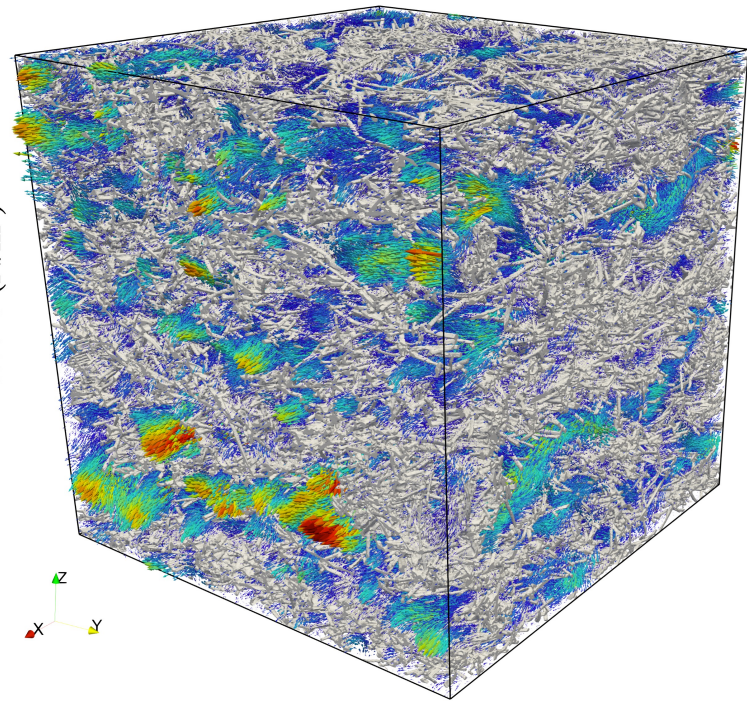
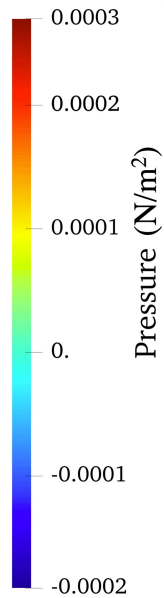
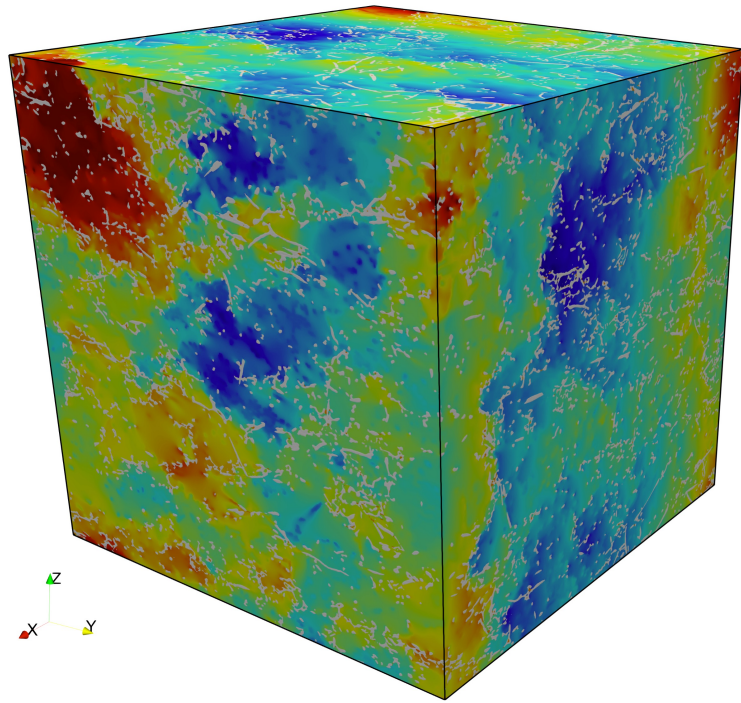
*Panerai, F., White, J.D., Cochell, T.J., Schroeder, O.M., Mansour, N.N., Wright, M.J., Martin, A., 2016. Experimental measurements of the permeability of fibrous carbon at high-temperature. *International Journal of Heat and Mass Transfer*, 101, pp.267-273.



*Pedro C. F. Lopes, Rafael S. Vianna, Victor W. Sapucaia, Federico Semeraro, Ricardo Leiderman, and Andre M. B. Pereira. Simulation Toolkit for Digital Material Characterization of Large Image-based Microstructures. *npj Computational Materials* (under review)

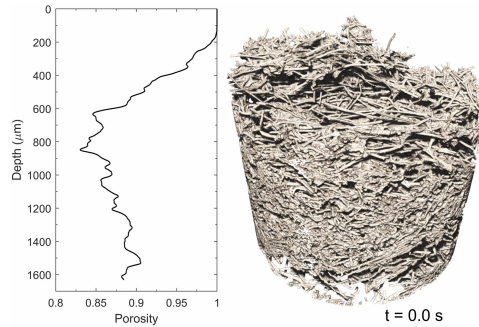


Velocity and Pressure Fields

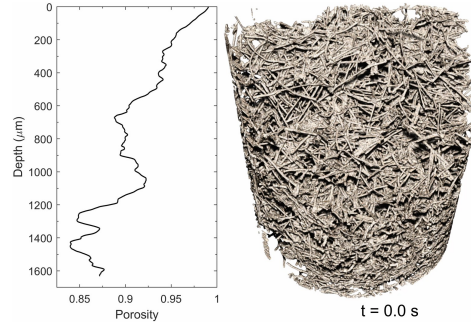




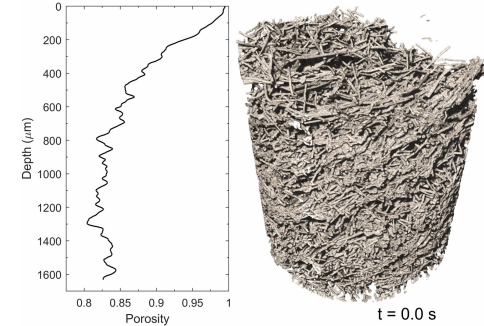
Time-dependent micro-CT of oxidizing Fiberform



Temp. (C)	Datasets
735	180



Temp. (C)	Datasets
875	67



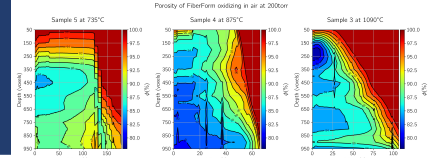
Temp. (C)	Datasets
1090	107

F. Semeraro, B. Ringel, F. Panerai

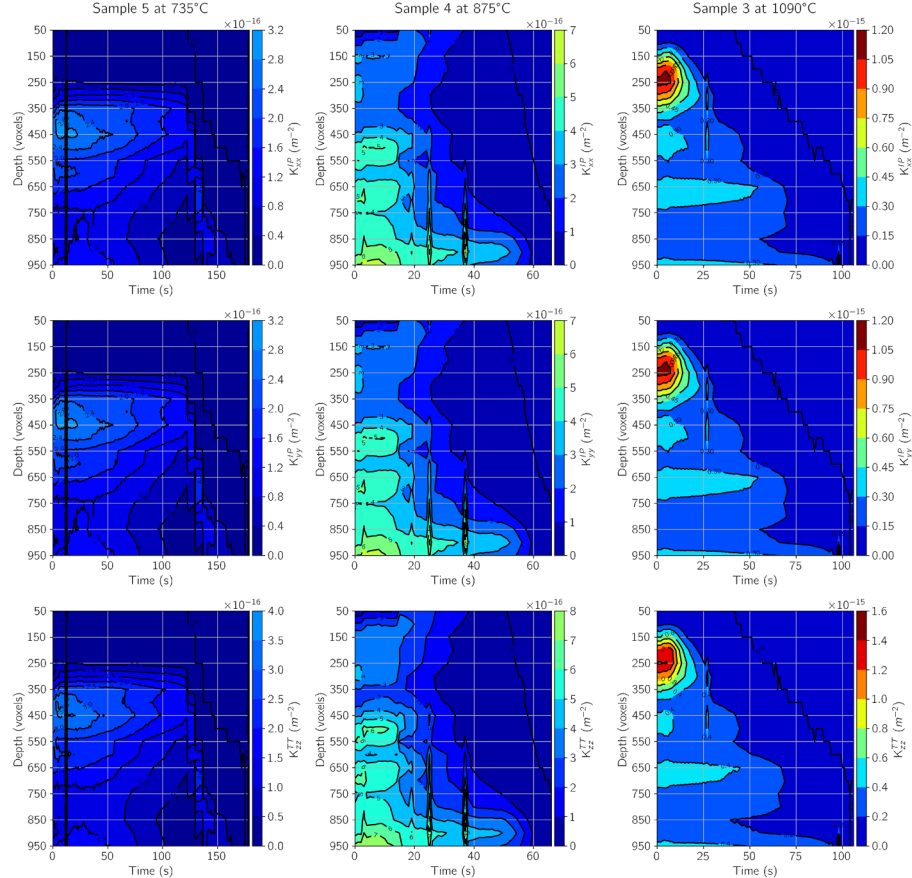
- 354 micro-CT datasets (2.5 TB) at 200 torr (0.26 atm)
- Dataset size: 700x700x1000 voxels, with resolution of 1.62 microns
- Each domain sub-divided into 19 different 700x700x100 voxels using a convolution window along Z
- Compute conductivity, elasticity, and permeability for all the subdivided datasets (i.e. 6,726 domains), to obtain them as a function of the samples' depth and time → 20,178 simulations on NAS
- Local Conductivity for two phases: $k_{\text{air}}=0.0257$, $k_{\text{fiber}}=13 \text{ W/(mK)}$



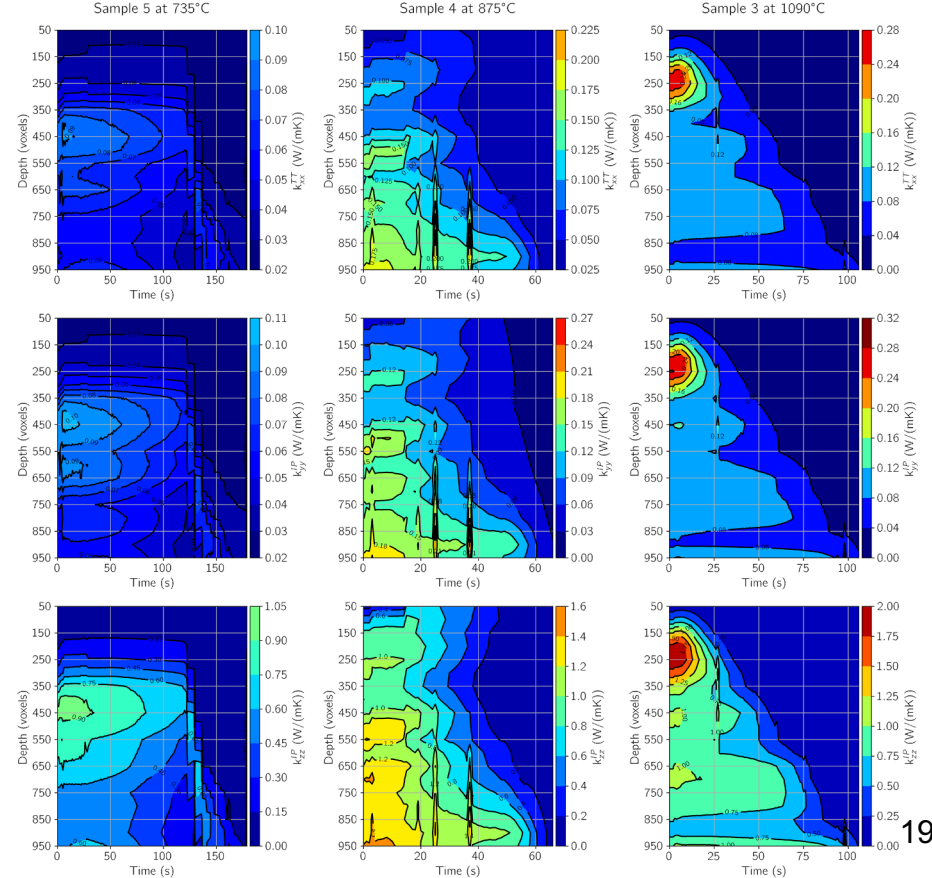
Conductivity and Permeability



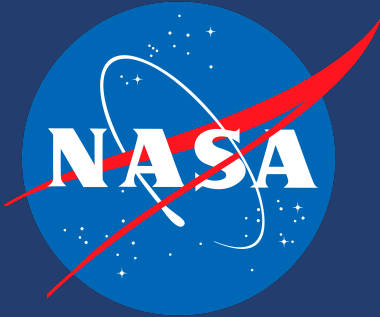
Permeability of FiberForm oxidizing in air at 200torr



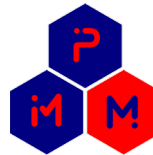
Thermal Conductivity of FiberForm oxidizing in air at 200torr



Questions?



Predictive Material Modeling (PMM) group



Entry System Modeling (ESM) project