Porous Microstructure Analysis (PuMA)

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AMA at Thermal Protection Materials Branch (ARC-TSM)

Lead Developers: J.C. Ferguson and F. Semeraro

Other Contributors: J. Thornton, F. Panerai, A. Borner, N.N. Mansour, S. Fraile Izquierdo, J.B.E. Meurisse

June 16th, 2022

Predictive Material Modeling (PMM) group

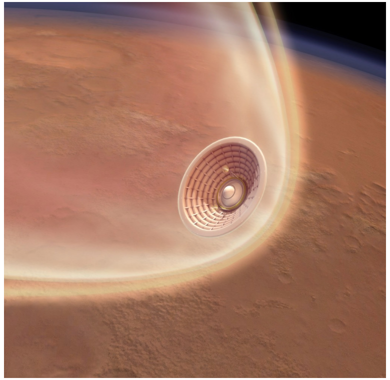
Entry System Modeling (ESM) project

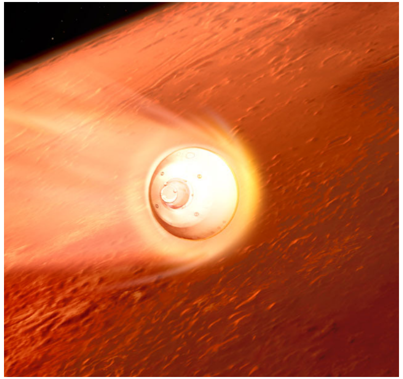
Content

- Motivation and objectives
- Overview of PuMA
  - Open-source release
  - Material properties computation
  - Artificial geometry generation
- Effective properties for anisotropic porous media
  - Fiber orientation
  - Conductivity
  - Elasticity
  - Permeability

Thermal Protection Systems (TPS)

Need for Thermal Protection Systems



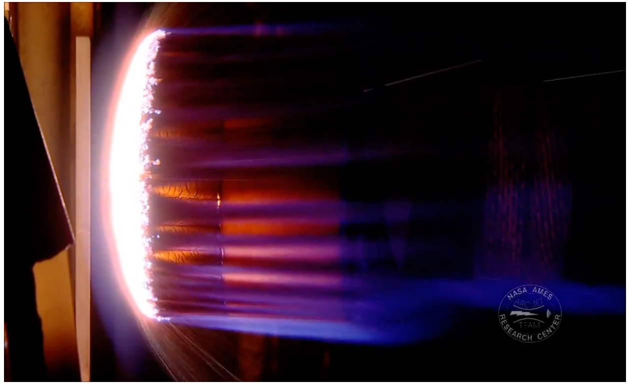


Ground-based Testing

P. Agrawal et. al. 2016.

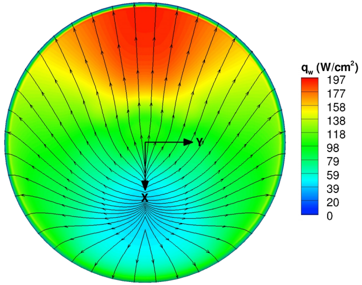
Virgin PICA Sample

Charred PICA Sample

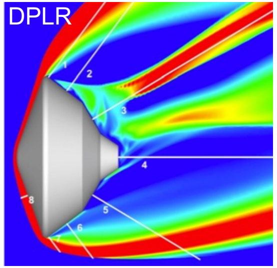


Arcjet Testing of TPS

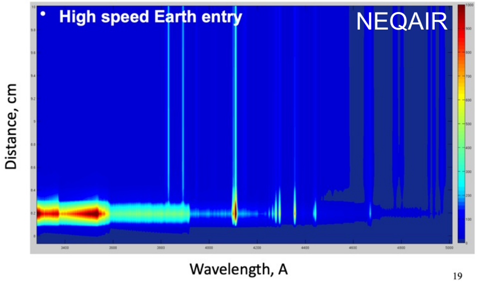
Computational Modeling



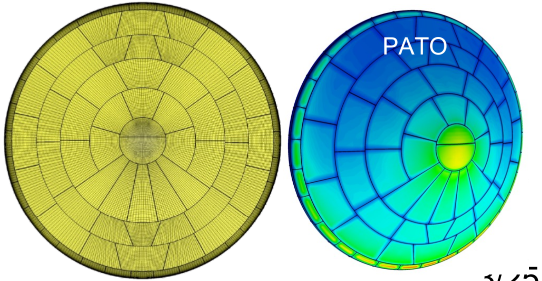
Hypersonic CFD



Radiation Analysis

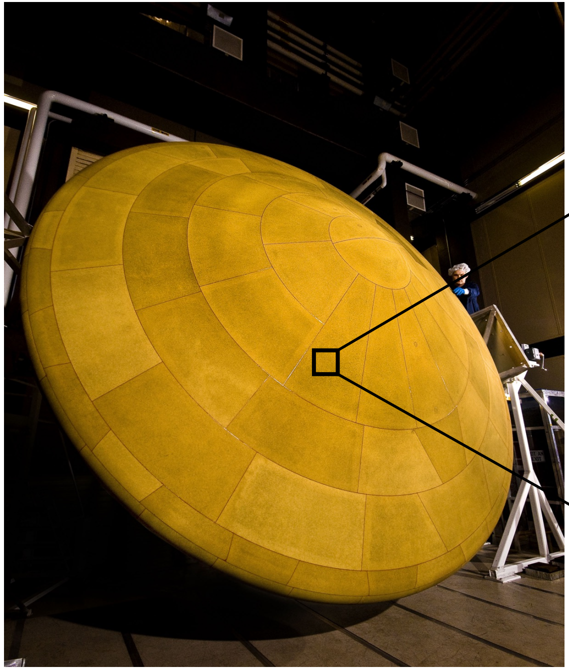


Material Response

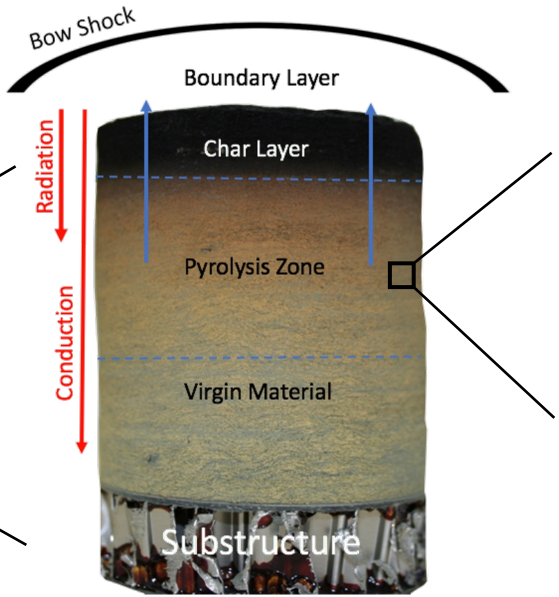


Modeling TPS

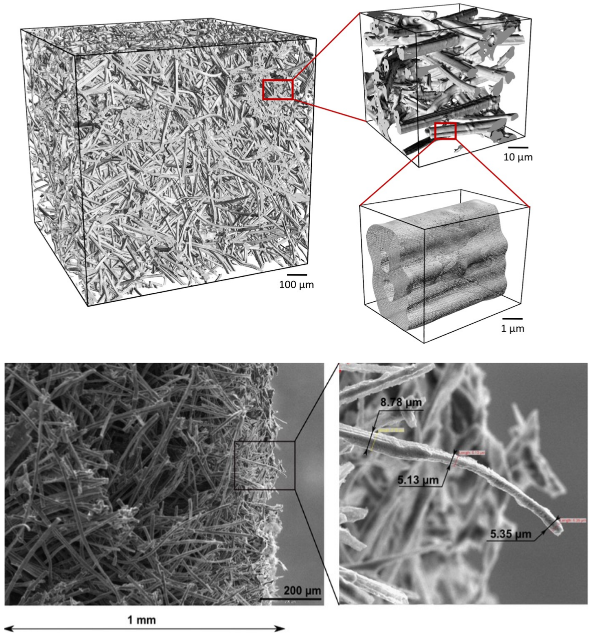
Full scale



Mars Science Laboratory (MSL) heat shield



Microscale



Carbon-fiber microstructure

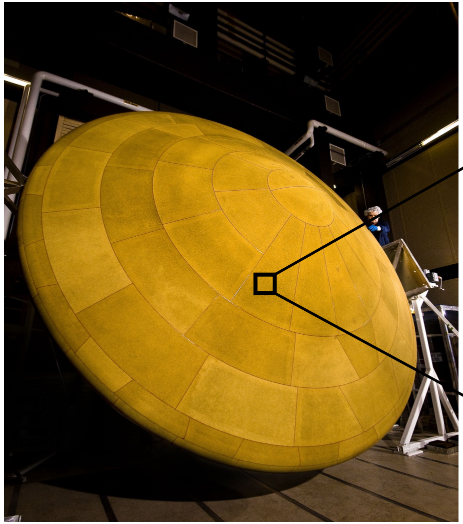
NASA Modeling Capabilities

FIAT | CHAR | Icarus | PATO

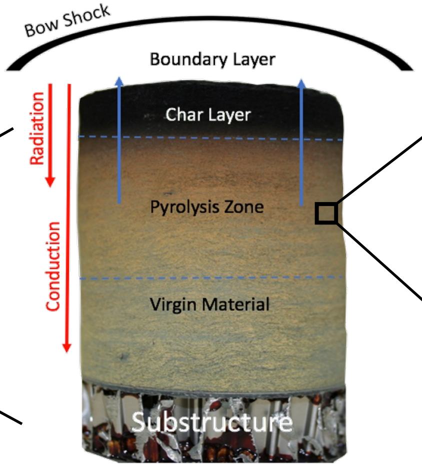
Full scale

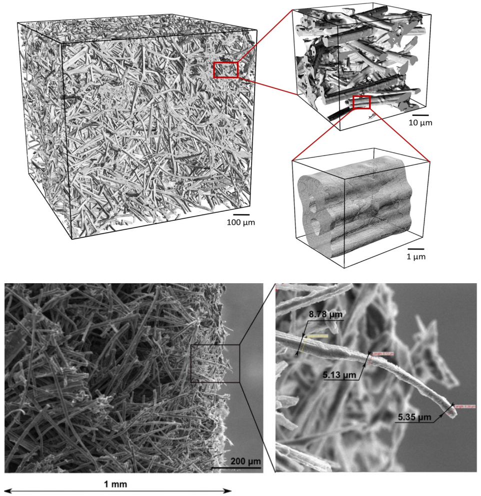
PuMA

Microscale



Mars Science Laboratory (MSL) heat shield

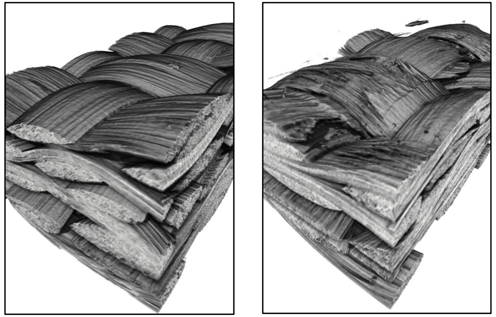




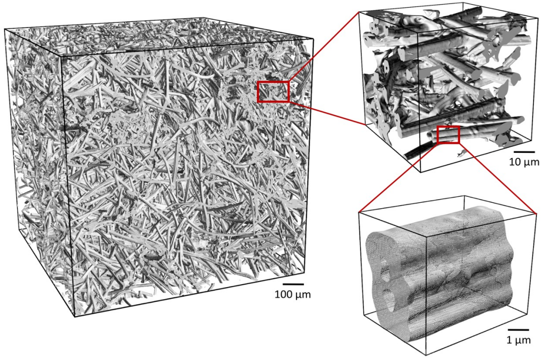
Carbon-fiber microstructure

Heat Shield Microstructures

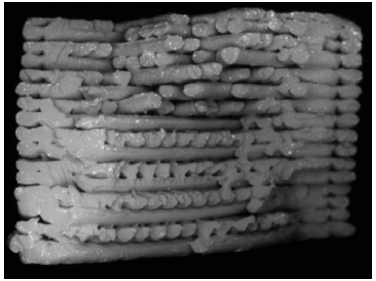
3D carbon fabric prior to (left) and after (right) Arcjet exposure



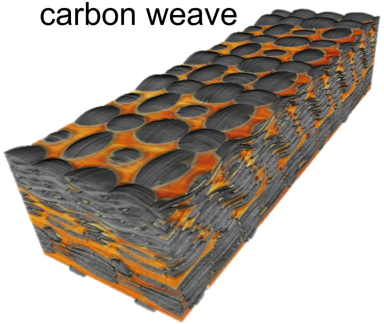
Fibrous architectures



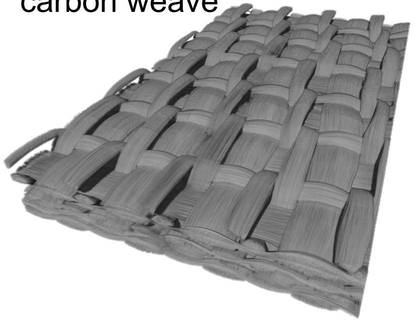
3D printed material



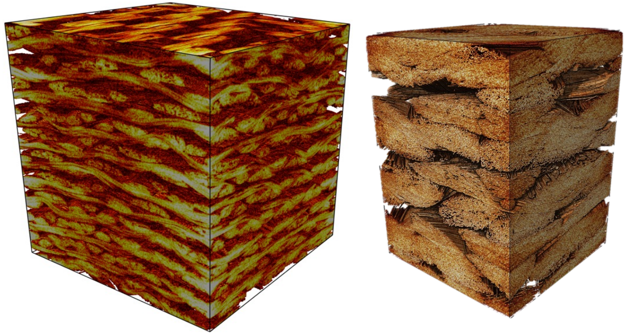
12-ply infused carbon weave



6-ply dry carbon weave

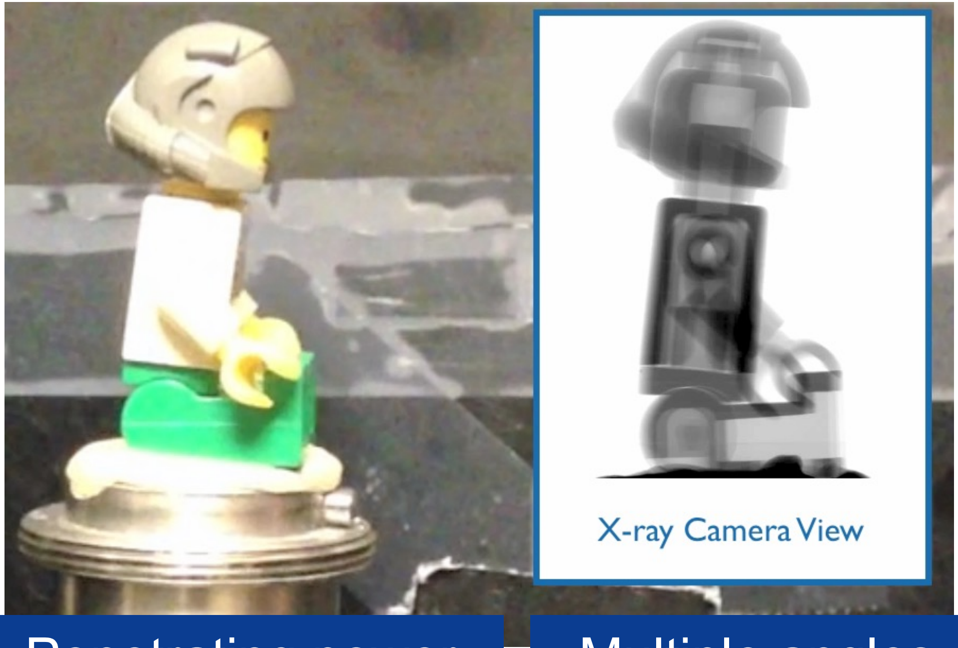


Multiscale imaging of silica weave



X-ray Microtomography

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



Penetrating power

Multiple angles

Use this series of images to “reconstruct” the 3D object

Courtesy of D. Parkinson (ALS)

Porous Microstructure Analysis (PuMA) v3 release

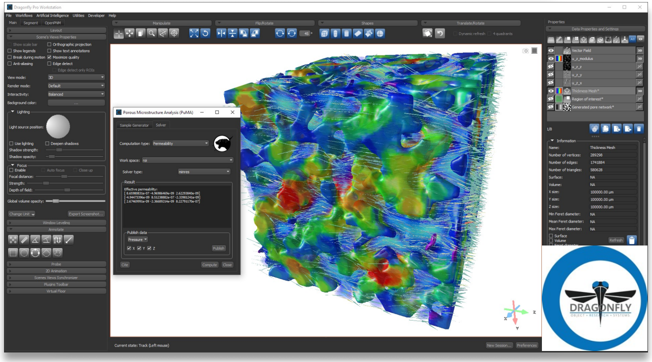
Installation: conda install -c conda-forge puma

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

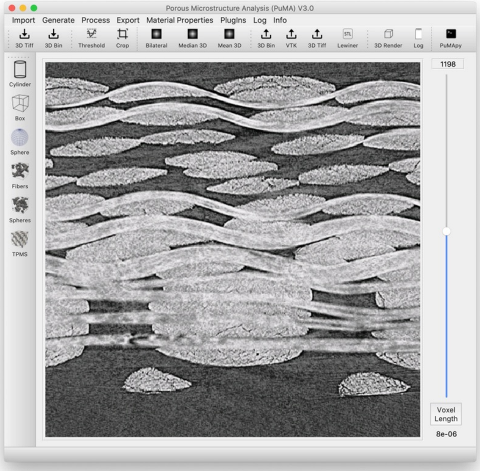
Documentation: https://puma-nasa.readthedocs.io

Community chat: https://gitter.im/puma-nasa/community

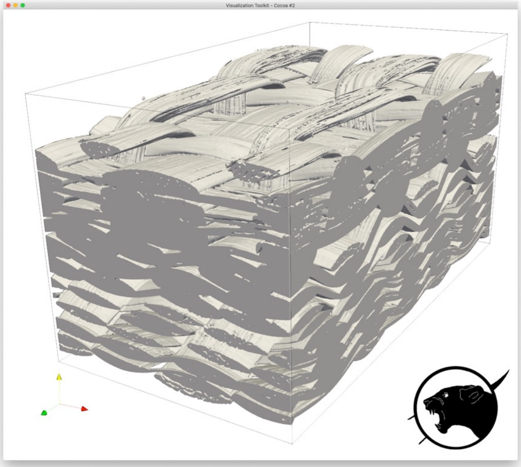
Tutorials: PuMA YouTube channel and online Colab notebook



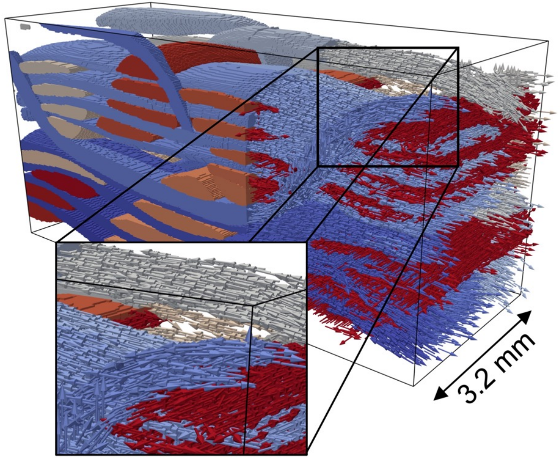
a)



b)

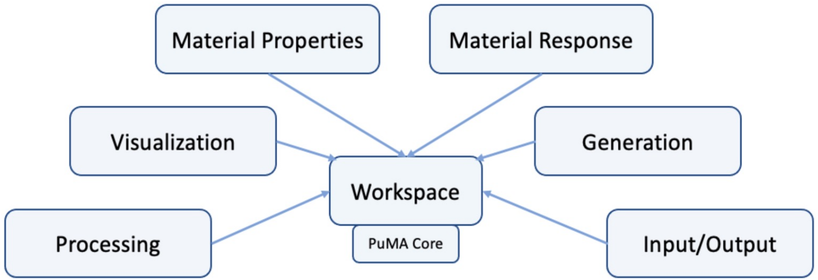


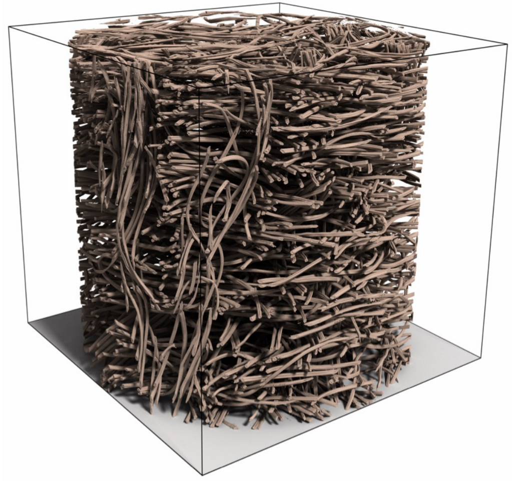
c)



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*

Behind the scenes





Porous Microstructure Analysis (PuMA)

Domain Generation
- ● X-ray Microtomography import / filtering
- ● Woven Material Generation (TexGen)
- ● Simplified Geometry Generation
  - ● Analytical shapes
  - ● Fibrous Materials
  - ● Sphere Beds
  - ● Triply Periodic Materials

Material Properties
- ● Porosity / Volume Fractions
- ● Specific Surface Area
- ● Pore Diameter
- ● Effective Thermal & Electrical Conductivity
- ● Anisotropic Thermal & Electrical Conductivity
- ● Anisotropic Elasticity
- ● Material Orientation
- ● Continuum Tortuosity
- ● Rarefied Tortuosity
- ● Permeability

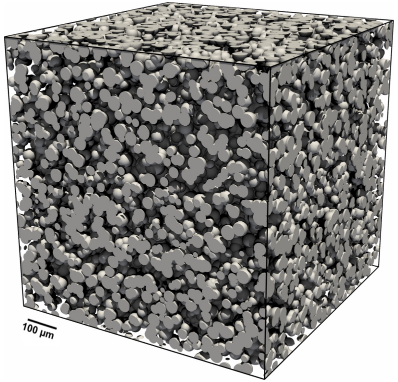
Shared Utilities
- ● Matrix & Vector data structures / operations
- ● Linear Solvers
- ● Iso-surface extraction
- ● Input/output utilities

Material Response
- ○ Microscale Oxidation
- ○ Hyperthermal Beam Simulations

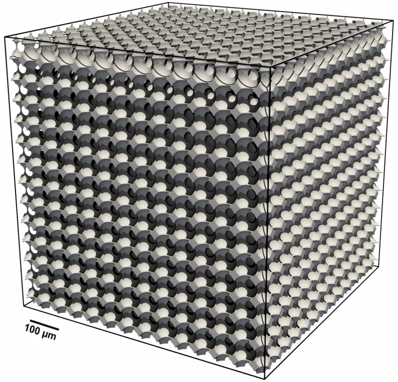
● Included in open-source release
○ Not included in open-source release

Artificial domain generation

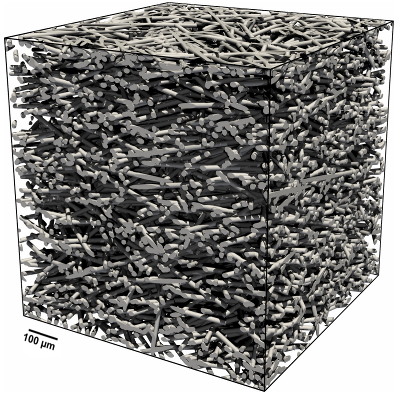
Packed Sphere Beds

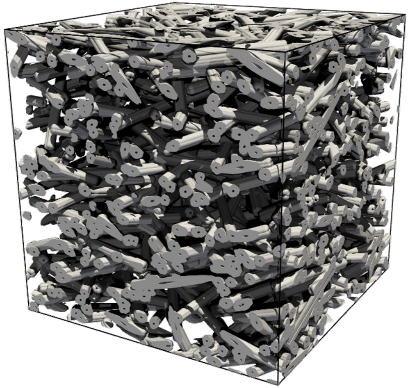


Periodic Foams

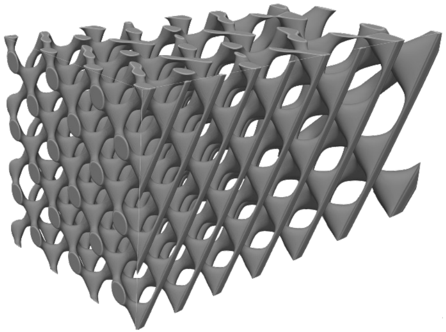


Fiber Structures

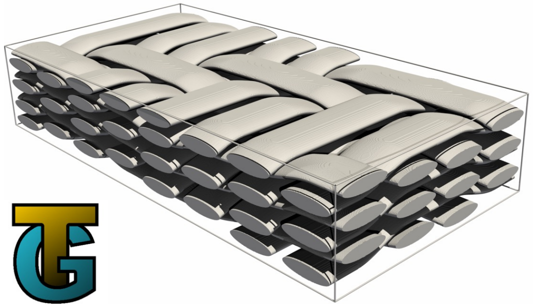




Triply Periodic Minimal Surface (TPMS)

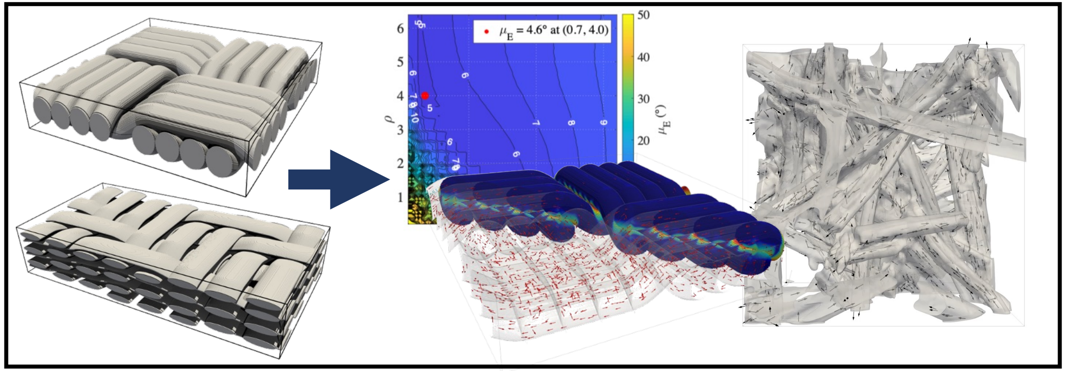


Woven geometries

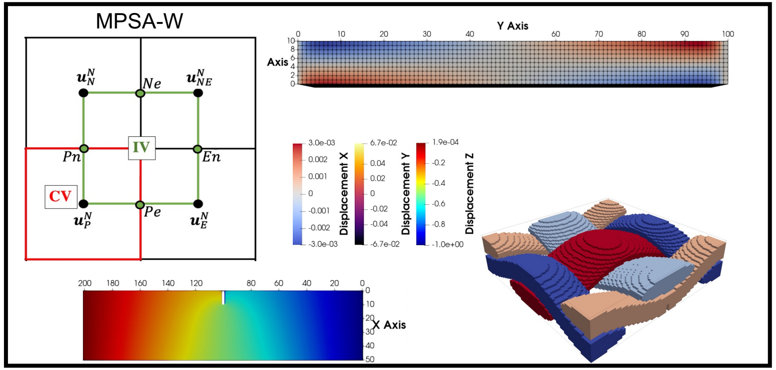


Advanced Material Property Computation

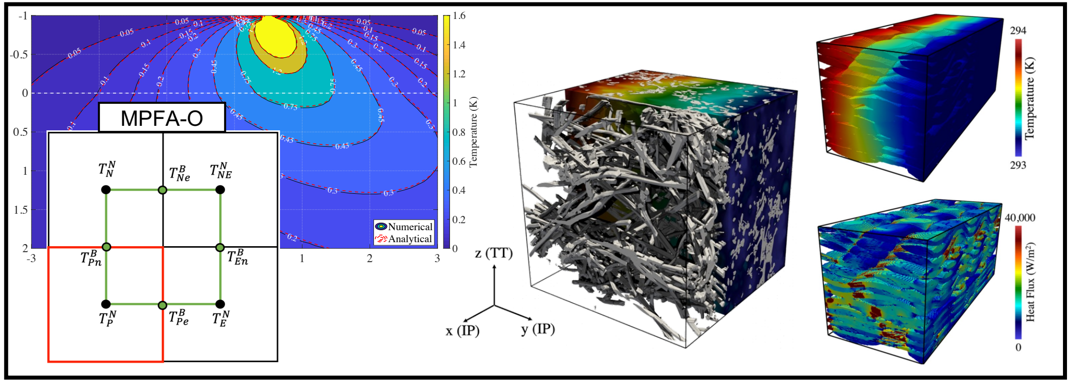
Local orientation. *Computational Materials Science* (2020)



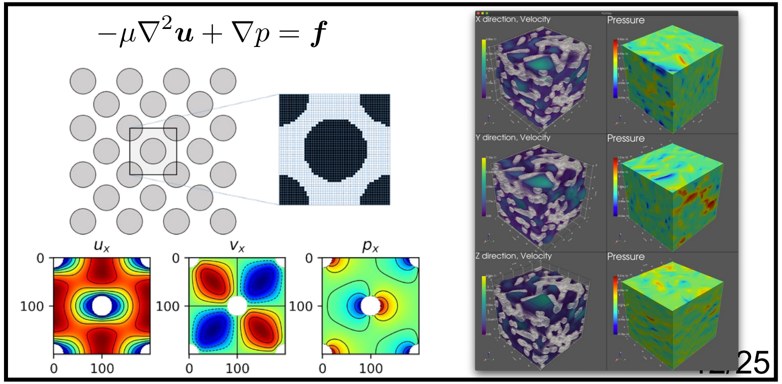
Effective elasticity. *AIAA Scitech Forum* (2022, 2023)



Effective conductivity. *Computational Materials Science* (2021)



Effective permeability. *npj Computational Materials* (2022)

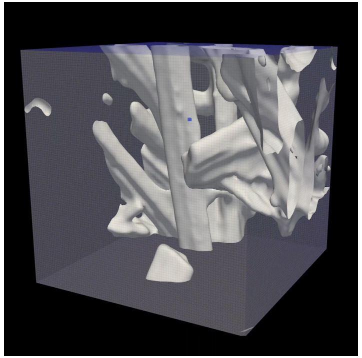


Particle Methods in PuMA

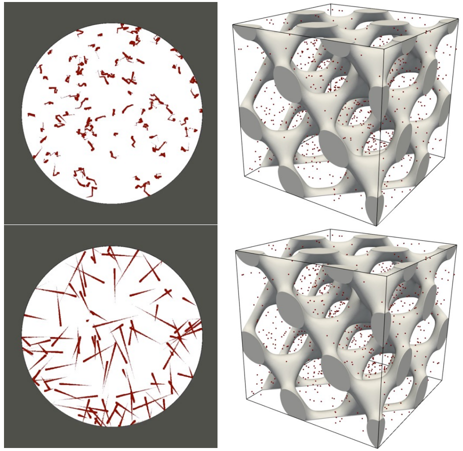
Oxidation

4D tomography

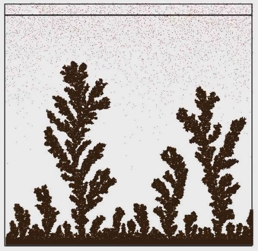
Radiative Conductivity



Tortuosity

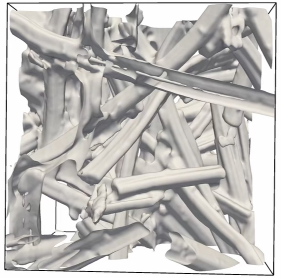


Dendrites in Batteries



Dendrite growth in lithium metal batteries. Wood et al. ACS Central Science. (2016)

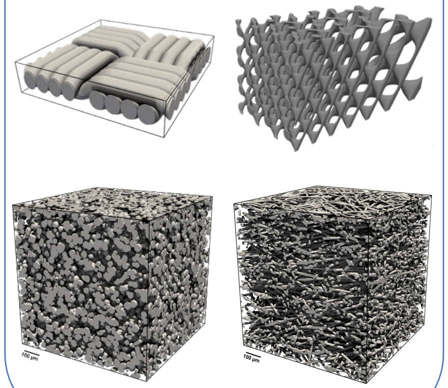
Material Orientation



Material Optimization

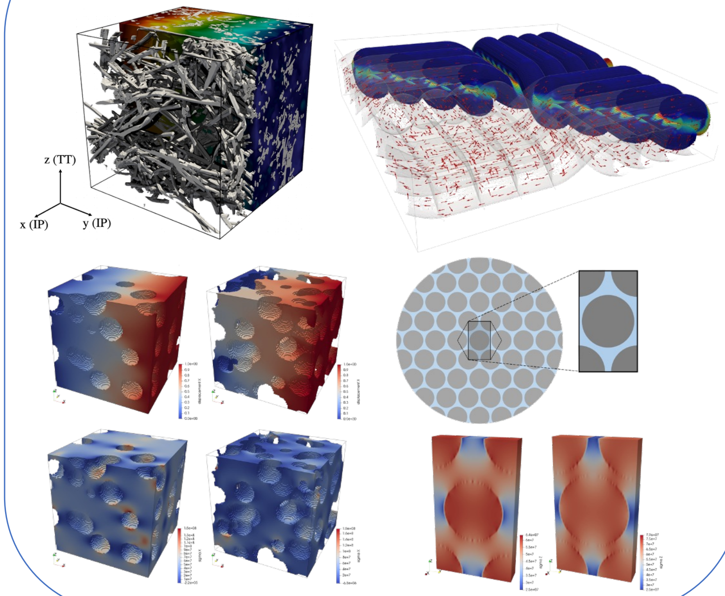
Compute Properties

Material Generation



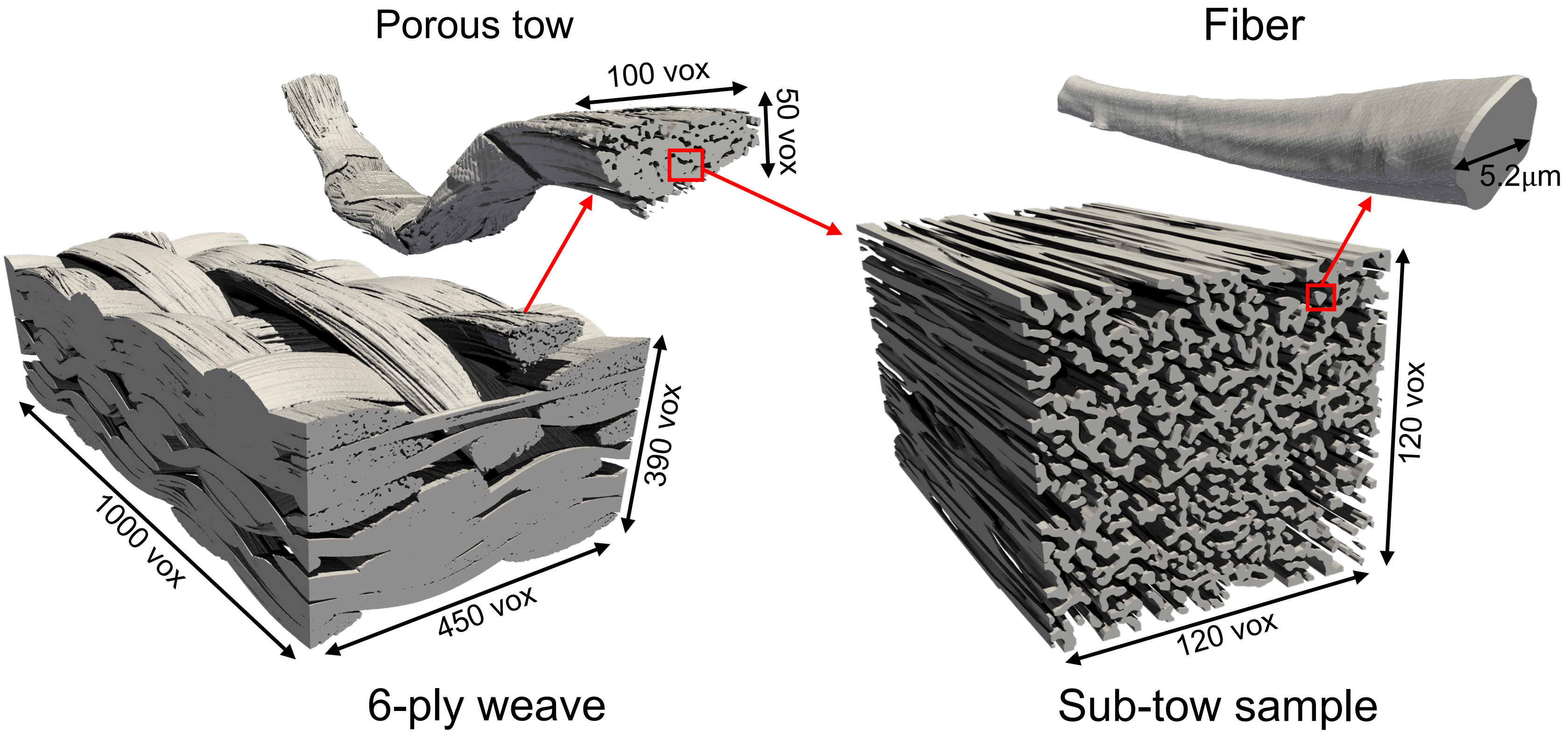
Optimization Toolbox

Material Properties



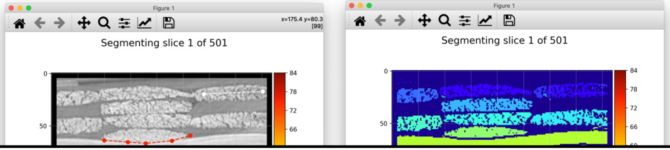
Update Geometry

Micro-CT weaves: anisotropic at multiple scales

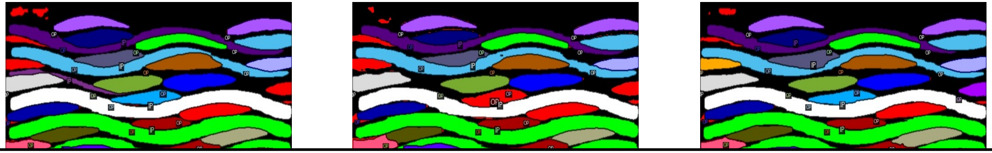


Weave segmentation and tow tracking

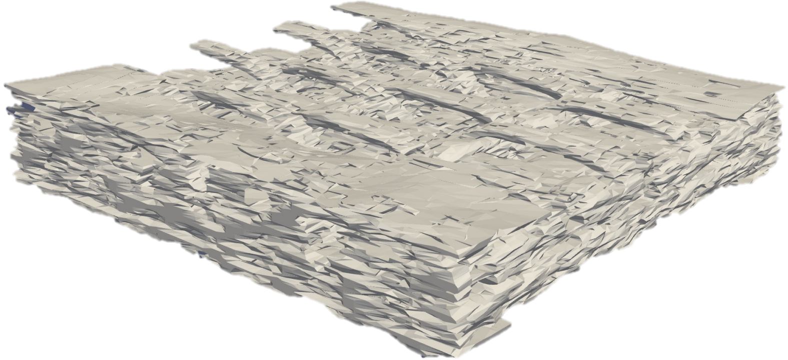
Manual labeling



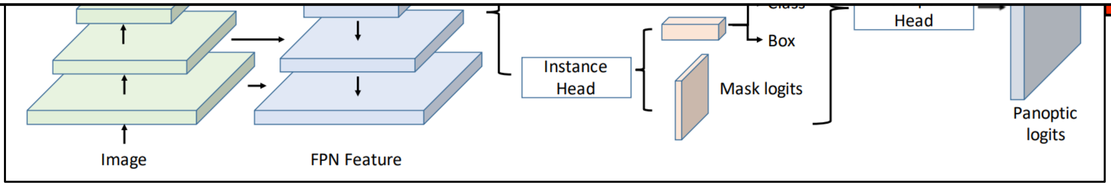
Tracking by IoU

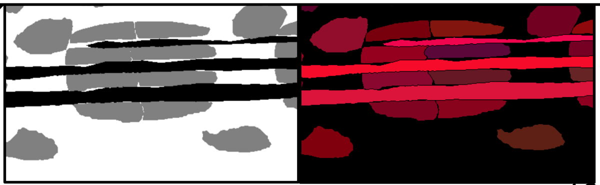


Naïve threshold of original Micro-CT weave



Fully segmented weave





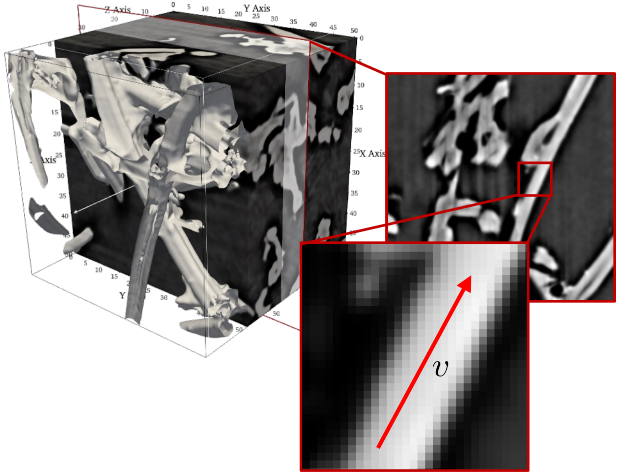
Semantic Classes

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* (accepted)

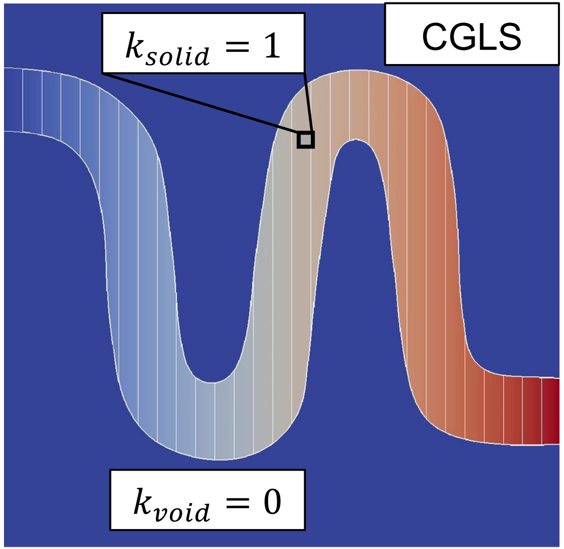
Orientation methods

Structure tensor

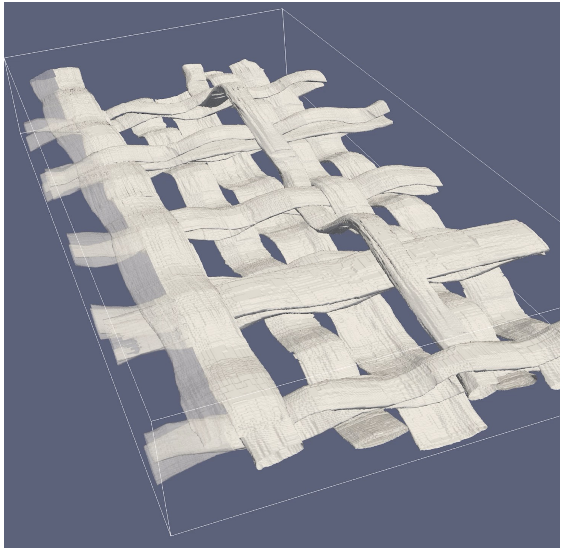


$$(I(x+v) - I(x))^2 \approx 0$$

Artificial flux



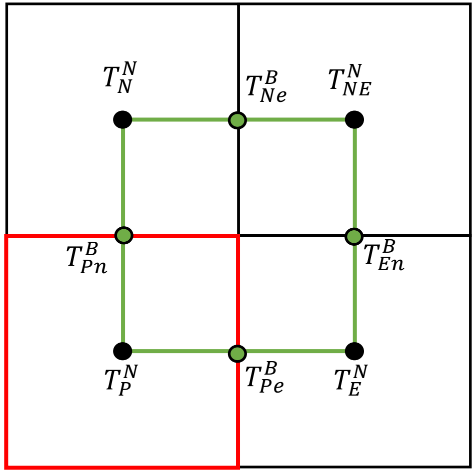
Ray casting



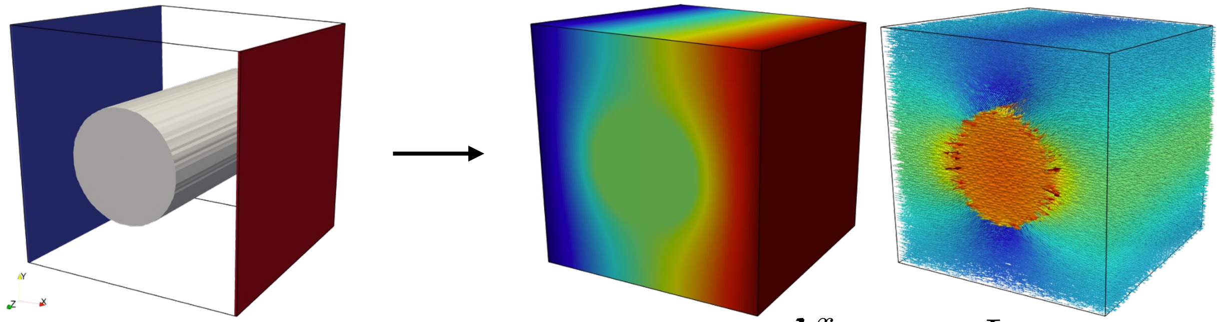
Semeraro, F., Ferguson, J.C., Panerai, F., King, R.J. and Mansour, N.N., 2020. Anisotropic analysis of fibrous and woven materials part 1: Estimation of local orientation. *Computational Materials Science*, *178*, p.109631.

Conductivity solver

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



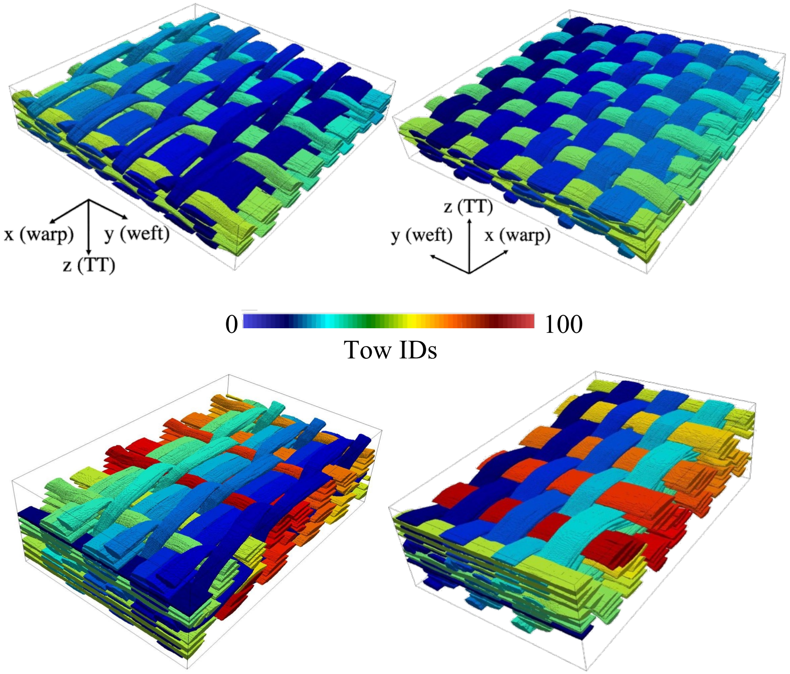
Multi-Point Flux Approximation (MPFA-O)*: $\boldsymbol{q} = \boldsymbol{E}\boldsymbol{T}^N$

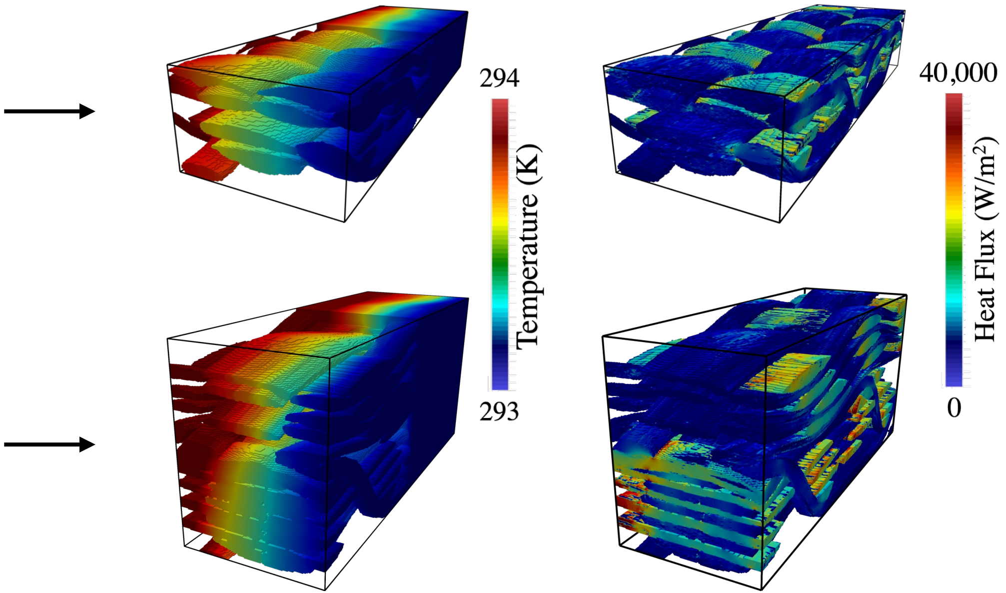


$$\boldsymbol{k}^x = -\boldsymbol{q} \cdot L_x$$

*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



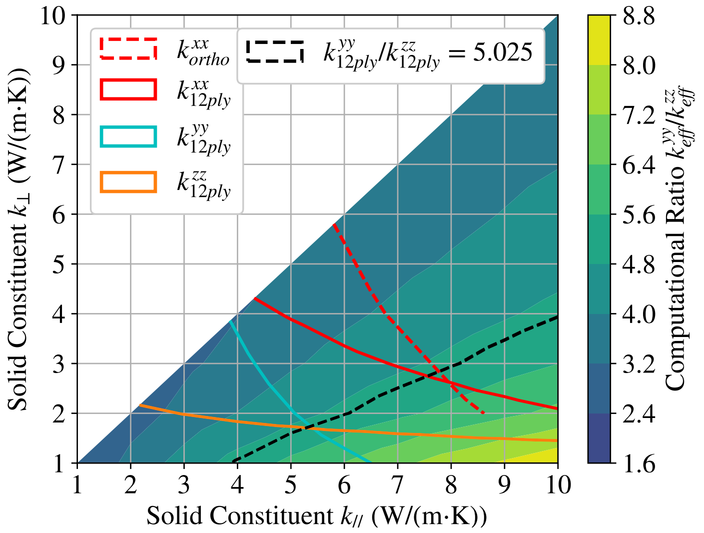


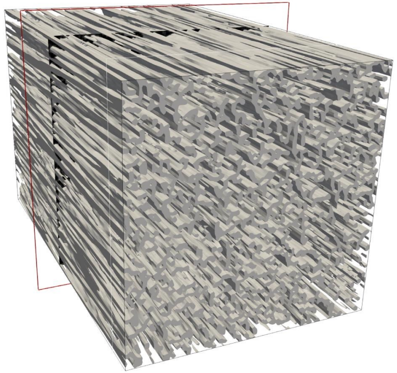
Semeraro, F., Ferguson, J.C., Acin, M., Panerai, F. and Mansour, N.N., 2021. Anisotropic analysis of fibrous and woven materials part 2: Computation of effective conductivity. Computational Materials Science, 186, p.109956.

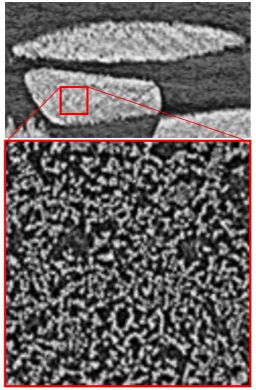
Single fiber conductivity estimation

Experimental value at room temperature:

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







Single fiber thermal conductivity

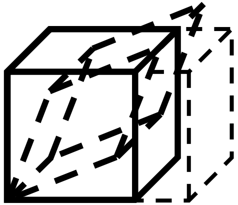
$$[k_{//}, k_{\perp}] = [9.7, 5.5]\frac{\text{W}}{\text{mK}}$$

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

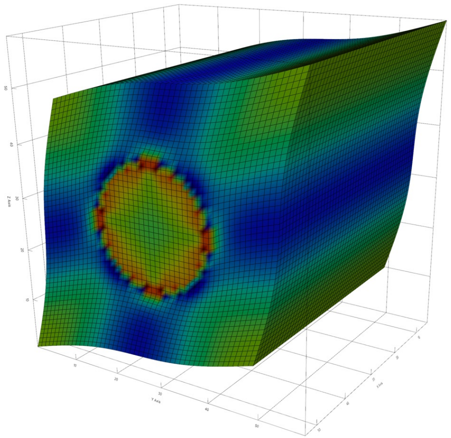
Elasticity solver

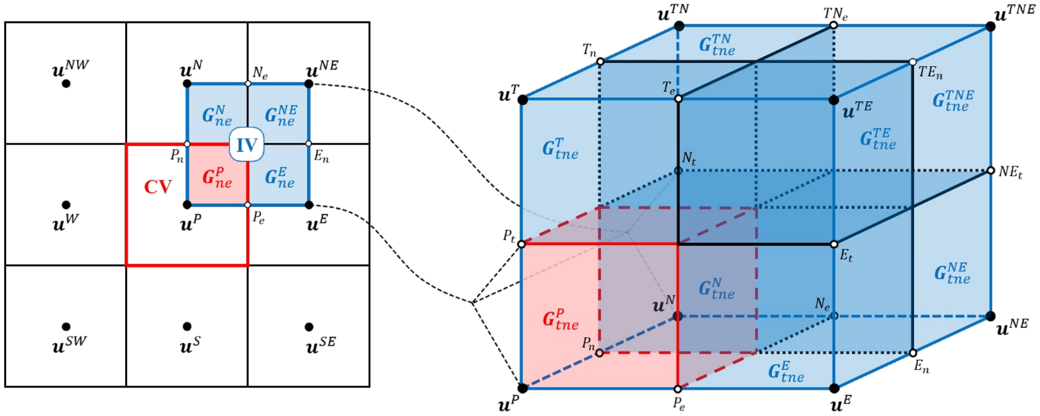
$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad \text{where} \quad \boldsymbol{\sigma} = \boldsymbol{C\varepsilon} = \begin{bmatrix} C^{11} & C^{12} & C^{13} & C^{14} & C^{15} & C^{16} \\ C^{12} & C^{22} & C^{23} & C^{24} & C^{25} & C^{26} \\ C^{13} & C^{23} & C^{33} & C^{34} & C^{35} & C^{36} \\ C^{14} & C^{24} & C^{34} & C^{44} & C^{45} & C^{46} \\ C^{15} & C^{25} & C^{35} & C^{45} & C^{55} & C^{56} \\ C^{16} & C^{26} & C^{36} & C^{46} & C^{56} & C^{66} \end{bmatrix} \frac{\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T}{2}$$

Multi-Point Stress Approximation (MPSA-W)*: $\boldsymbol{\sigma} = \boldsymbol{E}\,\boldsymbol{u}^N$



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



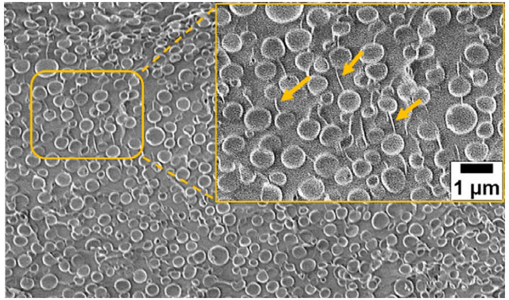


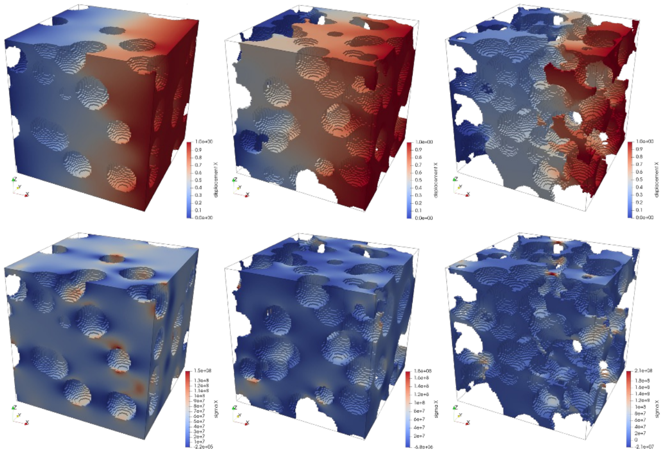
*Keilegavlen, E. and Nordbotten, J.M., 2017. Finite volume methods for elasticity with weak symmetry. Int. Journal for Numerical Methods in Engineering, 112(8), pp.939-962.

Elasticity solver validation: woven composite

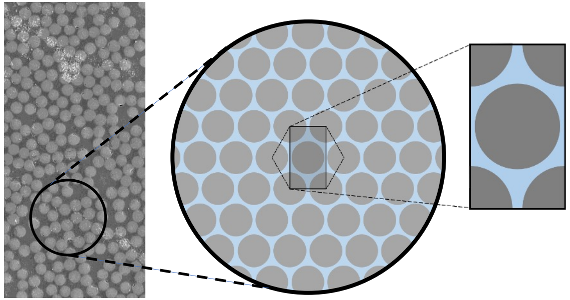
Fraile Izquierdo, S., Semeraro, F., Acin, M., 2022. Multi-Scale Analysis of Effective Mechanical Properties of Porous 3D Woven Composite Materials. *AIAA Scitech Forum*

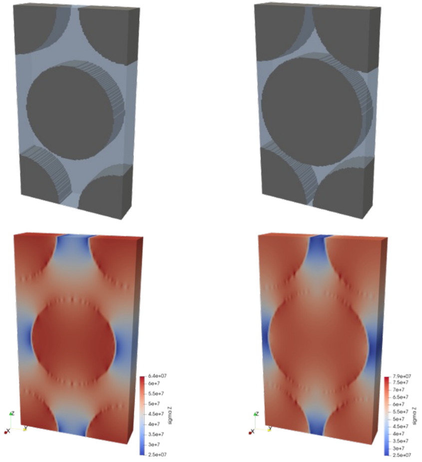
Matrix: porous phenolic resin



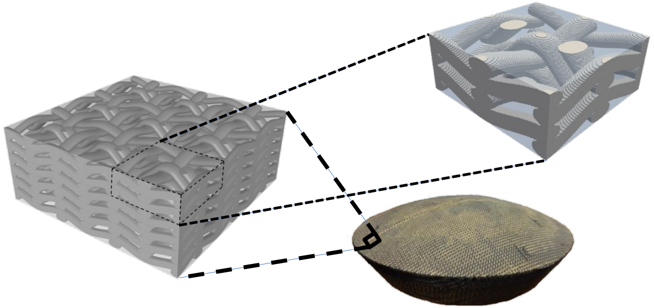


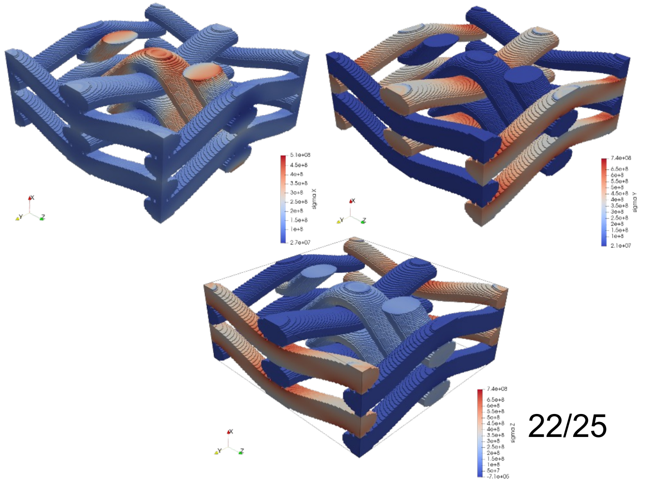
Intra-tow fiber packing





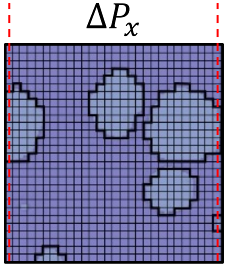
Woven unit cell



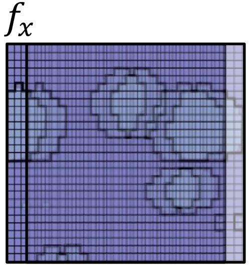


Permeability solver

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



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

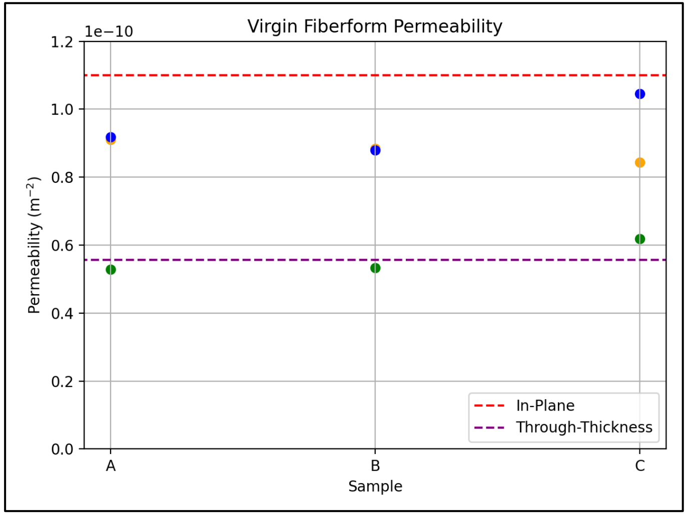


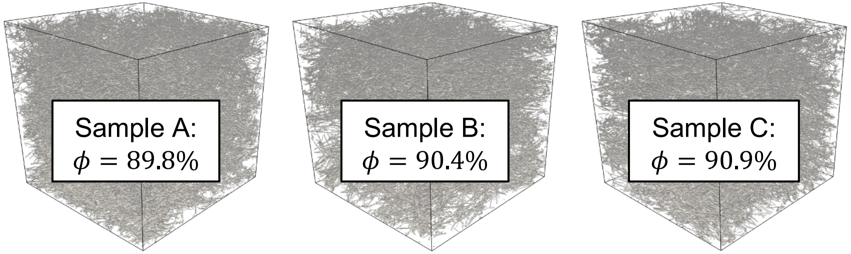
- Solved with Finite Element (FE) scheme with Q1-Q1 discretization in velocity and pressure (plus pressure stabilization) using Element-By-Element (EBE) technique
- By imposing a unit body force f_i in the three Cartesian directions, the permeability is homogenized as:

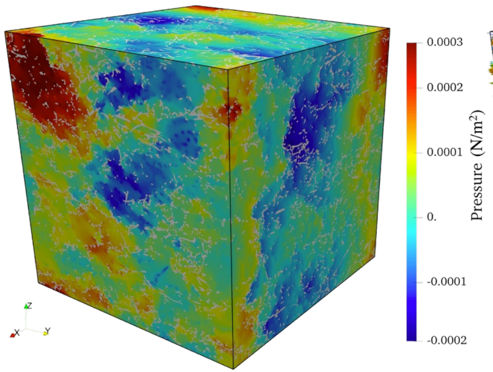
$$\begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{xy} & k^{yy} & k^{yz} \\ k^{xz} & k^{yz} & k^{zz} \end{bmatrix} = \frac{l^3}{|V|} \int^V u^i \, dV$$

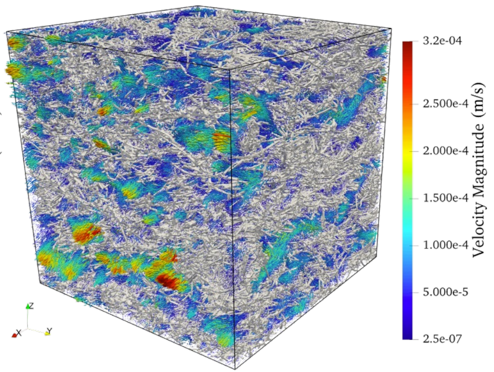
Permeability validation: Fiberform

- Three 500^3 samples with voxel size = 2.6μm
- Run on NVIDIA V100 GPUs with matrix-free PCG









*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)

Questions?

Predictive Material Modeling (PMM) group

Entry System Modeling (ESM) project