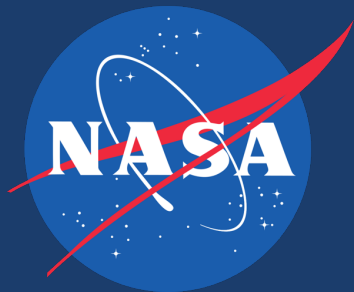


The Porous Microstructure Analysis (PuMA) software



Presented by: Federico Semeraro

NASA Ames Research Center, Moffett Field, CA

November 8th, 2023

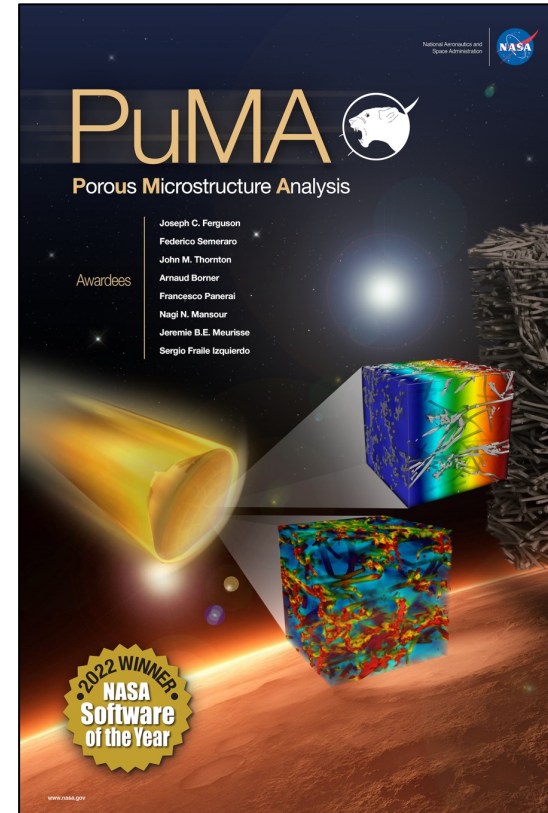
**Authors: Federico Semeraro¹, Joseph C. Ferguson^{1,2}, John Thornton¹, Francesco Panerai³, Arnaud Borner¹,
Nagi N. Mansour¹, Sergio Fraile Izquierdo¹, Jeremie B.E. Meurisse¹**





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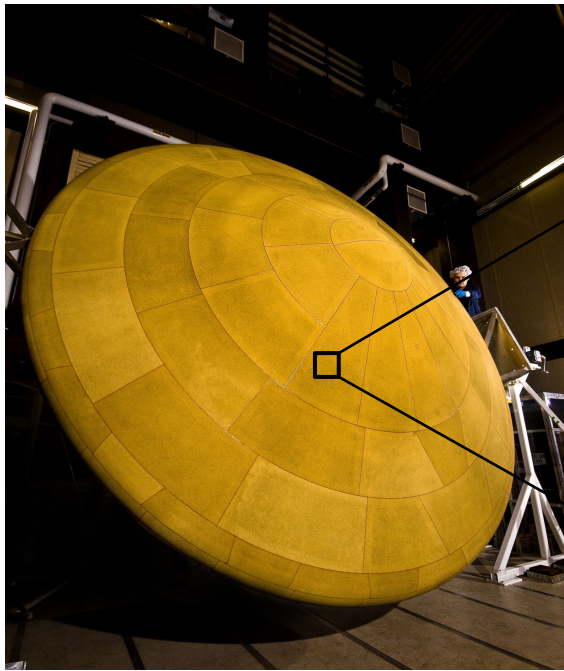
- Motivation
- Overview of PuMA
- MicroCT Workflow
- Tomography Segmentation
- Material Properties Computation



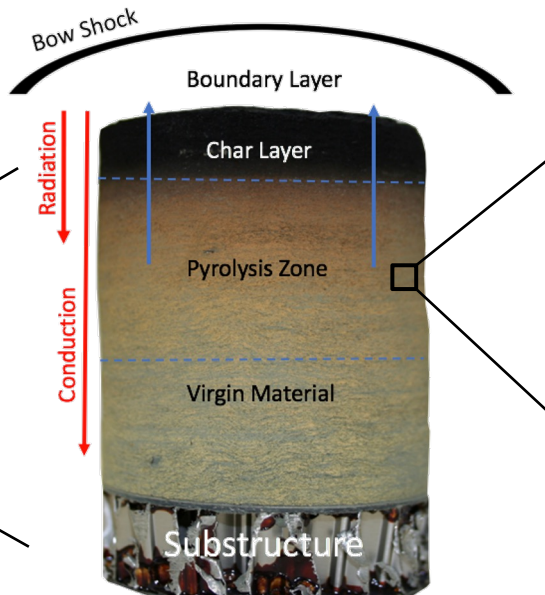


Modeling Thermal Protection Systems

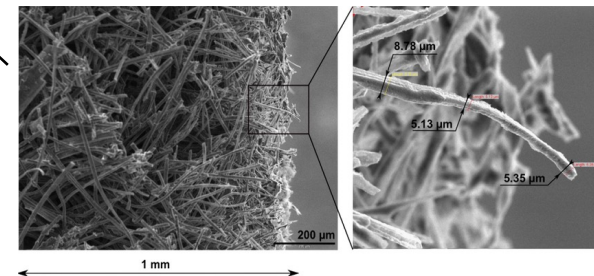
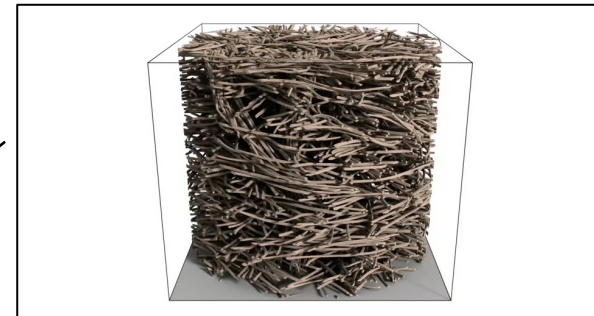
Full scale



Mars Science Laboratory (MSL) heat shield



Microscale



Carbon-fiber microstructure



Open-source Release v3.2



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

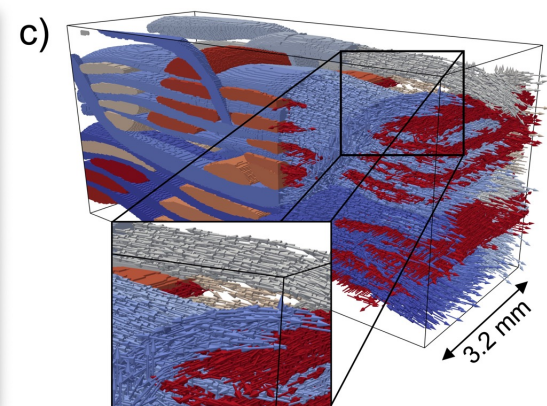
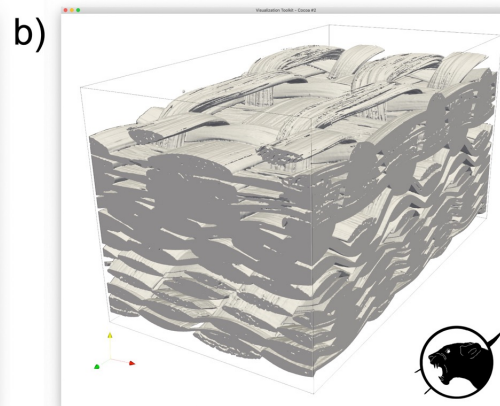
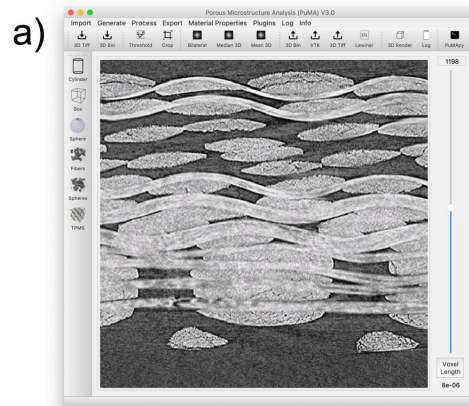
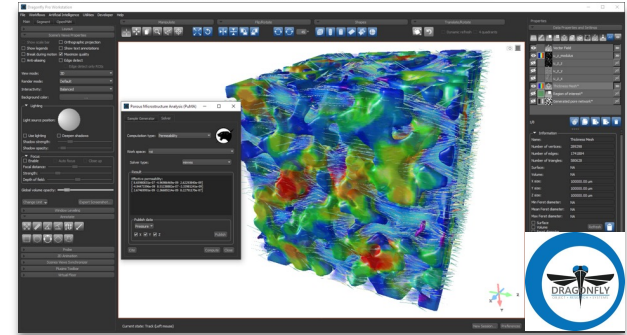
Installation: `conda install -c conda-forge puma`

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

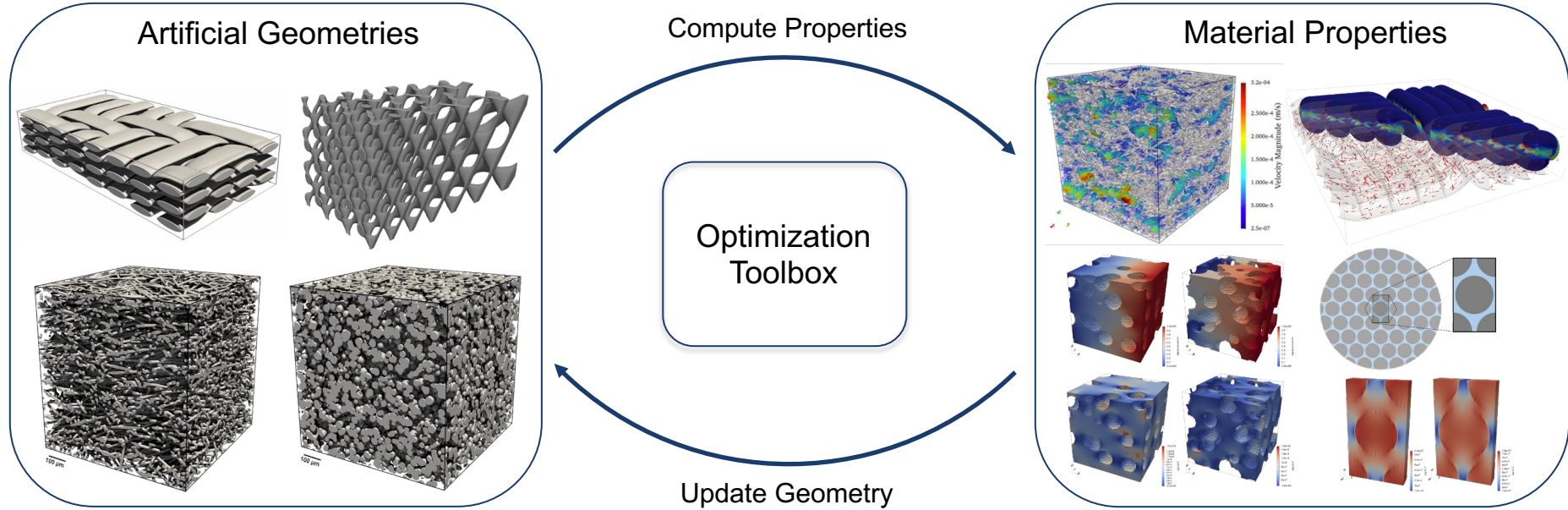
Documentation: <https://puma-nasa.readthedocs.io>

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

Tutorials: [PuMA YouTube channel](#) and [online Jupyter notebooks](#)



Material Generation



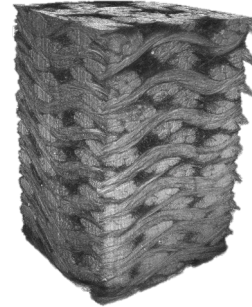
Micro-CT Workflow



TPS Sample



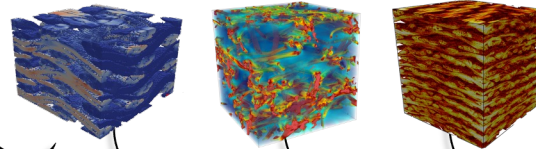
X-Ray Micro-CT



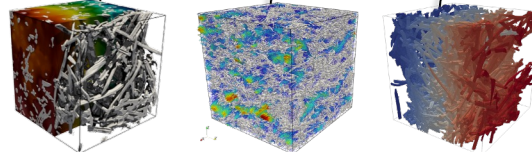
CT Reconstruction

Characterization

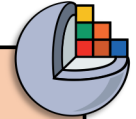
- Porosity Distribution
- Fiber Orientation
- Conductivity
- Tortuosity
- Elasticity
- Permeability



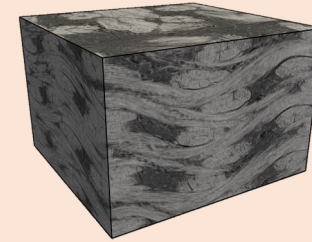
PuMA Physics Solvers



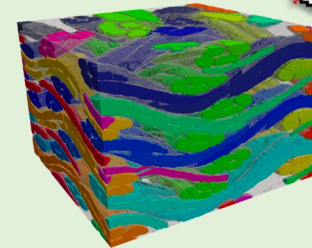
Post-Processing



REV Extraction

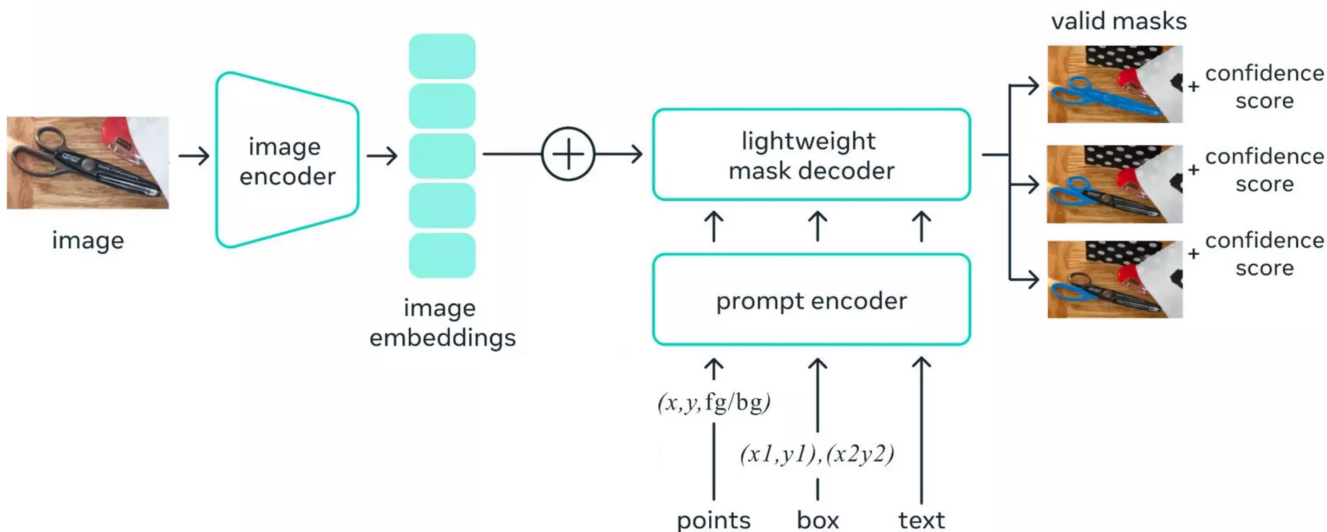


Segmentation

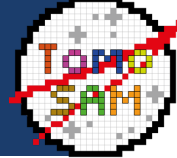


Segment Anything Model (SAM)

*Promptable segmentation system with zero-shot generalization



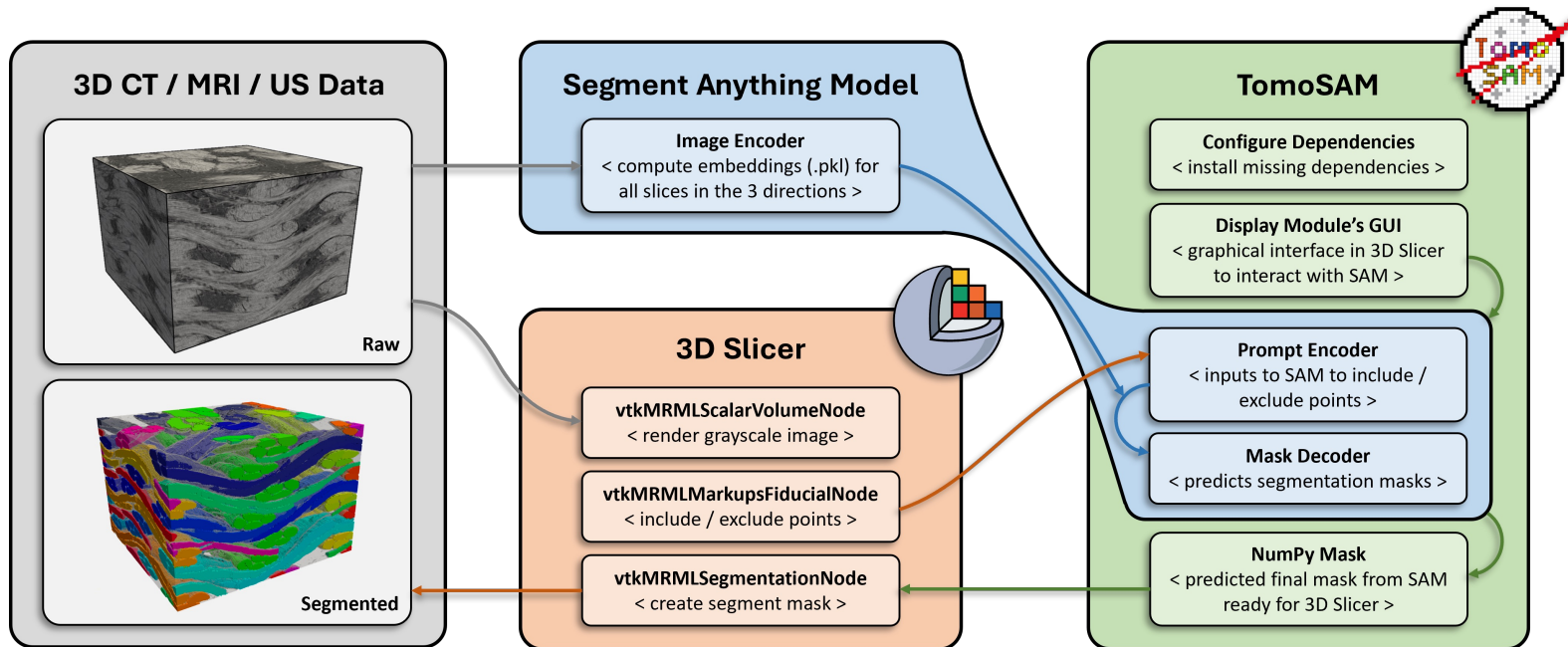
TomoSAM plugin

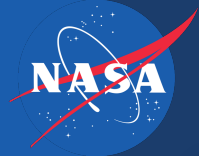


Semeraro, F., Quintart, A., Izquierdo, S.F. and Ferguson, J.C., 2023. TomoSAM: a 3D Slicer extension using SAM for tomography segmentation, *arXiv*

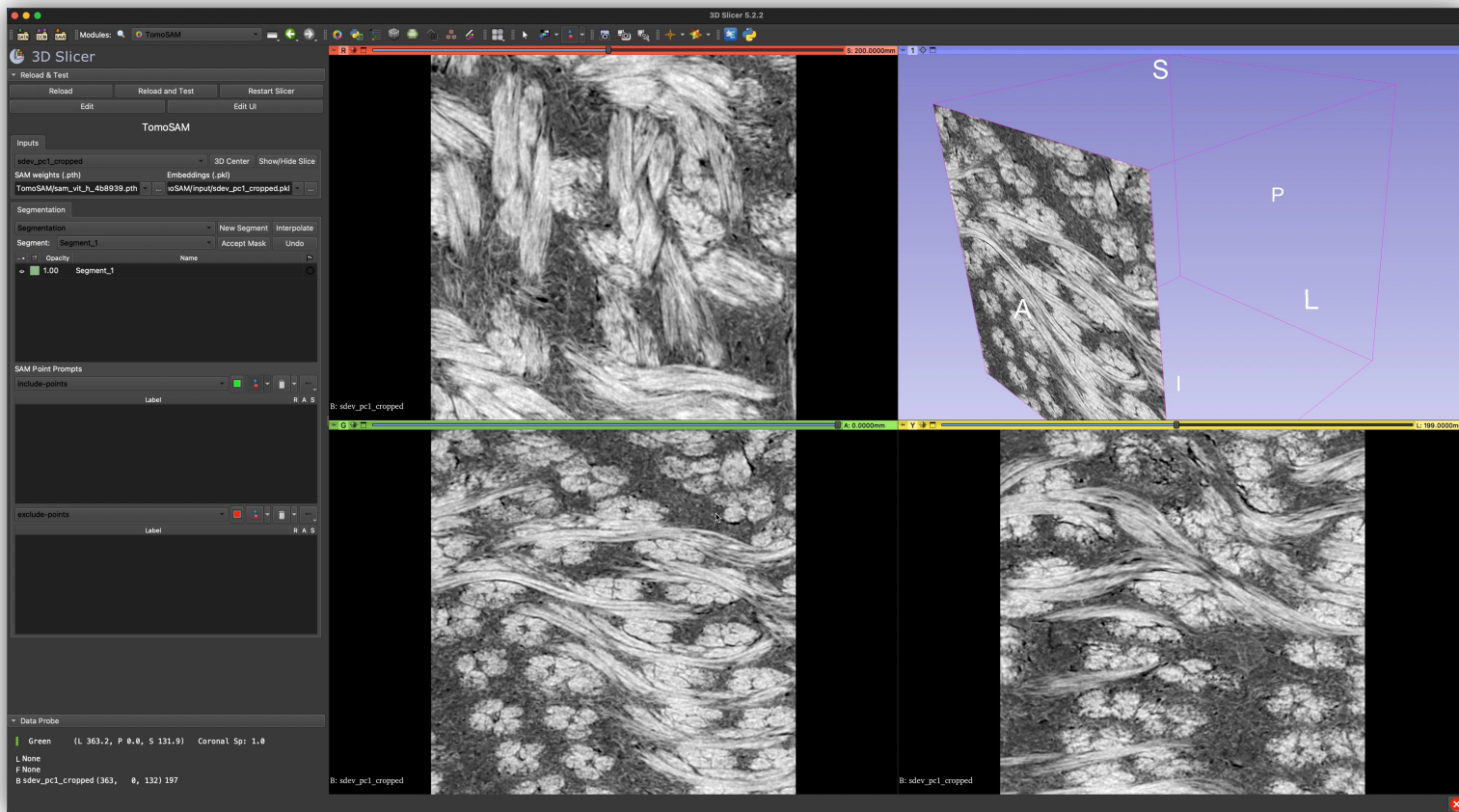
Open-source repository: <https://github.com/fsemerar/SlicerTomoSAM>

Tutorials: [YouTube demo](#) and [online Colab notebook](#)





Demo: segment tow of 3MDCP



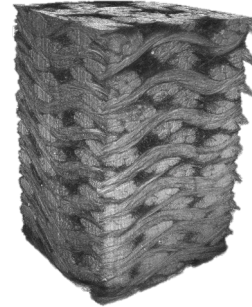
Micro-CT Workflow



TPS Sample



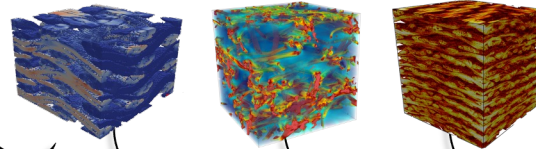
X-Ray Micro-CT



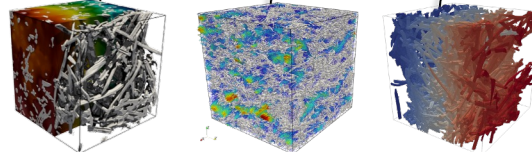
CT Reconstruction

Characterization

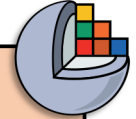
- Porosity Distribution
- Fiber Orientation
- Conductivity
- Tortuosity
- Elasticity
- Permeability



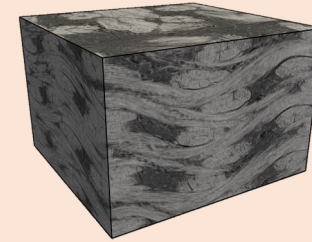
PuMA Physics Solvers



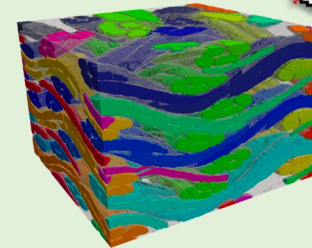
Post-Processing



REV Extraction

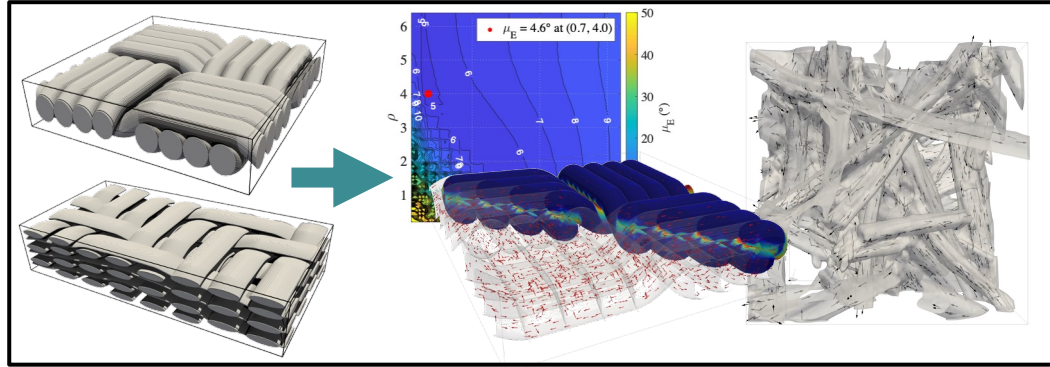


Segmentation

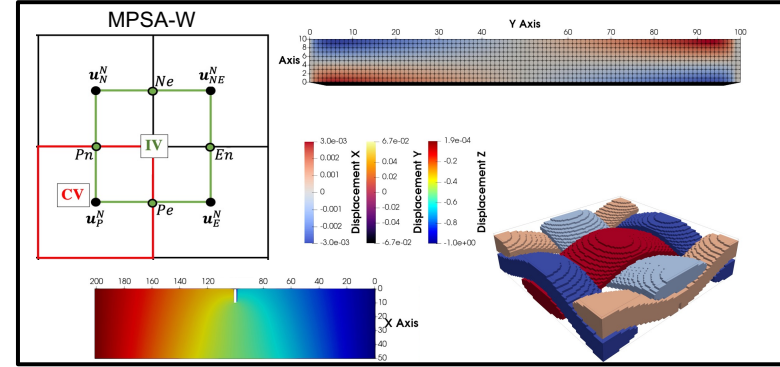


Material Property Computation

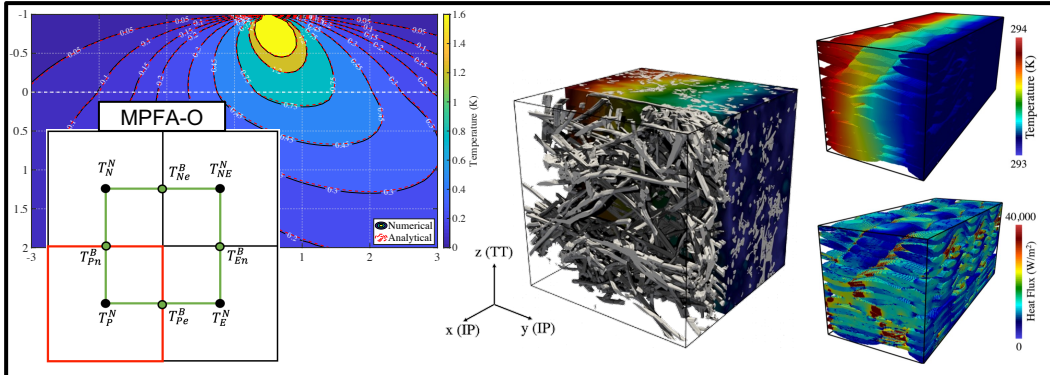
Material orientation. *Computational Materials Science (2020)*



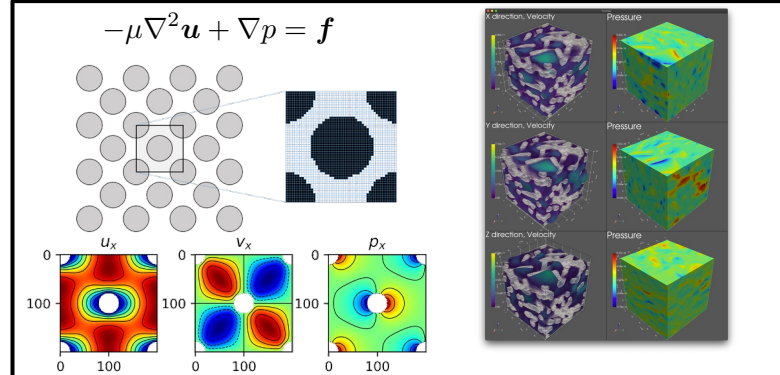
Effective elasticity. *AIAA SciTech Forum (2022)*



Effective conductivity. *Computational Materials Science (2021)*



Effective permeability. *Computational Materials Science (2023)*



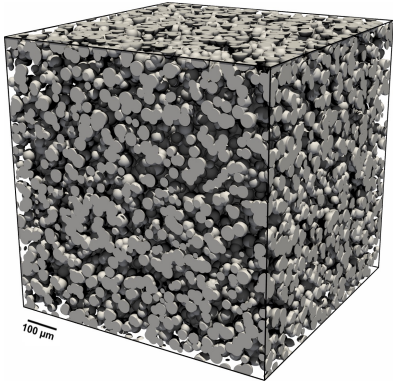


Thank you!

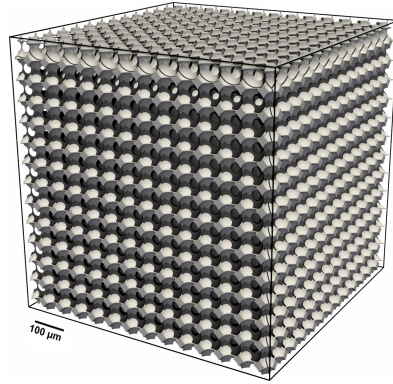


Artificial Domain Generation

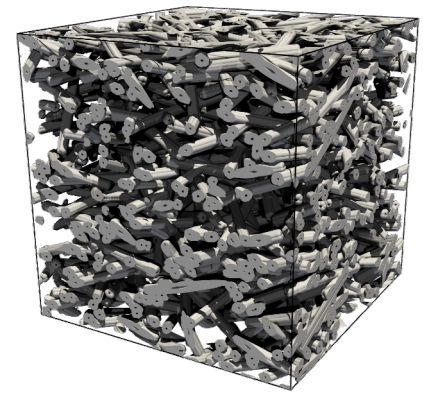
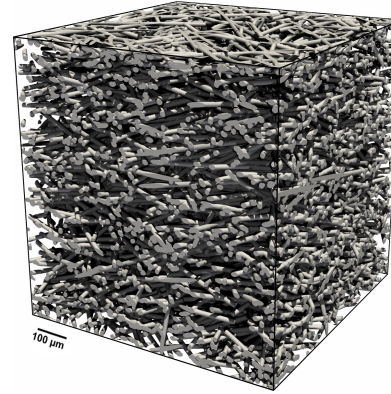
Packed Sphere Beds



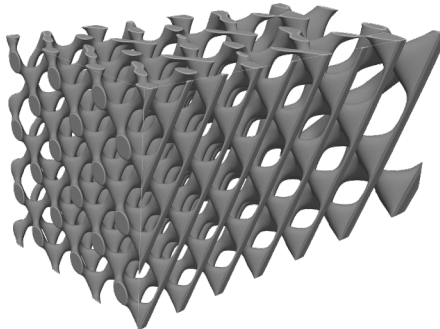
Periodic Foams



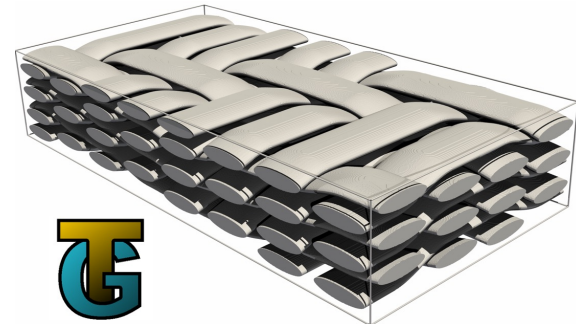
Fiber Structures



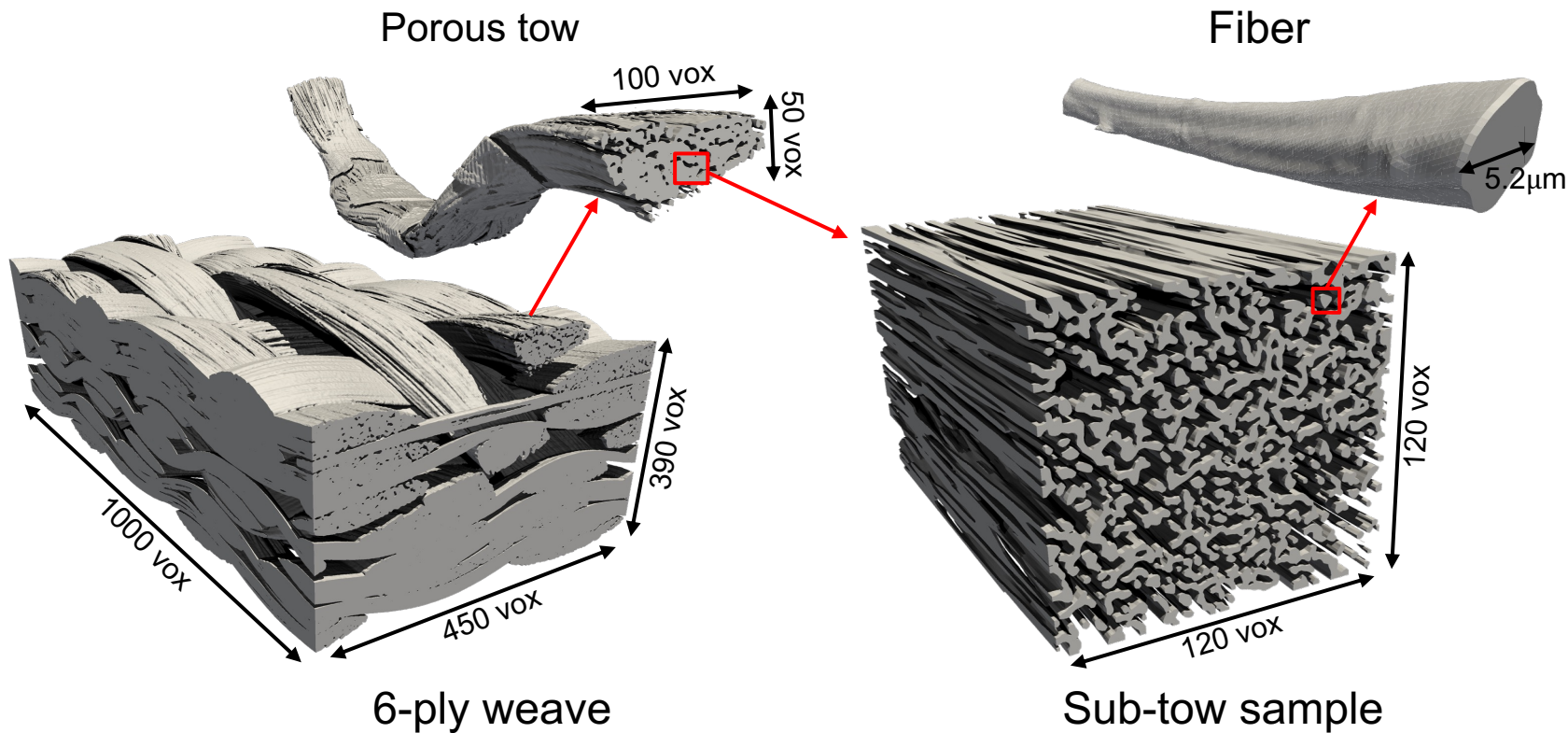
Triply Periodic Minimal Surface (TPMS)

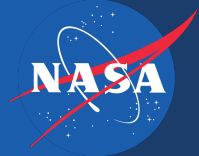


Woven geometries

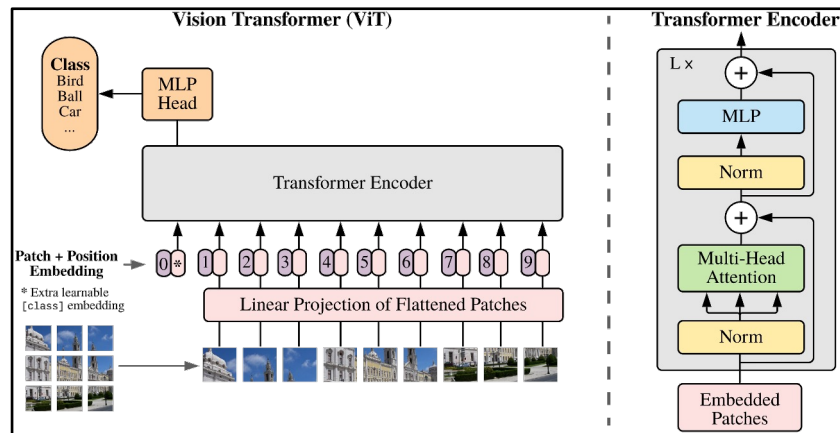
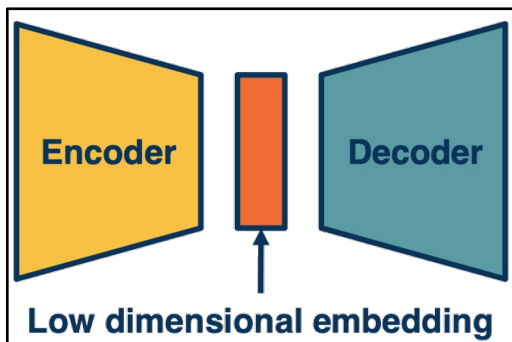
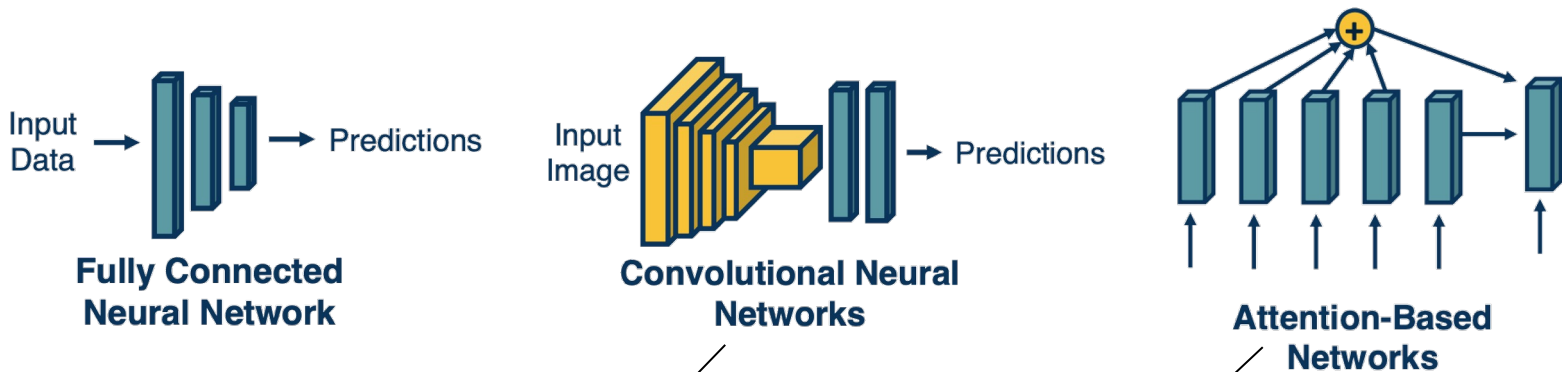


NASA Micro-CT weaves: anisotropic at multiple scales





Deep Learning Architectures



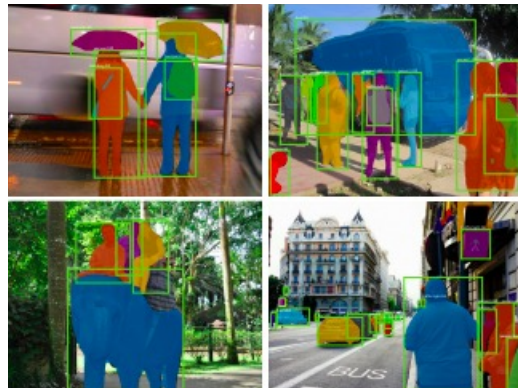


Types of Image Segmentation

Semantic



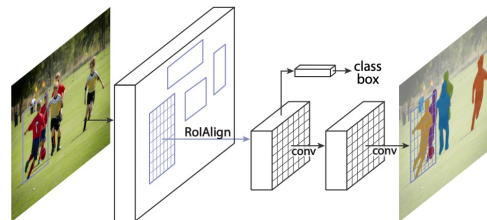
Instance



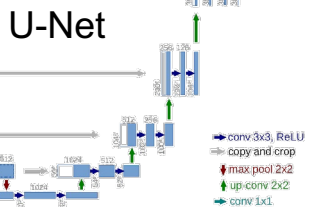
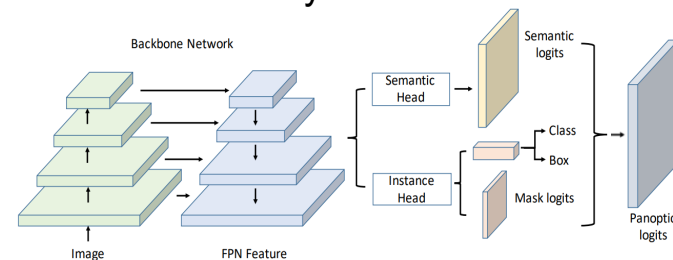
Panoptic



Mask R-CNN



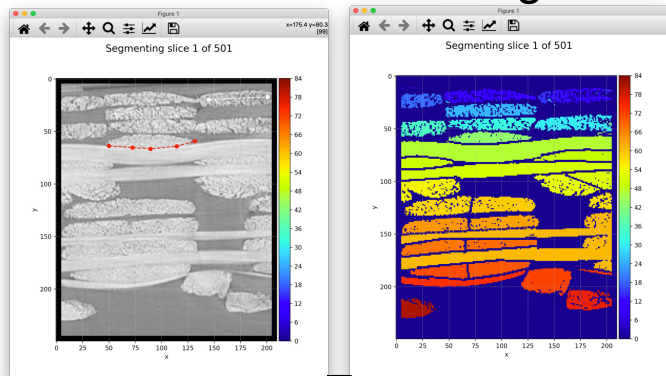
Feature Pyramid Network



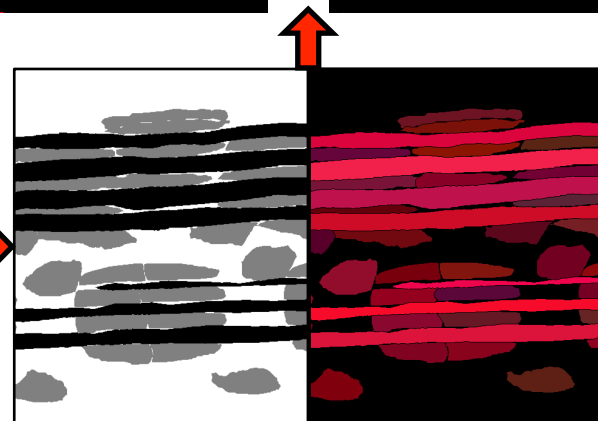
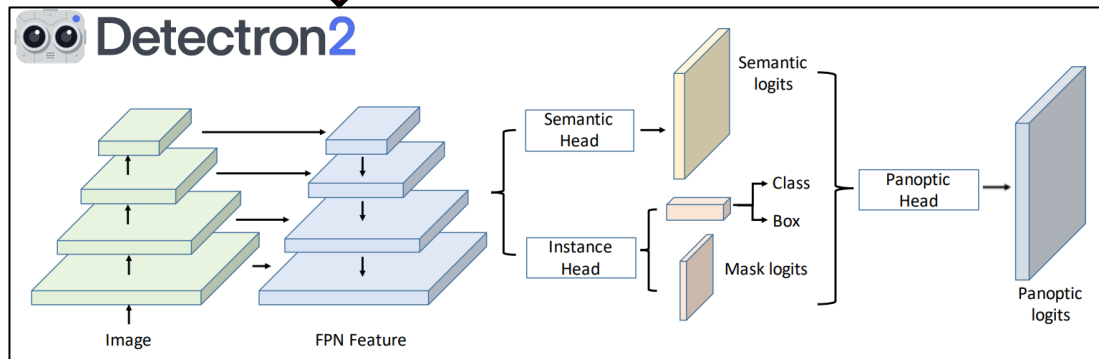
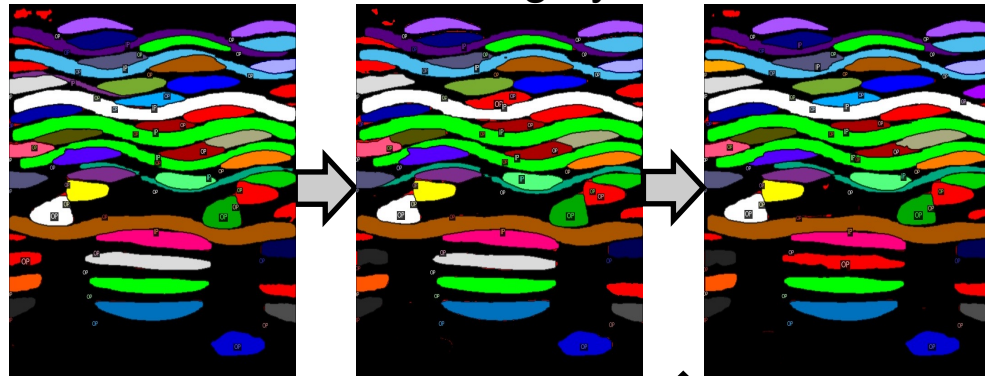


Tow Panoptic Segmentation and Tracking

Manual labeling



Tracking by IoU

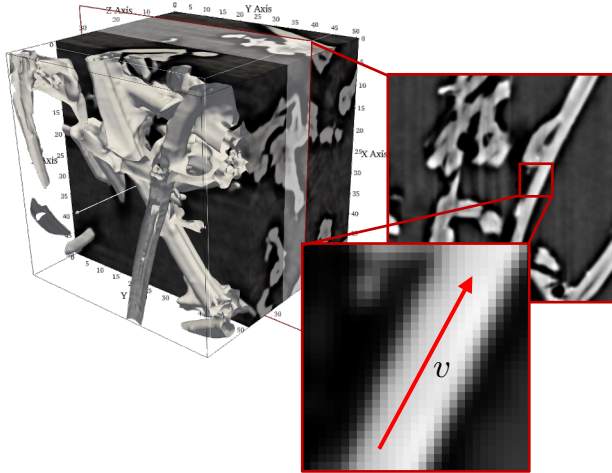


Semantic Classes

Instances

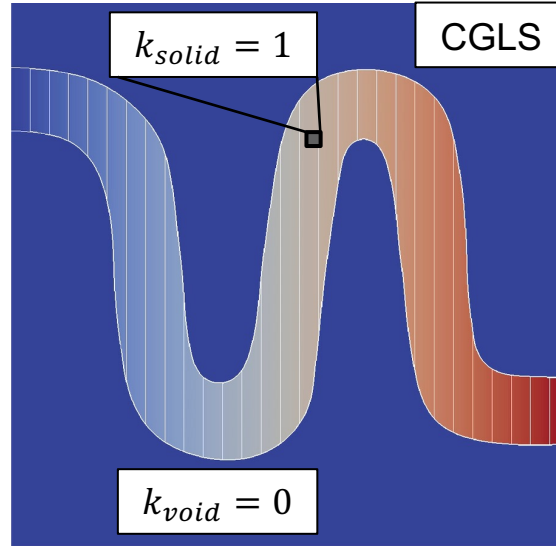
Orientation Methods

Structure tensor

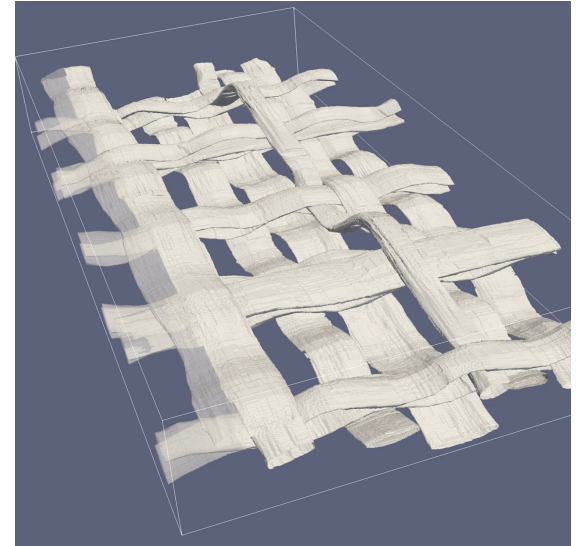


$$(I(x + v) - I(x))^2 \approx 0$$

Artificial flux

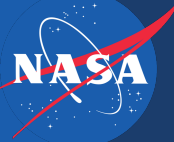


Ray casting



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

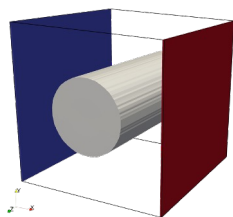
F. Semeraro, J.C. Ferguson, M. Acin, F. Panerai, N.N. Mansour, 2021. Anisotropic analysis of fibrous and woven materials part 2: Computation of effective conductivity. *Computational Materials Science*, 186, p.109956.



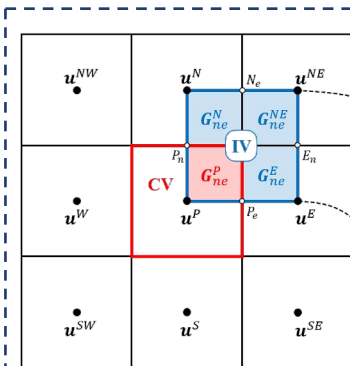
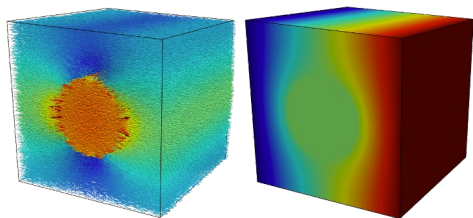
Conductivity and Elasticity Solvers

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

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



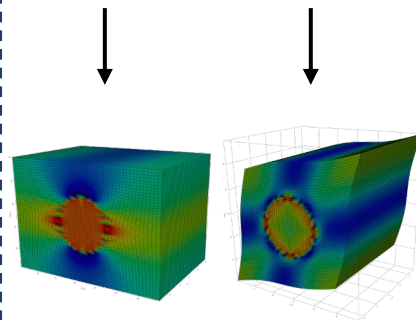
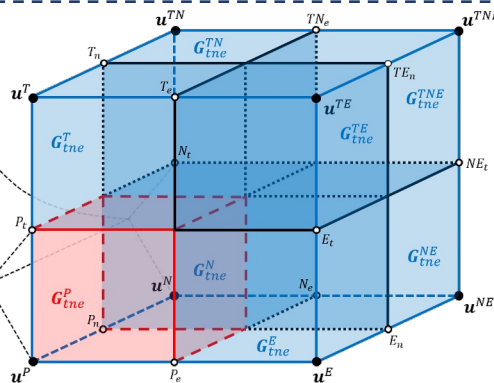
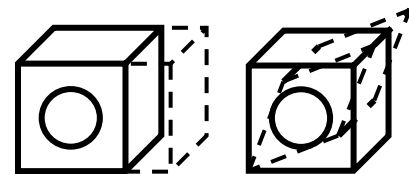
$$\mathbf{k}^x = -\mathbf{q} \cdot L_x$$



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

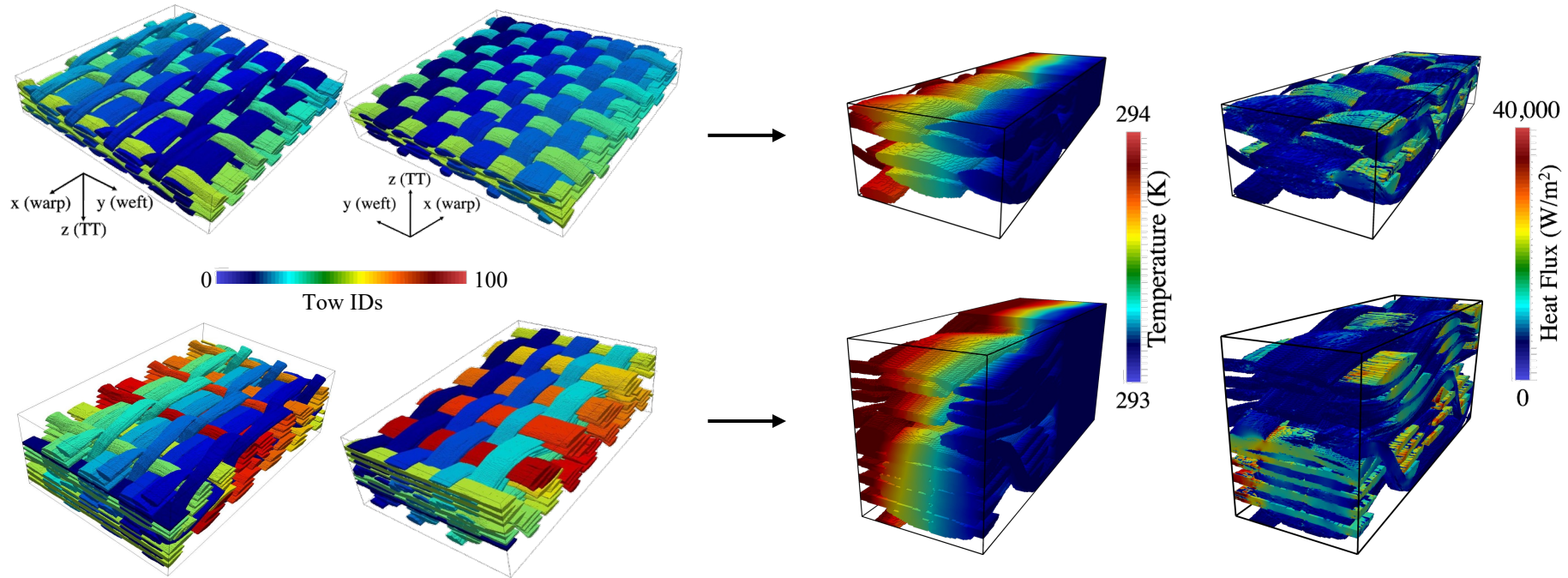
Multi-Point Stress Approximation (MPSA): $\boldsymbol{\sigma} = \mathbf{E} \mathbf{u}^N$

$$\mathbf{C}^1 = L_x \boldsymbol{\sigma} \quad \mathbf{C}^4 = \frac{2L_x L_y}{L_x + L_y} \boldsymbol{\sigma}$$





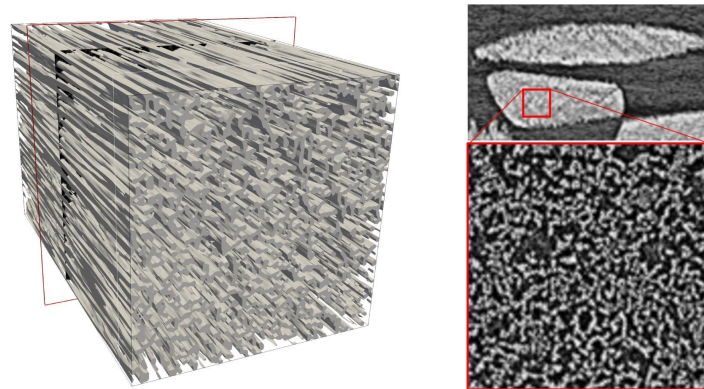
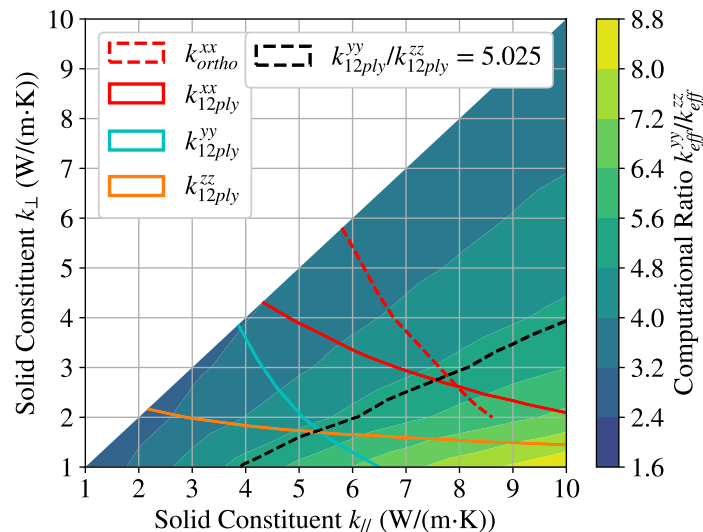
Conductivity solver validation: ADEPT



Single fiber conductivity estimation

Experimental value at room temperature:

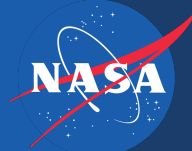
$$\mathbf{k}_{exp}^{12ply} = \begin{bmatrix} 2.184 & - & - \\ - & 1.980 & - \\ - & - & 0.394 \end{bmatrix}$$



Single fiber thermal conductivity

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

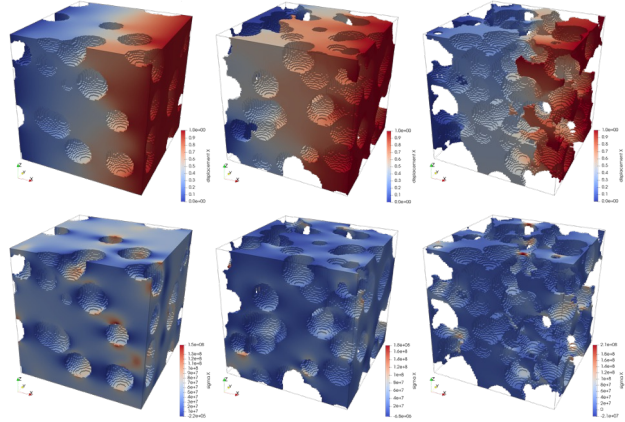
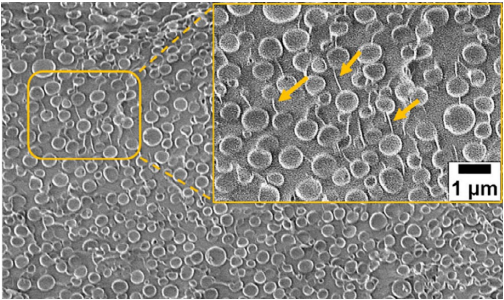
$$\mathbf{k}_{num}^{12ply} = \begin{bmatrix} 2.310 & -0.414 & 0.000 \\ -0.524 & 2.030 & 0.071 \\ 0.007 & 0.050 & 0.504 \end{bmatrix}$$



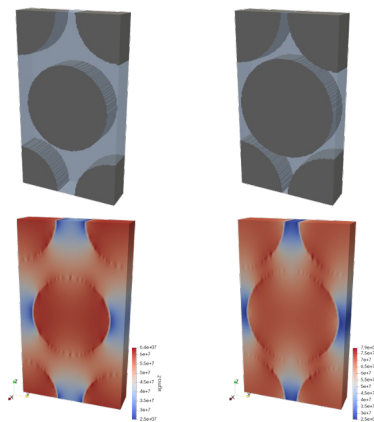
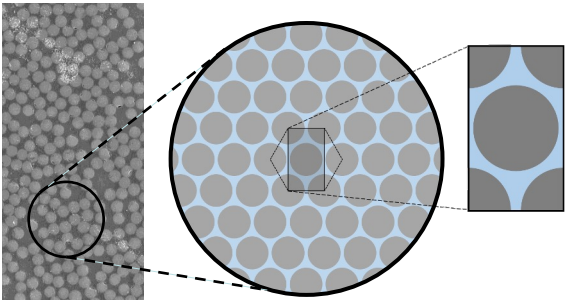
Elasticity Solver Validation: Woven Composite

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

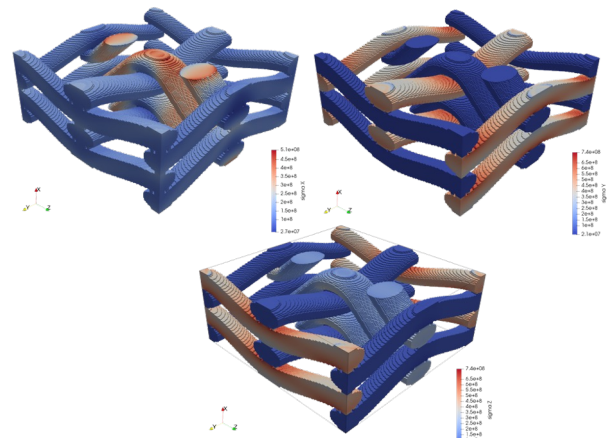
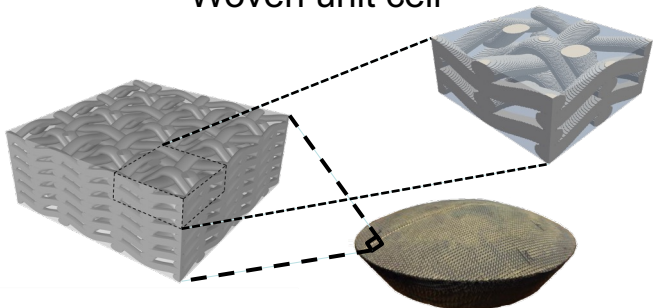
Matrix: porous phenolic resin



Intra-tow fiber packing

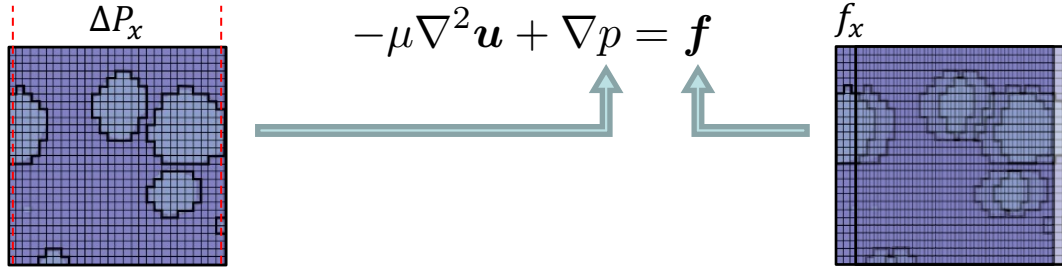


Woven unit cell

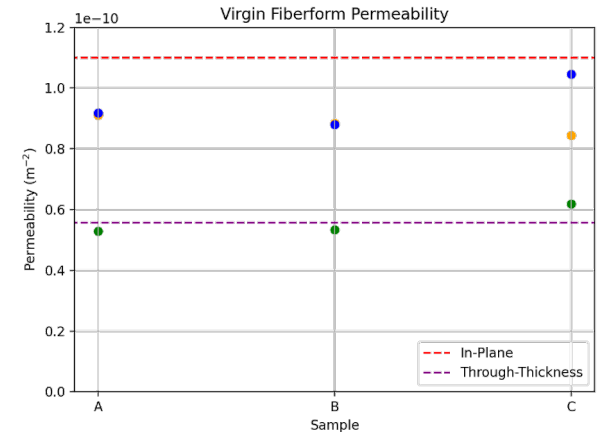
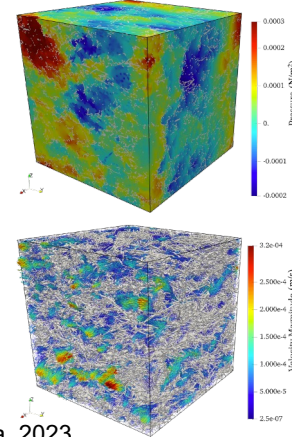
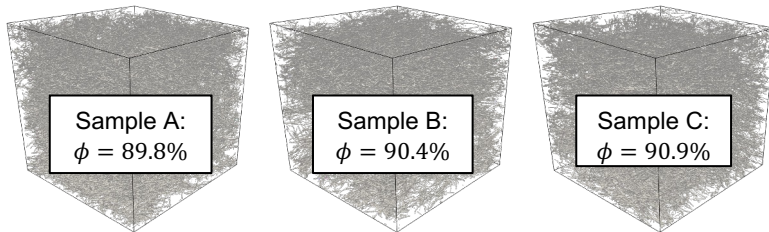


Permeability Solver

- Stokes flow ($Re \approx 0$) solved with Finite Element (FE) scheme with Q1-Q1 discretization:



- Validation on FiberForm (500^3 vox, $2.6\mu\text{m}$) run on NVIDIA V100s with matrix-free PCG



P.C.F. Lopes, R.S. Vianna, V.W. Sapucaia, F. Semeraro, R. Leiderman, A.M.B. Pereira. 2023
Simulation Toolkit for Digital Material Characterization of Large Image-based Microstructures. *Computational Materials Science*, 219, p.112021.