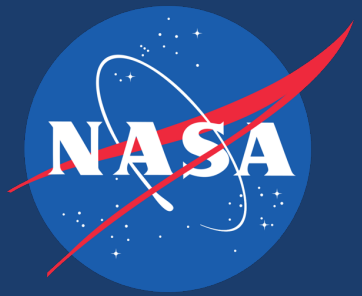
Porous Microstructure Analysis (PuMA) software



Presented by: Federico Semeraro
NASA Ames Research Center, Moffett Field, CA
AIAA SciTech Forum 2023, January 23rd - 27th
National Harbor, Maryland (USA)

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1. Analytical Mechanics Associates, Inc.
2. Stanford University
3. University of Illinois at Urbana-Champaign

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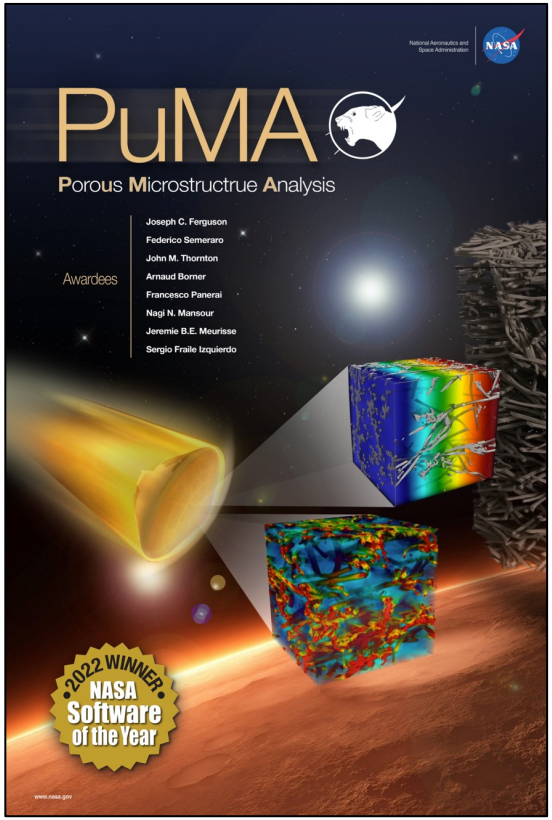
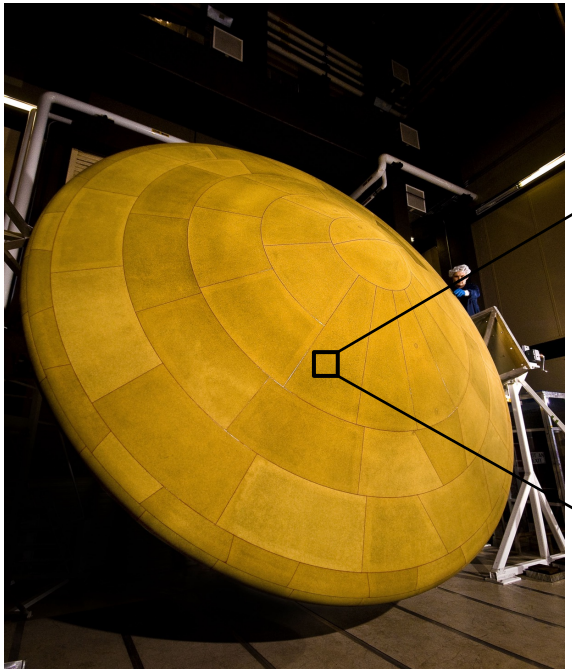
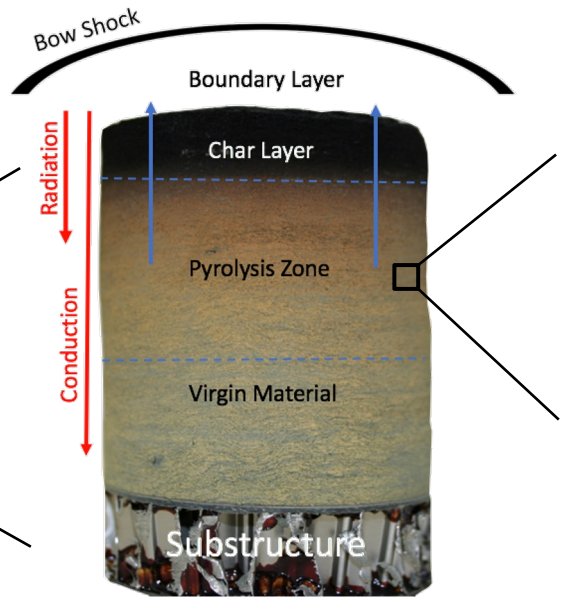


Modeling Thermal Protection Systems (TPS)

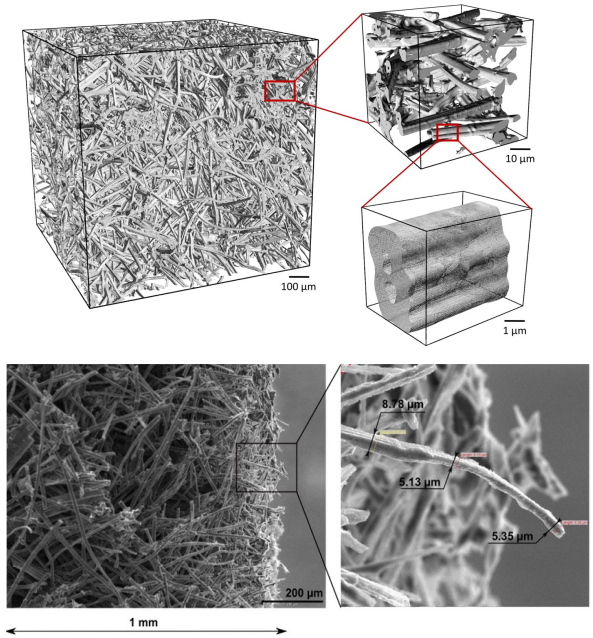
Full scale



Mars Science Laboratory (MSL) heat shield



Microscale



Carbon-fiber microstructure

PuMA v3.2 release

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*

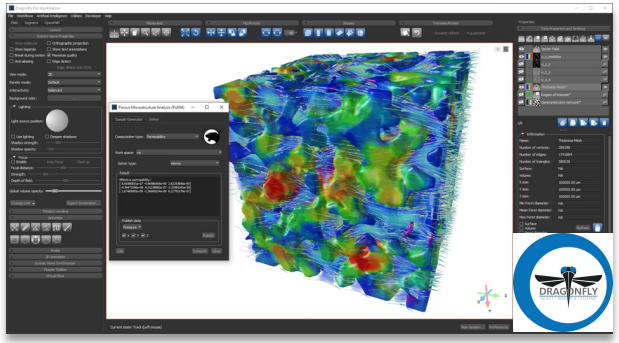
Installation: conda install -c conda-forge puma

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

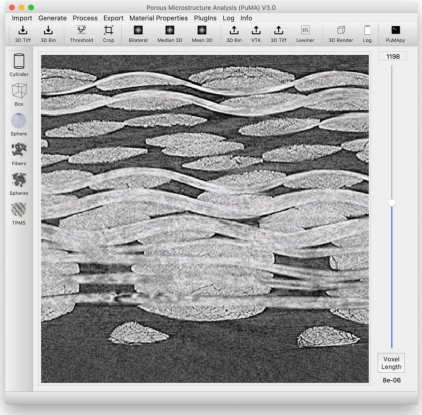
Documentation: https://puma-nasa.readthedocs.io

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

Tutorials: PuMA YouTube channel and online Jupyter notebooks



a)



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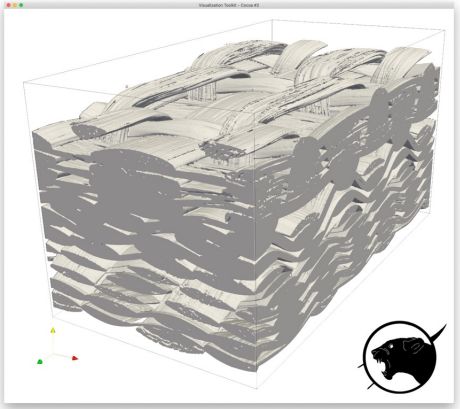

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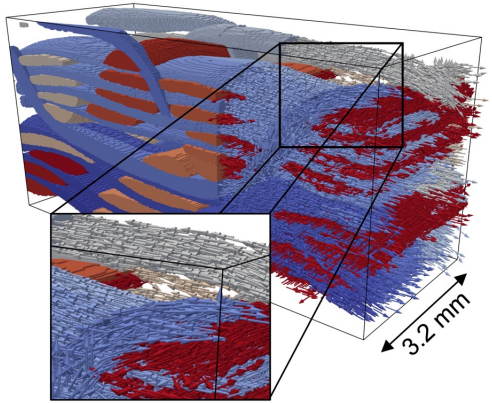
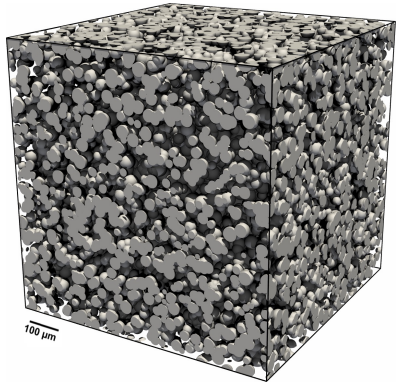
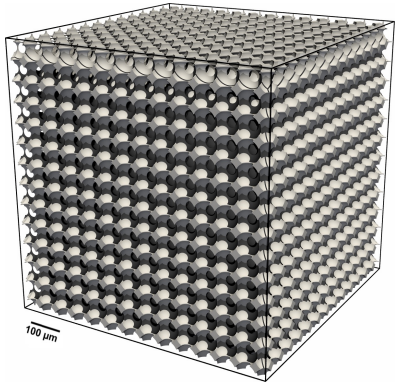


Artificial Domain Generation

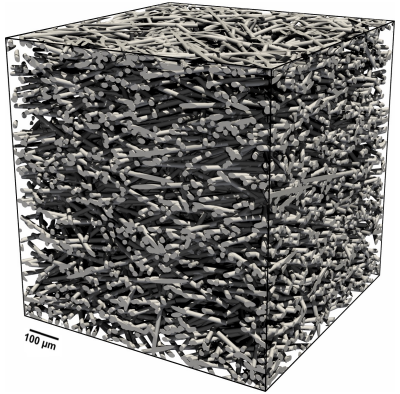
Packed Sphere Beds

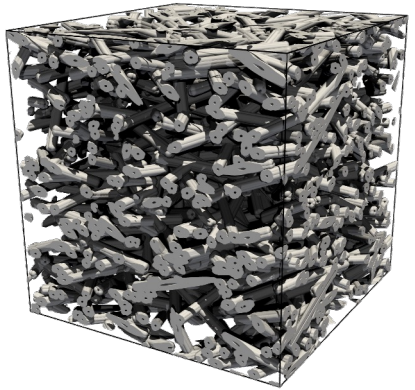


Periodic Foams

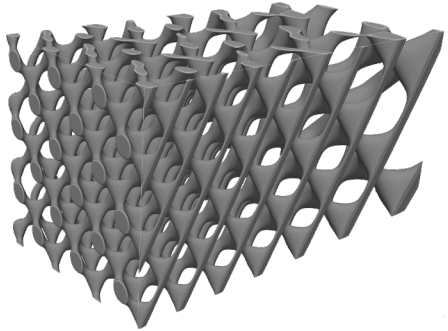


Fiber Structures

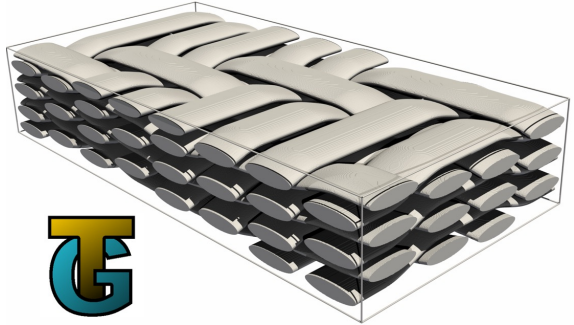




Triply Periodic Minimal Surface (TPMS)

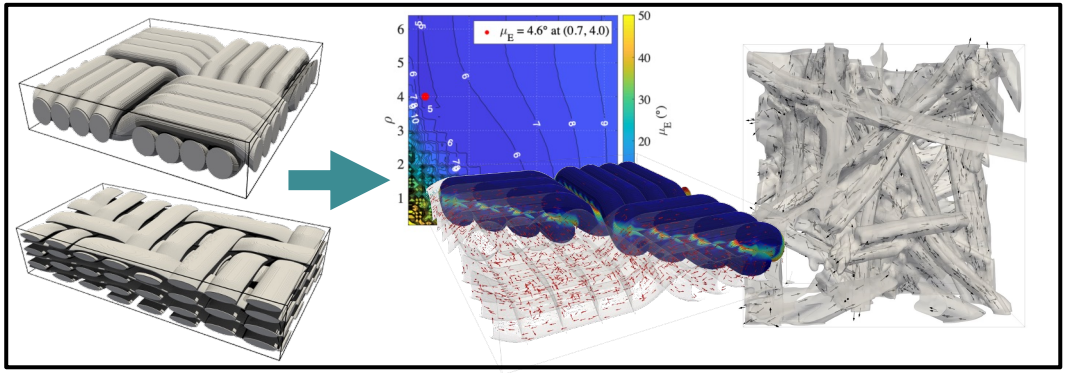


Woven geometries

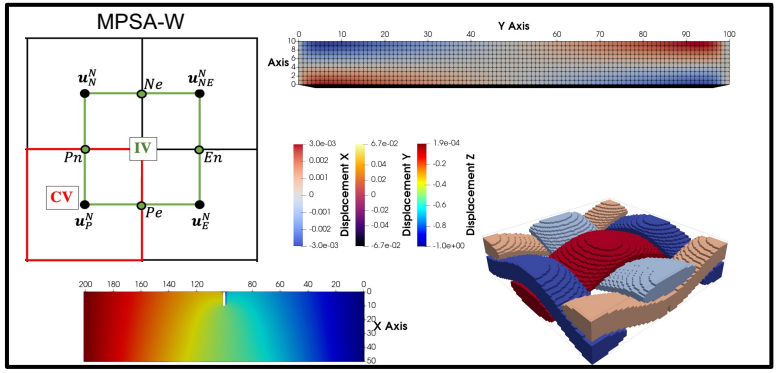


Advanced Material Property Computation

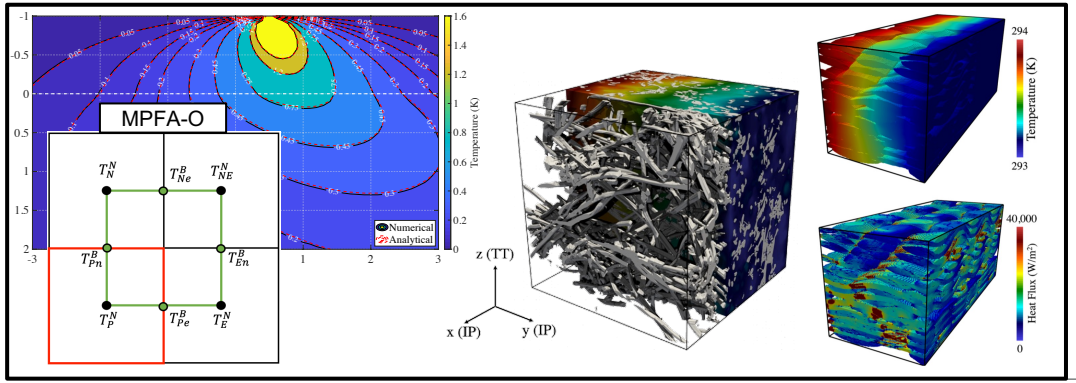
Material orientation. *Computational Materials Science* (2020)



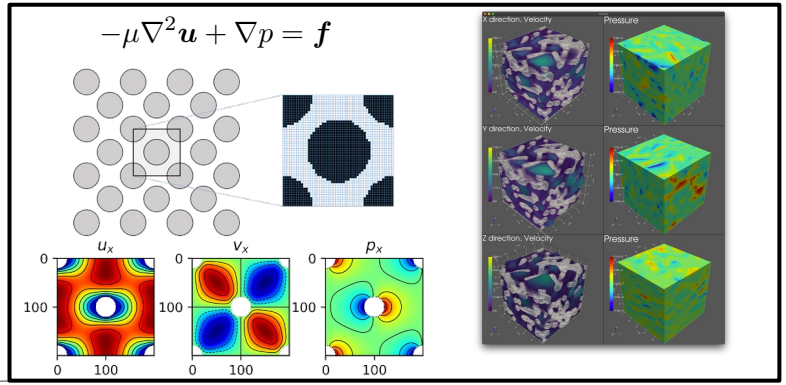
Effective elasticity. *Computational Materials Science* (*in progress*)



Effective conductivity. *Computational Materials Science* (2021)

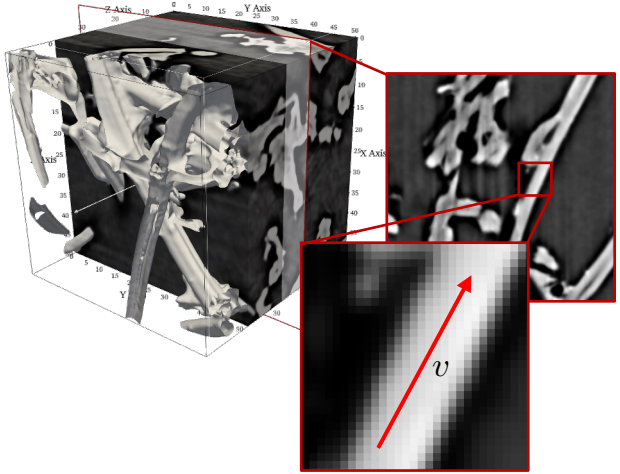


Effective permeability. *Computational Materials* Science (2022)



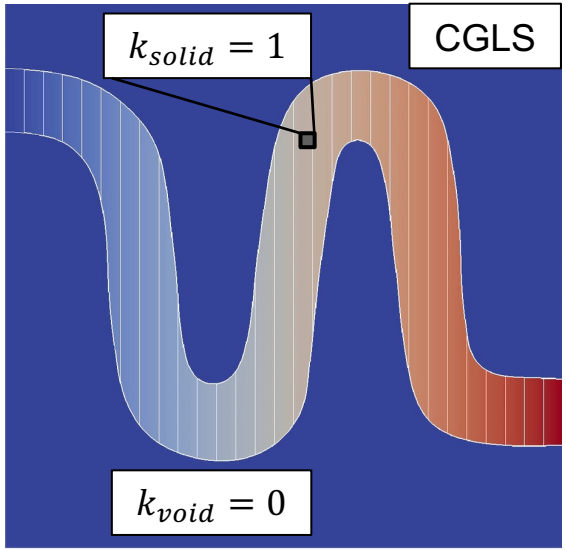
Orientation Methods

Structure tensor

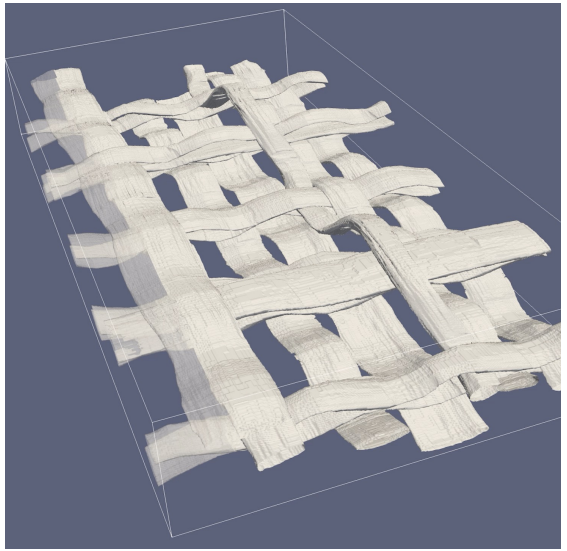


$$(I(x+v)-I(x))^2 \approx 0$$

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.

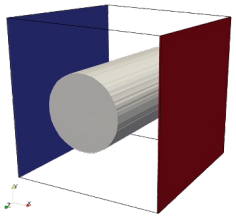
Conductivity and Elasticity Solvers

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

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

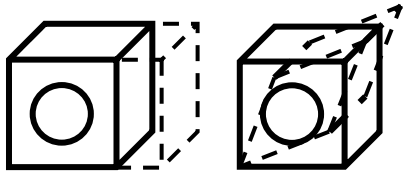
Multi-Point Flux Approximation (MPFA): $\boldsymbol{q} = \boldsymbol{E}\boldsymbol{T}^N$

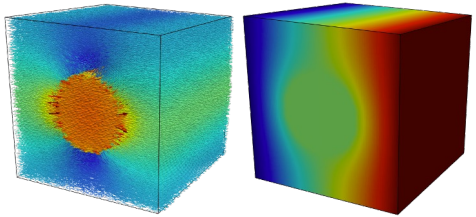
Multi-Point Stress Approximation (MPSA): $\boldsymbol{\sigma} = \boldsymbol{E}\,\boldsymbol{u}^N$

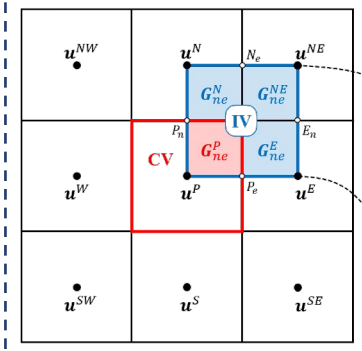


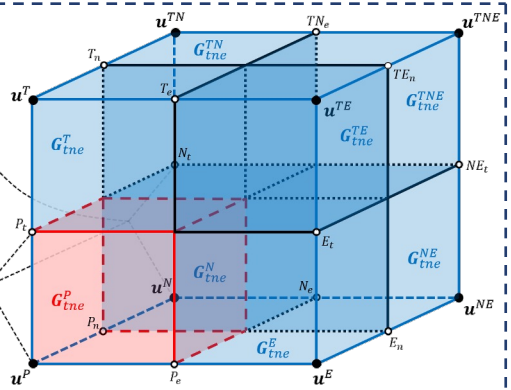
$$\boldsymbol{k}^x = -\boldsymbol{q} \cdot L_x$$

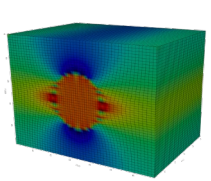
$$C^1 = L_x\,\boldsymbol{\sigma} \quad C^4 = \frac{2L_xL_y}{L_x + L_y}\boldsymbol{\sigma}$$

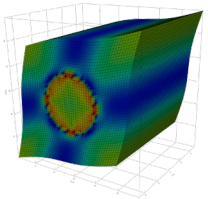








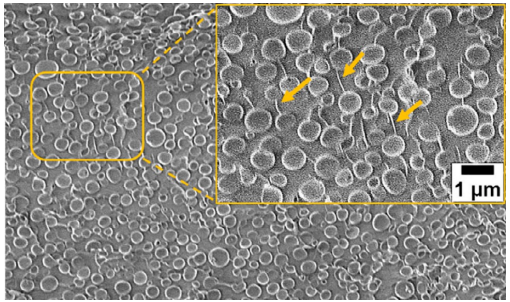


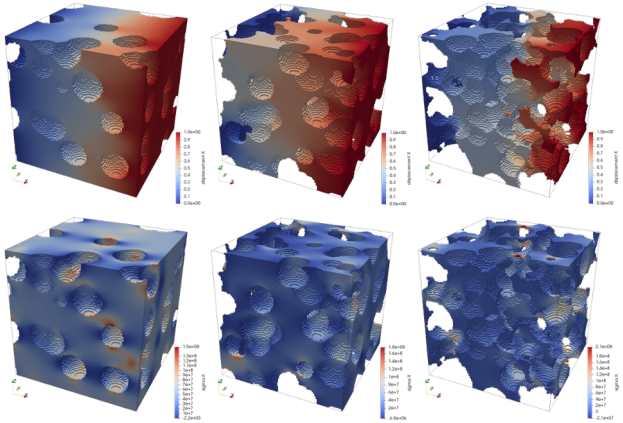


Elasticity Solver Validation: Woven Composite

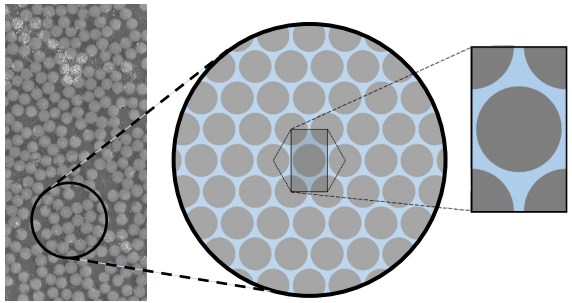
S. Fraile Izquierdo, F. Semeraro, M. Acin, 2022. Multi-Scale Analysis of Effective Mechanical Properties of Porous 3D Woven Composite Materials. *AIAA Scitech Forum*

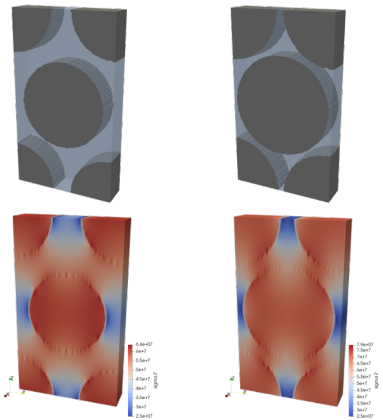
Matrix: porous phenolic resin



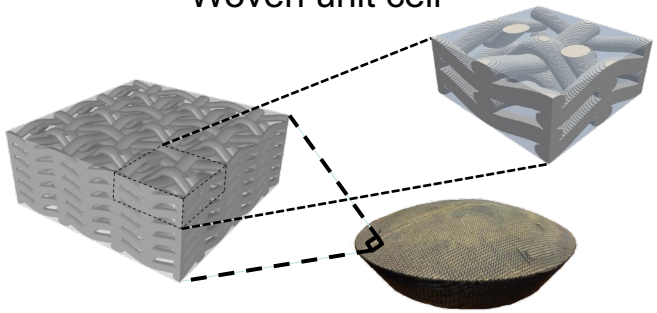


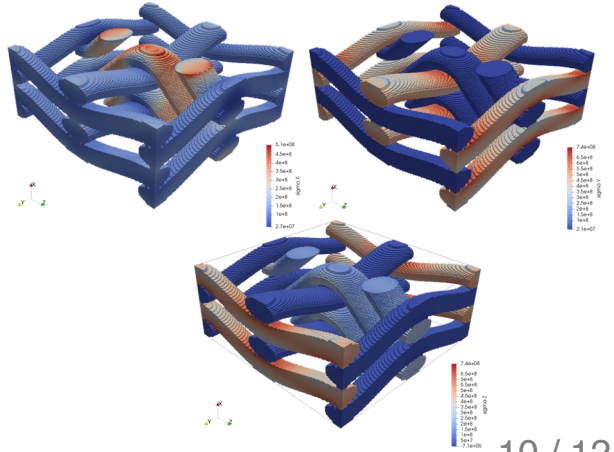
Intra-tow fiber packing





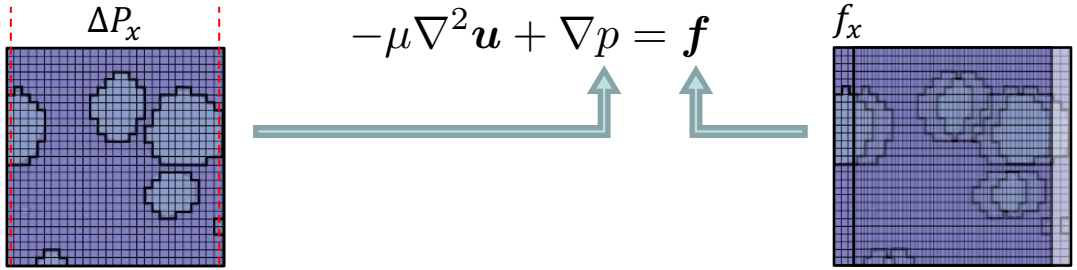
Woven unit cell



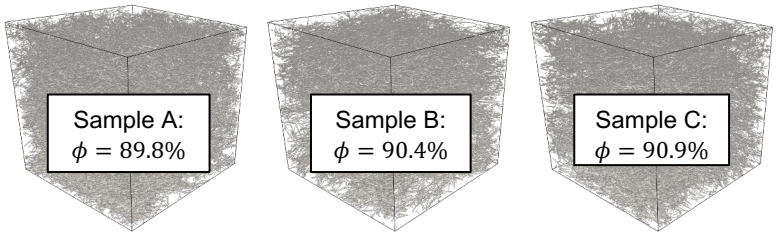


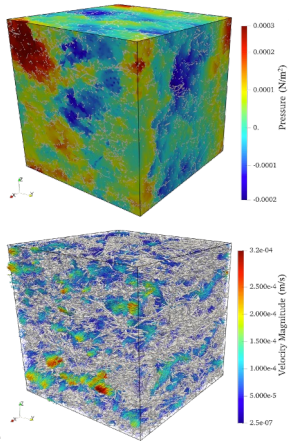
Permeability Solver

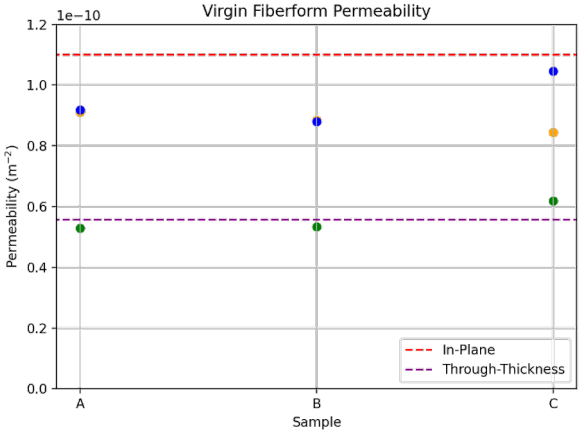
- Stokes flow ($Re \approx 0$) solved with Finite Element (FE) scheme with Q1-Q1 discretization:



- Validation on FiberForm (500^3 vox, 2.6μm) 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. Simulation Toolkit for Digital Material Characterization of Large Image-based Microstructures. *Computational Materials Science* (accepted)

Thank you!