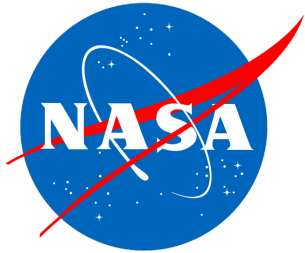


Recent Developments to the Porous Microstructure Analysis (PuMA) software



Presented by Joseph C. Ferguson
July 1st, 2024



Joseph C. Ferguson^{1}, Federico Semeraro¹, Arnaud Borner¹, Francesco Panerai²,
John M. Thornton¹, Sergio Fraile Izquierdo¹, Alexandre Quintart¹, Nagi N. Mansour²*

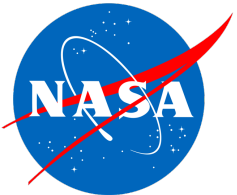
¹ AMA Inc. at NASA Ames Research Center

² Dept. of Aerospace Engineering, University of Illinois at Urbana-Champaign

* joseph.c.ferguson@nasa.gov

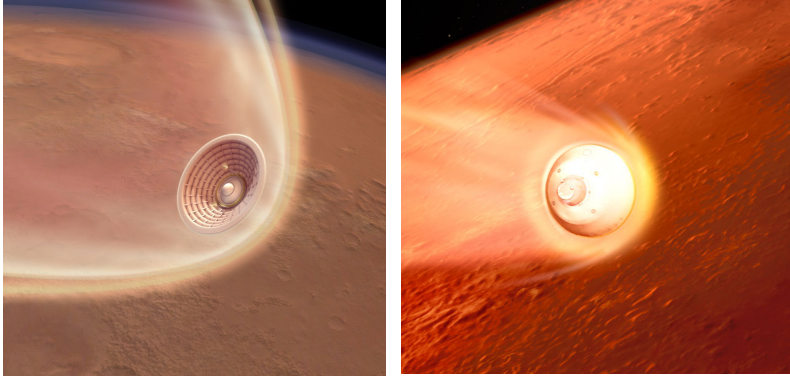
Presentation Outline

1. PuMA Introduction and Motivation
2. Overview of Capabilities
3. Recent PuMA Developments



Thermal Protection Systems (TPS)

Need for Thermal Protection Systems



Ground-based Testing

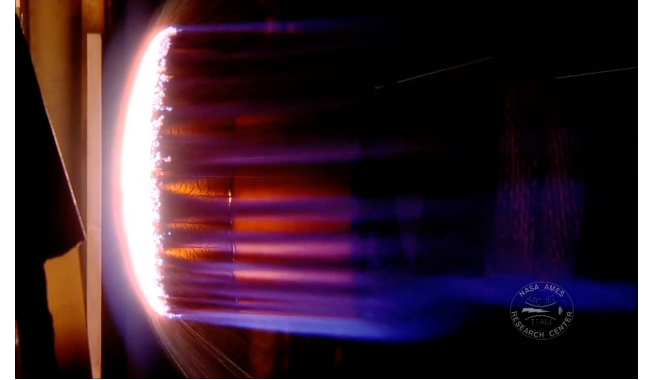
P. Agrawal et. al. 2016.



Virgin PICA Sample

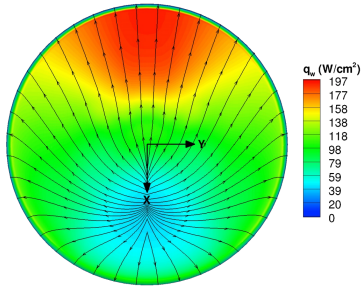


Charred PICA Sample

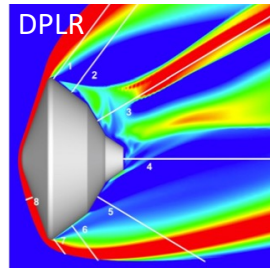


Arcjet Testing of TPS

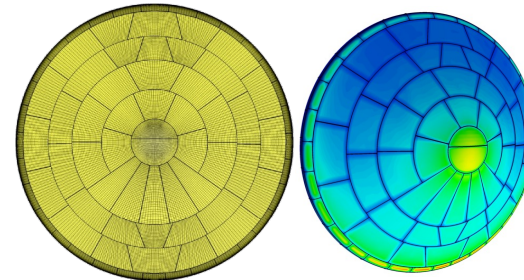
Computational Modeling



Hypersonic CFD

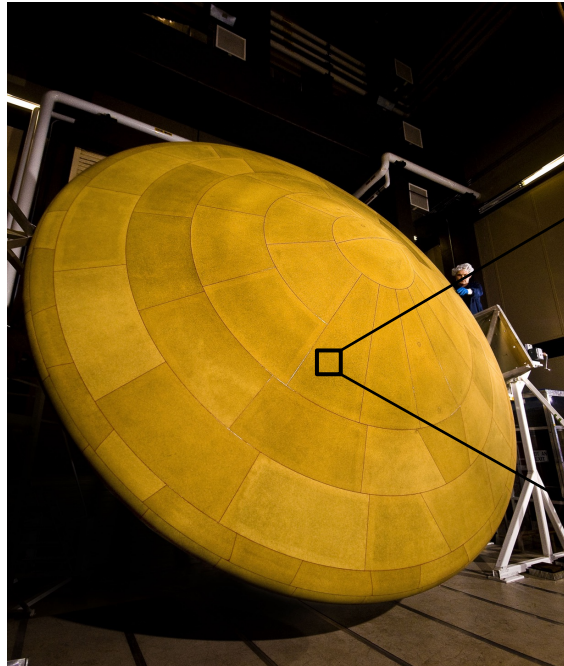


Material Response

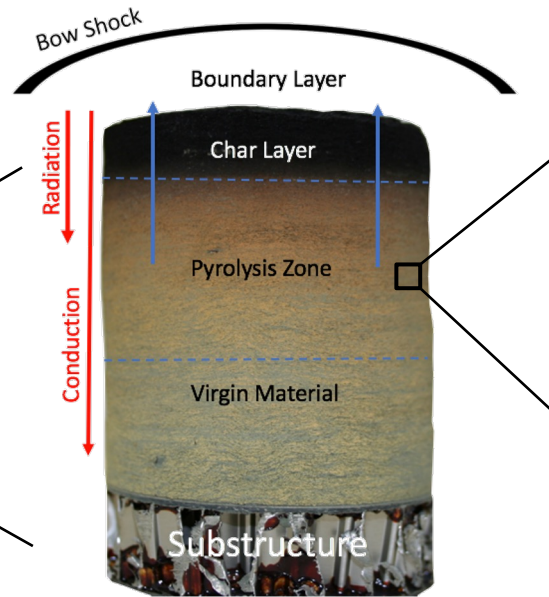


Heat Shields at Multiple Scales

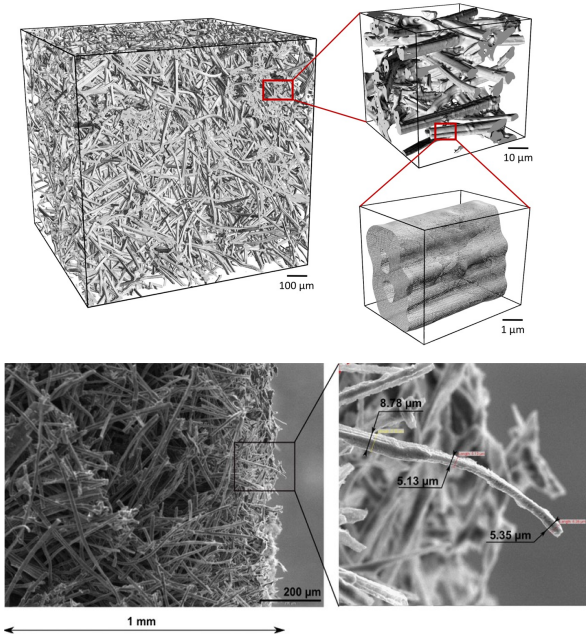
Full scale



Mars Science Laboratory (MSL) heat shield

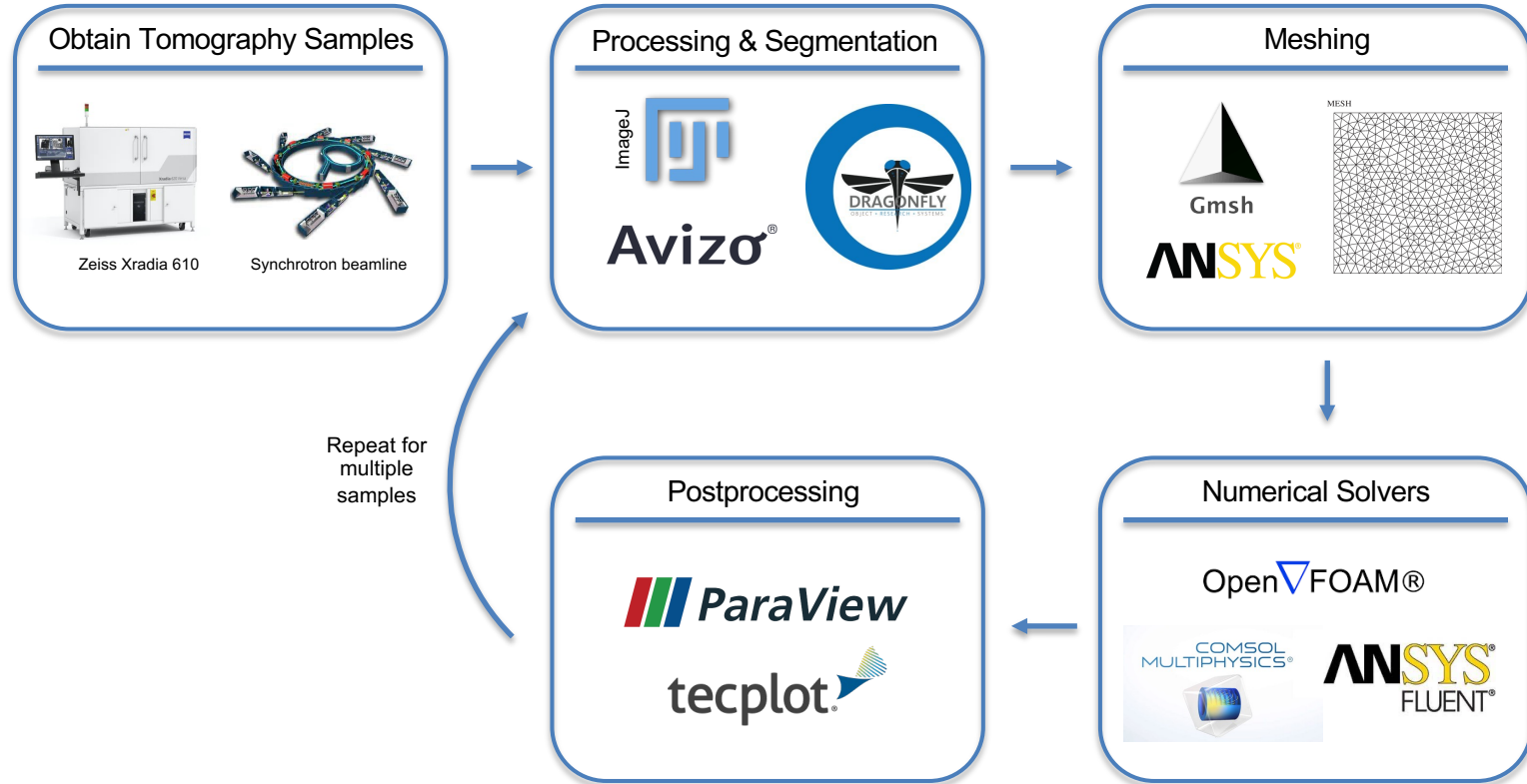


Microscale

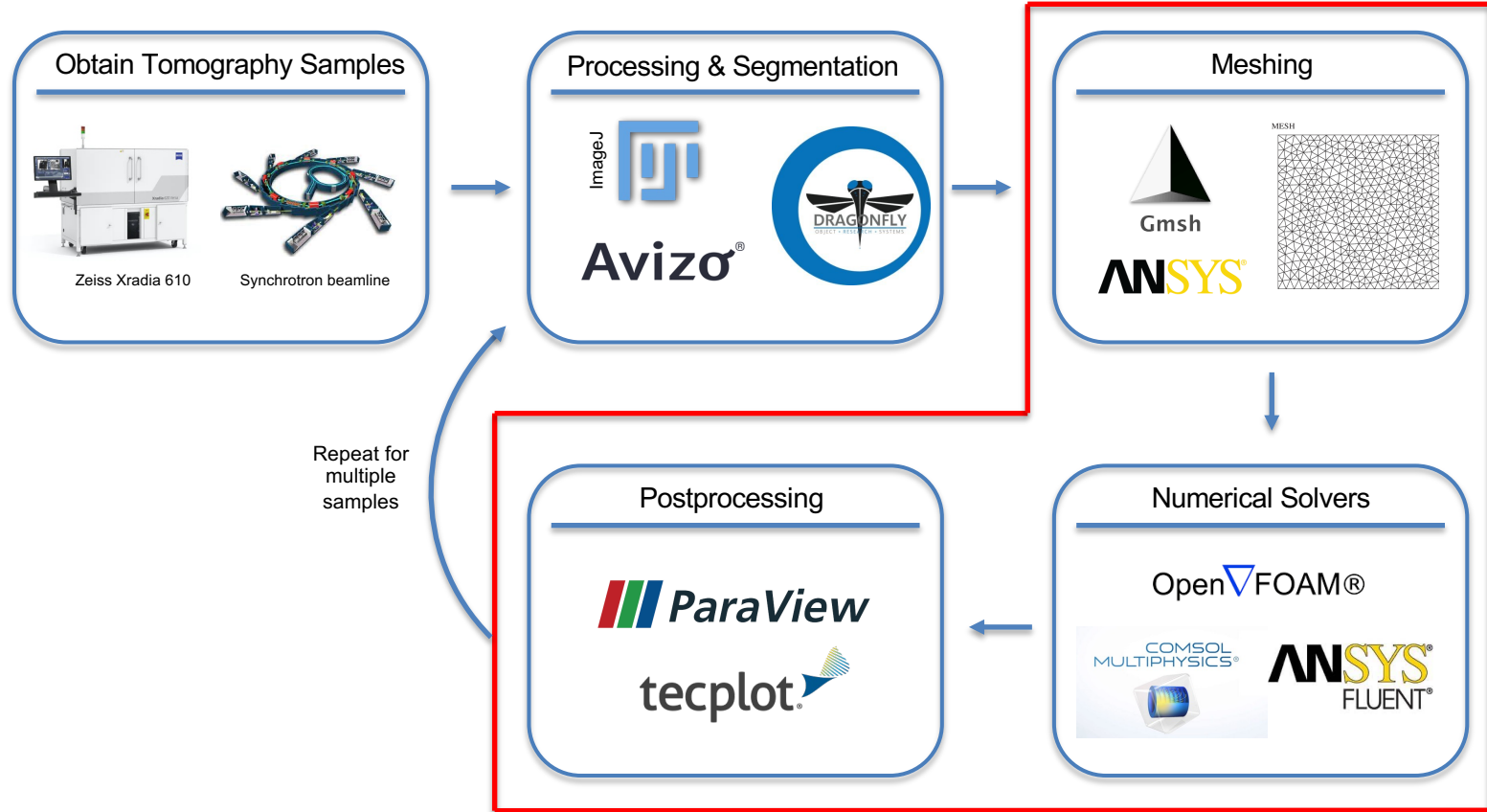


Carbon-fiber microstructure

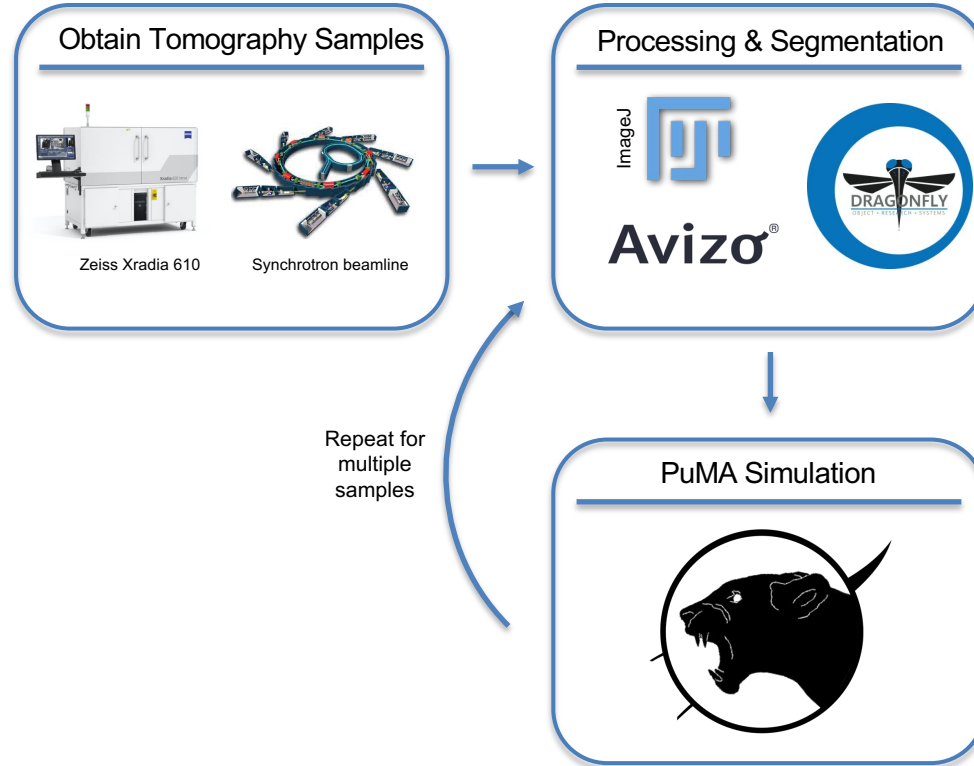
Typical Microscale Simulation Workflow



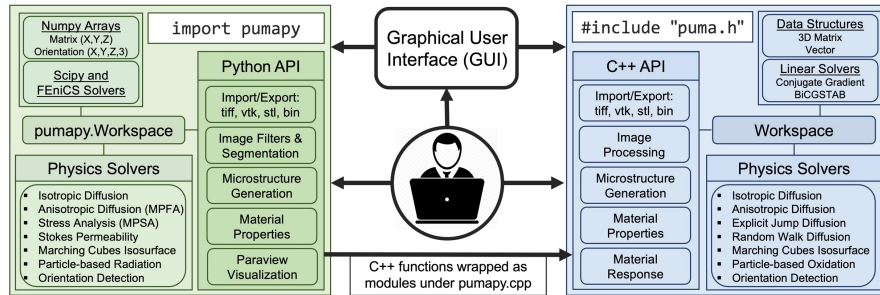
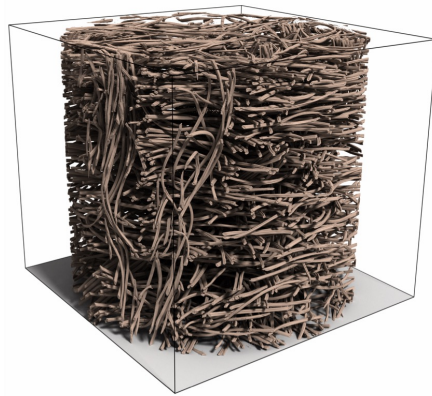
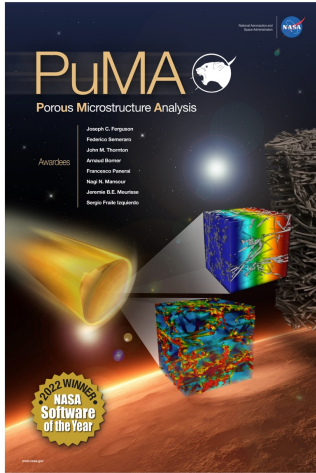
PuMA Workflow



PuMA Workflow



The PuMA software



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

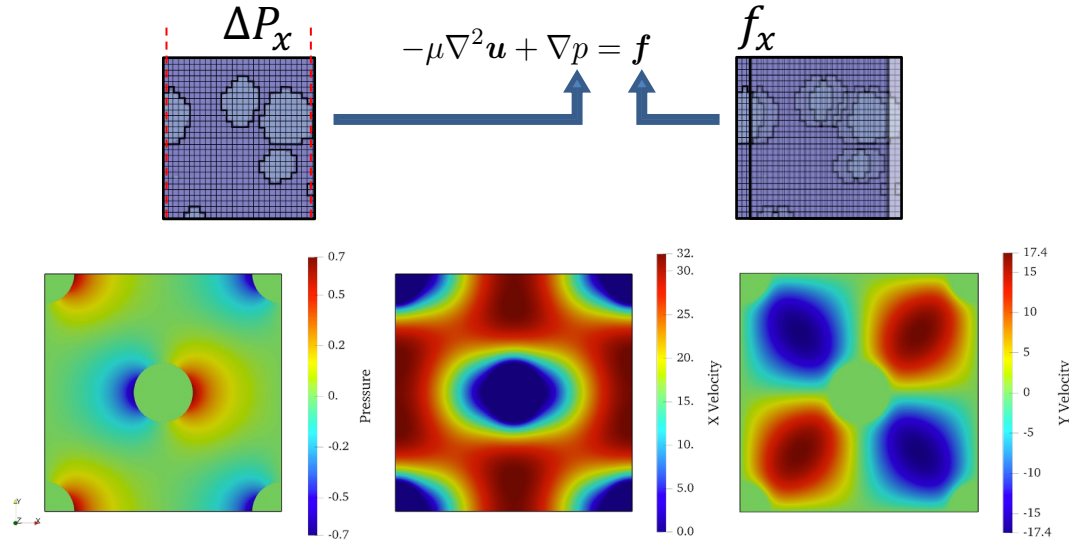
- Microscale Oxidation
- Hyperthermal Beam Simulations

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

[1] Ferguson JC, Panerai F, Borner A, Mansour NN. PuMA: *The Porous Microstructure Analysis software*. SoftwareX. 2018.

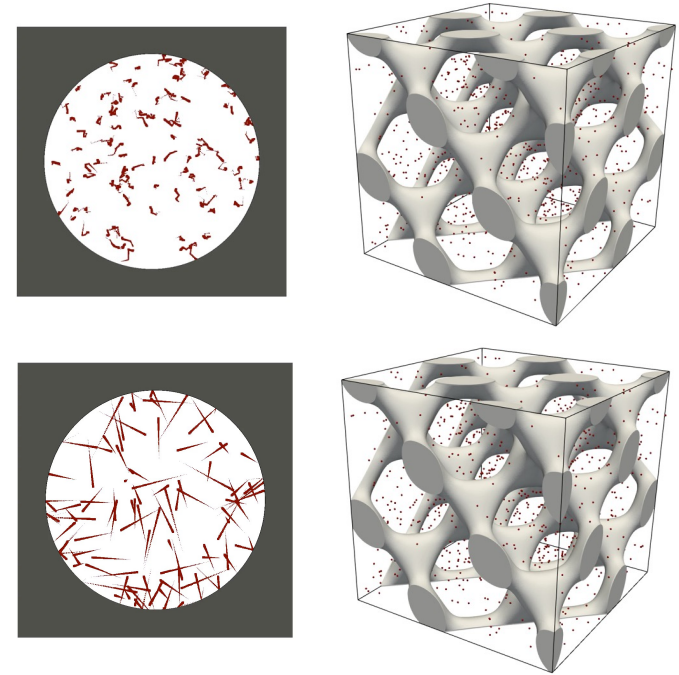
[2] Ferguson JC, Semeraro F, Thornton JM, Panerai F, Borner A, Mansour NN. Update 3.0 to "PuMA: The Porous Microstructure Analysis software", (PII: S2352711018300281). SoftwareX. 2021.

Permeability



Pressure driven Darcy flow through fibrous porous material [1]

Tortuosity

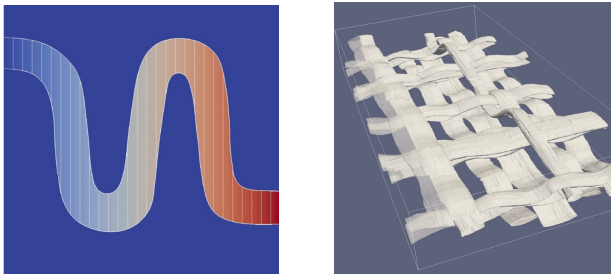


Continuum and Rarefied diffusion in porous media [2]

[1] Lopes PC, Vianna RS, Sapucaia VW, Semeraro F, Leiderman R, Pereira AM. *Simulation toolkit for digital material characterization of large image-based microstructures*. Computational Materials Science. 2023

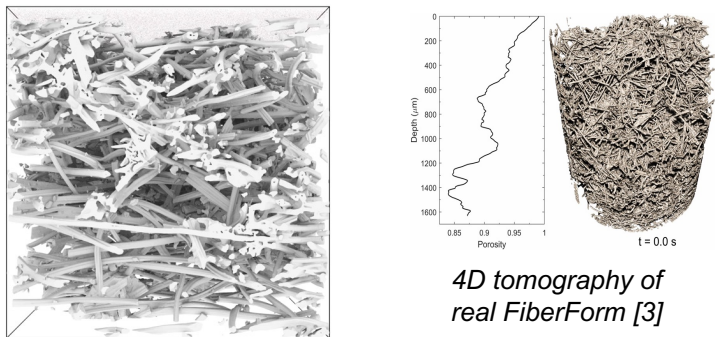
[2] Ferguson JC, Borner A, Panerai F, Close S, Mansour NN. *Continuum to rarefied diffusive tortuosity factors in porous media from X-ray microtomography*. Computational Materials Science. 2022

Orientation Estimation



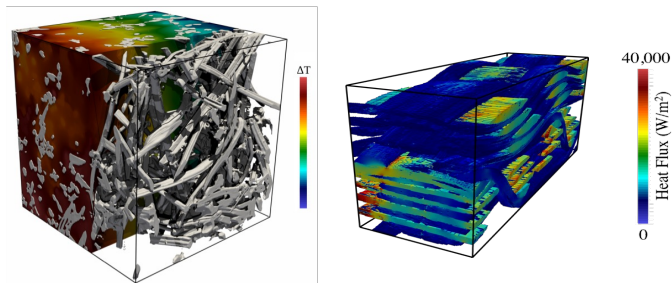
Predicting local orientation of weave from X-ray microtomography [1]

Microscale Oxidation [2]



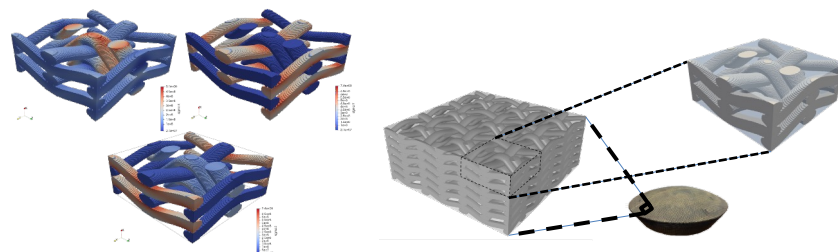
4D tomography of real FiberForm [3]

Effective Thermal Conductivity



Heat transfer in fibrous and woven materials [4]

Effective Elasticity



Elasticity of anisotropic porous 3D woven materials [5]

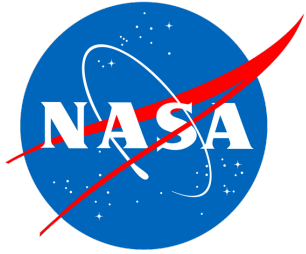
[1] Semeraro F et al. Computational Materials Science. 2020. (<https://doi.org/10.1016/j.commatsci.2020.109631>)

[2] Ferguson JC et al. Carbon. 2016 (<https://doi.org/10.1016/j.carbon.2015.08.113>)

[3] Ringel B et al. In preparation. 2024

[4] Semeraro F et al. Computational Materials Science. 2021 (<https://doi.org/10.1016/j.commatsci.2020.109956>)

[5] Fraile Izquierdo S et al. AIAA SciTech. 2016 (<https://doi.org/10.2514/6.2022-2281>)

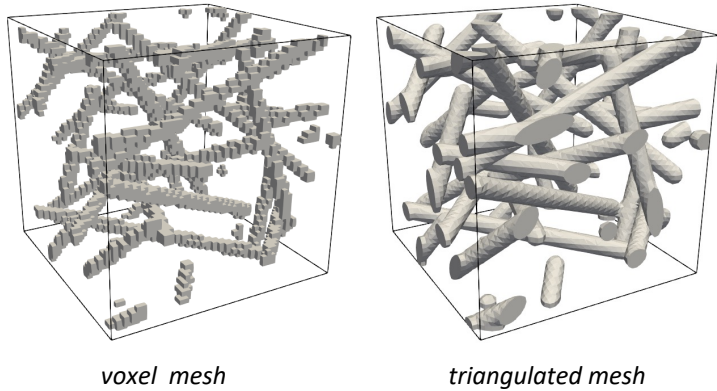


Recent Development #1:

Cut-Cell Poisson Solver for Effective Thermal Conductivity and Tortuosity

Surface Representation in Numerical Solvers

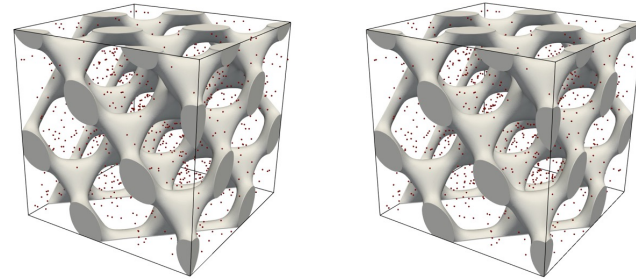
Voxel Mesh



- Simple to generate from X-ray microtomography datasets
- Relatively simple to implement numerical methods with low memory requirements
- Used in isotropic conductivity, continuum tortuosity, permeability, anisotropic conductivity, and elasticity solvers

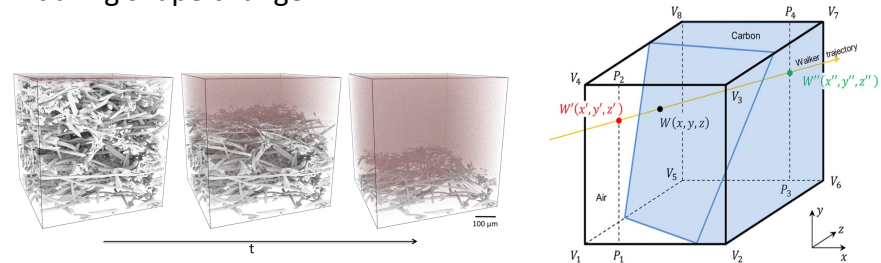
Triangulated Surface Mesh

- Useful for particle methods. Used in rarefied tortuosity solver



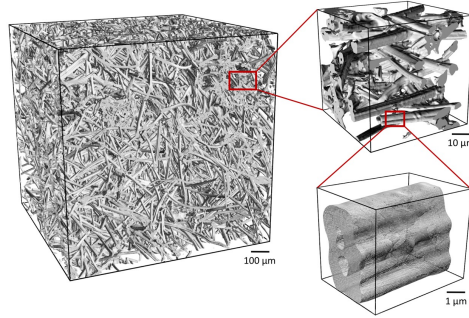
Interpolated Surface Mesh

- Used in microscale oxidation solver. Useful to avoid re-meshing during shape change

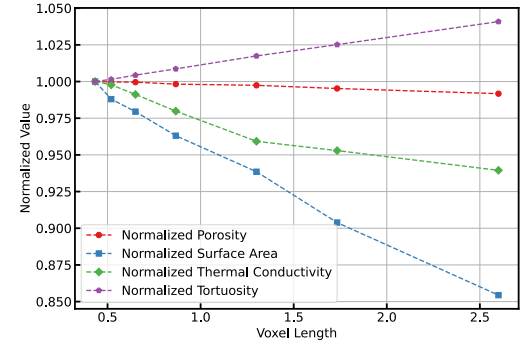


Voxel Mesh Accuracy

- Properties were computed for FiberForm as resolution was scaled from 0.325 μm to 2.6 μm voxel length
- The error caused by poor resolution is highly dependent on the specific microstructure

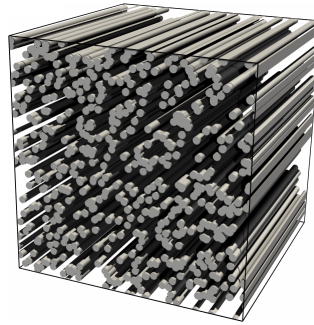


Large X-ray microtomography sample of FiberForm with voxel length 0.325 μm

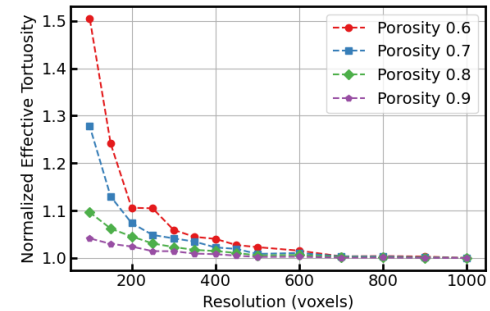


Relative error in effective material properties as resolution decreases

- For tortuosity, error increases dramatically with decreasing porosity (decreasing mean pore diameter)

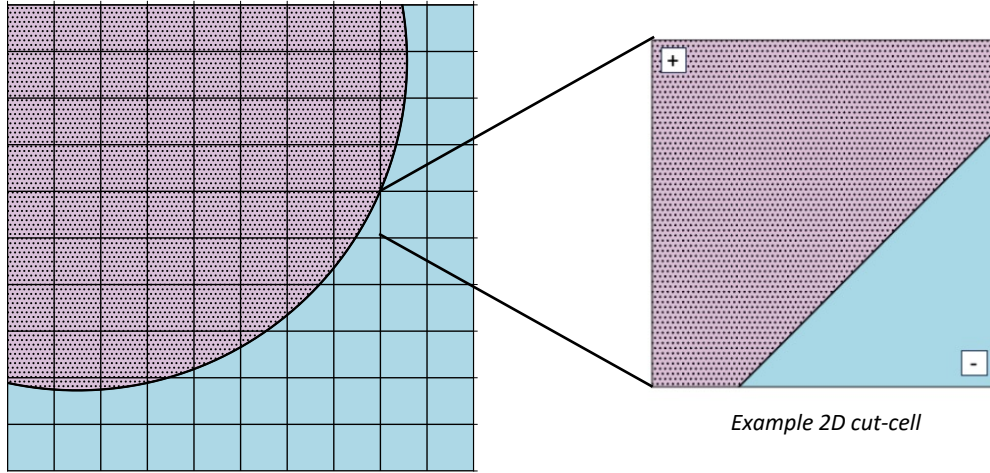


parallel fiber domains were tested between porosity of 0.6 and 0.9

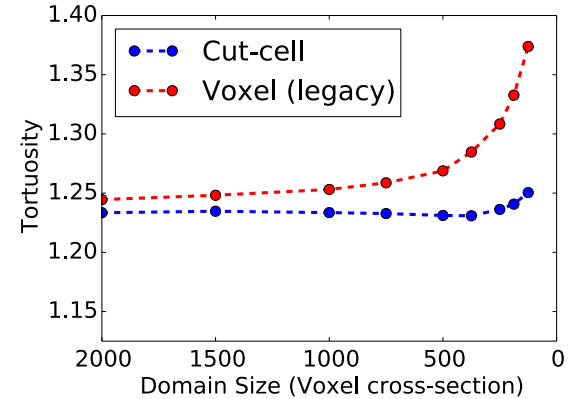


Relative error in continuum tortuosity as a function of domain size and porosity

Cut-Cell Poisson Solver



Example 2D cut-cell



Accuracy comparison between cut-cell and voxel PuMA solvers

Basic governing equation:

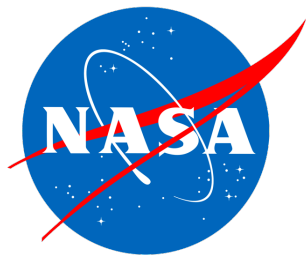
$$\sum_f \lambda A_f \cdot \nabla T \Big|_f = f(x, y, z)V$$

Sum of all the fluxes across the boundary faces is equal to the source term (usually zero) at steady state

λ = Thermal conductivity

A_f = Face area

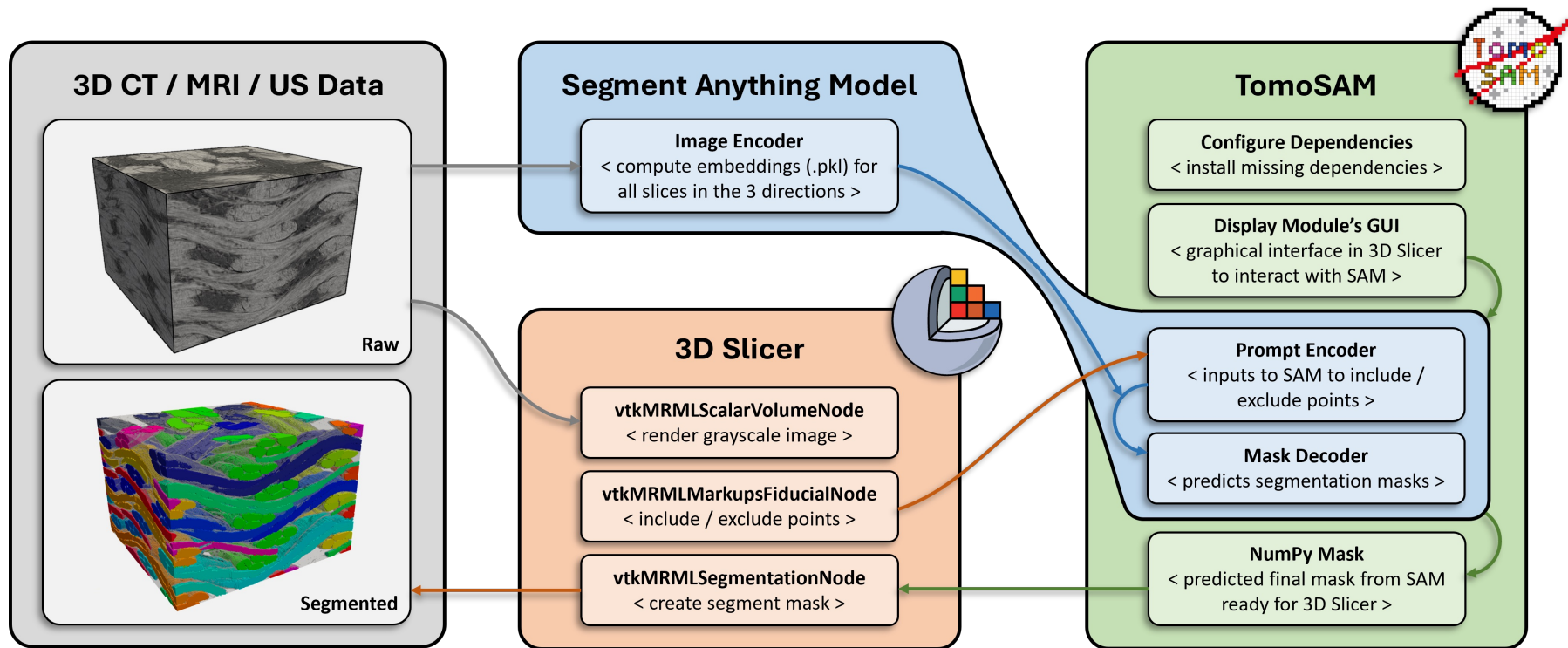
$\nabla T \Big|_f$ = Face temperature gradient



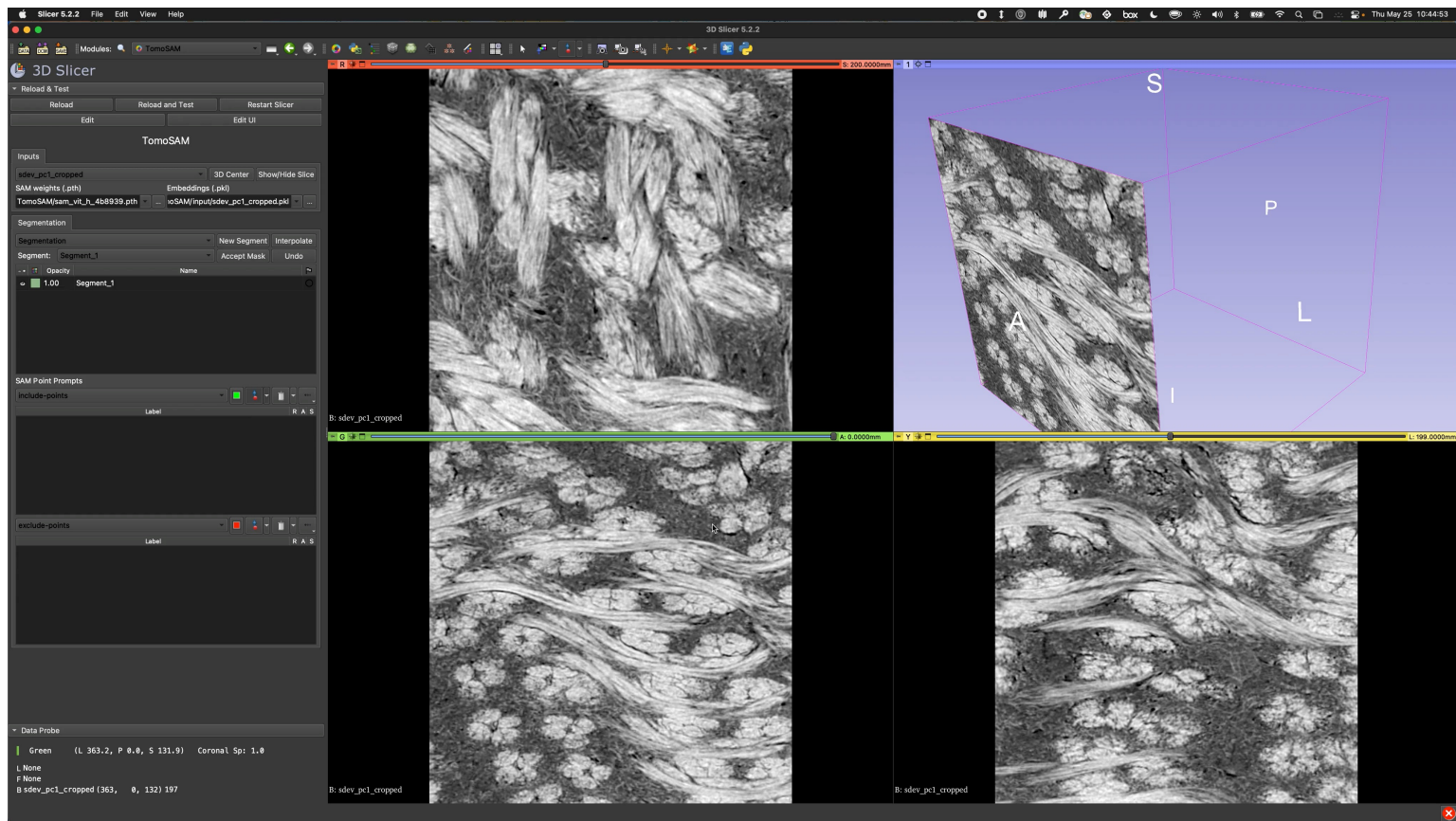
Recent Development #2:

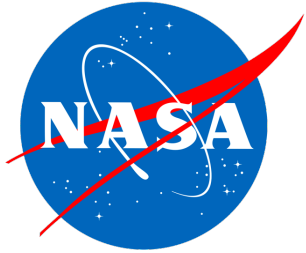
***TomoSAM: A Weave Segmentation Tool
Based on the Segment Anything Model
(SAM) from META***

TomoSAM: A Weave Segmentation Tool



TomoSAM Demo



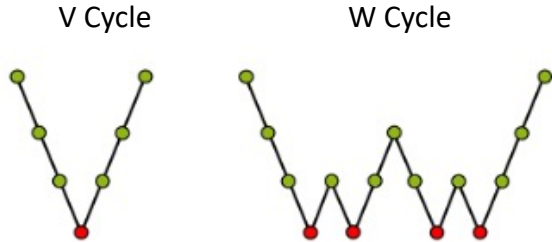


Recent Development #3:

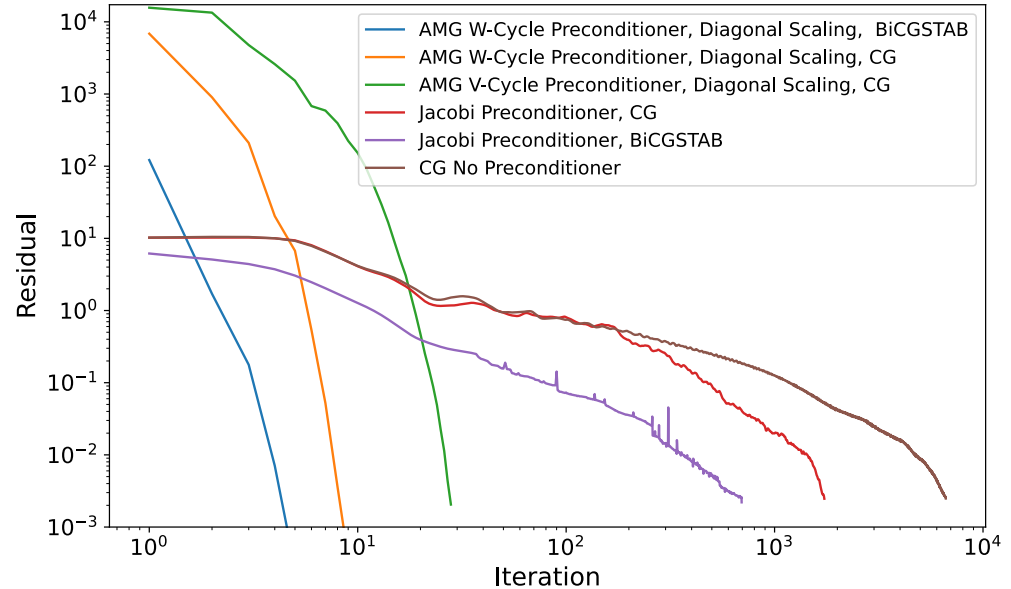
Multigrid Acceleration of PuMA Solvers

Multigrid Poisson Solver

- Multigrid methods can be used to significantly accelerate the convergence of PuMA solvers
- An initial prototype multigrid solver has been implemented, utilizing the pyAMG library and SciPy linear solvers
- Improved implementation is ongoing for the PuMA Poisson solver, allowing for multigrid acceleration to be used for large image-based simulations with only a slight increase in memory requirements over the legacy solver



Example V cycle and W cycle for a multigrid solver



Solver convergence for voxel isotropic conductivity solver in PuMA, demonstrating the significant solver performance improvement of multigrid preconditioning.

PuMA Resources



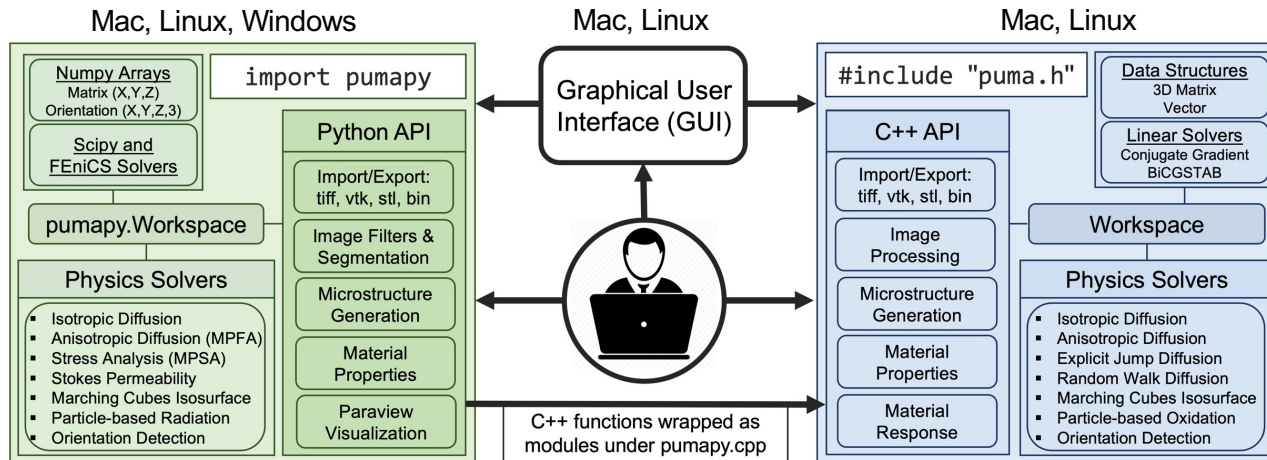
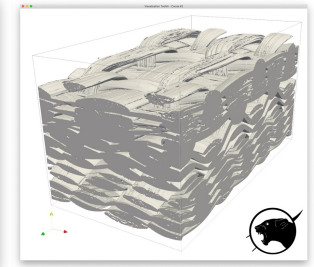
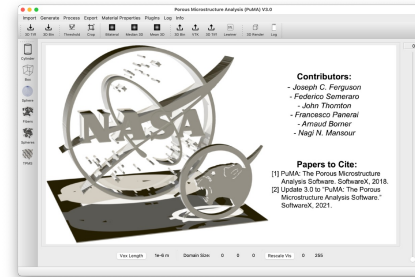
Installation: `conda install -c conda-forge puma`

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](#)



Youtube Channel



https://www.youtube.com/channel/UCBp_QC6ctwzdyxfZn7uHj0w/videos

PuMA: Porous Microstructure Analysis
61 subscribers

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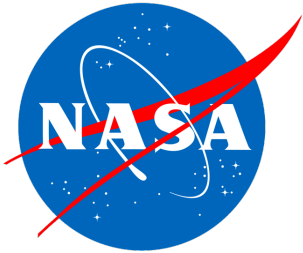
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The PuMA YouTube channel includes tutorials for all major software functionalities

Recent Developments to the Porous Microstructure Analysis (PuMA) software



Questions?



*Joseph C. Ferguson¹, Federico Semeraro¹, Arnaud Borner¹, Francesco Panerai²,
John M. Thornton¹, Sergio Fraile Izquierdo¹, Alexandre Quintart¹, Nagi N. Mansour^{1,2}*

¹ AMA Inc. at NASA Ames Research Center

² Dept. of Aerospace Engineering, University of Illinois at Urbana-Champaign

* joseph.c.ferguson@nasa.gov