



The Porous Microstructure Analysis (PuMA) software for high-temperature microscale modeling

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Overview



- Quick Description
- Motivation
- Capabilities
- Conclusions and Outlook

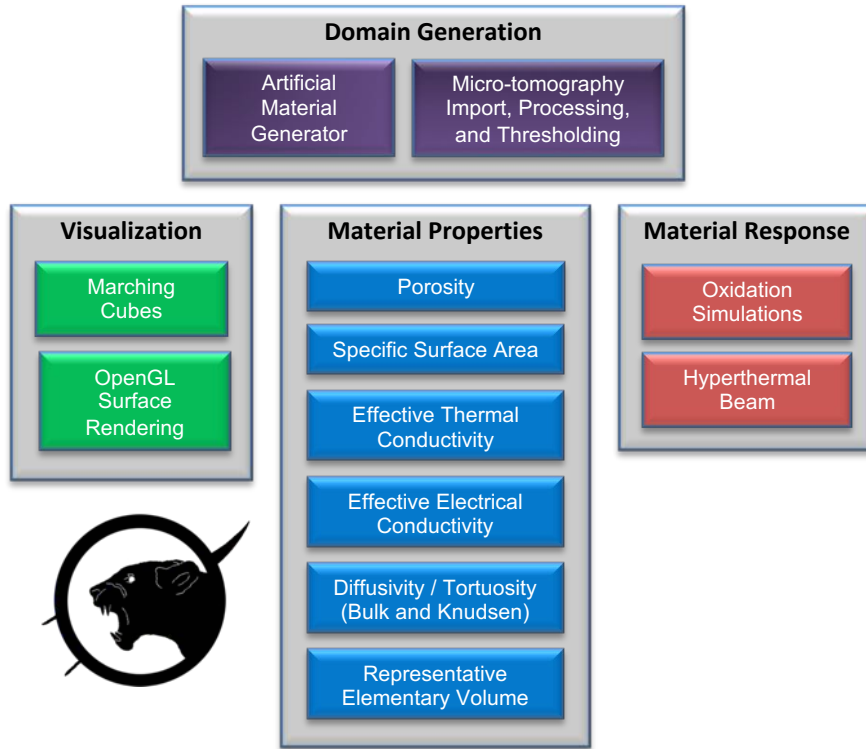


What is PuMA?



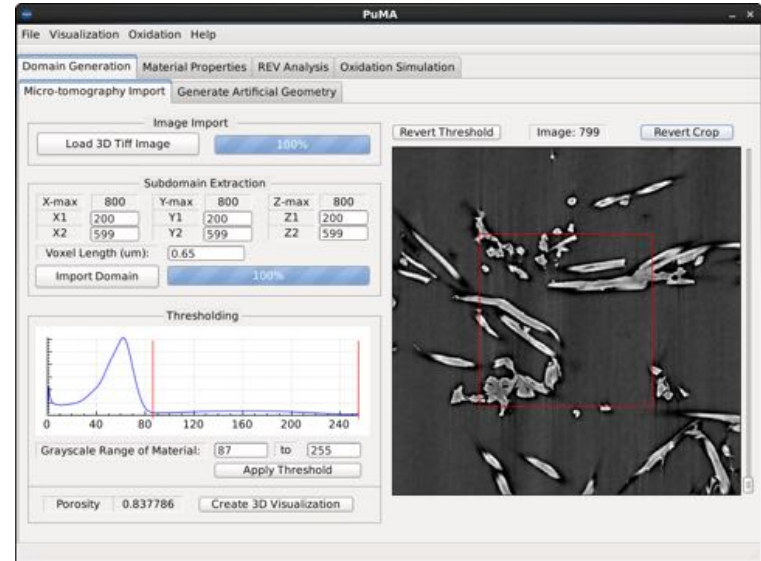
A collection of tools for the analysis of porous materials and generation of material microstructures

Porous Microstructure Analysis (PuMA)



Technical Specifications

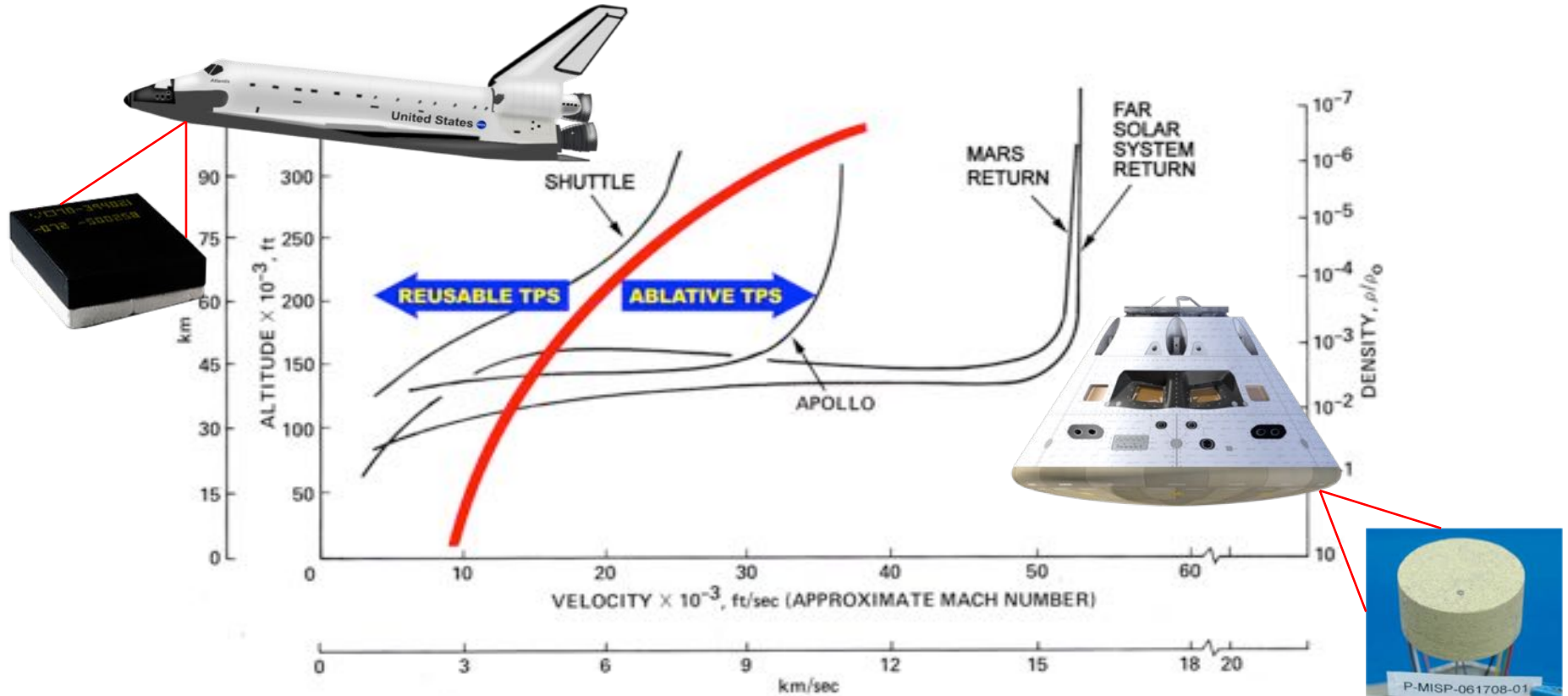
- Written in C++
- GUI built on QT
- Visualization module based on OpenGL
- Parallelized using OpenMP for shared memory systems





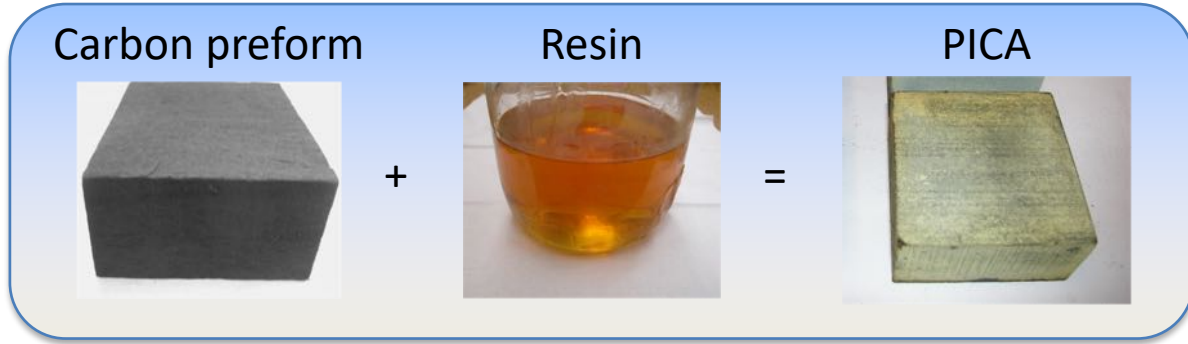
Motivation

Thermal Protection Systems (TPS)



NASA TM 101055, 1989

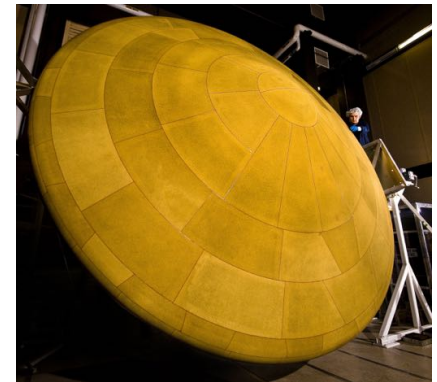
Ablative Thermal Protection Systems



Stardust Capsule

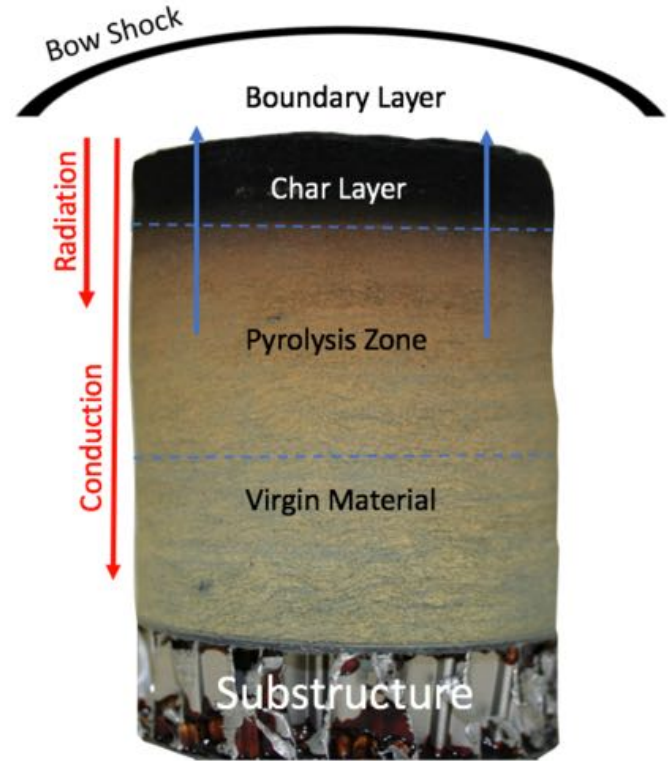
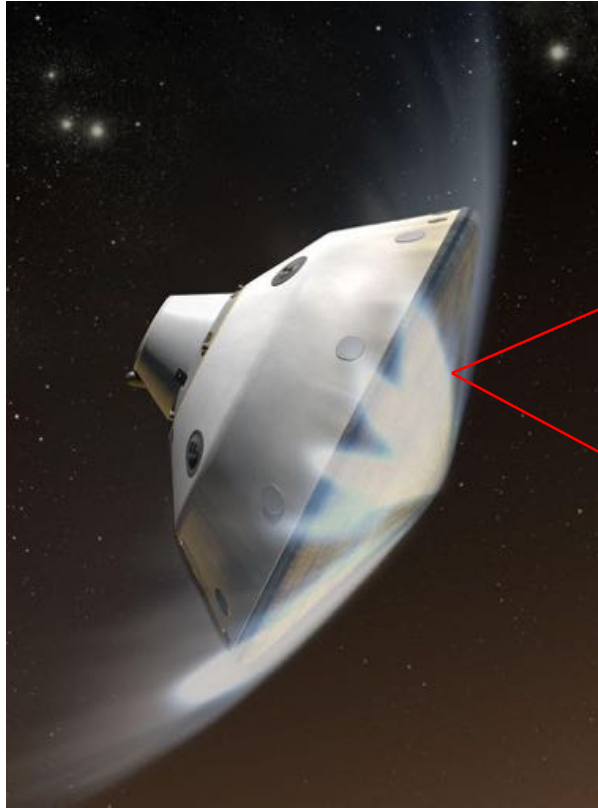


Dragon V1 & V2

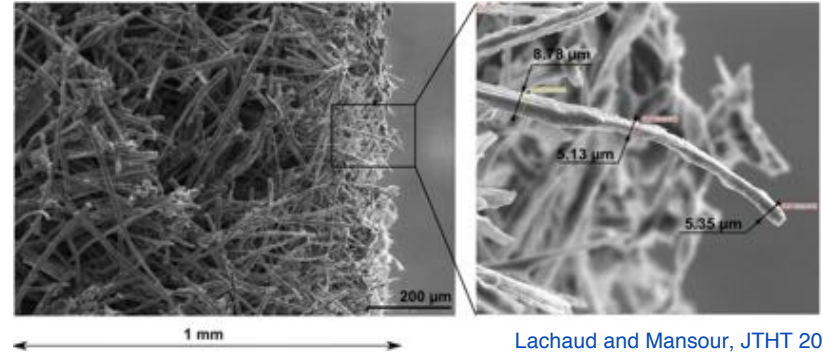
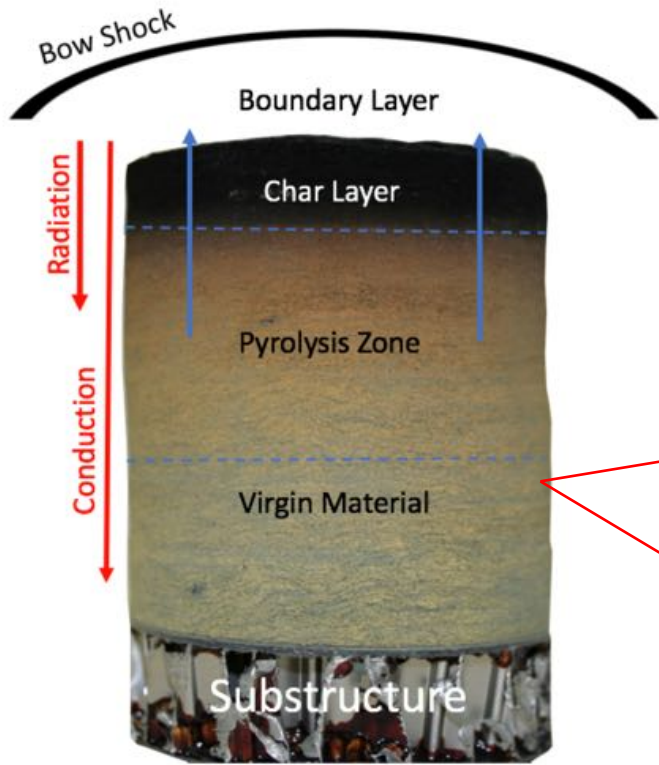


Mars Science Laboratory

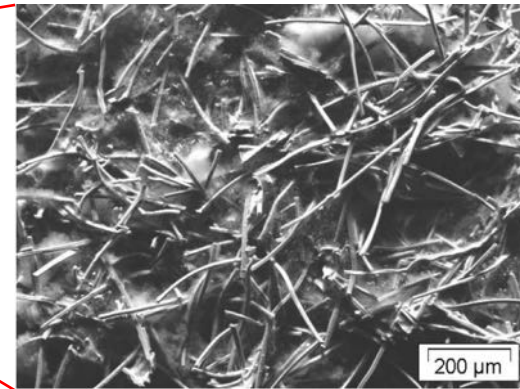
Material Design and Modeling



Material Design and Modeling



Lachaud and Mansour, JTHT 2013

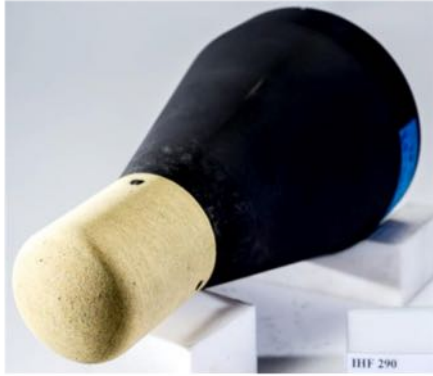


Lawson et. al. 2010

Material Design and Modeling



P. Agrawal et. al. 2016.



Virgin PICA Sample

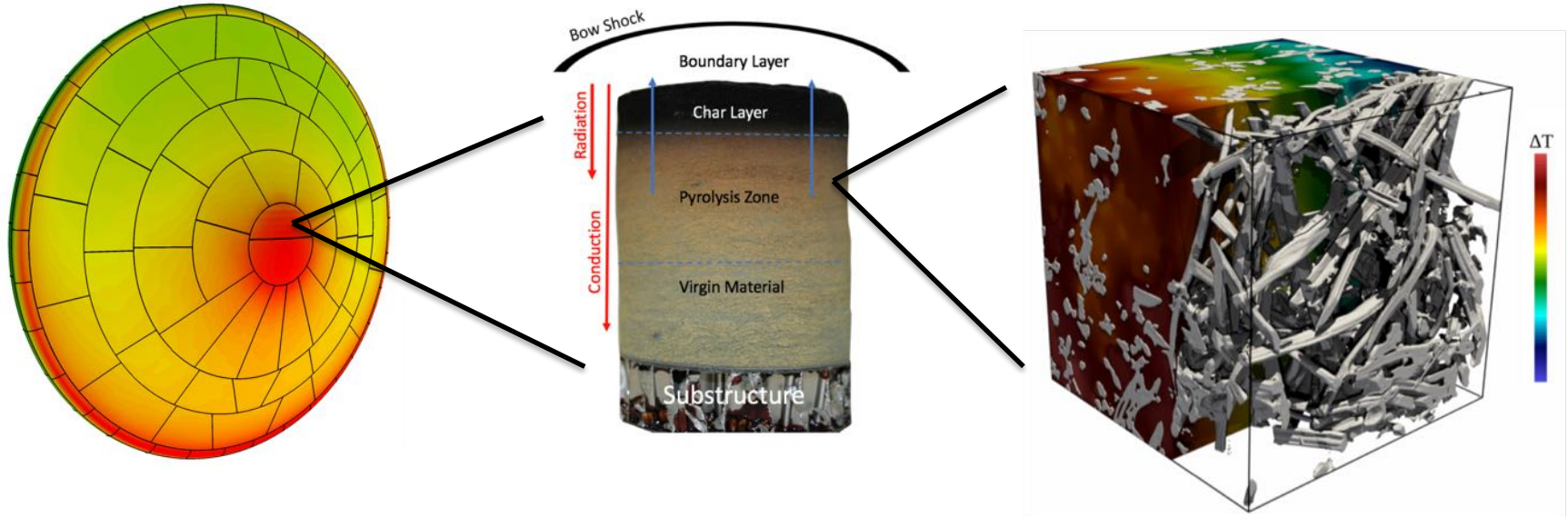


Charred PICA Sample



Arcjet Testing

Micro-scale modeling



1. Material Properties

1. Phenomenological Properties
2. Thermal transport
3. Mass transport

2. Material Decomposition

1. Oxidation
2. Sublimation
3. Spallation



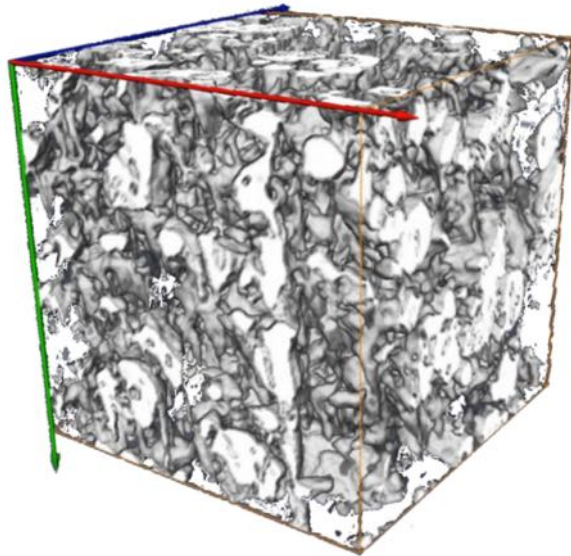
High fidelity characterization of heat shield materials in extreme environments is needed

Cannot be achieved with experiments alone

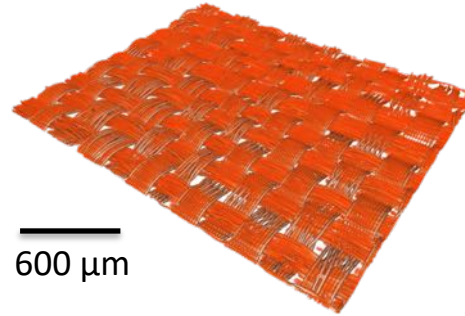
Other applications

- Main impact derives from the ubiquity of the underlying physics.

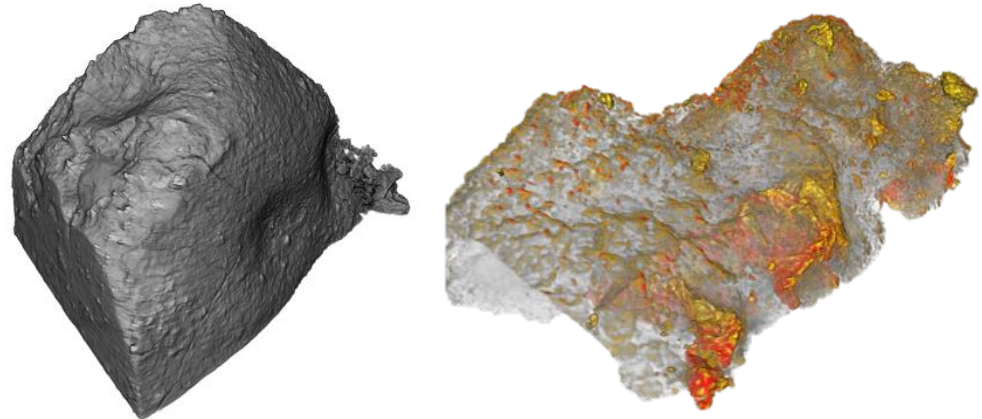
Plastic/Copper Composites



Parachute Materials



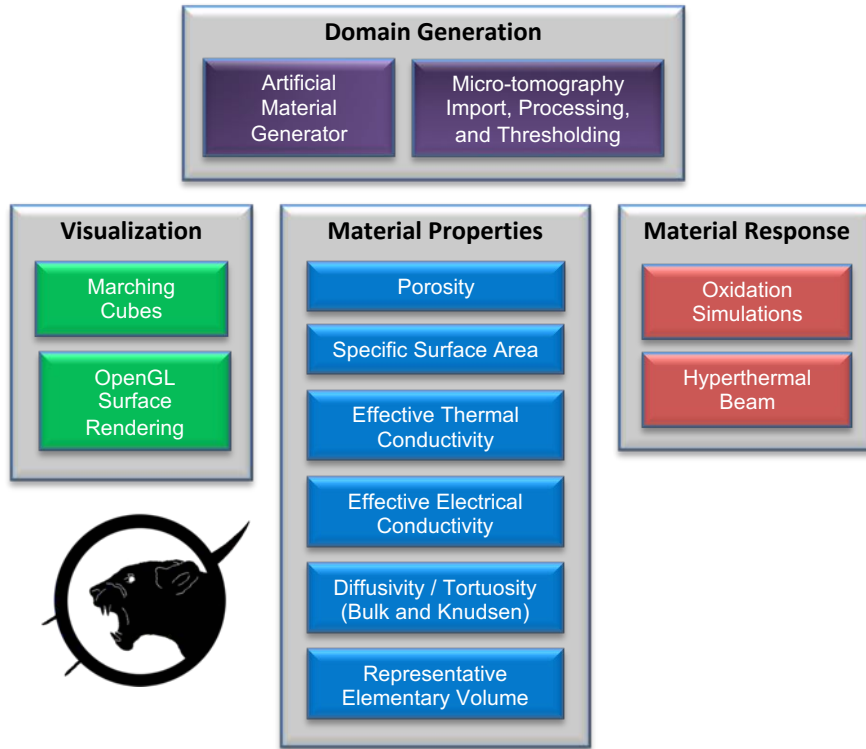
Meteorite Samples





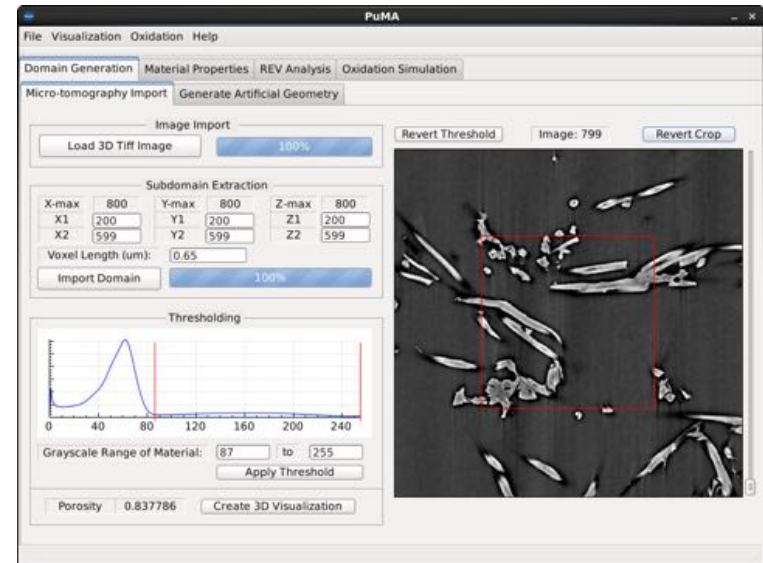
Capabilities

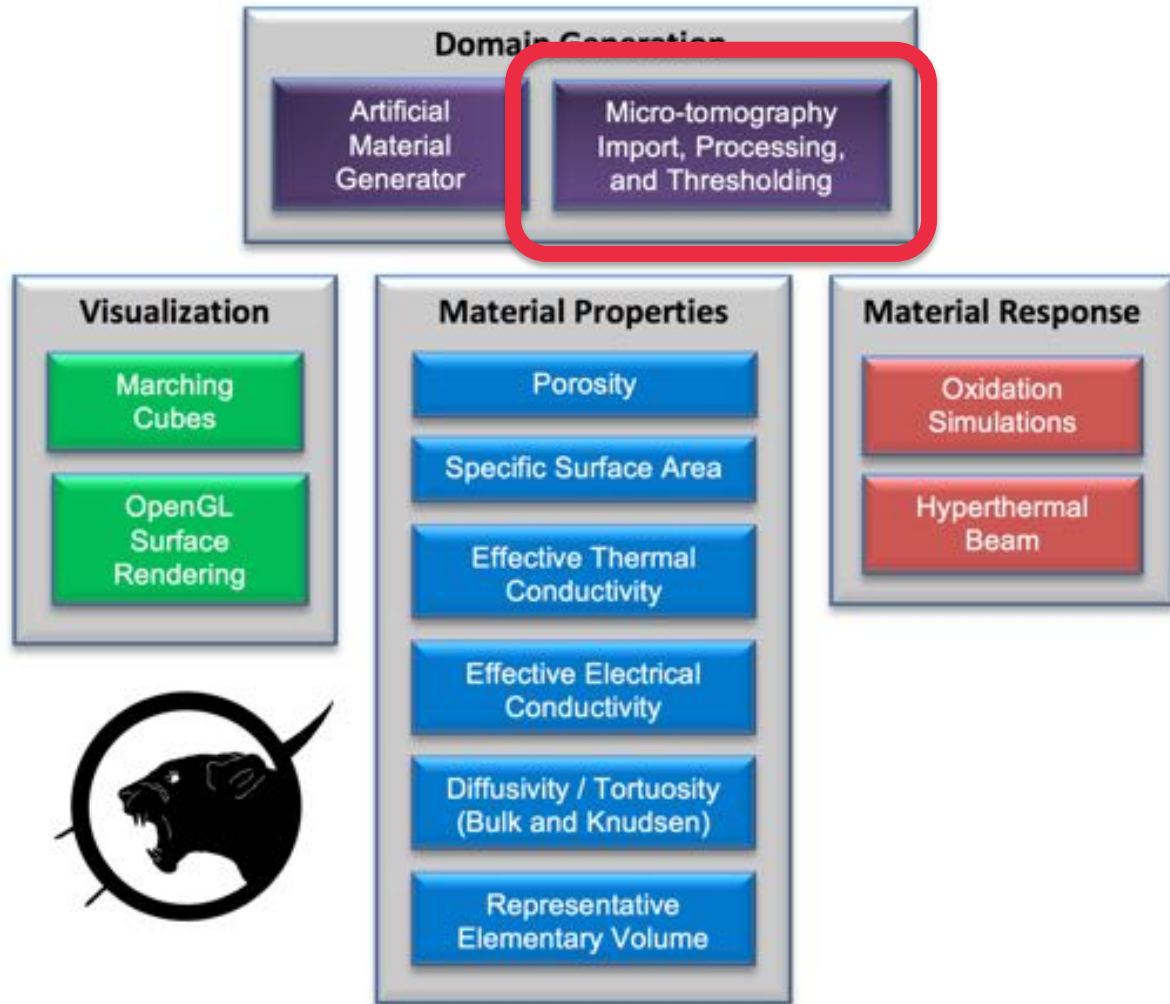
Porous Microstructure Analysis (PuMA)



Technical Specifications

- Written in C++
- GUI built on QT
- Visualization module based on OpenGL
- Parallelized using OpenMP for shared memory systems

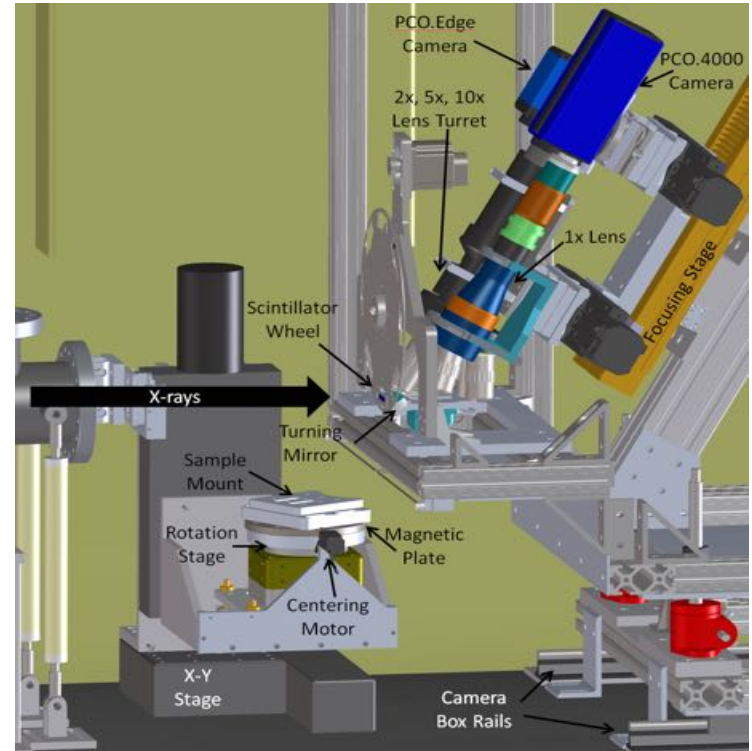




X-ray micro-tomography



- Advanced Light Source (ALS) at the Lawrence Berkeley Natl. Laboratory
- Synchrotron electron accelerator used to produce 14Kev X-rays
- Used for many research areas, including optics, chemical reaction dynamics, biological imaging, and **X-ray micro-tomography**.



<http://www2.lbl.gov/MicroWorlds/ALSTool>

Mansour et. al, A new approach to light-weight ablators analysis: from micro-tomography measurements to statistical analysis and modeling, 44th AIAA Thermophysics. (2013)

X-ray micro-tomography

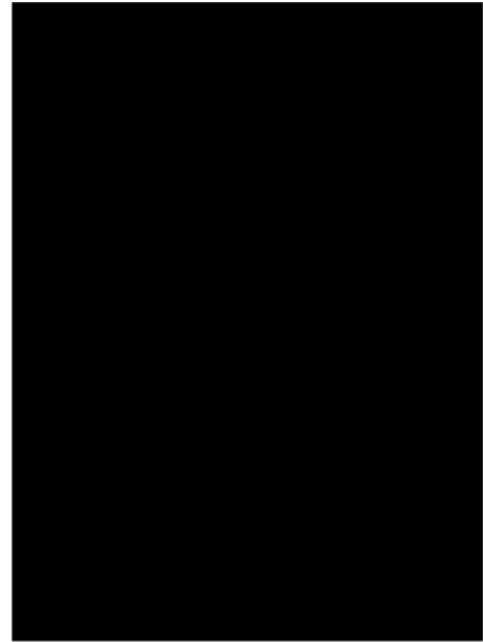
Collect X-ray images of the sample as you rotate it through 180°



Penetrating power

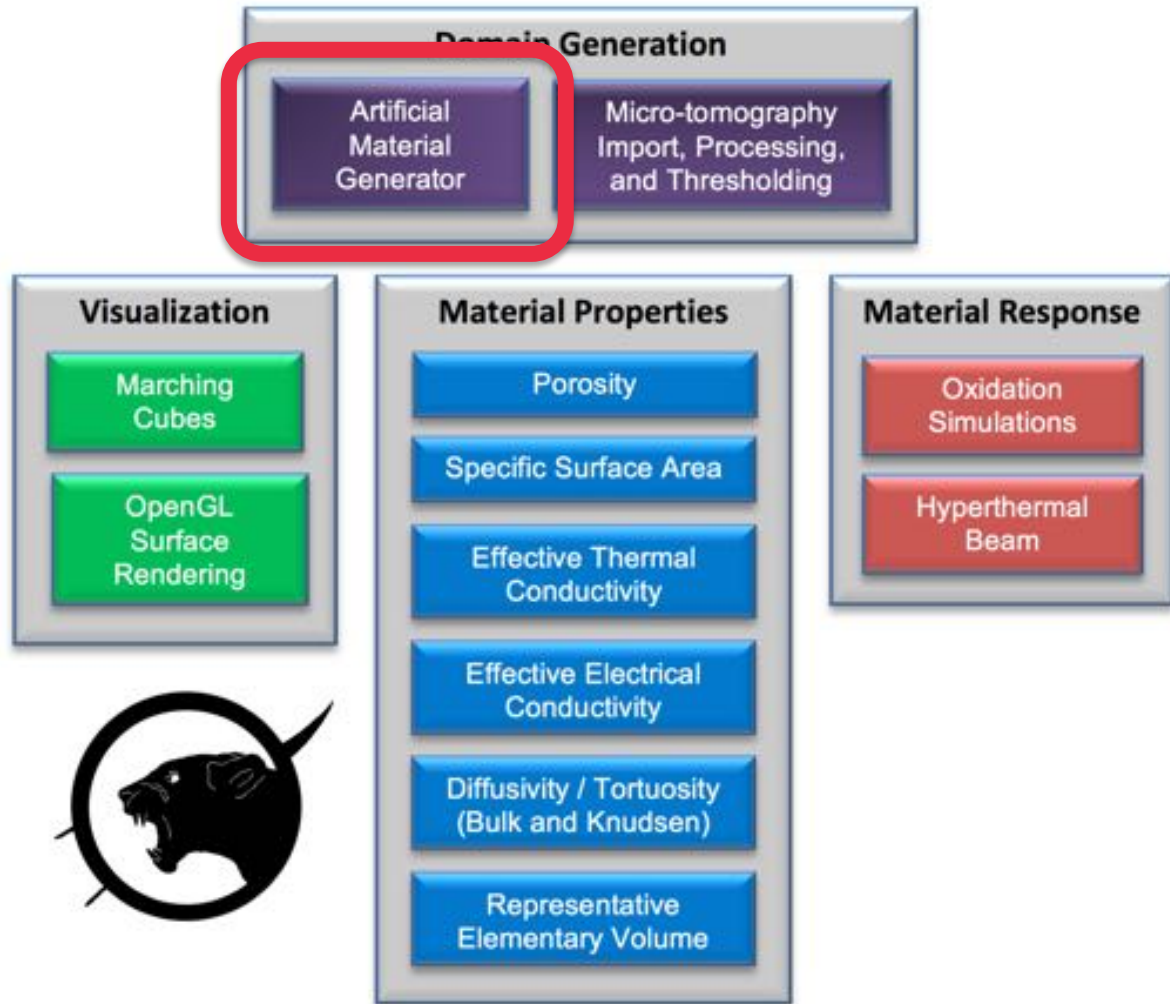
Multiple angles

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



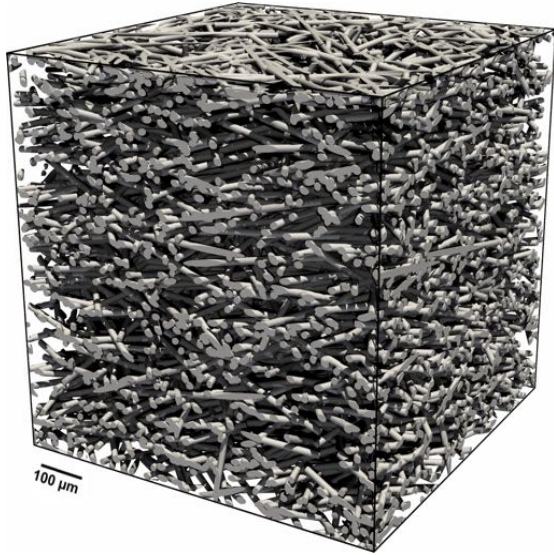
Courtesy of D. Parkinson (ALS)



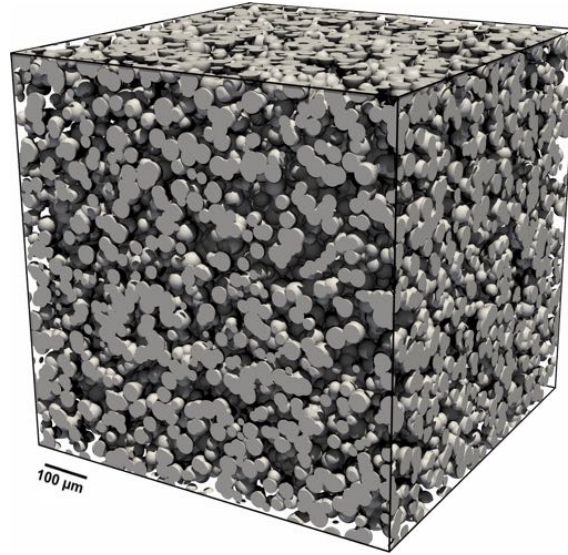


Material Generation

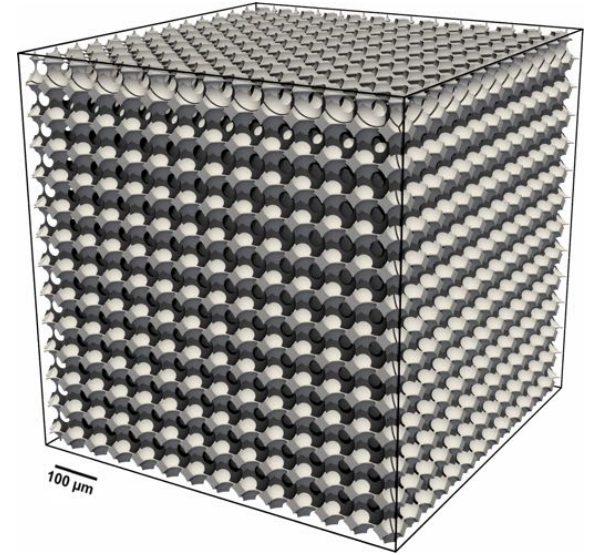
Random Fiber Structures



Packed Sphere Beds



Periodic Foams



Complex Fiber Generation



- Under Development for PuMA V3
- Capable of generating:
 - Curved fibers
 - Hollow fibers
 - Fibers with complex cross sections
- Degree of randomness can be specified to each of these parameters

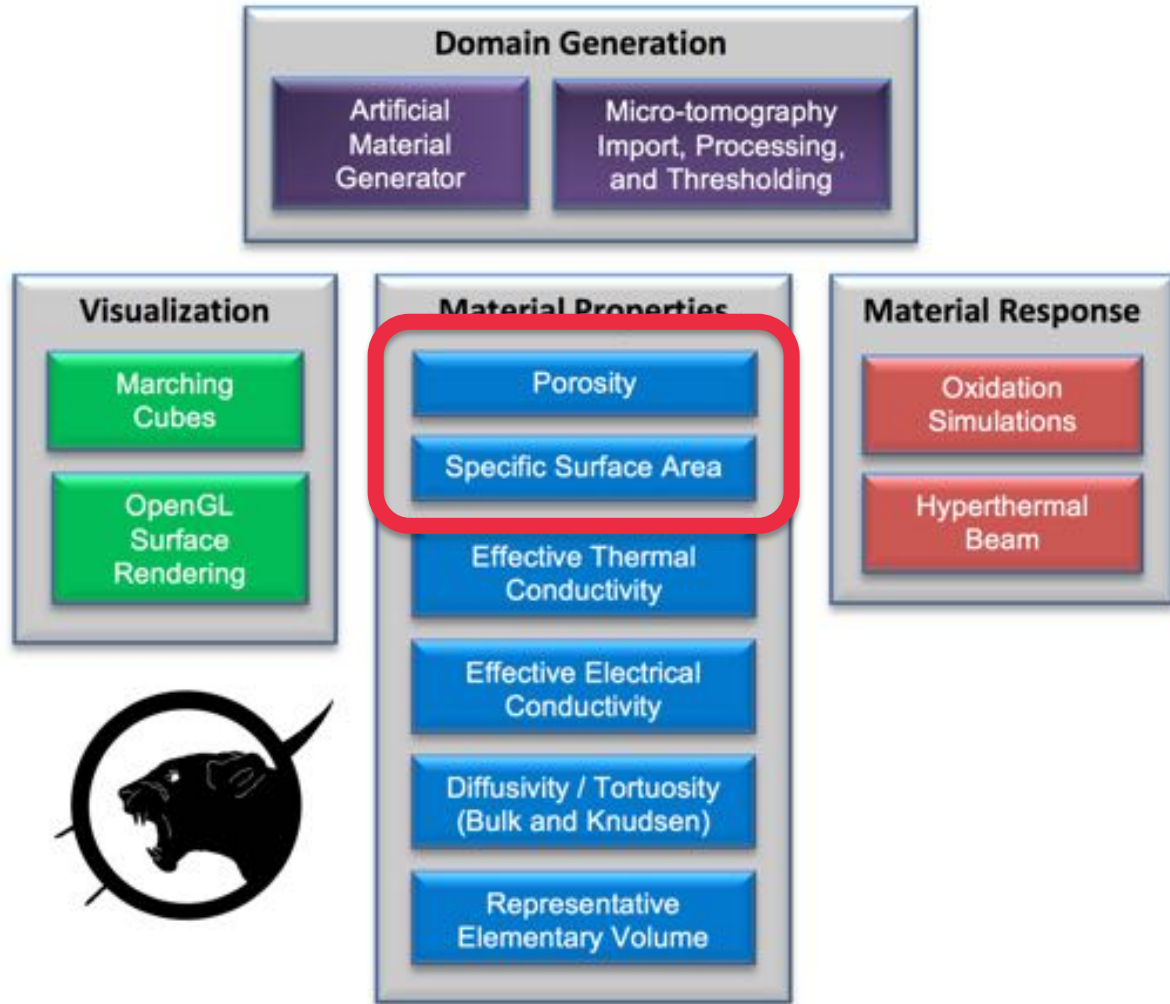


Weave Generation



- Under Development for PuMA V3
- TexGen library fully integrated





Effective Material Properties

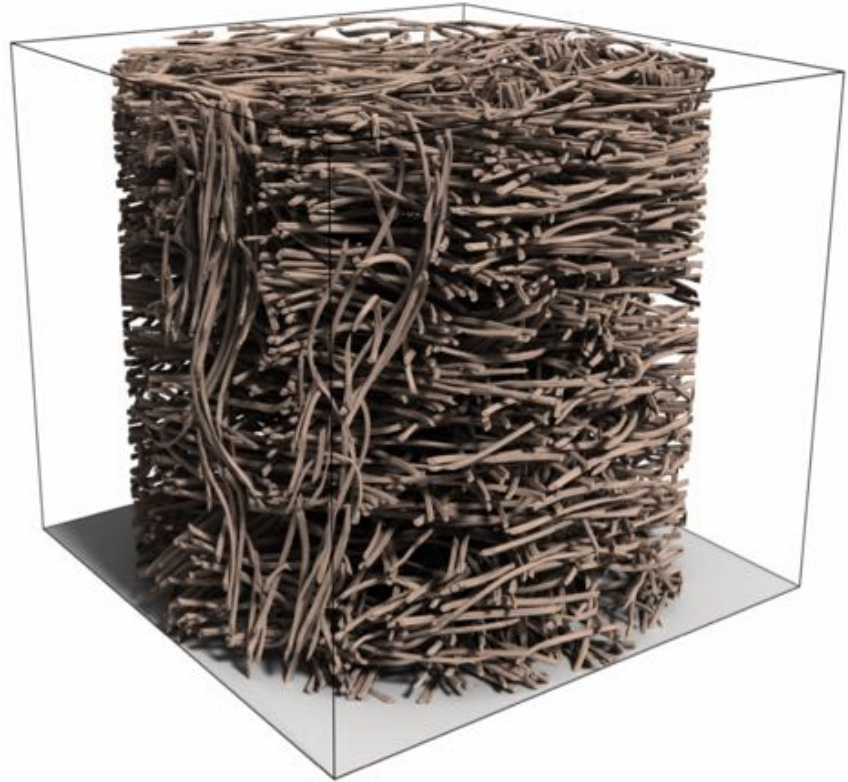


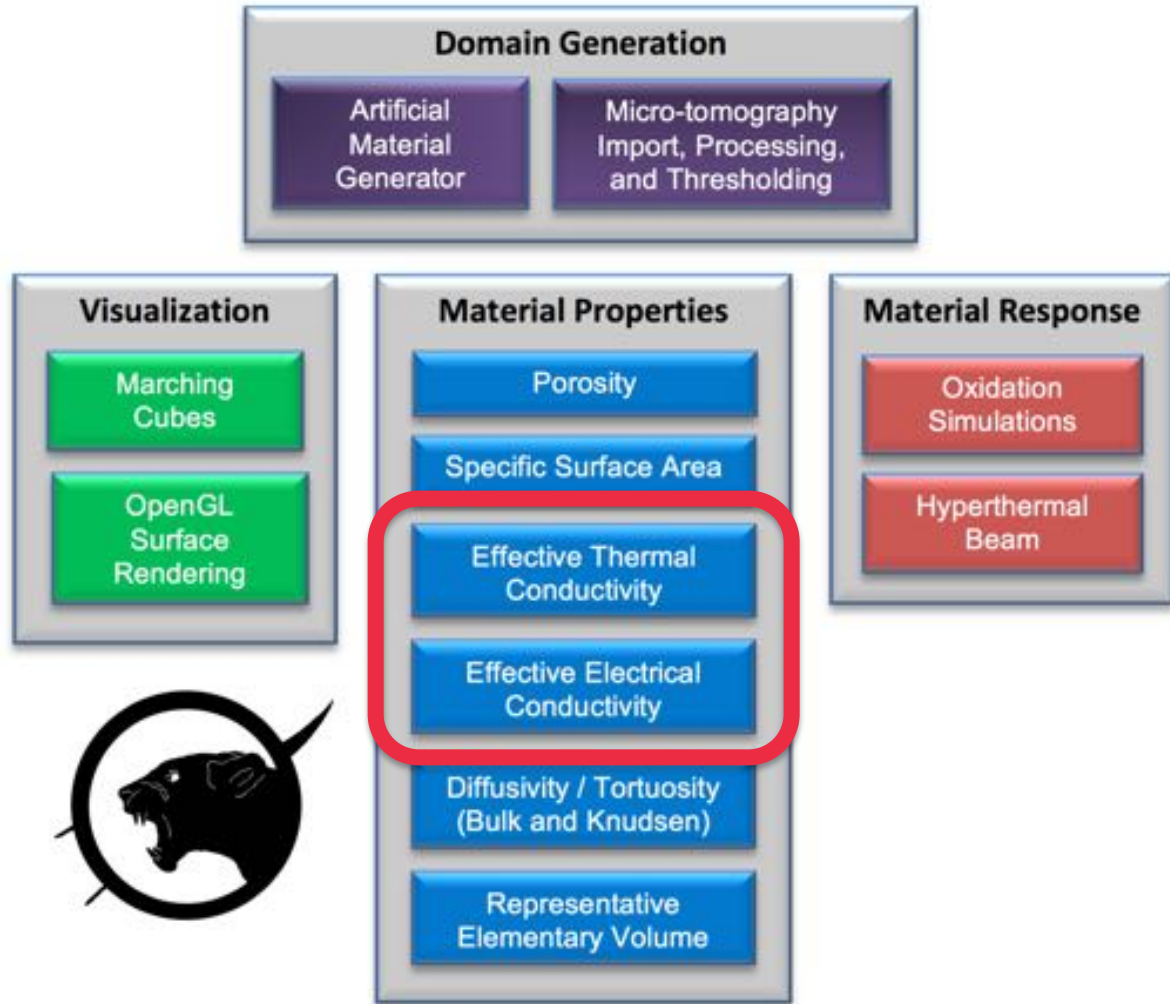
Porosity

- Based on the grayscale threshold
- Sum of all void voxels over the total volume

Specific Surface Area

- Based on the Marching Cubes algorithm
- Overall surface area computed as a sum of individual triangle areas

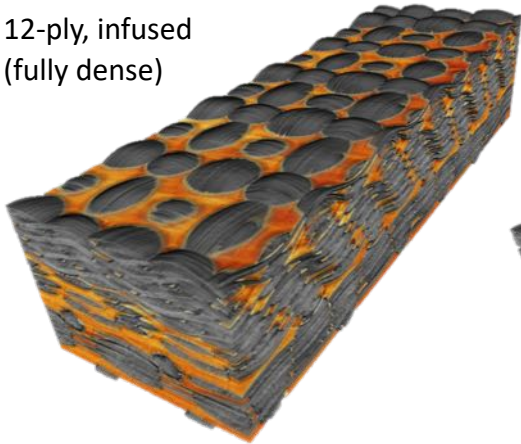




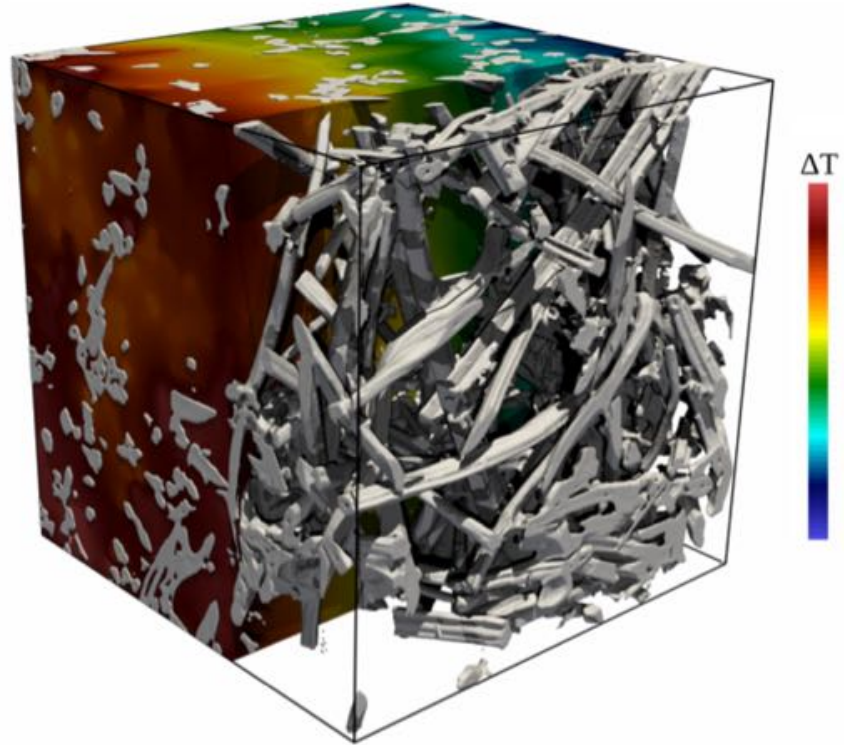
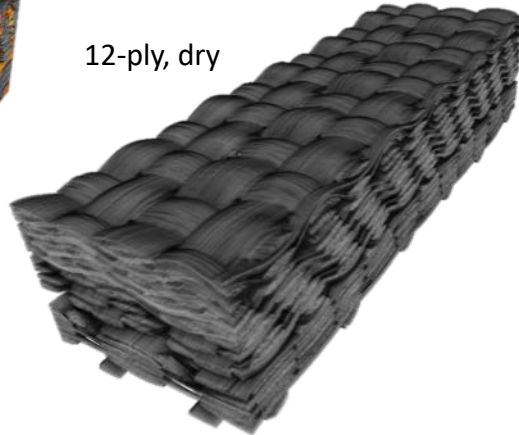
Effective Thermal Conductivity

- Computes effective thermal conductivity using a finite difference method [Weigmann, 2006]
- BicGStab iterative method and FFTW used to solve linear system of equations [Sleijpen, 1993]
- Parallelized based on OpenMP
- Verified against complex analytical solutions

12-ply, infused
(fully dense)

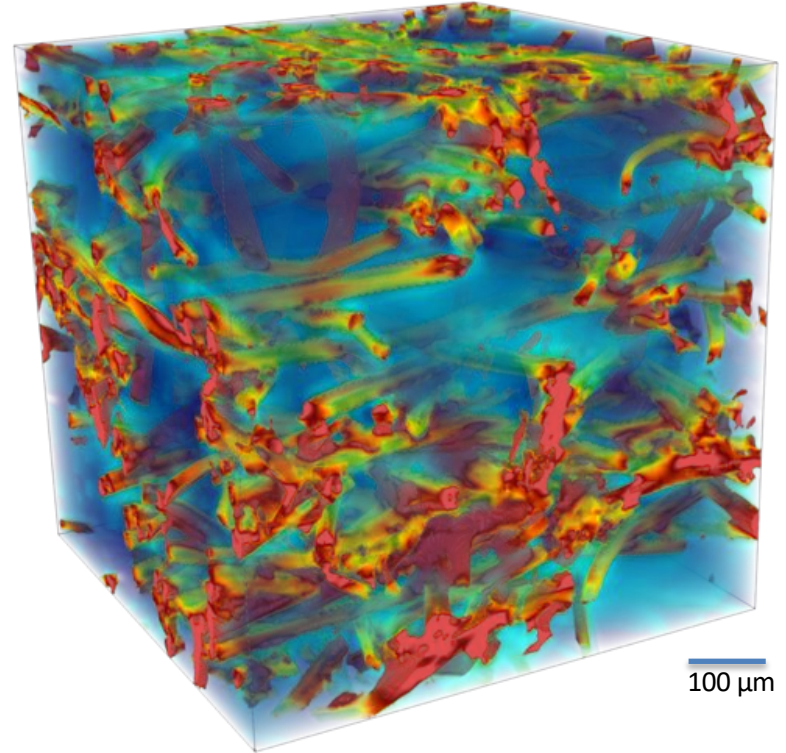


12-ply, dry



Effective Electrical Conductivity

- Computes effective electrical conductivity using a finite difference method [Weigmann, 2006]
- 1V voltage differential applied; solved with periodic boundary conditions
- BicGStab iterative method and FFTW used to solve linear system of equations [Sleijpen, 1993]
- Parallelized based on OpenMP
- Verified against complex analytical solutions
- Steady state current flow through a material can be determined

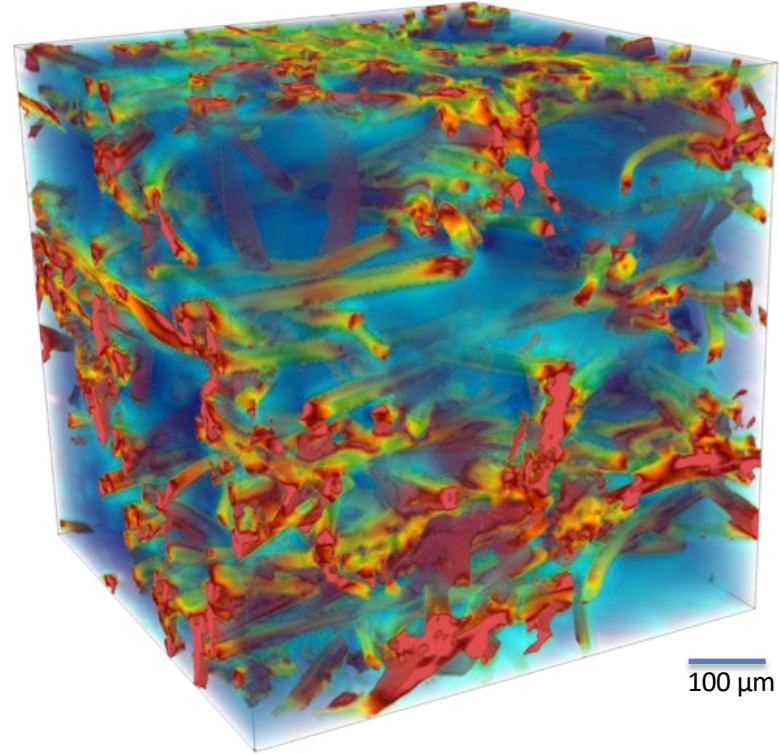


Steady state current flow through a carbon fiber material with an imposed voltage differential

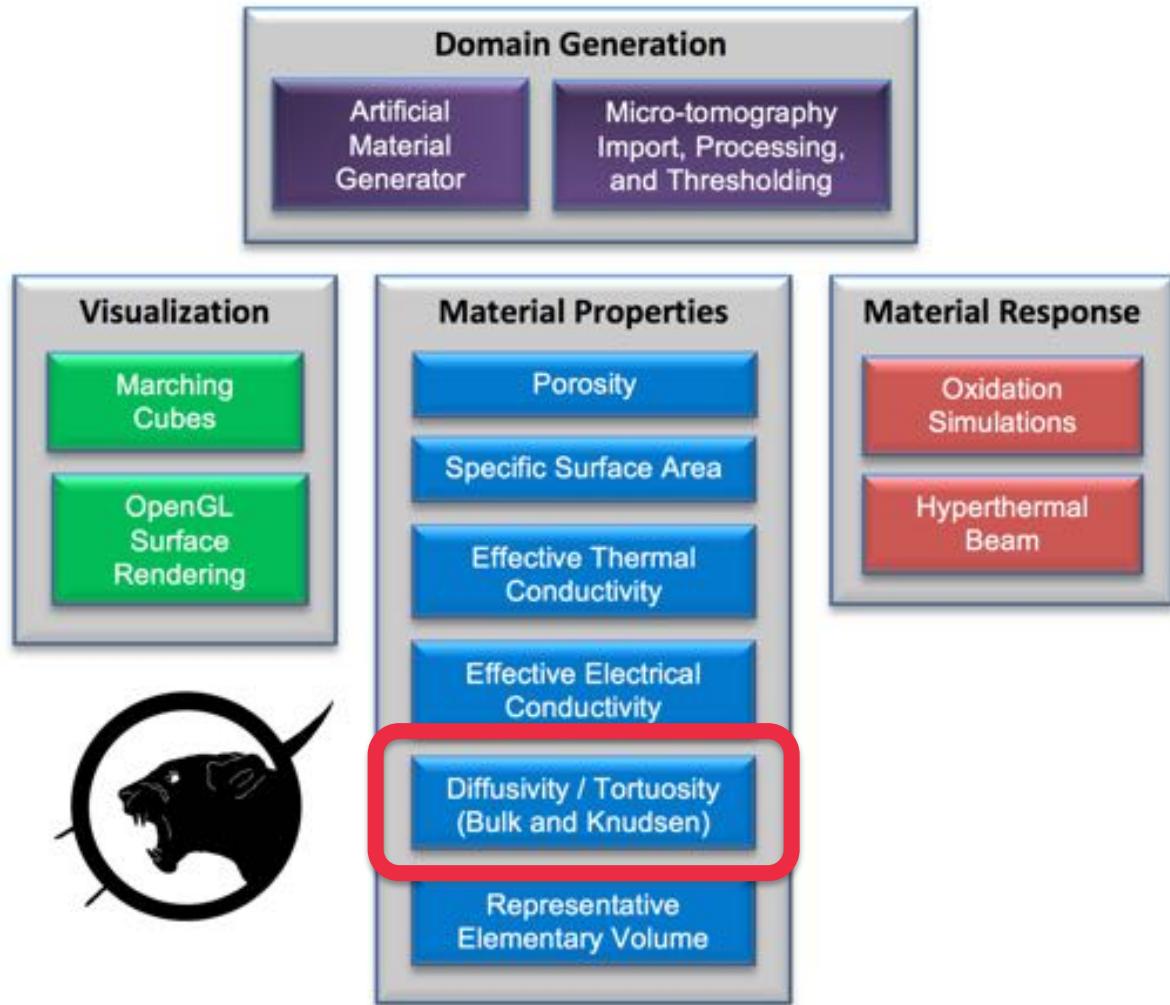
Anisotropic Thermal/Electrical Conductivity



- Allows for constituents with anisotropic thermal conductivities
- Method uses Multi-Point Flux Approximation (MPFA) which involves integrating over a control volume and enforcing continuity across separate interaction volume
- Solved with periodic boundary conditions
- Parallelized based on OpenMP
- Verified against complex analytical solutions



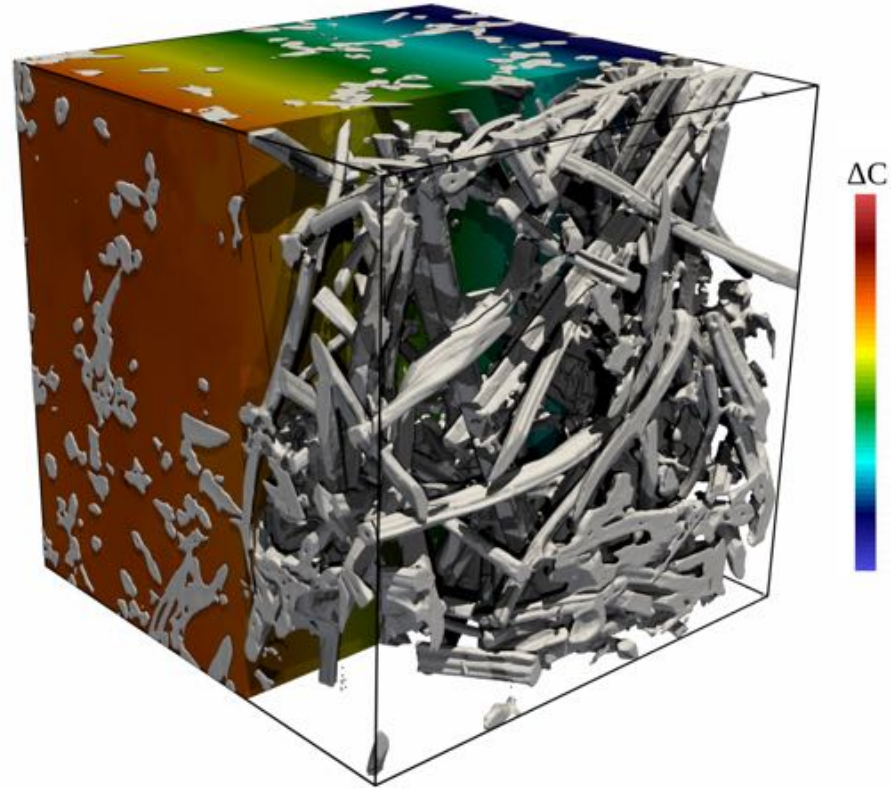
Steady state current flow through a carbon fiber material with an imposed voltage differential



Diffusivity / Tortuosity

Continuum

- Quantifies a materials resistance to a diffusive flux
- Solves for effective diffusivity using a finite difference method
- Valid for $Kn \ll 1$
- Solves diffusion equation using periodic boundary conditions



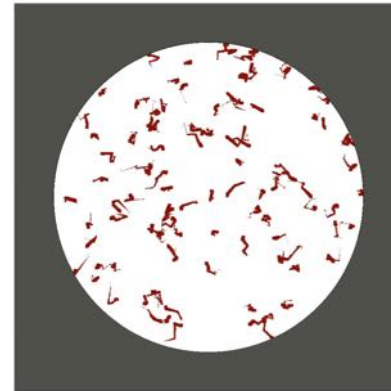
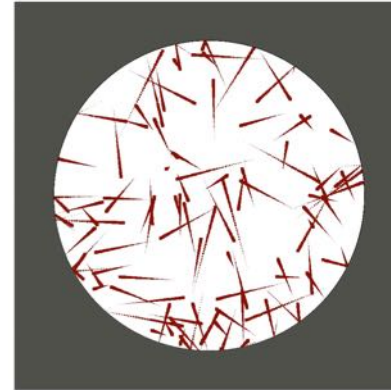
Diffusivity / Tortuosity – Random Walk

Transitional/Rarified

- Random walk method to simulate diffusion
- Mean square displacement method used to solve effective diffusion
- Valid for all Knudsen numbers.
- Knudsen number is varied by changing the molecular mean free path

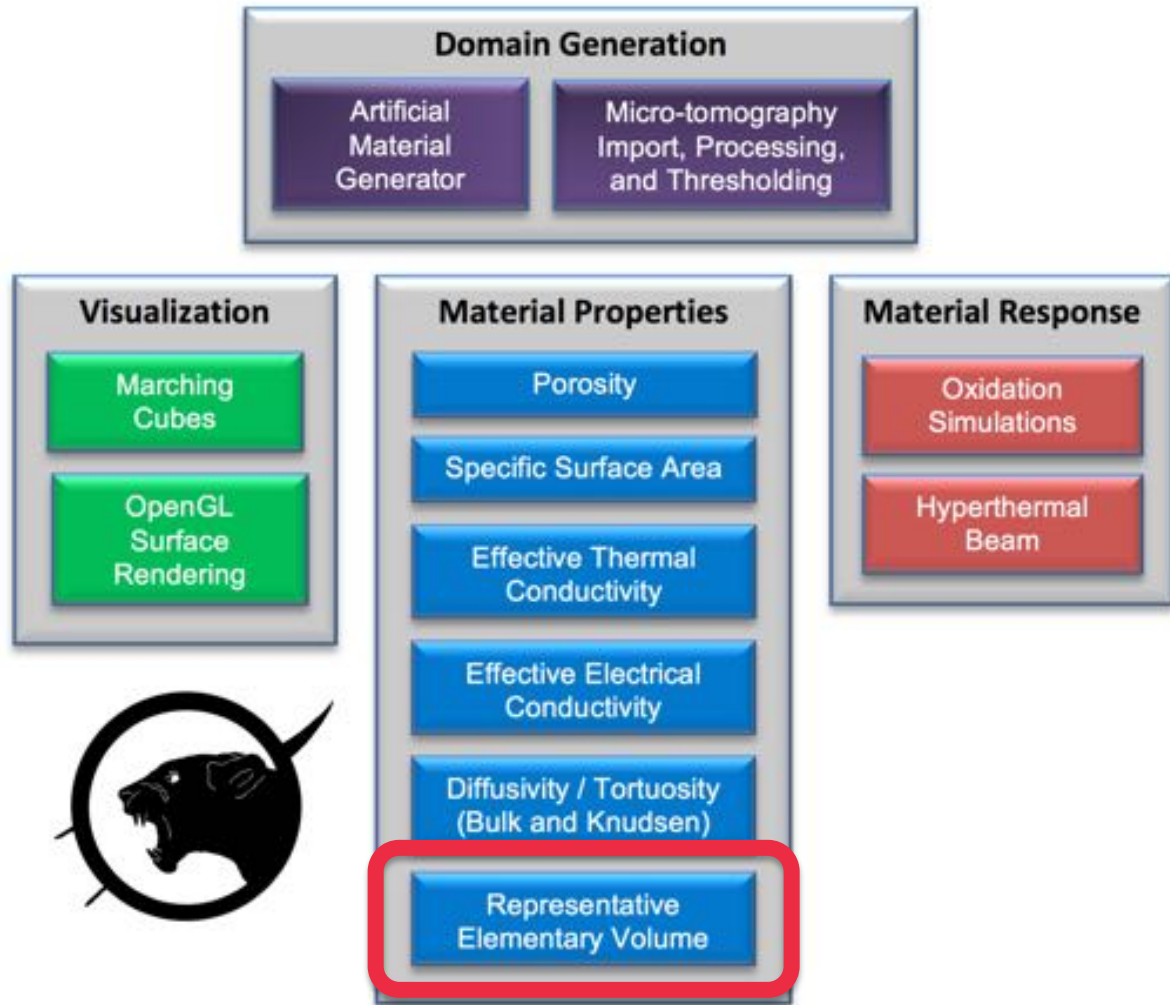
$$Kn = \frac{\bar{\lambda}}{\bar{d}} = \frac{\text{mean free path}}{\text{characteristic length}}$$

- Surface collisions based on marching cubes triangles with diffuse reflections used



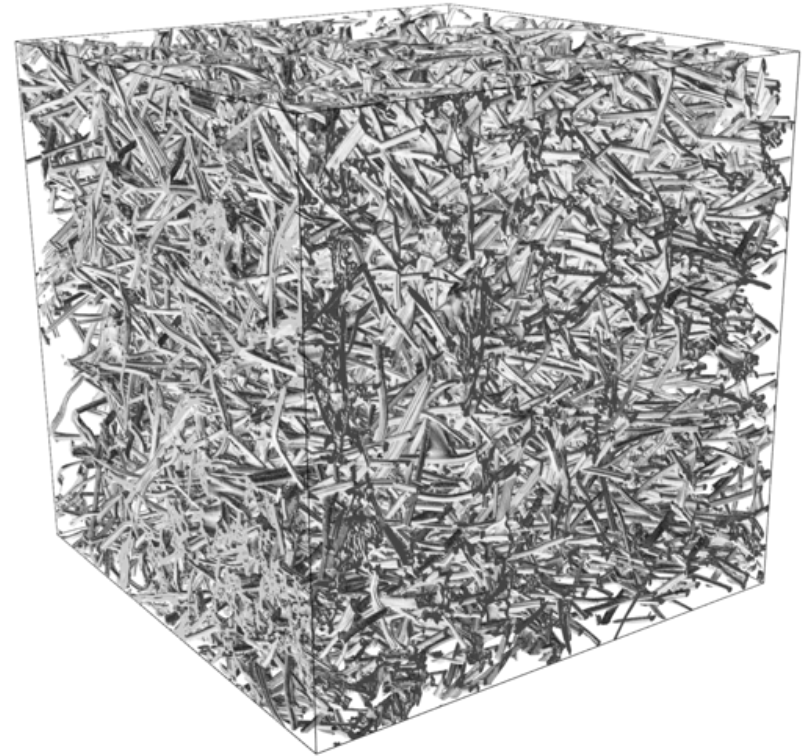
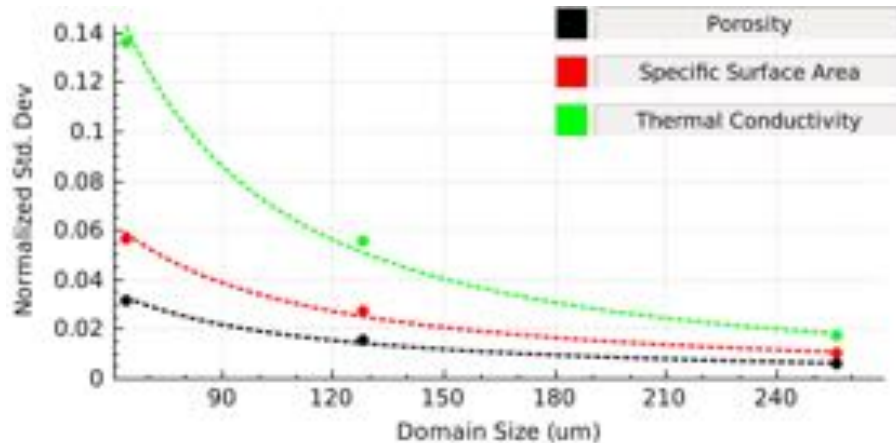
High Knudsen

Low Knudsen

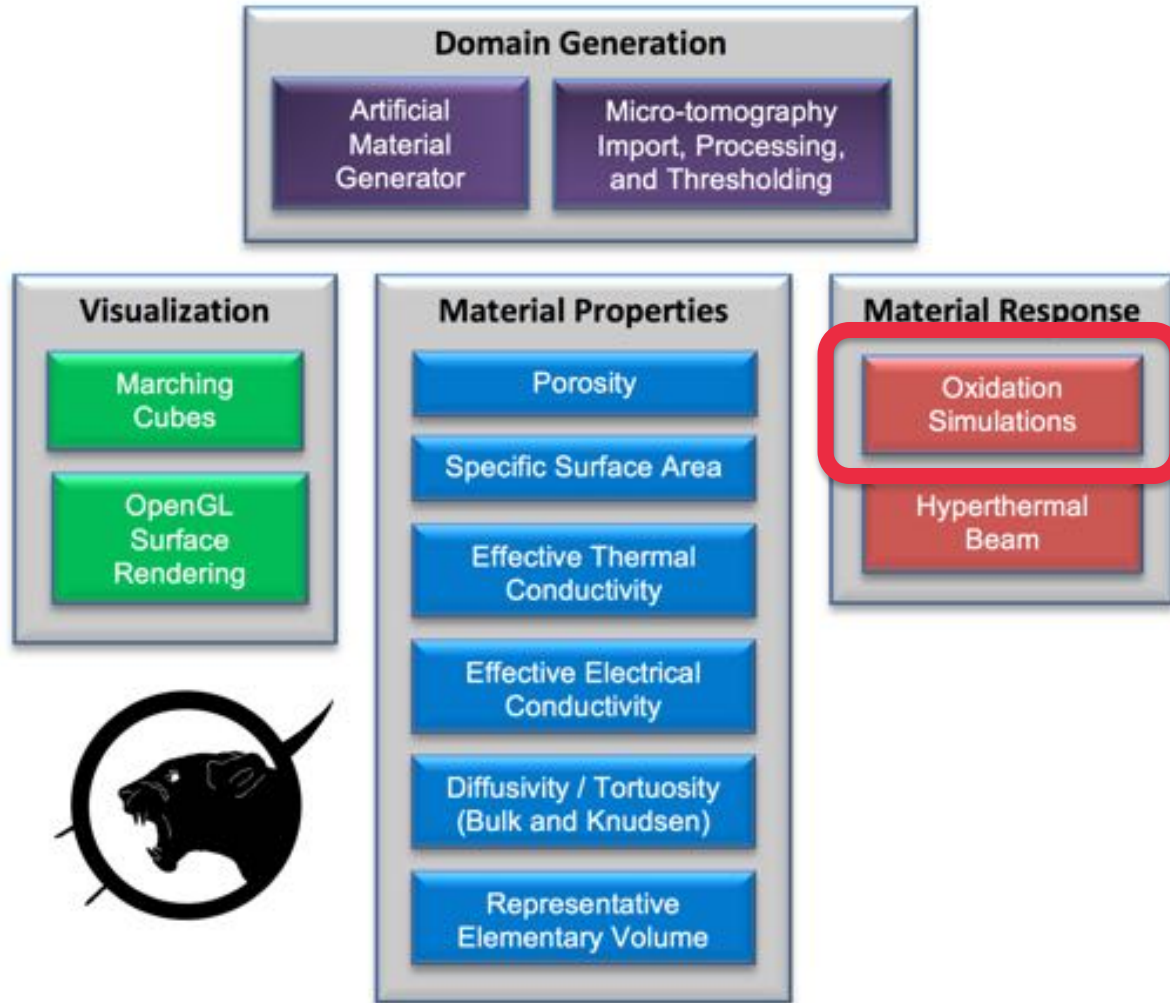


Representative Elementary Volume

- Defined in PuMA V2.1 as the size for which the std. dev. in a given property falls below a given threshold, usually 2%
- Power law used to interpolate/extrapolate REV
- Provides std. dev. of a given property as a function of sample size, helping to quantify the uncertainty in a calculation

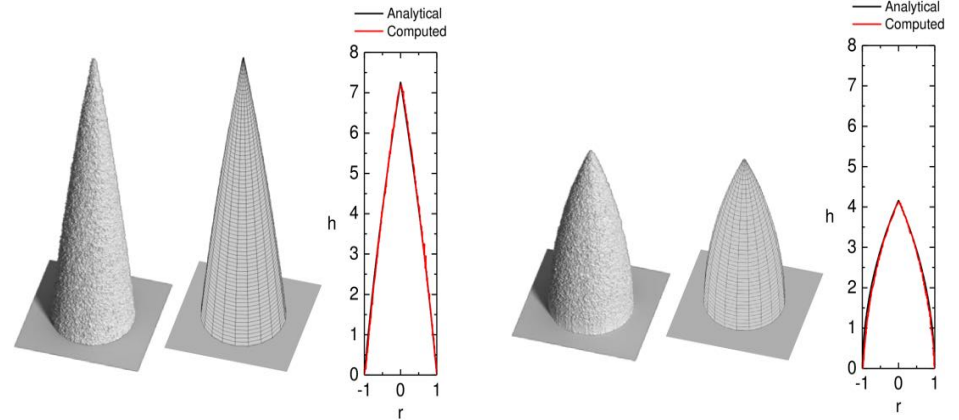
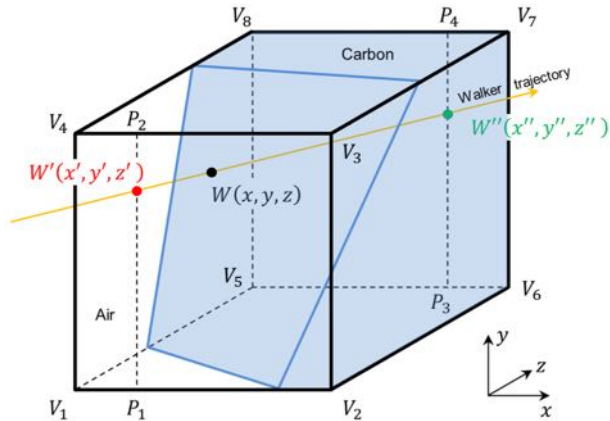
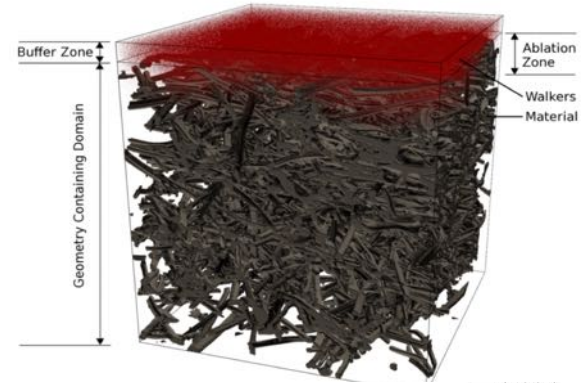


Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains \approx 500 million triangles.



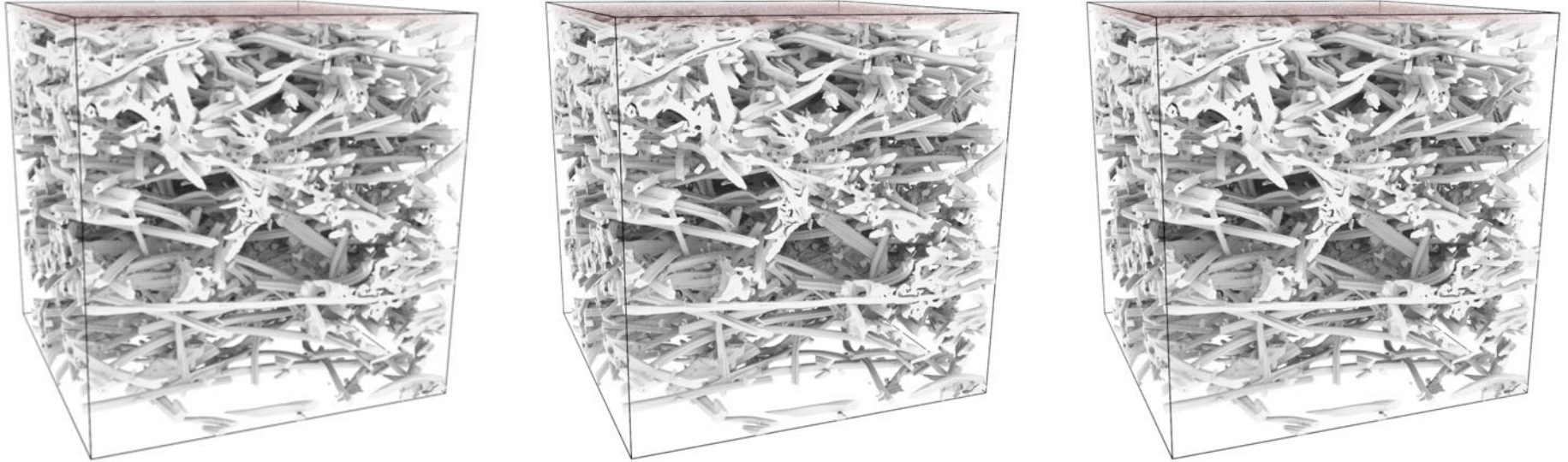
Micro-Scale Oxidation Simulations

- Particle-based oxidation method
- Diffusion simulated through random walks
- Collision detection with linear interpolation method
- Sticking probability method for material recession
- Verified against analytical solutions for single fiber



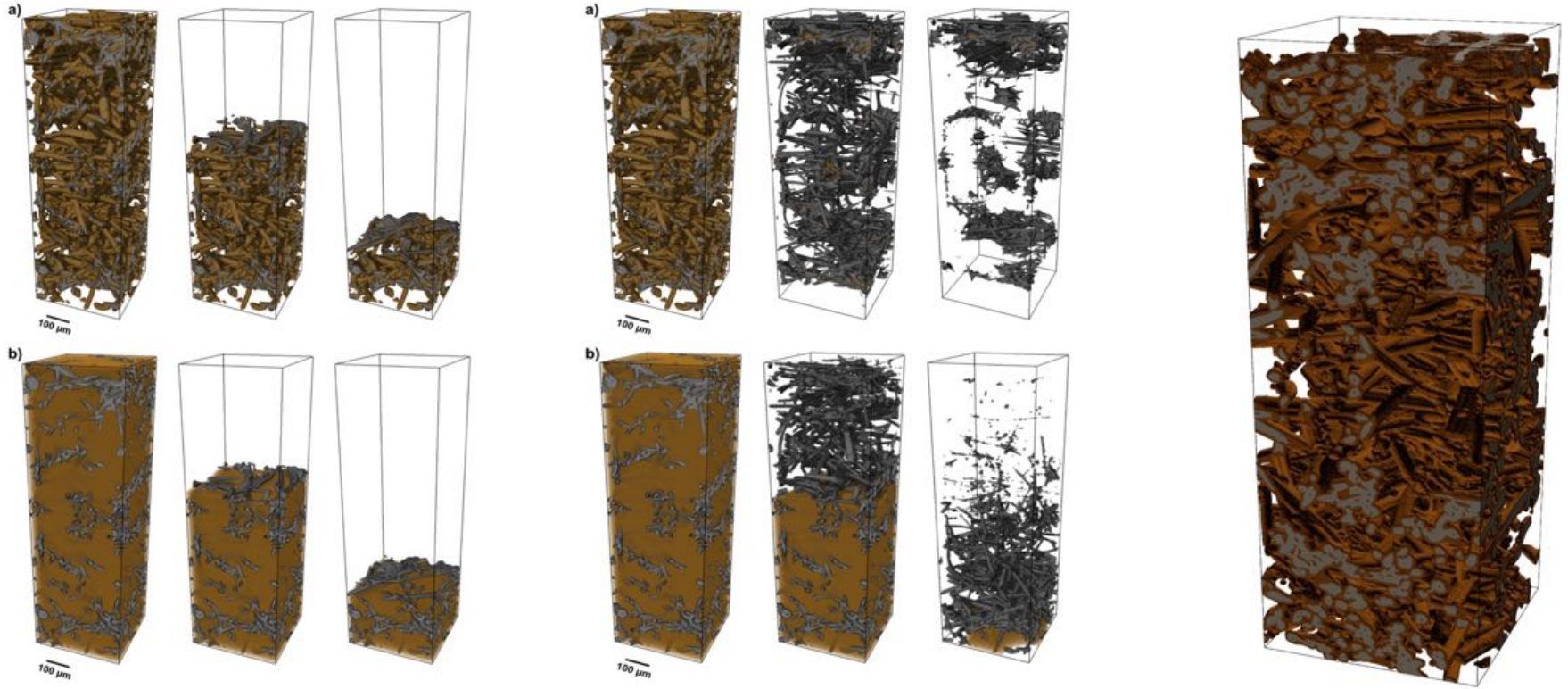


Micro-Scale Oxidation Simulations



Ferguson et. al, Modeling the oxidation of low-density carbon fiber materials based on micro-tomography, *Carbon*. (2016).
Ferguson et. al, Theoretical study on the micro-scale oxidation of carbon fiber materials, *Carbon*. (2017).

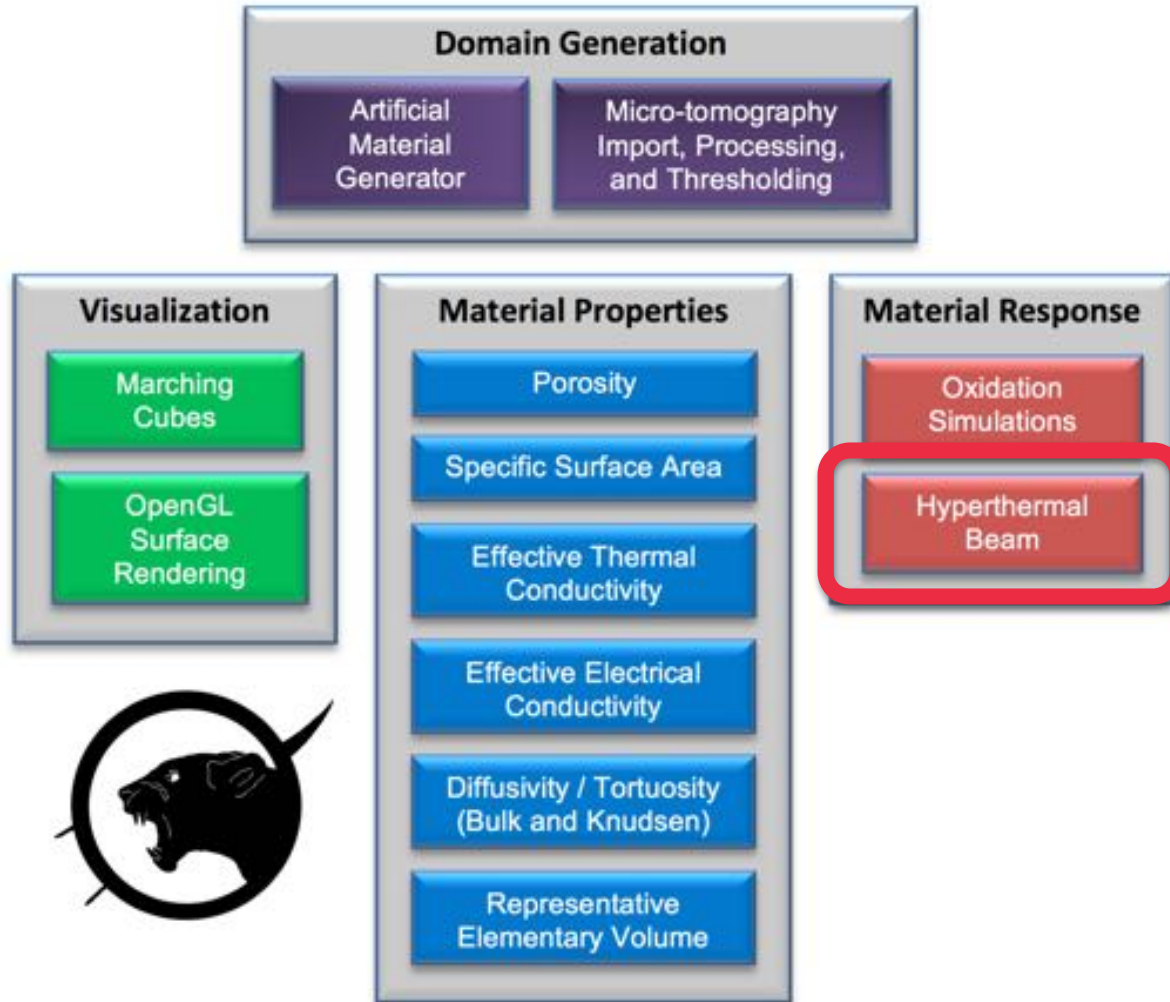
Micro-Scale Oxidation Simulations



Surface Ablation

Volume Ablation

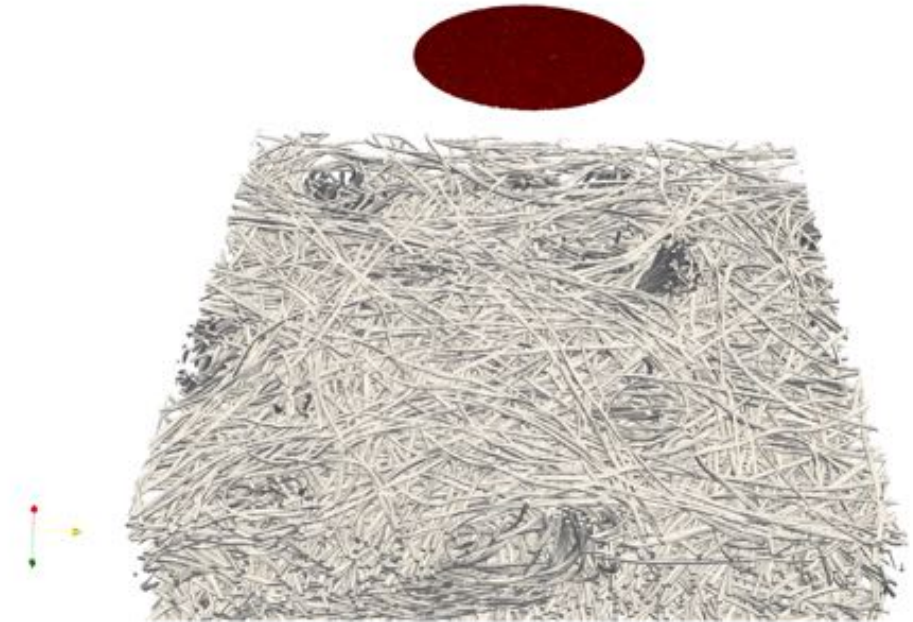
Ferguson et. al, Theoretical study on the micro-scale oxidation of carbon fiber materials, *Carbon*. (2017).



Molecular Beam Simulations

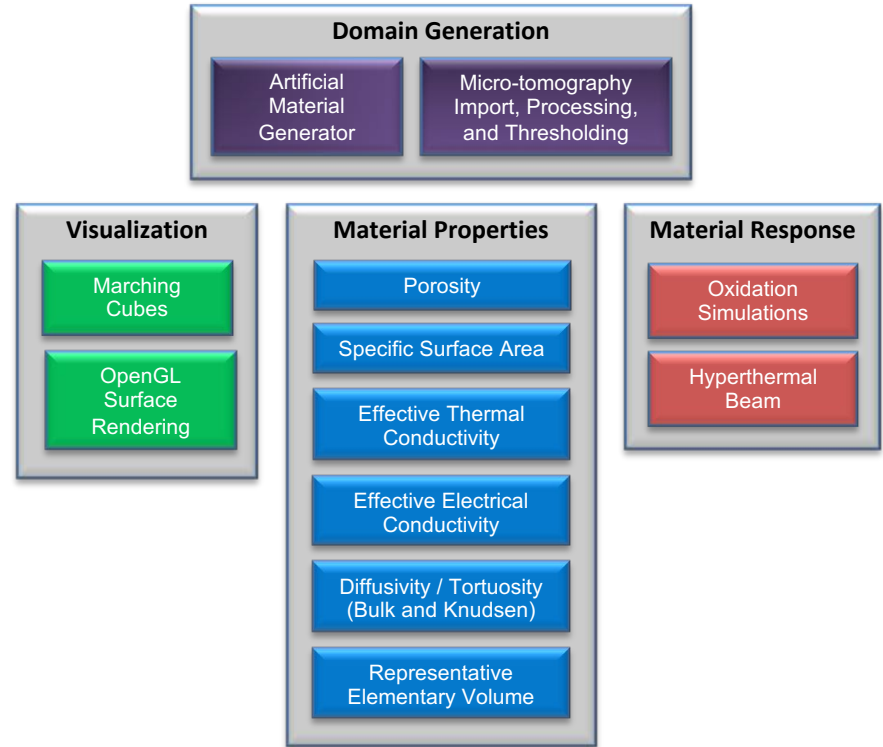


- Used in conjunction with molecular beam experiments [1] to calibrate finite rate chemistry models
- Particle-based method to solve transport of gas reactants and products
- Simulation of gas-surface collisions with complex, customizable reaction models
- Since particle-particle collisions are negligible, it provides a significant speed increase over DSMC simulations [2].



Conclusion and Outlook

- Future work will expand the material properties to include permeability and structural analysis
- Material generation will be expanded to allow realistic materials to be computationally designed, optimized over a set of characteristics
- **Need for good quality experimental data for model verification**



Microscale Modeling Research Group



Principle Investigator:



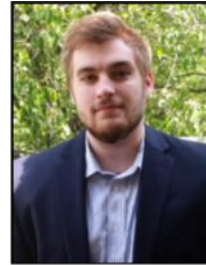
NN Mansour

Experimentalist:



F Panerai

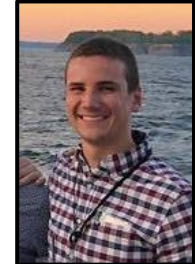
PuMA Development:



J Ferguson



F Semeraro



J Thornton

DSMC Development:



A Borner

X-Ray Microtomography:



A MacDowell



D Parkinson



H Barnard



Questions?

Point of Contact: John M. Thornton
john.m.thornton@nasa.gov

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InterPore 2019