https://ntrs.nasa.gov/search.jsp?R=20200000908 2020-03-28T19:05:39+00:00Z

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

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May 6th, 2019
InterPore 2019

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)

Domain Generation
- Artificial Material Generator
- Micro-tomography Import, Processing, and Thresholding

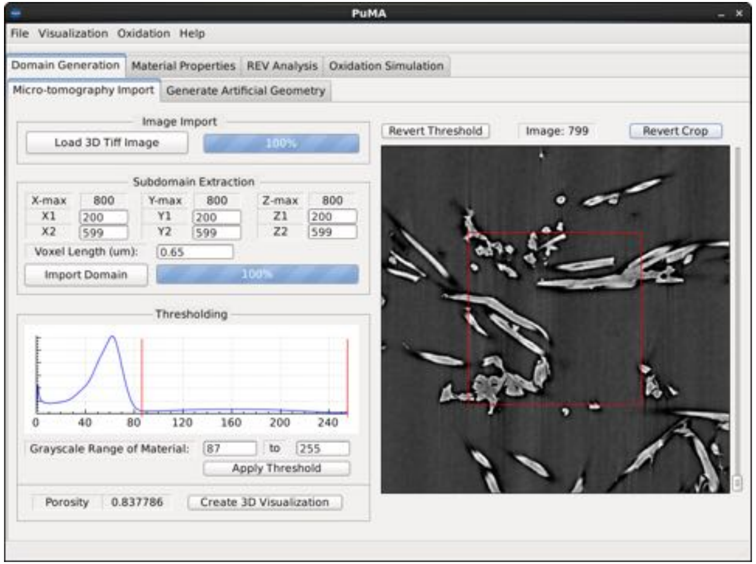
Visualization
- Marching Cubes
- OpenGL Surface Rendering

Material Properties
- Porosity
- Specific Surface Area
- Effective Thermal Conductivity
- Effective Electrical Conductivity
- Diffusivity / Tortuosity (Bulk and Knudsen)
- Representative Elementary Volume

Material Response
- Oxidation Simulations
- Hyperthermal Beam

Technical Specifications

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



X-max 800
X1 200
X2 599
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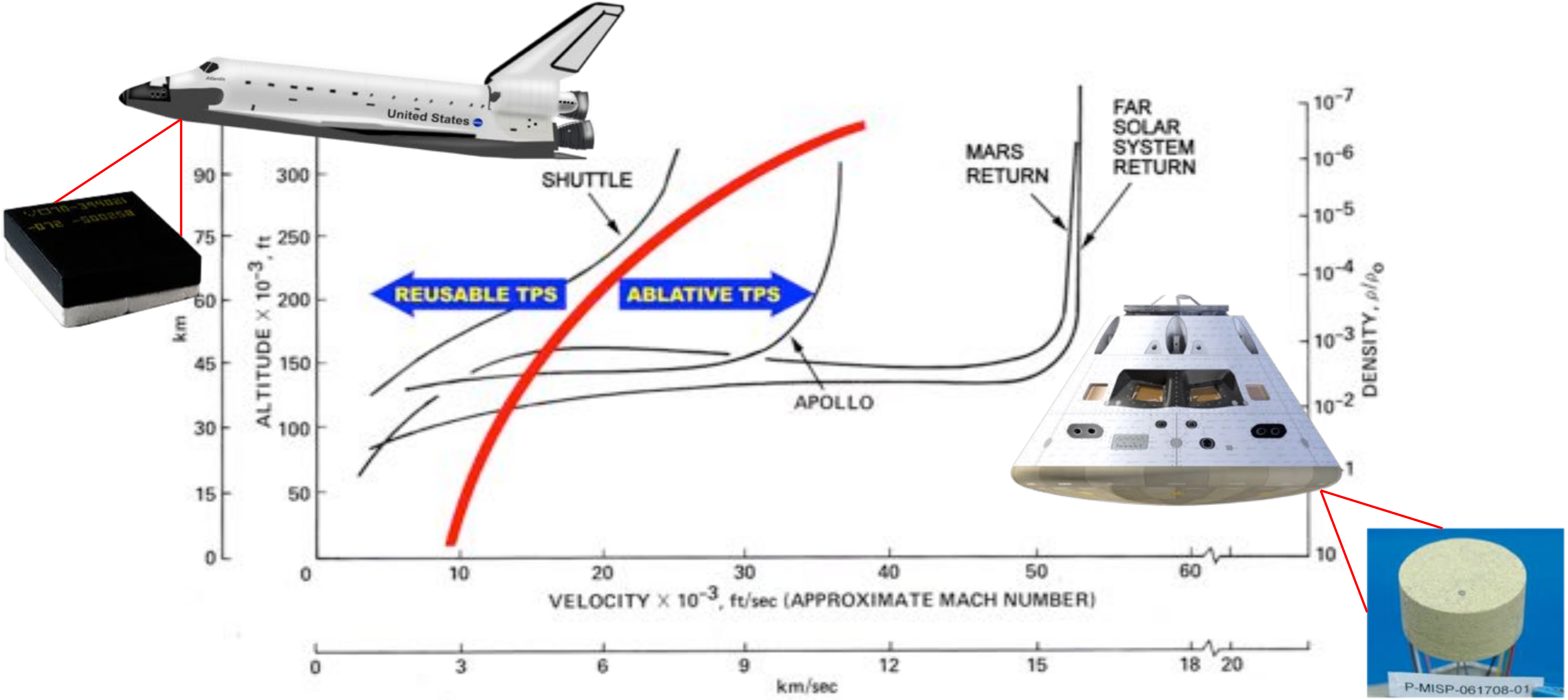
Z-max 800
Z1 200
Z2 599
Voxel Length (um): 0.65
Grayscale Range of Material: 87 to 255
Porosity 0.837786
Image: 799

Ferguson et. al, PuMA: the Porous Microstructure Analysis software. Submitted to SoftwareX (2017)

Motivation

Thermal Protection Systems (TPS)



NASA TM 101055, 1989

Ablative Thermal Protection Systems


Carbon preform

+


Resin

=

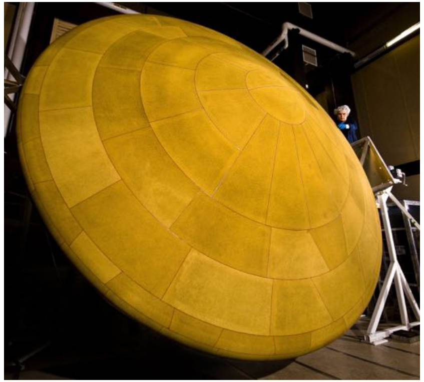

PICA


Stackpoole et al., *AIAA 2008-1202*

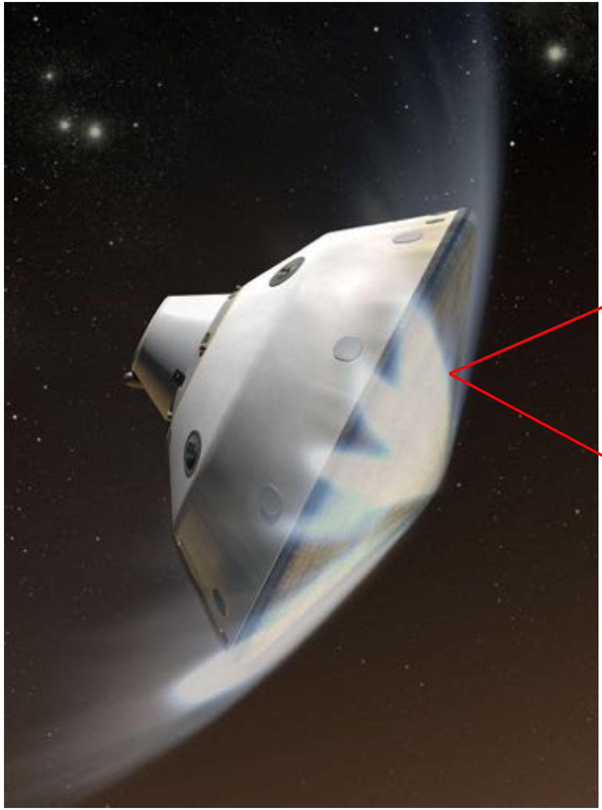
Stardust Capsule

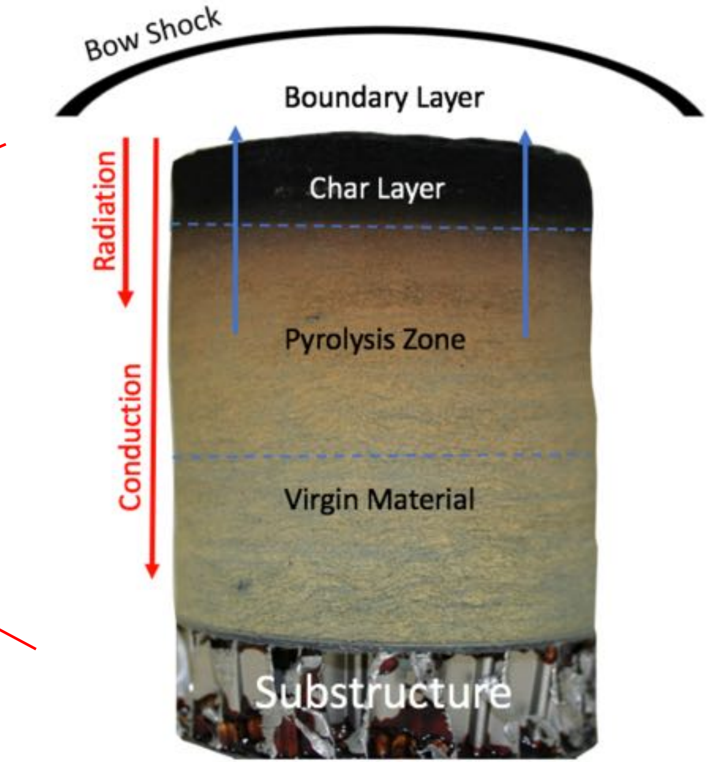

www.spacex.com

Dragon V1 & V2


Mars Science Laboratory

Material Design and Modeling





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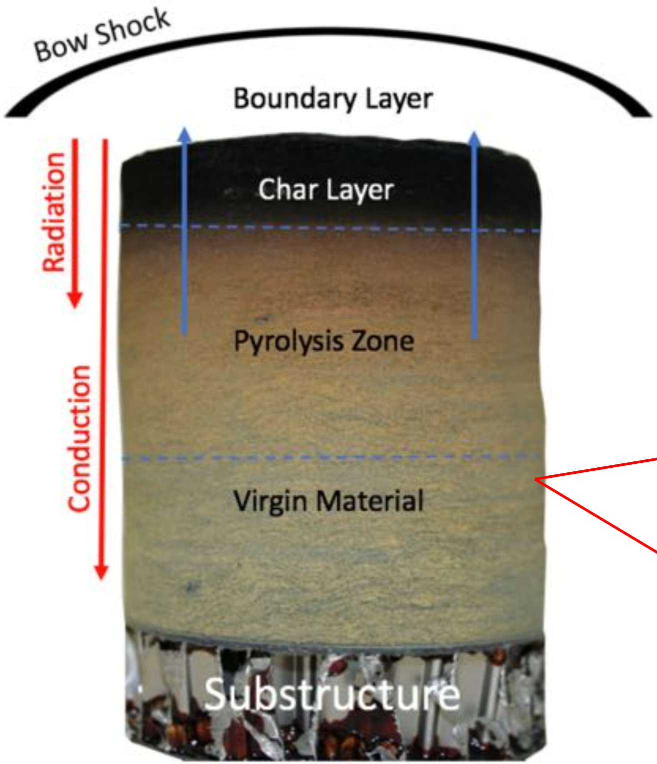
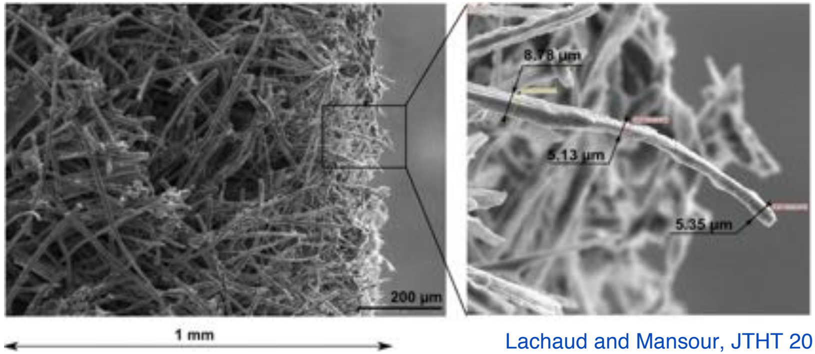
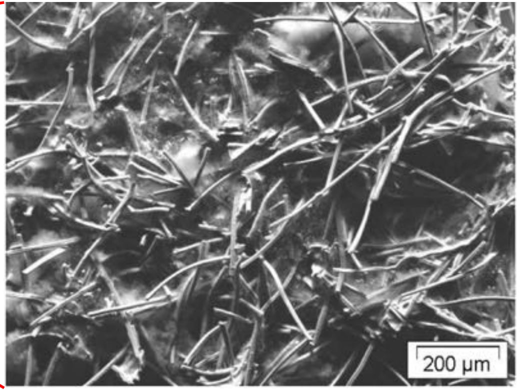




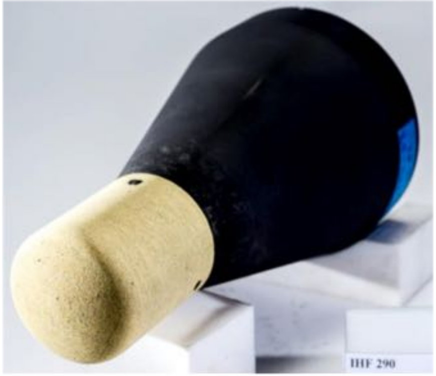
Lachaud and Mansour, JTHT 2013



Lawson et. al. 2010

Material Design and Modeling

P. Agrawal et. al. 2016.

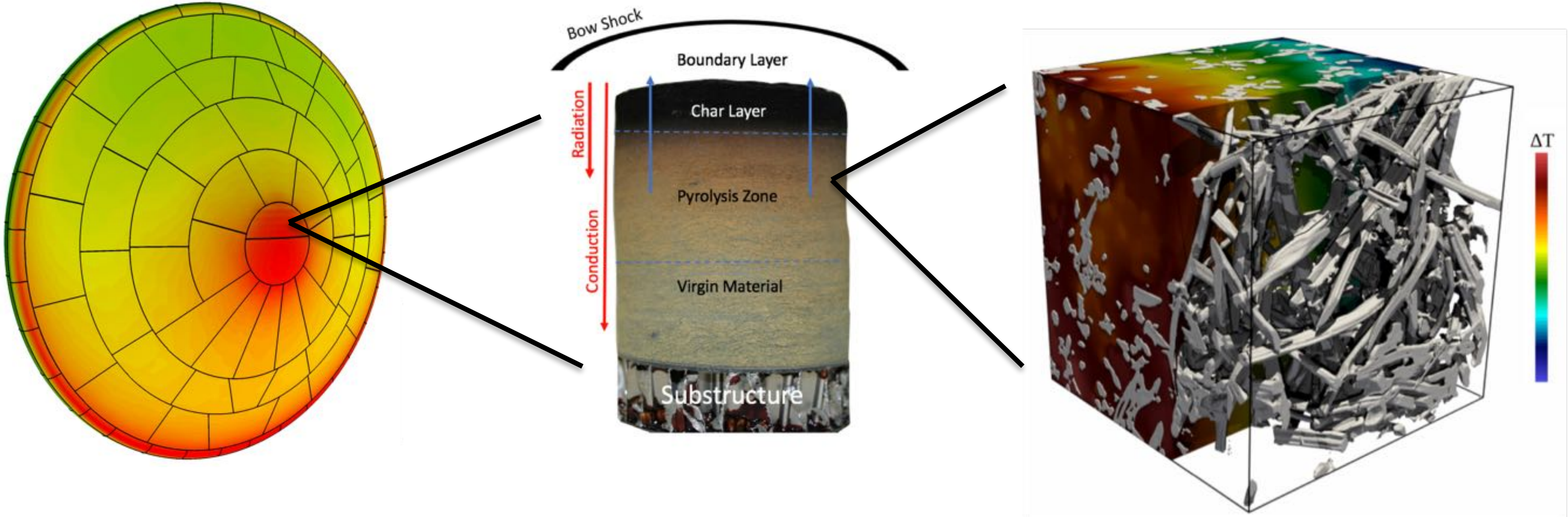


Virgin PICA Sample

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

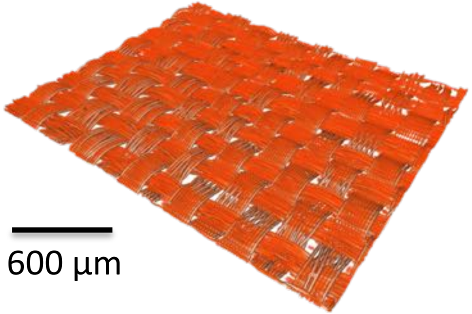
High fidelity characterization of heat shield materials in extreme environments is needed

Cannot be achieved with experiments alone

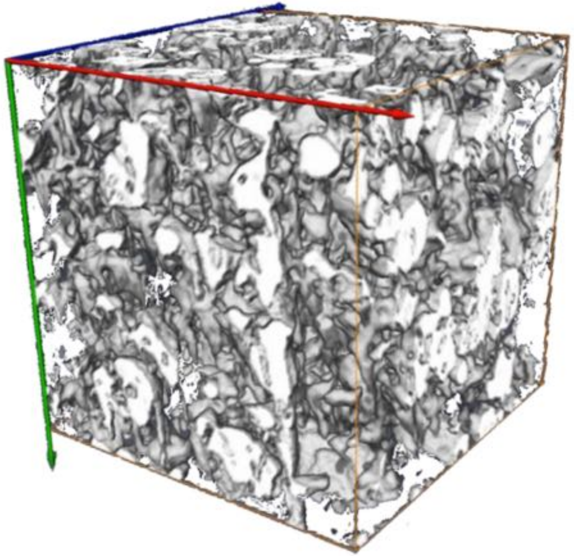
Other applications

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

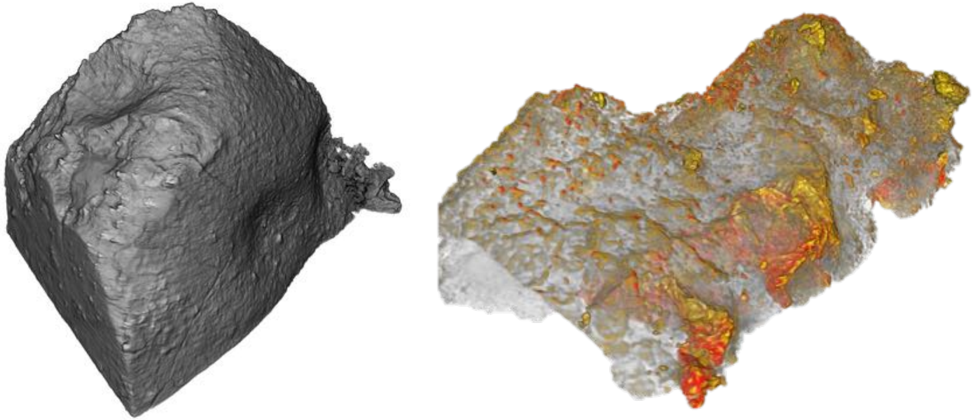
Parachute Materials



Plastic/Copper Composites



Meteorite Samples



Capabilities

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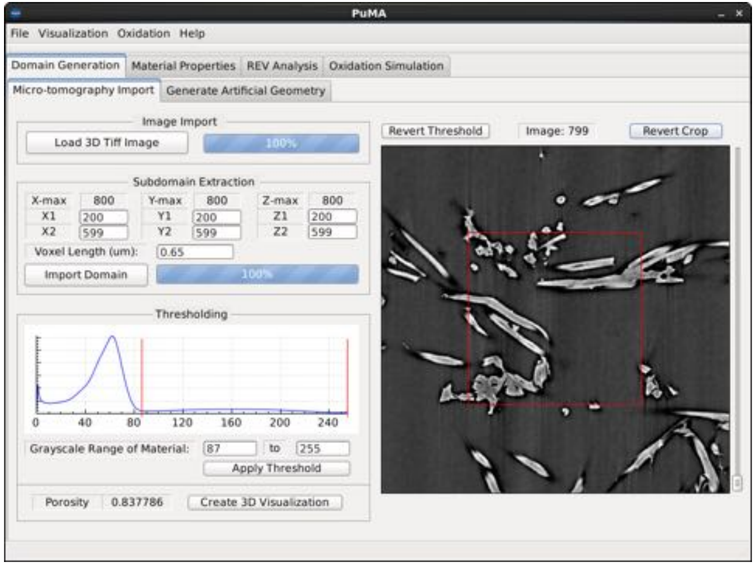

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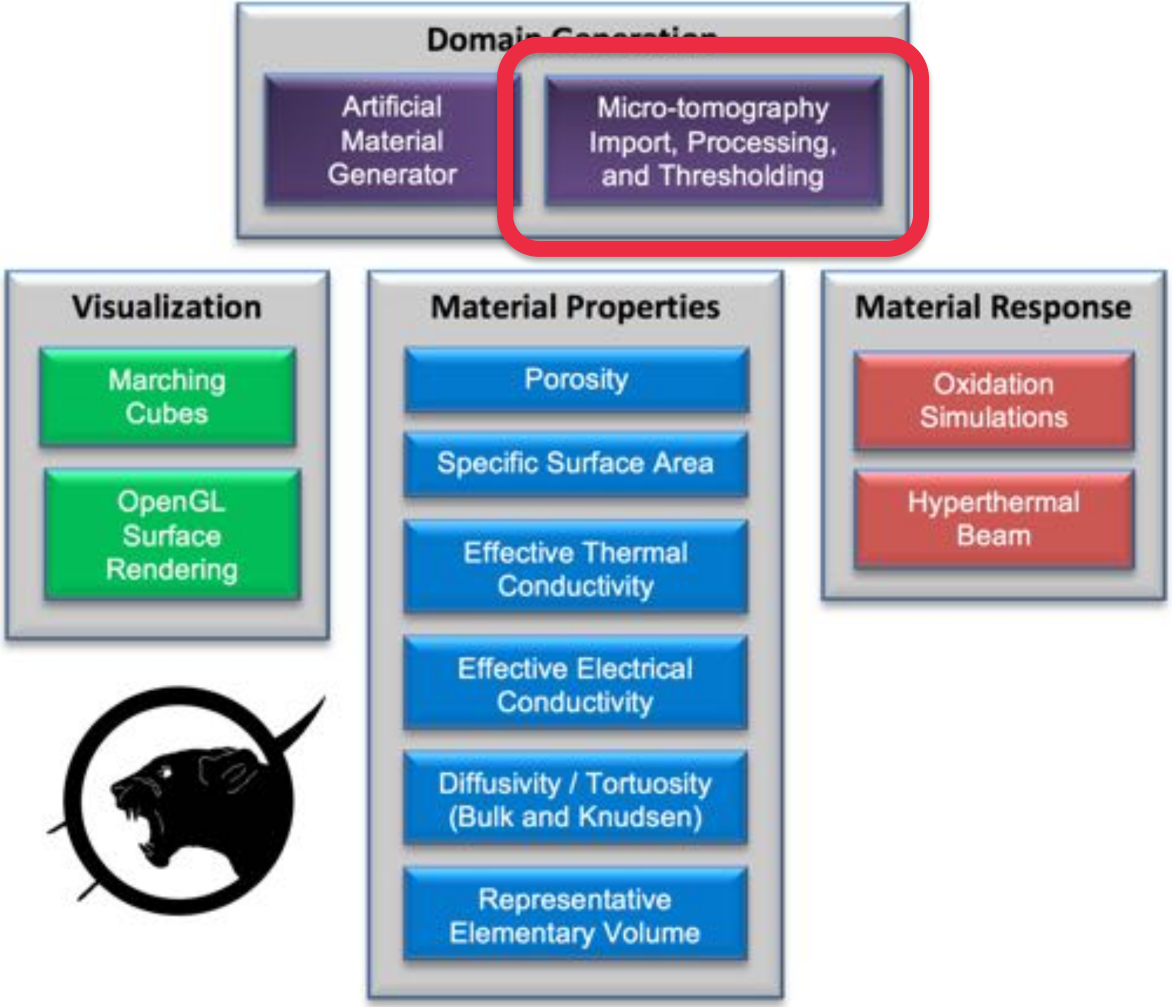

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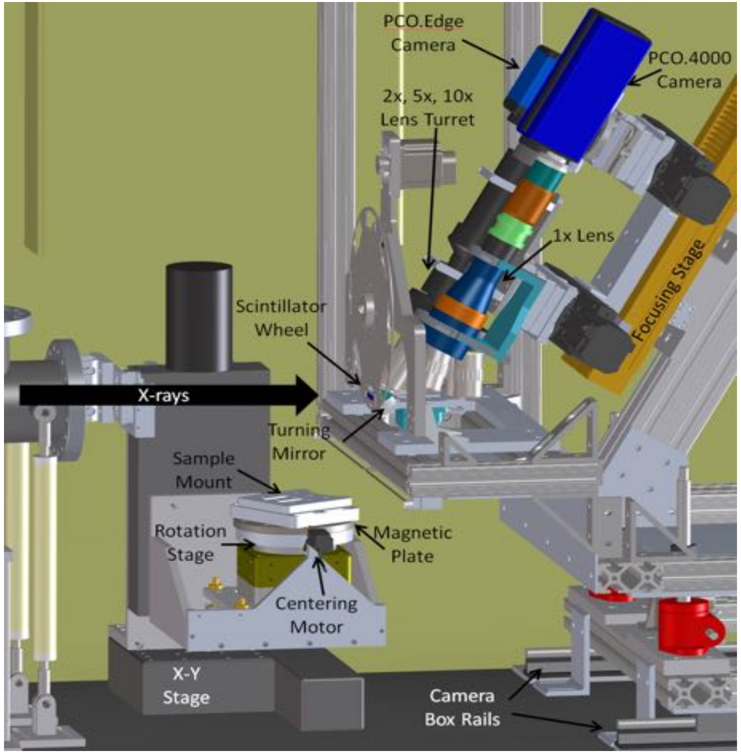
X-ray micro-tomography

- 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)

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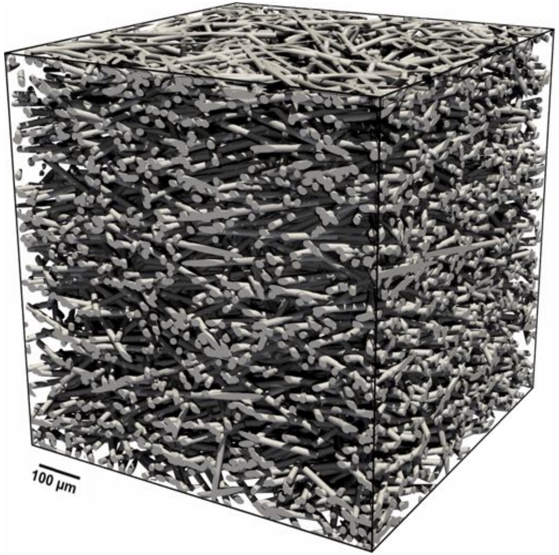
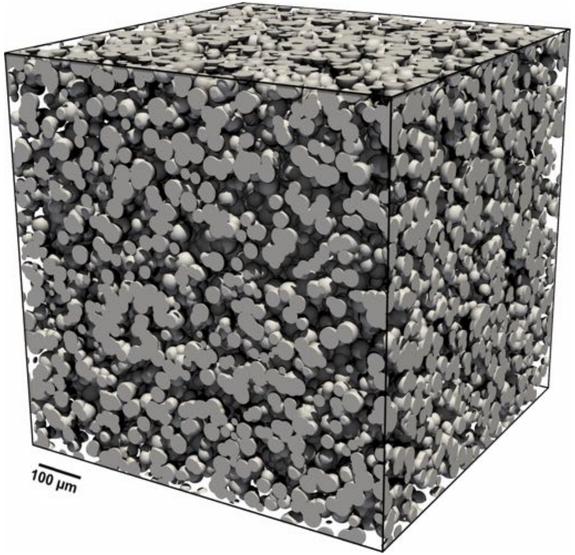
Material Generation

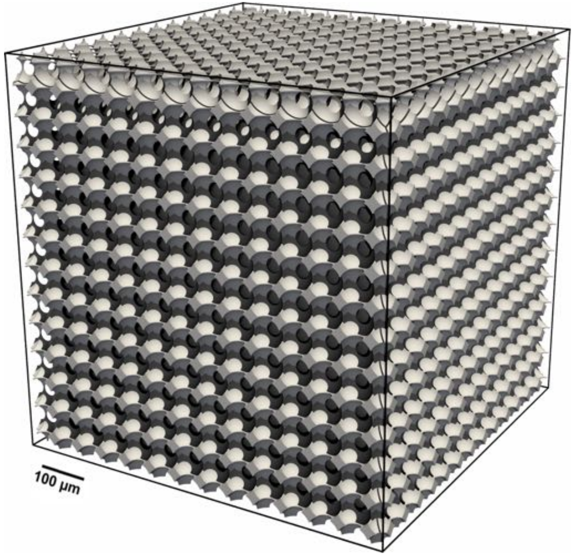
Random Fiber Structures



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

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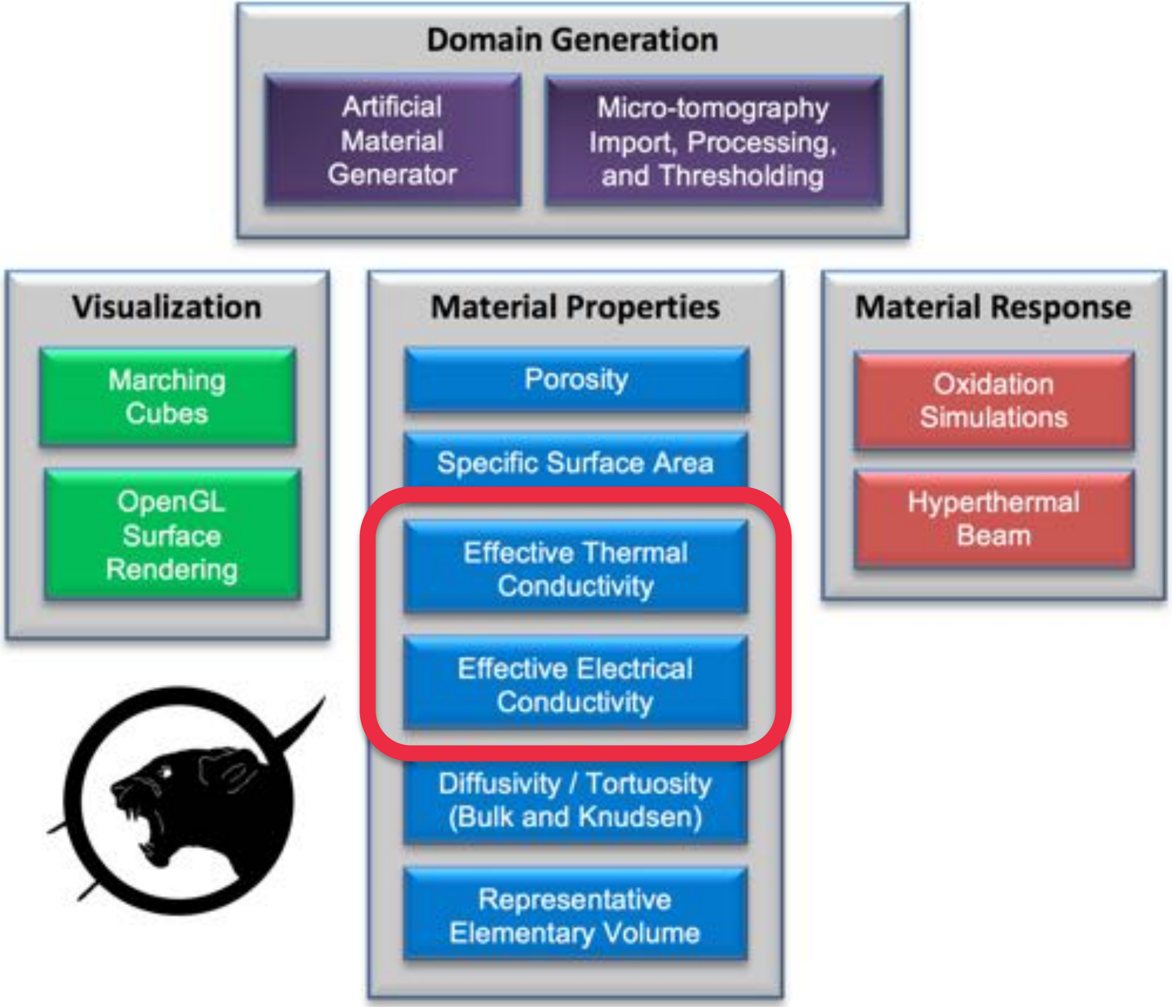
Effective Material Properties

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



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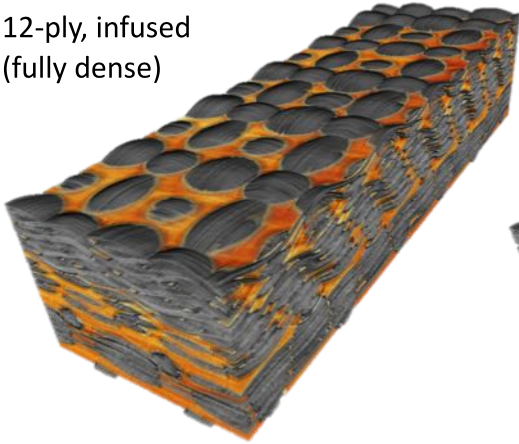
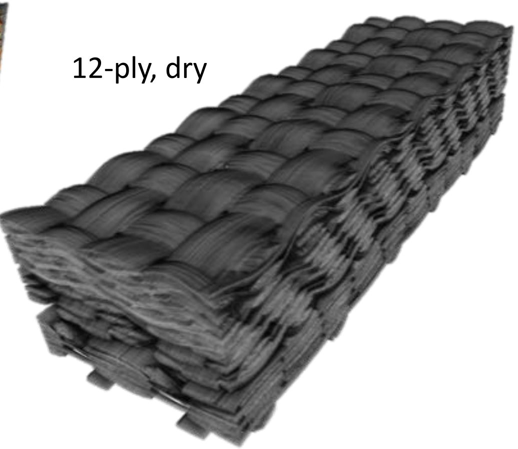
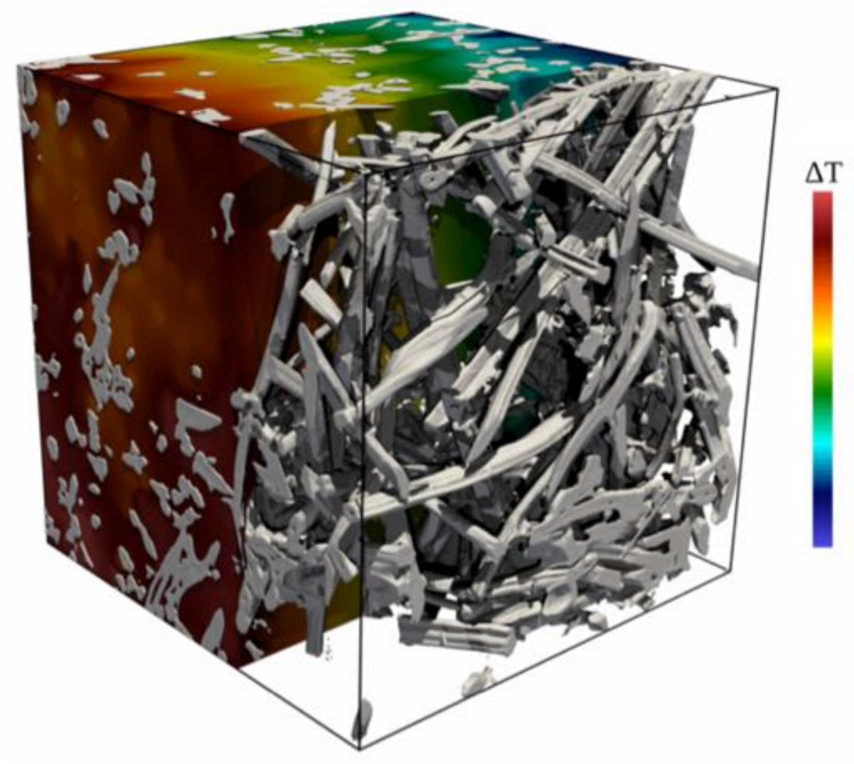
Effective Thermal Conductivity

- 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

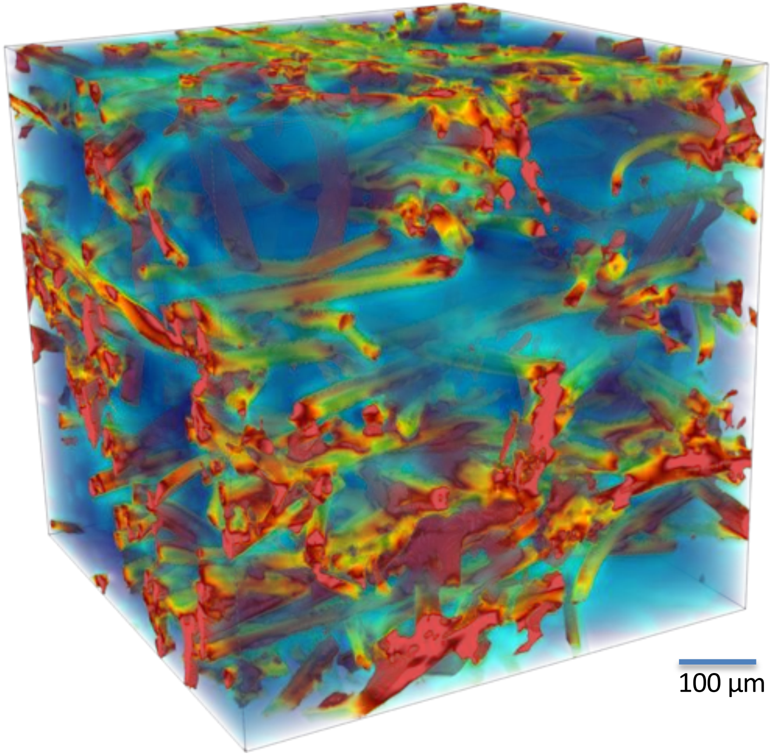

12-ply, infused (fully dense)


12-ply, dry



Effective Electrical Conductivity

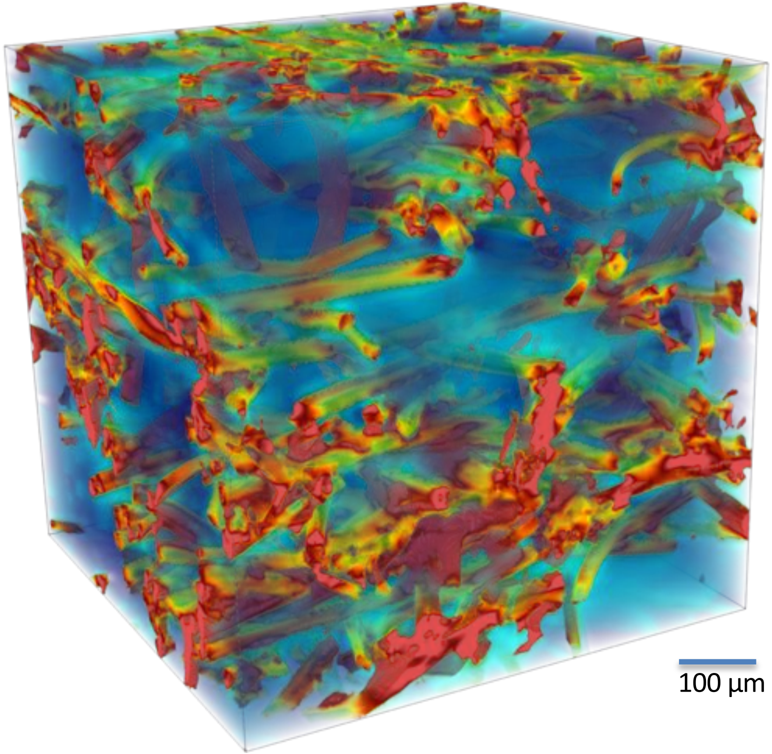
- Computes effective electrical conductivity using a finite difference method [Weigmann, 2006]
- 1V voltage differential applied; solved with periodic boundary conditions
- BicGStab iterative method and FFTW used to solve linear system of equations [Sleijpen, 1993]
- Parallelized based on OpenMP
- Verified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



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

Anisotropic Thermal/Electrical Conductivity

- Allows for constituents with anisotropic thermal conductivites
- 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



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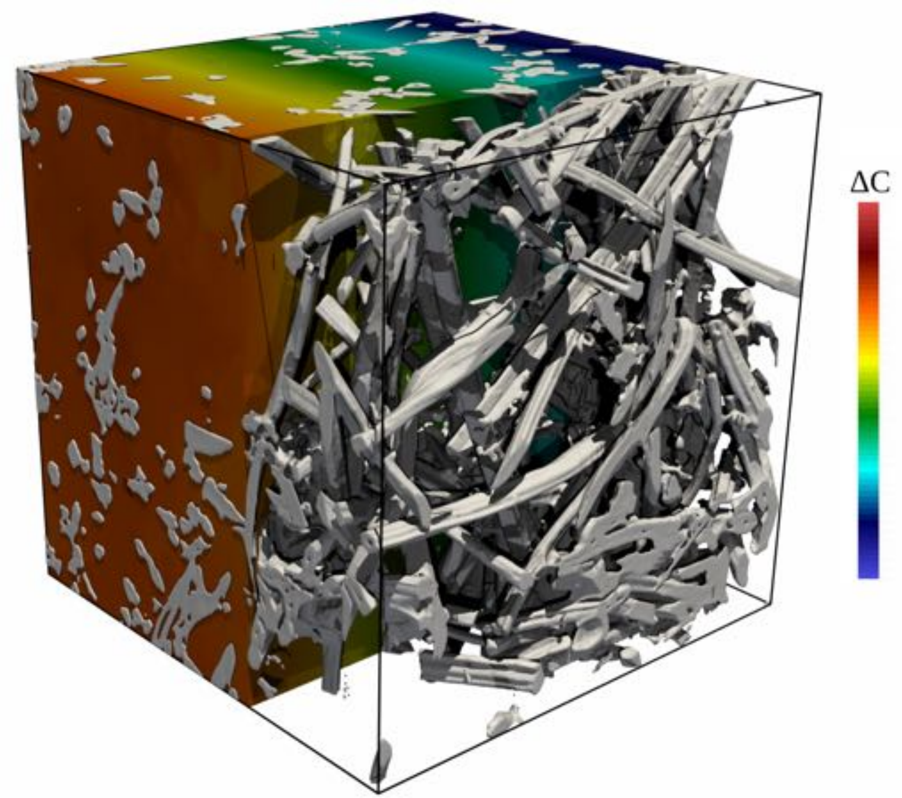
Diffusivity / Tortuosity

Continuum

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



Ferguson et. al, Particle methods for tortuosity factors in porous media, *9th Ablation Workshop, Bozeman MT. (2017).*

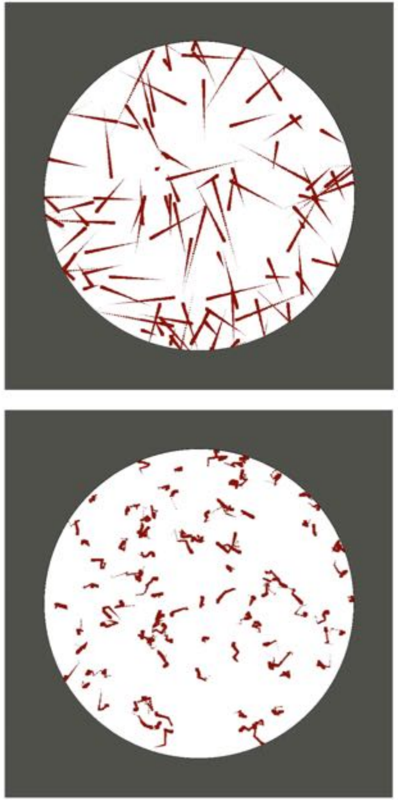
Diffusivity / Tortuosity – Random Walk

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

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

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



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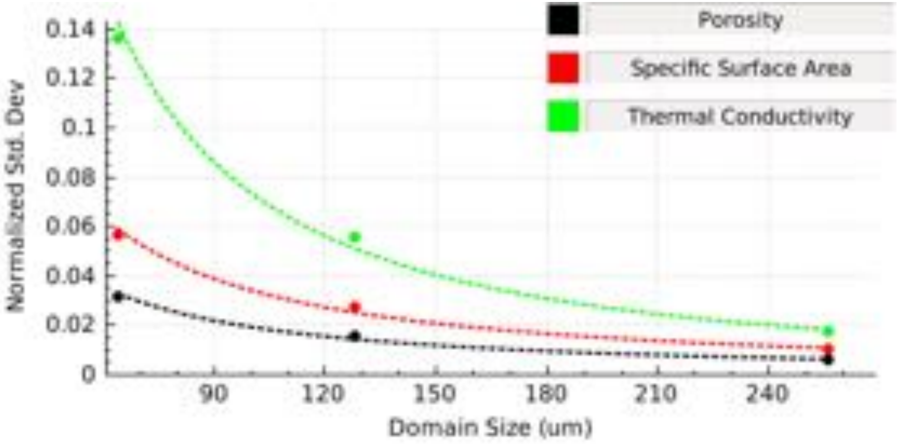
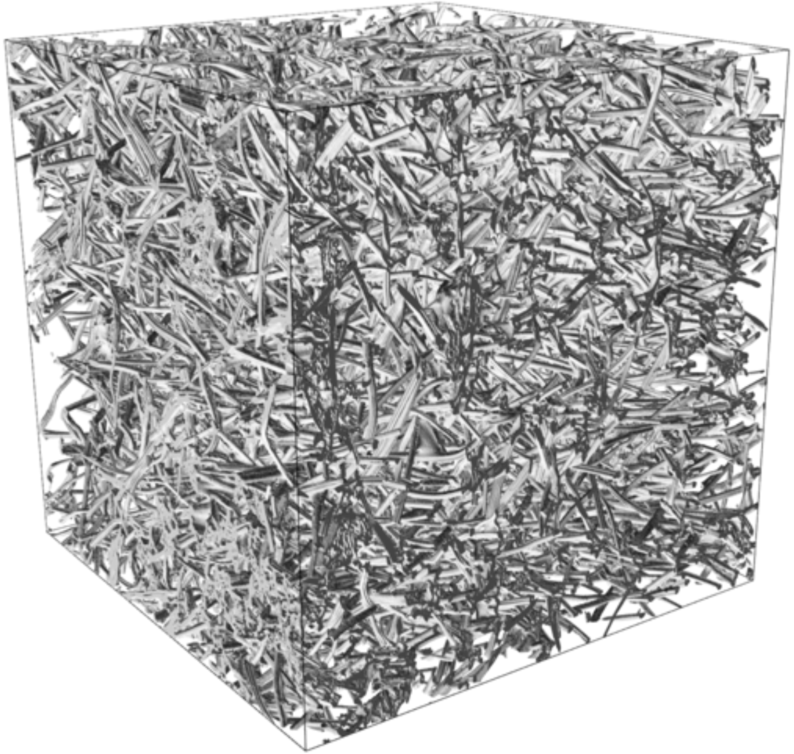
Representative Elementary Volume

- 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 ≈ 500 million triangles.

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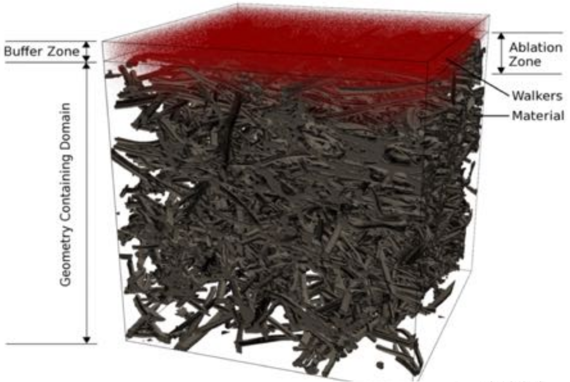
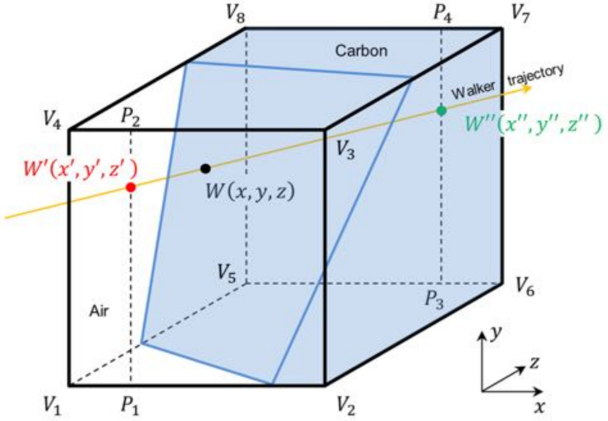
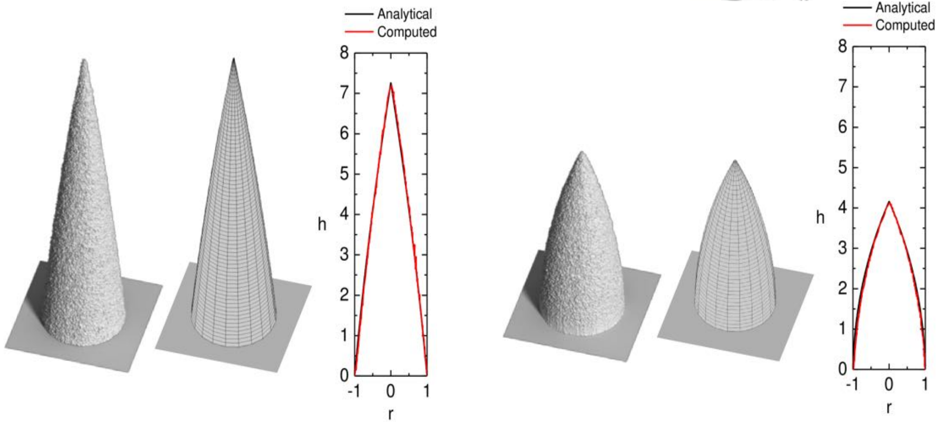
Micro-Scale Oxidation Simulations

- 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







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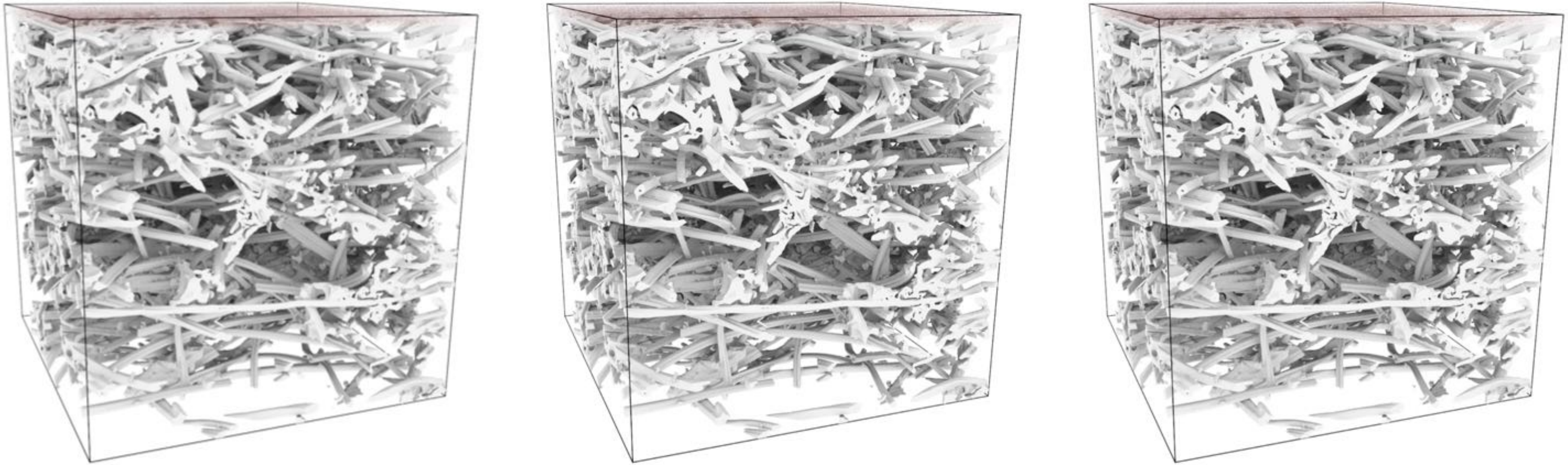
Micro-Scale Oxidation Simulations



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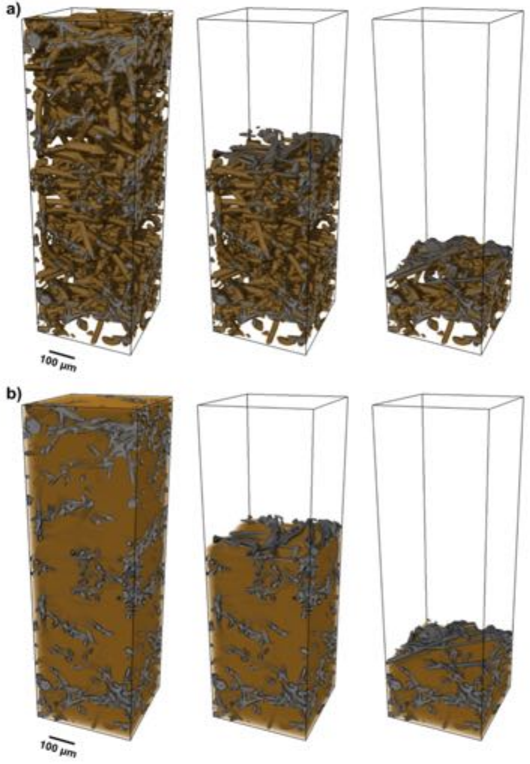
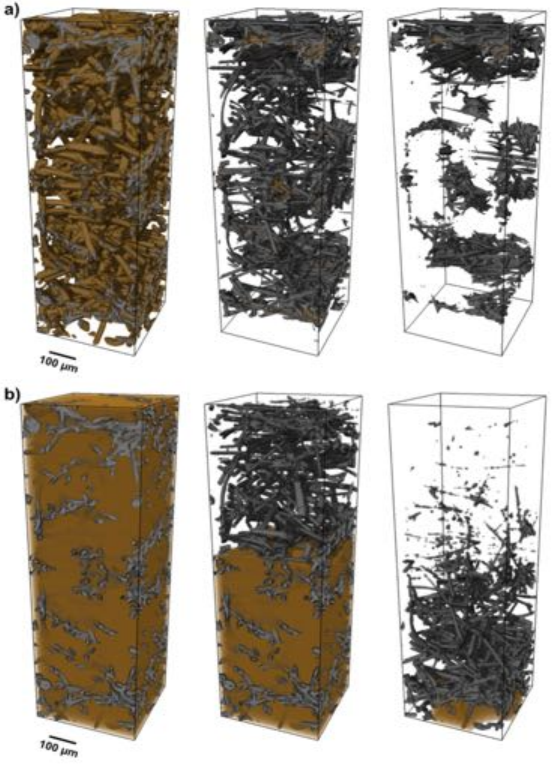


Surface Ablation



Volume Ablation

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

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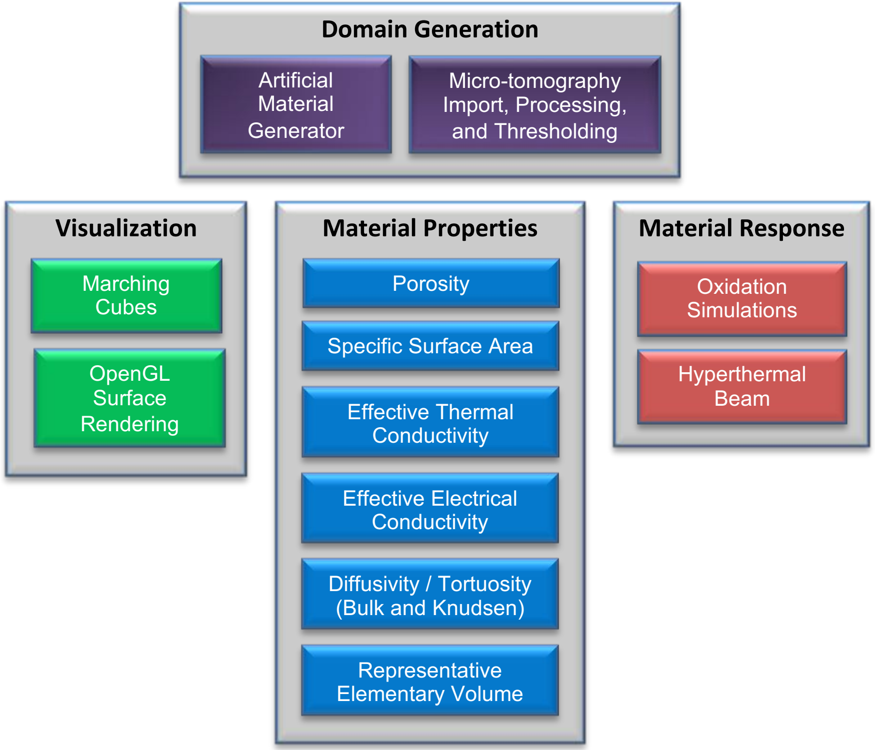
Molecular Beam Simulations

- 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].

[1] Murray V J., et al. Inelastic and Reactive Scattering Dynamics of Hyperthermal O and O2 on Hot Vitreous Carbon Surfaces. *The Journal of Physical Chemistry* C 119.26 (2015).
[2] Swaminathan-Gopalan K et. al. Development and validation of a finite-rate model for carbon oxidation by atomic oxygen, *Carbon* 137 (2018).

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
- **<u>Need for good quality experimental data for model verification</u>**



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Microscale Modeling Research Group

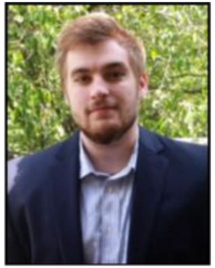
Principle Investigator:

NN Mansour

Experimentalist:

F Panerai

PuMA Development:



J Ferguson

F Semeraro

J Thornton

DSMC Development:

A Borner

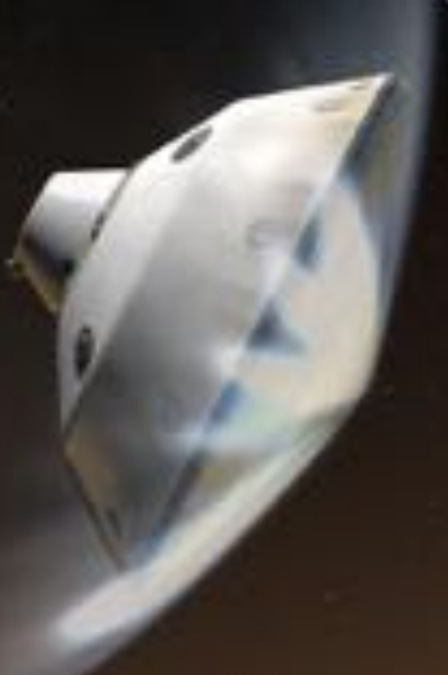
X-Ray Microtomography:

A MacDowell

D Parkinson

H Barnard

Questions?



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