Modeling of the fiber-scale oxidation of highly-porous carbon fiber materials based on synchrotron X-Ray Microtomography

Applied Modeling & Simulation (AMS) Seminar Series

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Thermal Protection Systems

Ceramic Tiles

- Used on the Space Shuttle
- Reusable
- Reentry from LEO

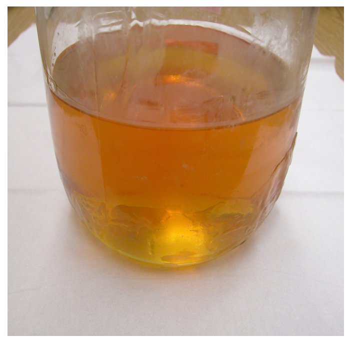
Ablative Heat Shields

- AVCOAT Ablative TPS used on the Apollo capsule
- Single use TPS
- High velocity reentry

Ablative TPS and PICA

FiberForm® Resin PICA

+



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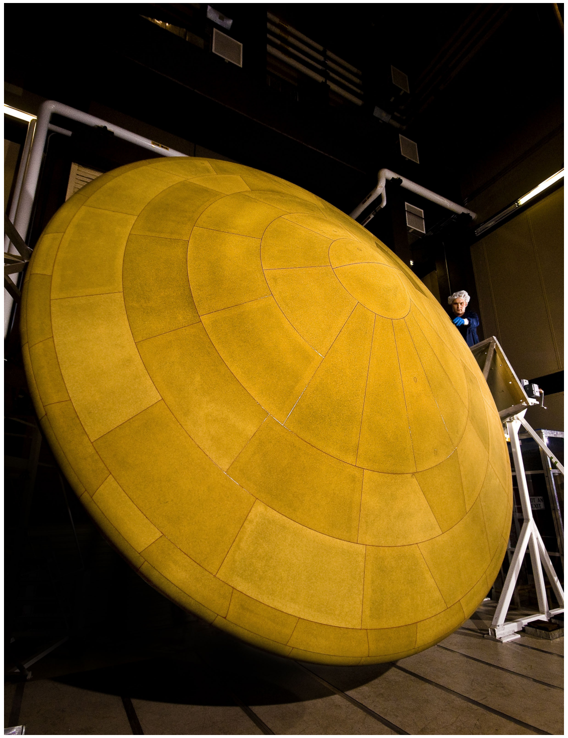
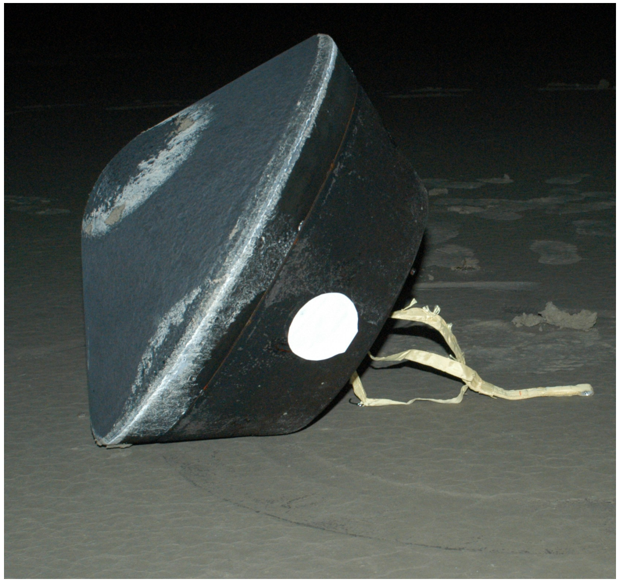
- Light weight Carbon / Phenolic Ablator
- Successfully flight tested
- SpaceX development of PICA - X

[Stackpoole *et al.*, AIAA 2008-1202]

PICA Flight Tests



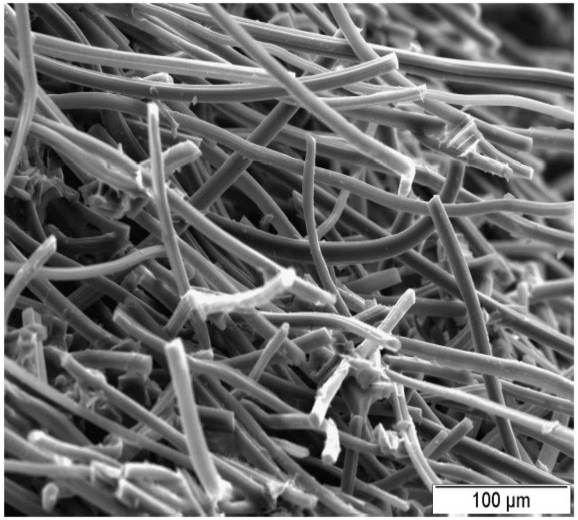
Mars Science Laboratory
(Curiosity Rover)



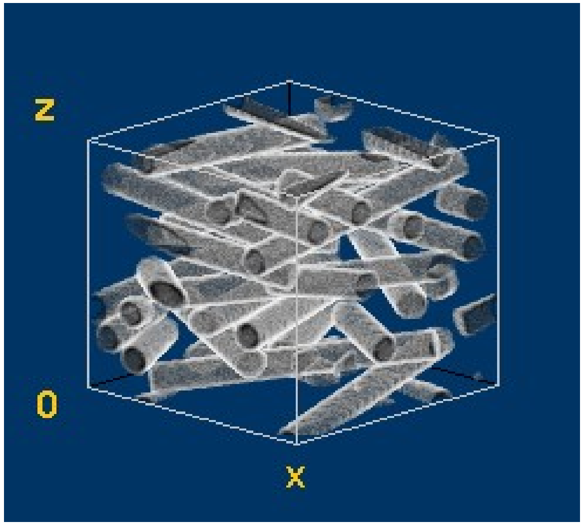
Stardust Capsule

SpaceX Dragon V1, V2

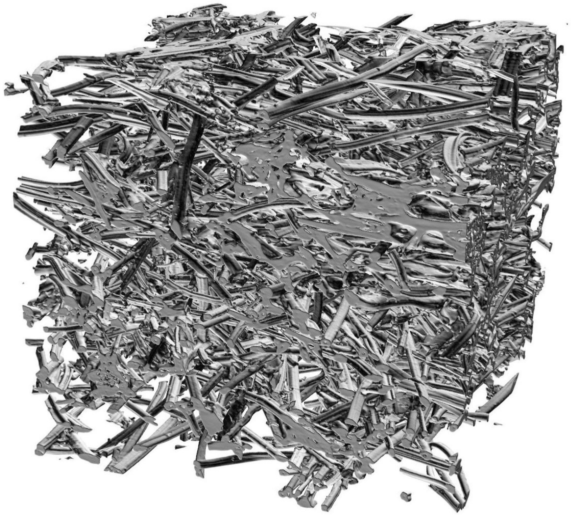
PICA Modeling



SEM Image of Fiberform



Artifically Generated Fiberform

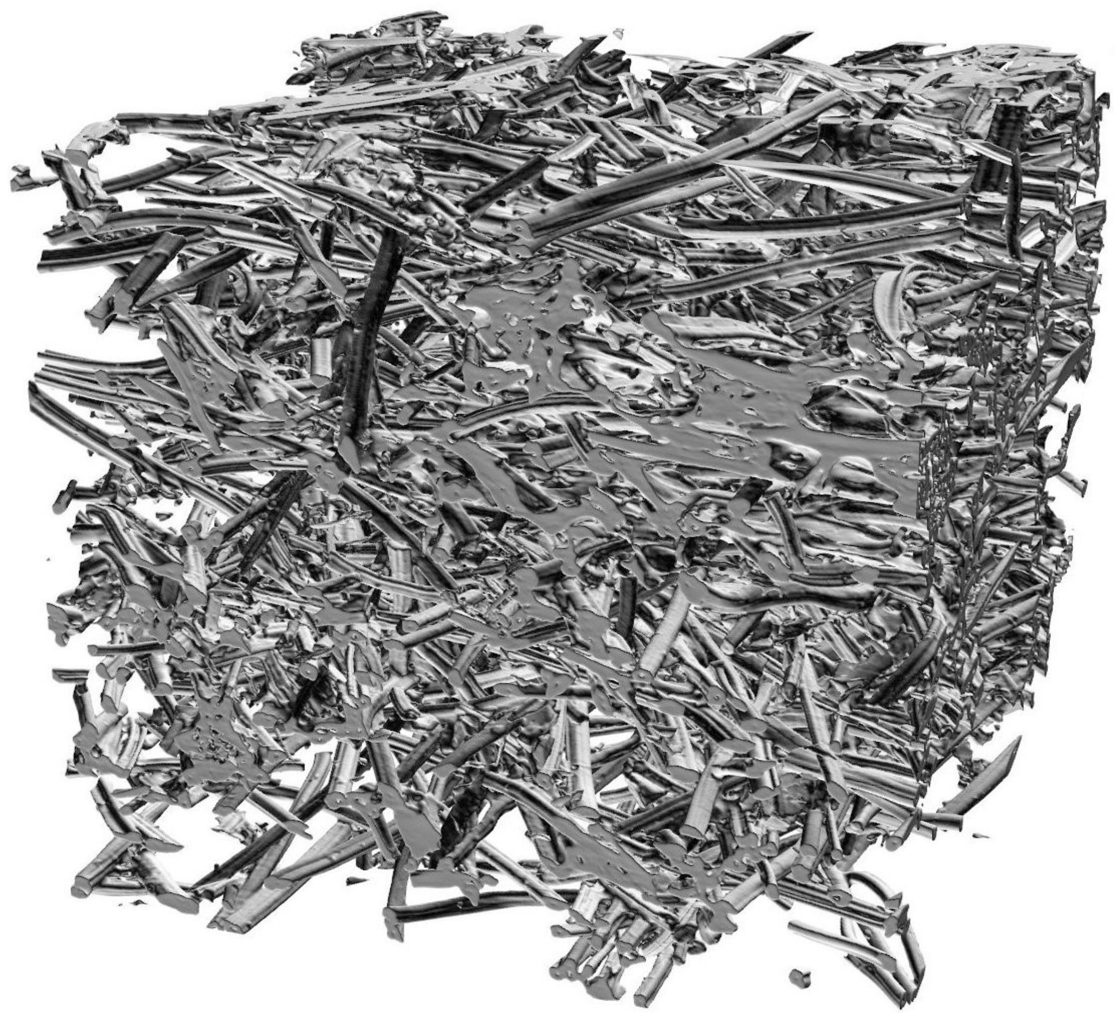


Surface Rendering of Microtomography Image

- Highly Porous Material
- Ablation can occur at a range of depths
- Models treat PICA as a solid material using a volume-averaged approach

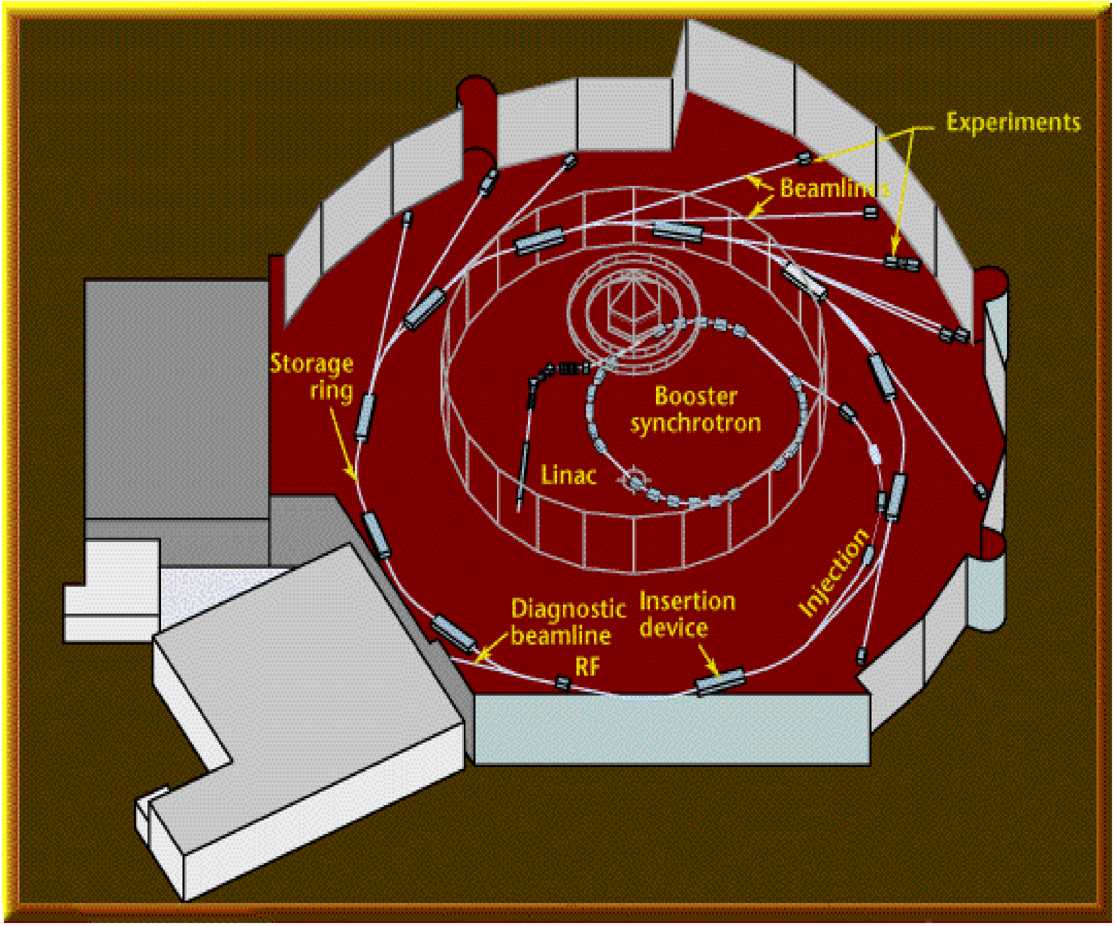
Objectives

- Handle Very Large Data sets of Microtomography
- Framework needed to analyze material properties and run simulations
- Desired Functionality:
  - Material Properties
  - Thermal phenomena
  - Mechanical phenomena
  - Transport phenomena

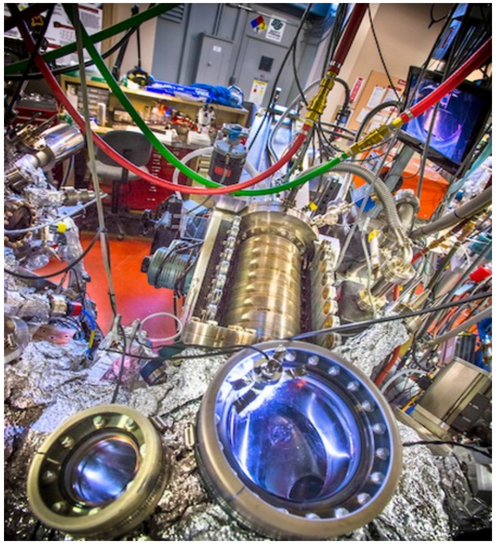


PuMA

Synchrotron Microtomography

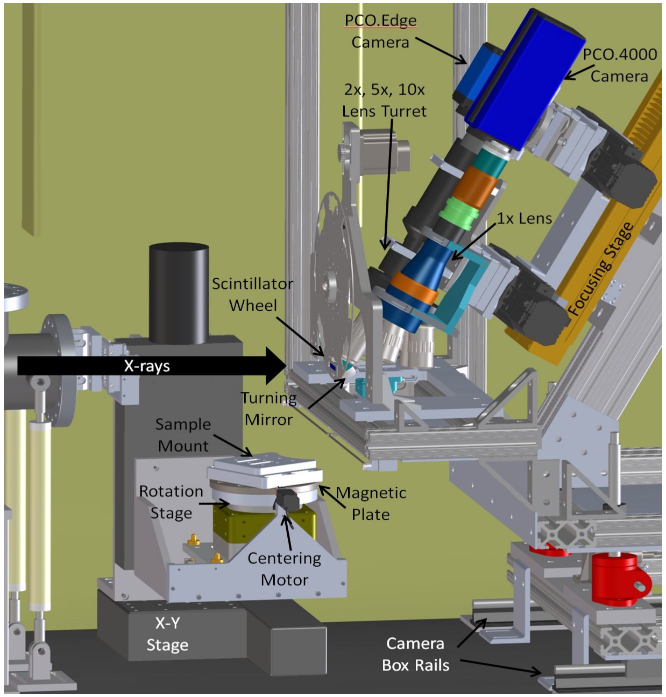


http://www2.lbl.gov/MicroWorlds/ALSTool/

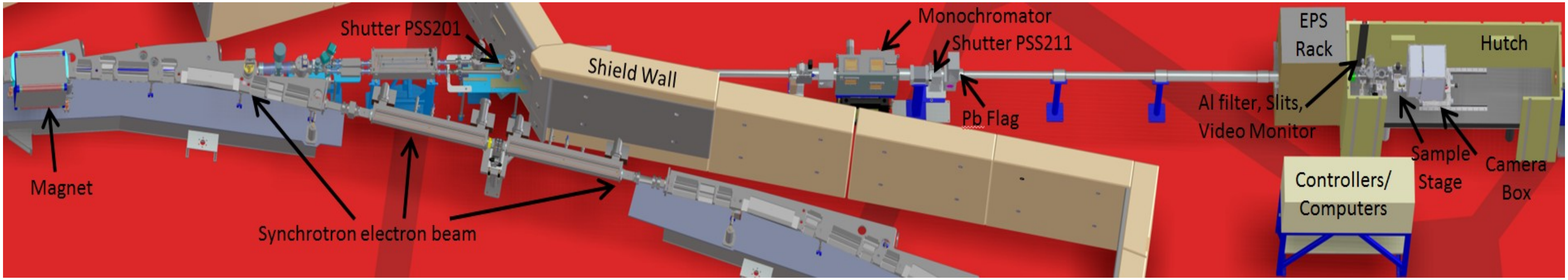


8.3.2 Beamline

- Hard X-ray microtomography
- 14 KeV X-rays
- Processed through scintillator, magnification lens, and a camera



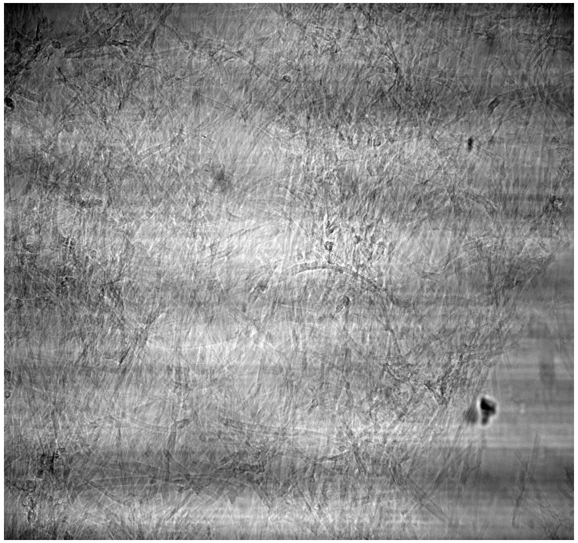
http://microct.lbl.gov/manual



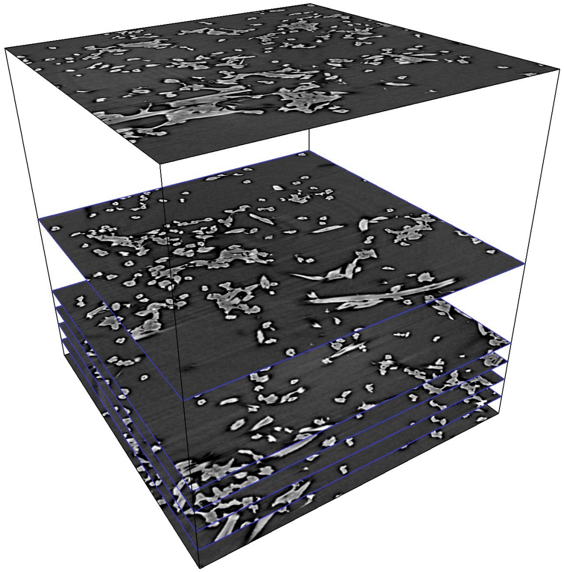
Projection processing

- Fiji plugin reconstruction algorithm.
- Converts 2048 projections into a 3D image stack

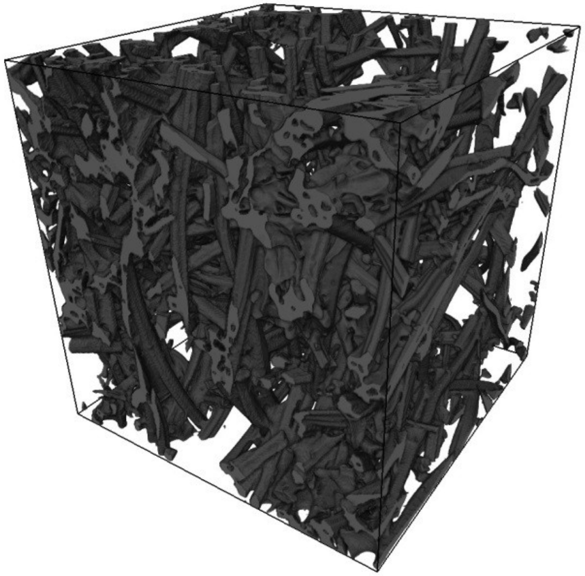
2048 Projections



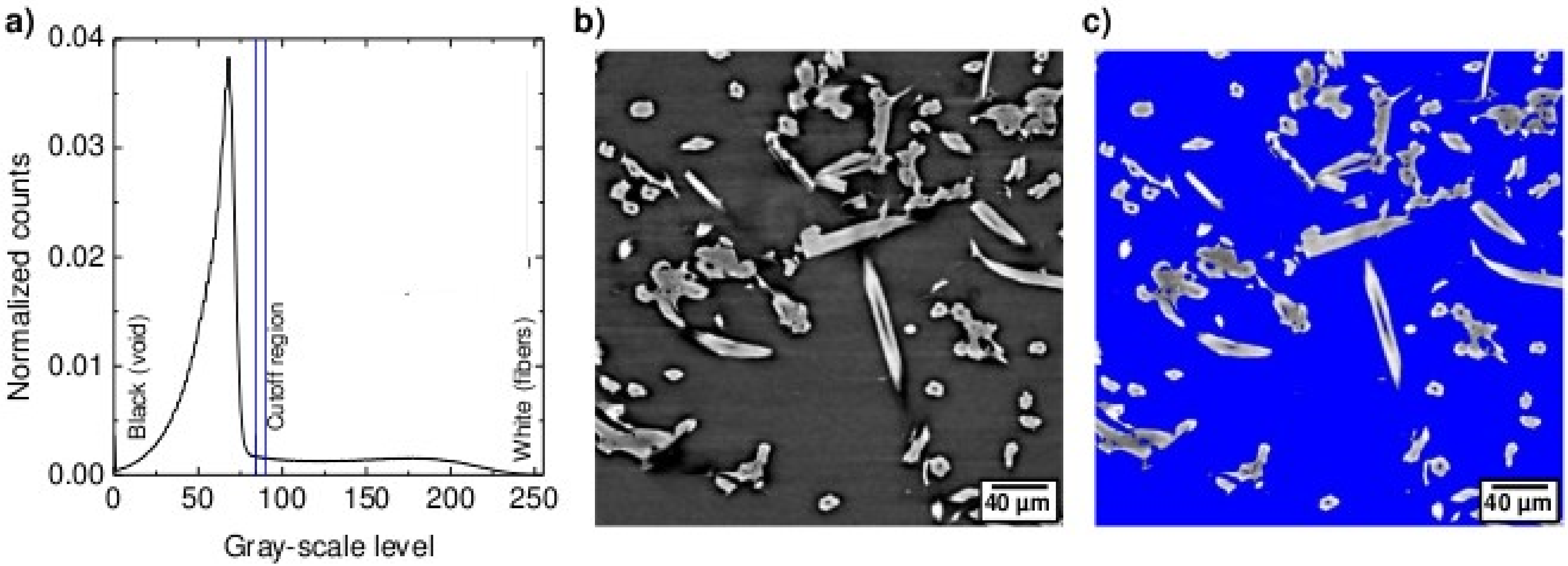
About 1600 Image Slices



Volume Rendering of Material



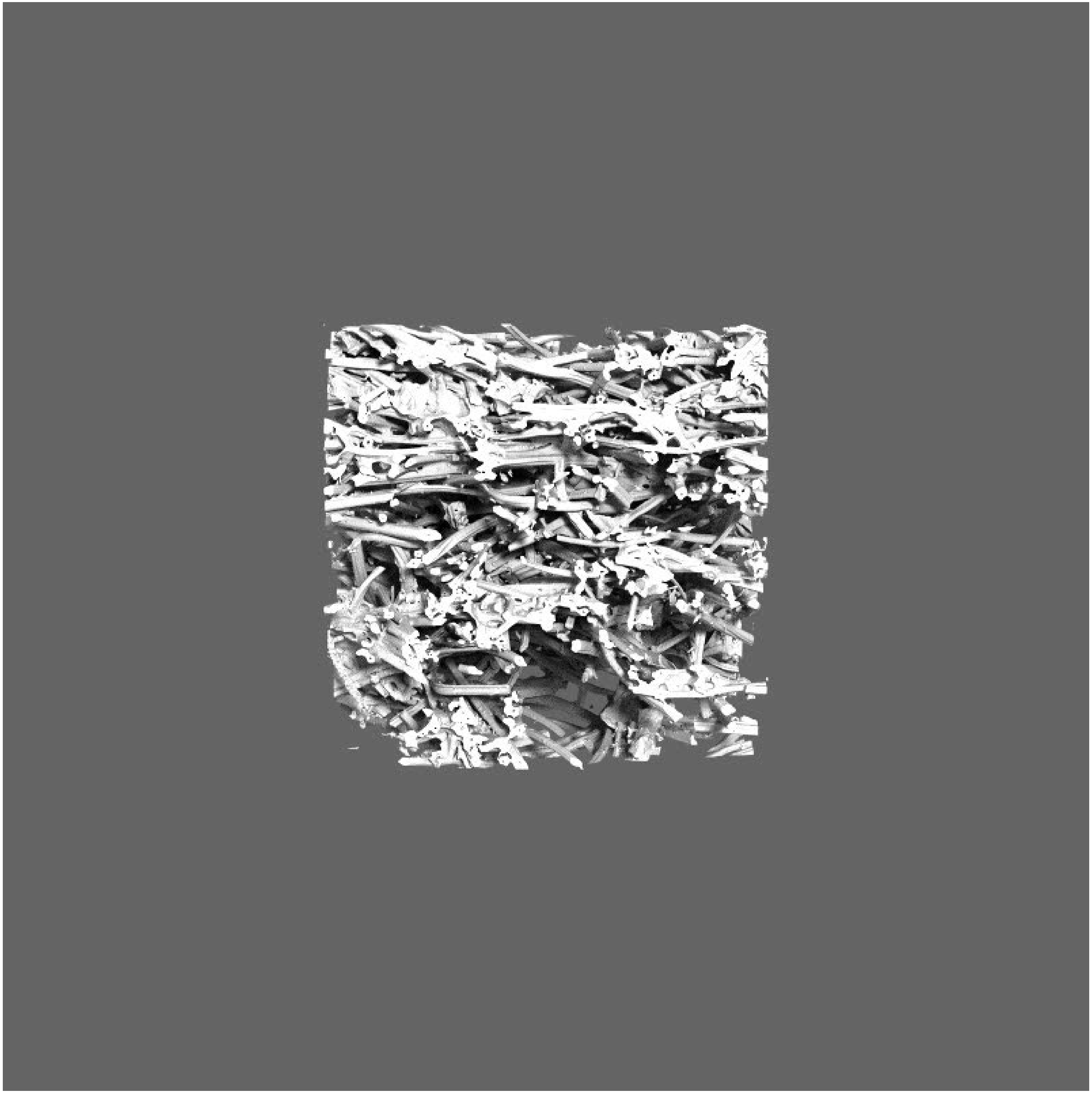
Grayscale Cutoff



Histogram of grayscale frequencies

Original Slice

Slice with threshold applied



Porous Media Analysis (PuMA)

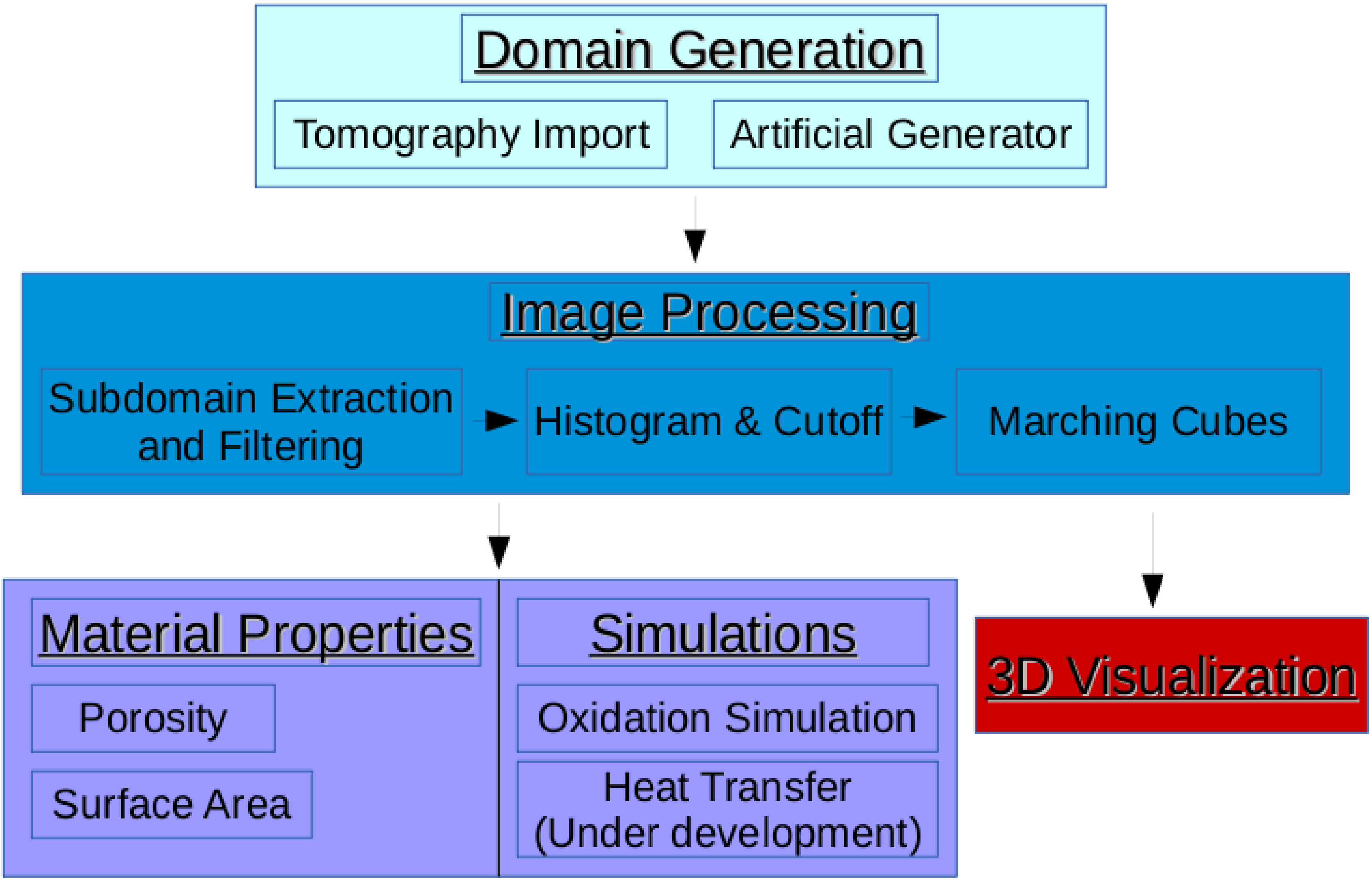
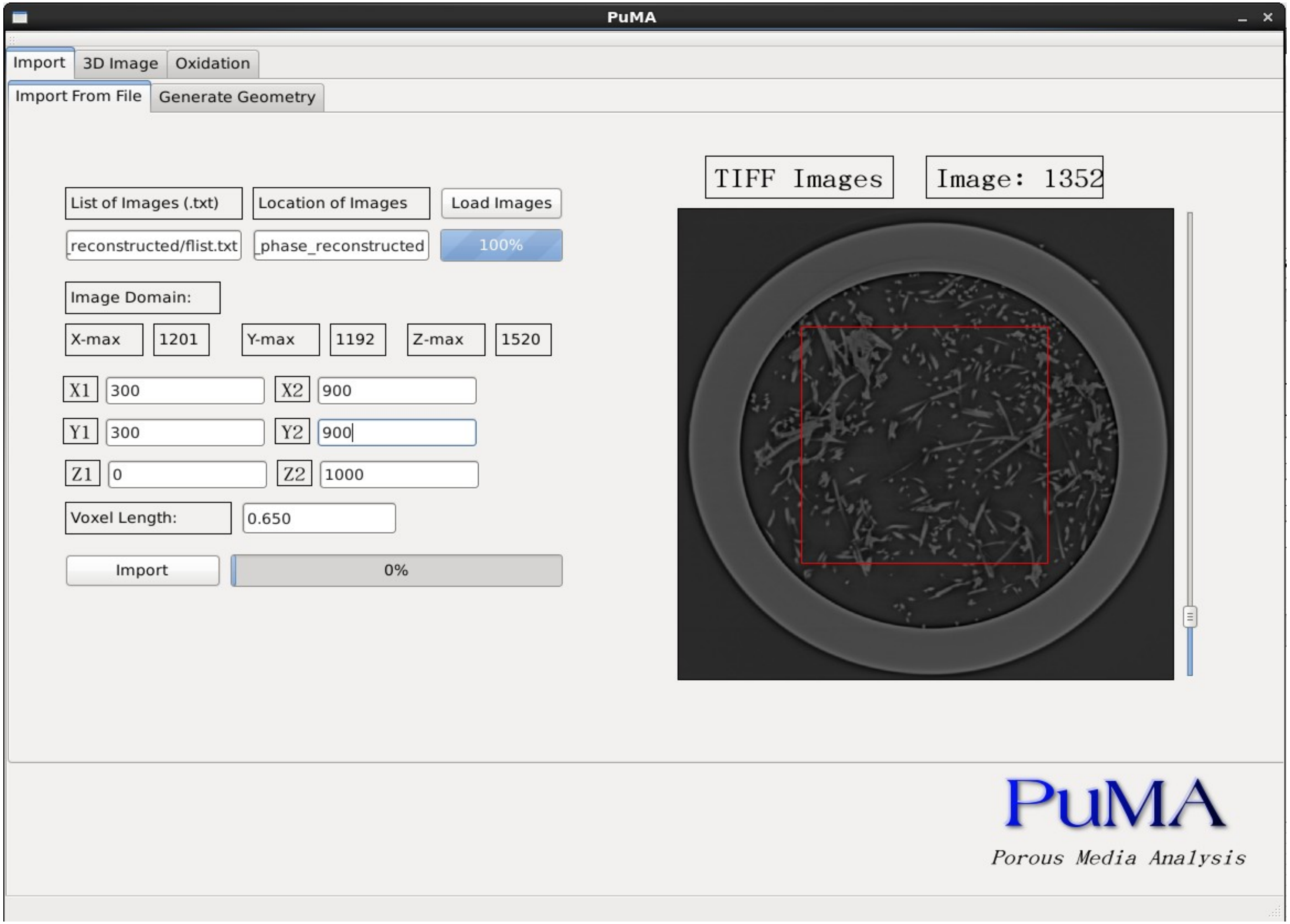
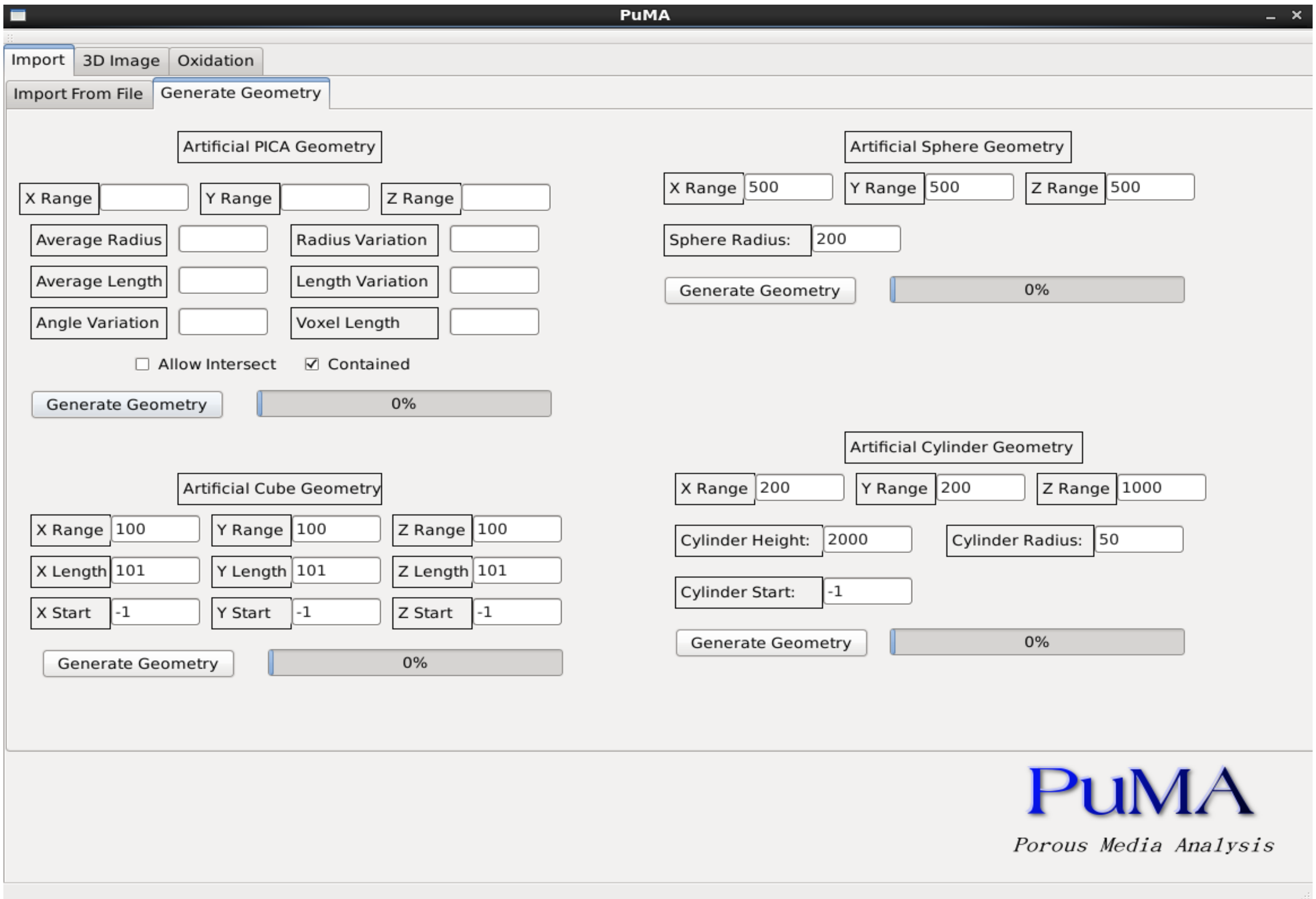


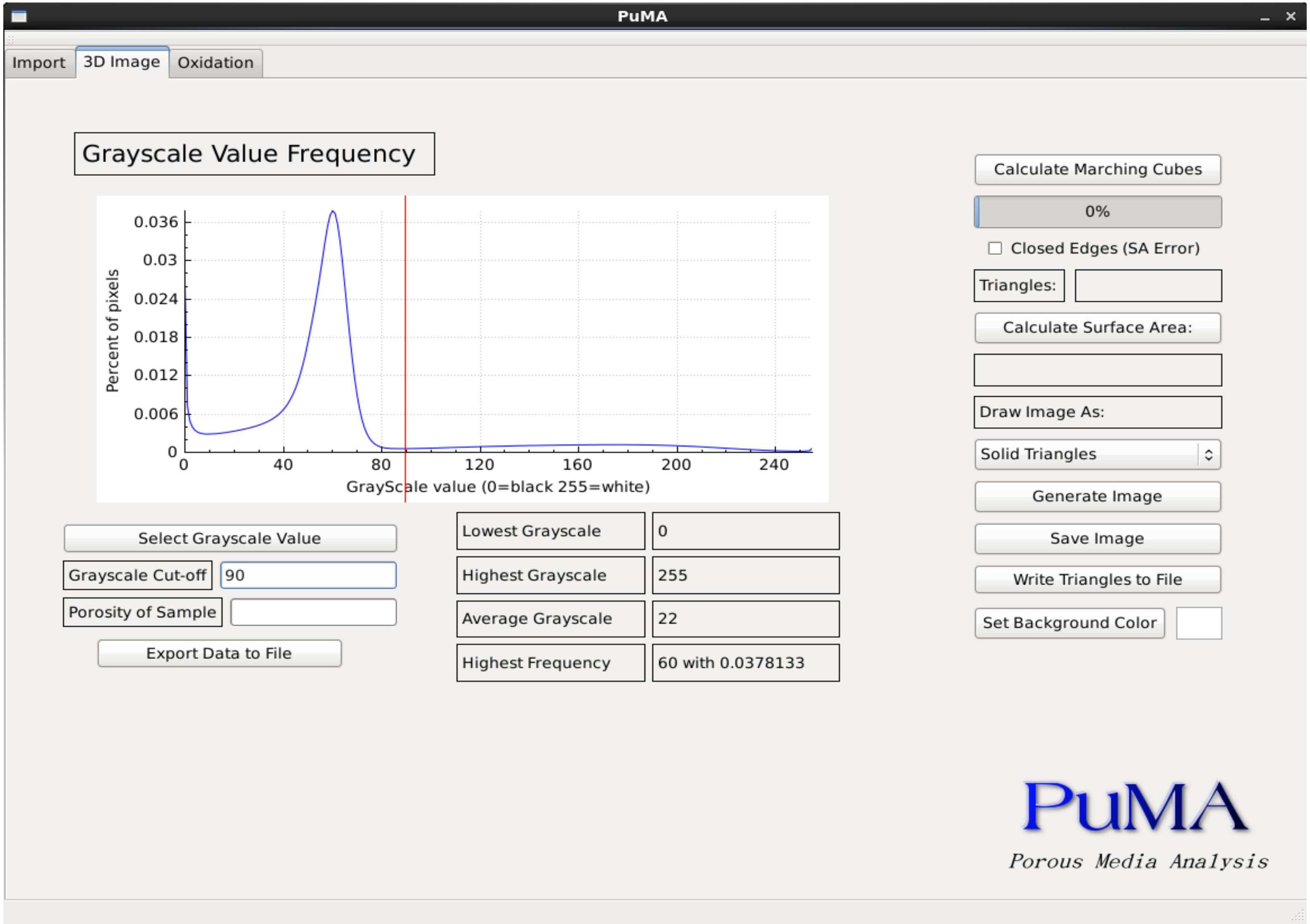
Image Import



Artificial Geometry Generator

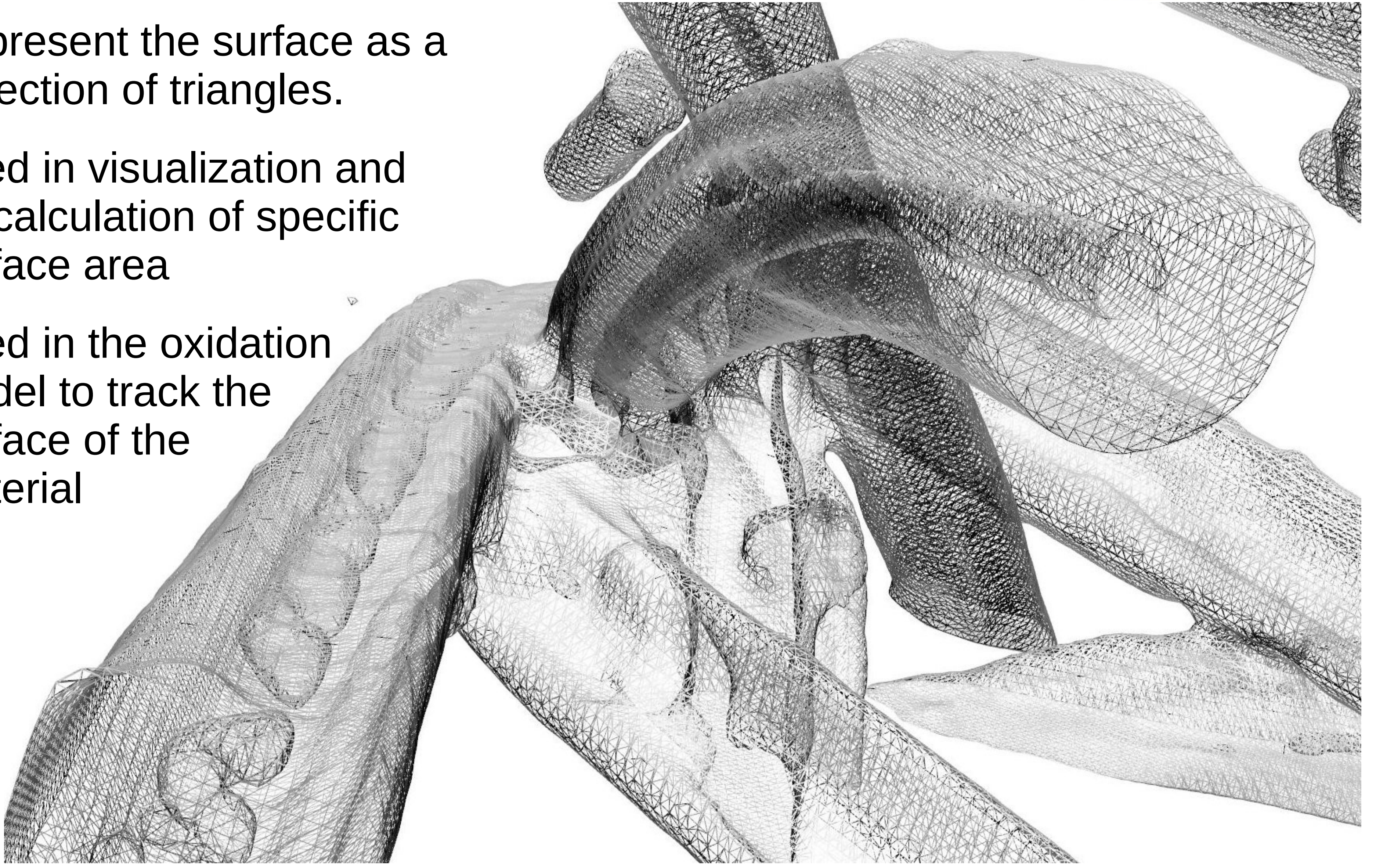


Histogram and Cutoff



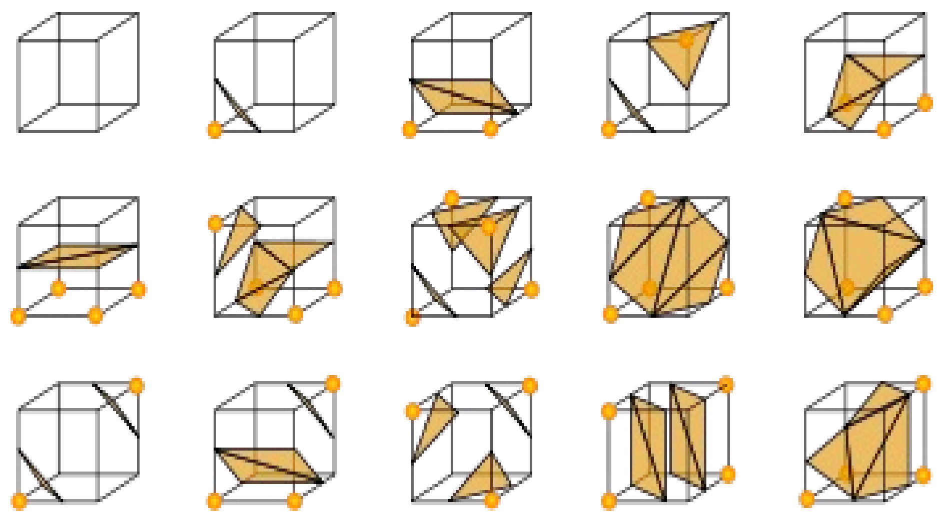
Marching Cubes Algorithm

- Represent the surface as a collection of triangles.
- Used in visualization and for calculation of specific surface area
- Used in the oxidation model to track the surface of the material



Marching Cubes Algorithm

- Marching Cubes Steps:
  - Define Space in X,Y, Z into voxels
  - Assign value to each voxel vertex
  - Compare each voxel to edge table to determine which edge case applies
  - Linearly interpolate triangle vertex positions
  - Use cross product to calculate normal vector

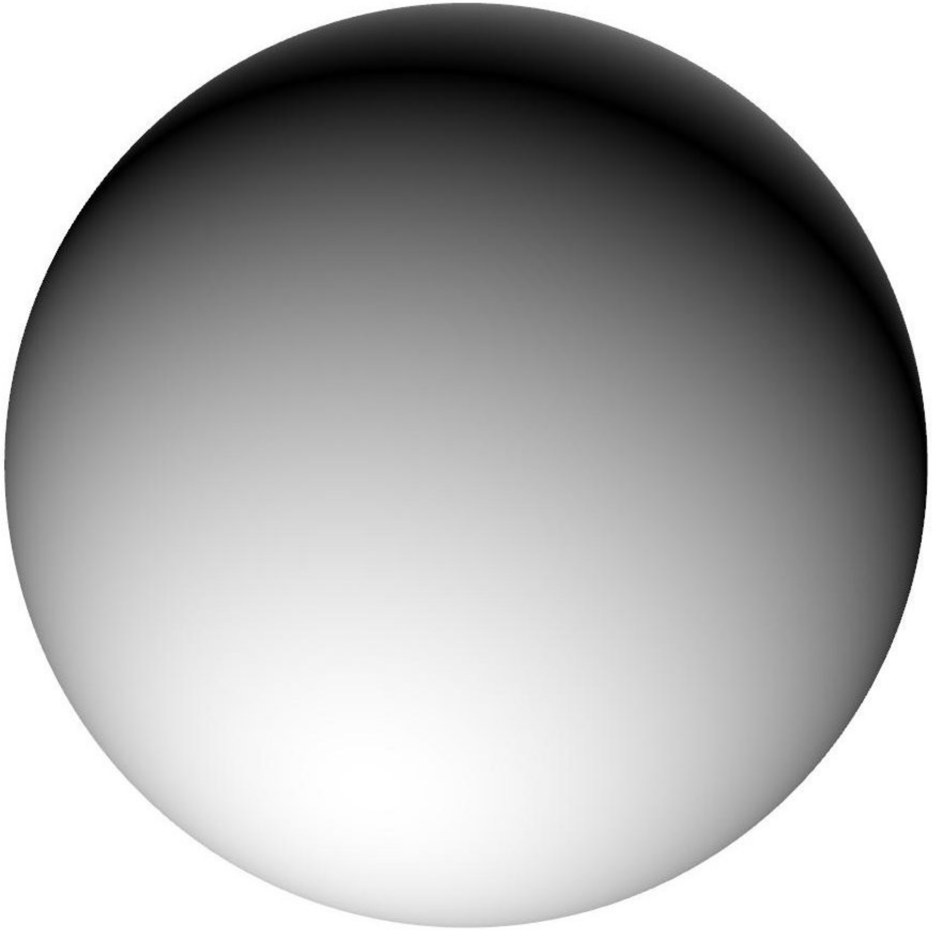


PuMA Visualization

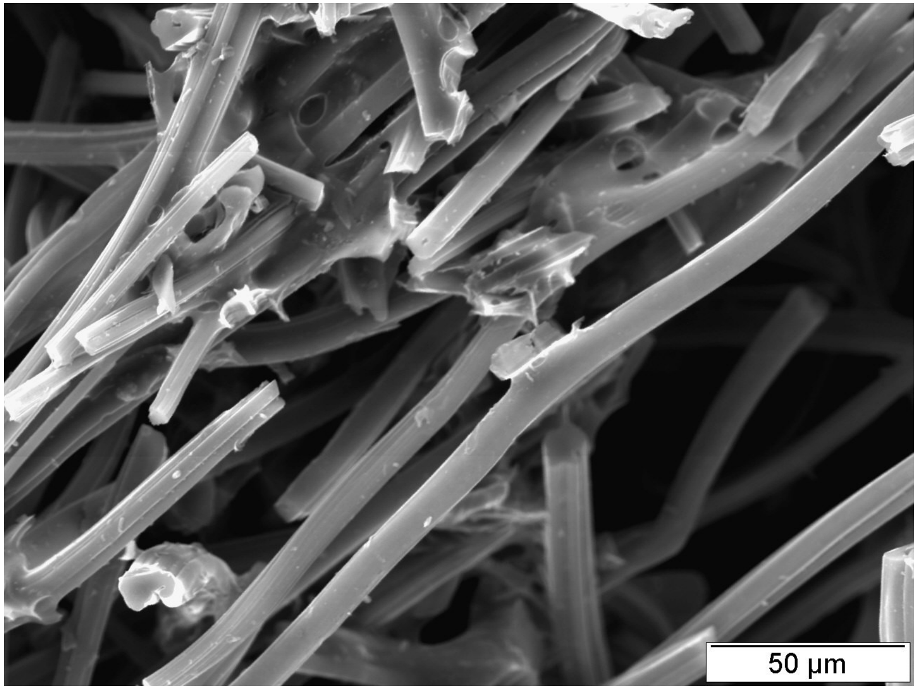
- Based upon an OpenGL framework written by Tim Sandstrom
- Uses triangle normals create an appropriate texture
- Capable of showing tomography images in good detail
- Can generate movies of material as well as movies of simulations progressing over time intervals

Material Properties

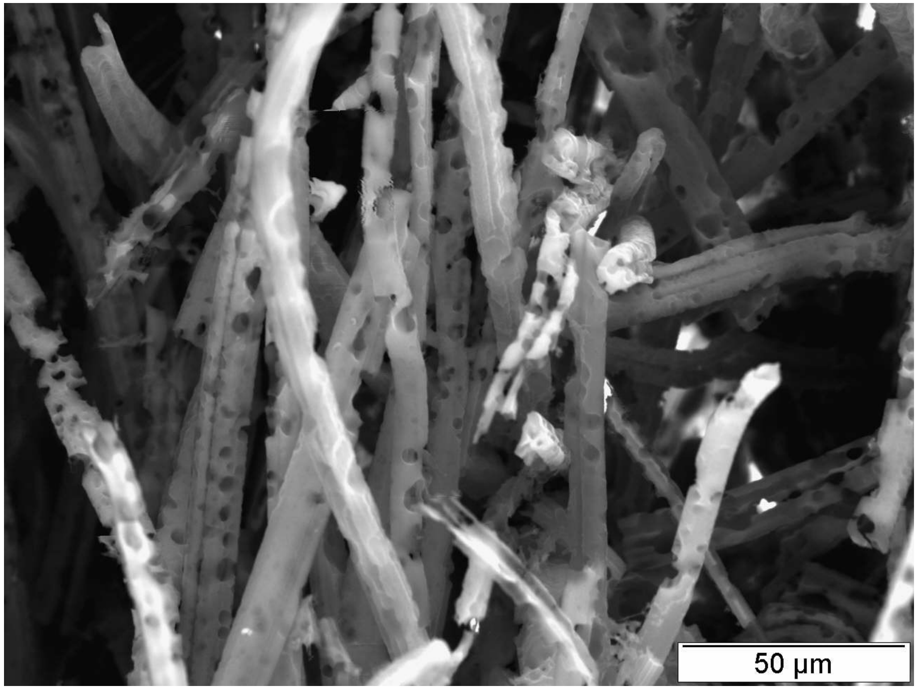
- Specific Surface Area
  - Requires Marching Cubes
  - Calculated as a sum of individual triangle areas
- Porosity
  - function of grayscale threshold



Oxidation



Virgin



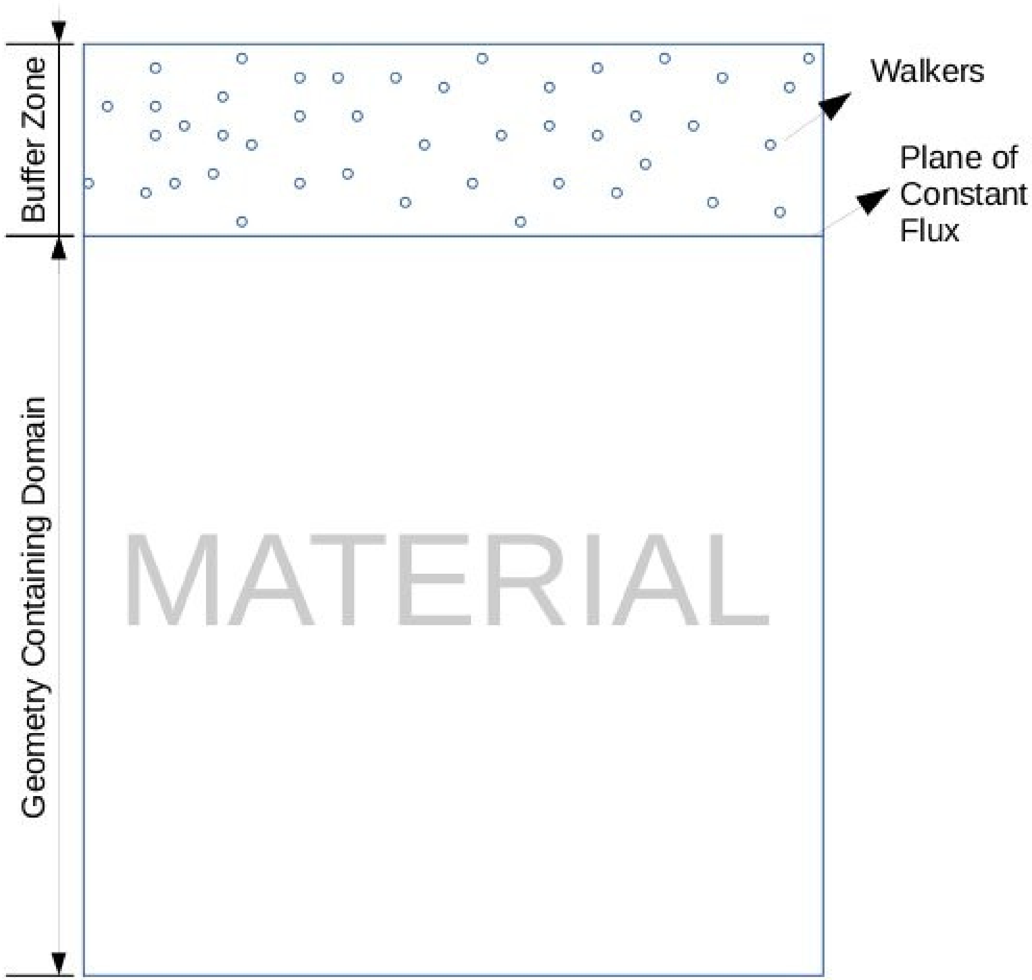
Tested

- How the material decomposes at the fiber scale
- Simulate this oxidation based upon the microtomography images.

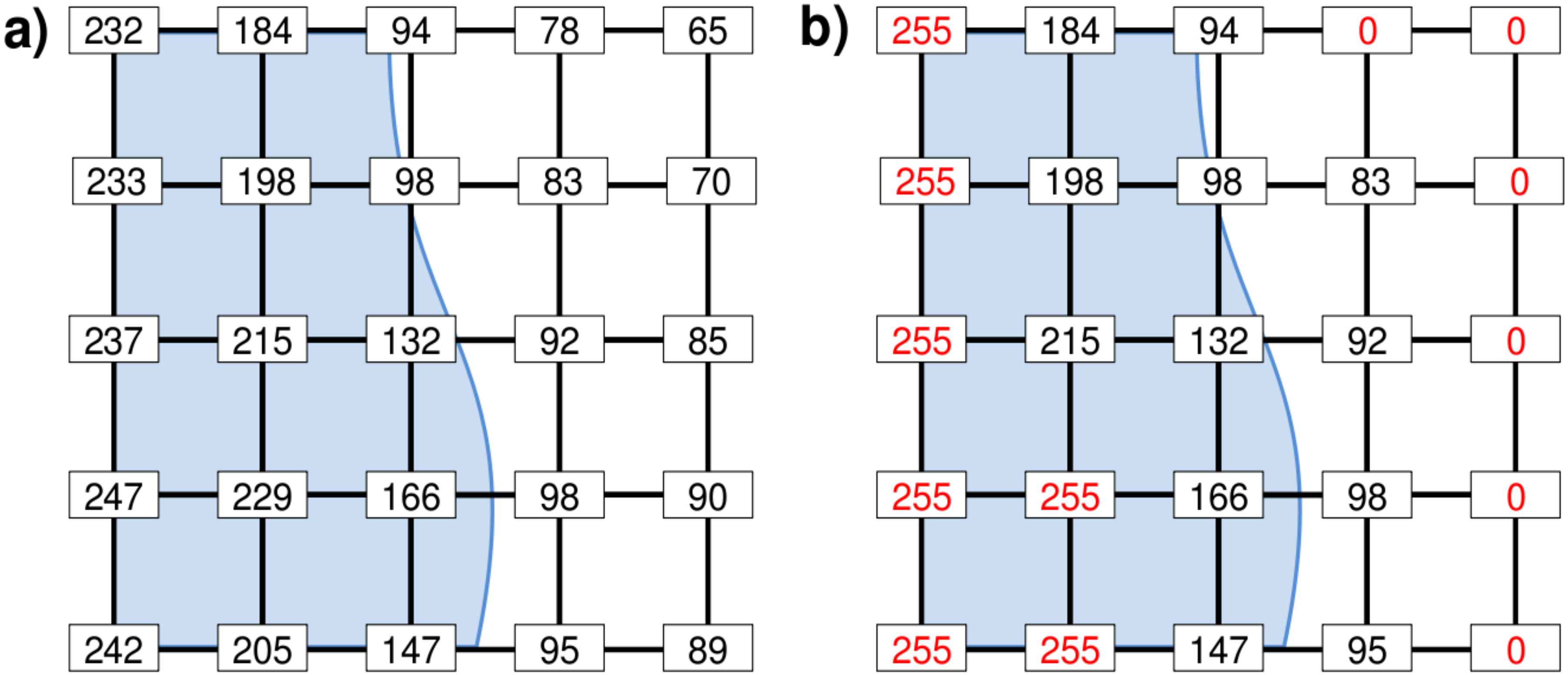
Oxidation Model

Lachaud *et al.*, *CMS*, 44 (2009]

Model Aspects:
- Material Storage
- Oxygen Storage
- Walker Movement
- Collision Handling
- Verification
- Application to Fiberform



Material Storage



Oxygen Storage

$$N_{walkers} = \frac{y_{O_2}\rho_g V}{n_w M_{O_2}}$$

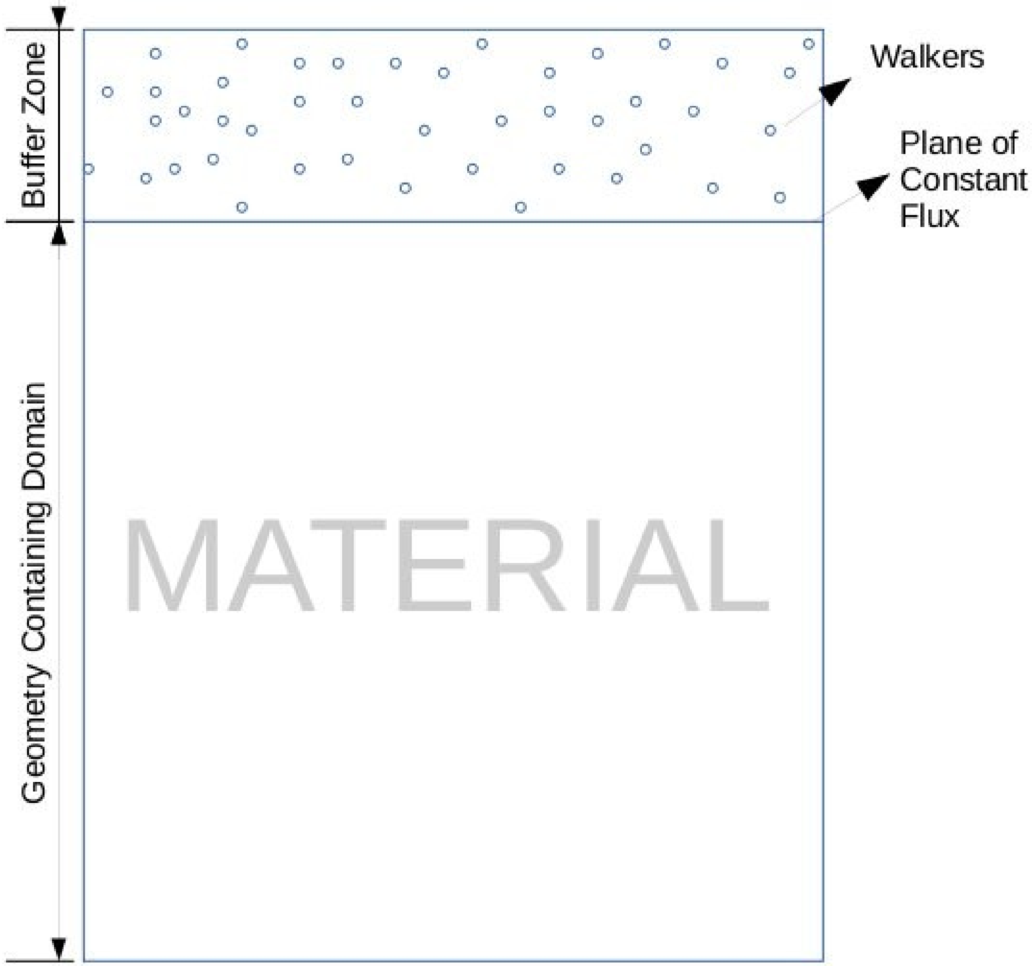
y_{O_2}: mass fraction of O_2

V: volume of the buffer zone

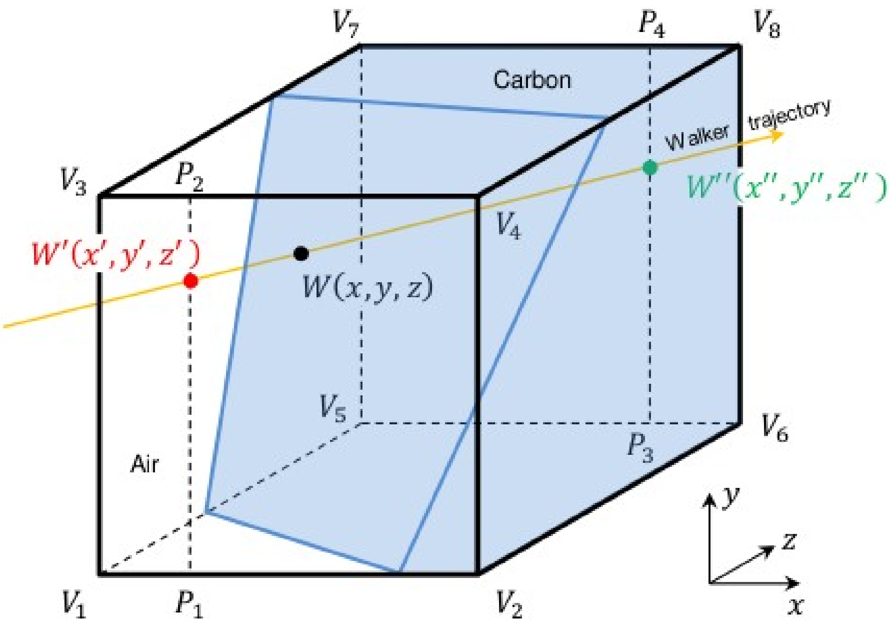
n_w: user-defined number of moles per walker

M_{O_2}: molar mass of oxygen

ρ_g: density of the gas mixture



Walker Movement



Movement of Walker through voxel containing material

$$\Delta t = \frac{\Delta r^2}{6D}$$

$$\Gamma' = a + bx' + cy' + dx'y'$$

$$a = \Gamma_1,\ b = \Gamma_2 - \Gamma_1,\ c = \Gamma_4 - \Gamma_1,\ d = \Gamma_1 - \Gamma_2 + \Gamma_3 - \Gamma_4.$$

$$(x, y, z) = (x', y', z') + \frac{\Gamma^* - \Gamma'}{\Gamma'' - \Gamma'}[(x'', y'', z'') - (x', y', z')]$$

Δt = time increment

$\Delta \mathrm{R}$ = random walk length

D = diffusion coefficient

$\Gamma_1 \ldots \Gamma_8$ = vertex grayscale values

Γ' = grayscale at entrance

Γ'' = grayscale at exit

Γ^* = grayscale threshold

Collision Handling

$$\tilde{P}_s = \frac{1}{1 + \frac{3\gamma D}{2k\Delta r_w}} \qquad \alpha = \frac{M_s n_w}{\rho_S \tilde{V}} 256$$

P_s = stsicking probability

D = diffusion coefficient

γ = sticking coefficient

Δr_w = walk length before collision

k = reactivity of material (fiber or matrix)

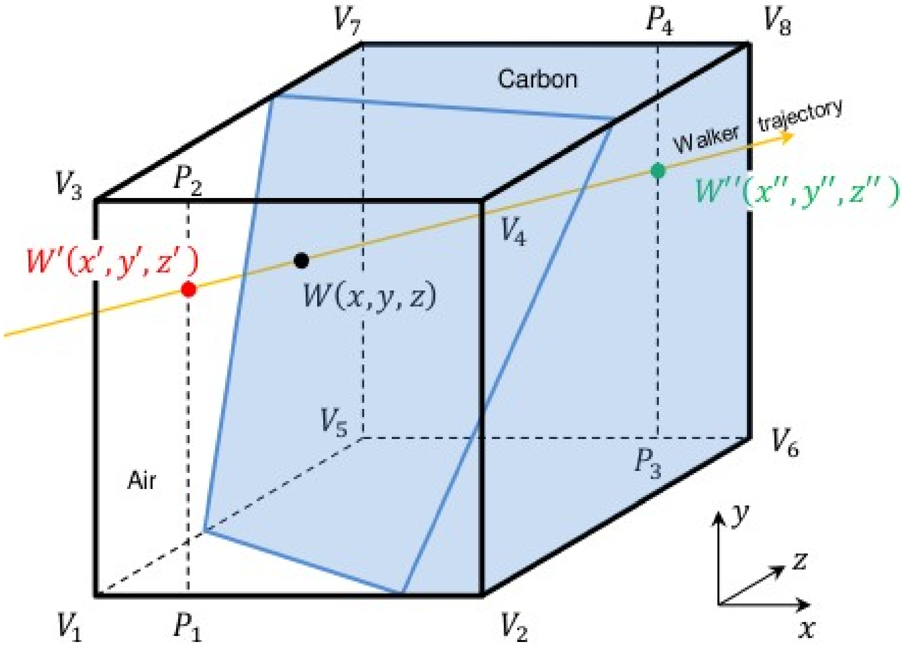
α = grayscale attenuation

M_S = molar mass of solid

ρ_s = density of solid

$\tilde{V}$ = voxel volume

n_w = mols of oxygen per walker



Verification

Exact solution Developed by Lachaud and Vingoles:

$$A = \frac{k_m \Omega_m}{k_f \Omega_f} \qquad Sh = \frac{k_m R_f}{D}$$

A = reactivity contrast

k_m = reactivity matrix

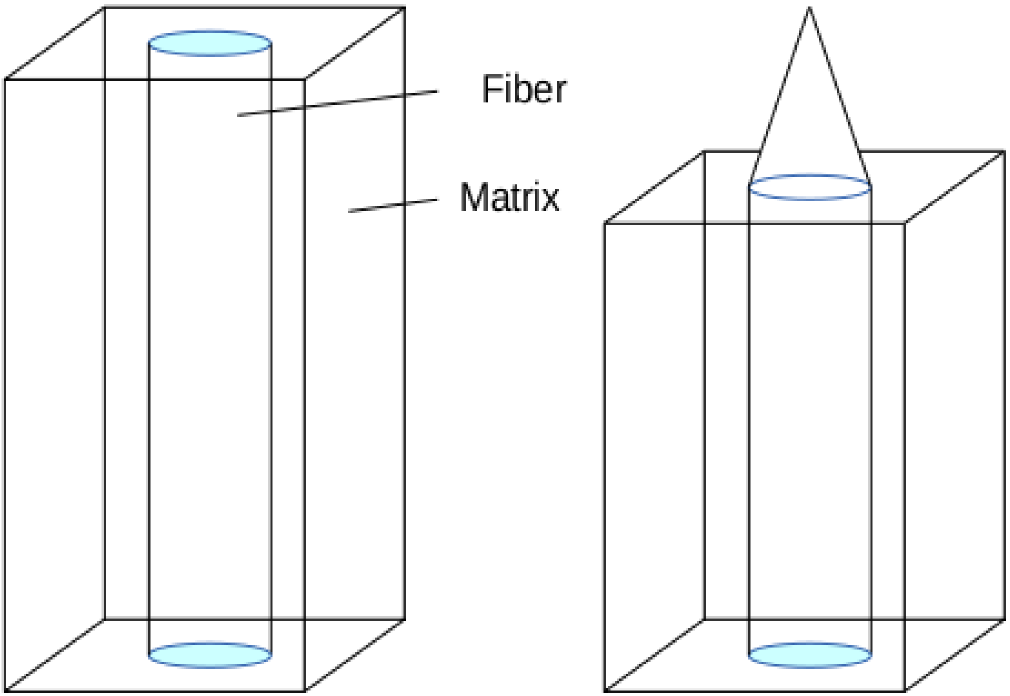
k_f = reactivity fiber

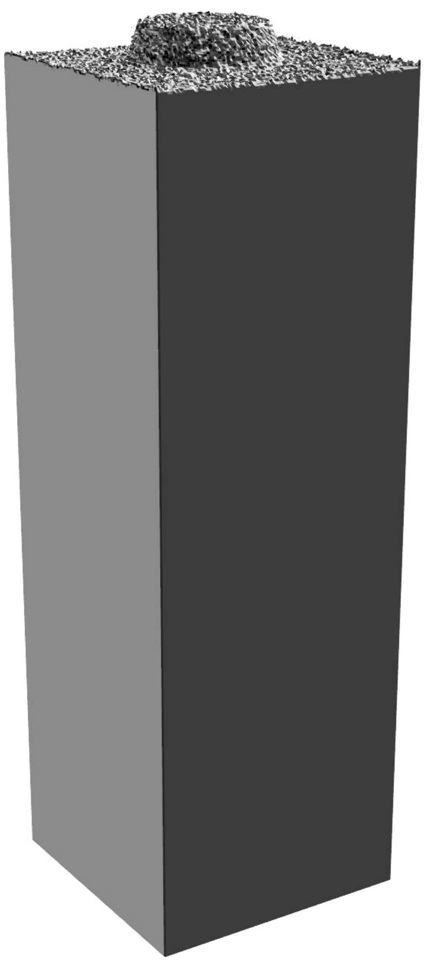
Ω_m = volume fraction matrix

Ω_f = volume fraction fiber

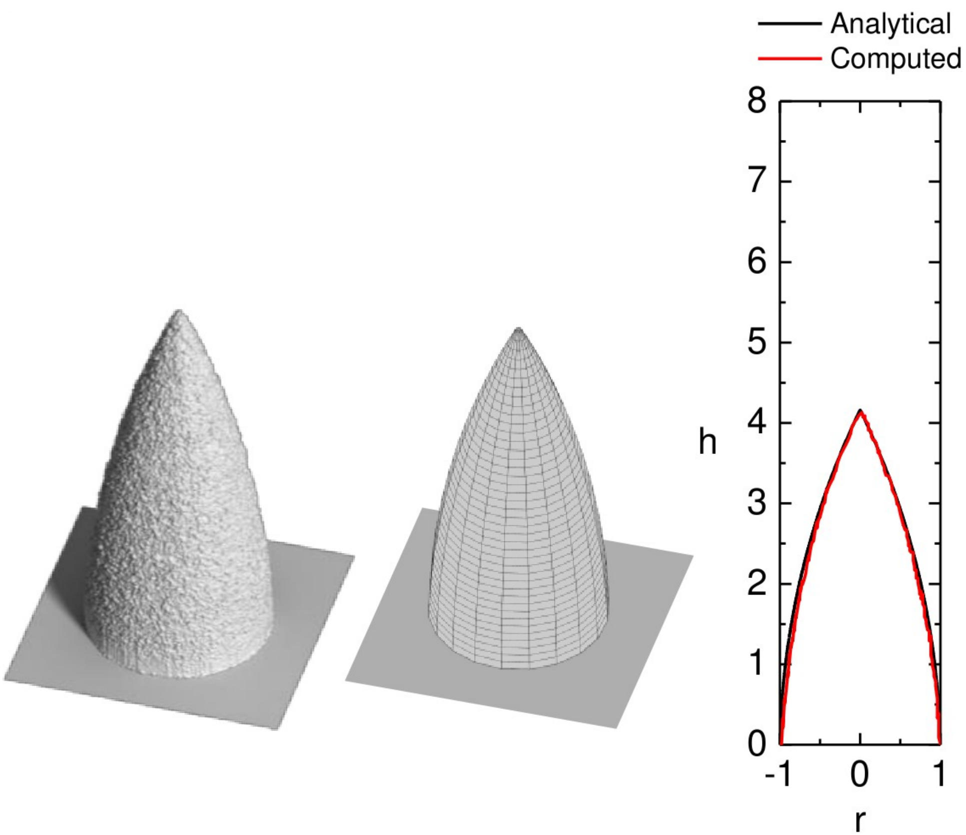
Sh = sherwood number

R_f = radius of fiber

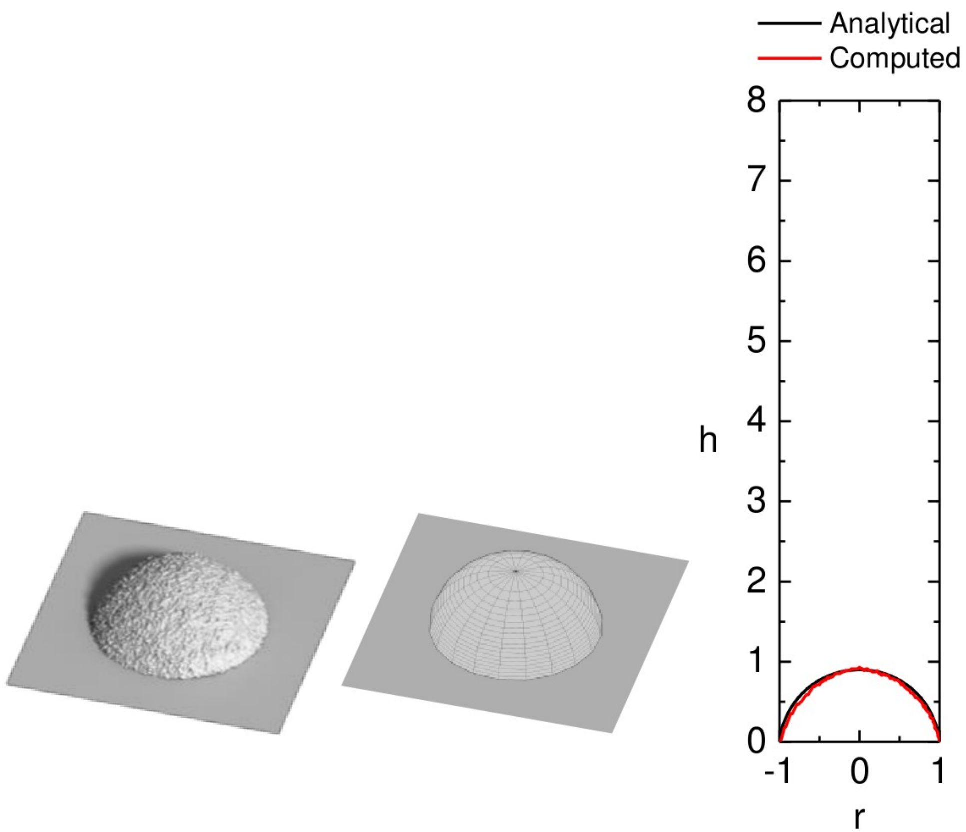




Diffusion Limited

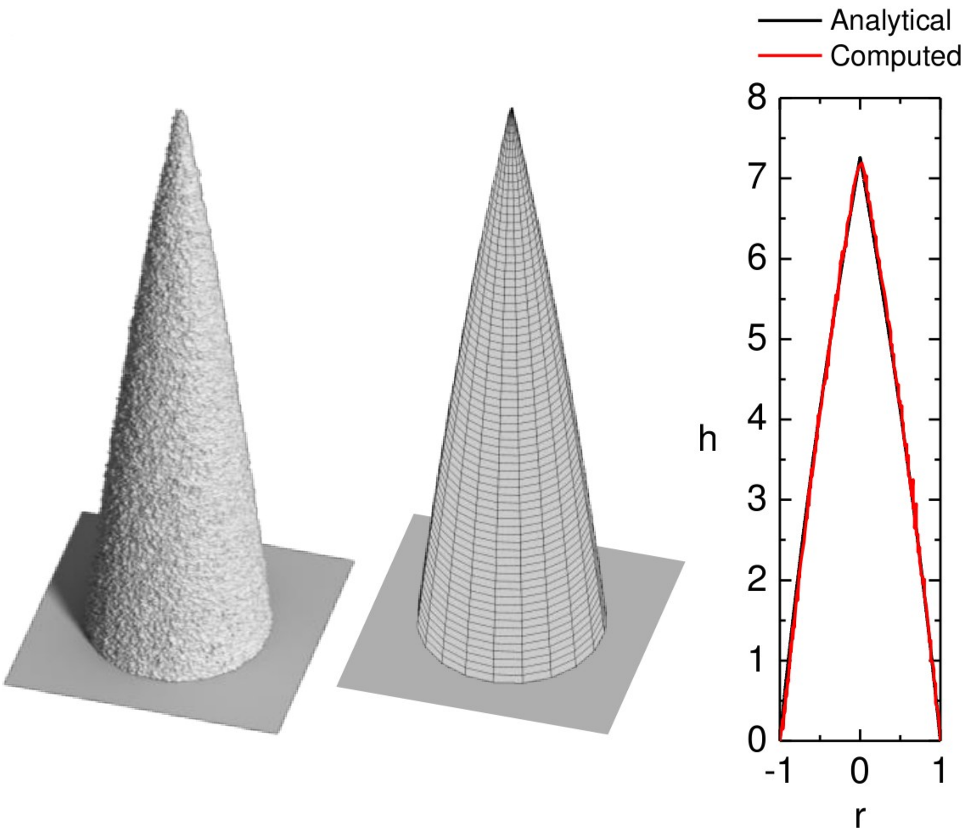


A = 50   Sh = 5

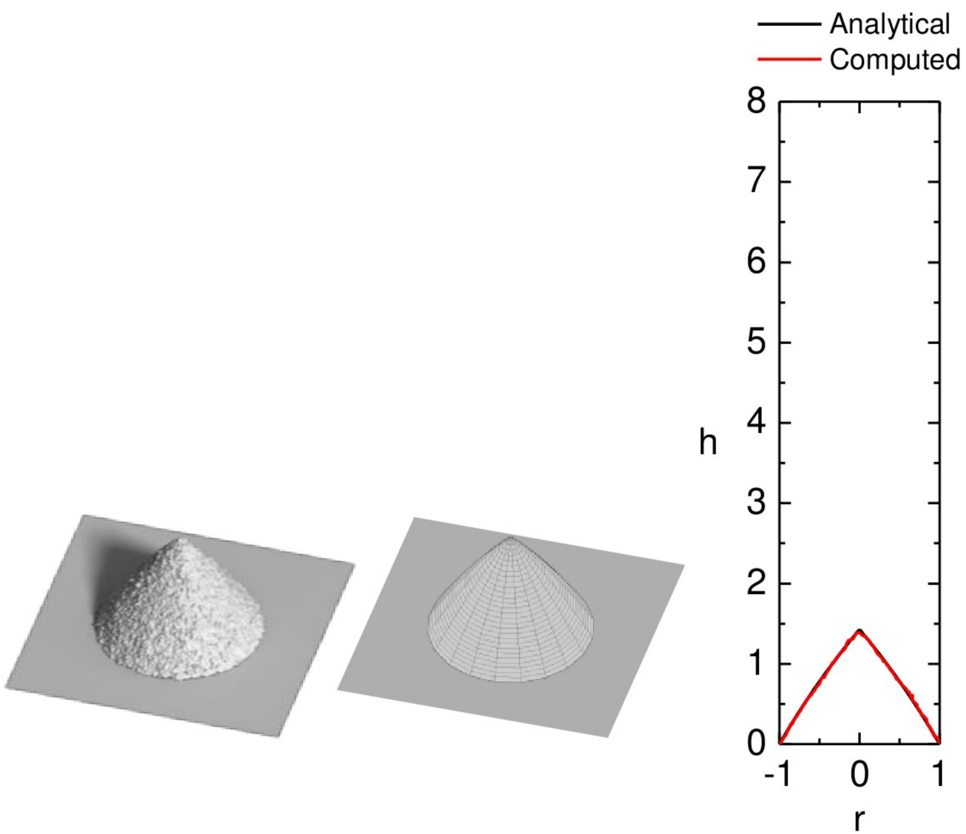


A = 10   Sh = 10

Reaction Limited



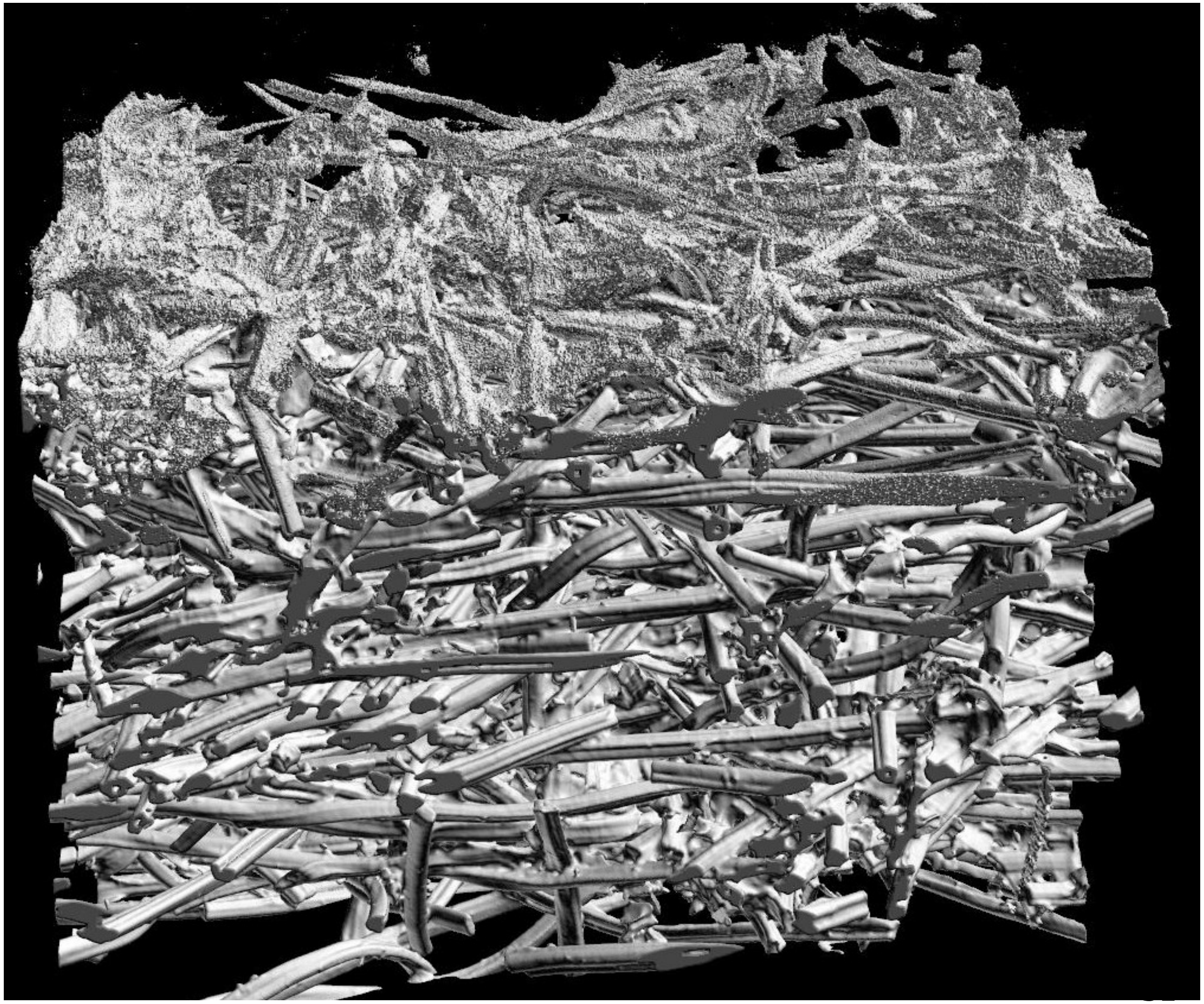
A = 10 Sh = 0.1

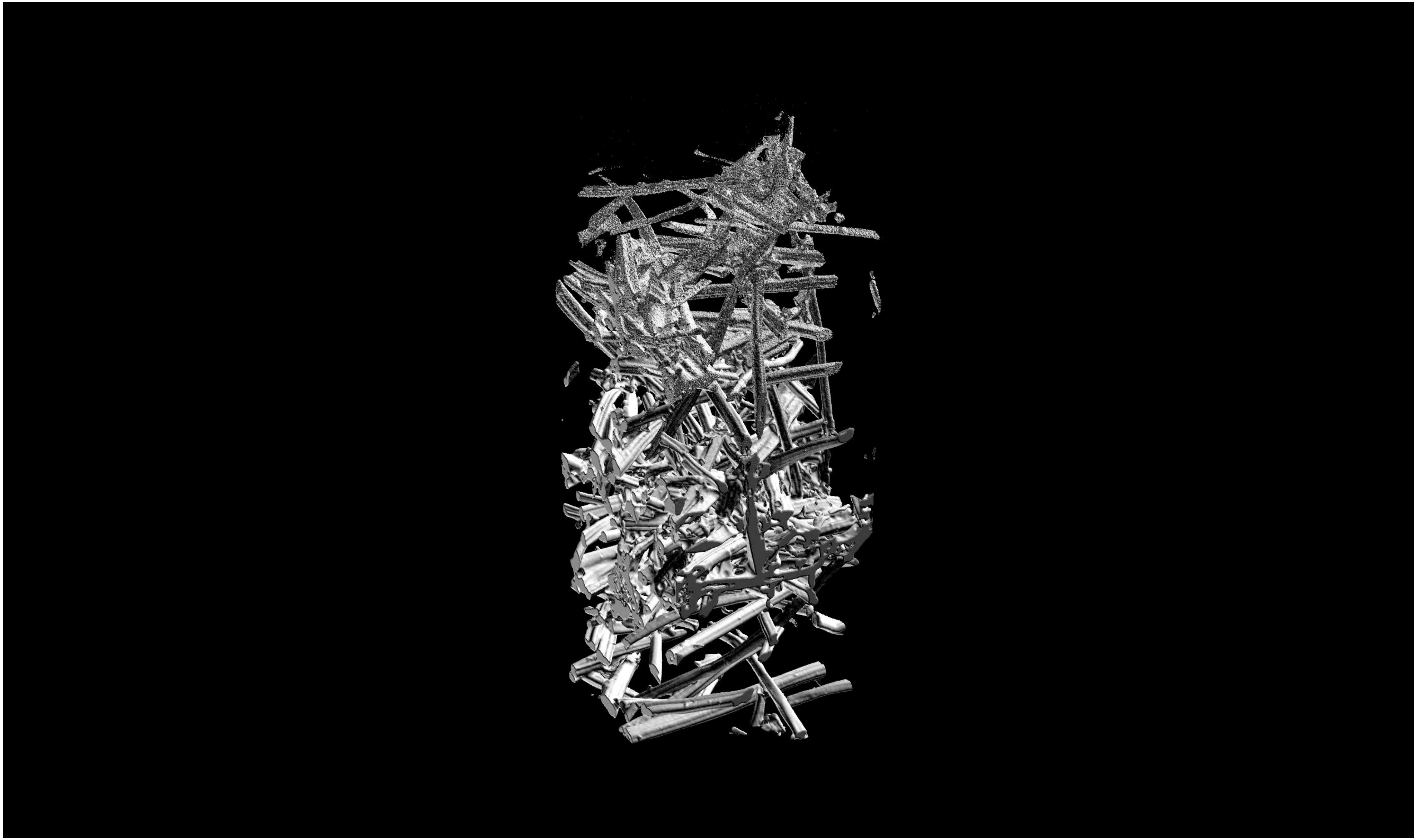


A = 2 Sh = 0.2

Oxidation applied to Fiberform

- Volume Ablation
  - High diffusion vs. reaction
- Surface Ablation
  - High reaction vs. diffusion
- Mixed Regime





Summary and Outlook

- Obtained microtomography images to use for material properties and simulations
- Developed framework to import and process images
- Calculation of basic material properties
- Completion of Oxidation simulation

Next Steps:

- Add artificially generation phenolic matrix for oxidation
- Parallelization of Oxidation Model
- Calculation of more material properties (tortuosity, mean pore diameter, etc)
- Module for thermal conductivity

Contributors

NASA

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LBNL

Alastair MacDowell

Dula Parkinson

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