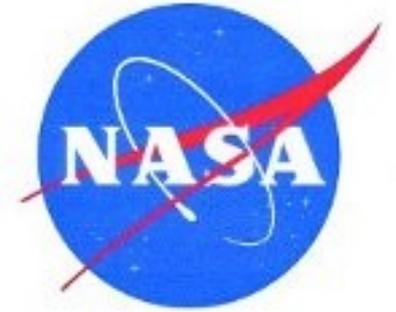


# Modeling of the fiber-scale oxidation of highly-porous carbon fiber materials based on synchrotron X-Ray Microtomography

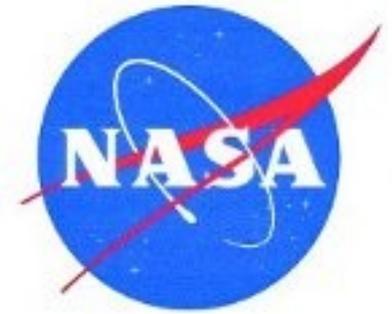


Applied Modeling & Simulation (AMS) Seminar Series

NASA Ames Research Center, 31 July 2014

Joseph Ferguson, Francesco Panerai, Timothy Sandstrom,  
Jean Lachaud, Alexandre Martin, Nagi Mansour

# Thermal Protection Systems



Ceramic Tiles



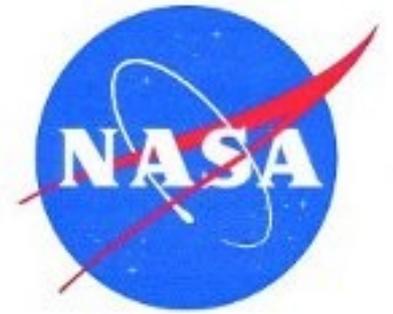
- Used on the Space Shuttle
- Reusable
- Reentry from LEO

Ablative Heat Shields



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

# Ablative TPS and PICA



FiberForm®



+

Resin



=

PICA

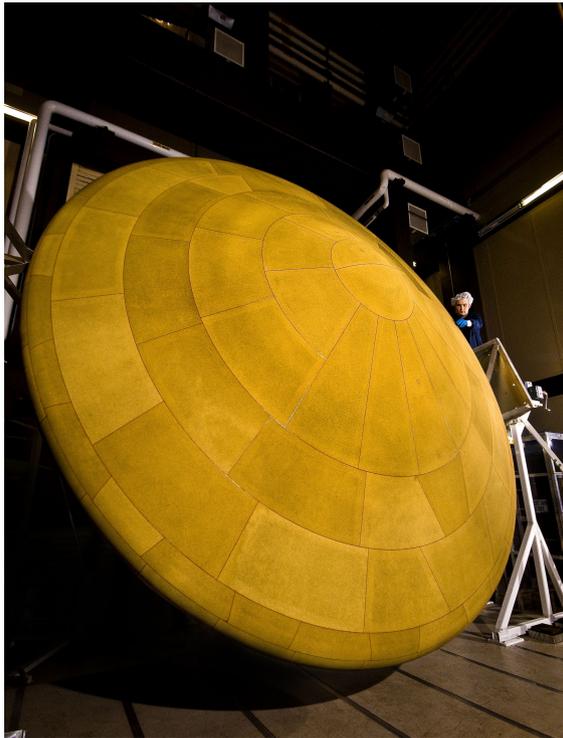
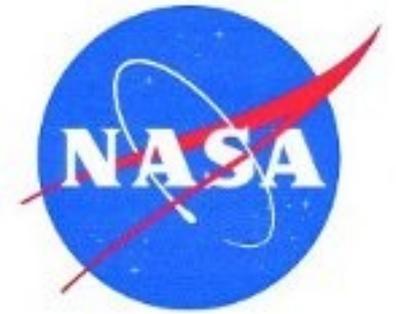


- Light weight Carbon / Phenolic Ablator
- Successfully flight tested
- SpaceX development of PICA - X



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

# PICA Flight Tests



Mars Science Laboratory  
(Curiosity Rover)

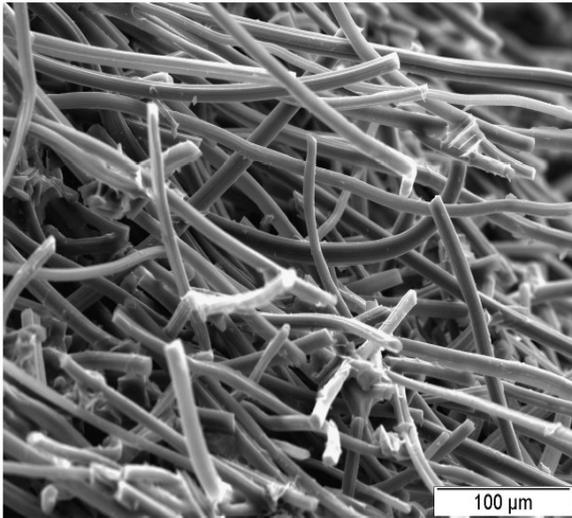
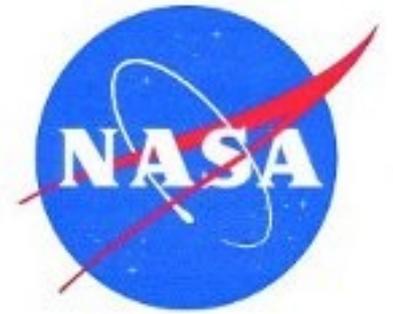


Stardust Capsule

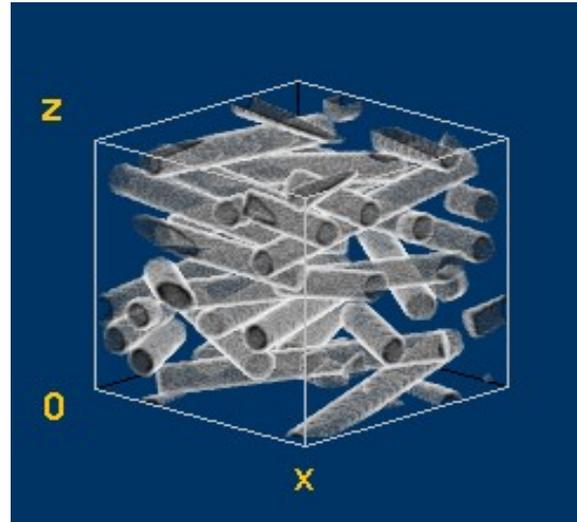


SpaceX Dragon V1, V2

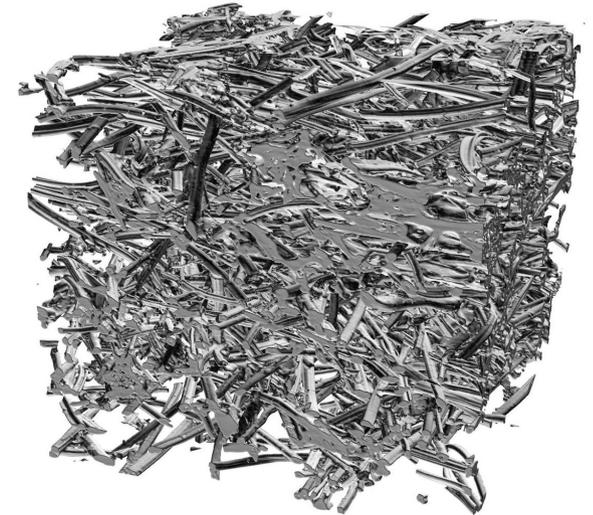
# PICA Modeling



SEM Image of Fiberform



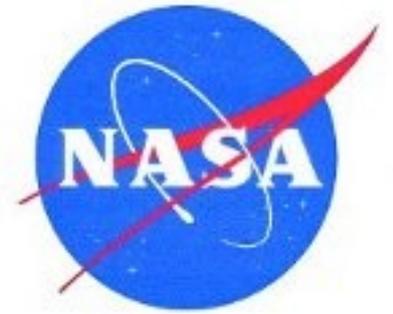
Artificially Generated Fiberform



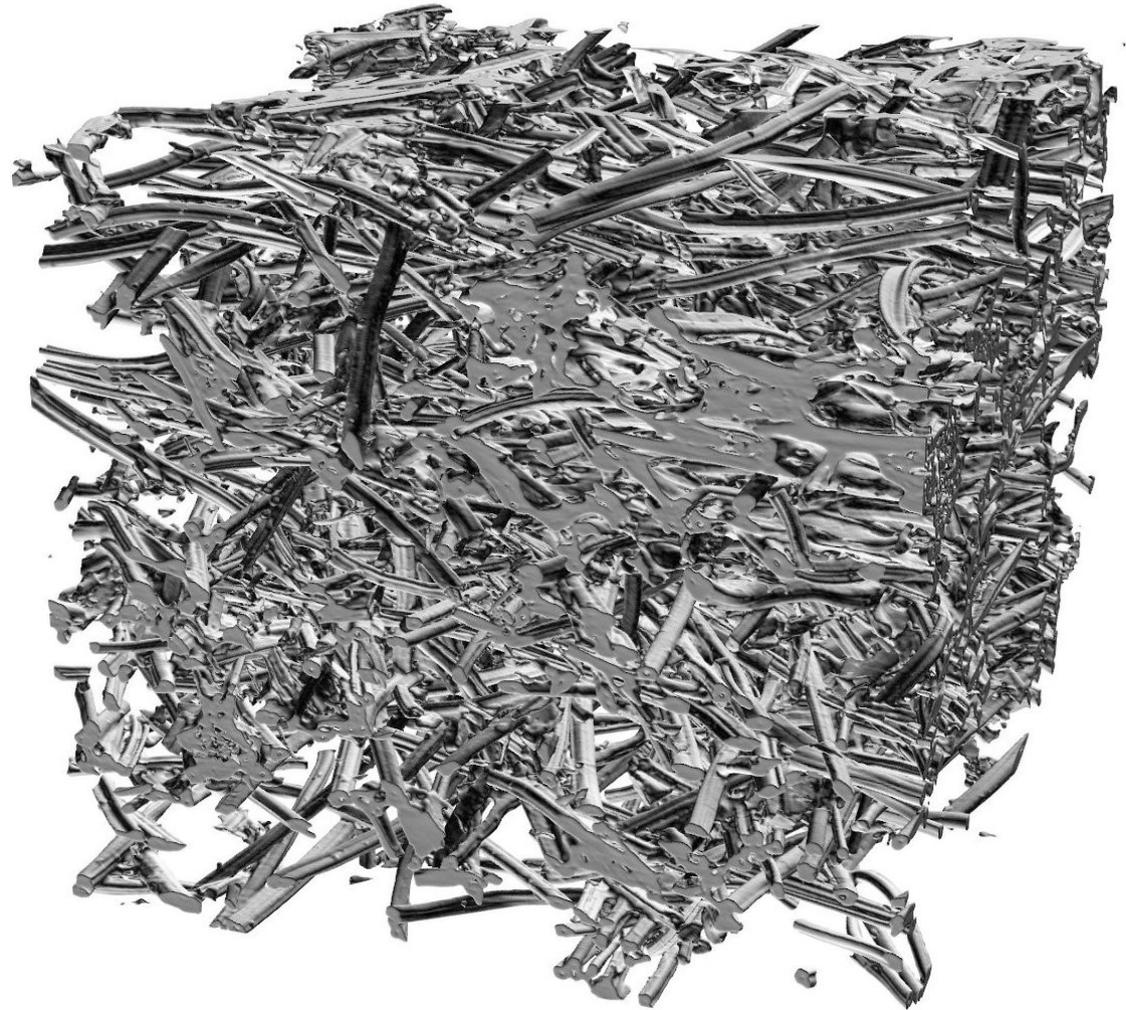
Surface Rendering of  
Microtomography Image

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

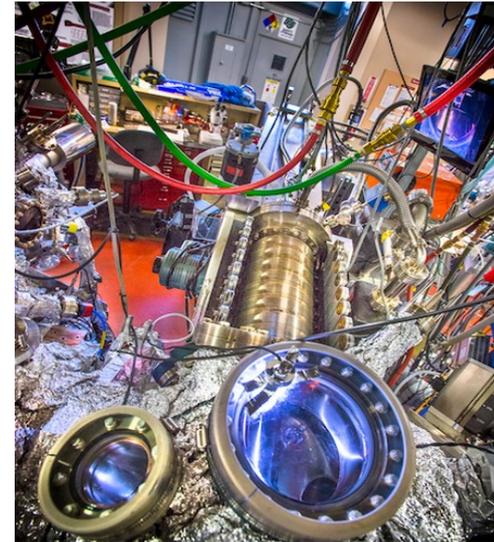
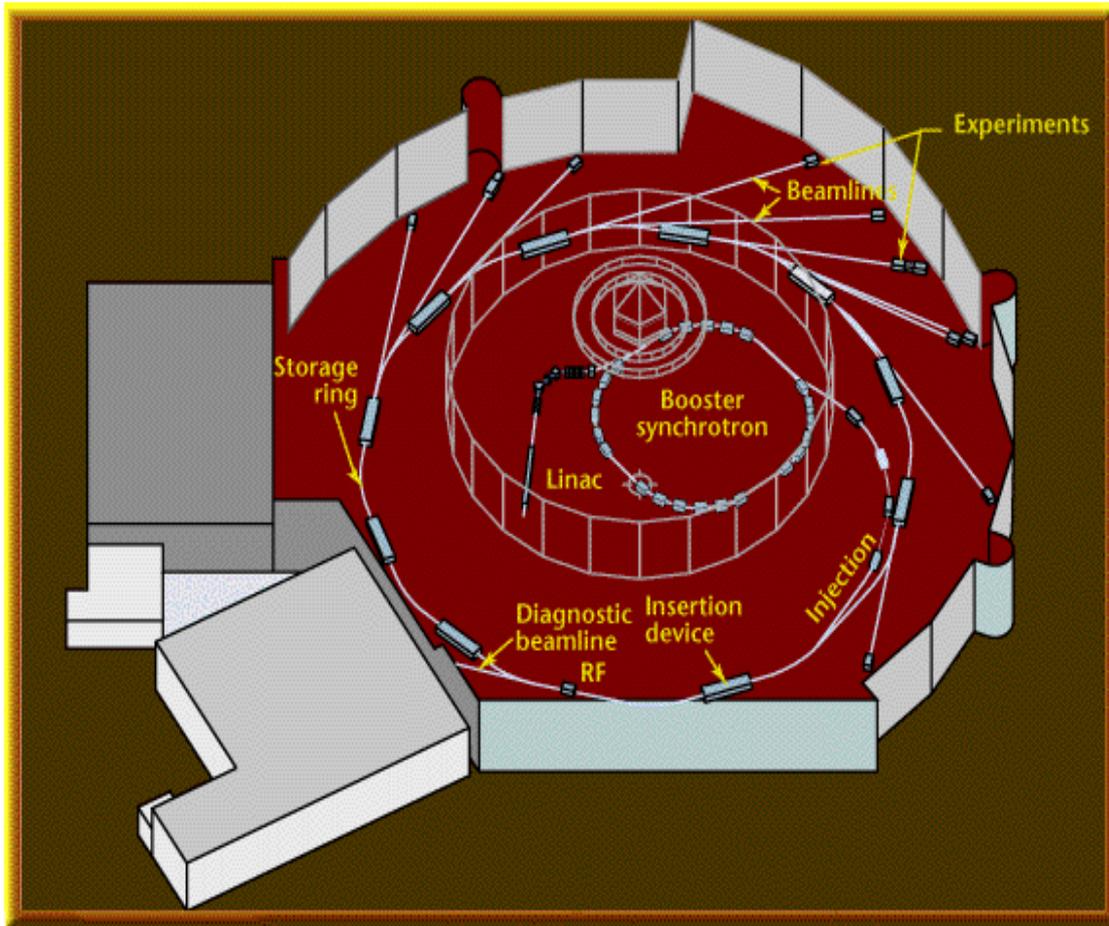
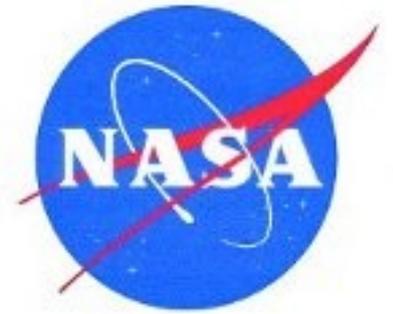
# Objectives



- 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

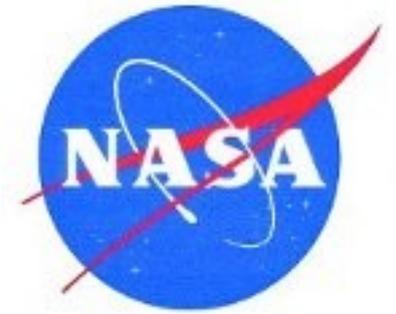


# Synchrotron Microtomography



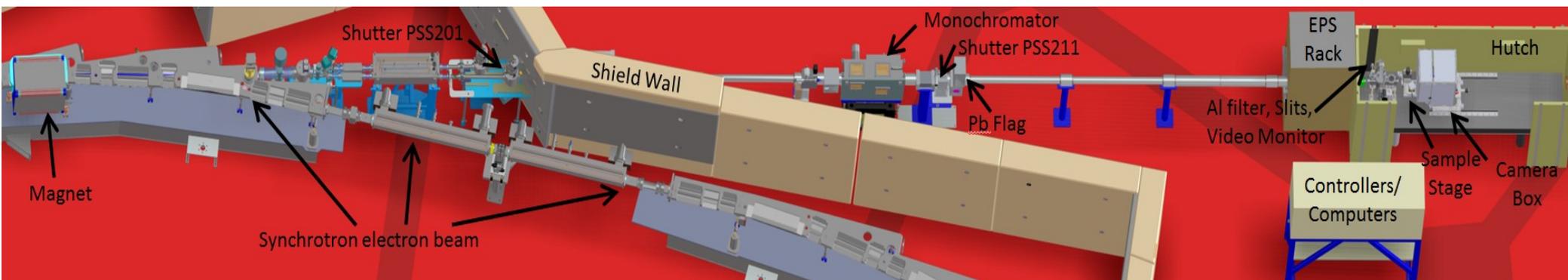
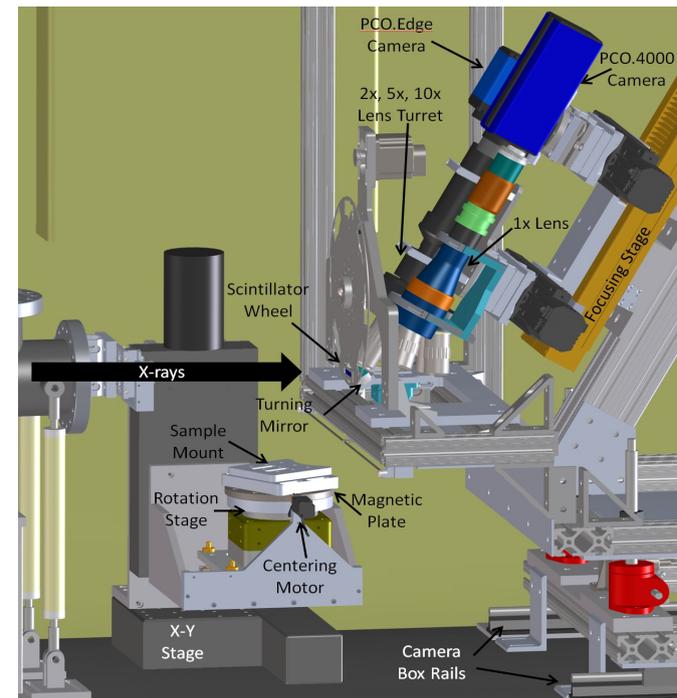
<http://www2.lbl.gov/MicroWorlds/ALSTool/>

# 8.3.2 Beamline

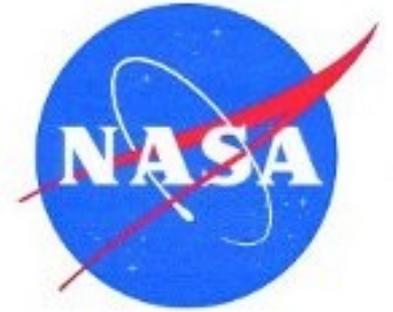


- Hard X-ray microtomography
- 14 KeV X-rays
- Processed through scintillator, magnification lens, and a camera

<http://microct.lbl.gov/manual>

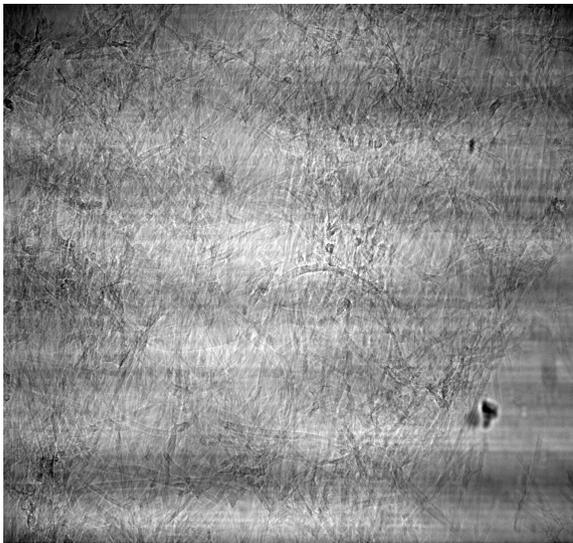


# Projection processing

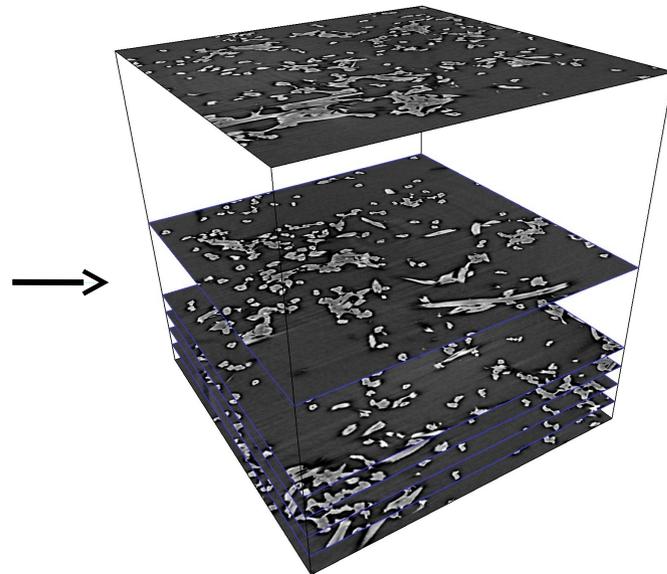


- Fiji plugin reconstruction algorithm.
- Converts 2048 projections into a 3D image stack

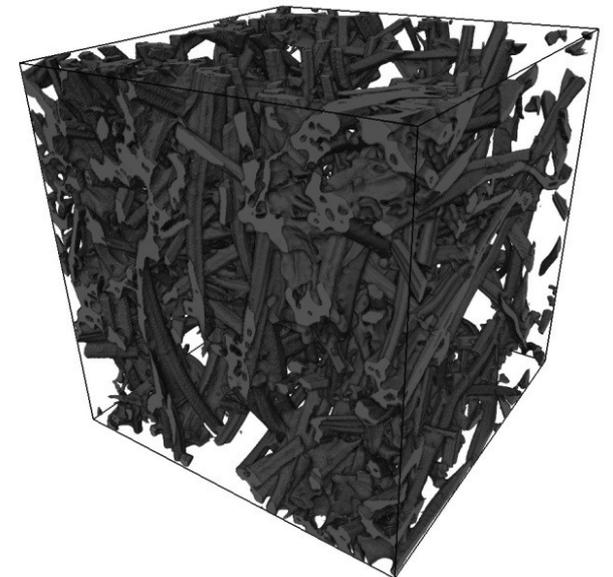
2048 Projections



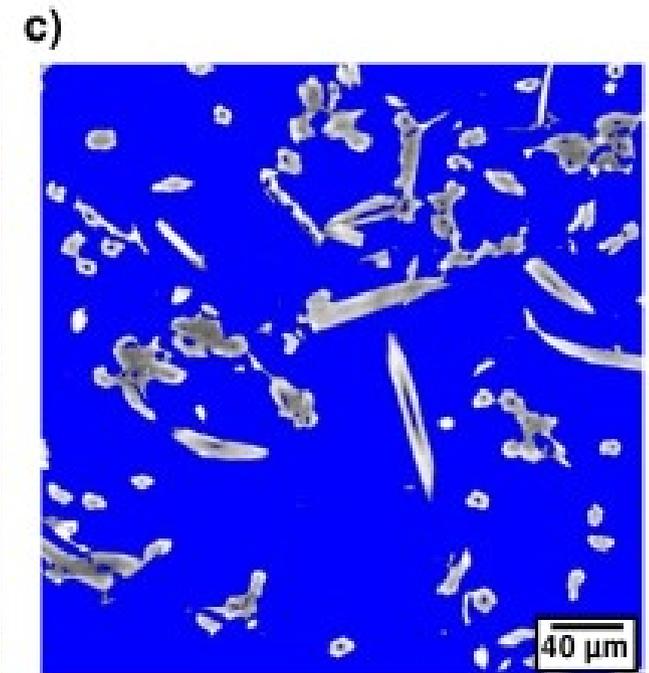
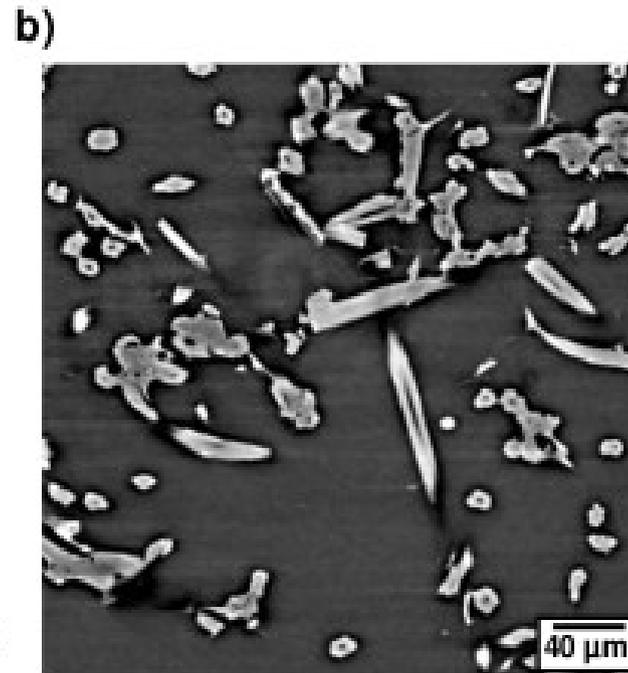
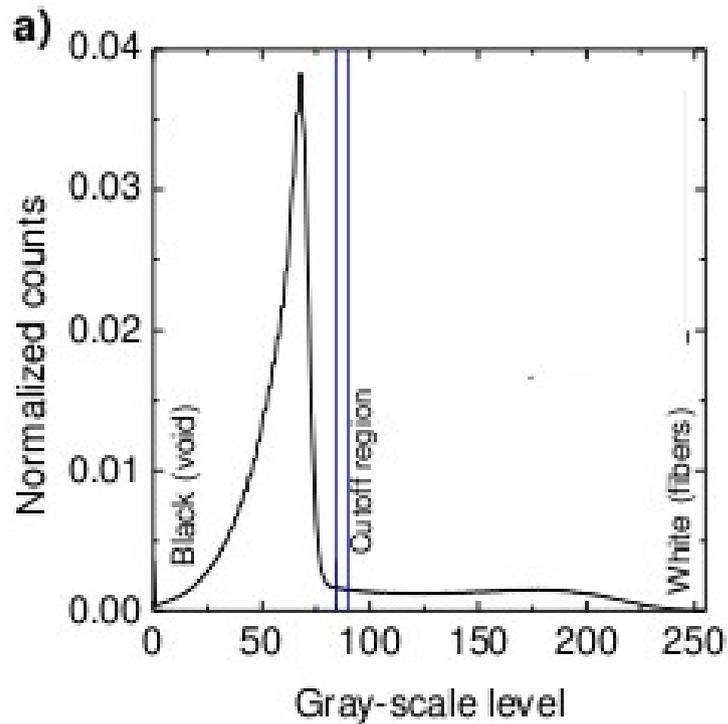
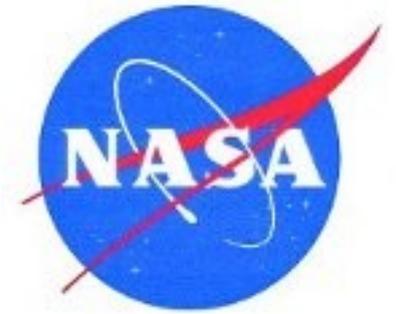
About 1600 Image Slices



Volume Rendering of Material



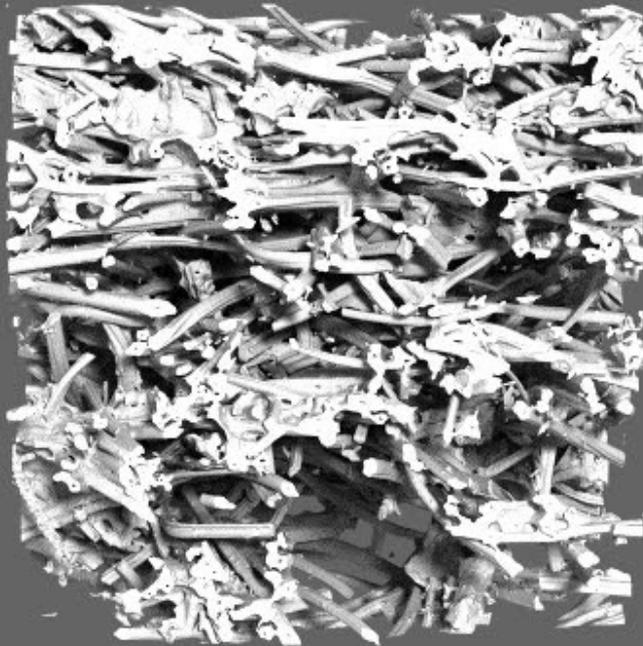
# Grayscale Cutoff



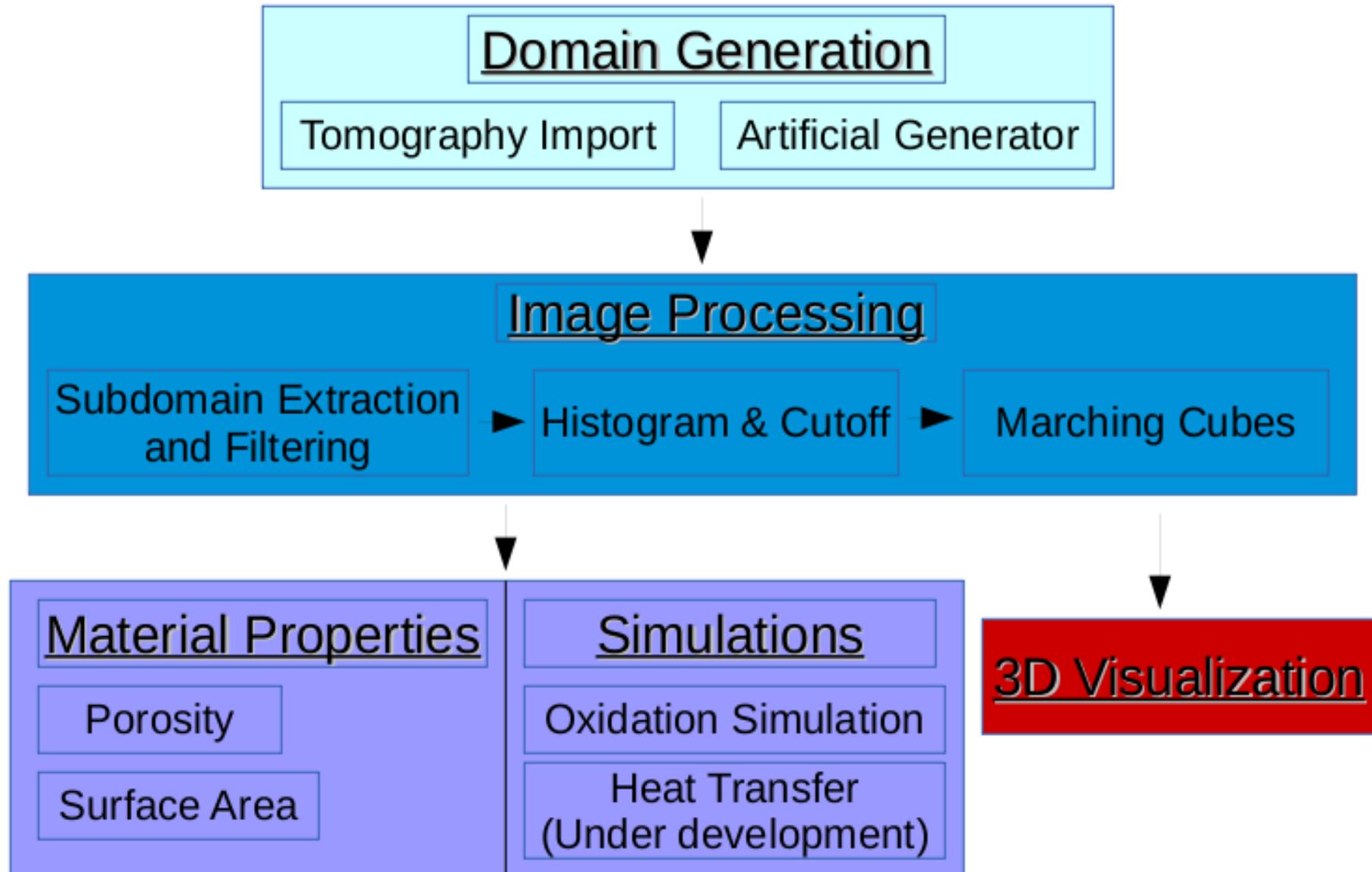
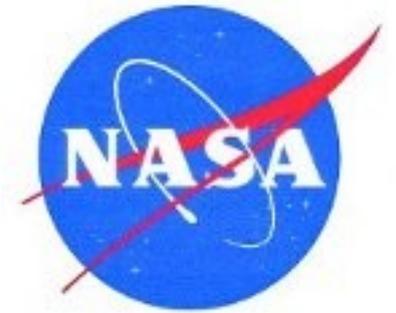
Histogram of grayscale frequencies

Original Slice

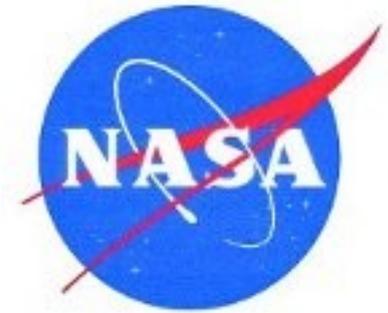
Slice with threshold applied



# Porous Media Analysis (PuMA)



# Image Import



PuMA

Import 3D Image Oxidation

Import From File Generate Geometry

List of Images (.txt) Location of Images Load Images

reconstructed/flist.txt phase\_reconstructed 100%

Image Domain:

X-max 1201 Y-max 1192 Z-max 1520

X1 300 X2 900

Y1 300 Y2 900

Z1 0 Z2 1000

Voxel Length: 0.650

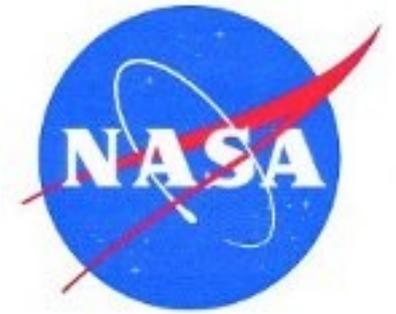
Import 0%

TIFF Images Image: 1352

A 3D visualization of a porous media structure, showing a dark, textured surface within a circular frame. A red rectangular bounding box is overlaid on the structure, indicating the selected region for import. The structure appears to be a complex, interconnected network of fibers or channels.

PuMA  
Porous Media Analysis

# Artificial Geometry Generator



**PuMA**

Import 3D Image Oxidation

Import From File Generate Geometry

**Artificial PICA Geometry**

X Range  Y Range  Z Range

Average Radius  Radius Variation

Average Length  Length Variation

Angle Variation  Voxel Length

Allow Intersect  Contained

Generate Geometry

**Artificial Sphere Geometry**

X Range  Y Range  Z Range

Sphere Radius:

Generate Geometry

**Artificial Cube Geometry**

X Range  Y Range  Z Range

X Length  Y Length  Z Length

X Start  Y Start  Z Start

Generate Geometry

**Artificial Cylinder Geometry**

X Range  Y Range  Z Range

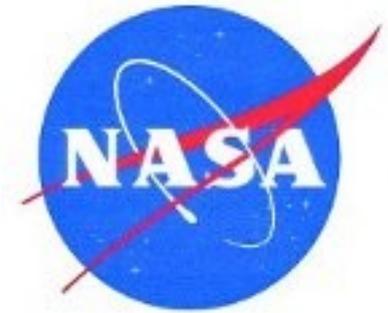
Cylinder Height:  Cylinder Radius:

Cylinder Start:

Generate Geometry

**PuMA**  
Porous Media Analysis

# Histogram and Cutoff



PuMA

Import 3D Image Oxidation

### Grayscale Value Frequency

Parameter	Value
Lowest Grayscale	0
Highest Grayscale	255
Average Grayscale	22
Highest Frequency	60 with 0.0378133

Select Grayscale Value

Grayscale Cut-off: 90

Porosity of Sample:

Export Data to File

Calculate Marching Cubes

0%

Closed Edges (SA Error)

Triangles:

Calculate Surface Area:

Draw Image As:

Solid Triangles

Generate Image

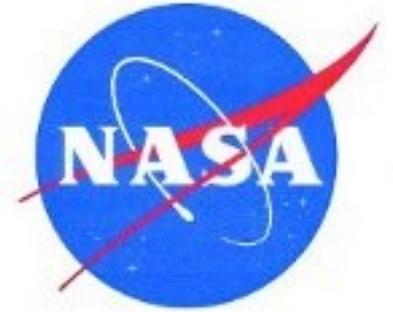
Save Image

Write Triangles to File

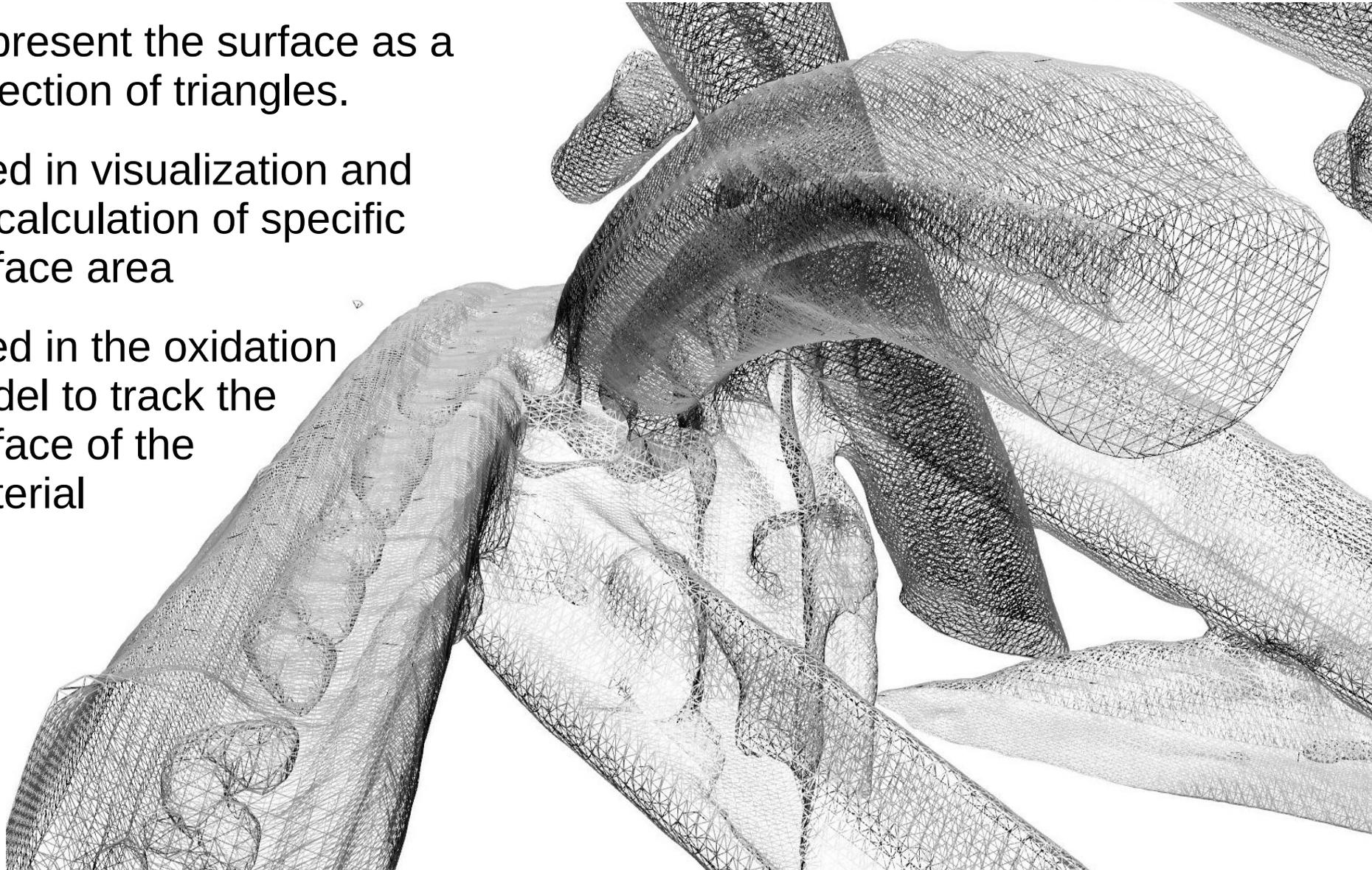
Set Background Color

**PuMA**  
*Porous Media Analysis*

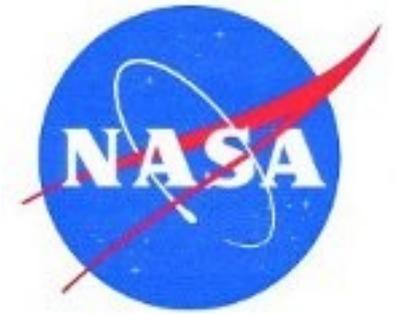
# Marching Cubes Algorithm



- 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

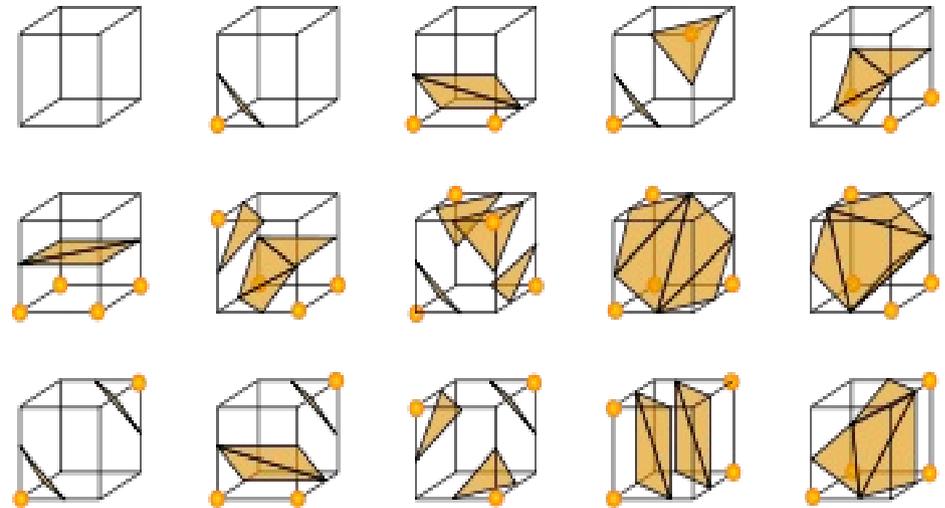


# Marching Cubes Algorithm

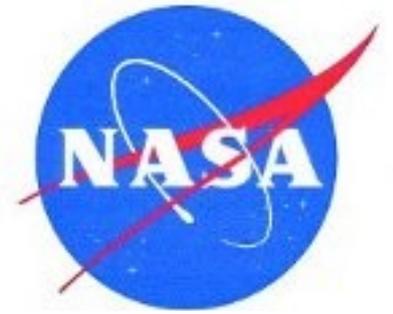


- Marching Cubes Steps:

- 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

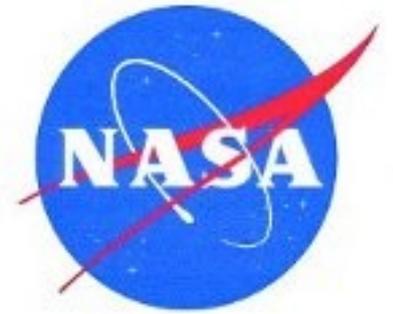


- Based upon an OpenGL framework written by Tim Sandstrom
- Uses triangle normals create an appropriate texture
- Capable of showing tomography images in good detail
- Can generate movies of material as well as movies of simulations progressing over time intervals

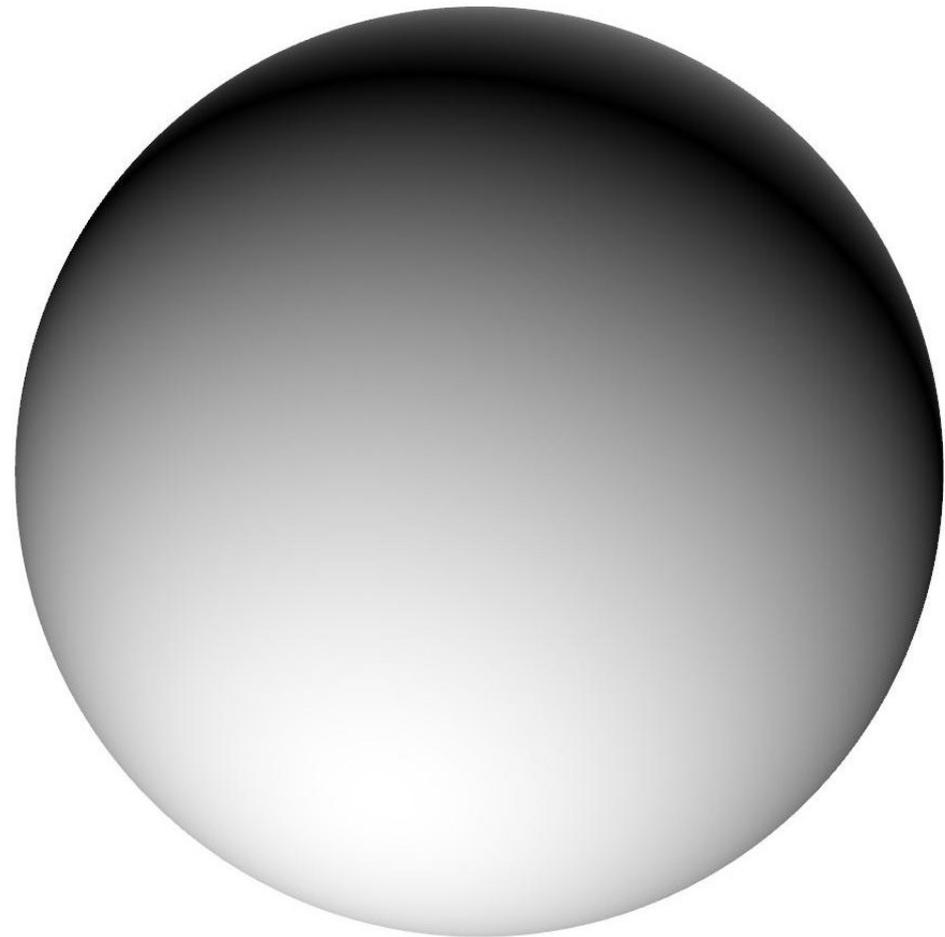




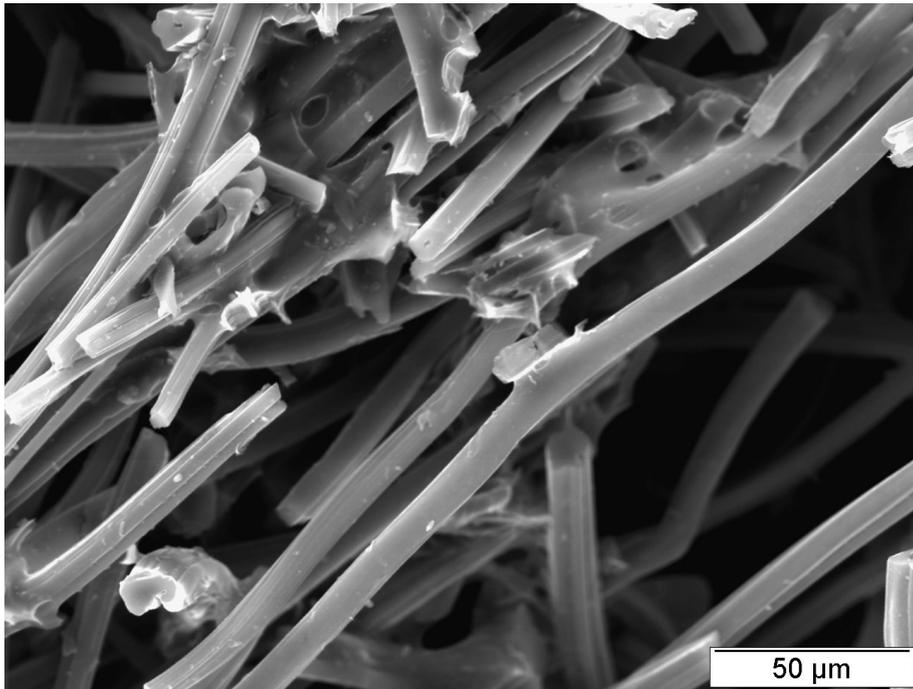
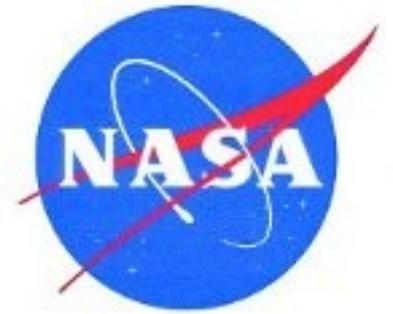
# Material Properties



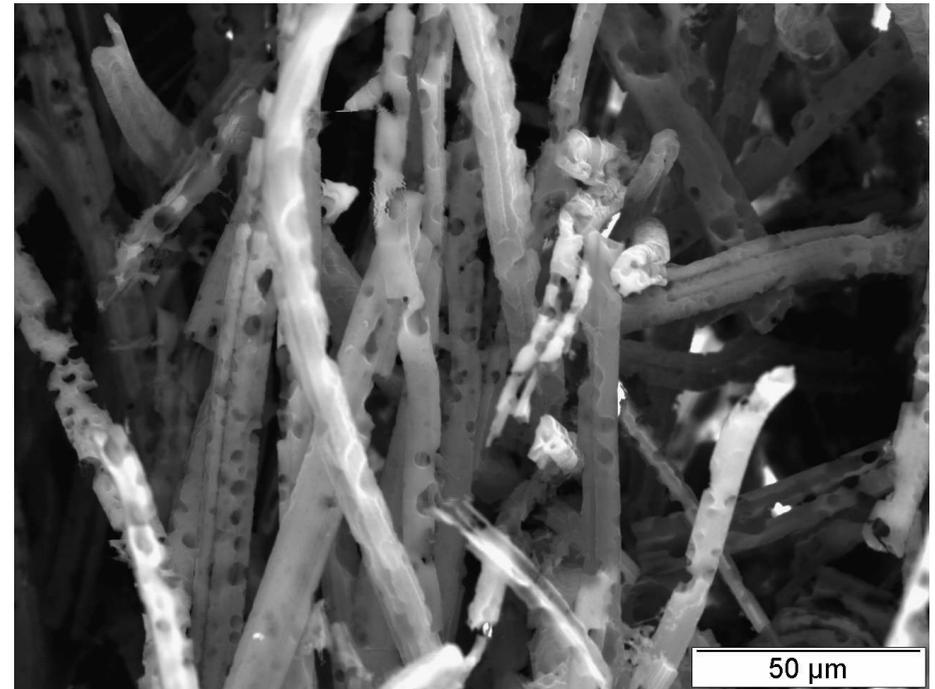
- Specific Surface Area
  - Requires Marching Cubes
  - Calculated as a sum of individual triangle areas
- Porosity
  - function of grayscale threshold



# Oxidation



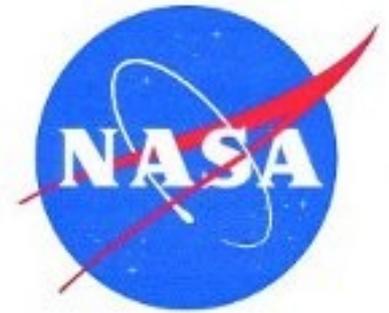
Virgin



Tested

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

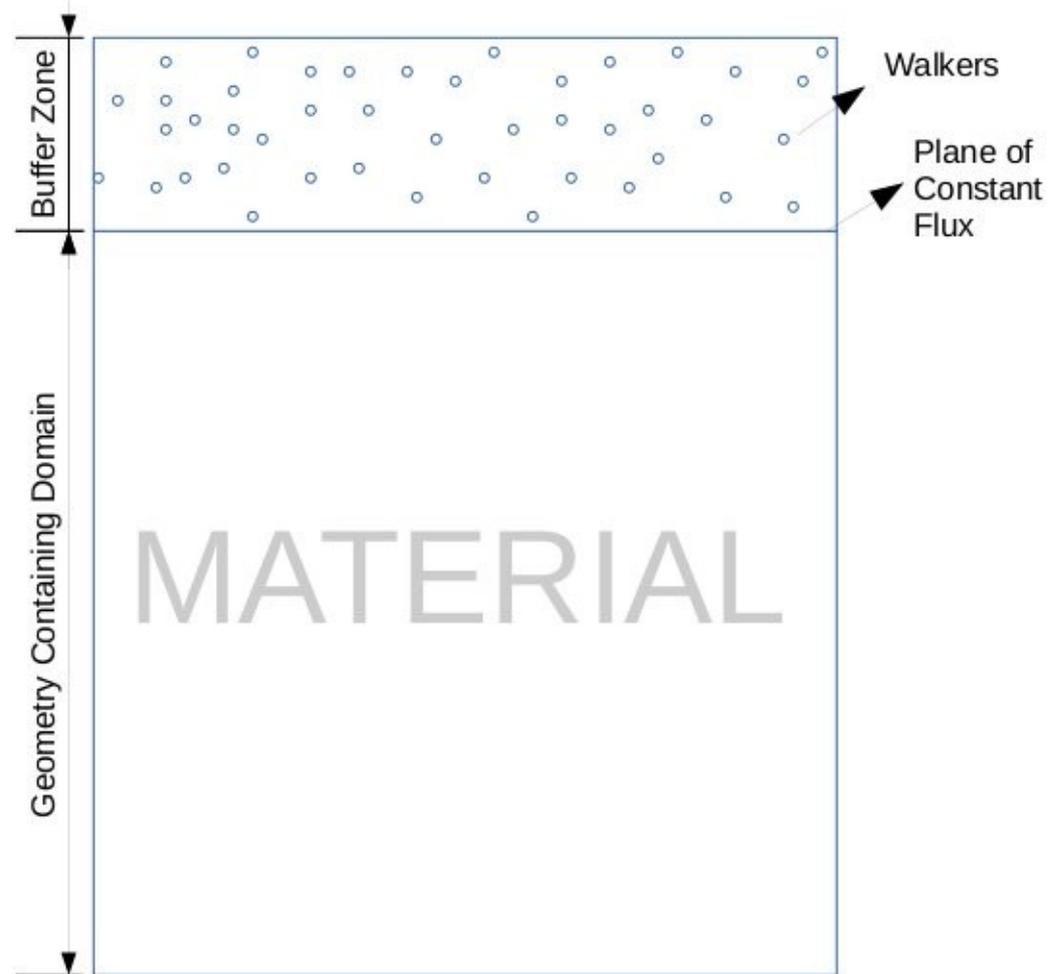
# Oxidation Model



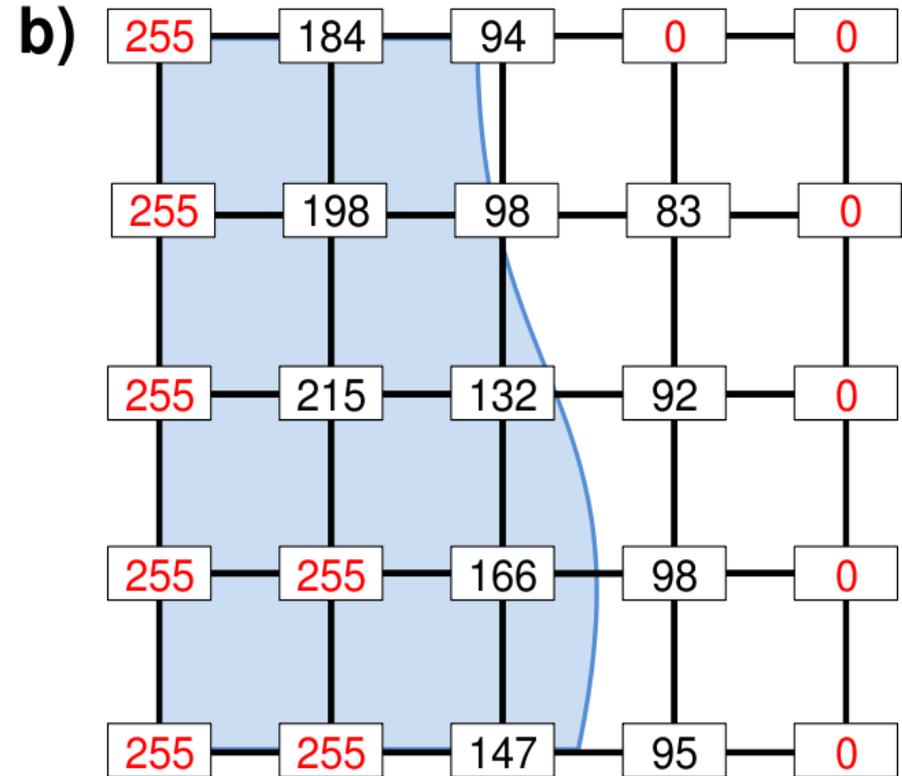
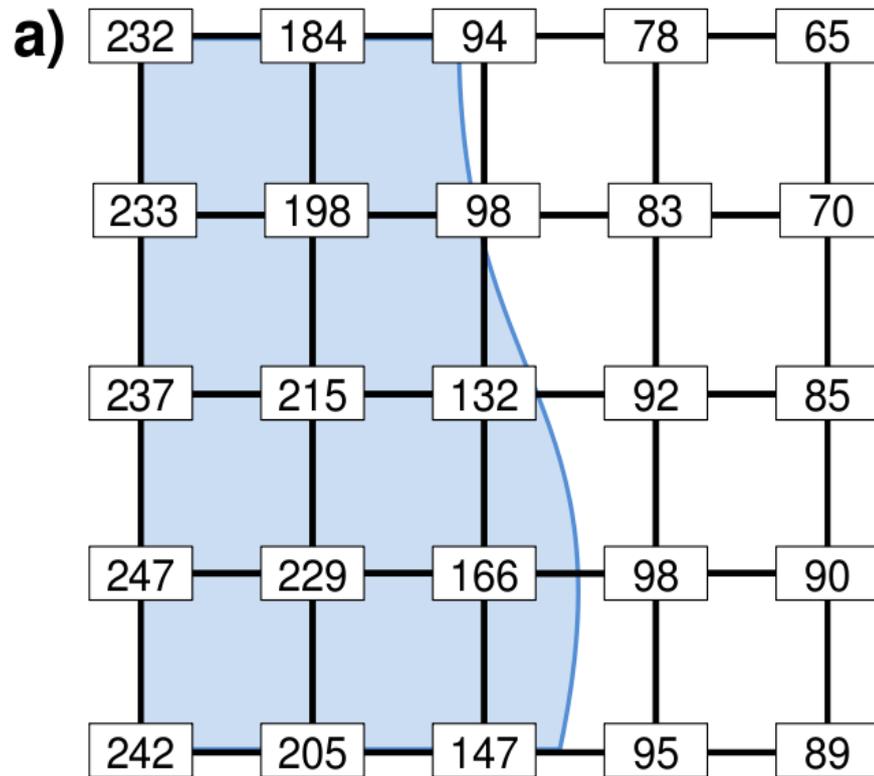
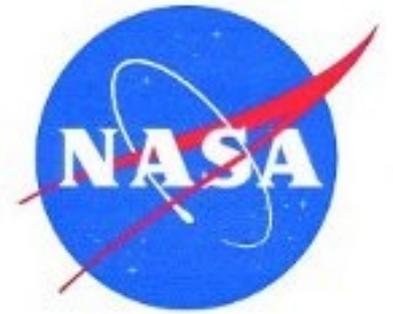
Lachaud *et al.*, *CMS*, 44  
(2009)

## Model Aspects:

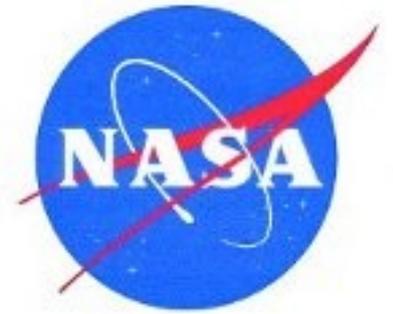
- Material Storage
- Oxygen Storage
- Walker Movement
- Collision Handling
- Verification
- Application to Fiberform



# Material Storage



# Oxygen Storage



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

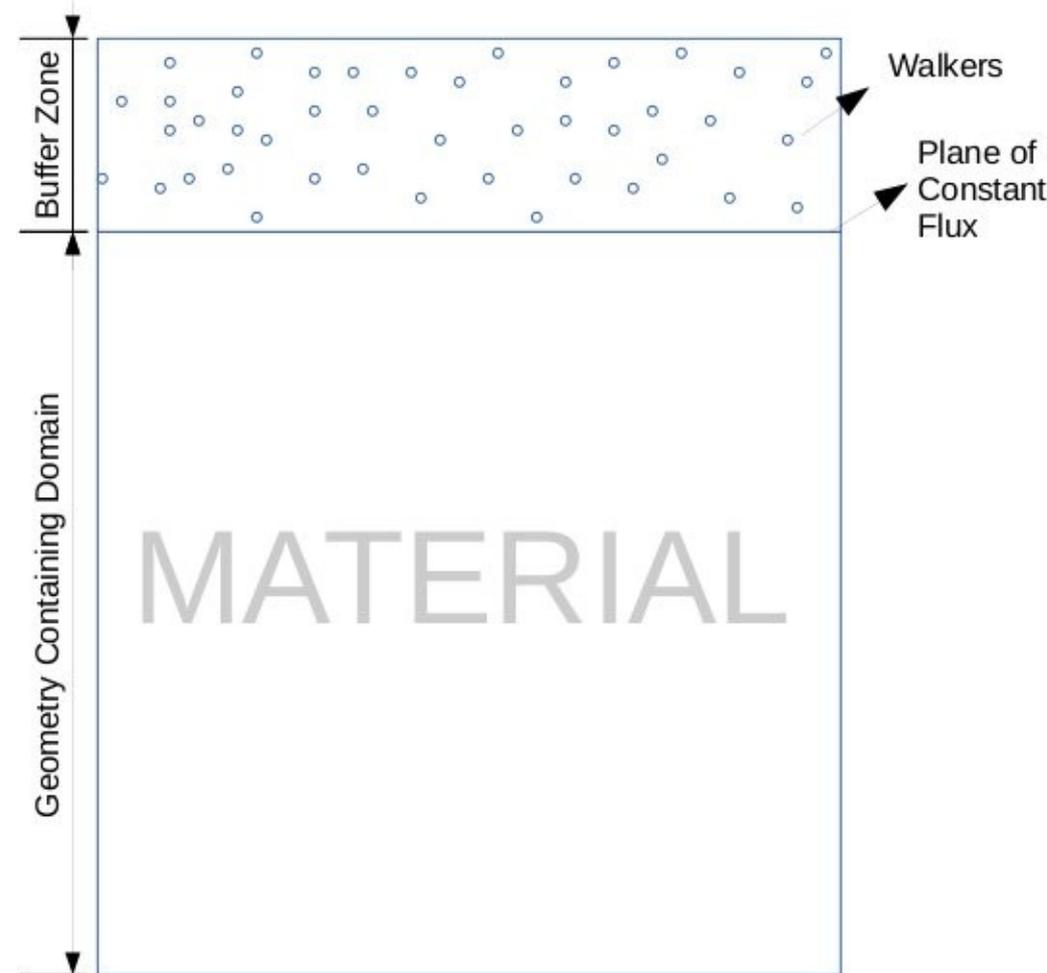
$y_{O_2}$ : mass fraction of  $O_2$

$V$ : volume of the buffer zone

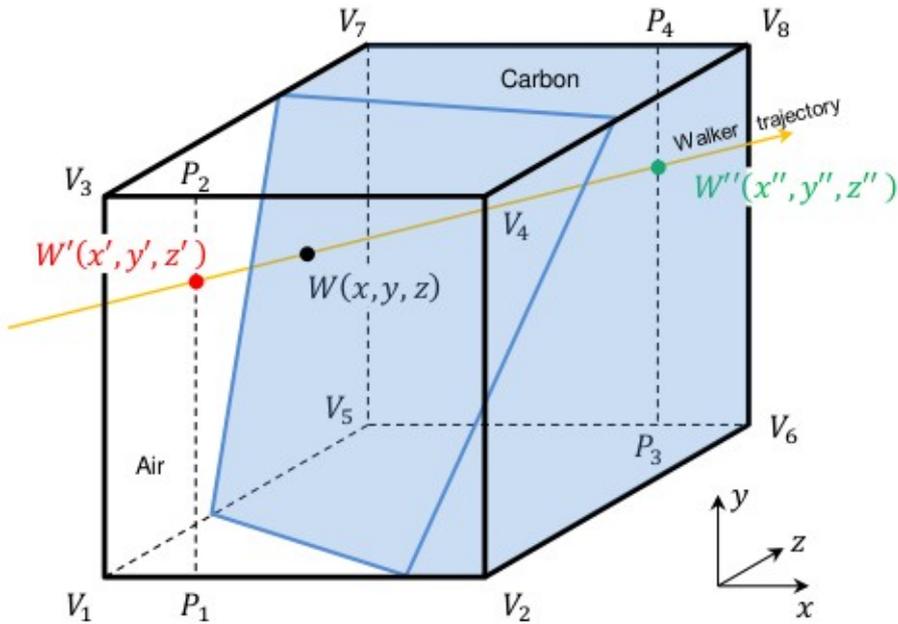
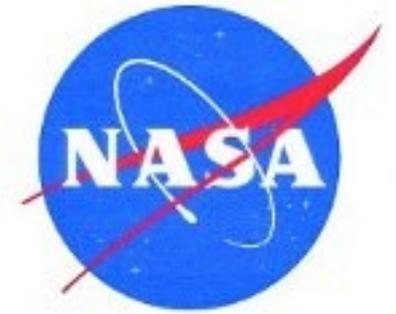
$n_w$ : user-defined number of moles per walker

$M_{O_2}$ : molar mass of oxygen

$\rho_g$ : density of the gas mixture



# Walker Movement



Movement of Walker through voxel containing material

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

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

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

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

$\Delta t$  = time increment

$\Delta R$  = random walk length

$D$  = diffusion coefficient

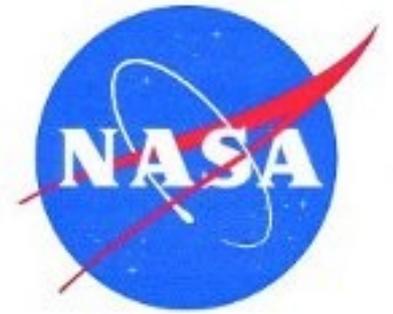
$\Gamma_1 \dots \Gamma_8$  = vertex grayscale values

$\Gamma'$  = grayscale at entrance

$\Gamma''$  = grayscale at exit

$\Gamma^*$  = grayscale threshold

# Collision Handling



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

$P_s$  = sticking probability

$D$  = diffusion coefficient

$\gamma$  = sticking coefficient

$\Delta r_w$  = walk length before collision

$k$  = reactivity of material (fiber or matrix)

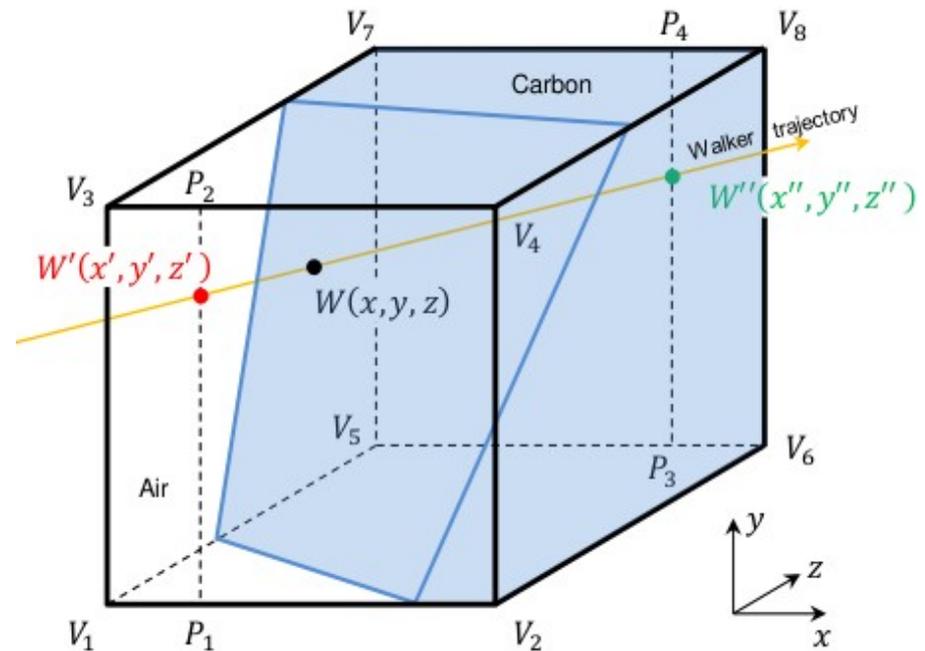
$\alpha$  = grayscale attenuation

$M_s$  = molar mass of solid

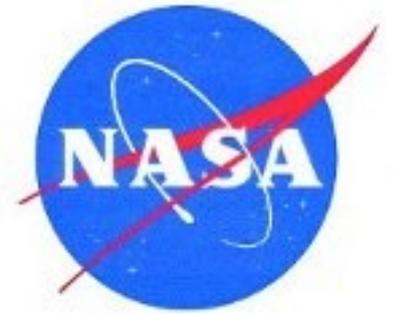
$\rho_s$  = density of solid

$\tilde{V}$  = voxel volume

$n_w$  = mols of oxygen per walker



# Verification



Exact solution Developed by Lachaud and Vingoles:

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

$A$  = reactivity contrast

$k_m$  = reactivity matrix

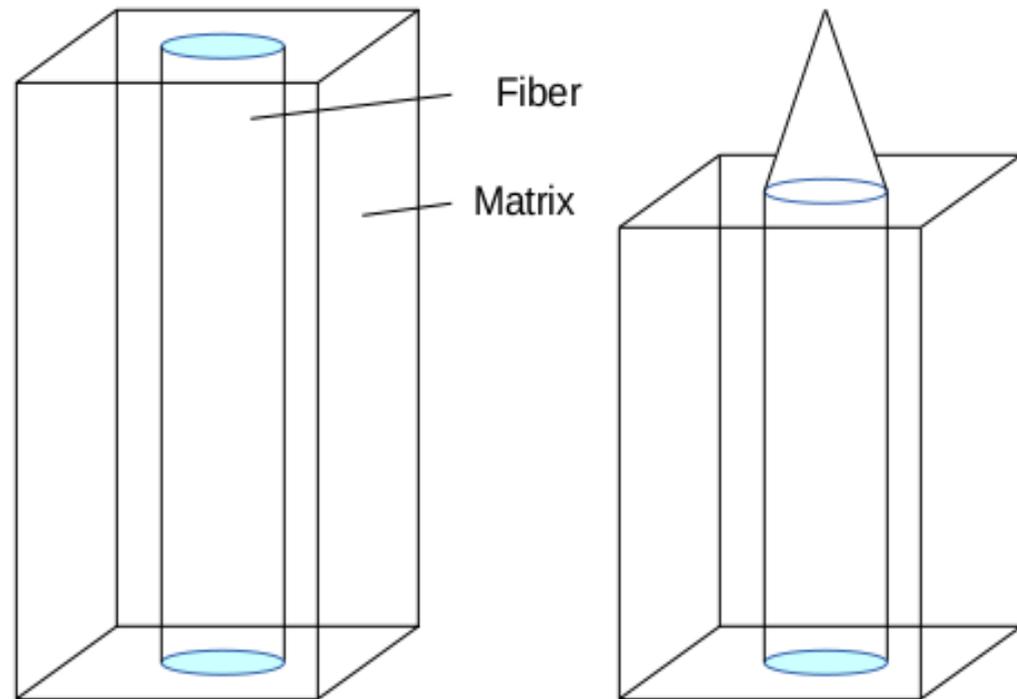
$k_f$  = reactivity fiber

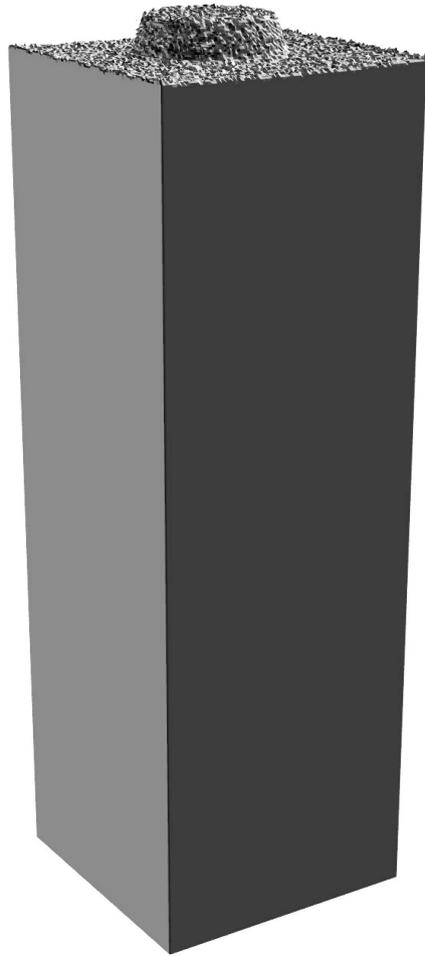
$\Omega_m$  = volume fraction matrix

$\Omega_f$  = volume fraction fiber

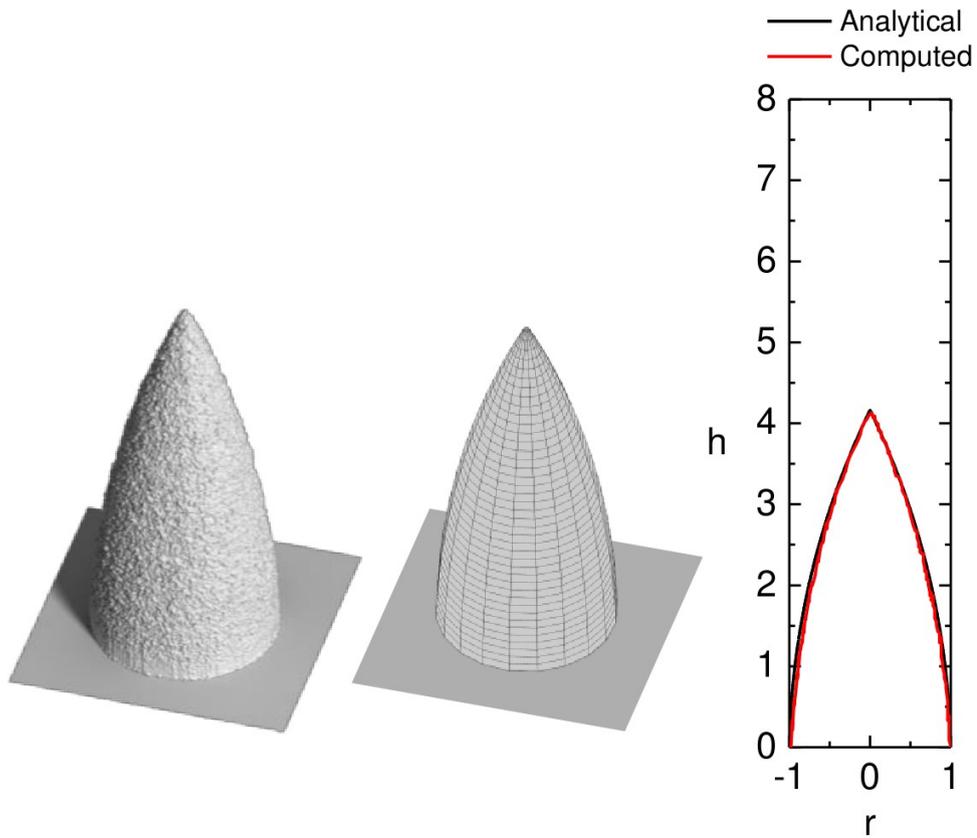
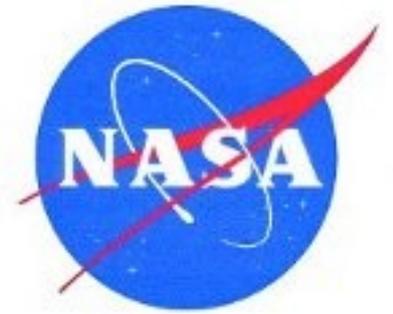
$Sh$  = sherwood number

$R_f$  = radius of fiber

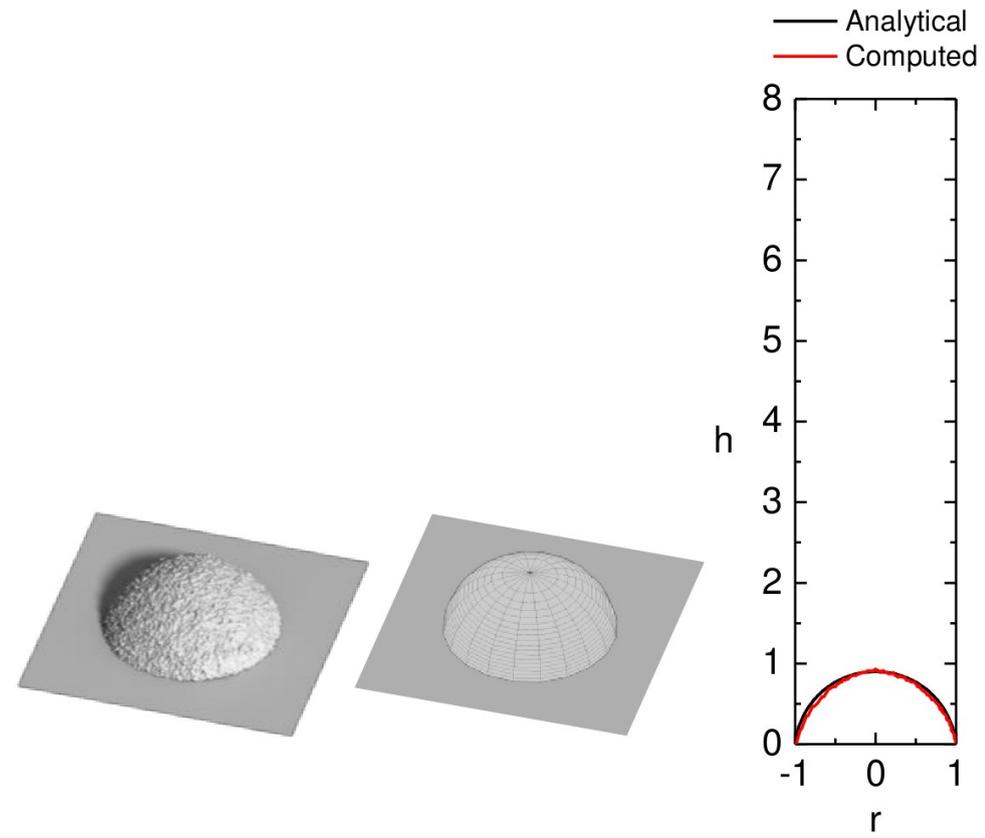




# Diffusion Limited

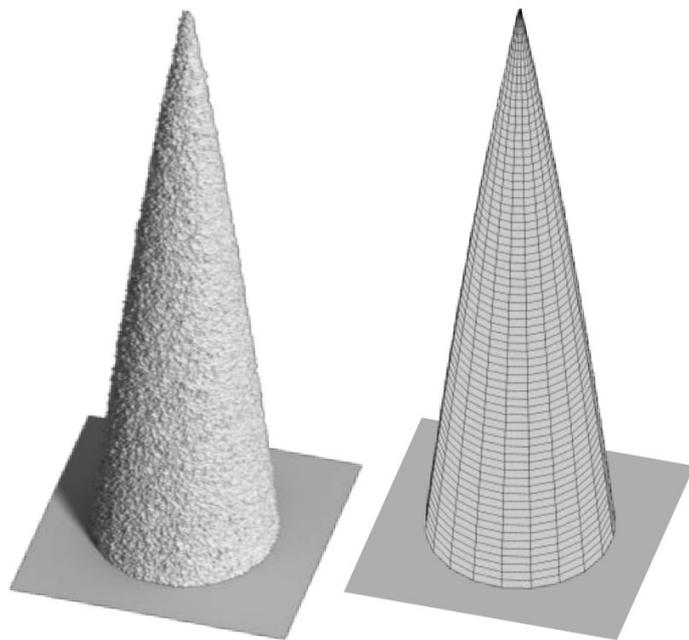
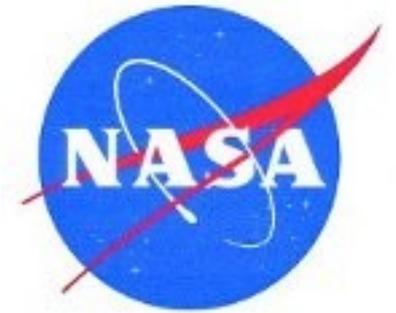


$A = 50$     $Sh = 5$

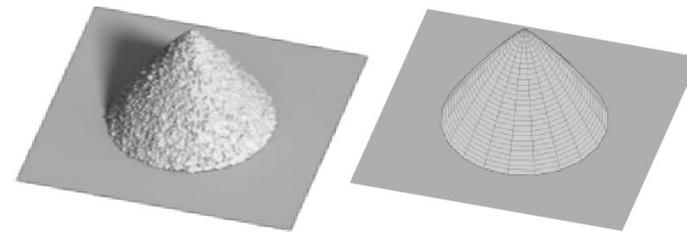
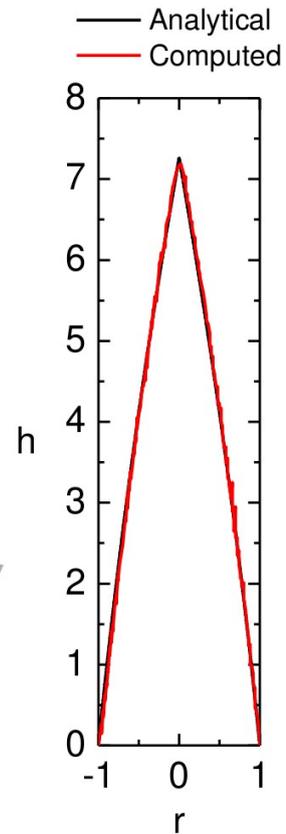


$A = 10$     $Sh = 10$

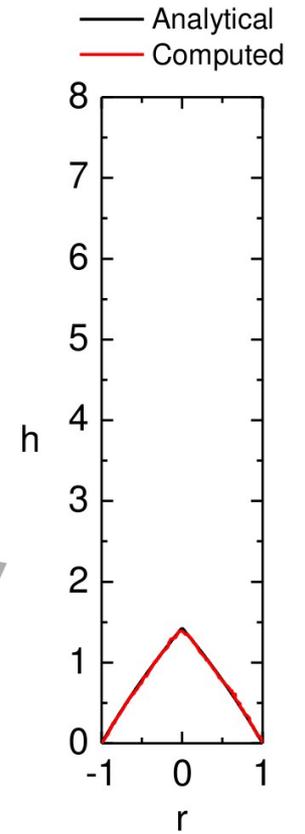
# Reaction Limited



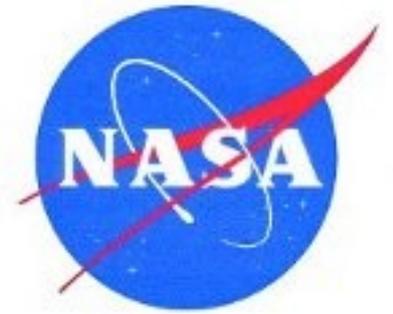
$A = 10$     $Sh = 0.1$



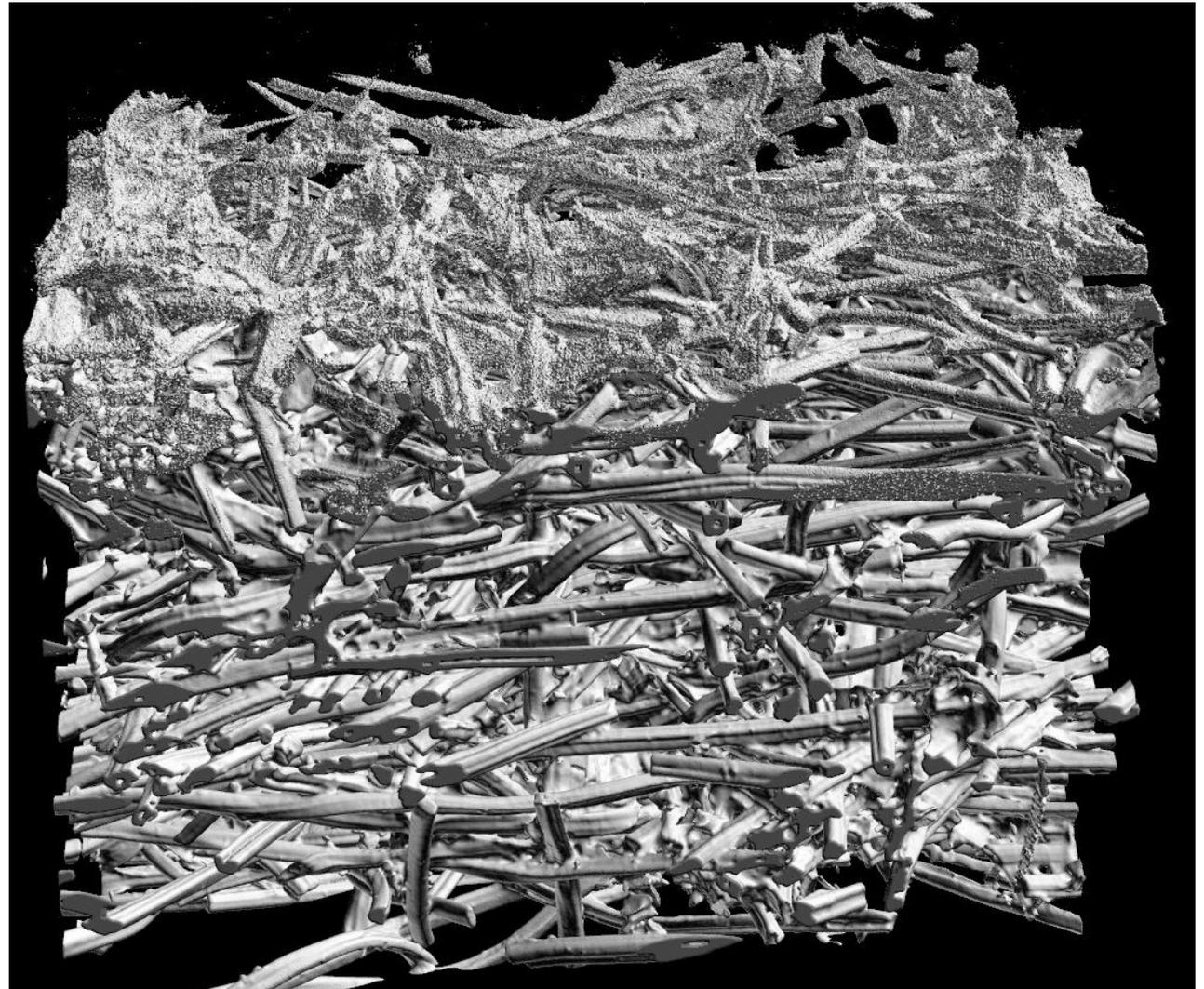
$A = 2$     $Sh = 0.2$



# Oxidation applied to Fiberform

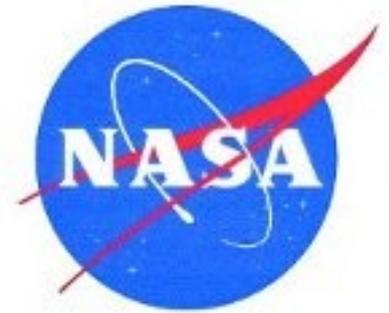


- Volume Ablation
  - High diffusion vs. reaction
- Surface Ablation
  - High reaction vs. diffusion
- Mixed Regime



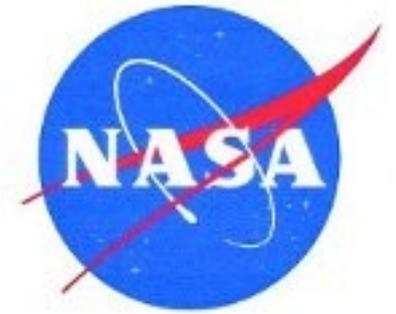


# Summary and Outlook



- 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



Nagi Mansour



Francesco Panerai



Tim Sandstrom

## LBL

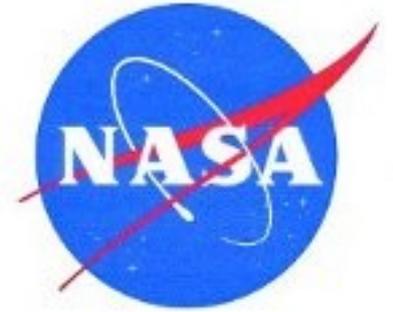


Alastair MacDowell



Dula Parkinson

# Acknowledgments



- Nagi Mansour and NASA Advanced Supercomputing Division for the opportunity to work at Ames and conduct the research
- Education Associates Program for hosting me as an intern
- The Lawrence Berkeley National Labs and the Advanced Light Source