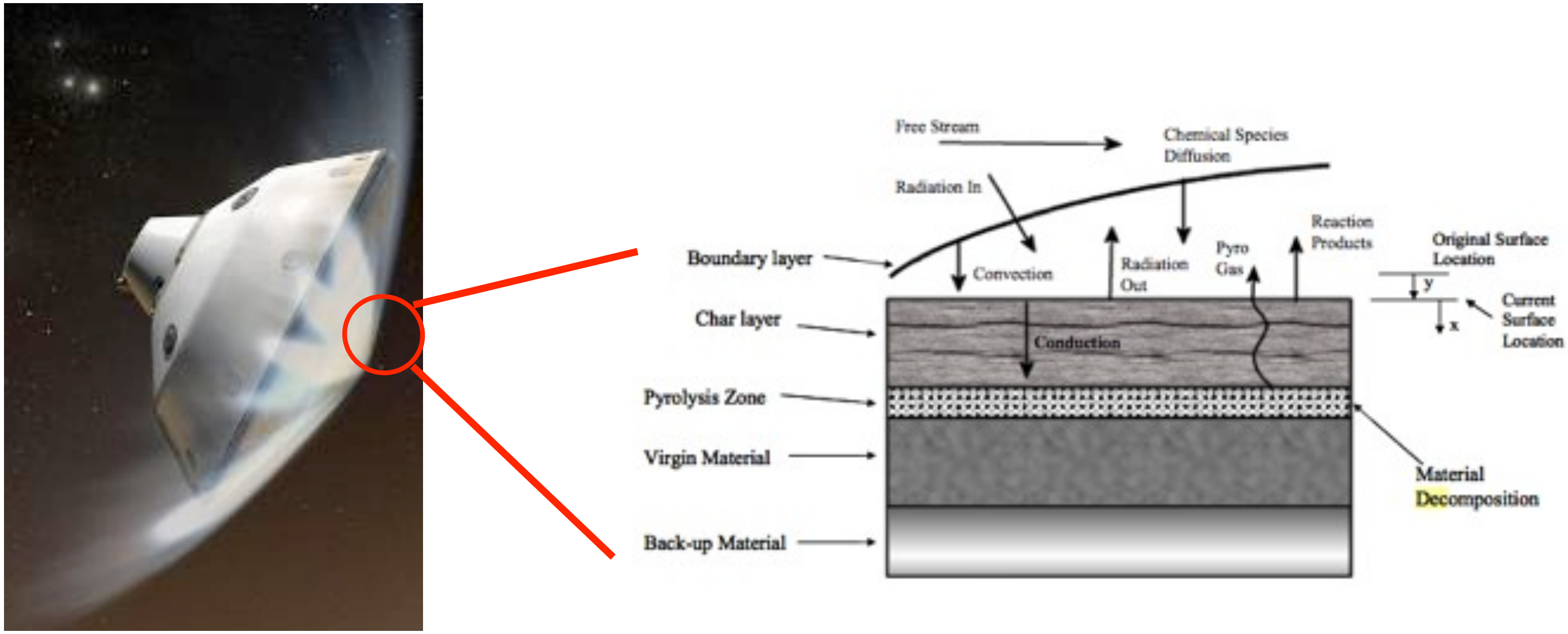
NASA Space Technology Research Fellowship

Microscale Modeling of Ablative Thermal Protection System Materials

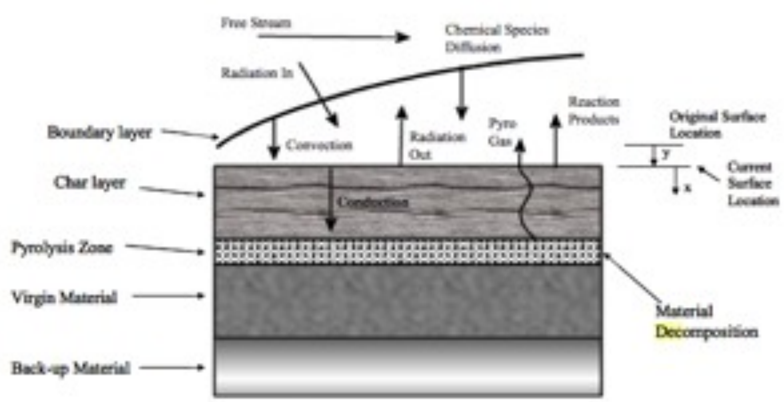
Eric Stern, Graham Candler, Tom Schwartzentruber, Ioannis Nompelis, Michael Barnhardt

Ablation Modeling



- **Engineering material response codes in use today take a macroscopic view of the TPS.**
- **Typically involve heavy empiricism, and many assumptions**

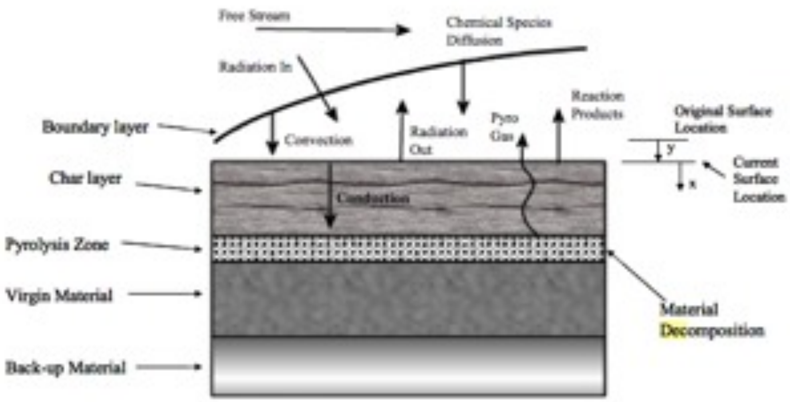
TPS Modeling



Lachaud, et al., JSR, 2010

- **The goal of this work is to better model processes at the micro-scale to inform macro-scale models.**
  - Volume averaging.
  - Model reduction!
- **This will attempt to build and expand on previous efforts in micro-scale modeling by enabling more physics**

TPS Modeling



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Lachaud, et al., JSR, 2010

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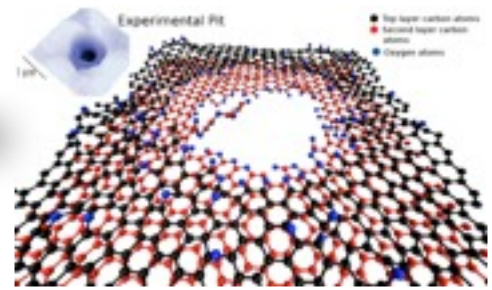


Poovathingal, et al., J. Phys. Chem., 2013

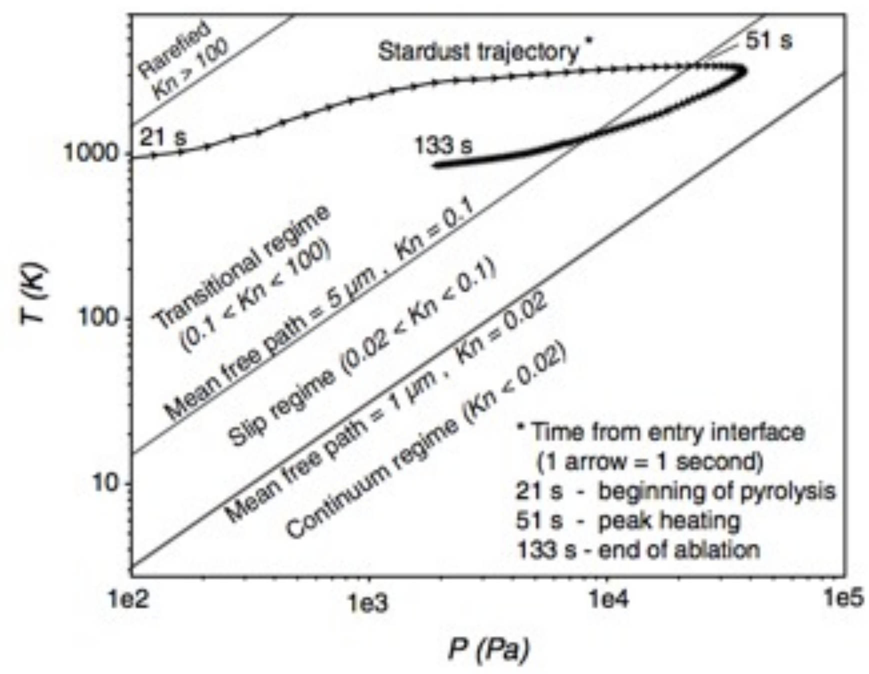
- **The goal of this work is to better model processes at the micro-scale to inform macro-scale models.**
- **...as well as build a framework where higher fidelity models can be incorporated from the nanoscale**

Outline

- **Methodology**
  - DSMC
  - Surface Generation and Movement
  - Coupled Ablation
- **Preliminary Validation and Applications**
  - Simplified Darcy Flow
  - Flow-tube Permeability Experiments
- **Future Work**

Why DSMC?

- **First: what is DSMC?**
- **Knudsen numbers in the porous medium range from high-slip to rarefied regimes.**
- **DSMC can (in principle) simulate all of the relevant physics.**
  - Convection
  - Multicomponent Diffusion
  - Gas-phase Kinetics
  - Sophisticated GSI Models
  - Non-equilibrium handled inherently
- **DSMC can simulate arbitrarily complex geometries**



Lachaud, et al., JSR, 2010

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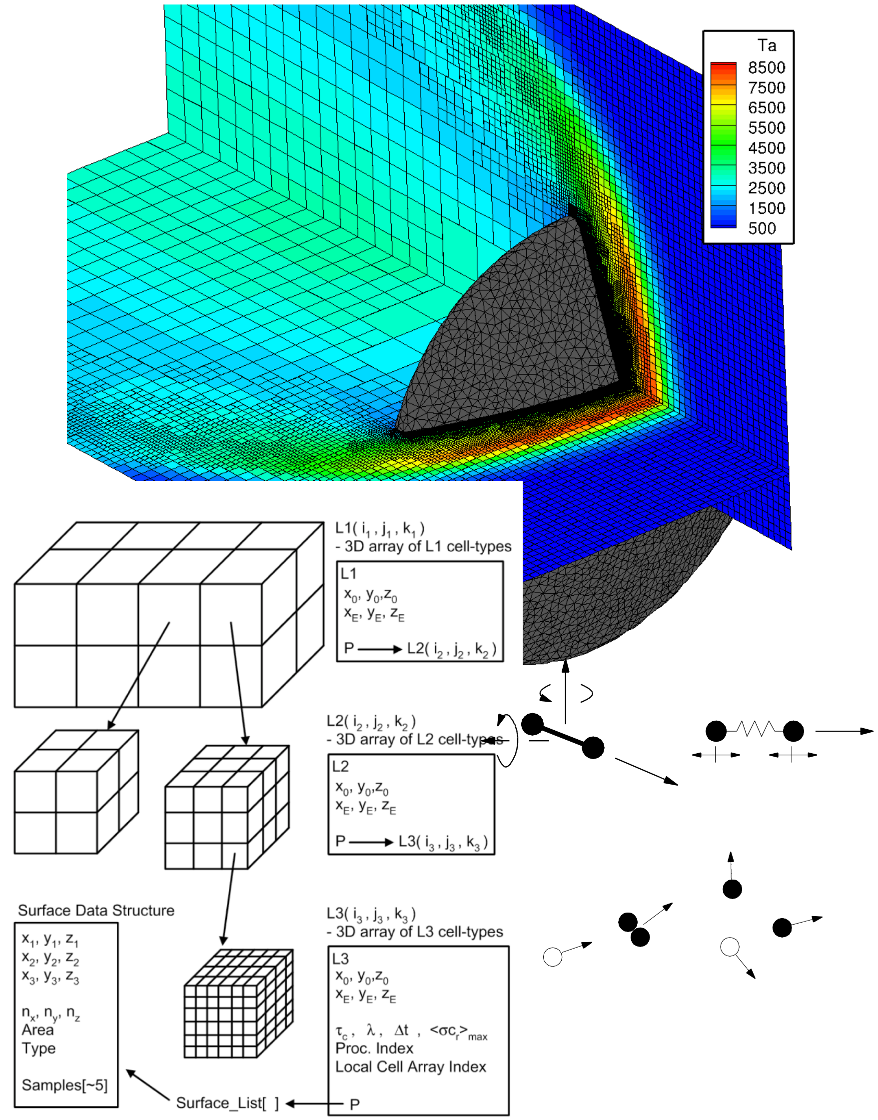
MGDS2

- **Parallel implementation of the DSMC method developed at the University of Minnesota.**
  - 3-Level Cartesian Mesh
  - Automated Mesh Refinement
  - Models for dissociation, vibrational/rotational relaxation.



1. *Zhang and Schwartzentruber., Comp. and Fluids, 2012*
2. *Nompelis and Schwartzentruber, AIAA Paper, 2014*

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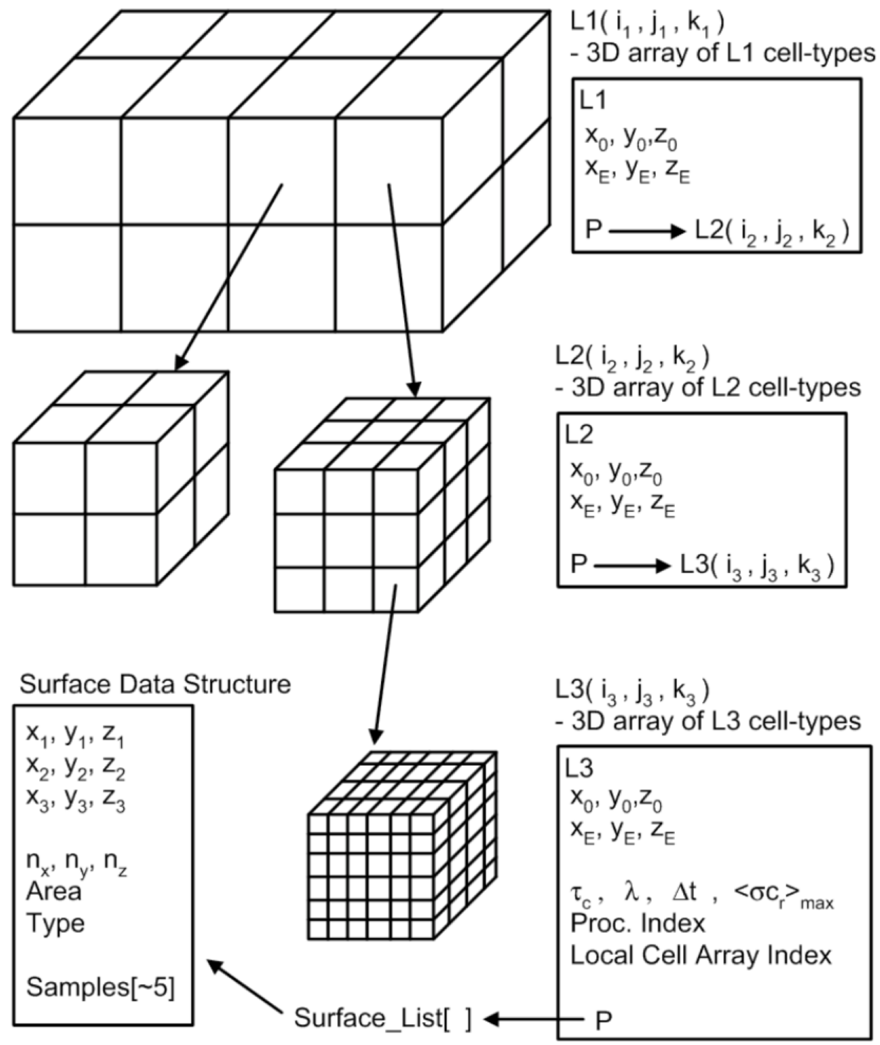

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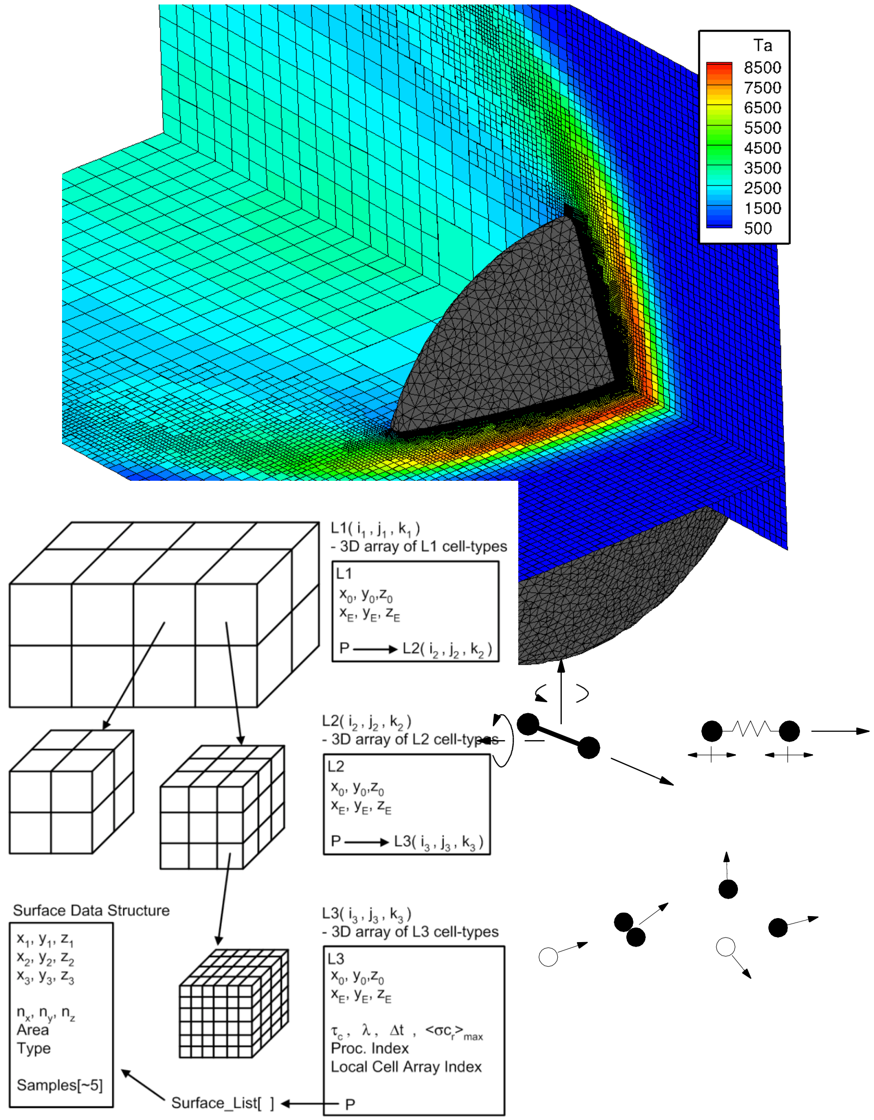

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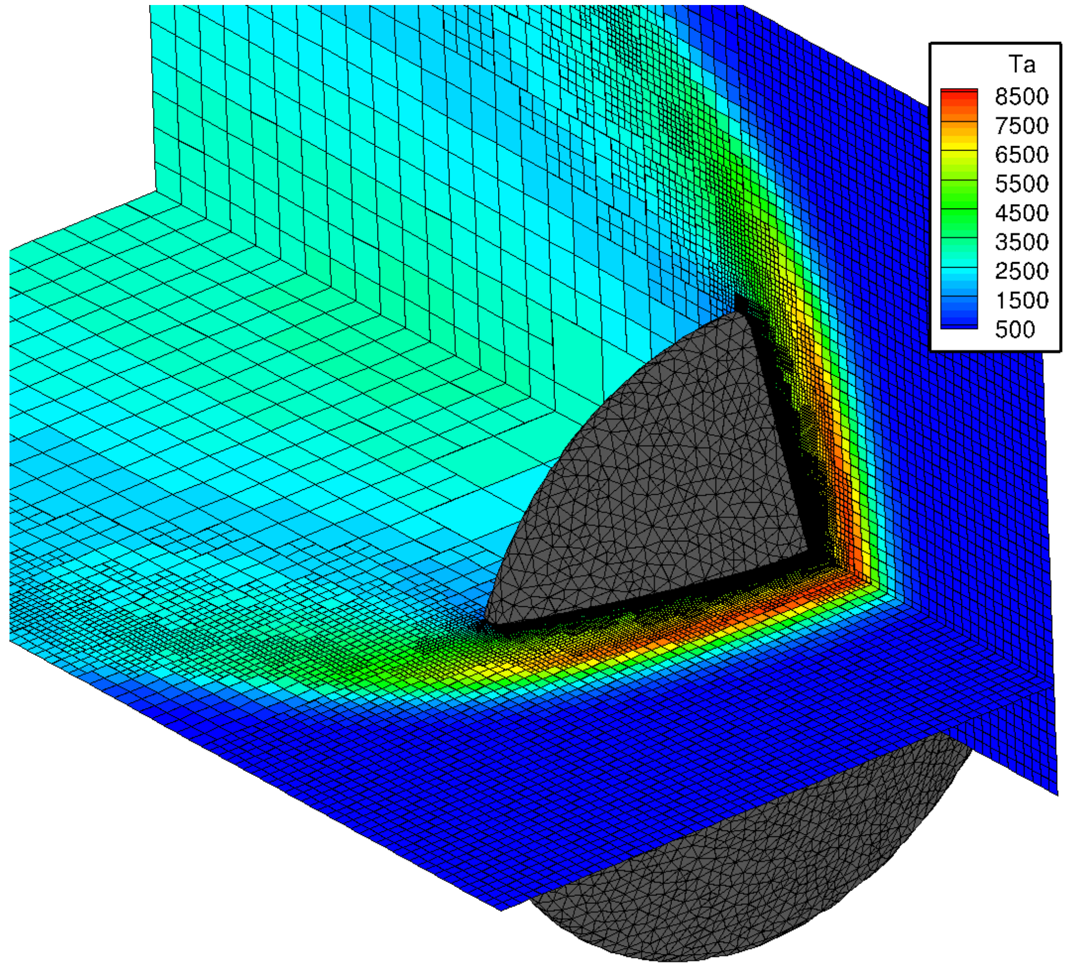

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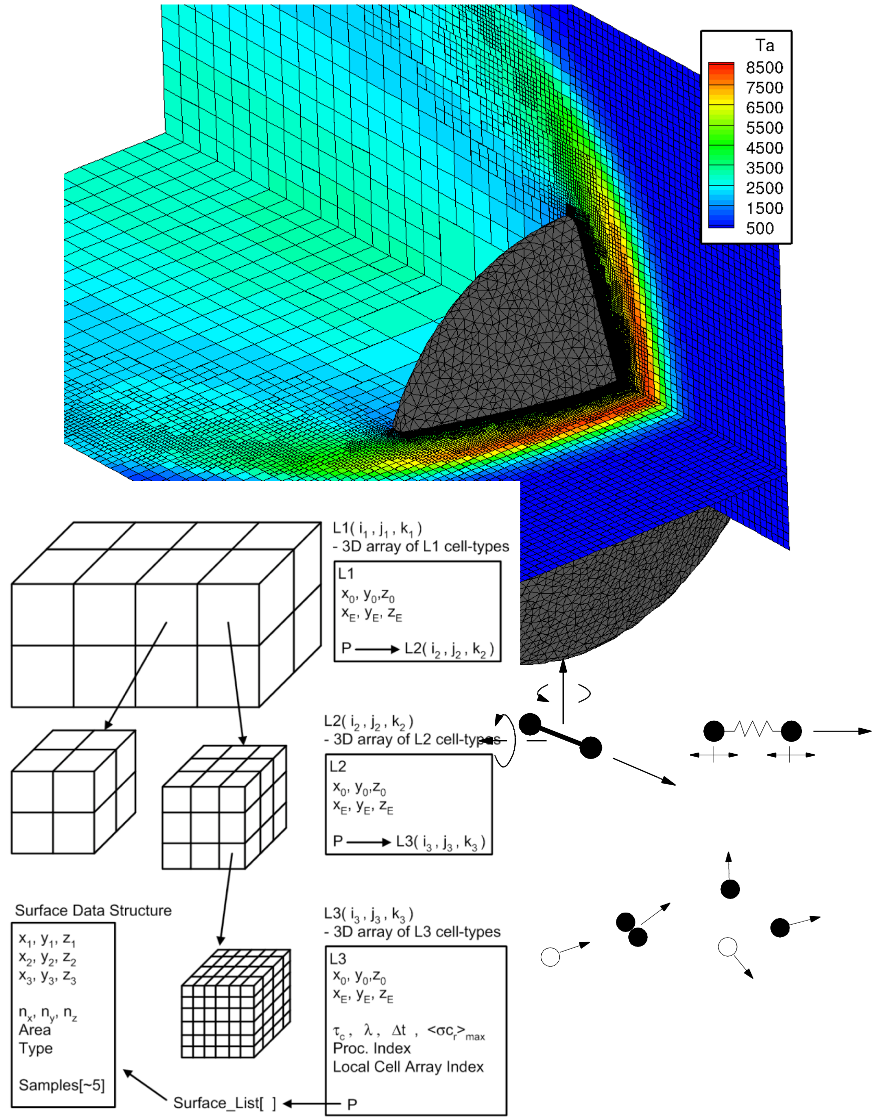

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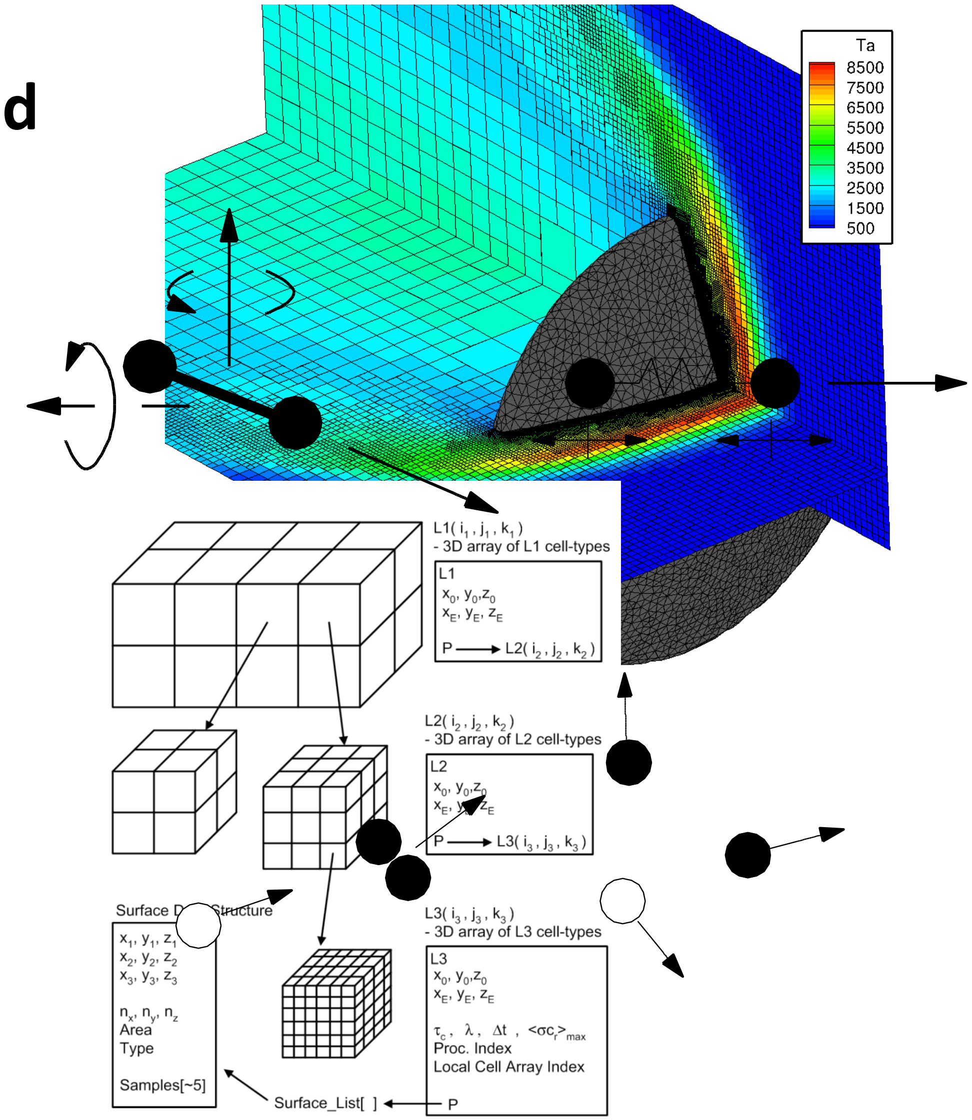

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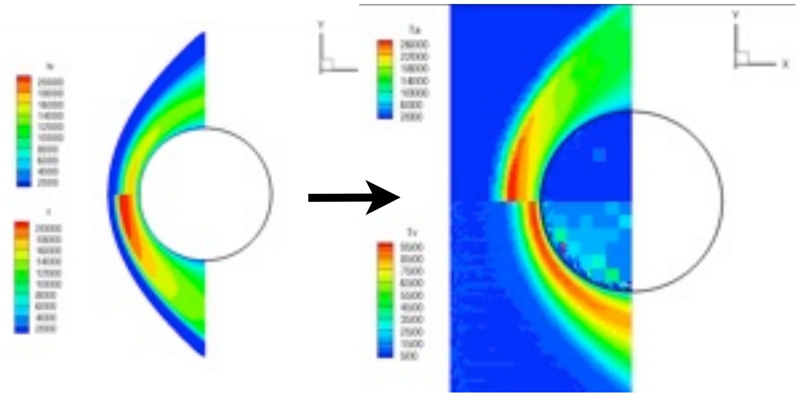
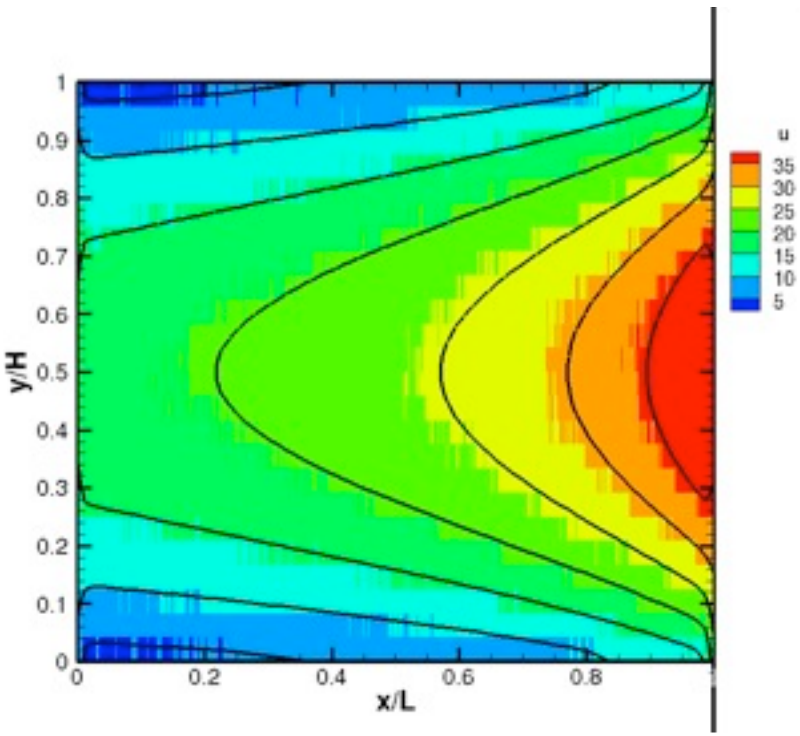
MGDS2

- **Some additional features have been added to the code specifically for this work.**
  - Initialization of simulation to CFD (using US3D).
  - Subsonic Boundary Conditions
  - Simple gas-surface interaction model
  - Ablation modules





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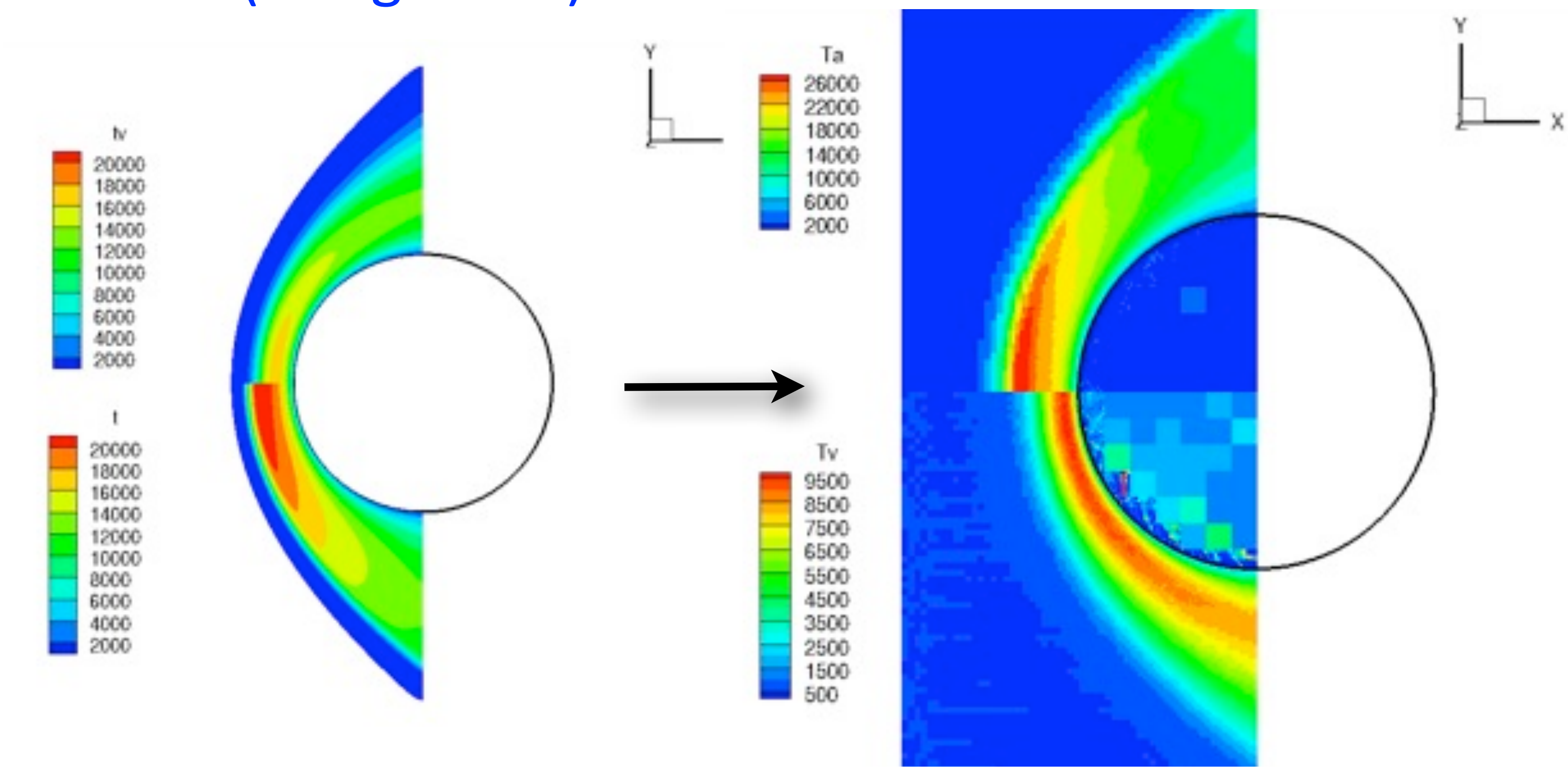

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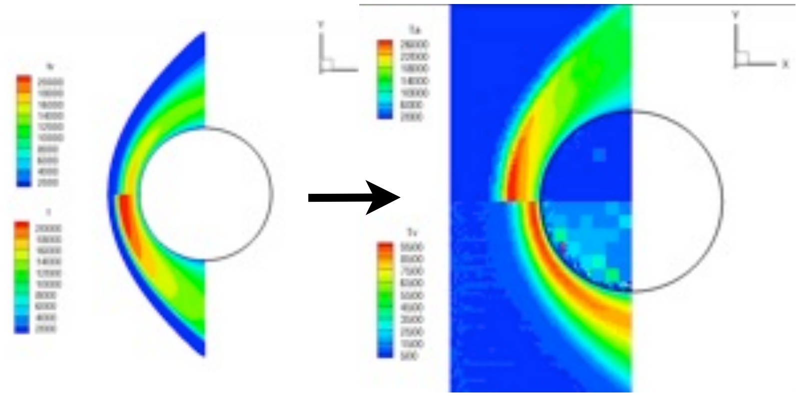

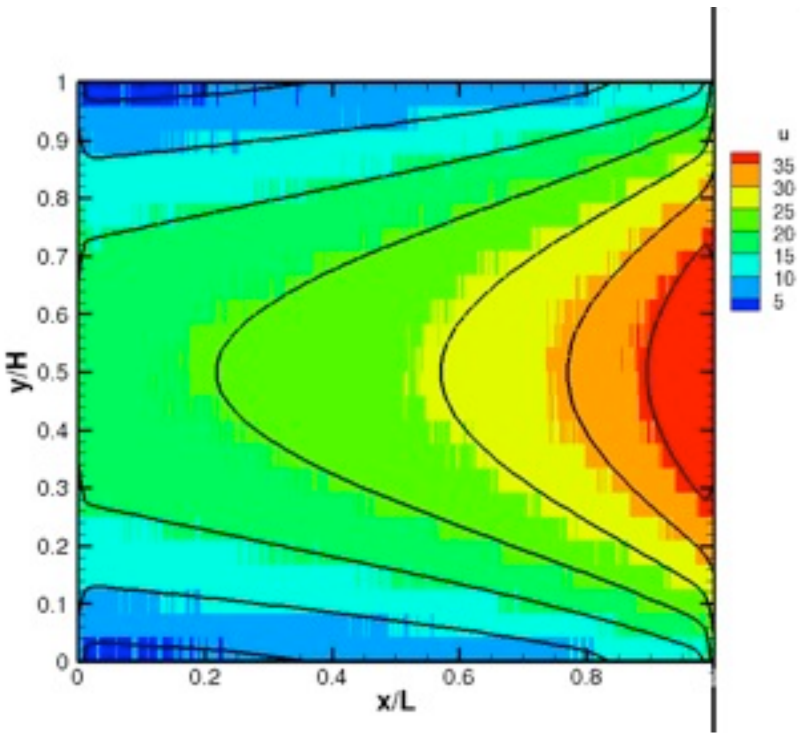

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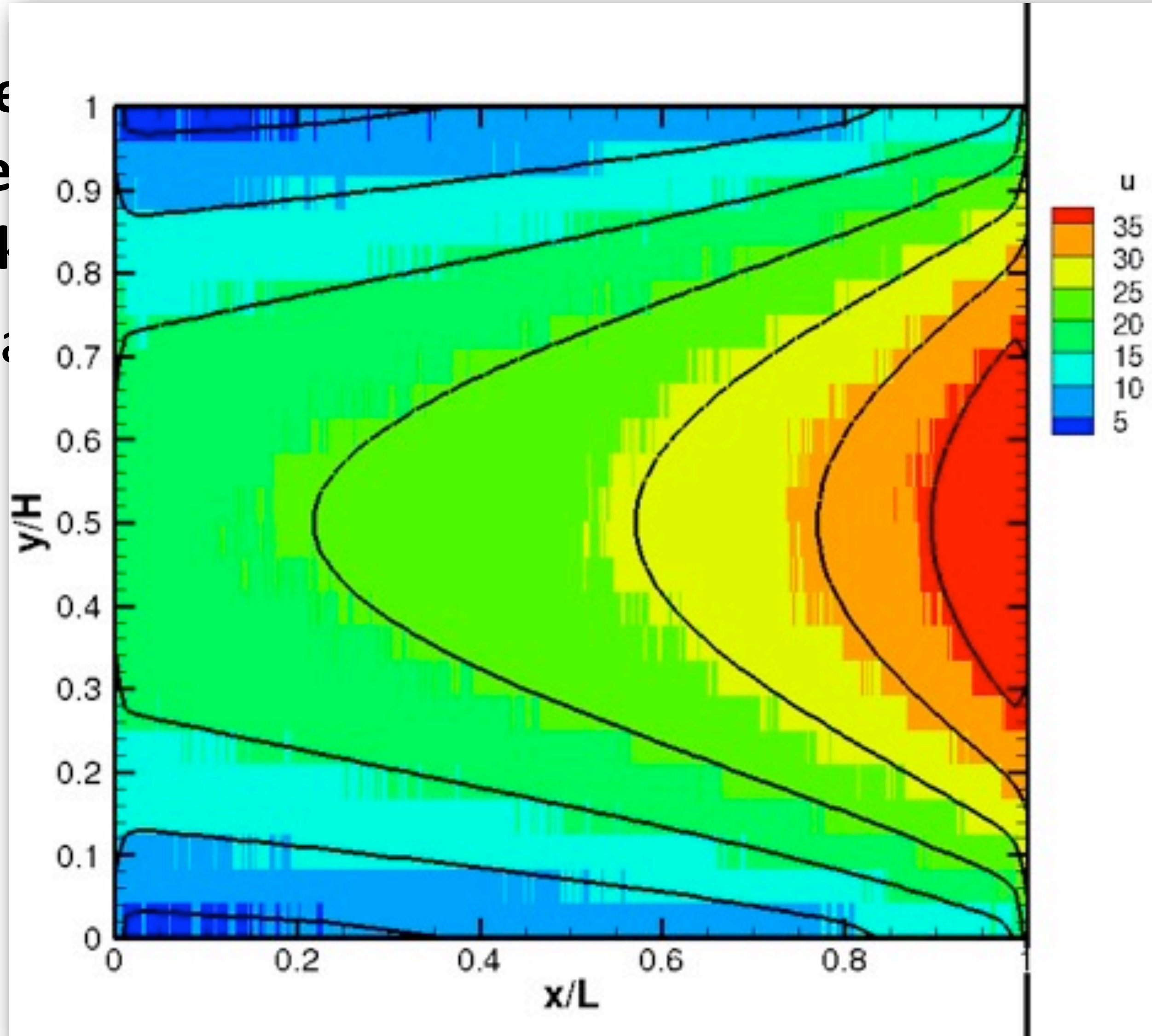

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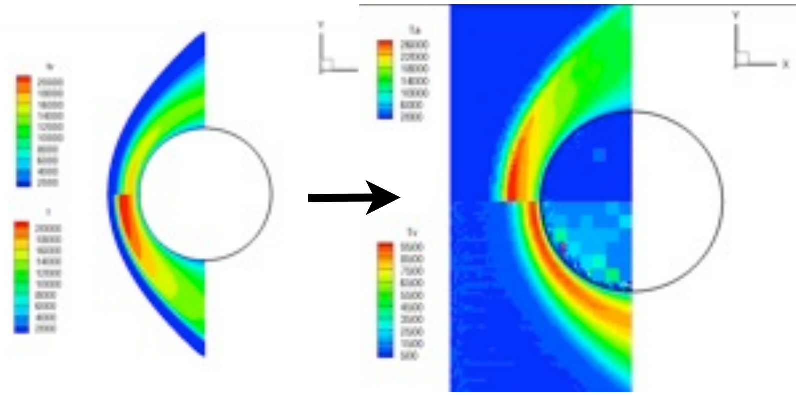

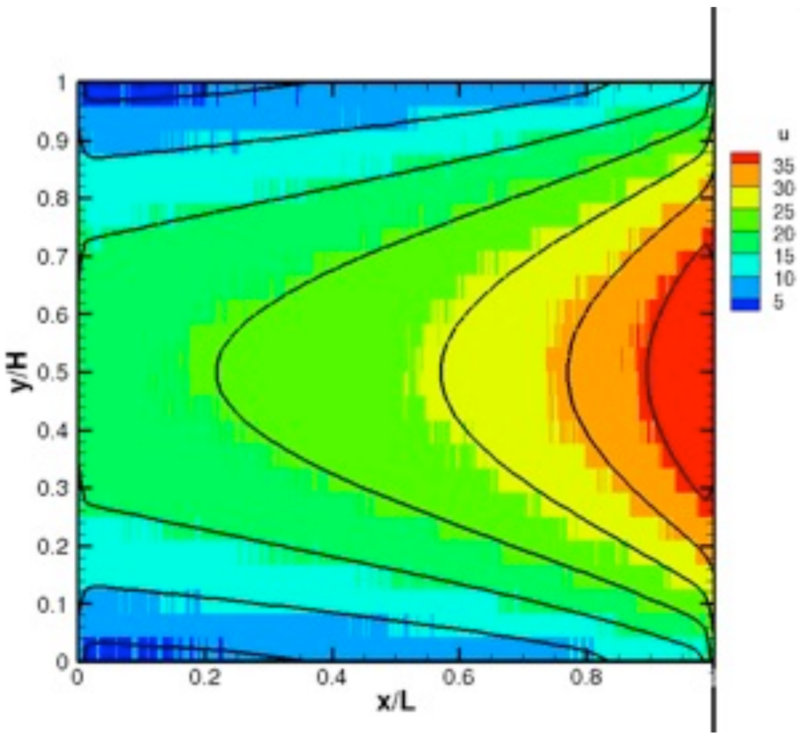

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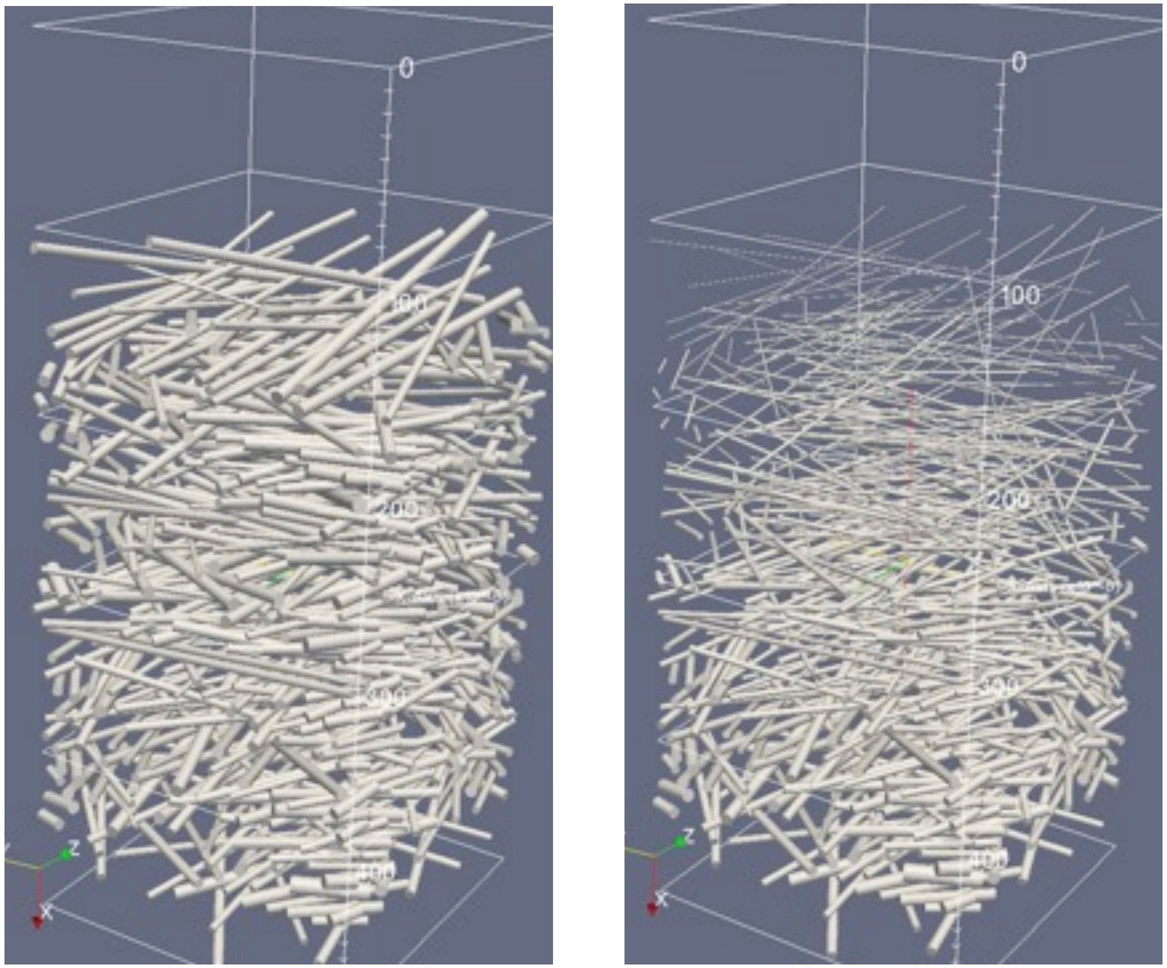
FiberGen

- **The objective is to develop a tool that is able to generate triangulated surface meshes of random arrays of "fibers" to use in microscale simulations.**
- **We have developed FiberGen with the following features:**
  - It can generate 2D and 3D, random and non-random arrays of cylindrical fibers.
  - The user specifies a box size to fill with fibers, and a target porosity.
  - The user can prescribe properties such as nominal fiber diameter, fiber length, angular biases (i.e. orthotropy), as well as variance and distribution in each.
  - Triangulated surface is output in STL format.
  - It also includes a post-processor for analyzing the geometry.

FiberGen



Example geometry having porosity of 0.85, and nominal fiber radius of 6 micron. The figure on the right is of the same geometry after having undergone a prescribed "ablation."

- **Additionally, the code creates data structures for the mesh which are used for evolving the surface.**
- **Fiber data structures are written to HDF5 format for efficient I/O in massively parallel applications.**

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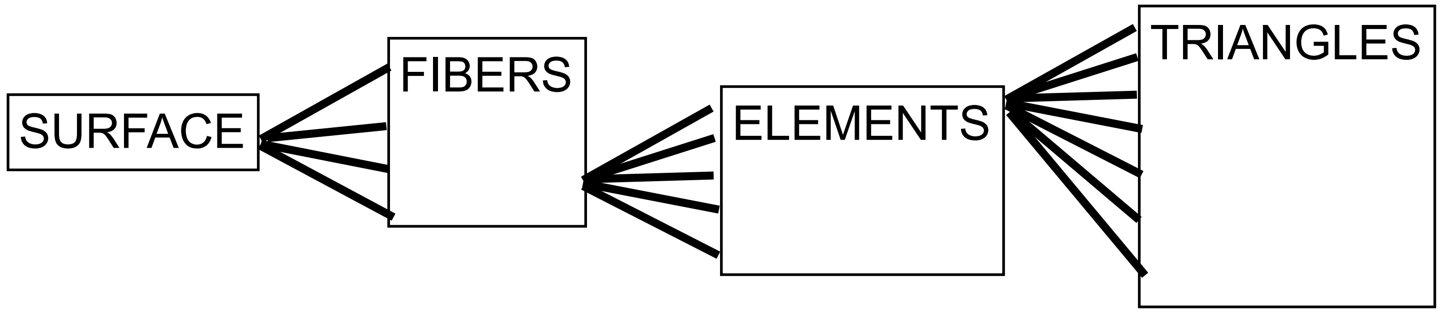
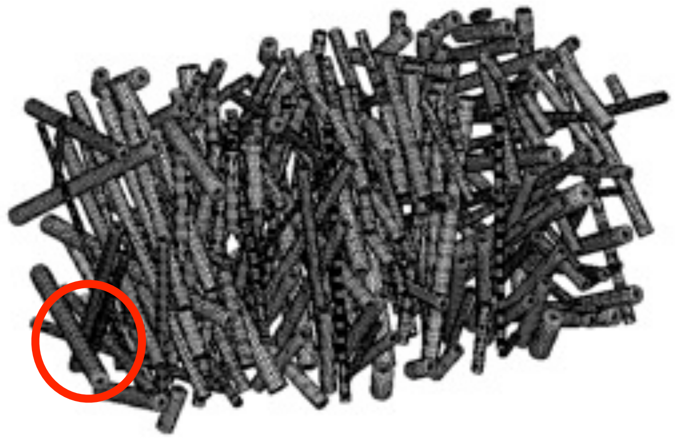
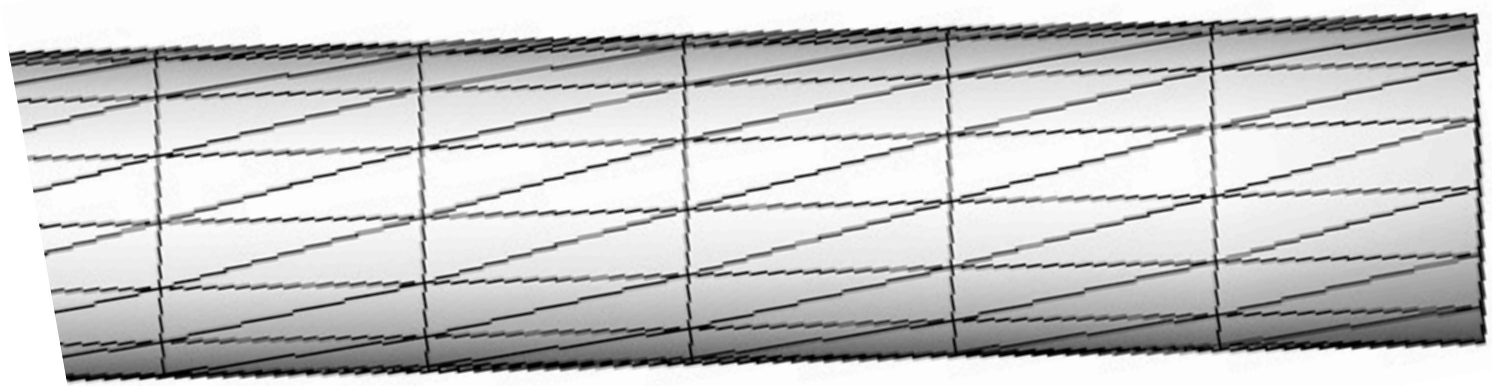
Surface Data Structure



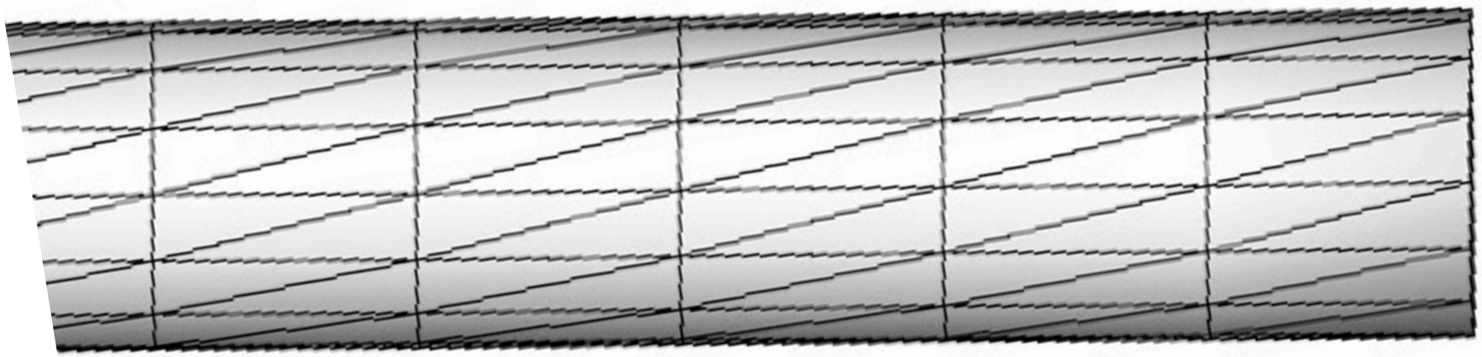


- The surface is composed of many *fibers*
- Each fiber is composed of discrete *elements* along the axis.
- Each element contains many *triangles* on their surface

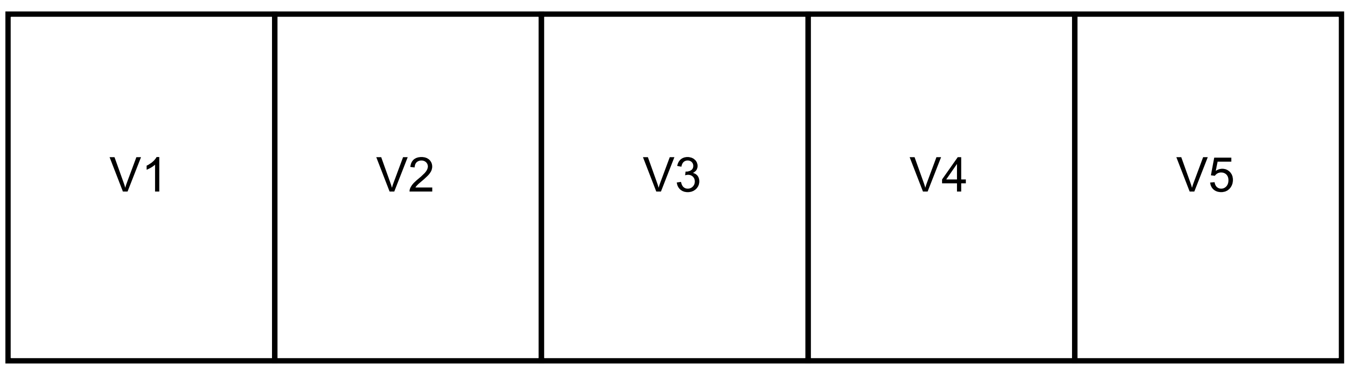


Surface Movement

- Now we would like to leverage this framework do develop an efficient method for evolving the surface under the influence of surface reactions (*ablation)*



- We begin by computing and storing the volume of each *element* for each fiber.



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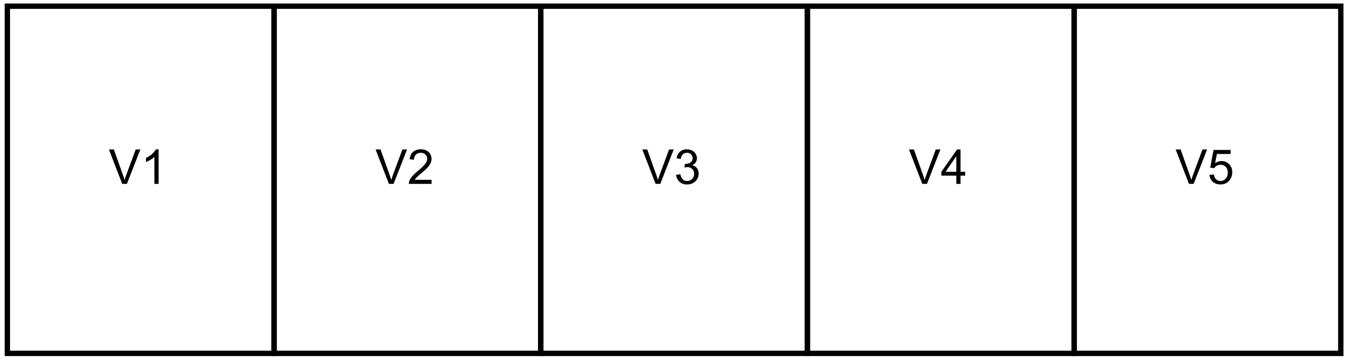
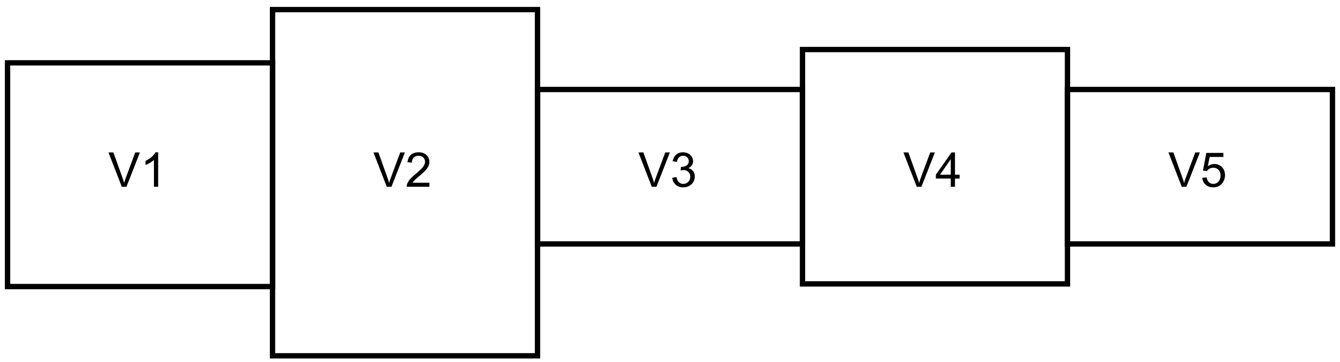
Surface Movement

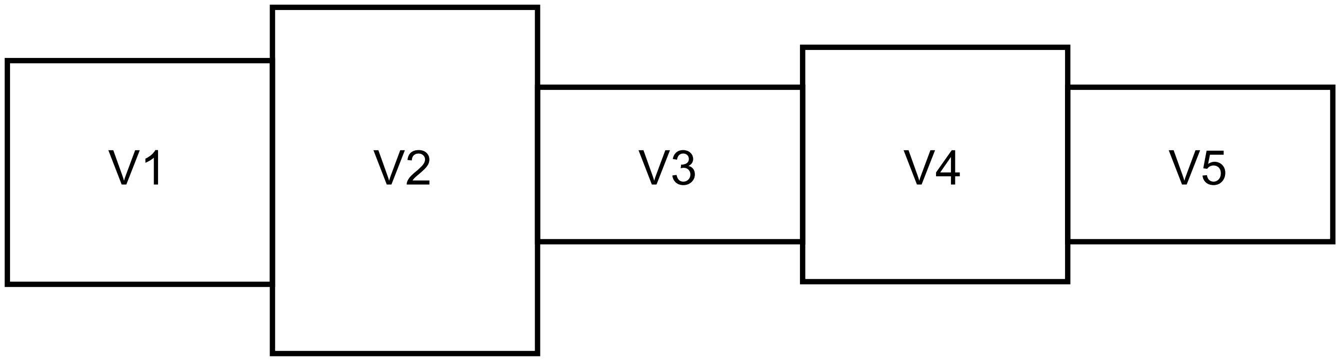


– We then update the *element* volumes as the simulation progresses, and reactions on the *triangles* remove material from the fibers.

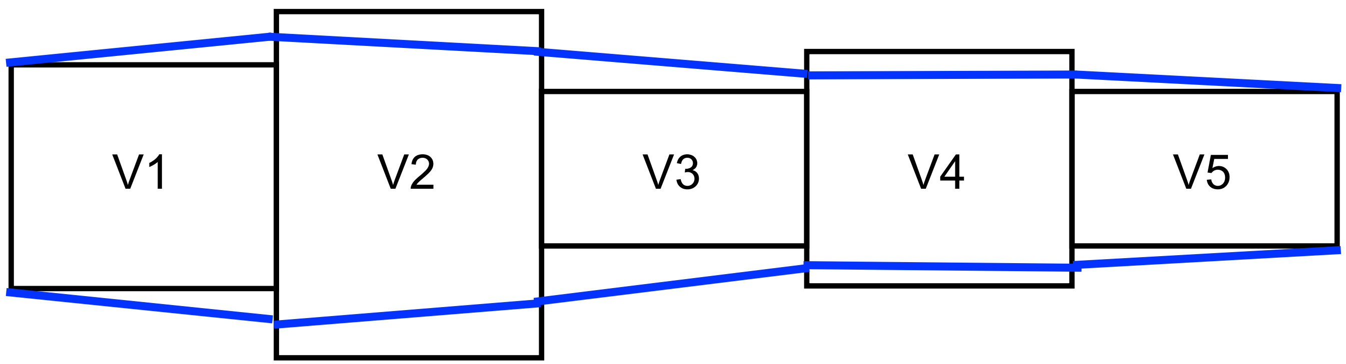


– An effective radius that yields a straight cylinder of the same volume is computed for each *element*.

Surface Movement

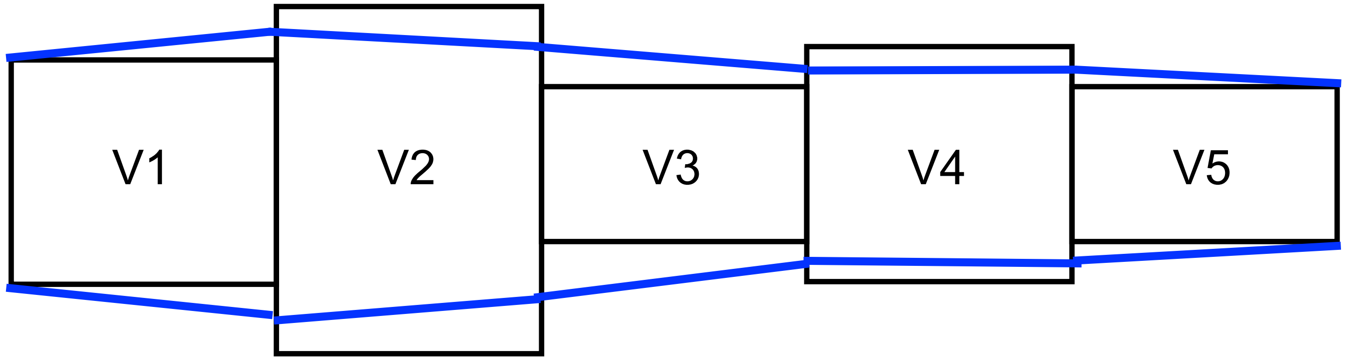


– The radius on each side of each element is then defined as the average between it and it's neighbor.



– The surface is then reconstructed from conical frustum segments.

Surface Movement



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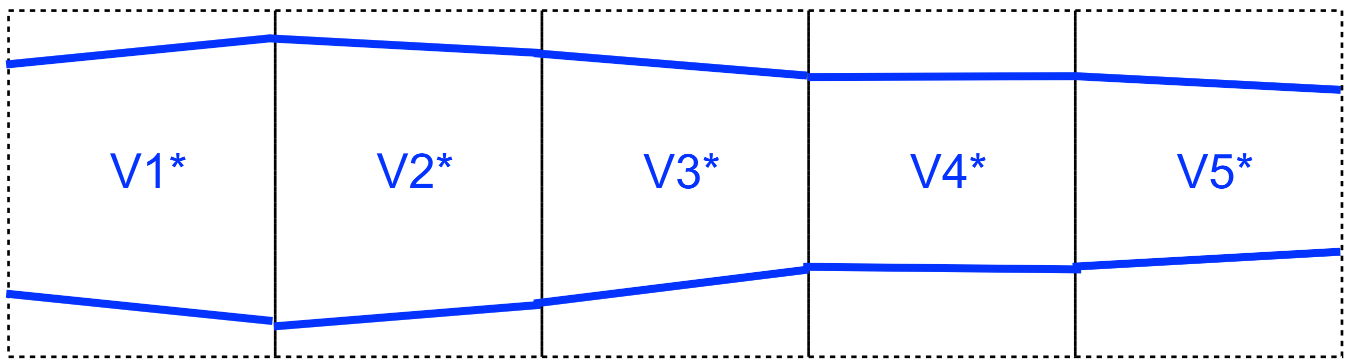
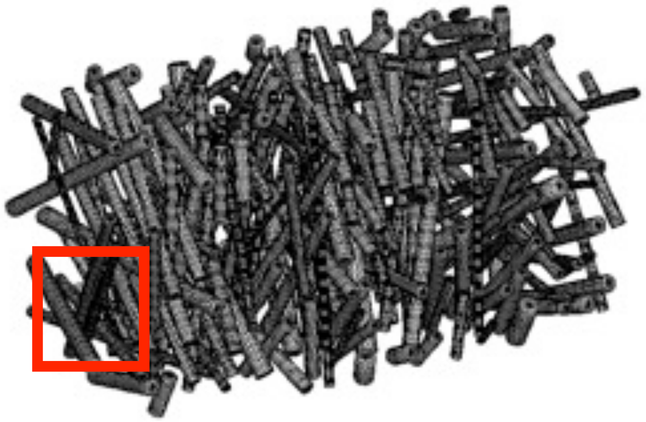


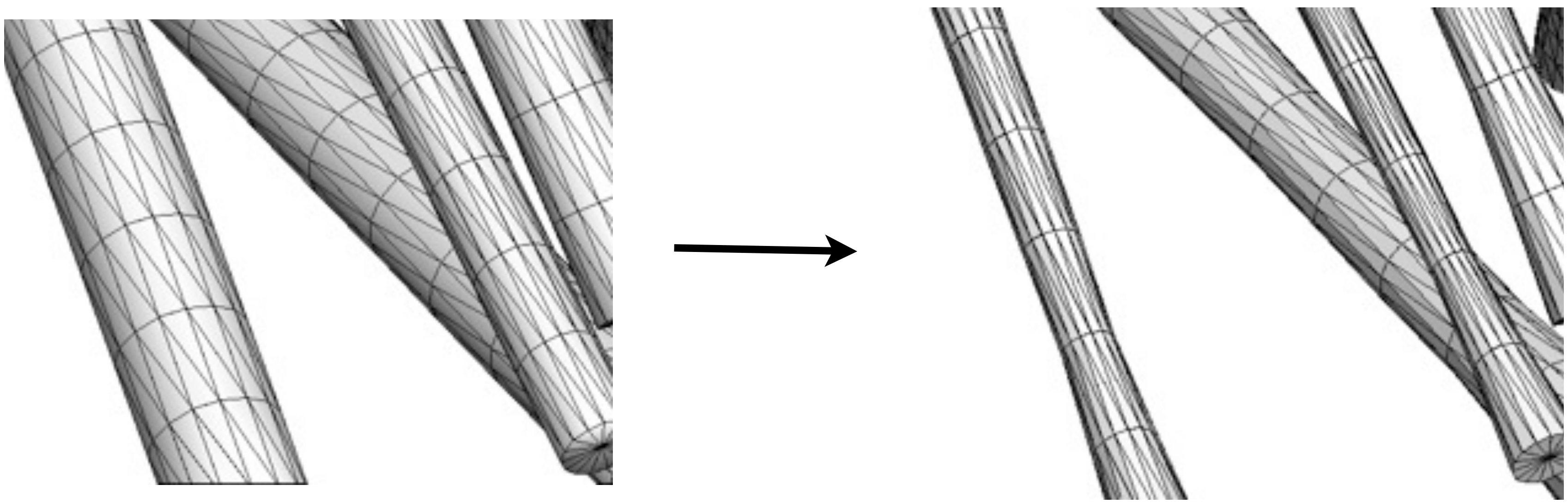
– Note: there is error in the volume of the reconstruction, however we always track and operate on the *actual* volume, so mass is conserved.

Surface Movement



This treatment is able to replicate some of the dominant morphologies we observe at the micro-scale.

– non-uniform thinning
– “needling”



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Surface Movement

- **This reconstruction method could be thought of as a Axisymmetric Volume of Fluid (VoF) approach.**
- **Benefits:**
  – Relatively easy to implement
  – Error in volume is small and bounded for our work (<1%)
  – Extending code to modeling fiber material response would be (fairly) straightforward (i.e. solving the heat conduction equation is quasi-1D).
  – Surface reconstruction is *very* fast
- **Limitations:**
  – Limited to axisymmetric shapes
  – Not easily extensible to tomography-generated surfaces

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  – Simplified Darcy Flow
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- **Future Work**
- **Conclusions**

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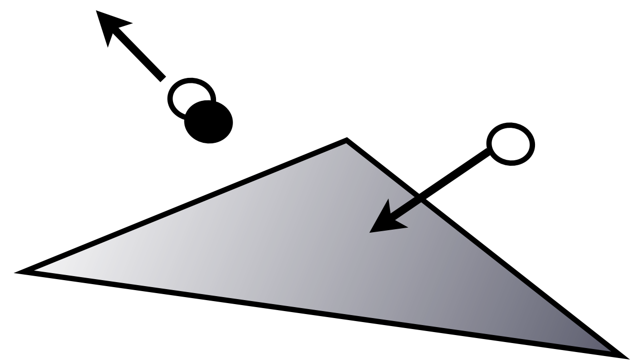
Gas-Surface Interaction Modeling

- **In DSMC, the gas surface interaction is modeled by determining the probability that a gas particle will react if it strikes a surface**
- **For our current analysis, we use a temperature dependent probability for carbon oxidation given by Park.**
- **Devising more sophisticated treatments for the GSI is an active area of research.**

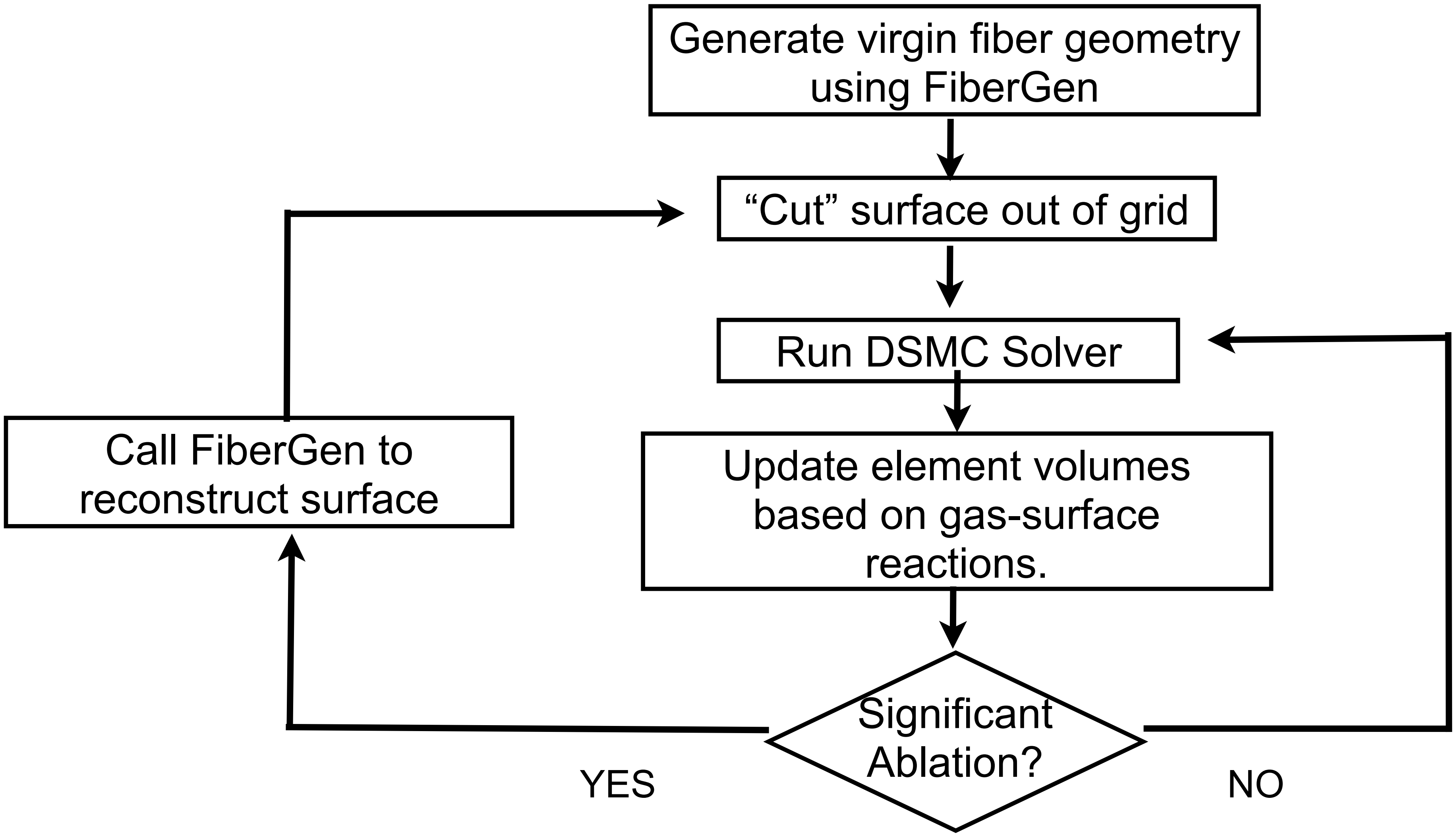
$$C(s) + O_2(a) \rightarrow CO(a) + O(a)$$



$$\alpha = \frac{1.43 \times 10^{-3} + 0.01 \exp(-1450/T)}{1 + 2 \times 10^{-4} \exp(13{,}000/T)}.$$

Park, Nonequilibrium Hypersonic Aerothermodynamics, 1991

Coupled Ablation



- **We have found (so far) that the surface update is generally very fast, therefore we update fairly frequently since there is little to no penalty**

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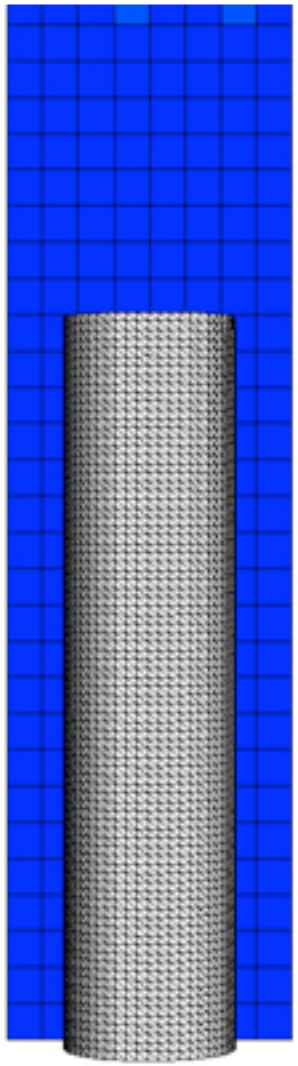
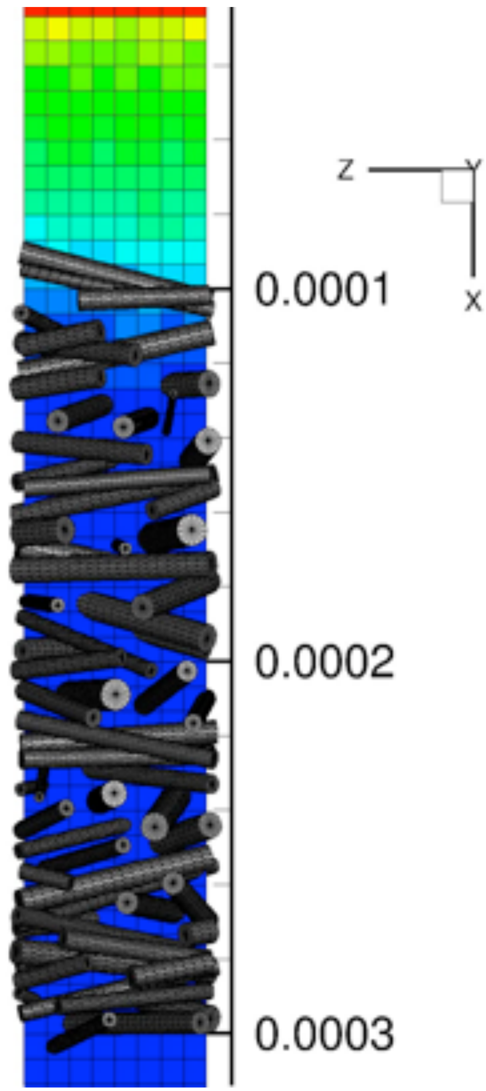
Movies



Ablation of a single fiber



Ablation of a porous geometry

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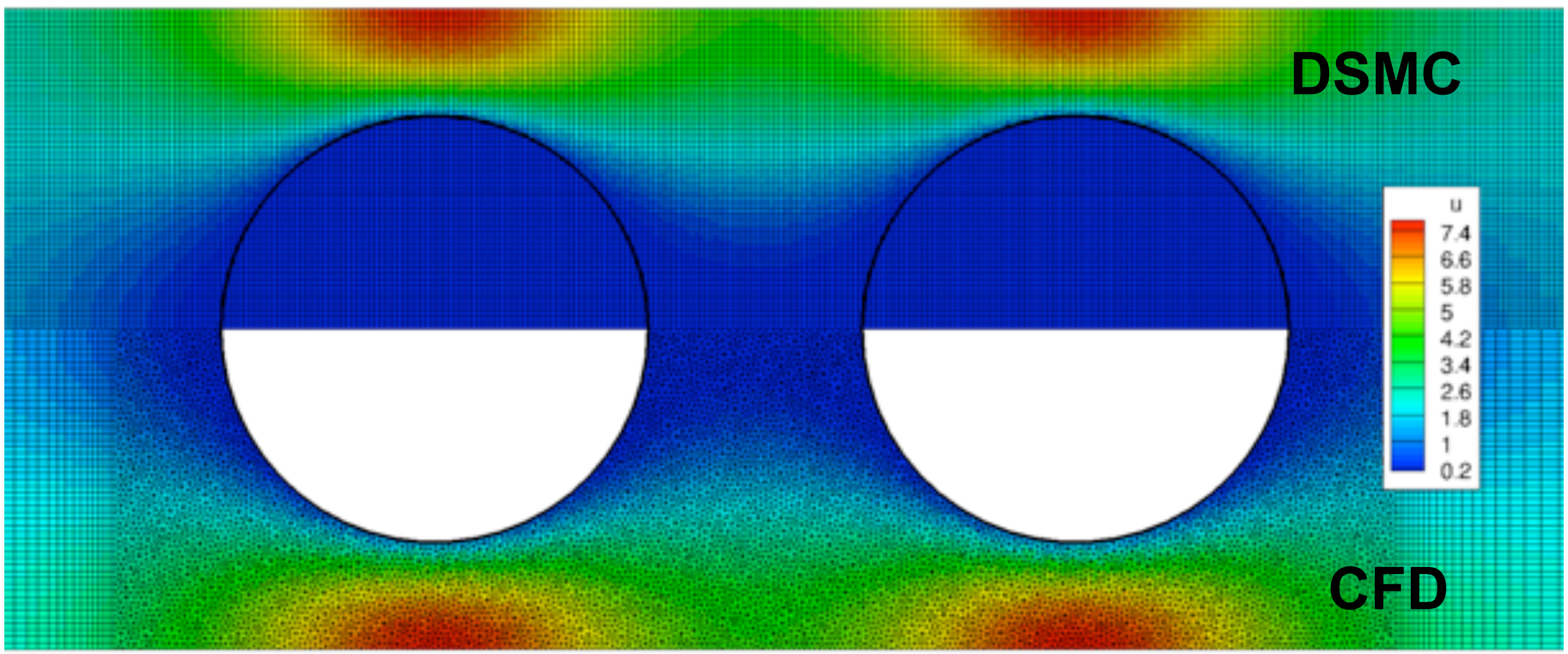
Simple Darcy Flow

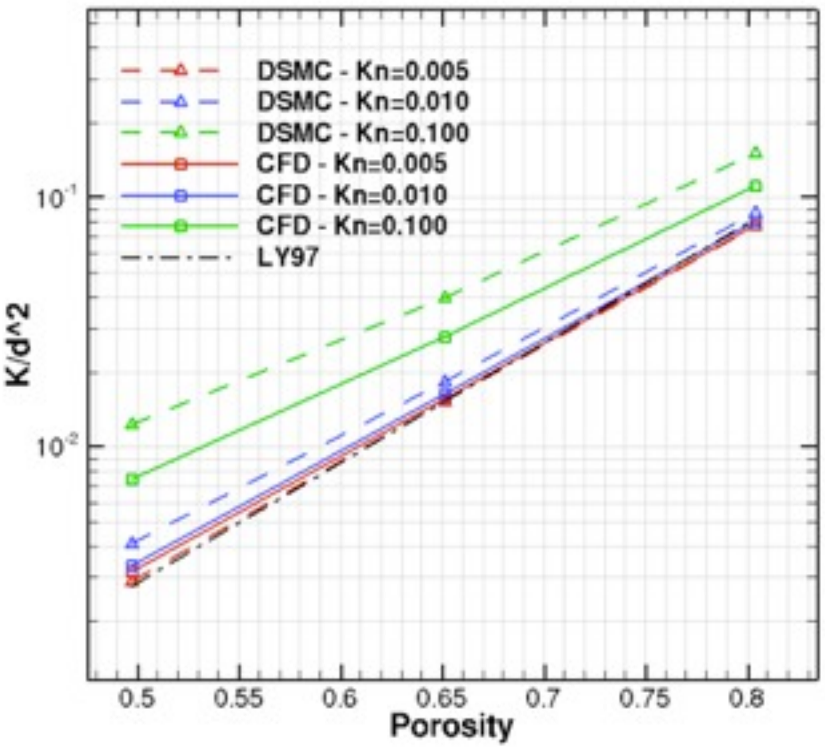
- **To begin, we seek to validate the approach for simple Stoke's flow through idealized porous medium.**
  - We compare to both CFD, and models (analytical and empirical) in the literature
  - CFD augmented with Maxwell slip model



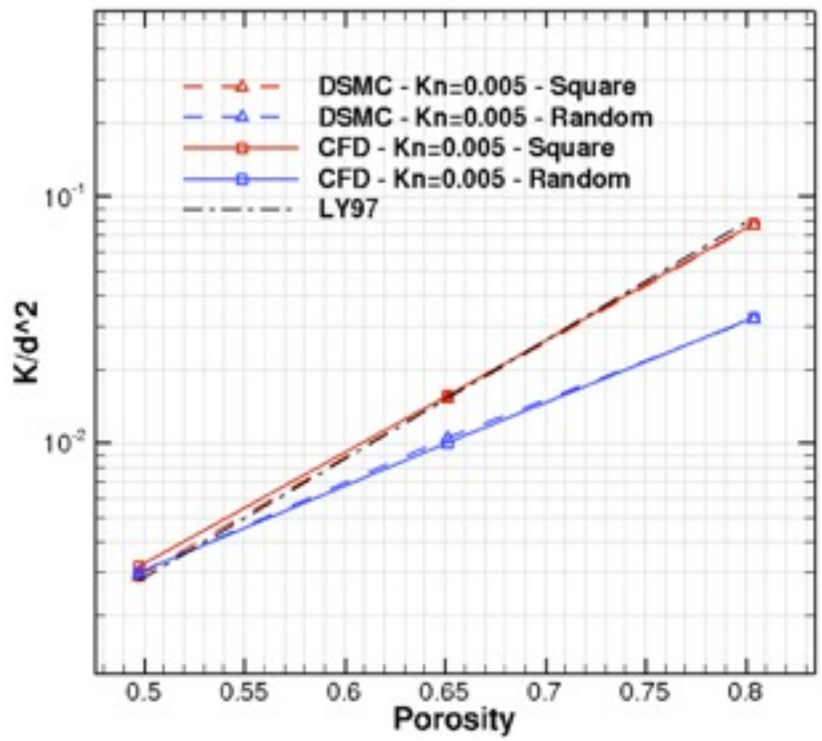
Simple Darcy Flow

- **Results show good agreement with literature.**
- **...as well as intuitive departures due to Knudsen number effects, as well as microstructure changes**

$$\frac{\partial p}{\partial x} = -\frac{\mu}{K} v_g'$$



Regular Array of Cylinders



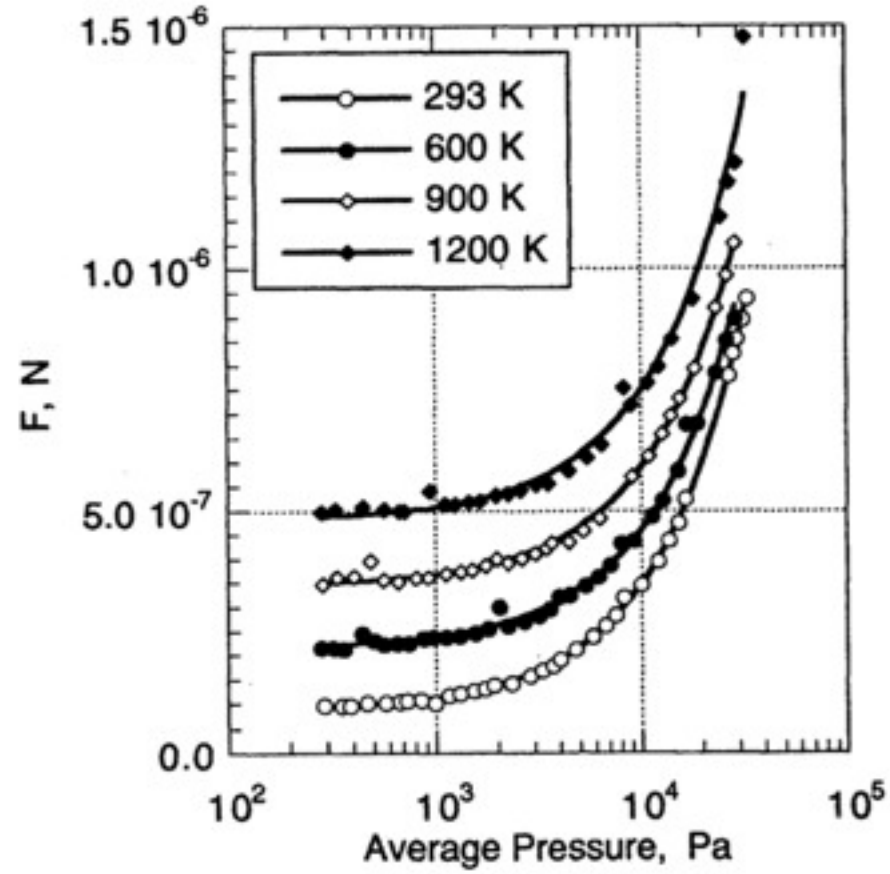
Random Array of Cylinders

Lee and Yang, JHMT, 1997

FiberForm Permeability

- Now we want to look at more relevant geometries and conditions.
- Flow-tube experiments performed at NASA Ames.
- Experimental data well-fit by Klinkenberg form of Darcy equation.
- Material permeability tested at various pressures and temperatures
- Significant variation in permeability observed due to rarefied effects.

$$F = \frac{4\mu \dot{m} RTL}{\pi D^2 M \Delta P} = K_0(P_{av} + b)$$



Marschall and Milos, JTHT, 1998

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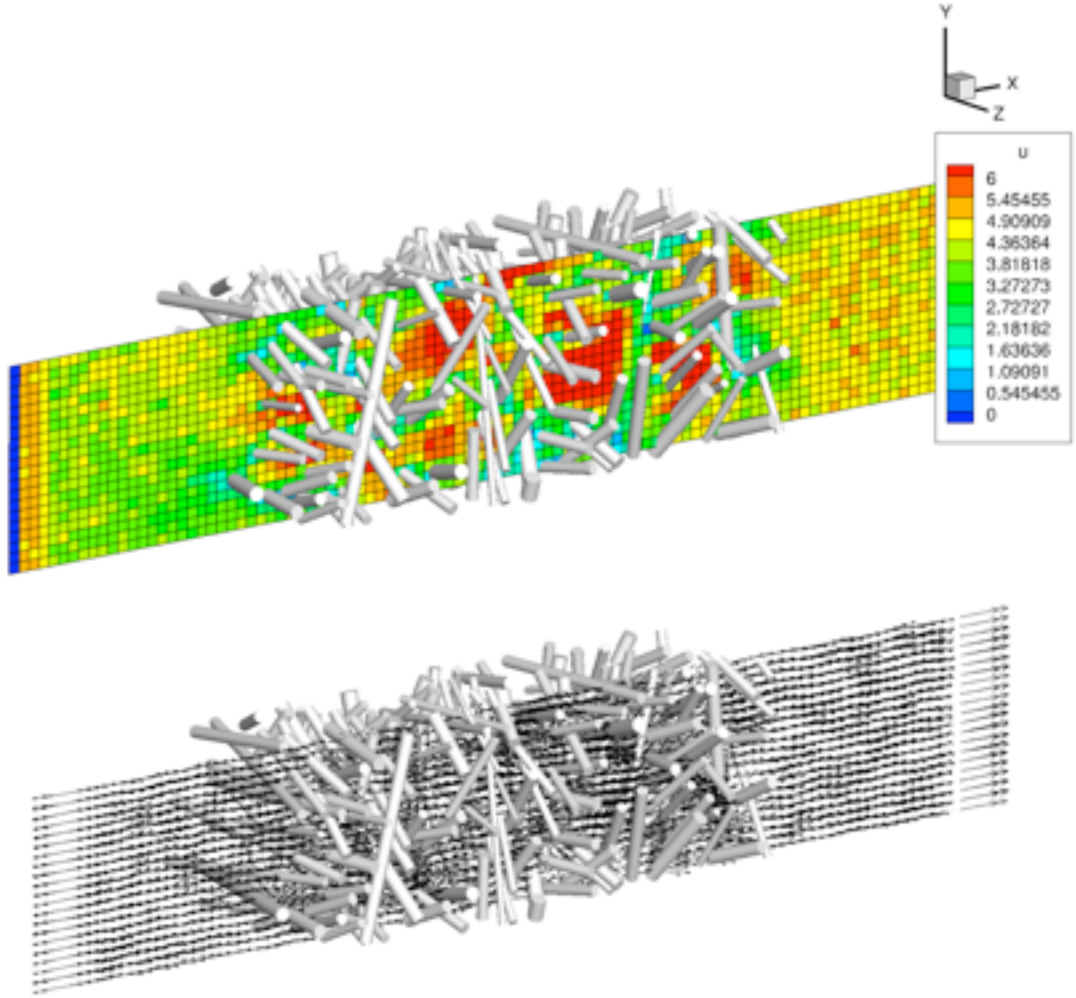
Preliminary Results

- **Simulations were performed near the low end of the pressure range (~ *1kPa*) of the experiments.**
- **Gas used was N2 at room temperature.**
- **Size of volume was 200x50x50 microns with a porosity of ~0.85**
- **Two nominal fiber radii were used**
  - 6 micron (*single fiber*)
  - 10 micron (*fiber bundle*)
- **Several fiber orientations were simulated**



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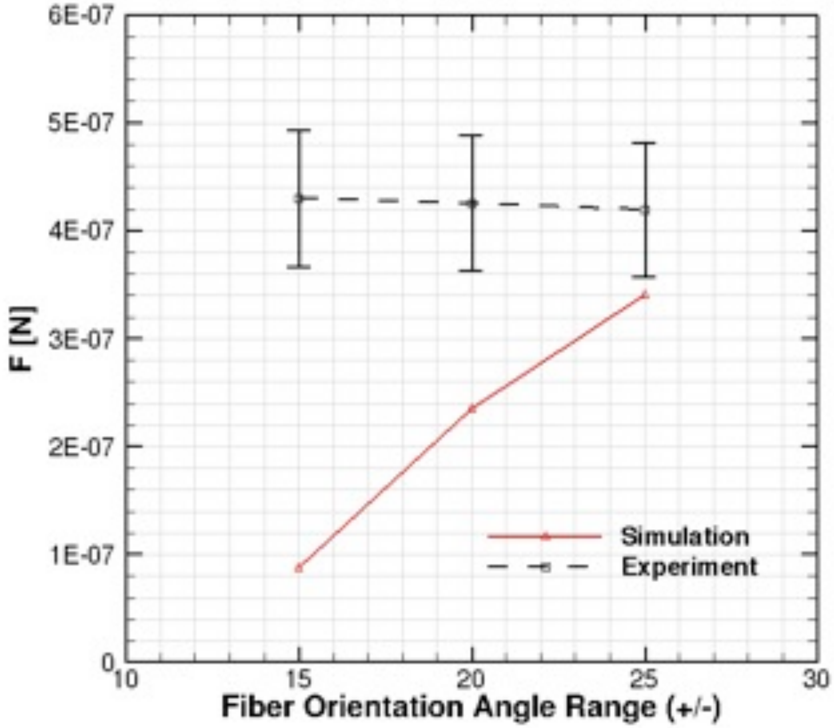
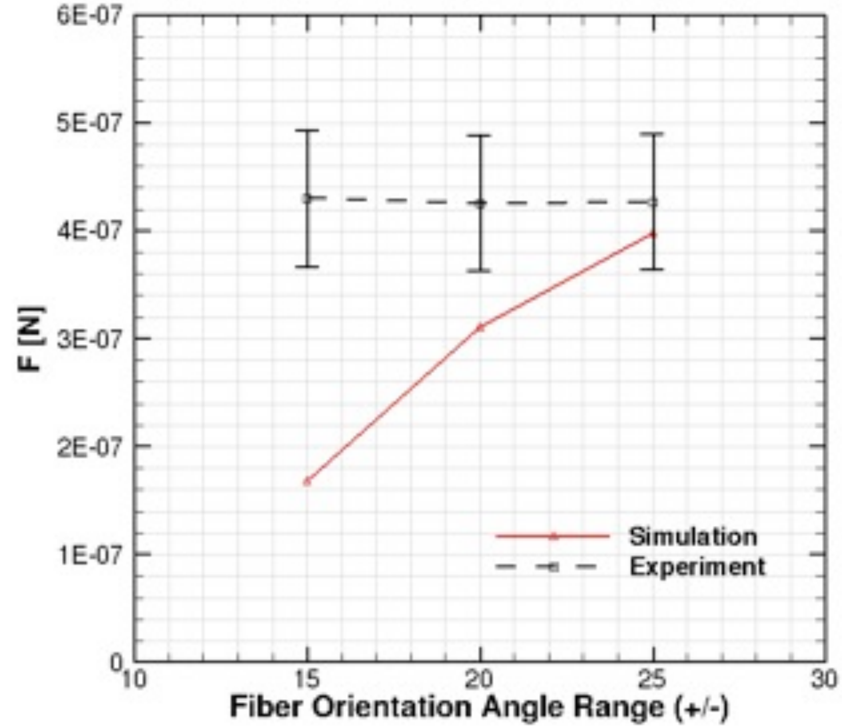
Preliminary Results

$D_f = 6\mu\text{m}$



$D_f = 10\mu\text{m}$



- **Fiber orientation is defined as the angle of the fiber with "pressing" plane.**
- **Error bars are those reported in the paper for *all* runs.**

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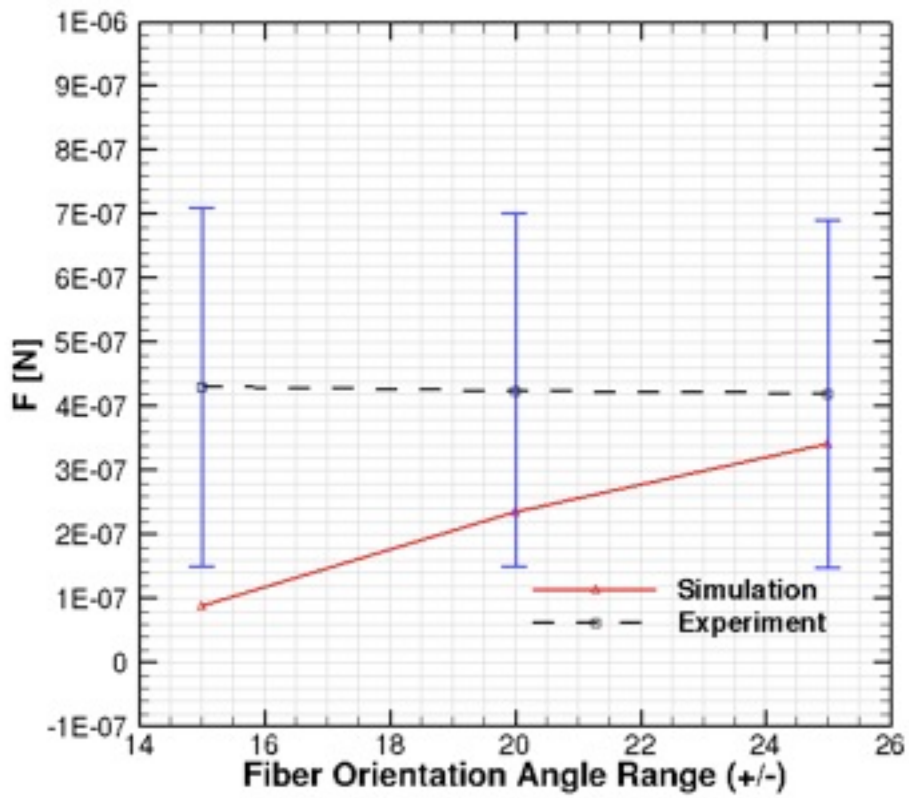
Permeability Results

- **Caveats:**
  - Seems to be large scatter in the experimental data

FiberForm	145	359	703
	149	323	877
	157	82.3	1100
	161	79.1	1150

  - Simulated geometry likely doesn't constitute a "representative volume element"
  - Experiment gas was air



- **Takeaways:**
  - Microstructure is important
  - We're in the ballpark!

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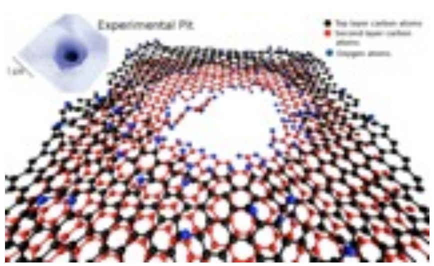
Future Work

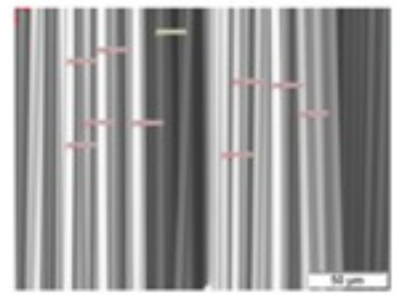
FiberGen
- Add analysis toolbox for computing geometric properties and statistics.
- Woven geometries

Gas-Surface Modeling
- Develop new gas-surface interaction model that takes better advantage of the improved fidelity of DSMC
  - "Active site" based approach
- Incorporate probabilities from Molecular Dynamics simulations

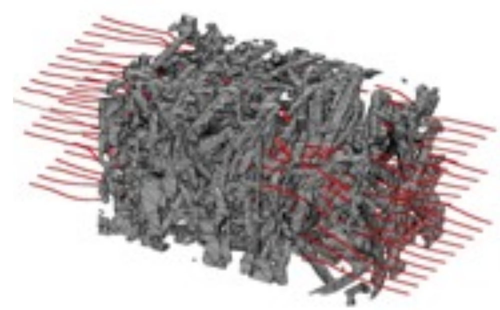


Poovathingal, et al., J. Phys. Chem., 2013

Experimental Validation
- Interested in performing targeted validation experiments in the NASA Flow-tube facility on "simple(r)" microstructure



Simulate Stuff!...(*cool stuff*)



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Questions?