

PuMA and Multiscale Modeling

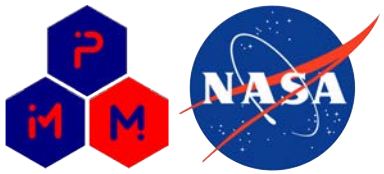
Presenters: Federico Semeraro

Krishnan Swaminathan Gopalan

Project contributors: Joseph C. Ferguson, Marcos Acin, Arnaud Borner, John Thornton Francesco Panerai, Nagi N. Mansour

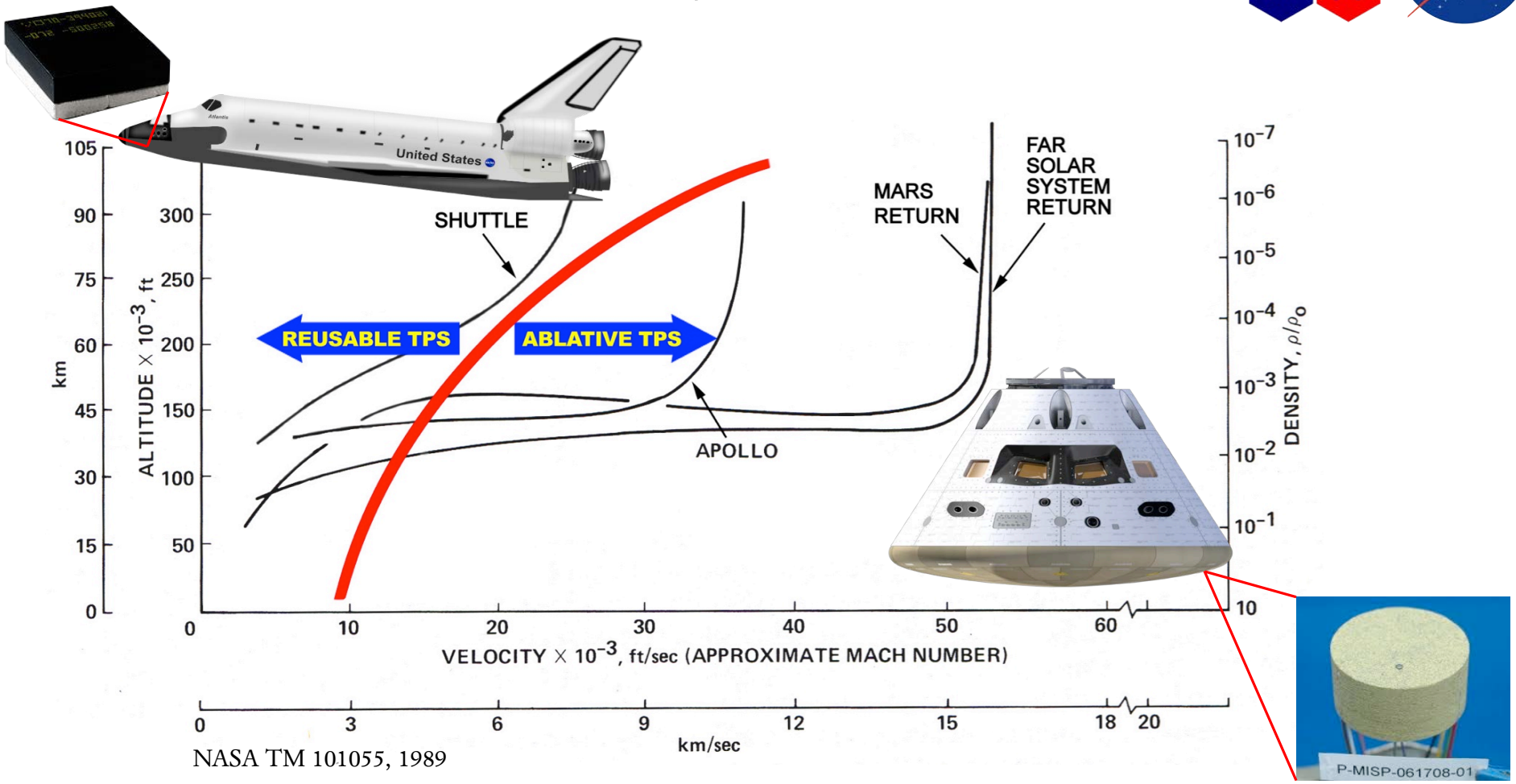
Advanced Modeling & Simulation (AMS) Seminar Series
NASA Ames Research Center, September 29th, 2020

Content



- Motivation
- Overview of PuMA
- Effective properties for fibrous media
  - ❖ Fiber orientation
  - ❖ Thermal conductivity
  - ❖ Elasticity
- Surface chemistry
  - ❖ Molecular beam
  - ❖ Oxidation model

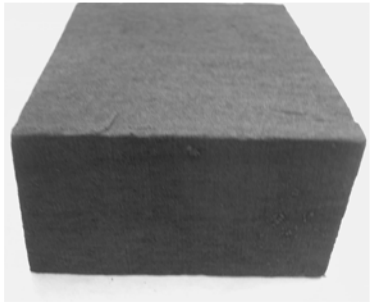
Thermal Protection Systems (TPS)



NASA TM 101055, 1989

Ablative TPS

Carbon preform + Phenolic Resin = PICA

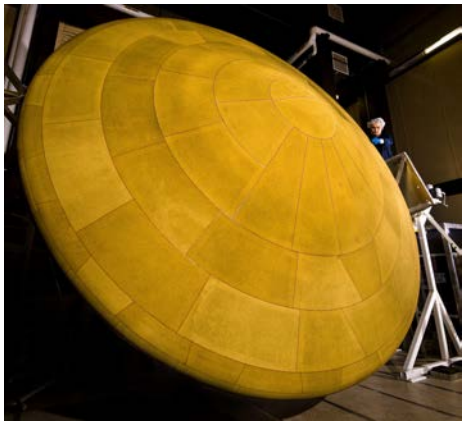








Stardust Capsule

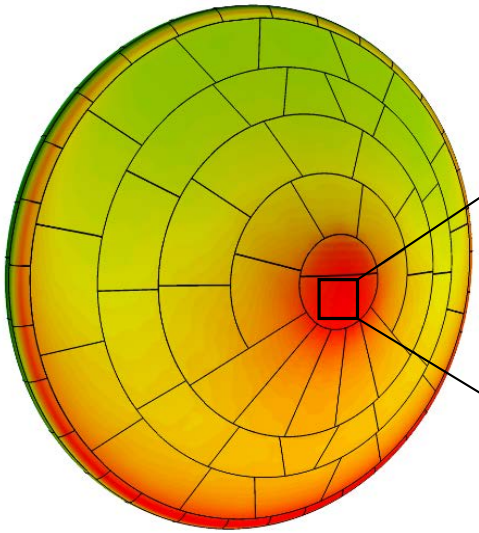


Mars Science Laboratory

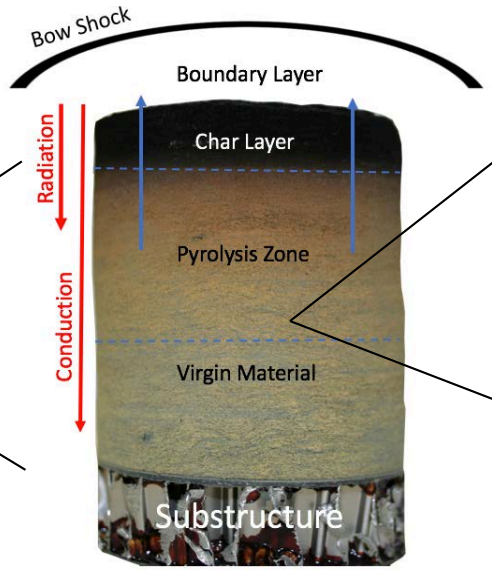
Modeling TPS

Macroscale Modeling

Full scale material response solvers, using volume-averaged techniques to solve conservation equations for ablation

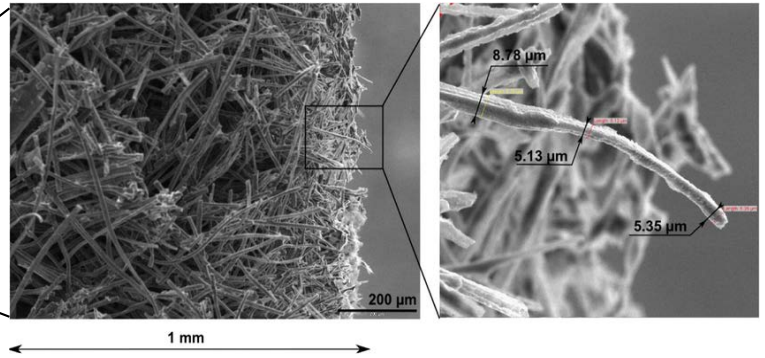


Simulation of surface temperature for MSL heatshield



Microscale Modeling

Used to inform material properties and material response parameters used in macro-scale modeling



Lachaud and Mansour, *JTHT* 2013

X-Ray Microtomography

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



Penetrating power

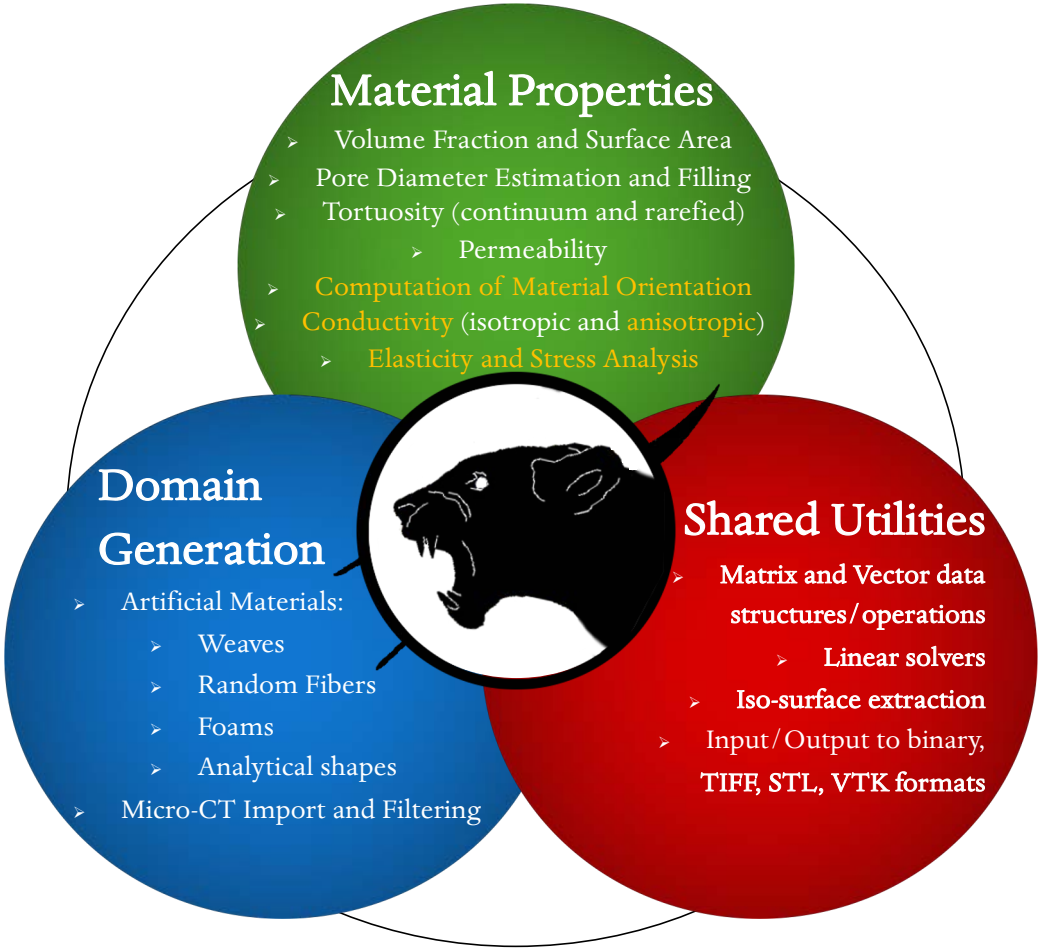
Multiple angles

Use this series of images to reconstruct the 3D object



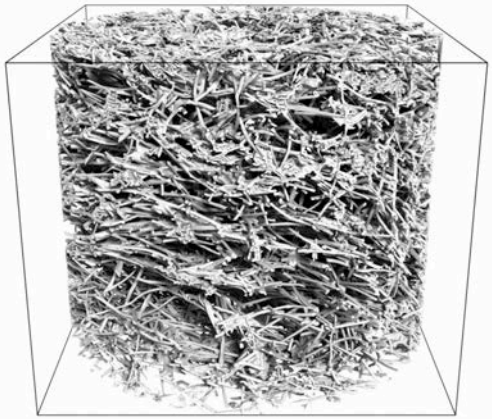
Courtesy of D. Parkinson (ALS)

Porous Microstructure Analysis (PuMA)



New features in Version 3:

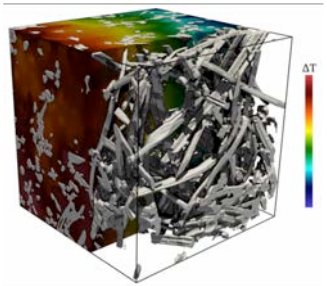
- Modular C++ library
- Redesigned GUI
- Wrapped as Python module
- Linux and Mac compatibility



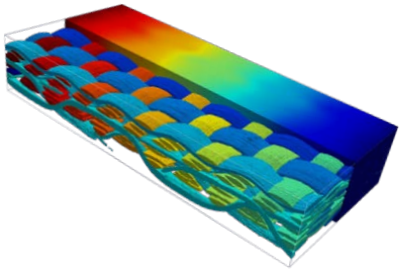
CT Reconstruction of FiberForm

Transport Properties in PuMA

Effective Thermal Conductivity



Conductivity of fibrous materials



Woven materials considering anisotropy

Tortuosity / Diffusivity

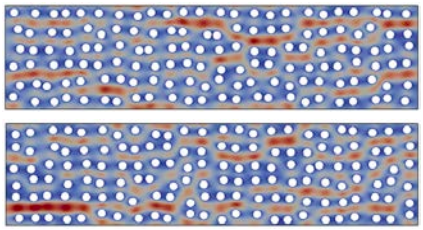


High Knudsen

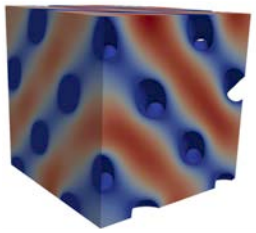


Low Knudsen

Permeability

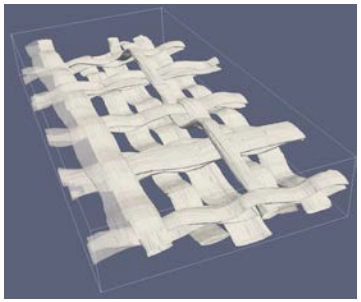


Pressure driven flow through 2D fibrous material

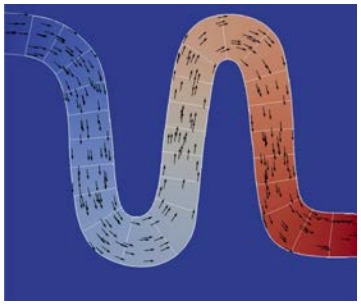


Pressure driven flow through 3D triply periodic material

Considering Anisotropy



Ray casting orientation

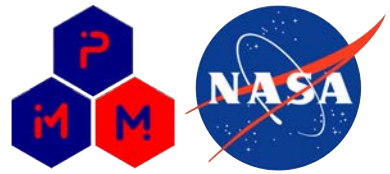


Heat flux orientation

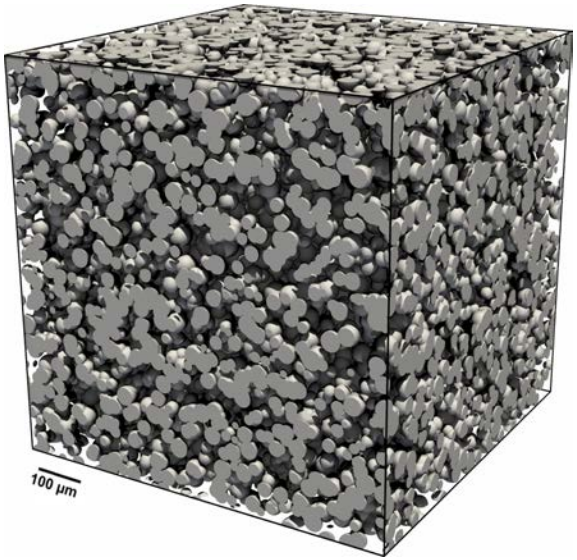
Material Response - Oxidation



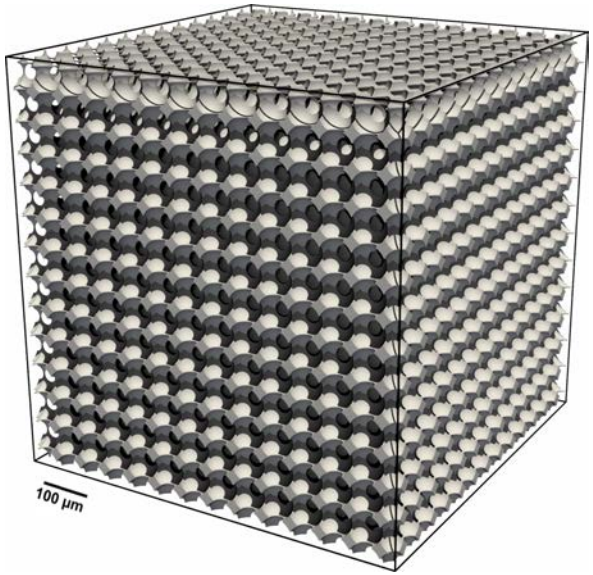
Advanced Domain Generation



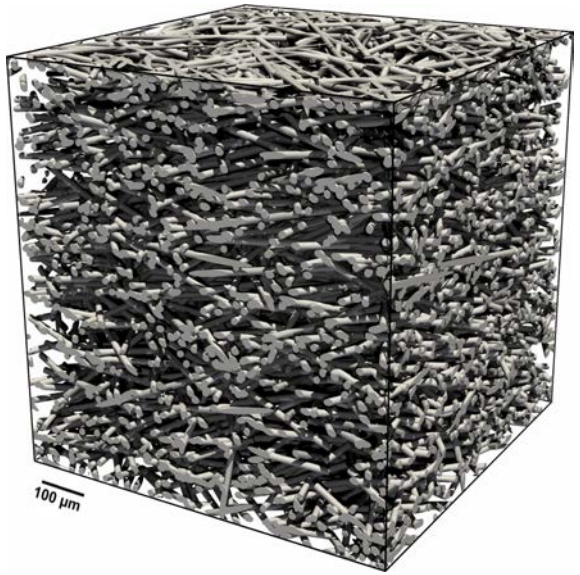
Packed Sphere Beds



Periodic Foams



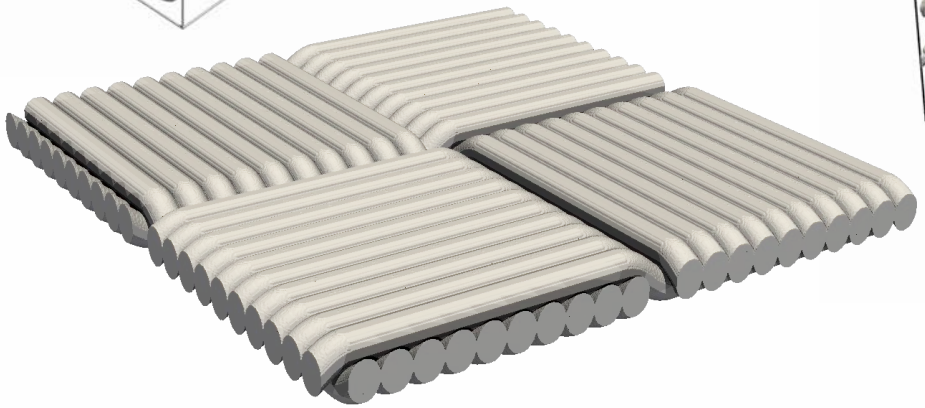
Fiber Structures



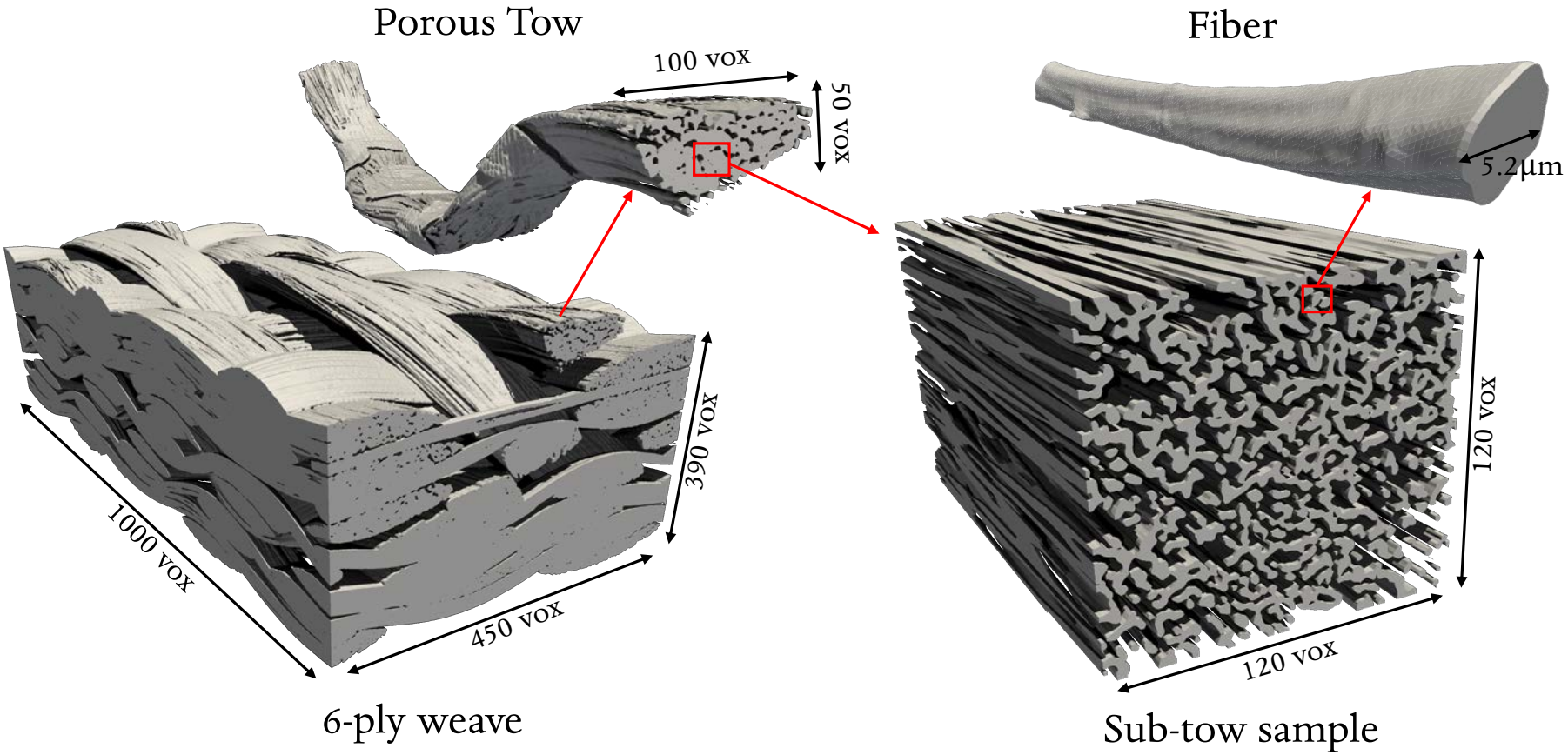
Fibers and Weaves Generator





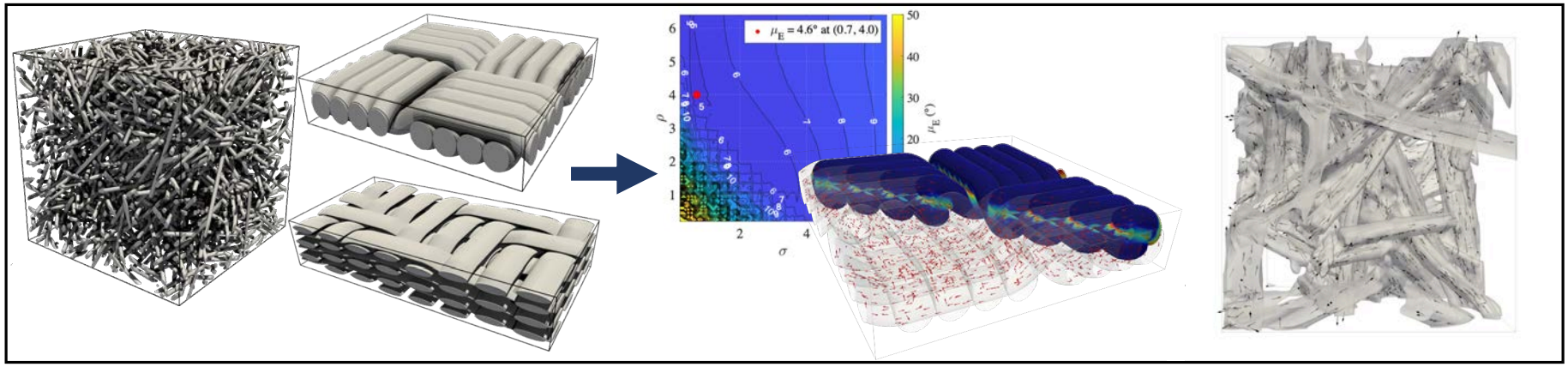


An Anisotropic and Multiscale Problem

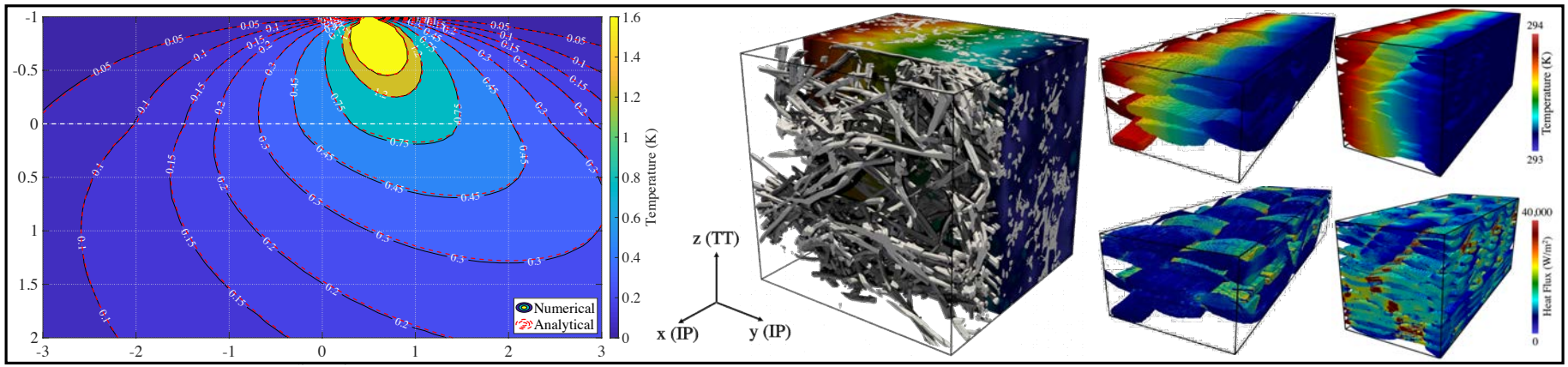


Effective properties for fibrous media

Semeraro, F., Ferguson, J.C., Panerai, F., King, R.J. and Mansour, N.N., Anisotropic analysis of fibrous and woven materials **part 1: Estimation of local orientation**. *Computational Materials Science*, 178, p.109631. (2020)

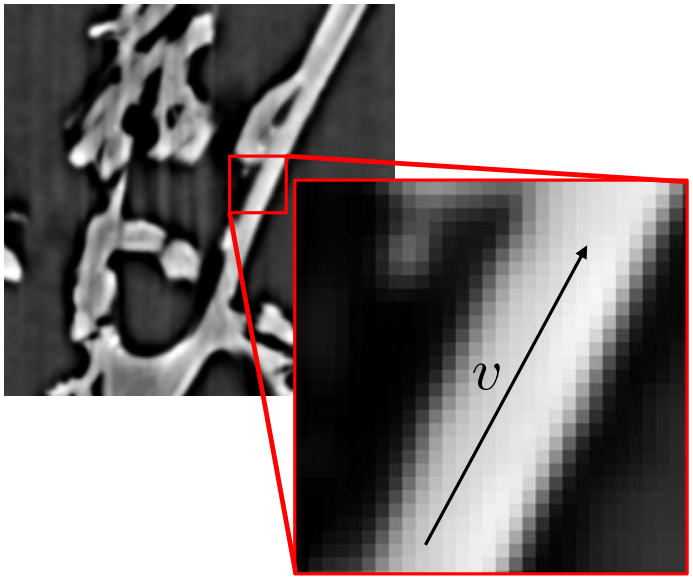


Semeraro, F., Ferguson , J.C, Acin, M., Panerai, F. and Mansour, N.N., Anisotropic analysis of fibrous and woven materials **part 2: Computation of effective conductivity**. *Computational Materials Science*, 186, p.109956. (2021)



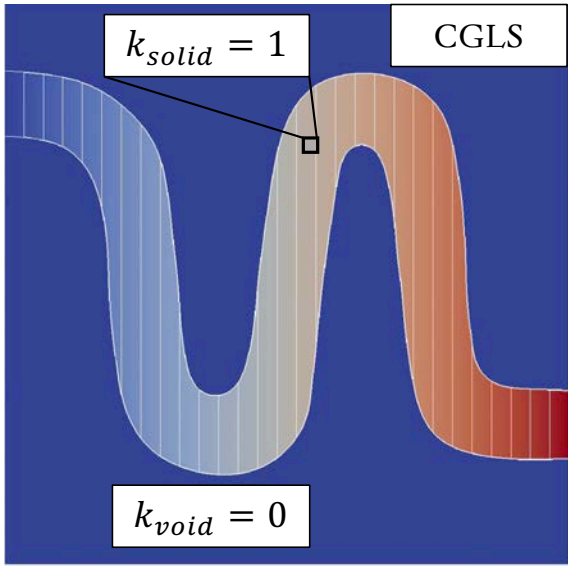
Fiber Orientation Methods

Structure Tensor

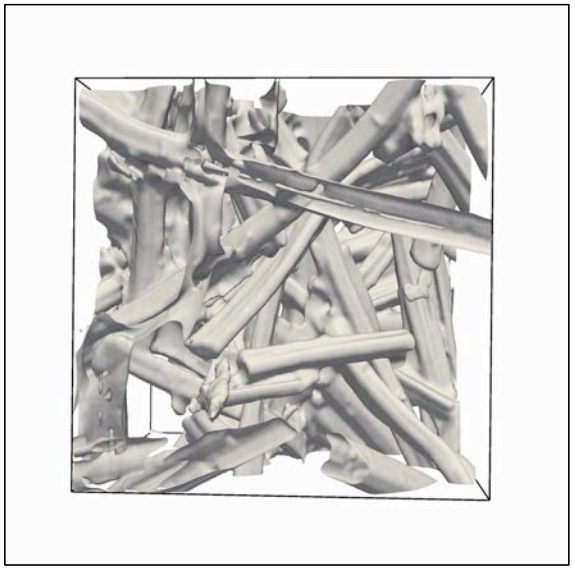


$$(I(x+v)-I(x))^2 \approx 0$$

Artificial Flux

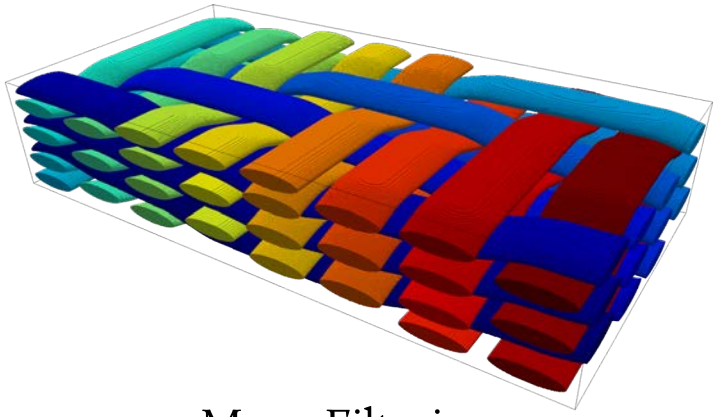


Ray Casting

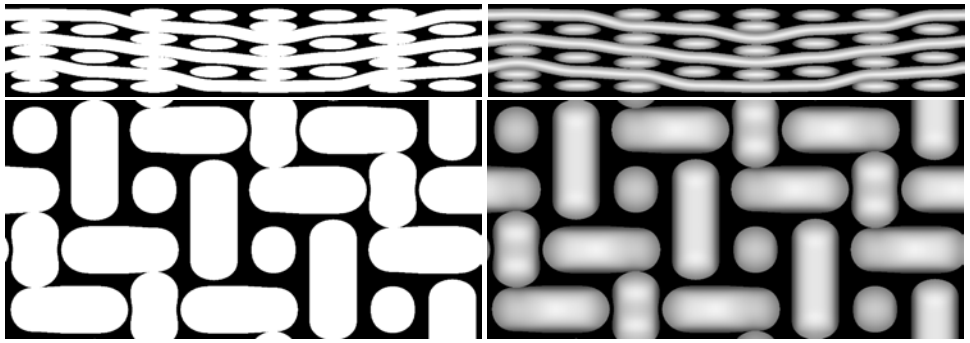


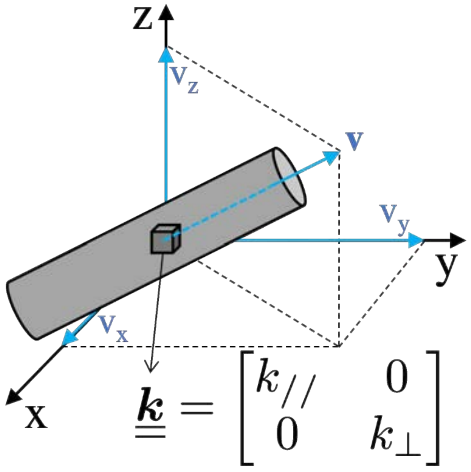
Workflow for Weave Orientation

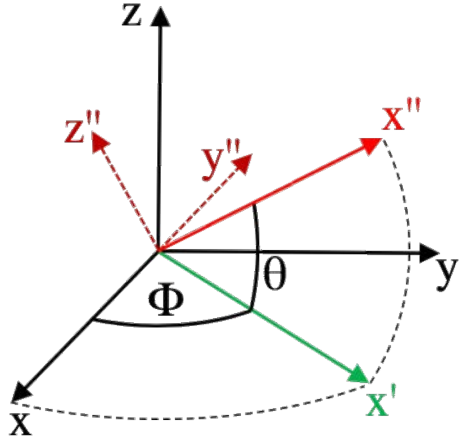
Individual tow segmentation and tracking



Mean Filtering



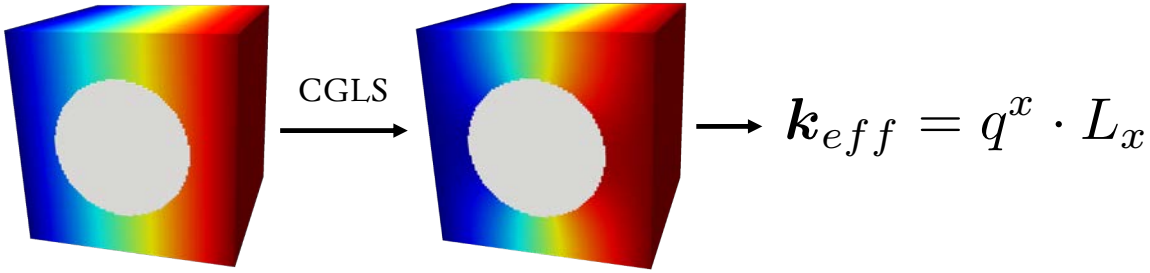




$$\boldsymbol{q} = \underbrace{\left[\boldsymbol{R}^{-1}\boldsymbol{k}''\boldsymbol{R}\right]}_{\boldsymbol{k}} \nabla T$$

$$\boldsymbol{R} = \begin{bmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

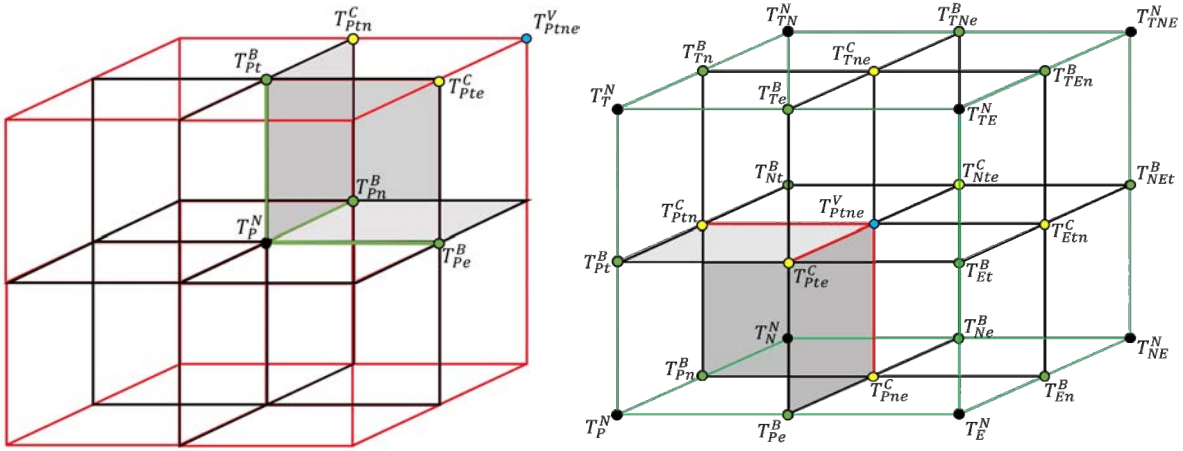
Effective Thermal Conductivity



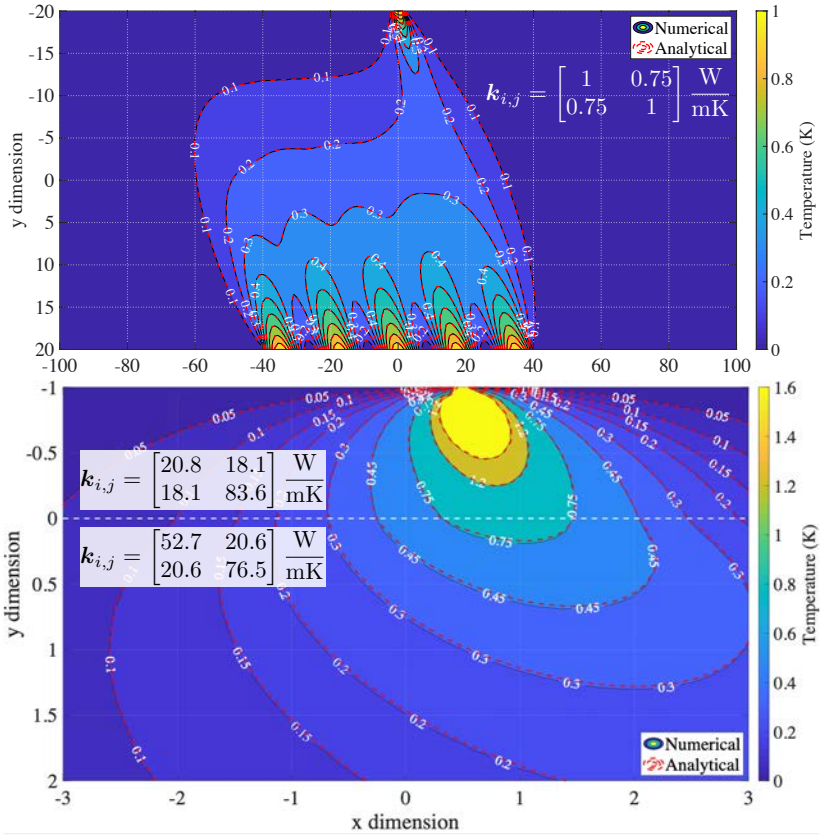
$$\boldsymbol{k}_{eff} = q^x \cdot L_x$$

$$\nabla \cdot \boldsymbol{q} = 0 \longrightarrow \boldsymbol{q}(x,t) = \boldsymbol{E}(x)\,\boldsymbol{T}^N(x,t)$$

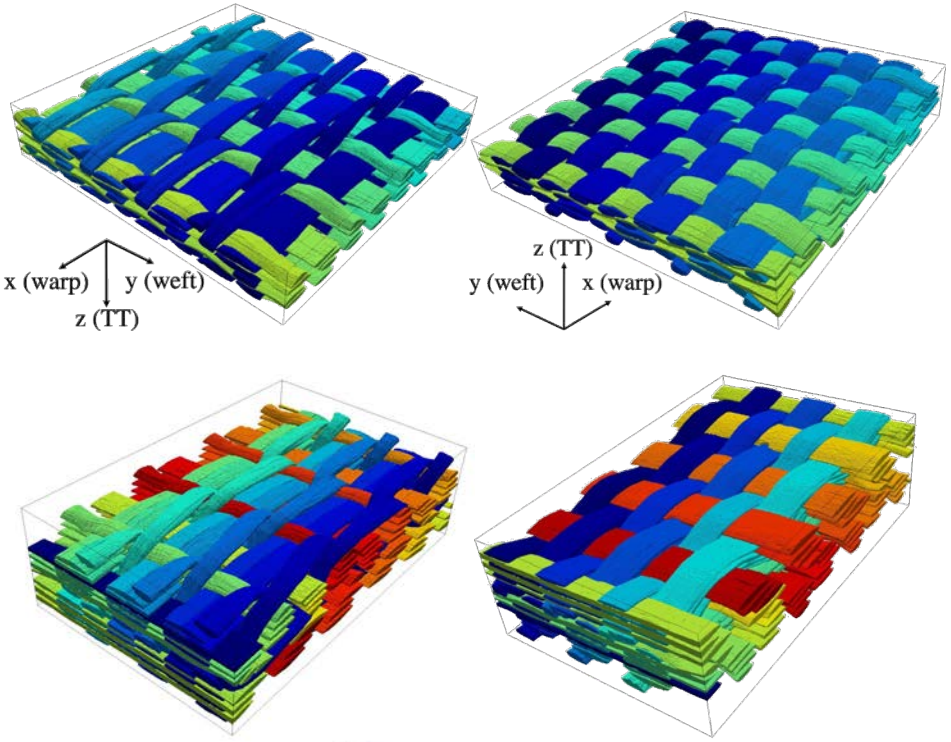
Multi-Point Flux Approximation (MPFA):

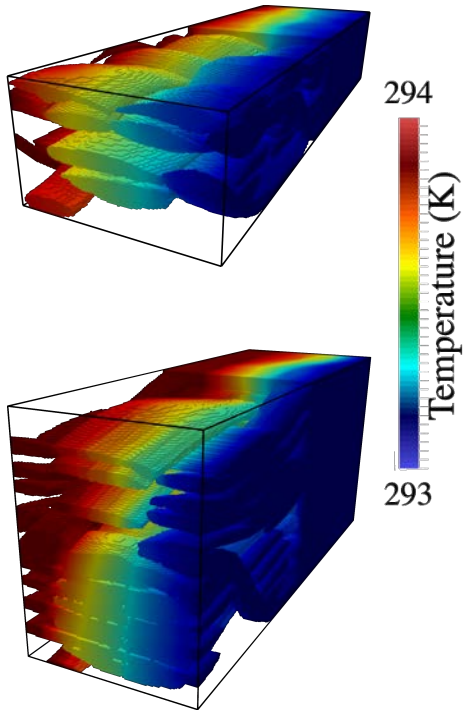


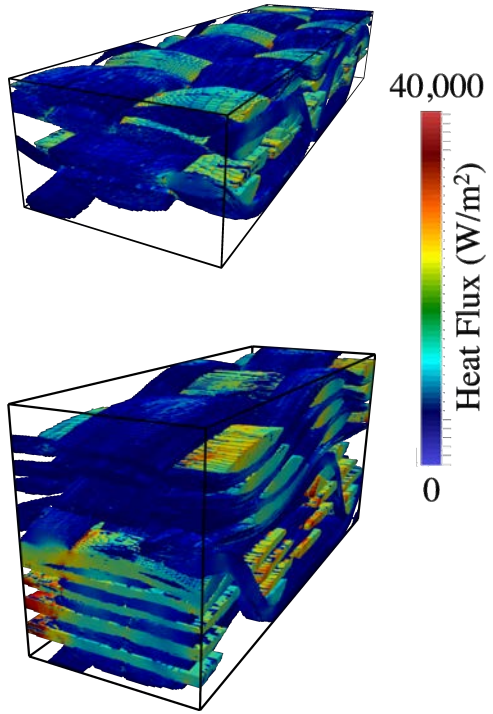
Verification against analytical solutions



ADEPT Validation



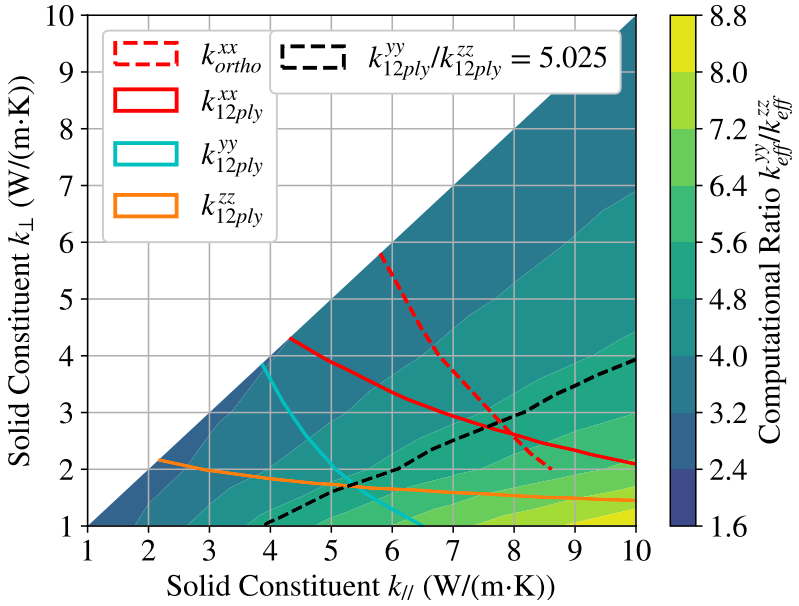




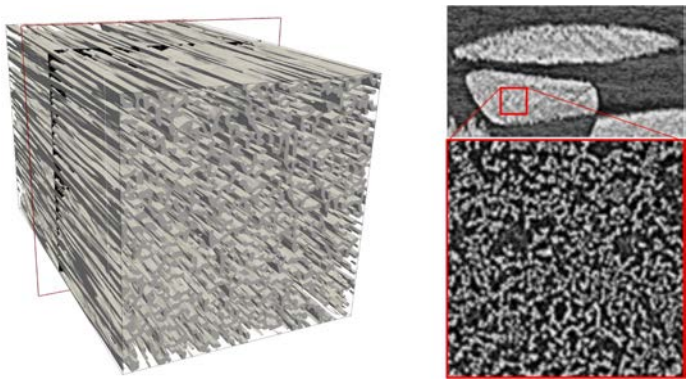
Single Fiber Conductivity Estimation

Two experimental values at Room Temperature:

$$\boldsymbol{k}_{eff}^{ortho} = \begin{bmatrix} 2.342 & - & - \\ - & 1.766 & - \\ - & - & 0.305 \end{bmatrix} \quad \boldsymbol{k}_{eff}^{12ply} = \begin{bmatrix} 2.184 & - & - \\ - & 1.980 & - \\ - & - & 0.394 \end{bmatrix}$$



$$[k_{//}^{weft}, k_{\perp}^{weft}] = [5.4, 1.8] \quad \text{and} \quad [k_{//}^{warp}, k_{\perp}^{warp}] = [7.7, 2.7] \frac{\text{W}}{\text{mK}}$$



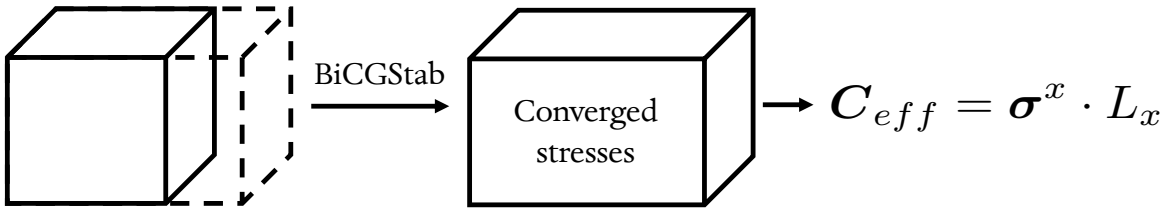
$$[k_{//}, k_{\perp}] = [9.7, 5.5] \frac{\text{W}}{\text{mK}}$$

$$\boldsymbol{k}_{eff}^{4ply} = \begin{bmatrix} 1.750 & -0.032 & -0.024 \\ -0.093 & 1.490 & 0.002 \\ 0.039 & 0.001 & 0.193 \end{bmatrix} \quad \boldsymbol{k}_{eff}^{6ply} = \begin{bmatrix} 1.740 & -0.141 & -0.020 \\ -0.105 & 1.710 & -0.005 \\ 0.091 & -0.023 & 0.200 \end{bmatrix}$$

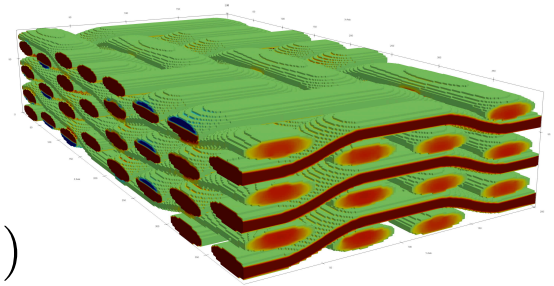
$$\boldsymbol{k}_{eff}^{8ply} = \begin{bmatrix} 1.830 & -0.244 & 0.016 \\ -0.192 & 1.510 & 0.005 \\ 0.039 & 0.000 & 0.231 \end{bmatrix} \quad \boldsymbol{k}_{eff}^{12ply} = \begin{bmatrix} 2.310 & -0.414 & 0.000 \\ -0.524 & 2.030 & 0.071 \\ 0.007 & 0.005 & 0.504 \end{bmatrix}$$

Effective Elasticity

Semeraro, F., Acin, M., Panerai, and Mansour, N.N., Anisotropic analysis of fibrous and woven materials **part 3: Computation of effective elasticity**. *Computational Materials Science*, (work in progress)

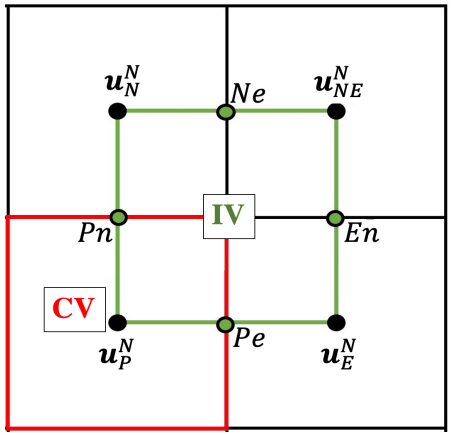


$$C_{eff} = \boldsymbol{\sigma}^x \cdot L_x$$

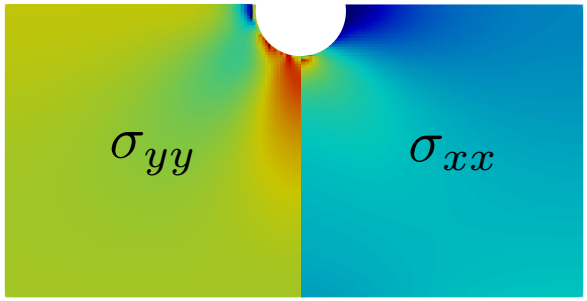


$$\nabla \cdot \boldsymbol{\sigma} = \nabla \cdot (\boldsymbol{C\varepsilon}) = 0 \longrightarrow \boldsymbol{\sigma}(x,t) = \boldsymbol{E}(x)\boldsymbol{D}^N(x,t)$$

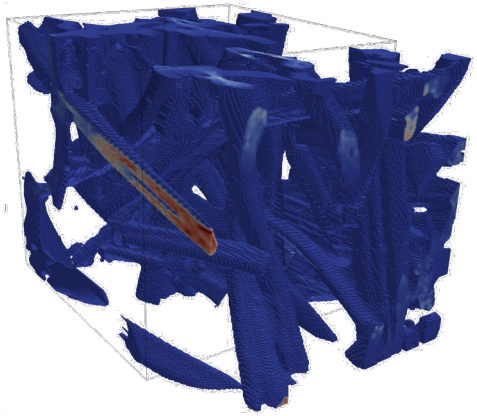
Multi-Point Stress Approximation (MPSA)



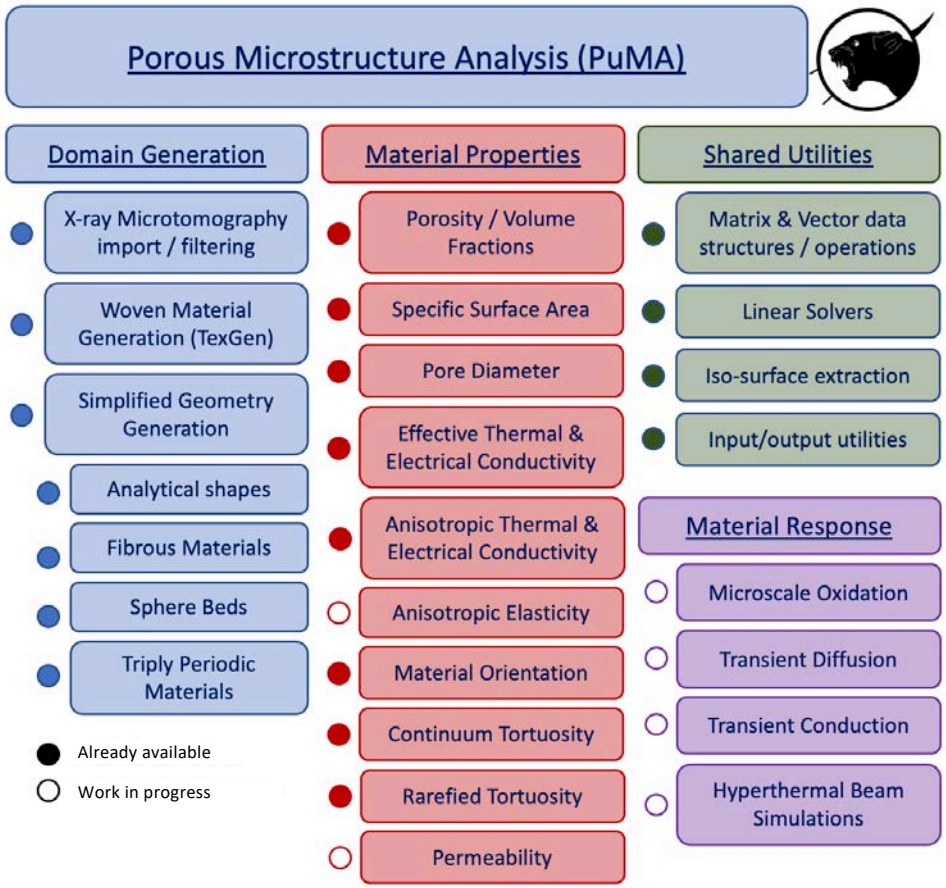
Verification against analytical solution



Validation on fibrous and woven media



Conclusion

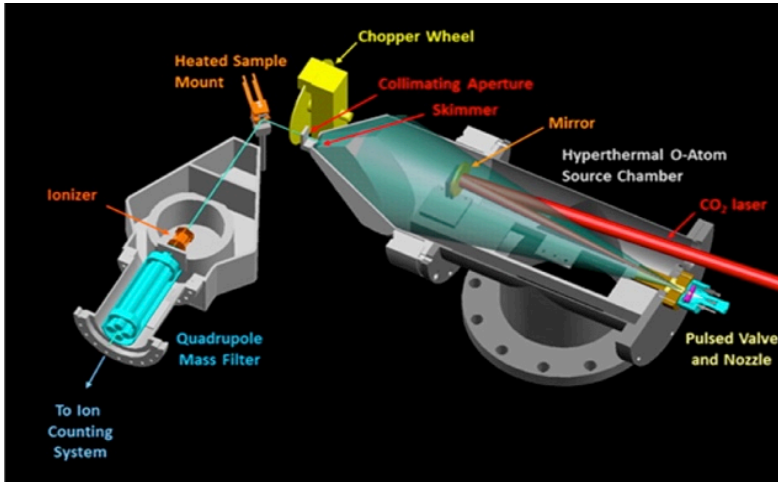

Porous Microstructure Analysis (PuMA)
Domain Generation
X-ray Microtomography import / filtering
Woven Material Generation (TexGen)
Simplified Geometry Generation
Analytical shapes
Fibrous Materials
Sphere Beds
Triply Periodic Materials
Material Properties
Porosity / Volume Fractions
Specific Surface Area
Pore Diameter
Effective Thermal & Electrical Conductivity
Anisotropic Thermal & Electrical Conductivity
Anisotropic Elasticity
Material Orientation
Continuum Tortuosity
Rarefied Tortuosity
Permeability
Shared Utilities
Matrix & Vector data structures / operations
Linear Solvers
Iso-surface extraction
Input/output utilities
Material Response
Microscale Oxidation
Transient Diffusion
Transient Conduction
Hyperthermal Beam Simulations
Already available
Work in progress



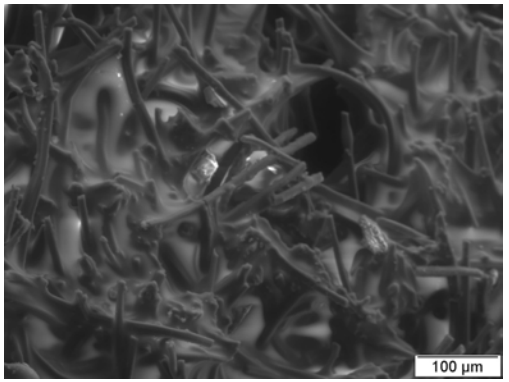
Application motivation

Objectives:

- Characterize recession/ablation of carbon surface coated with NuSil due to oxidation
- Develop a predictive model for use in microscopic (DSMC, PuMA) and macroscopic (CFD, MRC) solvers

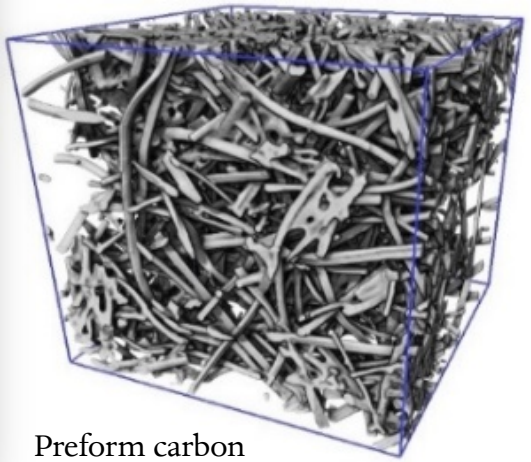


Murray, V J., et al. *The Journal of Physical Chemistry C* 119.26 (2015): 14780-14796.



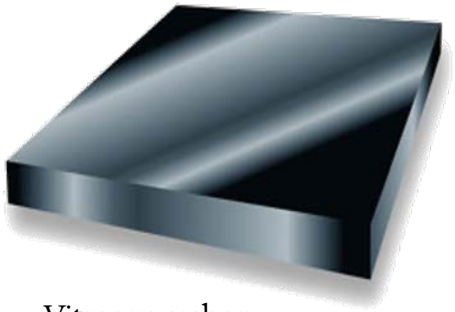
NuSil-coated FiberForm

Image courtesy: Dr. Bessire



Preform carbon

Image courtesy: Prof. Panerai

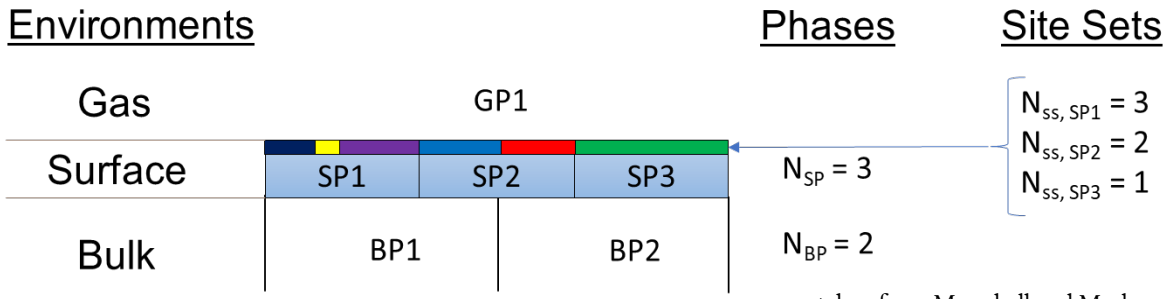


Vitreous carbon

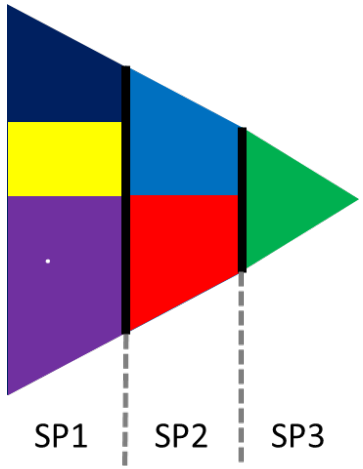
SPI Supplies

Surface chemistry framework

- Methodology to represent surface sites similar to Marschall, Maclean and Driver for CFD.
- Particles adsorbed (deleted) and desorbed (created), surface element stores adsorbed particle concentration.
- Surface reactions based on concentration within surface element.
- Multiple triangulated elements (like cells) on surfaces
- Langmuir model for surface sites.

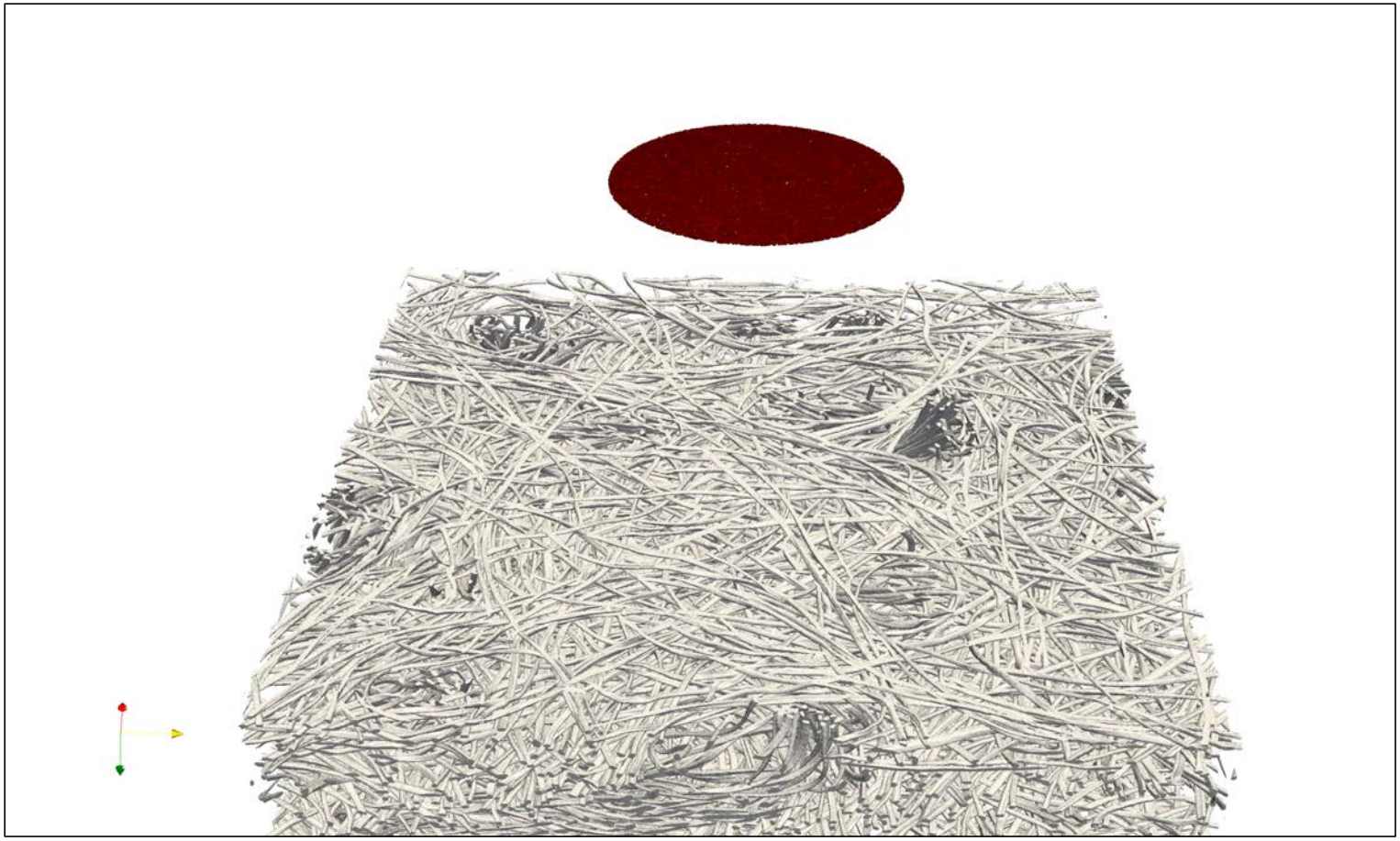


taken from Marschall and Maclean.

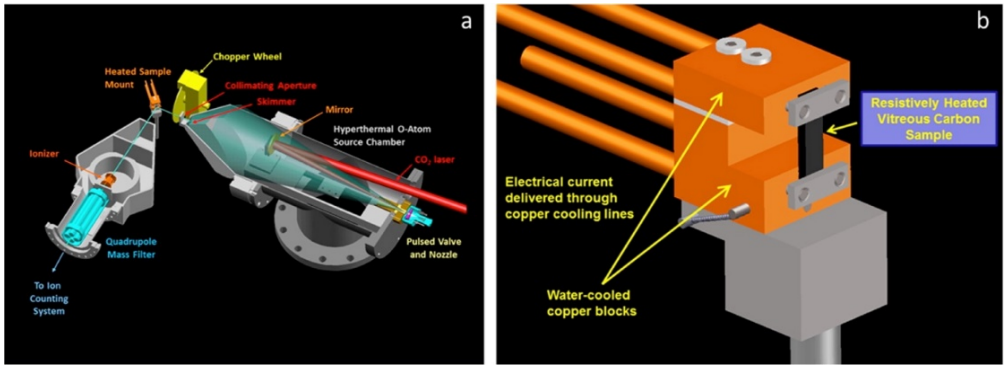


Marschall, J., & MacLean, M. (2011). Finite-rate surface chemistry model, I: Formulation and reaction system examples. AIAA Paper, 3783, 2011.

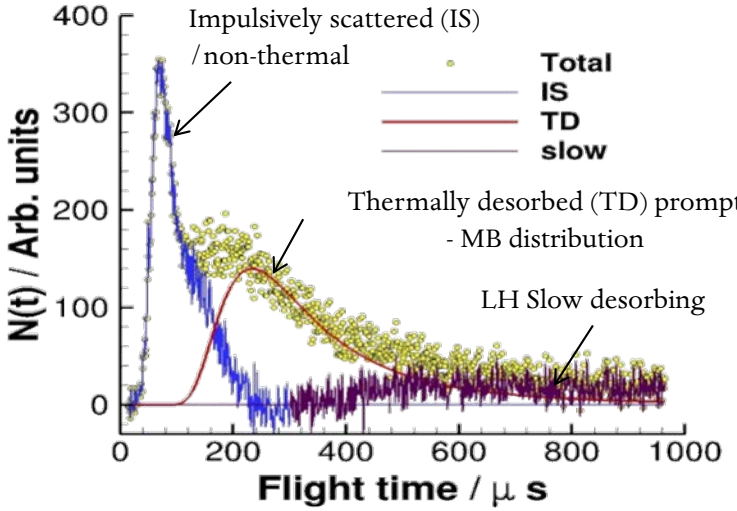
PuMA simulation

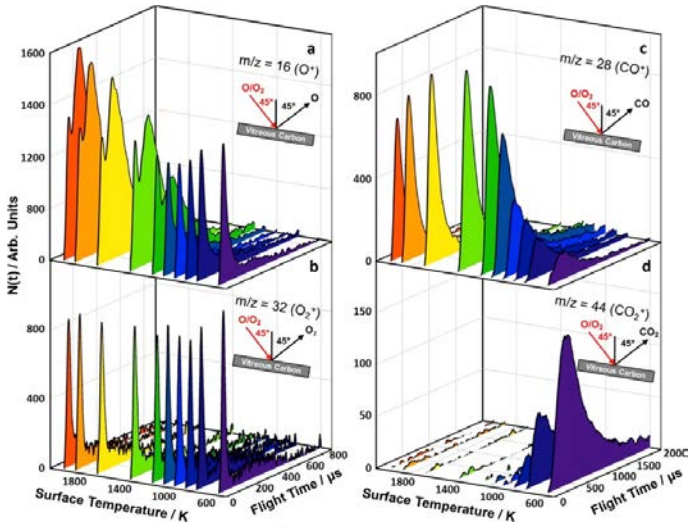


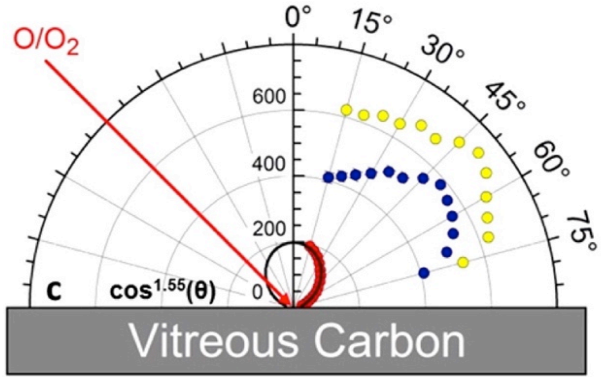
Molecular Beam Experimental Setup



Murray *et al*







Murray, V J., et al. *The Journal of Physical Chemistry C* 119.26 (2015): 14780-14796.

Carbon Oxidation Model

Type	Mechanisms	Reaction
Adsorption	Adsorption	$O(g) + (s) \longrightarrow O(ads)$
Adsorption-mediated GS reactions	TD O formation	$O(ads) \longrightarrow O(TD)(g) + (s)$
	TD CO formation	$O(ads) + C(b) + O'(ads) \longrightarrow CO(g) + (s) + O'(ads)$
	TD CO_2 formation	$O(ads)+O(s)+C(b)+4O'(ads) \longrightarrow CO_2(g)+2(s)+4O'(ads)$
	LH O{a} formation	$O(ads) \longrightarrow O\{a\}(s)$
	LH CO{a} formation	$O(ads) + C(b) + O'(ads) \longrightarrow CO\{a\}(s) + O'(ads)$
	LH CO{b} formation	$O(ads) + C(b) + O'(ads) \longrightarrow CO\{b\}(s) + O'(ads)$
PS reactions	LH O{a} desorption	$O\{a\}(s) \longrightarrow O(g) + (s)$
	LH CO{a} desorption	$CO\{a\}(s) \longrightarrow CO(g) + (s)$
	LH CO{b} desorption	$CO\{b\}(s) \longrightarrow CO(g) + (s)$

Fast TD reactions

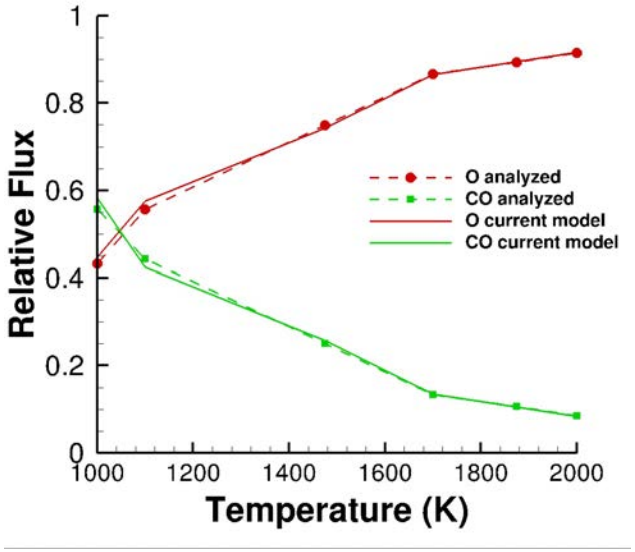
Slow formation reactions

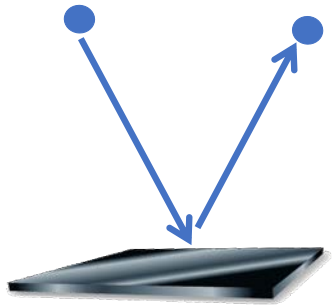
Desorption reactions

K. Swaminathan-Gopalan *et al.*, "***Development and validation of a finite-rate model for carbon oxidation by atomic oxygen.***" Carbon 137 (2018): 313-332.

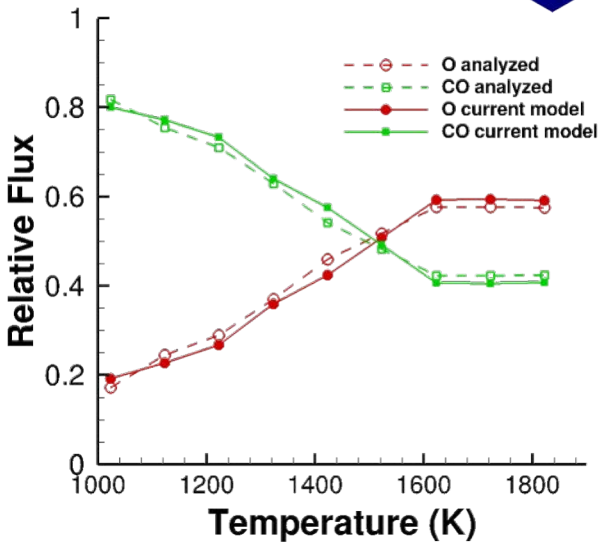
Vitreous and Preform Carbon model

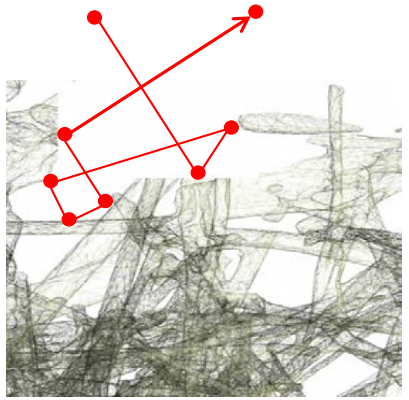
Vitreous carbon





FiberForm carbon





Effective model for macroscopic solvers

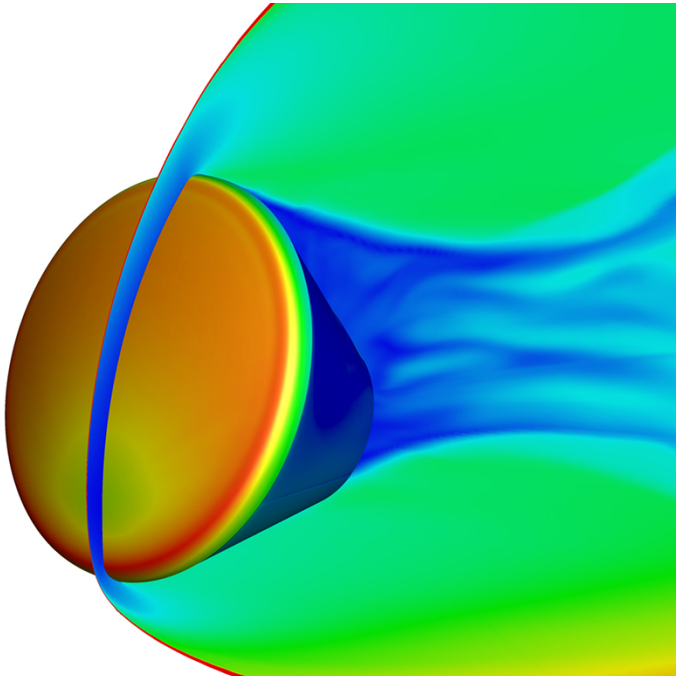
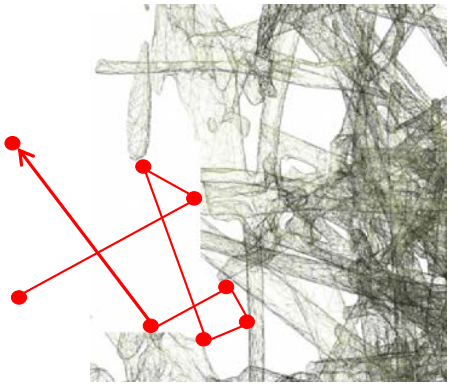
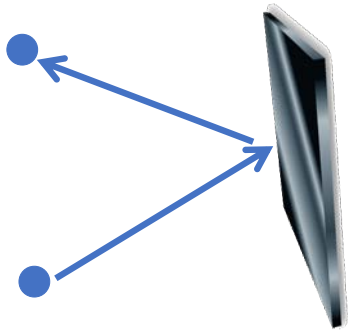


Image credit: NASA



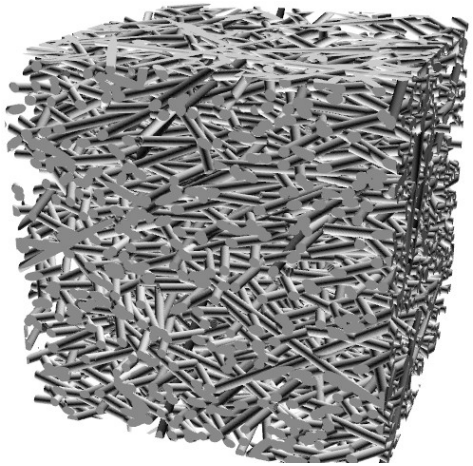
Real model
Rates → k



Effective model
Rates → k_{eff}

FiberForm – Varying Porosity

Varying porosity



$\epsilon = 0.84$

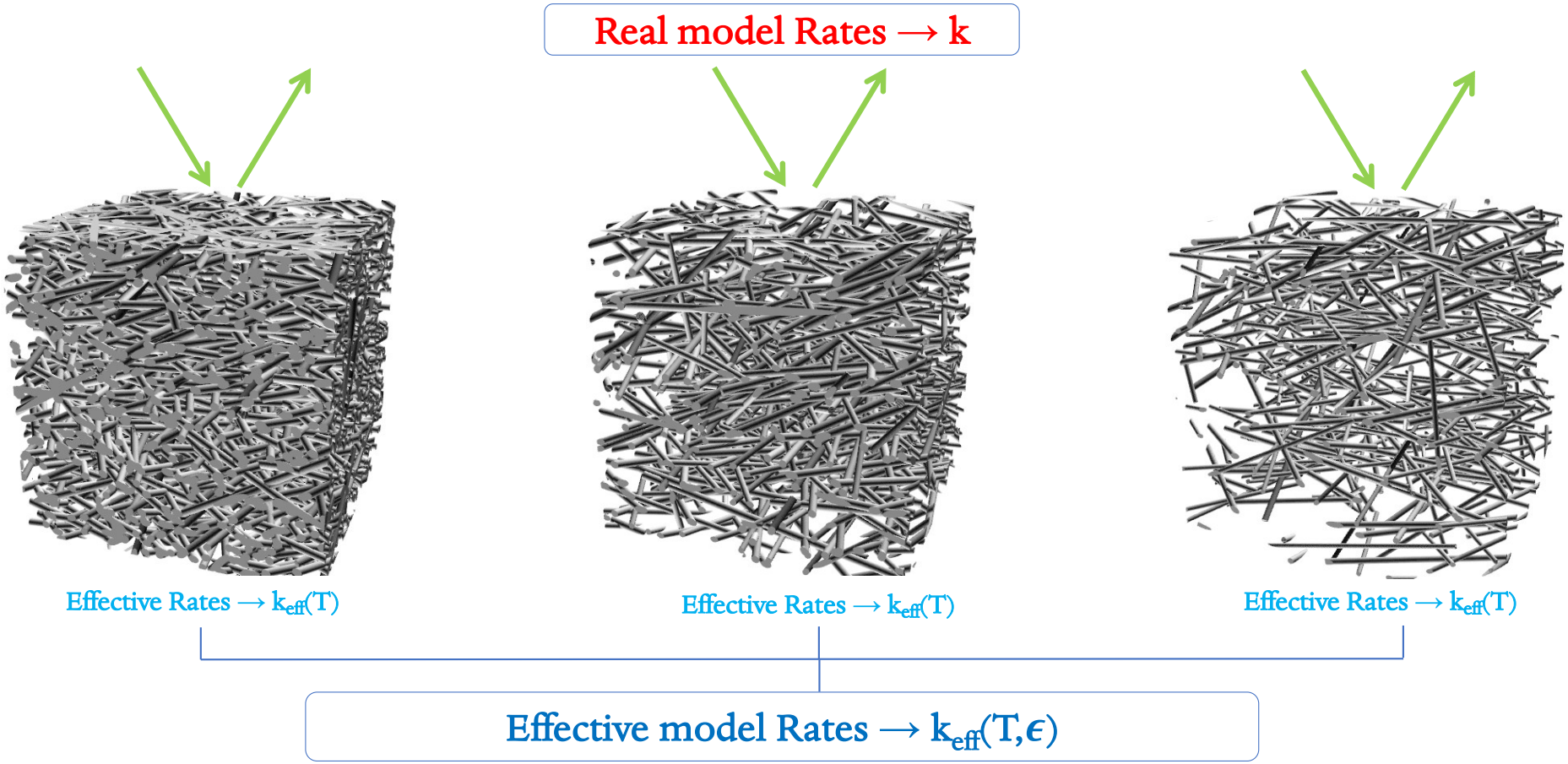


$\epsilon = 0.90$



$\epsilon = 0.96$

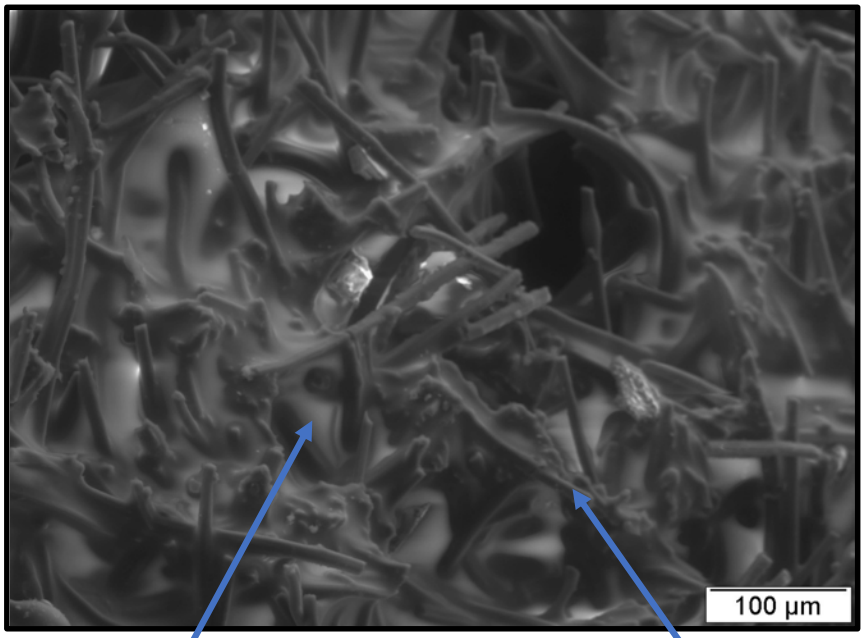
FiberForm – Varying Porosity



Effective model as a function of porosity

Mechanisms	Reaction	Rate constant $k = f(\Phi) * A * exp(-E/T)$				
		$f(\Phi)$	$A = a_0 + a_1 * \epsilon^1 + a_2 * \epsilon^2$			E
			a_0	a_1	a_2	
Adsorption	$O(g) + (s) \longrightarrow O(ads)$	$\frac{1}{\Phi} * \frac{1}{4}\sqrt{\frac{8k_bT_g}{\pi m}}$	+1.34E−1	+1.58E+0	−8.18E−1	0
LH1 O formation	$O(ads) \longrightarrow O(TD)(g) + (s)$	1	+6.30E+1	−1.15E+2	+5.94E+1	+6.16E+3
LH1 CO formation	$O(ads)+C(b)+O'(ads) \longrightarrow CO(g)+(s)+O'(ads)$	$\frac{1}{\Phi}$	−8.50E+6	+1.89E+7	−9.25E+6	+1.66E+4
LH3 O{a} formation	$O(ads) \longrightarrow O\{a\}(s)$	1	1	0	0	0
LH3 CO{a} formation	$O(ads) + C(b) + O'(ads) \longrightarrow CO\{a\}(s) + O'(ads)$	$\frac{1}{\Phi}$	−7.34E+4	+1.64E+5	−7.99E+4	+1.04E+4
LH3 CO{b} formation	$O(ads) + C(b) + O'(ads) \longrightarrow CO\{b\}(s) + O'(ads)$	$\frac{1}{\Phi}$	−5.09E+2	+1.13E+3	−5.55E+2	+2.91E+3

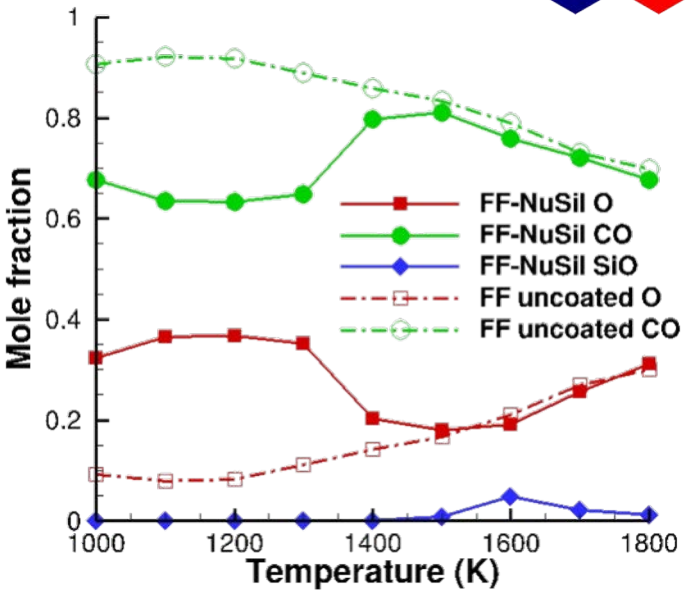
FiberForm-NuSil oxidation model



NuSil

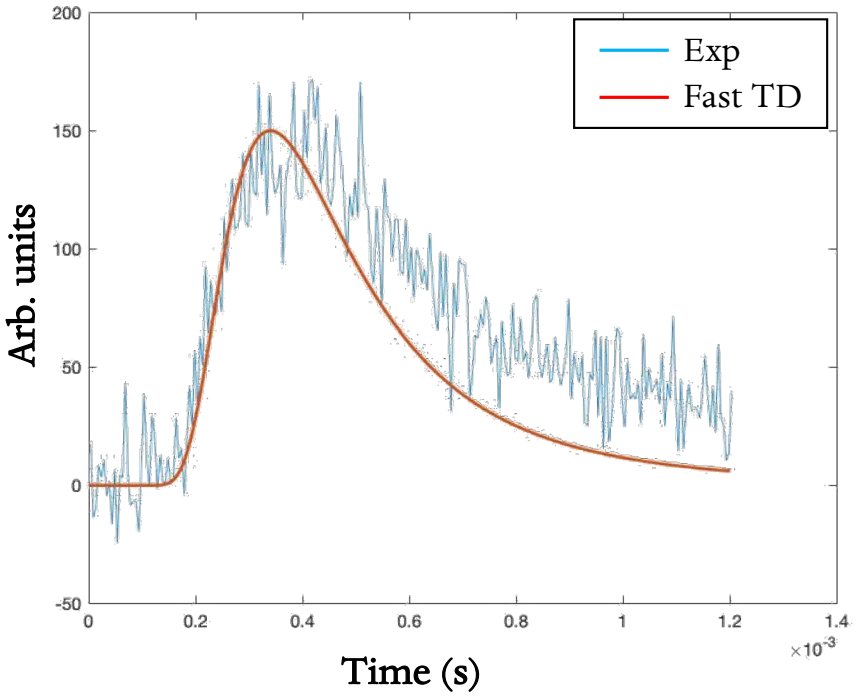
Preform carbon

2 phase model



- SiO additional product with NuSil.
- O mainly scatters non-reactively from NuSil.
- NuSil starts burning off ~ 1400 K.
- Higher fluxes of O and lower fluxes of CO on NuSil surfaces at lower temperatures.

SiO reactions

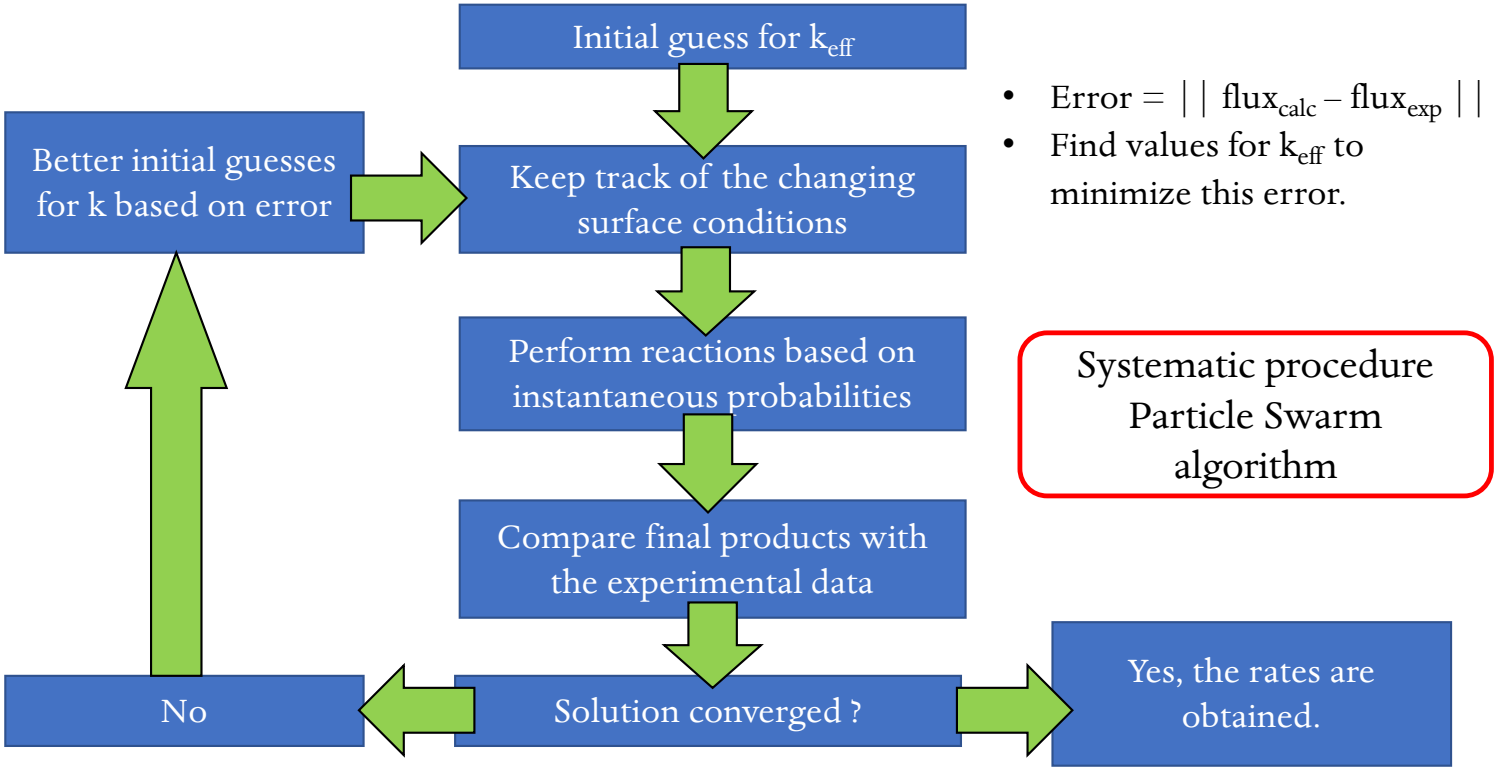


New reaction mechanisms for SiO

Mechanisms	Reaction
Scattering	$O(g) + Si(s) \longrightarrow O(g) + Si(s)$
fast SiO formation	$O(g) + Si(s) \longrightarrow SiO(g) + (s)$
slow SiO formation	$O(g) + Si(s) \longrightarrow SiO(s)$
slow SiO desorption	$SiO(s) \longrightarrow SiO(g) + (s)$

- SiO TOF has a fast TD and slow desorption component.

Reaction Rate Constants Fitting Method

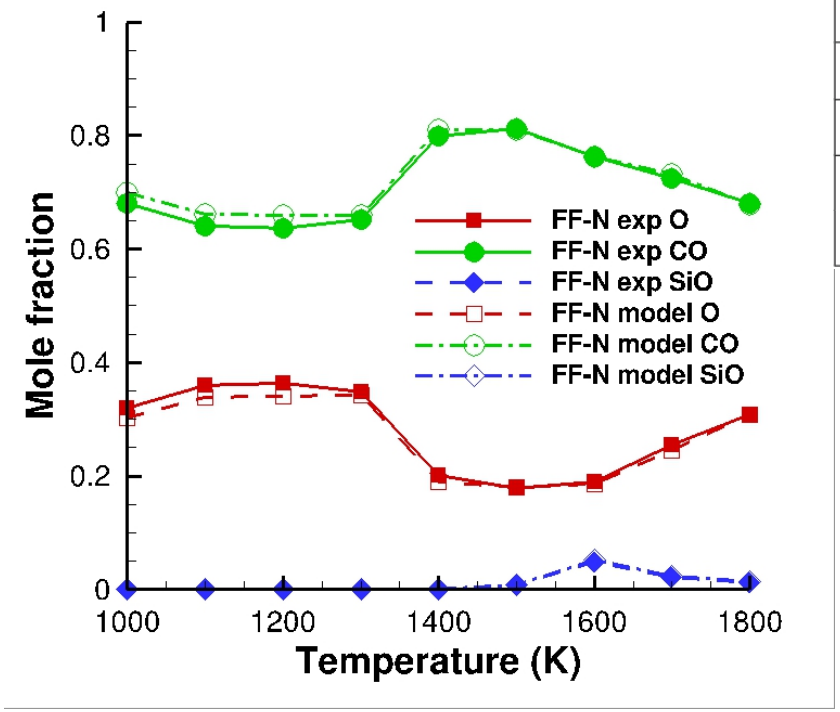


- Error = $|| flux_{calc} - flux_{exp} ||$
- Find values for k_{eff} to minimize this error.

Systematic procedure Particle Swarm algorithm

K. Swaminathan Gopalan and K. A. Stephani. In *47th AIAA Thermophysics Conference*, p. 4347. 2017.

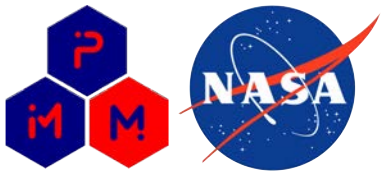
FiberForm-NuSil oxidation model



Mechanisms	Reaction	Rate constant (k)
Scattering	$O(g) + Si(s) \longrightarrow O(g) + Si(s)$	$\frac{1}{\Phi} * \frac{1}{4}\sqrt{\frac{8k_bT_g}{\pi m}} * 0.1$
fast SiO formation	$O(g) + Si(s) \longrightarrow SiO(g) + (s)$	$1.27E7 * exp(-\frac{26022.0}{T_s})$
slow SiO formation	$O(g) + Si(s) \longrightarrow SiO(s)$	1
slow SiO desorption	$SiO(s) \longrightarrow SiO(g) + (s)$	$1.12E6 * exp(-\frac{23718.8}{T_s})$

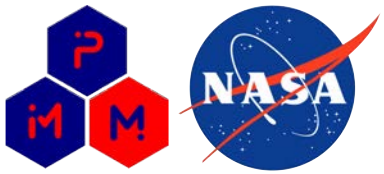
- New 2 phase model for FiberForm-NuSil
  - Phase 1: FiberForm – same rates as preform carbon model.
  - Phase 2: NuSil – new reactions and rates.
- Newly developed FiberForm-NuSil model agrees well with the experiments.

Summary



- Detailed surface chemistry framework was implemented in PuMA.
- The vitreous carbon (VC) oxidation model was developed and extended to FiberForm.
- Effective oxidation model for use in CFD was developed as a function of porosity k_{eff} (T,ϵ).
- Effective model was extended to NuSil-coated FiberForm.

- Future Work: extend to NuSil-coated PICA



Questions?

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