

# Microscale Modeling of High-temperature Heat Transfer in Anisotropic Porous Materials

Presented by Federico Semeraro  
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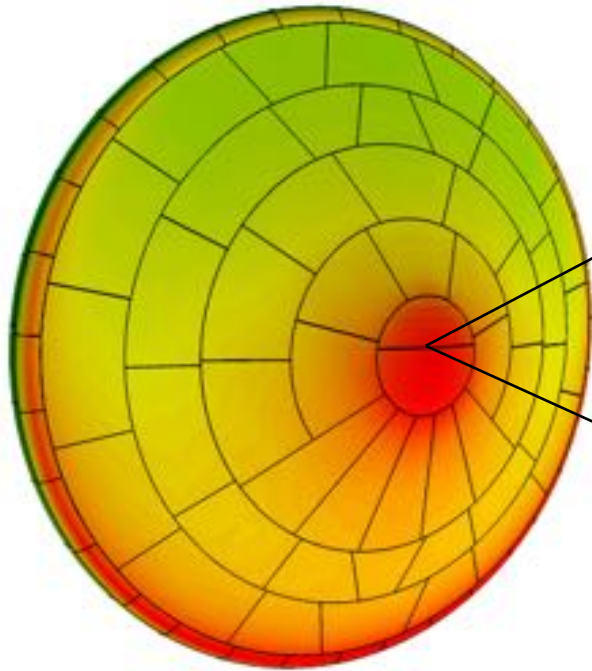
- Motivation & Objectives
- Solid Heat Conduction
- Fiber Orientation
- Radiative Heat Transfer

# MOTIVATION & OBJECTIVES

# Modeling Thermal Protection Systems (TPS)

## Macroscale Modeling

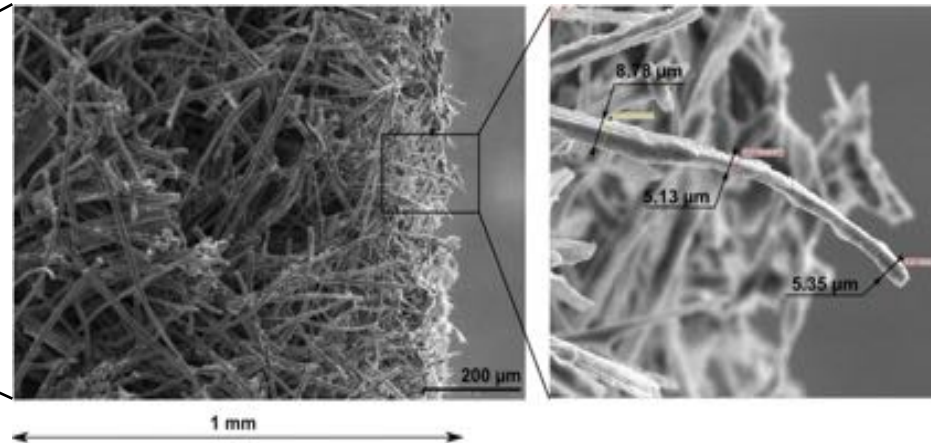
Full scale material response solvers, using volume-averaged techniques to solve conservation equations for ablation



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°

Use this series of images to reconstruct the 3D object

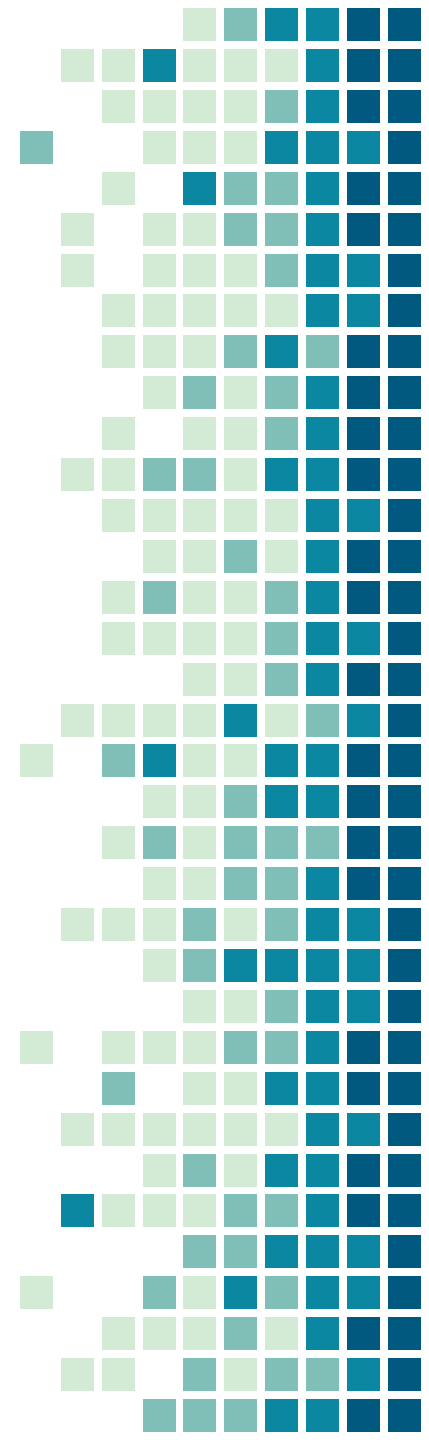


Penetrating power

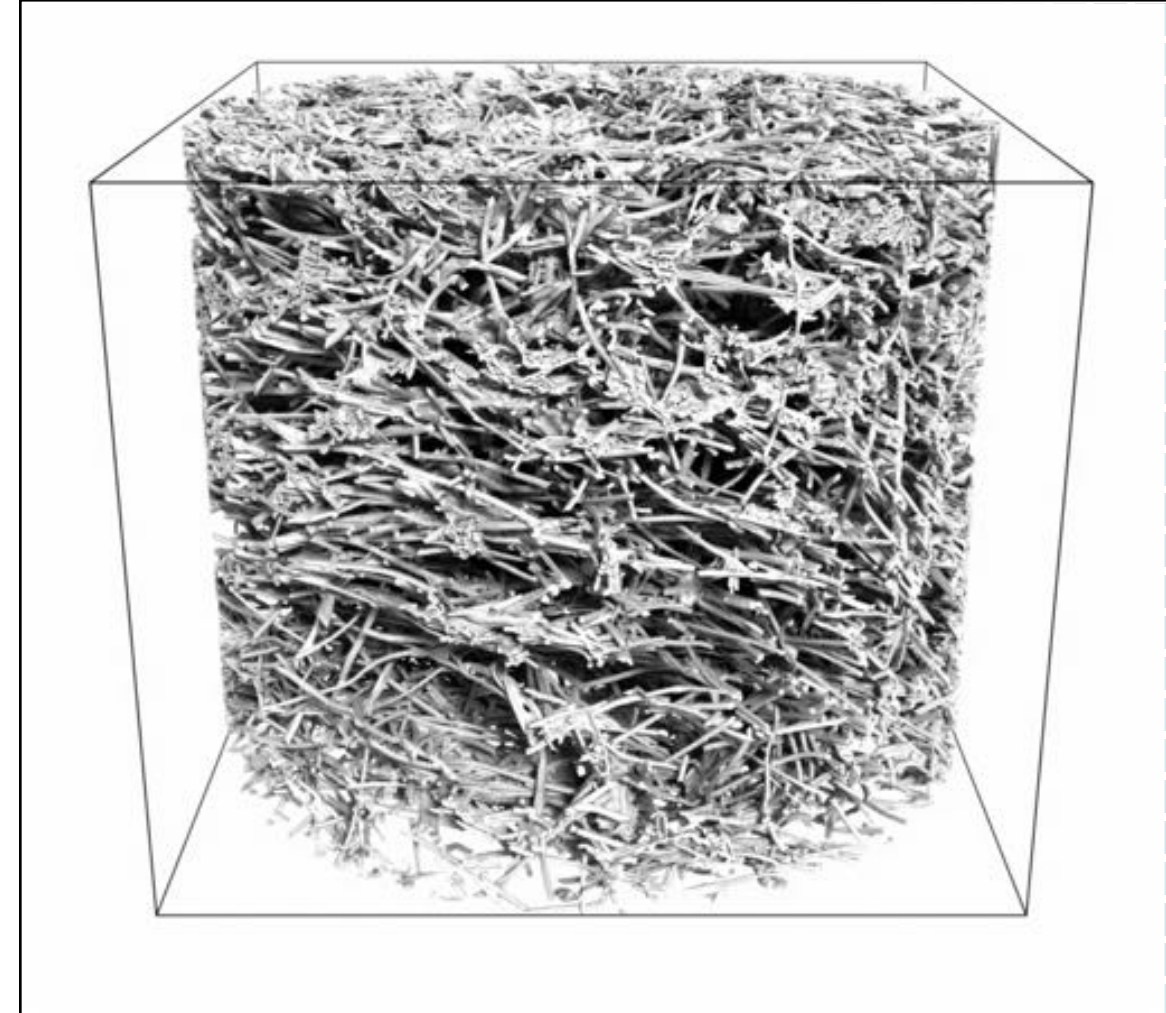
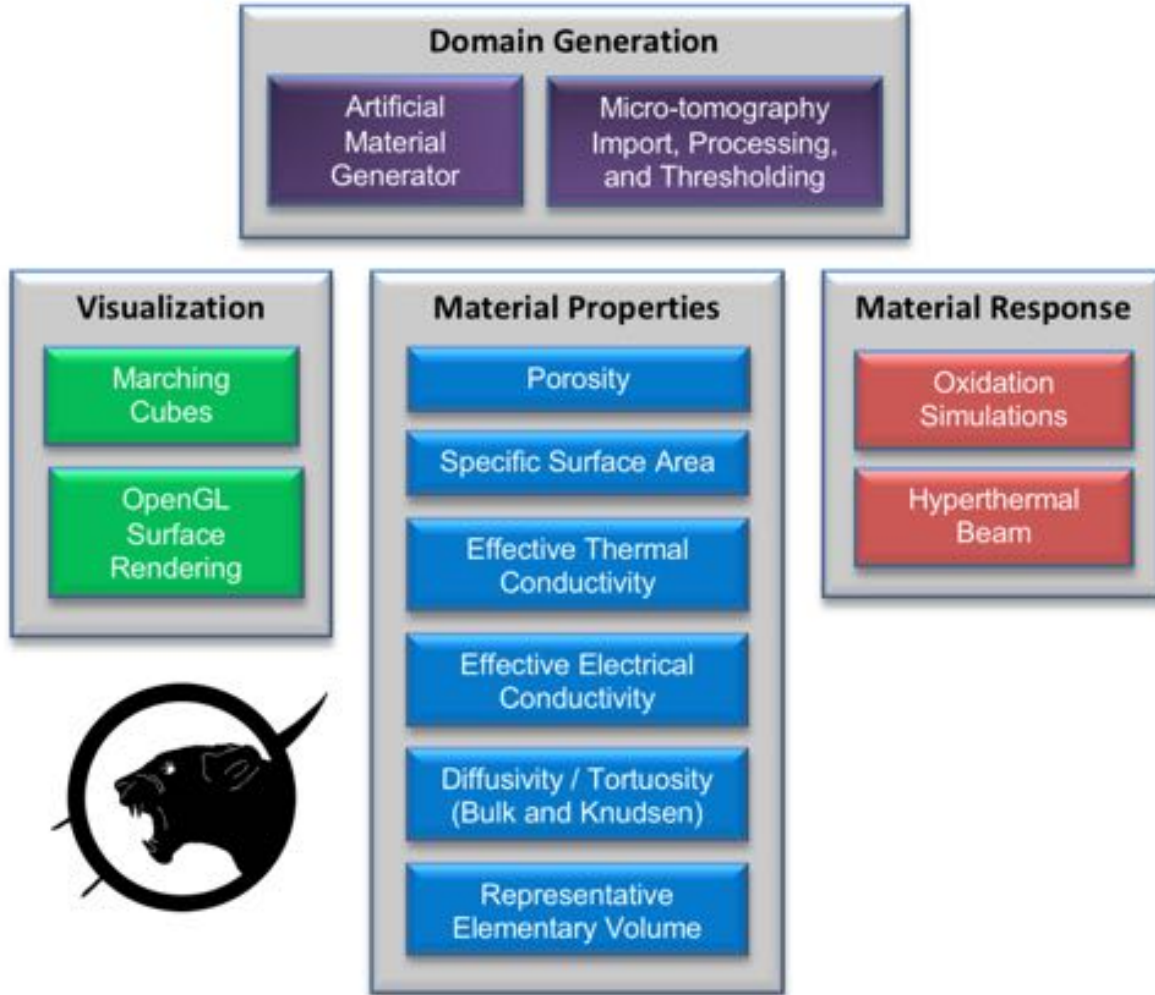
Multiple angles



Courtesy of D. Parkinson (ALS)



# Porous Microstructure Analysis (PuMA) software

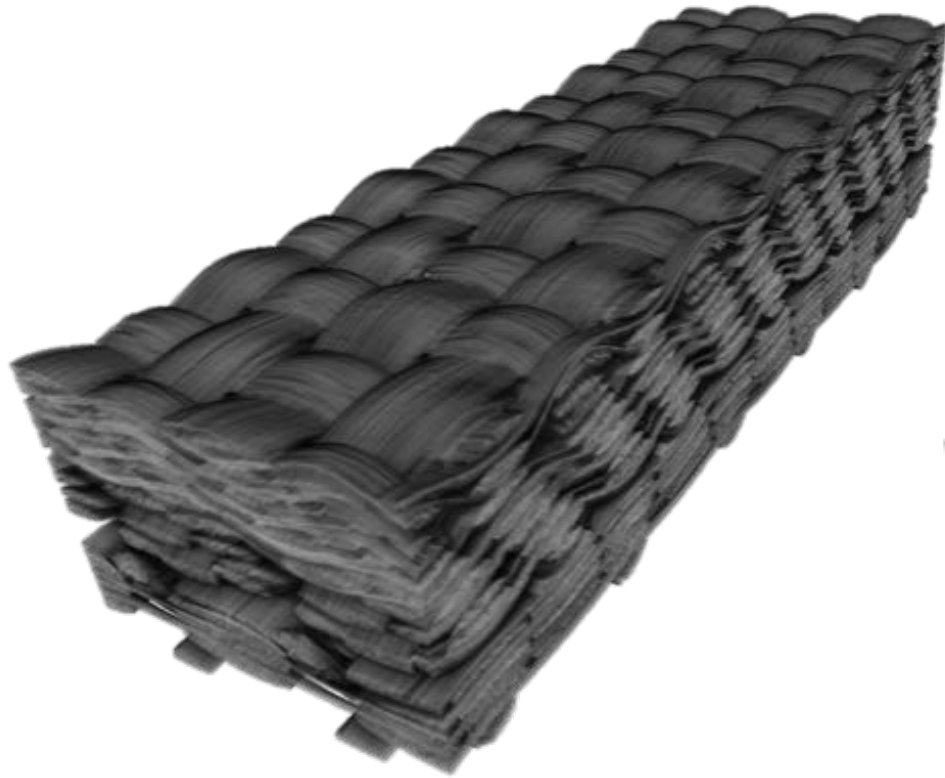


CT Reconstruction of FiberForm

Ferguson, J. C., Panerai, F., Borner, A., & Mansour, N. N. (2018). PuMA: the Porous Microstructure Analysis software. *SoftwareX*, 7, 81-87.

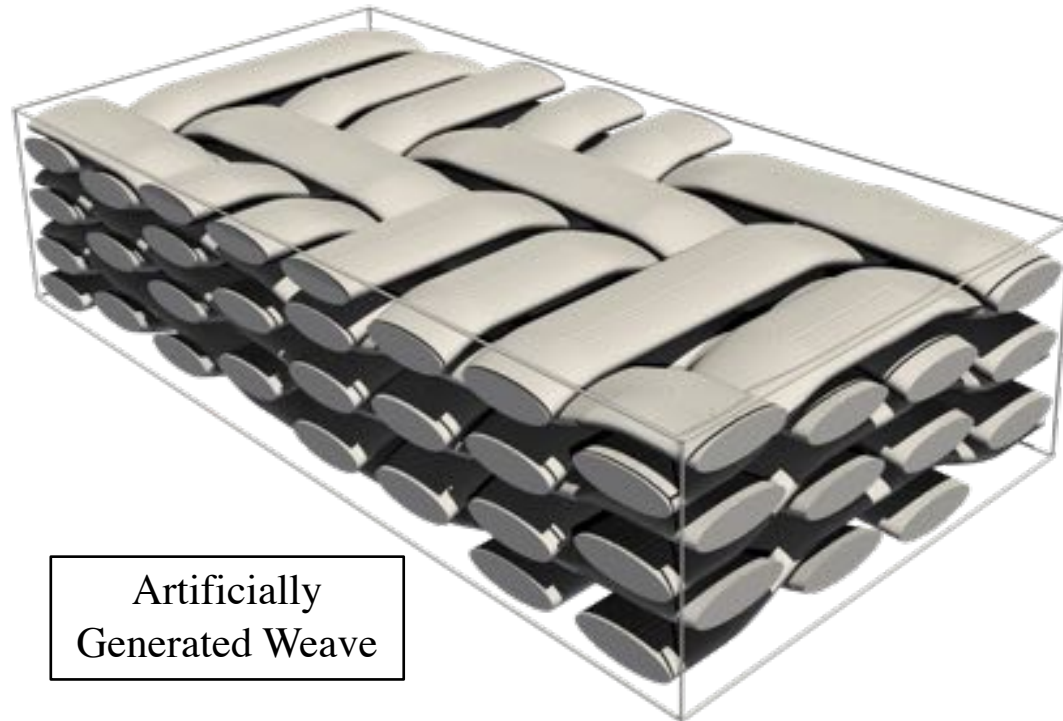
<https://software.nasa.gov/software/ARC-17920-1>

# Challenges in Micro-scale modeling

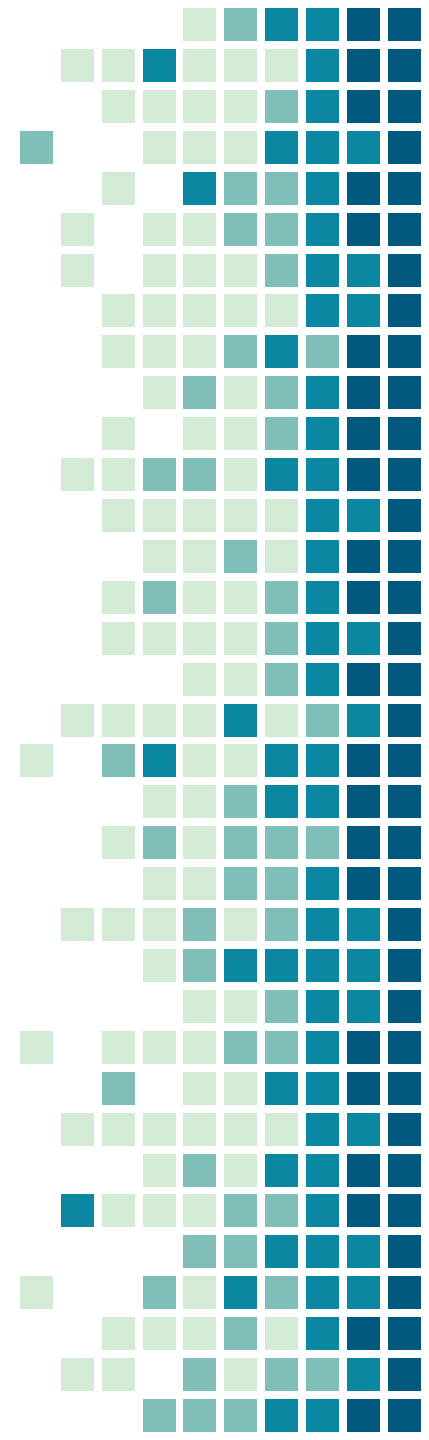


12- ply real  
TPS weave

As NASA moves towards  
woven TPS materials, our  
modeling must adapt



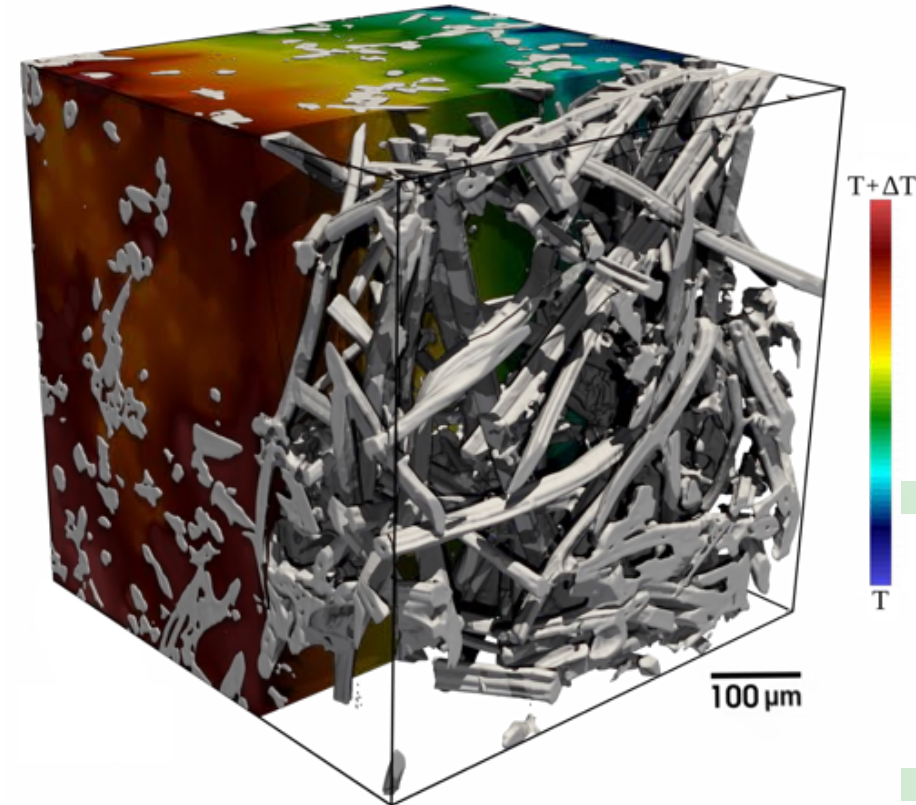
Artificially  
Generated Weave



# Objectives

Formulate, implement and validate:

1. Finite Volume (FV) method to find the effective thermal conductivity due to anisotropic solid heat conduction
2. Ray Casting method for estimating the fiber orientation in CT reconstructions
3. Collision based Monte-Carlo method to find the View Factors (VF) to compute the effective radiative coefficient



$$q = (\underbrace{k_c}_{\text{conduction}} + \underbrace{k_r}_{\text{radiation}}) \nabla T$$

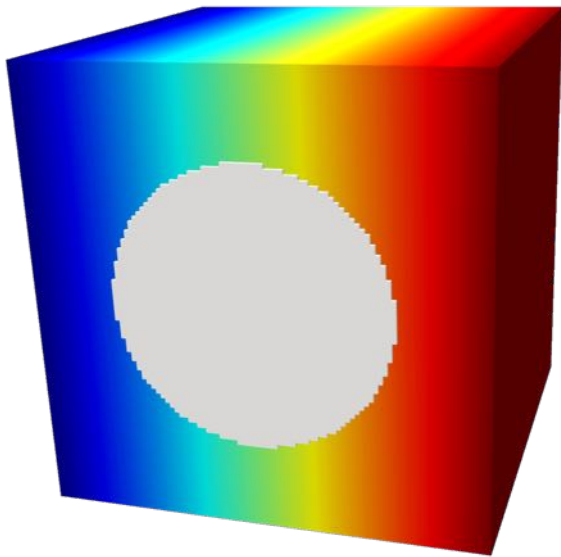




# SOLID HEAT CONDUCTION

# Computing the effective thermal conductivity

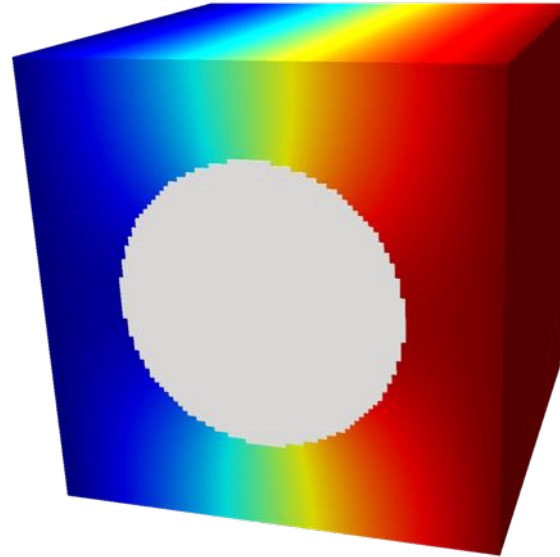
Impose initial linear  
Temperature profile



$$T_{i,j,k} = \frac{i}{L_x}$$

CGLS  
→

Temperature converged  
to Steady State



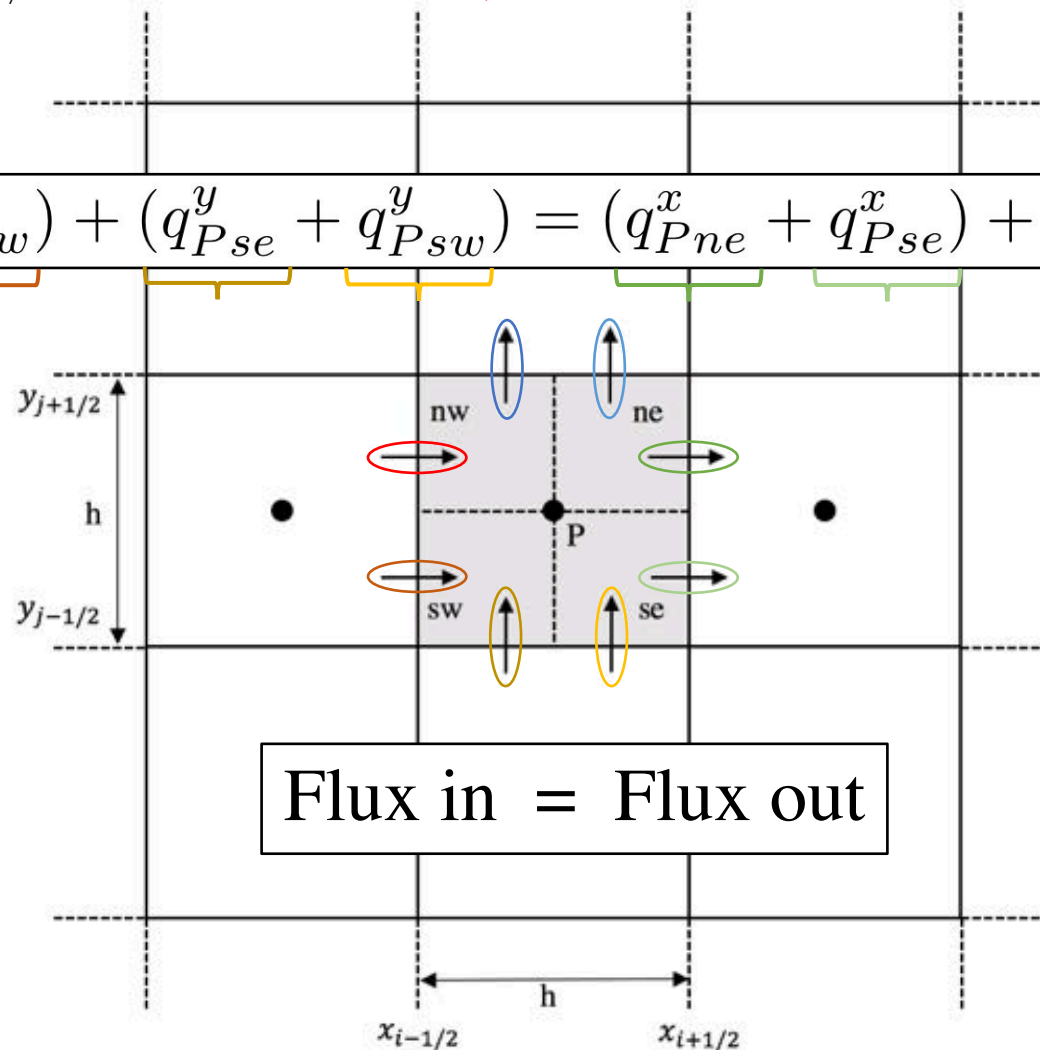
Compute Effective  
Thermal Conductivity

$$k_{c,eff} = \mathbf{q}^x \cdot L_x$$

# Finite Volume Method

$$\int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \left( \frac{\partial q^x}{\partial x} + \frac{\partial q^y}{\partial y} + \frac{\partial q^z}{\partial z} \right) dx dy dz = 0 \quad \text{where } \mathbf{q} = \begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{yx} & k^{yy} & k^{yz} \\ k^{zx} & k^{zy} & k^{zz} \end{bmatrix} \begin{bmatrix} \partial T / \partial x \\ \partial T / \partial y \\ \partial T / \partial z \end{bmatrix}$$

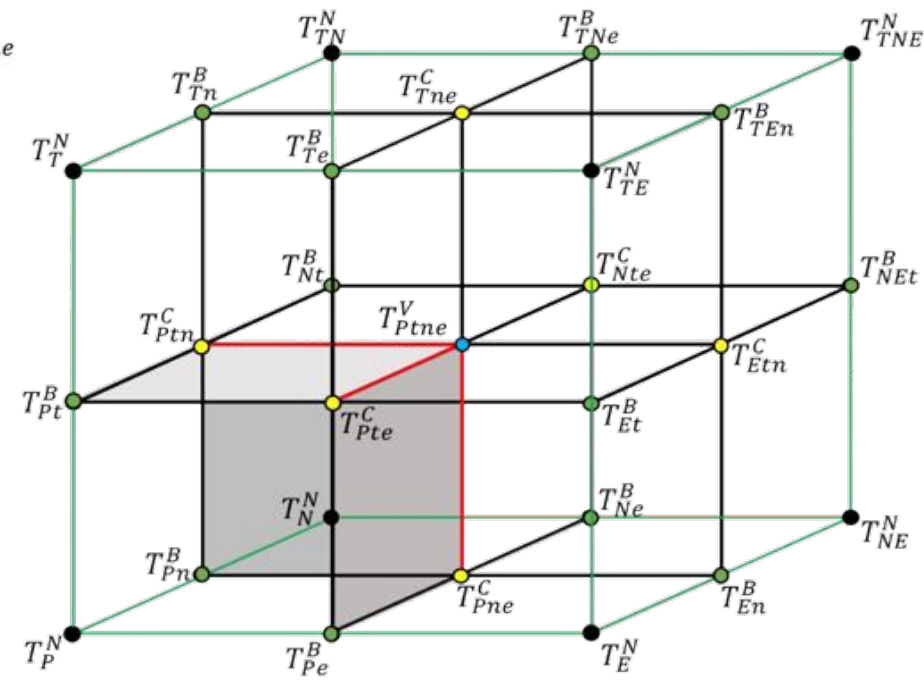
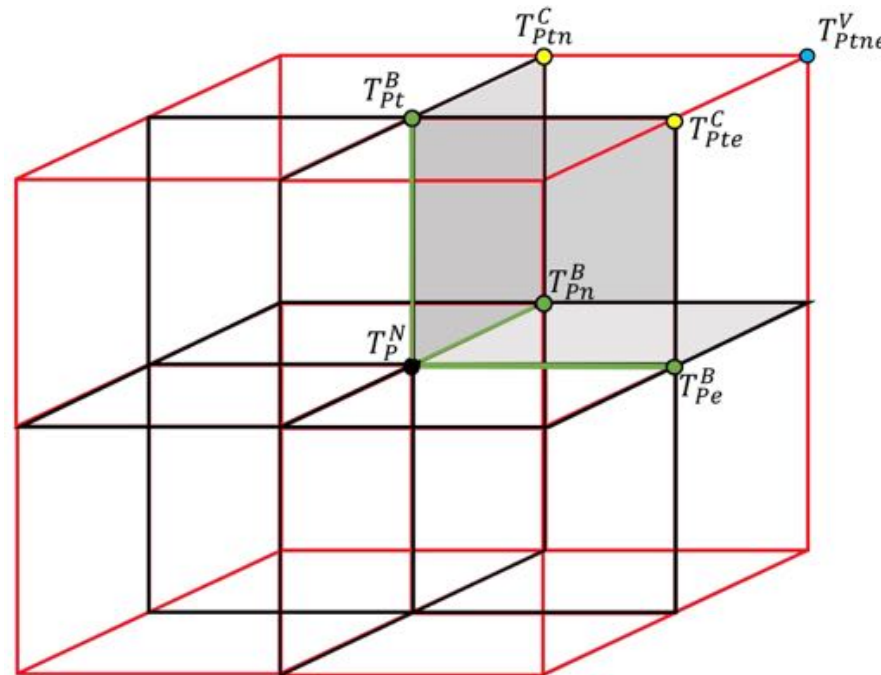
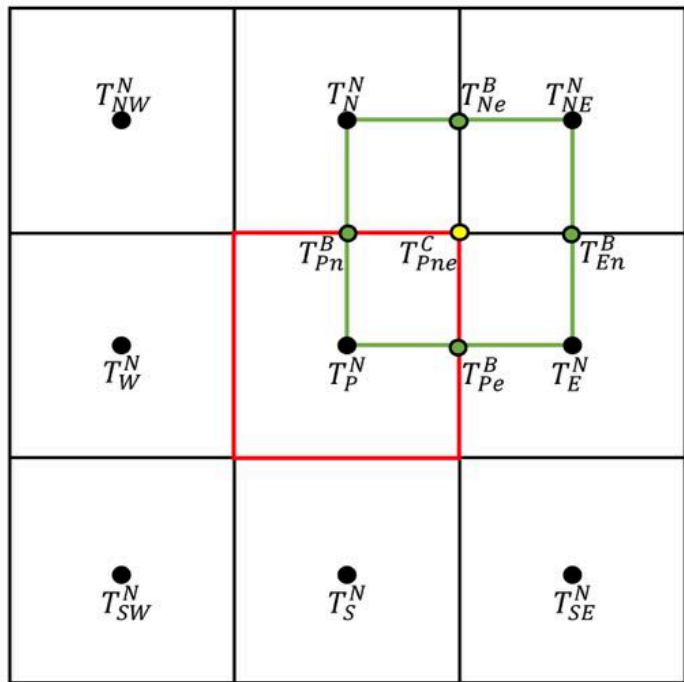
$$\underbrace{(q_{Pnw}^x + q_{Psw}^x)}_{\text{red}} + \underbrace{(q_{Pse}^y + q_{Psw}^y)}_{\text{orange}} = \underbrace{(q_{Pne}^x + q_{Pse}^x)}_{\text{yellow}} + \underbrace{(q_{Pne}^y + q_{Pnw}^y)}_{\text{green}} + \underbrace{(q_{Pnw}^z + q_{Psw}^z)}_{\text{blue}}$$



Flux in = Flux out

# Multi-Point Flux Approximation (MPFA\*)

- Integration carried out inside Control Volume (CV)
- Continuity of flux enforced inside Interaction Volume (IV)



\*Ivar Aavatsmark. Multipoint flux approximation methods for quadrilateral grids. *9<sup>th</sup> International forum on reservoir simulation, Abu Dhabi*, pages 9–13, 2007.

# Transmissibility Matrix

$$q_{Pne}^x = k_P^{xx} \overbrace{\frac{T_{Pe}^B - T_P^N}{h/2}} + k_P^{xy} \overbrace{\frac{T_{Pn}^B - T_P^N}{h/2}}$$

$$\mathbf{T}^N = [T_P^N, T_E^N, T_N^N, T_{NE}^N]^T \quad \mathbf{T}^B = [T_{Pe}^B, T_{Ne}^B, T_{Pn}^B, T_{En}^B]^T$$

$$\mathbf{q} = \mathbf{A} \mathbf{T}^B + \mathbf{B} \mathbf{T}^N$$

$$\mathbf{C} \mathbf{T}^B = \mathbf{D} \mathbf{T}^N \rightarrow \mathbf{T}^B = \mathbf{C}^{-1} \mathbf{D} \mathbf{T}^N$$

$$\mathbf{q} = \mathbf{E} \mathbf{T}^N \quad \text{where} \quad \mathbf{E} = \mathbf{B} + \mathbf{A} \mathbf{C}^{-1} \mathbf{D}$$

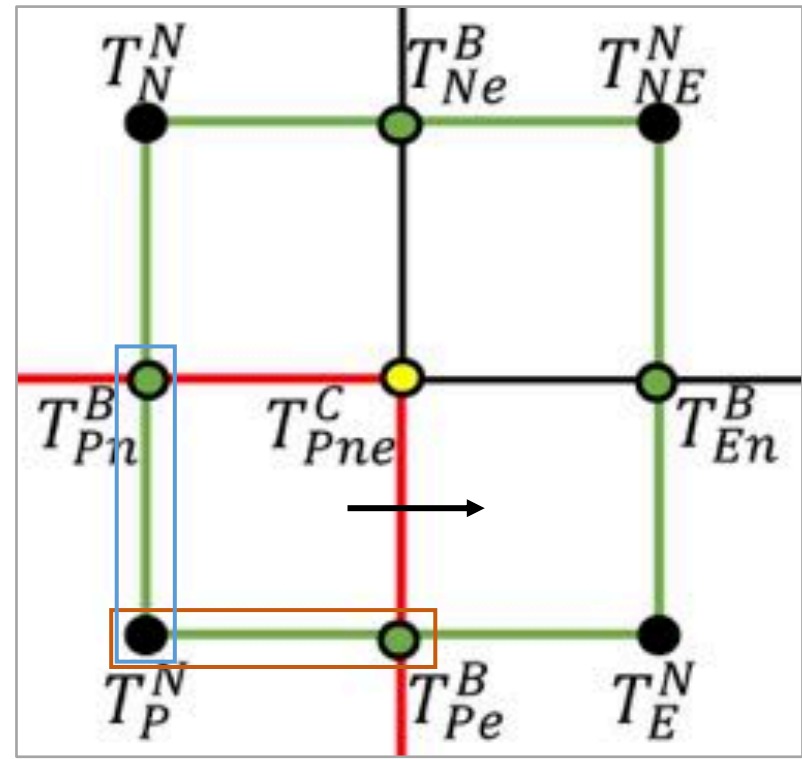
$$\mathbf{q}(x, t) = \mathbf{E}(x) \mathbf{T}^N(x, t)$$

$$q_{Pne}^x = q_{Enw}^x$$

$$q_{Nse}^x = q_{NEsw}^x$$

$$q_{Pne}^y = q_{Nse}^y$$

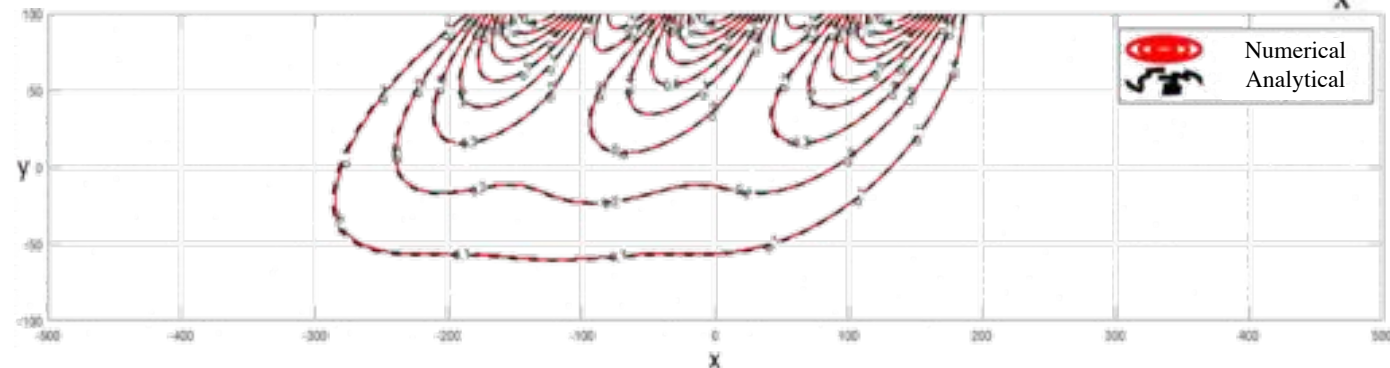
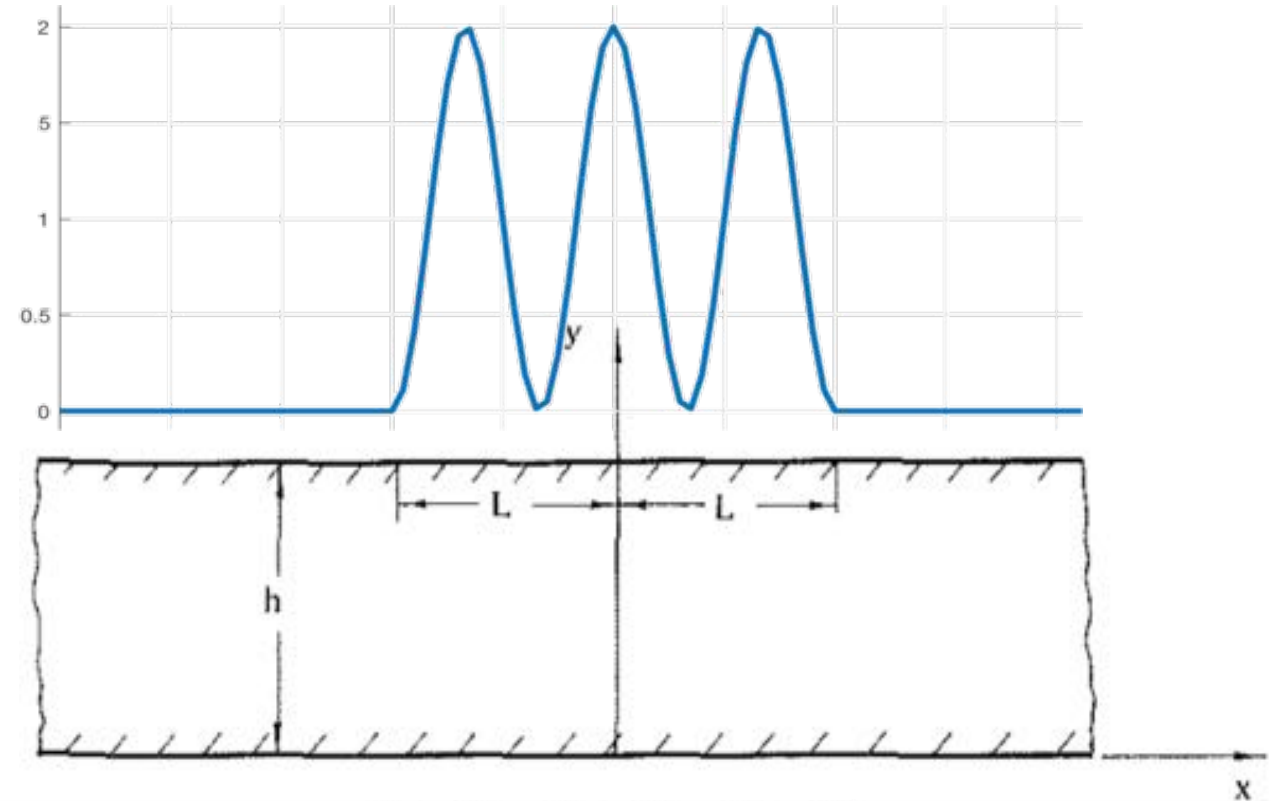
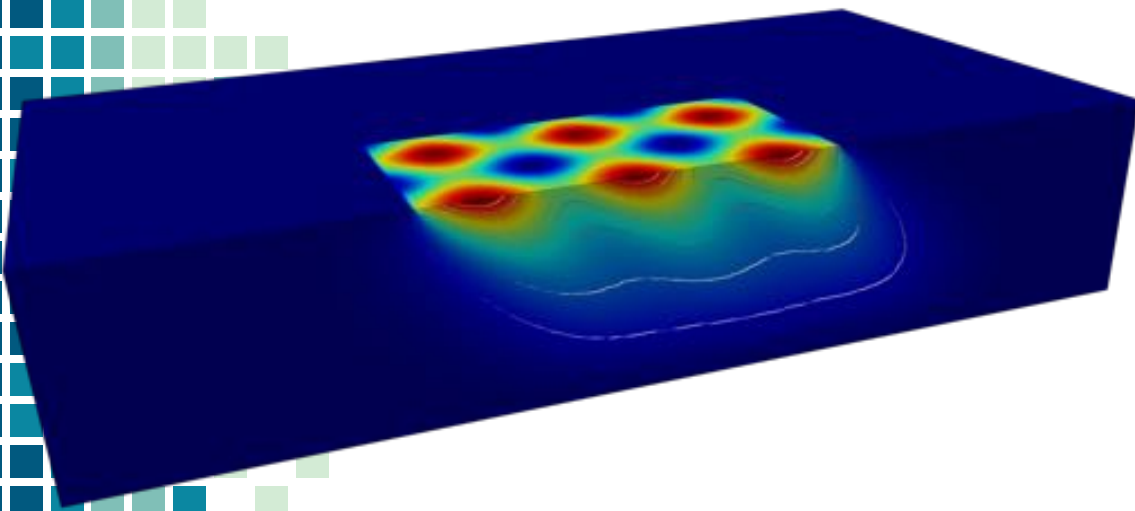
$$q_{Enw}^y = q_{NEsw}^y$$



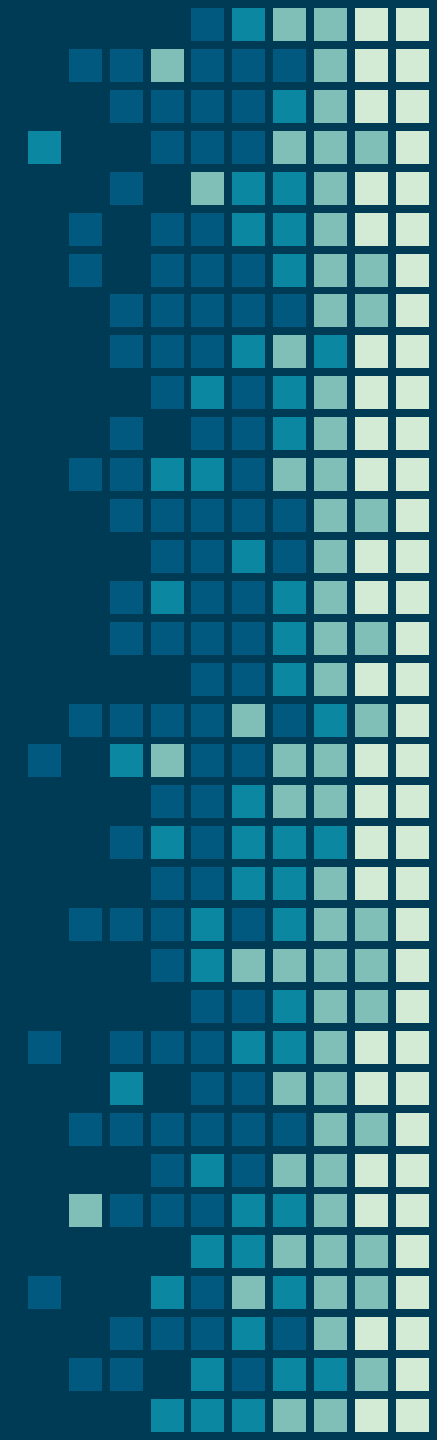
# Analytical Case for Anisotropic sample

$$T_{i,j,k} = \begin{cases} 0, & x < -L \\ \cos(3\pi/h x) + \cos(3\pi/h z), & -L \leq x \leq L \\ 0, & x > L \end{cases}$$

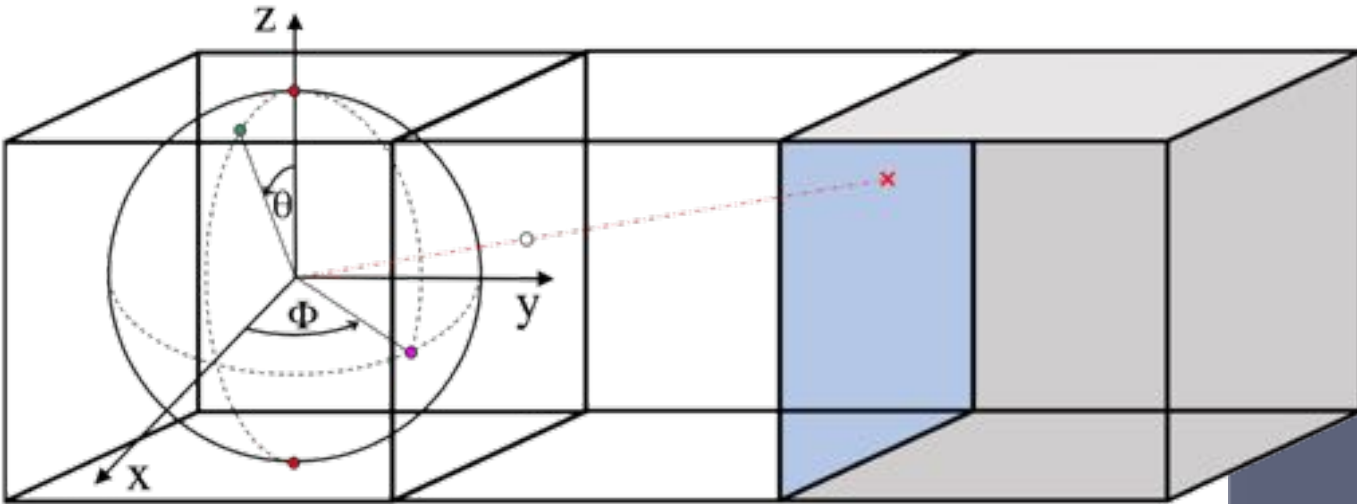
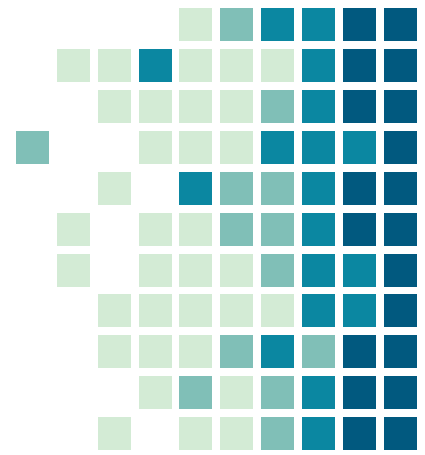
$$k_{i,j,k} = \begin{bmatrix} 1 & 0.75 & 0.75 \\ 0.75 & 1 & 0.75 \\ 0.75 & 0.75 & 1 \end{bmatrix}$$



# FIBER ORIENTATION



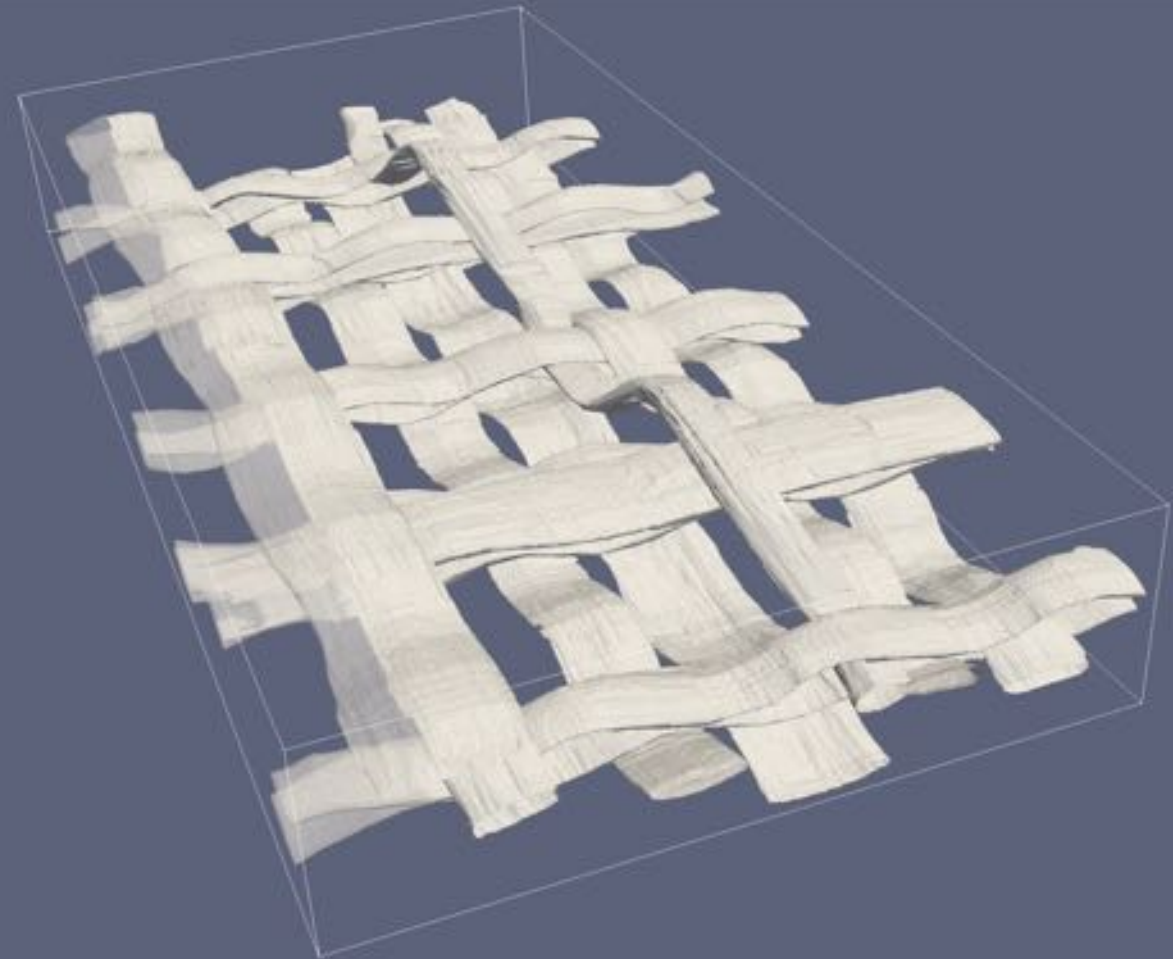
# Ray Casting Method



$$\theta \in [0, 180^\circ) \quad \phi \in [0, 360^\circ)$$

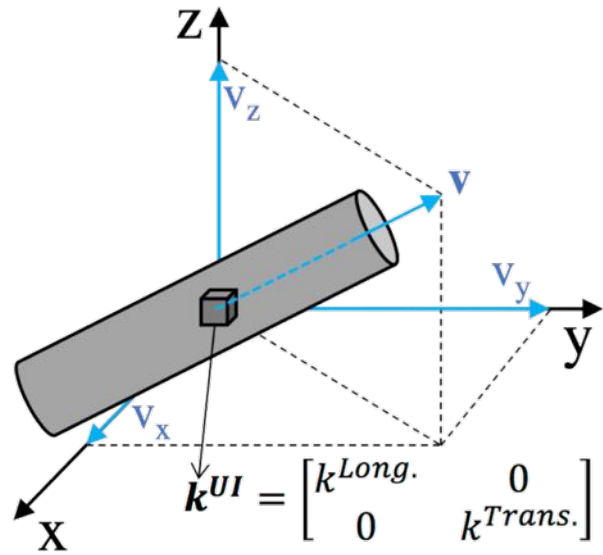
$$N = \left( \frac{180^\circ}{d\psi} - 1 \right) \left( \frac{360^\circ}{d\psi} \right) + 2$$

$$\mathbf{v} = v_x \mathbf{i} + v_y \mathbf{j} + v_z \mathbf{k}$$





# Conductivity Tensor Rotation



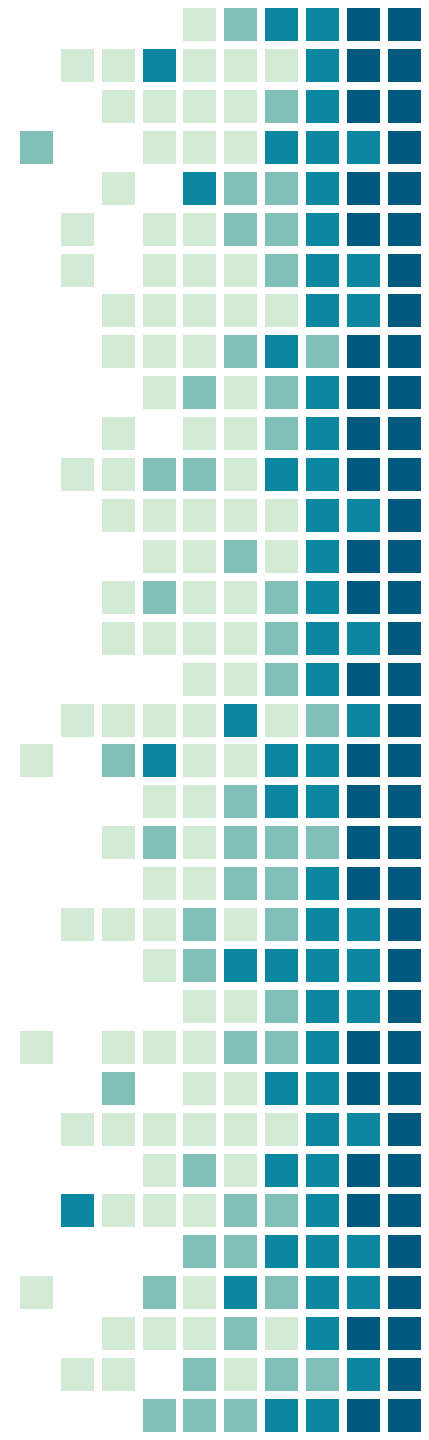
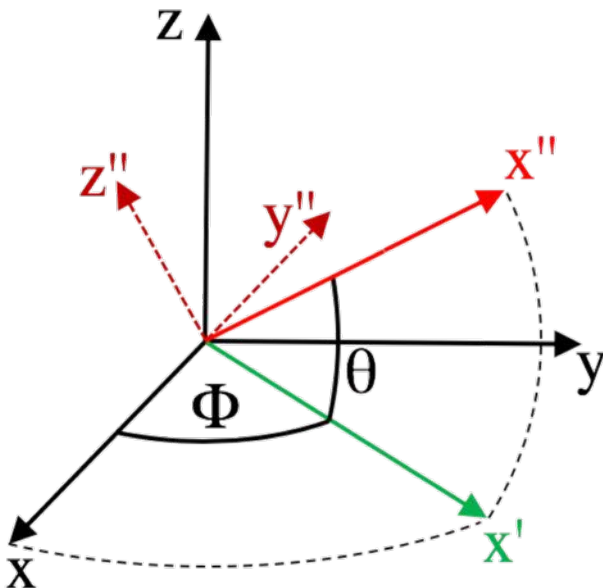
$$\mathbf{v} = v_x \mathbf{i} + v_y \mathbf{j} + v_z \mathbf{k}$$

$$\mathbf{k}'' = \begin{bmatrix} k^{Long.} & 0 & 0 \\ 0 & k^{Trans.} & 0 \\ 0 & 0 & k^{Trans.} \end{bmatrix}$$

$$\theta = \arcsin v_z \quad \phi = \arctan \frac{v_y}{v_x}$$

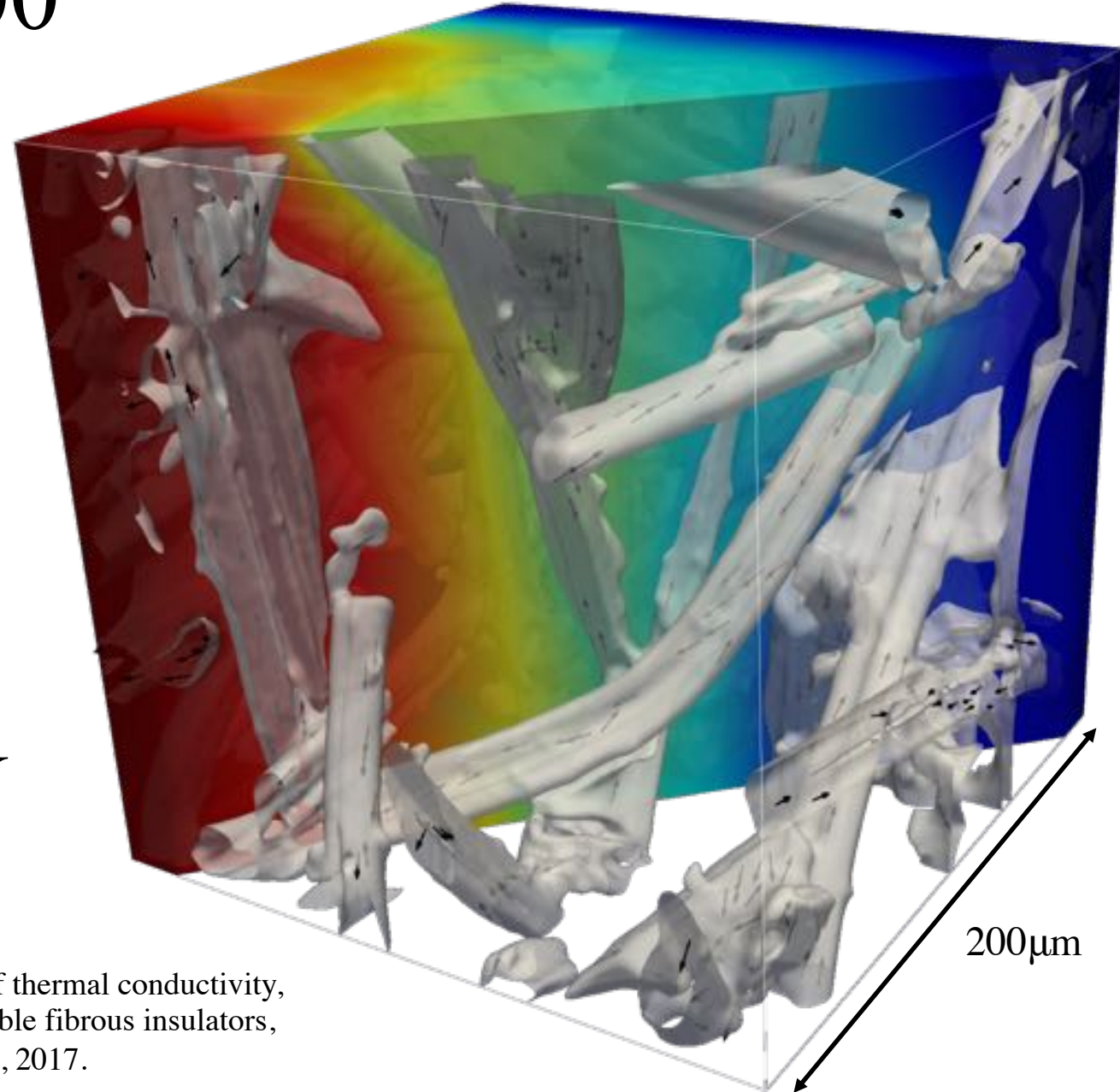
$$\mathbf{q} = \underbrace{[\mathbf{R}^{-1} \mathbf{k}'' \mathbf{R}]}_{\mathbf{k}} \nabla T$$

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



# FiberForm 800<sup>3</sup>

$$\mathbf{k}^{UI} = \begin{bmatrix} 12 & 0 \\ 0 & 1.2 \end{bmatrix} W/mK$$



F. Panerai et al., Micro-tomography based analysis of thermal conductivity, diffusivity and oxidation behaviour of rigid and flexible fibrous insulators, *Int. Journal of Heat and Mass Transfer*, 108-801-811, 2017.



# RADIATIVE HEAT TRANSFER

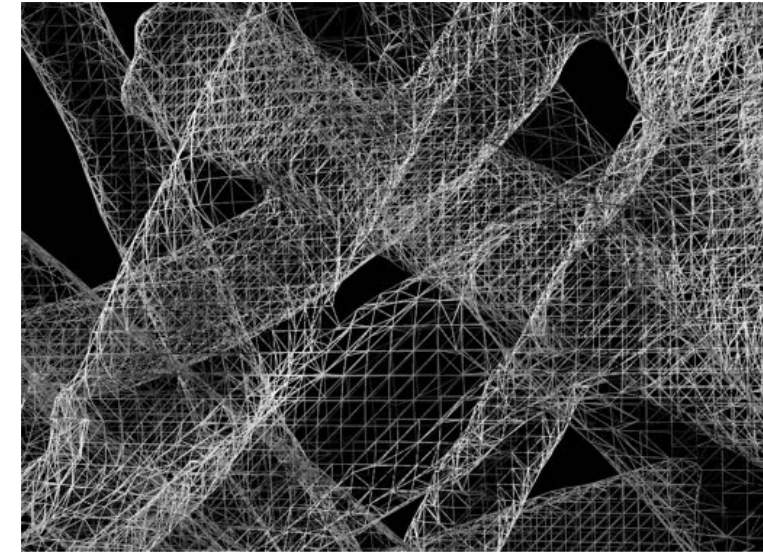
# Radiation Model

- Marching Cubes for surface triangulation
- The total heat flux is computed by iteratively solving the sparse coupled linear system:

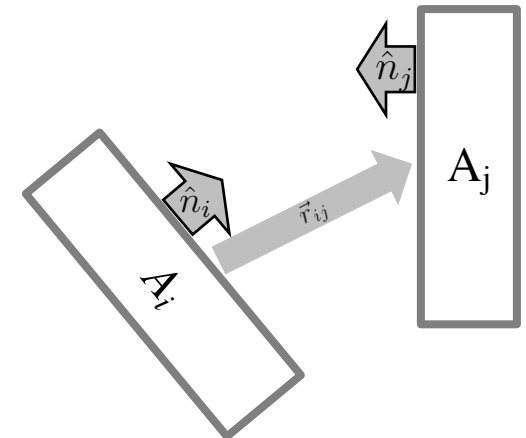
$$\underbrace{J_i}_{\text{Total radiation from surface } i} = \underbrace{\epsilon_i \sigma T_i^4}_{\text{Emitted radiation}} + \underbrace{(1 - \epsilon_i) \sum_j \boxed{F_{ij}} J_j}_{\text{Reflected radiation}}$$

- View Factors are determined by projecting rays from each surface as:

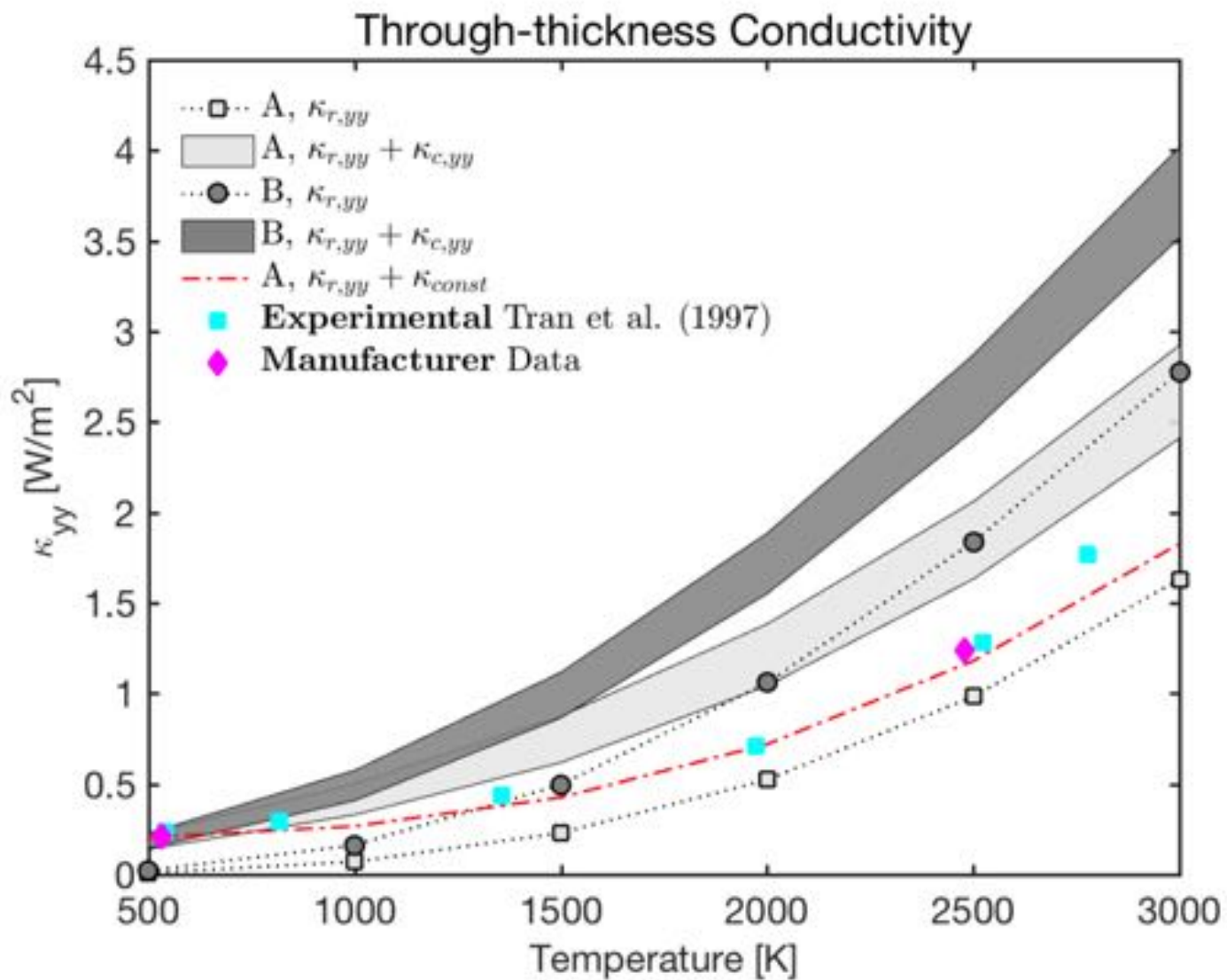
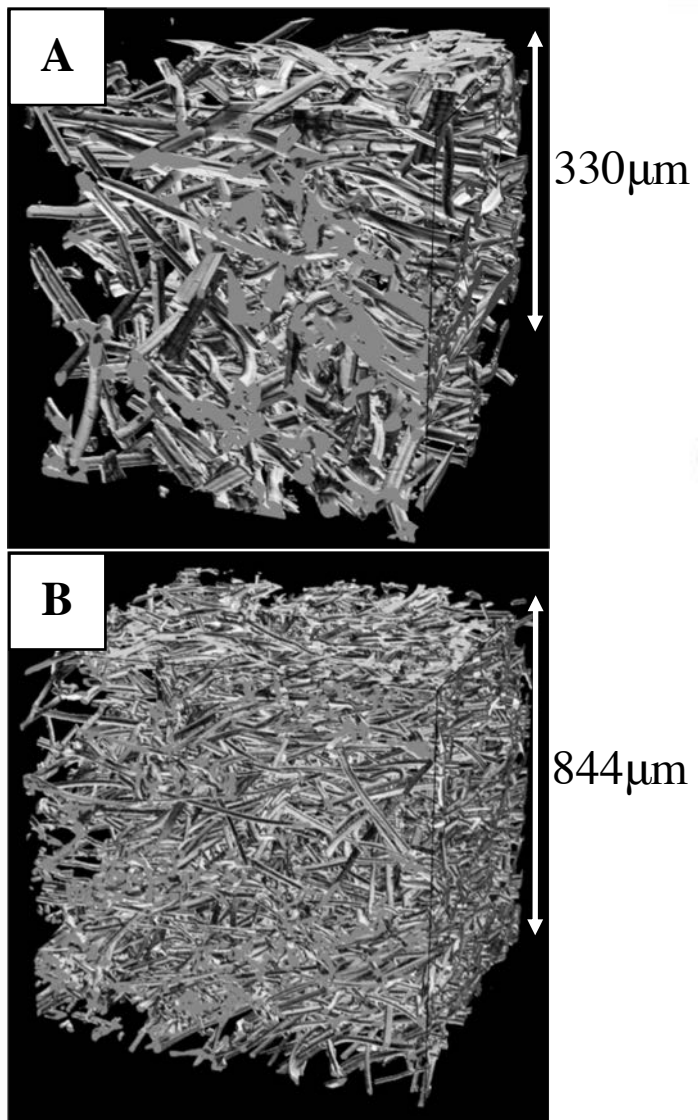
$$F_{ij} = \frac{1}{A_i} \int_{A_i} \int_{A_j} \frac{|\hat{n}_i \cdot \hat{r}_{ij}| |\hat{n}_j \cdot \hat{r}_{ij}|}{|\vec{r}_{ij}|^2} dA_j dA_i$$



$T_i$ : Temperature of surface  $i$   
 $\epsilon_i$ : Emissivity of surface  $i$   
 $F_{ij}$ : **View Factor, fraction of radiation from surface  $j$  reaching surface  $i$**



# Heat Transfer Calculation



Thank you

