Computing the effective thermal conductivity of anisotropic porous media from micro-Computed Tomography

Presented by Federico Semeraro
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Minisymposium #1301: Image-Based Simulation

MOTIVATION & OBJECTIVES

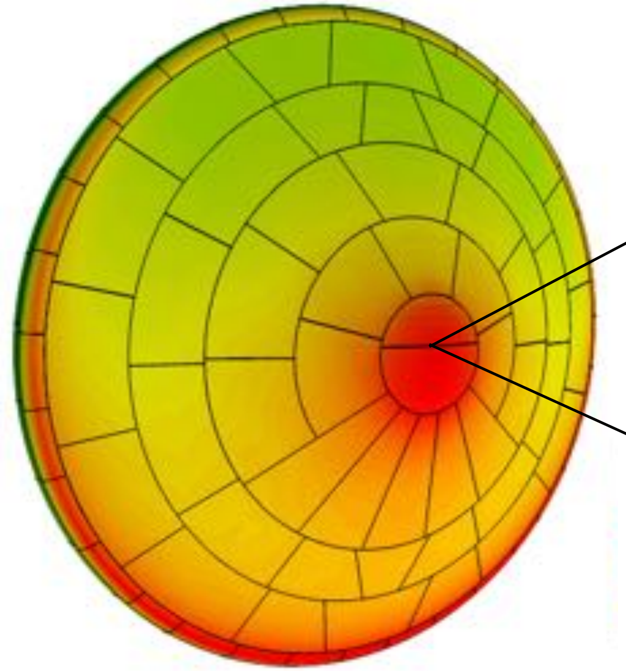
Modeling Thermal Protection Systems (TPS)

Macroscale Modeling

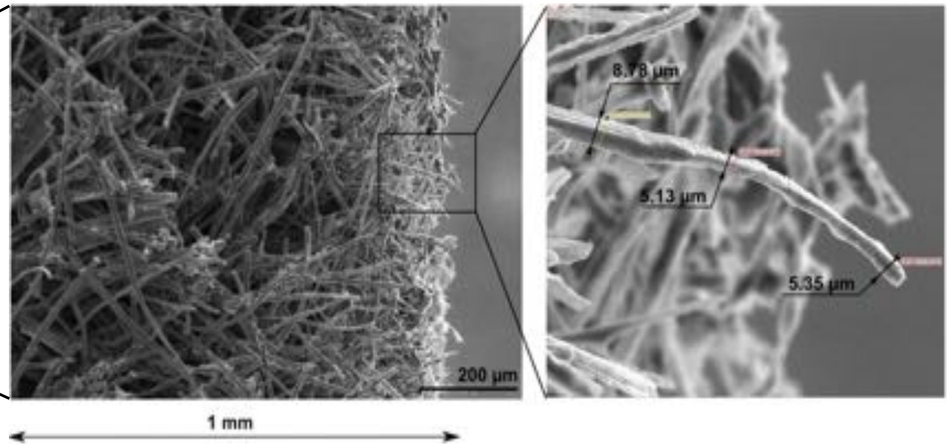
Full scale material response solvers, using volume-averaged techniques to solve conservation equations for ablation

Microscale Modeling

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



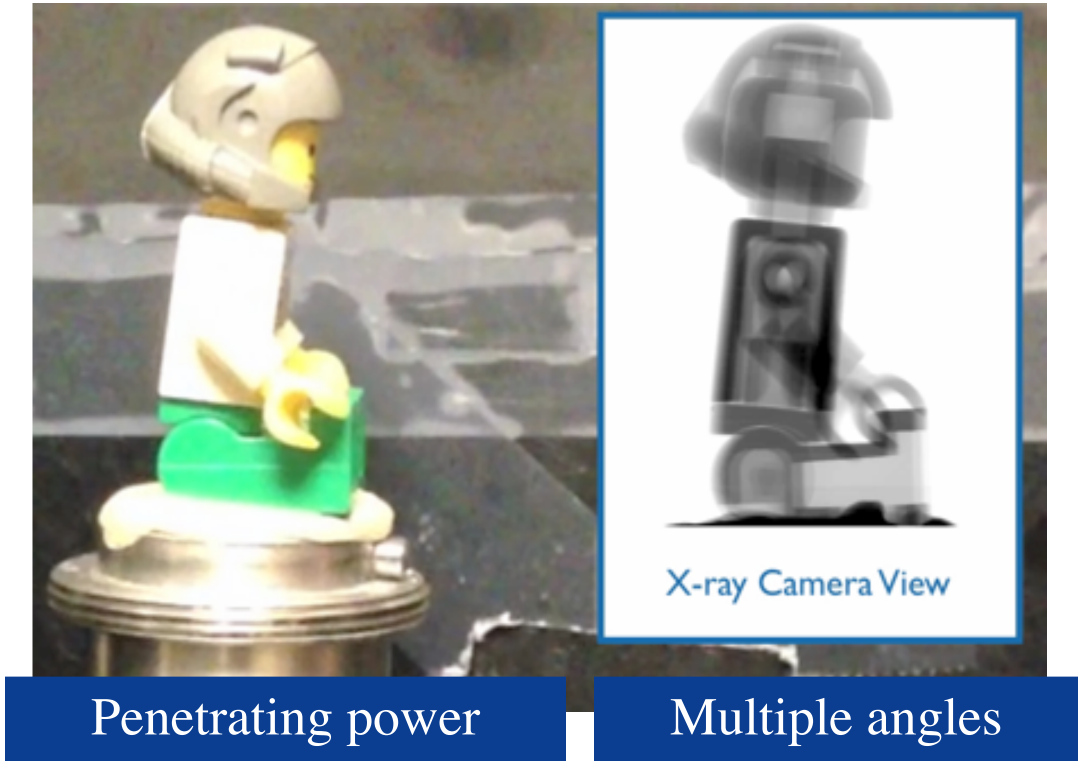
Simulation of surface temperature for MSL heatshield



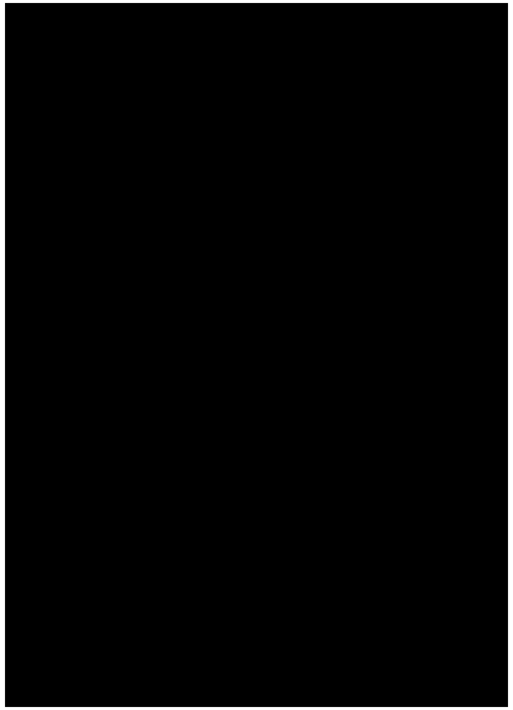
Lachaud and Mansour, *JTHT* 2013

X- Ray Microtomography

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

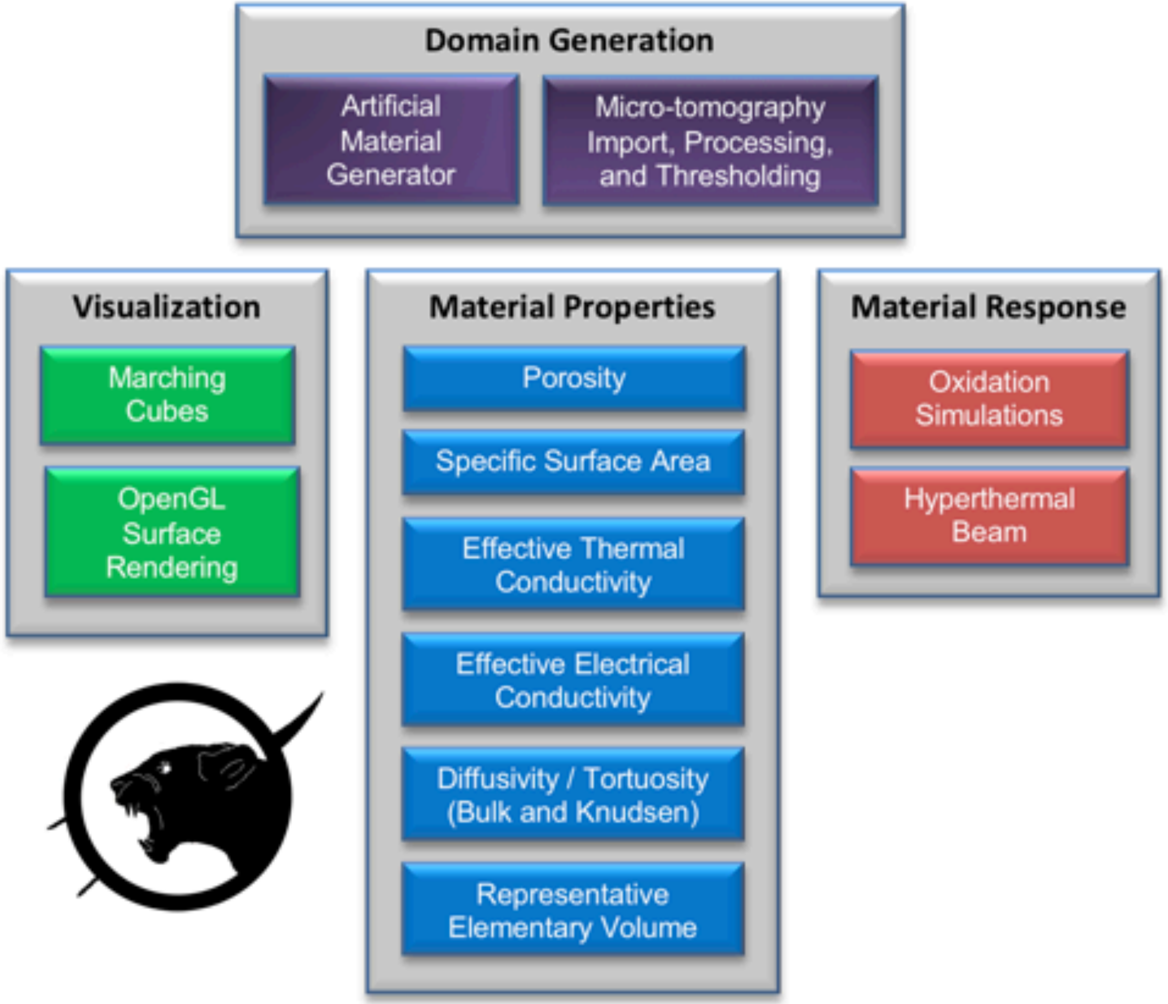


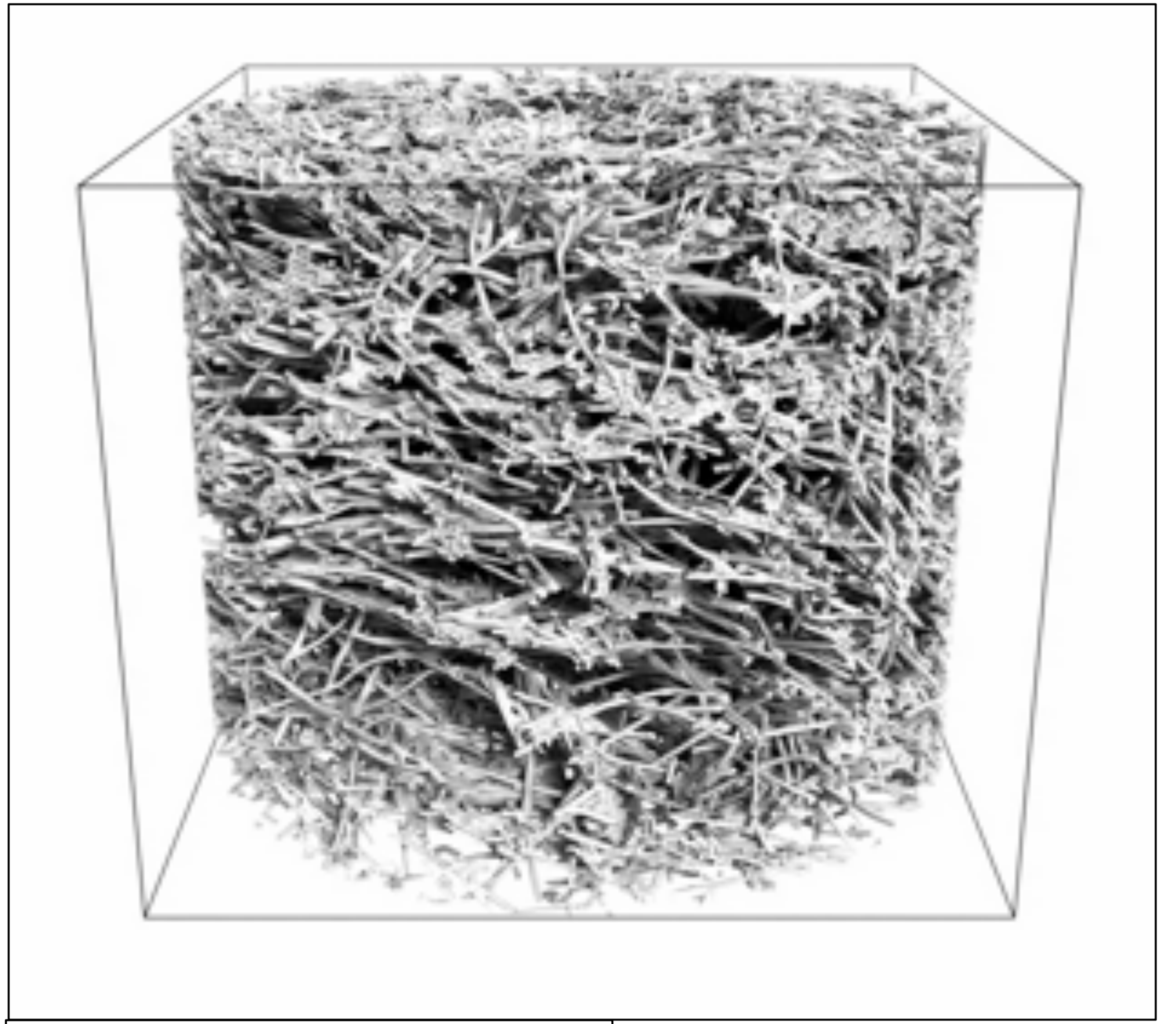
Use this series of images to reconstruct the 3D object



Courtesy of D. Parkinson (ALS)

Porous Microstructure Analysis (PuMA)



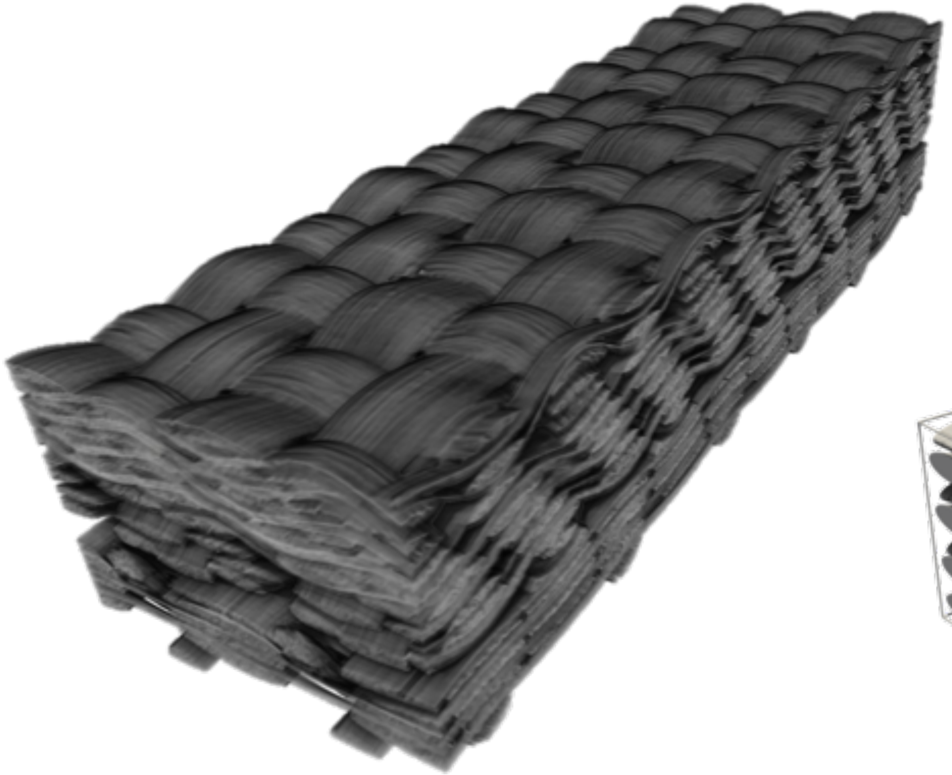


CT Reconstruction of FiberForm

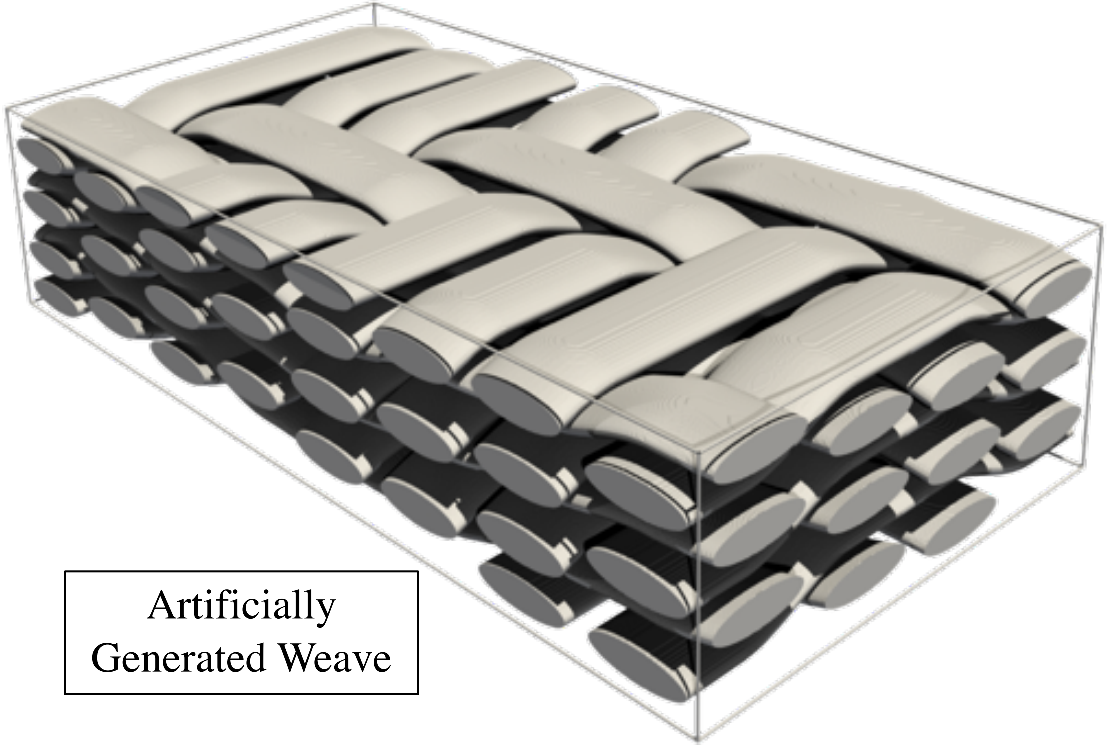
Ferguson, J. C., Panerai, F., Borner, A., & Mansour, N. N. (2018). PuMA: the Porous Microstructure Analysis software. *SoftwareX*, *7*, 81-87.
https://software.nasa.gov/software/ARC-17920-1

Challenges in Micro-scale modeling

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



12-ply real TPS weave

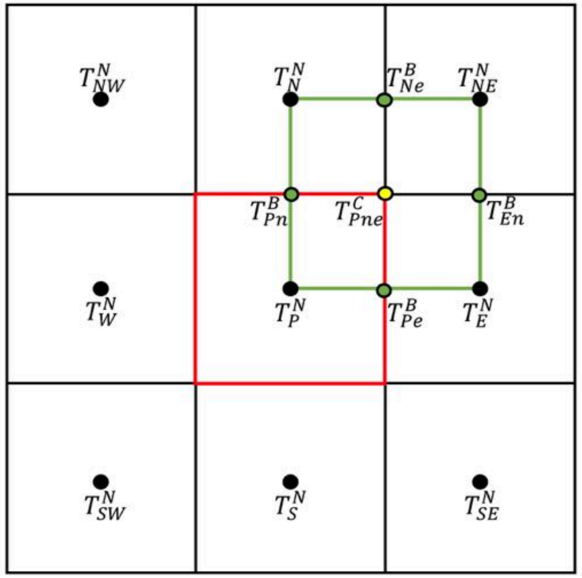


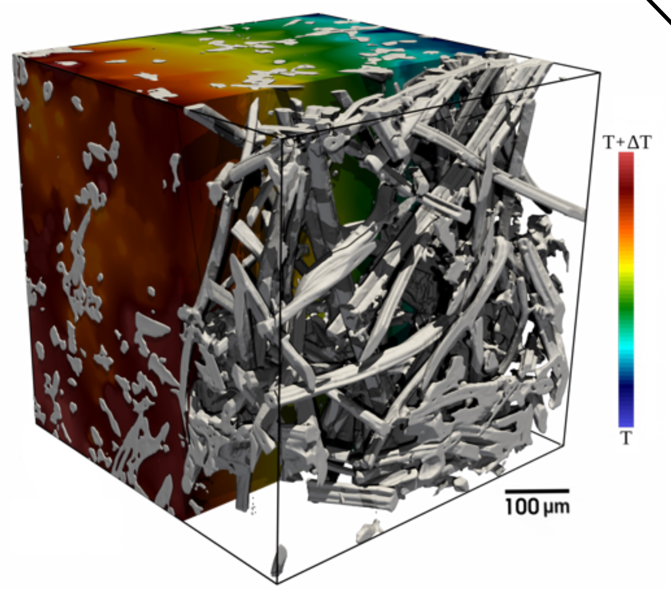
Artificially Generated Weave

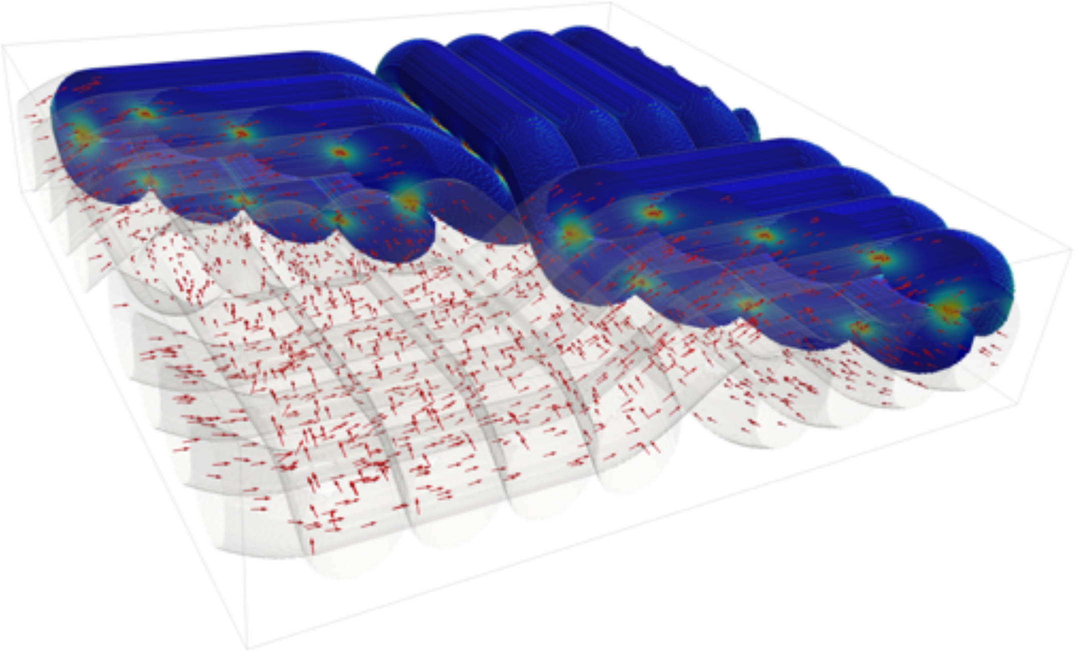
Objectives

Model Anisotropic Heat Conduction

1. Physical and Numerical Model
2. Fiber Orientation Estimation



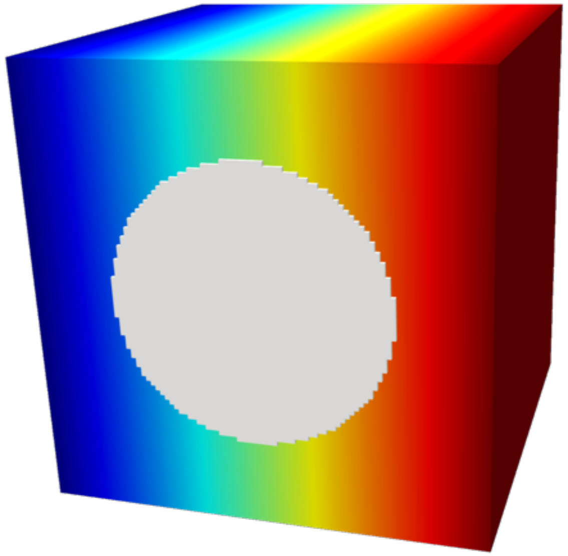




PHYSICAL & NUMERICAL MODEL

Computing the effective thermal conductivity

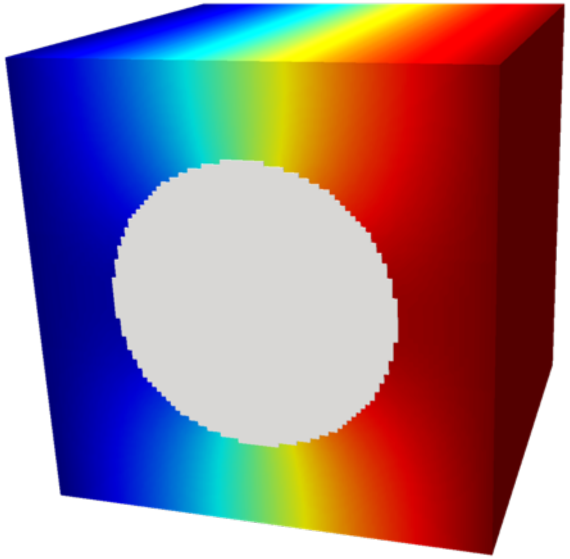
Impose initial linear Temperature profile



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

CGLS →

Temperature converged to Steady State

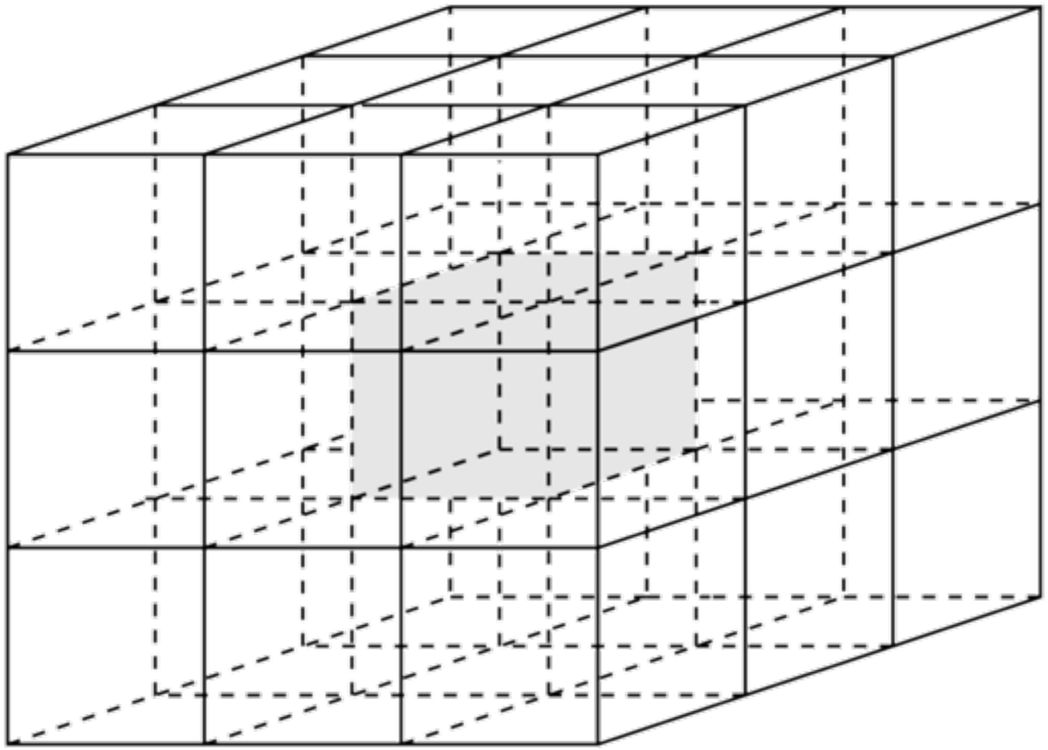


→ Compute Effective Thermal Conductivity

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

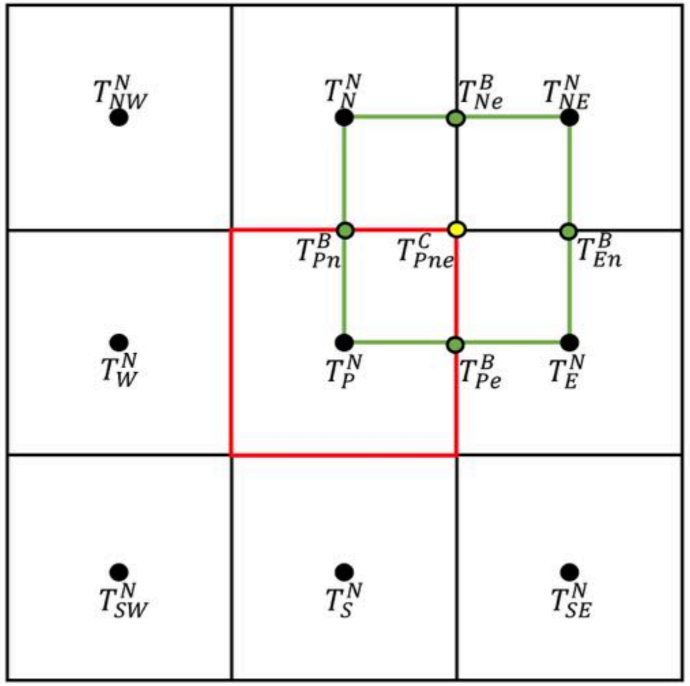
Finite Volume Method

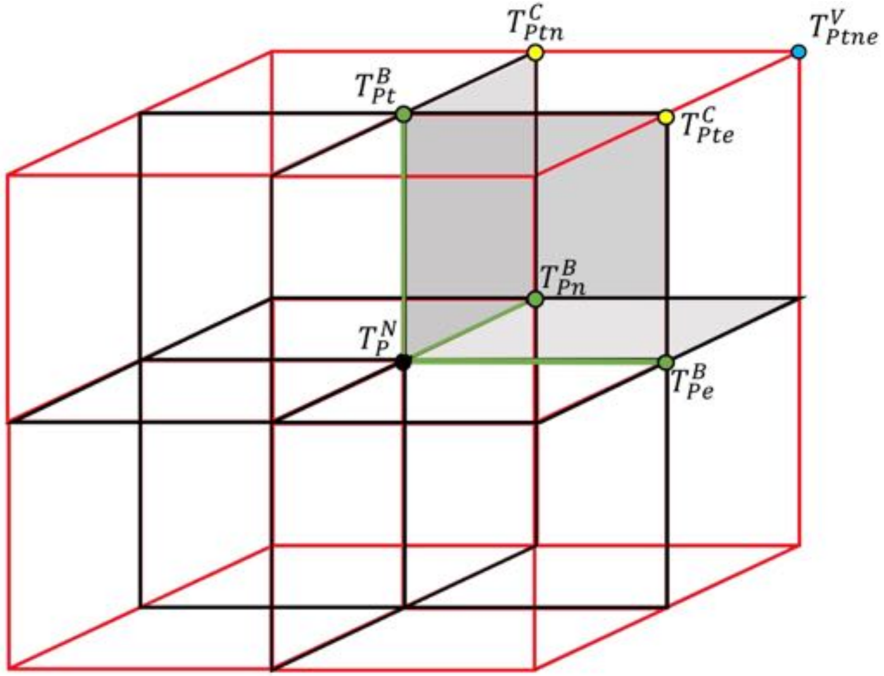
$$\int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\frac{\partial q^x}{\partial x} + \frac{\partial q^y}{\partial y} + \frac{\partial q^z}{\partial z} \right) dxdydz = 0 \;\; \text{where} \;\; \boldsymbol{q} = \begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{yx}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

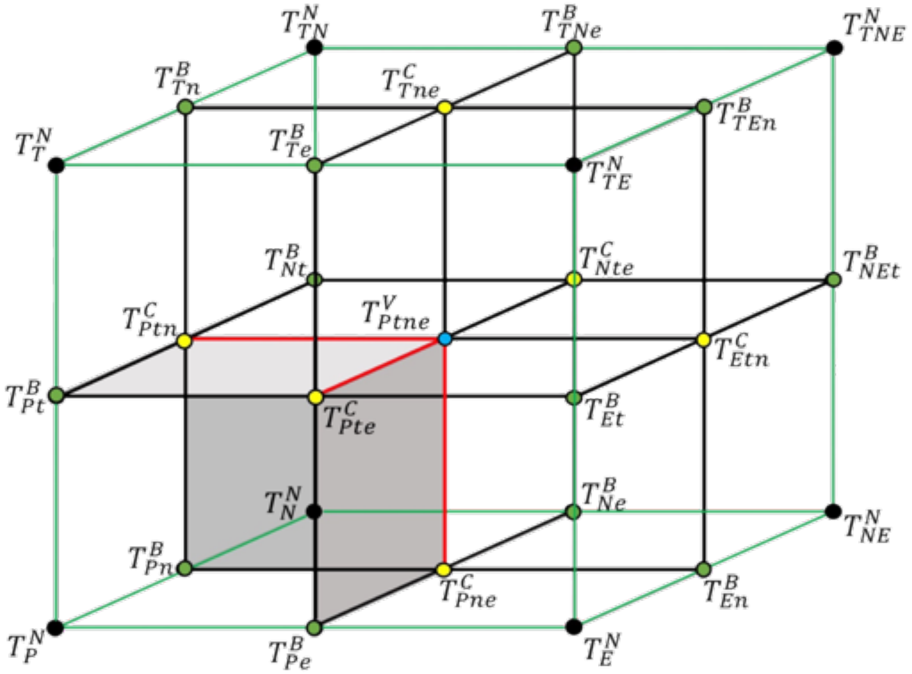


Multi-Point Flux Approximation (MPFA*)

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





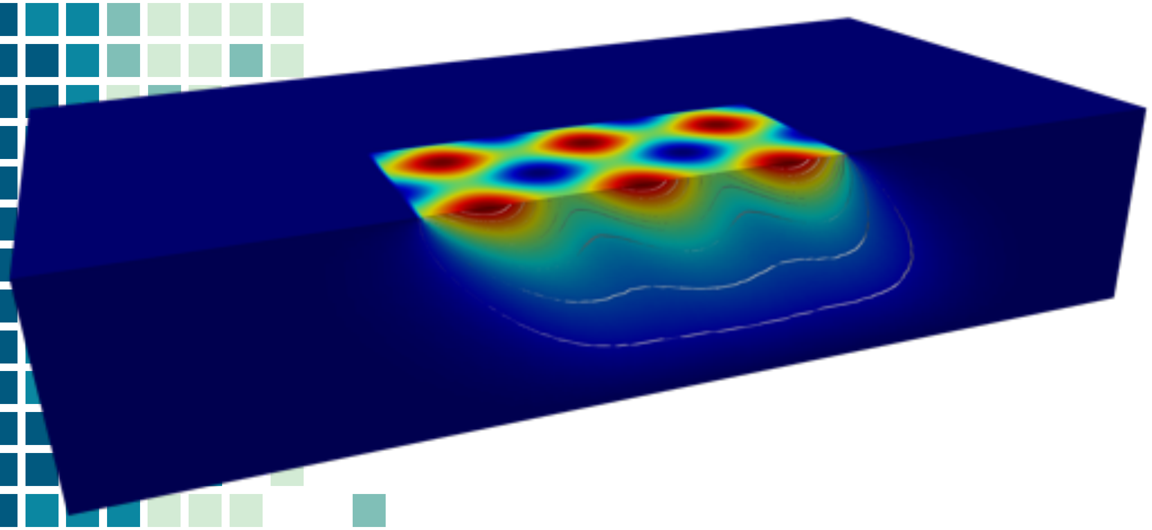


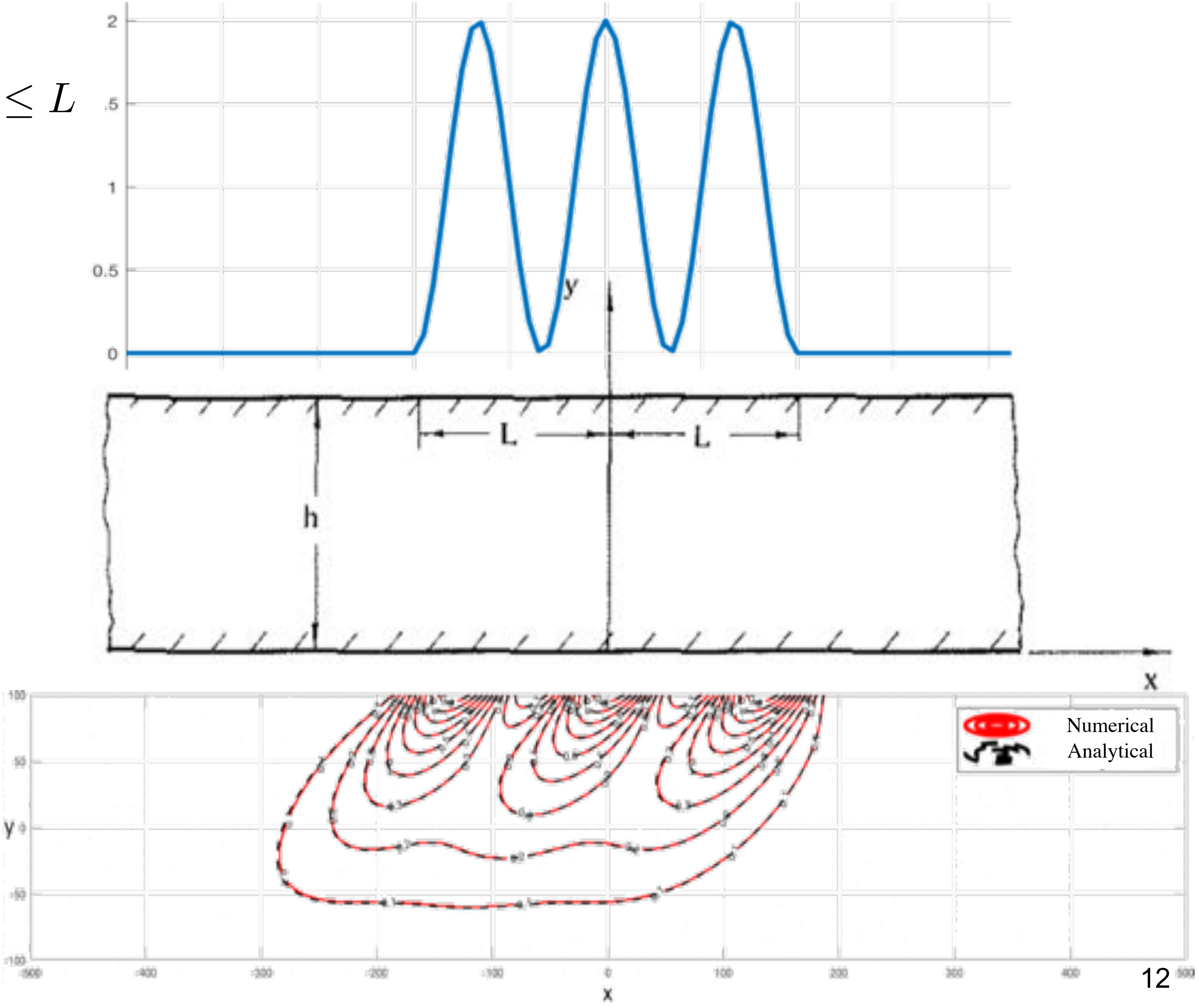
*Ivar Aavatsmark. Multipoint flux approximation methods for quadrilateral grids. *9th International forum on reservoir simulation 2007*, *Abu Dhabi*, pages 9–13.

Analytical Case* for Anisotropic sample

$$
\boldsymbol{T}_{i,j,k} = \begin{cases} 0, & [x,z] < -L \\ \cos\left(\frac{3\pi}{h}x\right) + \cos\left(\frac{3\pi}{h}z\right), & -L \le [x,z] \le L \\ 0, & [x,z] > L \end{cases}
$$

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



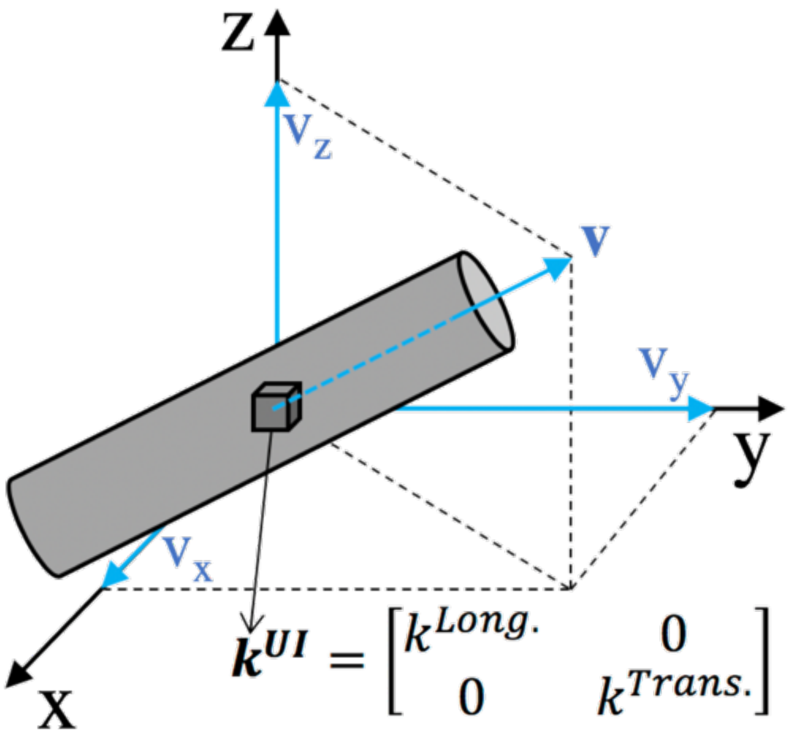


* Zhang Xiangzhou, Steady-State Temperatures in an Anisotropic Strip, *ASME Journal of Heat Transfer 1990*, 112(1), pp. 16-20.

FIBER ORIENTATION ESTIMATION

Overview of methods

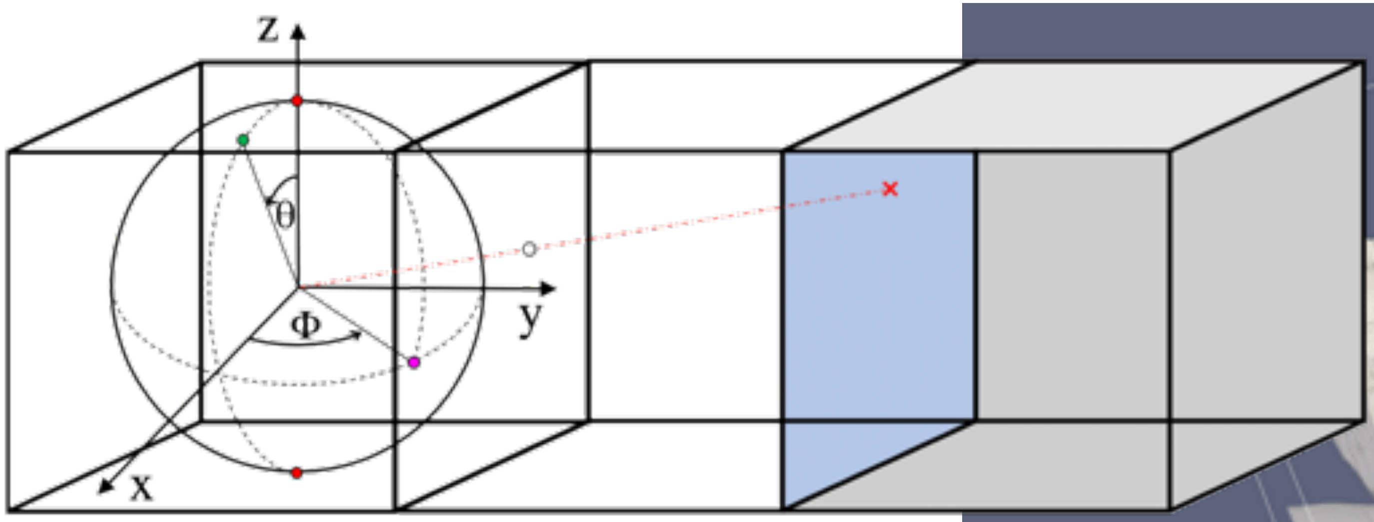
- Ray casting (novel)
- Artificial heat flux *1
- Structure tensor *2

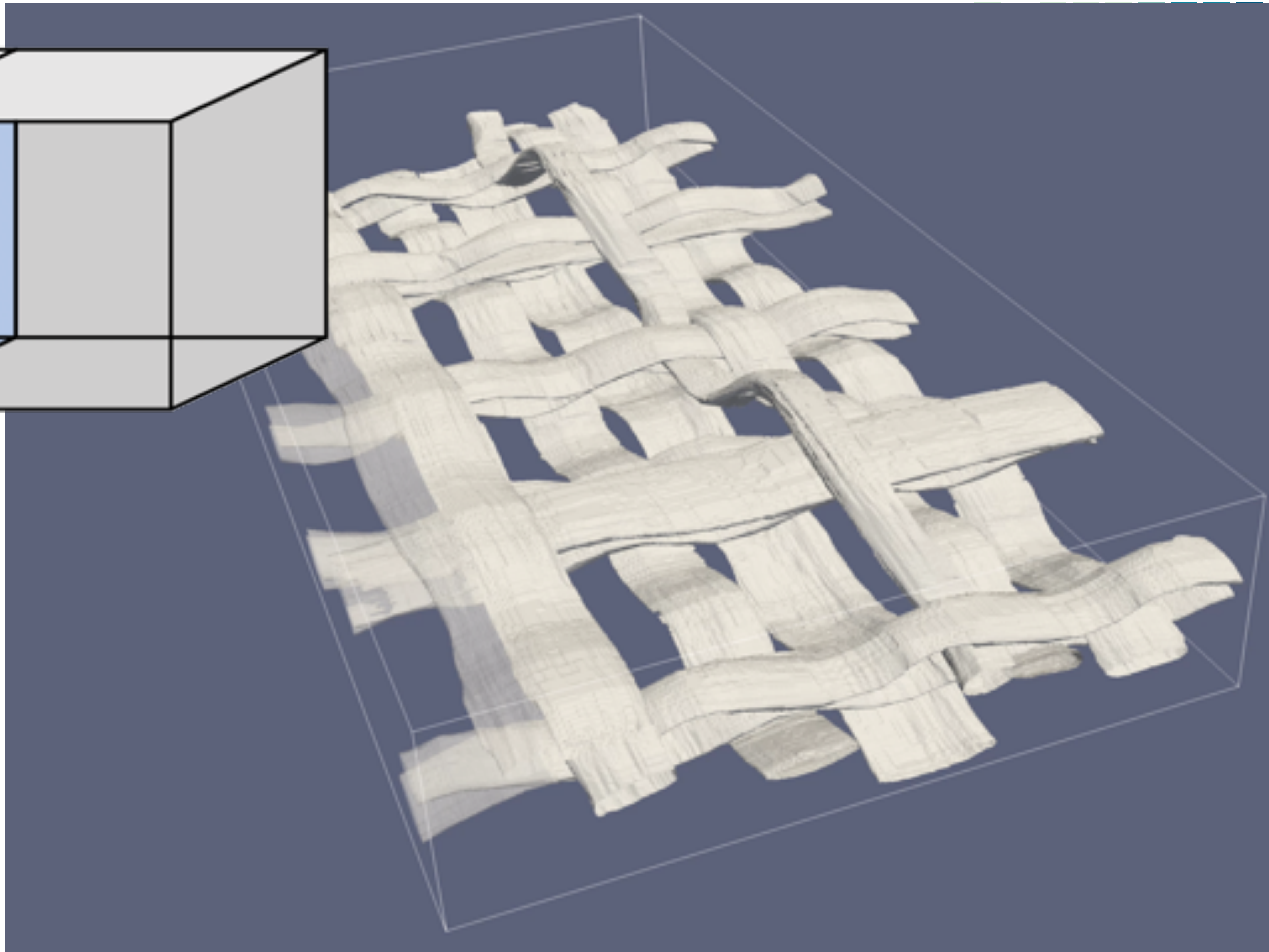


*1 Matti Schneider, Matthias Kabel, Heiko Andrä, et al. Thermal fiber orientation tensors for digital paper physics. *International Journal of Solids and Structures 2016*; 100-101 234

*2 Krause M, Hausherr JM, Burgeth B, Herrmann C, Krenkel W. Determination of the fibre orientation in composites using the structure tensor and local x-ray transform. *J Mater Sci 2010*; 45(4):888–96.

Ray Casting

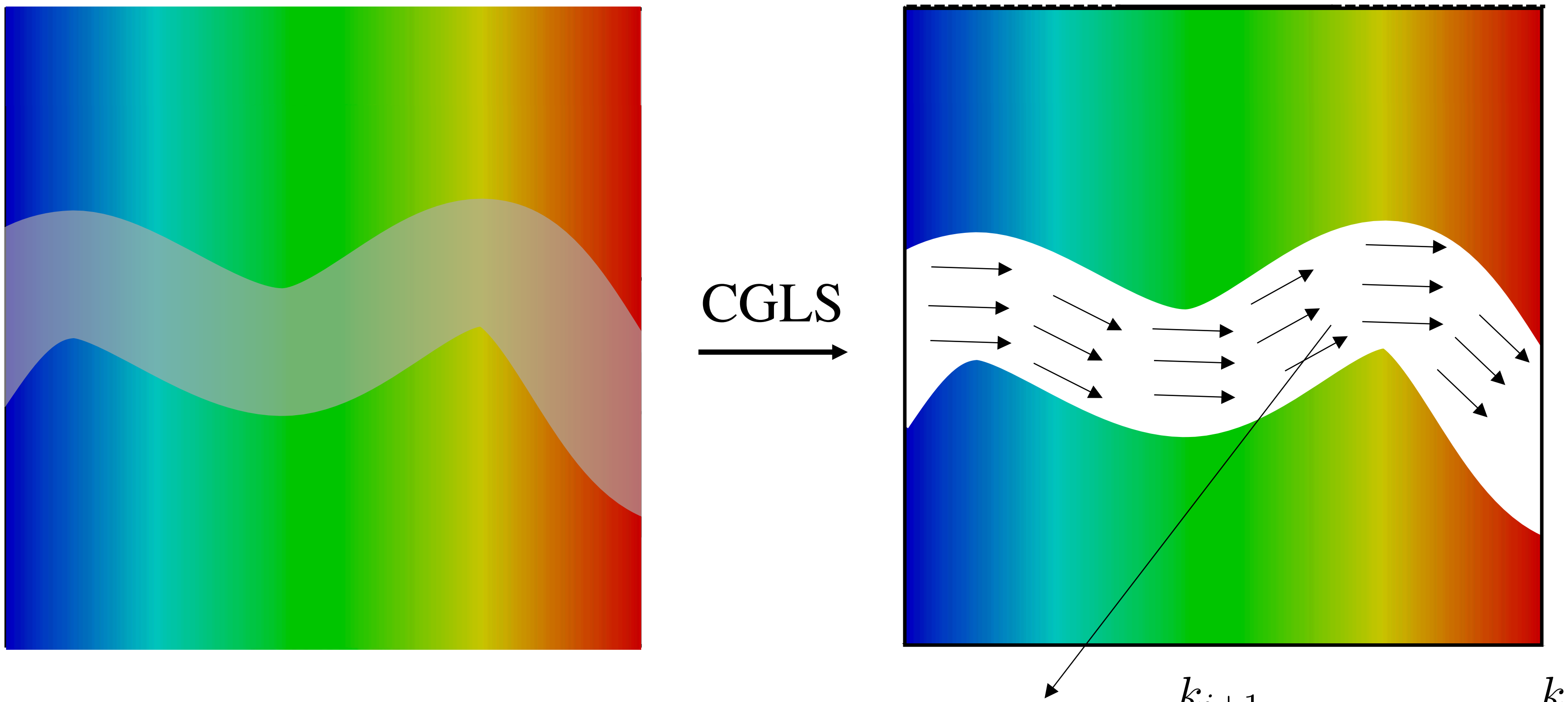




$$\theta \in [0, 180^\circ) \qquad \phi \in [0, 360^\circ)$$

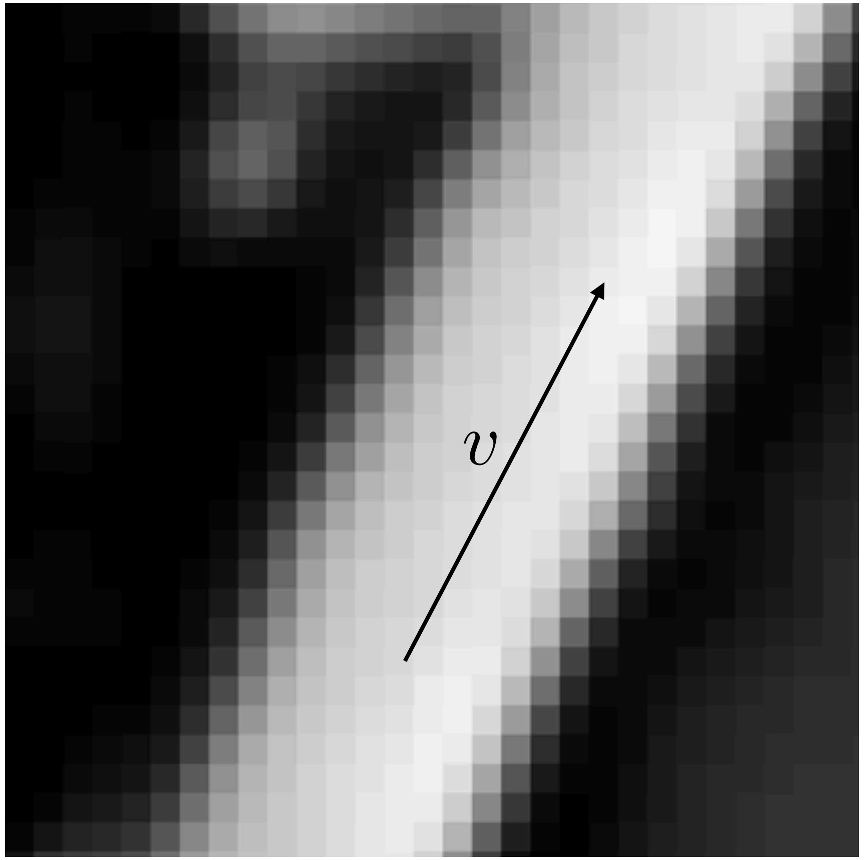
$$N = \left(\frac{180^\circ}{d\psi} - 1\right)\left(\frac{360^\circ}{d\psi}\right) + 2$$

Artificial Heat Flux



$$T_{i+1/2} = \frac{k_{i+1}}{k_i + k_{i+1}} T_{i+1} + \frac{k_i}{k_i + k_{i+1}} T_i$$

Structure Tensor

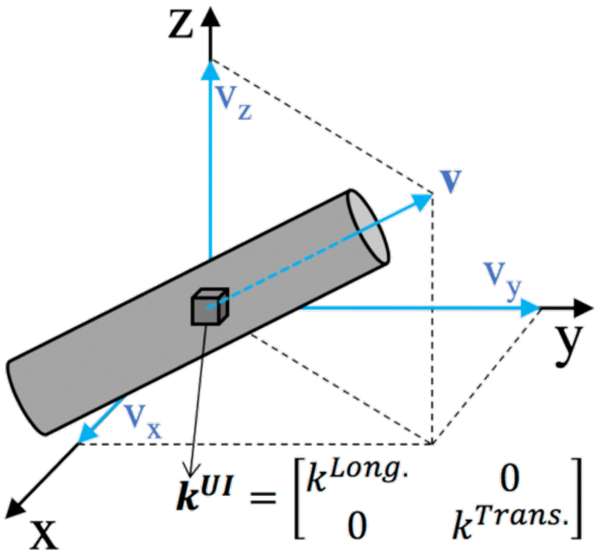


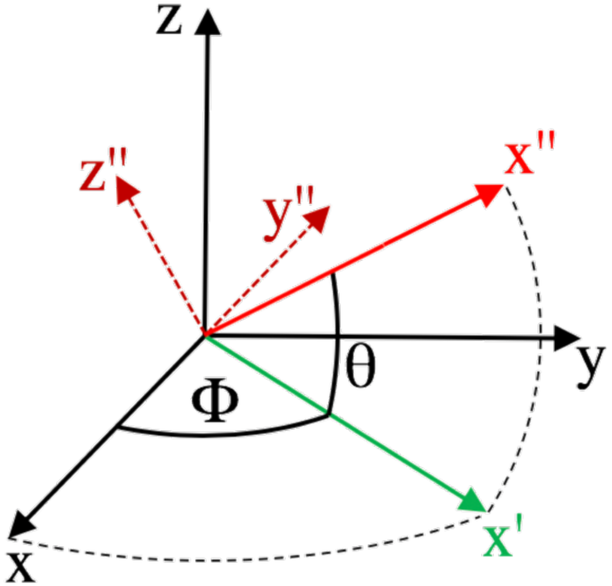
$$(I(x+v) - I(x))^2 \approx 0$$

4 Steps:

1. $\nabla I_\sigma(x) = \nabla(\sigma * I(x))$
2. $\nabla I_\sigma \nabla I_\sigma^T = \begin{pmatrix} I_x^2 & I_x I_y & I_x I_z \\ I_x I_y & I_y^2 & I_y I_z \\ I_x I_z & I_y I_z & I_z^2 \end{pmatrix}$
3. $J_\rho(x) = \rho * (\nabla I_\sigma \nabla I_\sigma^T)$
4. Local orientation vector v is the eigenvector related to the smallest eigenvalue of $J_\rho(x)$

Conductivity Tensor Rotation





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

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

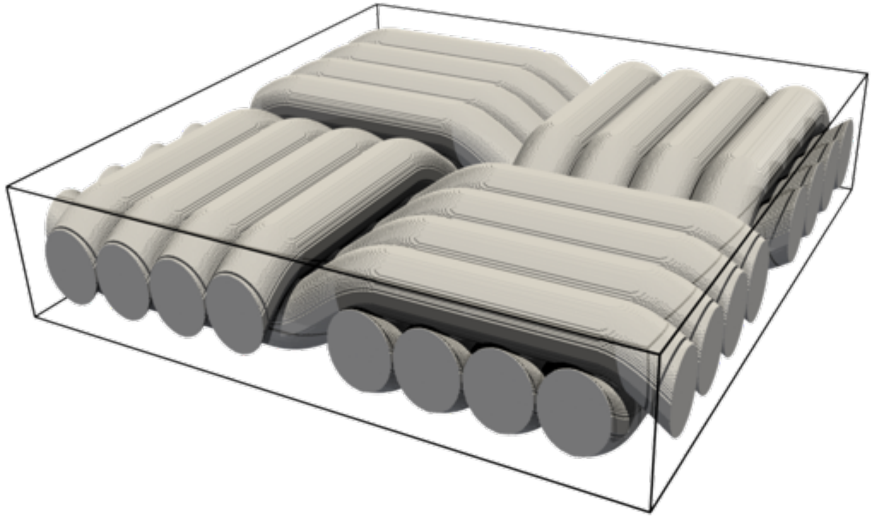
$$\theta = \arcsin v_z \quad \phi = \arctan \frac{v_y}{v_x}$$

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

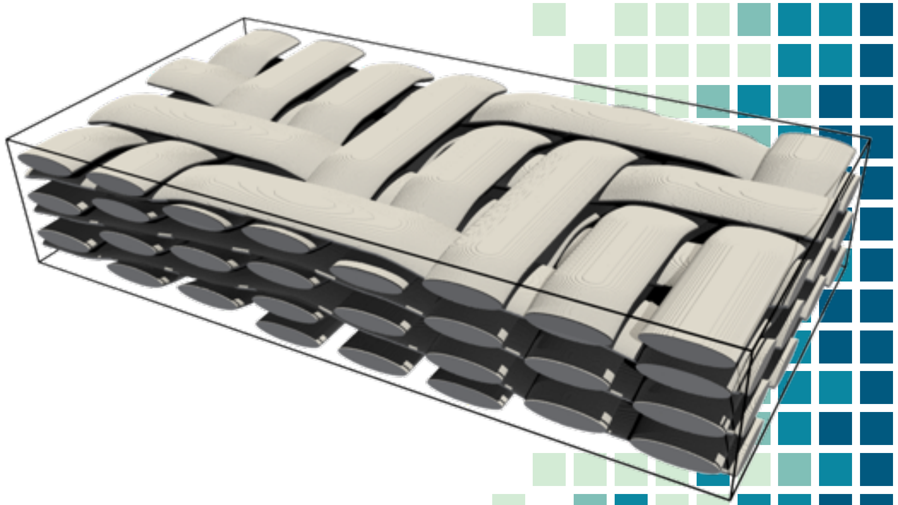
$$\boldsymbol{R} = \begin{bmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Parametric Study

Artificial Straight Fibers



Parachute Weave



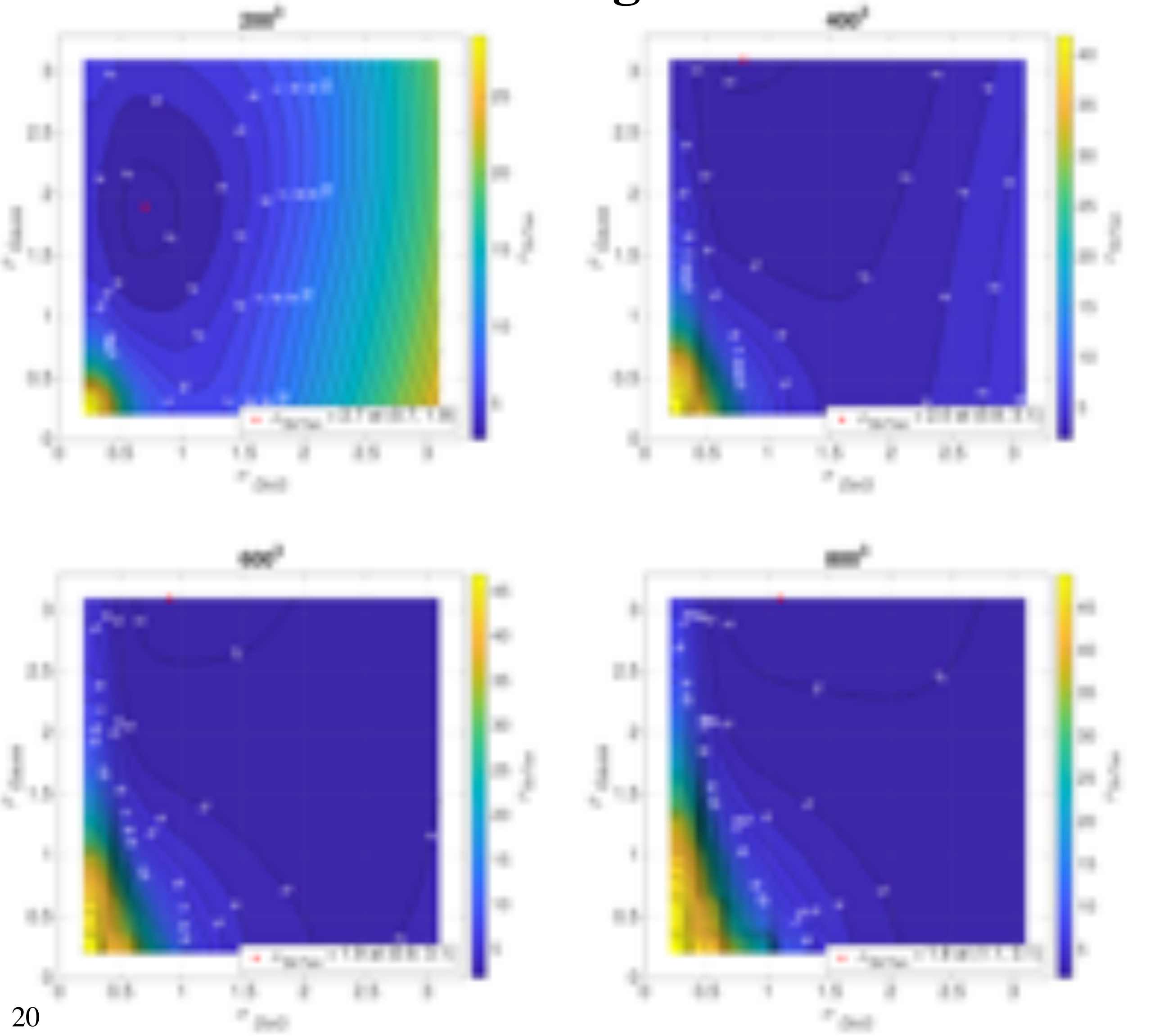
Adept Weave

Degrees of Freedom

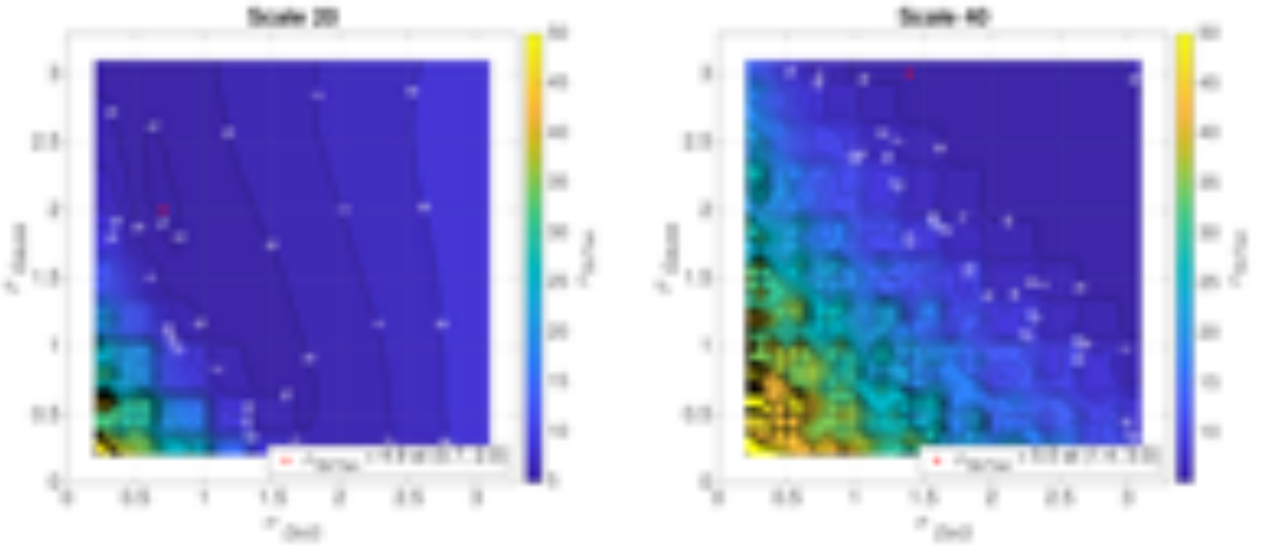
Ray casting	Artificial heat flux	Structure tensor
1. Ray angle separation $d\psi$	None	Kernel window sizes: 1. σ 2. ρ

Parametric Study : Gaussian Filters

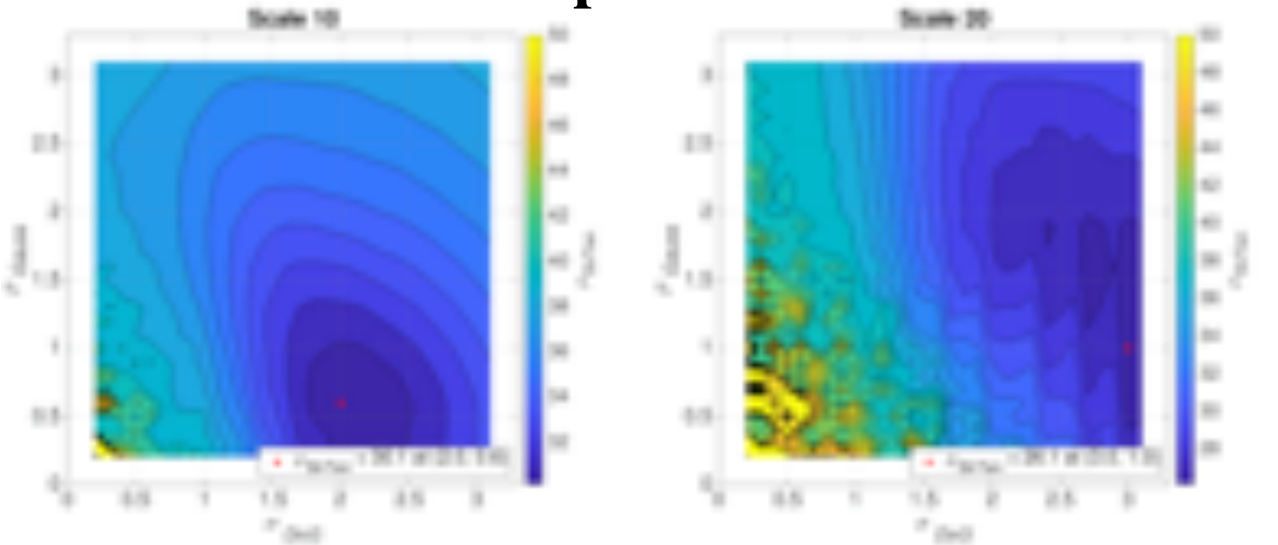
Artificial Straight Fibers



Parachute weave



Adept weave



Methods Performance

1. Ray casting:
   - Performs well on artificial straight fibers ($\mu \sim 3 - 5°$) and similar to other methods on woven structures ($\mu \sim 10 - 15°$)
   - Limitation: Computationally very expensive
2. Heat flux:
   - Easy to use because independent on inputs. Performs similar to other methods on weaves ($\mu \sim 15°$)
   - Limitation: Performs poorly on artificial straight fibers due to regions not being in the path of heat flux through the material ($\mu \sim 15 - 20°$)
3. Structure tensor:
   - Performs effectively on artificial straight fibers ($\mu \sim 1 - 5°$) and similar to other methods on weaves ($\mu \sim 20°$)
   - Limitation: hard to define optimal window a priori. For binary images, window must be sufficiently large, which can be expensive

Summary

Formulated, implemented and validated:

1. Finite Volume method based on the MPFA technique to find the effective thermal conductivity due to anisotropic solid heat conduction

2. Fiber orientation estimation based on:
    1. Ray casting technique
    2. Artificial heat flux
    3. Structure tensor method

Thank you. Questions?