Modeling the Effective Thermal Conductivity of Anisotropic Porous Materials

Presented by Federico Semeraro
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Authors: Federico Semeraro, Joseph Ferguson, Francesco Panerai, Nagi N. Mansour

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

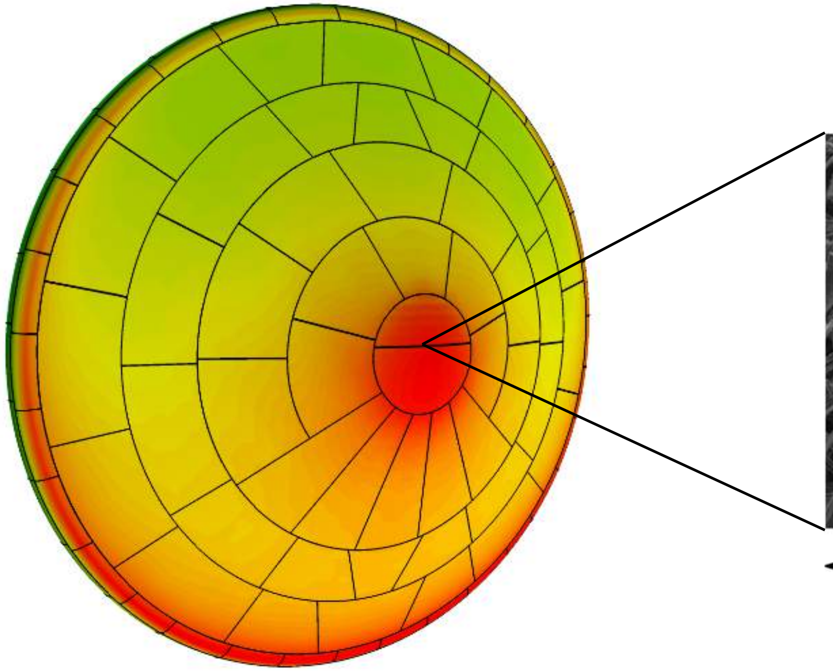
Contents

MOTIVATION & OBJECTIVES

Modeling Thermal Protection Systems (TPS)

Macroscale Modeling

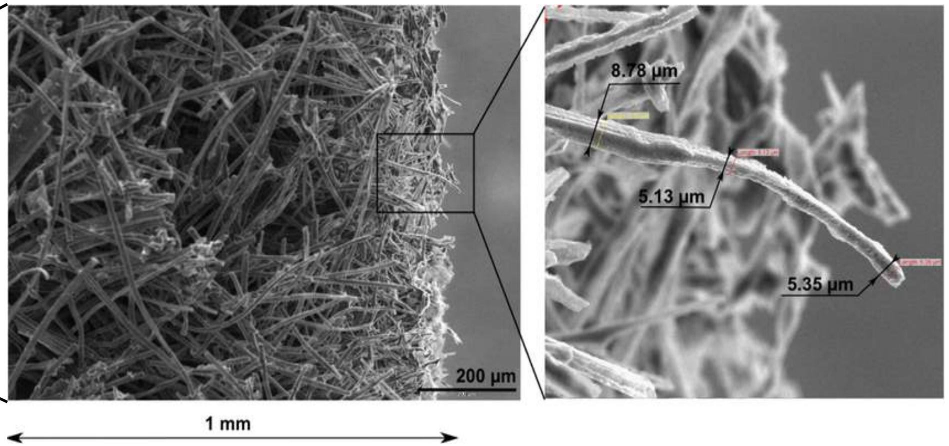
Full scale material response solvers, using volume-averaged techniques to solve conservation equations for ablation



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

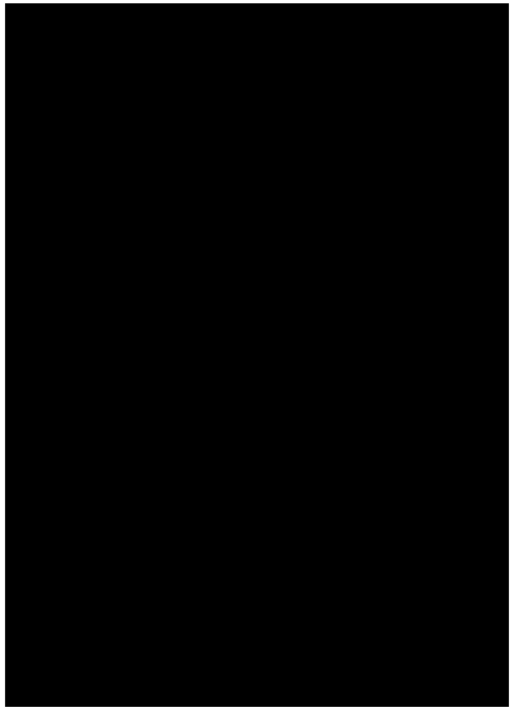
X- Ray Microtomography

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

Use this series of images to reconstruct the 3D object

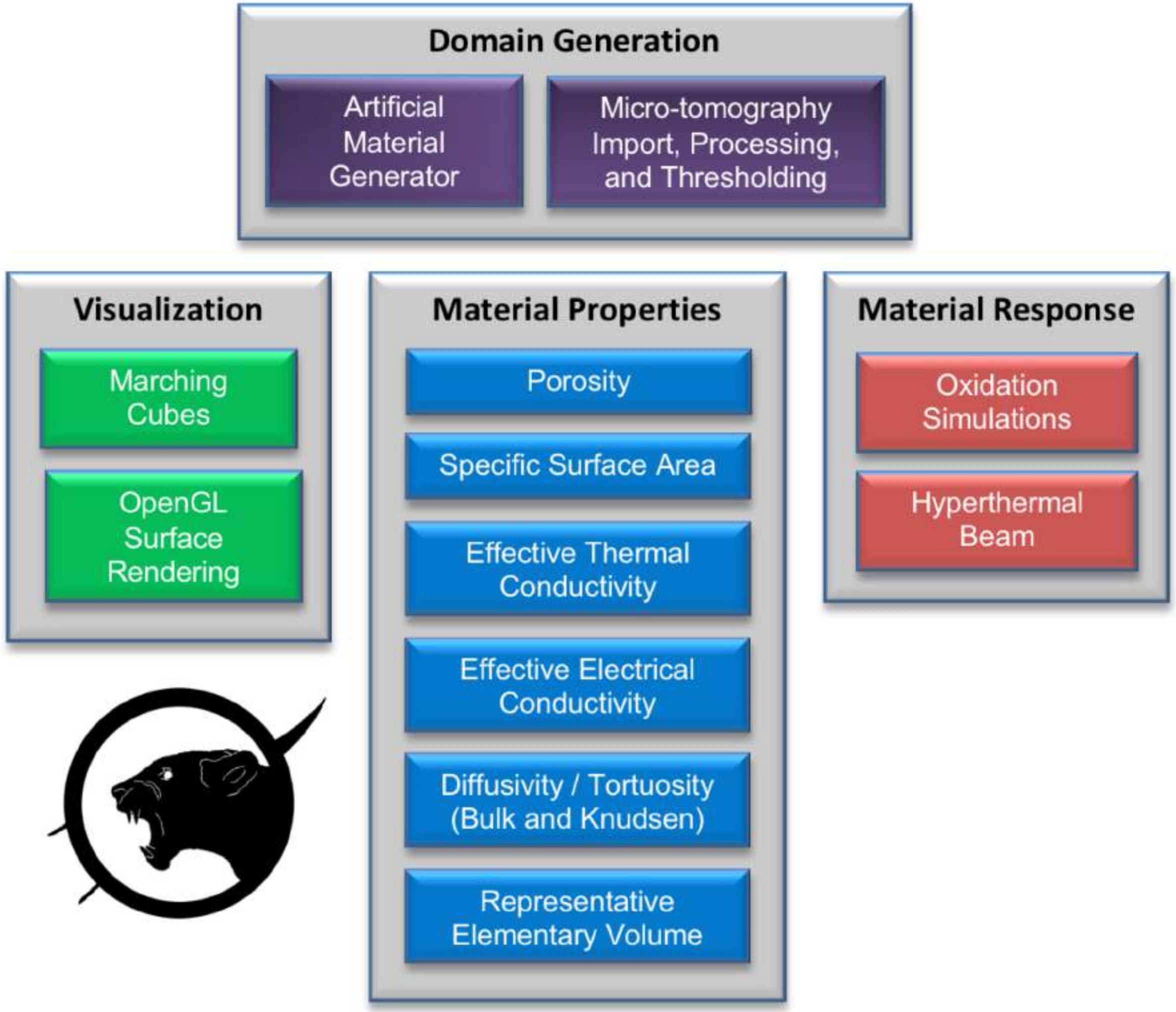
Penetrating power

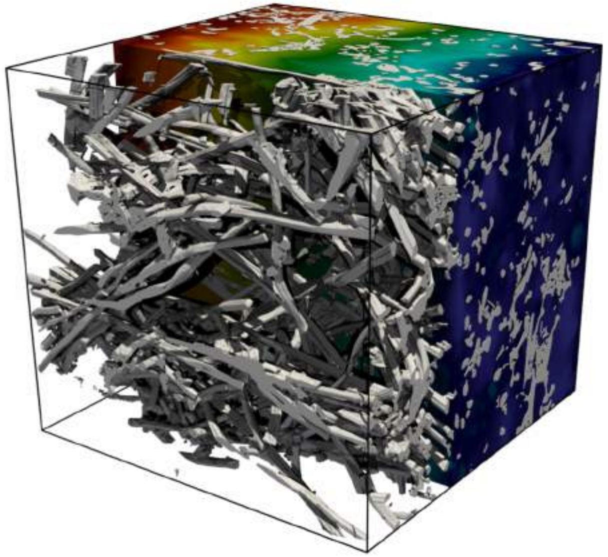
Multiple angles



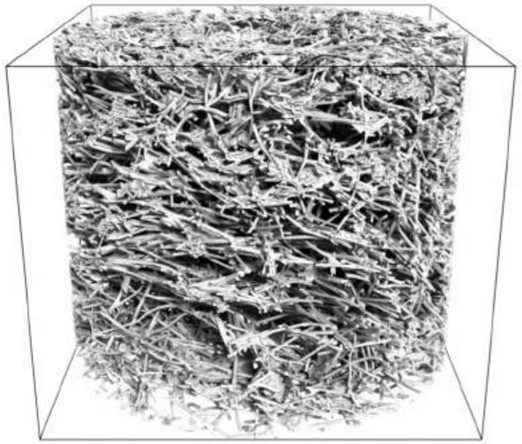
Courtesy of D. Parkinson (ALS)

Current Microscale Modeling





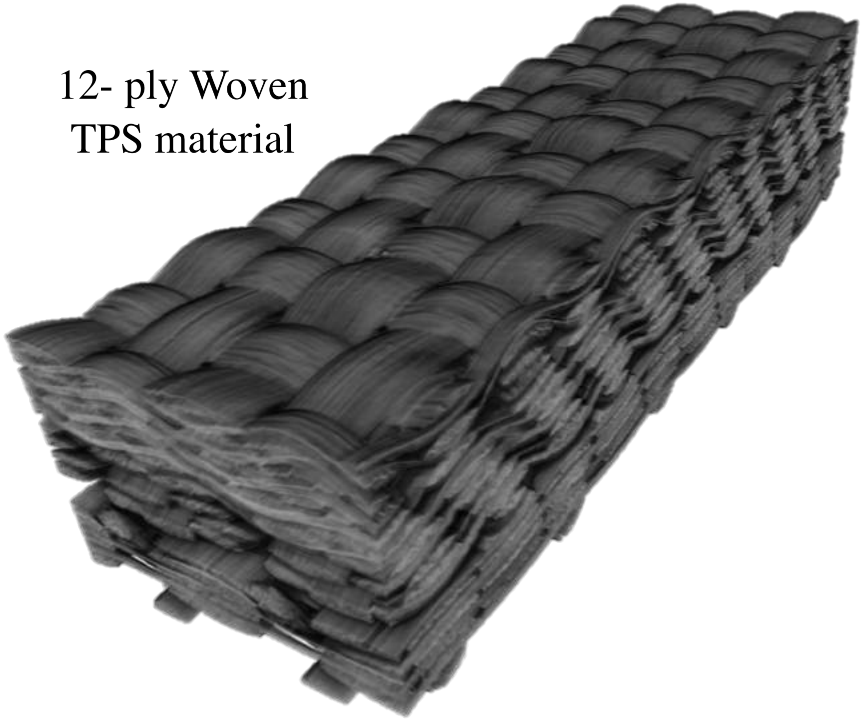
Effective Thermal Conductivity



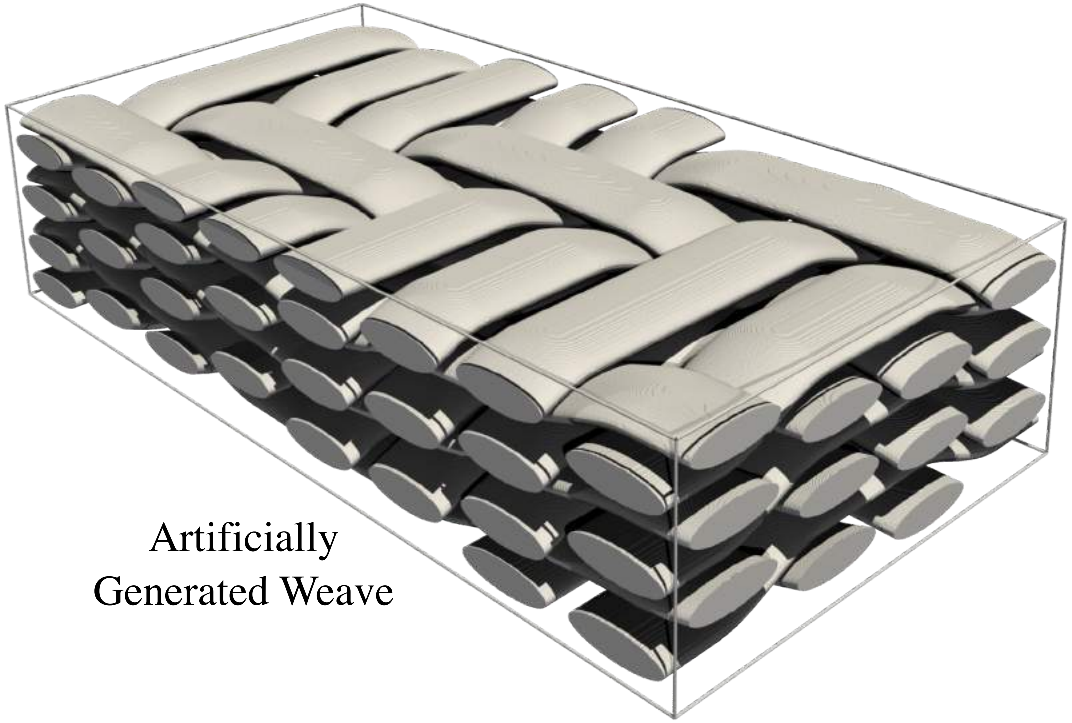
Ferguson, J. C., Panerai, F., Borner, A., & Mansour, N. N. (2018).
PuMA: the Porous Microstructure Analysis software. *SoftwareX*, *7*, 81-87.
https://software.nasa.gov/software/ARC-17920-1

Challenges in Micro-scale modeling

12- ply Woven
TPS material



Current modeling based on assumption that material constituents are isotropic

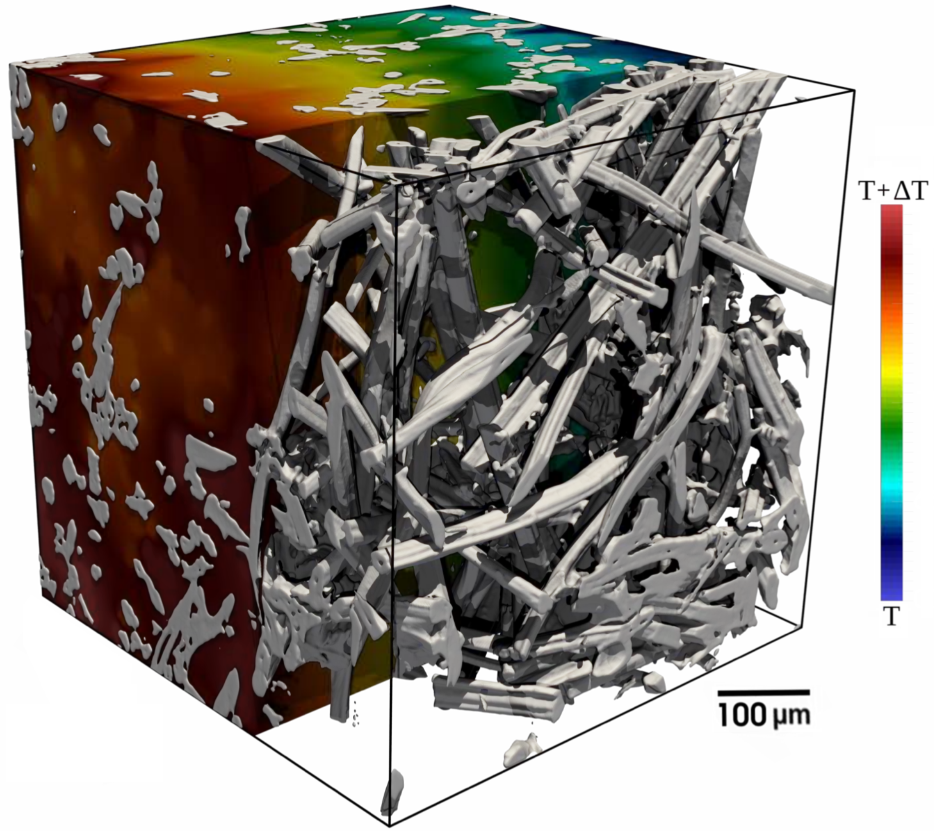


Artificially
Generated Weave

As NASA moves towards woven materials, our modeling must adapt

Summary of Objectives

1. Extend the current formulation of thermal conductivity for anisotropic constituents
2. Evaluate suitability of numerical methods for anisotropic heat transfer
3. Implement the developed formulations in C++ to be integrated in PuMA
4. Conduct a verification campaign for the developed numerical models

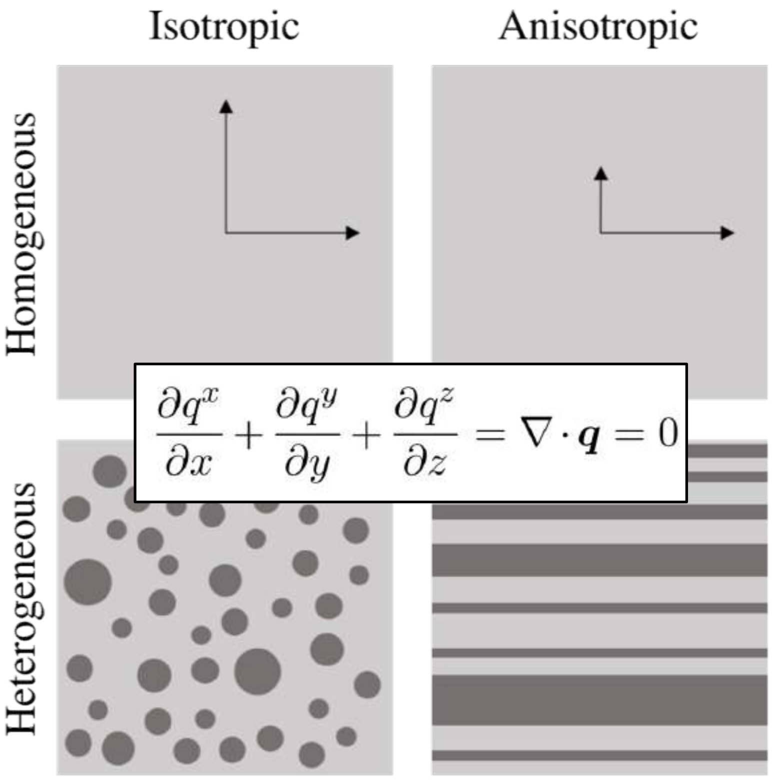


PHYSICAL & NUMERICAL MODEL

Problem Statement

Homogeneous Isotropic:

$$k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)=k\nabla^2 T=(\rho c_p)\frac{\partial T}{\partial t}$$



$$\frac{\partial q^x}{\partial x}+\frac{\partial q^y}{\partial y}+\frac{\partial q^z}{\partial z}=\nabla\cdot\boldsymbol{q}=0$$

Homogeneous Anisotropic:

$$k=\begin{bmatrix}k_{xx} & k_{xy} & k_{xz}\\ k_{yx} & k_{yy} & k_{yz}\\ k_{zx} & k_{zy} & k_{zz}\end{bmatrix}$$

$$k_{xx}\frac{\partial^2 T}{\partial x^2}+k_{xy}\frac{\partial^2 T}{\partial y^2}+k_{xz}\frac{\partial^2 T}{\partial z^2}+$$
$$k_{xy}\frac{\partial^2 T}{\partial x^2}+k_{yy}\frac{\partial^2 T}{\partial y^2}+k_{yz}\frac{\partial^2 T}{\partial z^2}+$$
$$k_{xz}\frac{\partial^2 T}{\partial x^2}+k_{yz}\frac{\partial^2 T}{\partial y^2}+k_{zz}\frac{\partial^2 T}{\partial z^2}=0$$

Heterogeneous Isotropic:

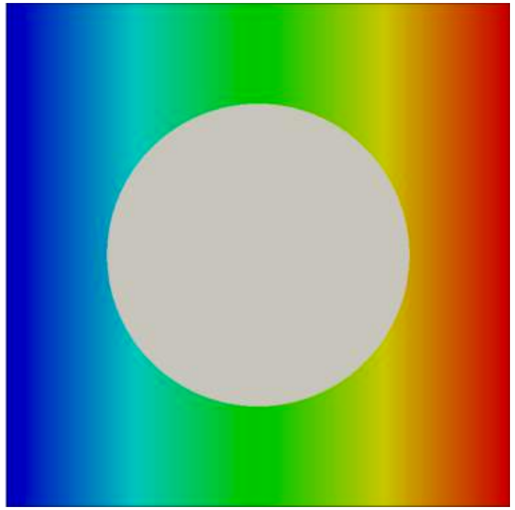
$$\frac{\partial}{\partial x}\left(k(x,y,z)\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k(x,y,z)\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k(x,y,z)\frac{\partial T}{\partial z}\right)=0$$

Heterogeneous Anisotropic:

$$\frac{\partial}{\partial x}\left(k_{xx}(x,y,z)\frac{\partial T}{\partial x}+k_{xy}(x,y,z)\frac{\partial T}{\partial y}+k_{xz}(x,y,z)\frac{\partial T}{\partial z}\right)+$$
$$\frac{\partial}{\partial y}\left(k_{xy}(x,y,z)\frac{\partial T}{\partial x}+k_{yy}(x,y,z)\frac{\partial T}{\partial y}+k_{yz}(x,y,z)\frac{\partial T}{\partial z}\right)+$$
$$\frac{\partial}{\partial z}\left(k_{xz}(x,y,z)\frac{\partial T}{\partial x}+k_{yz}(x,y,z)\frac{\partial T}{\partial y}+k_{zz}(x,y,z)\frac{\partial T}{\partial z}\right)=0$$

Computing the effective thermal conductivity

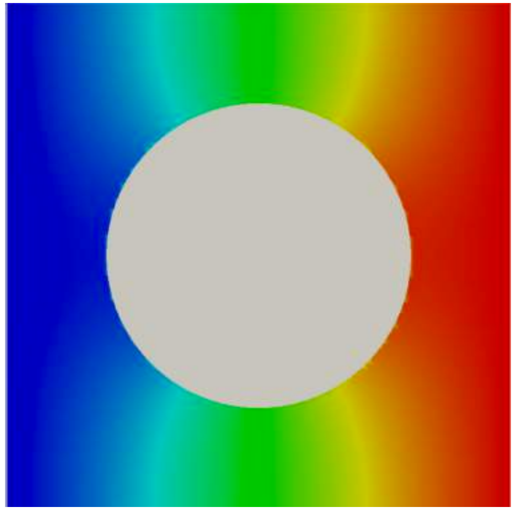
Impose initial linear
Temperature profile



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

CGLS →

Temperature converged
to Steady State



→

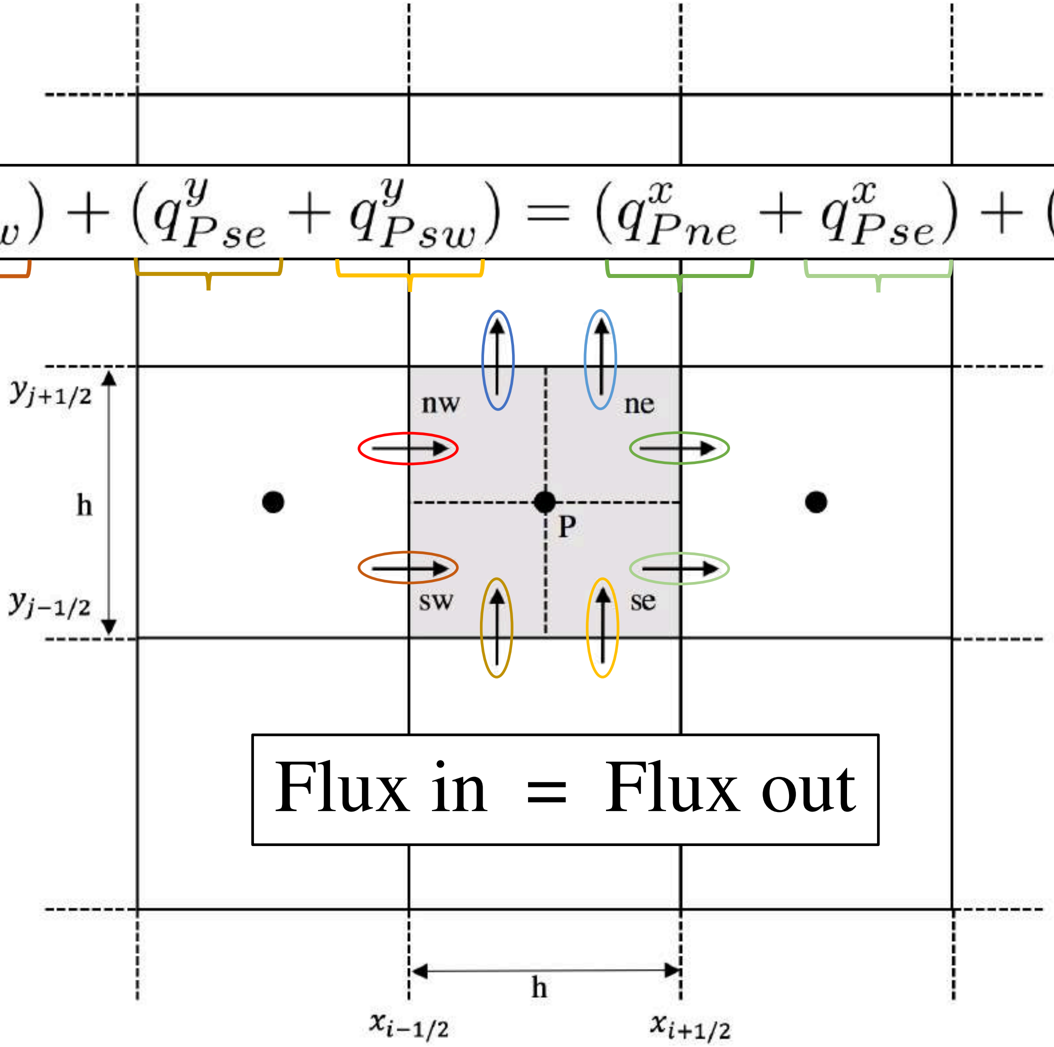
Compute Effective
Thermal Conductivity

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

Finite Volume Method

$$\int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial}{\partial x}\left(k^{xx}\frac{\partial T}{\partial x} + k^{xy}\frac{\partial T}{\partial y}\right) dxdy + \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial}{\partial y}\left(k^{xy}\frac{\partial T}{\partial x} + k^{yy}\frac{\partial T}{\partial y}\right) dxdy = 0$$

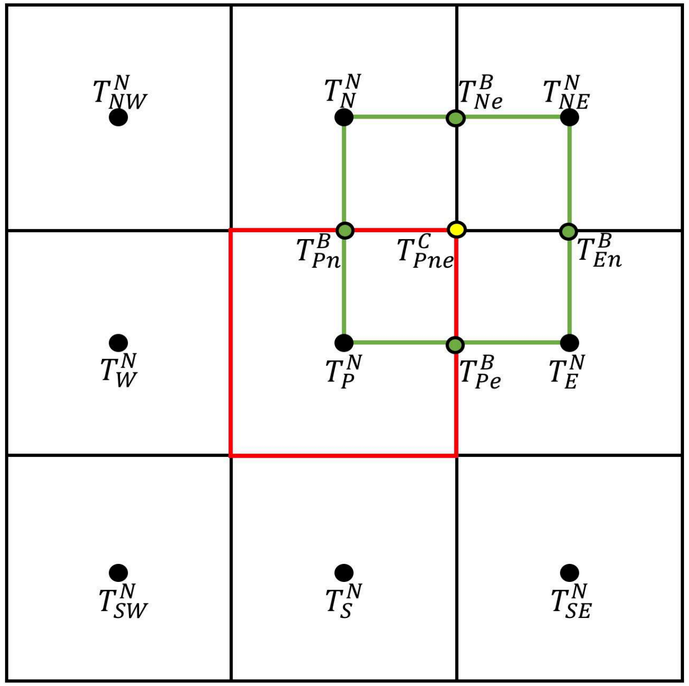
$$(q^x_{Pnw} + q^x_{Psw}) + (q^y_{Pse} + q^y_{Psw}) = (q^x_{Pne} + q^x_{Pse}) + (q^y_{Pne} + q^y_{Pnw})$$

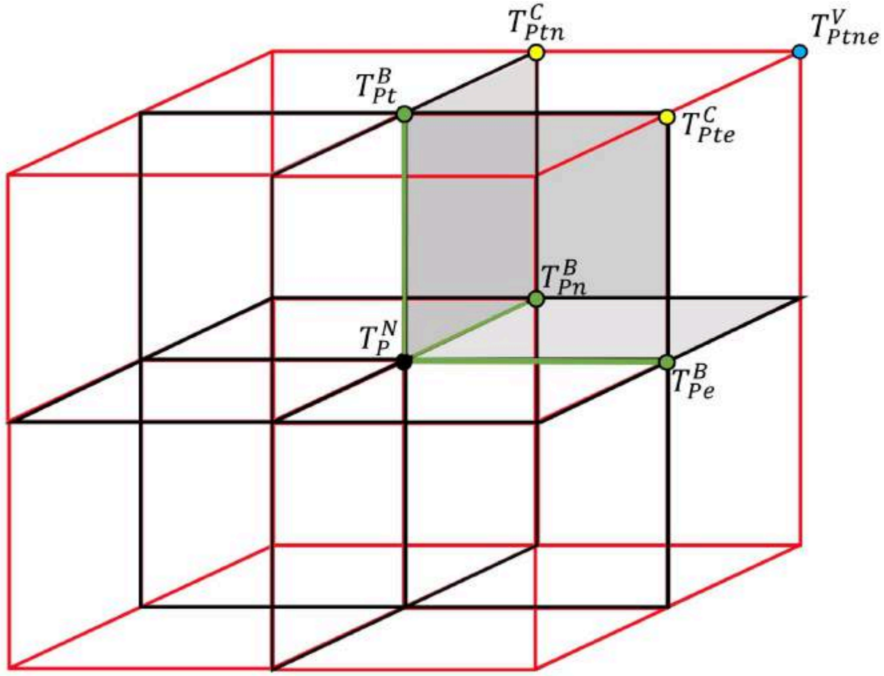


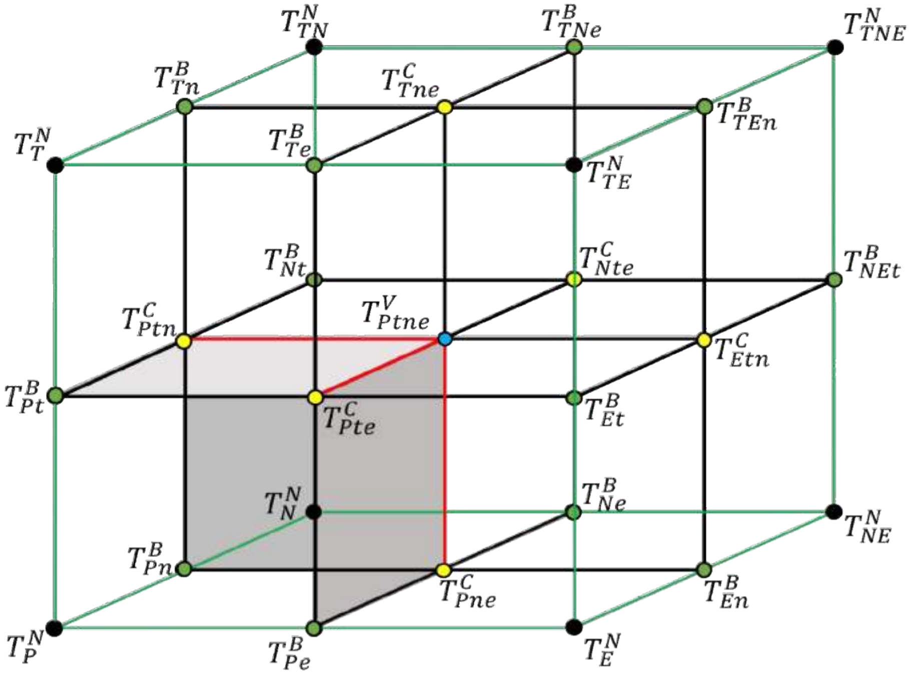
Flux in = Flux out

Multi-Point Flux Approximation (MPFA)

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







Auxiliary Temperatures Elimination

$$\boxed{q^x_{Pne}} = k^{xx}_P \overbrace{\frac{T^B_{Pe} - T^N_P}{h/2}} + k^{xy}_P \overbrace{\frac{T^B_{Pn} - T^N_P}{h/2}}$$

$$\boxed{q^x_{Pne}} = q^x_{Enw}$$
$$q^x_{Nse} = q^x_{NEsw}$$
$$q^y_{Pne} = q^y_{Nse}$$
$$q^y_{Enw} = q^y_{NEsw}$$

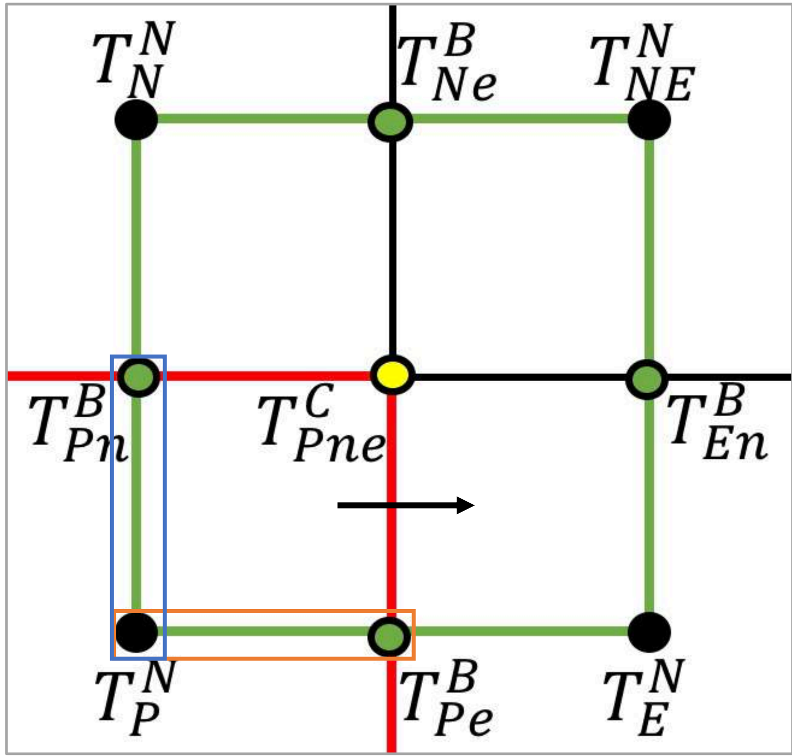
$$\boldsymbol{T}^N = \left[T^N_P, T^N_E, T^N_N, T^N_{NE}\right]^T \qquad \boldsymbol{T}^B = \left[T^B_{Pe}, T^B_{Ne}, T^B_{Pn}, T^B_{En}\right]^T$$

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

$$\boldsymbol{C}\,\boldsymbol{T}^B = \boldsymbol{D}\,\boldsymbol{T}^N \quad \rightarrow \quad \boldsymbol{T}^B = \boldsymbol{C}^{-1}\boldsymbol{D}\,\boldsymbol{T}^N$$

$$\boldsymbol{q} = \boldsymbol{E}\,\boldsymbol{T}^N \qquad \text{where} \qquad \boldsymbol{E} = \boldsymbol{B} + \boldsymbol{A}\boldsymbol{C}^{-1}\boldsymbol{D}$$

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



MPFA Improvements

Multi-Point Flux Approximation (**MPFA**)

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

Ivar Aavatsmark, *Center for International Forum on Reservoir Simulation*, 2007

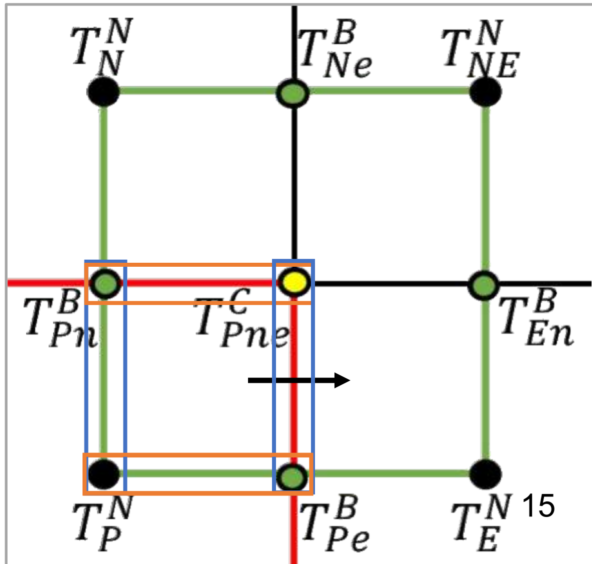
Simplified Enhanced Multi-Point Flux Approximation (**eMPFA**)

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

Wenjuan Zhang, *Computational Geoscience*, 2017

Refined Simplified Enhanced Multi-Point Flux Approximation (**ReMPFA**)

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

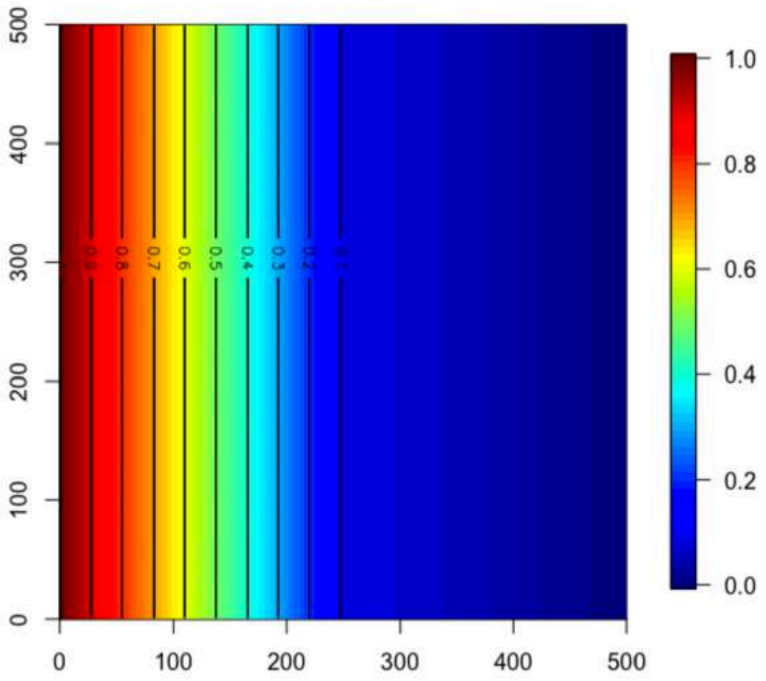


RESULTS & VERIFICATION

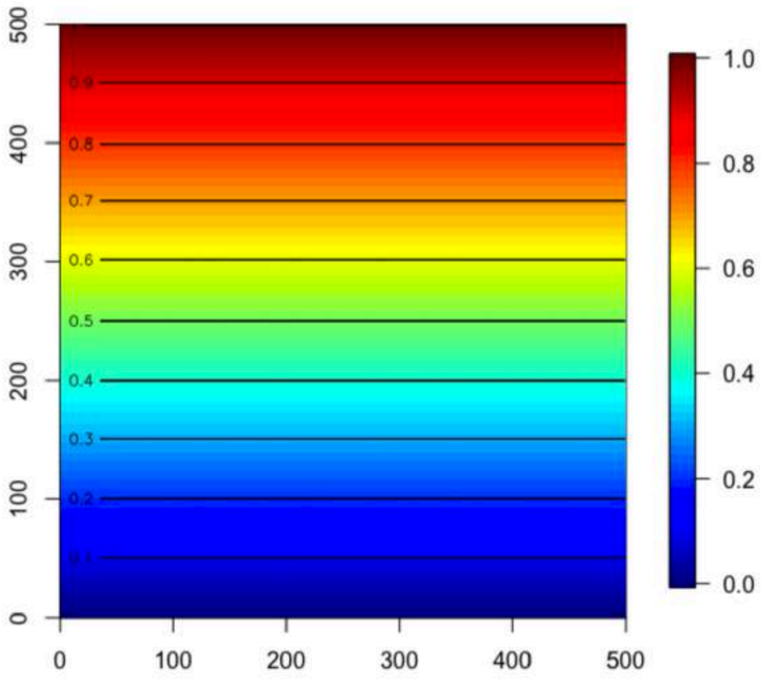
Test Case 1

$$\boldsymbol{k} = \begin{cases} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, & 0 < x \leq X/2 \\ \begin{bmatrix} 10 & 0 \\ 0 & 10 \end{bmatrix}, & X/2 < x < X \end{cases}$$

$$\xrightarrow{\text{CGLS}} \quad \boldsymbol{k} = \begin{bmatrix} 1.\overline{81} & 0 \\ 0 & 5.5 \end{bmatrix}$$

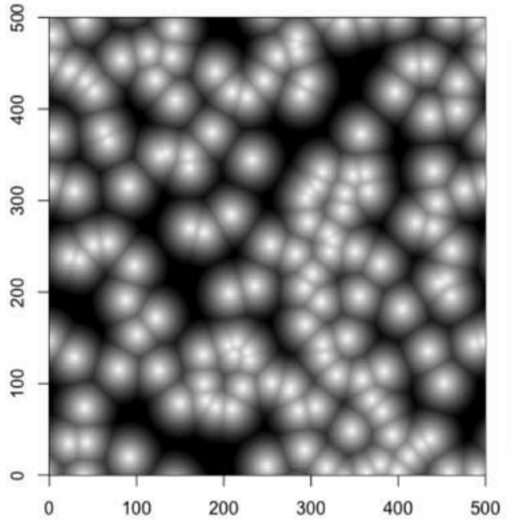


(a) x temperature gradient

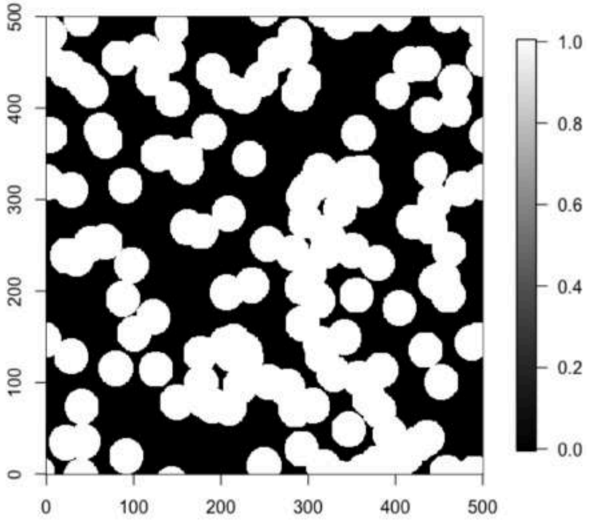


(b) y temperature gradient

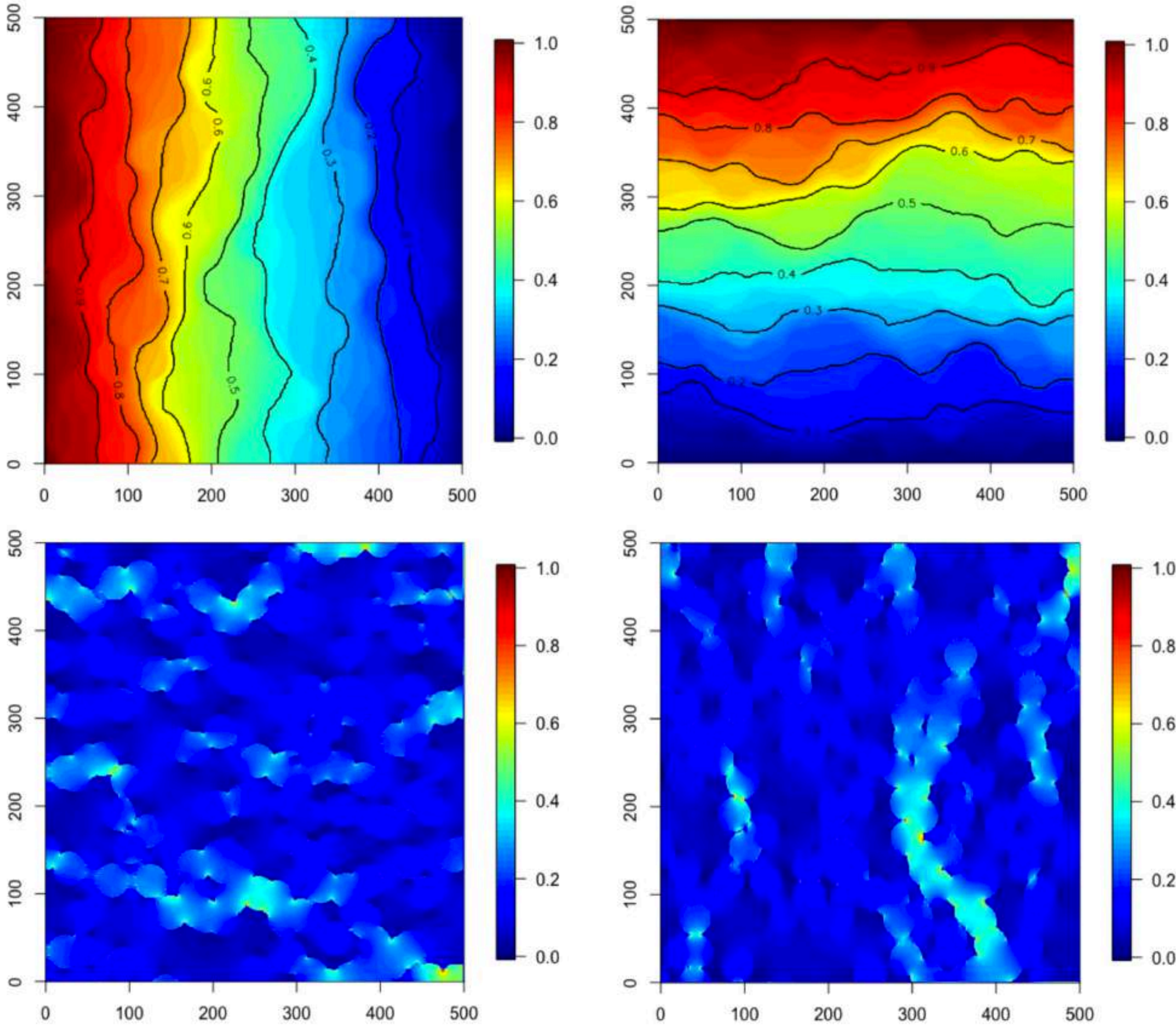
Test Case 2



(a) Gray-scale values



(b) Segmentation by thresholding

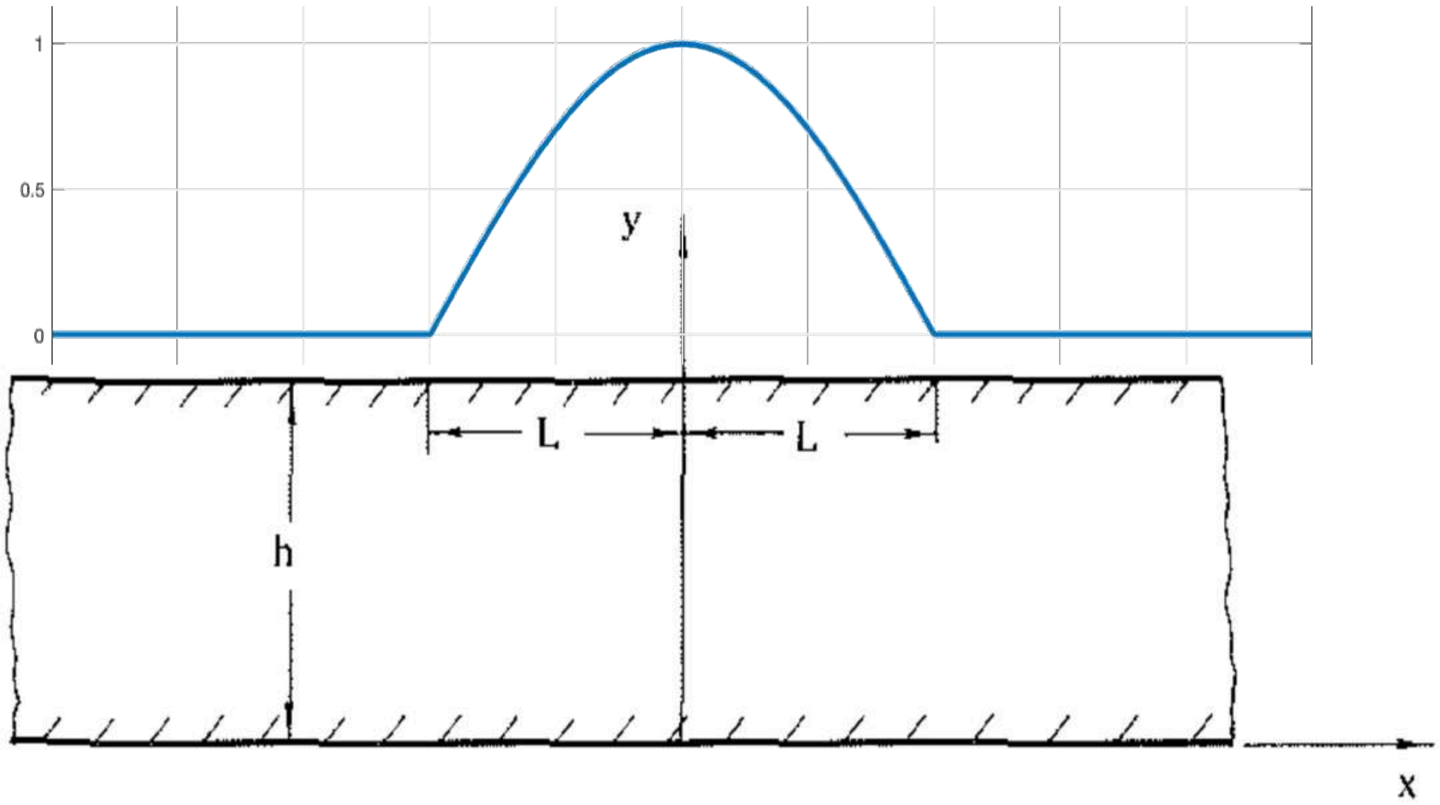


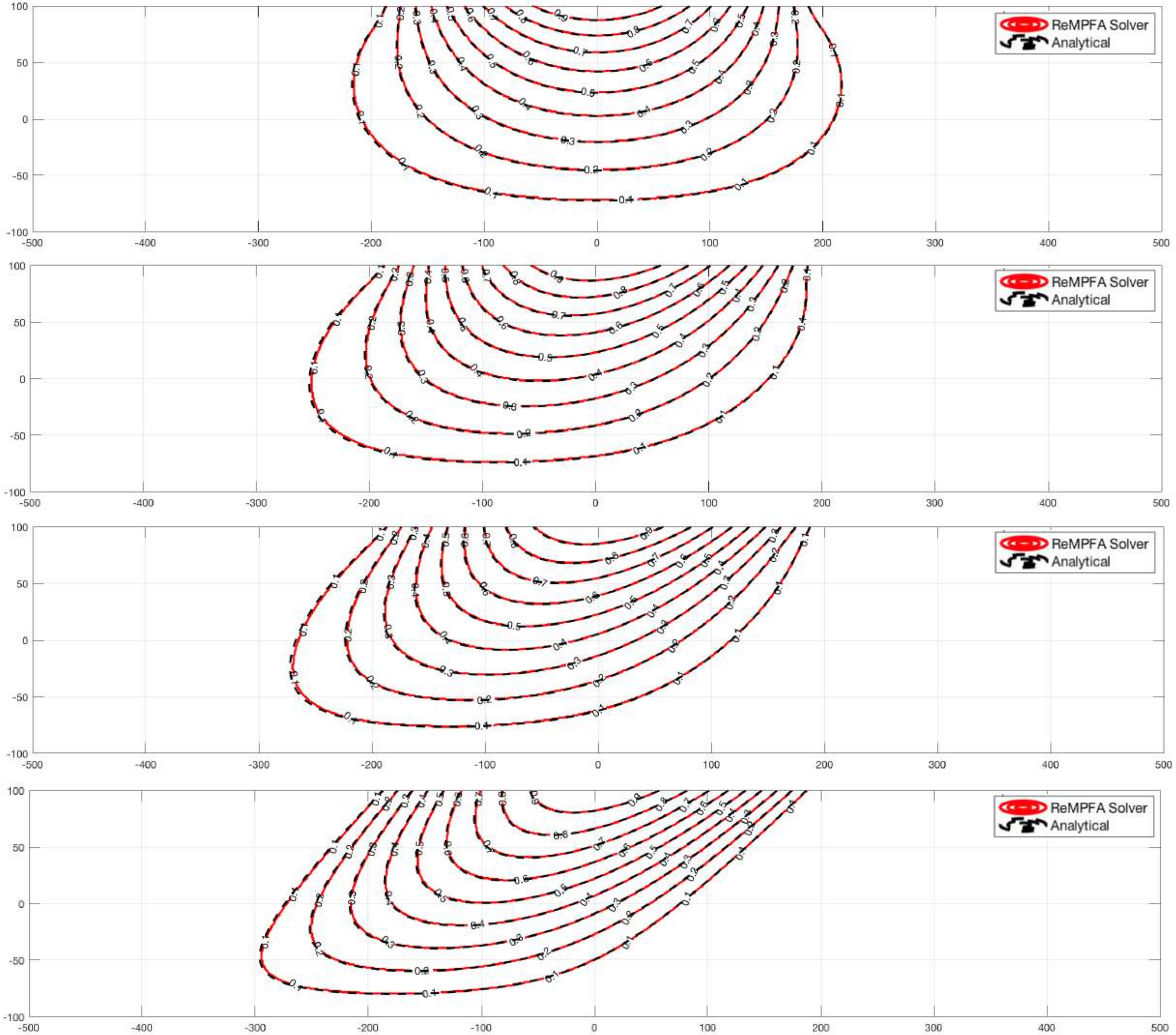
Test Case 3

$$\boldsymbol{k}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \boldsymbol{k}_2 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix} \quad \boldsymbol{k}_3 = \begin{bmatrix} 1 & 0.75 \\ 0.75 & 1 \end{bmatrix} \quad \boldsymbol{k}_4 = \begin{bmatrix} 1 & 0.99 \\ 0.99 & 1 \end{bmatrix}$$

Zhang Xiangzhou. Steady-state temperatures in an anisotropic strip. *Journal of heat transfer*

$$\boldsymbol{T} = \begin{cases} 0, & x < -L \\ \cos(cx), & -L \leq x \leq L \\ 0, & x > L \end{cases} \quad \text{where} \quad c = \frac{\pi x}{2h}$$

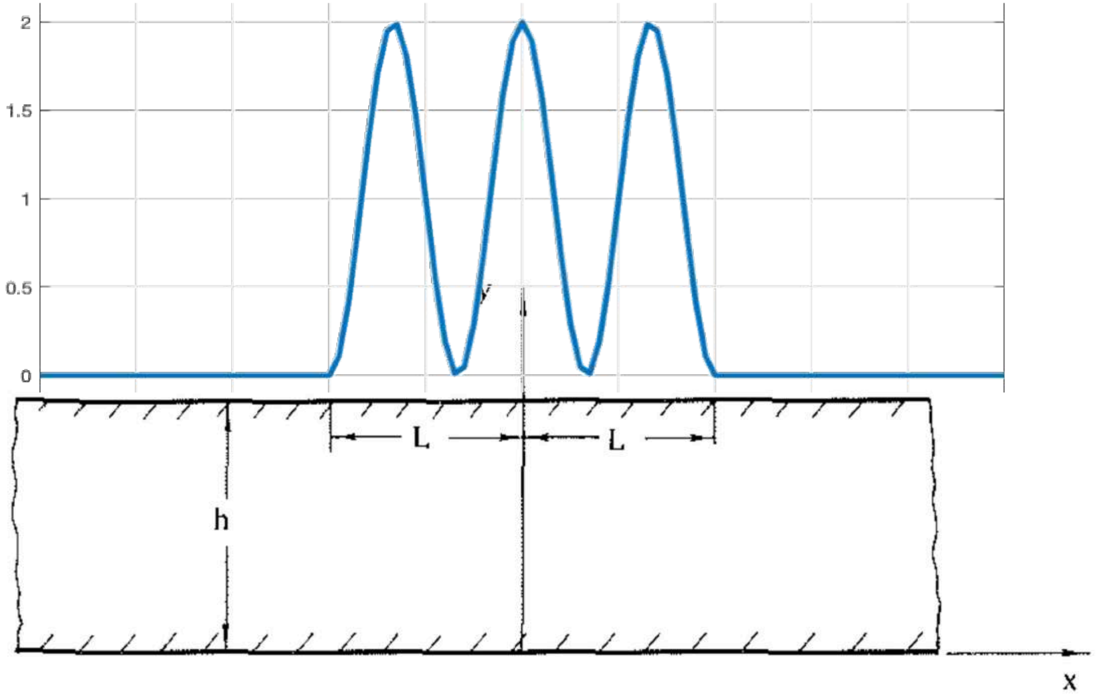


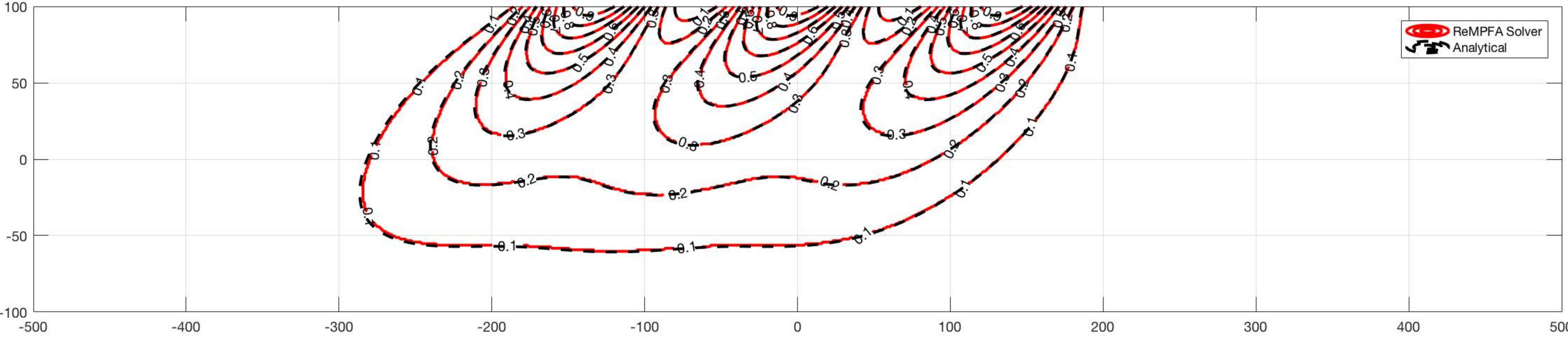

ReMPFA Solver
Analytical
100
50
0
-50
-100
-500
-400
-300
-200
-100
0
100
200
300
400
500

Test Case 4

$$\boldsymbol{T} = \begin{cases} 0, & x < -L \\ \cos(6cx) + 1, & -L \le x \le L \\ 0, & x > L \end{cases}$$

$$\boldsymbol{k} = \begin{bmatrix} 1 & 0.75 \\ 0.75 & 1 \end{bmatrix}$$





CONCLUSION & FUTURE WORK

Next Steps

- 3D implementation
- Fiber tracking (ML, ray casting, flux vector…)
- Multigrid methods to accelerate convergence
- Validation on experimental data

Thank you