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Geometry modeling of open-cell foams for efficient fluid flow and heat transfer computations using modified Kelvin cells

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Outline

(1) Introduction
CFD modeling of heat transfer and fluid flow in open-cell foams

(2) Geometry modeling
Analysis of the reference foam
Generation of modified Kelvin cells

(3) Determination of effective properties
Finite volume method for effective thermal conductivity
Lattice-Boltzmann method for permeability

(4) Results
Representative volume element (RVE)
Effective thermal conductivity
Permeability

(5) Conclusions & outlook

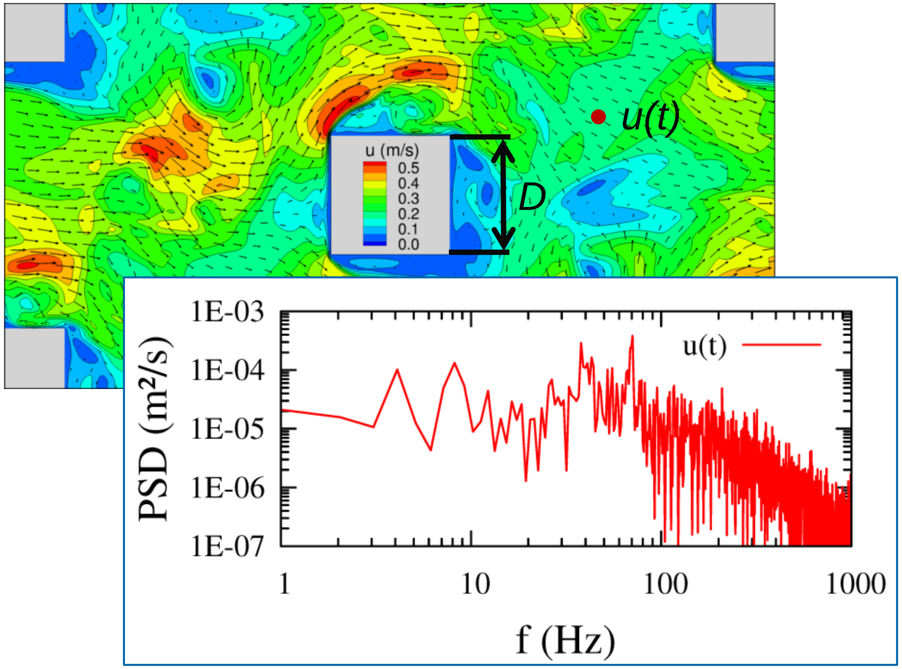
CFD modeling of open-cell foams

Two major classes of approaches

1. macroscopic modeling: volume-averaged equations using eff. properties
2. microscopic modeling: taking into account the intricate geometry
   → computationally expensive for the entire physical domain

Alternative method

- approximation of geometry using idealized structure with same geometric properties, e.g. array of cylinders, Weaire-Phelan structures, Kelvin cells, ...
- periodicity reduces the size of the computational domain
- allows extended parametric studies or complete resolution of small-scale structures



DNS inside idealized porous medium (Re_D = 400) [Werzner et al., 2013]

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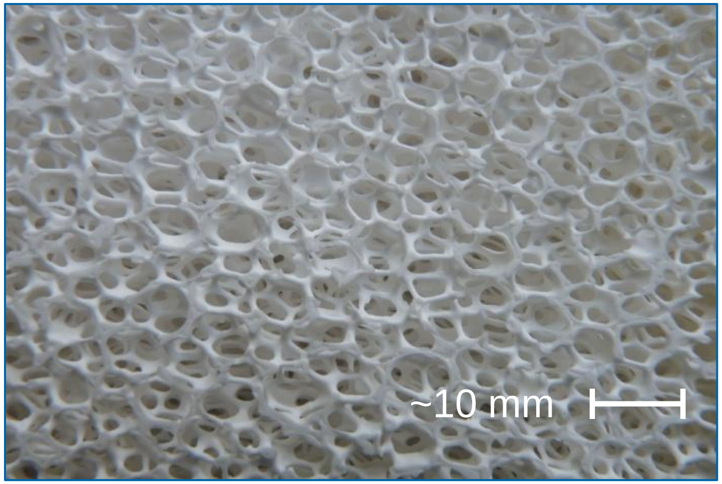
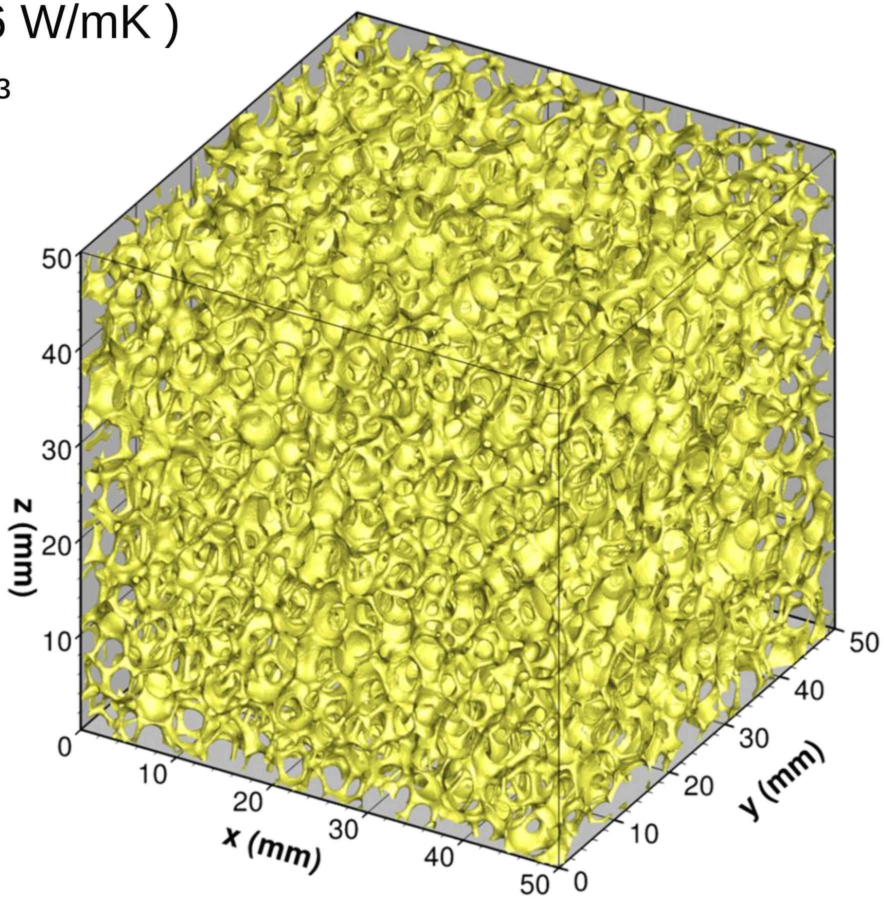
Reference foam

- manufactured using the replica technique on the basis of a polyurethane sponge [Schwartzwalder and Somers, 1963]
- material: Al_2O_3 (k = 18.66 W/mK)
- dimensions: 121 x 121 x 58 mm³
- pore density: 10 ppi
- voxel representation available from 3D computed-tomography scan (resolution Δx =70 µm)



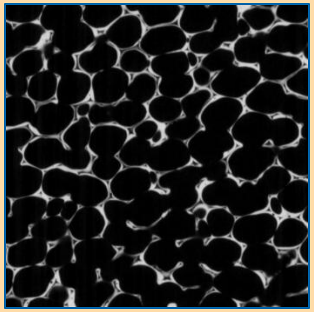
photograph



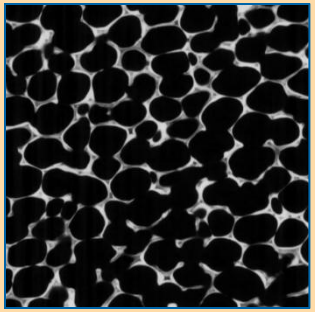
selection considered for the simulations ($718^3 \approx$ 370 million voxels)

Morphology of the reference foam

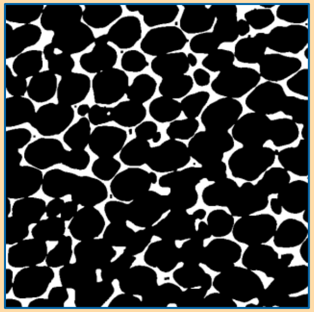
CT geometry analysis using 3D image analysis software MAVI



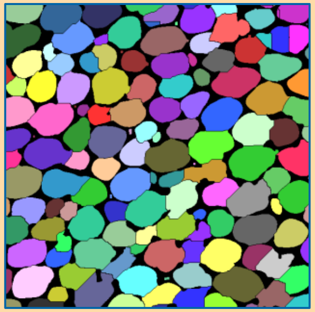
1. raw data



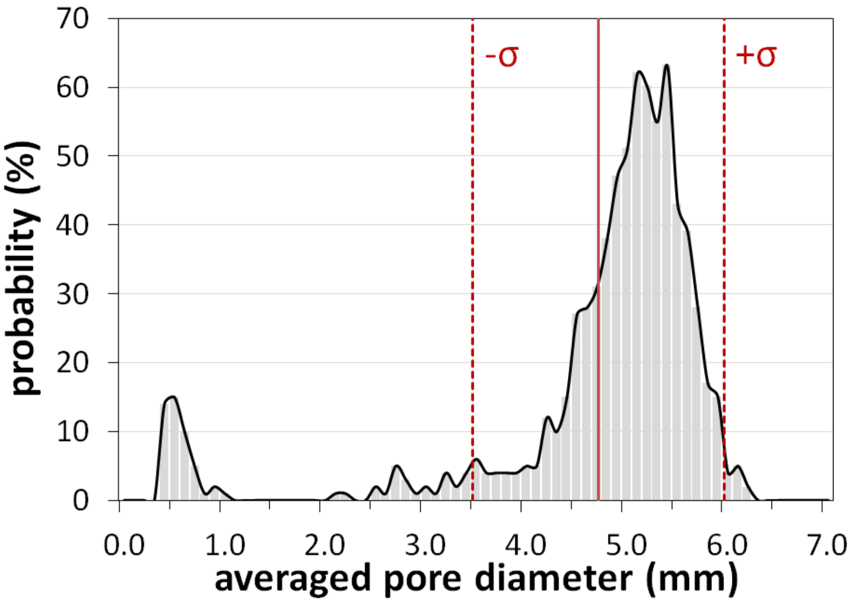
2. closure



3. binarization



4. watershed transformation



Results

- porosity: 85.56 %*
- number of pores: 11,693
- pore diameter: 4.77* ± 1.13 mm
- facets per pore: 15.08 ± 2.07
- av. strut width: 6.80 mm

(parameters used for generation of Kelvin cells)*

[Rößger and Jorschick, 2014]

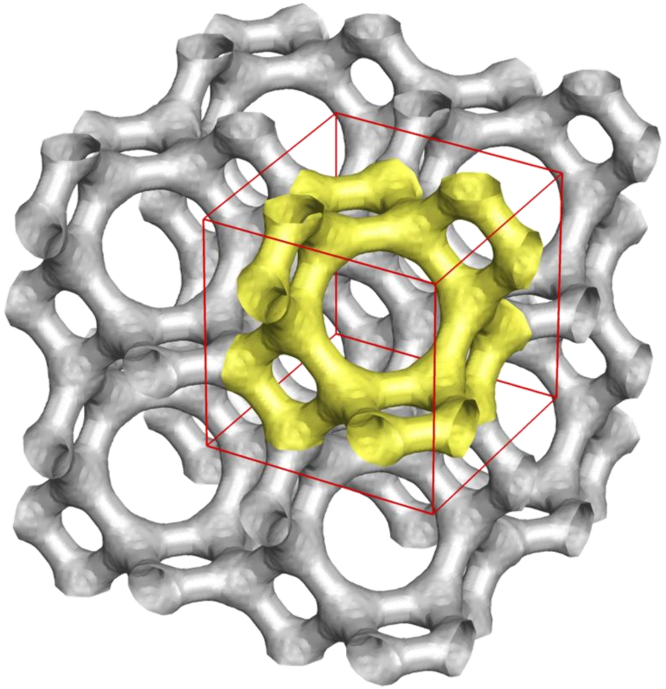
Generation of modified Kelvin cells

The Kelvin cell [Thomson, 1887]

- polyhedron consisting of 14 faces: 8 hexagons and 6 squares
- space-filling unit-cell with lowest surface area
- resembles the polyhedra encountered in reticulate foams

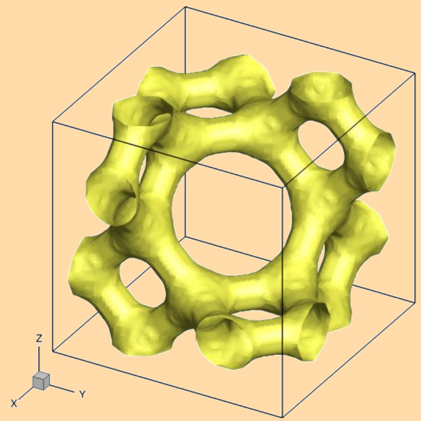
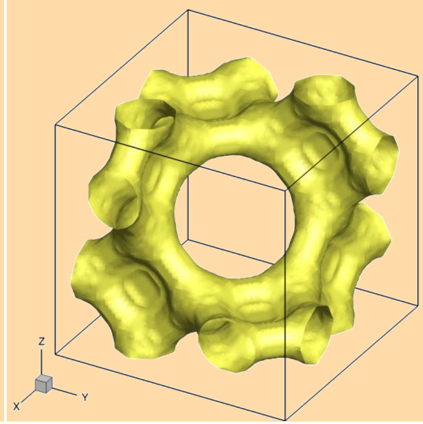
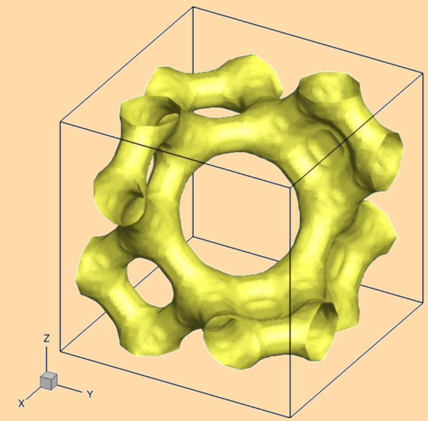
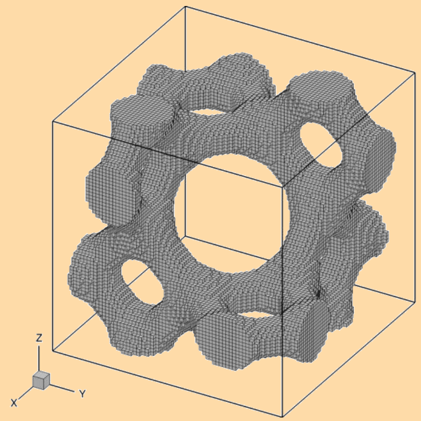
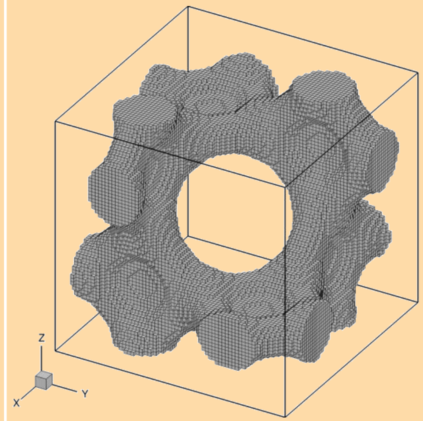
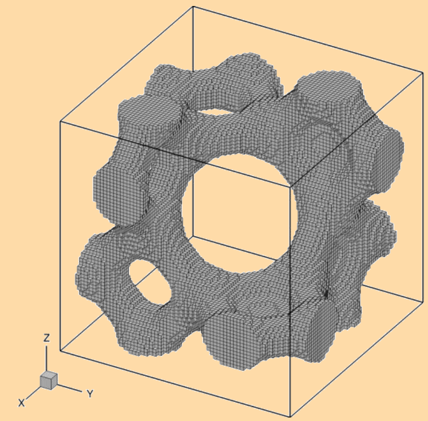
Model generation

- three types are considered:
  - open square windows (o)
  - closed square windows (c)
  - half-closed square windows (hc)
- ligaments and closed faces are modeled by cylinders using implicit functions
- connections are rounded using the Blinn transformation [Storm et al., 2013]



homogenous lattice of Kelvin cells and periodic unit cell

Overview of considered Kelvin cells

nr. of closed windows	0 [o]	6 [c]	3 [hc]
pore diameter		4.77 mm	
porosity	85.98 %	85.05 %	85.51 %
iso-surface representation			
voxel mesh used for the simulations (69 x 69 x 69)			

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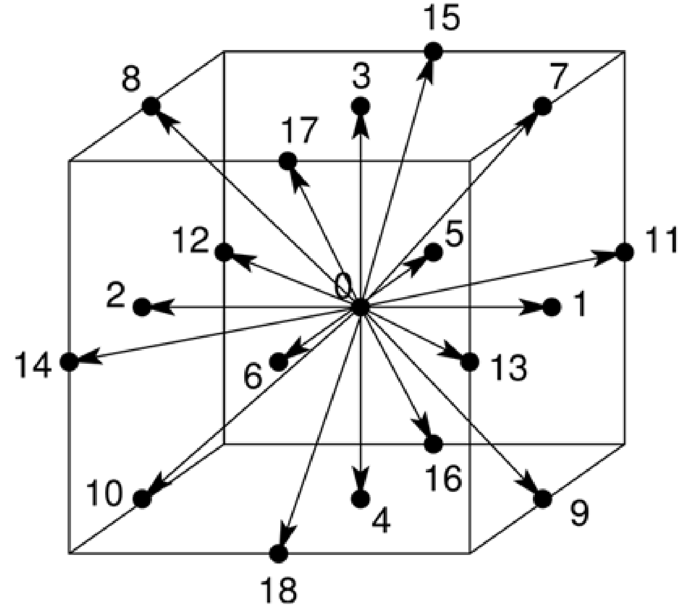
Modeling of fluid flow

Lattice-Boltzmann method (LBM)

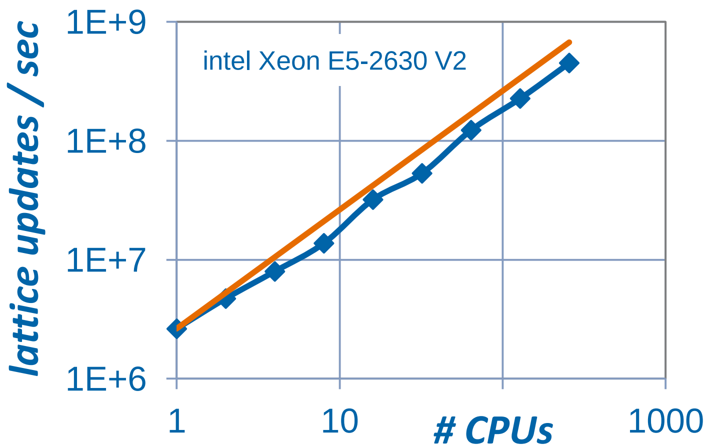
- LBM is used to obtain solutions of the mass and momentum conservation equations
- physical domain is discretized into a uniform voxel mesh
- fluid flow is treated as movement of particle populations, which undergo consecutive streaming and collision processes over a discrete lattice
- macroscopic properties are obtained as moments of particle distributions

Boundary conditions

- periodicity on all domain boundaries
- no-slip on all solid voxels



possible velocities in D3Q19 phase space around a single lattice node



Scaling of LBM code

Evaluation of permeability tensor and extreme values

Determination of permeability tensor

- evaluated at Darcy flow condition: $\mathrm{Re}_k = u_D \sqrt{\kappa} / \nu \leq 1 \ (\approx 0.2)$
- Darcy's law: $$\begin{pmatrix} \kappa_{xx} & \kappa_{xy} & \kappa_{xz} \\ \kappa_{yx} & \kappa_{yy} & \kappa_{yz} \\ \kappa_{zx} & \kappa_{zy} & \kappa_{zz} \end{pmatrix} \cdot \begin{pmatrix} \partial p / \partial x \\ \partial p / \partial y \\ \partial p / \partial z \end{pmatrix} = -\mu \begin{pmatrix} \bar{u}_x \\ \bar{u}_y \\ \bar{u}_z \end{pmatrix}$$

Eigenvalues and eigenvectors

- eigenvalues are defined by a homogenous linear system:

$$\left(\mathrm{K} - \lambda\, \mathrm{I}\right) \cdot \vec{v} = 0$$

- solution consists of three eigenvalues λ and corresponding eigenvectors v, which form an orthogonal system
- min., max. and average permeability are obtained as:

$$\kappa_{\min} = \min(\lambda) \qquad \kappa_{\max} = \max(\lambda) \qquad \kappa_{avg} = \frac{1}{3} \sum \lambda$$

Modeling of heat transfer and determination of ETC

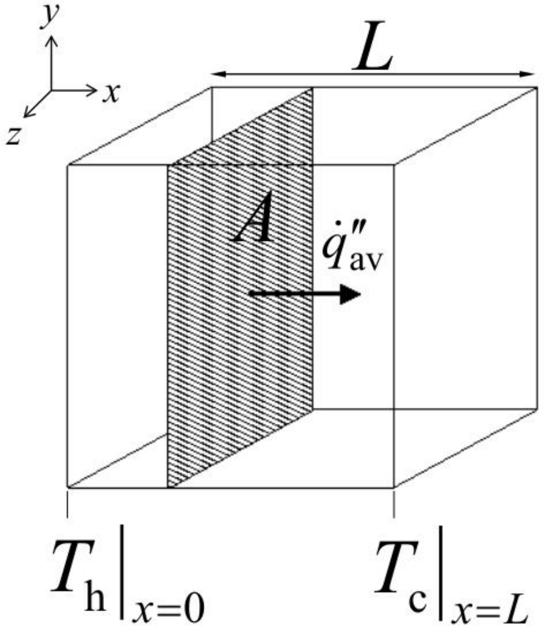
Governing equation

- steady-state heat conduction equation for heterogeneous materials, without heat source:

$$\nabla \cdot (k \nabla T) = 0$$

Boundary conditions

- different temperatures on two opposite walls
- remaining walls adiabatic



Determination of effective thermal conductivity

- after convergence of the temperature field, the average steady-state heat flux is evaluated over a plane of the computational domain :
- ETC is obtained using averaged Fourier's law of heat conduction:

$$\dot{q}''_{av} = \frac{\int \dot{q}'' \mathrm{d}A}{\int \mathrm{d}A}$$

$$\dot{q}''_{av} = k_{eff} \frac{T_h - T_c}{L}$$

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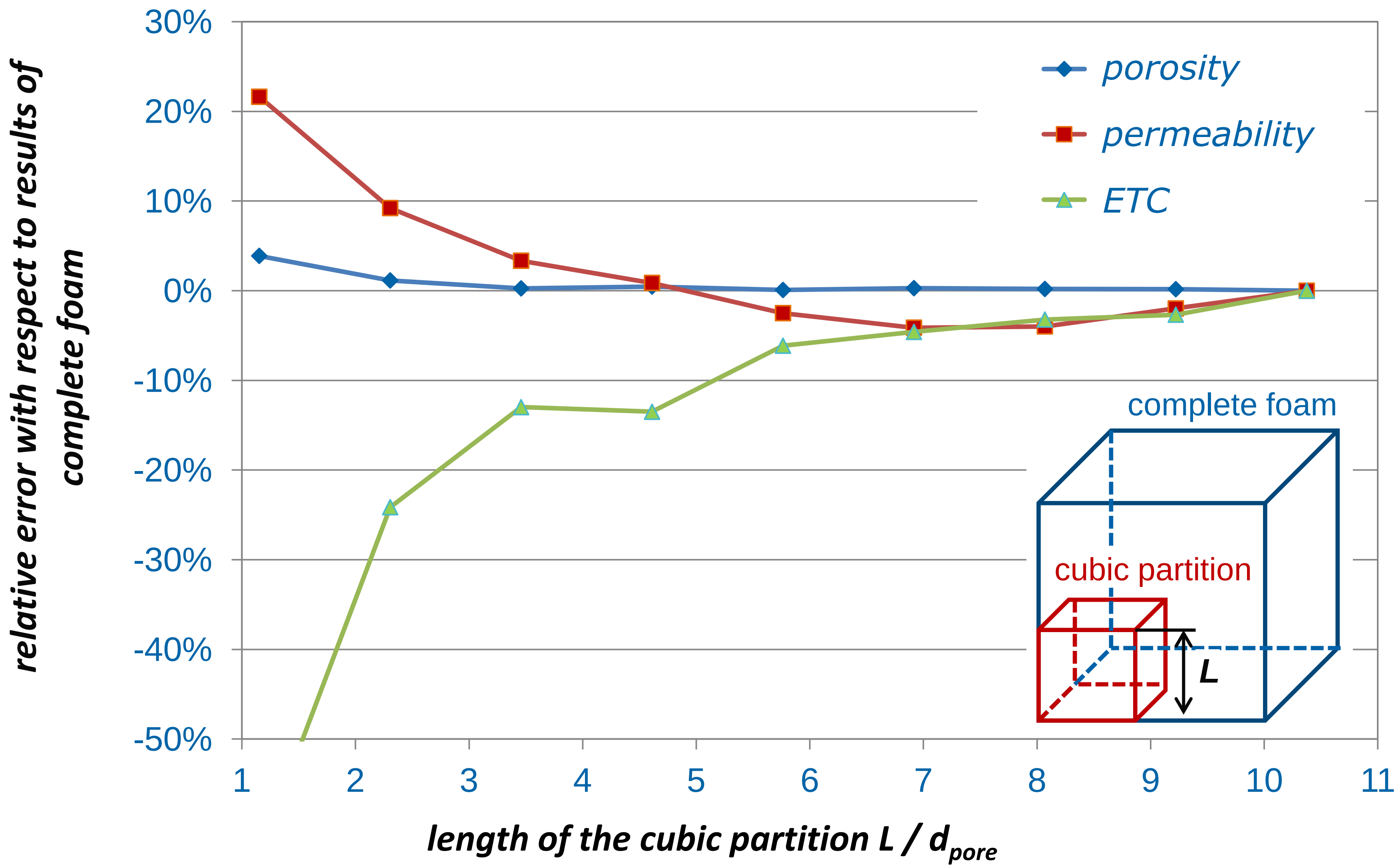
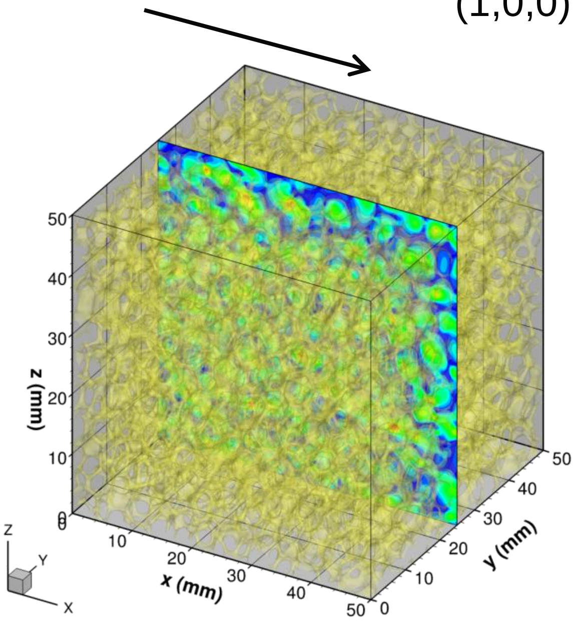
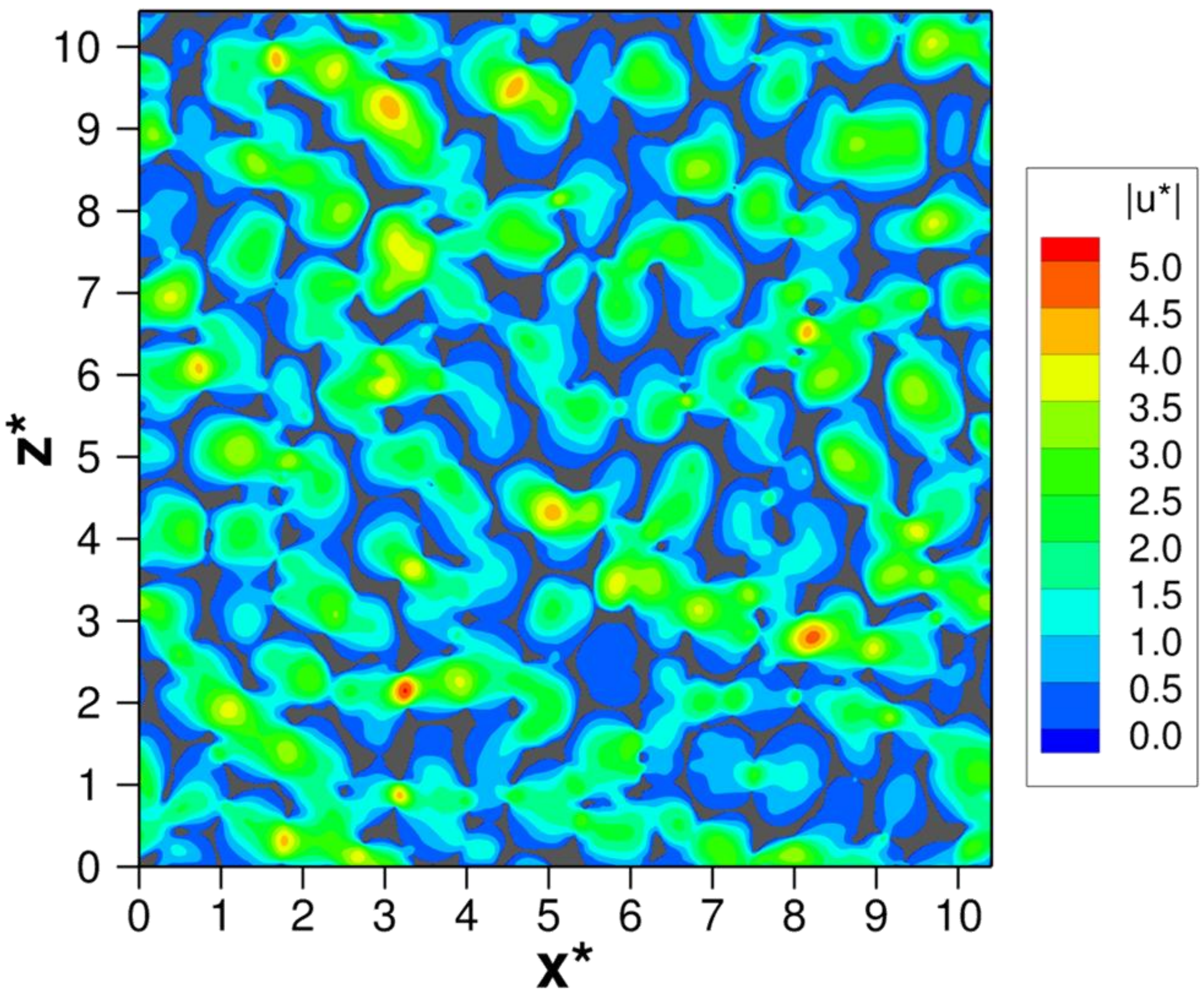
Results: representative volume element (RVE)



foam sample – velocity magnitude (1,0,0)

direction of pressure gradient (1,0,0)

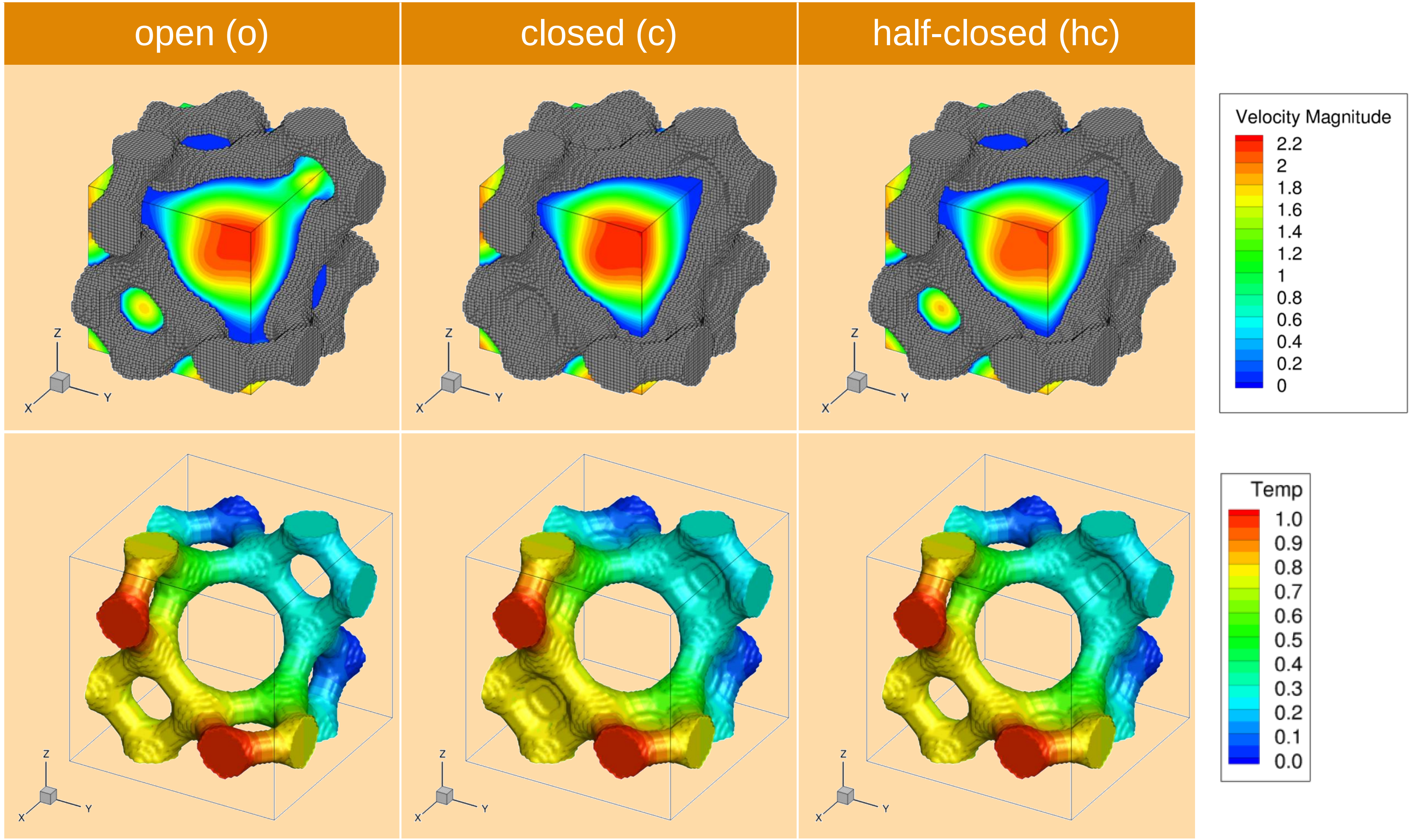




- inhomogenous distribution of velocity magnitude
- preferential paths with high velocities

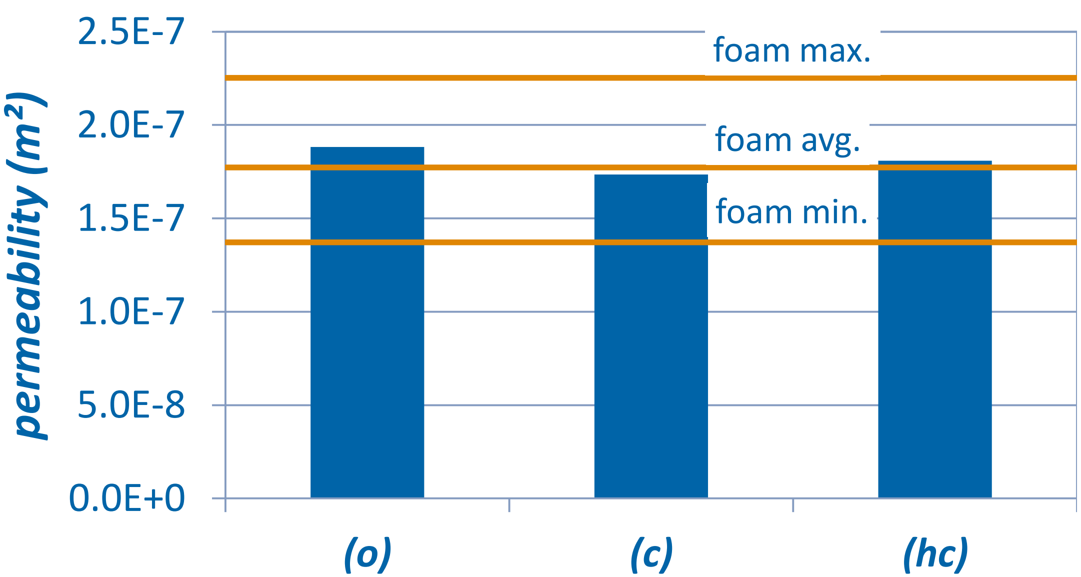
contour plot of velocity magnitude at a plane y = 25 mm

Kelvin cells – velocity magnitude and temperature (1,0,0)



Comparison for permeability

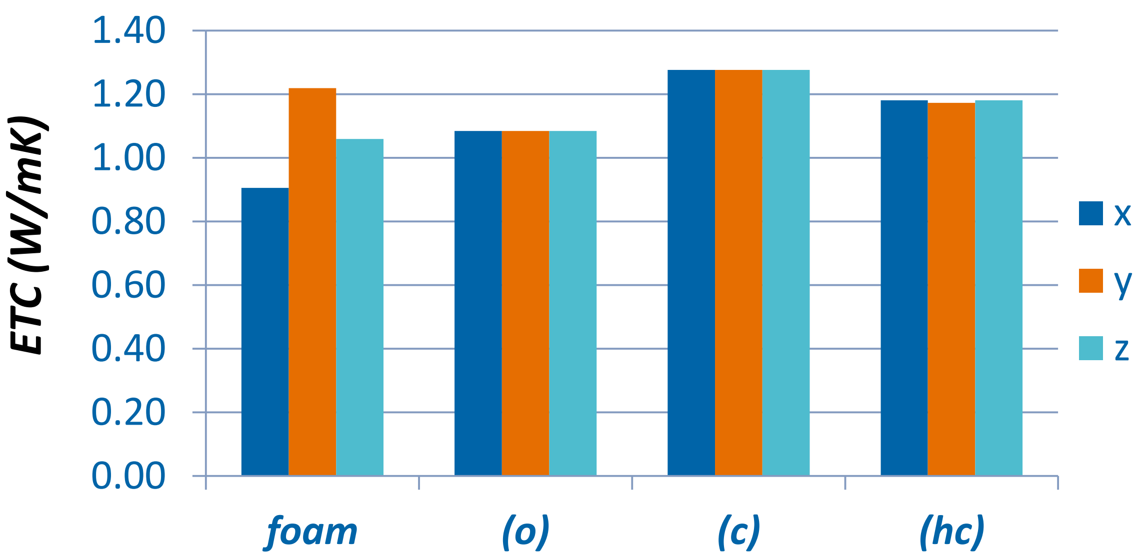
structure		permeability (10^{-7} m²)			
		minimum	maximum	average	av. error
foam sample		1,37	2,25	1,77	-
Kelvin cell	open (o)	1,88			+6 %
	closed (c)	1,73			+2 %
	half-closed (hc)	1,81			-2 %



- foam exhibits anisotropy (Kelvin cells are isotropic)
- Kelvin cells with half-closed and closed windows give good prediction of average permeability
- effect of closed square windows is small

Comparison for effective thermal conductivity

structure		effective thermal conductivity (W/mK)				
		x	y	z	average	av. error
foam sample		0.91	1.22	1.06	1.06	-
Kelvin cell	open (o)	1.08			1.08	+2.2 %
	closed (c)	1.28			1.28	+20.3 %
	half-closed (hc)	1.18	1.17	1.18	1.18	+11.0 %



- anisotropy of permeability and ETC correlate
- Kelvin cell with open windows gives best prediction of average ETC
- position of closed windows causes slight anisotropy for the half-closed Kelvin cells

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Conclusions

- accurate prediction of permeability and eff. thermal conductivity of open-cell foams require large computational domain: RVE ≈ $(10\ D_P)^3$
- optimal model structure depends on the property of interest:
  - eff. thermal conductivity: Kelvin cell with open windows (+2 %)
  - permeability: Kelvin cell w. half-closed windows (-2 %)
- idealized foam structures can reduce the computational effort by $O(10^3)$ or allow high-res simulations, e.g. for the DNS of turbulent flows

Outlook

- inclusion of additional geometric parameters to consider anisotropy:
  - anisotropy of pores by elongated Kelvin cells
  - statistics on number and orientation of closed windows
- DNS of higher *Re* flows: inertial coefficient and turbulence spectra
- applicability of turbulence models for turbulence inside porous media

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