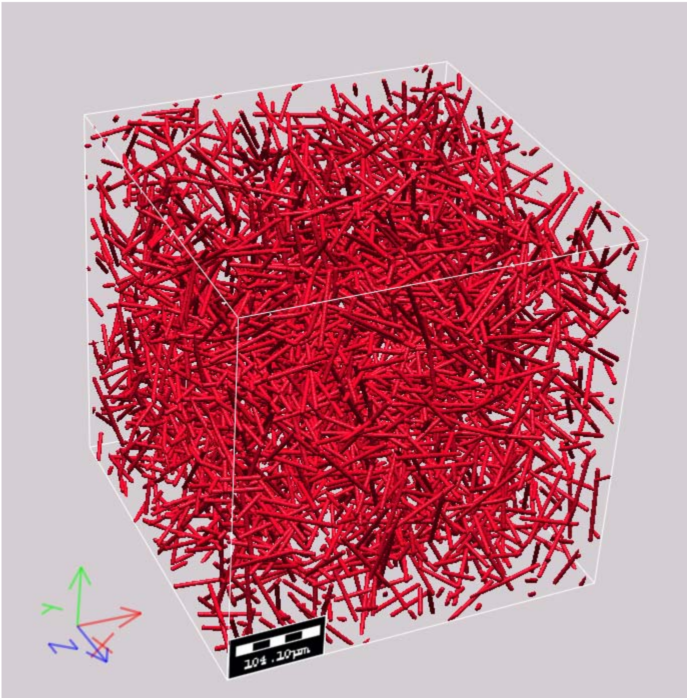
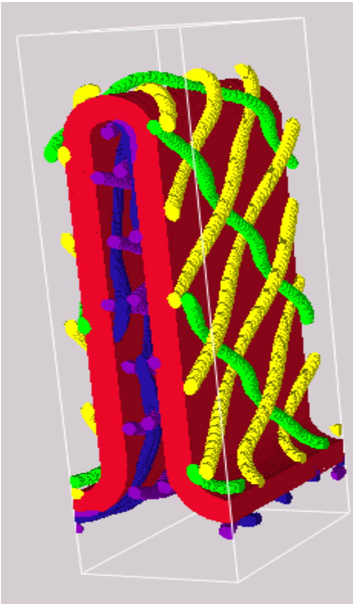
Microstructure Simulation and Virtual Material Design



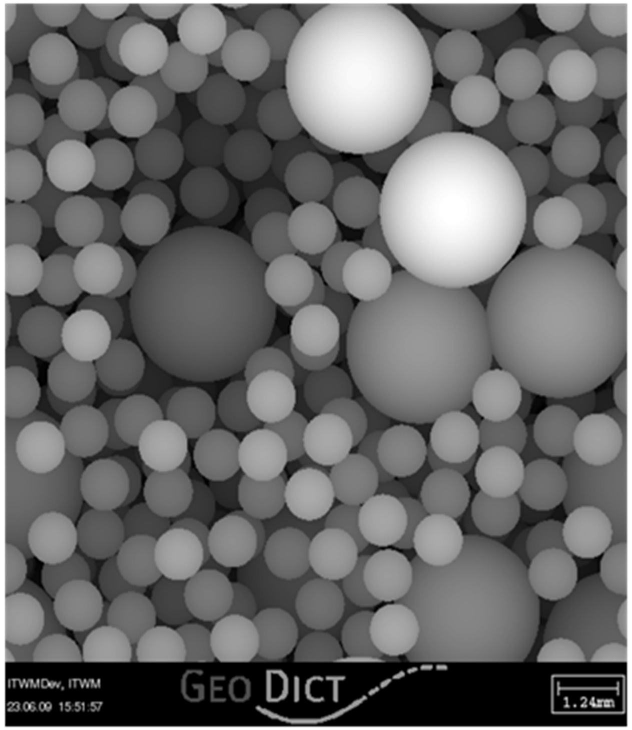
Andreas Wiegmann

Fraunhofer ITWM

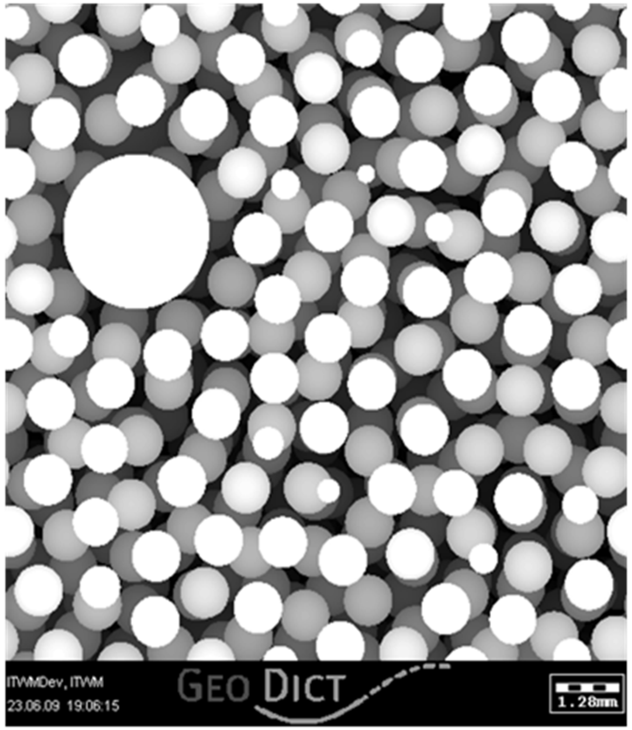


1. Microscopic geometry governs macroscopic properties
    - Permeability depends on the pores in fibrous media
    - Conductivity depends on connectivity of the fibers
2. Some times, only 3d models will do
    - Flow through densely packed spheres or circles
    - Supporting mesh in a filter pleat
3. Materials are random
    - Under microscope , details at different locations are different
    - Multiple experiments yield mean value and standard deviation
    - Capture this in geometric models and property predictions
4. Computations must be fast and completely automatic
    - Materials are “cheap” and no CAD data exist
    - For material design, many simulation runs may be necessary

Packed bed of spheres and floating spheres



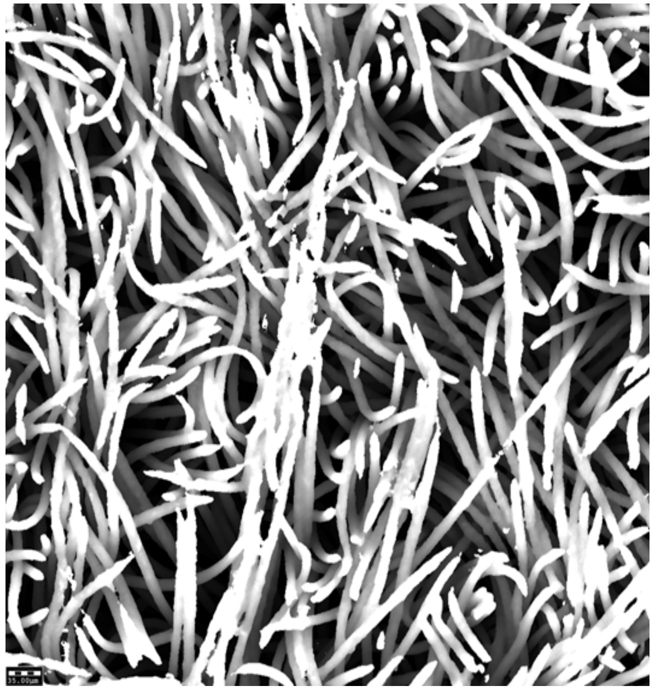
svf 0.64



svf 0.30

Option a): import 3d image of existing media

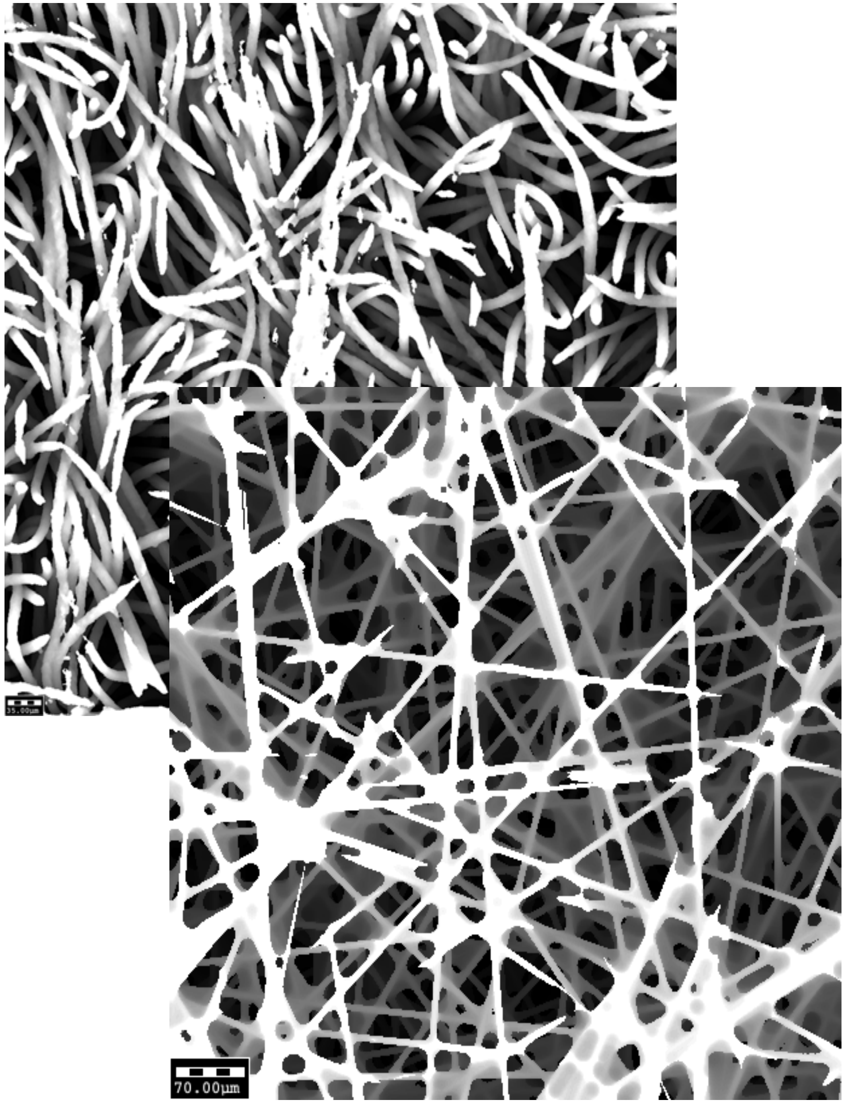
- Input: 3d gray-valued image obtained by DVI, tomography or similar 3d imaging method
- Options:
  - choice of threshold
  - filtering
  - edge smoothing

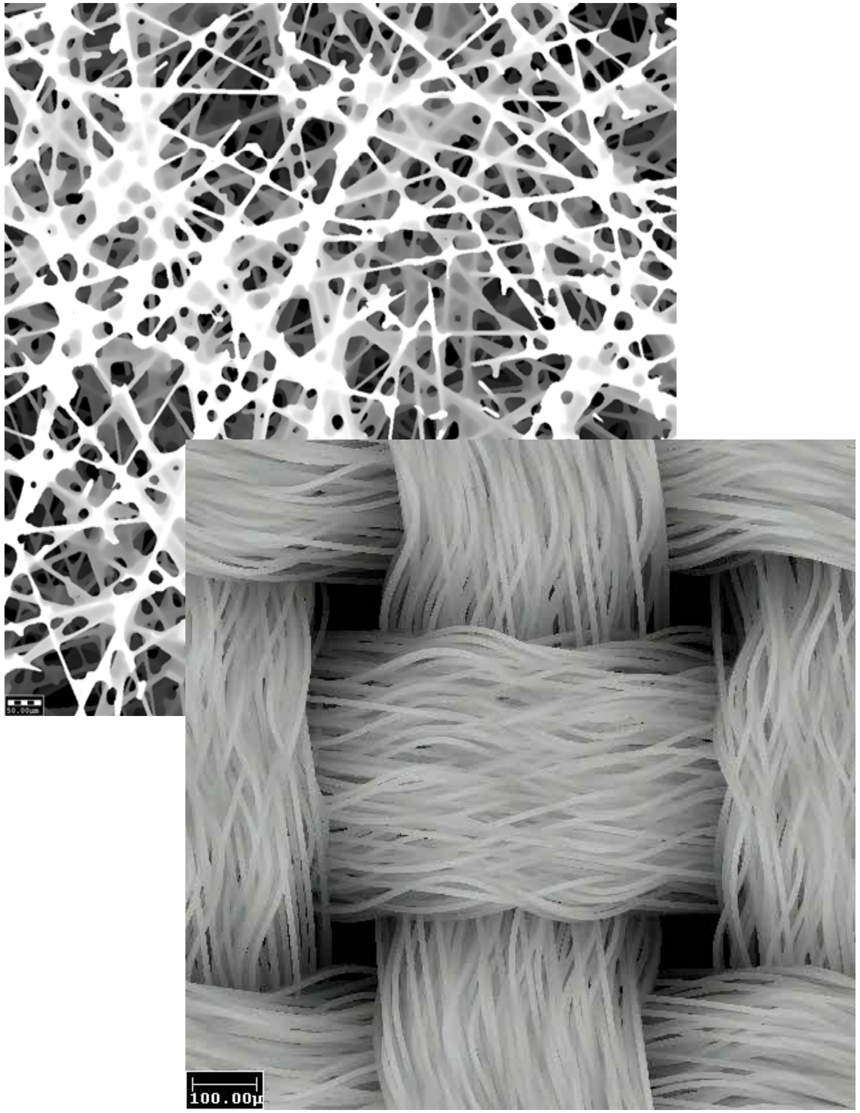


Typical voxel length: 1µm

Current µCT images: up to 3mm x 3mm x 3mm voxels, *a 128 GB drive*

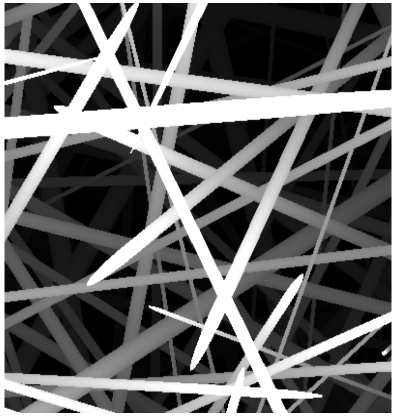
Virtual Textile Generation

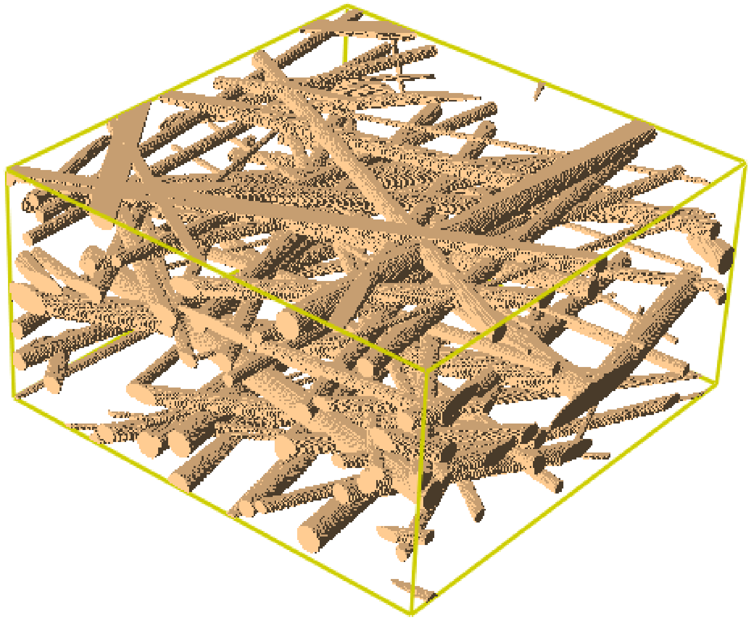




Option b): Virtually Generated Nonwoven: Input Parameters

- Porosity
- Fiber orientation distribution (anisotropy)
- Fiber diameter (distribution)
- Fiber cross sectional shape
- Fiber length (distribution)



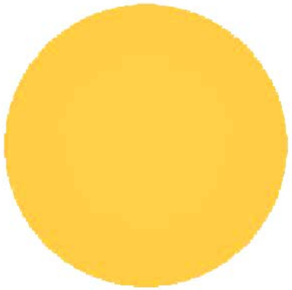


In the "overlapping" model, fibers are placed at random positions with appropriately randomized orientation and without consideration of each other

It is a surprise that such a simple model works!

Fiber anisotropy:

orientation parameter β



$\beta_1 = \beta_2 = 1$

$\beta_1 = \beta_2 > 1$

$$
\begin{aligned}
\xi &\in [-1, 1]\,, \text{ uniformly distributed,}\\
\Phi &\in [0, 2\pi)\,, \text{ uniformly distributed,}\\
u &= \frac{\beta_1 \cos\Phi \sqrt{1-\xi^2}}{\sqrt{\xi^2 + (1-\xi^2)\left\{\beta_1^2 \cos\Phi + \beta_2^2 \sin\Phi\right\}}},\\
v &= \frac{\beta_2 \sin\Phi \sqrt{1-\xi^2}}{\sqrt{\xi^2 + (1-\xi^2)\left\{\beta_1^2 \cos\Phi + \beta_2^2 \sin\Phi\right\}}},\\
w &= \frac{\xi}{\sqrt{\xi^2 + (1-\xi^2)\left\{\beta_1^2 \cos\Phi + \beta_2^2 \sin\Phi\right\}}}.
\end{aligned}
$$

Uniform distribution of directions gets mapped to non-uniform one by picking point with uniform ξ and ϕ on $(\beta_1, \beta_2, 1)$ ellipsoid and pulling it back to the unit sphere.

K. Schladitz, S. Peters, D. Reinel-Bitzer, A. Wiegmann and J. Ohser, *Design of acoustic trim based on geometric modelling and flow simulation for non-woven*, Computational Materials Science, Volume 38, Issue 1, 2006, pp 56-66.

Solving the Poisson equation on a 3d image

$$\mathrm{div}\,(\beta(\vec{x})\nabla\bar{U}_3) = \mathrm{div}\,(\beta(\vec{x}))\cdot\nabla\bar{U}_3 + \beta(\vec{x})\mathrm{div}\,(\nabla\bar{U}_3) = 0, \quad \vec{x} \in \Omega = (0,d_1)\times(0,d_2)\times(0,d_3),$$

with boundary conditions

$$\begin{aligned}
\bar{U}_3(x_1,x_2,0) &= \bar{U}_3(x_1,x_2,d_3) - d_3, \\
\bar{U}_3(x_1,0,x_3) &= \bar{U}_3(x_1,d_2,x_3), \\
\bar{U}_3(0,x_2,x_3) &= \bar{U}_3(d_1,x_2,x_3), \\
\beta(x_1,x_2,0)\frac{\partial\bar{U}_3(x_1,x_2,0)}{\partial x_3} &= \beta(x_1,x_2,d_3)\frac{\partial\bar{U}_3(x_1,x_2,d_3)}{\partial x_3}, \\
\beta(x_1,0,x_3)\frac{\partial\bar{U}_3(x_1,0,x_3)}{\partial x_2} &= \beta(x_1,d_2,x_3)\frac{\partial\bar{U}_3(x_1,d_2,x_3)}{\partial x_2}, \\
\beta(0,x_2,x_3)\frac{\partial\bar{U}_3(0,x_2,x_3)}{\partial x_1} &= \beta(d_1,x_2,x_3)\frac{\partial\bar{U}_3(d_1,x_2,x_3)}{\partial x_1}.
\end{aligned}$$

A. Wiegmann and A. Zemitis, *EJ-HEAT: A Fast Explicit Jump Harmonic Averaging Solver for the Effective Heat Conductivity of Composite Materials*, Bericht des Fraunhofer ITWM, Nr. 94, 2006.

Discretization by harmonic averaging

Uniform Cartesian grid (mesh width h) on box domain results in "simple" discretization of $\operatorname{div}\left(\beta(\vec{x})\nabla\bar{U}_3\right)$:

$$
\begin{aligned}
&\frac{1}{h}\Bigg(\left(\frac{\beta_{i+1,j,k}+\beta_{i,j,k}}{2\beta_{i+1,j,k}\beta_{i,j,k}}\right)^{-1}\frac{u_{i+1,j,k}-u_{i,j,k}}{h}-\left(\frac{\beta_{i,j,k}+\beta_{i-1,j,k}}{2\beta_{i,j,k}\beta_{i-1,j,k}}\right)^{-1}\frac{u_{i,j,k}-u_{i-1,j,k}}{h}\\
&+\left(\frac{\beta_{i,j+1,k}+\beta_{i,j,k}}{2\beta_{i,j+1,k}\beta_{i,j,k}}\right)^{-1}\frac{u_{i,j+1,k}-u_{i,j,k}}{h}-\left(\frac{\beta_{i,j,k}+\beta_{i,j-1,k}}{2\beta_{i,j,k}\beta_{i,j-1,k}}\right)^{-1}\frac{u_{i,j,k}-u_{i,j-1,k}}{h}\\
&+\left(\frac{\beta_{i,j,k+1}+\beta_{i,j,k}}{2\beta_{i,j,k+1}\beta_{i,j,k}}\right)^{-1}\frac{u_{i,j,k+1}-u_{i,j,k}}{h}-\left(\frac{\beta_{i,j,k}+\beta_{i,j,k-1}}{2\beta_{i,j,k}\beta_{i,j,k-1}}\right)^{-1}\frac{u_{i,j,k}-u_{i,j,k-1}}{h}\Bigg) = 0
\end{aligned}
$$

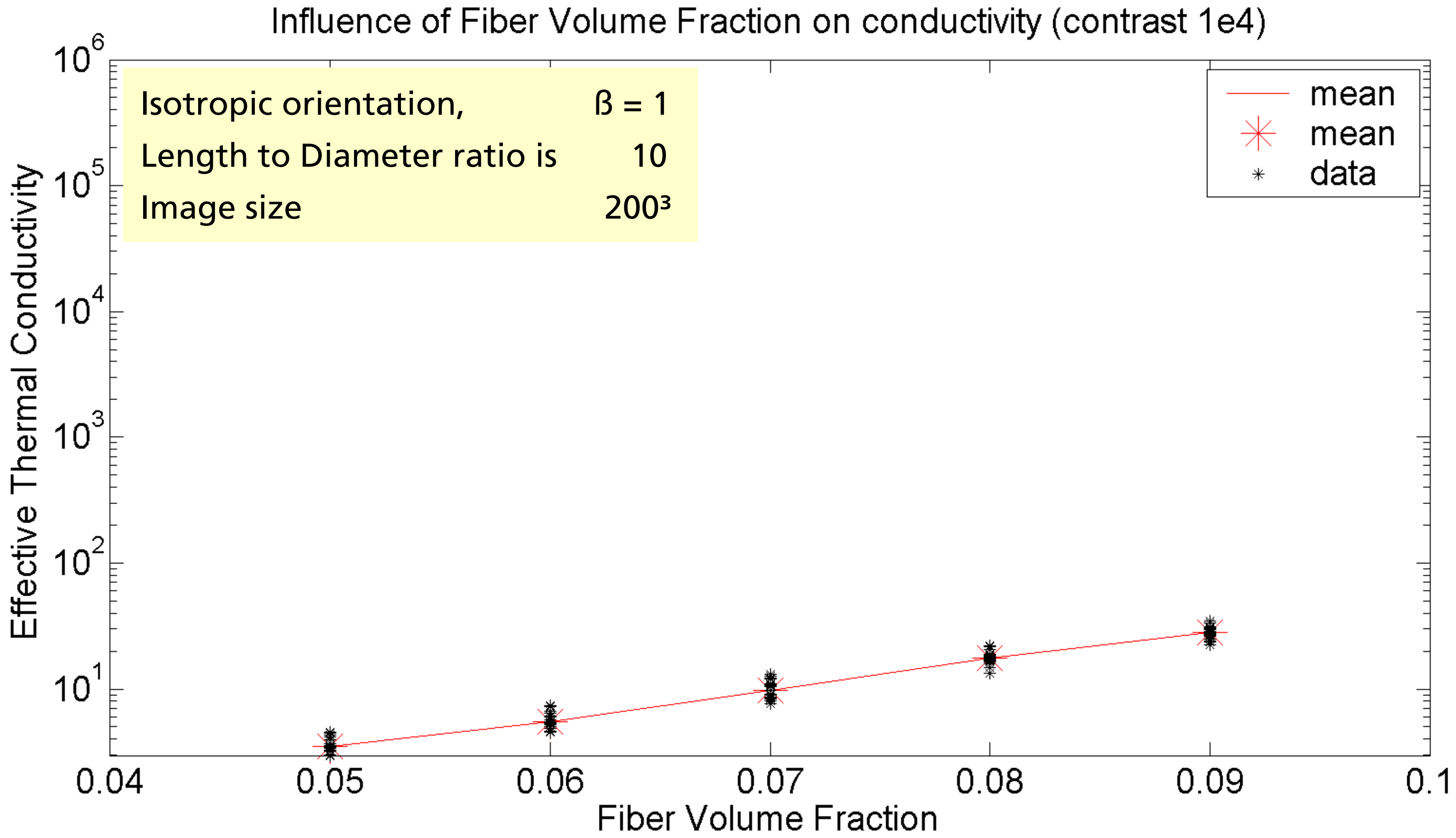
Regions of repeating coefficients create shifted identical rows in the matrix – devise implicit solvers that takes less memory than it would take to store the matrix!

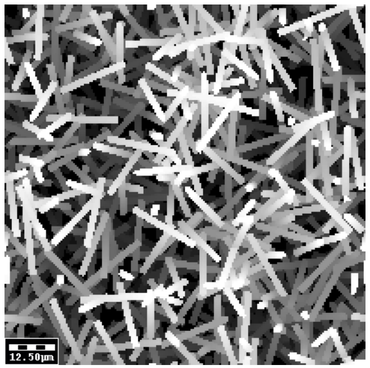
Effective conductivity via homogenization

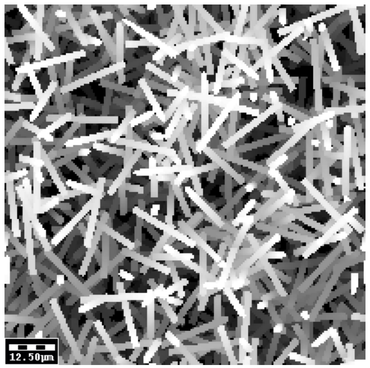
$$\begin{aligned} \nabla \cdot (\beta(\vec{x})(\nabla U_l + \vec{e}_l)) &= 0, \quad \vec{x} \in \Omega, \\ U_l(\vec{x} + id_1\vec{e}_1 + jd_2\vec{e}_2 + kd_3\vec{e}_3) &= U_l(\vec{x}), \quad i,j,k \in \mathbb{Z}, l = 1,2,3 \end{aligned}$$

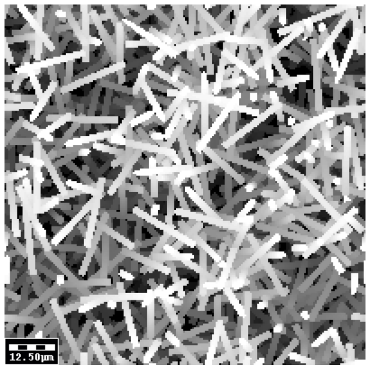
$$\beta^*_{ml} = \frac{1}{d_1 d_2 d_3} \int_\Omega \langle \vec{e}_m, \beta(\vec{x})(\nabla U_l + \vec{e}_l)\rangle d\vec{x}, \quad l = 1,2,3; \quad m = 1,2,3,$$

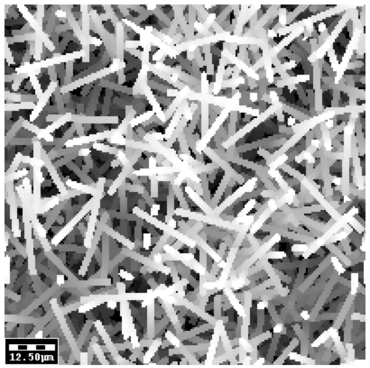
U_l has kinks where β is discontinuous – must be careful evaluating ∇U_l.

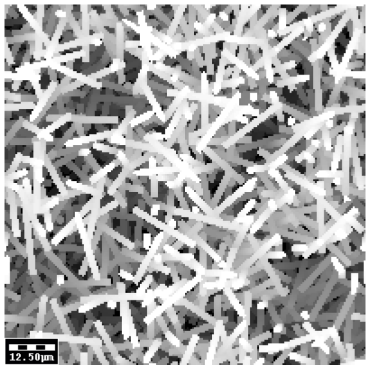

Influence of Fiber Volume Fraction on conductivity (contrast 1e4)
Isotropic orientation, ß = 1
Length to Diameter ratio is 10
Image size 200³
mean
mean
data
Effective Thermal Conductivity
Fiber Volume Fraction
0.04
0.05
0.06
0.07
0.08
0.09
0.1
10^1
10^2
10^3
10^4
10^5
10^6

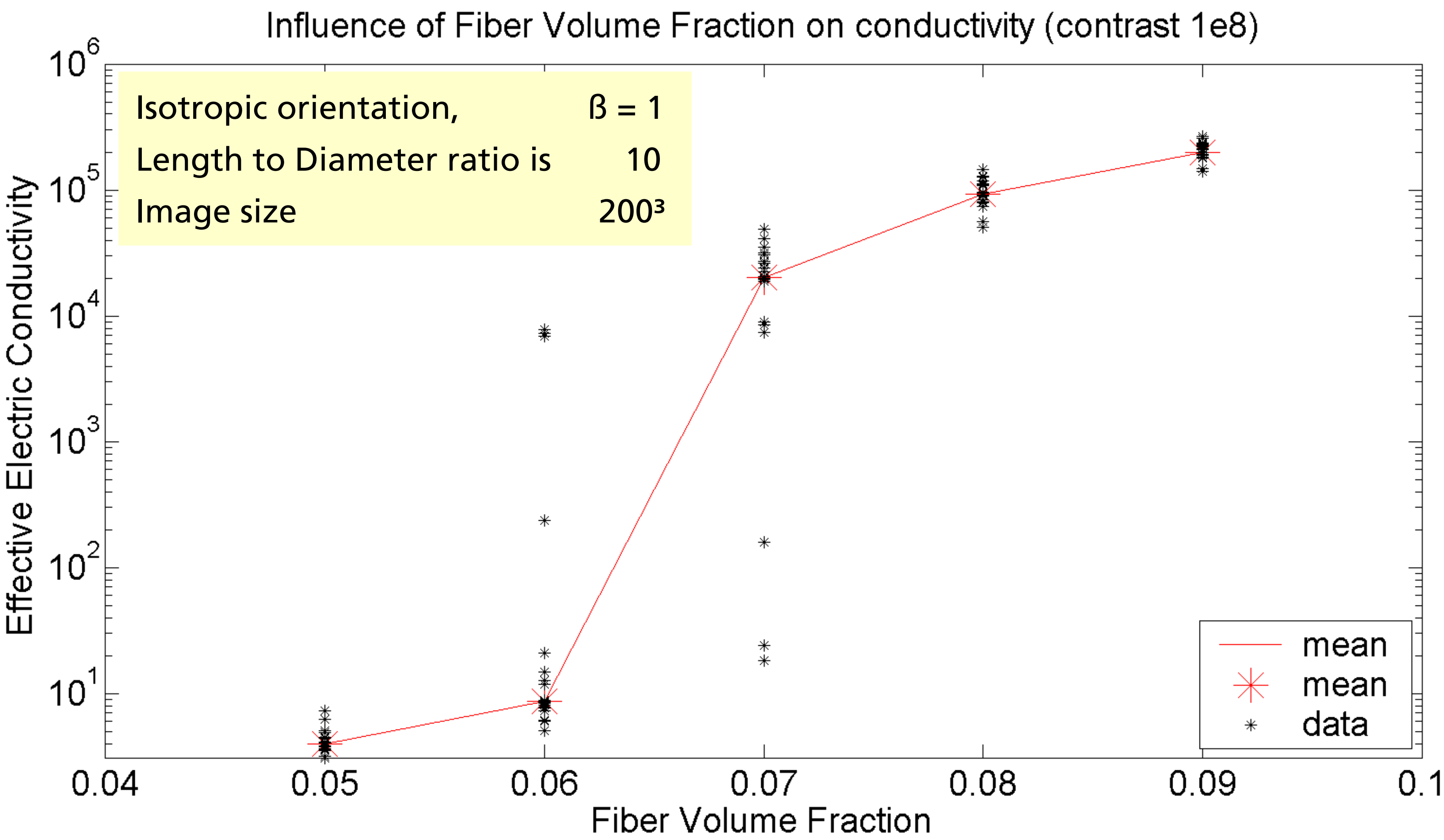




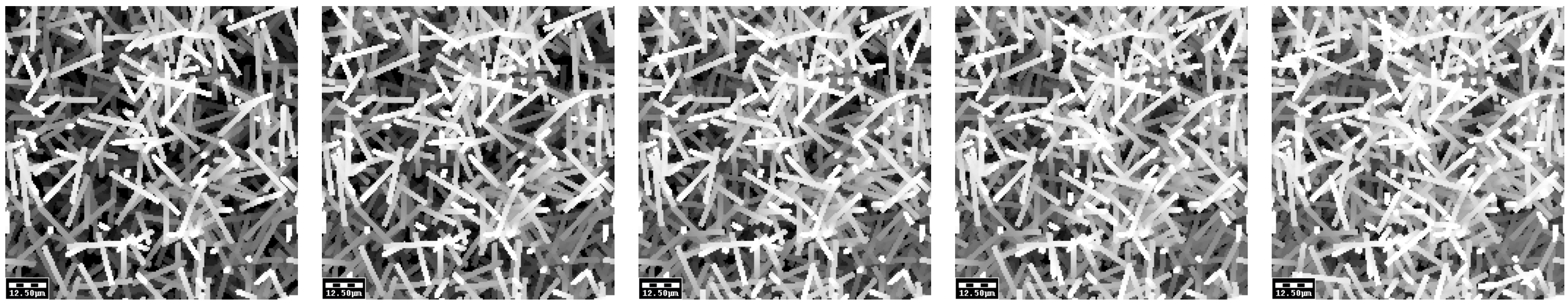






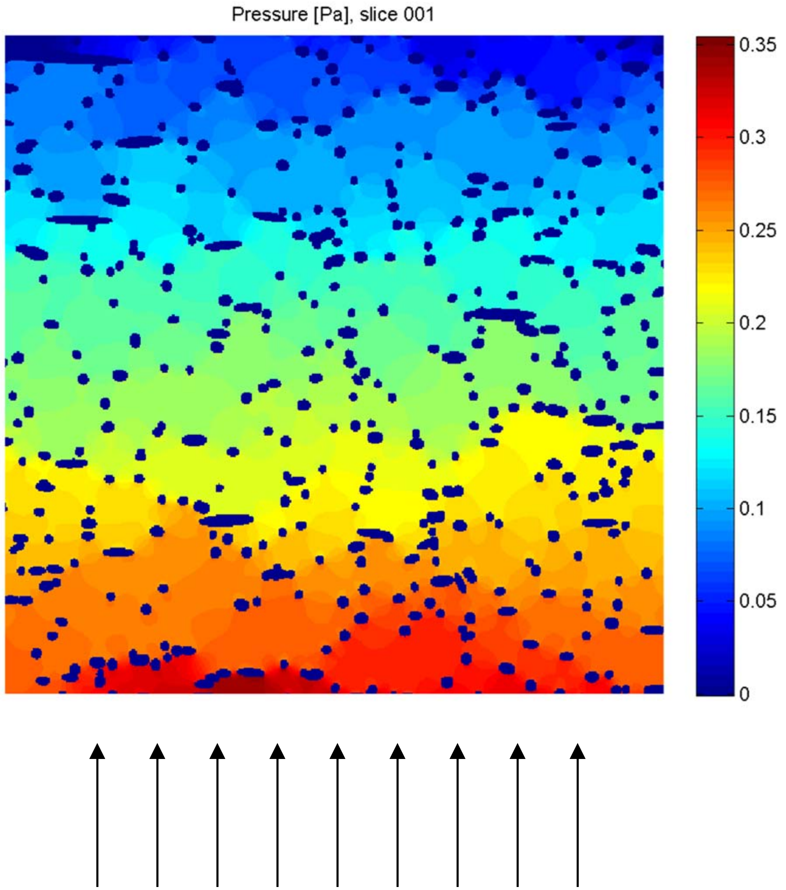


Influence of Fiber Volume Fraction on conductivity (contrast 1e8)
Isotropic orientation, ß = 1
Length to Diameter ratio is 10
Image size 200³
Effective Electric Conductivity
Fiber Volume Fraction
mean
mean
data

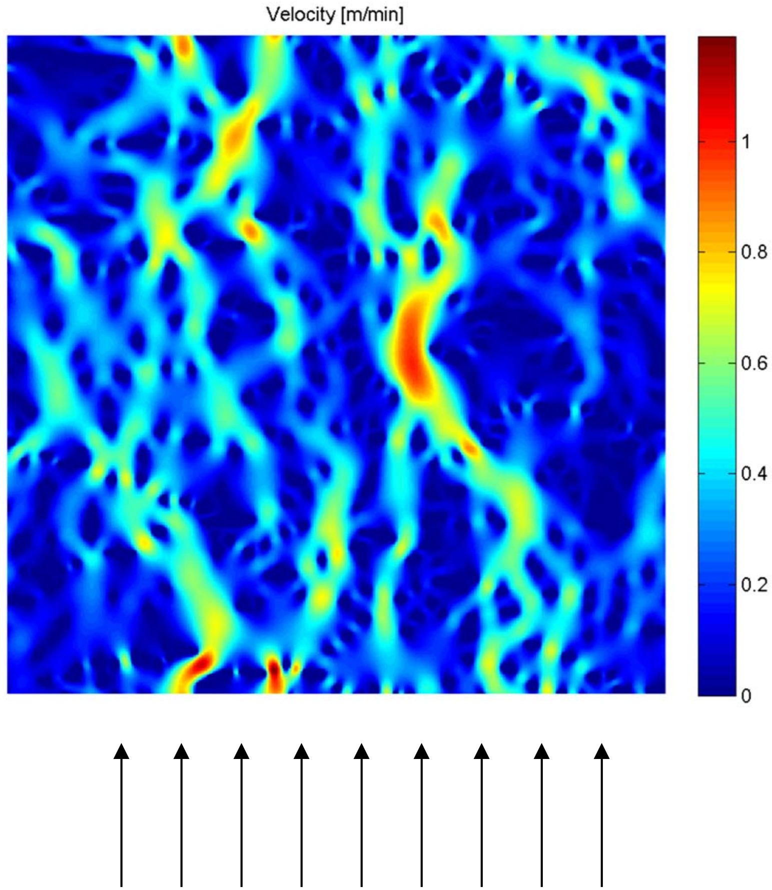


Pressure and velocity

Pressure (p)



Velocity ($\vec{u}$)

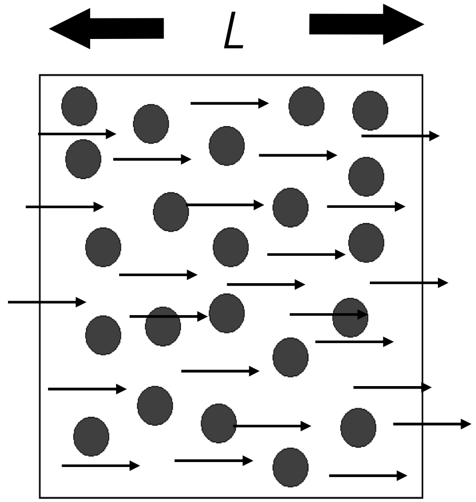


Computation of permeability

$\overline{\mathbf{u}}$: Macroscopic (creeping) flow velocity

$\mathbf{K}$: Permeability tensor

$\Delta\mathbf{p}$: Pressure difference

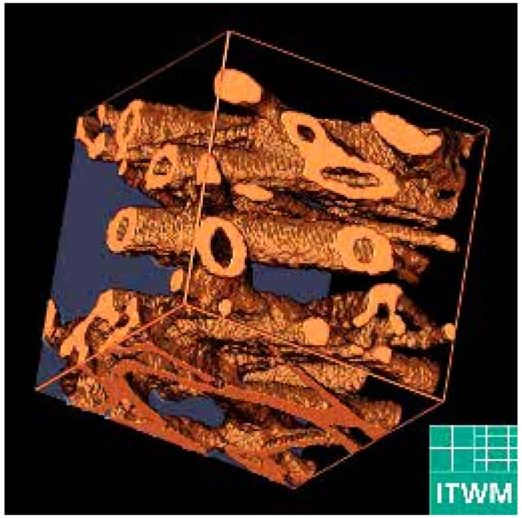


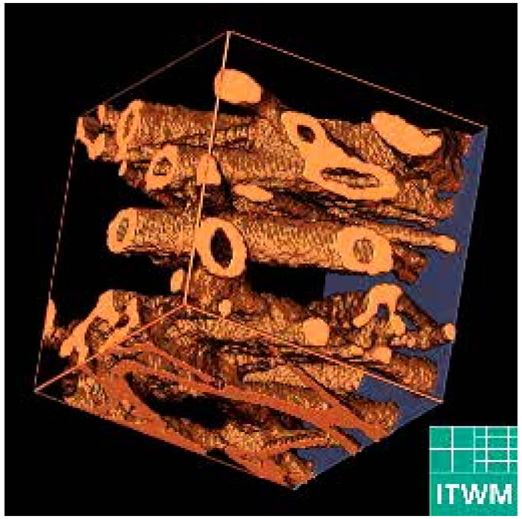
The flow solver provides the microscopic flow field for $\overline{\mathbf{u}}$ a given pressure difference, averaging yields

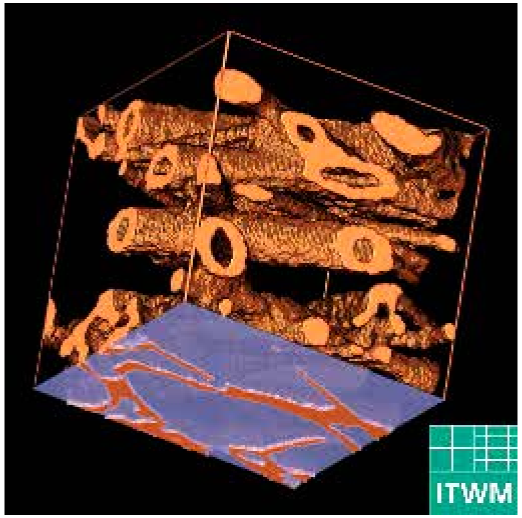
Darcy-Law: $\overline{\mathbf{u}} = \frac{1}{L}\mathbf{K} \cdot \Delta\mathbf{p}$ Generalized: $\vec{\mathbf{u}} = -\kappa \cdot \nabla\mathbf{p}$

Computation of permeability

Permeability tensor: $\mathbf{K} = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{32} & k_{32} & k_{33} \end{pmatrix}$ → Find anisotropic material behavior

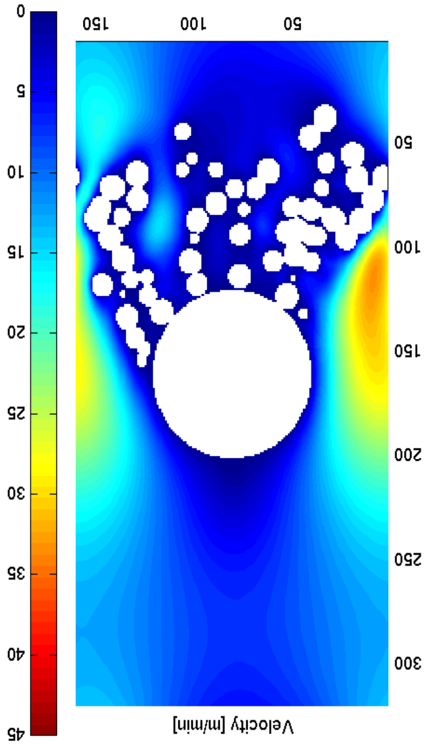


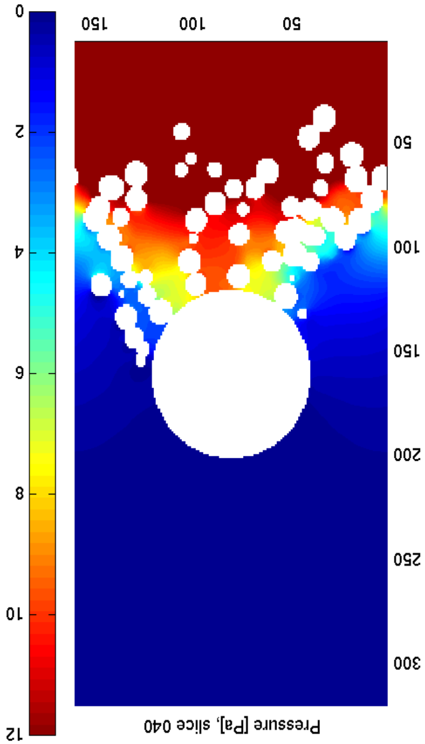


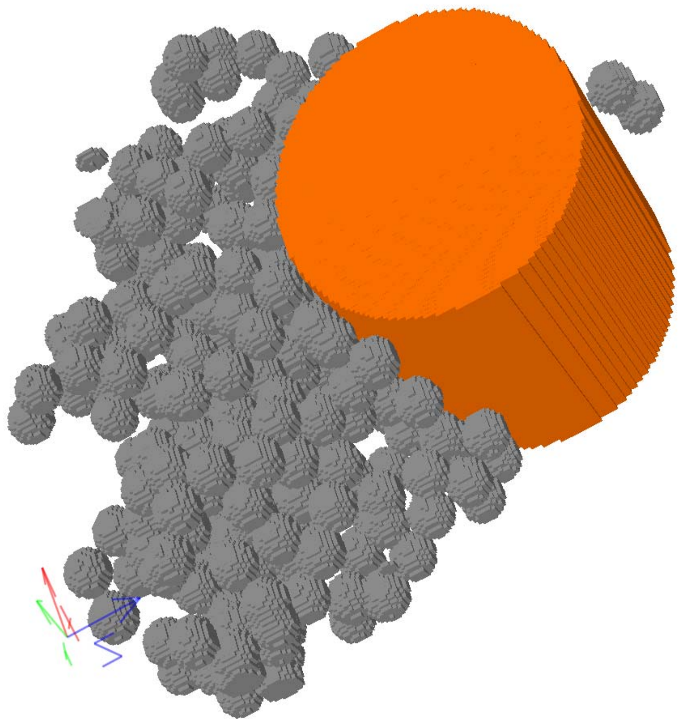


Pressure and Velocity in Clogging Simulation

Filtration is multiple physics!

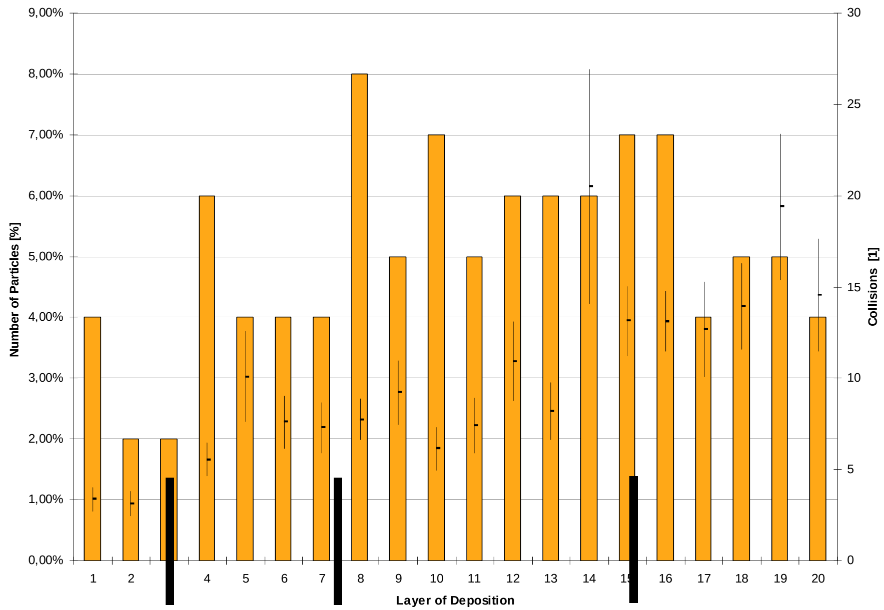


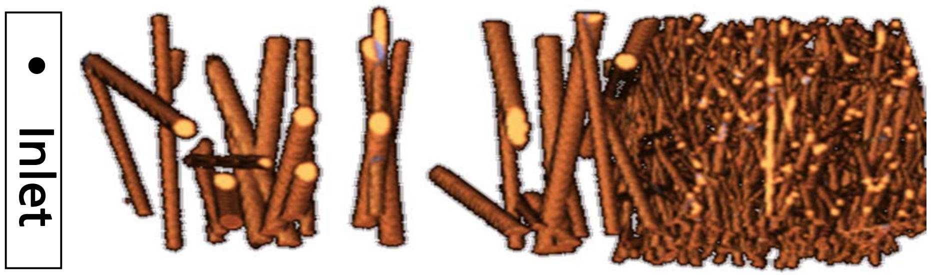




Deposition Diagram

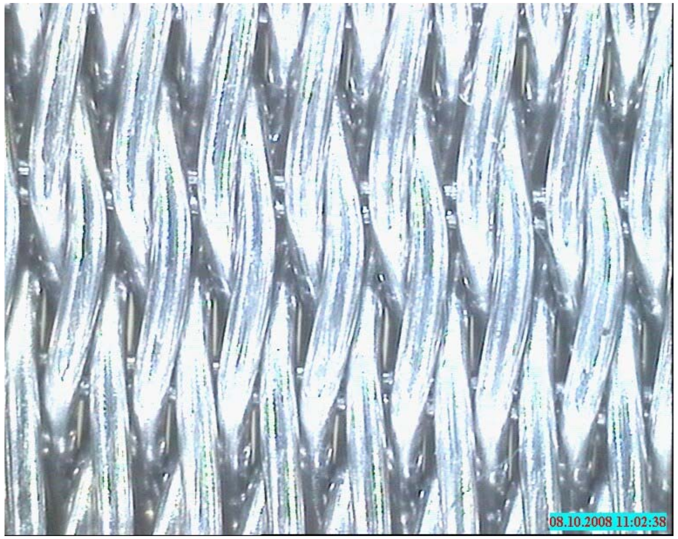
- Deposition locations are 20 64µm layers.
- Orange: particle numbers
- Lines: mean value and standard deviation of number of collisions
- Example: Layer 15 contains 7% of the filtered particles. Those had on average 13.15 collisions with standard deviation 1.9
- 4 layers of gradient material indicated by thick black lines:

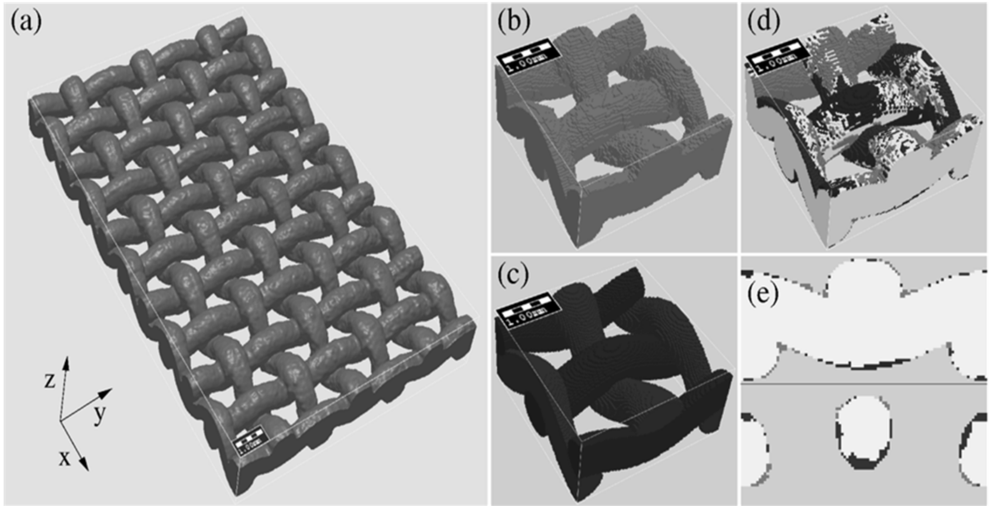




On 8 cores 64GB Linux desktop:
400 x 400 x 1200 filter media

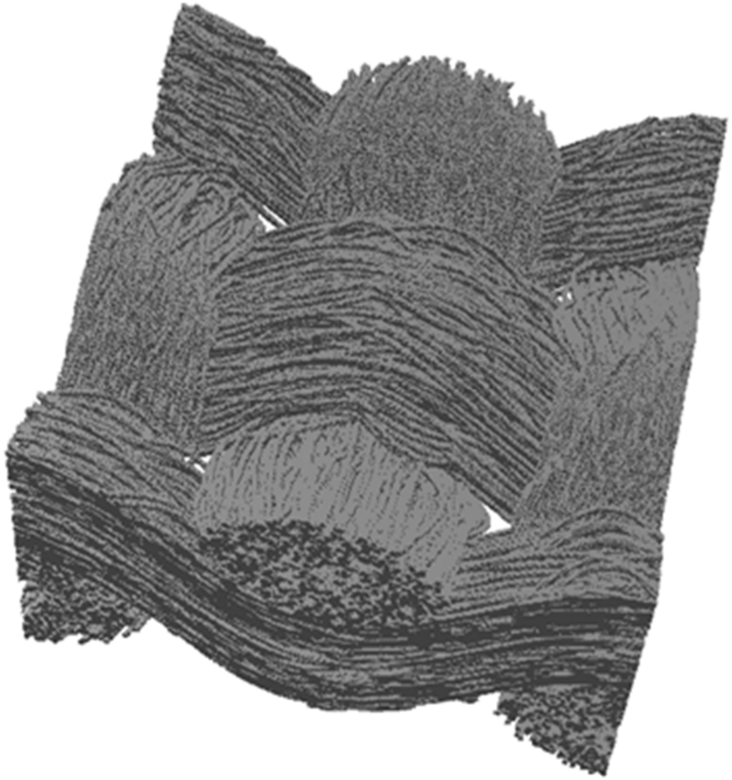
Reconstruction of Woven





Microscopy Courtesy M. Knefel, Gebr. Kufferath AG.

Carbon fiber multi-filament woven



3D Visualization (generated)

SEM (real)

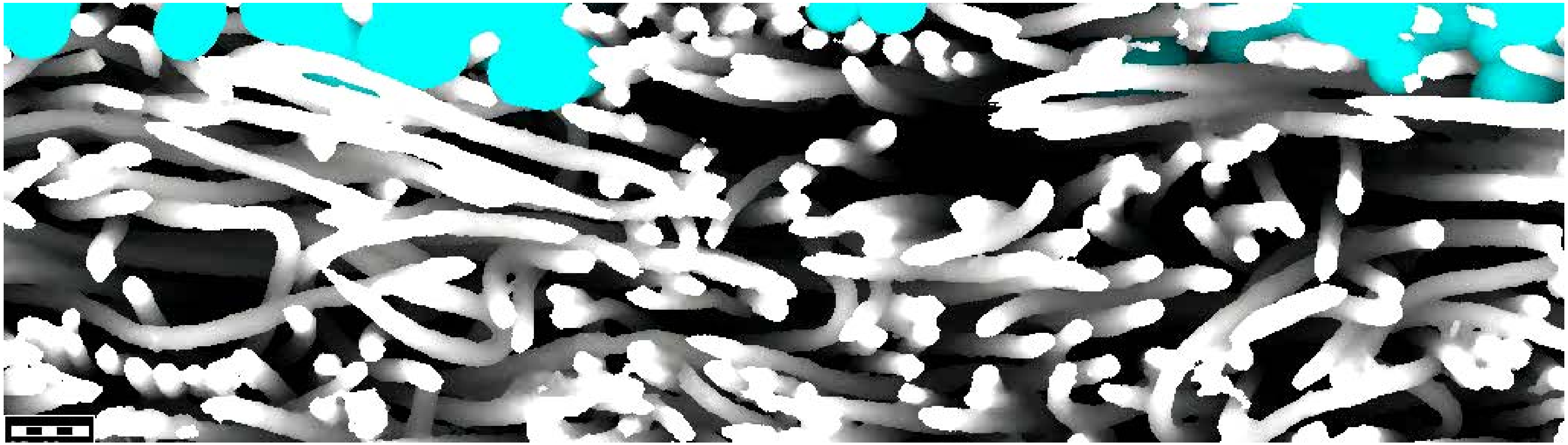
(courtesy of Jeff Gostick, Univ. of Waterloo)

V.P. Schulz, P.P. Mukherjee, J. Becker, A. Wiegmann and C.Y. Wang, *Modeling of Two-phase Behavior in the Gas Diffusion Medium of Polymer Electrolyte Fuel Cells via Full Morphology Approach*, Journal of the ECS, Issue 4, Vol. 154, 2007, pp B419-B426.

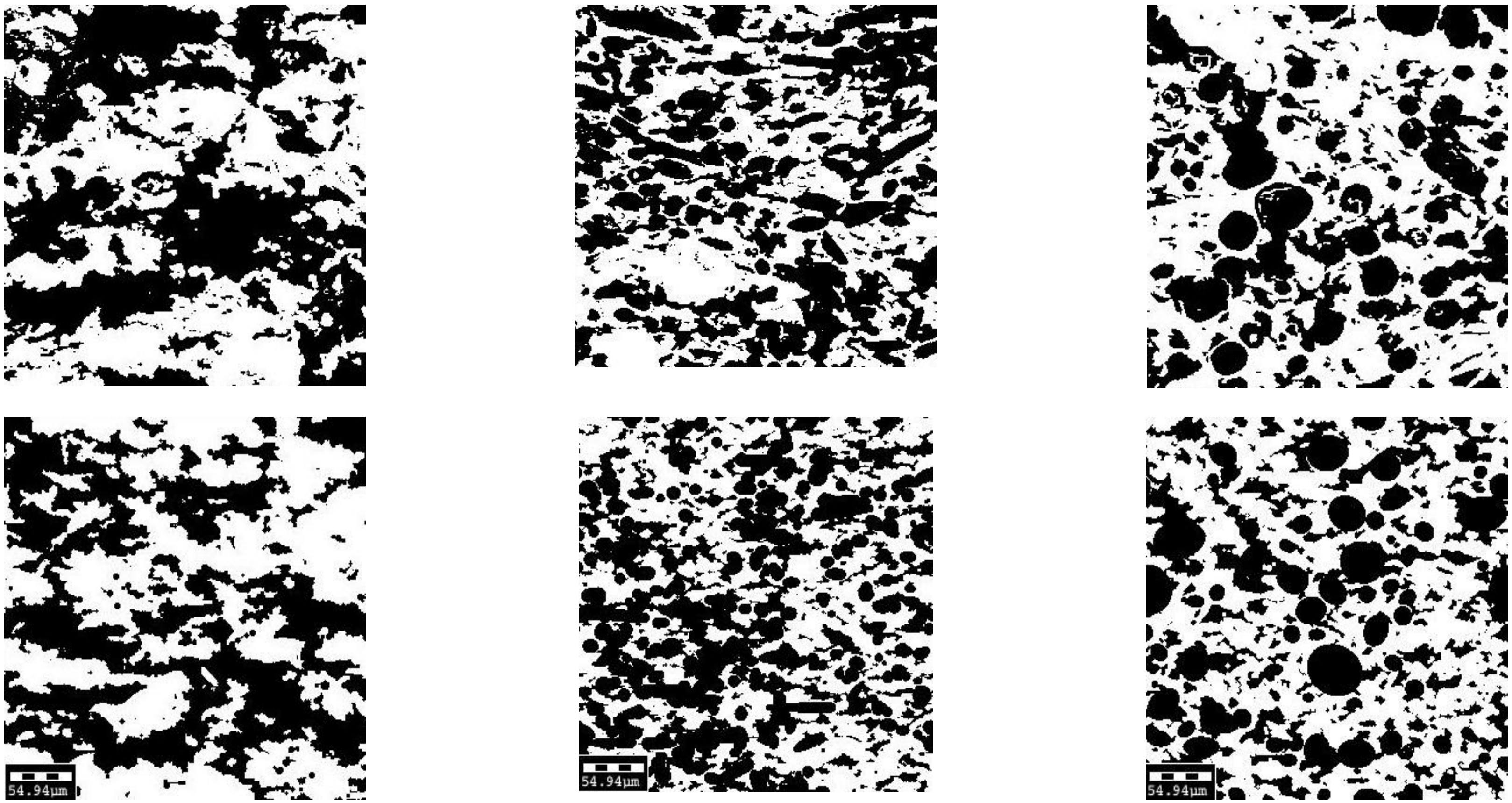
Simulated mercury Distribution at Bubble Point in tomography

pc= 10.6 kPa

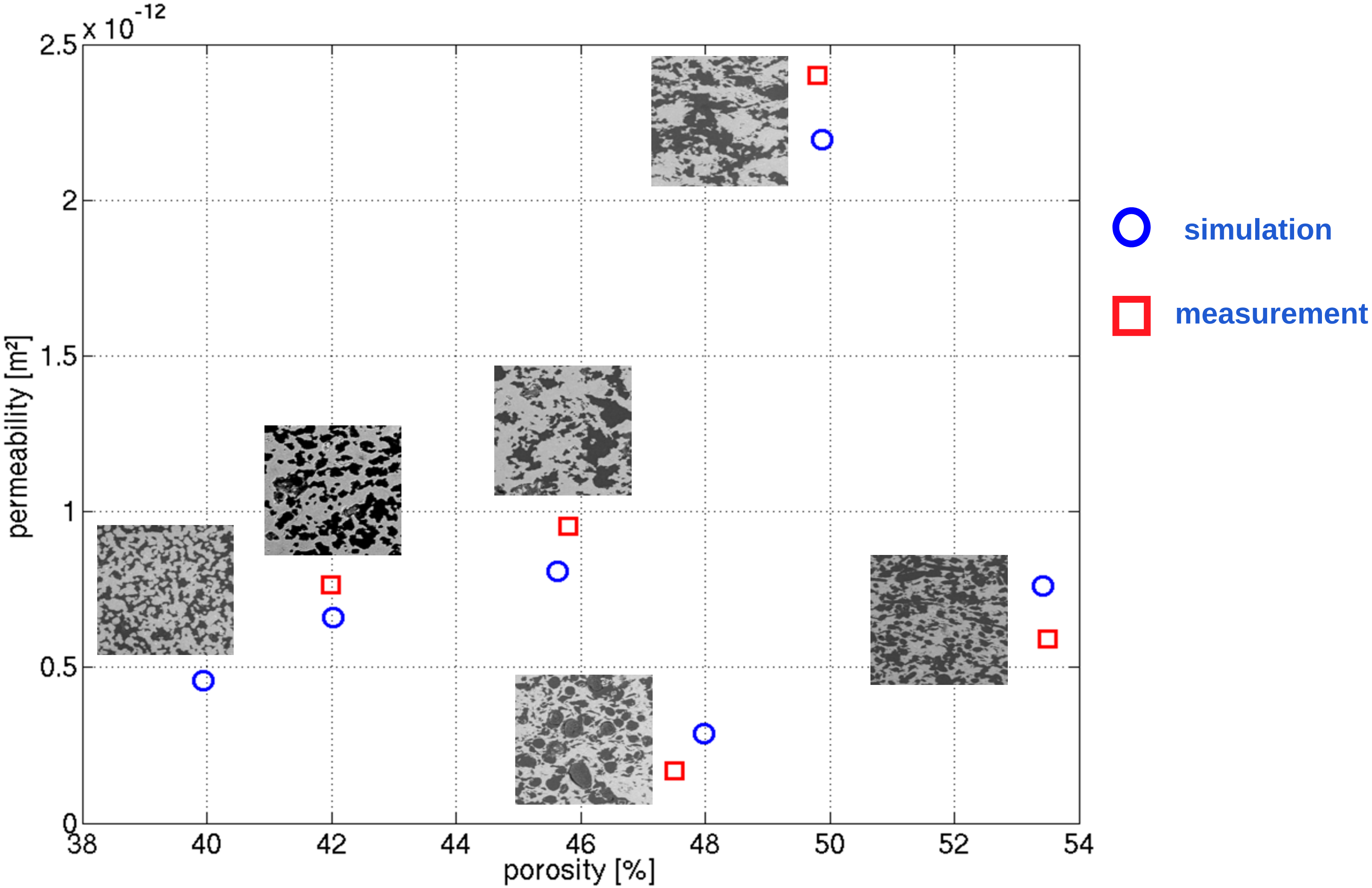
(r=10.5 μm)



Binarized SEM (top) and virtual sintered ceramics (bottom)



Computed vs measured porosities and permeabilities



CAE of Materials – Modules of the GeoDict Software

- FiberGeo, SinterGeo, WeaveGeo, GridGeo, PackGeo, PleatGeo , PaperGeo (structure generators)
- ProcessGeo (3d image processing)
- LayerGeo (layered media)
- ImportGeo (e.g. tomographie, STL, .gad)
- ExportGeo (e.g. Fluent, Abaqus)
- FlowDict (single phase flow properties)
- PleatDict (porous media flow)
- ElastoDict (effective elastic properties)
- ThermoDict (effective conductivity)
- DiffuDict (effective diffusivity)
- FilterDict (pressure drop, efficiency, life time)
- SatuDict (two phase flow properties)
- PoroDict (pore size measures)
- AcoustoDict (acoustic absorption)

Target hardware:

Solver: Workstation or cluster

Pre + Post: Laptop

GeoDict contributors: 2001 - 2010

GeoDict
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Jürgen Becker
Erik Glatt
Stefan Rief
Heiko Andrä
Sven Linden
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Ashok Kumar Vaikuntam
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PoroDict
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PleatDict
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FlowDict Lattice Boltzmann
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WeaveGeo
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Jürgen Becker

PackGeo
Erik Glatt
Andreas Wiegmann
Joachim Seibt

GridGeo
Erik Glatt
Liping Cheng
Andreas Wiegmann
Rolf Westerteiger

RenderGeo
Matthias Groß
Sven Linden
Carsten Lojewski
Rolf Westerteiger

PaperGeo
Erik Glatt

Conclusions and Restrictions

- Materials random – no CAD but 3d digital images (CT) available, segment into ST
- Optimize meaningful design variables, not voxels
- Generators convert design variables into random realizations (ST)
- Solving pde on ST avoids meshing step
- Solution of pde can be
  - averaged for effective property
  - used as flow field for particle tracking
- Requests repeat – developed software tool GeoDict
- Must be able to solve pde on very large 3d images
- Voxels do not allow boundary layers
- Large contrast deteriorates performance
- …

Find out more:

Demo from
www.geodict.com

Thank you for your attention

www.itwm.fhg.de

GEO DICT