
PEFC Gas Diffusion Layer: Effective Properties and Compression Effect

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Motivation

- MEA is an assembly of porous layers: GDL, MPL, CL, membrane
- Each layer need to have optimal properties
- Properties of a porous medium are influenced by
 - Material
 - Pore structure

Our goal: enable virtual material design by

- *Creation of 3D pore structure models*
- *Numerical determination of effective properties (diffusivity, permeability, etc.)*

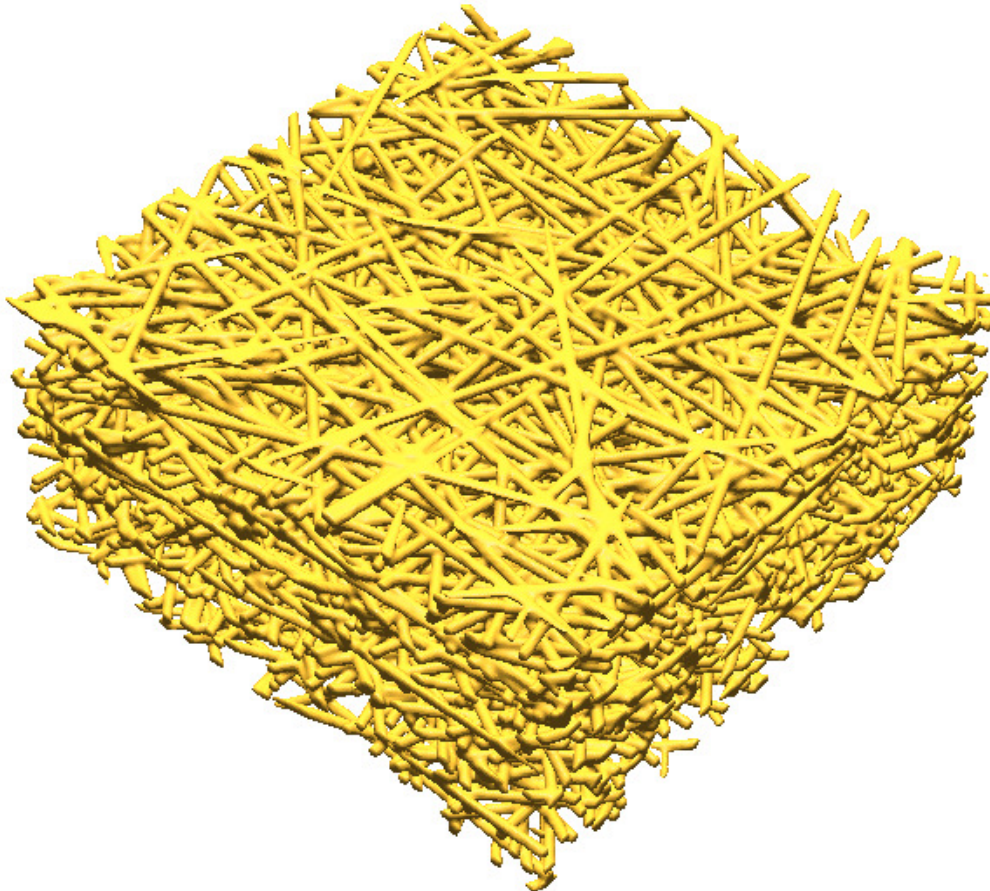
Outline

- 3D structure models
- Compression
 - Reduced Model
 - FE Model
- Effective (two-phase) parameters

Model: Straight Fibers

Poisson line process using:

- fiber diameter
- anisotropy
- porosity



GEO DICT

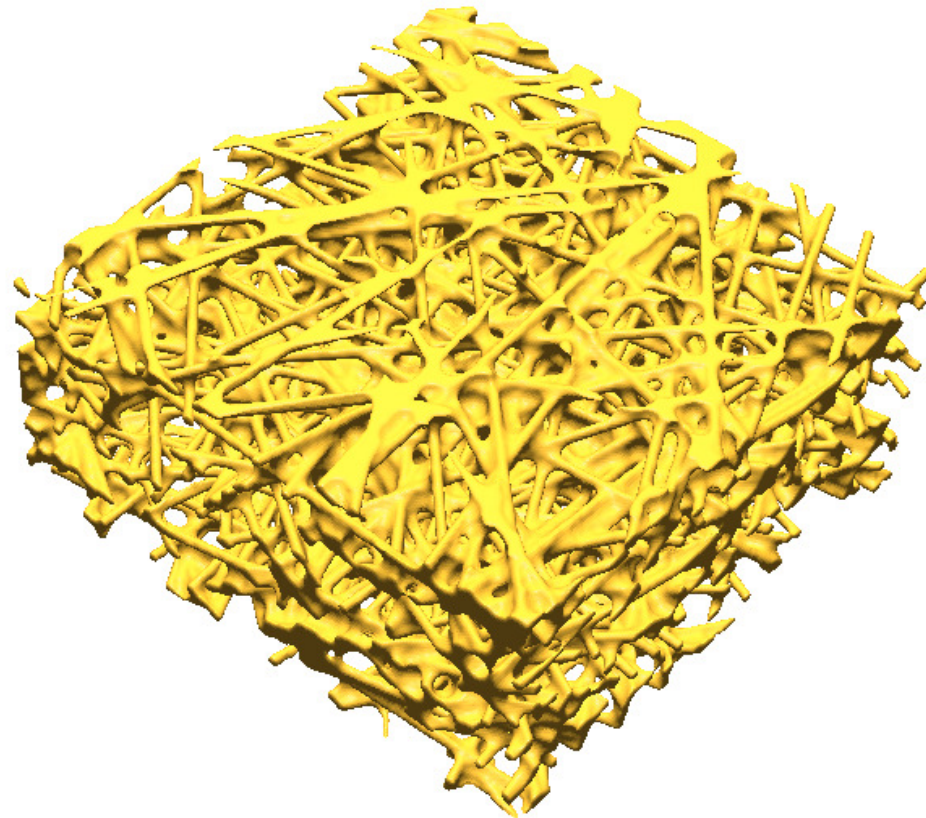
Model: Straight Fibers and Binder

Poisson line process using:

- fiber diameter
- anisotropy
- porosity

Second step:

- fill small pores with binder
- smallest pores first



GEO DICT

Model: Curved Fibers

Process:

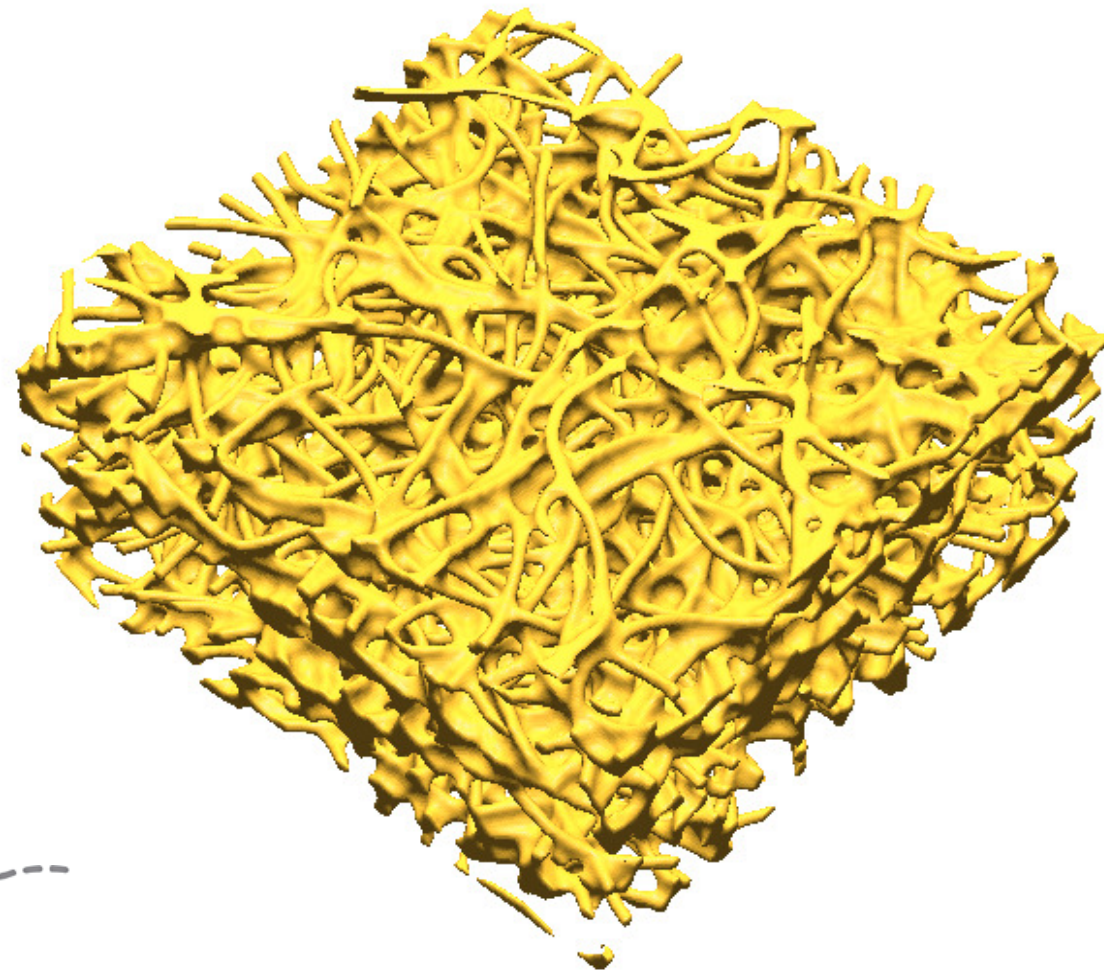
- fibers consist of straight segments
- start with one segment, then add segments
- direction of added segment:
 - direction of prev. segment + random disturbance
 - direction of first segment + random disturbance
 - keep current curvature + random disturbance



GEO DICT

Model: Curved Fibers and Binder

- create fibers
- add binder



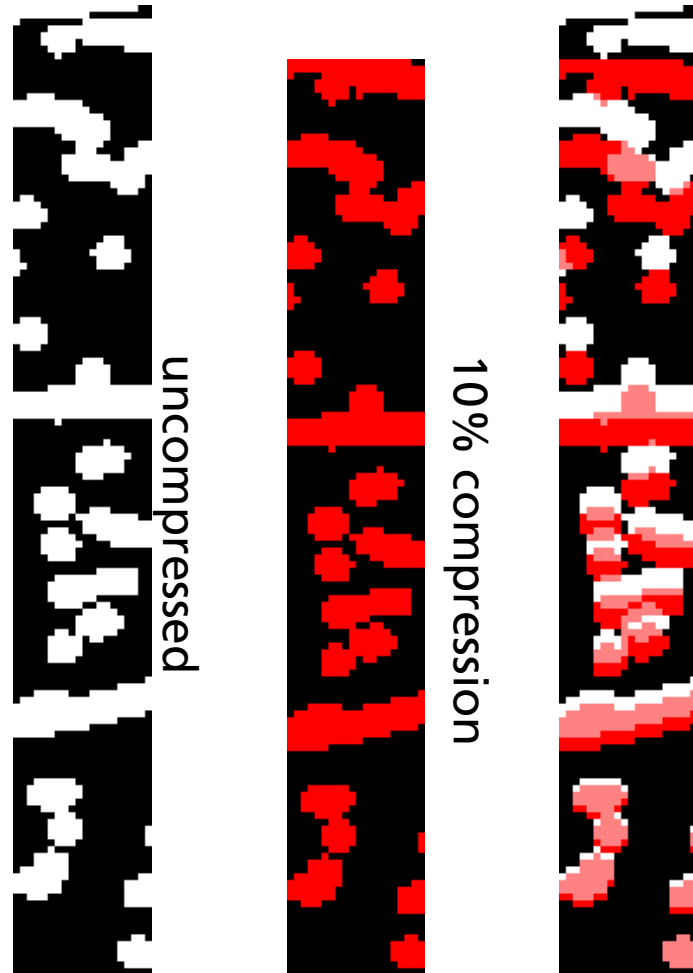
GEO DICT

Compression

Why?

- GDL is compressed
- Compression changes the effective properties of the layer: reduced permeability and diffusivity, enhanced conductivity

Compression: Reduced Model



Algorithm:

(Schulz, Becker, Wiegmann, Mukherjee, Wang, *J. Electrochem Soc.* 154, 2007)

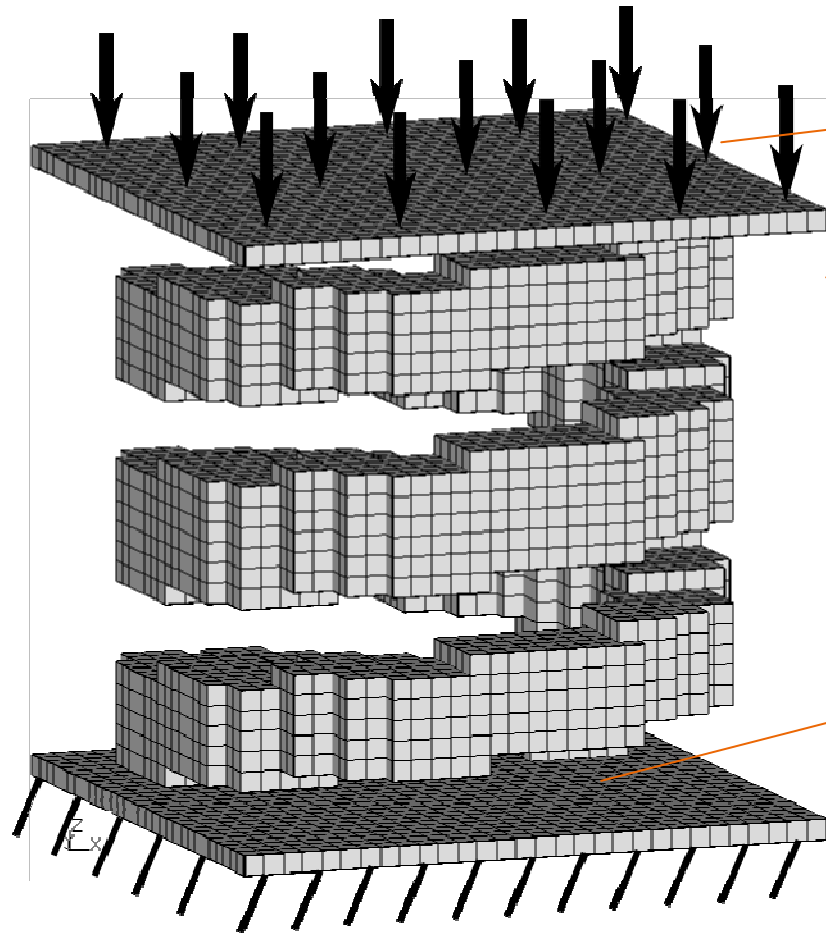
- compression in z-direction
- handles each z-column separately
- mass is kept by shifting solid blocks

Problems

- fibers cannot bend
- only works for small compression ratio and low porosity



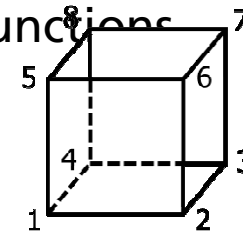
Compression: FE Model



Area load implemented as nodal forces at the upper boundary

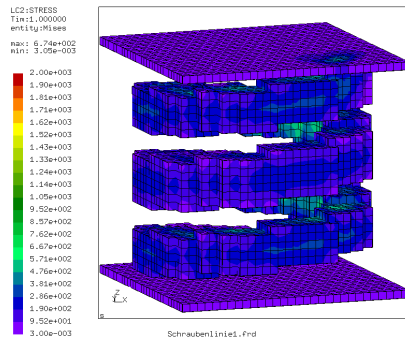
Microstructure is clamped between two plates. The lower plate is fixed while the upper plate can move vertically only

For the μ FE-calculation the voxels are treated as 8 node brick elements with linear ansatz functions

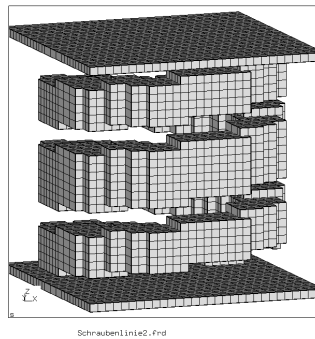


Example: Helix under compression

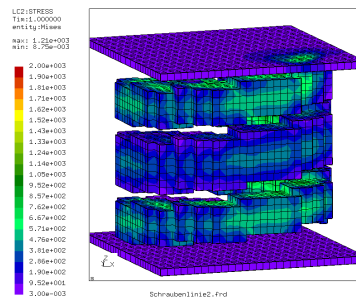
FE Compression Model: Iterative Approach



Calculation of displacements, stress and strains by standard FE software such as Abaqus or Calculix. Limitation of the load such that the deformed bricks do not pervade each other.



Remeshing by a conversion of the deformed bricks into a voxel mesh (undeformed brick elements). Calculated stresses are interpolated as initial conditions on the new mesh.

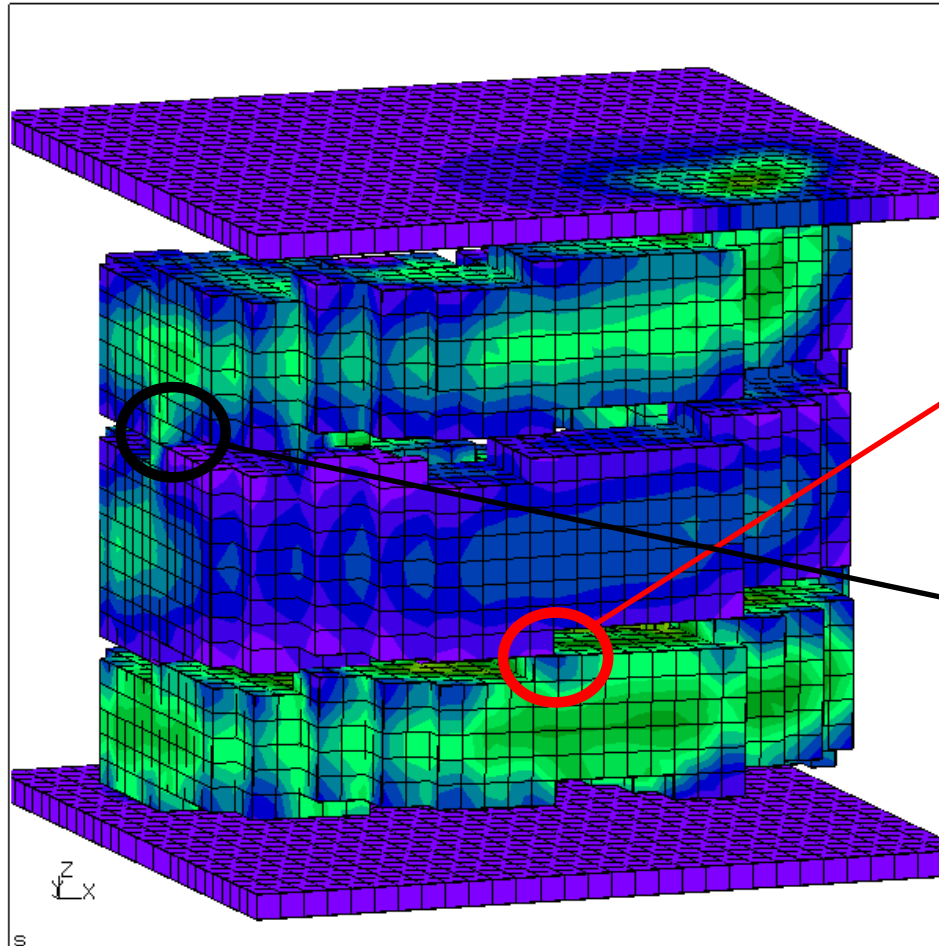
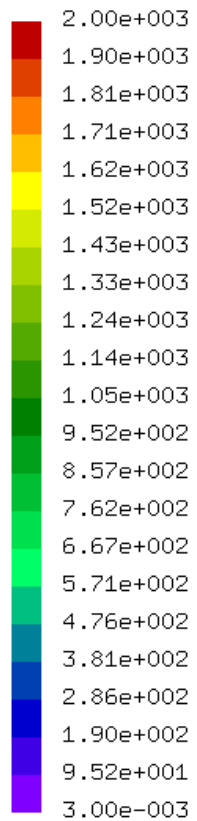


Recalculation using the FE solver.

...

Remeshing

LC2:STRESS
Tim:1.000000
entity:Mises
max: 2.00e+003
min: 2.33e-003



Schraubenlinie3.frd

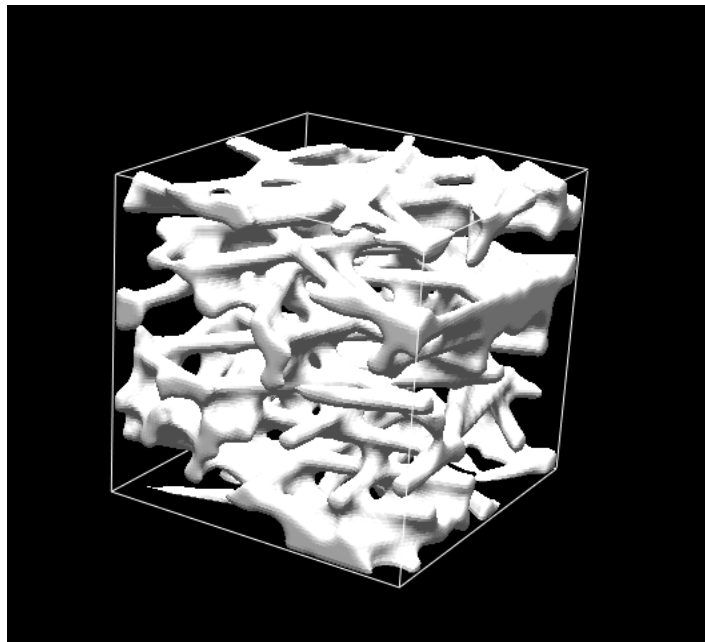
Why do we remesh after each iteration step?

We avoid the penetration of initially separated parts

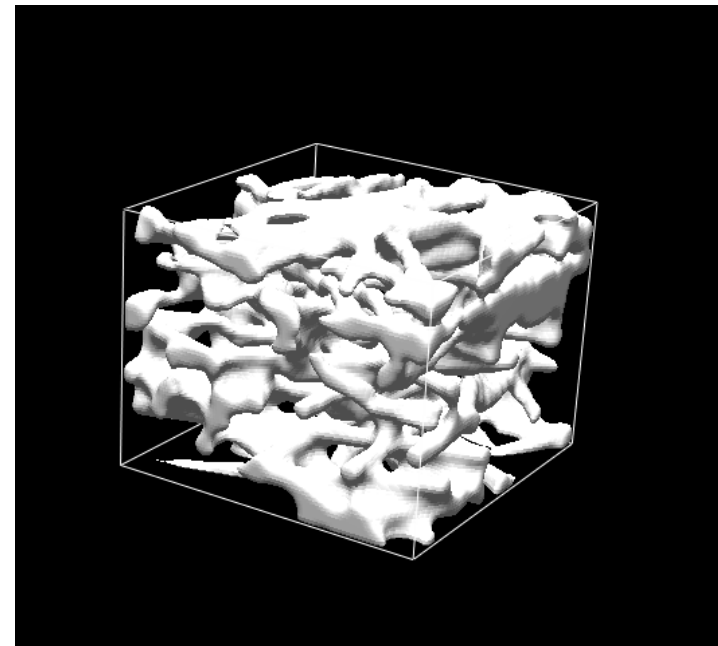
Touching elements can easily treated as adhesive

Compression Example: FE model

Model: straight fibres with binder, 100x100x100 cutout



uncompressed

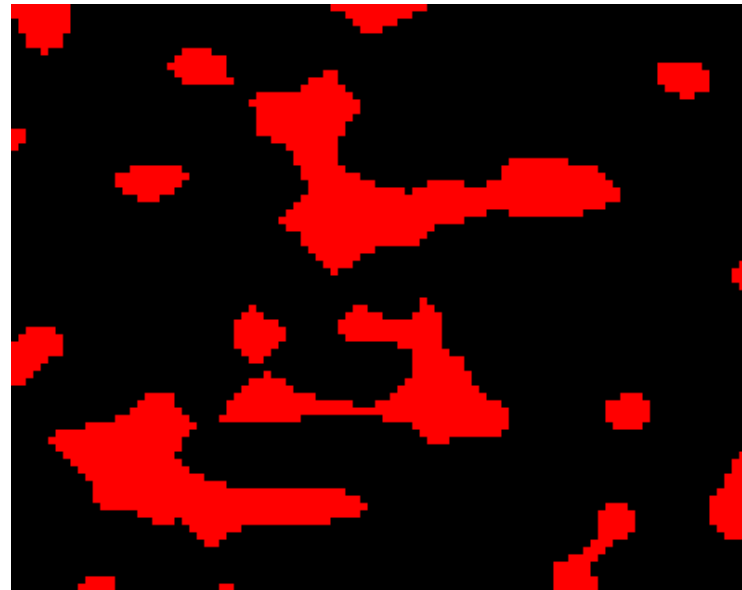


compressed (20%)

Comparison of the Two Models



uncompressed



compressed (20%, Edmundo) $\epsilon = 0.01$
computation time: 0.25ys

FE compression model: Advantages and drawbacks

- + Calculation of the compression ratio as a function of the external load
- + Beside local stresses, we get the entire deformed microstructure
- + Iterative remeshing is an efficient way in order to detect penetrating elements. Touching elements are treated as adhesive
- + Remeshing shows artifacts locally but is mass conservative
- Approach is limited by the capacity of the FE solver. Currently, image sizes of about 100x100x100 voxels are possible (no REV properties!)
- Corresponding to the FE solver, the computation times are significant

Effective Parameters

Common approach:

1. Start with a 3D voxel structure given
2. Find effective properties based on the geometrical structure
 - a) Geometrical properties:
 - pore size distribution, pore morphology, surface area
 - b) Transport properties:
 - i. Solve PDE on the voxel grid
 - ii. Find effective property by upscaling / averaging

(Becker, Wiegmann, Schulz, J. Fuel Cell Sci. Technol. 5, 2008)

(Becker, Flückiger, Reum, Büchi, Marone, Stampanoni, J. Electrochem. Soc 156, 2009)

Compression Effect on Pore Size Distribution

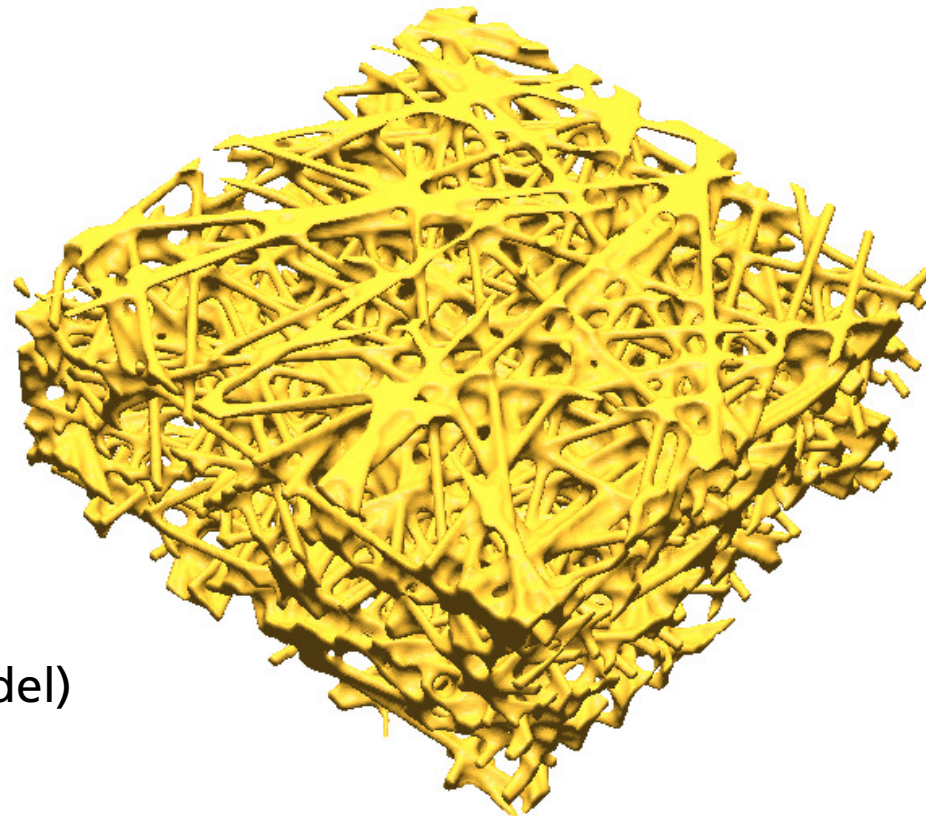
Example geometry:

- straight fibers with binder
- 420 x 420 x 200 μm
- voxel length 1.4 μm

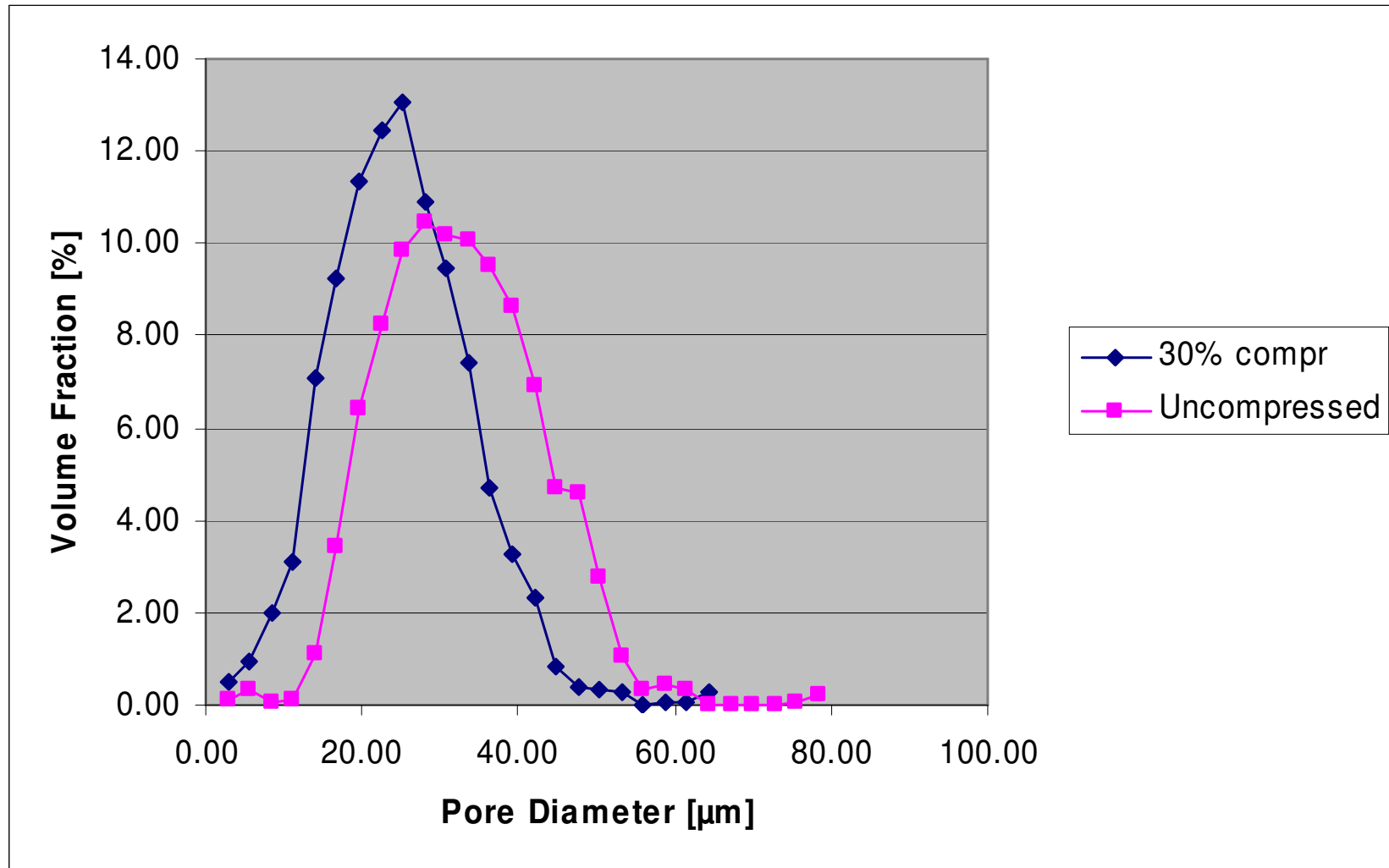
Compressed with:

- Reduced Model

(structure too large for FE Model)



Compression Effect on Pore Size Distribution



Permeability

- Macroscopic description (hom. porous media model)

Darcy's law :

$$u = -\frac{1}{\mu} \kappa \nabla p$$

u : average flow velocity

κ : permeability tensor *unknown*

μ : viscosity

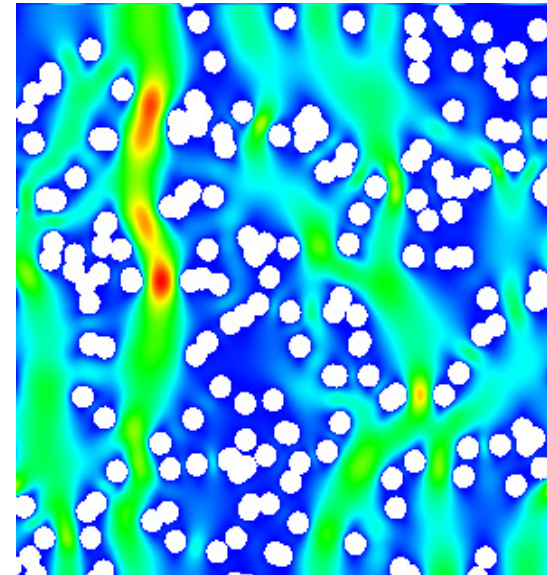
p : pressure

- Microscopic description (pore structure model)

Stokes equation: $-\mu \Delta u + \nabla p = 0$

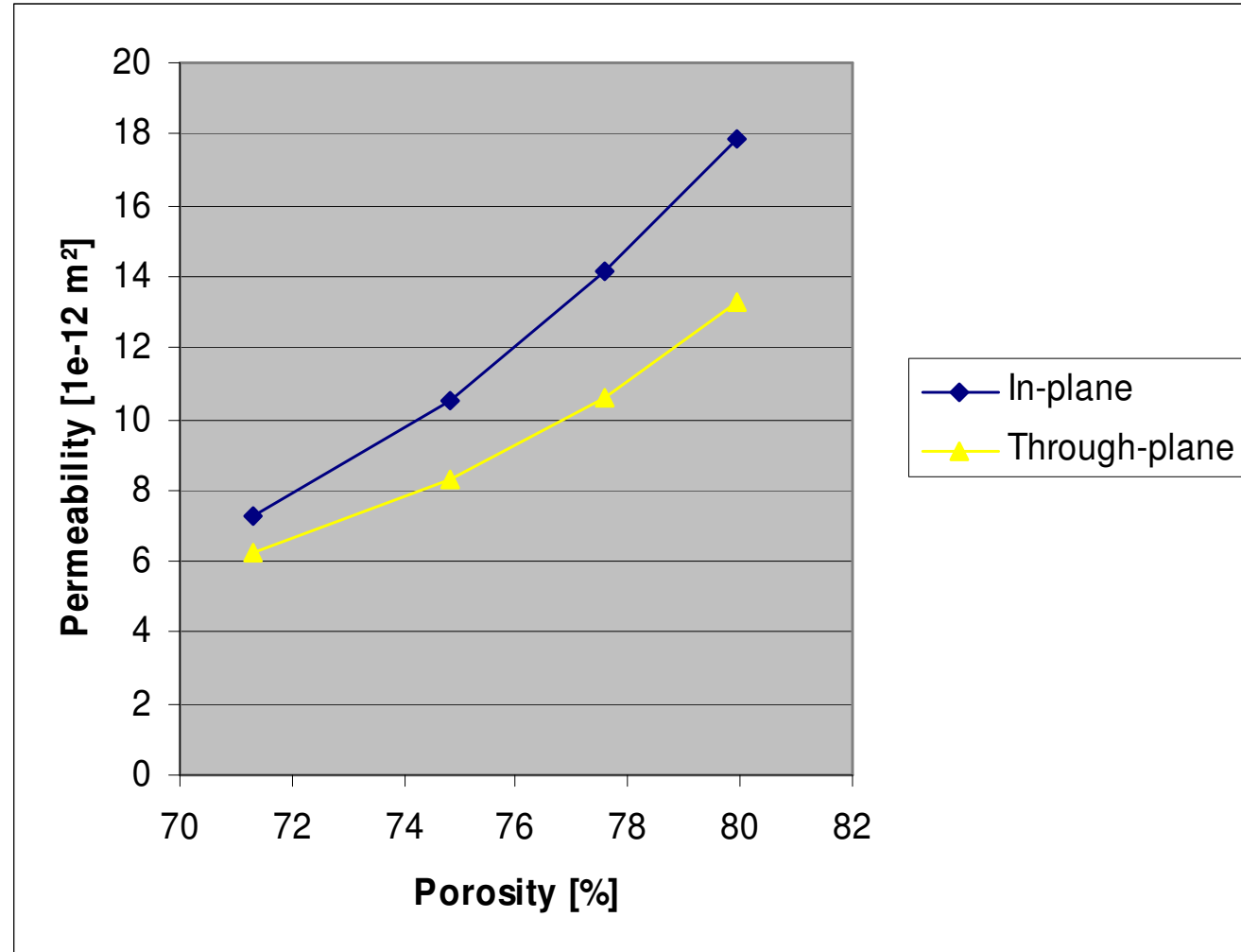
Boundary conditions: no-slip on fibre surface, pressure drop

κ can be determined from the solution!



Compression Effect on Permeability

- calculated for 0%, 10%, 20%, 30% compression

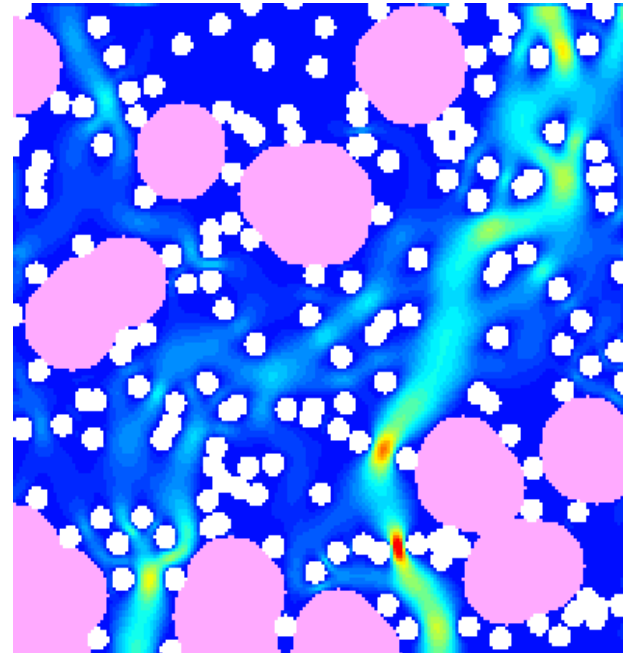
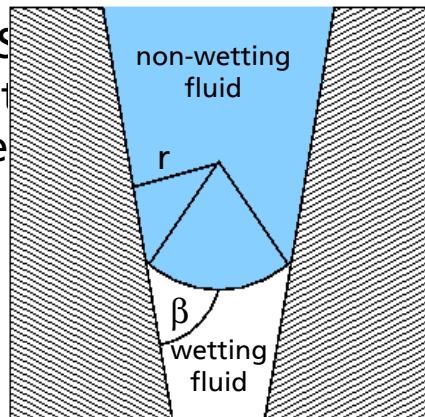


Relative Permeability

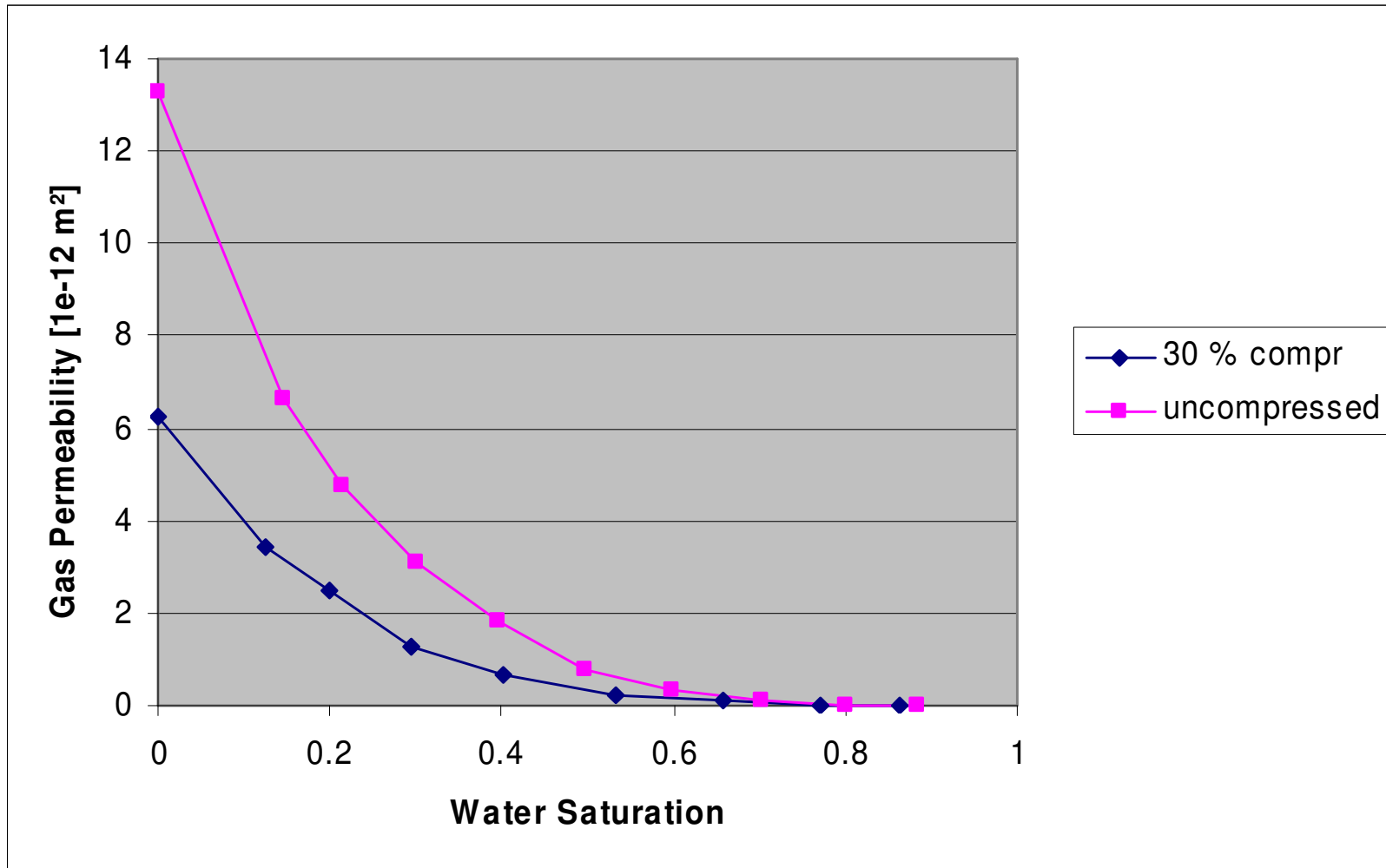
Two-step approach:

1. Use pore morphology method (Hilpert, 2001) to determine distribution of air and water phase.
 - Idea: a pore is filled with the non-wetting fluid (=water), if $p_c \geq \frac{2\sigma}{r} \cos \beta$

2. Solve for space permeability of the remaining pore phase (=air)



Compression Effect on Relative Permeability



Conclusions and Outlook

- Virtual created 3D structure models
- Two compression models
- Effective (two-phase) parameters

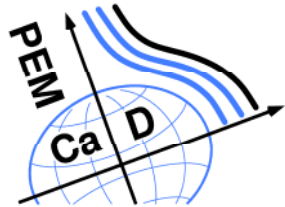
Key problem: speed of FE solver (Abaqus and Calculix are not able to solve REV problem)

- replace FE solver by own FE solver ?
- replace FE solver by FFTW based solver ?
 - elasticity eq. (FE) on 100^3 grid points: ~ 2h, 4 GB RAM
 - Stokes eq (FFTW) on 100^3 grid points: ~ 2 min, 90 MB RAM

Thank You

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BMBF project PemCaD



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