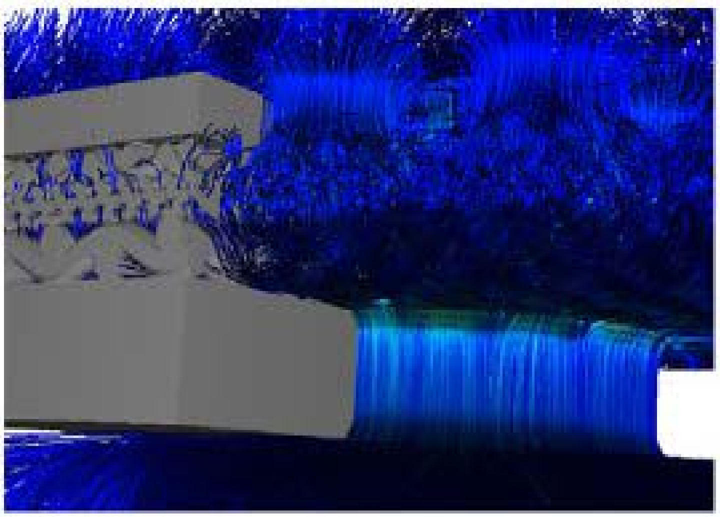
Software – centered approach to the simulation of thin porous media and their properties



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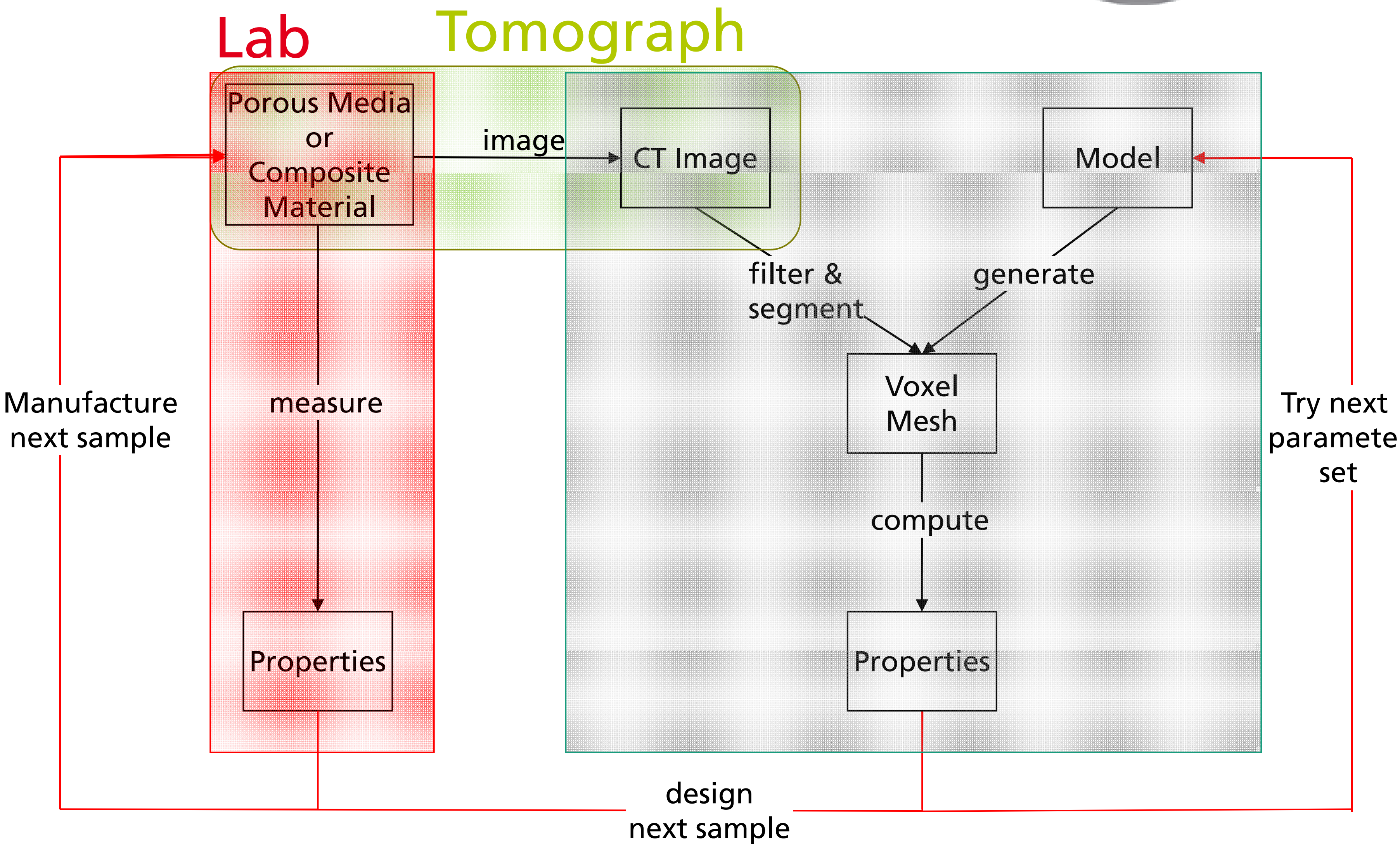
Outline

- **GeoDict in general**
- Thin porous Media
- Material properties
- GeoDict: Software for Virtual Material Design

Computer Aided Material Engineering

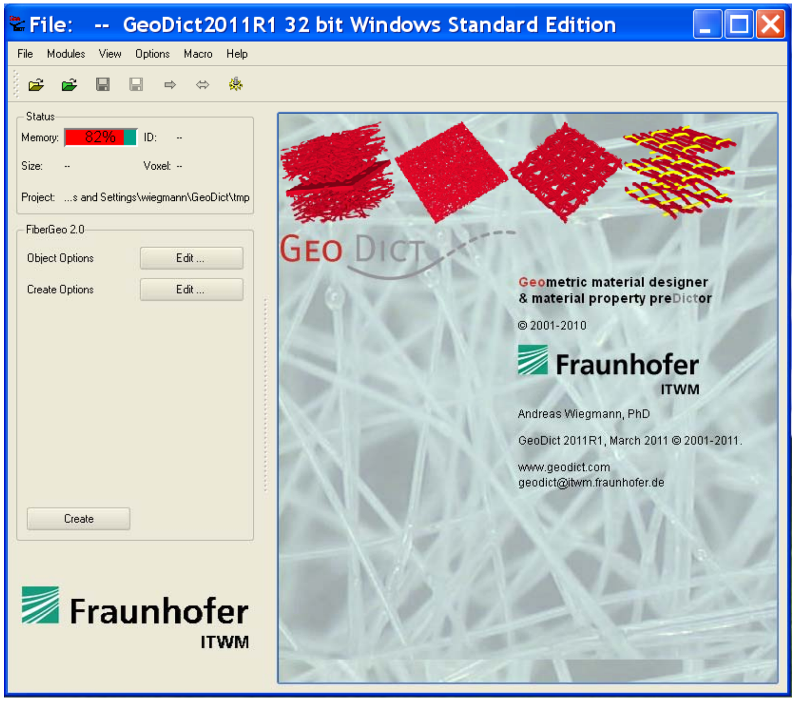
GeoDict



Modules

GEO DICT

- FiberGeo, SinterGeo, WeaveGeo, GridGeo, PackGeo, PaperGeo, PleatGeo,
- DpfGeo, LungGeo , UserGeo , GadGeo (structure generators)
- ProcessGeo (3d image processing)
- LayerGeo (layered media)
- ImportGeo (e.g. tomography, STL, .gad)
- ExportGeo (e.g. Fluent, Abaqus)
- FlowDict (single phase flow properties)
- PleatDict (porous media flow)
- ElastoDict (effective elastic properties)
- ConductoDict (effective conductivity)
- DiffuDict (effective diffusivity)
- FilterDict (pressure drop, efficiency, capacity)
- SatuDict (two phase flow properties)
- PoroDict (pore size measures)
- AcoustoDict (acoustic absorption)
- GadDict (Analysis and export of analytic descriptions)



Modules

GEO DICT

- FiberGeo, SinterGeo, WeaveGeo, GridGeo, PackGeo, PaperGeo, PleatGeo,

Every structure
• tomogram or
• generated
is compatible with every
property simulation!

- GadDict (Analysis and export of analytic descriptions)

Outline

- GeoDict in general
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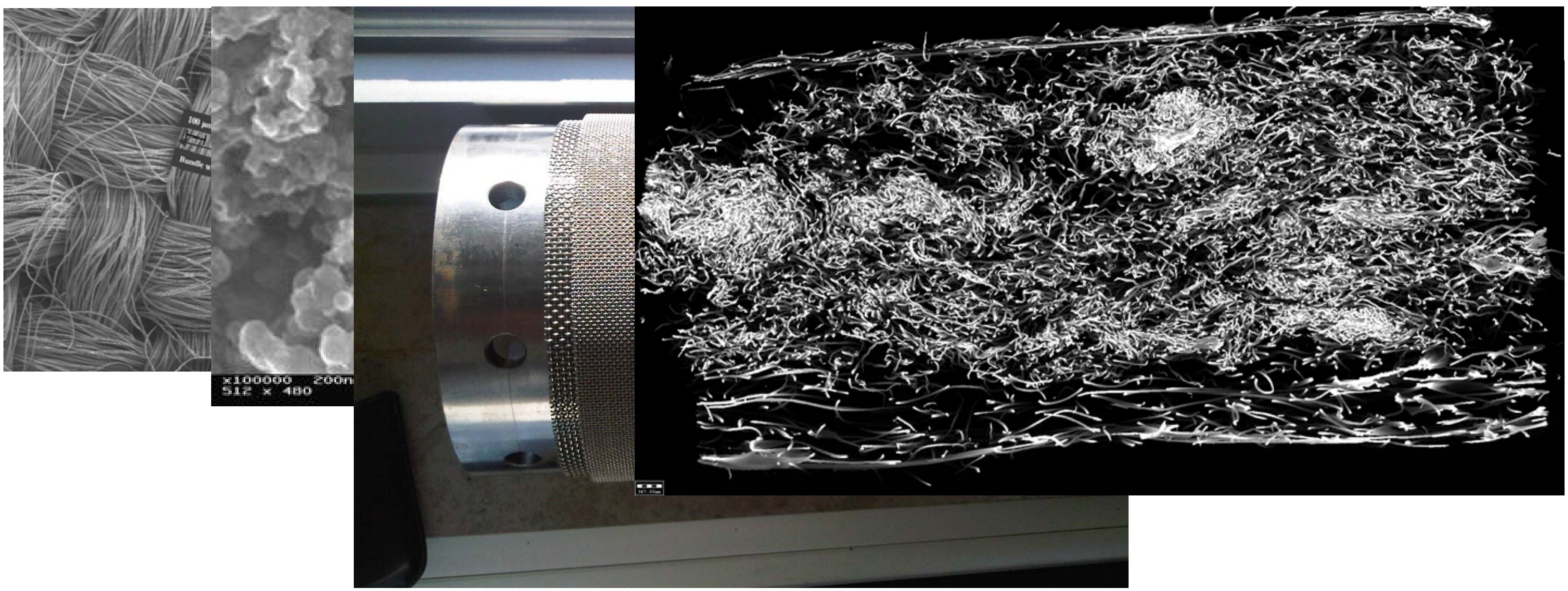
Scanning Electron Microscopy, photo & tomogram of thin porous media

GEO DICT

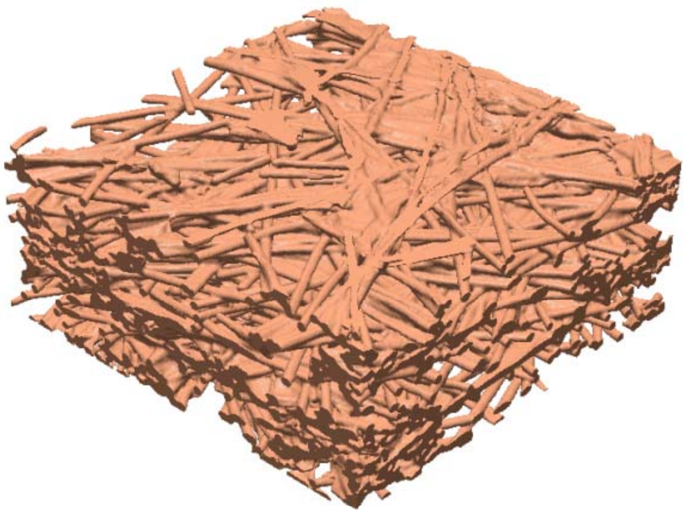
- Gas Diffusion Layer, Micro Porous Layer, Metal wire mesh and Cellulose media

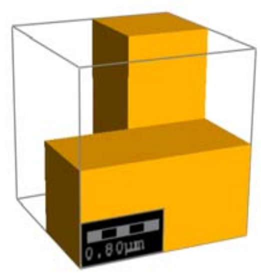


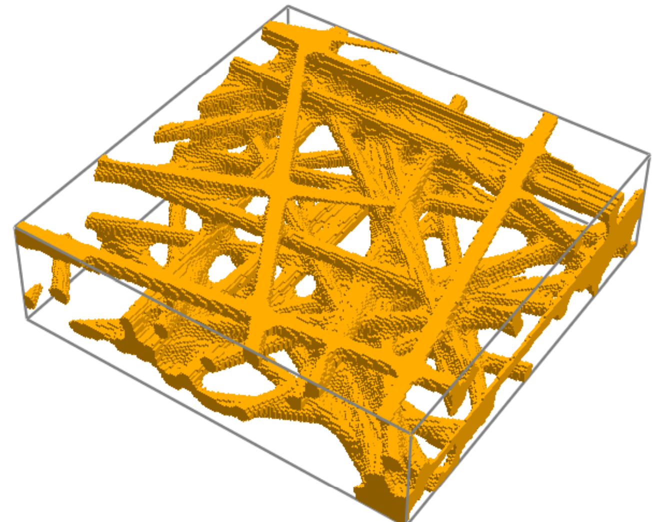
3d structure idea

- Two sources:
- 1) tomography image (segmentation)

2) virtually generated
(stochastic geometry)





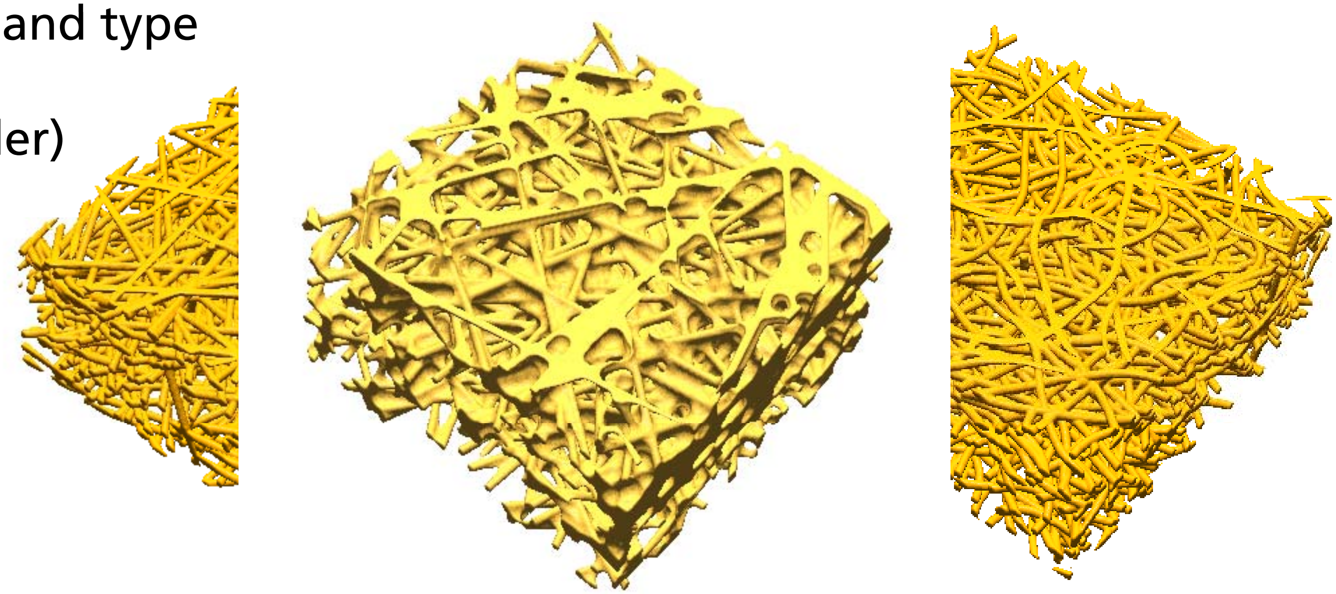


all structure models:
cubic voxels (voxel = volume celll)

3D Models:
Gas Diffusion Layer (GDL)

- Typically: nonwoven fibre structures plus binder

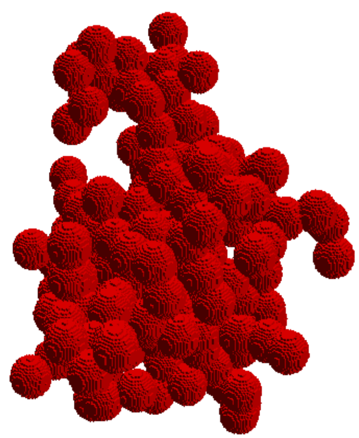
- Input:
  - Porosity
  - Fibre diameter and type
  - Anisotropy
  - (Weight% binder)
  - (Fibre crimp)

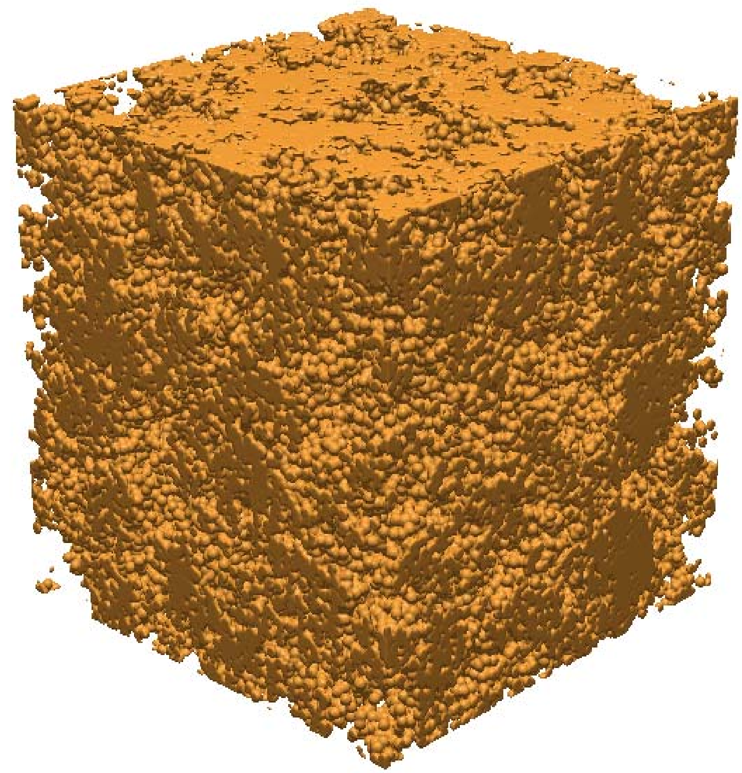


3D Models:
Microporous Layer (MPL)

GEO DICT

- Typically: carbon agglomerates
- Input:
  - Particle size
  - Particles per Agglomerate
  - Porosity

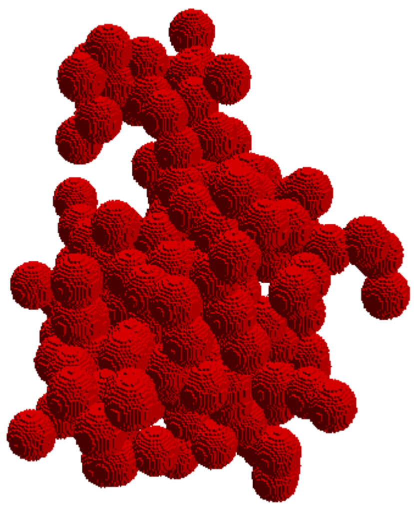


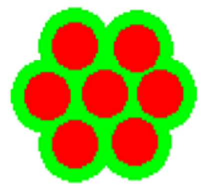


Becker, Wieser, Fell, Steiner, 2011, to appear

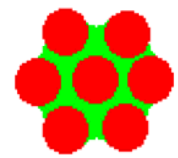
3D Models: Catalyst Layer (CL)

- Carbon agglomerates plus elektrolyte





Elekt. surrounds C. Partikels



Elekt. between C. Partikels

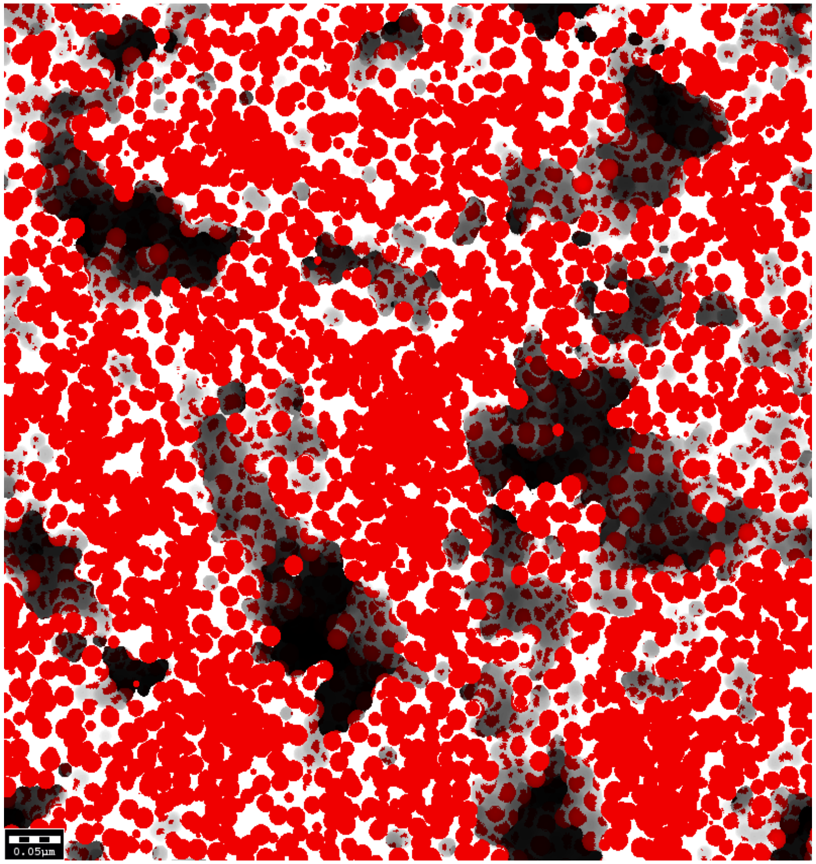
Elekt. surrounds C. Partikels but not in between

3D Models: Catalyst Layer (CL)

- Model example:

- Porosity 33.3 %
- Carbon/Pt 50.1 vol%
- Elektrolyte 16.6 vol%

- Size: (800 nm)³, voxel length 1 nm



GDL model(fuel cell)

GEO DICT

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.

Pipeline model (Oil & Gas)

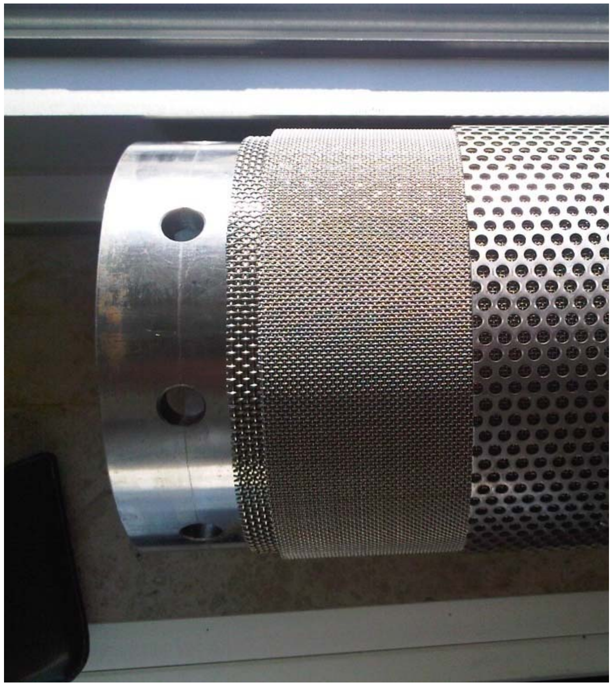
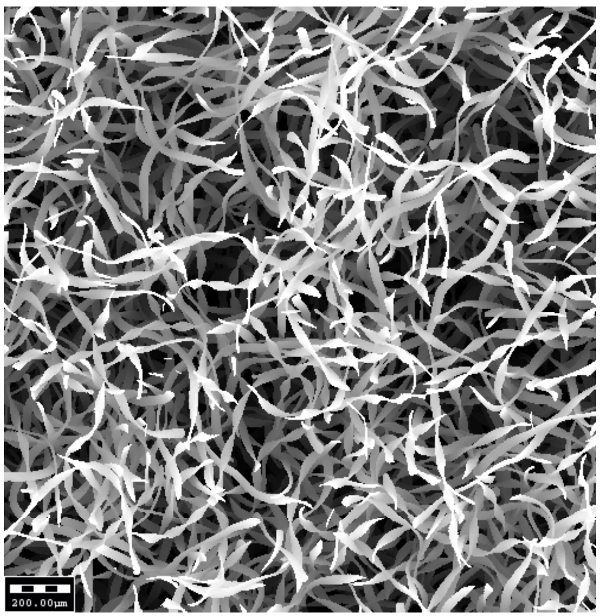
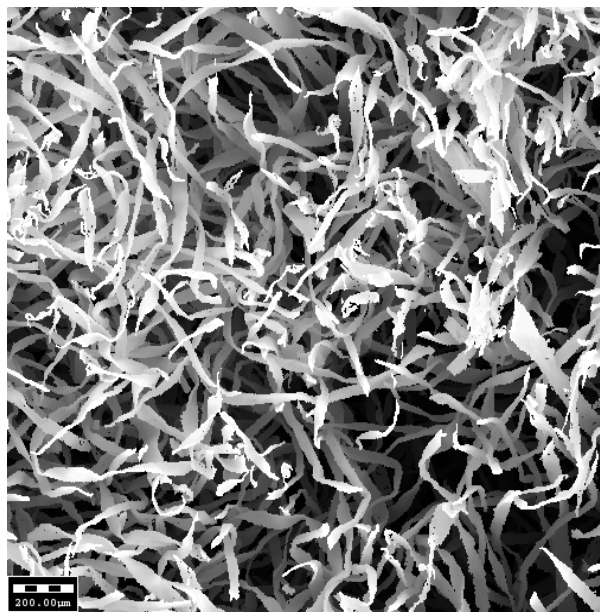
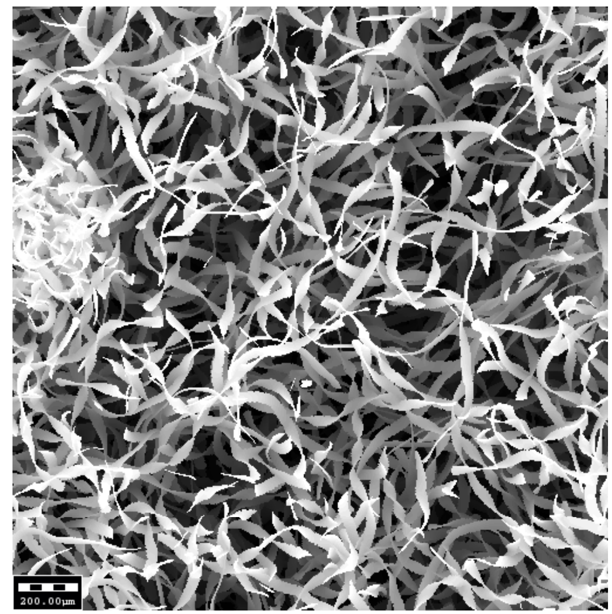


Photo: M. Knefel Gebrüder Kufferath, Düren,
Modell: E. Glatt, Fraunhofer ITWM, with GeoDict

Nonwoven model

GEO DICT

Homogeneous	Tomogram	Inhomogeneous
		

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Determination of Effective Properties

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

- 3d Image ***is*** the computational grid
- Grid from µCT by segmentation
- Grid for models by discretization (vCT)
- Memory: factor 30 over Fluent
- Run-time: FFT-methods possible
- Simple visualization: structure, solution

Geometric analysis

GeoDict

- Connectivity
- Pore size distribution
- Tortuosity
- **Anisotropy**
- Specific surface area
- Triple lines
- Etc. etc

Cross section of resin-embedded fleece, in plane

GEO DICT

In plane,
1,1mm x 1,1mm
magnification: 10x

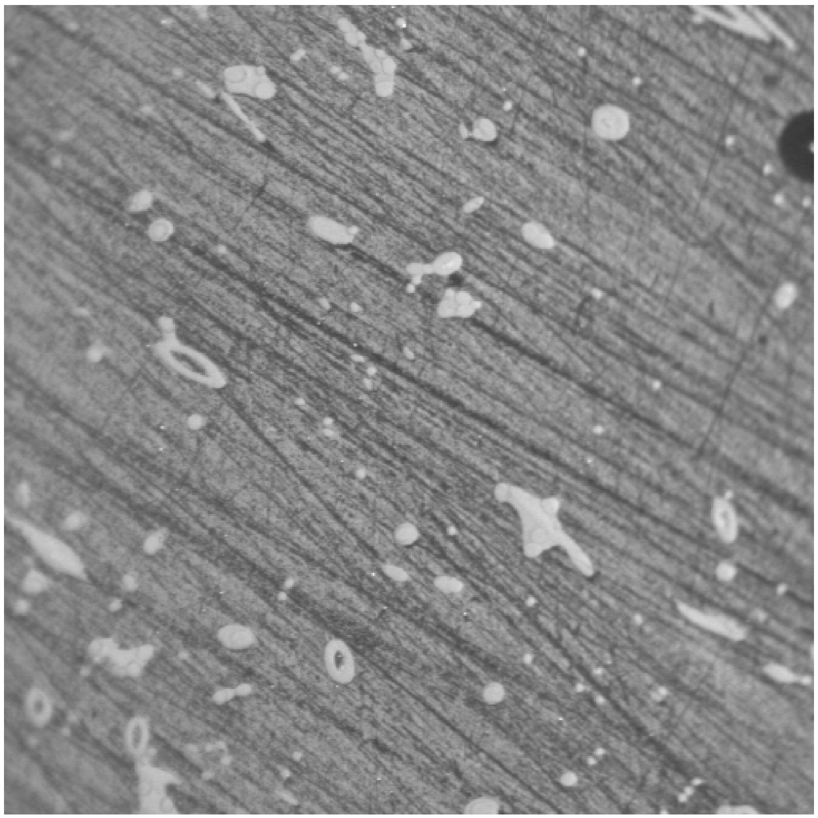
Cross section of resin-embedded fleece, in plane

In plane,
1,1mm x 1,1mm
magnification: 10x

Cross section of resin-embedded fleece, in plane

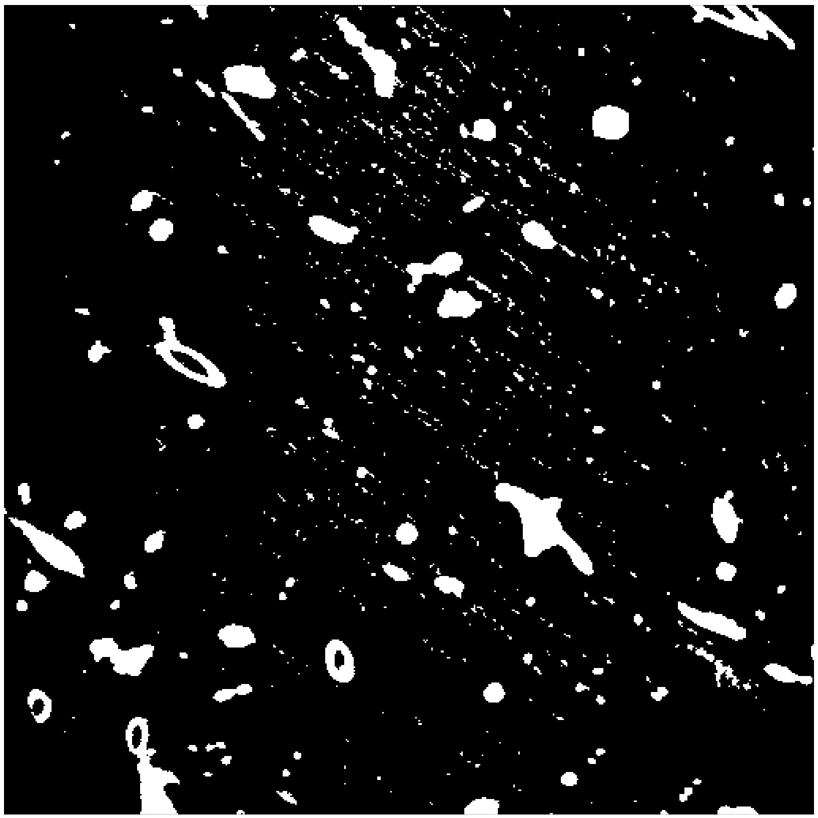
In plane,
1,1mm x 1,1mm
magnification: 10x

Cross section of resin-embedded fleece, through plane



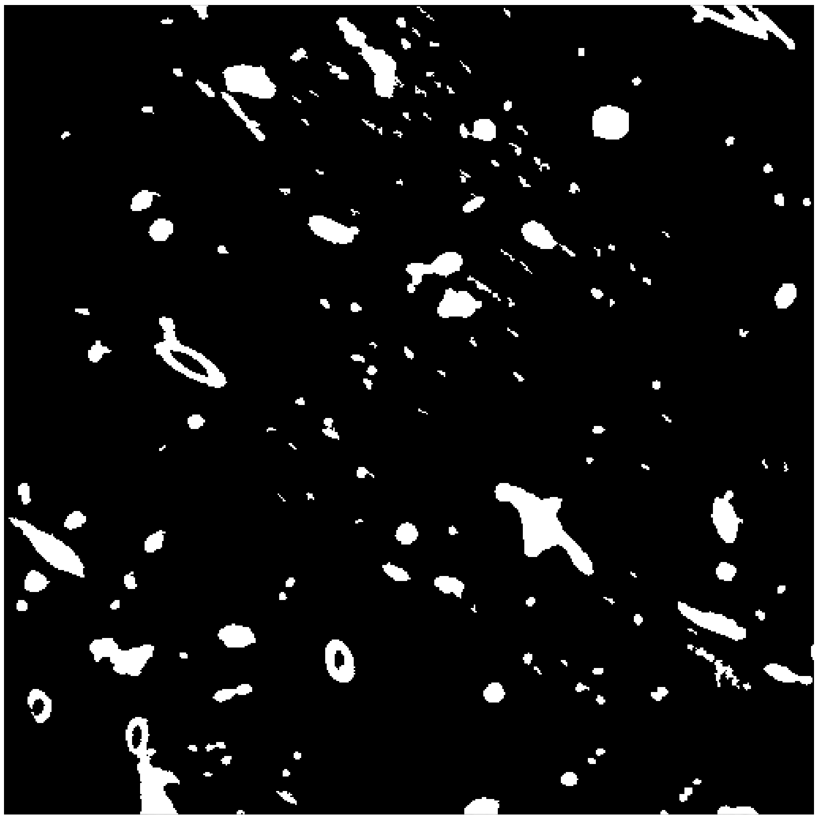
Through plane,
1,1mm x 1,1mm
magnification: 10x

Cross section of resin-embedded fleece, through plane



Through plane,
1,1mm x 1,1mm
magnification: 10x

Cross section of resin-embedded fleece, through plane

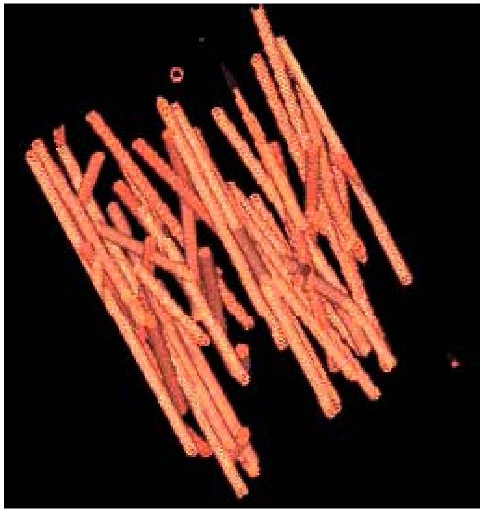


Through plane,
1,1mm x 1,1mm
magnification: 10x

Estimation of the anisotropy:

GEO DICT

Can estimate the anisotropy from the number of connected white components in the images



Use 5 images each:

IP: 35, 36, 48, 79, 61 -- 52

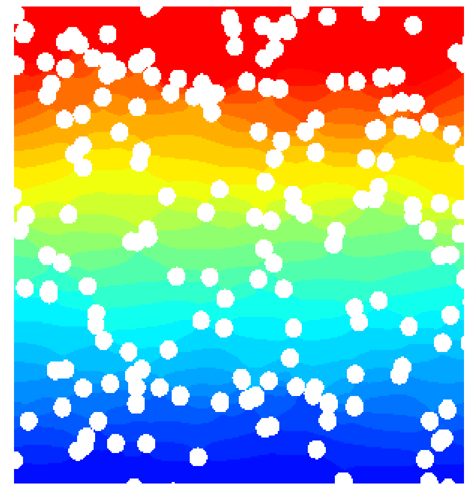
TP: 164, 144, 158, 170, 168 -- 161

find ß ~4,1 for the original (uncompressed) fleece.

Effective diffusivity

- **Macroscopic description (homogenized porous media model)**
- Fick's first law: $j = -D^* \nabla c$
- D^* : effective diffusivity [m²/s] ***unknown***
- j : diffusion flux [mol/m²/s]
- c : concentration [mol/m³]
- **Microscopic description (pore structure model)**
- Laplace equation: $-\Delta c = 0$
- Boundary conditions: no-flux on fibre surface, concentration drop
- D^* can be determined from the solution!

c=1

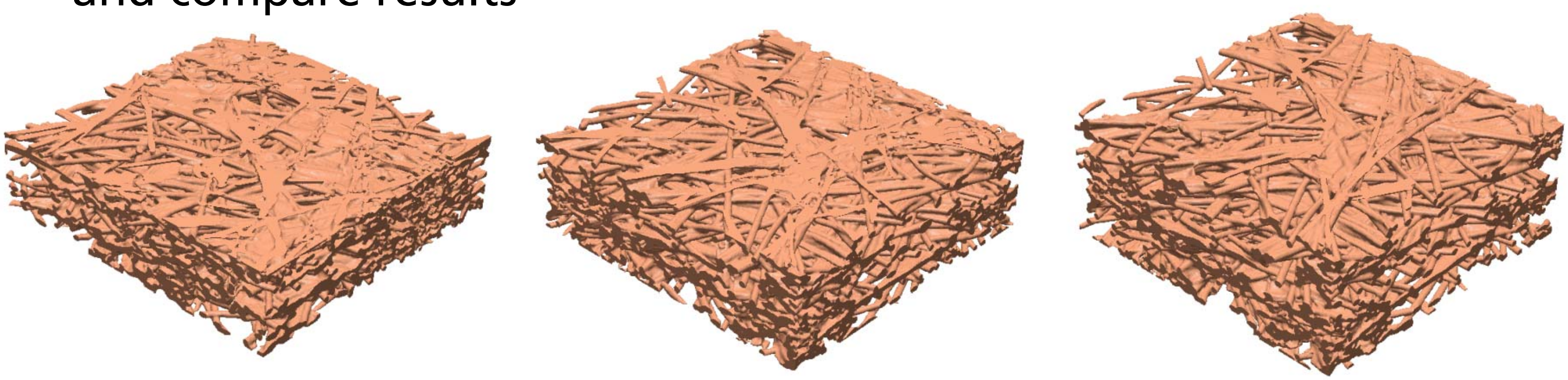


c=0

Validation:
Toray TGP H 060 Gas Diffusion Layer

- Data from PSI:
- Tomography images of Toray TGP H 060 at different compression levels
- Diffusivity, permeability and conductivity were measured at different compression levels experimentally

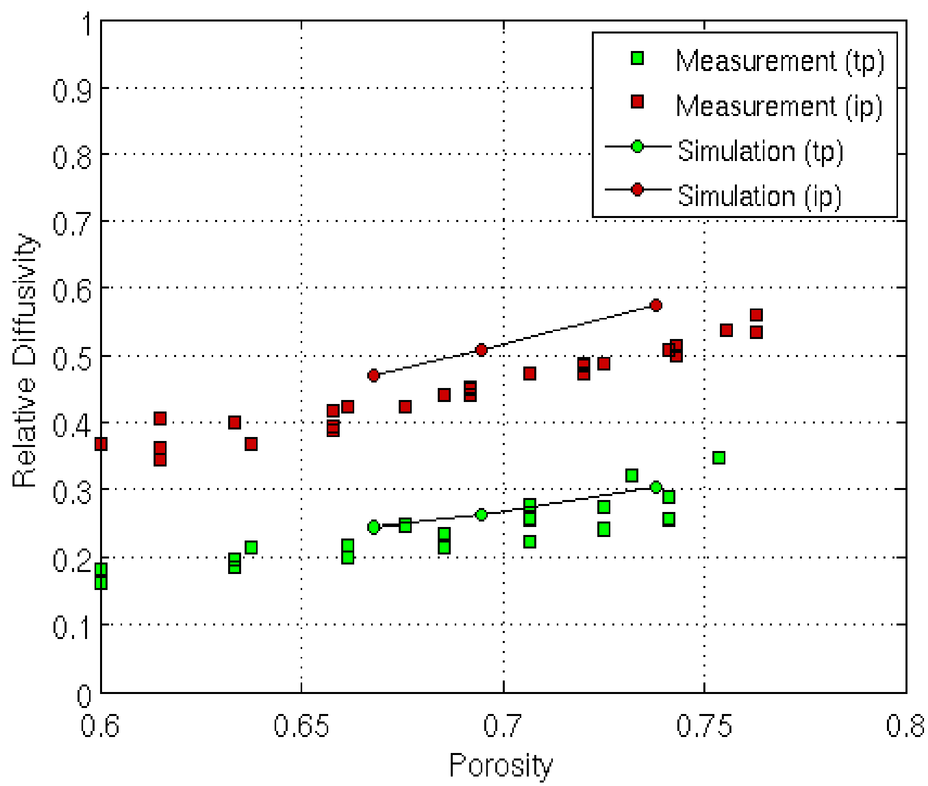
- Now: compute diffusivity, permeability and conductivity numerically and compare results



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

Diffusivity

GEO DICT

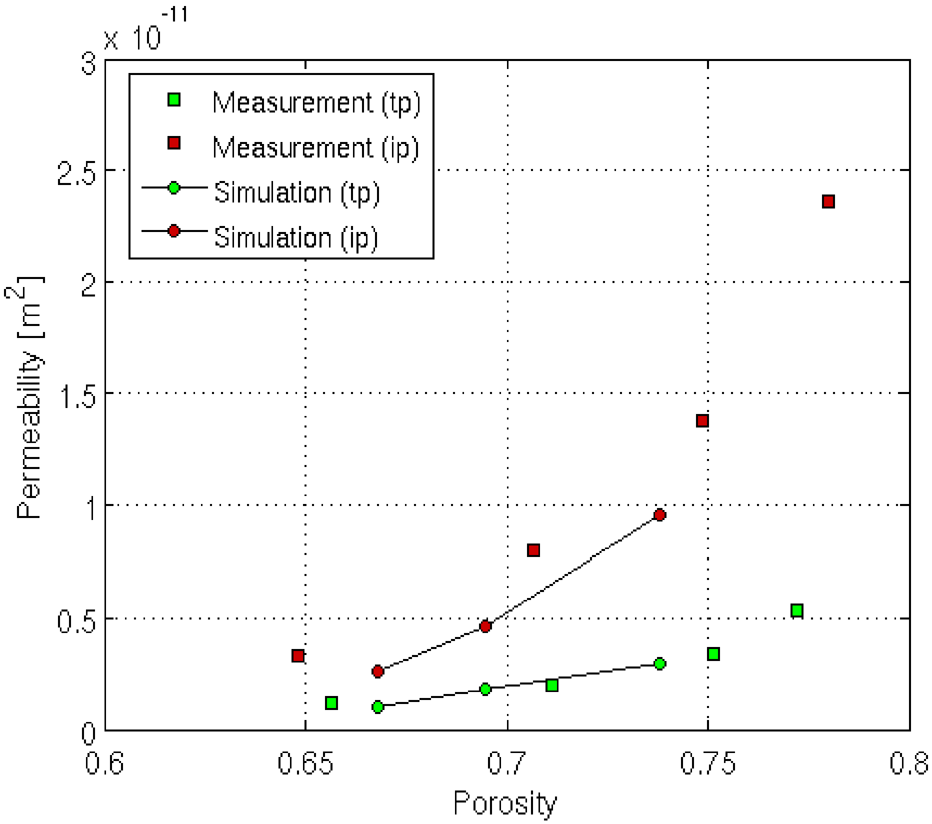


Perfect in tp-direction

Small differences in ip-direction

1. ip-measurememts performed on a stack of GDLs
2. tomography image shows single layer between sample holder

Permeability

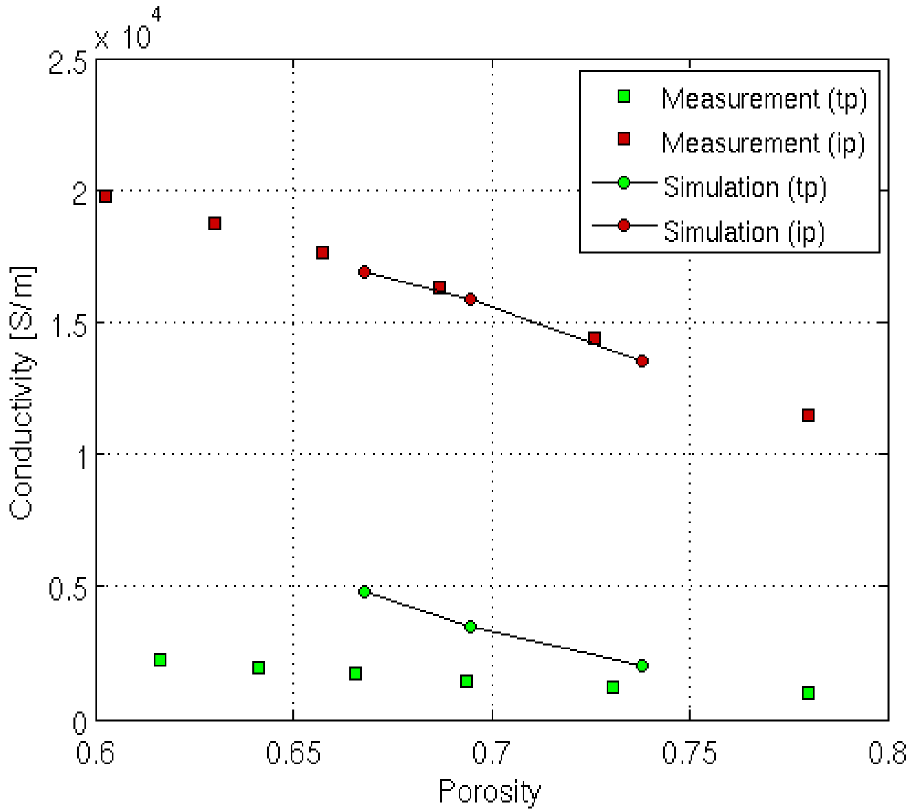


Perfect in tp-direction

Small differences in ip-direction

1. ip-measurememts performed on a stack of GDLs
2. tomography image shows single layer between sample holder

Electric Conductivity

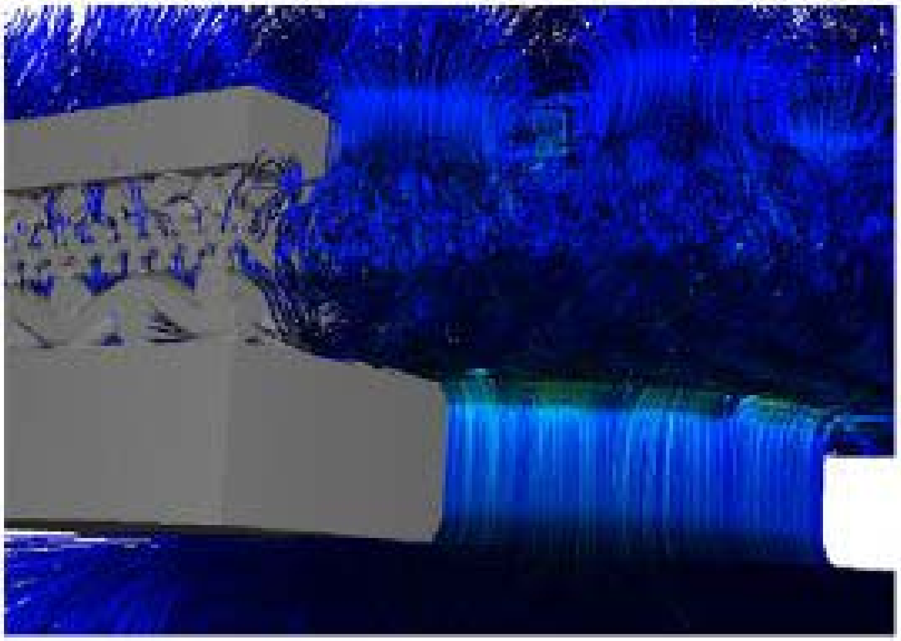


Tp-conductivity too high!

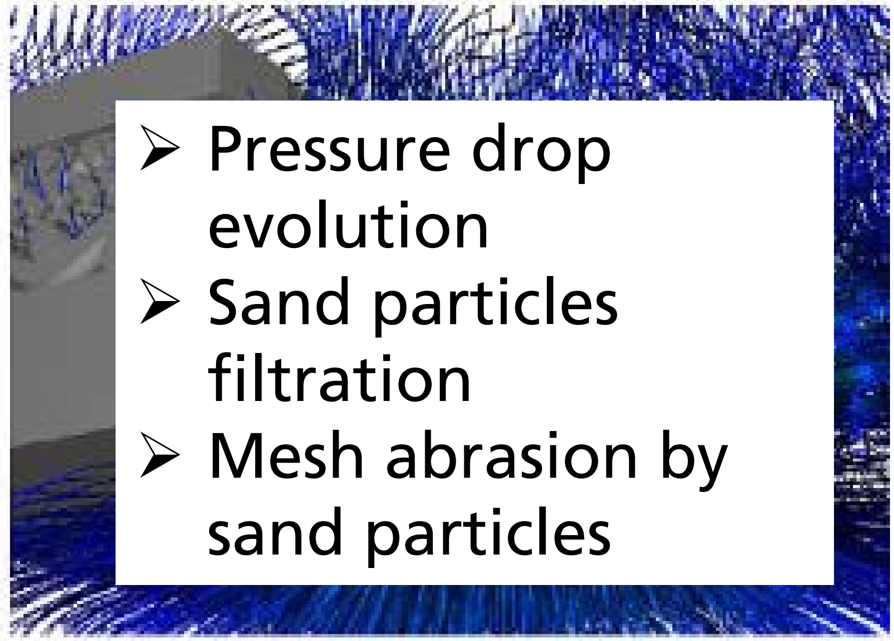
Reason: model assumes a perfect contact between the fibres (and the binder)

Pipeline model

GEO DICT



Picture 5: 3D visualisation of the flowlines.

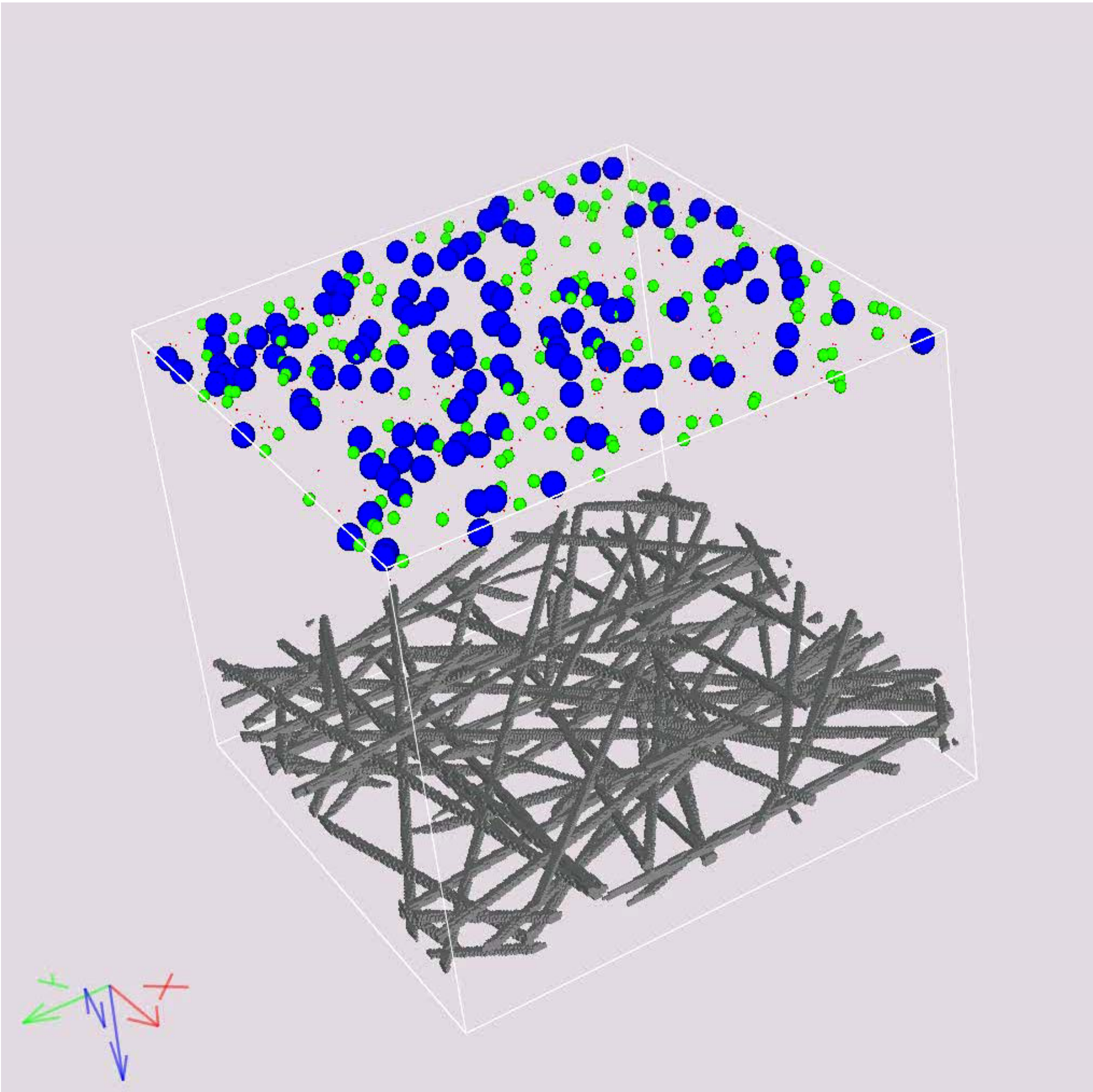


- Pressure drop evolution
- Sand particles filtration
- Mesh abrasion by sand particles

Picture 6: Simulation of the multilayer mesh with a reduced number of flowlines.

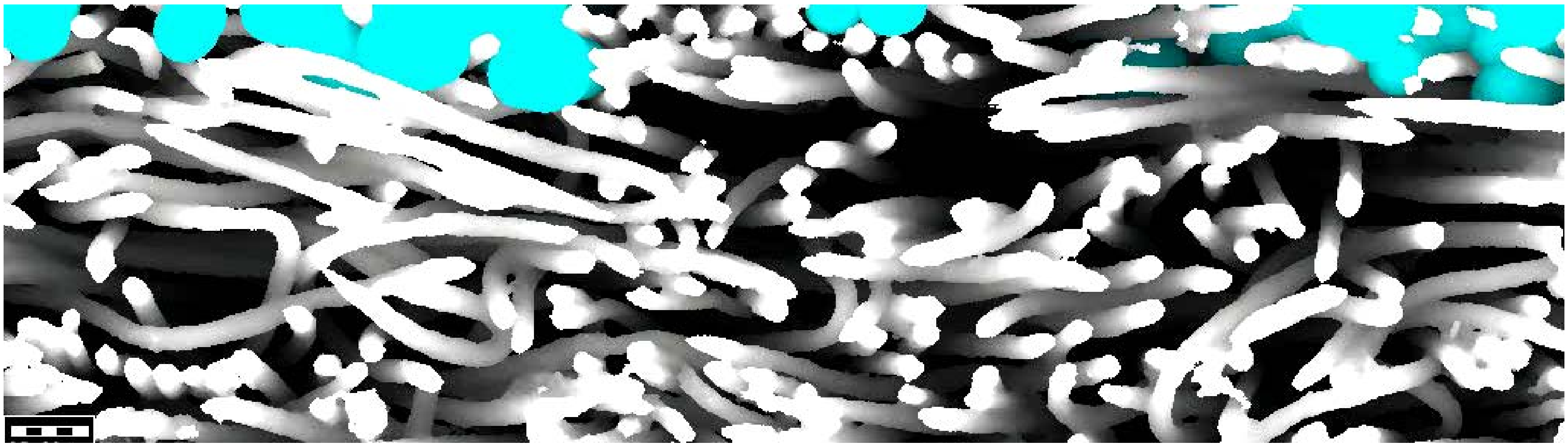
Flow simulations and Visualizations: M. Knefel, Gebrüder Kufferath, Düren, using GeoDict and built-in *ParPac* Lattice-Boltzmann solver

Filtration: Cake formation



- Filter Efficiency evolution
- Pressure drop evolution

Bubble point

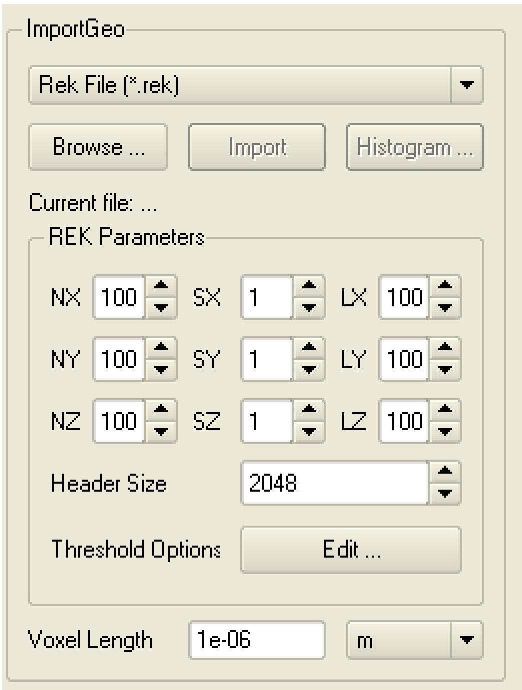


- Pressure at which break through occurs

Outline

- GeoDict in general
- Thin porous Media
- Material properties
- **GeoDict: Software for Virtual Material Design**

Pre-processing:
Import & Structure Generation



Import + segmentation
or structure generation
both yield segmented 3d image

Input parameters are measurables like porosity, fiber orientation, fiber diameter distribution

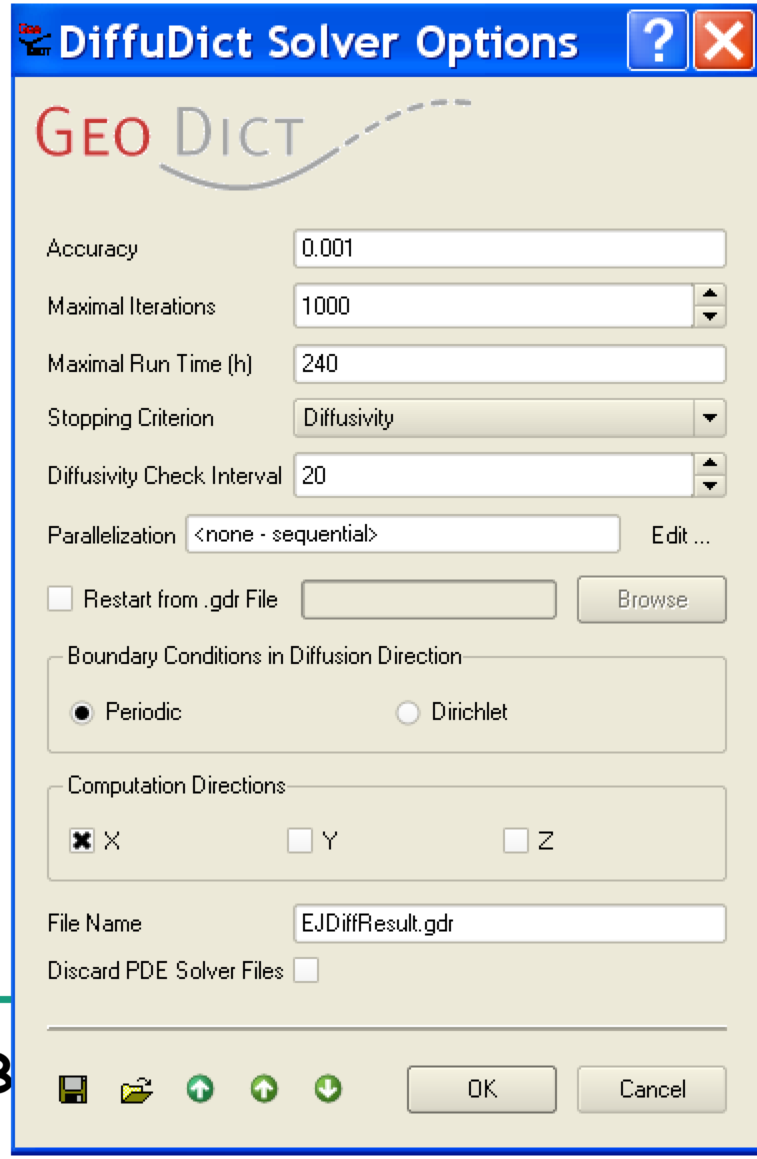
Randomness reproducible via random seeds

Solve: Standardized Property Computation

GEO DICT

For any pde, the solver options always have similar options and meaning

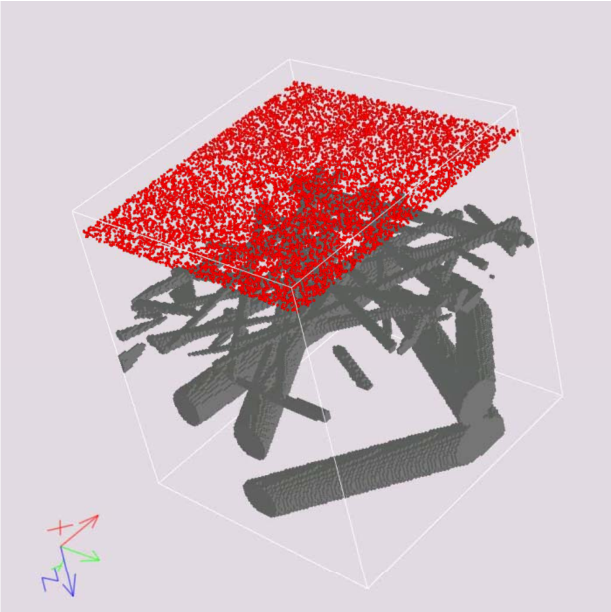
The results are available as detailed solution and aggregated into effective properties like diffusivity, filter efficiency, etc.



Postprocessing:
Visualization, Animation, Dexcel & MATLAB

- Structures and result fields can be visualized and animated in 2d and 3d, as slices, virtual REM or vCT
- Analysis available in Excel or MATLAB
- All operations are scriptable / reproducible
- Software runs in Linux and Windows
- All codes use common framework 3d structure classes, settings classes, etc. etc.

- All animations / visualizations done with GeoDict



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Rolf Westerteiger

PaperGeo
Erik Glatt

Find out more:

www.geodict.com

www.itwm.fhg.de

live demo outside

GeoDict Mission

- To help our industrial partners reduce R&D cost in terms of time and money for their ***material analysis, material developments and product developments***.
- To save our academic partners time to ***focus on research in their own discipline*** and not on the details of Mathematics or Computer Science.
- To minimize the need for real experiments by providing software. GeoDict ***performs standardized computer simulations*** yielding results on tomograms and model structures that are ***directly comparable to experiments***.