Numerical Determination of Effective Material Properties of Porous Media

MMM, Freiburg, 08.10.2010

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- Fraunhofer Institute for Industrial Mathematics ITWM
- Kaiserslautern, Germany

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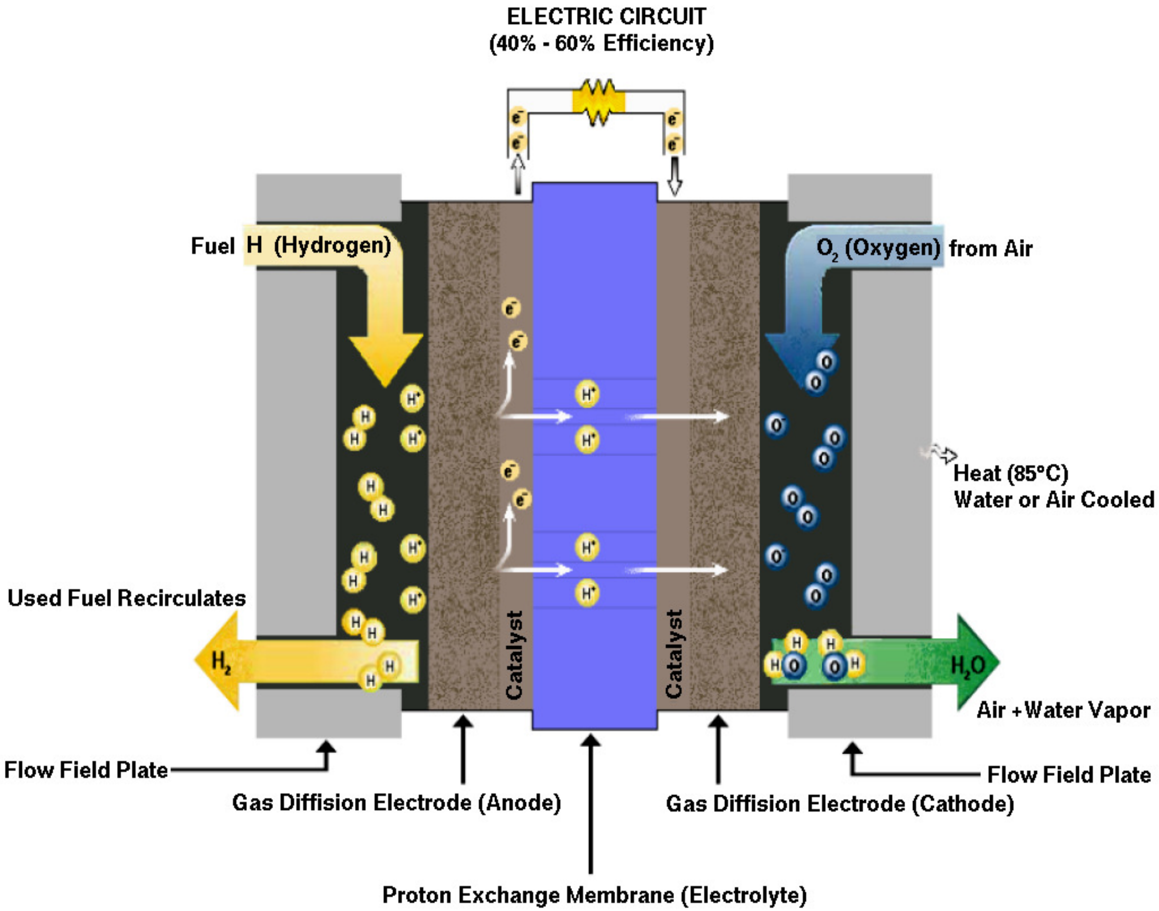
Application Example:
Porous Layers inside PEM Fuel Cell



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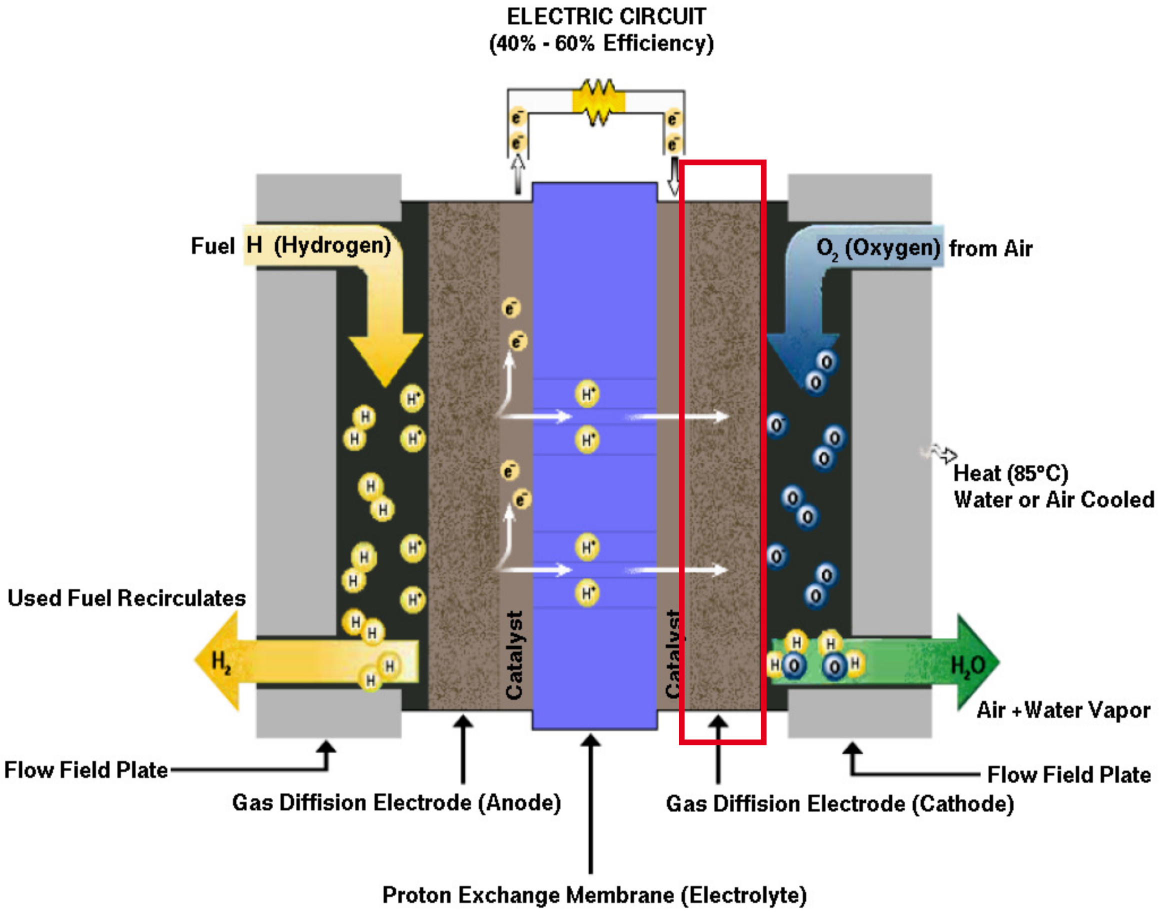
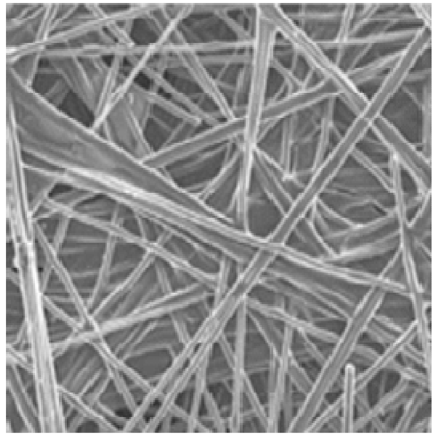
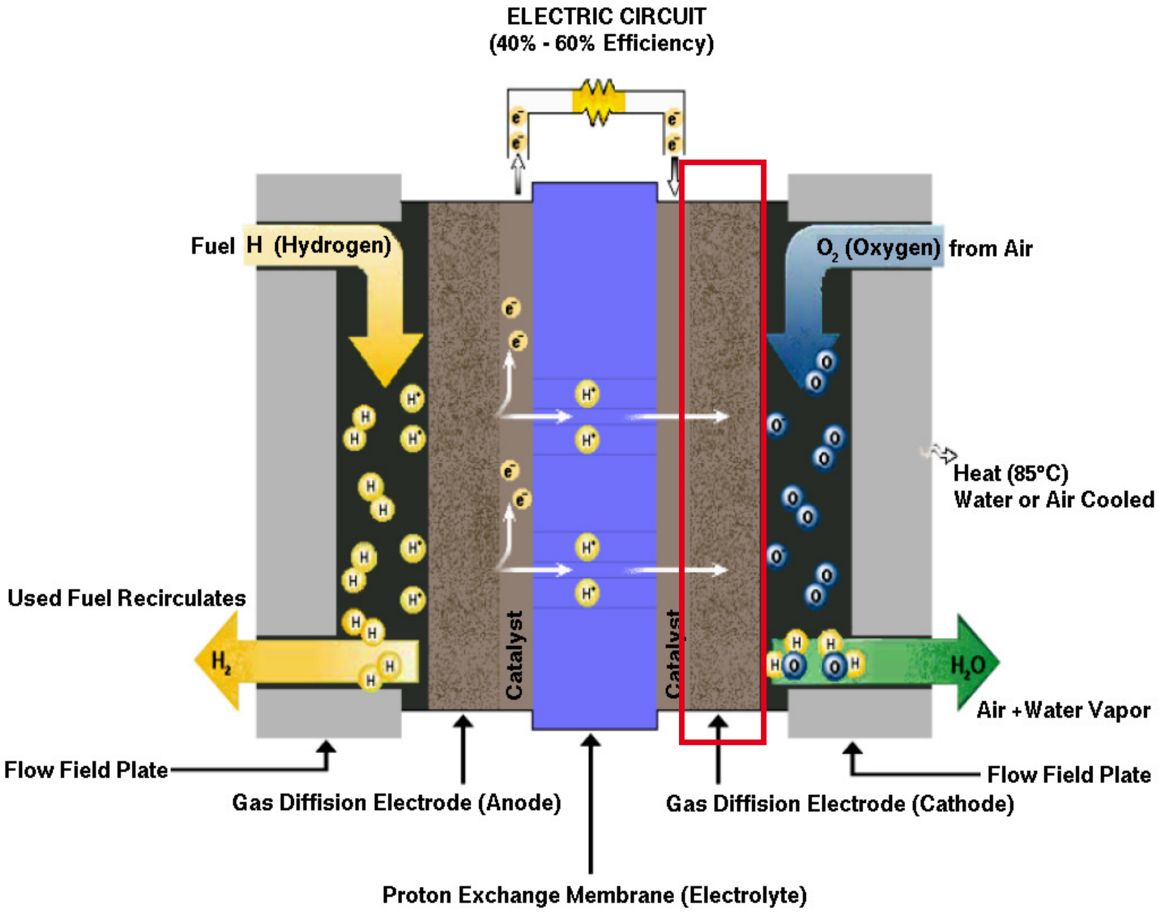
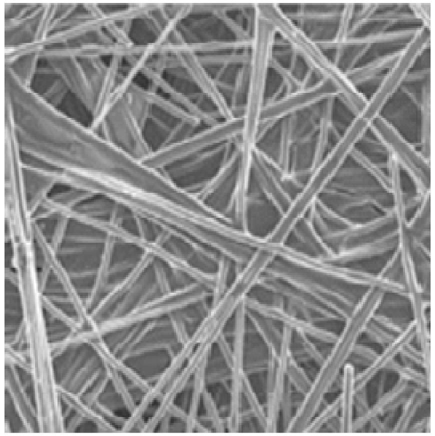




Gas Diffusion layer

Application Example:
Porous Layers inside PEM Fuel Cell





Gas Diffusion layer

Aim: engineer a better GDL !

Better ?
- higher electronic conductivity
- higher diffusivity
- higher stability
- ??

Properties are dependent on
- material type
- pore structure

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Computer Aided Material Engineering

1. General Approach

2. Applications
   - PEM Fuel Cell Gas Diffusion Layer
   - Others

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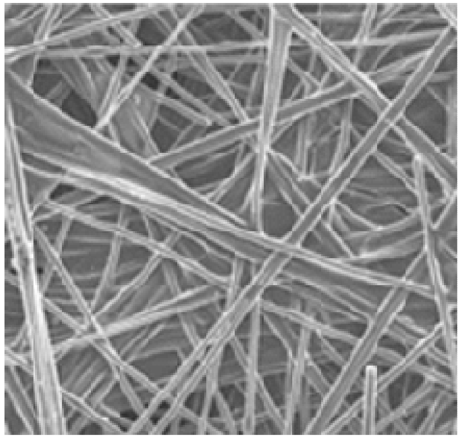
Aim: Computer Aided Material Engineering

Lab

Porous Material



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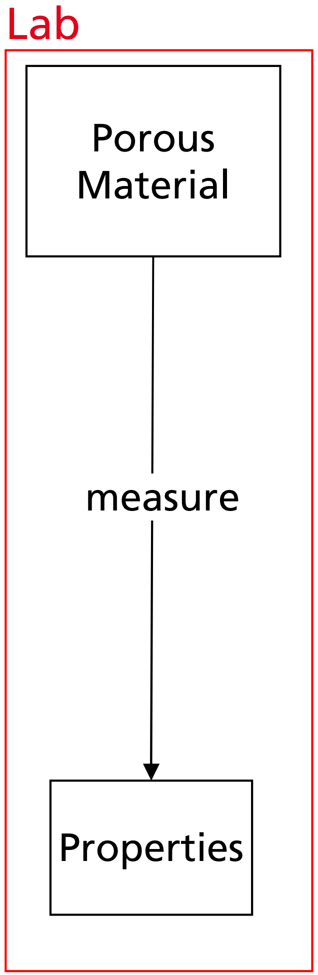
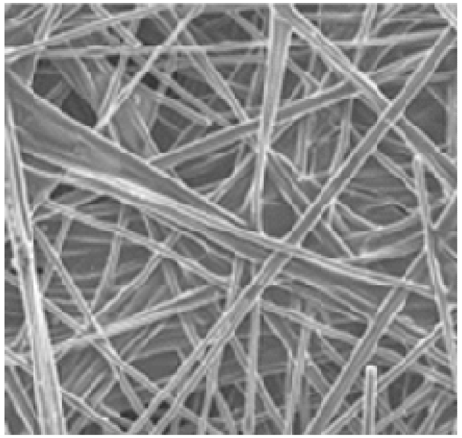
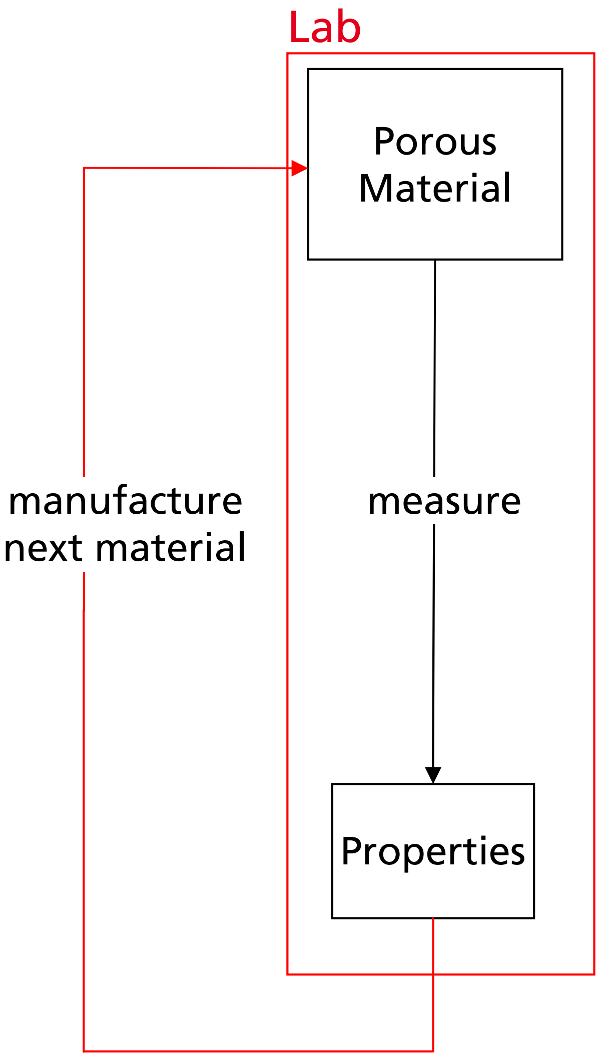


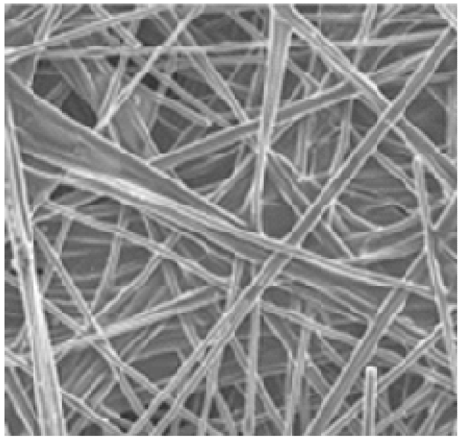


Properties are:

- pore size distribution
- permeability
- diffusivity
- capillary pressure curve
- ...

Aim: Computer Aided Material Engineering





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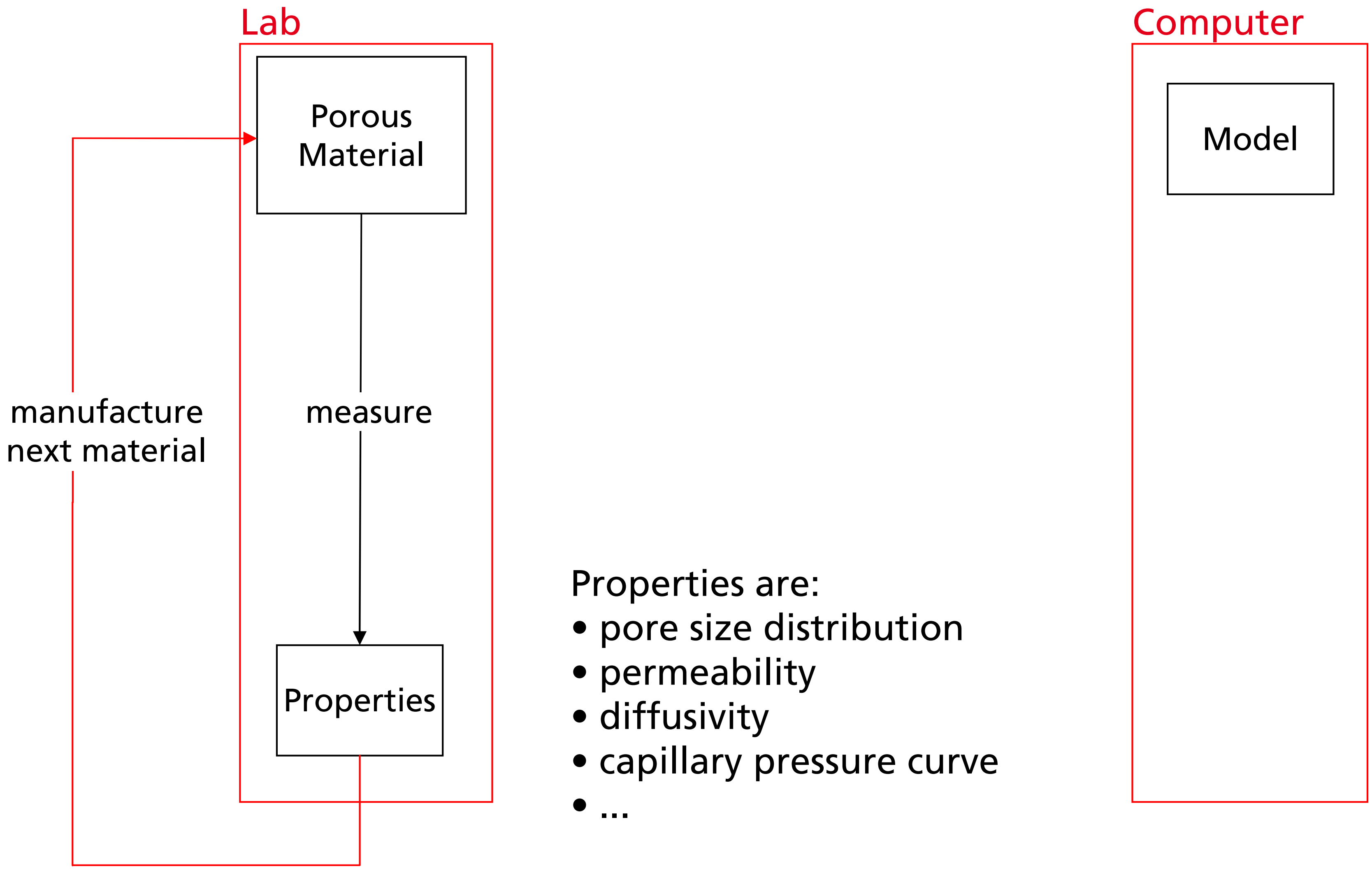

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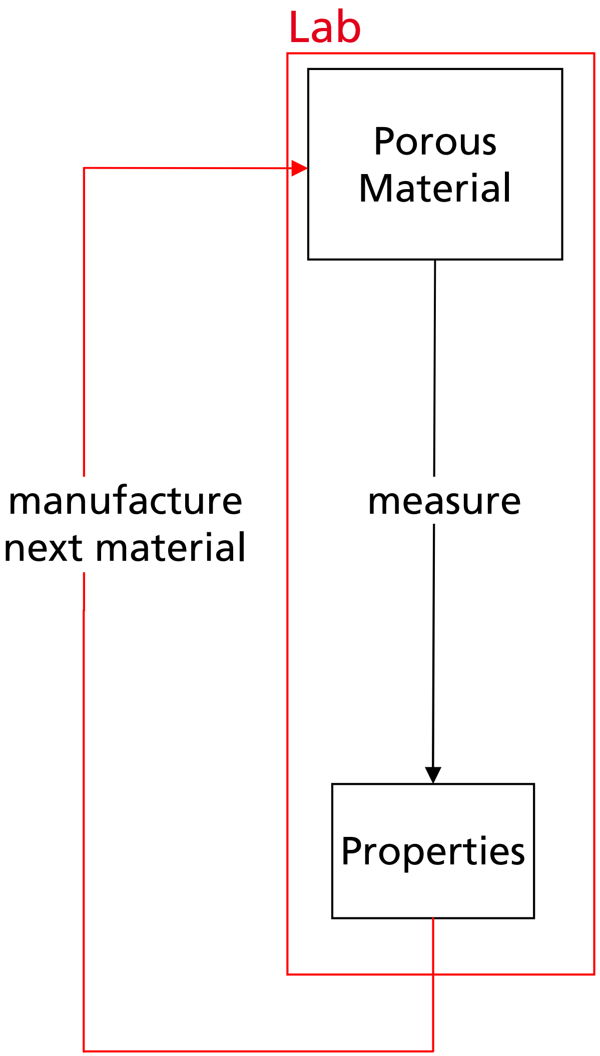

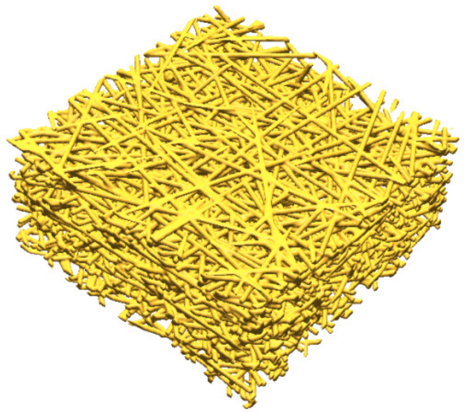

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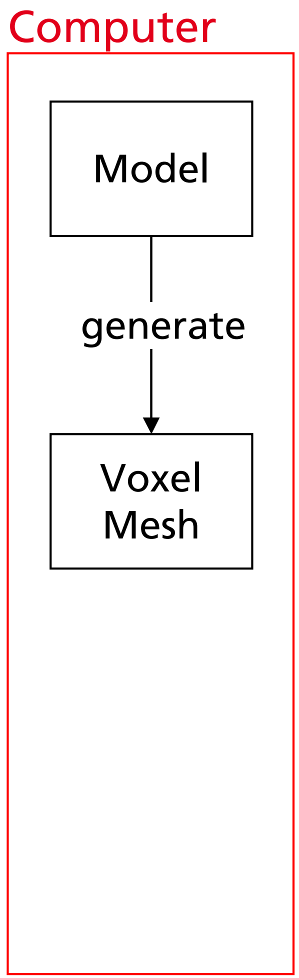


Aim: Computer Aided Material Engineering

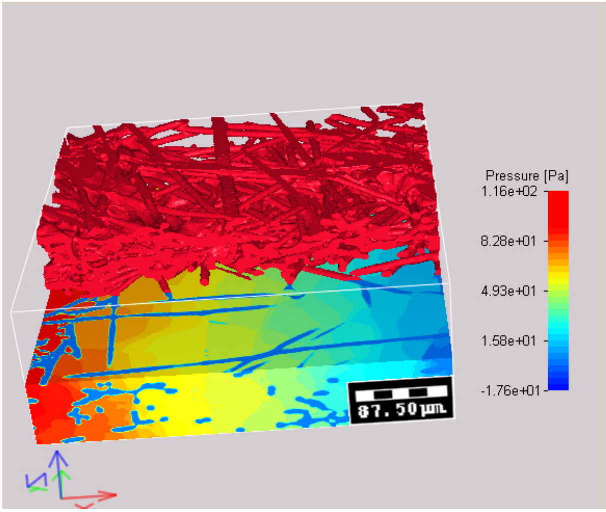
Lab

Porous Material

measure

Properties

manufacture next material



Properties are:
- pore size distribution
- permeability
- diffusivity
- capillary pressure curve
- ...

Computer

Model

generate

Voxel Mesh

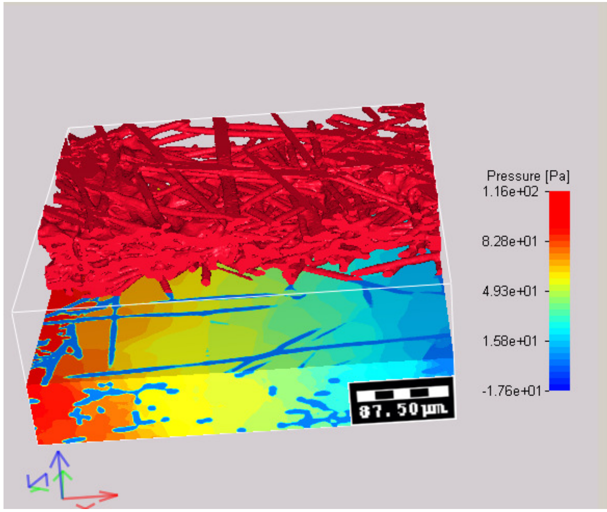
compute

Properties

Aim: Computer Aided Material Engineering

Lab

Porous Material → measure → Properties → manufacture next material



Properties are:
- pore size distribution
- permeability
- diffusivity
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- ...

Computer

Model → generate → Voxel Mesh → compute → Properties → try next set of parameters

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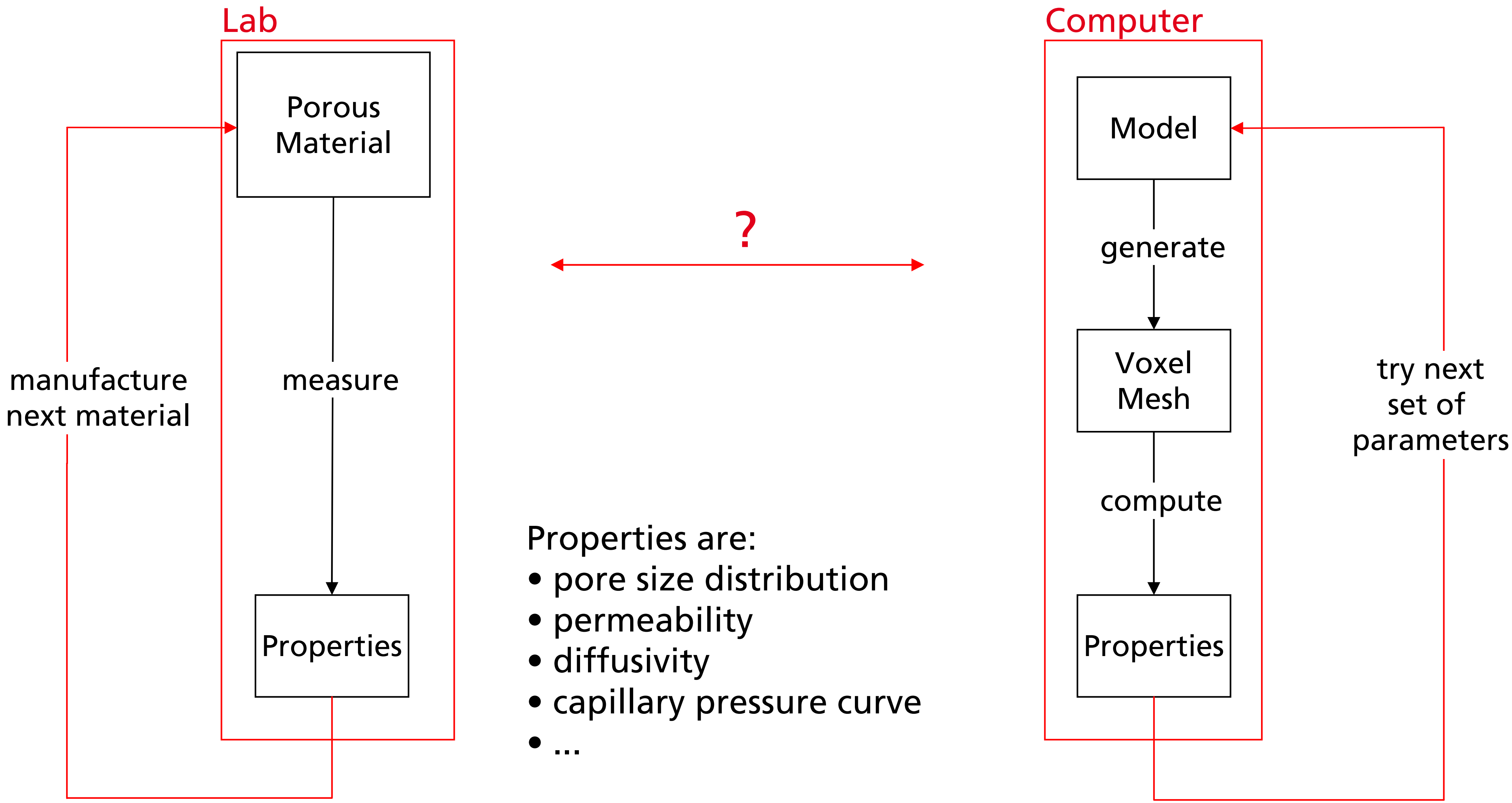
Aim: Computer Aided Material Engineering



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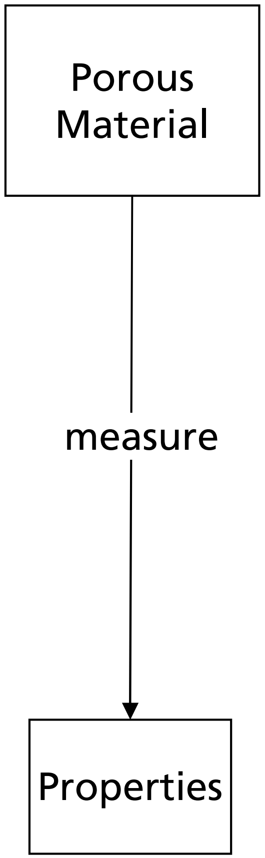
Validation - Step 1: Property Computations



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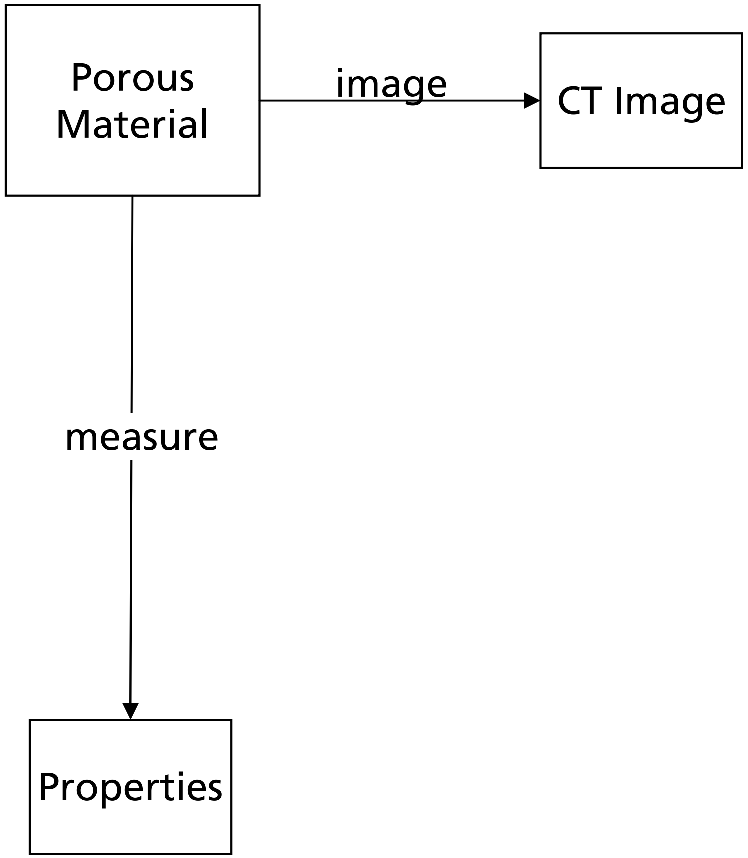

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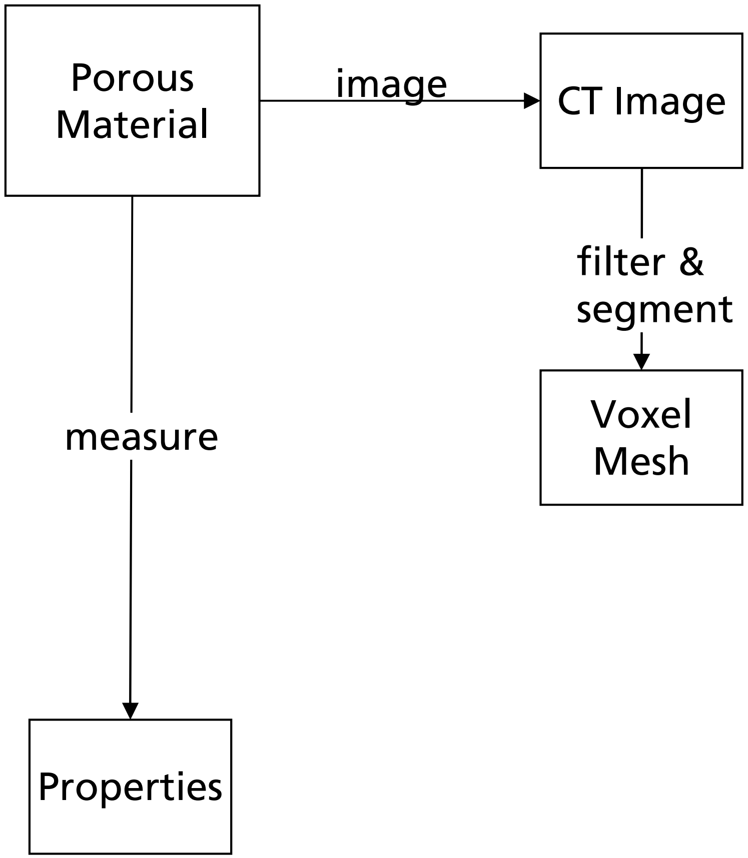

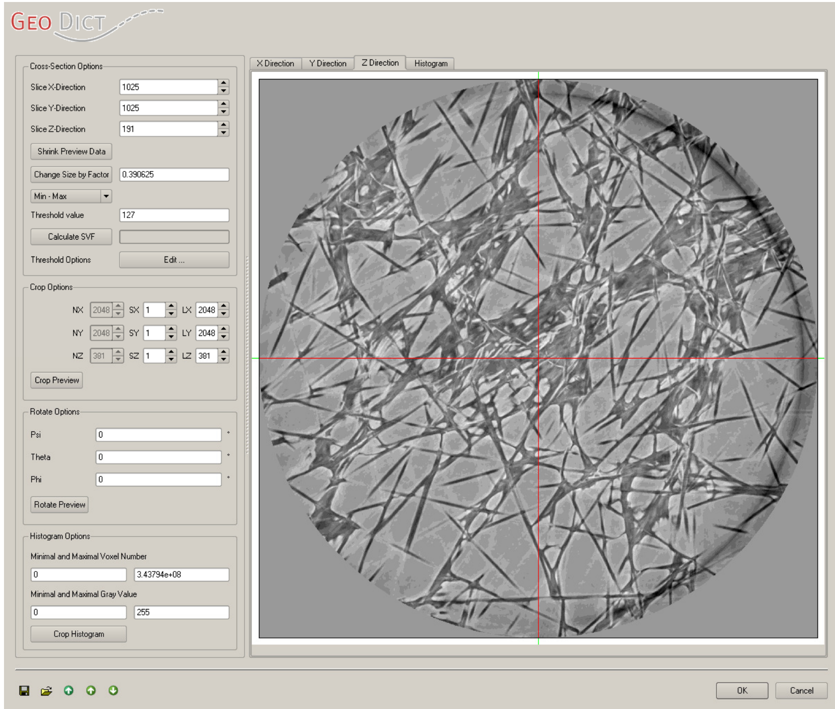

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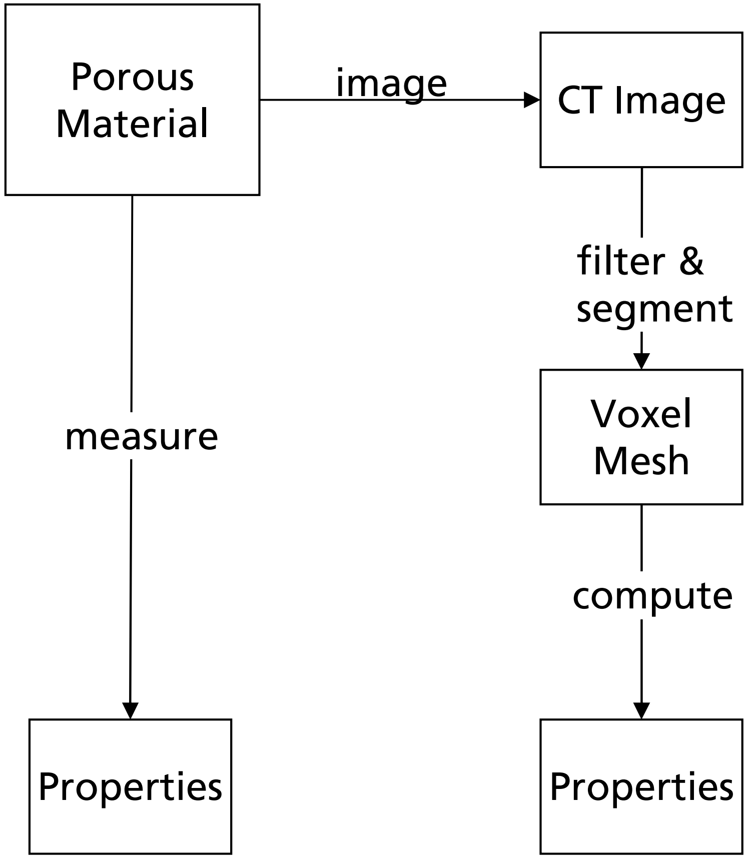

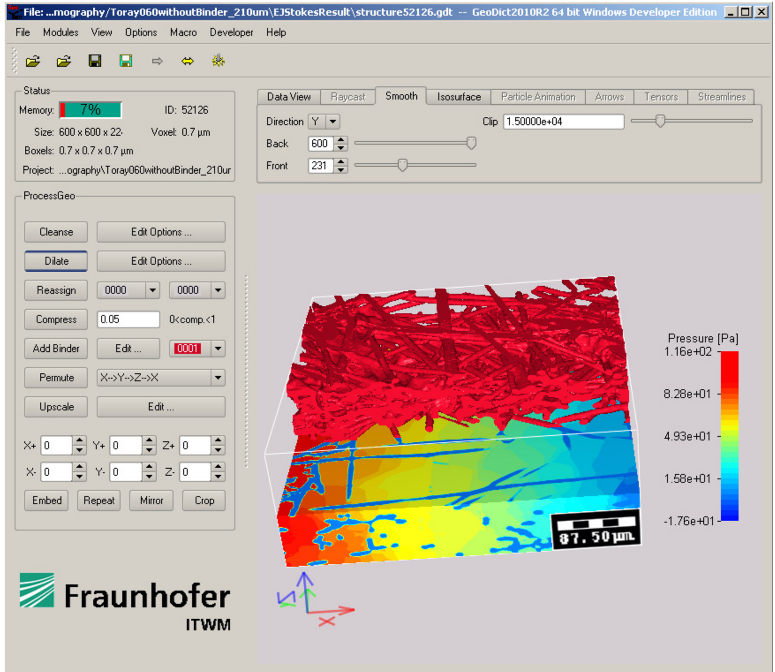

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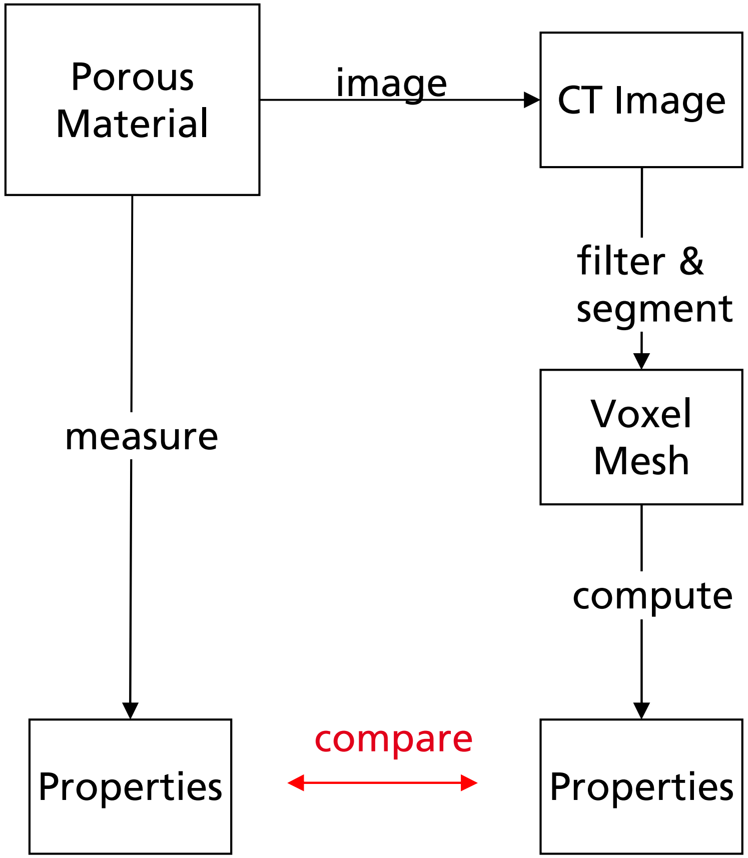

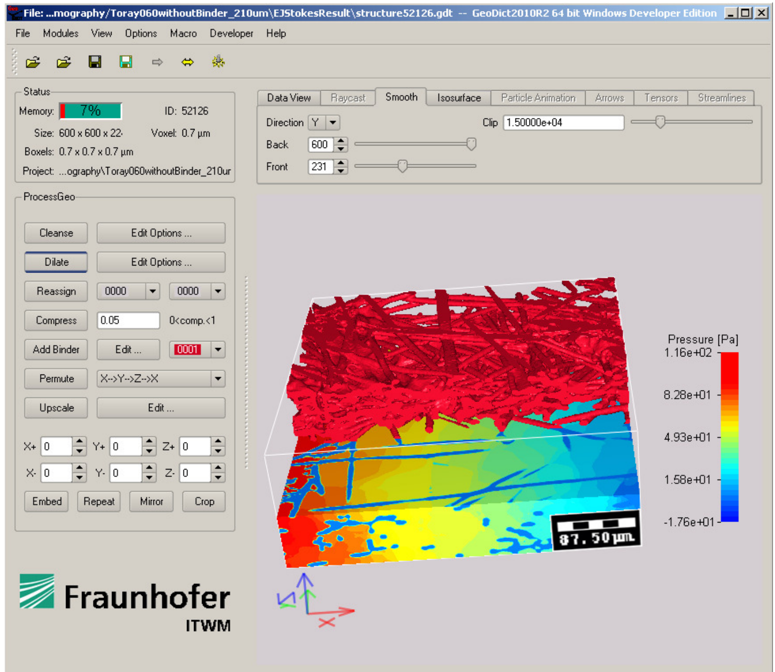

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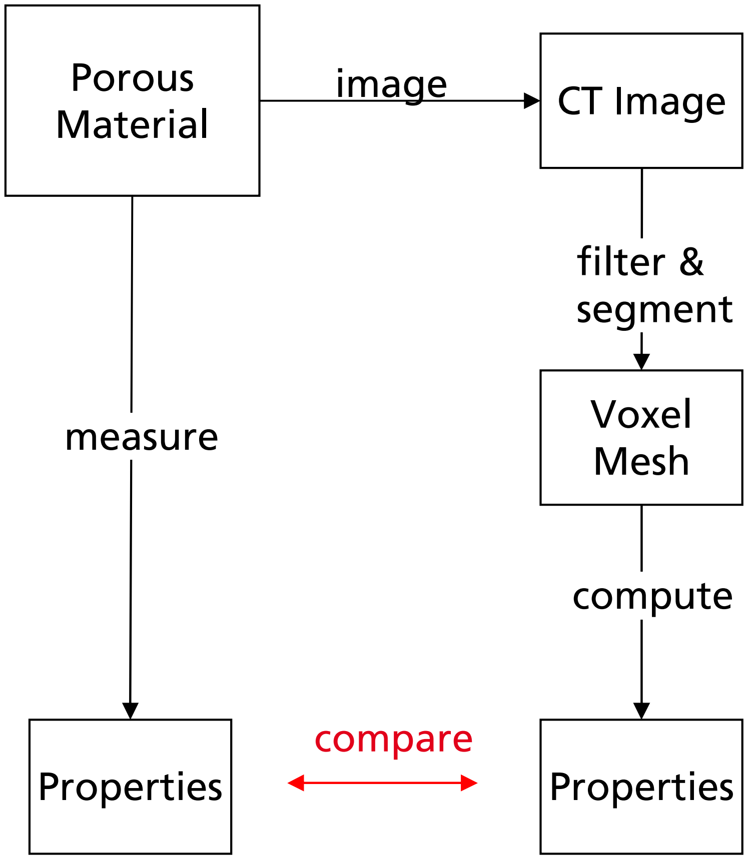
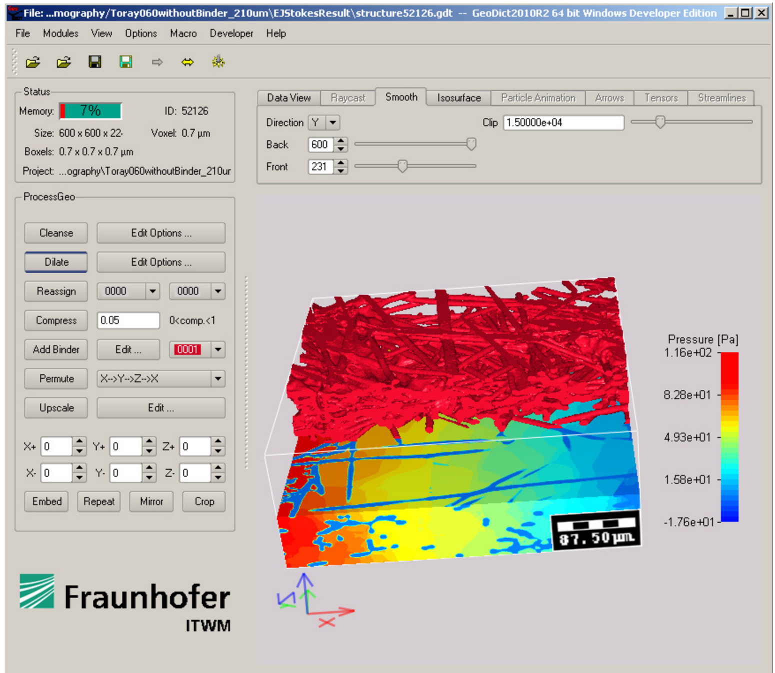
Validation - Step 1: Property Computations

... and image acquisition
... and image processing
... and measurements





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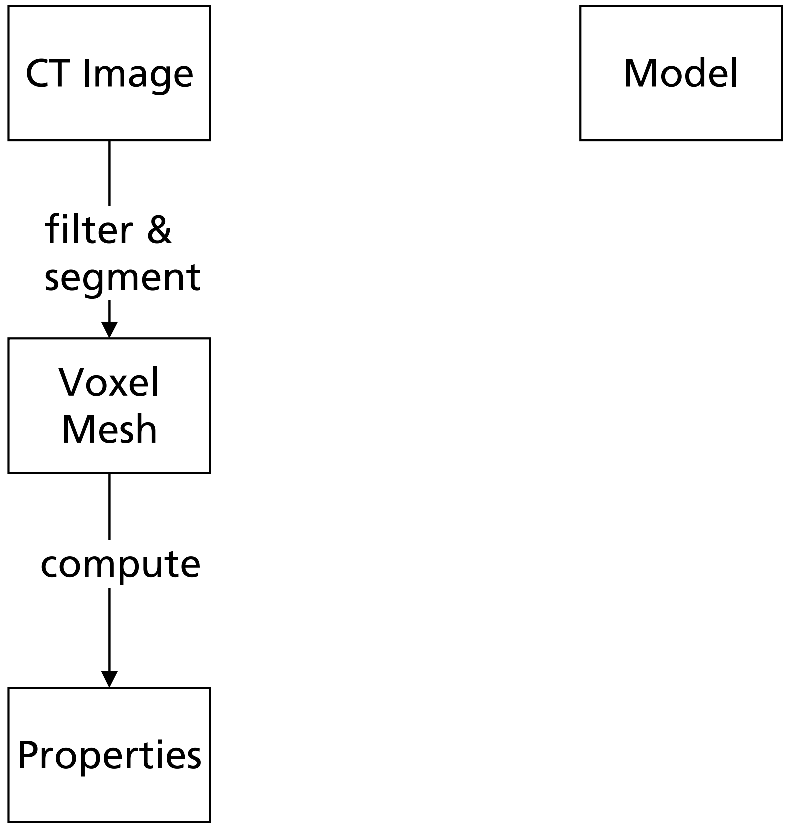
Validation - Step 2: Material Models



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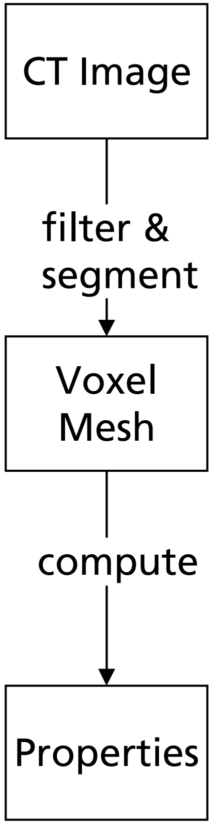

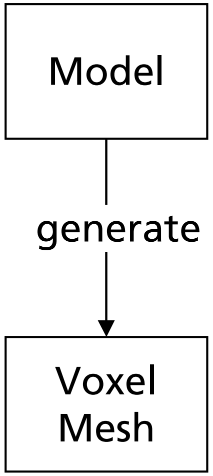

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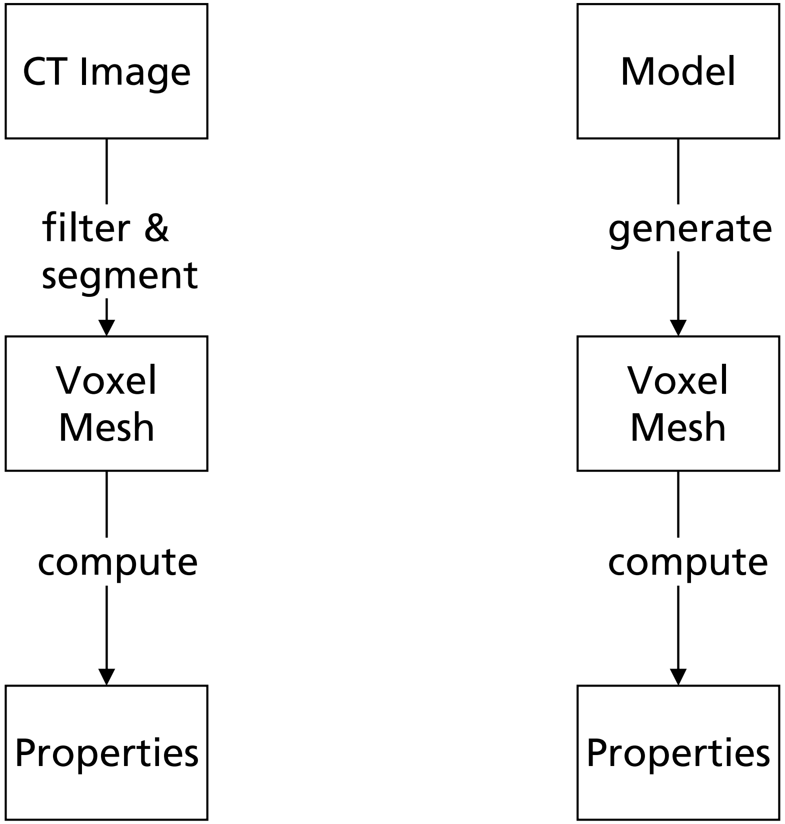

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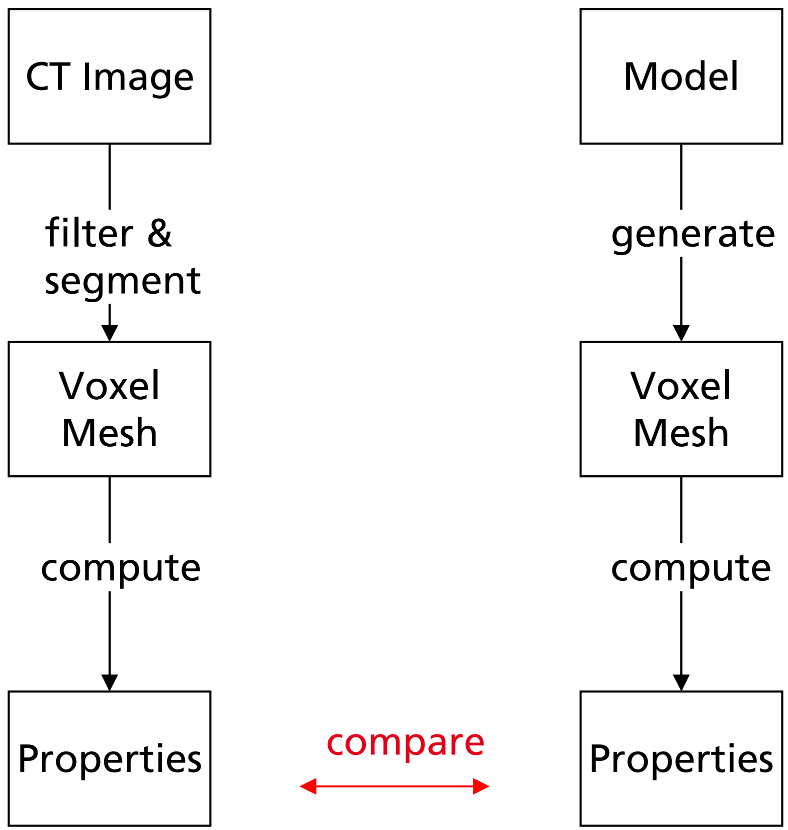

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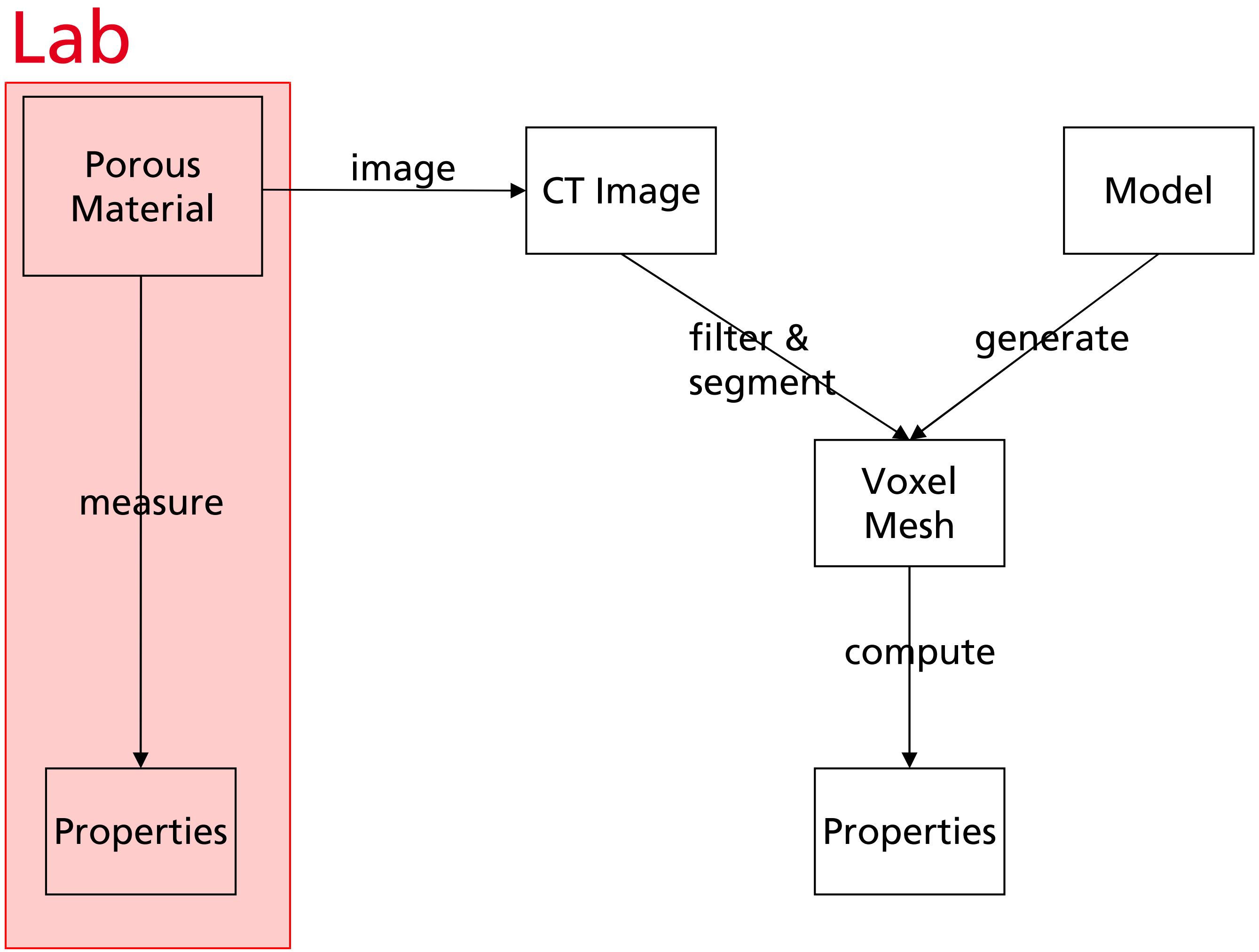
Computer Aided Material Engineering



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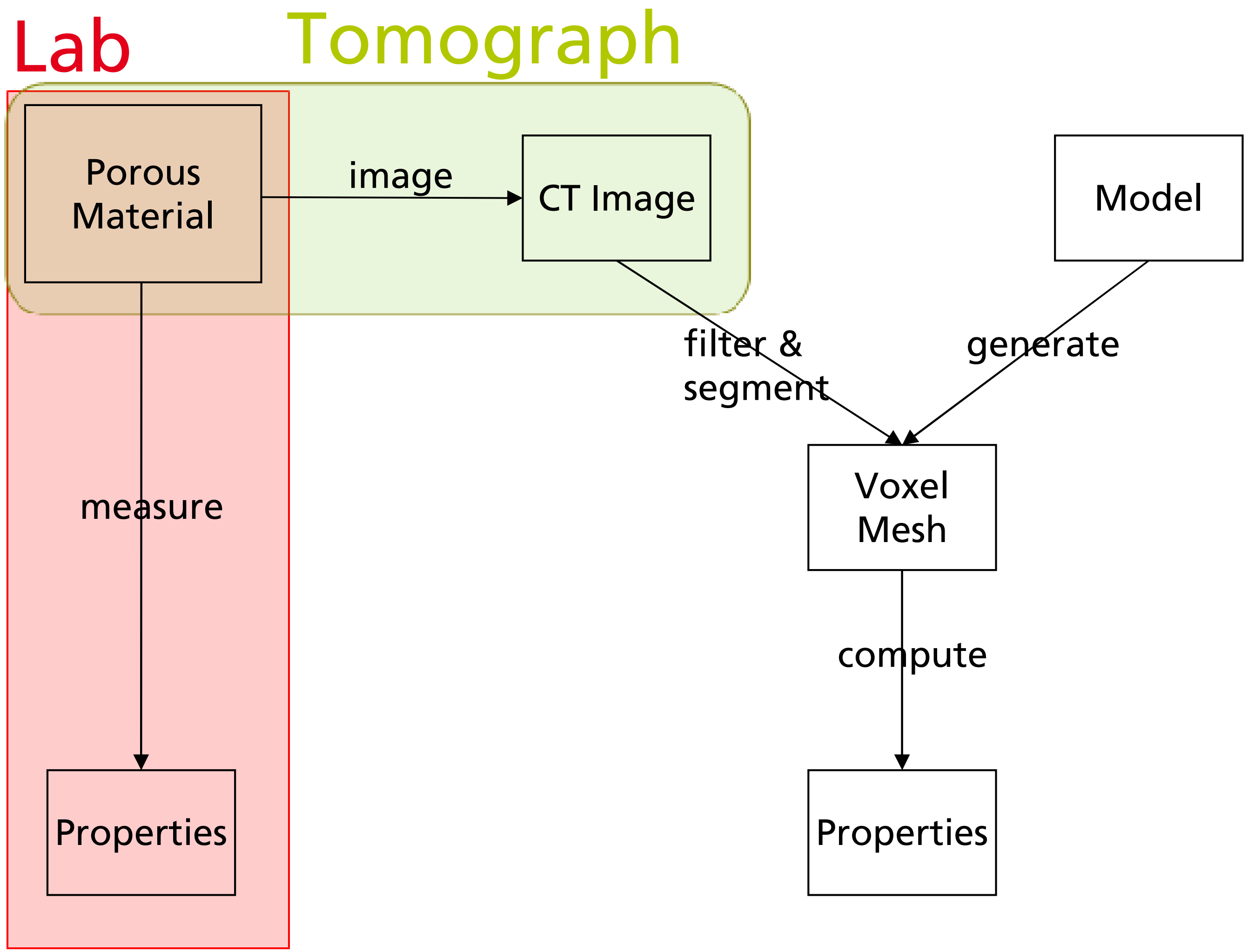

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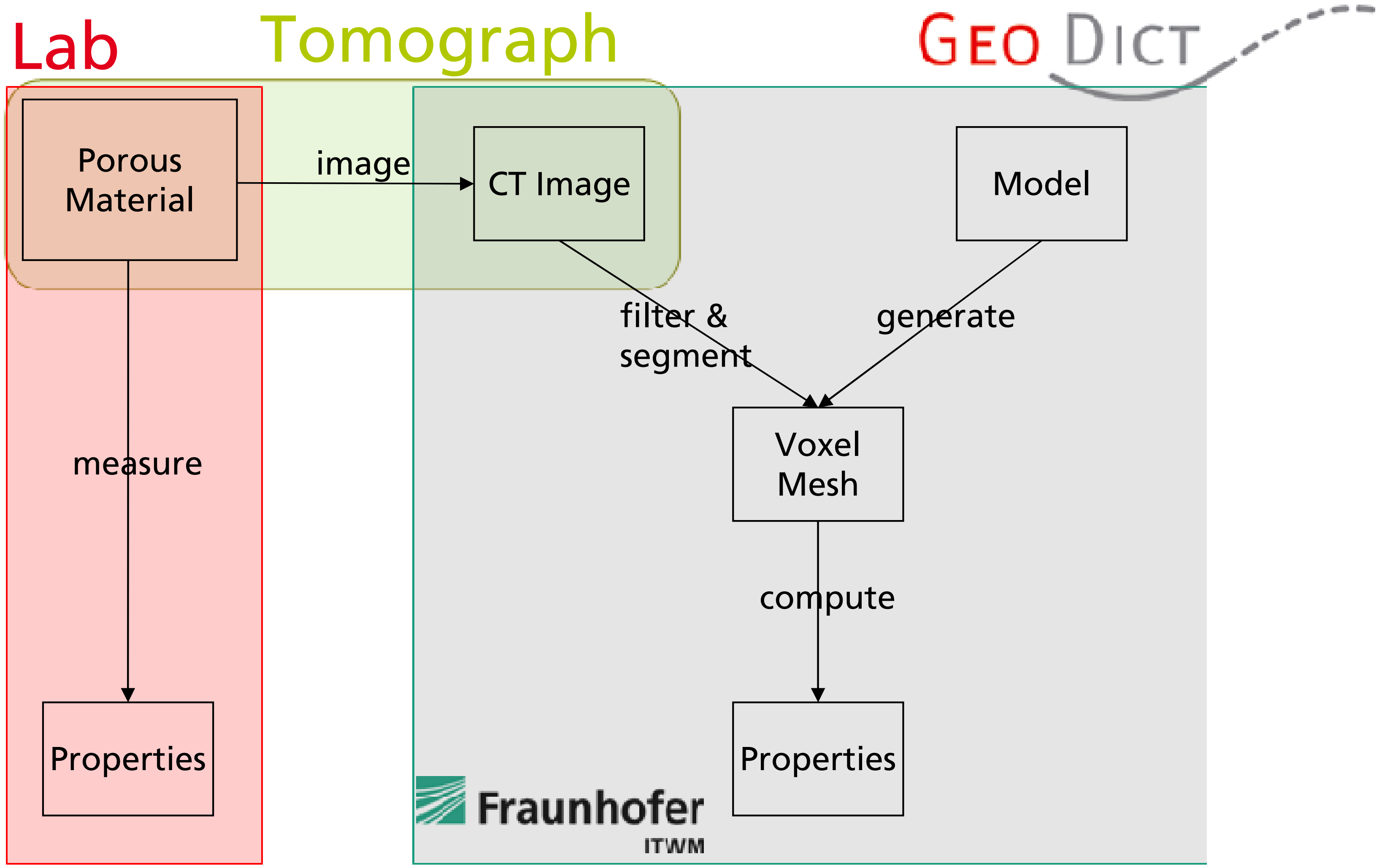

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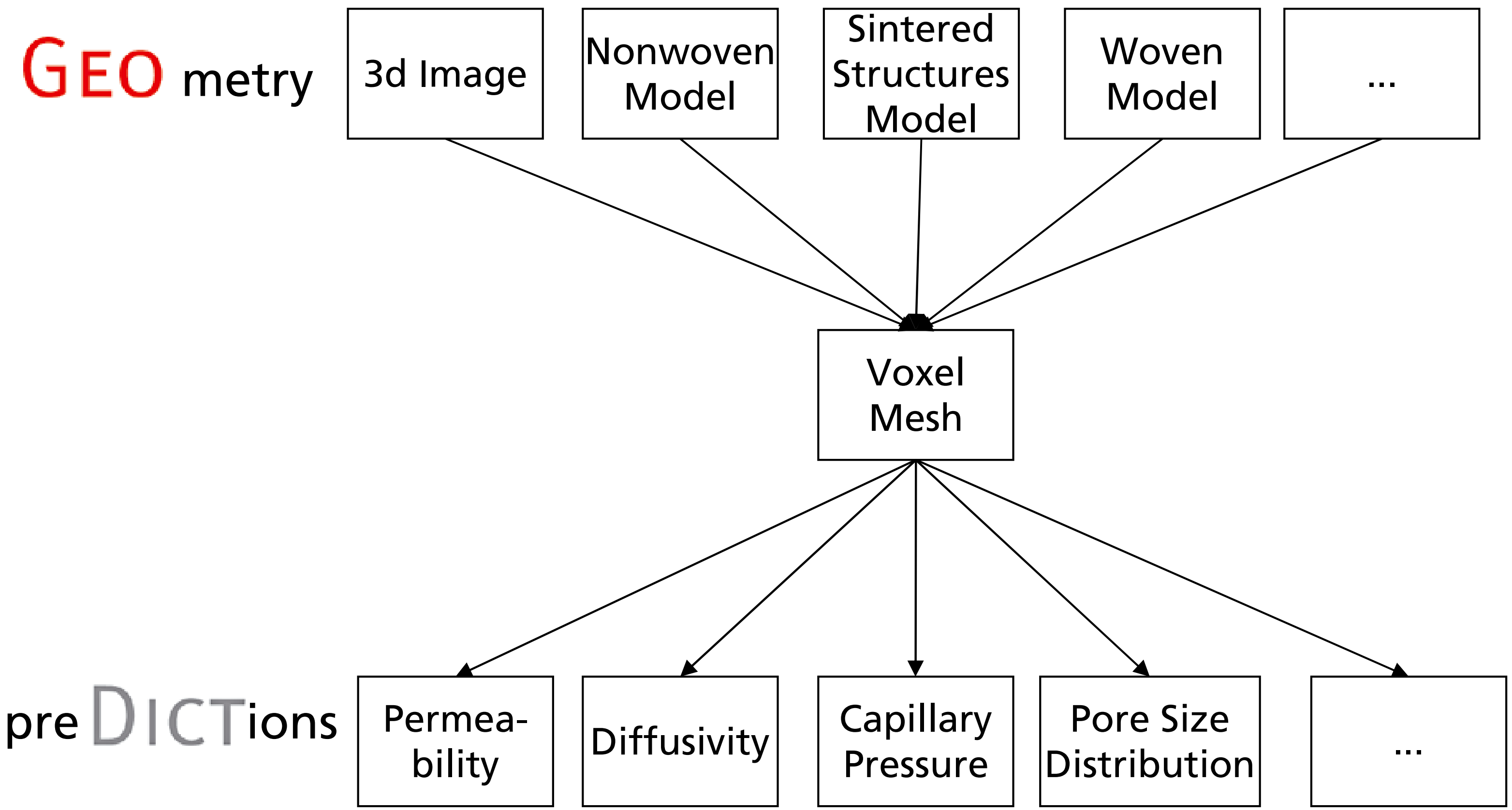
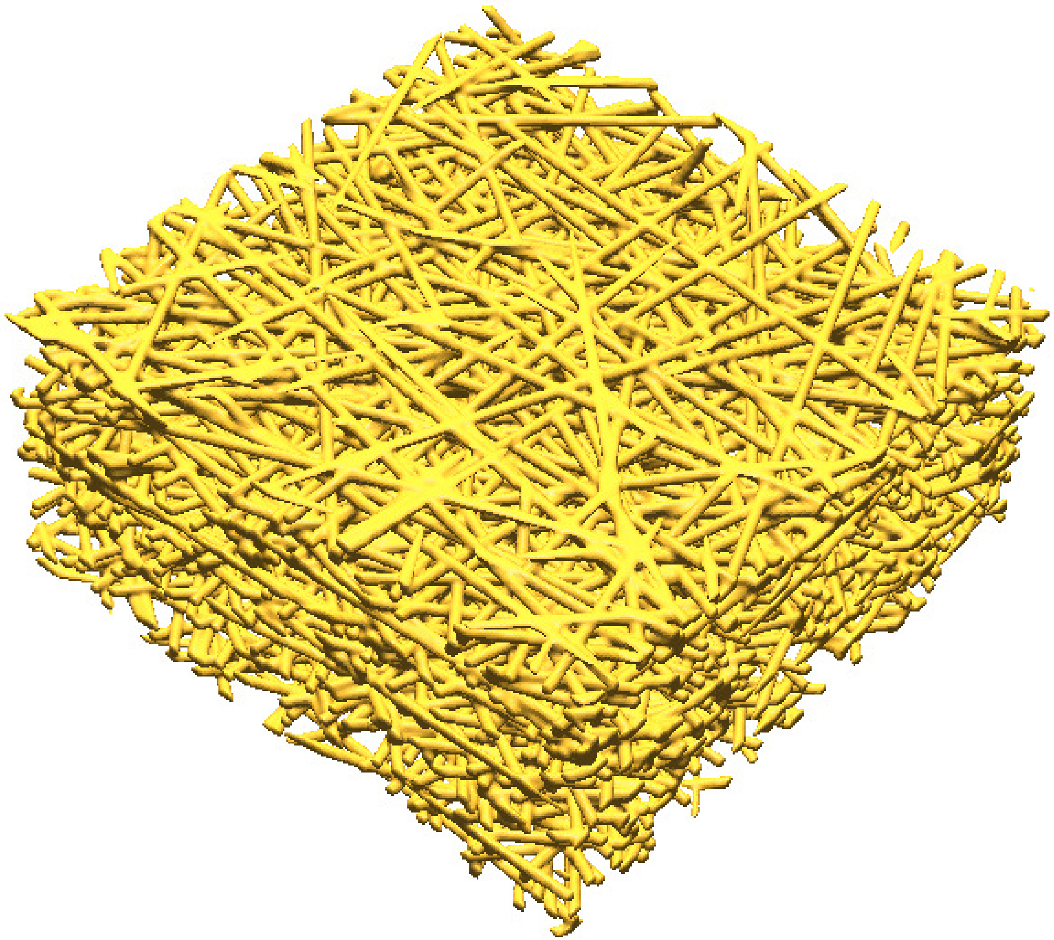
The GeoDict Software



Model: Nonwovens - Straight Fibres

Poisson line process using:

- fibre diameter
- fibre cross sectional shape
- anisotropy
- porosity



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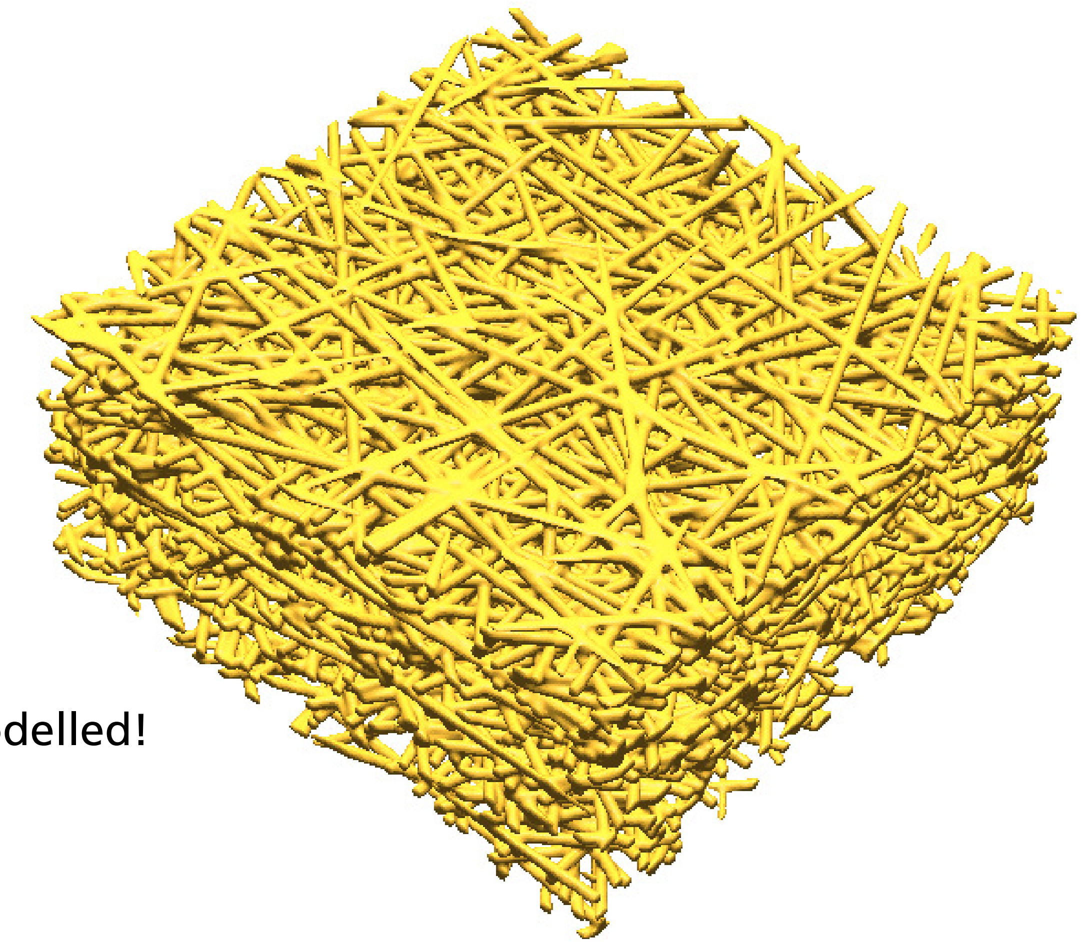

Production process is not modelled!

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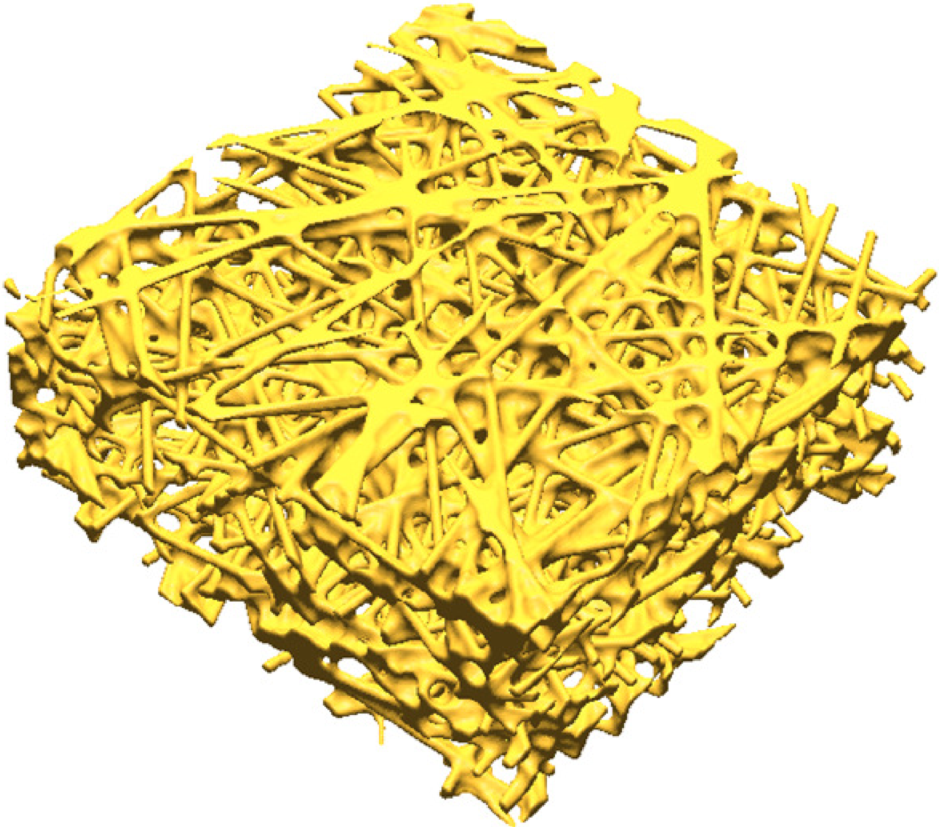
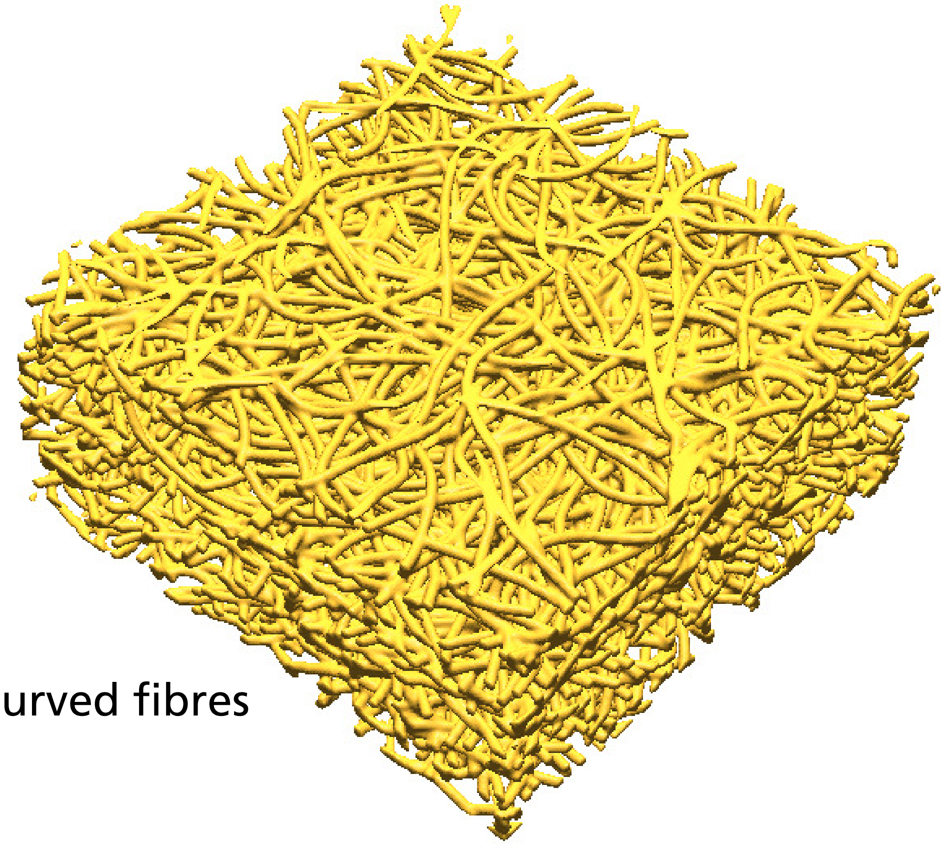
Model: Nonwovens - Some Variants



Straight fibres plus binder



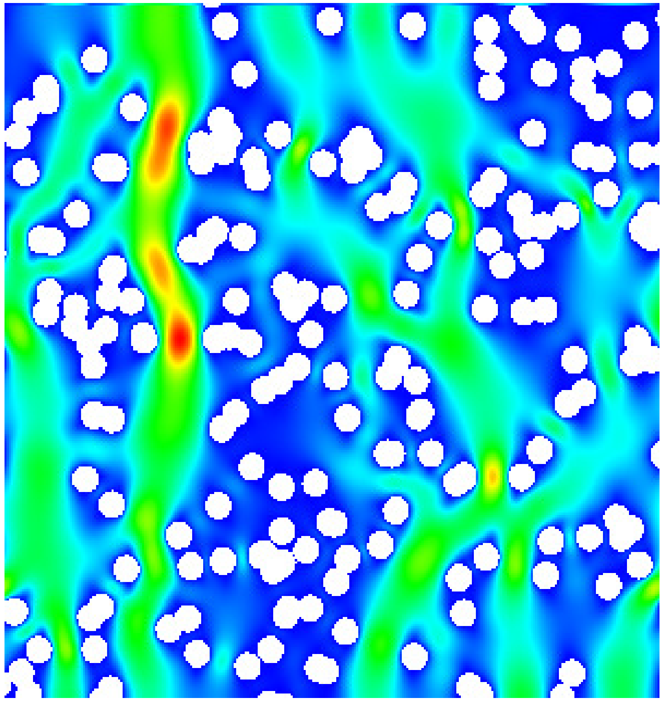
Curved fibres

Property: Permeability

Macroscopic description (homogenized 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!

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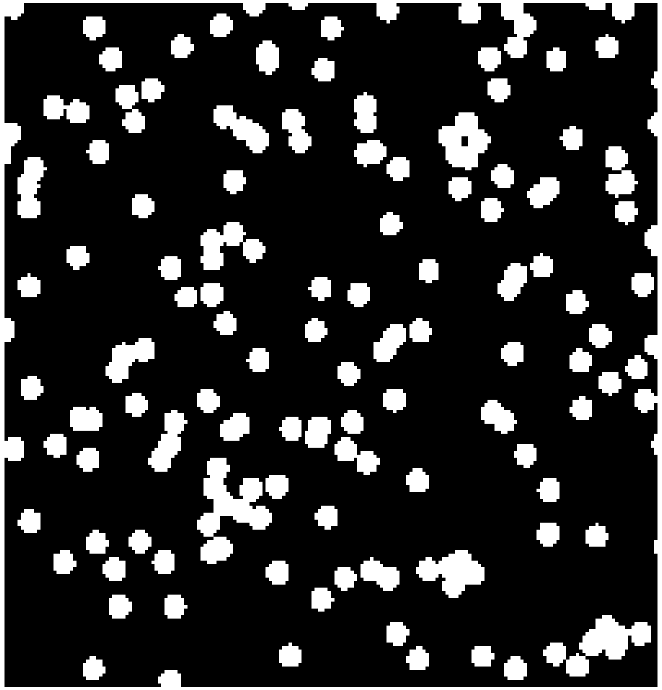
Property: Relative Permeability

Two-step approach:

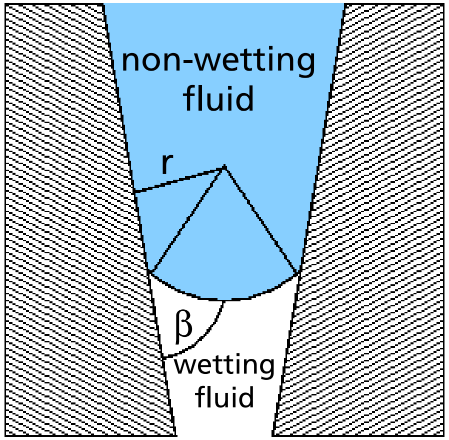


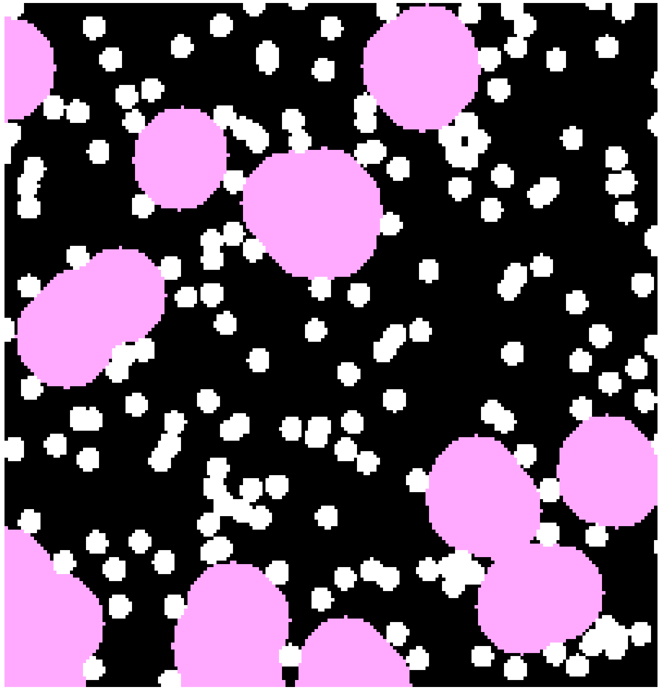
Property: Relative Permeability

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 $p_c \geq \frac{2\sigma}{r} \cos \beta$





Property: Relative Permeability

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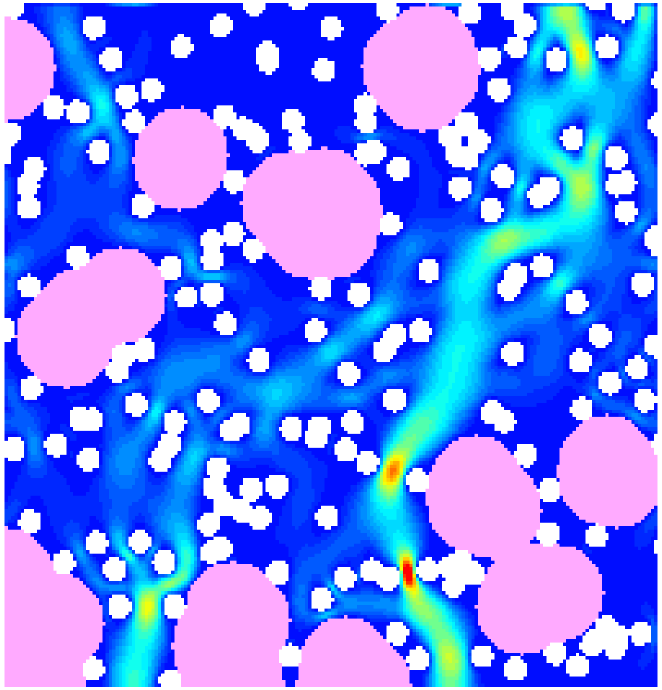
2. Solve Stokes equation on the remaining pore space to determine wetting phase (=air) permebility



Property: 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]

Property: Diffusivity

Macroscopic description
(homogenized porous media model)
Fick's first law: $j = -D^* \nabla c$

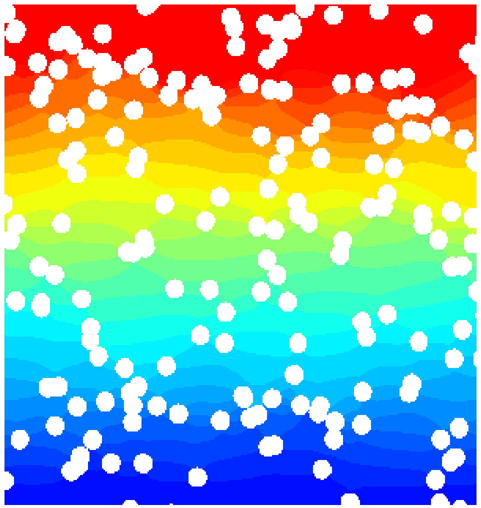
D^* : effective diffusivity [m²/s] ***unknown***
j : diffusion flux [mol/m²/s]
c : concentration [mol/m³]

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

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Summary Part I

Models:

- CT Images

- Fibrous
- *Woven*
- *Spheres*
- *Sintered*
- *Patterns*

- *Layered structures*

Properties:

- *Pore size distribution*
- *Surface area*
- *Largest Through Pore*

- *(Knudsen)* Diffusivity
- Permeability
- *Electric conductivity*
- *Thermal conductivity*
- *Stiffness*

- *Capillary pressure curve*
- *Bubble point*
- Relative (= saturation dependent) permeability
- *Relative (= saturation dependent) diffusivity*

- *Filter efficiency and life time*

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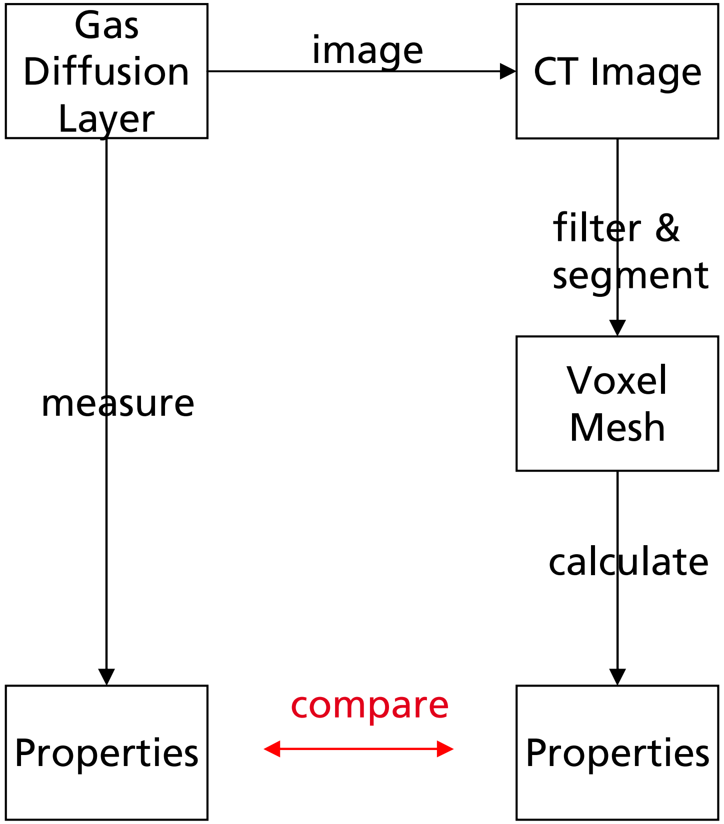
Application: Gas Diffusion Layer of PEM Fuel Cell



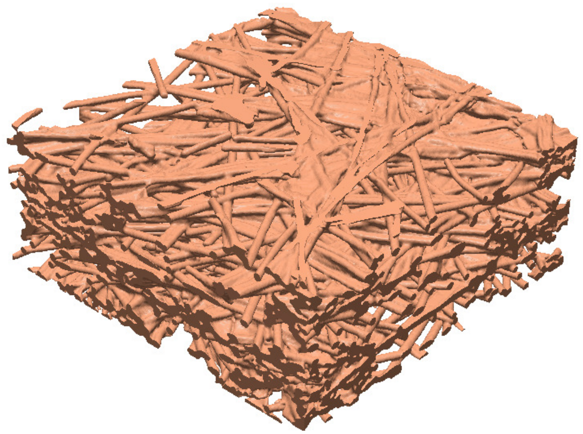
Joint work

PSI:

- CT Images of Toray paper at different compression levels
- Diffusivity and permeability measure-ments at different compression levels

ITWM:

- Compute diffusivity and permeability



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

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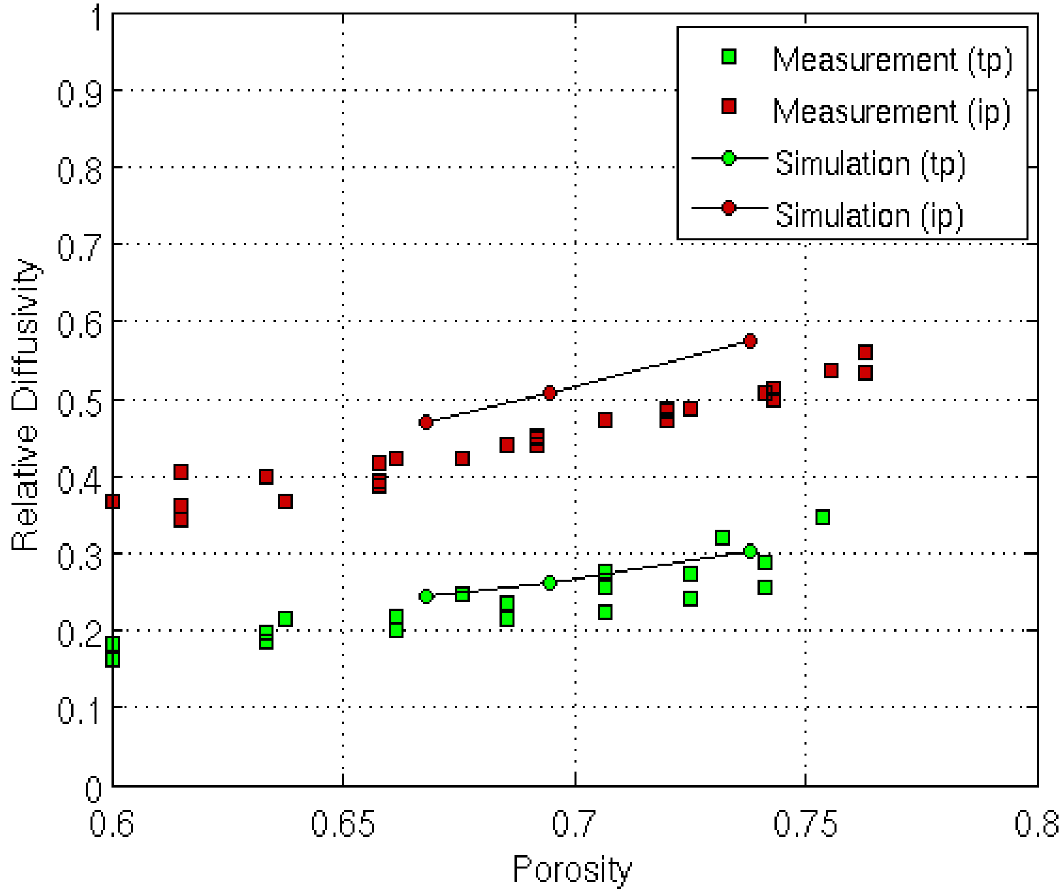
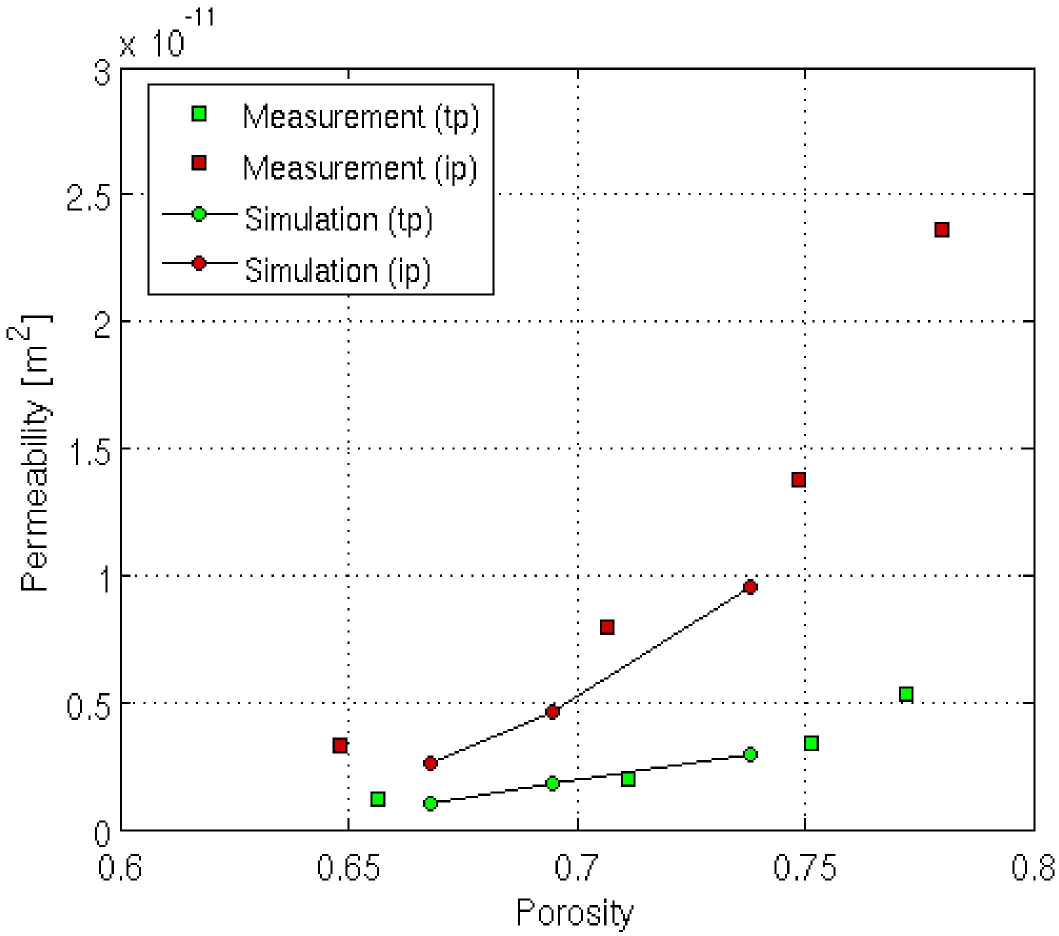
Diffusivity



Perfect in tp-direction

Small differences in ip-direction
- ip-measurememts performed on a stack of GDLs
- tomography image shows single layer between sample holder

Permeability



Perfect in tp-direction

Small differences in ip-direction
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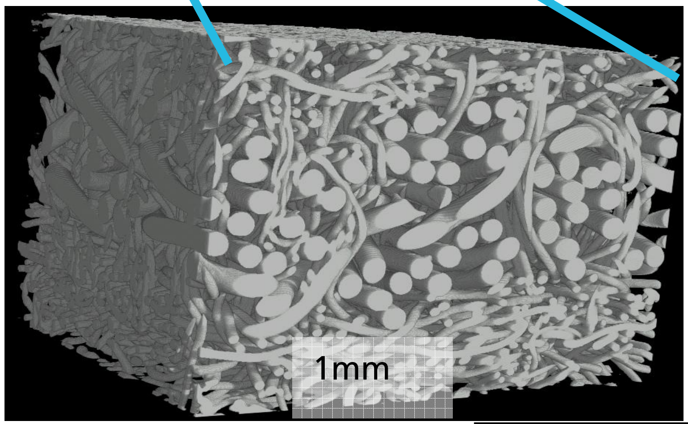
Other Applications

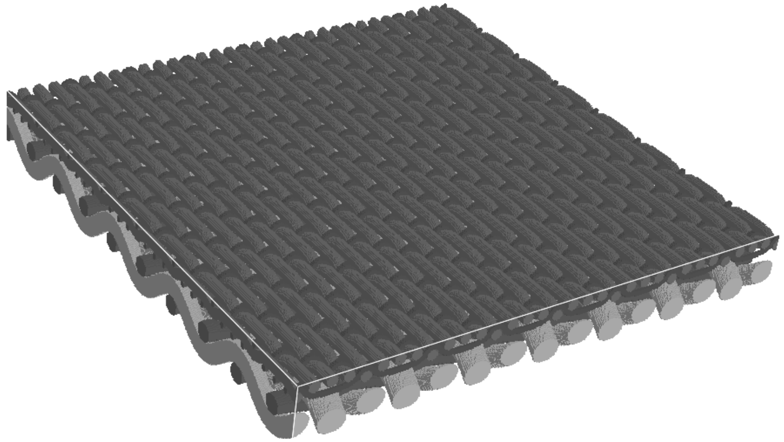
- Woven metal wire meshes
- Filtration
- Paper dewatering felts
- Permeability of rocks
- Diapers
- Sintered ceramics

Tomography and Models of Felts

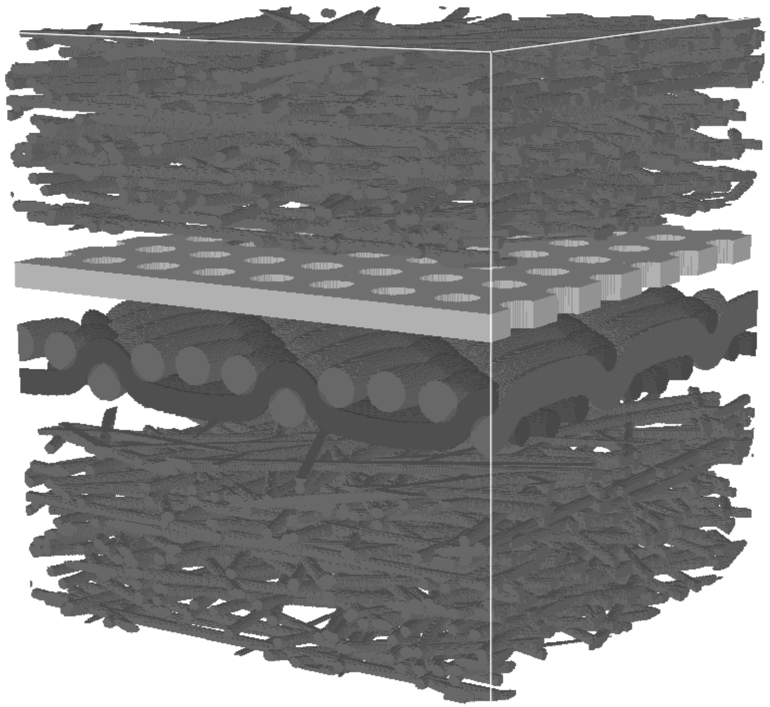
Paper machine



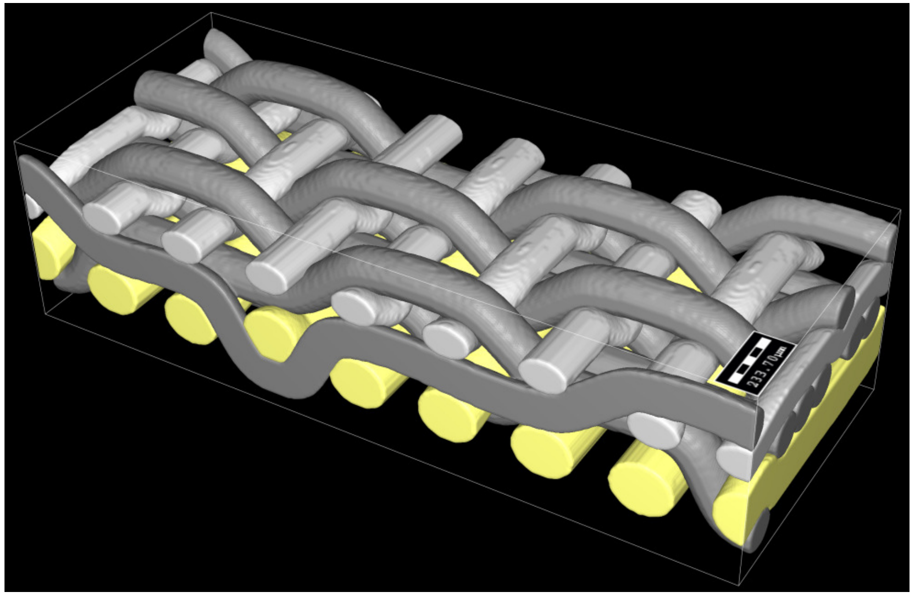
Tomography

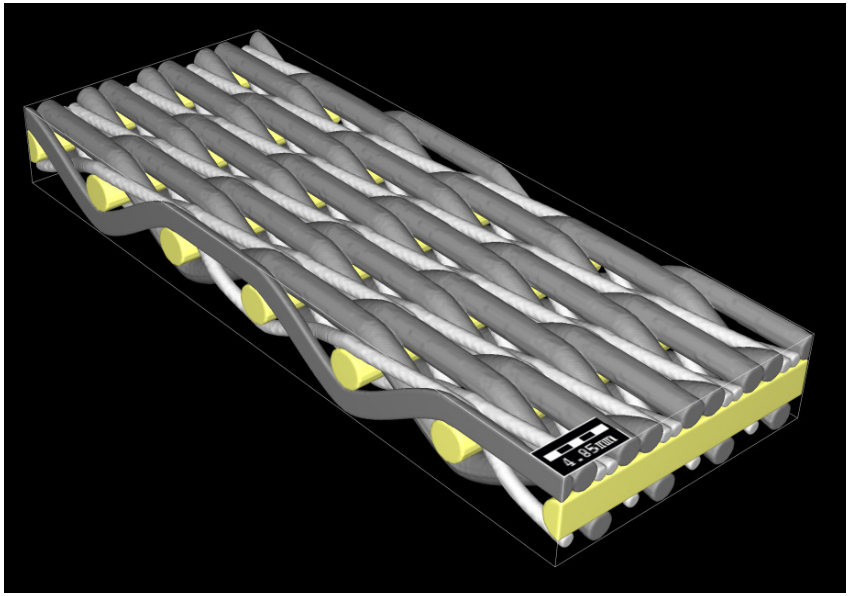


Forming fabric and dewatering felt



Woven Metal Wire Meshes: Complex weave models





Left: Model of a two-layer weave based on a CT-scan.
Right: Model of a complex one-layer twill Dutch-weave.

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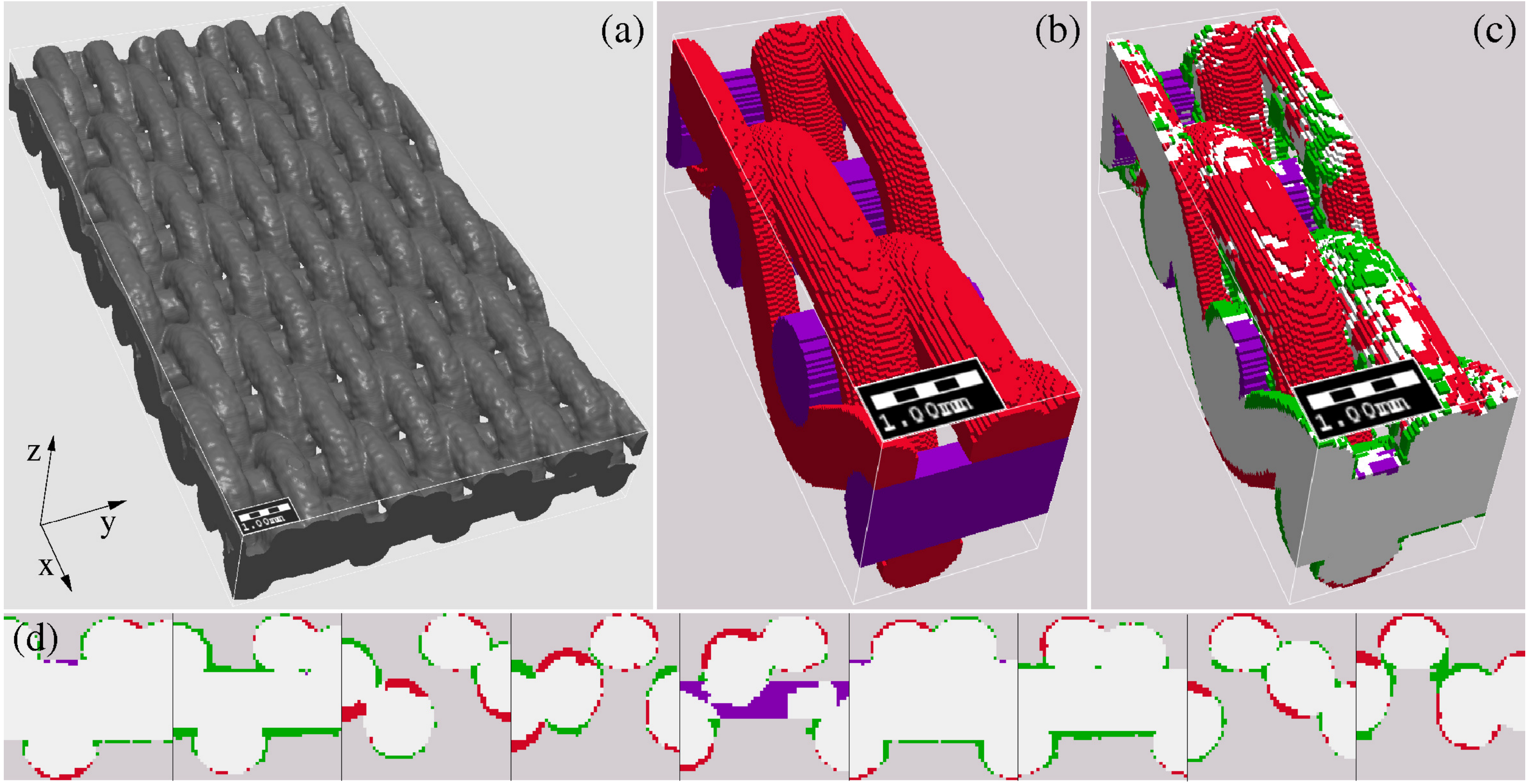
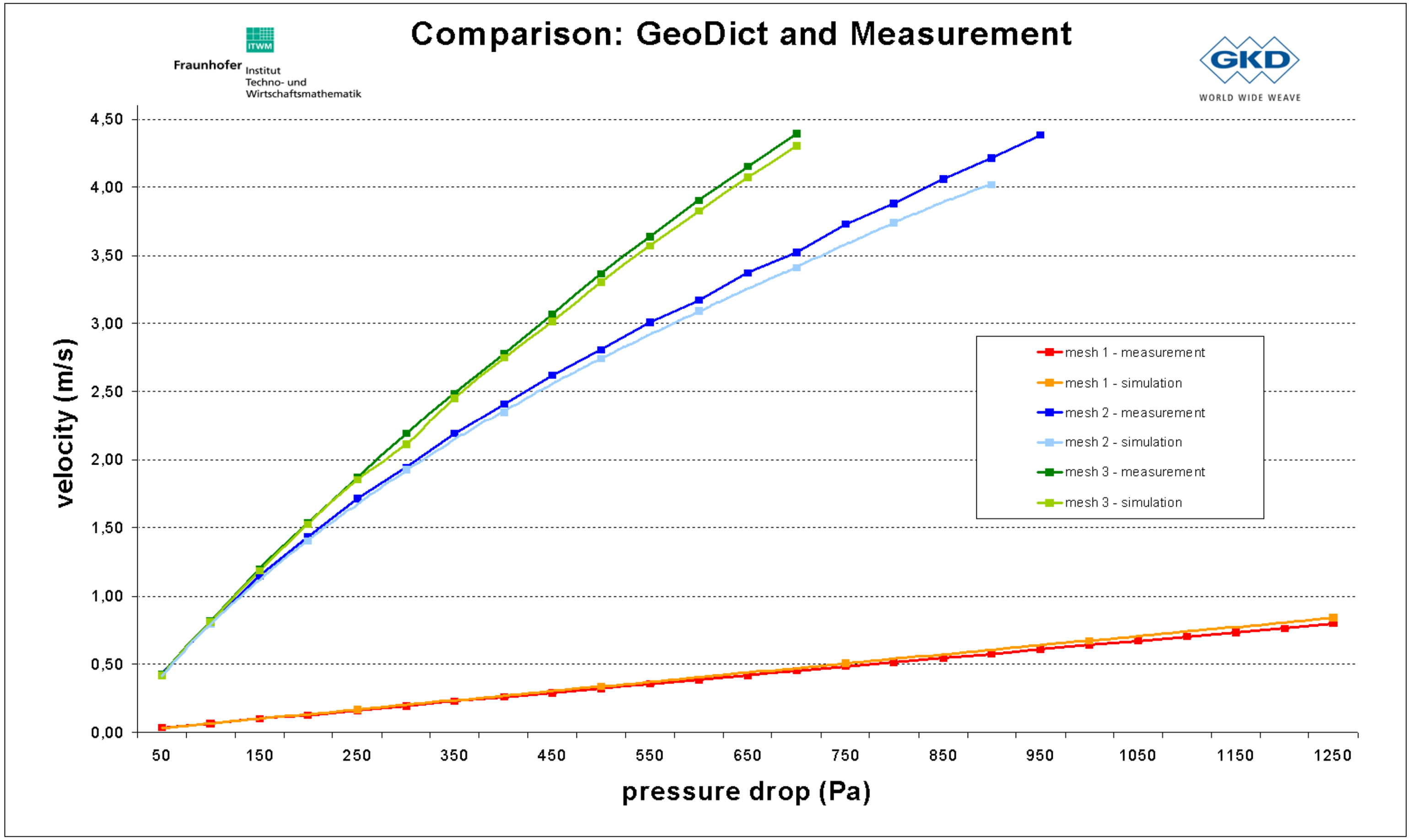
Woven Metal Wire Meshes: Geometric Validation



(a): CT of a twill Dutch-weave. (b): Geometry model.
(c)-(d): Geometric validation.

Woven Metal Wire Meshes: Measurement and Simulation



Velocity dependent pressure drop: Comparison between measurements and simulations on corresponding geometry models.

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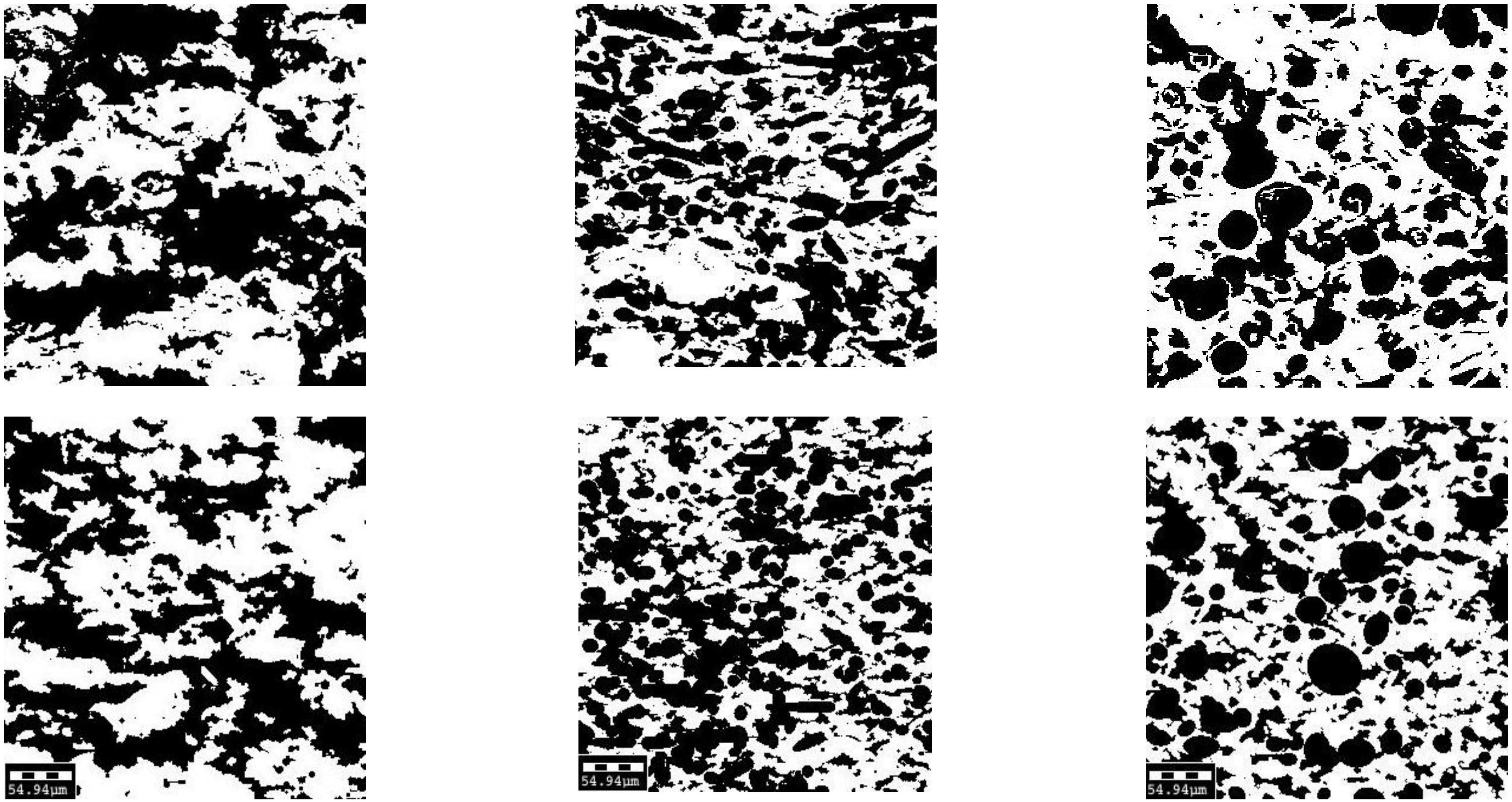
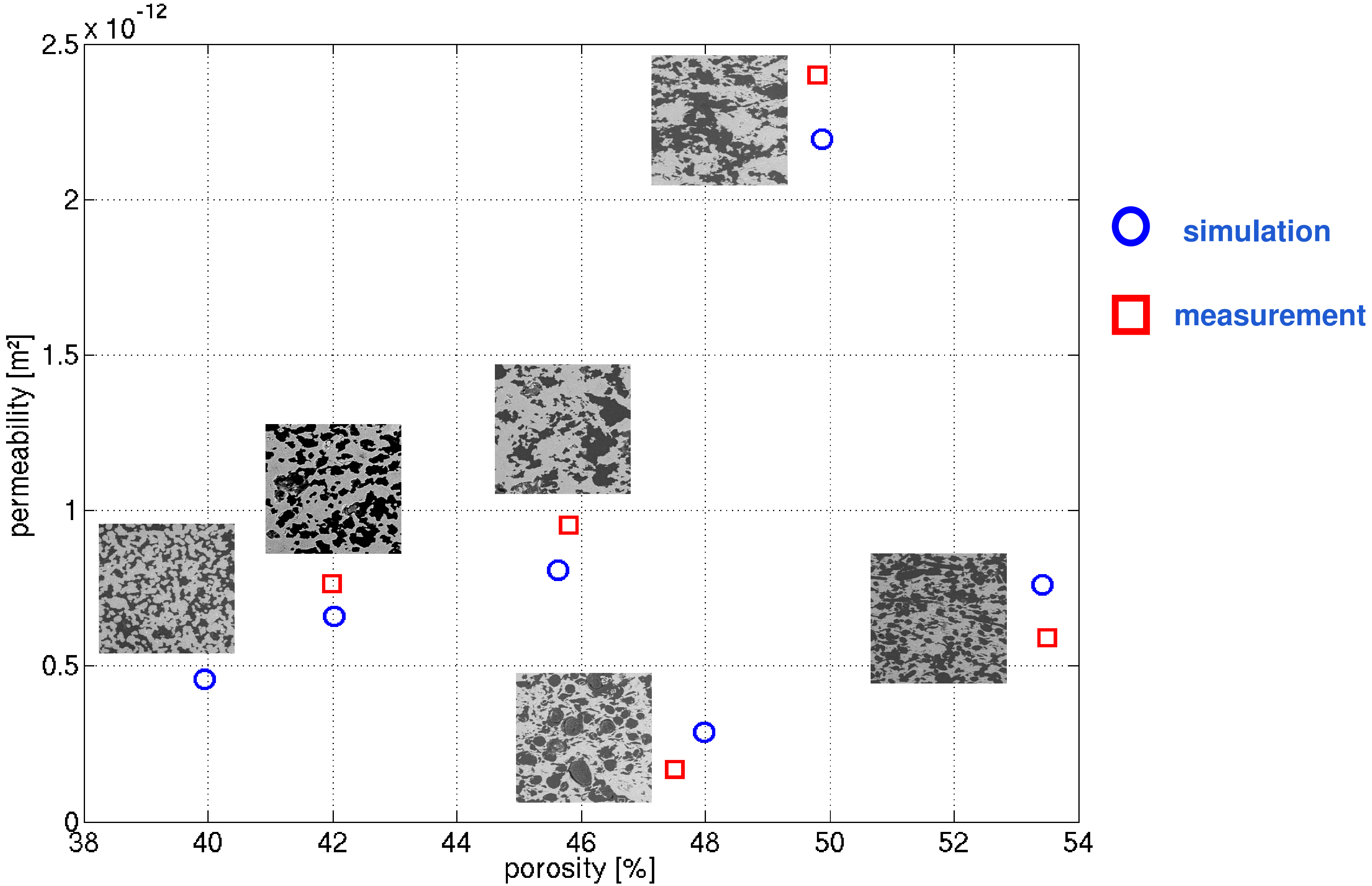
Sintered Ceramics

- top: binarized SEM image
- bottom: cross section through virtually created medium



Computed vs measured porosities and permeabilities



Fraunhofer ITWM

Conclusions

Two validation steps to enable Computer Aided Material Engineering:

- validate property computations
- validate virtual structure models

Many fields of applications

Thank You !

Geometry generator,
property predictor and
virtual material designer

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