Predicting Transport Properties of Porous Layers Based on Pore-Scale Models

Transpore, Villigen, 19.08.2010

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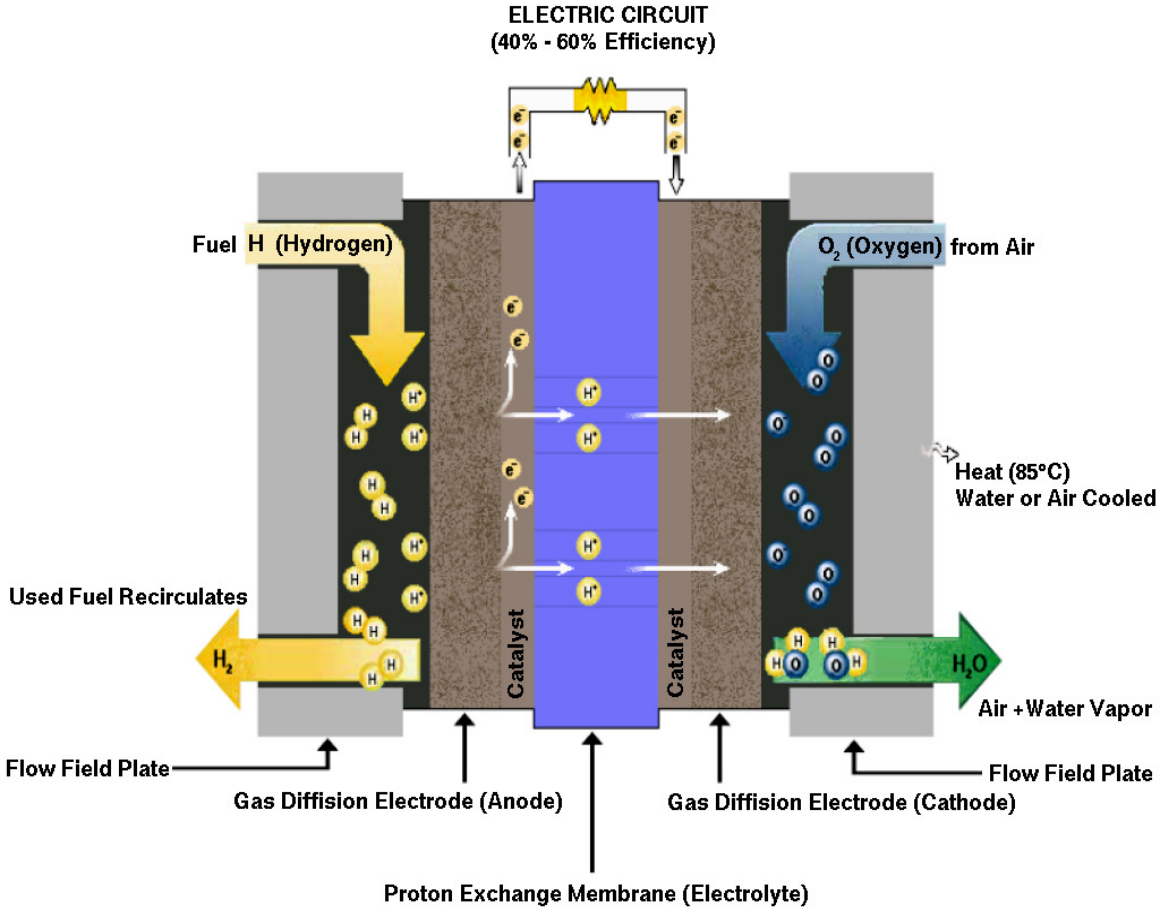
PEM Fuel Cell



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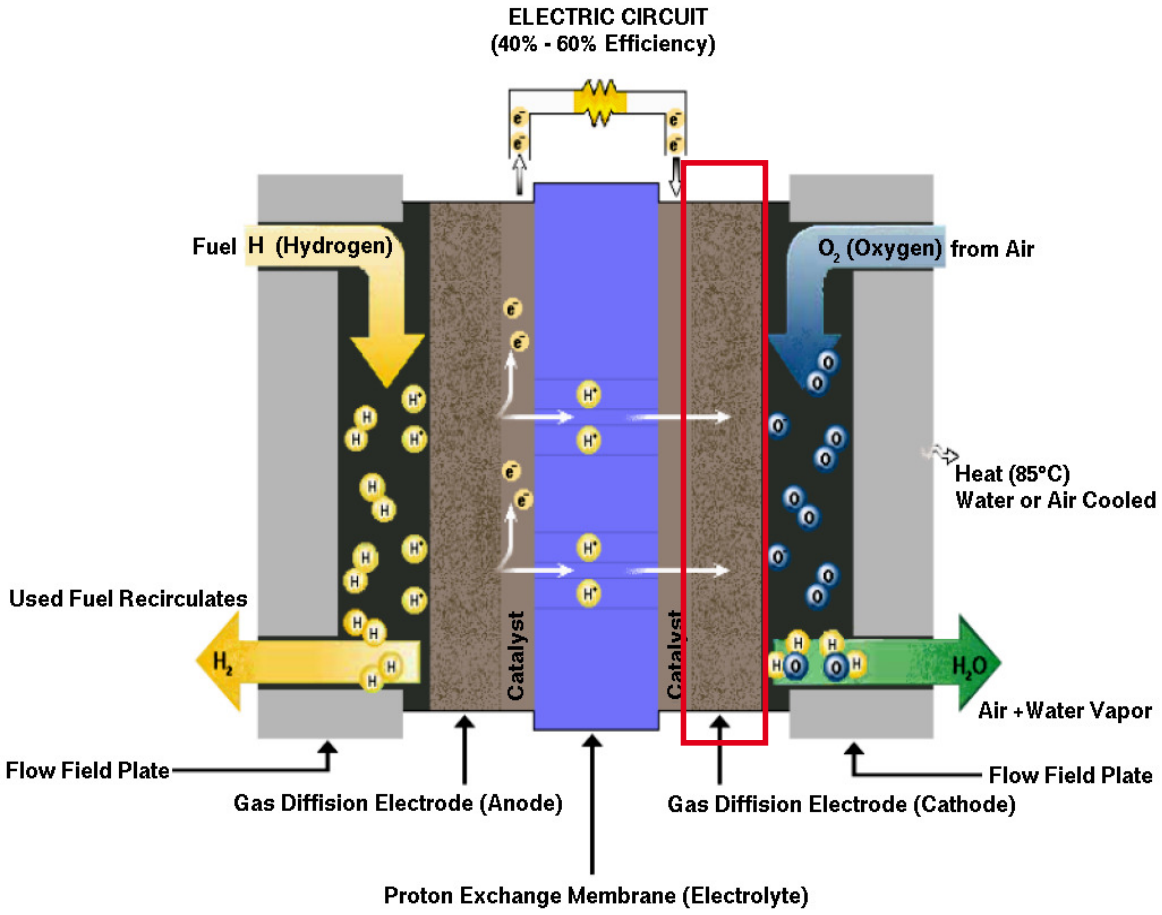
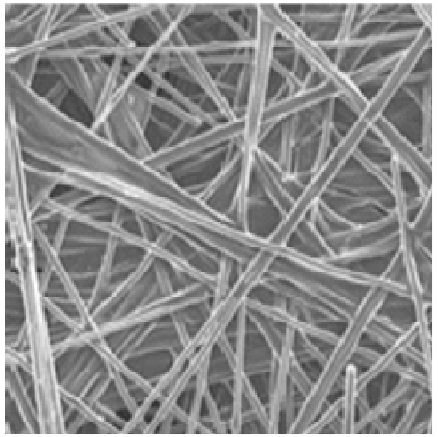
PEM Fuel Cell





Gas Diffusion layer

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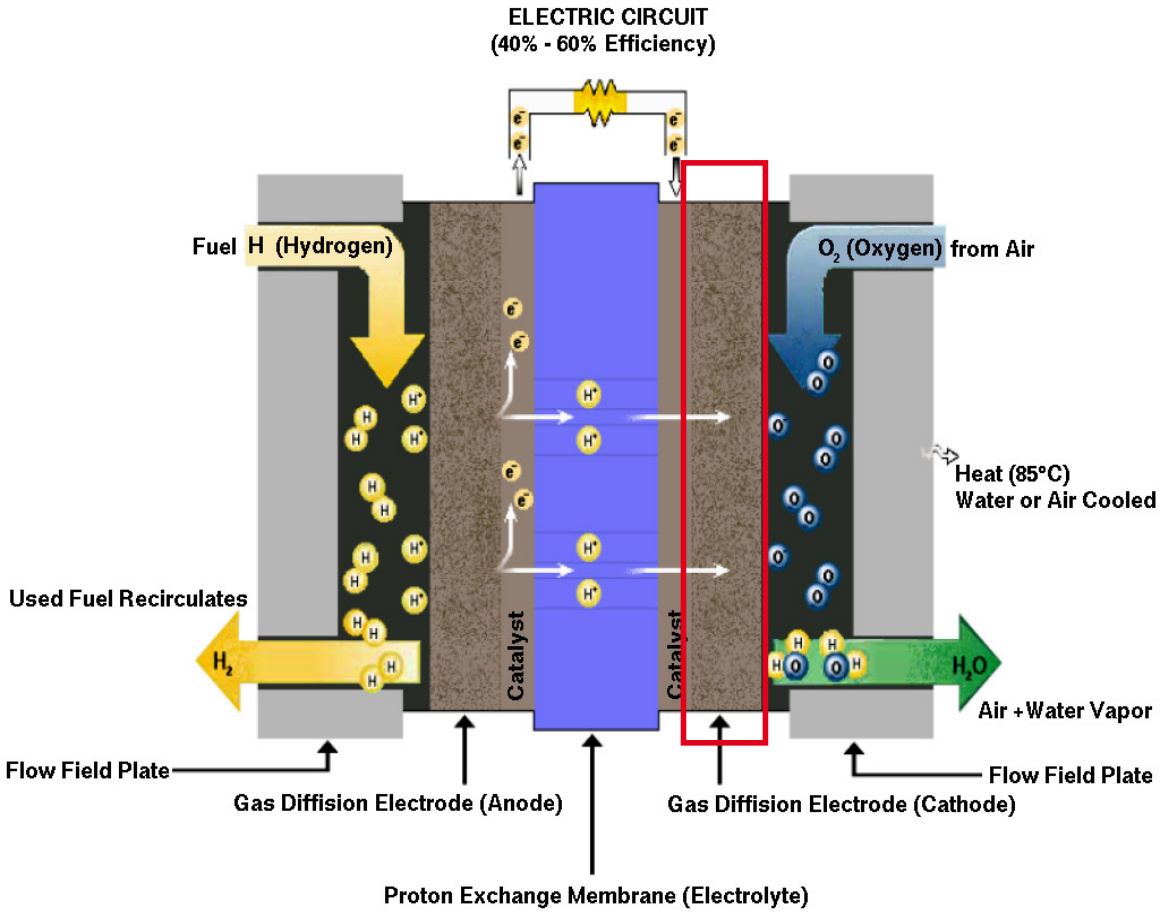
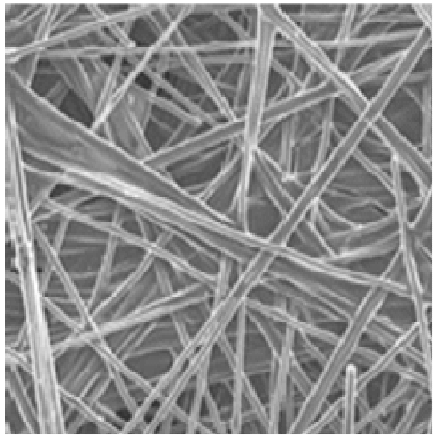
PEM Fuel Cell





Gas Diffusion layer

Aim: engineer a better GDL !

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

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Predicting Transport Properties of Porous Layers Based on Pore-Scale Models

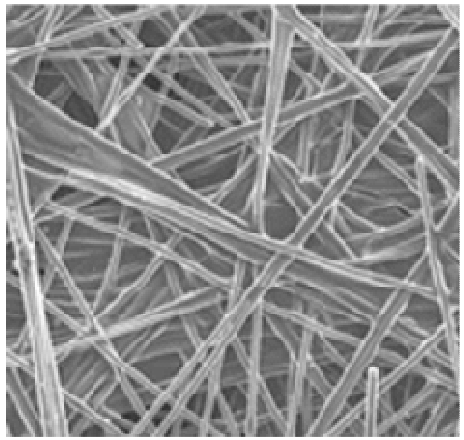
1. General Approach

2. Application to PEM fuel cells
   - Gas Diffusion Layer
   - Catalyst Layer

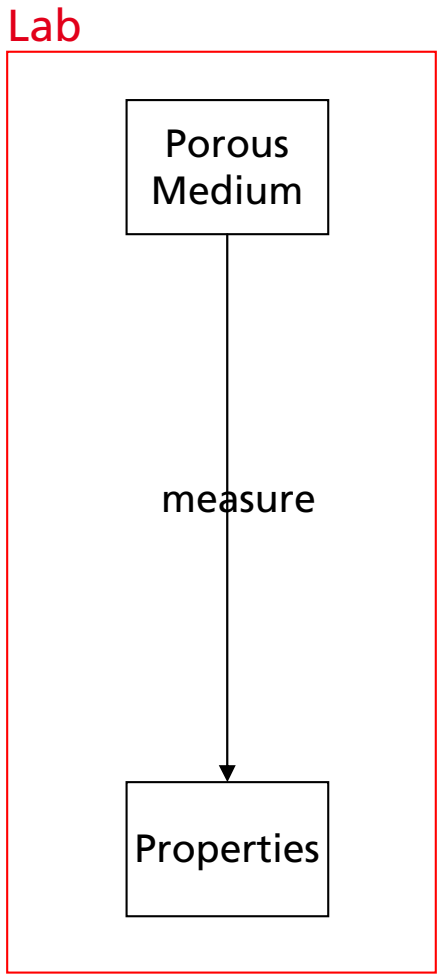
Aim: Virtual Material Design

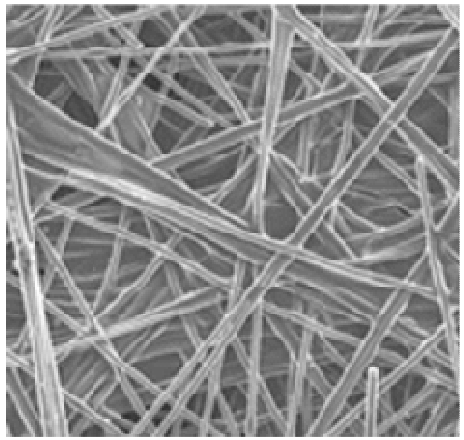
Lab

Porous Medium



Aim: Virtual Material Design





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

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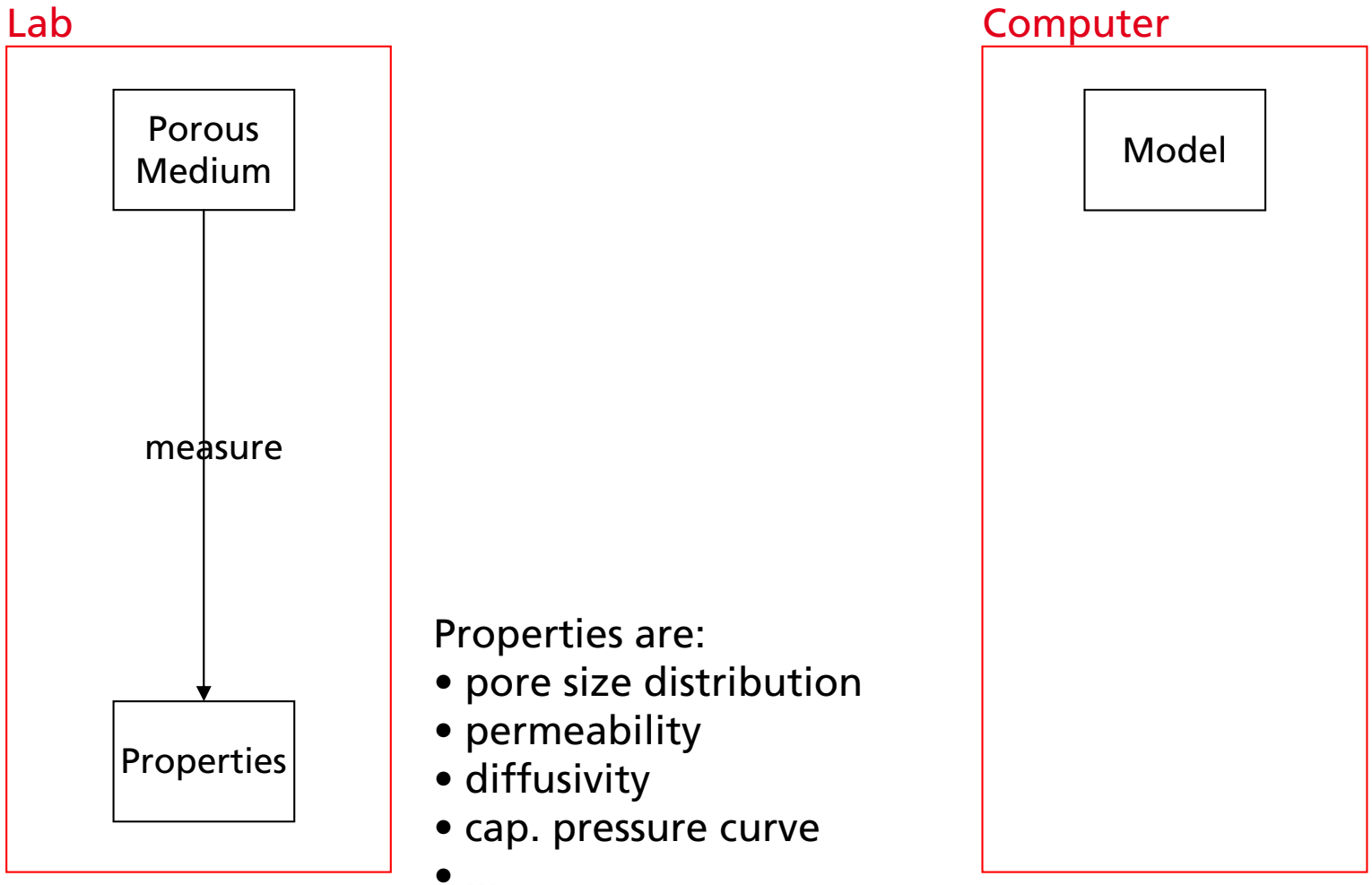
Aim: Virtual Material Design



Properties are:
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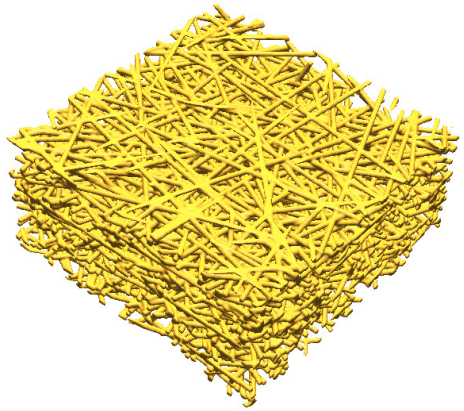
Aim: Virtual Material Design

Lab

Porous Medium

measure

Properties



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

Computer

Model

generate

Voxel Mesh

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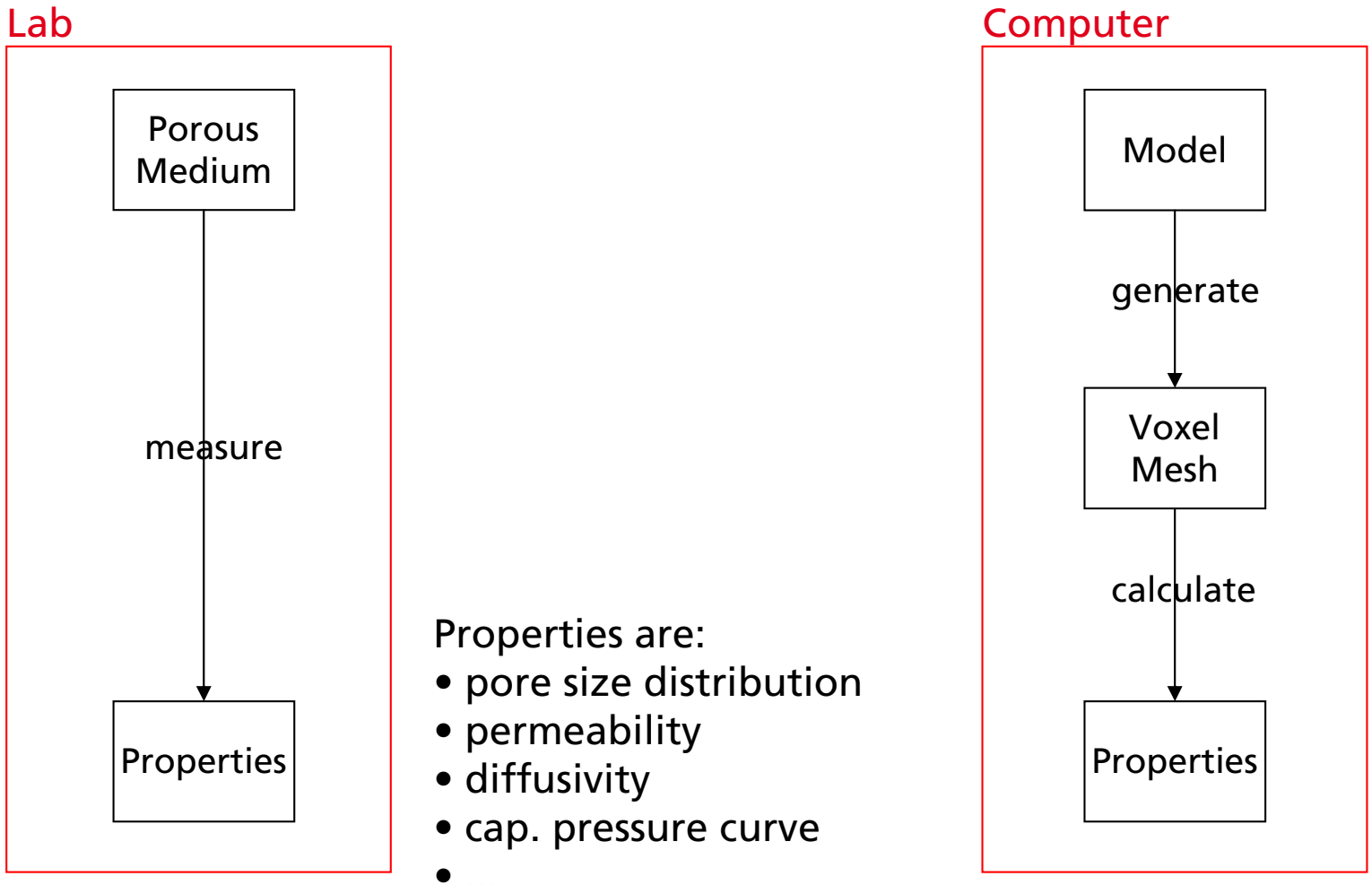
Aim: Virtual Material Design



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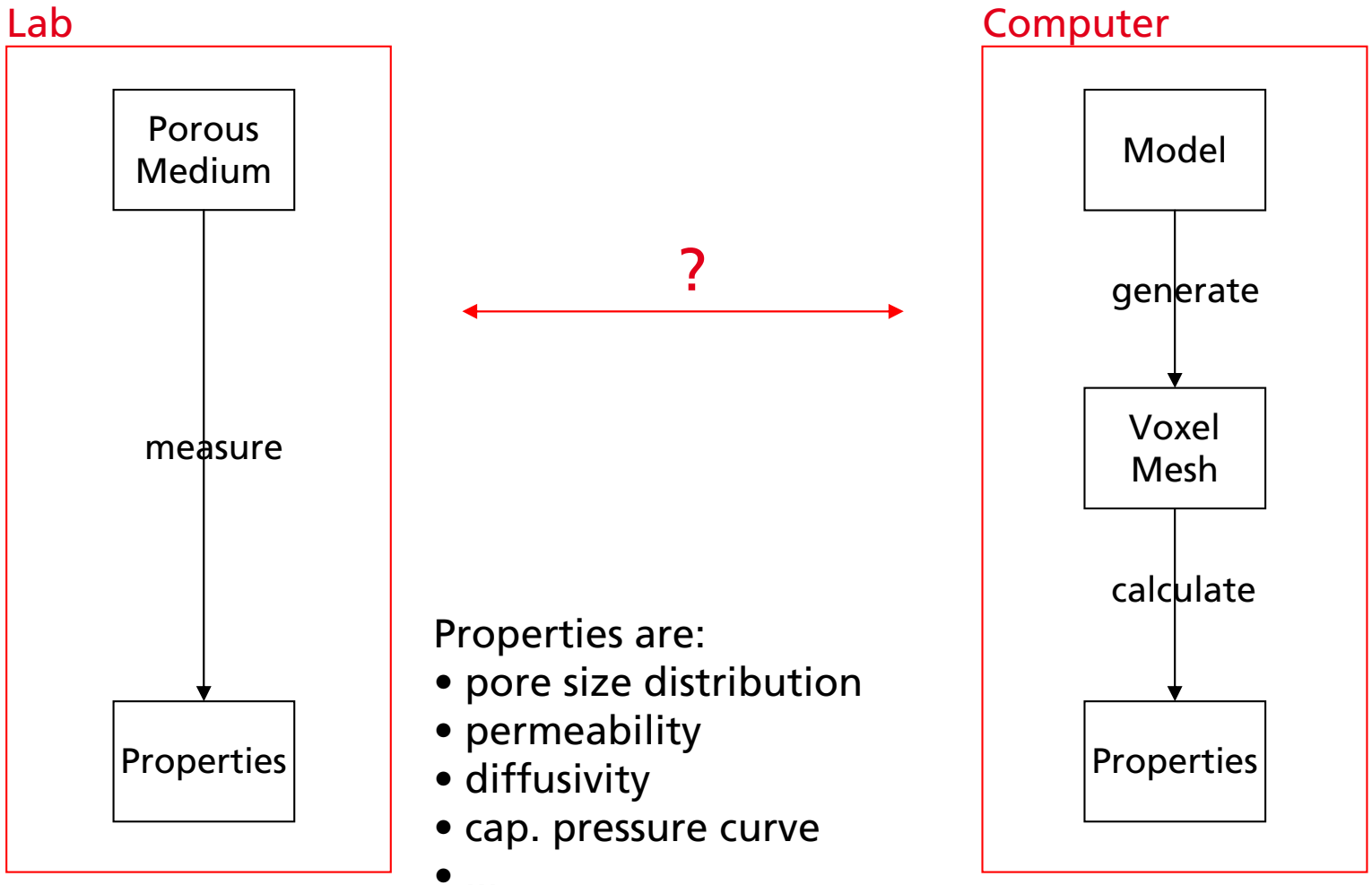
Aim: Virtual Material Design



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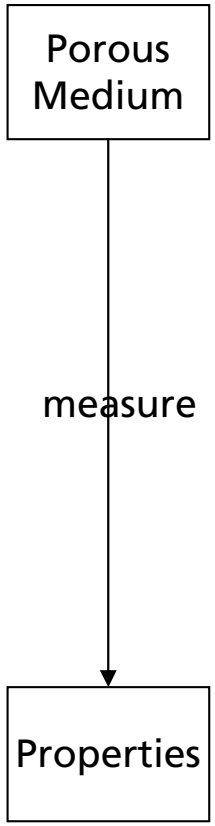
Bridge the Gap - Step 1: Validate Calculations



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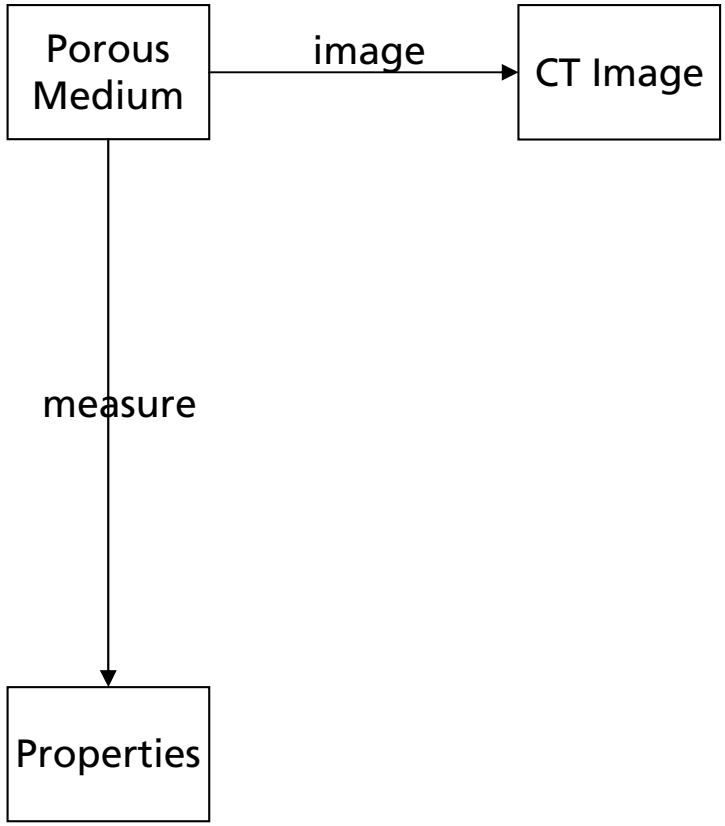
Bridge the Gap - Step 1: Validate Calculations



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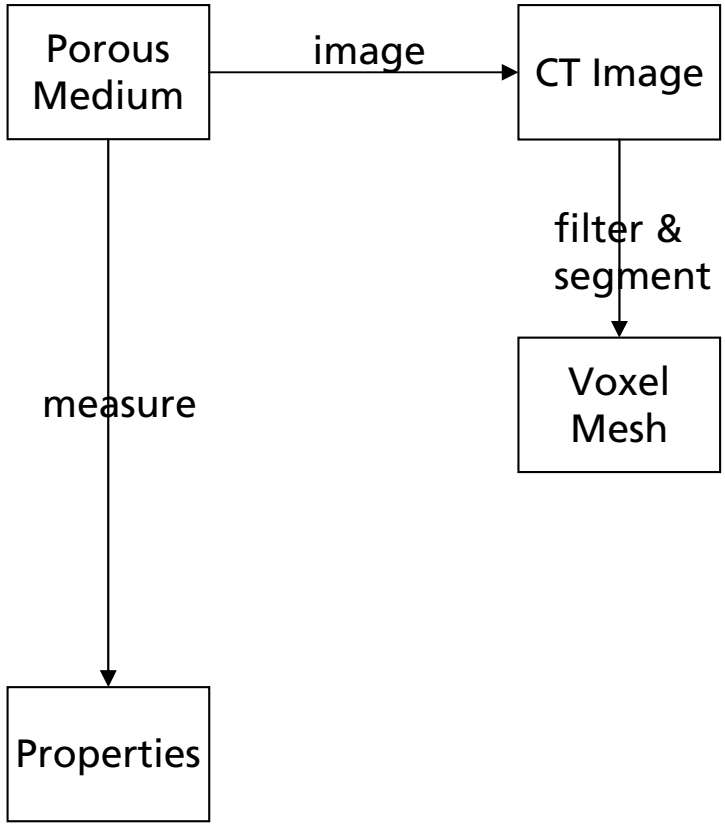

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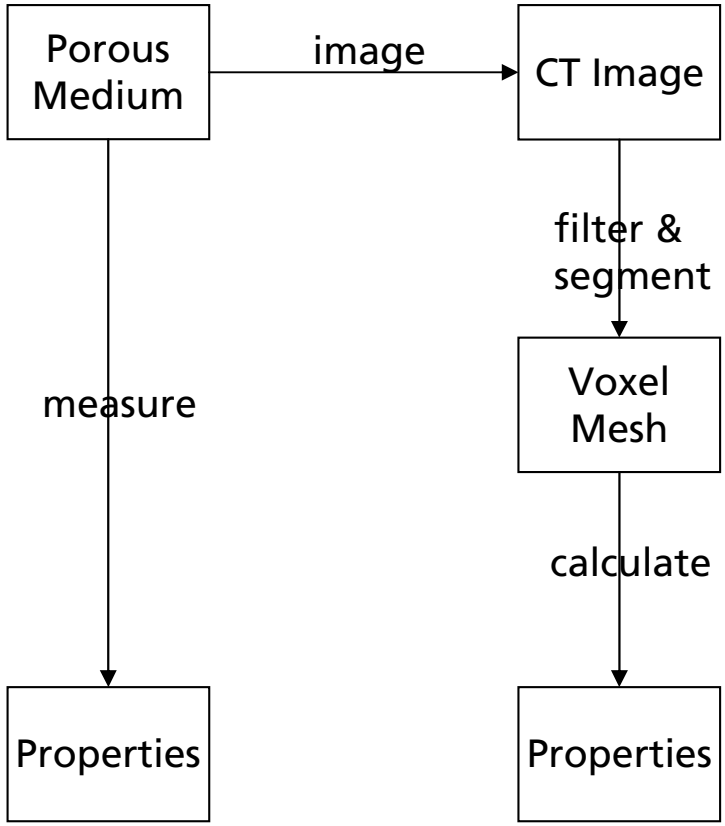

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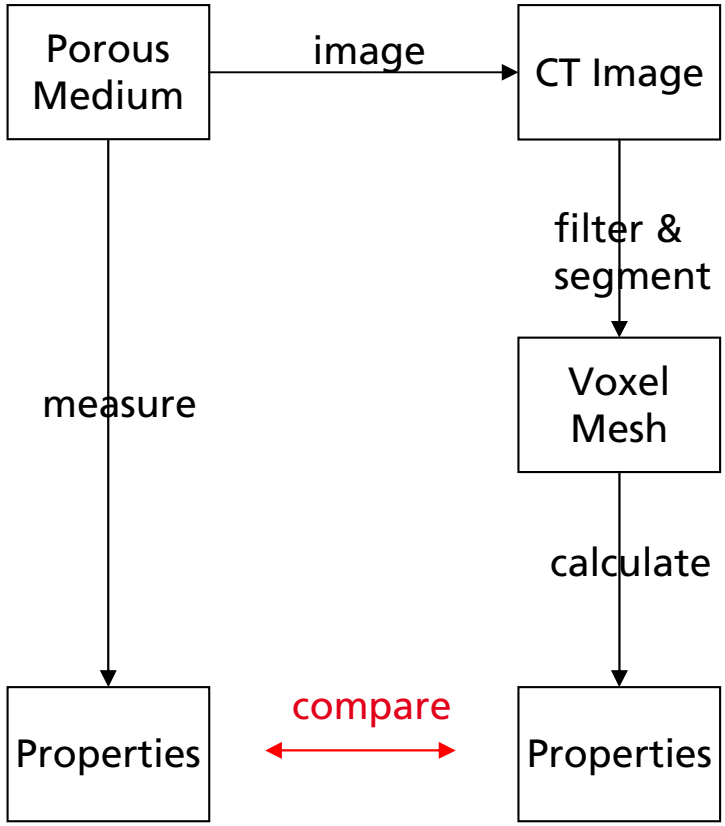

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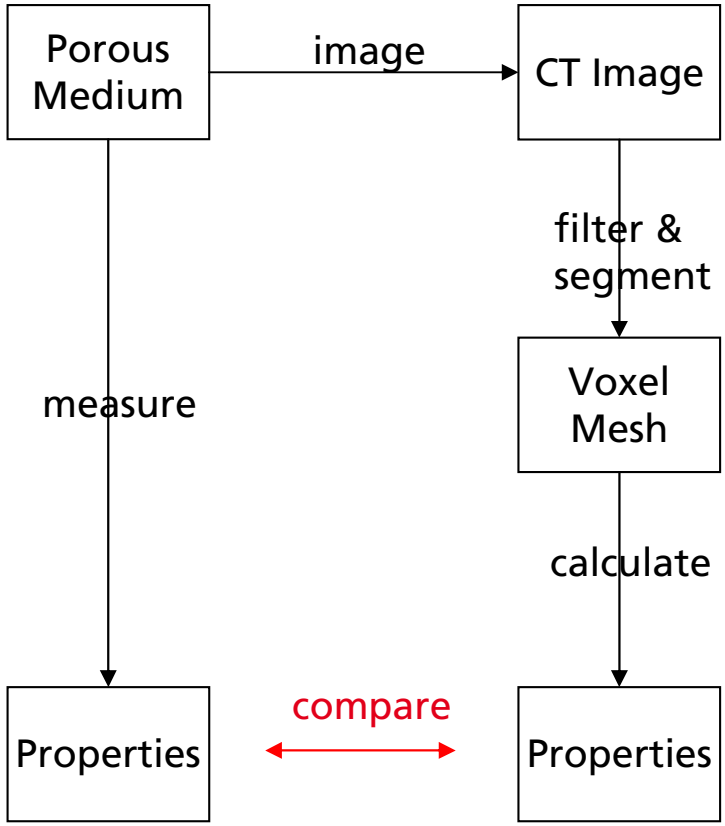
Bridge the Gap - Step 1: Validate Calculations
... and Measurements
... and Imaging



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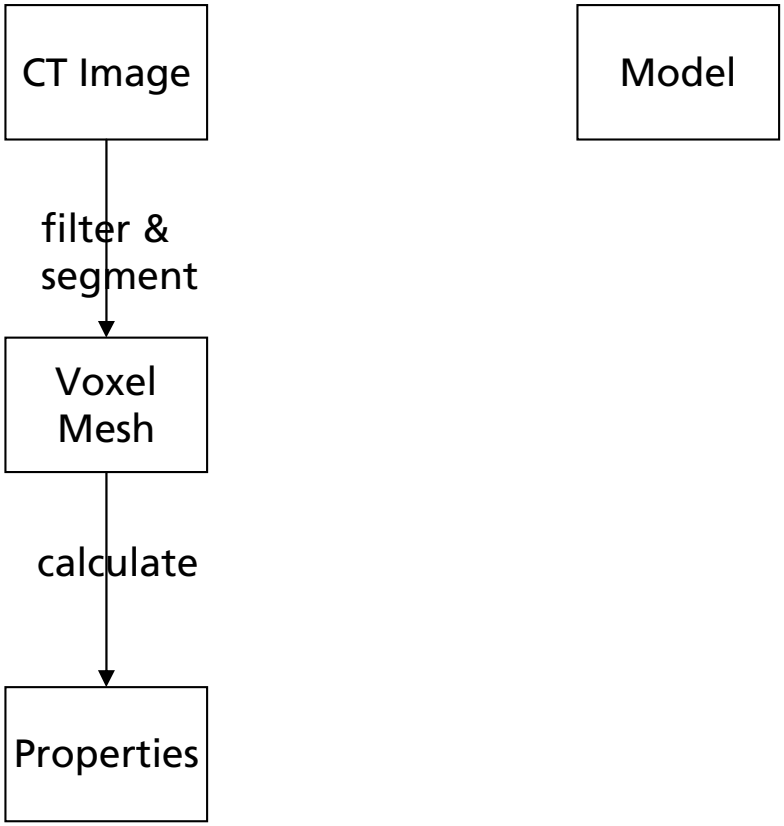
Bridge the Gap - Step 2: Validate Modeling



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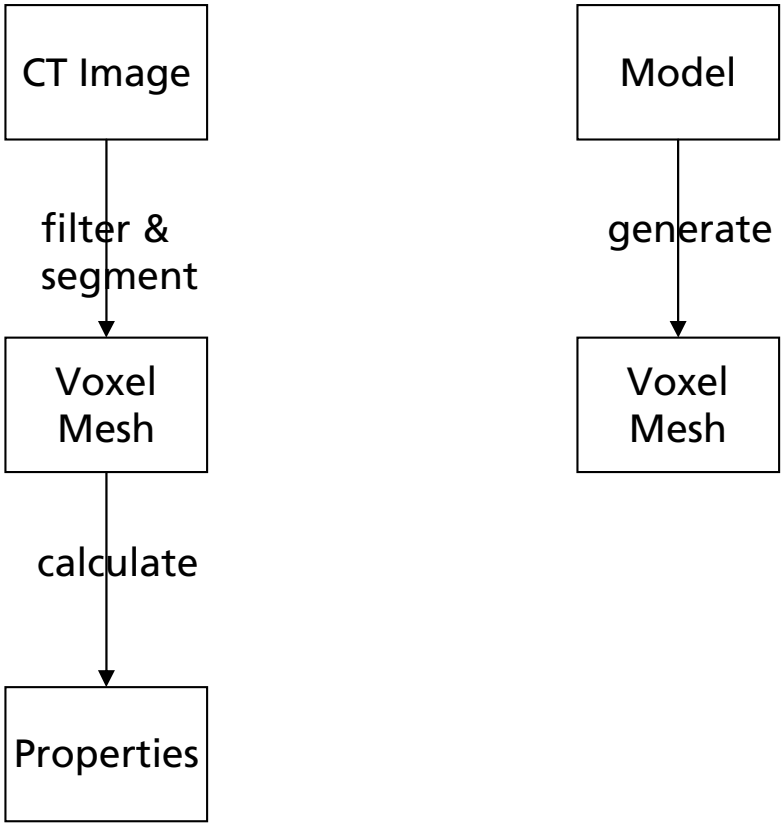
ITWM

Bridge the Gap - Step 2: Validate Modeling



Fraunhofer
ITWM

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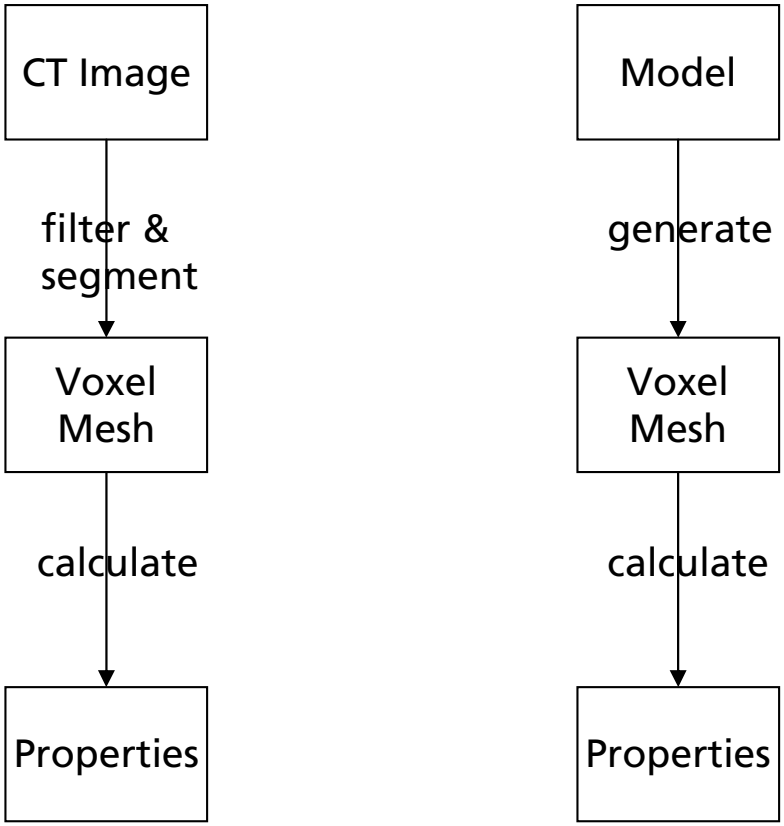

Fraunhofer ITWM

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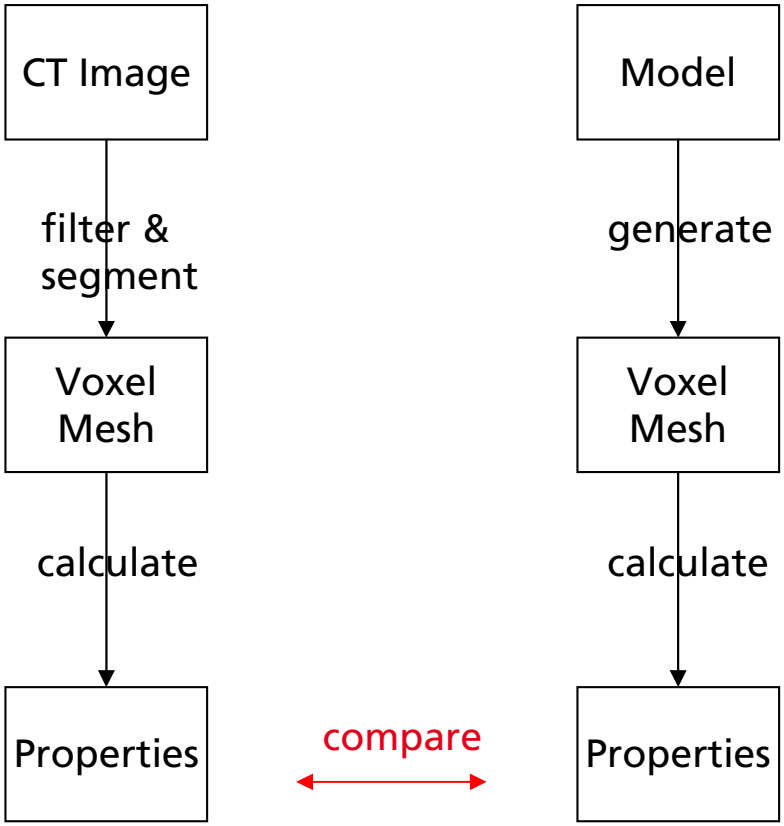

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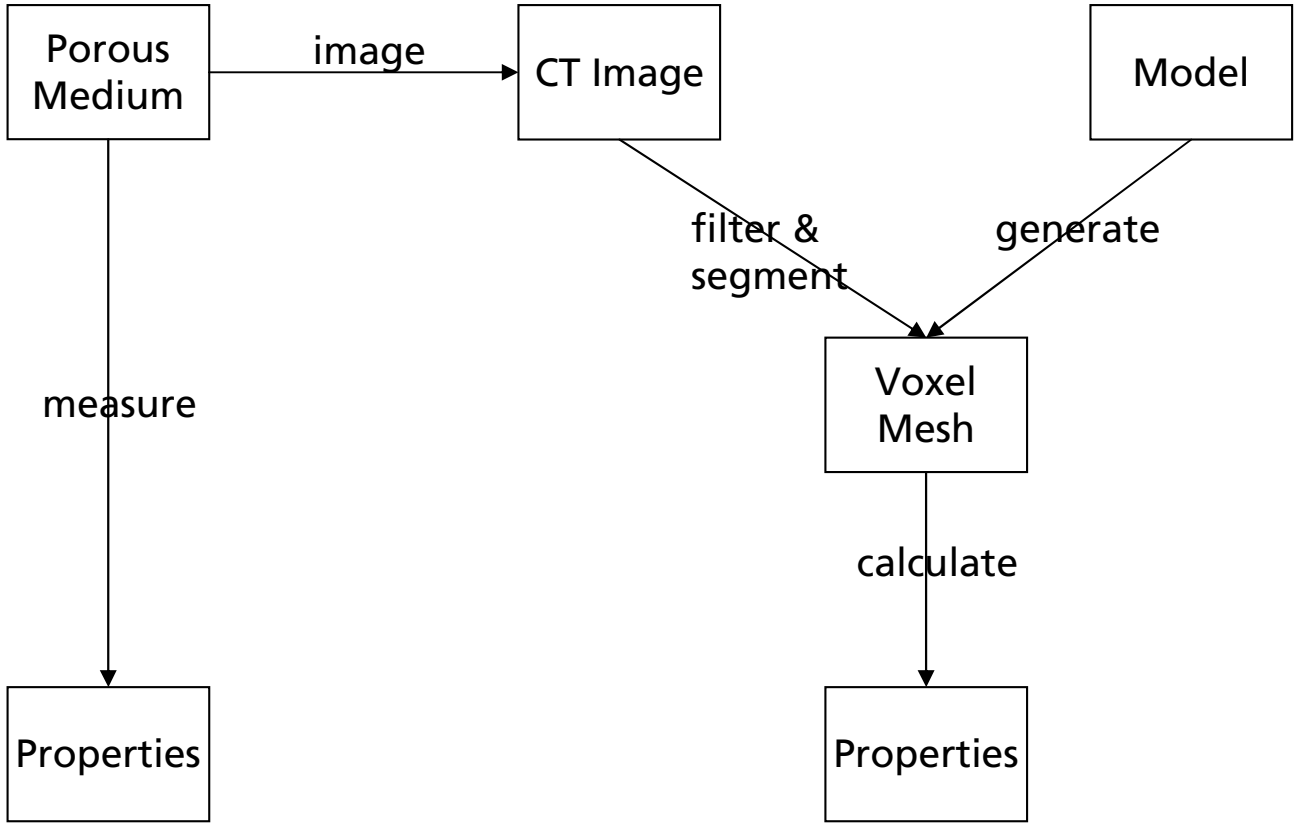
The GeoDict Idea



Fraunhofer ITWM

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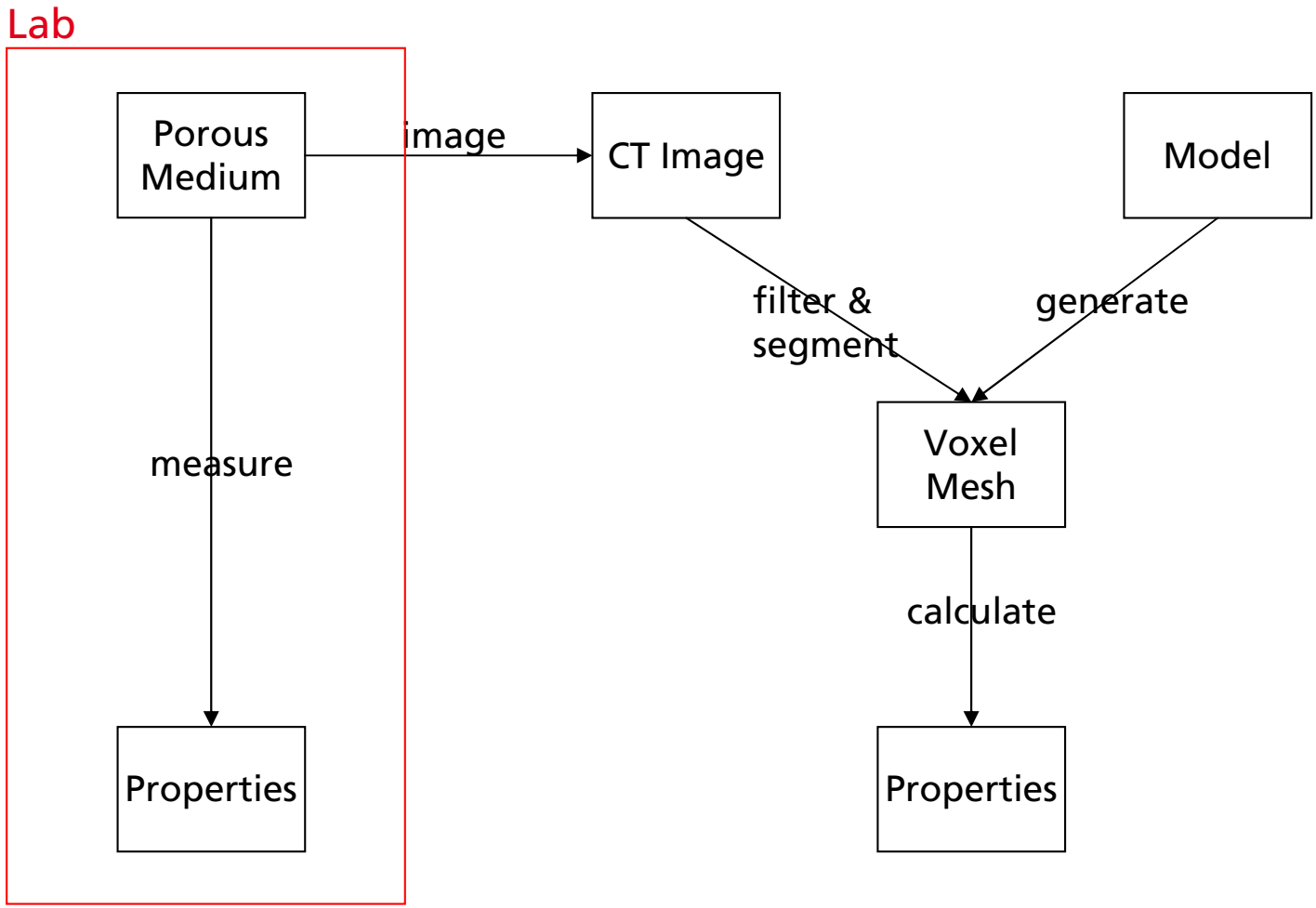

Fraunhofer ITWM

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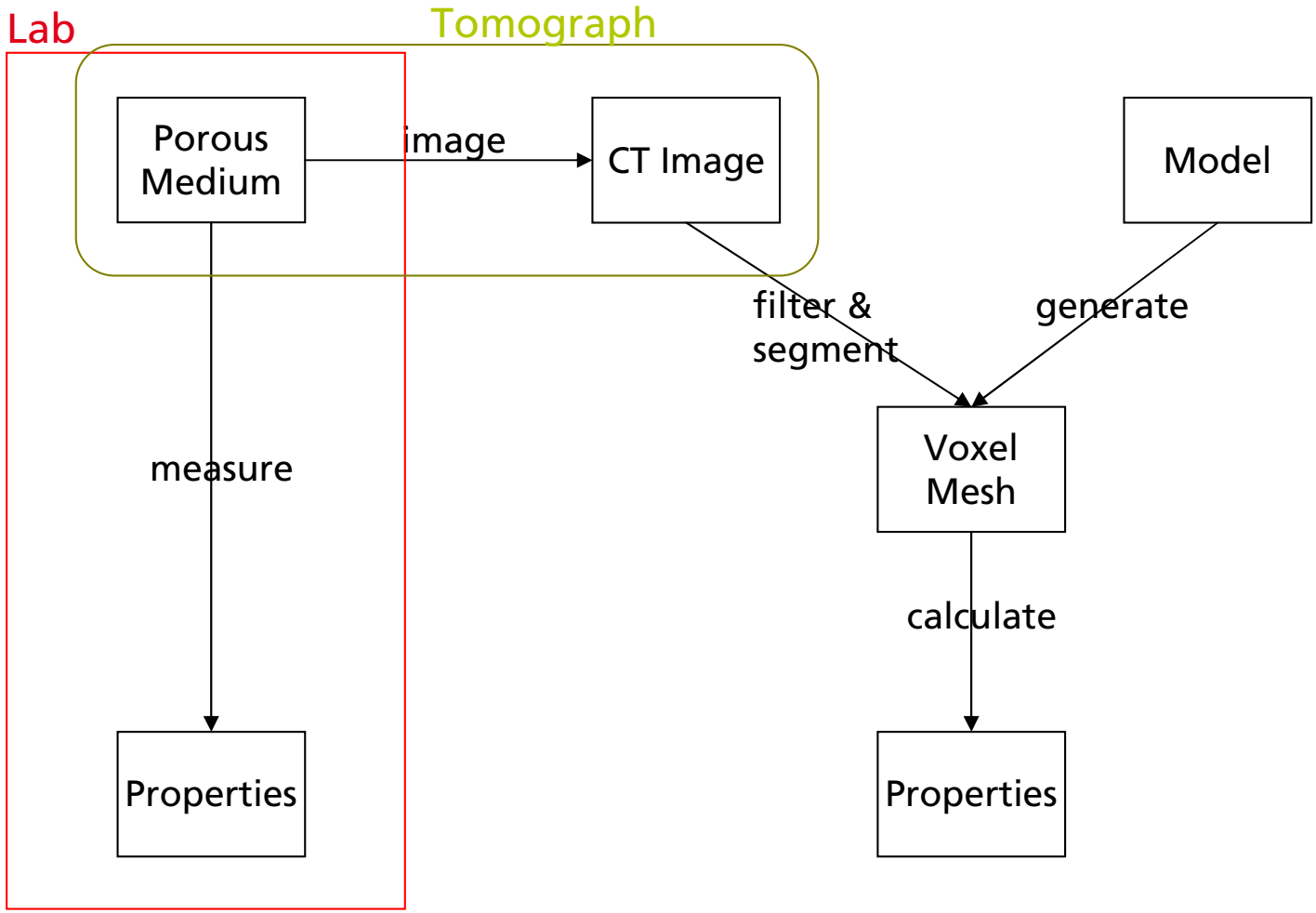

Fraunhofer ITWM

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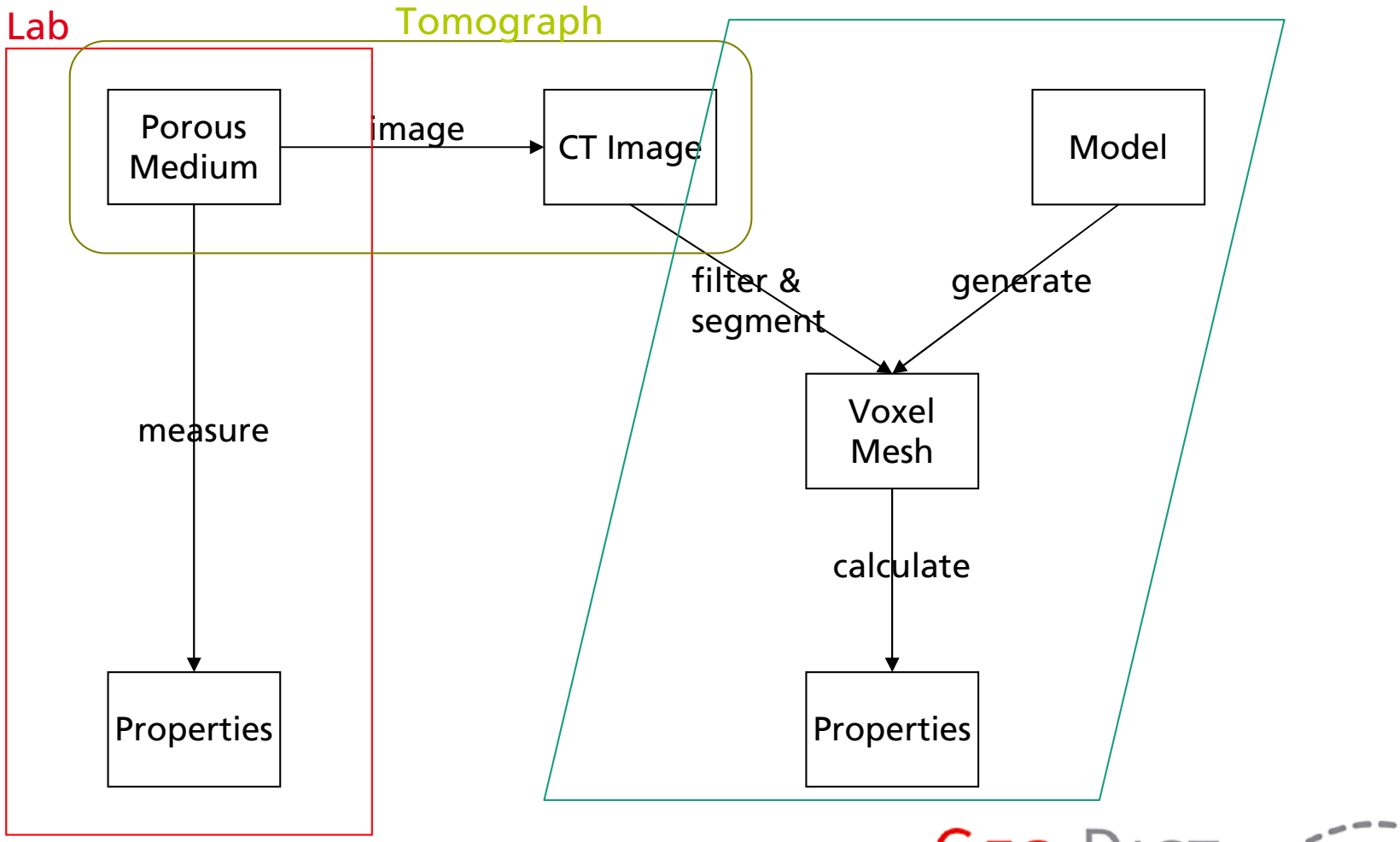
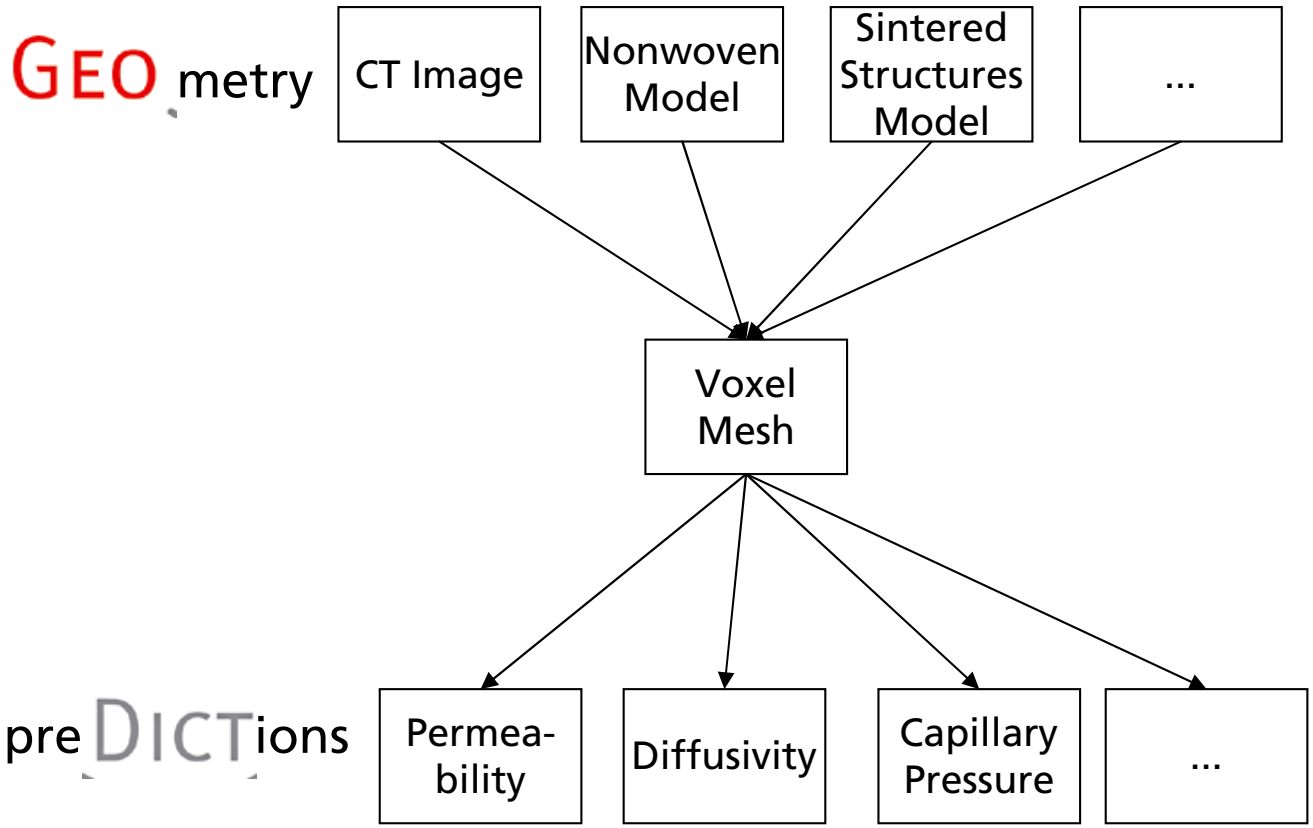


GEO DICT

Fraunhofer ITWM

The GeoDict Software



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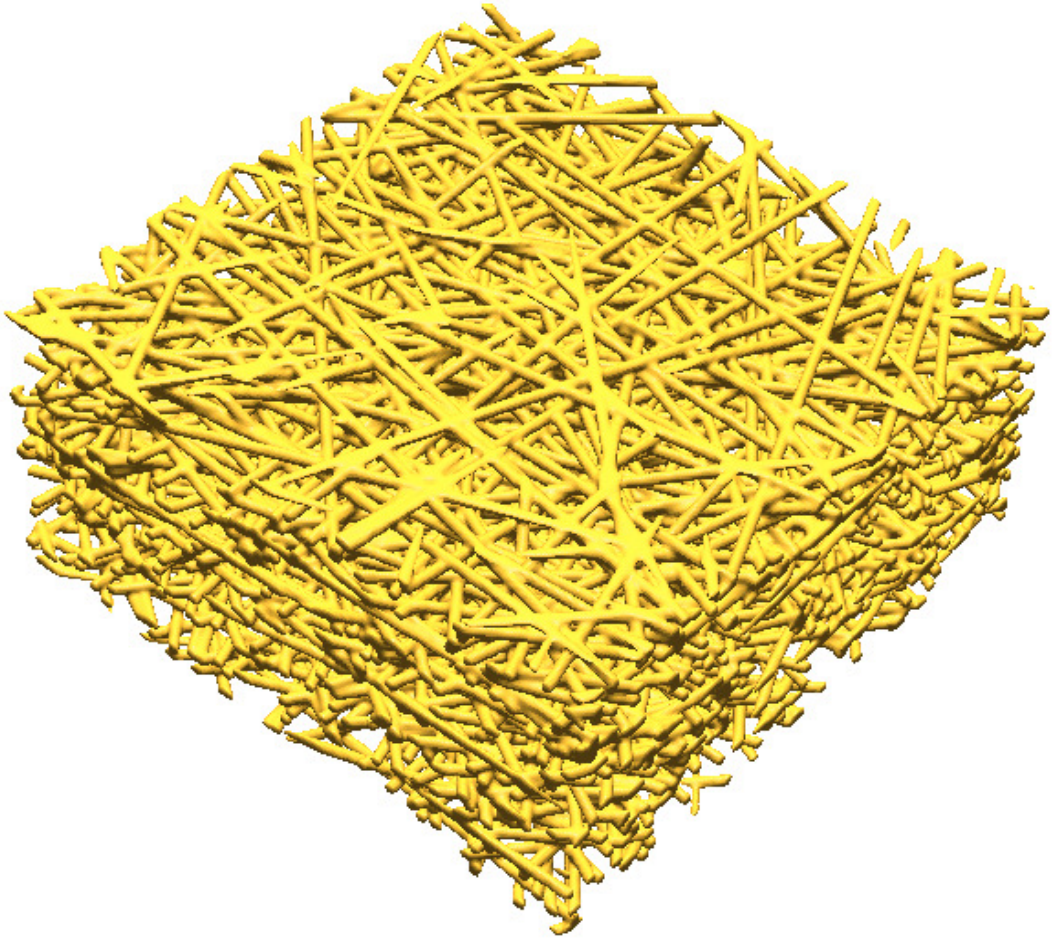
Model: Nonwovens - Straight Fibres

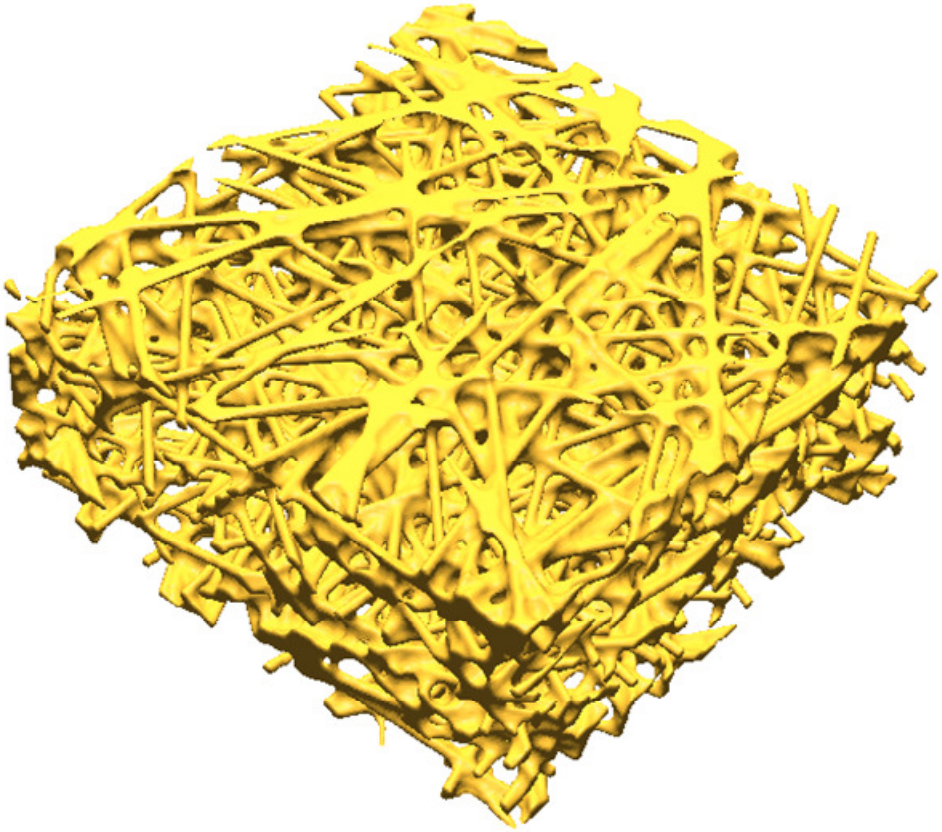
Poisson line process using:

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

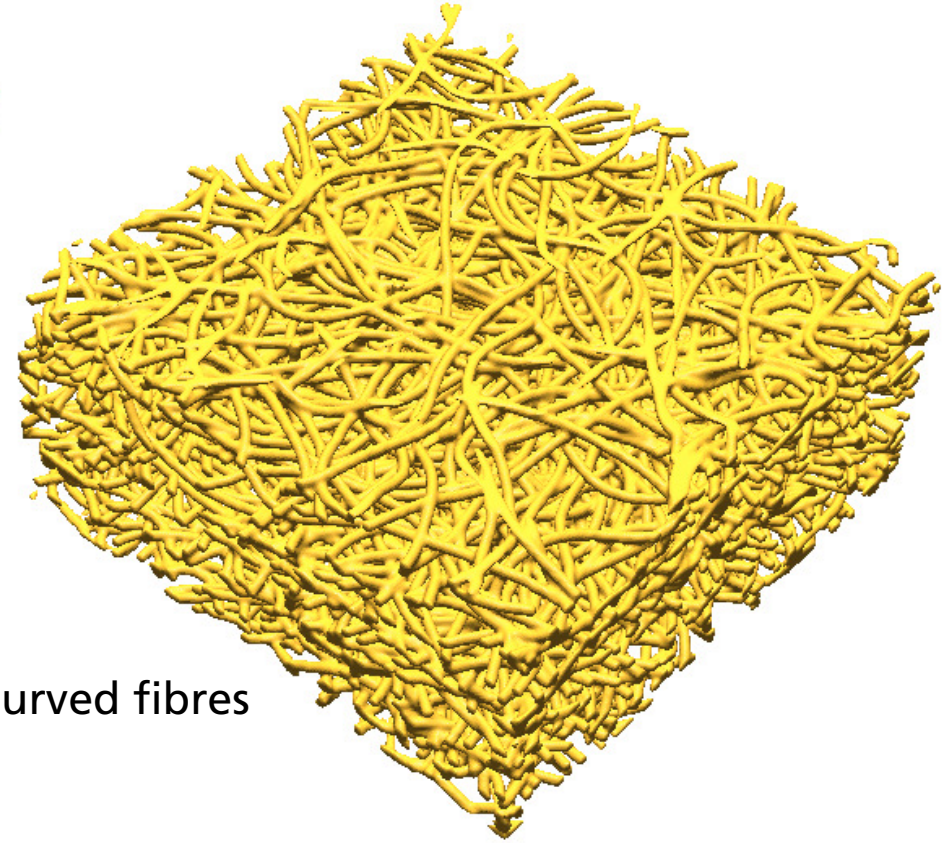


Fraunhofer ITWM

Model: Nonwovens - Some Variants

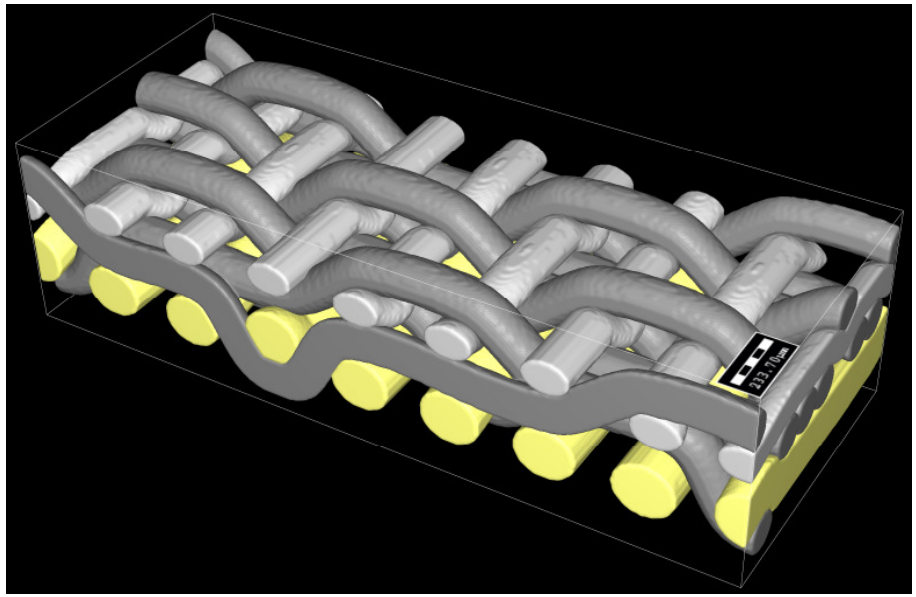


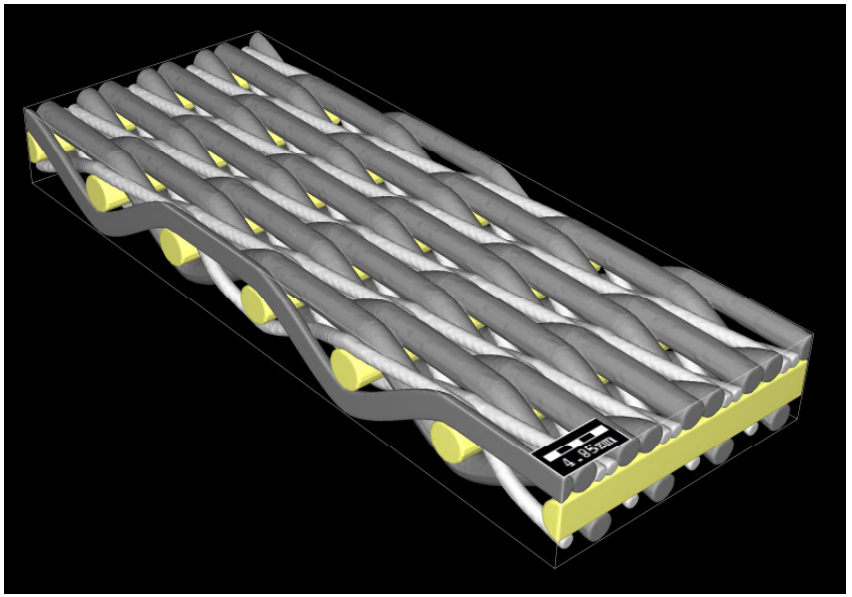
Straight fibres plus binder



Curved fibres

Model: Woven Fabric





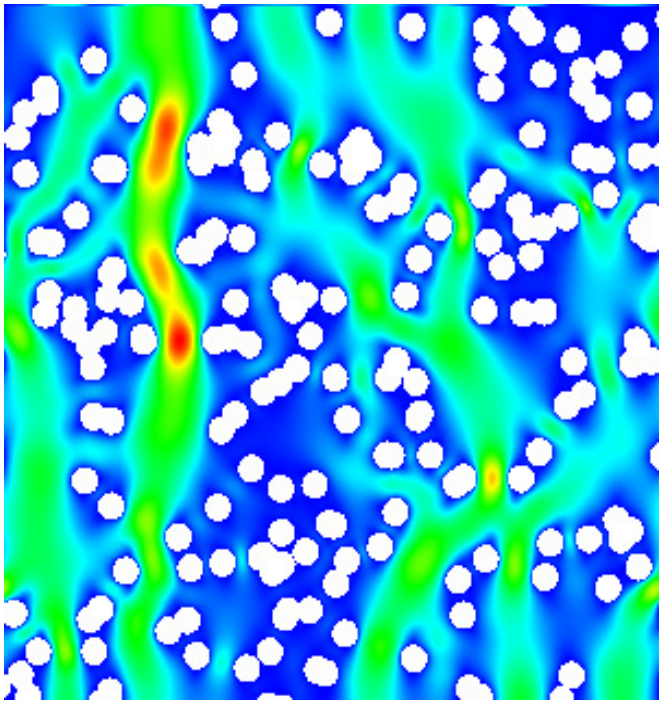
Fraunhofer ITWM

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



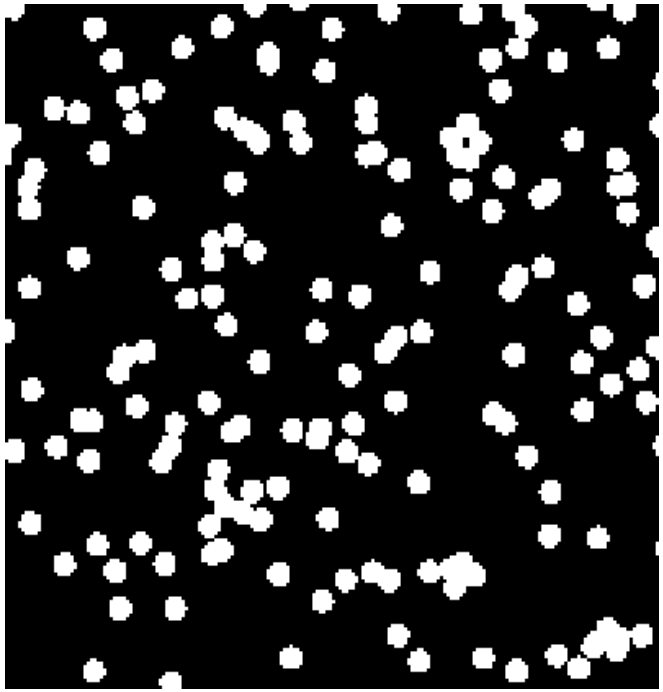
Microscopic description
(pore structure model)

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

Boundary conditions: no-slip on fibre surface, pressure drop
κ can be determined from the solution!

Property: Relative Permeability

Two-step approach:

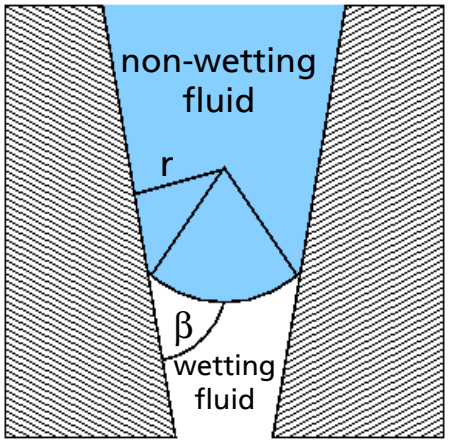


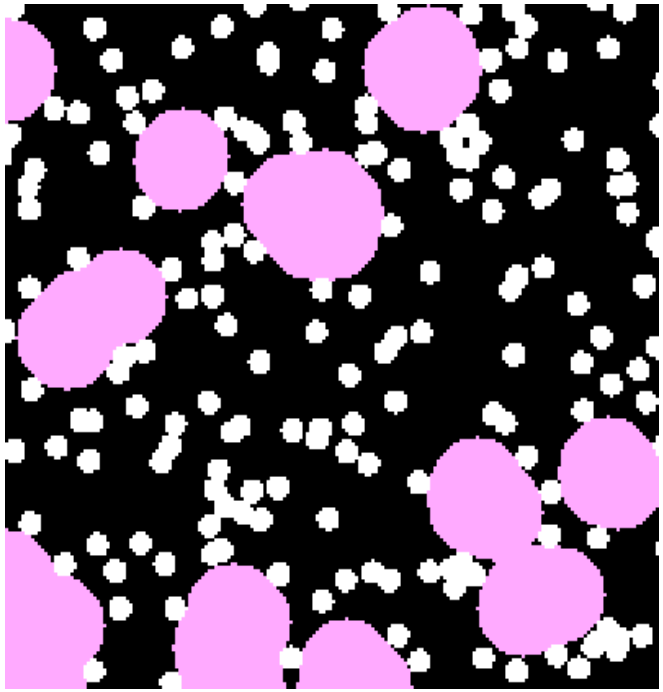
Property: Relative Permeability

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





Fraunhofer ITWM

Property: Relative Permeability

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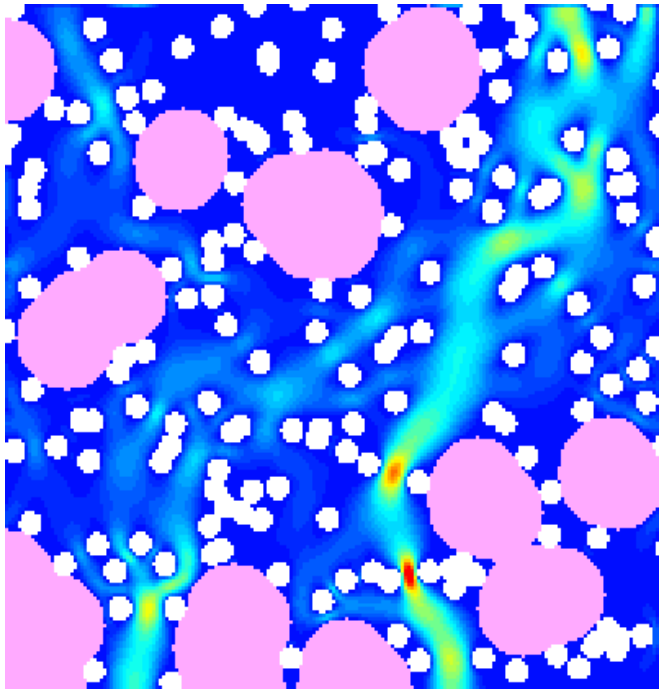
   - Idea: a pore is filled with the non-wetting fluid (=water), if $p_c \geq \frac{2\sigma}{r} \cos\beta$

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

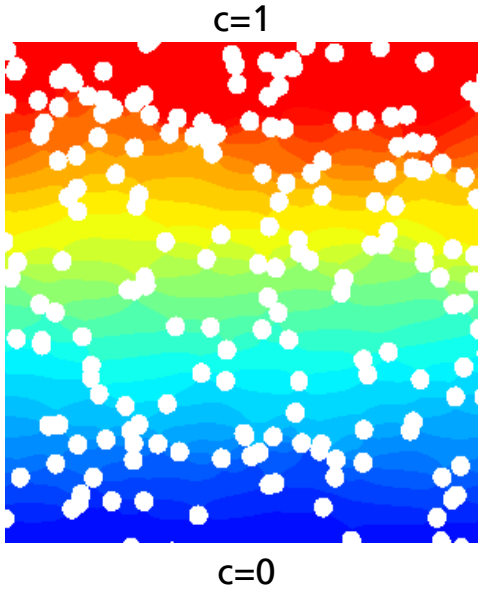
Macroscopic description
(homogenized porous media model)
Fick's first law: $j = -D^* \nabla c$

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!



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Summary Part I

Models:

- CT Images

- Fibrous nonwovens
- Woven structures
- Sintered structures
- Sphere packings

- Layered structures

Properties:

- Pore size distribution
- Surface area

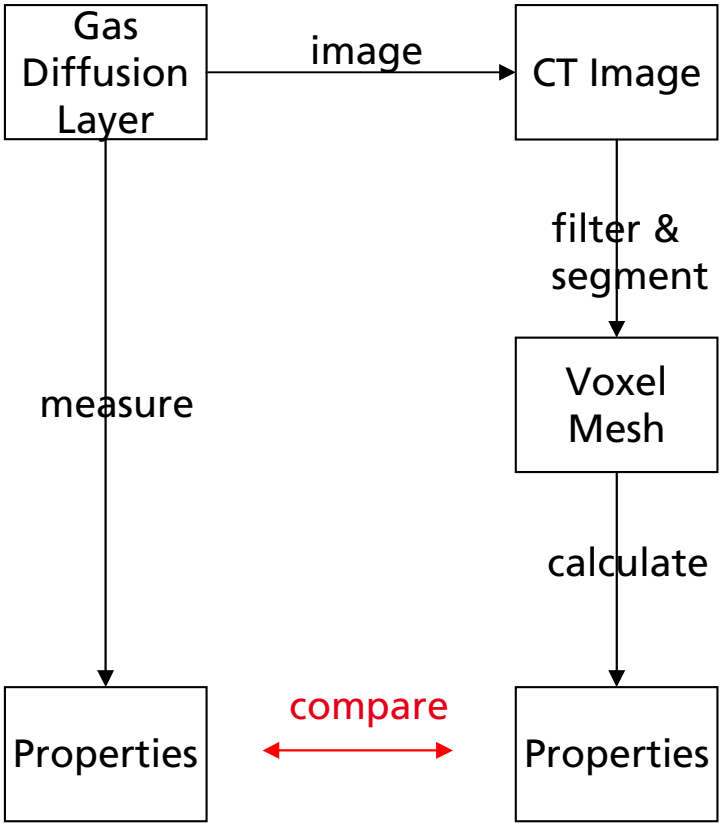
- (Knudsen) Diffusivity
- Permeability
- Electric conductivity
- Heat conductivity

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

- Filter efficiency and life time

Fraunhofer ITWM

Application: Gas Diffusion Layer of PEM Fuel Cell



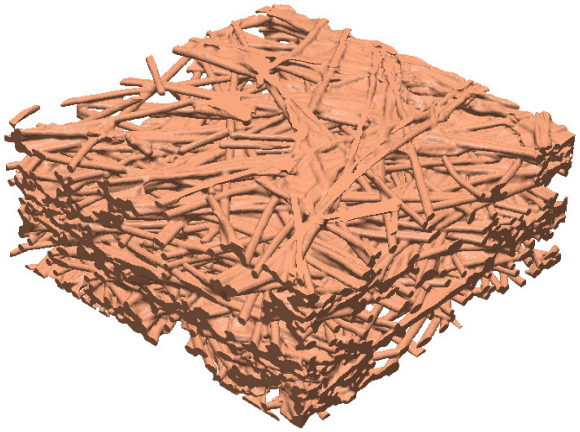
Joint work

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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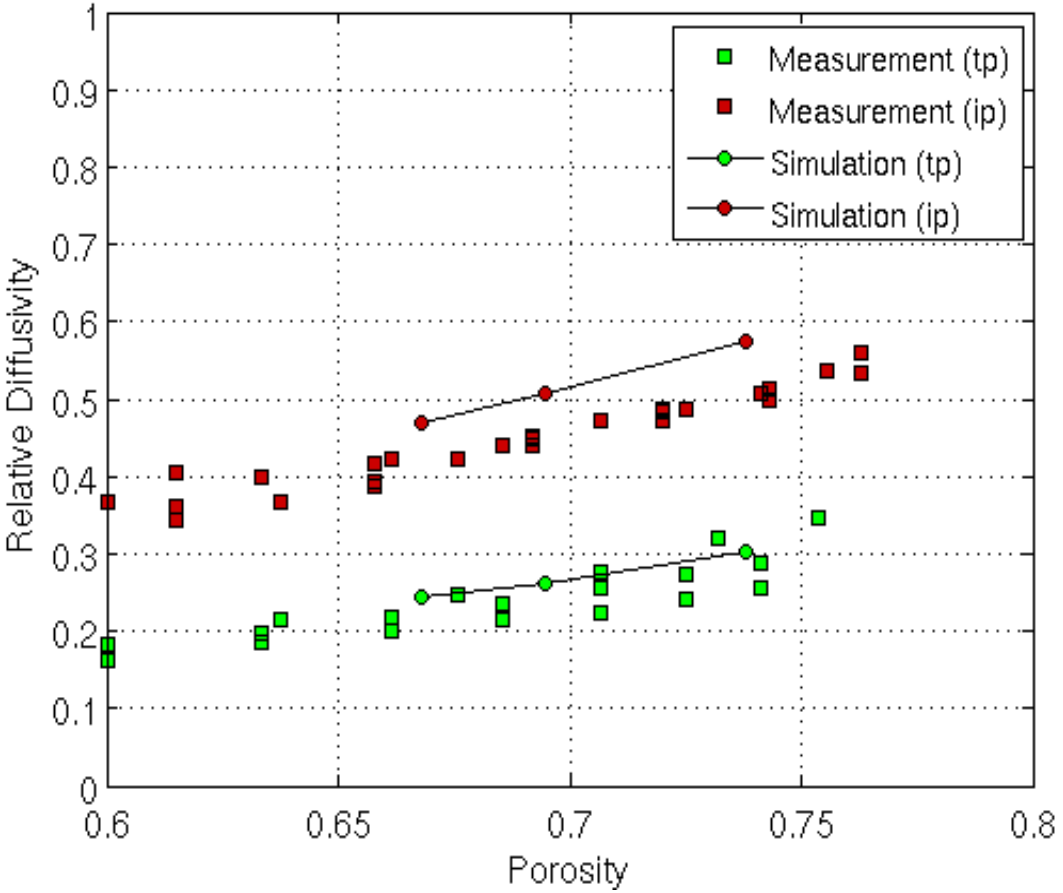
Diffusivity



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

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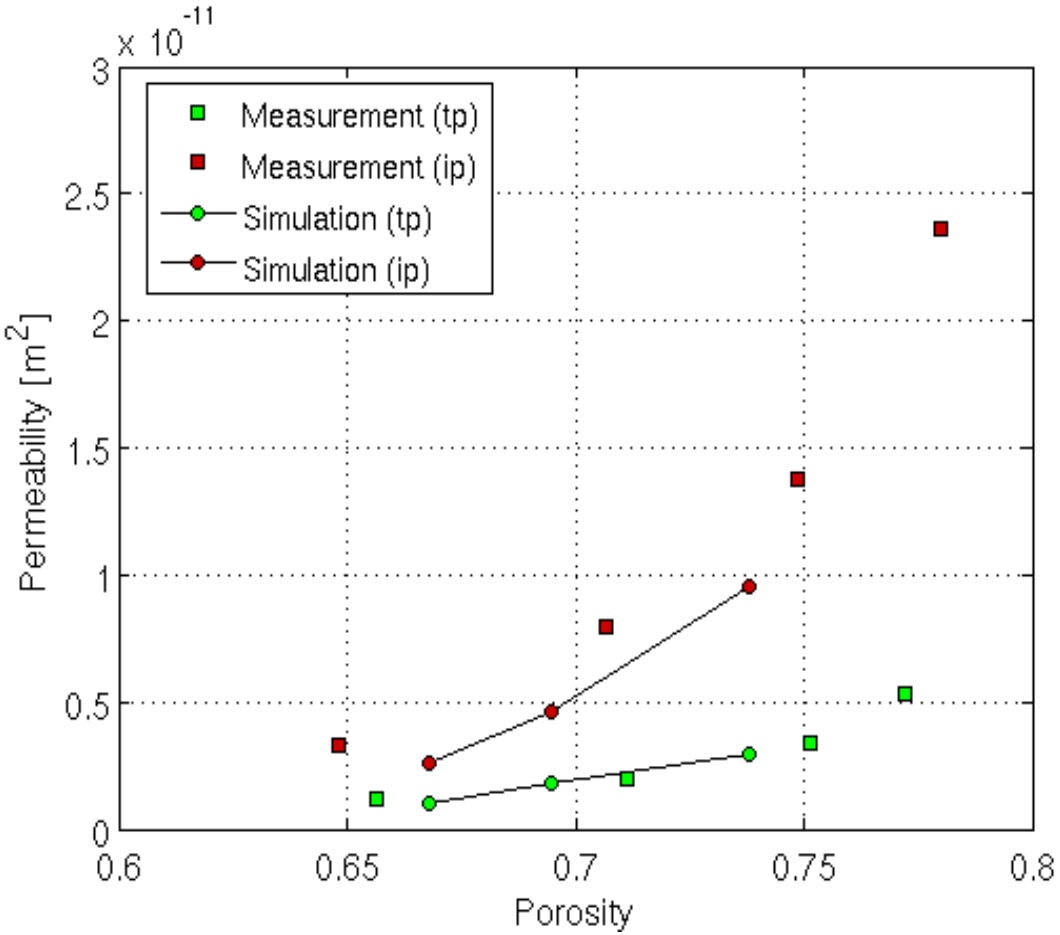
Permeability



Perfect in tp-direction

Small differences in ip-direction
- ip-measurememts performed on a stack of GDLs
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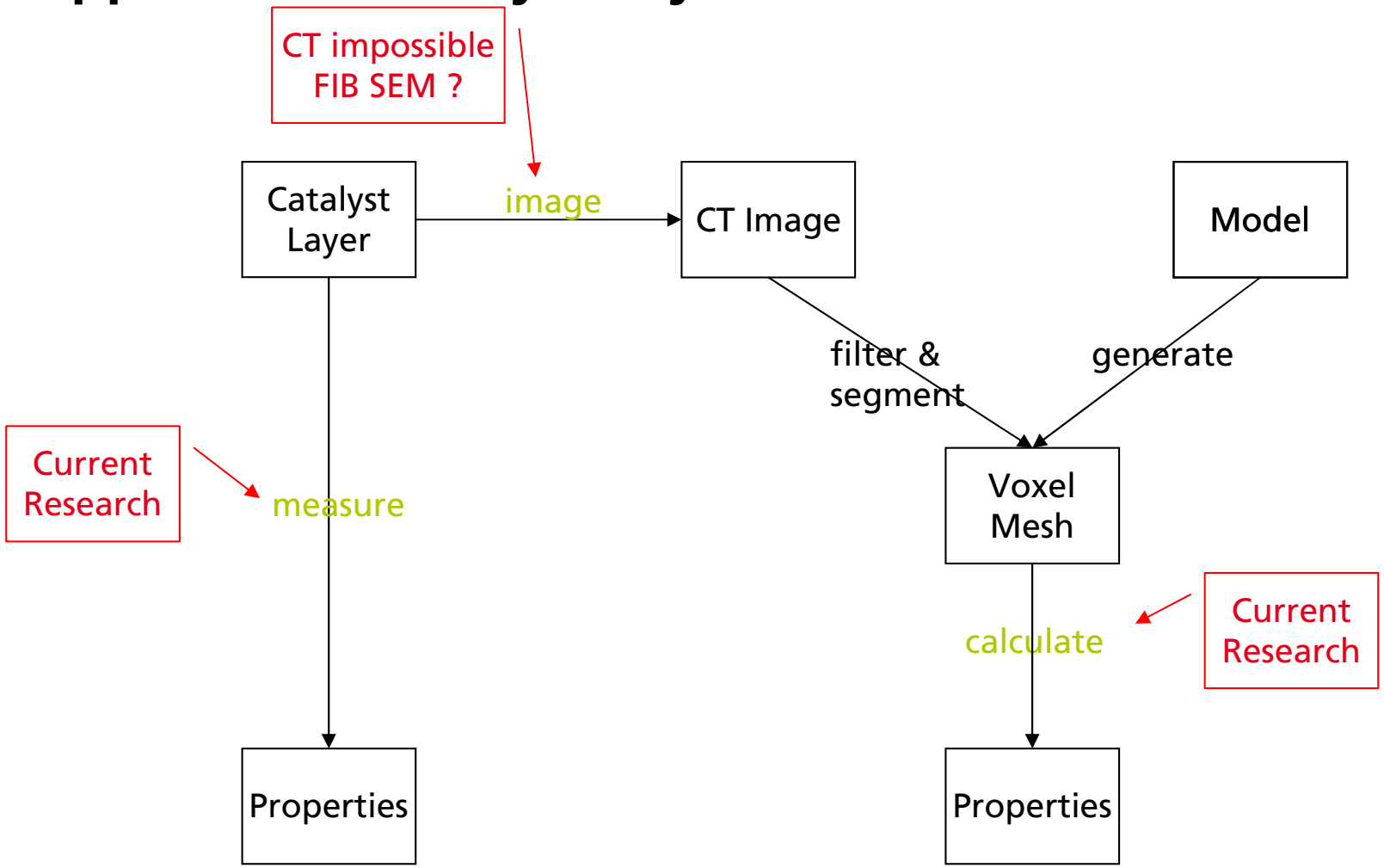
Application: Catalyst Layer of PEM Fuel Cell



Problem: pore sizes < 100 nm

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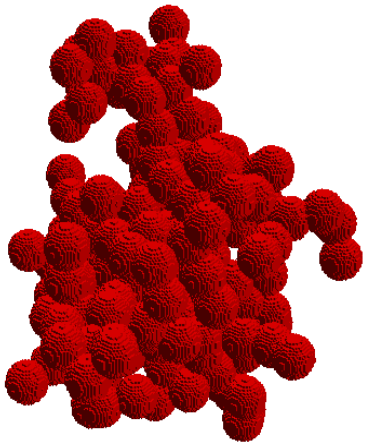
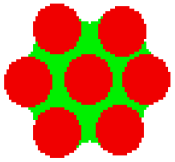
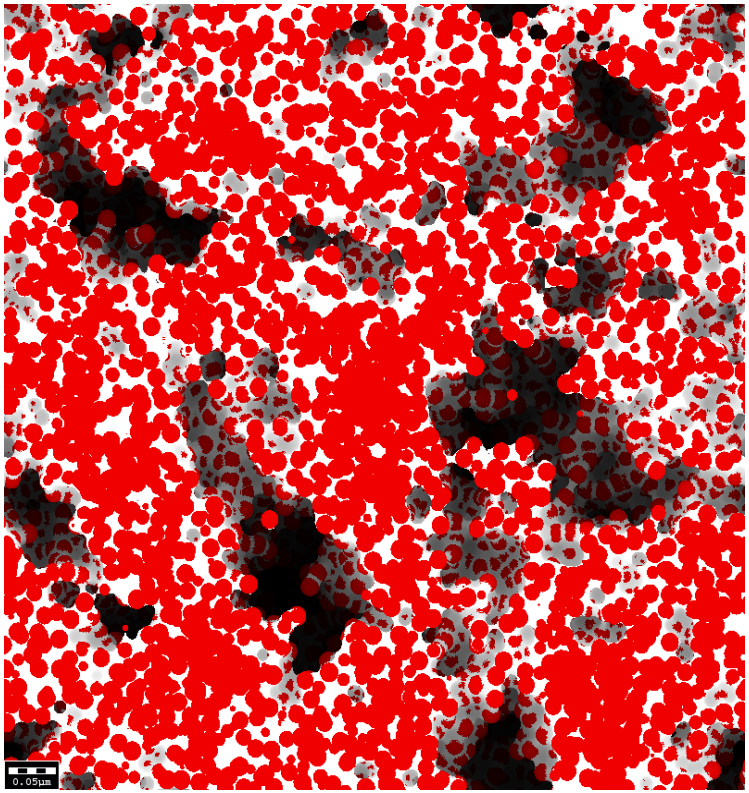
Catalyst Layer Model

Carbon agglomerates plus electrolyte





Elect. between
Carbon Partikels



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Conductivity

Compare models with varying carbon and electrolyte volume fractions

Vol% Carbon	Vol% Electrolyte	Porosity	Electronic Conductivity	Protonic Conductivity
35.4	12.2	52.4	6.6 %	1.1 %
40.9	5.2	53.9	9.7 %	none
40.9	13.8	45.3	9.7 %	1.6 %
40.9	20.7	38.3	9.7 %	4.9 %
40.9	26.3	32.8	9.7 %	8.2 %
45.1	15.2	39.8	13.4 %	1.9 %
50.1	16.6	33.3	17.6 %	2.2 %

Summary Part II

Gas diffusion layer:

- validated method to determine diffusivity and permeability

Catalyst layer:

- no validation possible until 3D images are available

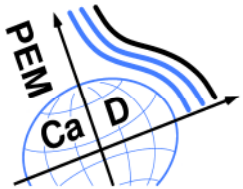
Thank You !

GEO DICT

Geometry generator,
property predictor and
virtual material designer

www.geodict.com

BMBF project PemCaD



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