The Influence of Variable Wettability on Mass Transport Properties of GDLs

Jürgen Becker, Christian Wagner, Sven Linden,
Andreas Wiegmann

ModVal Lausanne, 23.03.2016

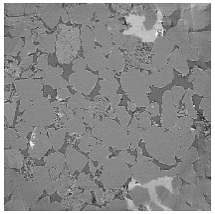
Who is Math2Market ?

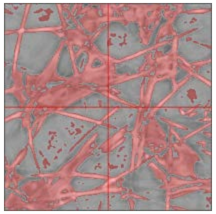
- Math2Market GmbH was founded 2011 in Kaiserslautern.
- Spin-off of Fraunhofer Institute for Industrial Mathematics, ITWM.
- Today: 12 full-time, 6 part-time employees, turnover >2 Mio € / year

- Our product: GeoDict software
  - Sales
  - Development and Customization
  - Consulting

What can GeoDict do?

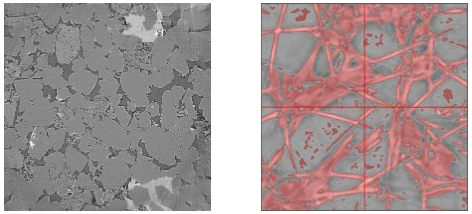
What can GeoDict do?



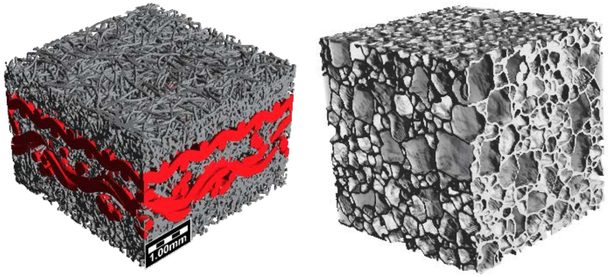


Import of CT Scans

What can GeoDict do?

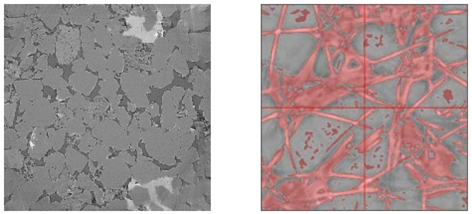


Import of CT Scans

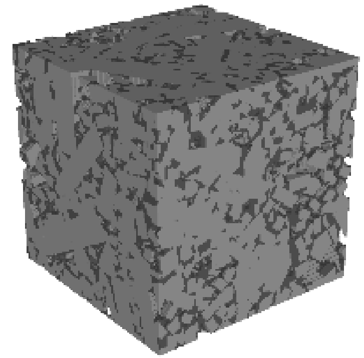


Create 3D Models of Microstructures

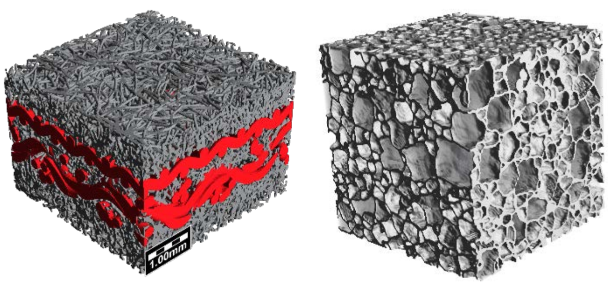
What can GeoDict do?



Import of CT Scans

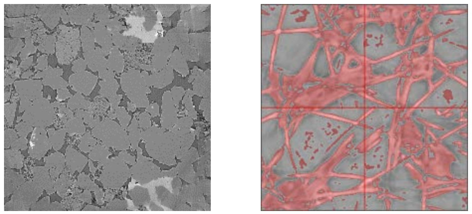


Geometric Analysis of 3D Structures

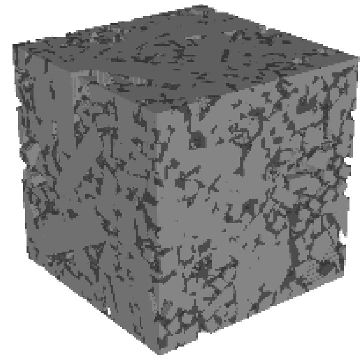


Create 3D Models of Microstructures

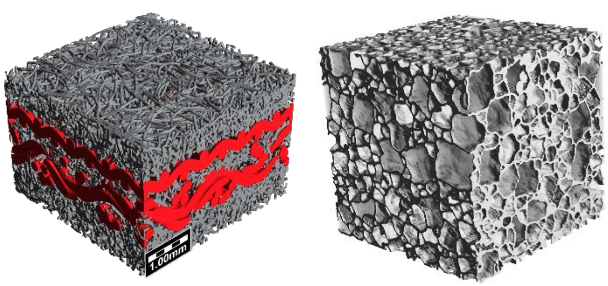
What can GeoDict do?



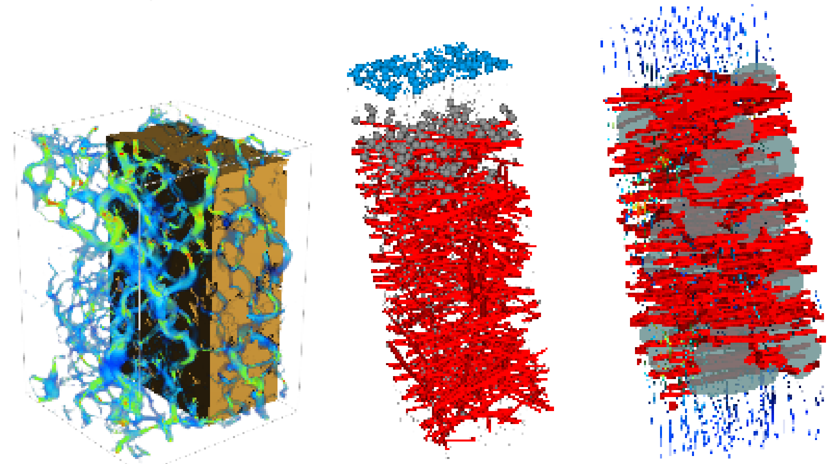
Import of CT Scans



Geometric Analysis of 3D Structures



Create 3D Models of Microstructures



Simulate advection, diffusion particle transport, stiffness

… with applications in:

Filtration	Mostly automotive, filter media & filters
Personal Care	Wipes, Feminine Care, Baby Care
Electrochemistry	Fuel cell media & battery materials
Weaves and Paper	Paper forming and dewatering, Metal Wire Mesh
Composites	Mostly automotive, lightweight materials
Oil and Gas	Digital rock physics, digital sand control

The Influence of Variable Wettability on Mass Transport Properties of GDLs

Overview:

1. 3D GDL model and compression
2. Computing permeability
3. Capillary pressure and saturation with variable wettability
4. Effect on relative permeability

3D GDL Model and Compression

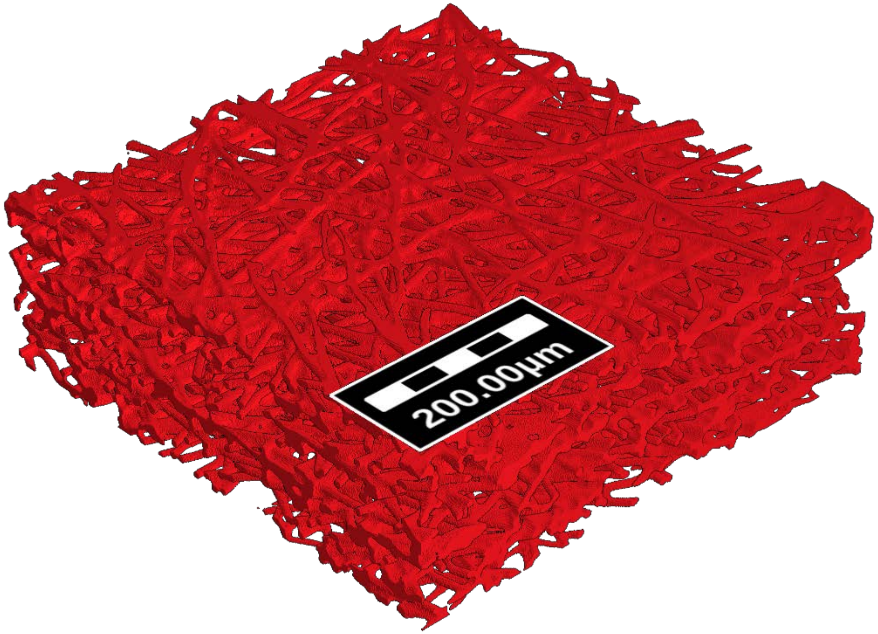
Structure Model

GDL:

- Carbon fibers, 7 µm diameter
- 20 wt% binder
- 200 µm thickness

Model

- 1 µm resolution
- Voxel grid
- 600x600x200 = 72 Mio. cells
- Stochastic process



Compression Simulation

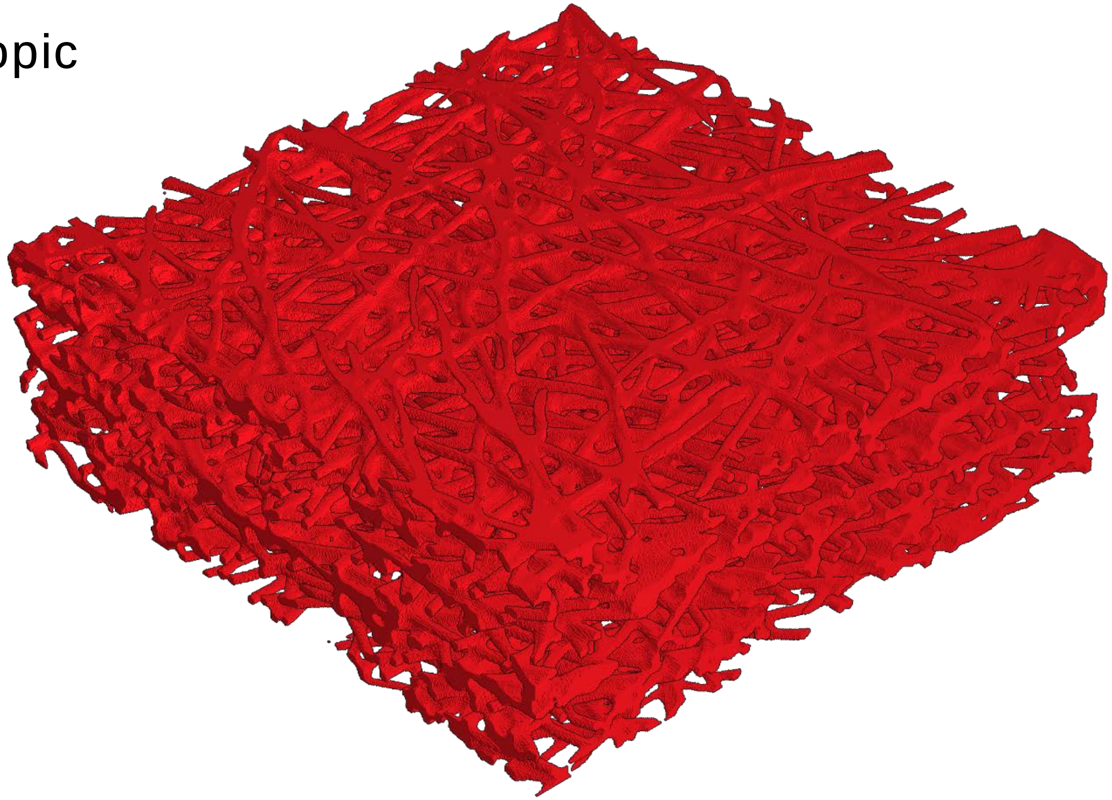
Fibers: linear elastic, transverse isotropic

Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM



Runtime: 1h 17 min (8x)

Compression	0	0.05	0.1	0.15	0.2	0.25

Compression Simulation

Fibers: linear elastic, transverse isotropic

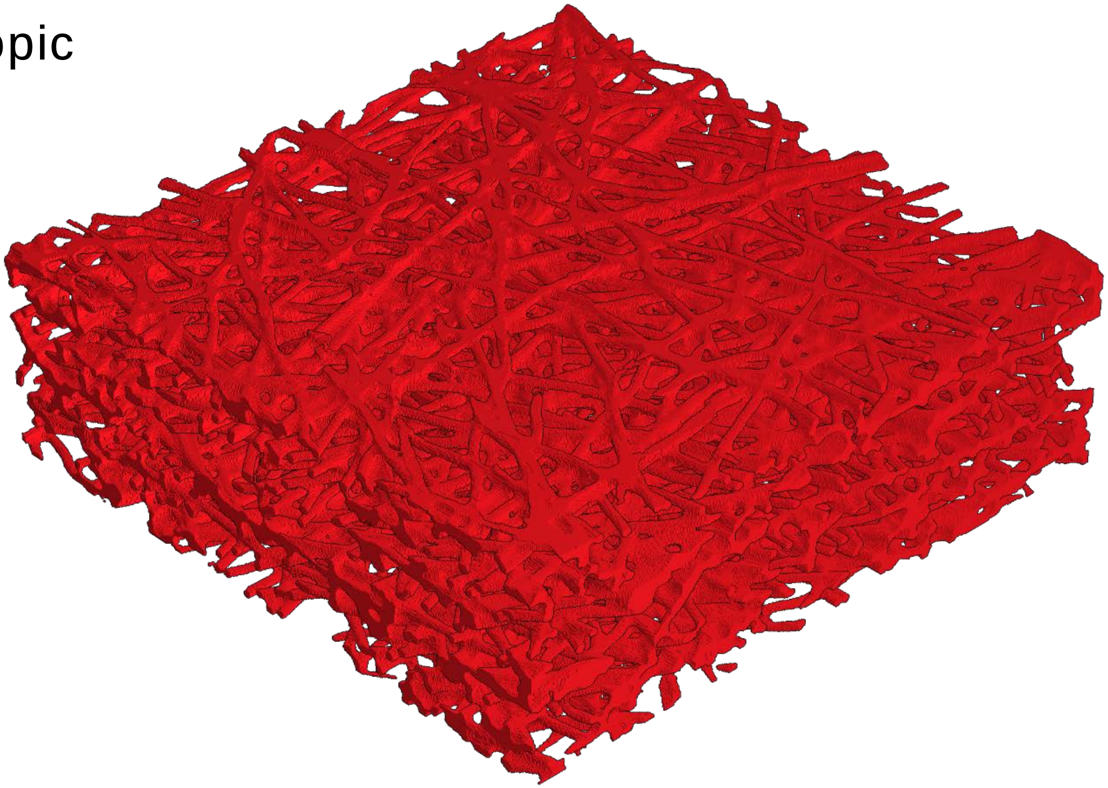
Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM

Runtime: 1h 17 min (8x)



Compression	0	0.05	0.1	0.15	0.2	0.25

Compression Simulation

Fibers: linear elastic, transverse isotropic

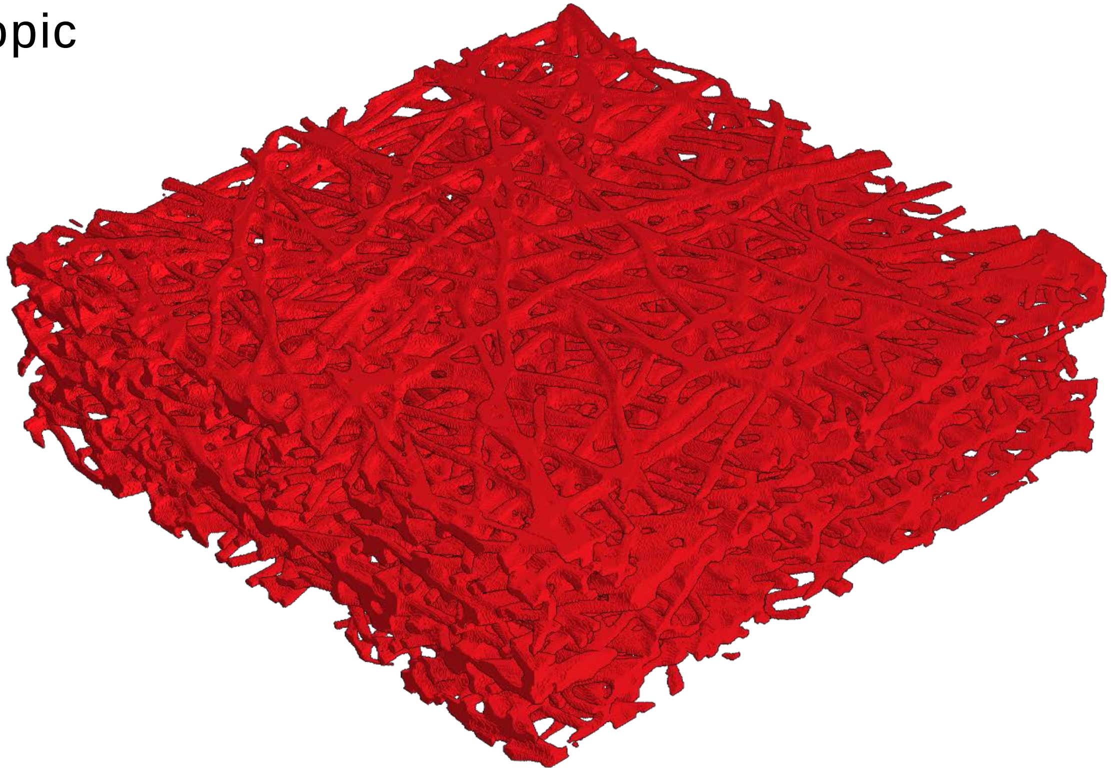
Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM

Runtime: 1h 17 min (8x)



Compression	0	0.05	0.1	0.15	0.2	0.25

Compression Simulation

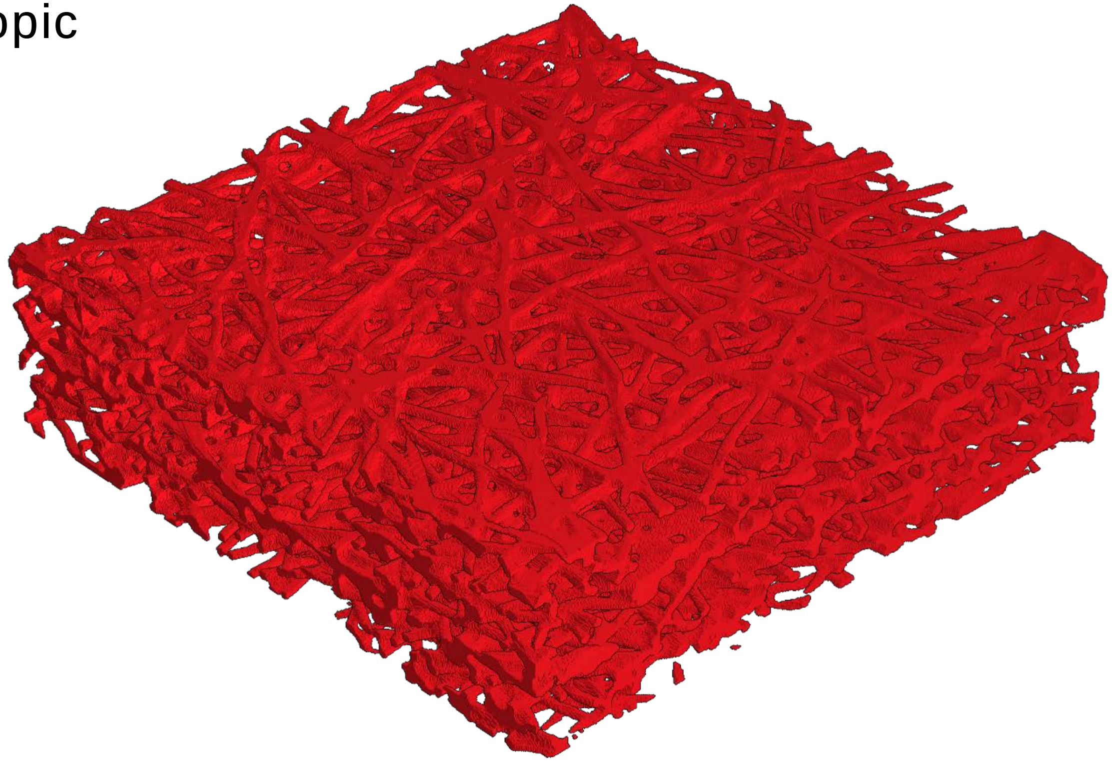
Fibers: linear elastic, transverse isotropic

Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM



Runtime: 1h 17 min (8x)

Compression	0	0.05	0.1	0.15	0.2	0.25

Compression Simulation

Fibers: linear elastic, transverse isotropic

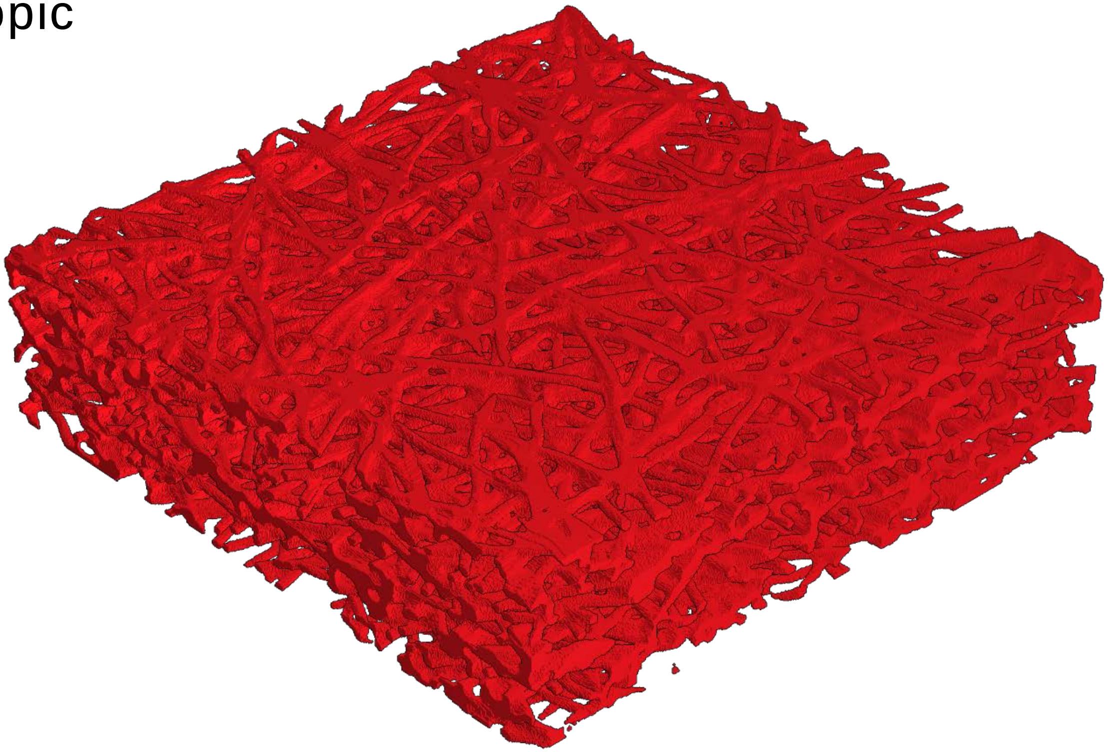
Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM

Runtime: 1h 17 min (8x)



Compression	0	0.05	0.1	0.15	0.2	0.25

Compression Simulation

Fibers: linear elastic, transverse isotropic

Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM

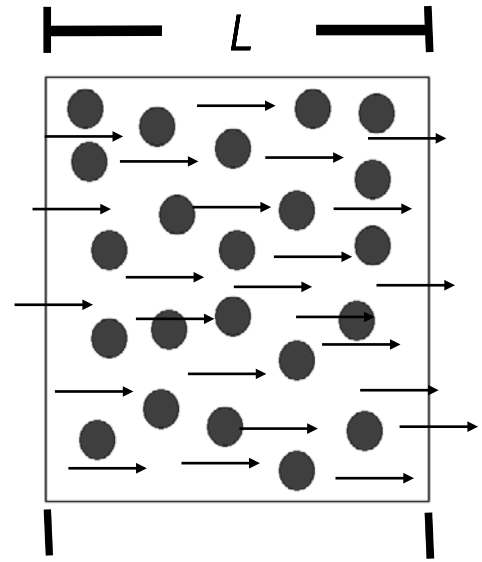
Runtime: 1h 17 min (8x)

Compression	0	0.05	0.1	0.15	0.2	0.25

Computing Permeability

Flow solver finds interstitial flow field **u**.

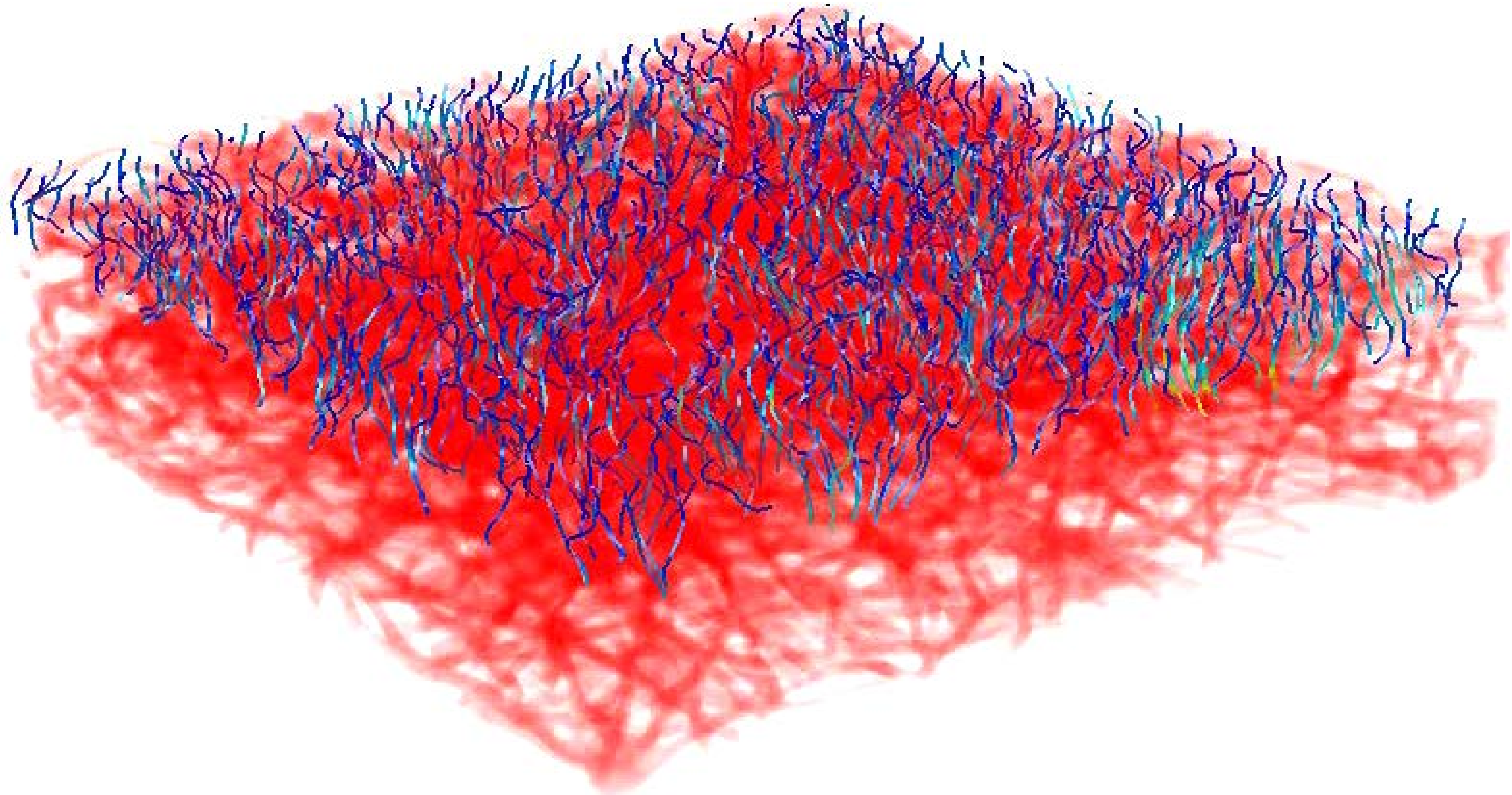
- $\bar{\mathbf{u}}$: Average (superficial) flow velocity
- P_1: Pressure average over inflow plain
- P_2: Pressure average over outflow plain
- $\mathbf{K}$: Permeability tensor



Pressure P_1 Pressure P_2

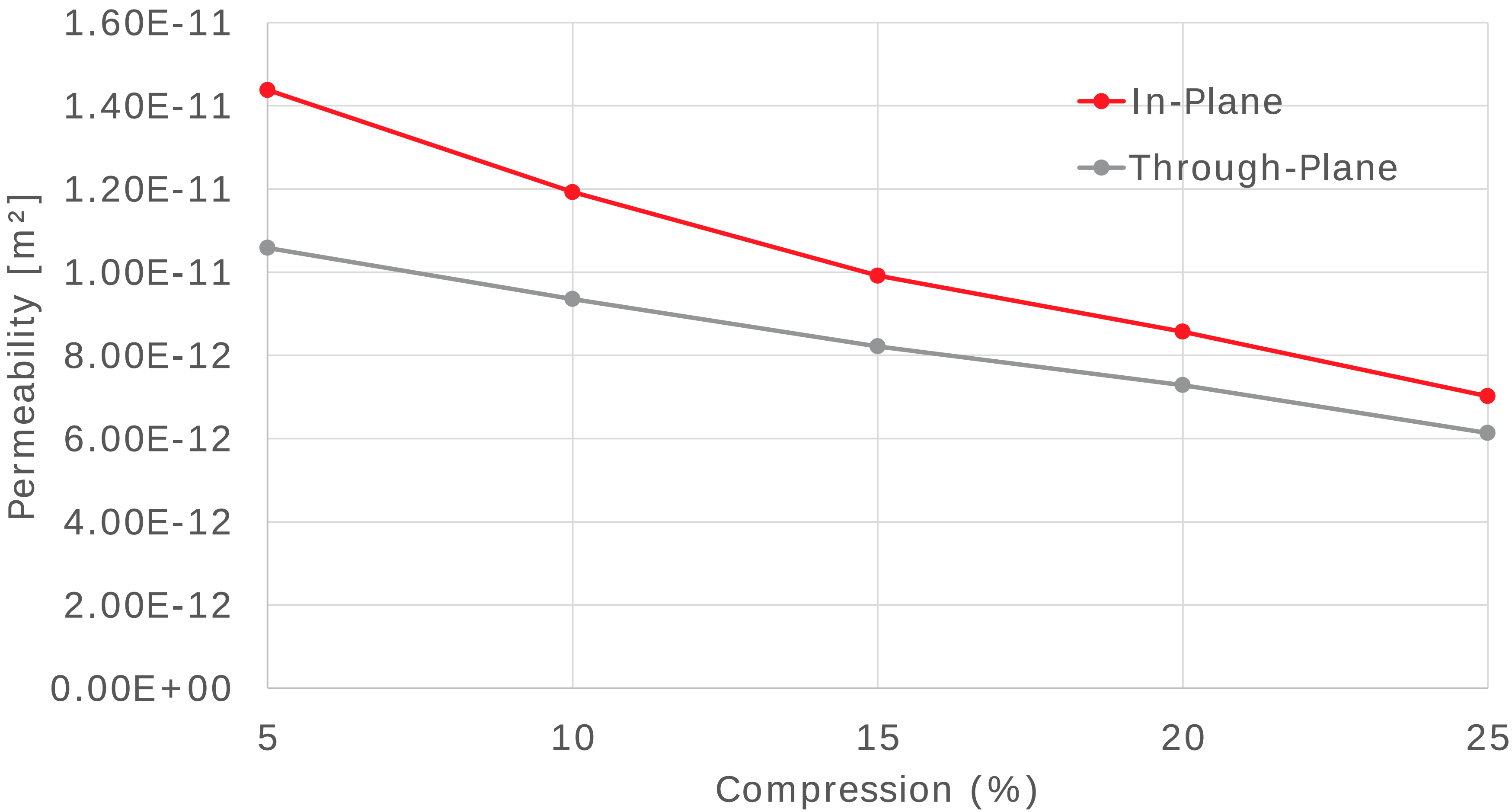
Darcy-Law: $\bar{\mathbf{u}} = -\frac{\mathbf{K}}{\mu}\frac{(P_2 - P_1)}{L}$

Flow Simulation



Solver runtime (12x parallel): 5 min 41 s

Compression and Permeability



Capillary Pressure and Saturation with Variable Wettability

Capillary Pressure

When does the gas enter a cylindrical capillary?

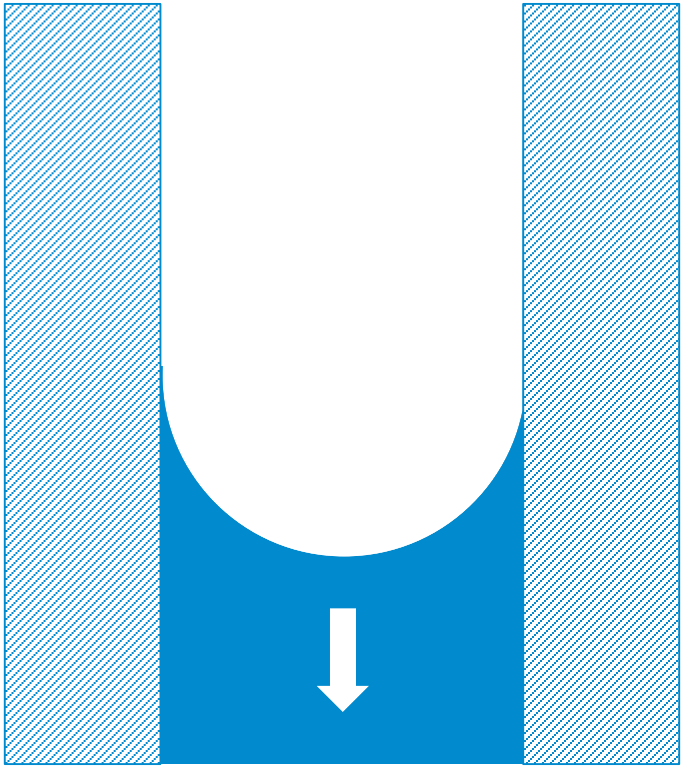
$$p = \frac{4\,\sigma}{d}$$

p differential pressure

d pore diameter

σ surface tension

complete wetting $\beta = 0$



Capillary Pressure

When does the gas enter a cylindrical capillary?

$$p = \frac{4\,\sigma}{d}\cos\beta$$

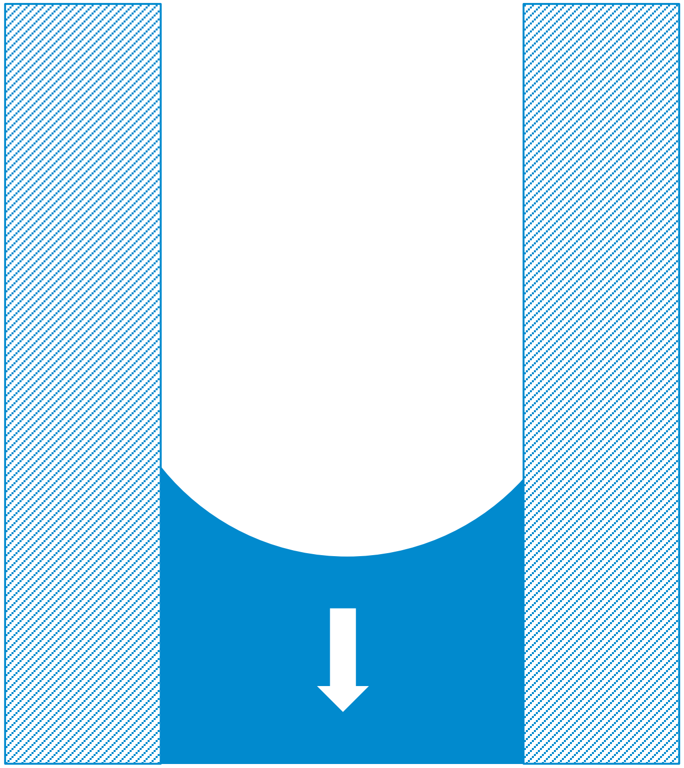
p differential pressure

d pore diameter

σ surface tension

β contact angle

partial wetting $0° < \beta < 90°$



Can we have variable contact angles?

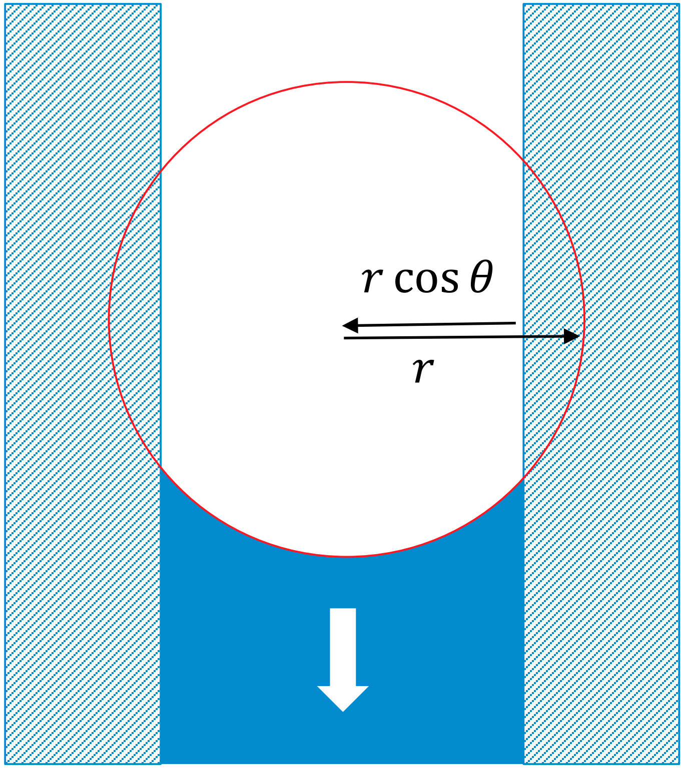
Idea (Schulz et al, 2014)

- dilate by $r \cos\theta$
- erode by r

Result: contact angle θ on pore wall

Young-Laplace: $p = \frac{2\sigma}{r}$

r: sphere radius ($\neq$ pore radius)

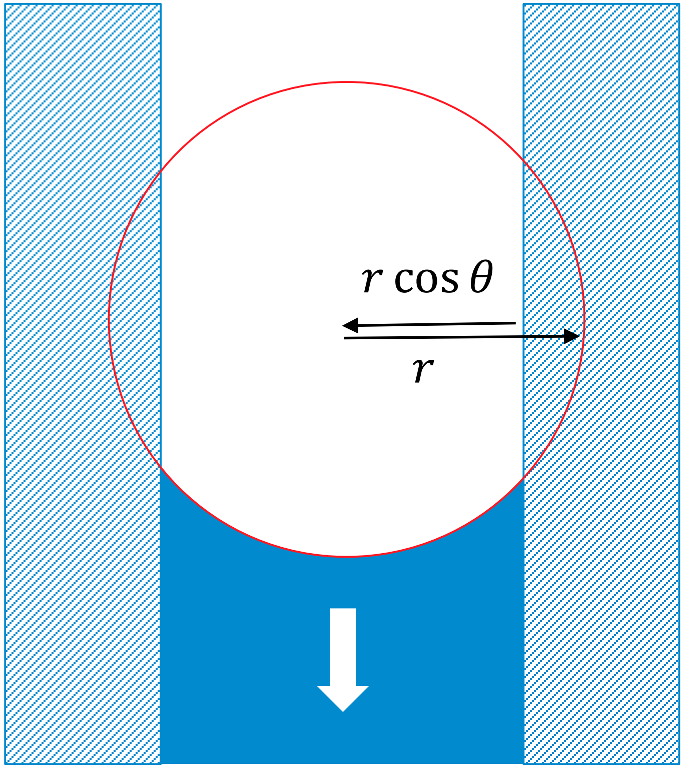


V.P. Schulz, E. A. Wargo, E. Kumbur, Pore-Morphology-Based Simulation of Drainage in Porous Media Featuring a Locally Variable Contact Angle, Transport in Porous Media, 2014.

Can we have variable contact angles?

Restriction on possible contact angles:

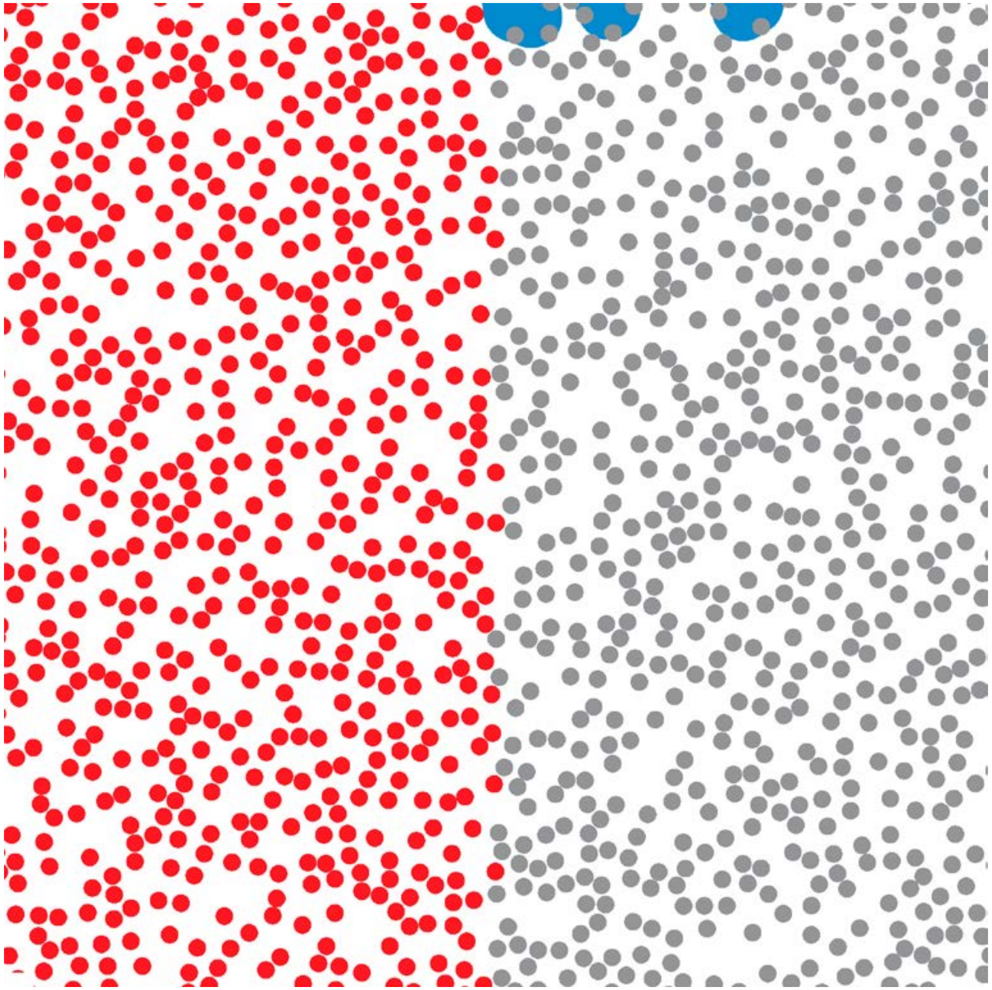
- If the difference between $r\cos\theta$ and r is larger than the fiber diameter (or wall thickness), the method produces artifacts.
  $\Rightarrow$ Contact angles should not be too close to 90°
- No mixed (hydrophobic-hydrophilic) wettability possible.



V.P. Schulz, E. A. Wargo, E. Kumbur, Pore-Morphology-Based Simulation of Drainage in Porous Media Featuring a Locally Variable Contact Angle, Transport in Porous Media, 2014.

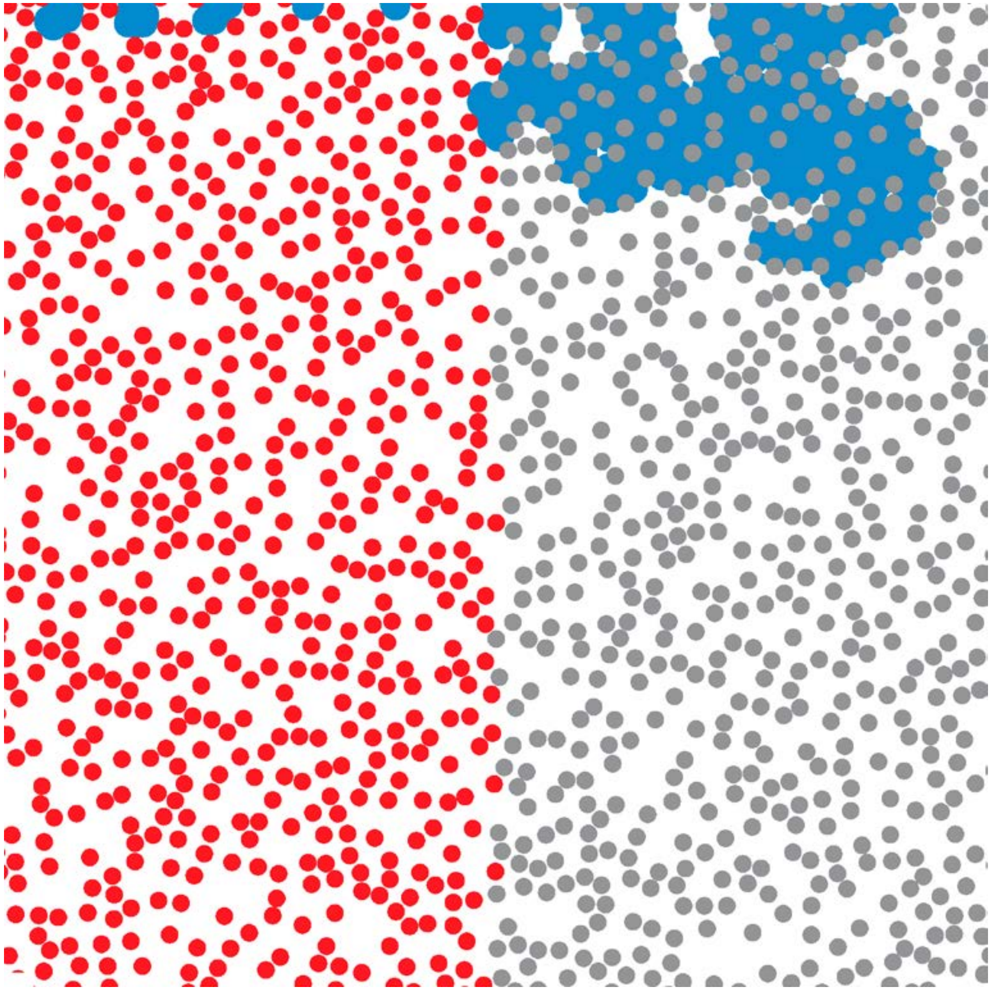
2D Example

- Contact angle 0°
- Contact angle 40°
- Water (non-wetting)
- Air (wetting)



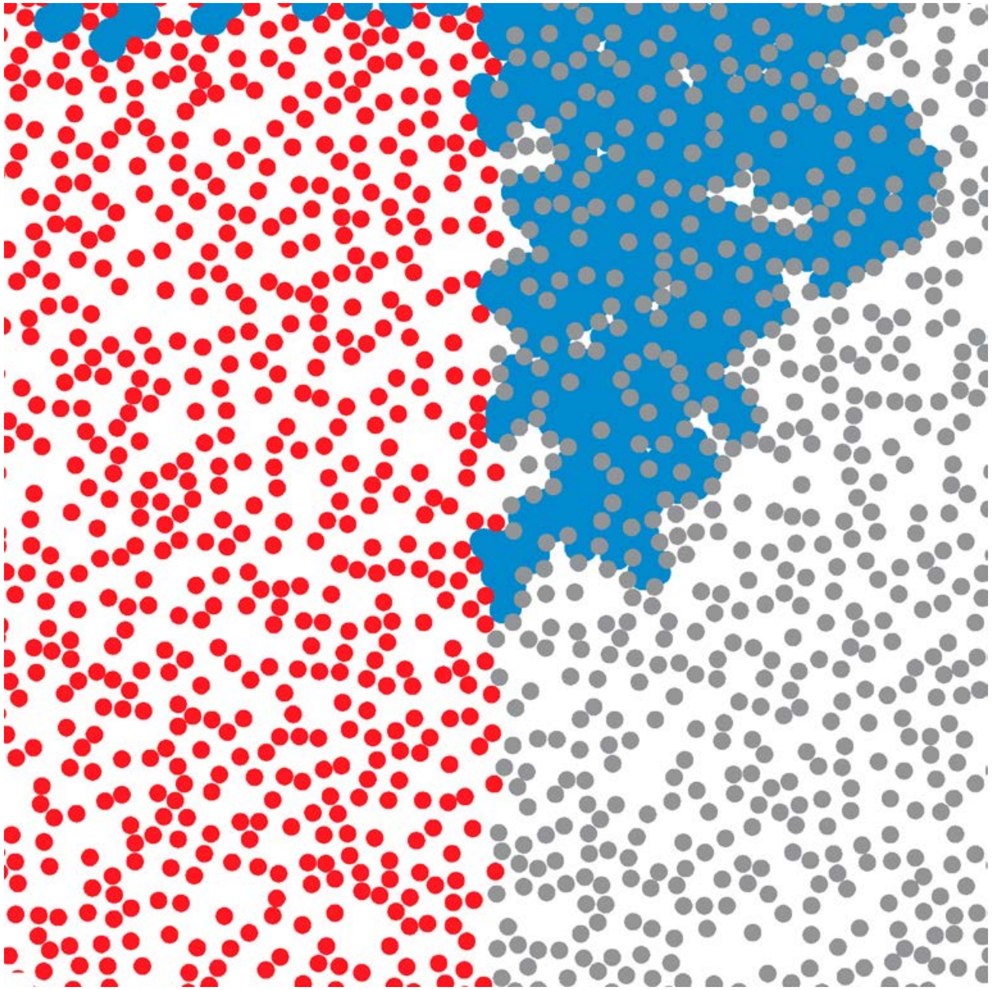
2D Example

- Contact angle 0°
- Contact angle 40°
- Water (non-wetting)
- Air (wetting)



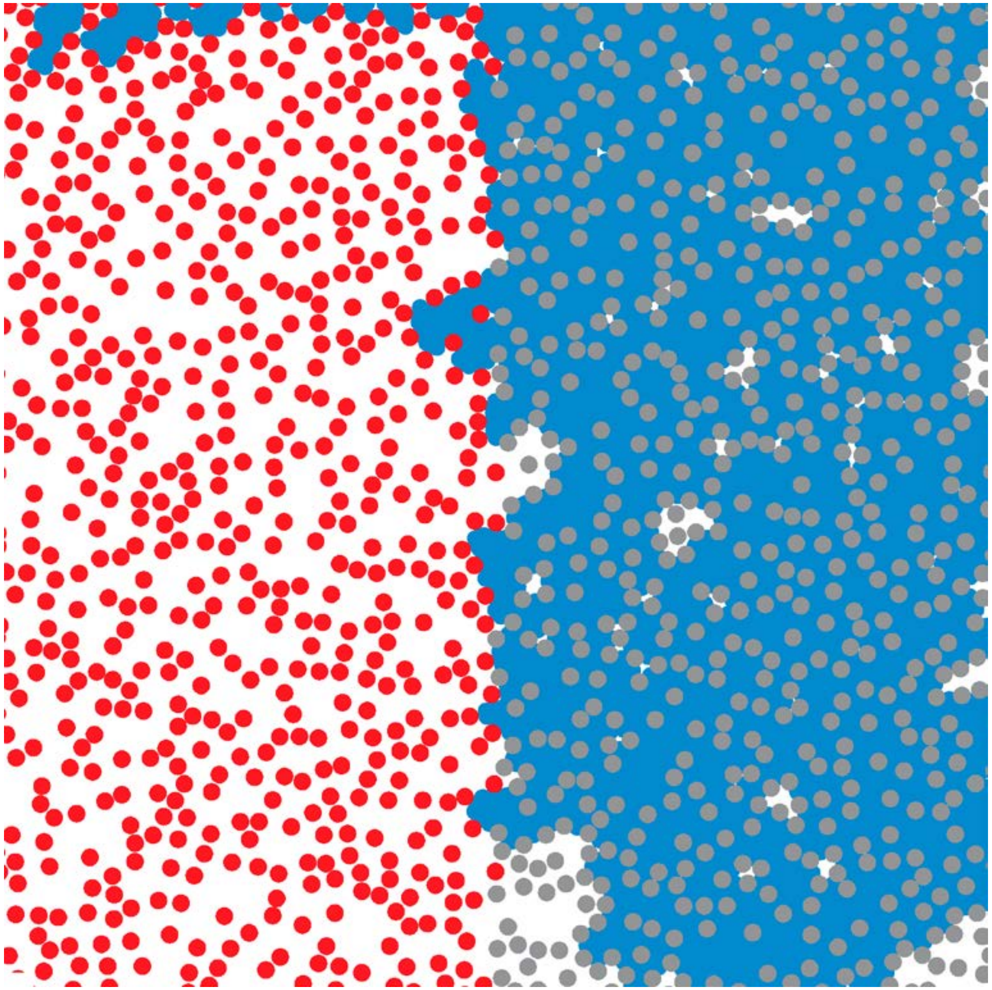
2D Example

- Contact angle 0°
- Contact angle 40°
- Water (non-wetting)
- Air (wetting)



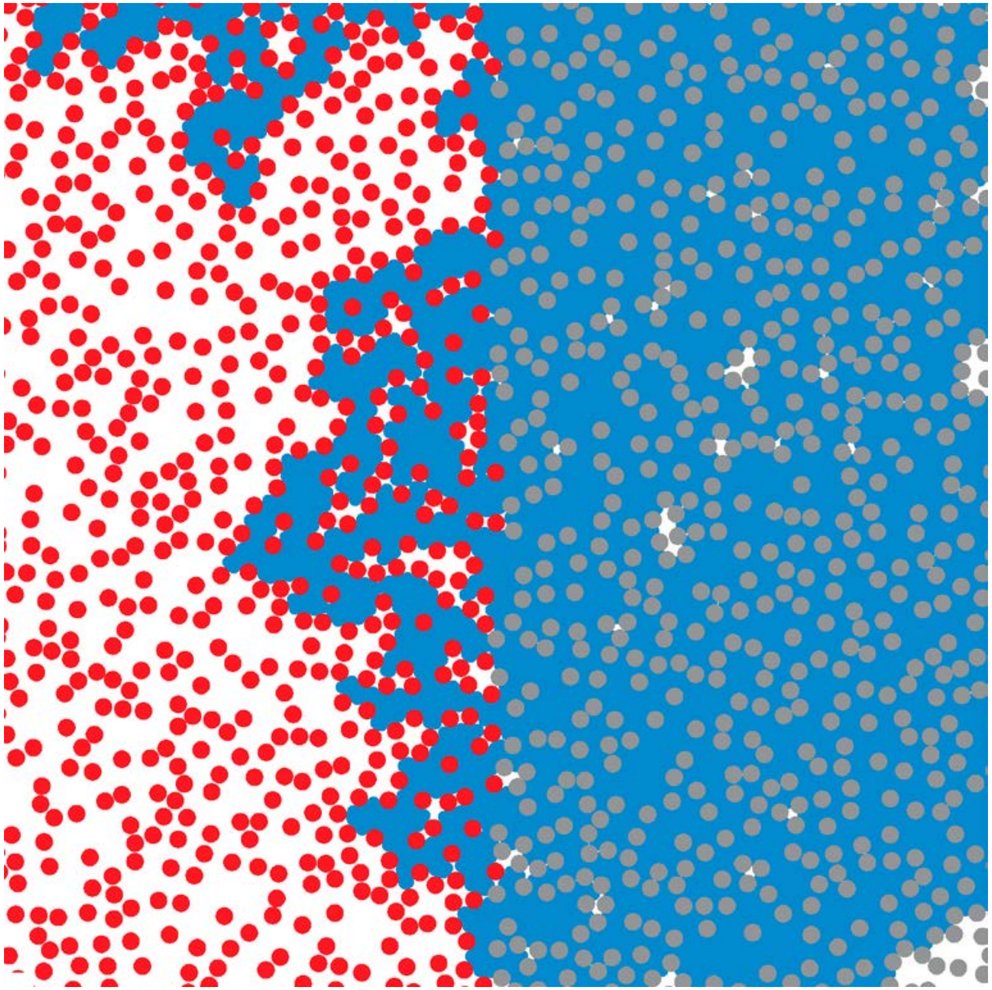
2D Example

- Contact angle 0° (red)
- Contact angle 40° (grey)
- Water (non-wetting) (blue)
- Air (wetting) (white)



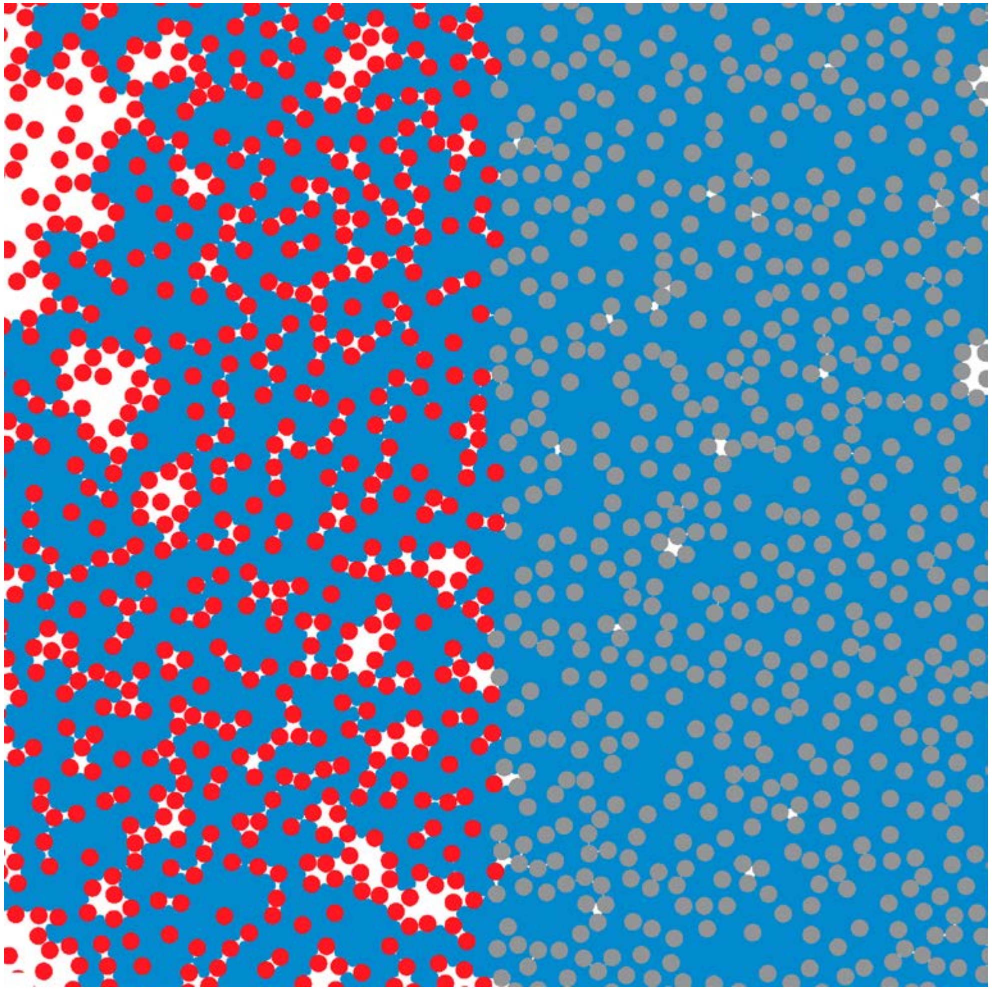
2D Example

- Contact angle 0°
- Contact angle 40°
- Water (non-wetting)
- Air (wetting)



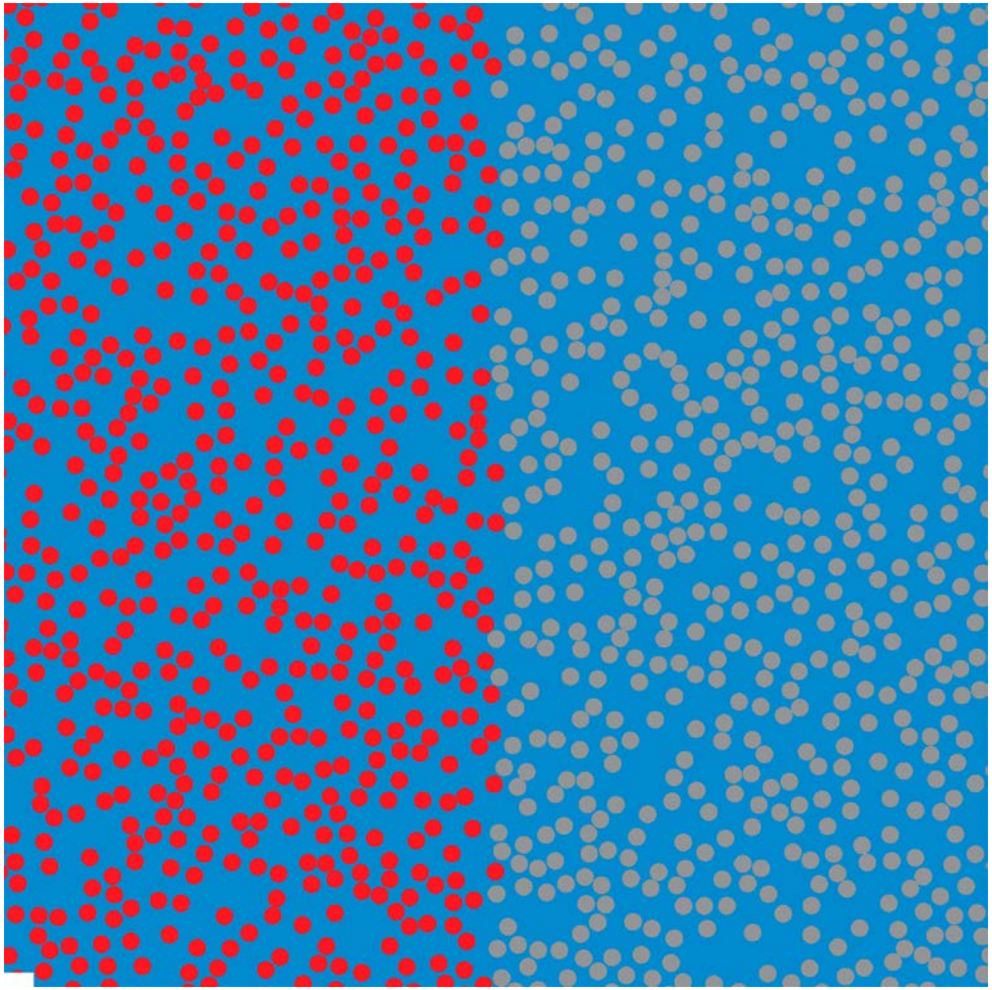
2D Example

- Contact angle 0°
- Contact angle 40°
- Water (non-wetting)
- Air (wetting)



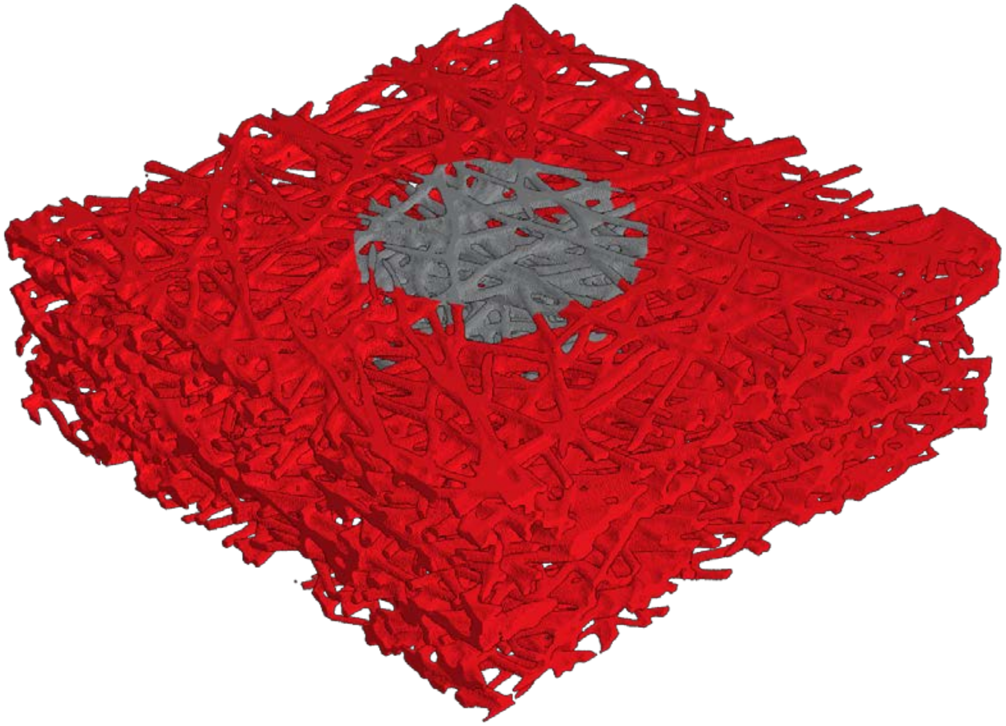
2D Example

- Contact angle 0°
- Contact angle 40°
- Water (non-wetting)
- Air (wetting)



Structure with Variable Wettability

- Marked a cylinder as area with higher wettability

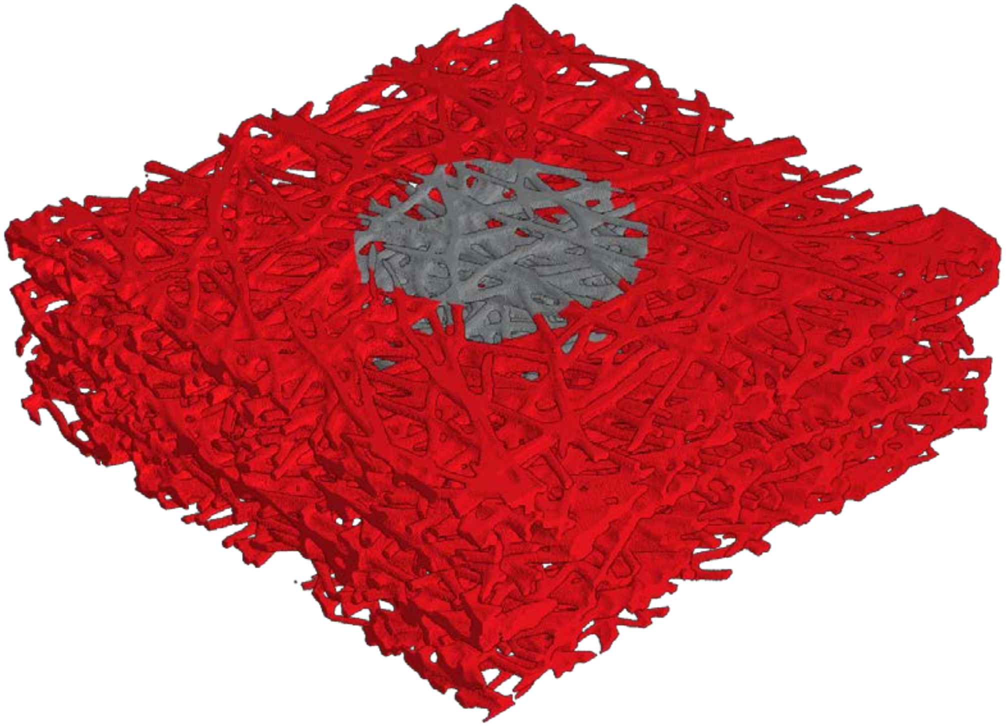


Structure with Variable Wettability

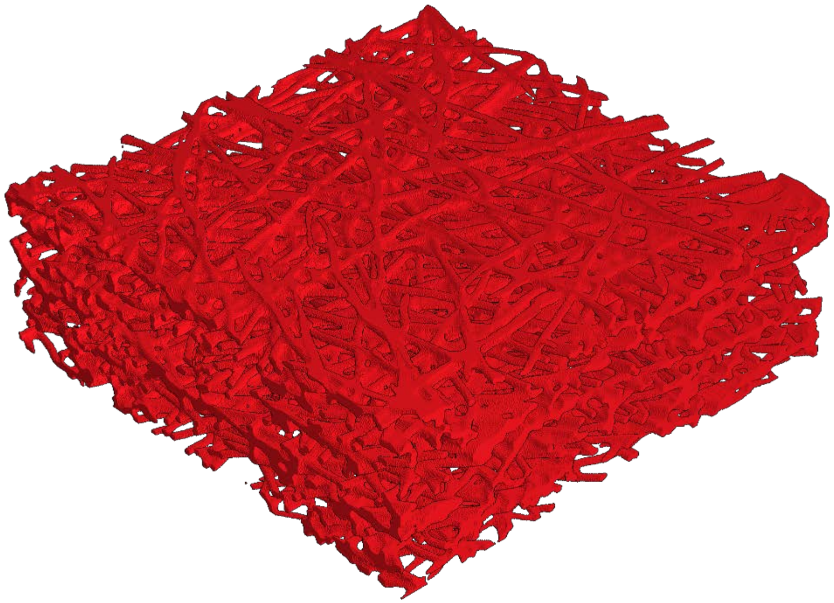
- Marked a cylinder as area with higher wettability

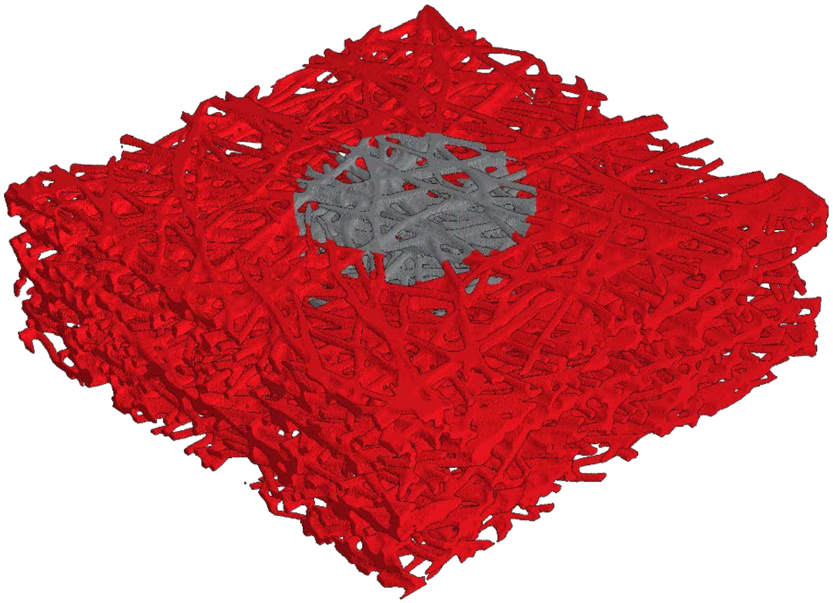
Other options:

- distinguish between binder and fibers
- mark individual fibers
- ...



GDL Models





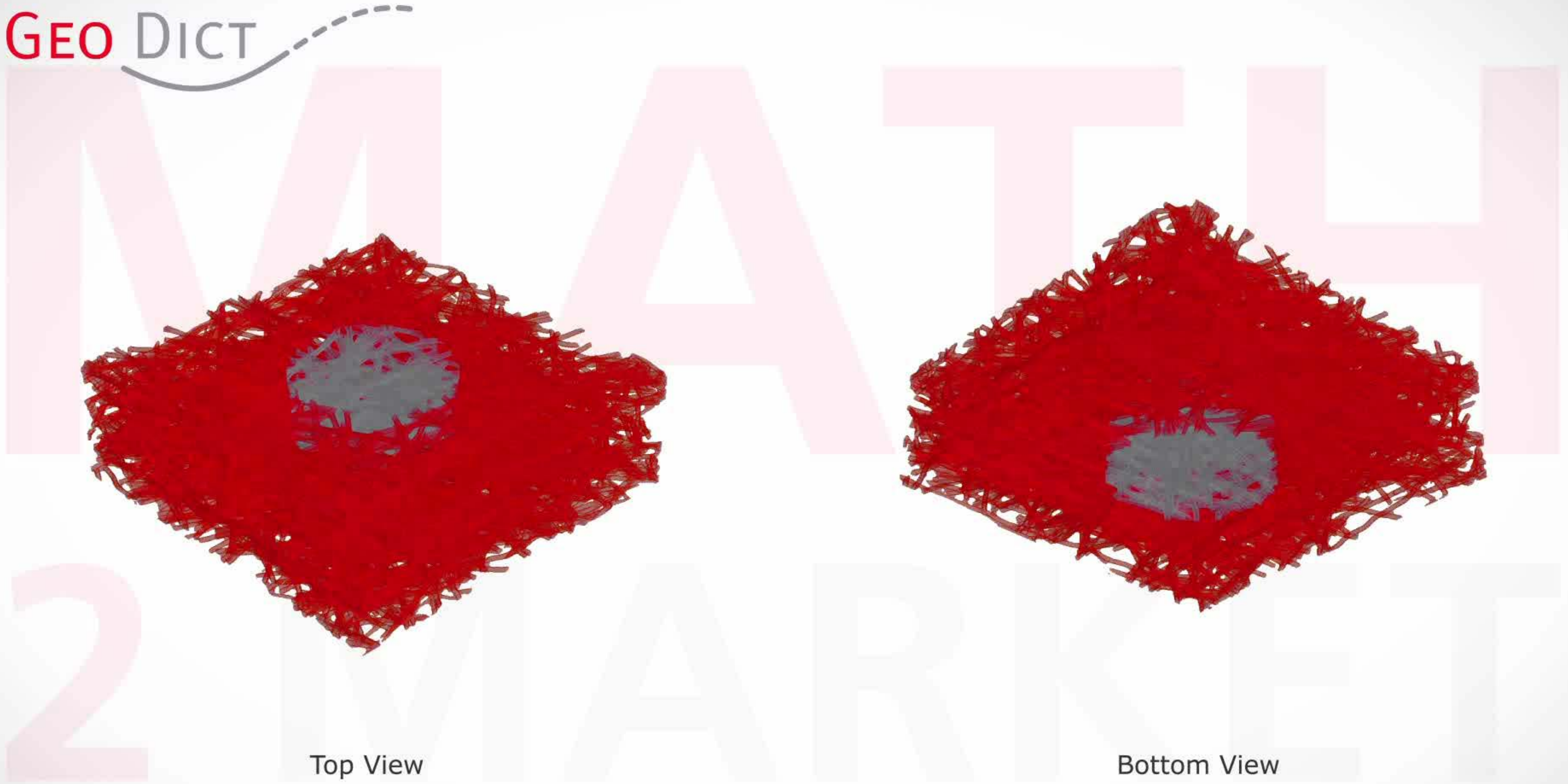
Constant Contact Angle

Two Different Contact Angles

Water Entering into the GDL

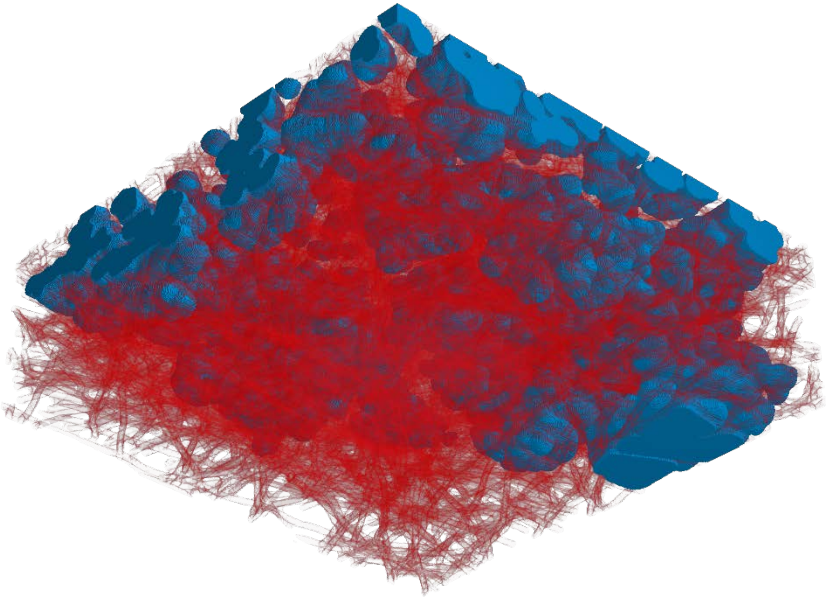
SatuDict Simulation with constant contact angle; uncompressed

Water Entering into the GDL

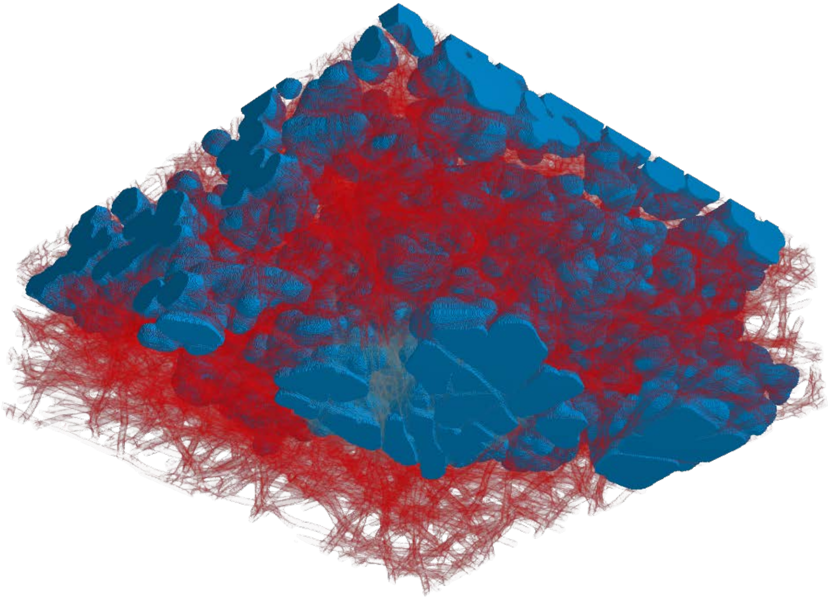


SatuDict Simulation with two different contact angles; uncompressed

Comparison



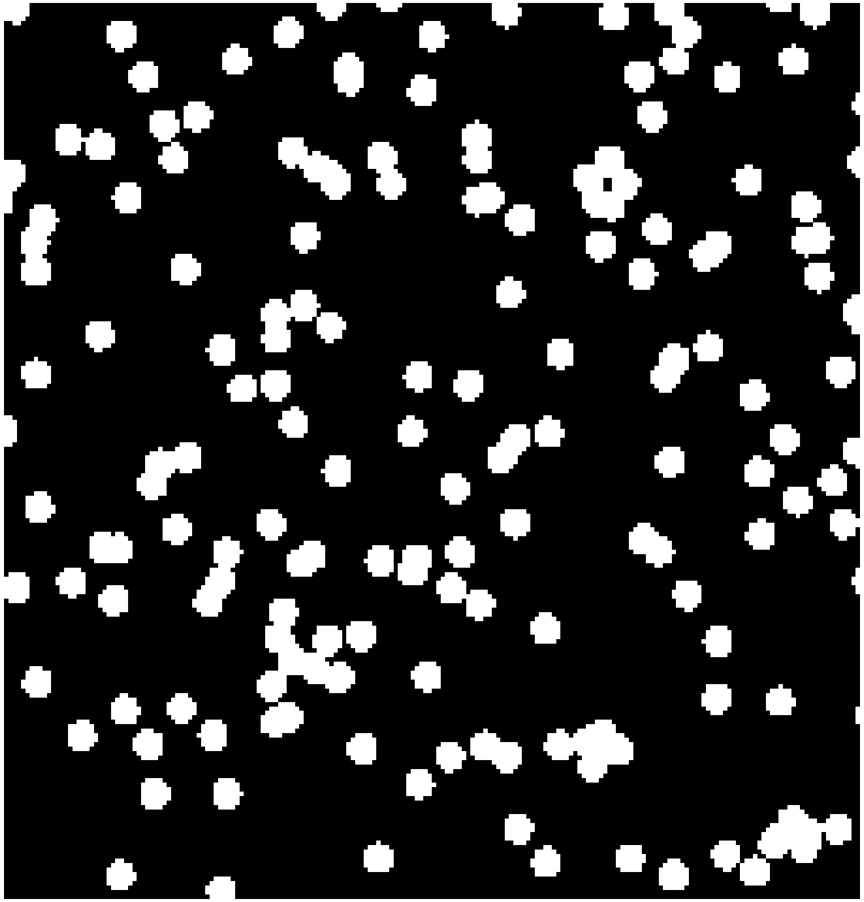
Constant Contact Angle



Two Different Contact Angles

Relative Permeability

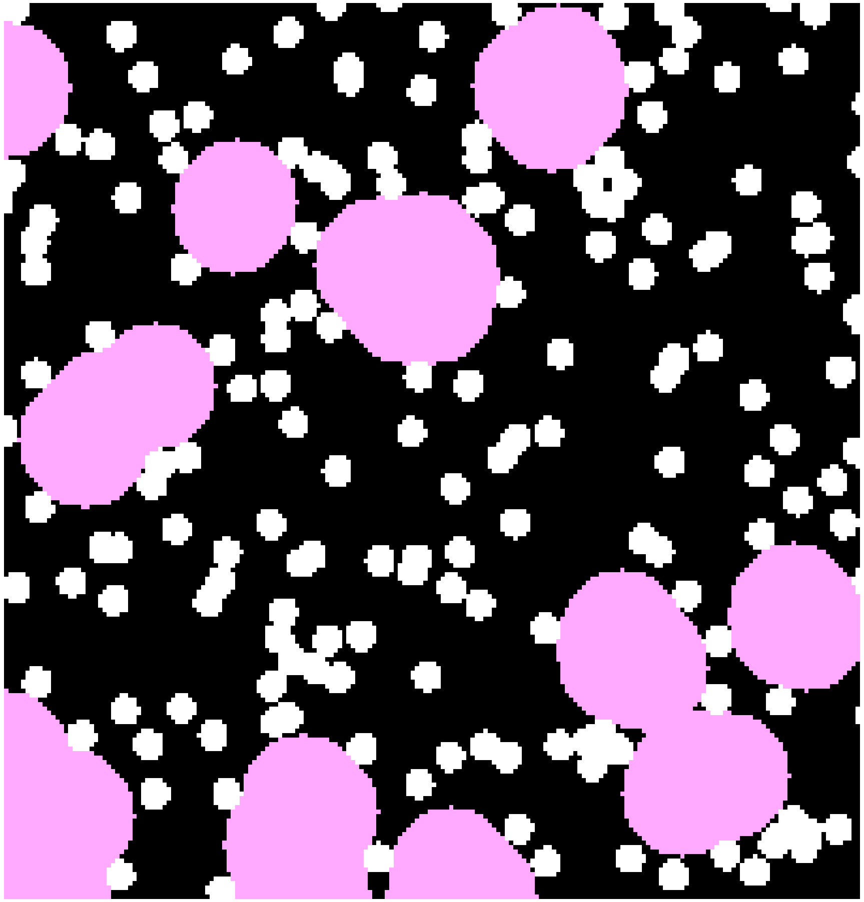
Saturation Dependent Permeability



Saturation Dependent Permeability

For each saturation:

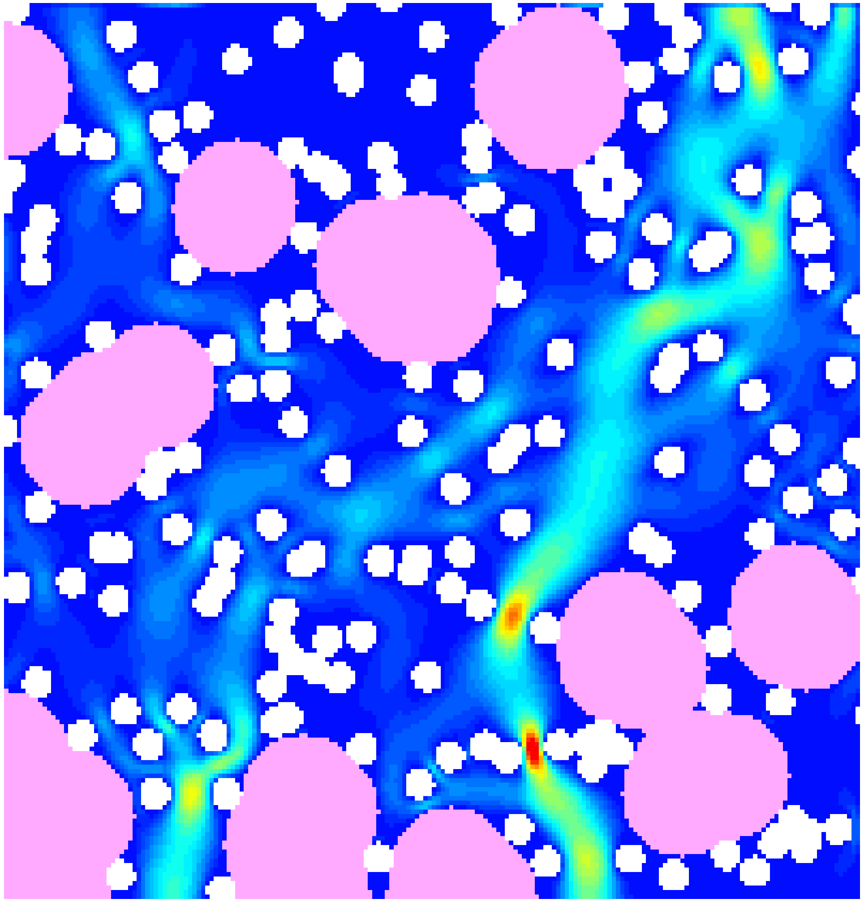
1. Determine phase distribution



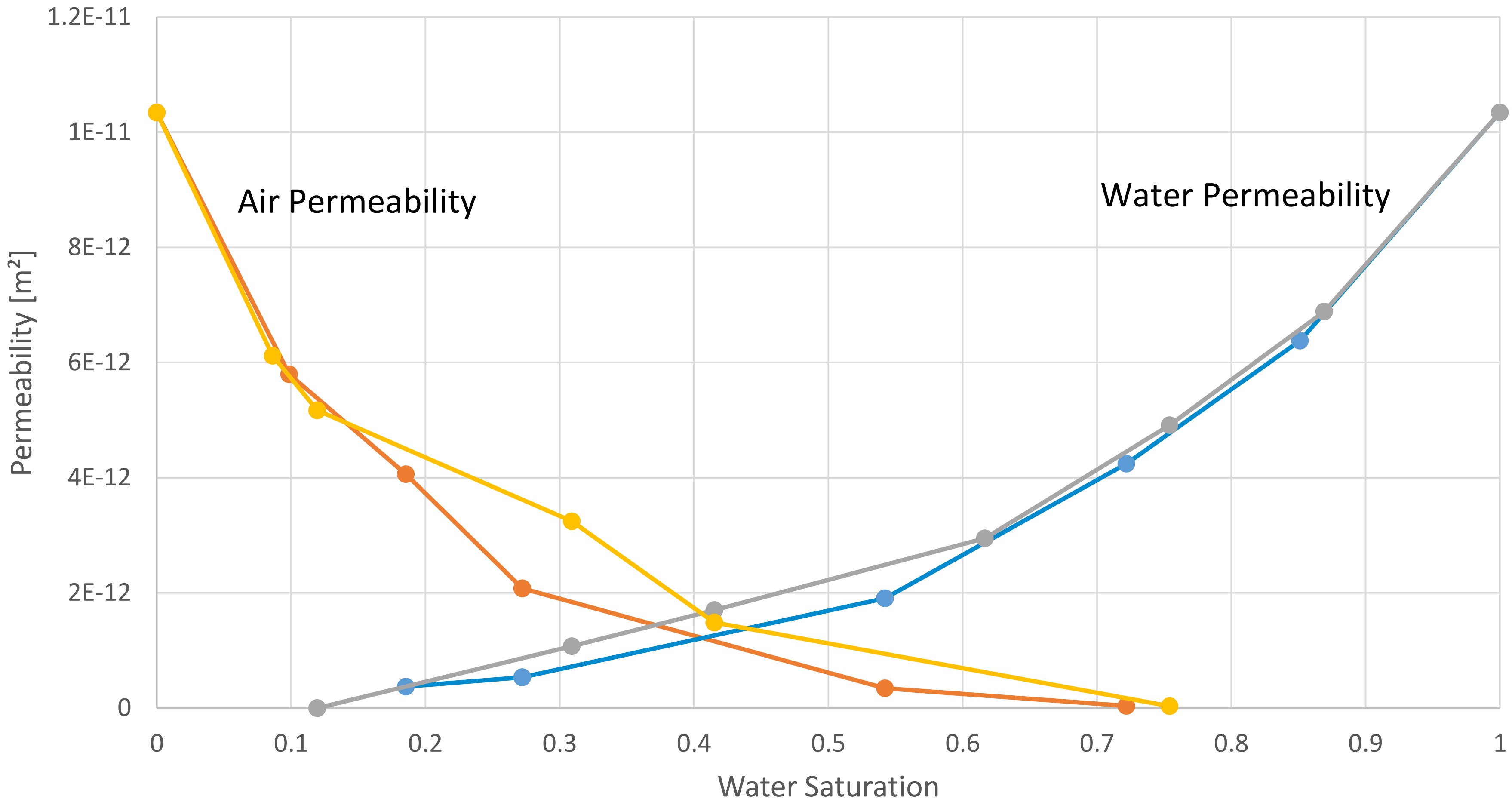
Saturation Dependent Permeability

For each saturation:

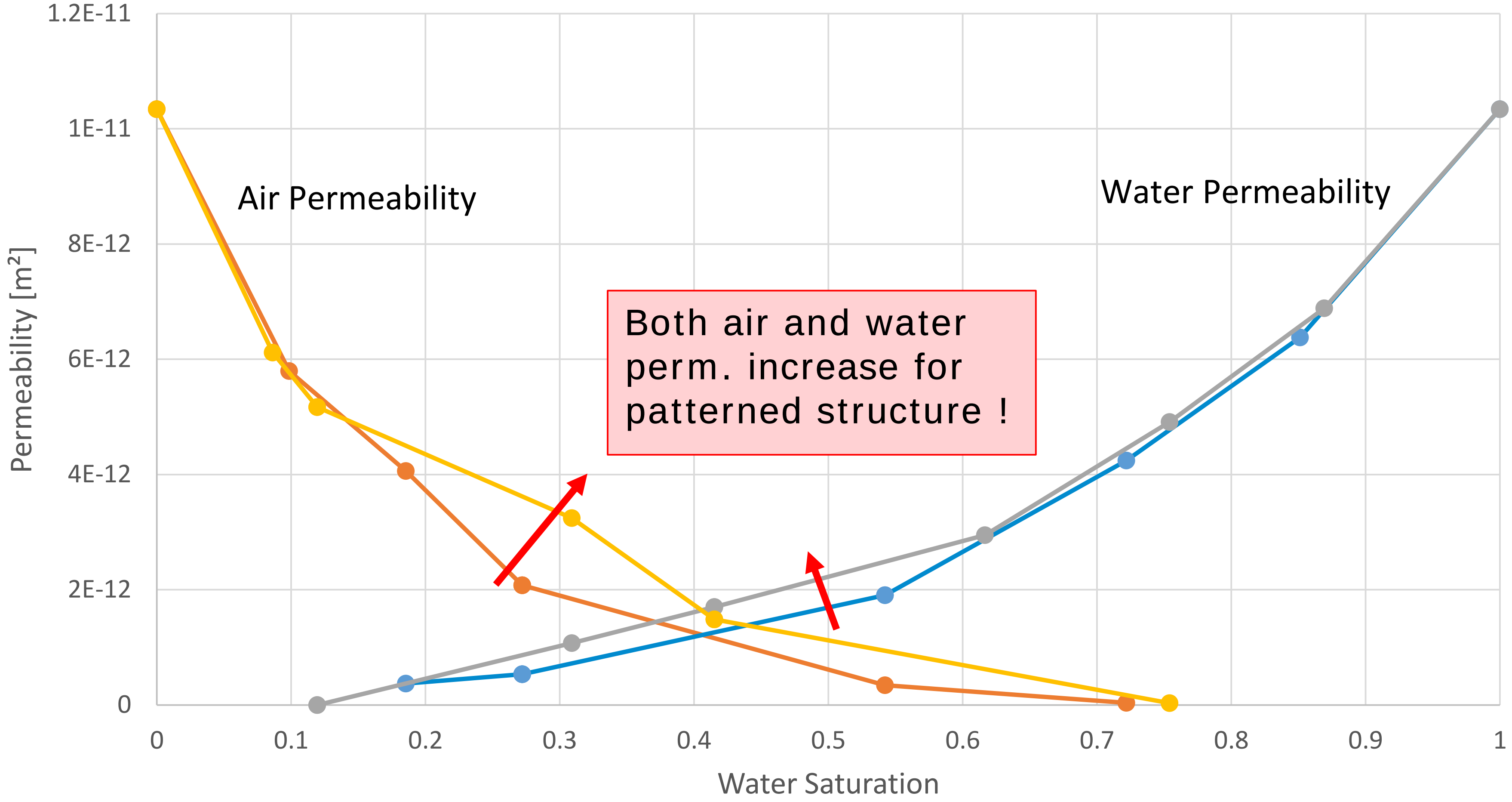
1. Determine phase distribution
2. Calculate single-phase flow (solve Stokes equation)
3. Find permeability (average flow velocity)



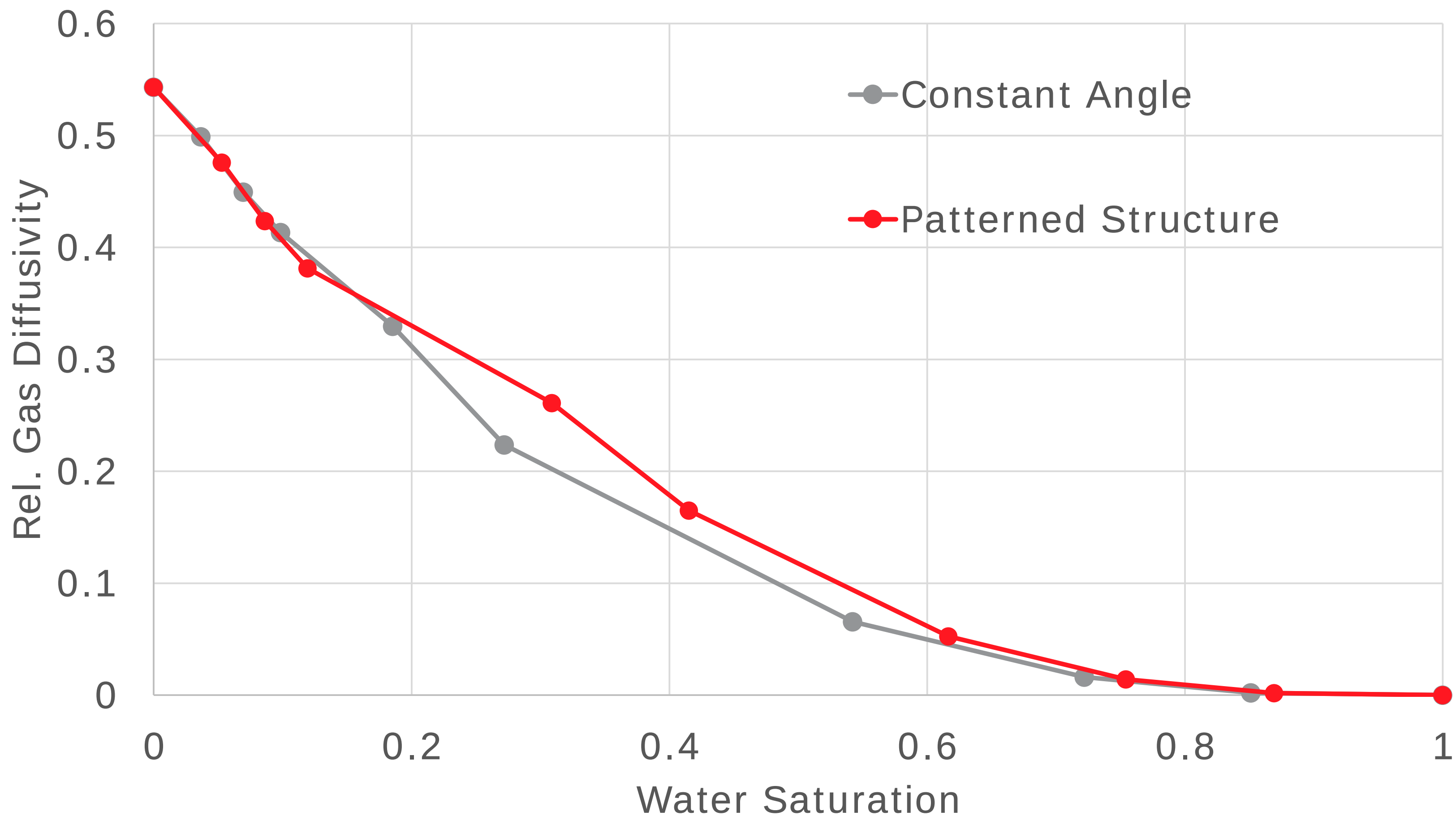
Through-Plane Permeability (Uncompressed GDL)



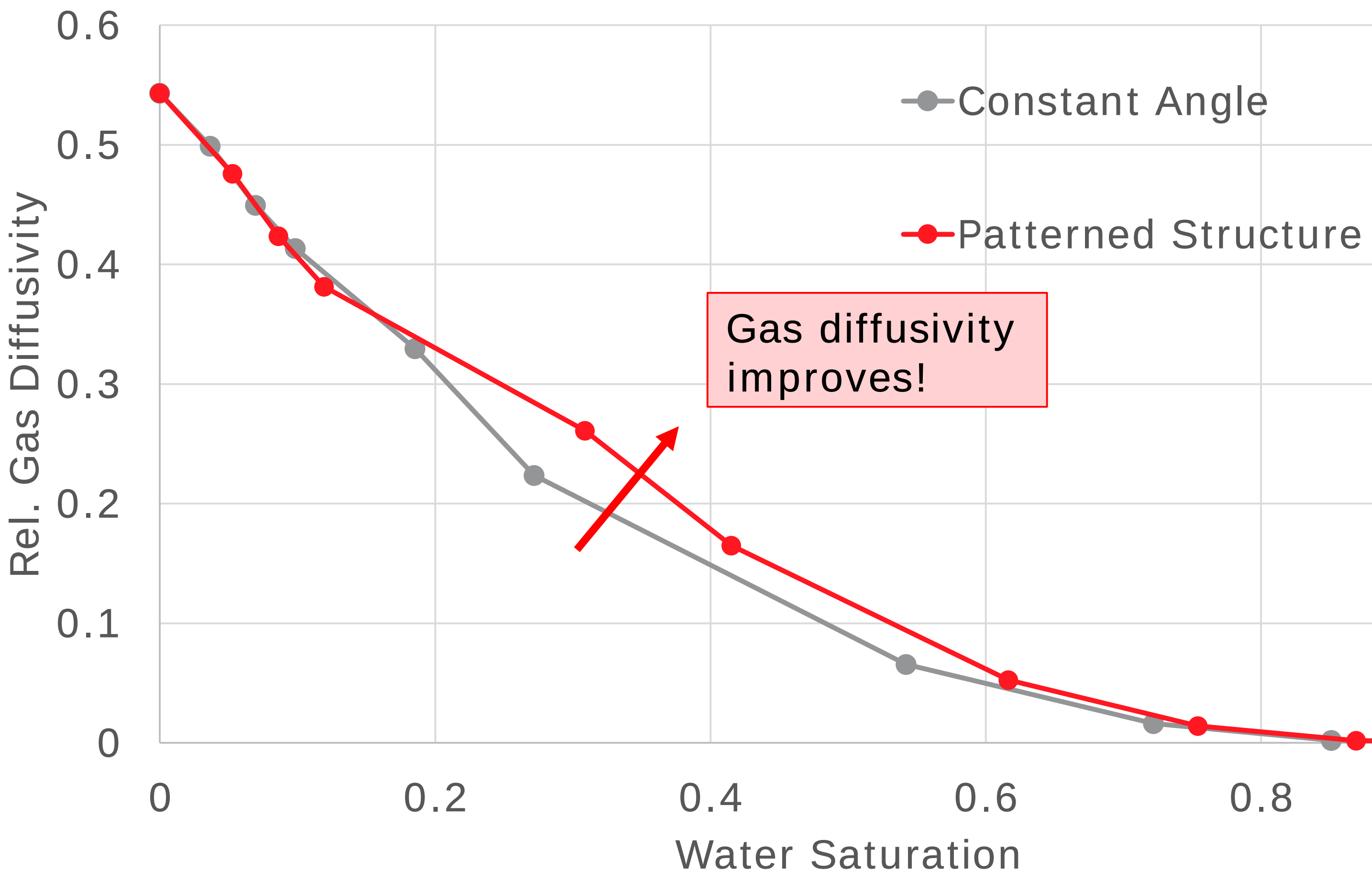
Through-Plane Permeability (Uncompressed GDL)



Through-Plane Diffusivity (Uncompressed GDL)



Through-Plane Diffusivity (Uncompressed GDL)



Relative Permeability – Computational Costs

Challenge:

- Parameter that is most expensive to compute:
  - Requires to solve one flow problem per saturation level

Observation:

- Low saturation states are computationally most expensive

Relative Permeability – Computational Costs

Challenge:

- Parameter that is most expensive to compute:
  - Requires to solve one flow problem per saturation level

Observation:

- Low saturation states are computationally most expensive

Improvements:

- Restart of computations
  - Compute permeability from highest to lowest saturation state
  - Use result from previous computation to speed up the next one

Relative Permeability – Computational Costs

Challenge:

- Parameter that is most expensive to compute:
  - Requires to solve one flow problem per saturation level

Observation:

- Low saturation states are computationally most expensive

Improvements:

- Restart of computations
  - Compute permeability from highest to lowest saturation state
  - Use result from previous computation to speed up the next one
- New stopping criterion:
  - Relative error compared to the permeability of the fully saturated state

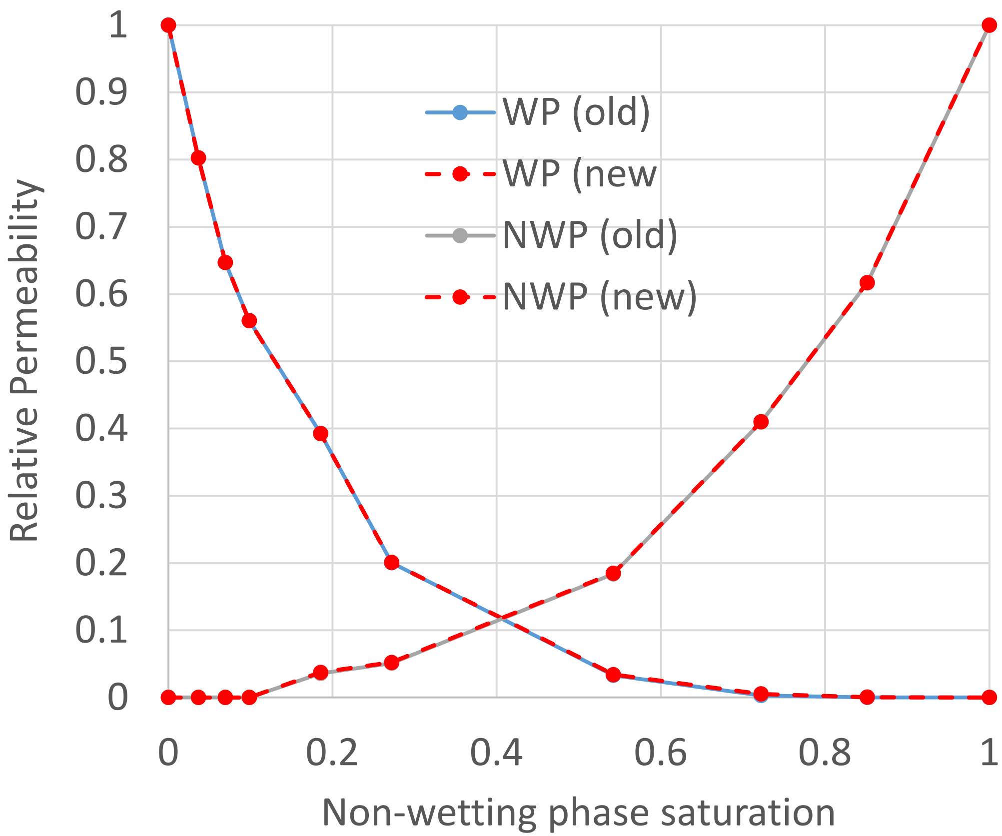
Speed-Up

Comparison:

- Uncompressed GDL
- 600 x 600 x 200 Voxels
- 10 Saturation levels each
- Parallelization: 12x

Runtime needed:

- Old: 6h 22 min
- New: 58 min



Summary

1. Generated a 3D GDL model
2. Computed compressed structure
3. Computed permeability
4. Computed water saturation with different contact angles
5. Computed transport properties for different water saturations
6. Speed-up of permeability computations

Thank You!

Thanks to:

- Steffen Schwichow (Math2Market)
- Volker Schulz (DHBW Mannheim)
- Funding through OptiGaaII project

Visit us @ www.geodict.com