Mass Transport in a GDL with Variable Wettability

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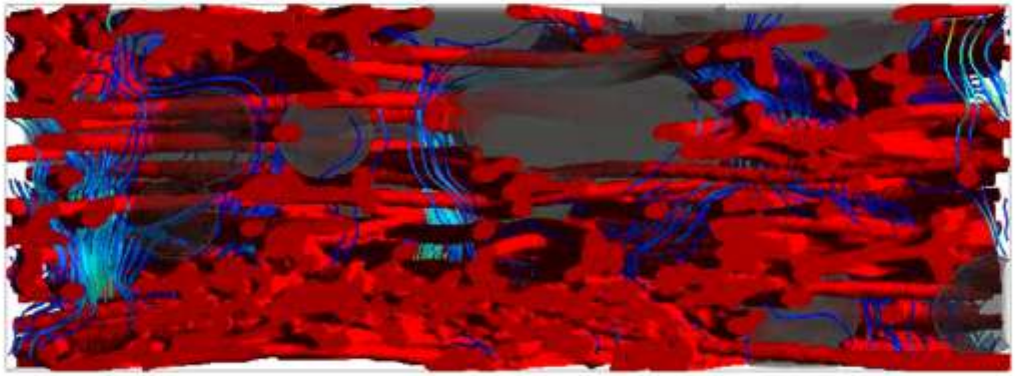

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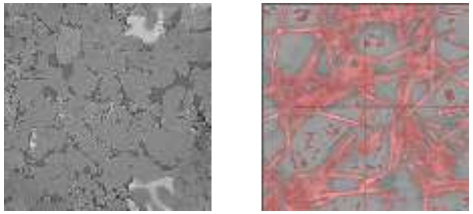
Who is Math2Market?

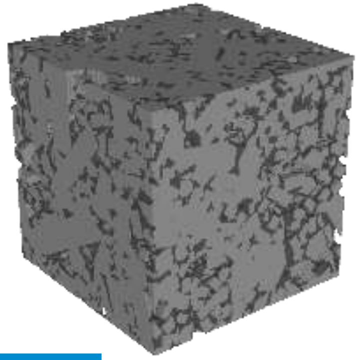
- Math2Market GmbH was founded September 2011 in Kaiserslautern.
- Spin-off of Fraunhofer Institute for Industrial Mathematics, ITWM.

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

What is GeoDict ?

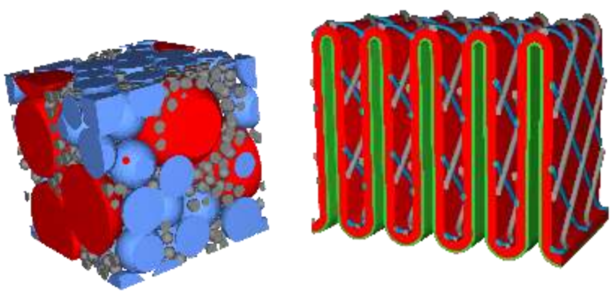


Import of CT Images

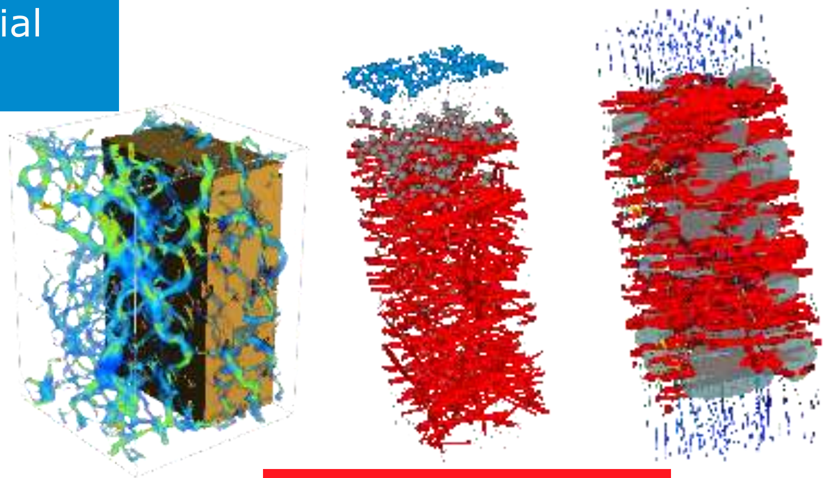


Geometric Analysis

Virtual Material Laboratory



Create 3D Models of Microstructures



Analyze Properties

Mass Transport in a GDL with Variable Wettability

Overview:

1. 3D GDL model and compression
2. Capillary pressure and saturation with variable wettability *New!*
3. Effect on relative permeability

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3D GDL Model and Compression

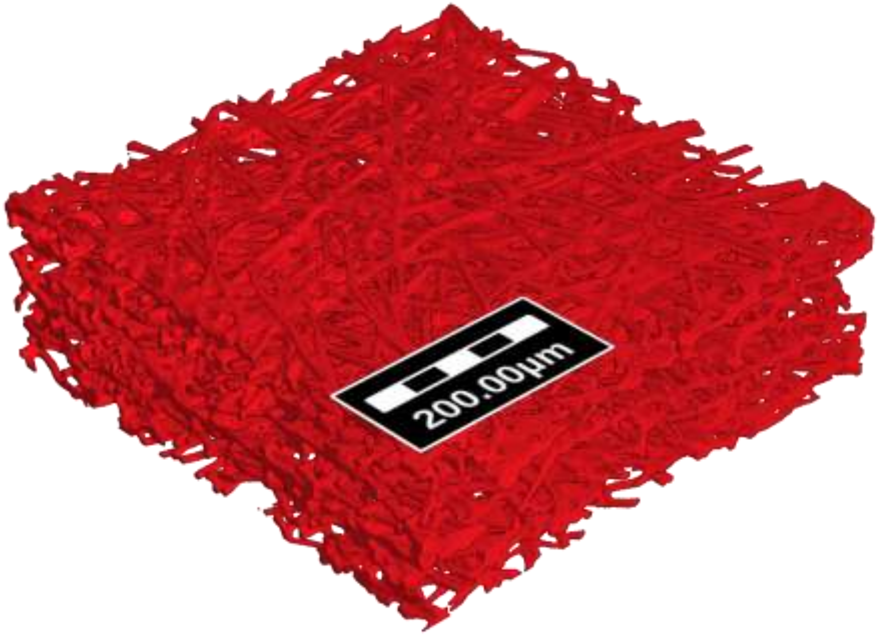
Structure Model

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

Fibers: linear elastic, transverse isotropic

Binder: linear elastic, isotropic

Solver:

FeelMath

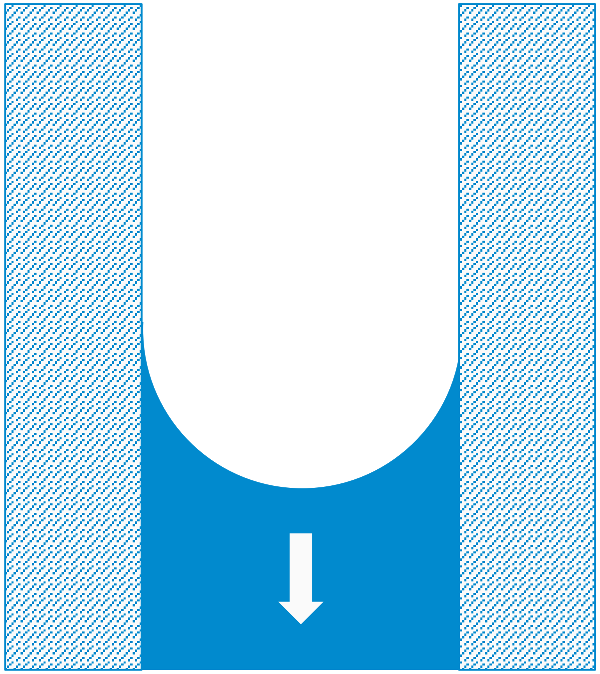
Fraunhofer ITWM

Runtime: 1h 17 min (8x)

Compression	0	0.05	0.1	0.15	0.2	0.25

Capillary Pressure and Saturation with Variable Wettability

Capillary Pressure



When does the gas enter a cylindrical capillary?

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

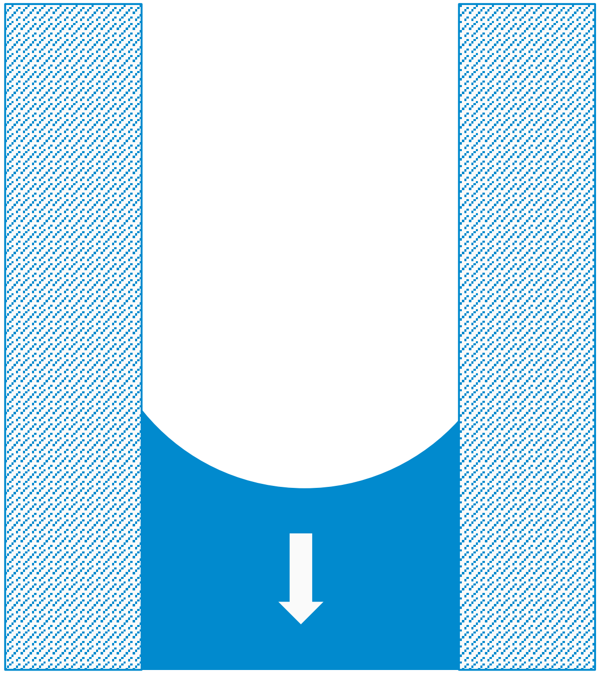
p differential pressure

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 $0° < \beta < 90°$

The Idea of SatuDict (State-of-the-art)

Use this relation between pore size and capillary pressure to predict the distribution of the phases

Advantage:

- purely geometrical (fast calculations)

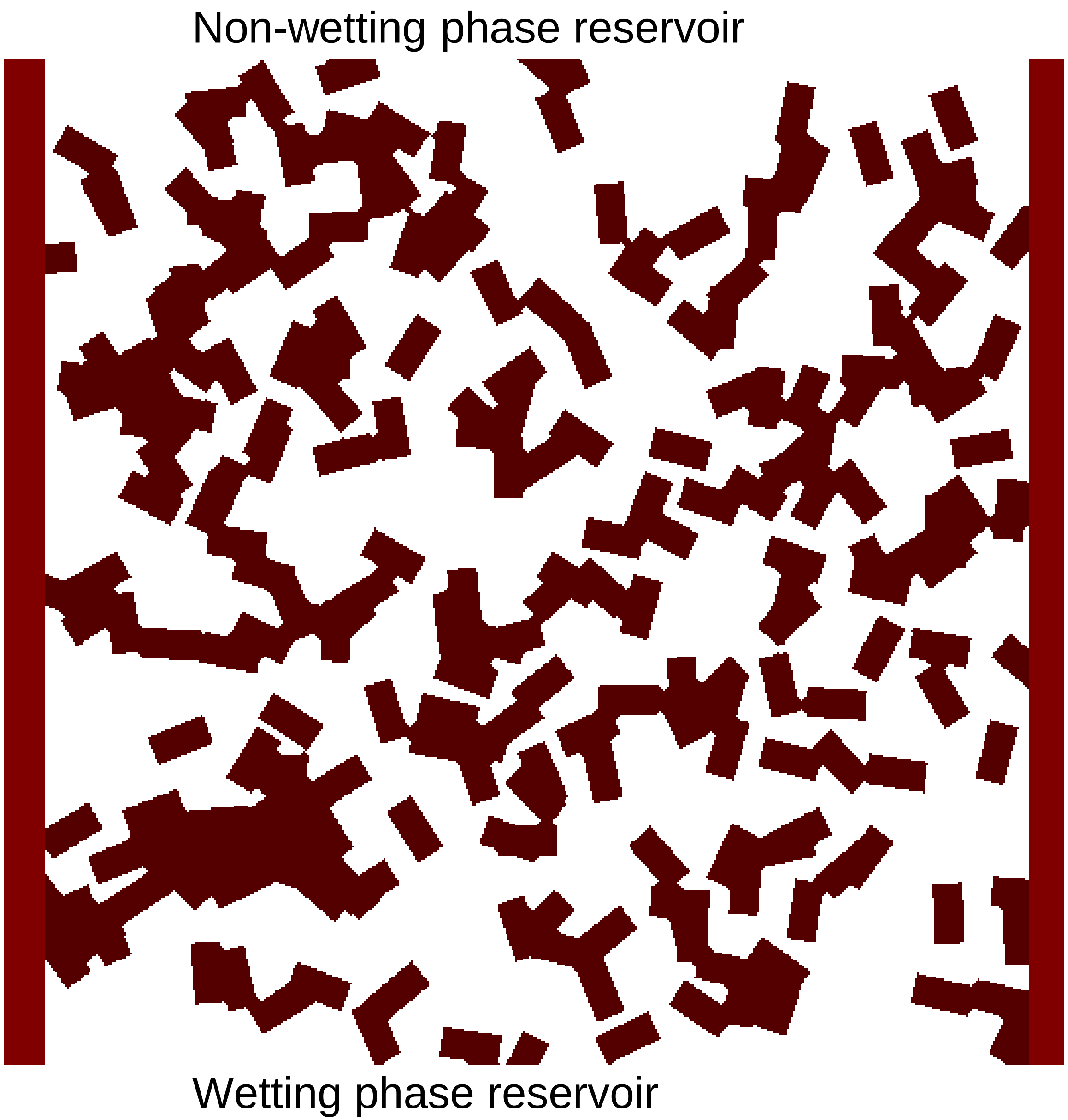
Assumption:

- quasi-stationary phase distribution
- fixed contact angle
- cylindrical pores

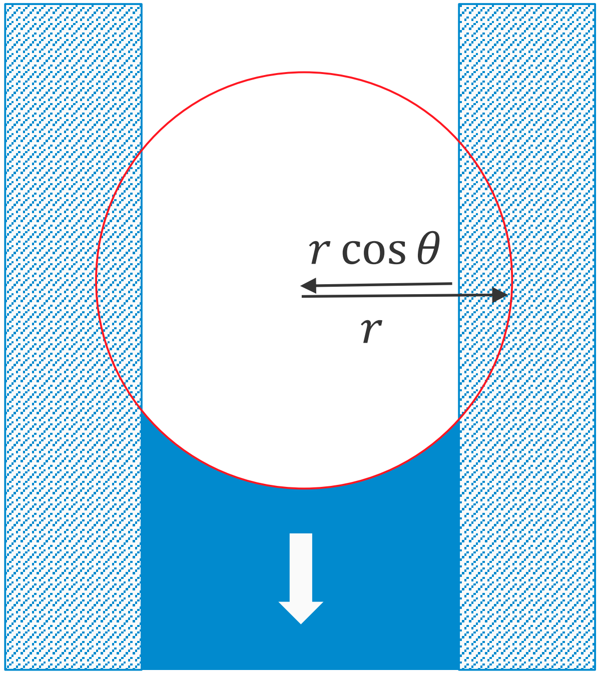
Pore Morphology: Drainage

- Assure connectivity of NWP to reservoir

- Start: completely wet
- Start: large radius (i.e. small p_c)
- Steps: smaller radius (higher p_c)



New Idea:
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

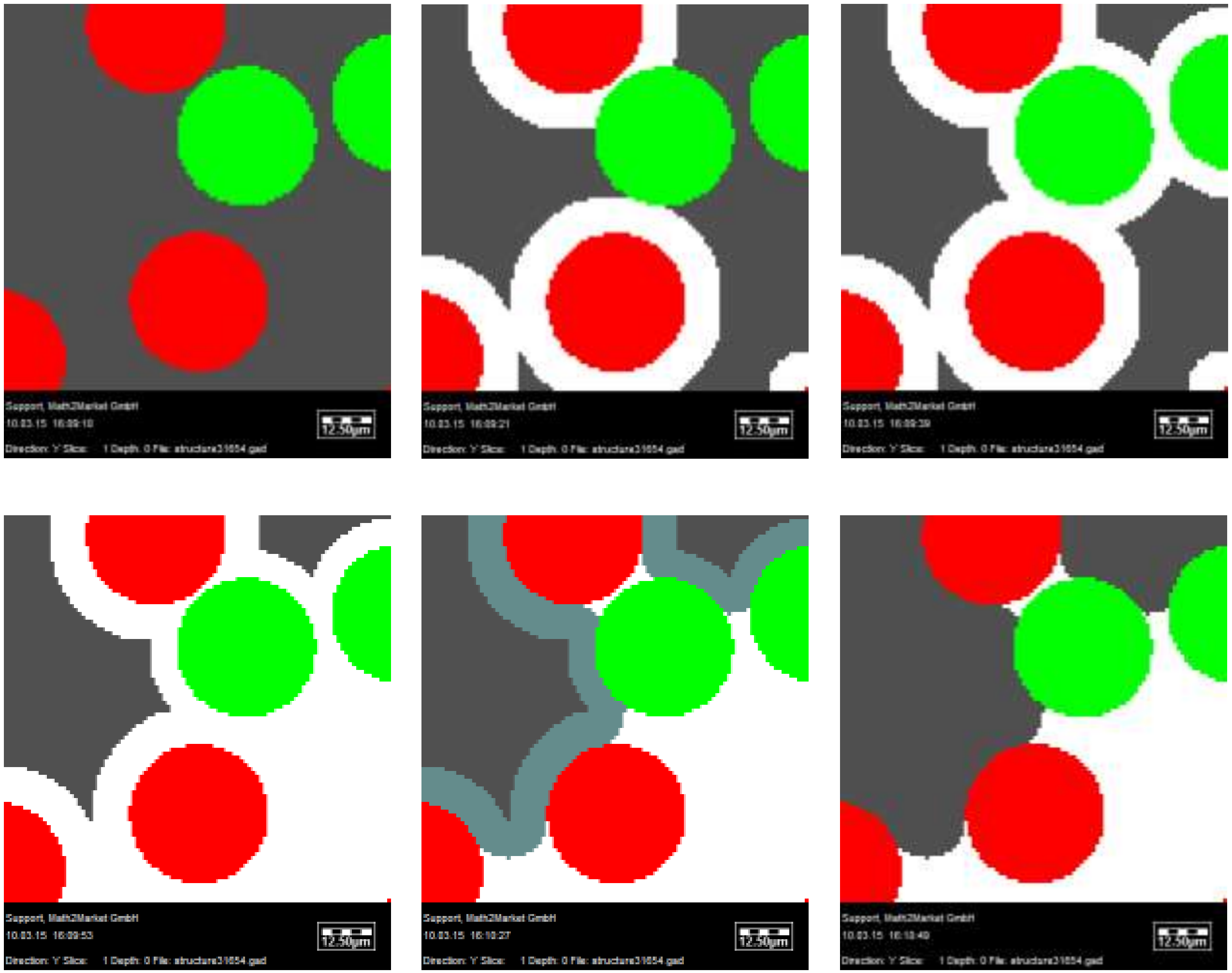
Young-Laplace: $p = \frac{2\,\sigma}{r}$

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.

Multiple Contact Angles

SatuDict



1. Dilate material 1
2. Dilate material 2
3. Check connectivity
4. Erode
5. Final result

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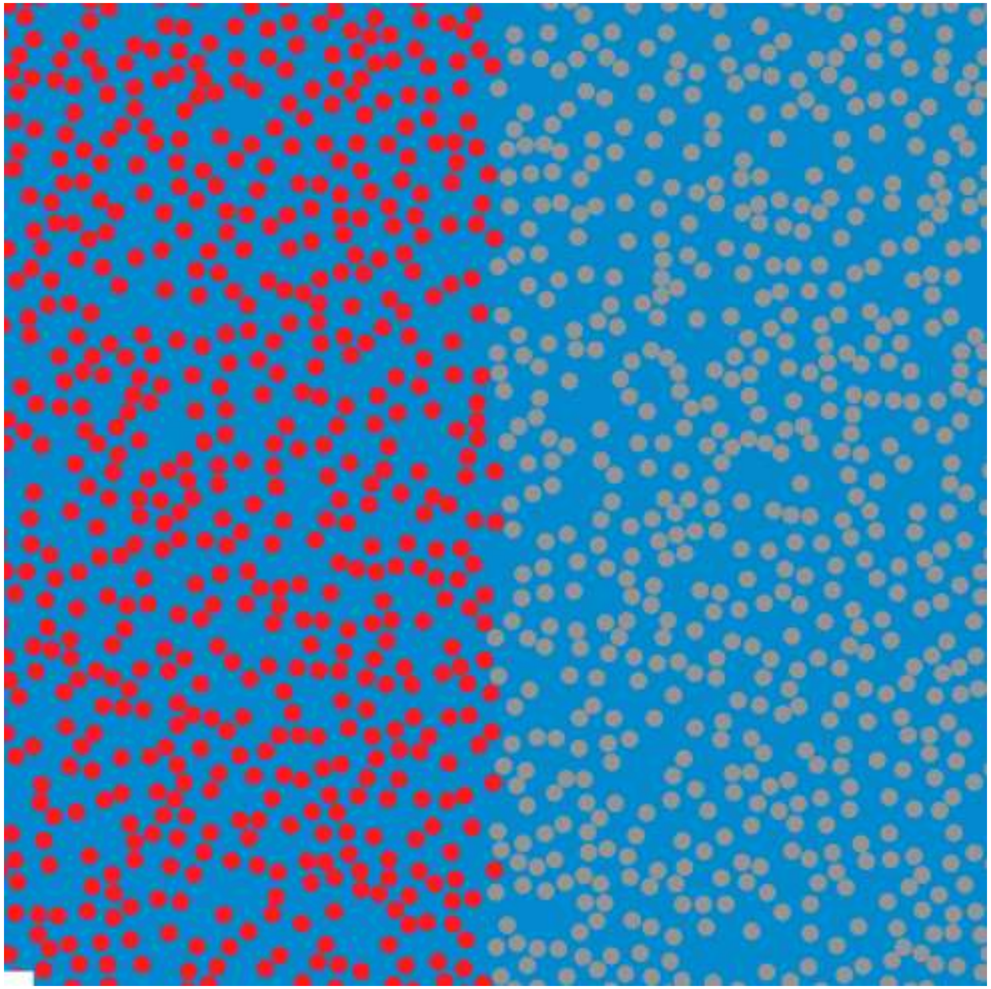
2D Example

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

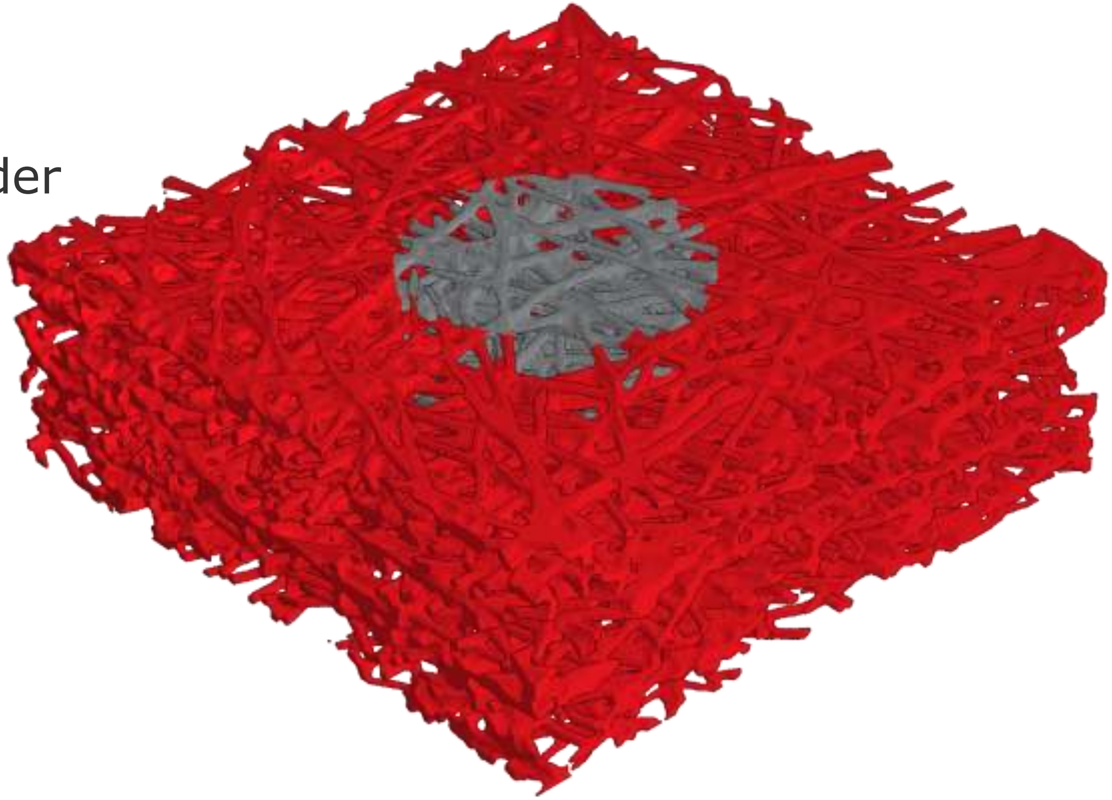


Structure with Variable Wettability

- Marked a cylinder as area with higher wettability

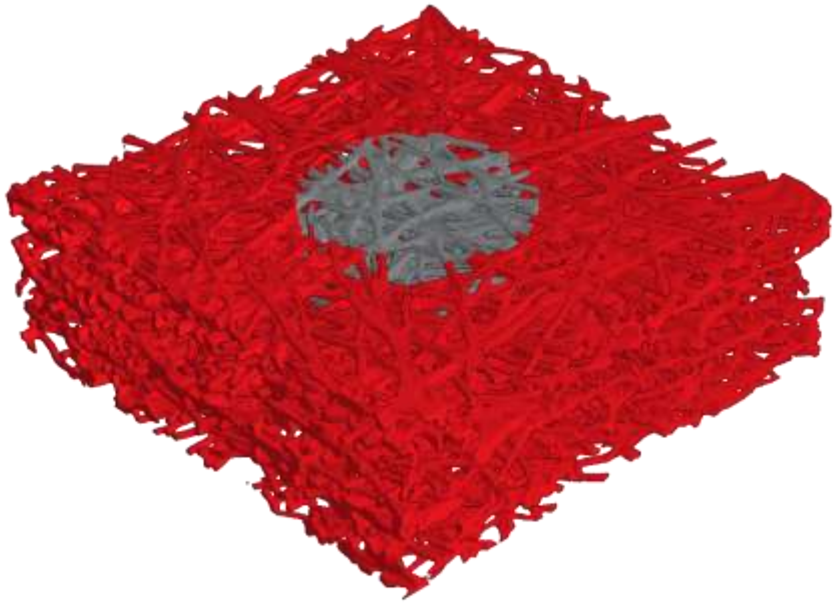
Other options:

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



GDL Models

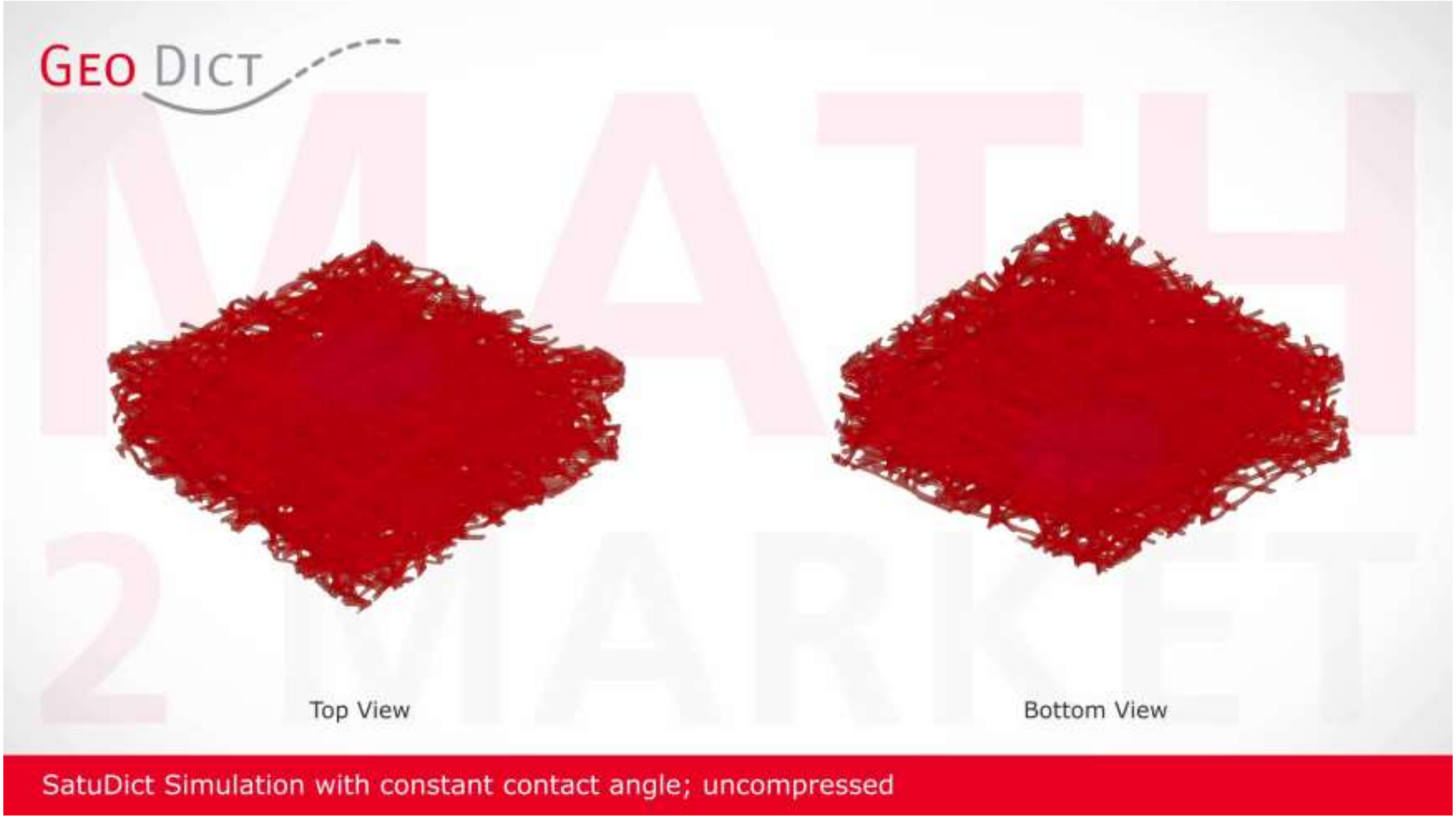
Constant Contact Angle



Two Different Contact Angles

Water Entering into the GDL

SatuDict



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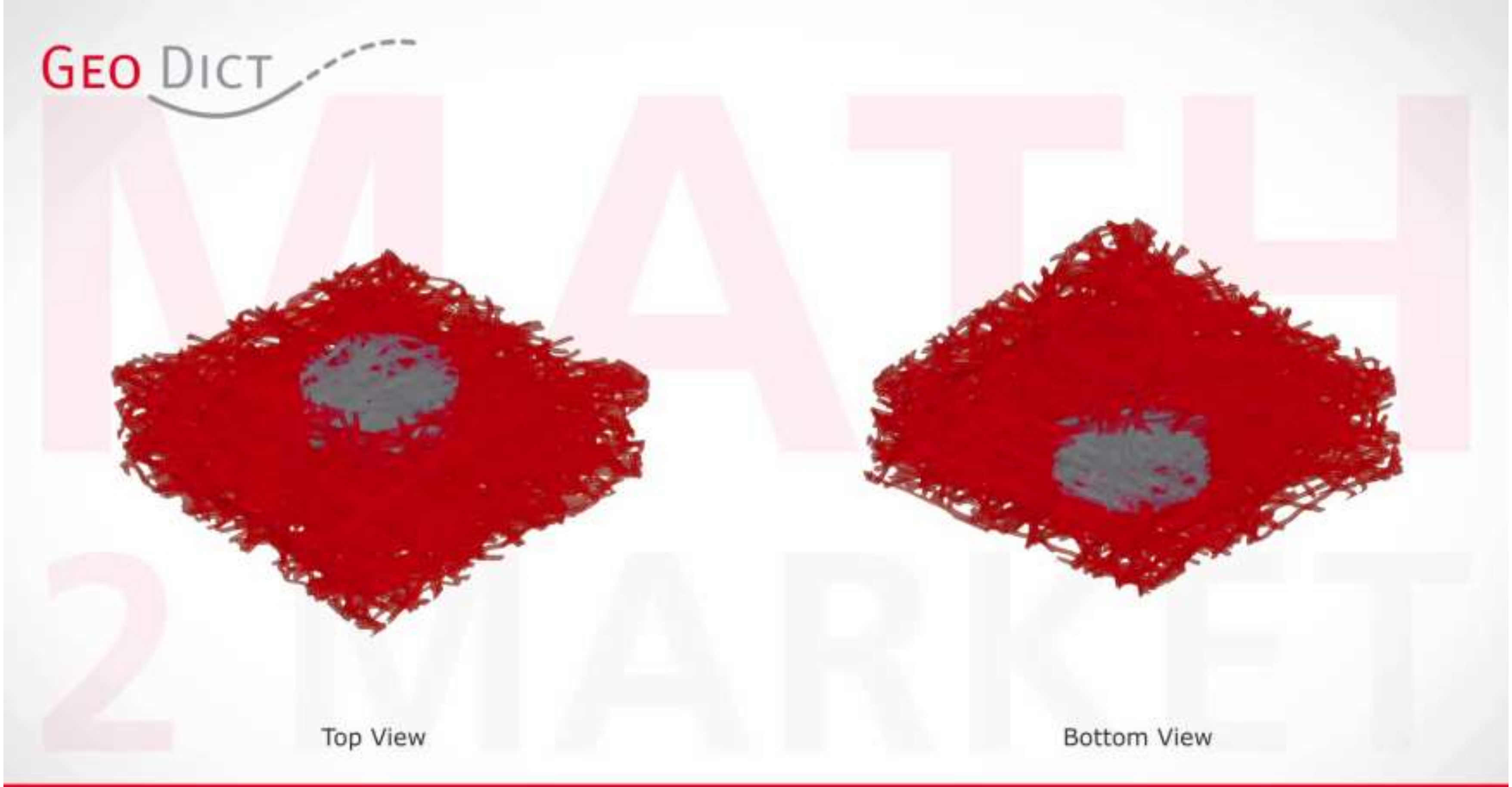
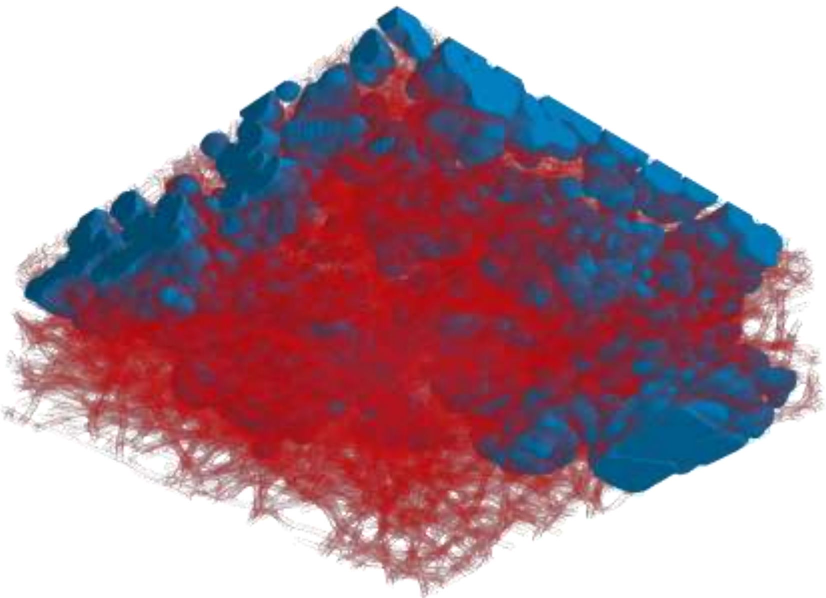
Water Entering into the GDL

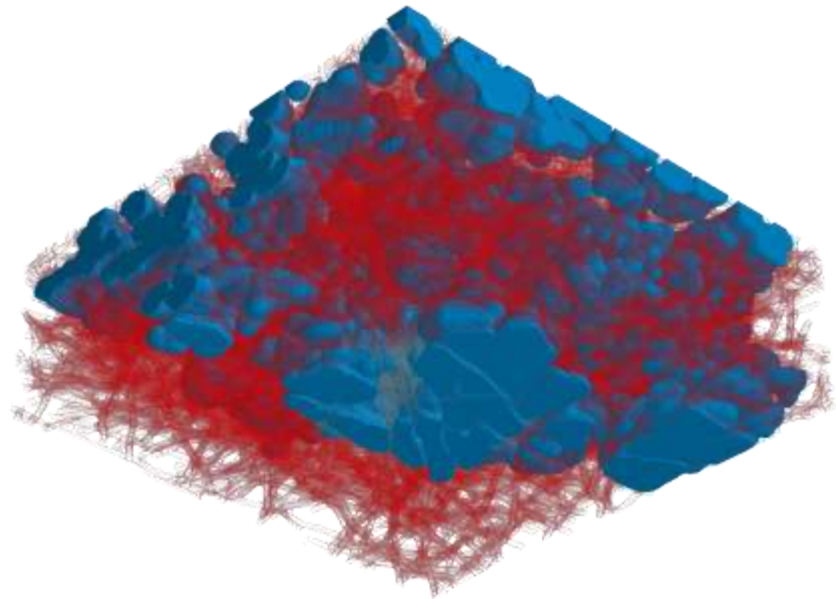
SatuDict



SatuDict Simulation with two different contact angles; uncompressed

Comparison





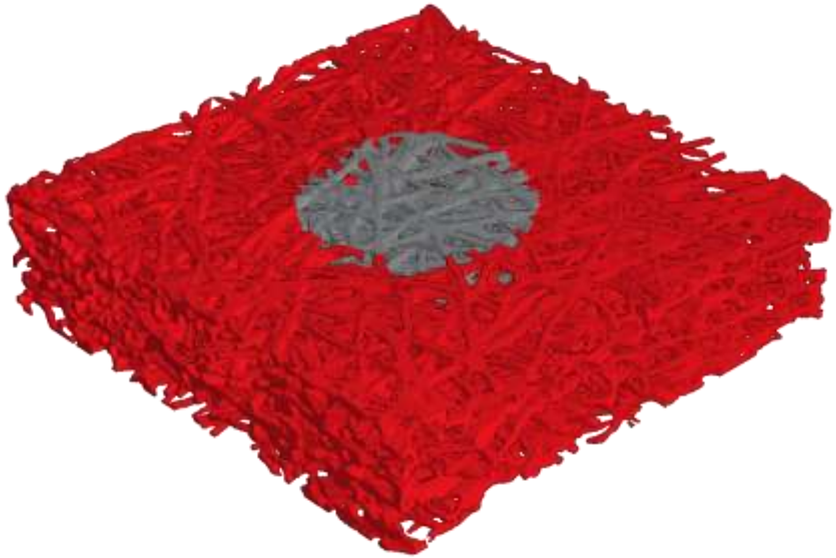
Constant Contact Angle

Two Different Contact Angles

Compressed GDL Models

SatuDict

Constant Contact Angle



Two Different Contact Angles

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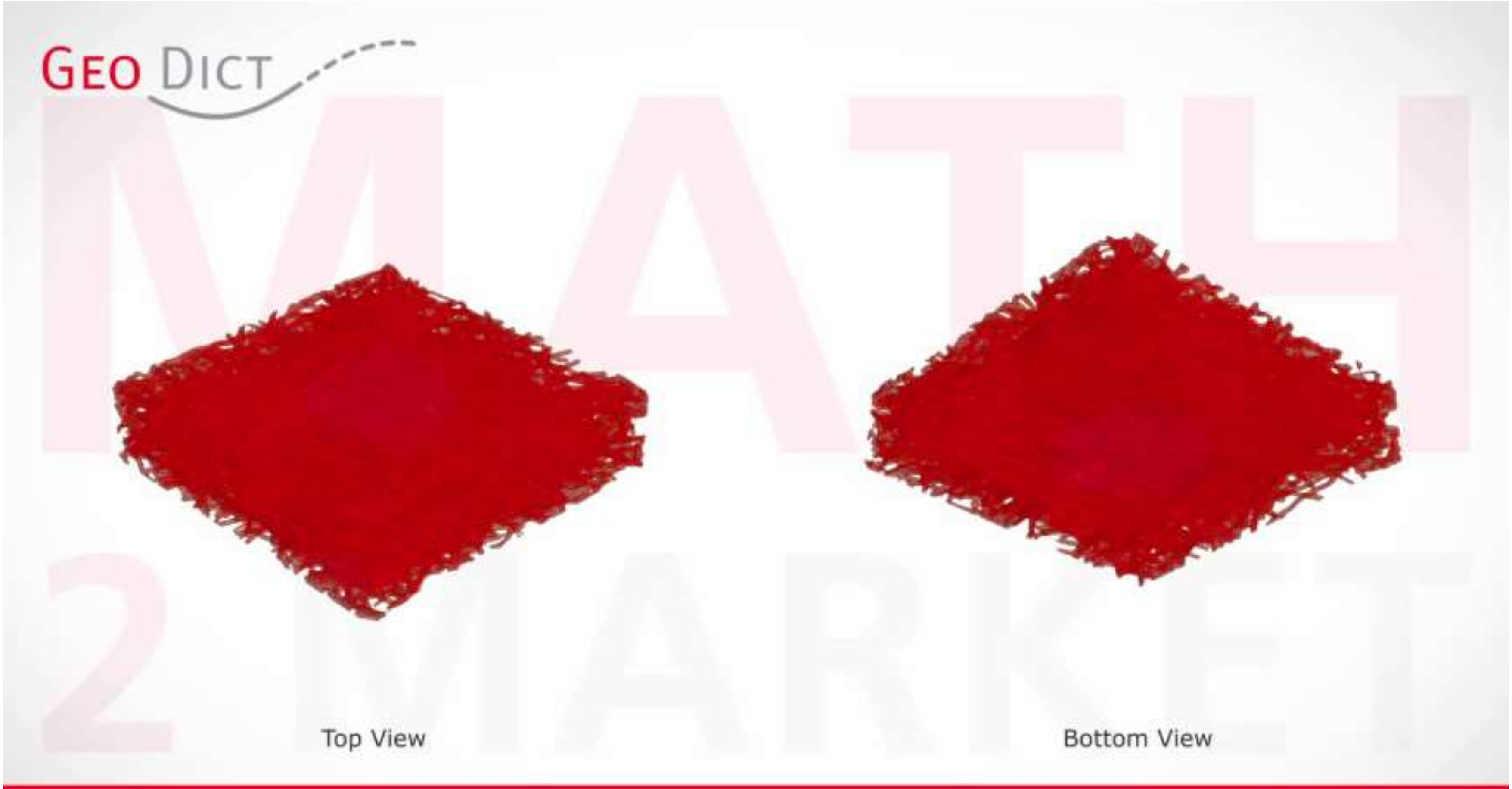
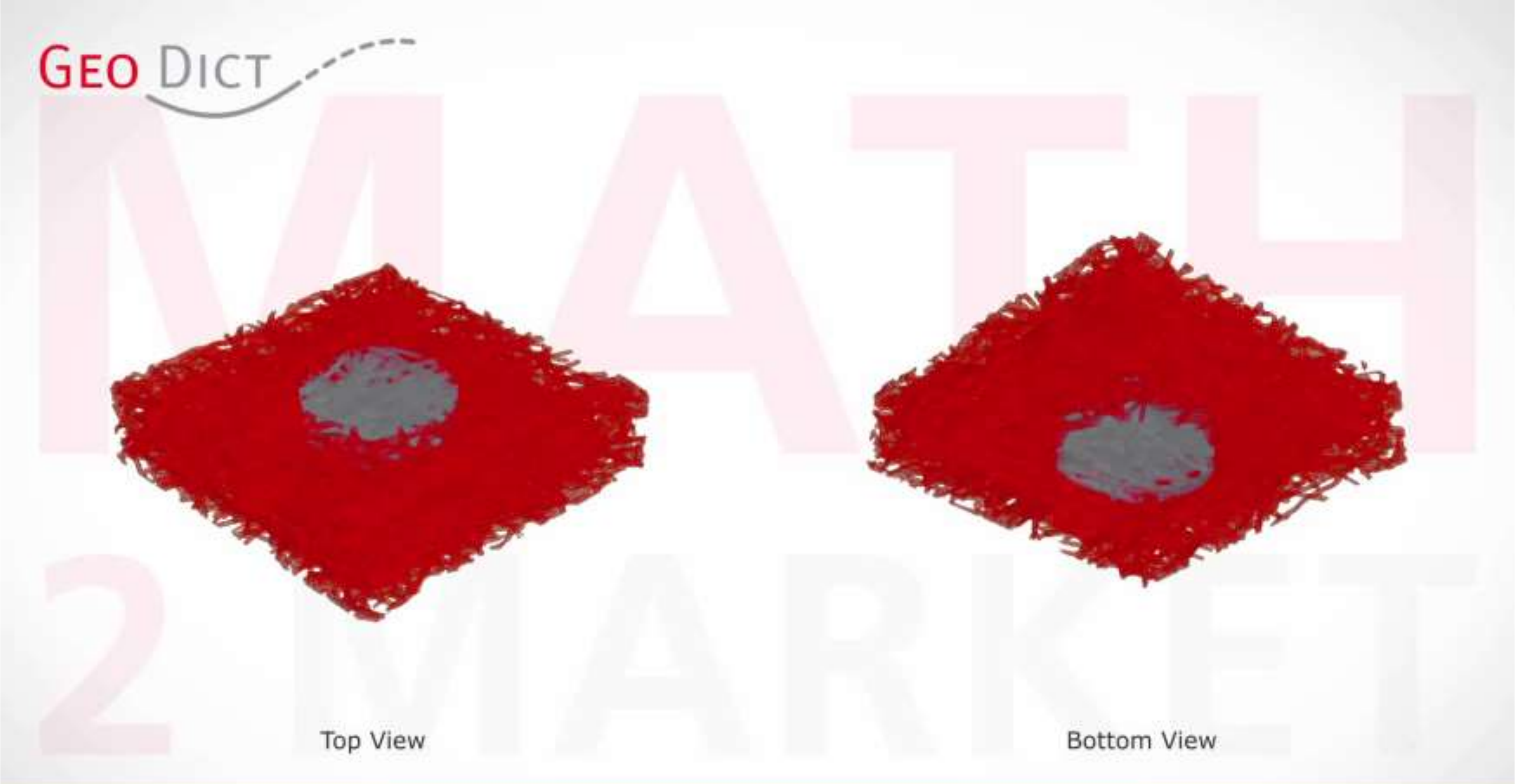
Water Entering Compressed GDL



SatuDict Simulation with constant contact angle; compressed 25%

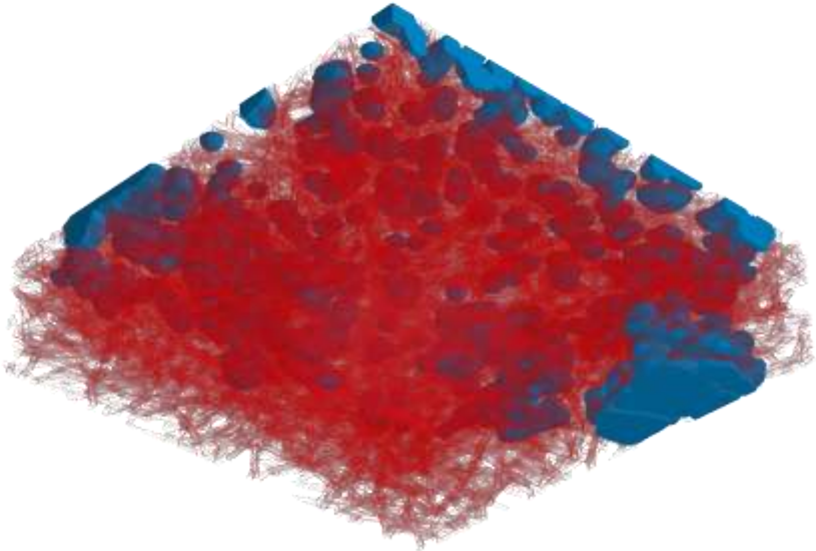
Water Entering Compressed GDL

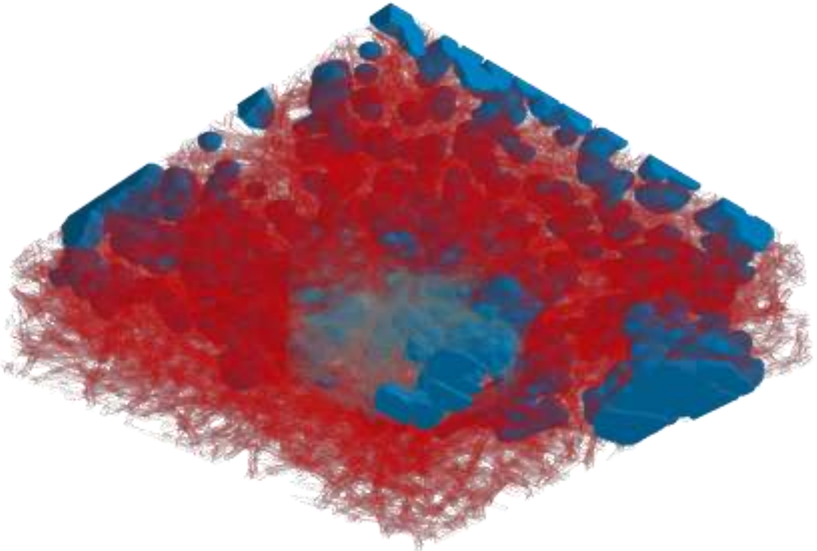
SatuDict



SatuDict Simulation with two different contact angles; compressed 25%

3D Example with Compression





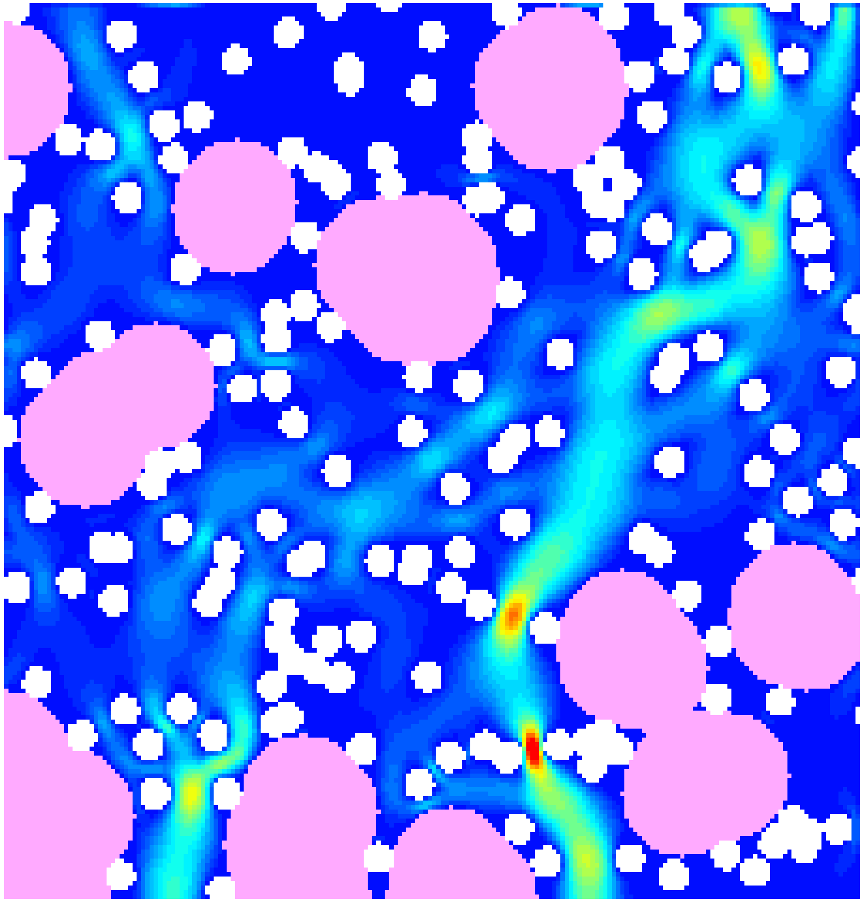
Constant Contact Angle	Two Different Contact Angles

Relative Permeability

Two-phase parameters

For each saturation:

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



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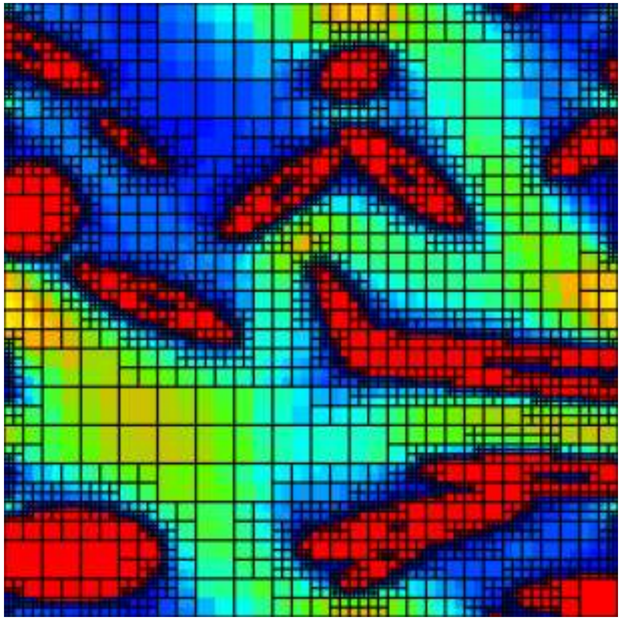
New: Speed-up through Adaptive Grid

New solver in GeoDict 2014: LIR

- Solves the Stokes equation
- On adaptive grid structure

Benefits

- Very low memory usage
- Very low runtime in high porosity geometries
- Runtime-optimized version LIR-Speed
- Memory-optimized version LIR-Memory



Benchmark (1024x1024x1200 voxels, ϕ = 88%)

Methods	LIR-Speed	LIR-Memory	SIMPLE-FFT	EJ
PermZ $[10^{-11} m^2]$	5.04	5.04	5.03	5.04
Runtime [h]	1.3	2.3	37.2	16.0
Memory [GB]	14.3	7.2	93.3	70.1

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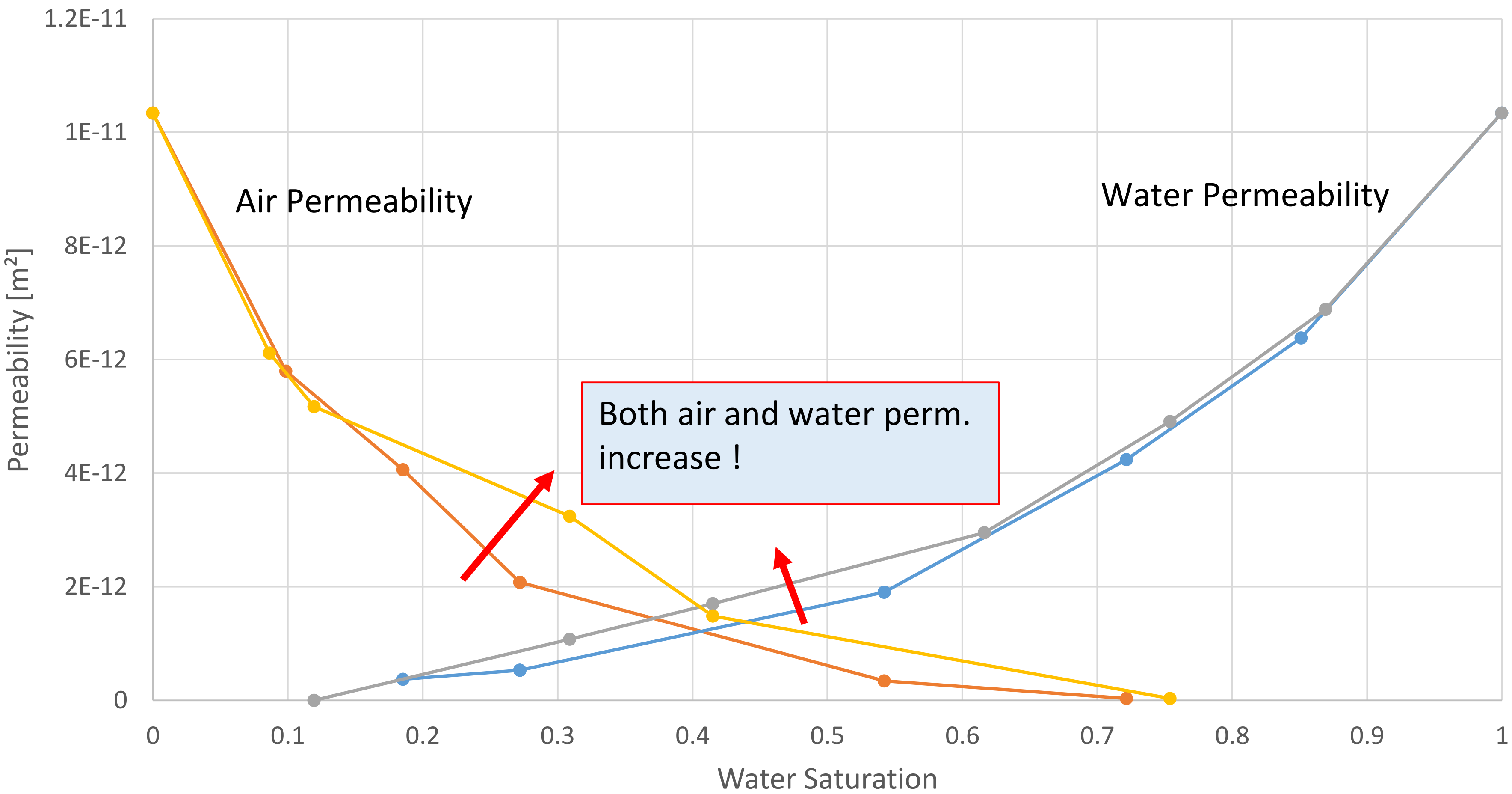
Relative Permeability (Uncompressed GDL)

SatuDict



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Summary

1. Added a model for variable contact angles
2. Demonstrated effect on relative permeability

Limitation: restriction on possible contact angles:

- If the difference between $r \cos \theta$ and r is larger than the fiber diameter, the method produces artifacts.

  $\Rightarrow$ Contact angles should not be close to 90°
  (for a GDL model it works until 50°)
- No mixed (hydrophobic-hydrophilic) wettability possible.

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Thank You!

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