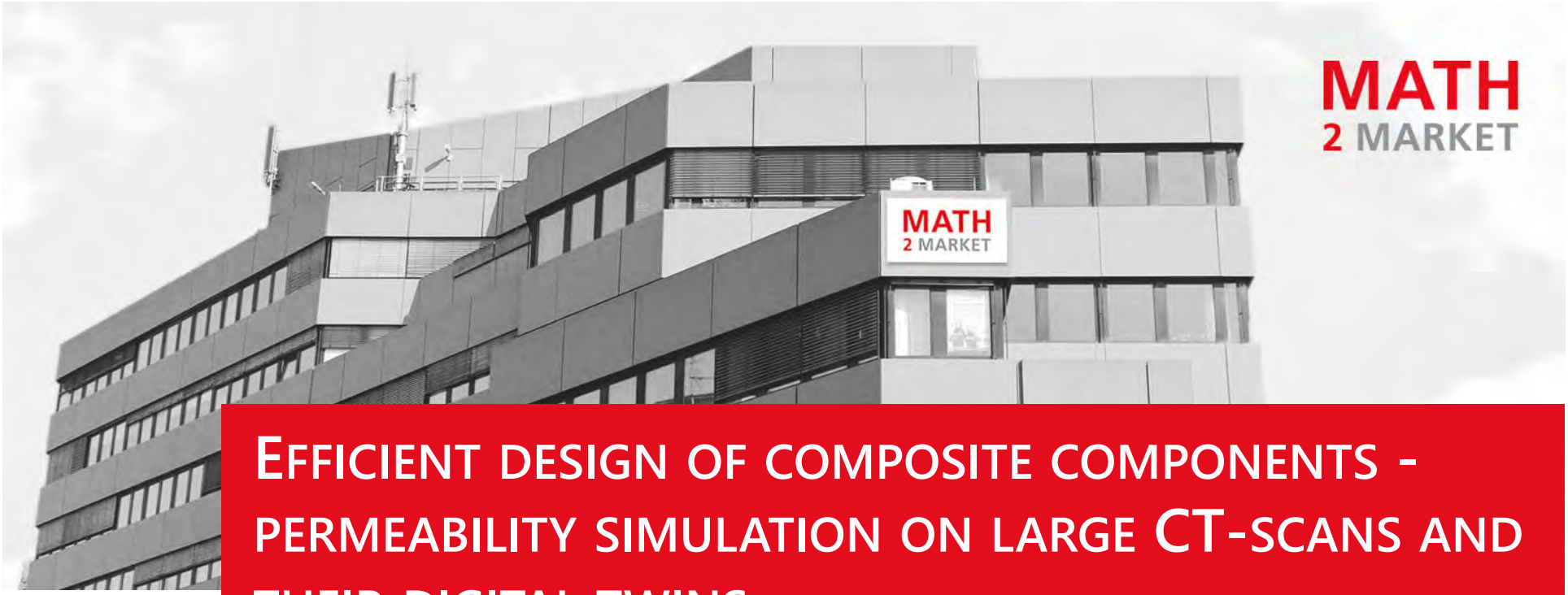


EFFICIENT DESIGN OF COMPOSITE COMPONENTS - PERMEABILITY SIMULATION ON LARGE CT-SCANS AND THEIR DIGITAL TWINS

JEMP 2018, Nantes, October 9th, 2018

Andreas Wiegmann, Constantin Bauer, Aaron Widera (Math2Market GmbH)

Tim Schmidt, David May (Institute for Composite Materials GmbH)

MATH
2 MARKET

OUTLINE

GEODICT

01 What are Math2Market & GeoDict?

02 Research Project “Math2Composites”

03 Flow Simulations on Large Structures

MATH 2 MARKET

Math2Market GmbH

- creates and markets the scientific software GeoDict®.
- was spun off in 2011 from Fraunhofer ITWM in Kaiserslautern.
- is an privately owned company based in Kaiserslautern, Germany.

GeoDict® - The Digital Material Laboratory

- is a software tool to analyze and design porous media and composites.
- works on
  - µCT and FIB-SEM 3D images or
  - random geometric material models.

GeoDict® Solutions for ...

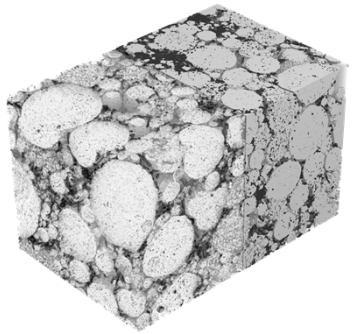
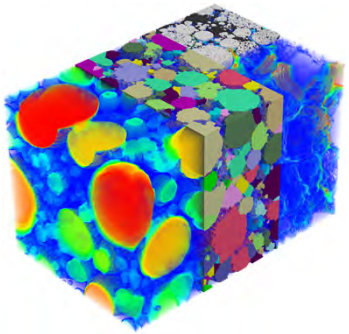
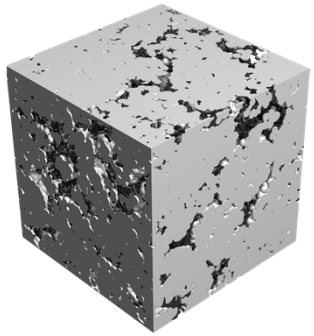
GeoDict

Filtration	Mostly automotive, filter media & filters for water, sludge, oil, air and fuel
Electrochemistry	Fuel cell media & battery materials, catalyst materials
Composites, Ceramics & Metals	CFRP, GFRP, mostly automotive, lightweight materials
Digital Rock Physics	Digital rock physics, digital sand control

MATH 2 MARKET

The Workflow for Digital Material Design with GeoDict®

GeoDict

Import	Analyze	Model	Design	Next Generation Material
				
The idea is the beginning. Design a material from scratch or import images from an existing material to create a digital model.	Discover the geometric properties and compute the physical properties of the material. This is the start of creating a Digital Twin.	A Digital Twin is the statistical representation of the material in the digital world. Here begins the design process.	Digital prototypes are easily and rapidly created. Simulate and evaluate in a loop to find the material with the desired properties.	The materials of the future are within reach and we help you find them faster.
Digital Material	Statistical Model	Digital Twin	Digital Prototypes	This is innovation through simulation.

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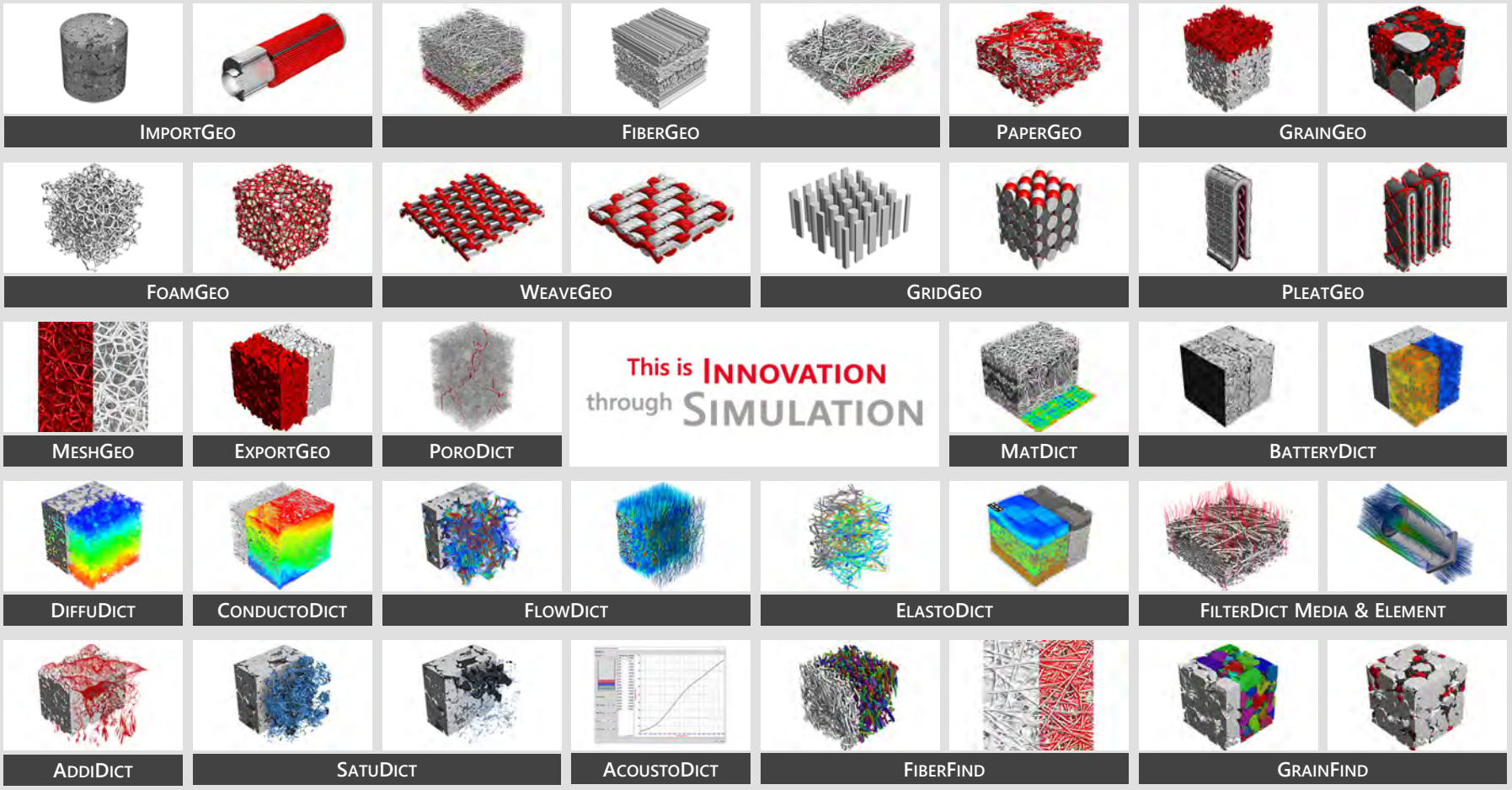
GeoDict® Module Overview

GeoDict



MATH 2 MARKET

Outline

GeoDict

01 What are Math2Market & GeoDict?

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MATH 2 MARKET

Our dreams in short

GeoDict

- The usual idea of Digital Material Design:

1. First make sure 3-D imaging of **existing materials** + property computation agrees with experiments.
2. Then model **new materials** as 3-D images and compute their properties until you **find a better material**.

- In the Math2Composites project, there is a twist:

1. First make sure 3-D imaging + property computation agrees with ***easy / cheap*** experiments
2. Infer that property computation is also correct for ***difficult / expensive*** experiments

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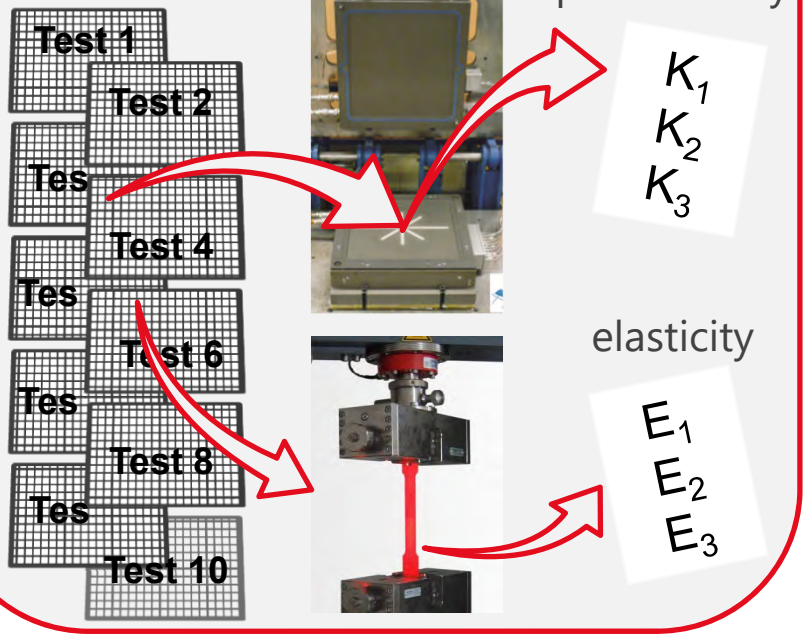
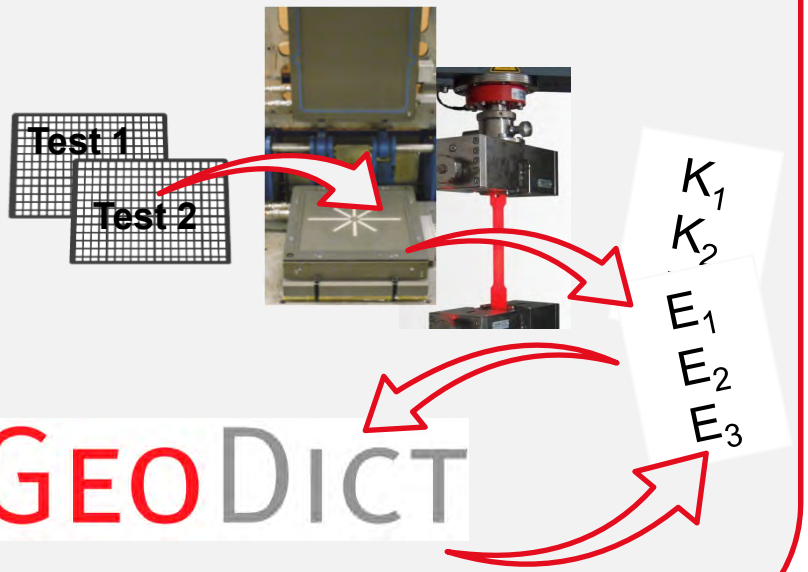
Research Project "Math2Composites"

GeoDict

Large amount of experiments for the determination of material properties



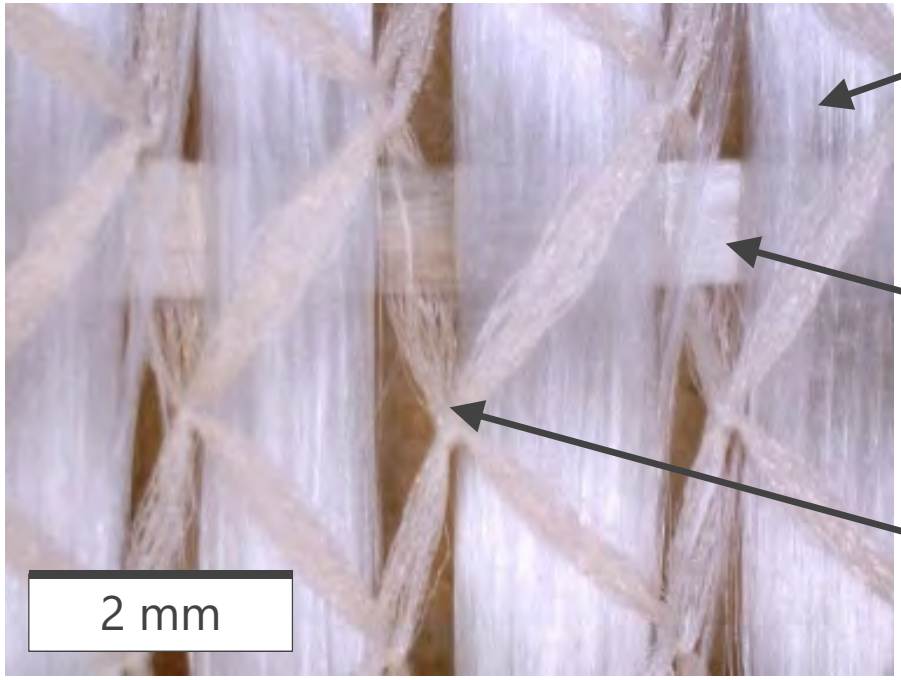
Novel simulative-experimental approach for the determination of material properties



Replace a large amount of experiments by validated simulations

MATH 2 MARKET

- Structure of the non-crimped fabric Hacotech G300U-1270mm



0° glass fiber roving
(80% of fiber volume fraction)

90° glass fiber roving
(20% of fiber volume fraction)

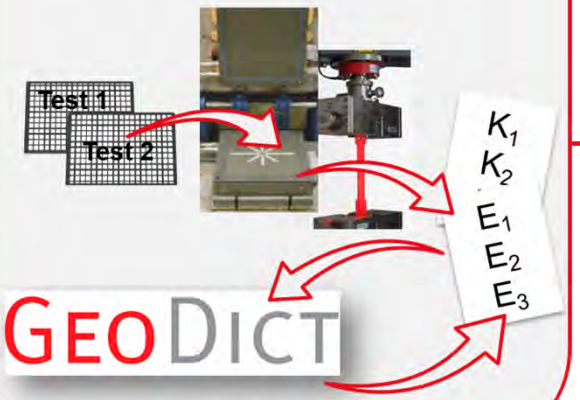
PET stitching

HACOTECH
HANSEATIC COMPOSITES TECHNOLOGIES

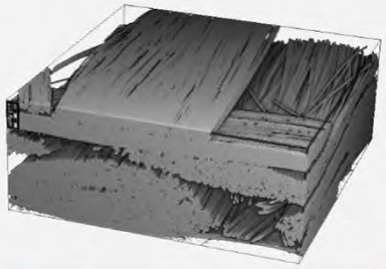
Research Project "Math2Composites"

GeoDict

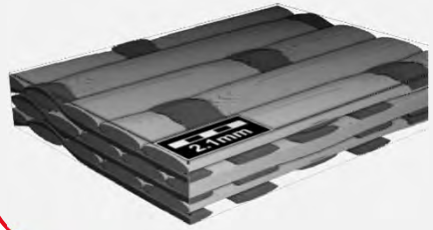
Novel simulative-experimental approach for the determination of material properties



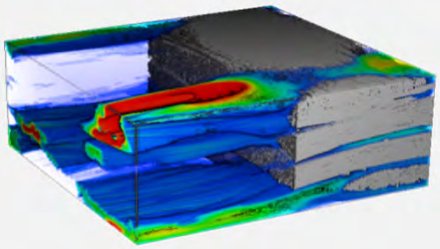
µCT-Scan

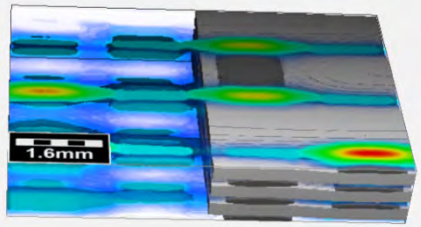


Model



Simulation





calibration of the simulation → validated simulation → **PREDICTION**

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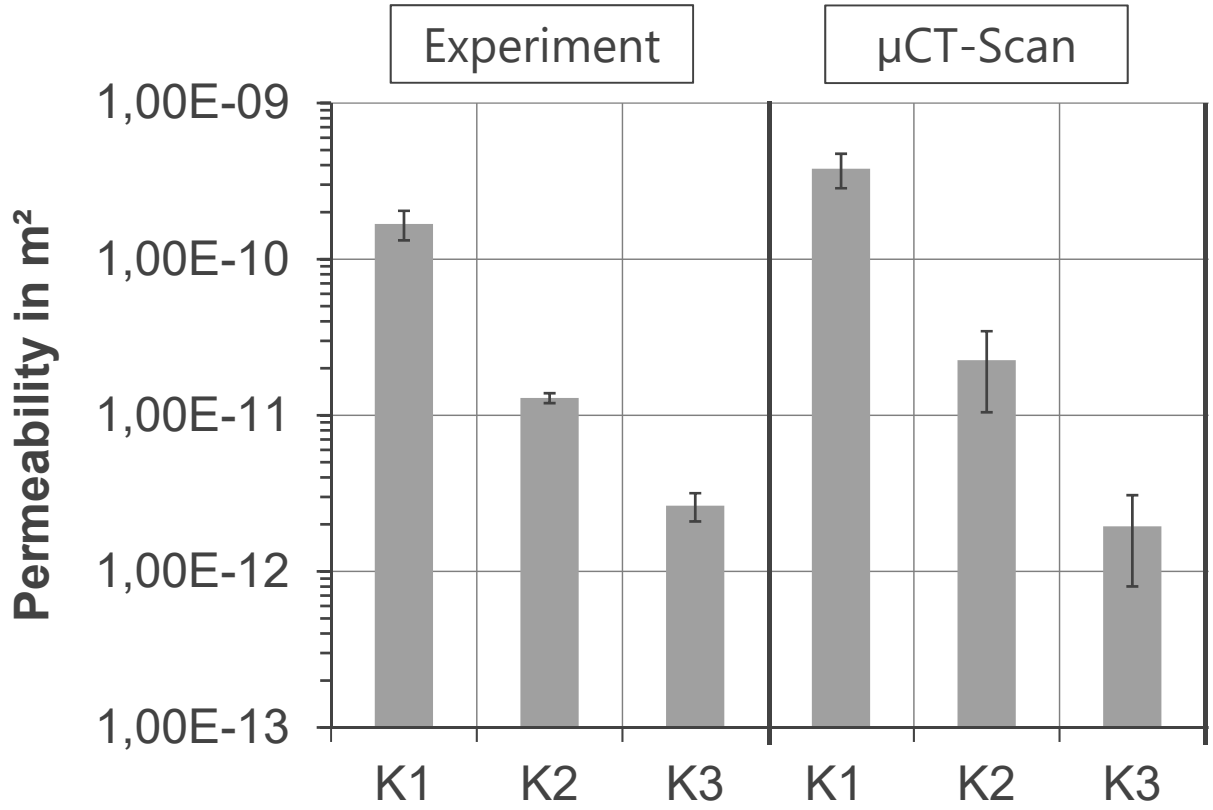
Research Project "Math2Composites"

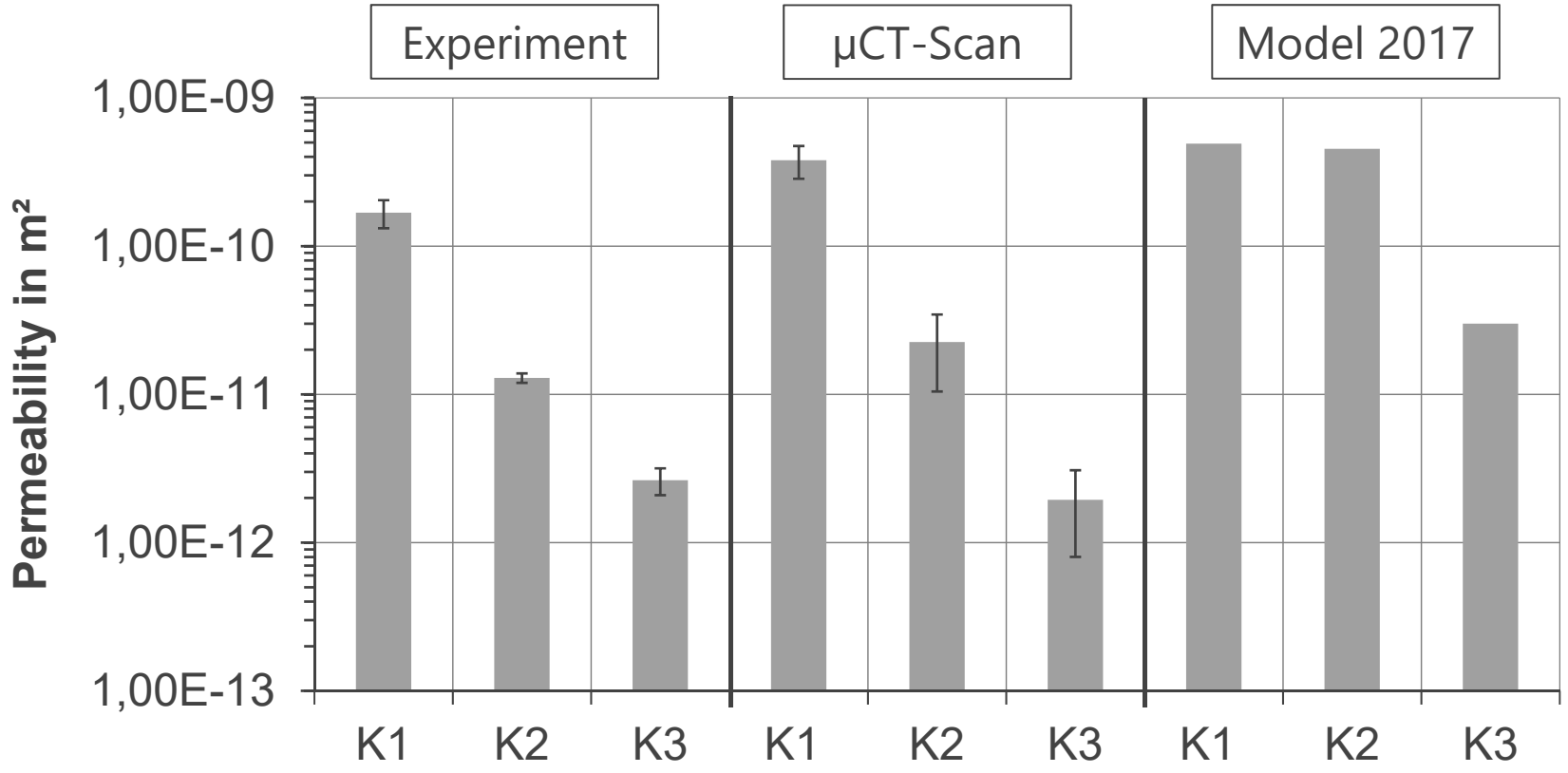
GeoDict

- Results of the permeability calculation 2017



MATH 2 MARKET

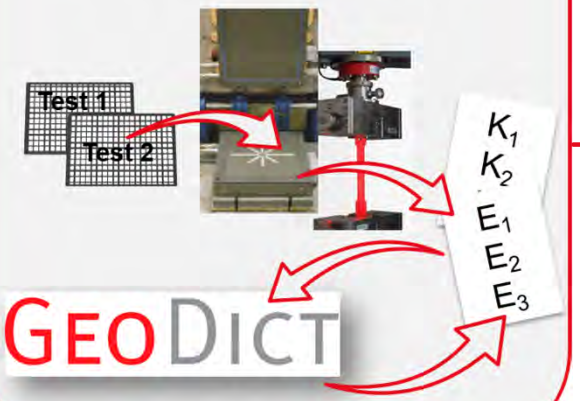
- Results of the permeability calculation 2017



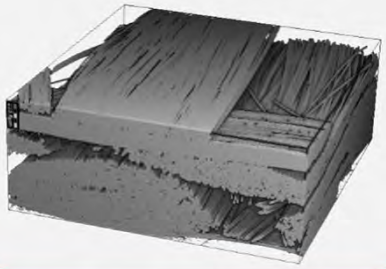
Research Project "Math2Composites"

GeoDict

Novel simulative-experimental approach for the determination of material properties



µCT-Scan

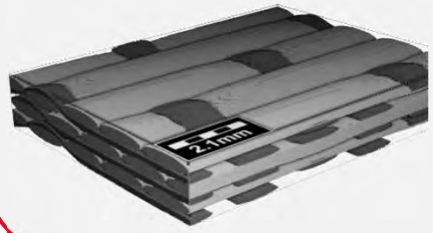


✓ good simulation results

✗ huge experimental effort

→ can't be reduced

Model



✓ low experimental effort

✗ deviation from simulation and experiment too high

→ can be reduced by improved modeling techniques

Digital Twin

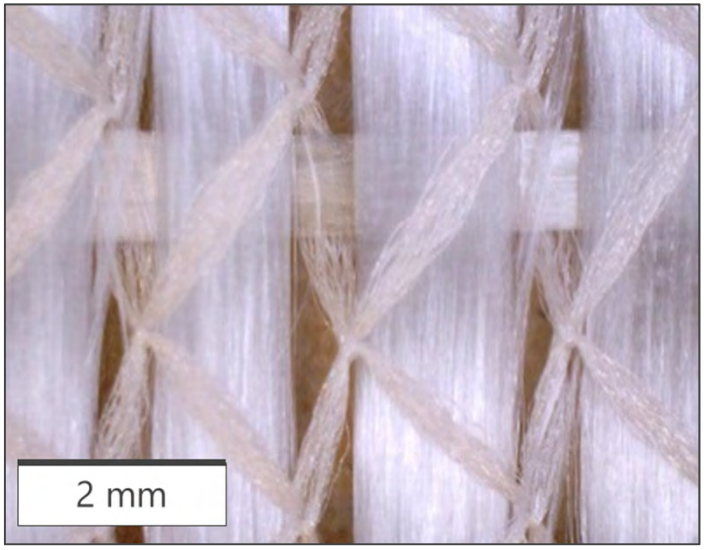
MATH 2 MARKET

Research Project "Math2Composites"

GeoDict

- Structure of the non-crimped fabric Hacotech G300U-1270mm

µCT-Scan



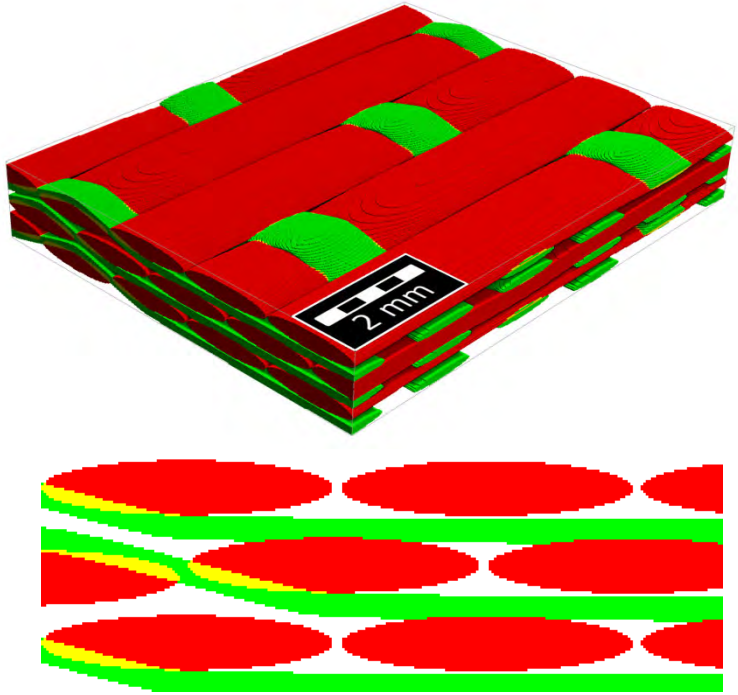
Microscopy

MATH 2 MARKET

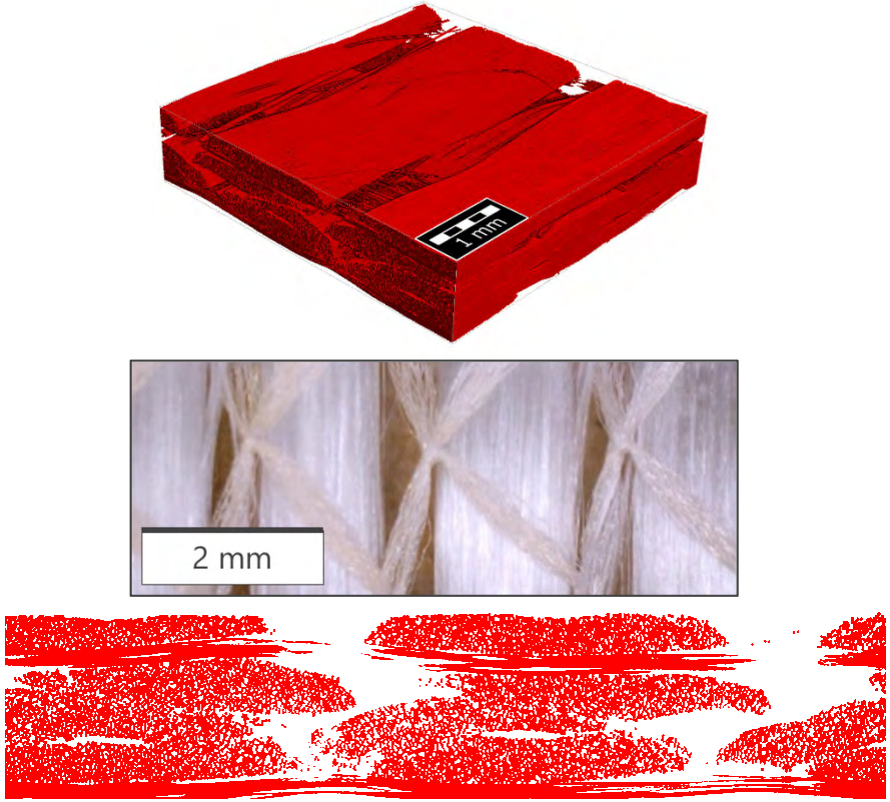
Research Project "Math2Composites"

GeoDict

- modeling with WeaveGeo



Model 2017



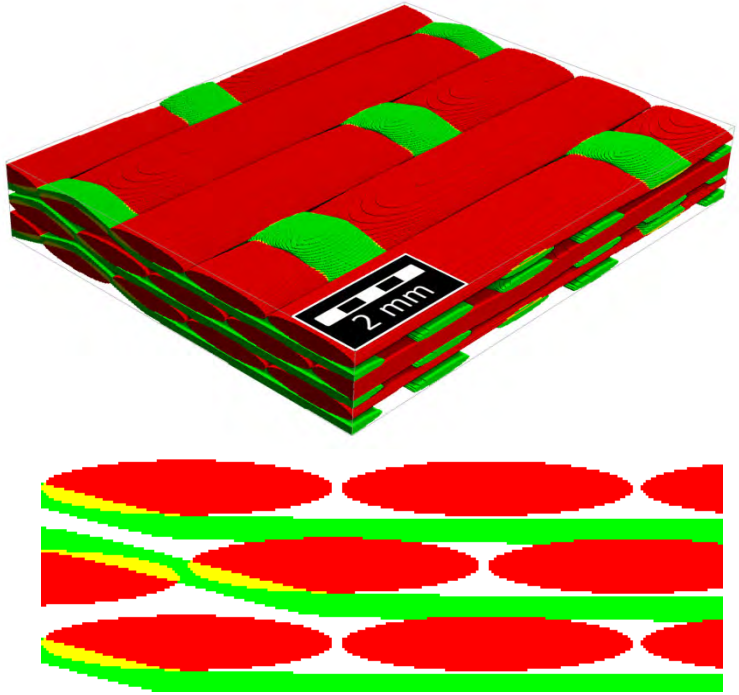
µCT-Scan

MATH 2 MARKET

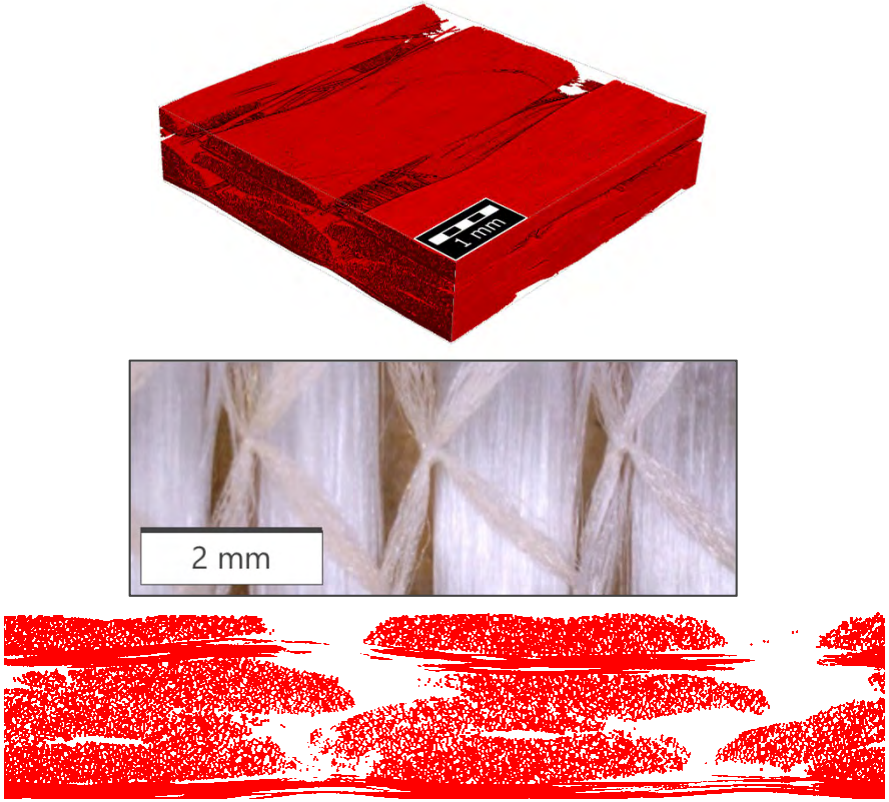
Research Project "Math2Composites"

GeoDict

- modeling with WeaveGeo



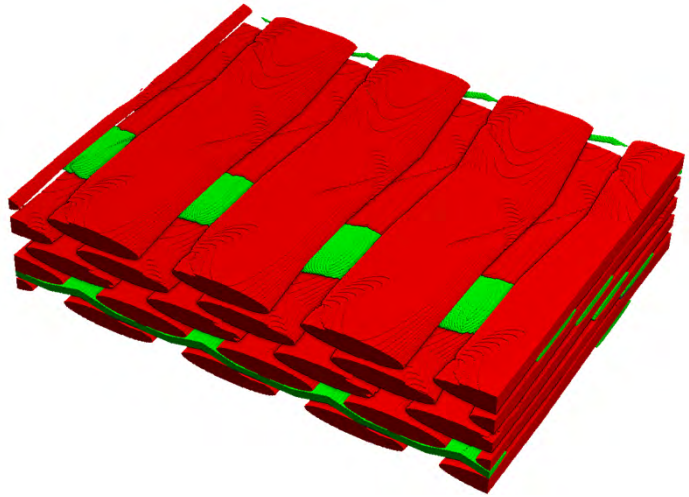
3rd cousin



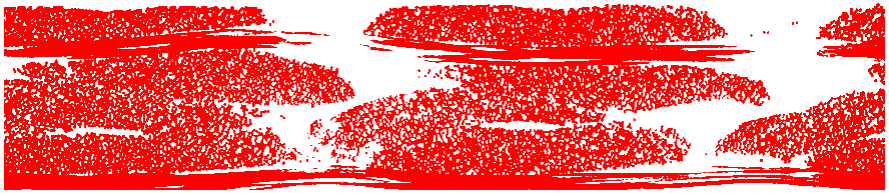
µCT-Scan

MATH 2 MARKET

- Implementation of roving undulation



2nd cousin

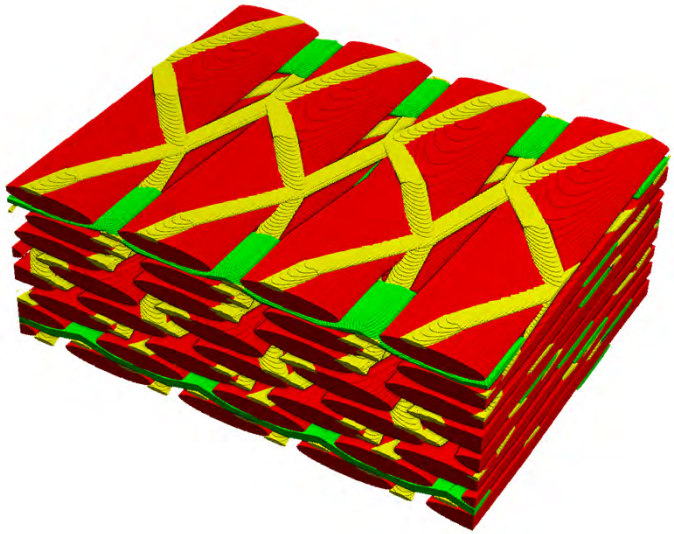


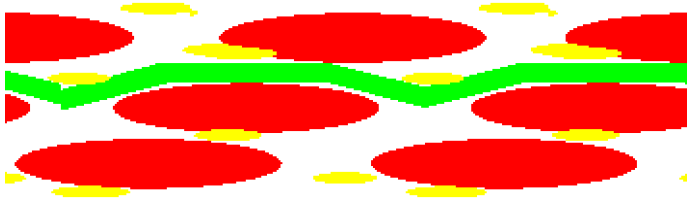
µCT-Scan

Research Project "Math2Composites"

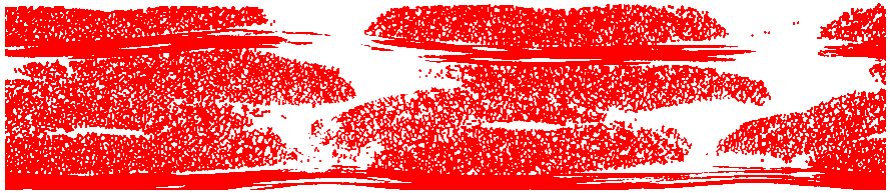
GeoDict

- modeling the PET stitching (yellow)





1st cousin



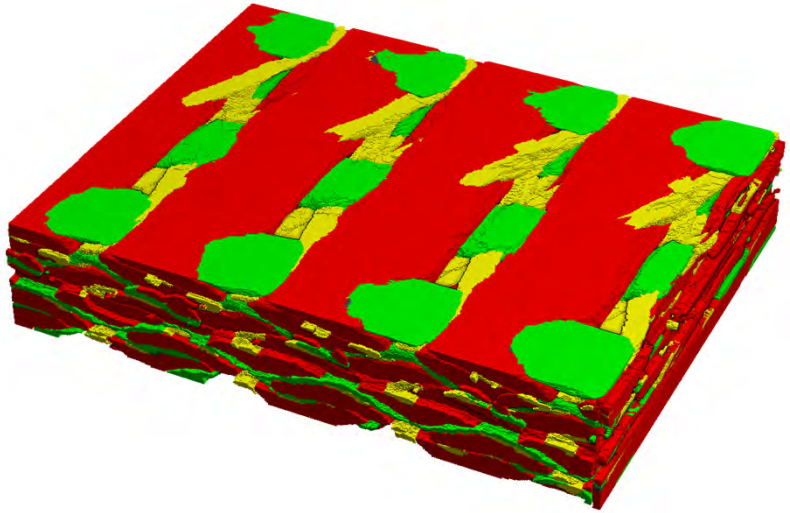
µCT-Scan

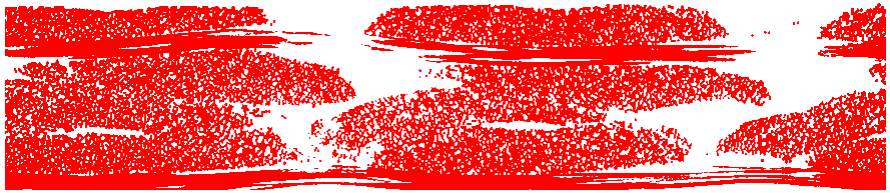
MATH 2 MARKET

Research Project "Math2Composites"

GeoDict

- Compaction of the modeled structure with ElastoDict-LD





brother / sister

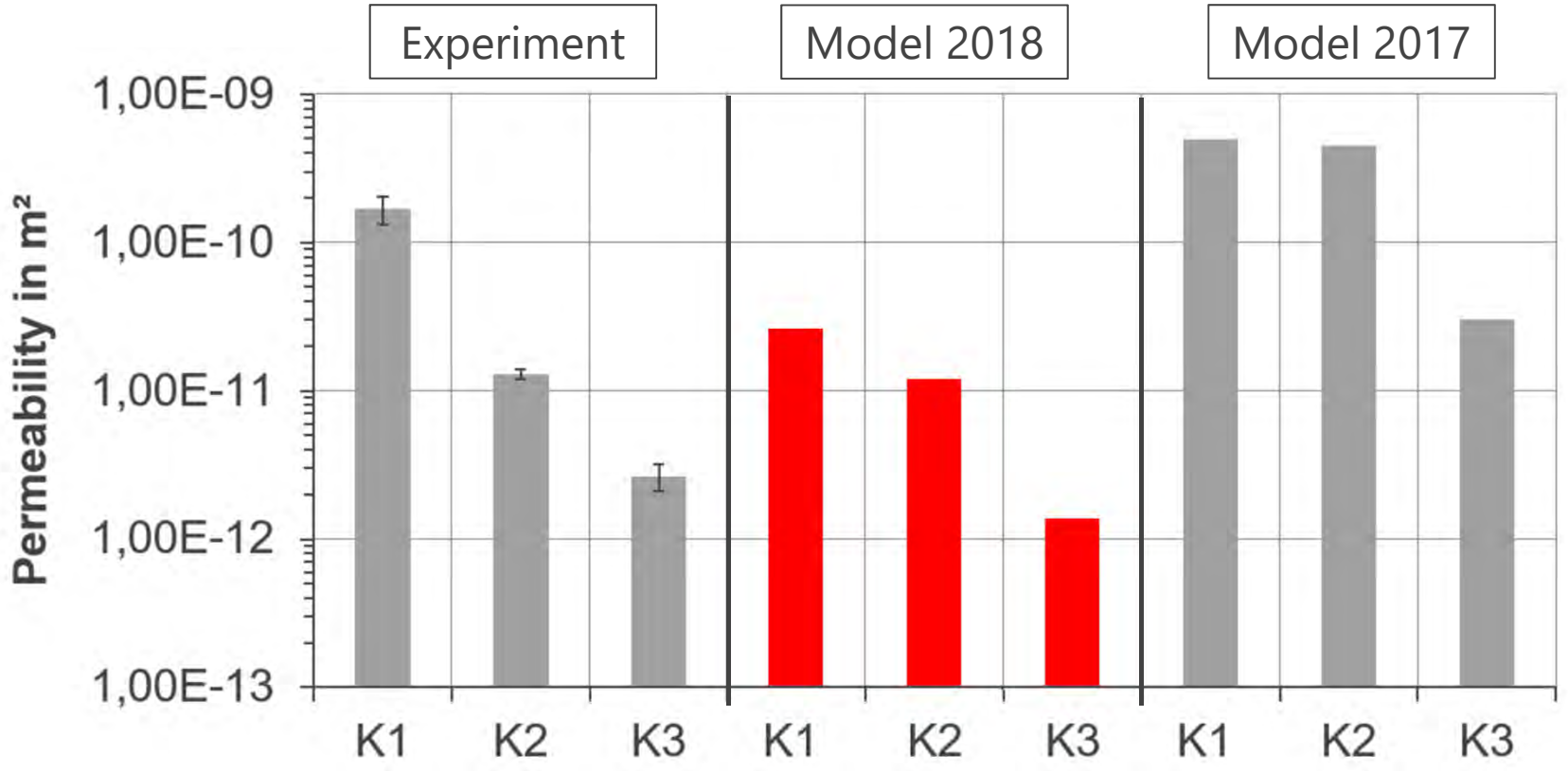
µCT-Scan

MATH 2 MARKET

Research Project "Math2Composites"

GeoDict

- Calculation of the permeability with FlowDict



➡ **next step:** using anisotropic permeabilities for the roving material

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SUMMARY

GEODICT

- Calculated permeabilities by flow simulation on µCT-scan show very good agreement with experiments.
- Elevated effort to obtain µCT-scan.
- Modeled structures for permeability calculation must take material imperfections into account
  - fiber undulation
  - PET stitching
  - roving deformation through compaction
- Flow simulations on the new modeled structure with material imperfections show only small deviations from experiment.

MATH 2 MARKET

Research Project "Math2Composites"

GeoDict

- Acknowledgement

The project "Math2Composites" is funded by the ZIM program of the Federal Ministry for Economic Affairs and Energy (BMWi), funding reference: ZF40523110EB6

Supported by:

Federal Ministry for Economic Affairs and Energy

on the basis of a decision by the German Bundestag

ZIM Zentrales Innovationsprogramm Mittelstand

MATH 2 MARKET

Outline

GeoDict

01 What are Math2Market & GeoDict?

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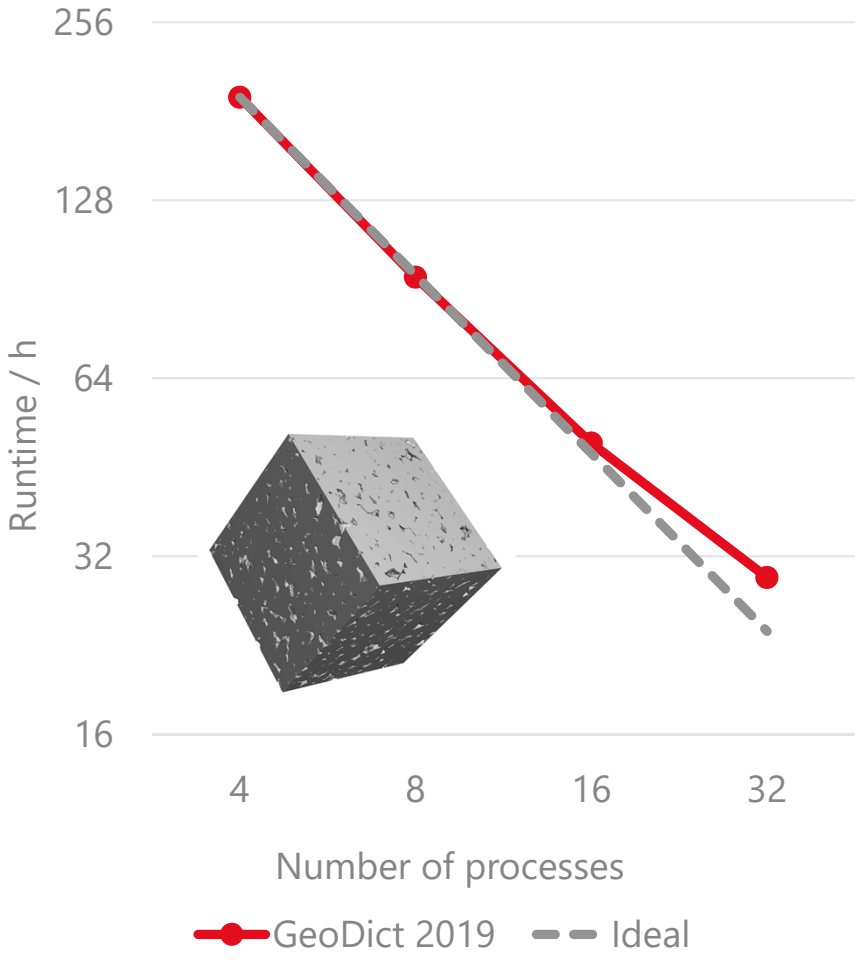
MATH 2 MARKET

Flow Computation with LIR solver

GeoDict

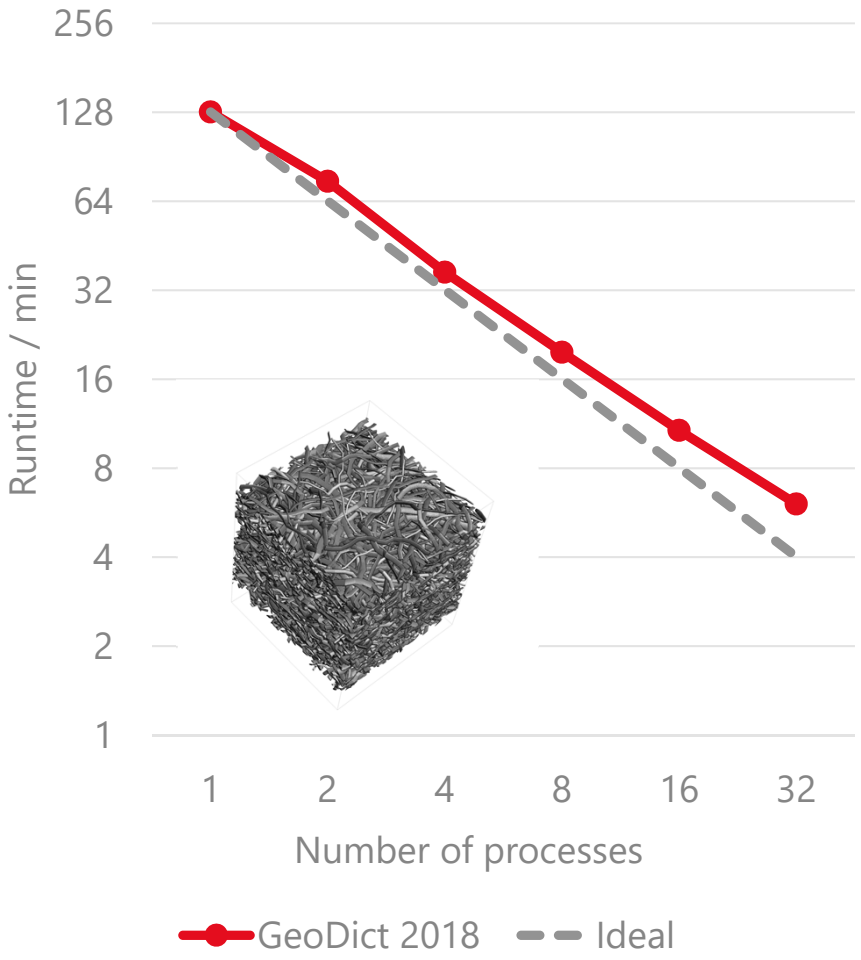


- Rock structure
- Structure size 3072x3072x3072 ~30 billion voxels
- 21% porosity
- Stokes solver
- Error bound = 0.01
- Memory usage
  - Optimized for speed: 636GB
  - Optimized for memory: 371GB

MATH 2 MARKET

Flow Computation with LIR solver

GeoDict

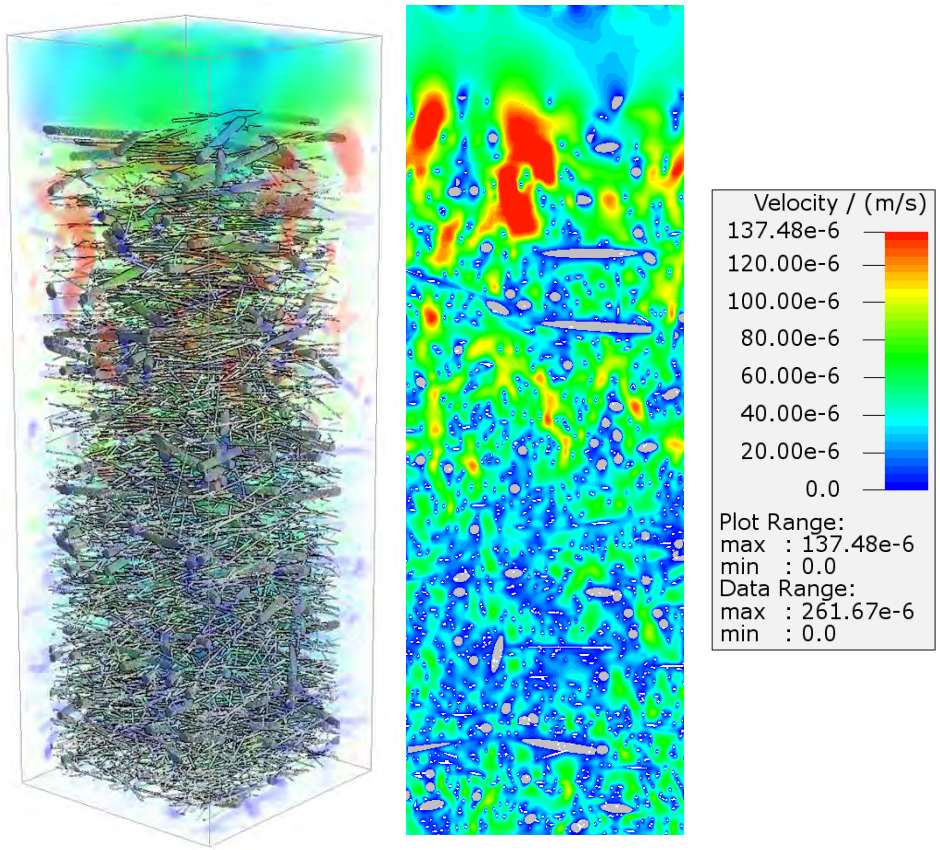


- Paper structure
- Structure size 1024x1024x1200 ~1.3 billion voxels
- 89% porosity
- Stokes solver
- Fixed number of iterations
- Memory usage <16GB

MATH 2 MARKET

Filter Simulation with GeoDict

GeoDict



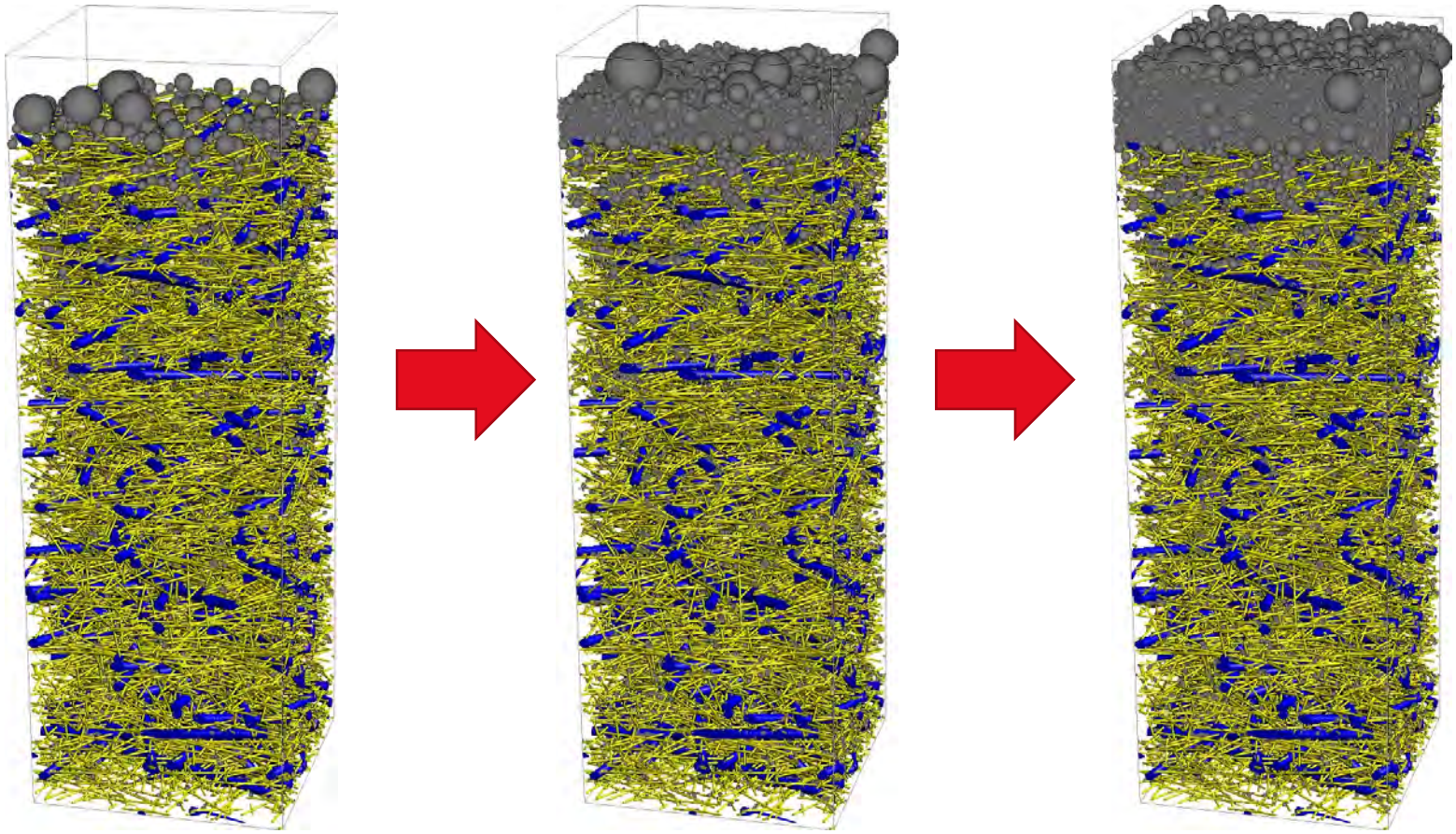
- Fibrous oil filter media
- Structure size 600x600x1800
  ~0.7 billion voxels
- 94.1% porosity
- Filtration simulation
  - flow simulation
  - particle tracking
  - flow simulation....
- 230 batches (simulation runs)

MATH 2 MARKET

Filter Simulation with GeoDict

GeoDict

- Transient filtration simulation



2650 s

8733 s

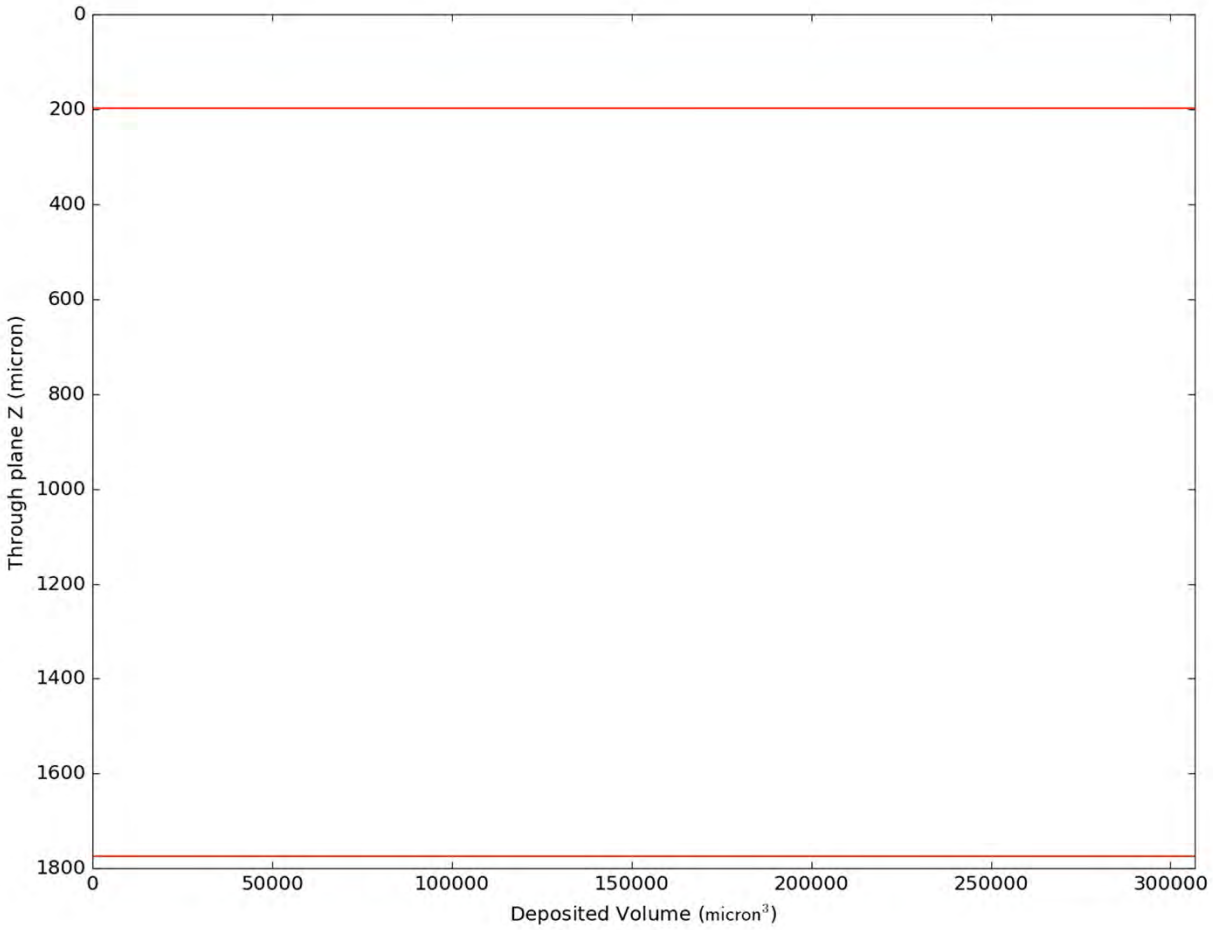
11340 s

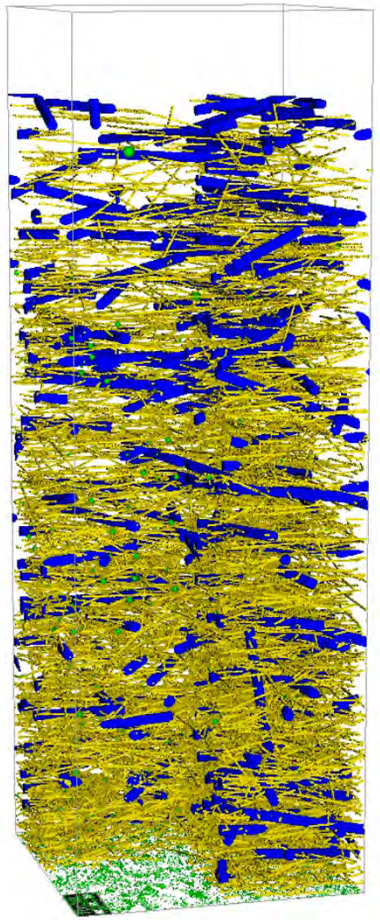
MATH 2 MARKET

Filter Simulation with GeoDict

GeoDict

- Transient filtration simulation

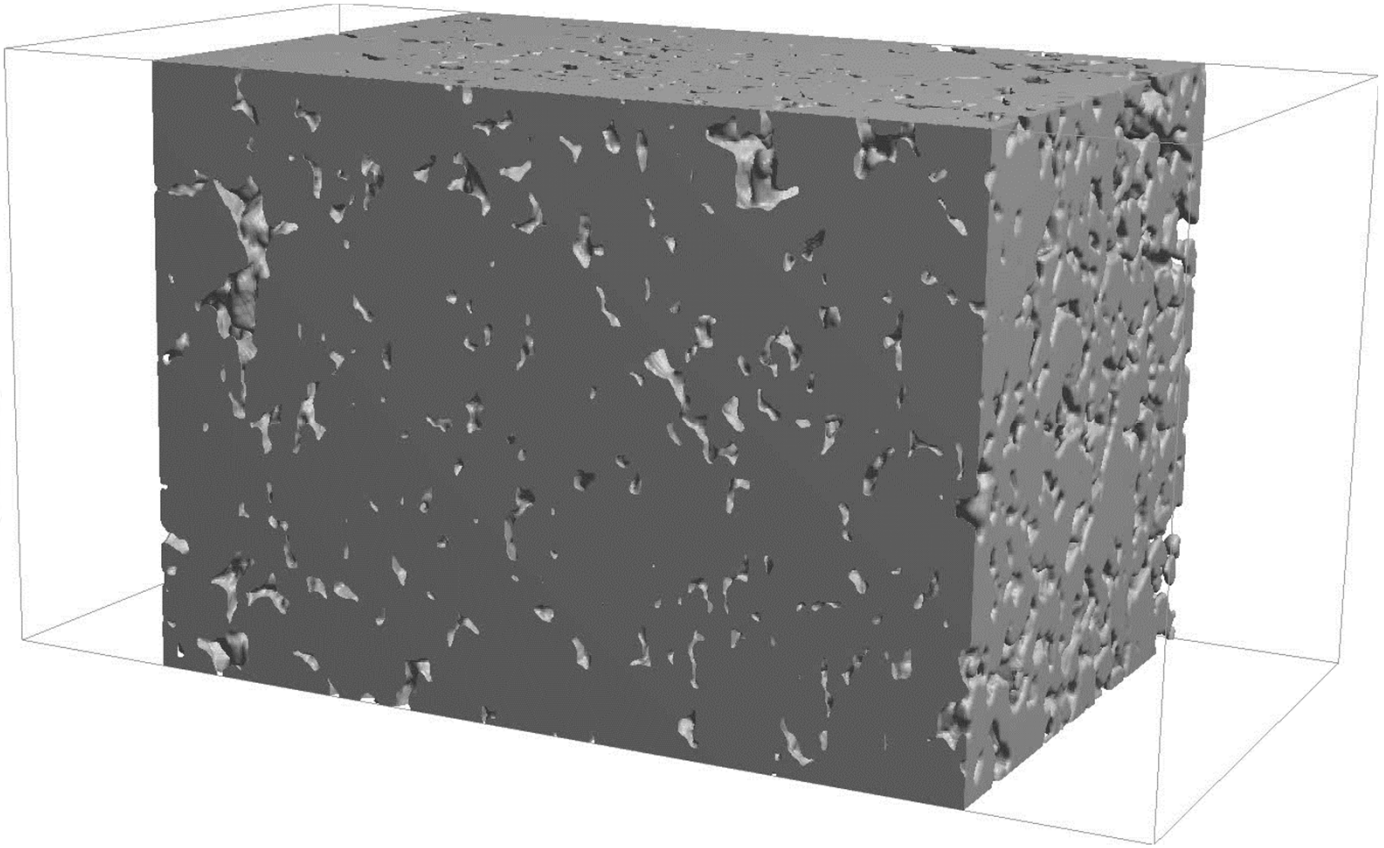




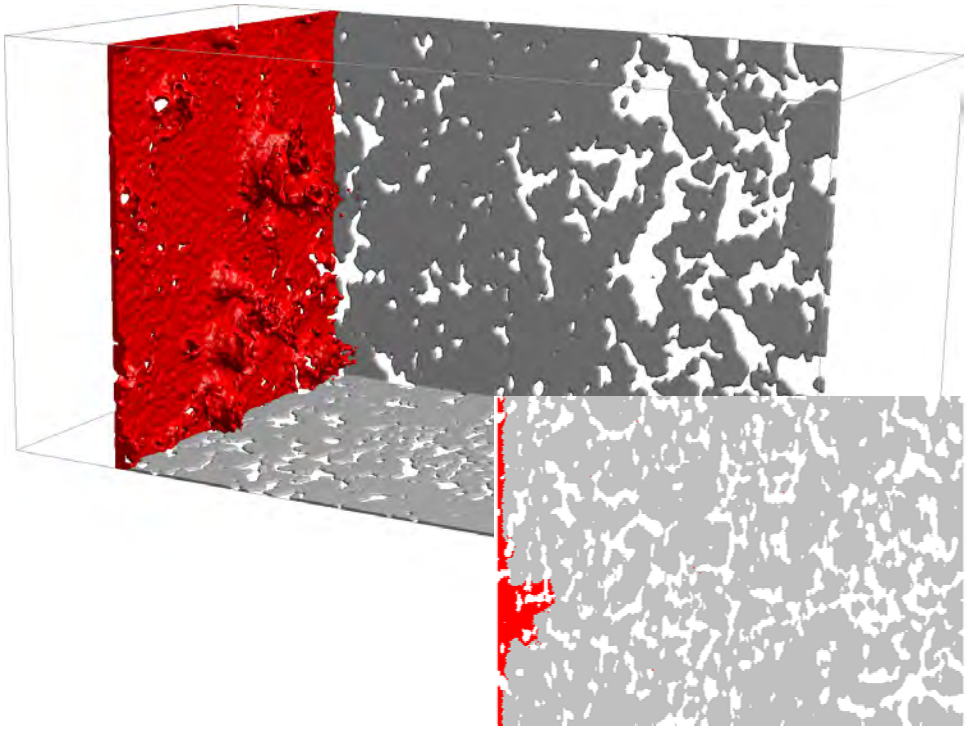
MATH 2 MARKET

Dissolution pattern – Face dissolution

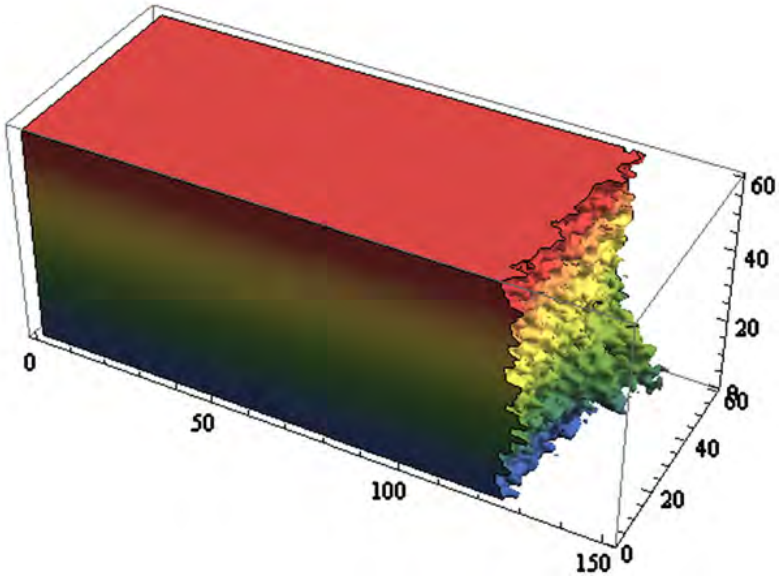
Simulation settings:
Domain: 256x256x512 voxel
Runtime: 50 h
Average velocity: 0.001 m/s
pH value: 3.2
Simulation time: 700s
Number of particles: ~2000



Comparison face dissolution pattern

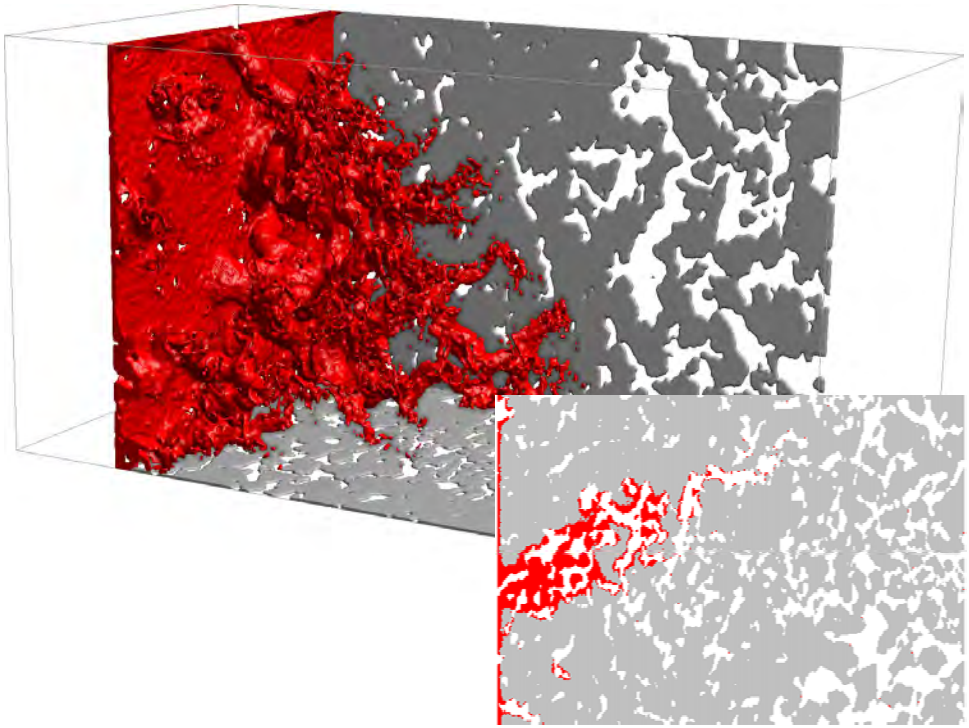


GeoDict simulation

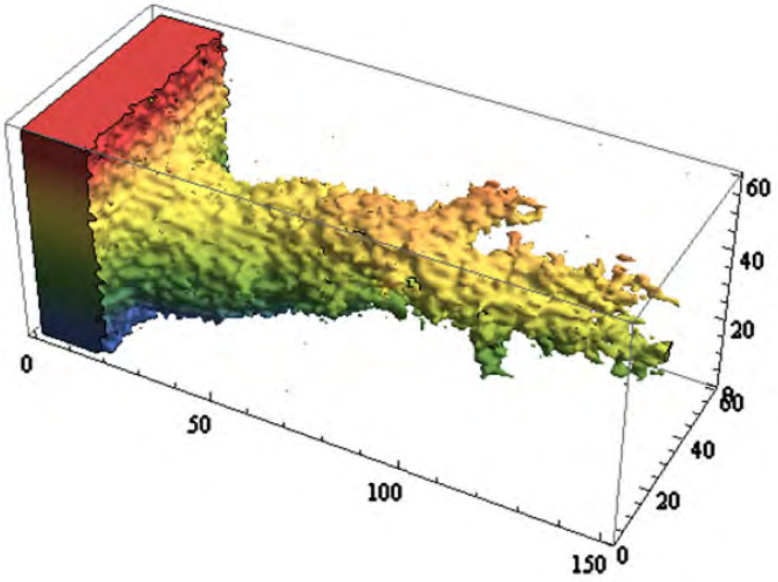


Maheshwari et al. 2013

Comparison Conical Wormhole pattern

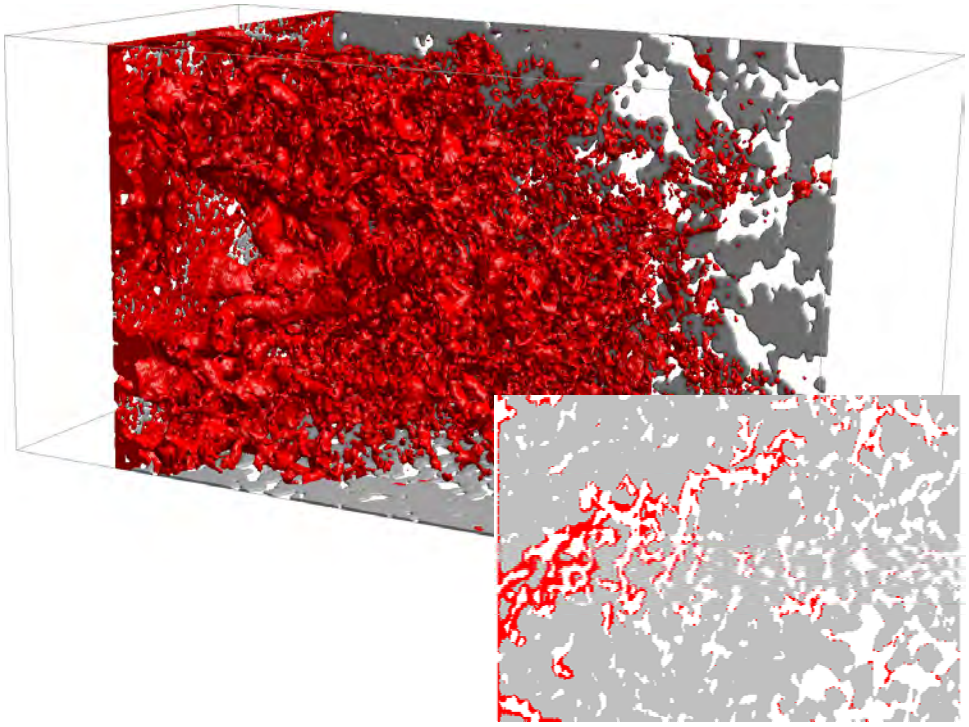


GeoDict simulation

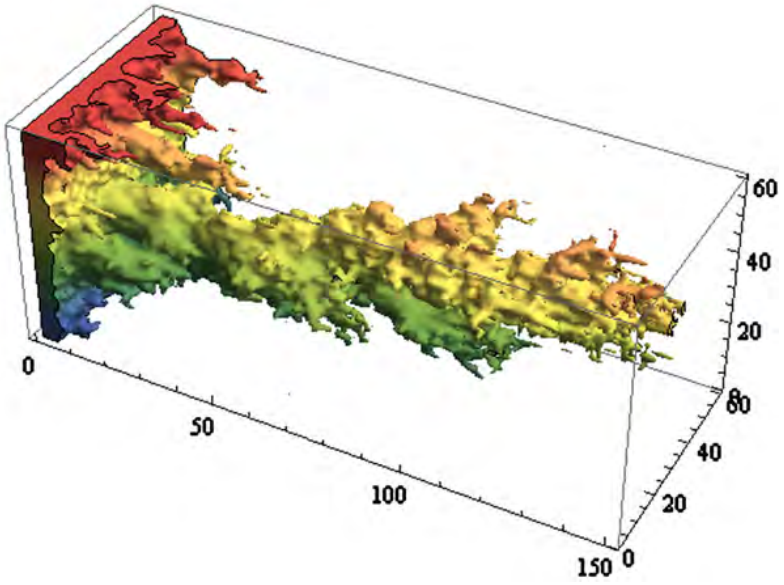


Maheshwari et al. 2013

Comparison Wormhole pattern

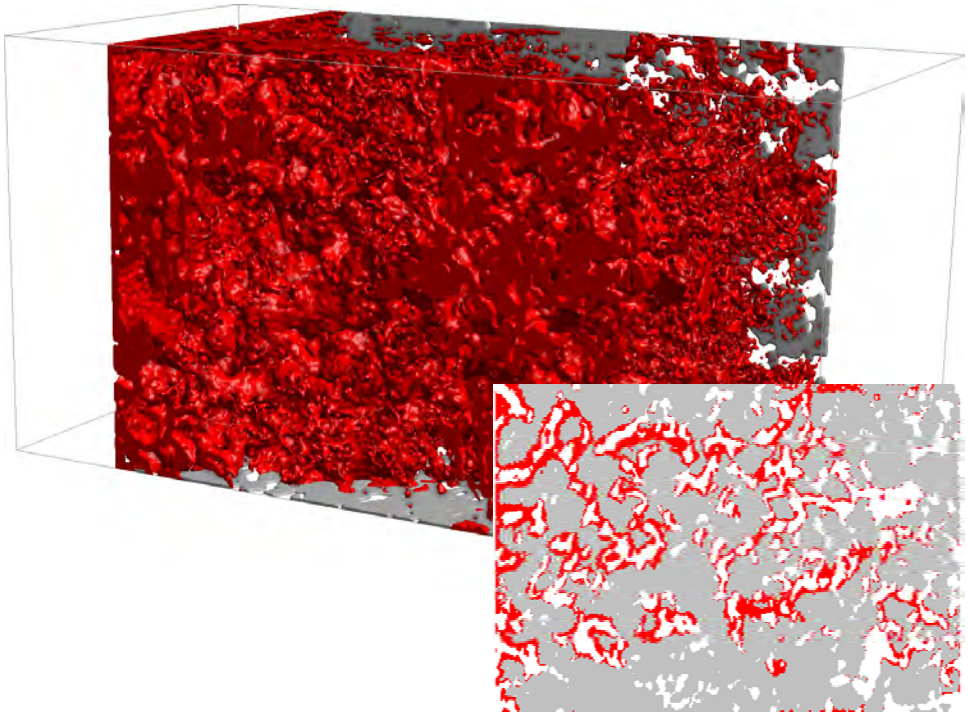


GeoDict simulation

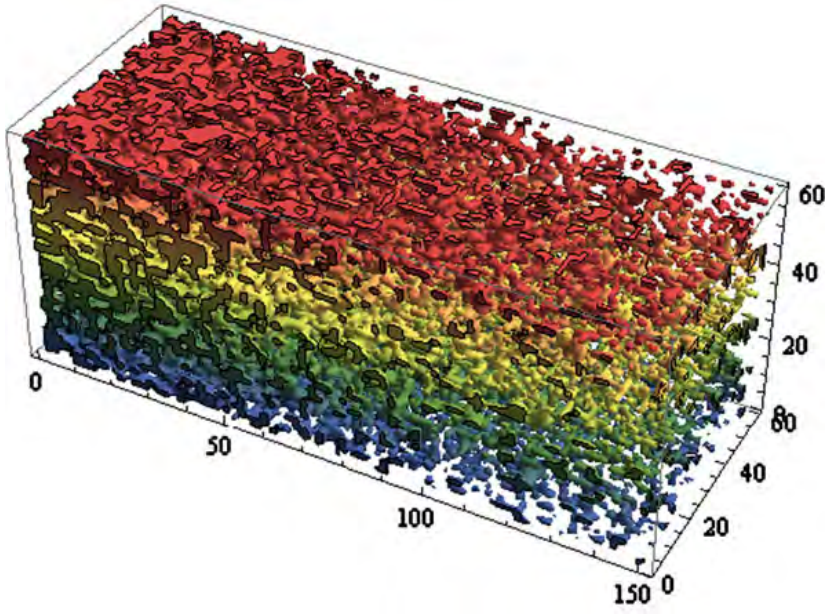


Maheshwari et al. 2013

Comparison uniform dissolution pattern

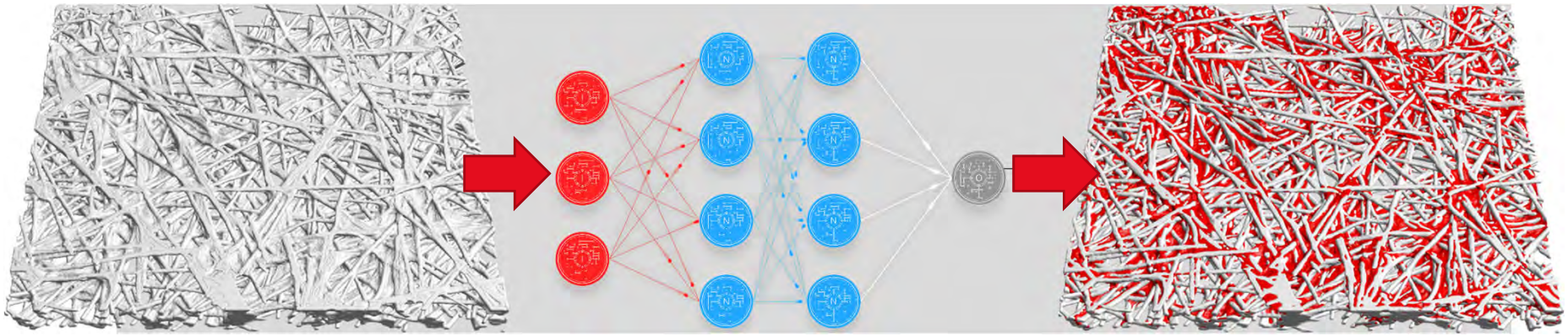


GeoDict simulation



Maheshwari et al. 2013

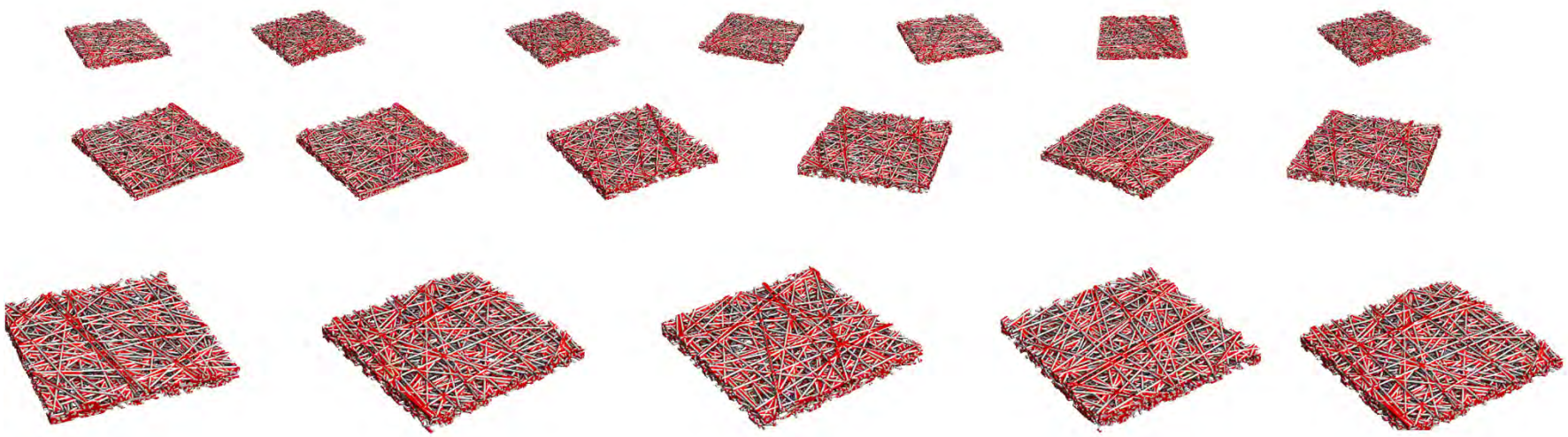
Machine Learning-based Binder identification



- Training phase: neural network sees input and output image pairs
  - input: segmented black&white image
  - output: same image but with binder and fibers distinguished (labeled)
  - network learns to transform input to output images
- Application phase:
  - network transforms segmented µCT data into labeled output image

SYNTHETIC TRAINING DATA GENERATION

MATH
2 MARKET

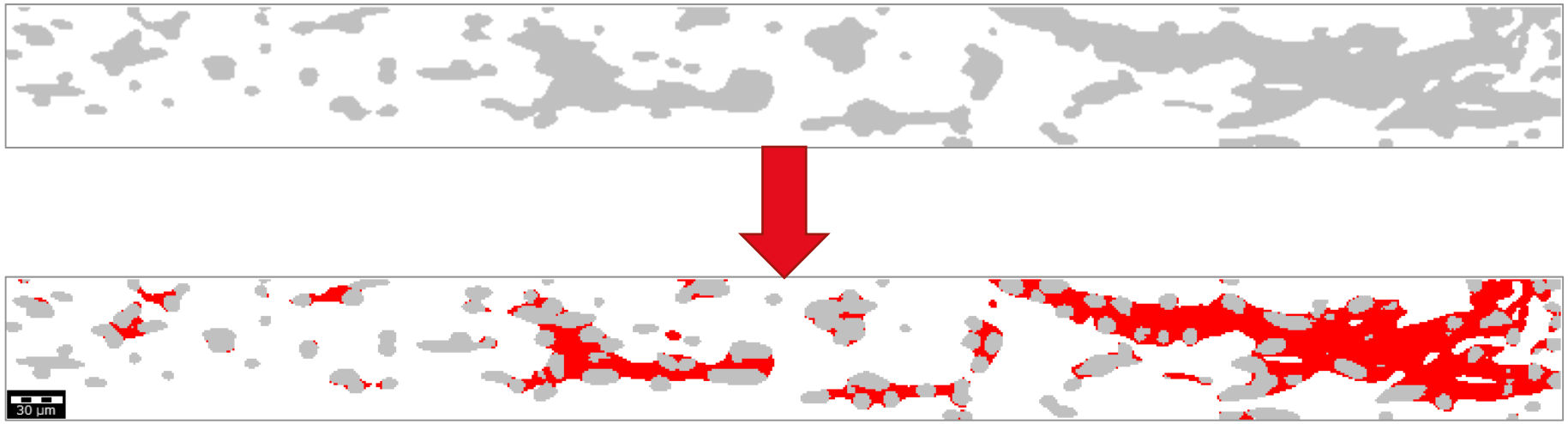


- modeled 18 GDL structures (512x512x256 voxels each) as training data
- varied porosity and binder volume fraction
- corresponds to ~800 million solid voxels as training data points

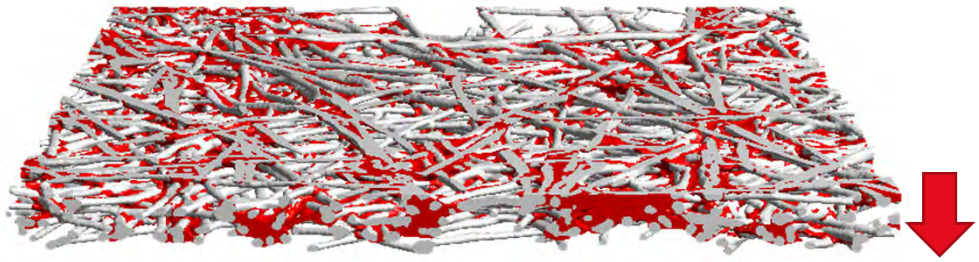
Binder identification in Gas Diffusion Layer

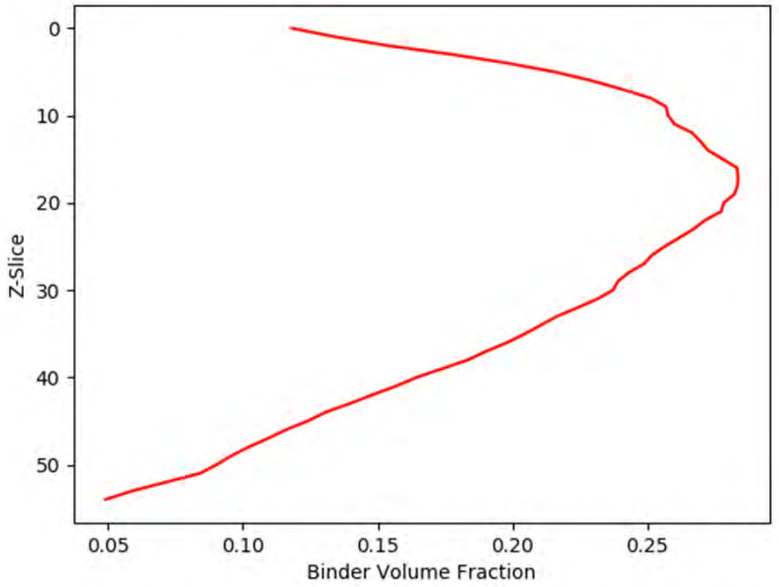
MATH 2 MARKET

Cross-section in X-Direction:



Binder Distribution in through (Z) direction (MatDict)





- In production, binder is applied to the top of the paper and, then, intrudes into deeper layers
- After labelling binder voxels, we can compute the distribution of binder in through direction (right)