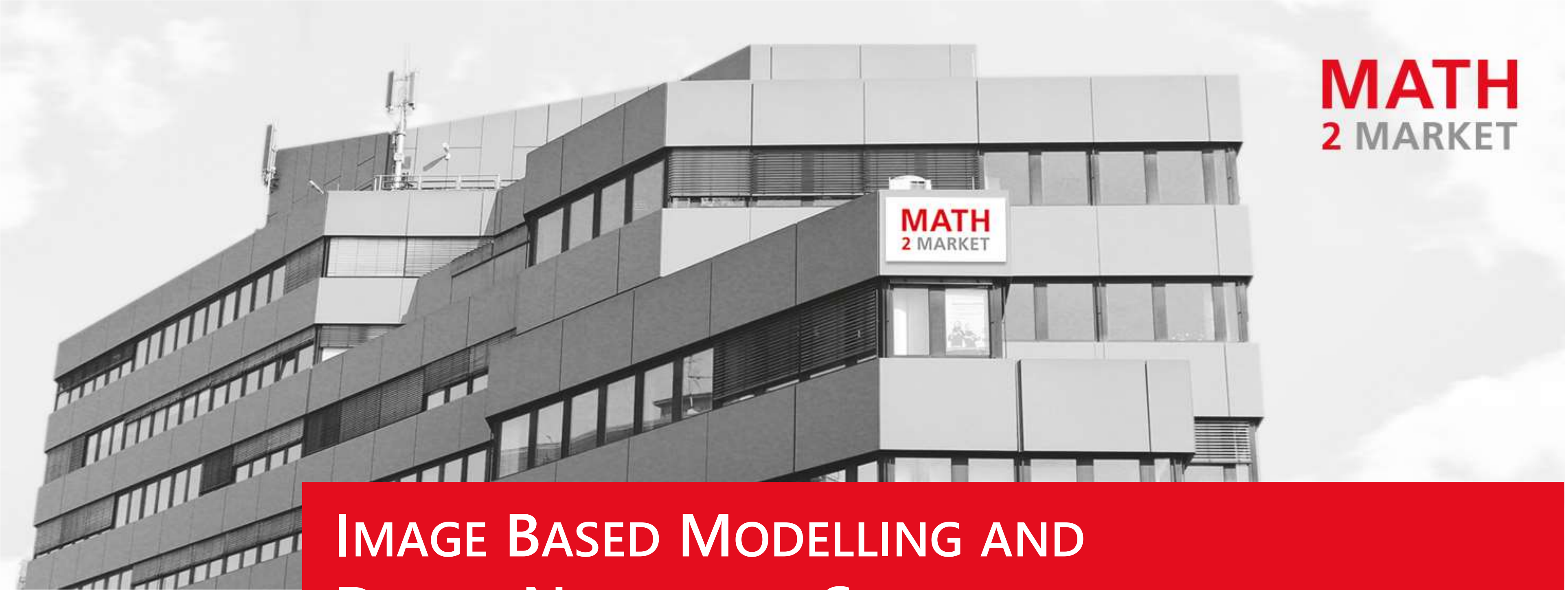


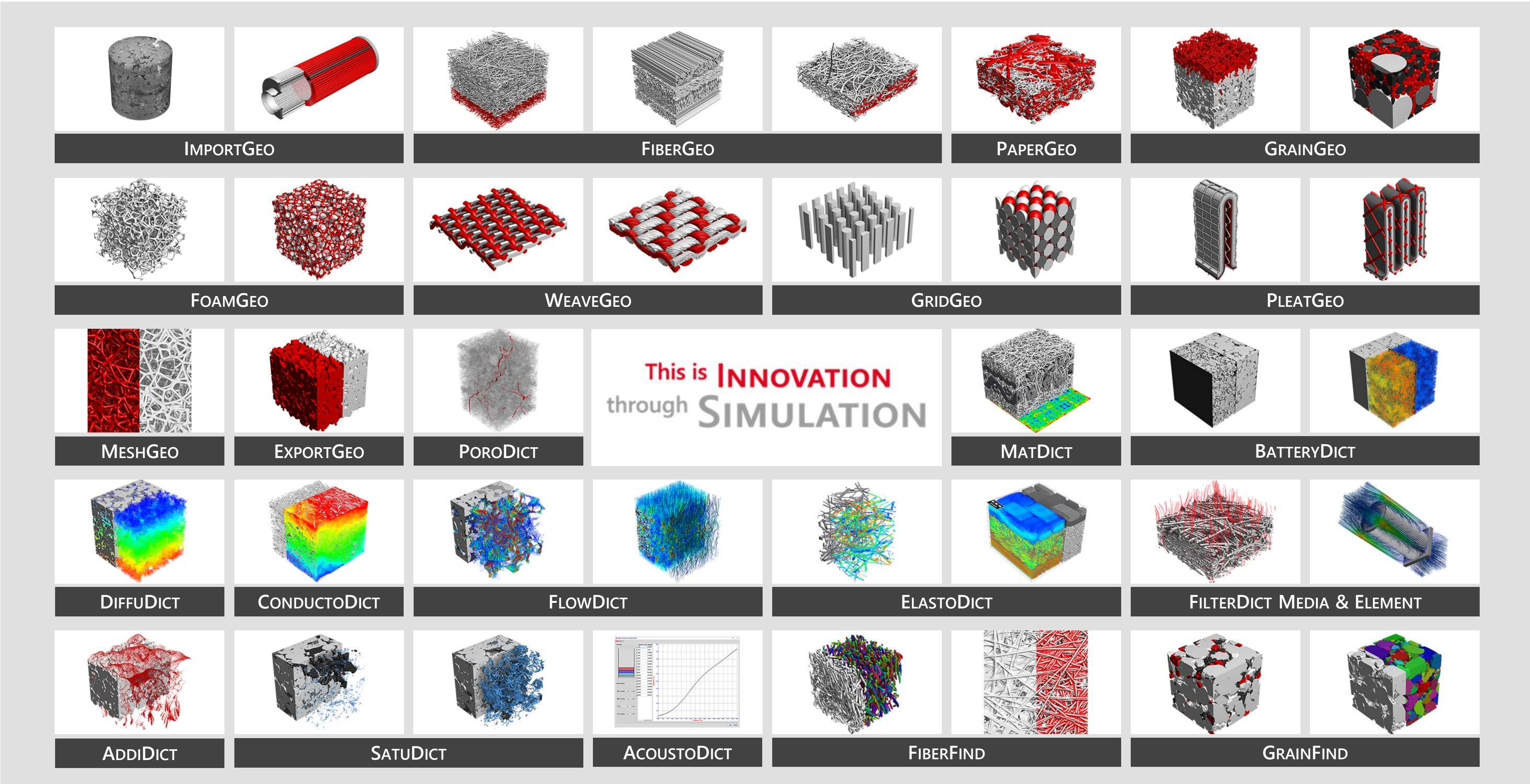

# Image Based Modelling and Direct Numerical Simulations with GeoDict, the Digital Material Laboratory

**IBFEM-4i**

Swansea, September 12th, 2019

Andreas Wiegmann

# GeoDict® Module Overview



# GeoDict® Solutions for ...

| | |
|---|---|
| Filtration | For a clean environment |
| Electrochemistry | For electromobility |
| Structural materials | For lightweight applications |
| Digital Rock Physics | For efficient energy production |

# Distributors Worldwide

MATH
2 MARKET

| BRAZIL | GERMANY | SOUTH KOREA | CHINA | JAPAN |
| --- | --- | --- | --- | --- |
| TENNESSINE Instrumentação Analítica | MATH 2 MARKET | TRINITY Engineering Co., Ltd. | FLight 晶飞科技<br>PAN-i 磐翼信息科技(上海)有限公司 | SCSK |

# Selected Clients of a total of ~150 clients

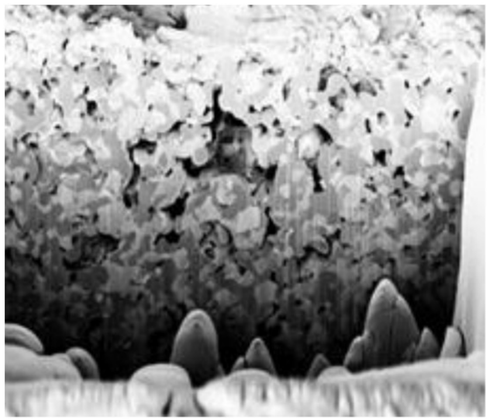
MATH 2 MARKET

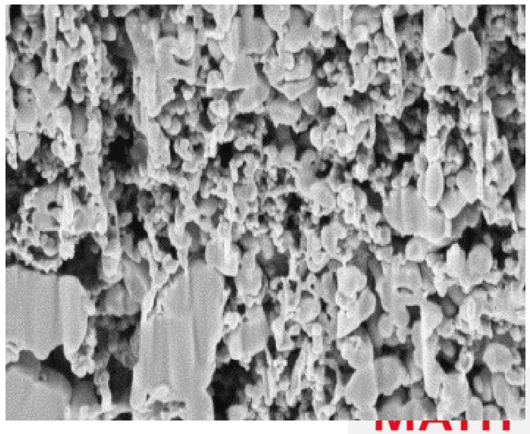
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Shell | Opel – Wir leben Autos. | GKD – World Wide Weave | Bosch | TU Clausthal | Haver & Boecker | IMTEK | Voith |
| Freudenberg – Innovating Together | Toyota | Volkswagen Aktiengesellschaft | Mann+Hummel | Croft Additive Manufacturing | NASA | Jülich Forschungszentrum | Toray |
| ETH – Eidgenössische Technische Hochschule Zürich, Swiss Federal Institute of Technology Zurich | PF | Zeiss | NRC-CNRC – From Discovery to Innovation… | Purdue University | BASF – We create chemistry | JRC – European Commission | UNSW Sydney |
| Fleetguard | Fraunhofer | DHBW – Duale Hochschule Baden-Württemberg | DLR | Huyck.Wangner | Johannes Gutenberg Universität Mainz | RWTH Aachen University | NTNU – Norwegian University of Science and Technology |
| Bulgarian Academy of Sciences 1869 | Chalmers | TTRI – Taiwan Textile Research Institute | The University of Texas at Austin | cea | Indian Institute of Technology | Paul Scherrer Institut – PSI | The Nonwovens Institute |
| Uppsala Universitet | Universitas Bergensis | KIT – Karlsruher Institut für Technologie | Technische Universität Kaiserslautern | Université Joseph Fourier Grenoble | KAUST | Universität des Saarlandes | 九州大学 Kyushu University |

# Typical Artifacts



- Image Alignment
- Brightness
  - changes in cutting direction and in single images
  - Curtaining-effect / streaking, sensor dependent
  - Local charging leads to local change in brightness
- Non-invaded pores after resin infiltration

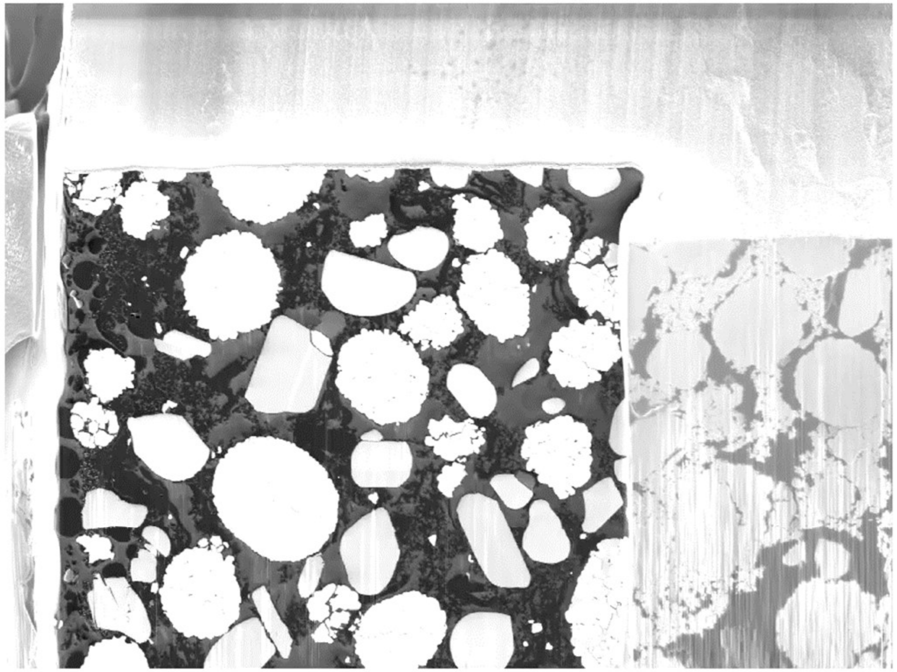


# FIB-SEM IMAGE ALIGNMENT

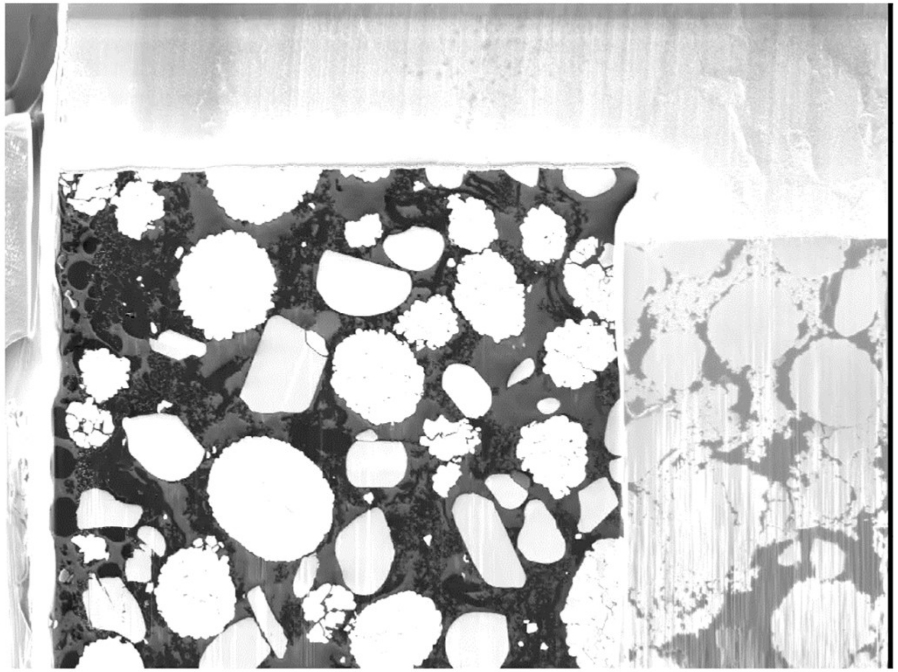
GeoDict

**Image Stack Alignement - Aligned by Region**

Unaligned image stack, image #1



Aligned image stack, image #1





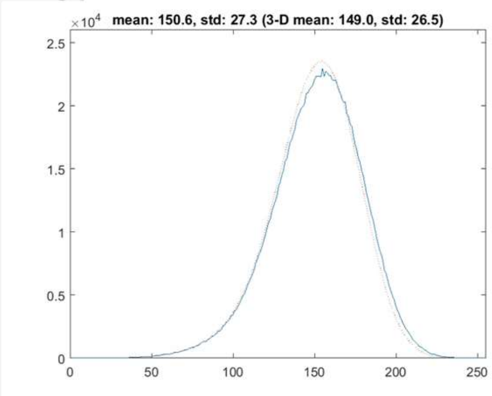


MATH 2 MARKET

# NANO-CT GRAY-VALUE CORRECTION

GEODICT

- Images can have changes in brightness
- Can be adjusted for each direction, x-, y-, and z-
- Can be beneficial in other use cases as well
  - Here: brightness correction of a nanoCT scan

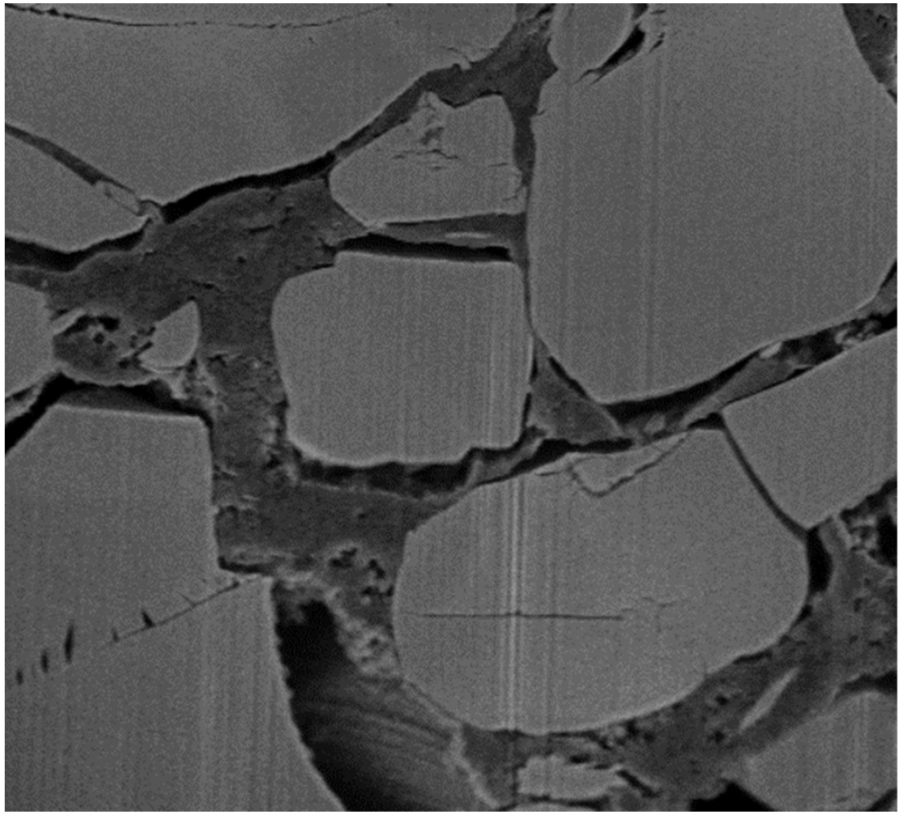





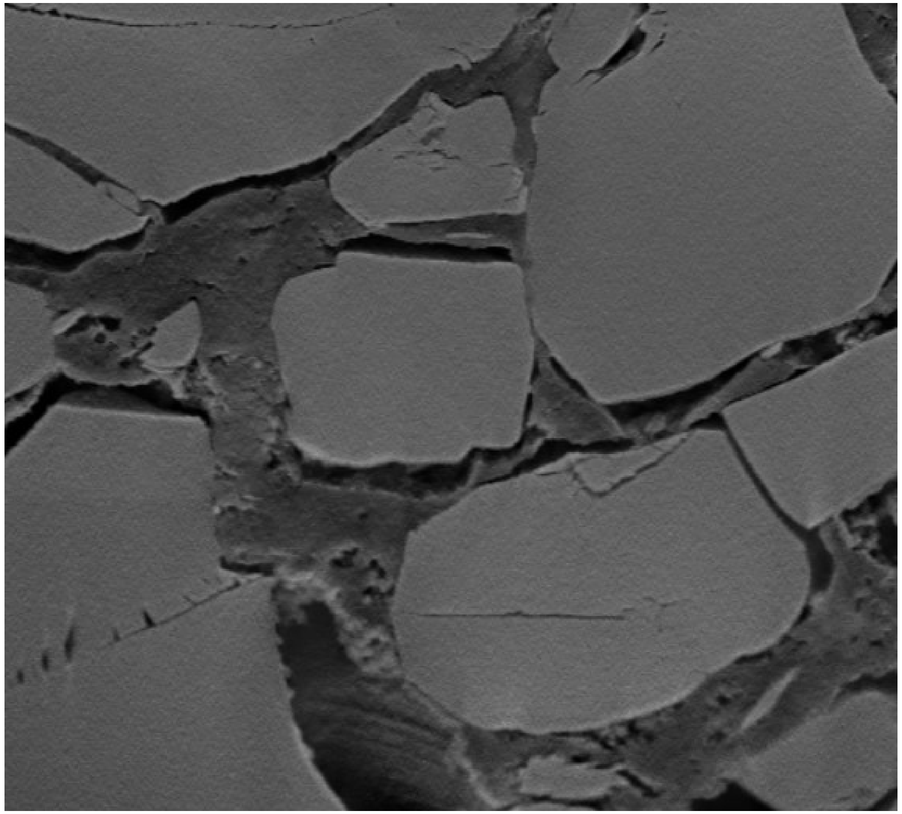

MATH 2 MARKET

# Curtain Filter



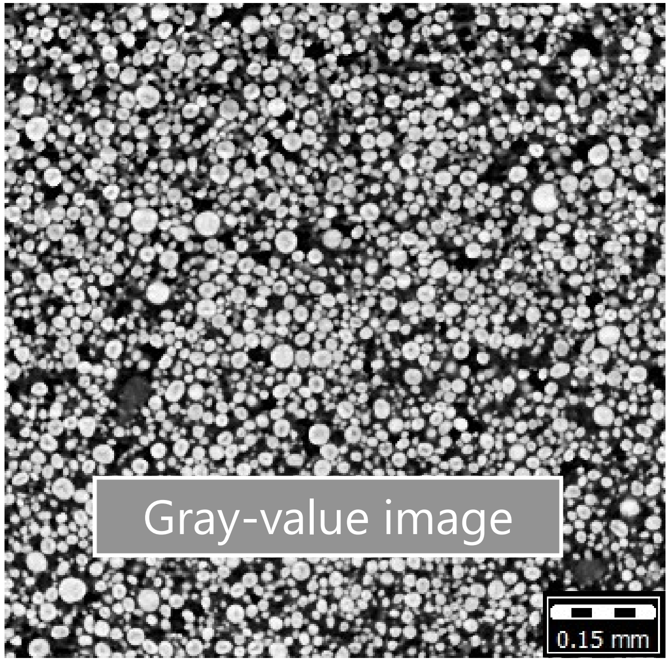


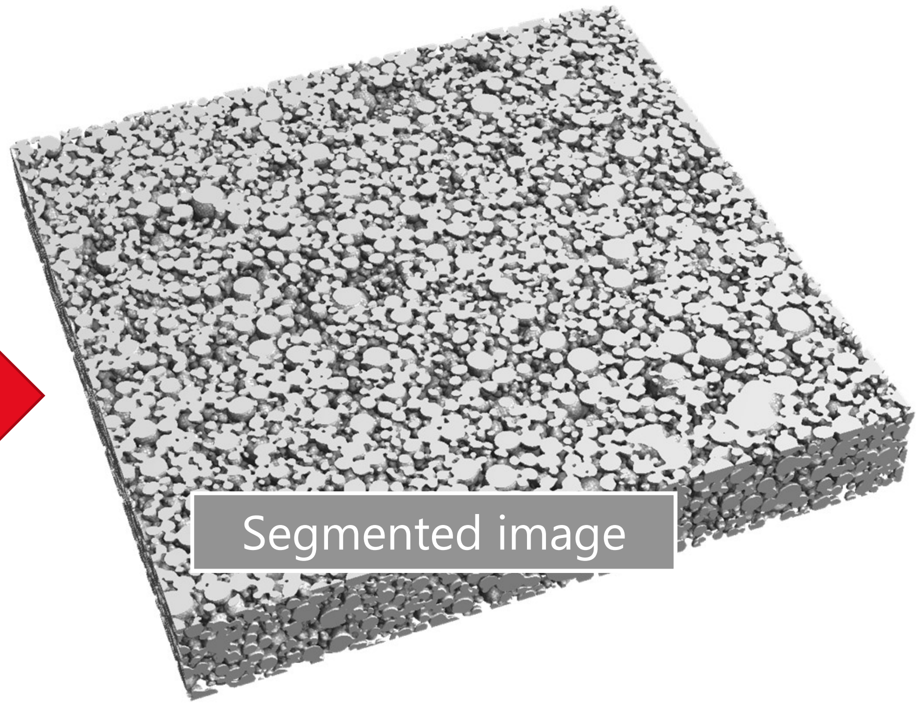
Original
SEM



SEM
after applying the curtain filter

# IMPORTGEO

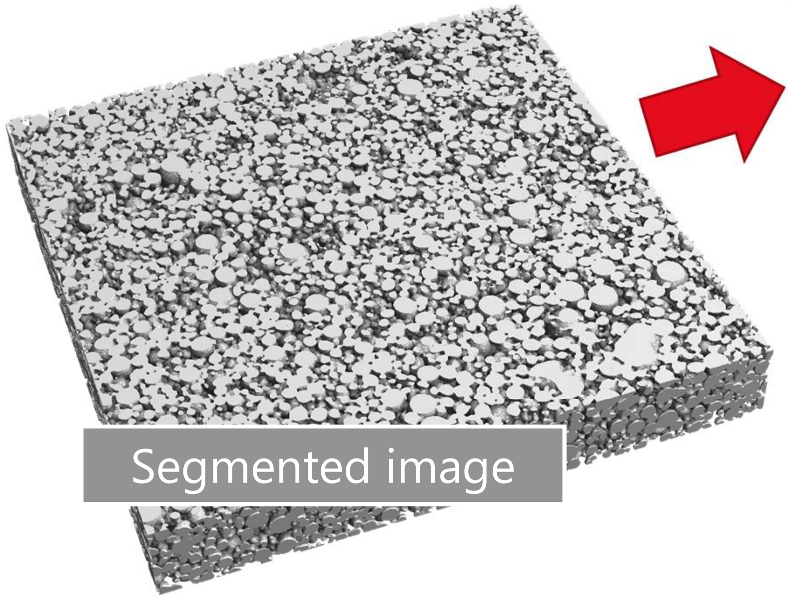


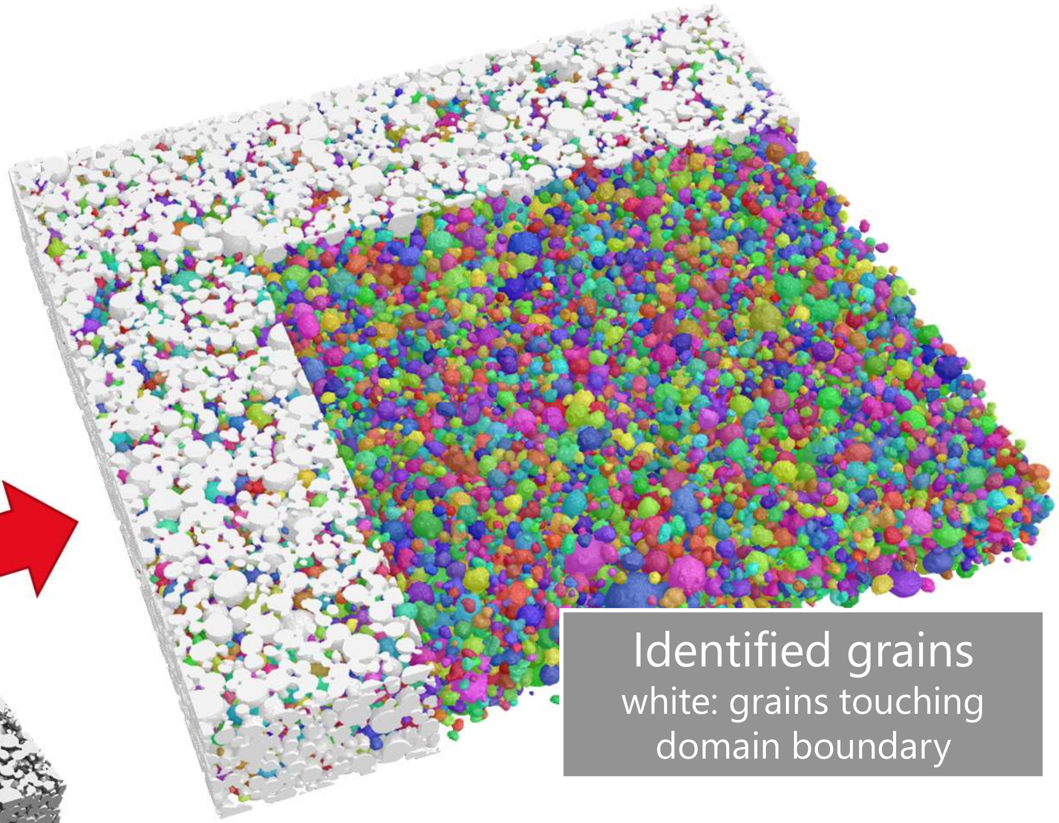




Applied Filters:

- Non-Local Means Filter
- Sharpen Filter

# GRAINFIND

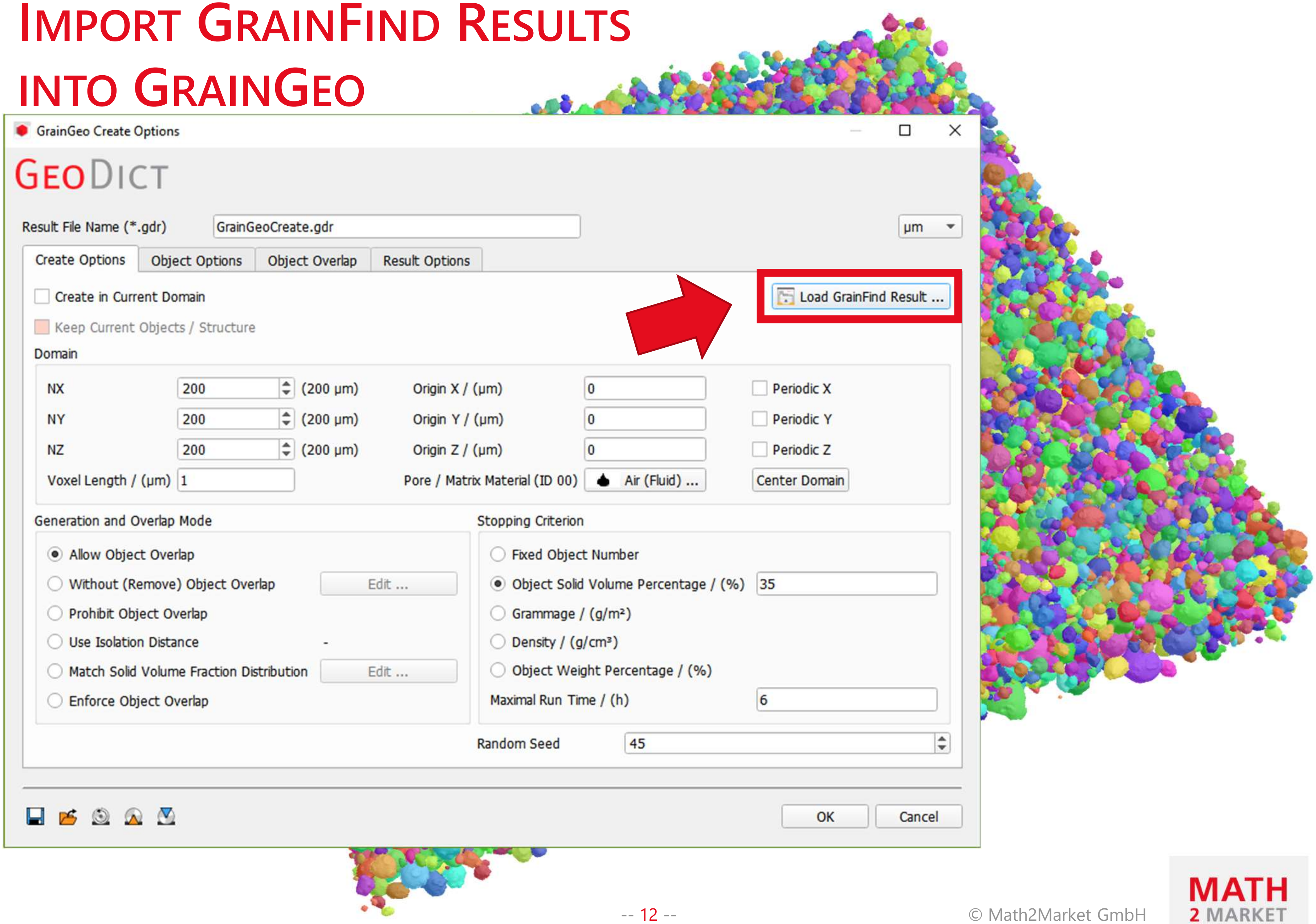



- Identified grains using specialized watershed and subsequent grain reconnection.
- Removed grains at the domain boundary

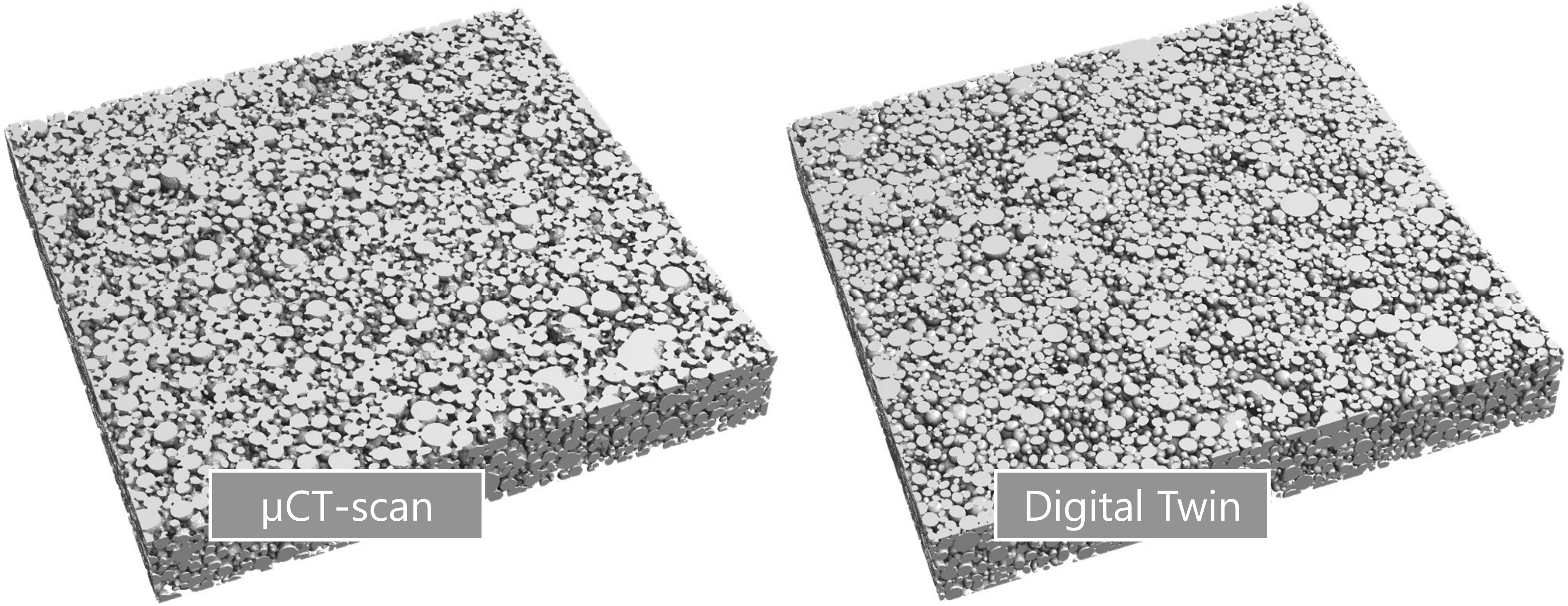
## Statistical twin using GrainGeo

# Import GrainFind Results into GrainGeo



# GRAINGEO

GEODICT



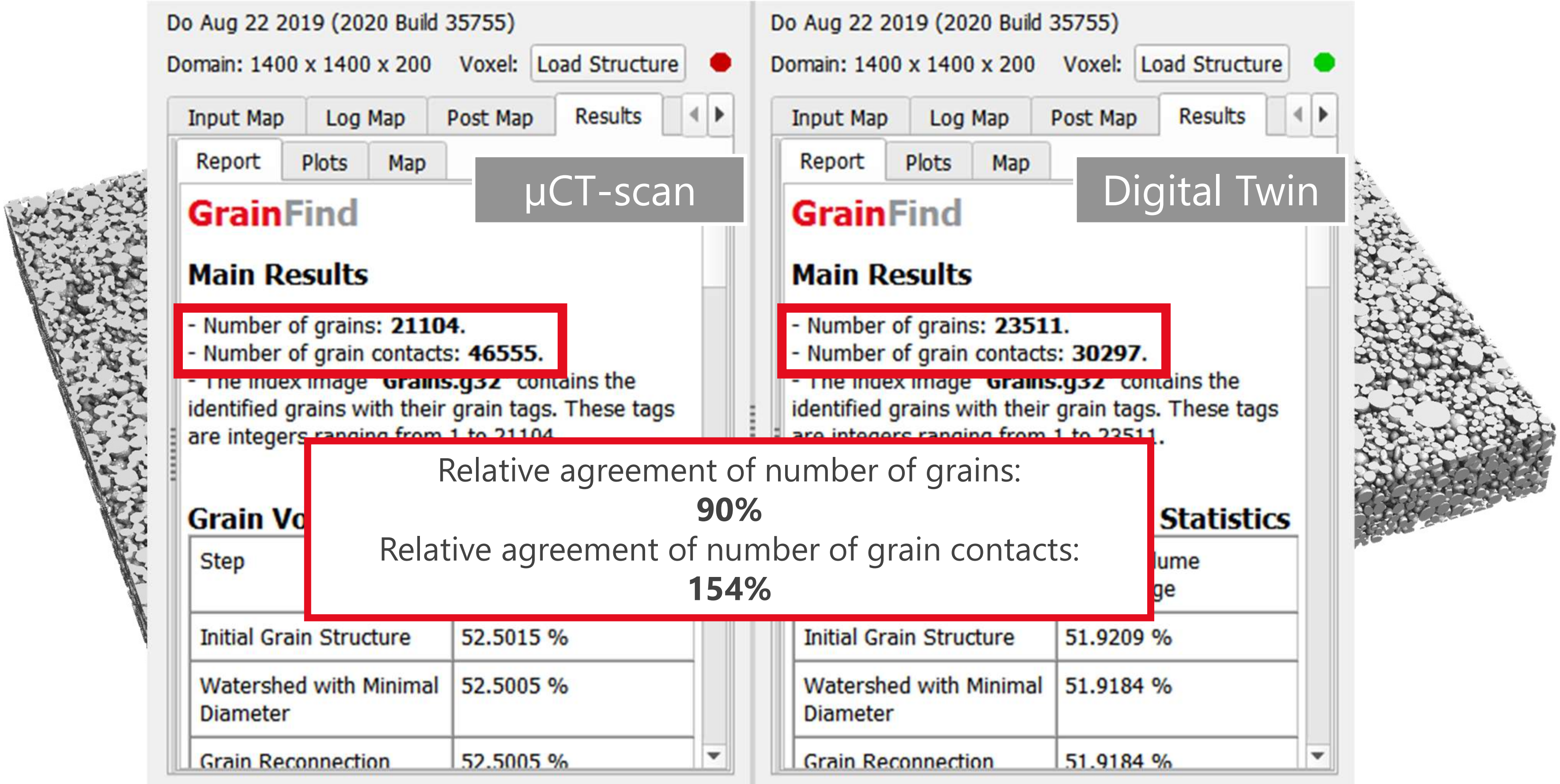

- Used GrainGeo's "Create Grains"
- Visual comparison is good



MATH 2 MARKET

# COMPARISON OF STATISTICS

GEODICT




- Used GrainGeo's "Create Grains"
- Visual comparison is good
- However, statistics do not match perfectly

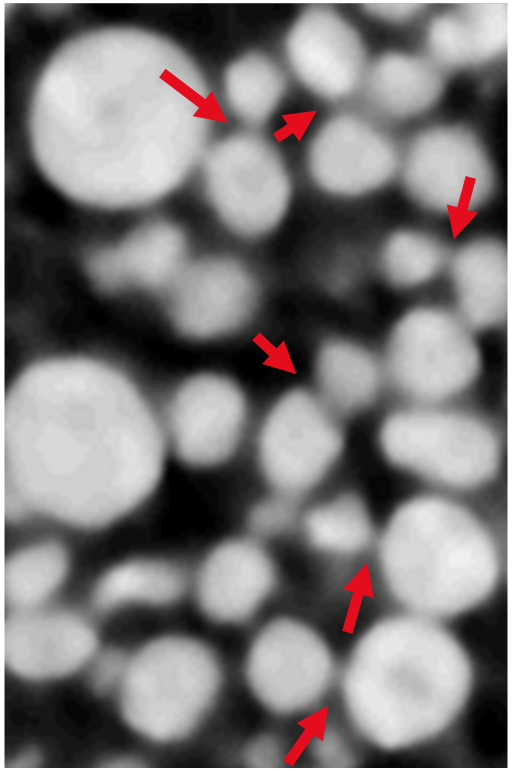




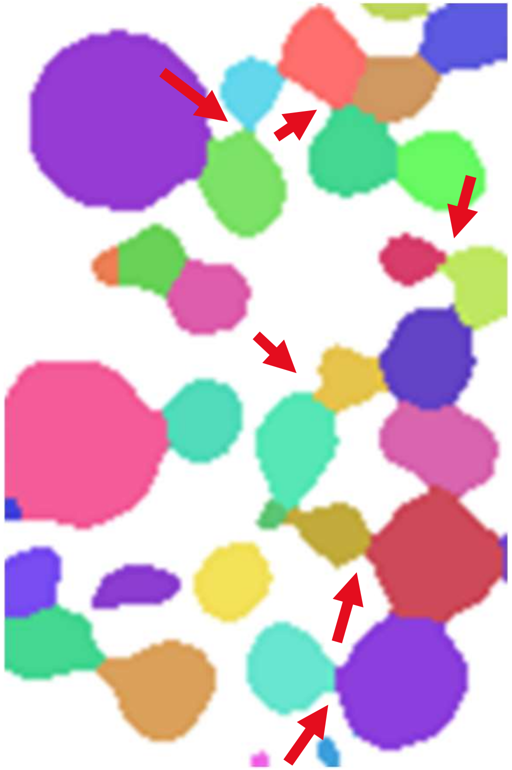
MATH 2 MARKET

# GRAINGEO: ADD BINDER!

GEODICT



Slice from



Slice from Grain Identification





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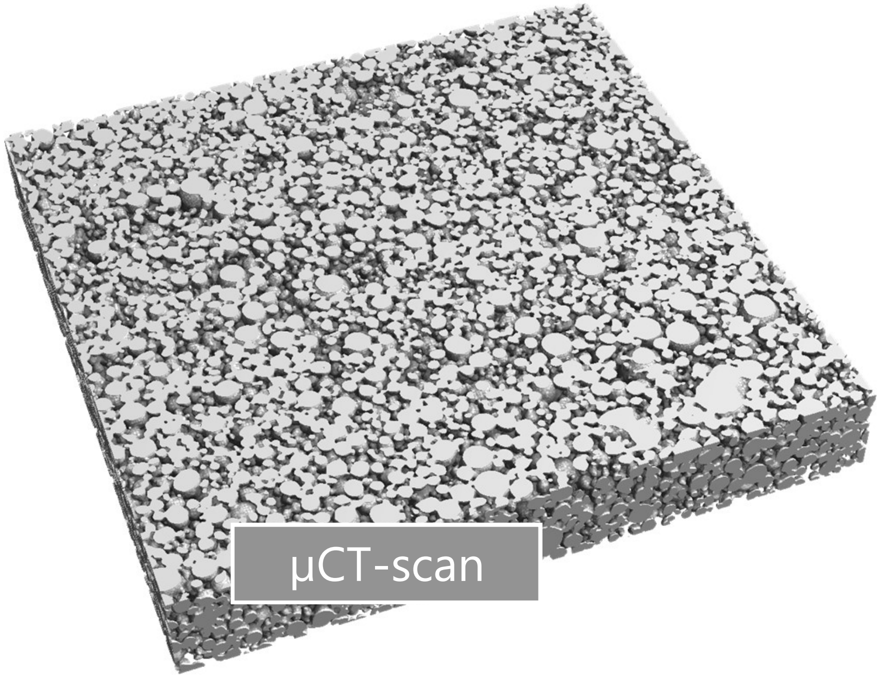
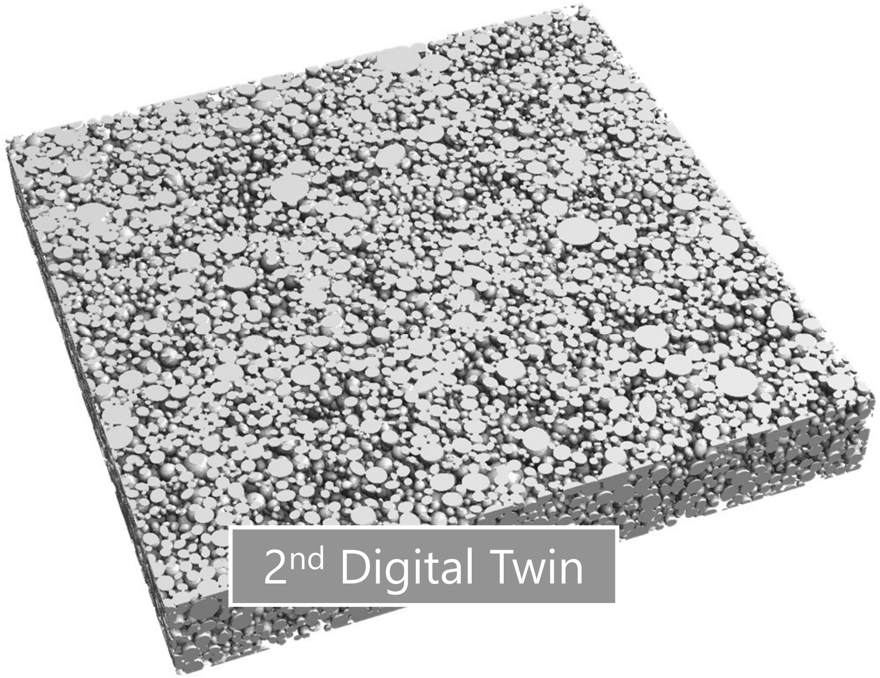
# Visual Comparison

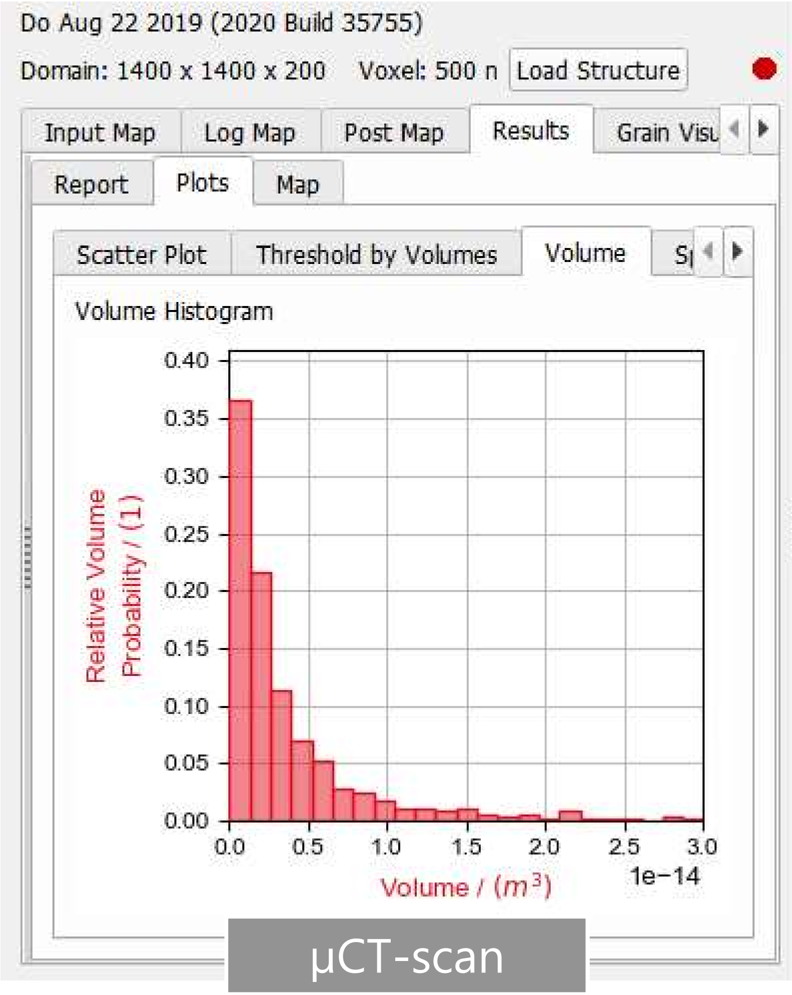


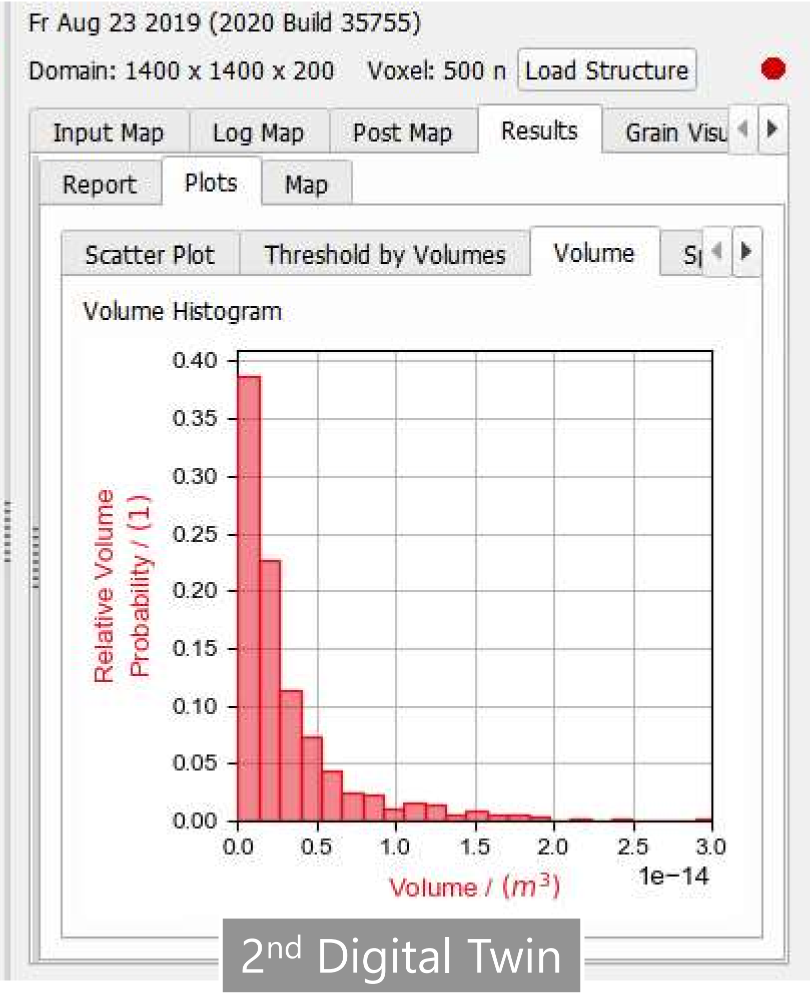




- Used GrainGeo's "Create Grains" and GrainGeo's "Add Binder"
- Visual comparison is good

# COMPARISON PLOTS

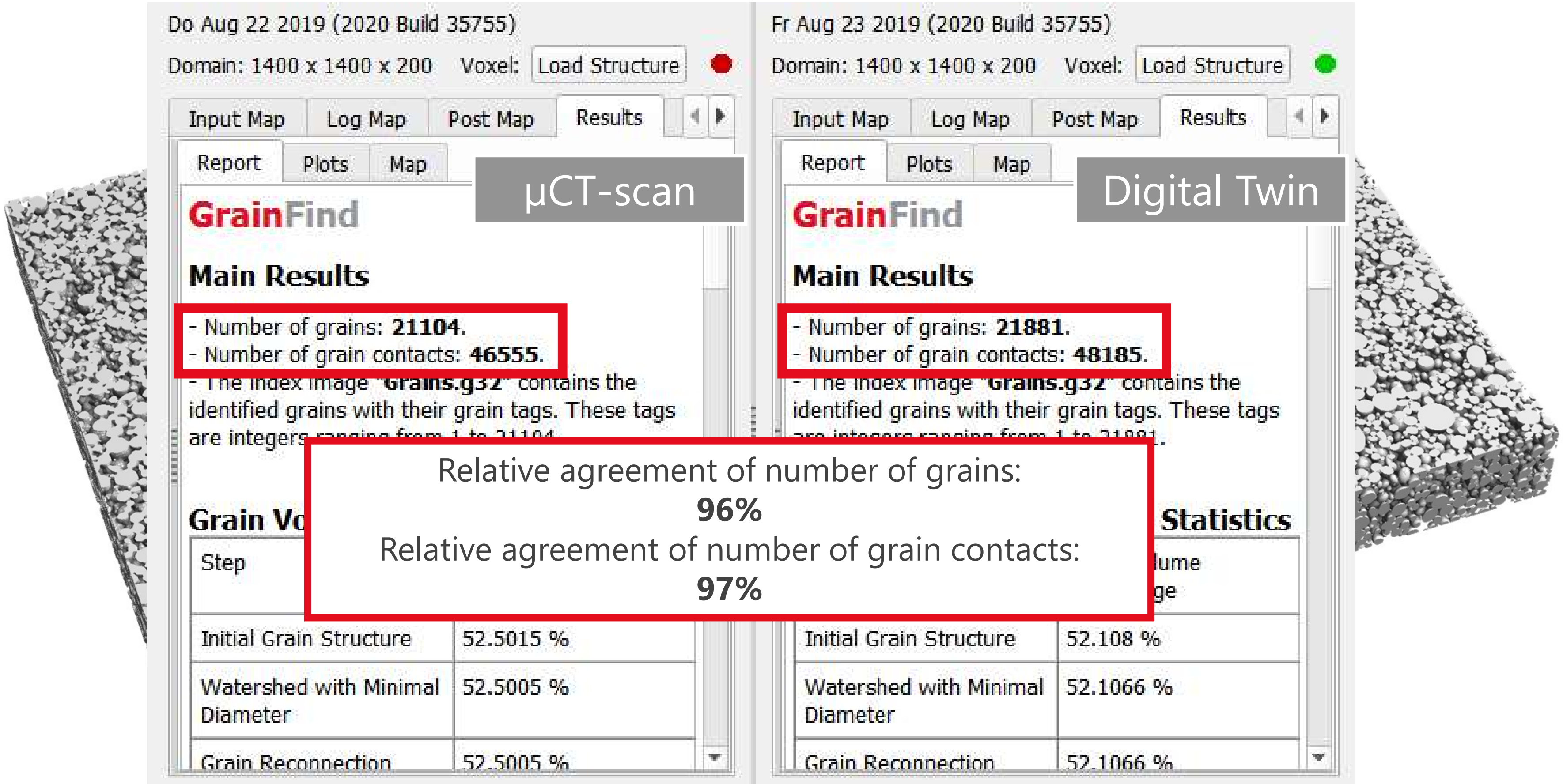




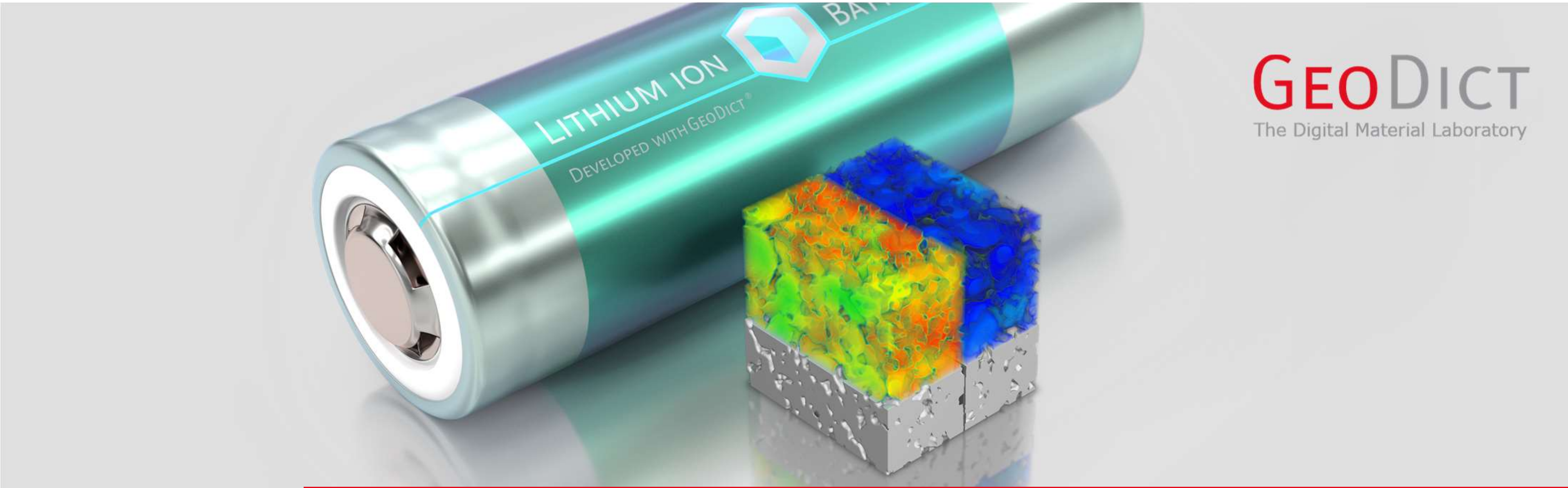



# VISUAL COMPARISON






- Used GrainGeo's "Create Grains" and GrainGeo's "Add Binder"
- Visual comparison is good
- Statistics match nicely




# DIGITAL BATTERY DEVELOPMENT

## Solutions with GeoDict®

**Dr. Ilona Glatt**, Dr. Mathias Fingerle, Dr. Fabian Biebl, Sebastian Rief, Franziska Arnold, Steffen Schwichow, Dr. Barbara Planas



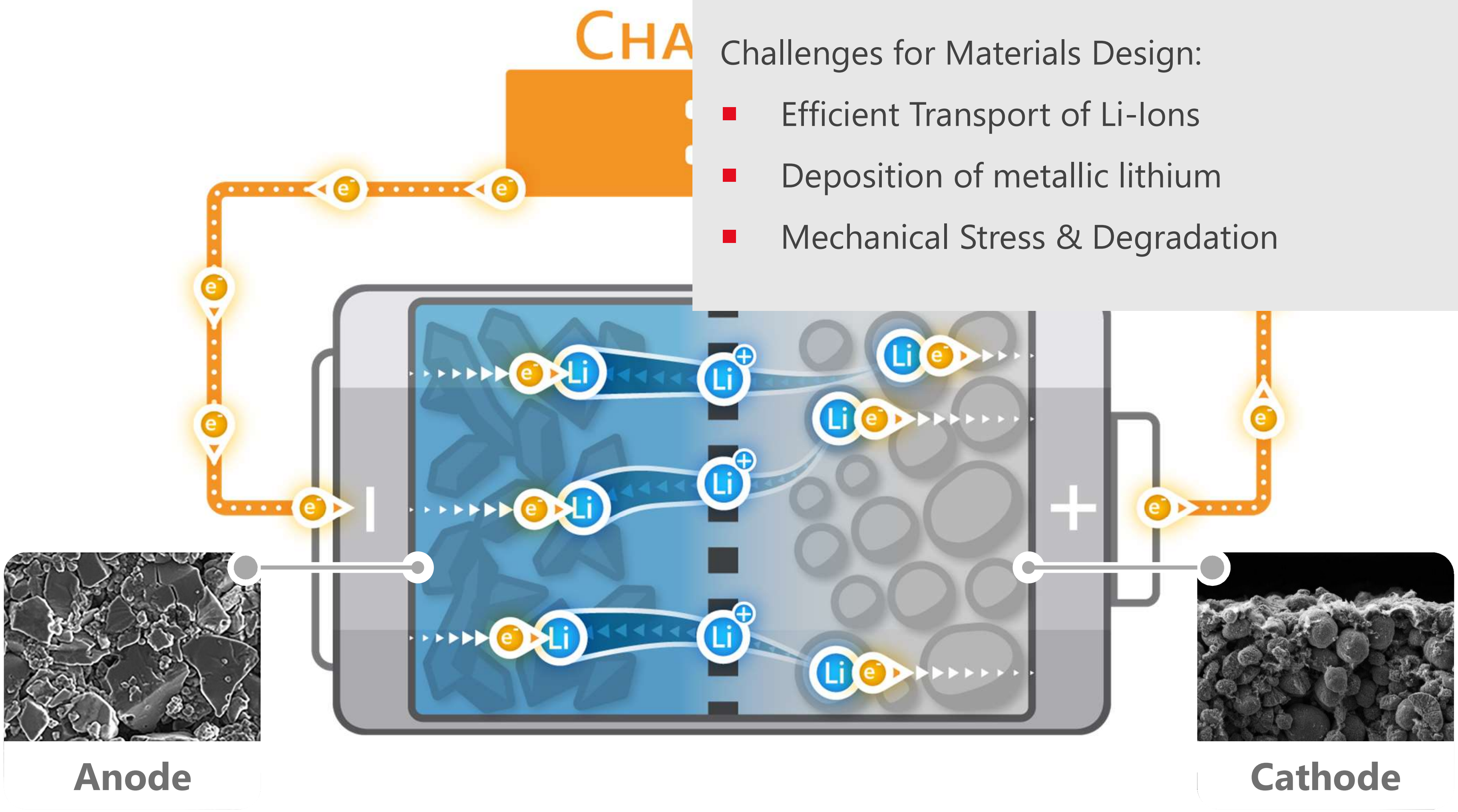
MATH 2 MARKET

# Li-Ion Battery

GeoDict

Challenges for Materials Design:

- Efficient Transport of Li-Ions
- Deposition of metallic lithium
- Mechanical Stress & Degradation






MATH 2 MARKET

# Microstructure of a Li-Ion – Cathode

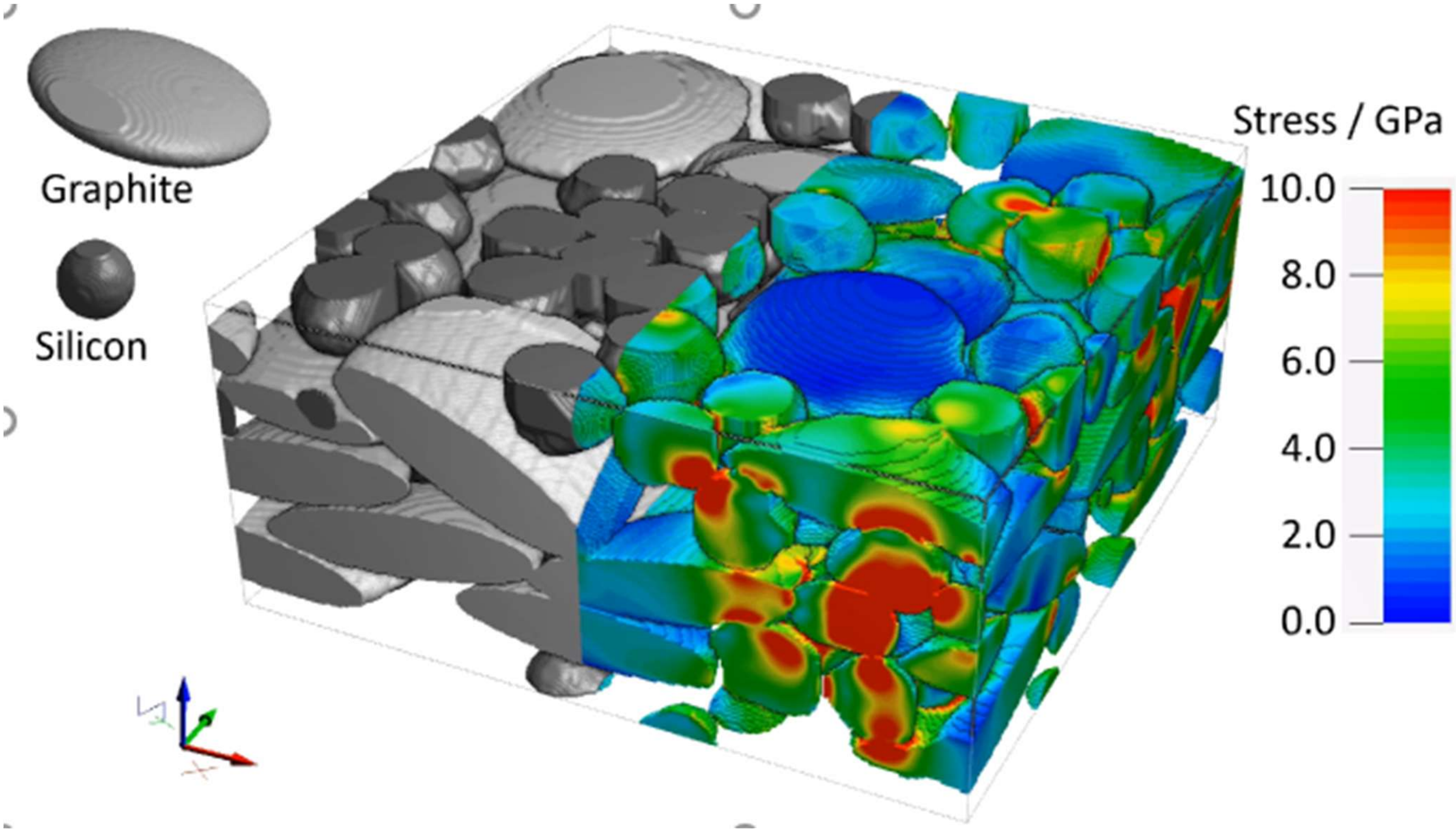
GeoDict

Scan and segmentation: by courtesy of J. Joos, KIT

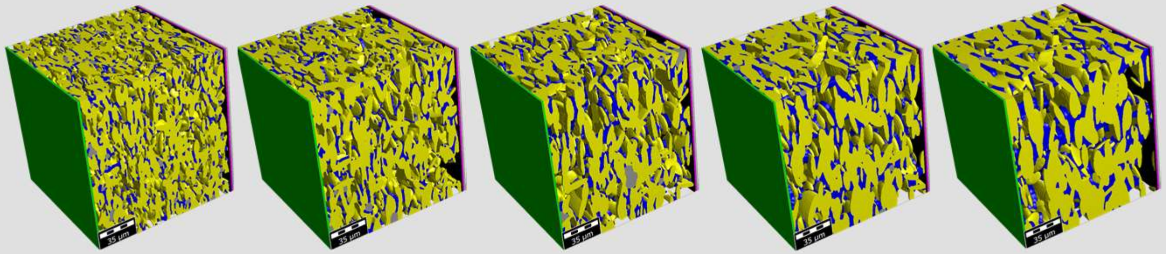
LiFePO$_4$ Cathode

MATH 2 MARKET

# Particle Expansion due to Li-Intercalation

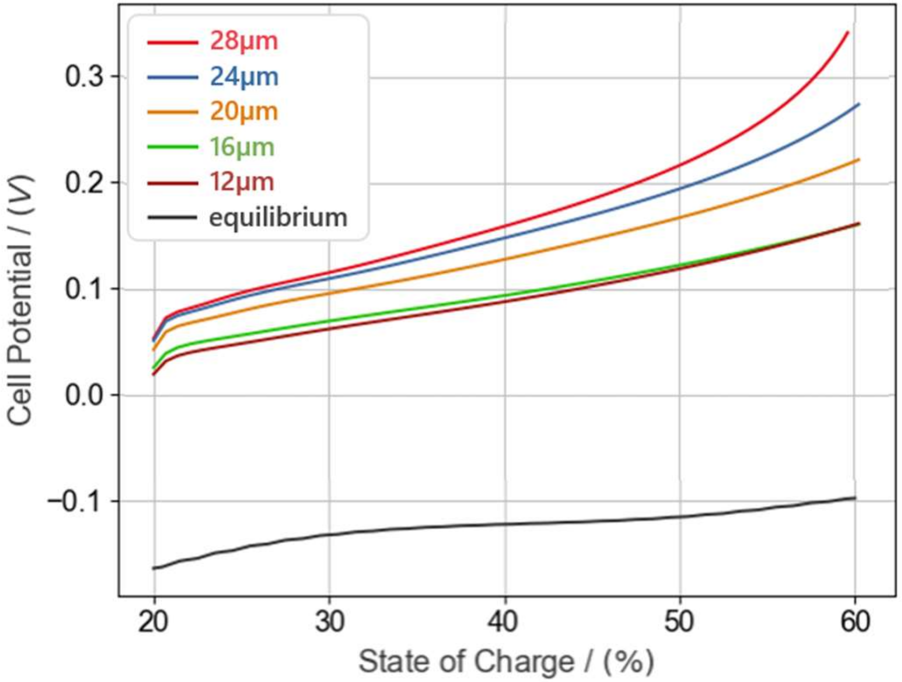


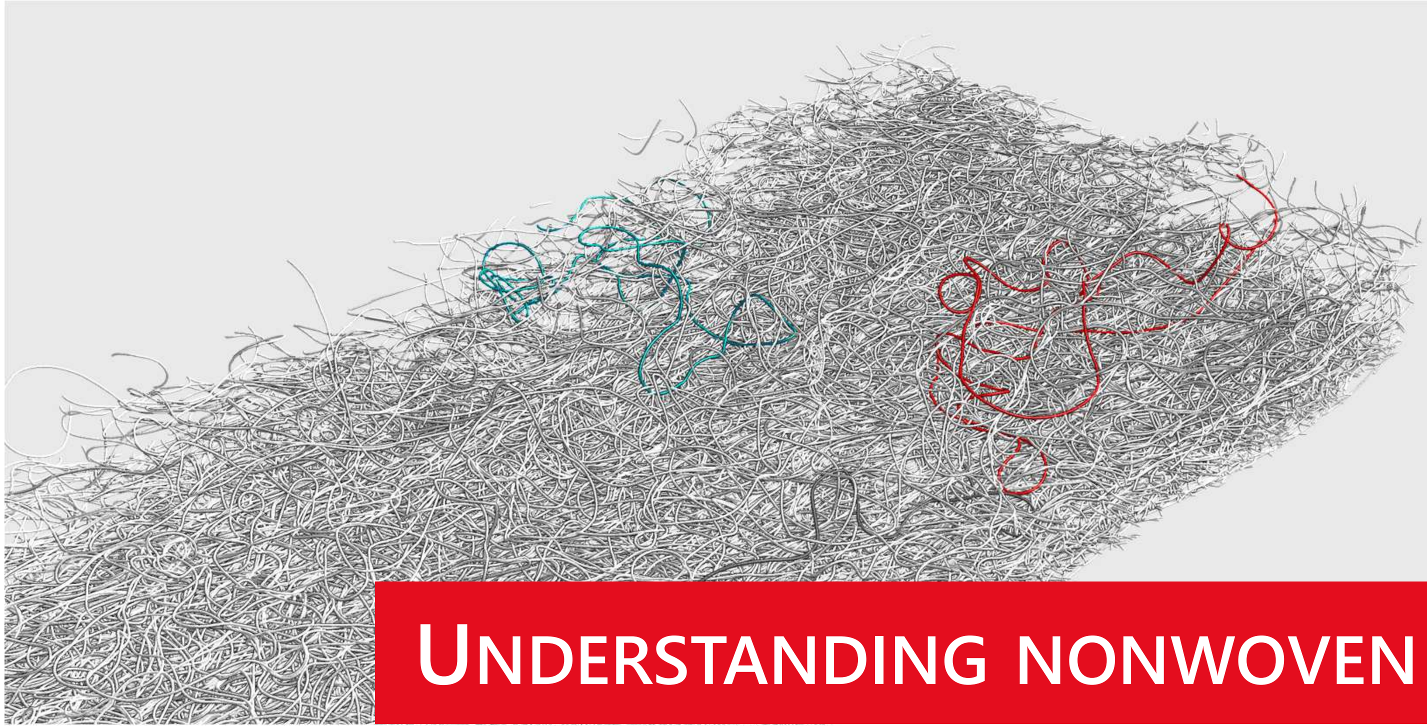
# INFLUENCE OF ANODE GRAIN SIZE:
# BATTERYDICT HALF-CELL SIMULATION



Largest Diameter: 12µm 16µm 20µm 24µm 28µm

- Charging of an anode with different grain sizes
- Identical porosity, amount of connected active material and electrolyte
- At 2.5 C, charging gets harder with larger particles





GEODICT
The Digital Material Laboratory

# UNDERSTANDING NONWOVEN

## Analysis of µCT scans of nonwoven samples

Andreas Grießer, Rolf Westerteiger, Steffen Schwichow, Andreas Wiegmann, Math2Market

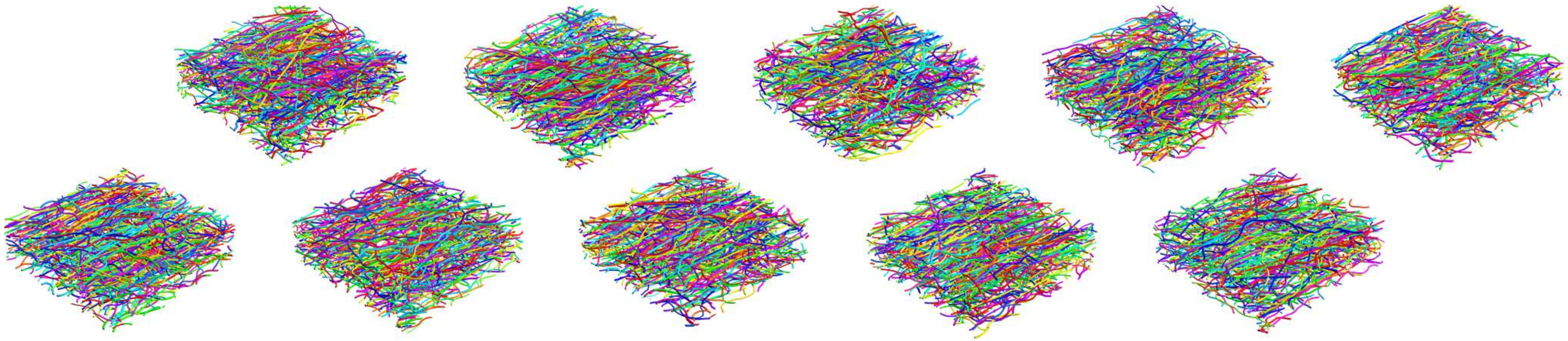
Wesley DeBoever, Bruker µCT



MATH 2 MARKET

# DIGITAL TWINS PROVIDE GROUND TRUTH

GEODICT



**Training Data: Use GeoDict's unique fiber modelling capabilities:**

- Modeled 10 Digital siblings (512x512x256 Voxels) as training data
- Varied fiber curvature, orientation, length and diameter
- Corresponded to ~1 billion solid voxels as training data points

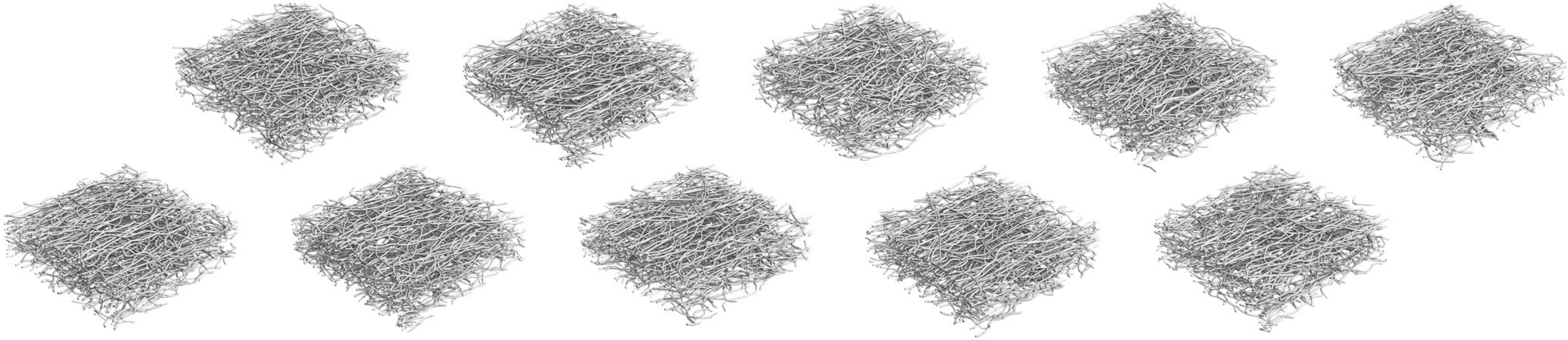




MATH 2 MARKET

# Digital Twins looking like scans

GeoDict



**Training Data: Then make the models look like binarized scans!**

- All fibers in the models get the same gray value, just as in the segmented 3D scans

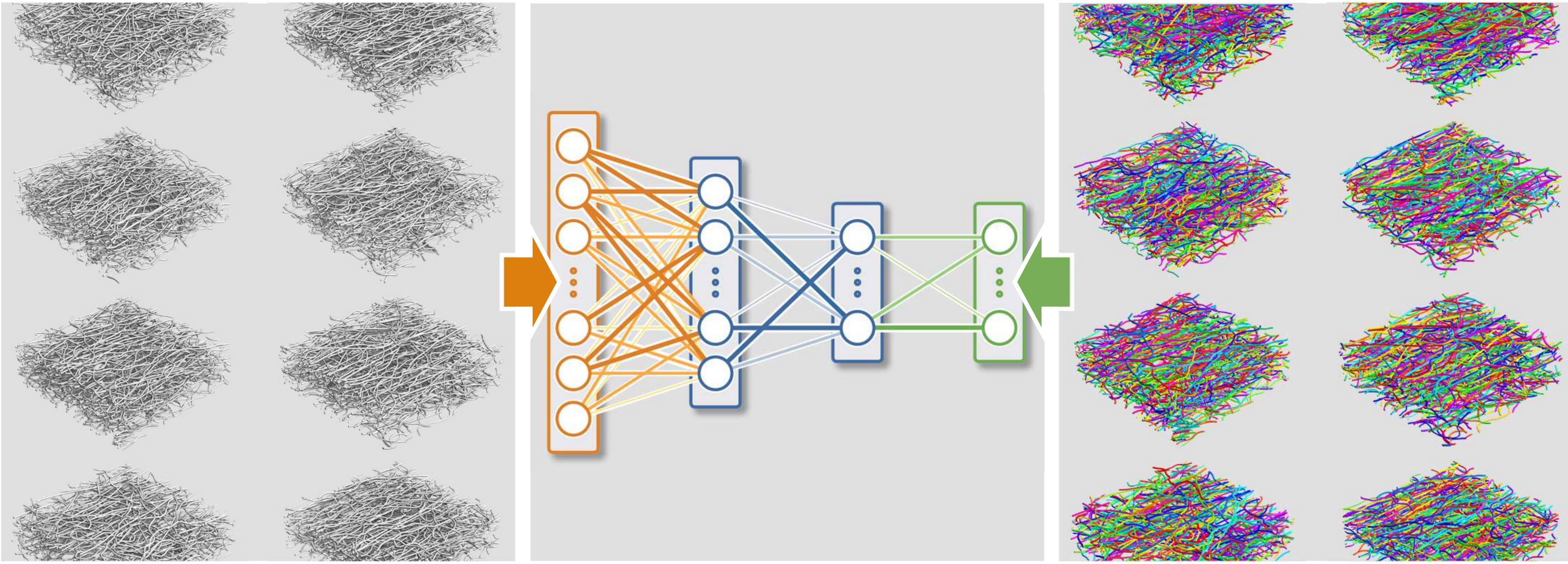




MATH 2 MARKET

# Training Phase of NN

GeoDict



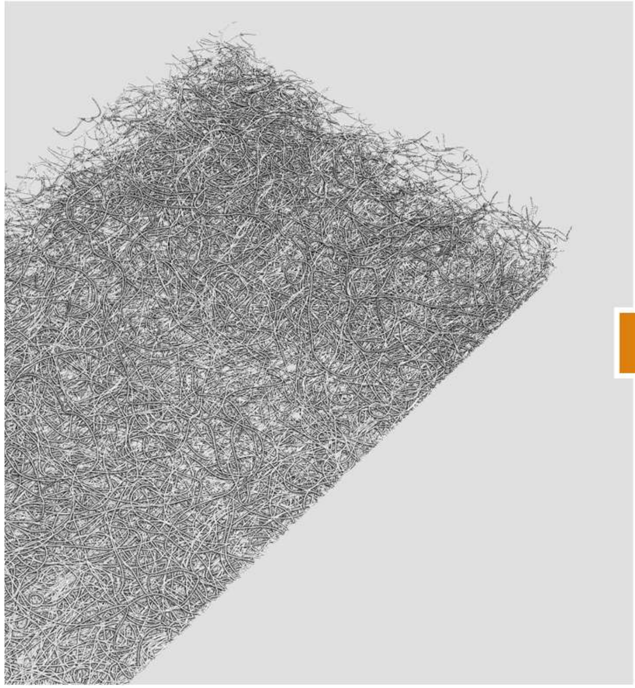
Dozens of Binarized GeoDict models

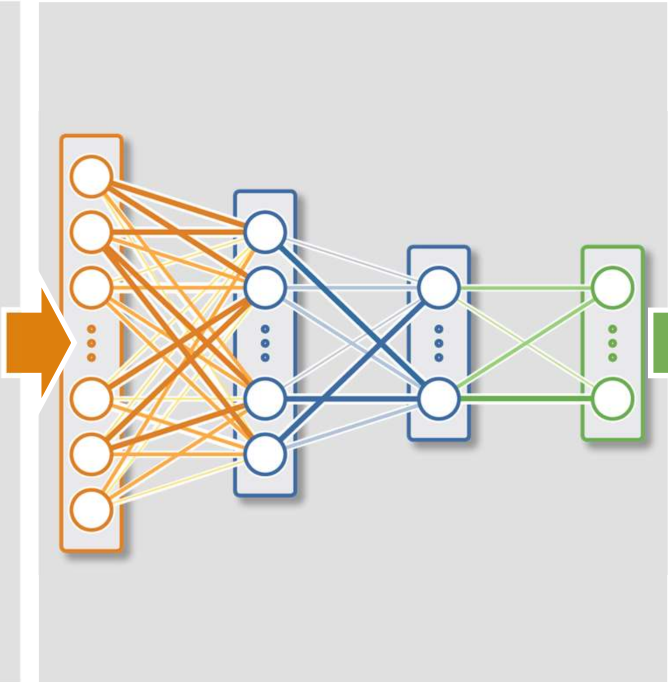
Neural Network learns weights for edges

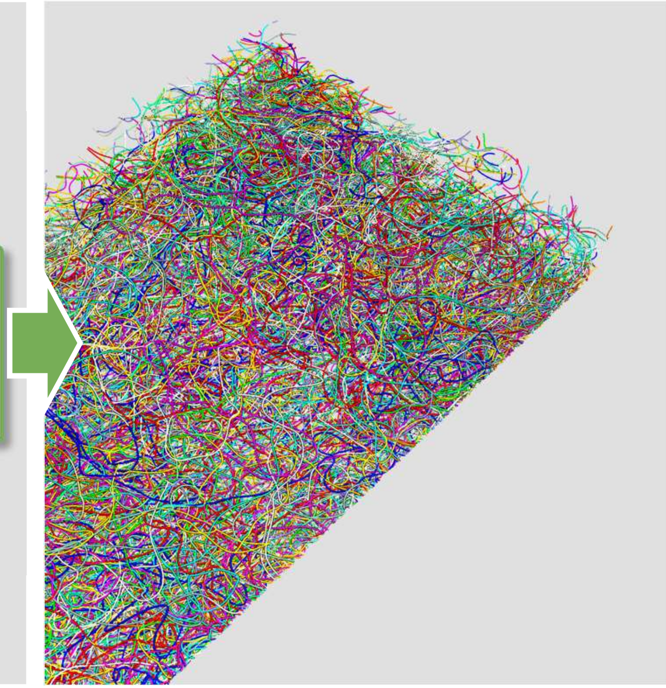
Dozens of Original GeoDict models

# Usage Phase of NN









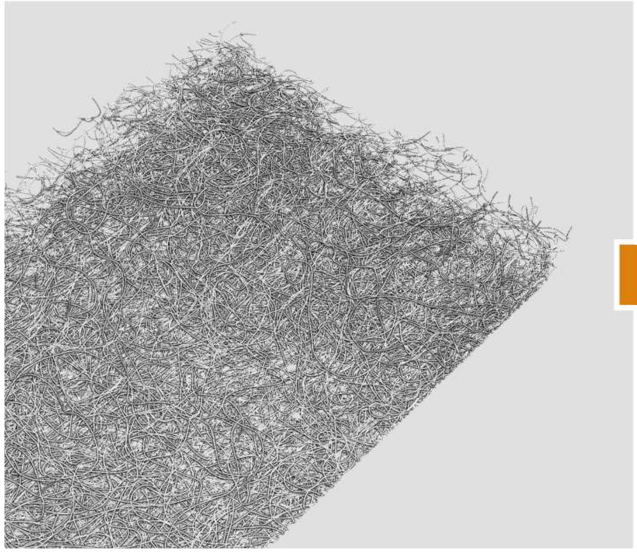
Segmented 3D scan

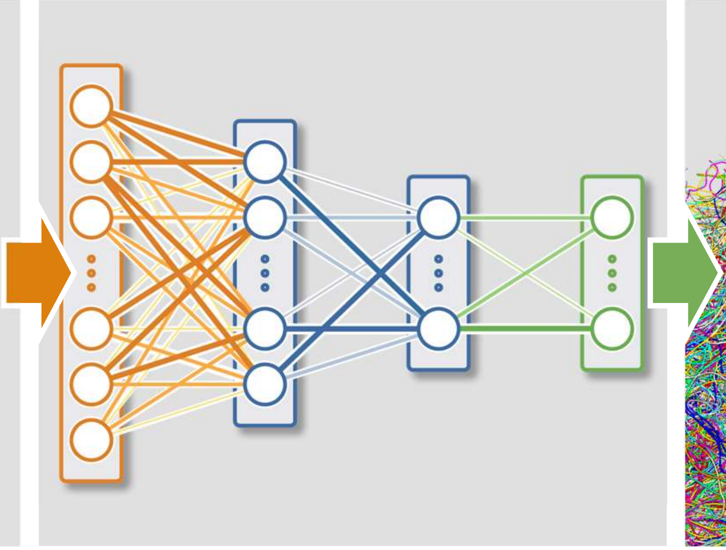
Neural Network with weights on edges

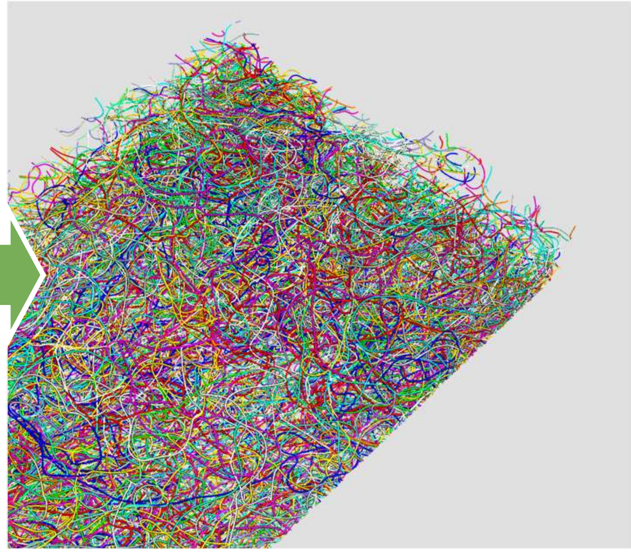
Labeled fibers for 3D scan

# Fiber identification by NN: Summary

GeoDict







**Training: NN learns edge weights from input and output**

- input: GeoDict Model: binarized version
- output: GeoDict Model: labeled fibers

**Usage: NN predicts labeled output from input using weights**

- input: Synchrotron / µCT data: binarized version
- output: Synchrotron / µCT data: labeled fibers





MATH 2 MARKET

# Overview of Sample Structures

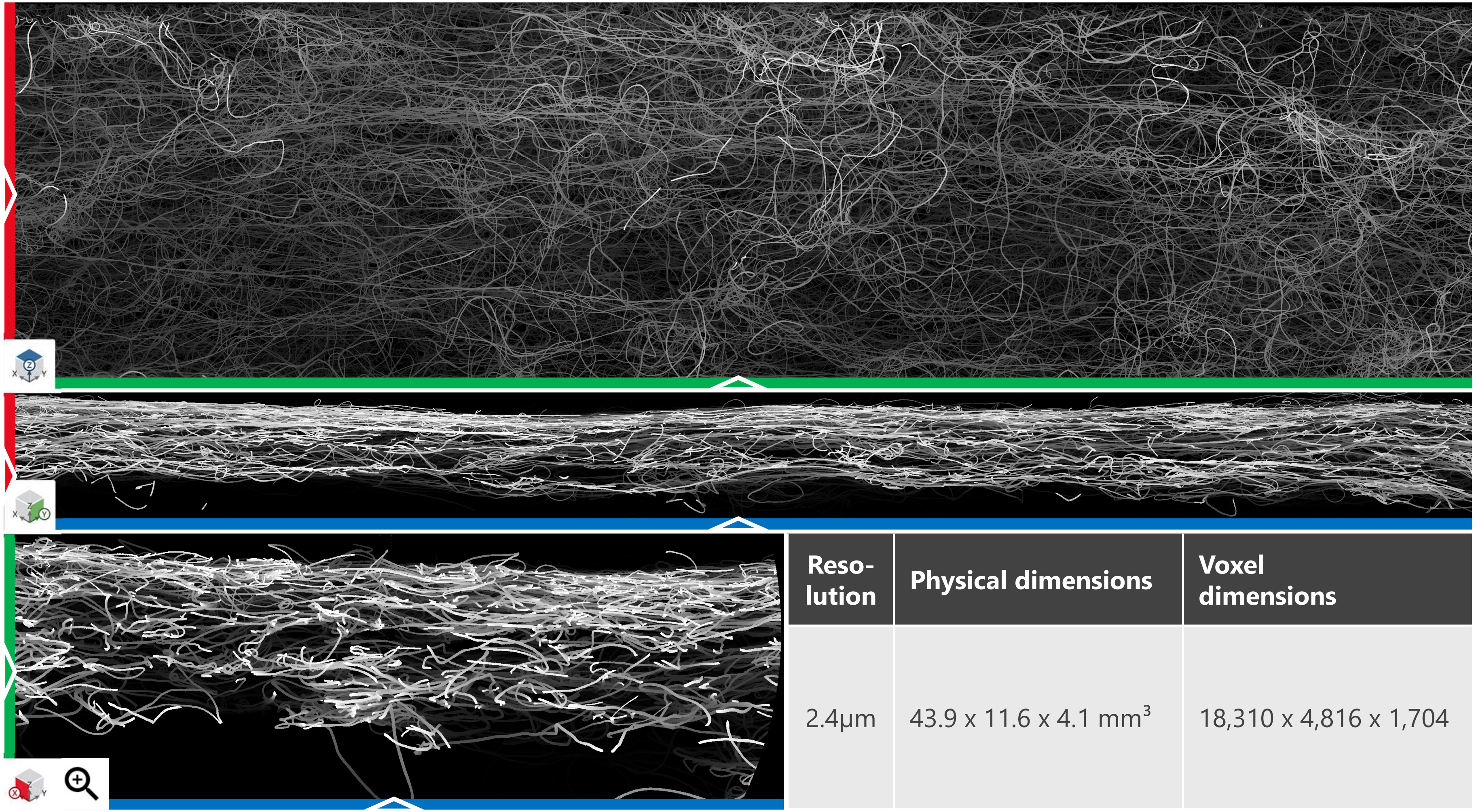
GeoDict

| Sample Name | Resolution | Physical dimensions | Voxel dimensions |
|---|---|---|---|
| **A** | 2.4µm | 43.9 x 11.6 x 4.1 mm | 18,310 x 4,816 x 1,704 |
| **B** | 2.7µm | 42.2 x 10.9 x 4.8 mm | 15,619 x 4,032 x 1,796 |

- Carded nonwoven samples
- Scanned and stitched together by Bruker microCT
- Analyzed by Math2Market using GeoDict

# Sample A – SEM view

GeoDict



| Reso-lution | Physical dimensions | Voxel dimensions |
|---|---|---|
| 2.4µm | 43.9 x 11.6 x 4.1 $mm^3$ | 18,310 x 4,816 x 1,704 |

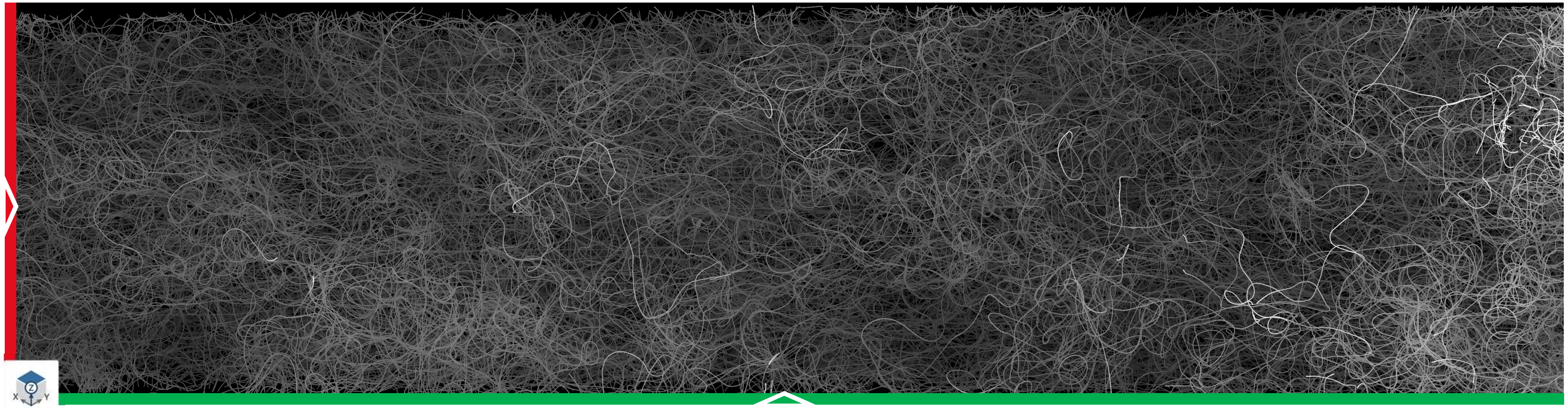




MATH 2 MARKET

# SAMPLE B – SEM VIEW

GEODICT



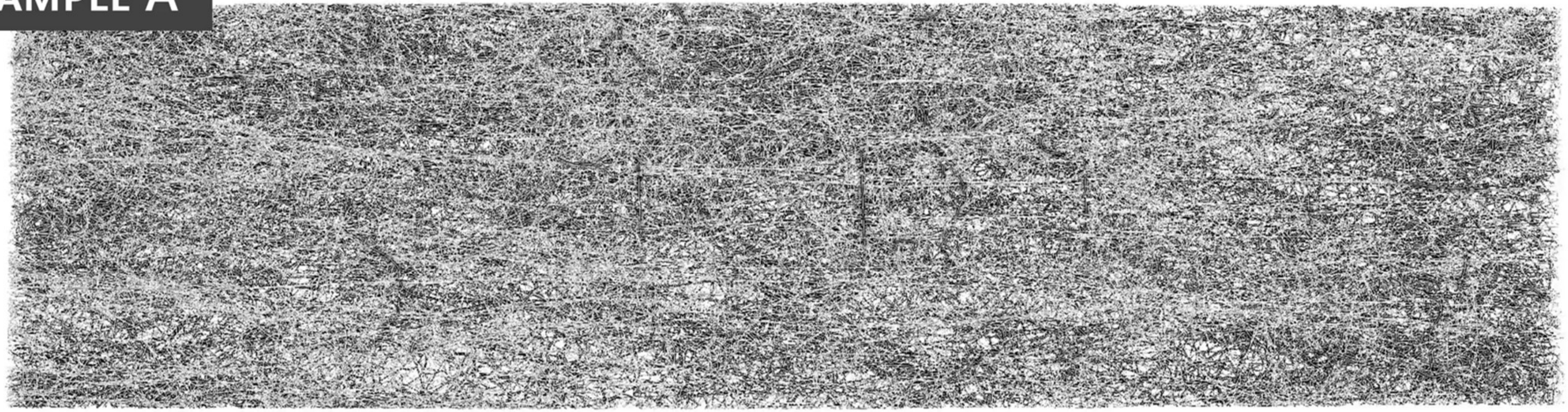
| Resolution | Physical dimensions | Voxel dimensions |
|---|---|---|
| 2.7µm | 42.2 x 10.9 x 4.8 $mm^3$ | 15,619 x 4,032 x 1,796 |



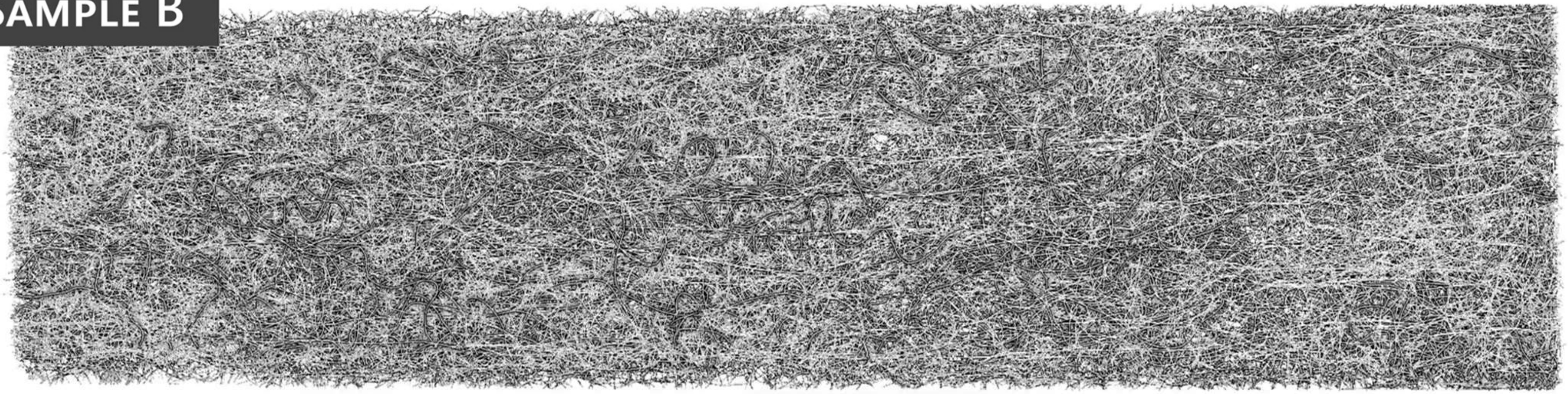


MATH 2 MARKET

## Sample A



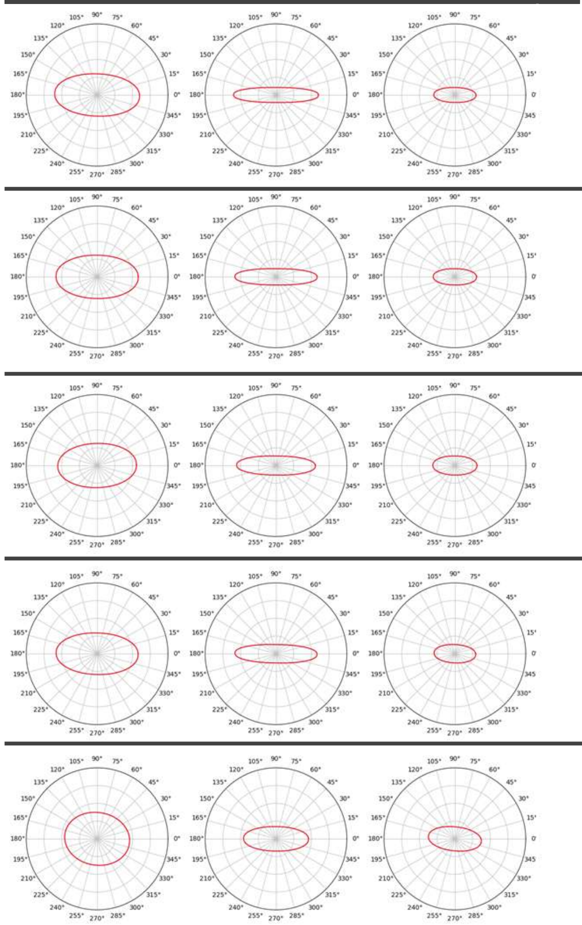
## Sample B

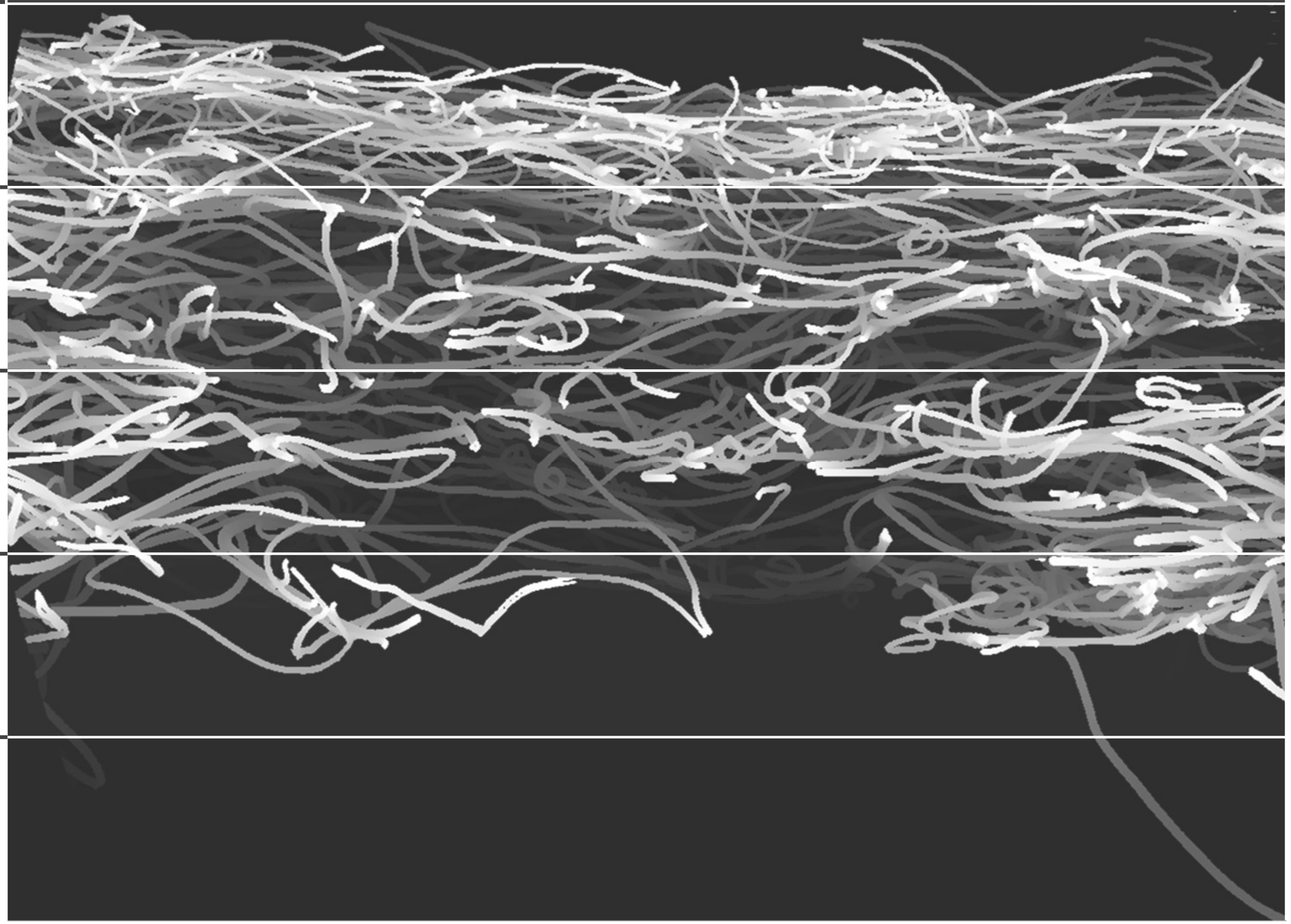


# FIBER ORIENTATIONS – SAMPLE A

GEODICT

| XY | XZ | YZ | View of a section of the surface in the direction of the X axis. |
|---|---|---|---|







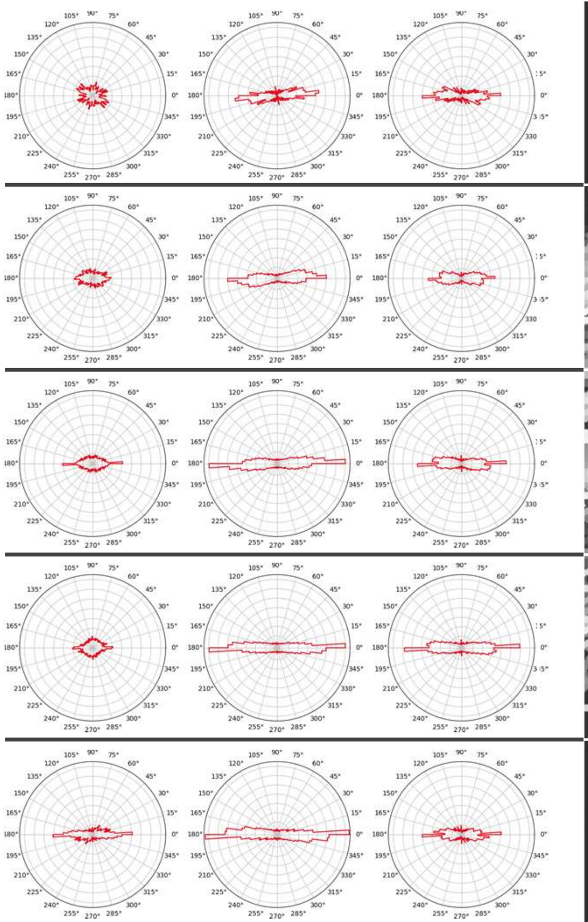


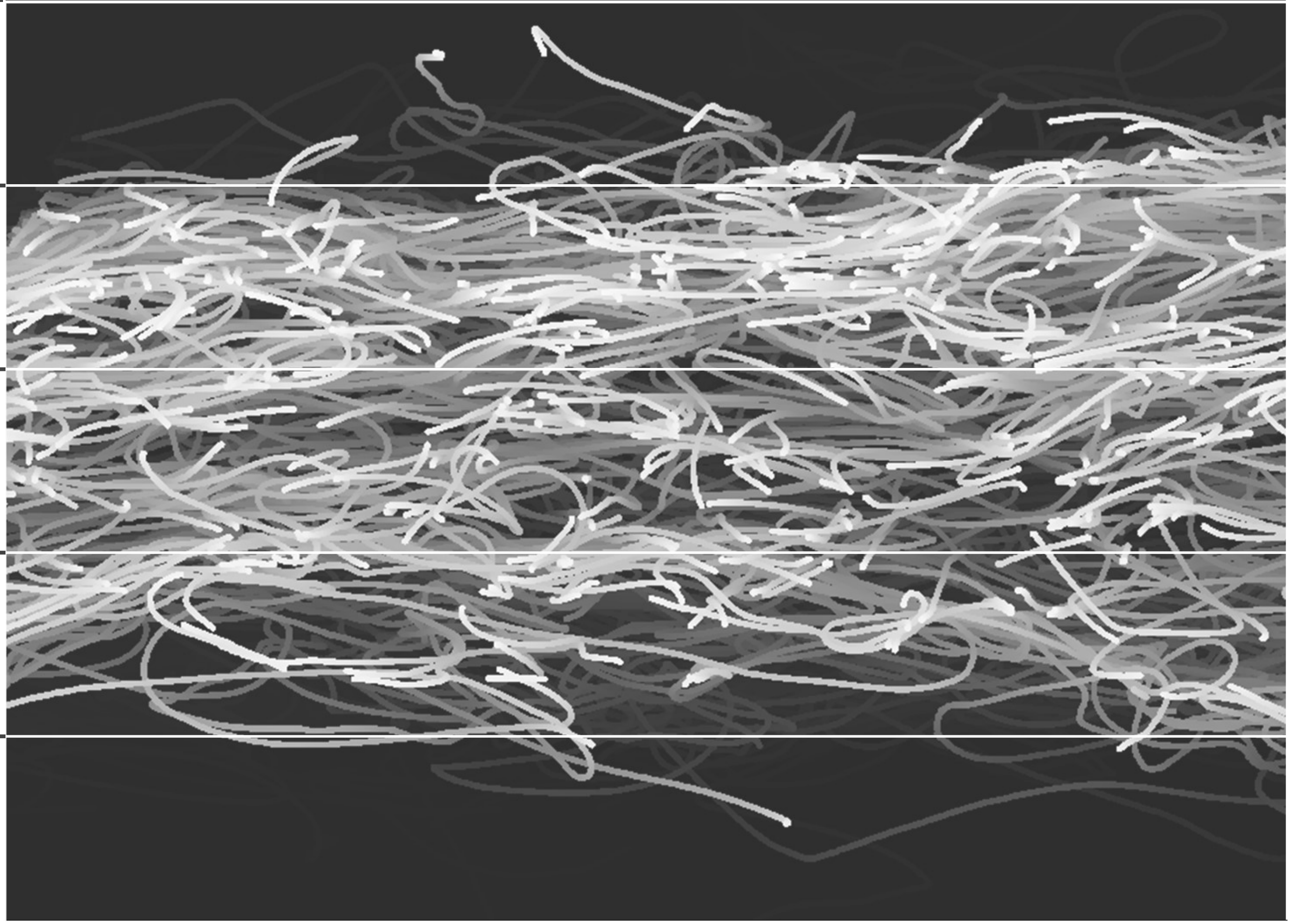
MATH 2 MARKET

# FIBER ORIENTATIONS – SAMPLE B

GEODICT

| XY | XZ | YZ | View of a section of the surface in the direction of the X axis. |
|---|---|---|---|







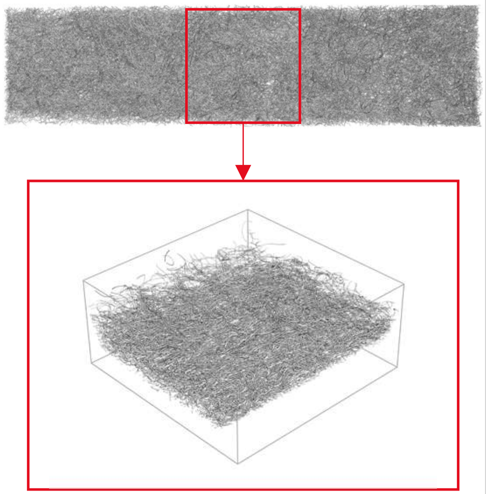


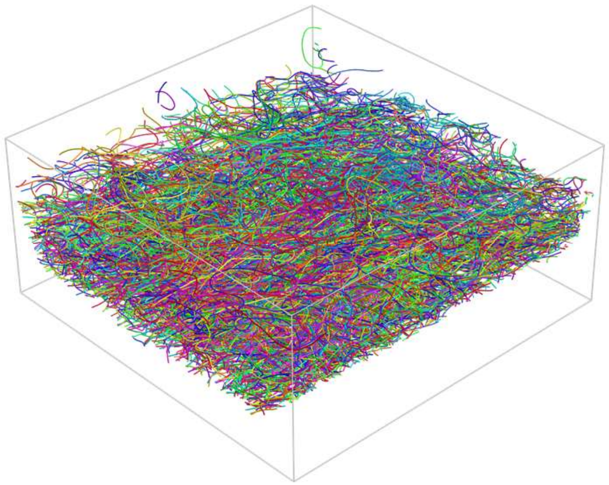
MATH 2 MARKET

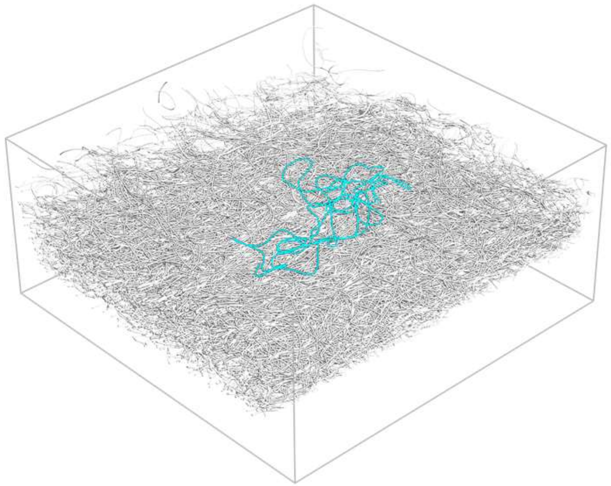
# FIBER IDENTIFICATION ON SAMPLE B

GeoDict

| Sample B | Labeling of fibers | Data becomes information |
| --- | --- | --- |
| FiberFind was used on the complete sample.<br>Process is explained on a smaller cutout | The artificial intelligence separates the solid voxels in the image data into individual fibers.<br>Each fiber becomes an independent, modifiable object which can be treated independently. | Geometric information, such as fiber length, fiber segment orientation and fiber diameter, can be read directly from the object. |



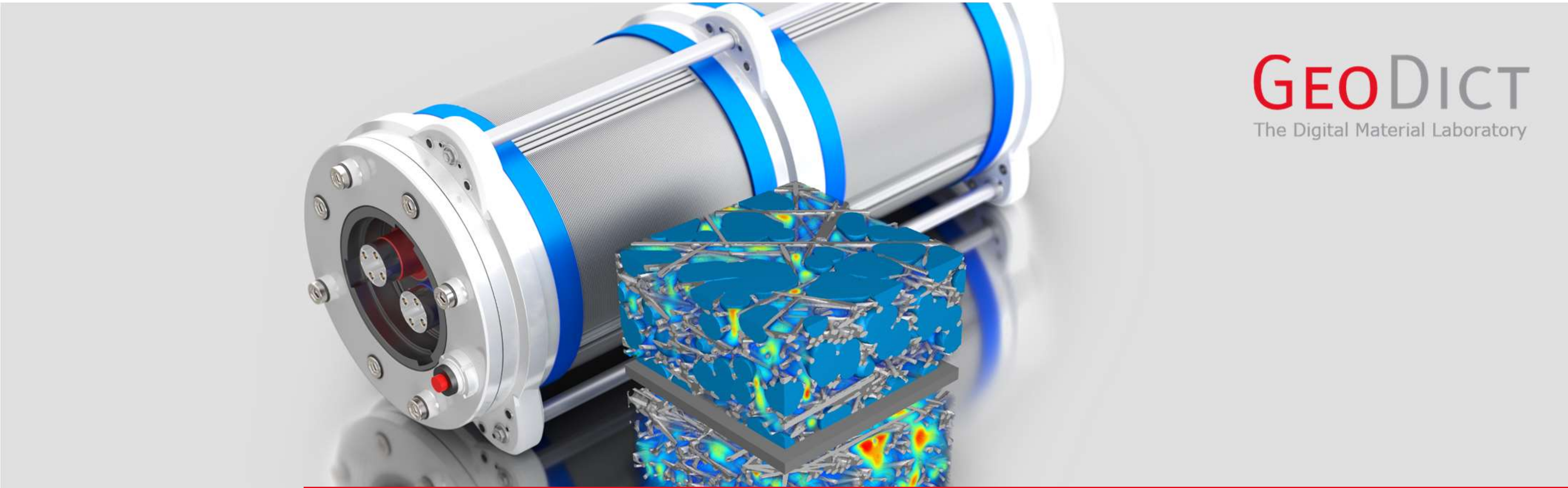








MATH 2 MARKET




# DIGITAL PEM FUEL CELL DEVELOPMENT

Solutions with GeoDict®

**Dr. Mathias Fingerle**, Dr. Ilona Glatt, Dr. Jürgen Becker, Sebastian Rief, Andreas Grießer, Steffen Schwichow, Franziska Arnold

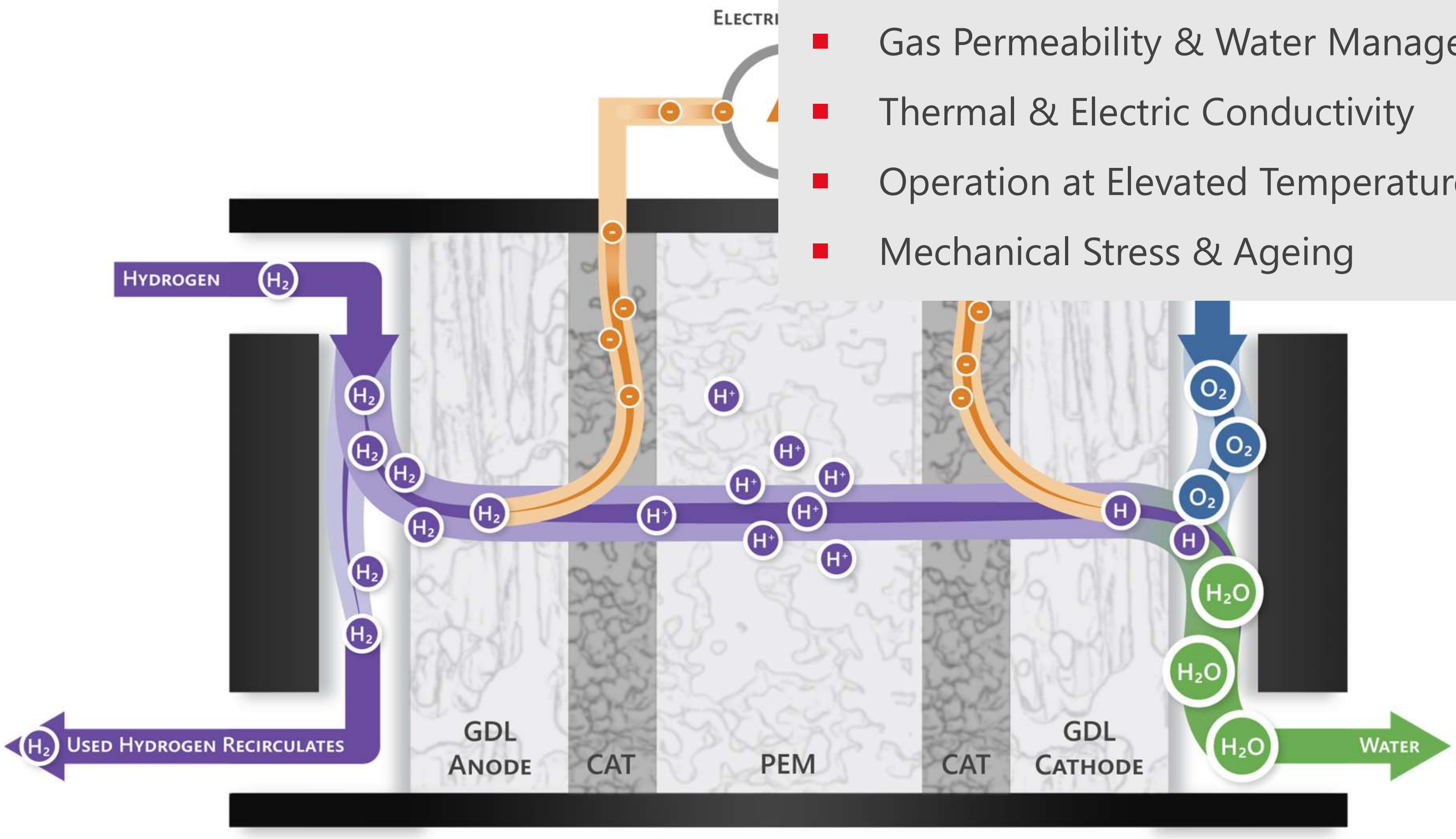


MATH
2 MARKET

# PEM Fuel Cell

Challenges for Materials Design:

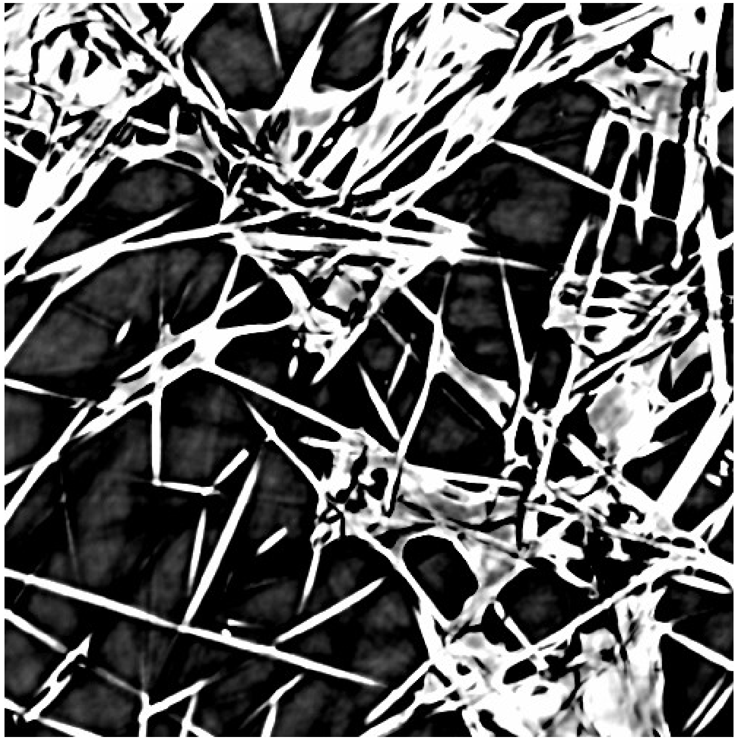
- Gas Permeability & Water Management
- Thermal & Electric Conductivity
- Operation at Elevated Temperatures (350 K)
- Mechanical Stress & Ageing



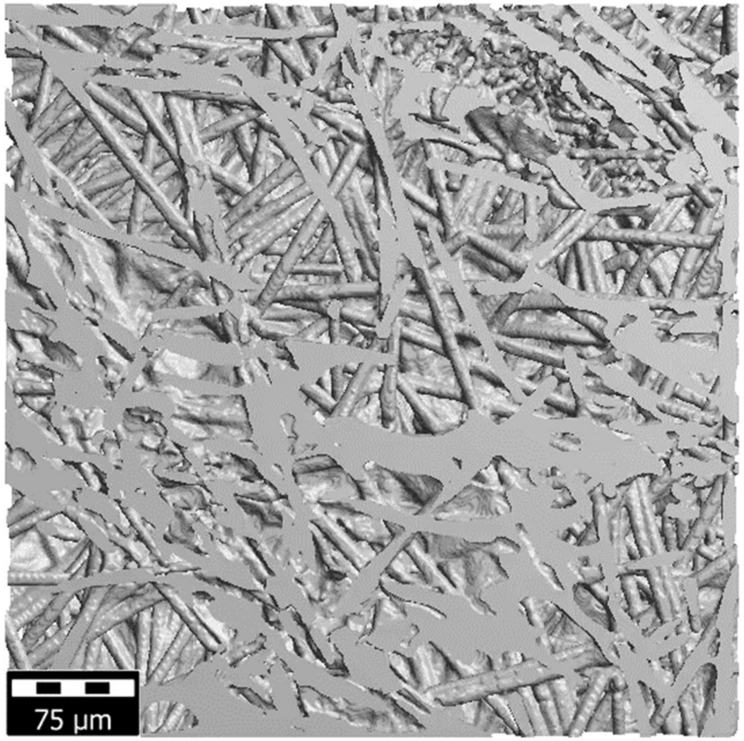
# Import of a $\mu$CT Scan with GeoDict®

GeoDict

1. Import 2. Analyze 3. Model 4. Design



Data: $\mu$CT Scans of Toray TGP H 060, PSI Villingen (CH)




Segmentation with ImportGeo-Vol



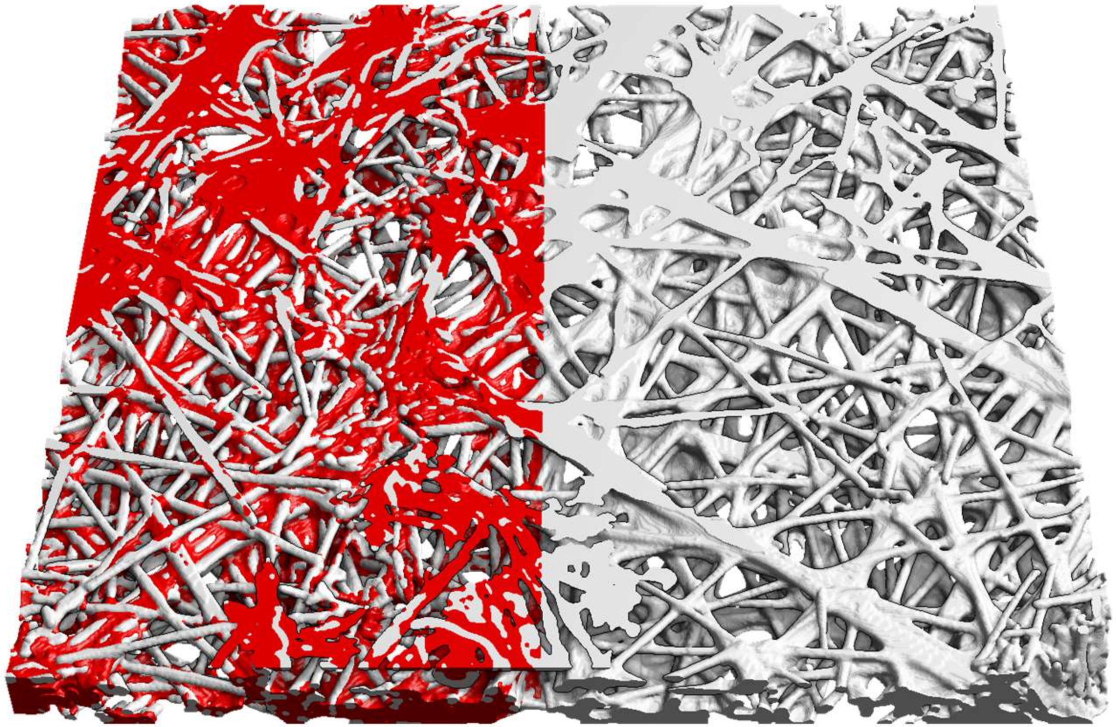


MATH 2 MARKET

# Segmentation of a GDL with FiberFind-AI*

GeoDict

1. Import »  2. Analyze »  3. Model »  4. Design »



Fibers: 14.0%
Binder: 18.3%

The neural network in FiberFind-AI, can distinguished fiber and binder of a Toray Paper



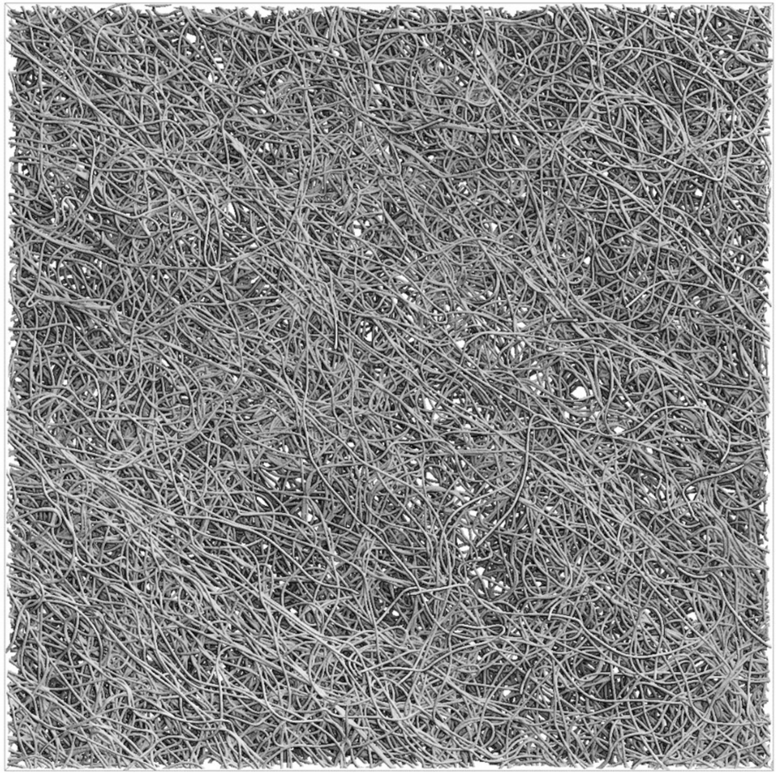


MATH 2 MARKET

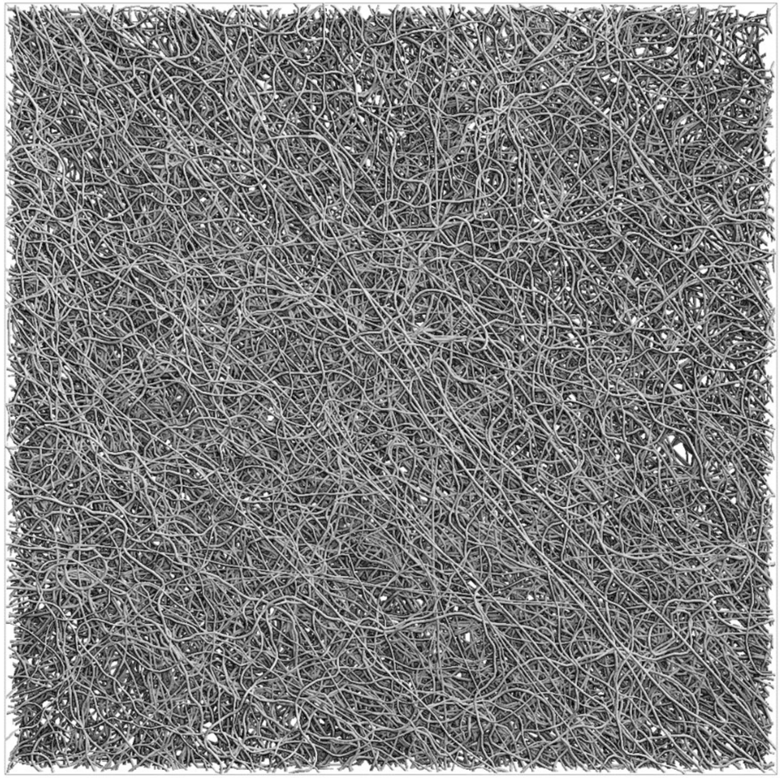
# CT-scan vs Digital Twin generated in GeoDict®

GeoDict

1. 2. 3. Model 4. Design



µCT-scan



Digital Twin





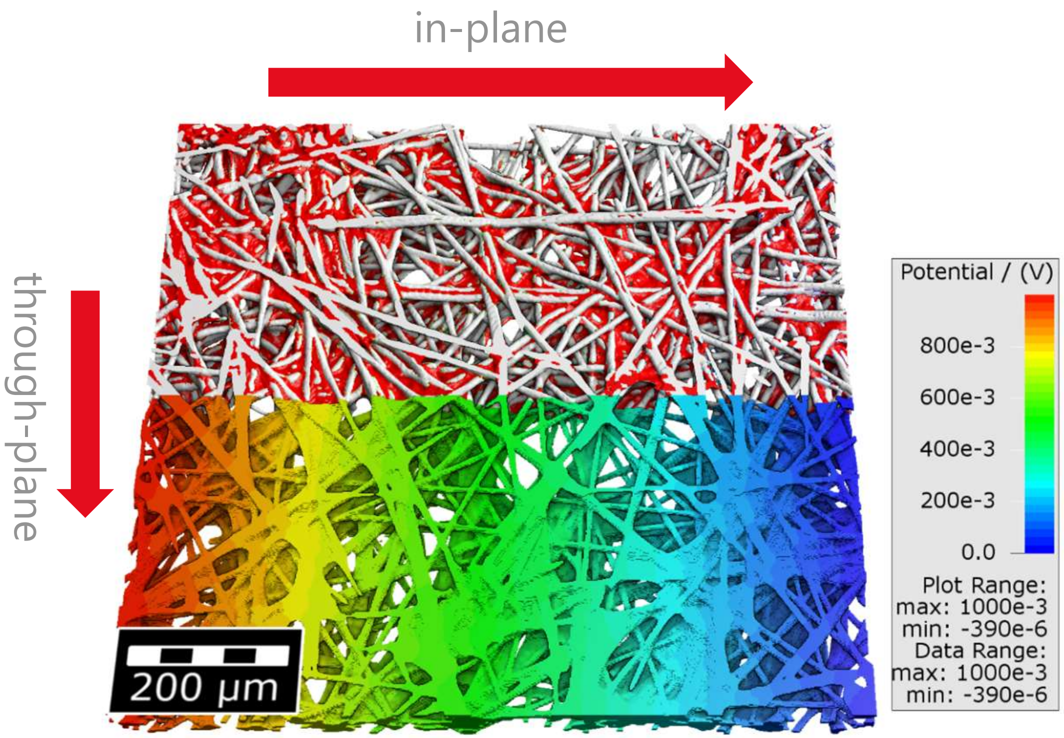
MATH 2 MARKET

# SIMULATION OF ELECTRICAL CONDUCTIVITY*

GEODICT

Conductivity in experiments did not fit conductivity in simulations. [1]

- Reason: fibers and binder could not be differentiated. [1]
- Solution: After identifying fiber and binder with **FiberFind-AI**, we can now run simulations where binder and fibers have different conductivity




[1] J. Becker et. al.: Determination of Material Properties of Gas Diffusion Layers: Experiments and Simulations Using Phase Contrast Tomographic Microscopy, Journal of The Electrochemical Society, 2009.





MATH 2 MARKET

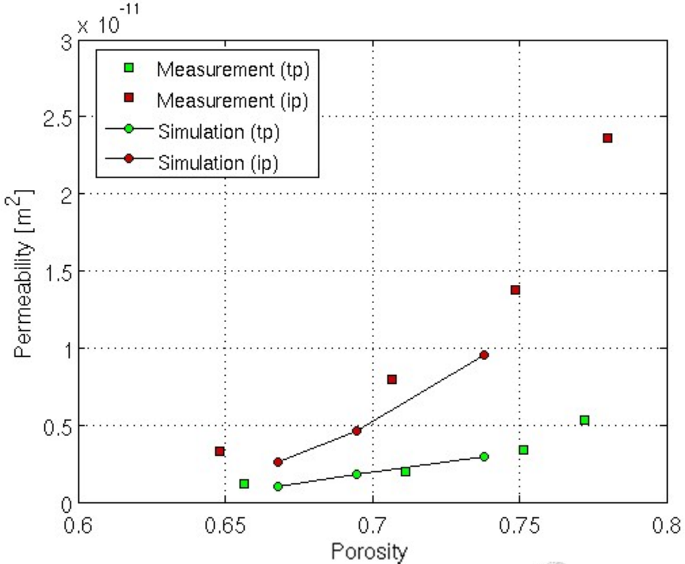
# Transport Properties at Different Compression Levels

GeoDict

1. | 2. Analyze | 3. Model | 4. Design

GeoDict simulations with PoroDict & DiffuDict:

- Diffusivity and permeability calculated on Toray TGP H 060 at different compression level
- Comparison to experimental results in through plane (tp) and in plane (ip) direction




*J. Becker et. al.: Determination of Material Properties of Gas Diffusion Layers: Experiments and Simulations Using Phase Contrast Tomographic Microscopy, Journal of The Electrochemical Society, 2009.*



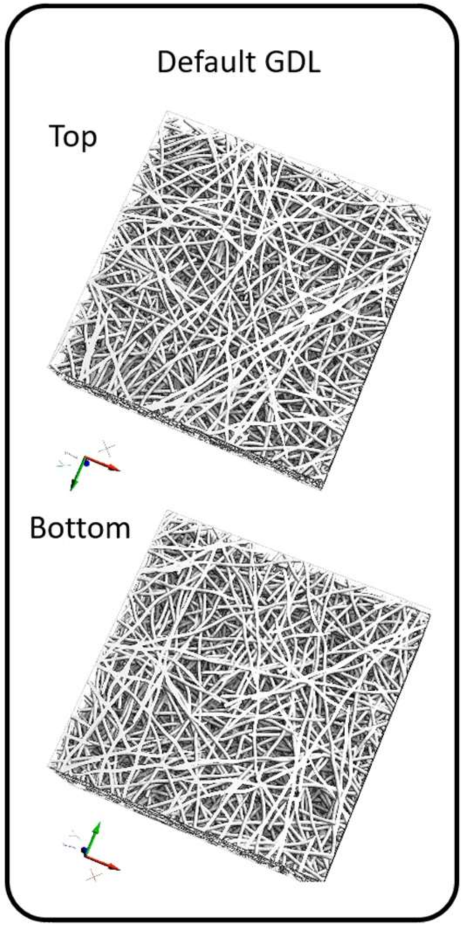


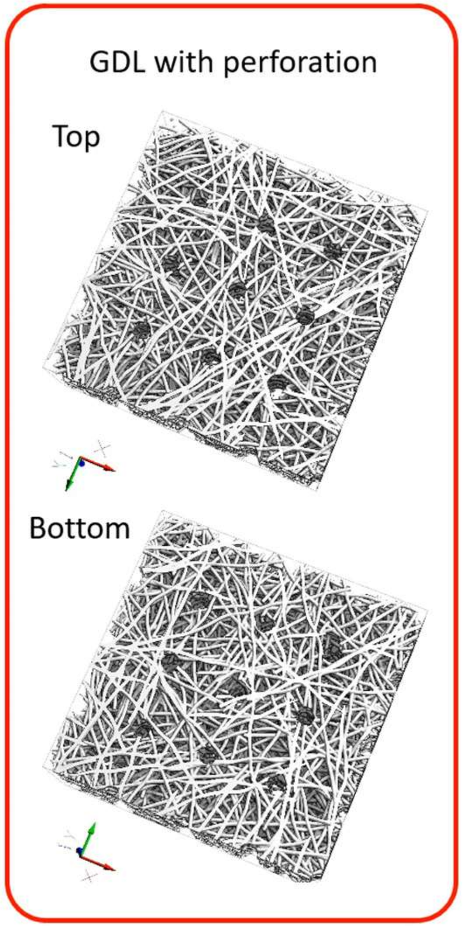
MATH 2 MARKET

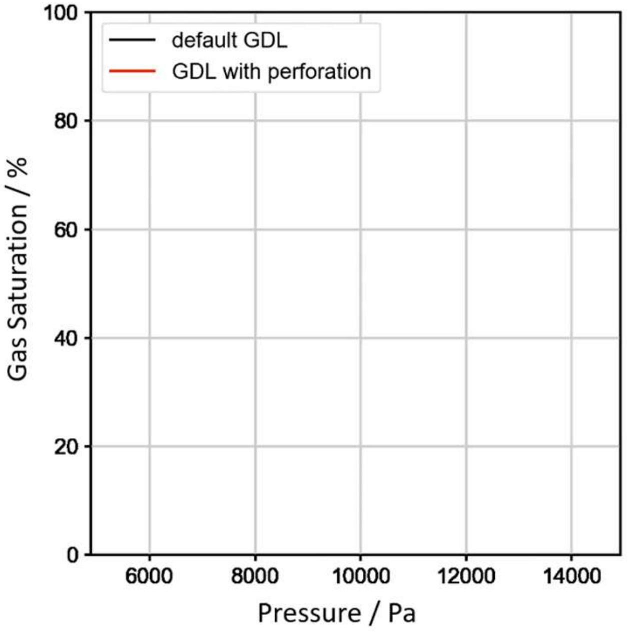
# Water Saturation of a GDL simulated with SatuDict

GeoDict

1. | 2. Analyze | 3. Model | 4. Design







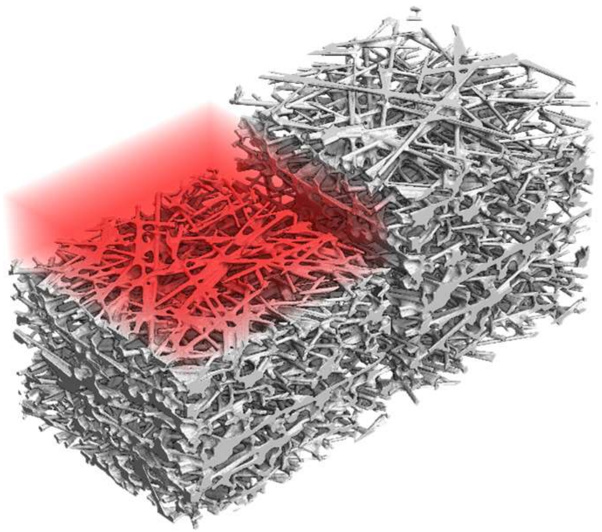

MATH 2 MARKET

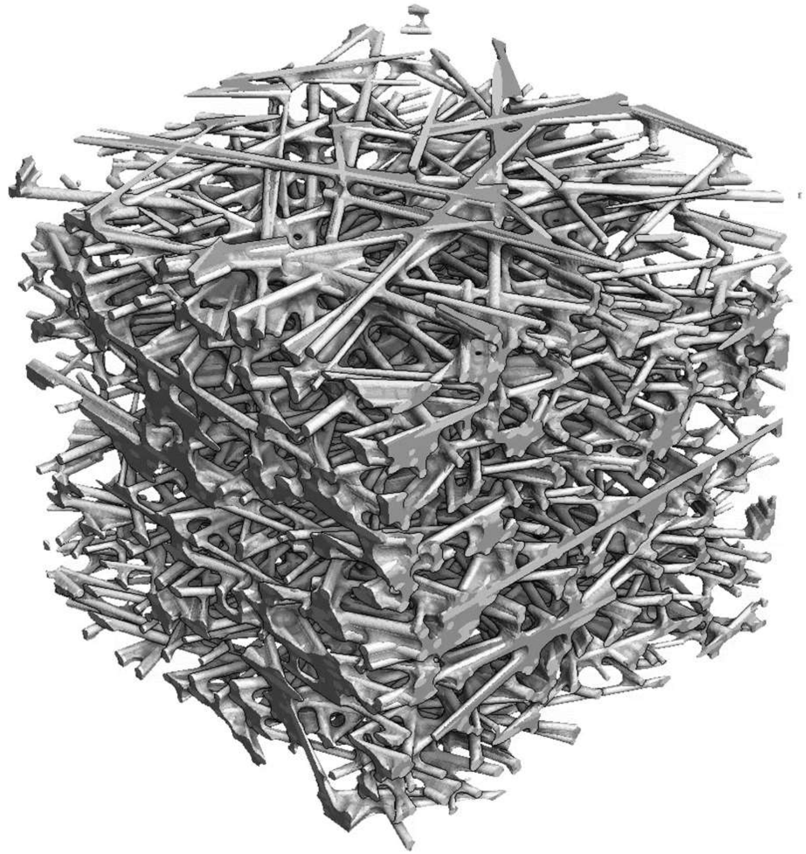
# Mechanical Properties: Compression of GDL Determined with ElastoDict

GeoDict

1. | 2. Analyze | 3. Model | 4. Design

- Transverse isotropic elastic modulus for fibers
- Isotropic elastic modulus for binder
- 30% compression





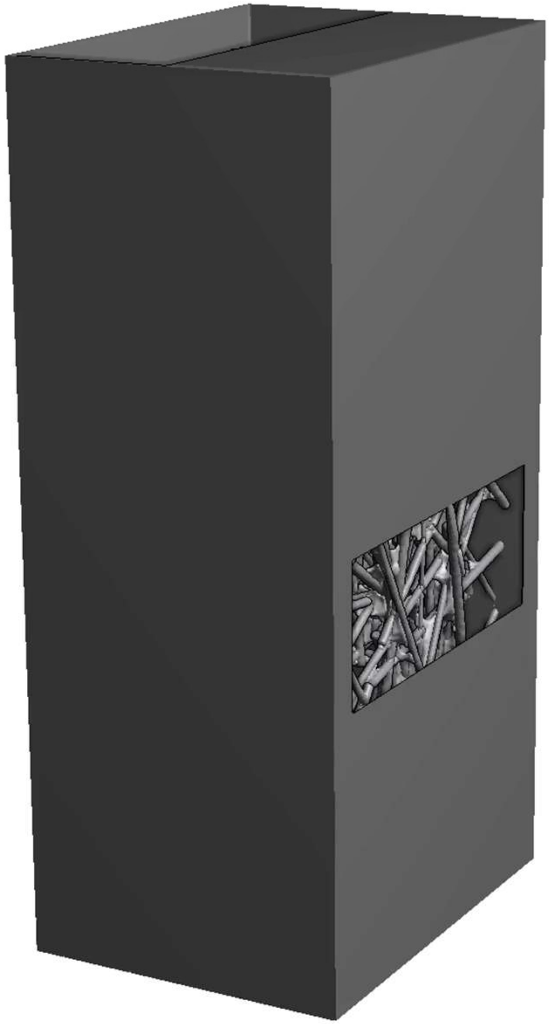




MATH 2 MARKET

# Optimize Water Management with GeoDict®*

GeoDict



Motivated by Jens Eller, Paul Scherrer Institut





MATH 2 MARKET

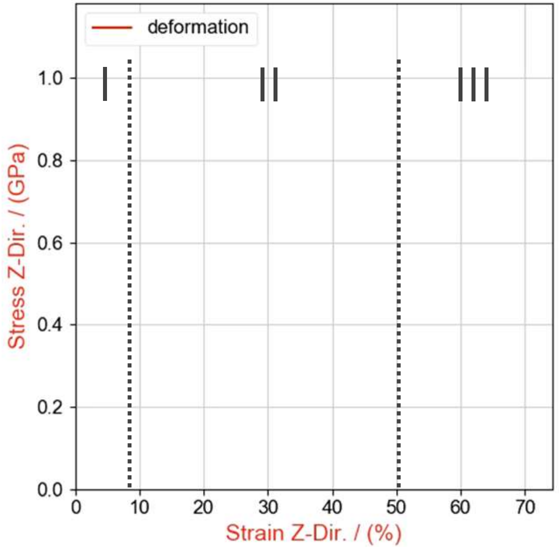
# Compression of Porous Media with GeoDict

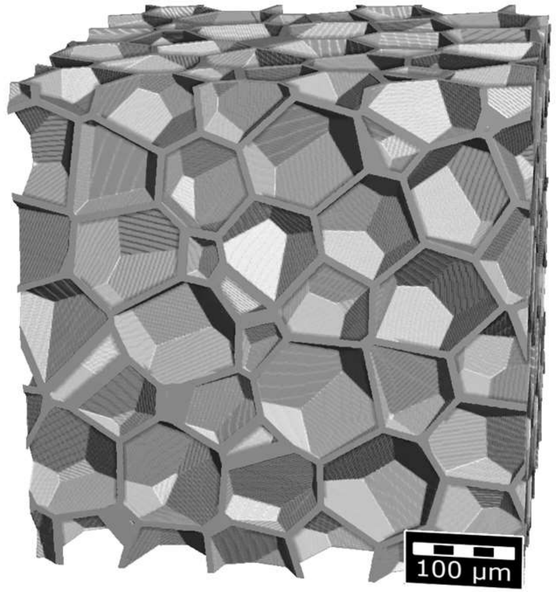
µCT scans and alignment by Stefan Probst-Schendzielorz, Voith Paper, Heidenheim

# COMPRESSION OF GENERATED FOAMS

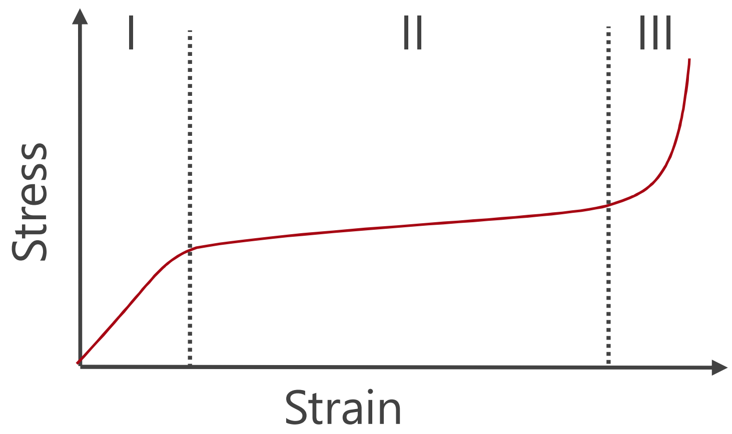
GEODICT

Stress-strain curve calculated with GeoDict




Theoretical stress strain curve




I. Linear elasticity,
II. Plateau
III. Densification

- Foam generated with FoamGeo
- 80 % compression (on deformed geometry)
- Buckling of cell walls can be observed
- Characteristical stress strain curve
- Constant positive pore pressure

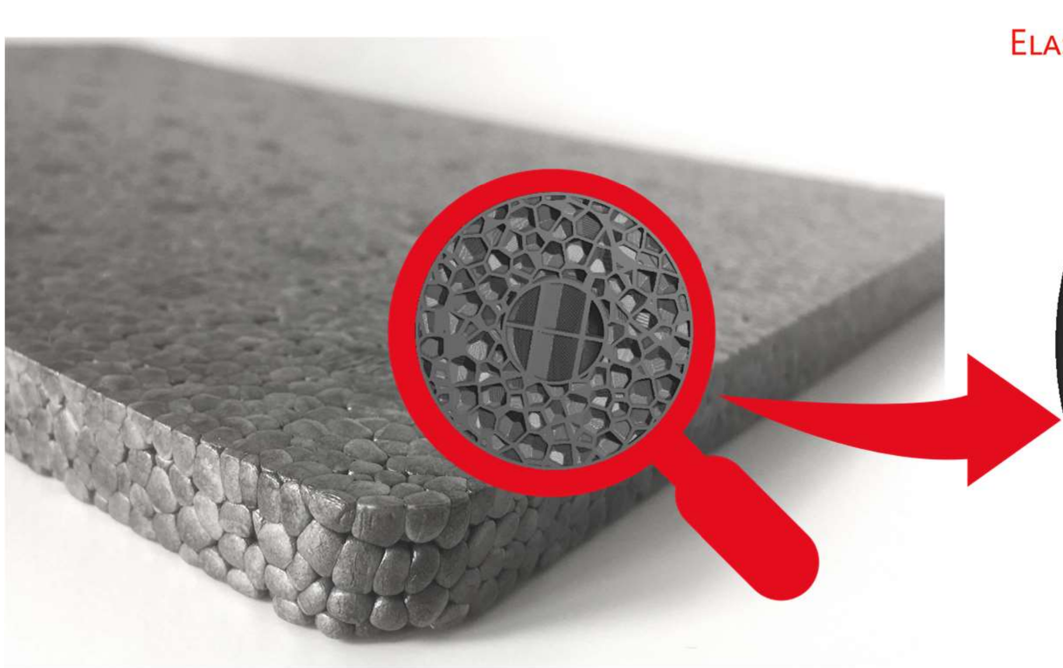


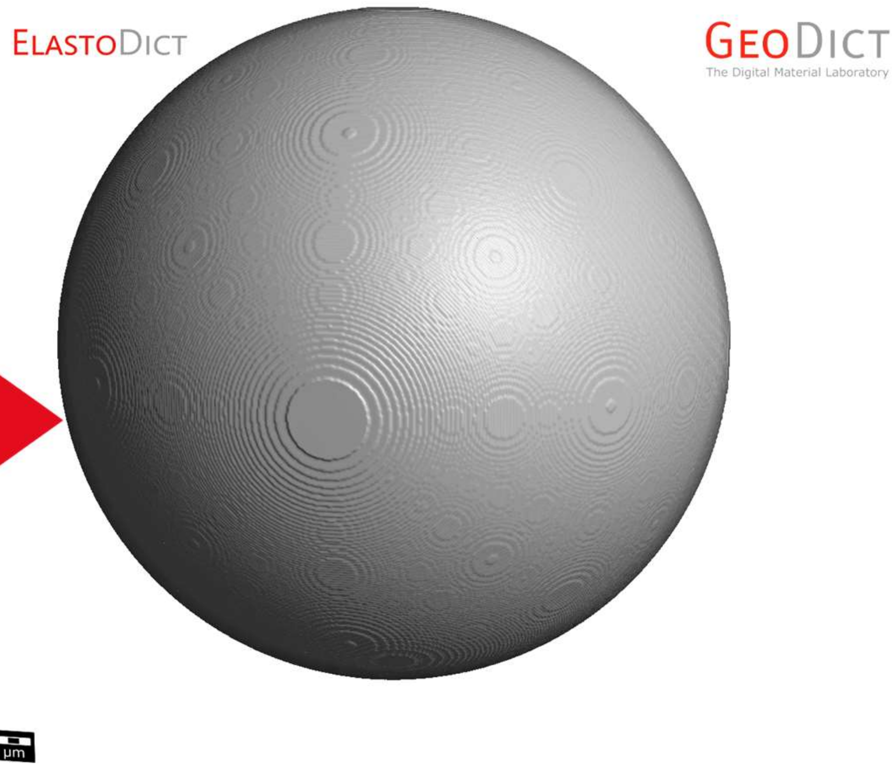


MATH 2 MARKET

# COMPRESSION OF A SINGLE BEAD

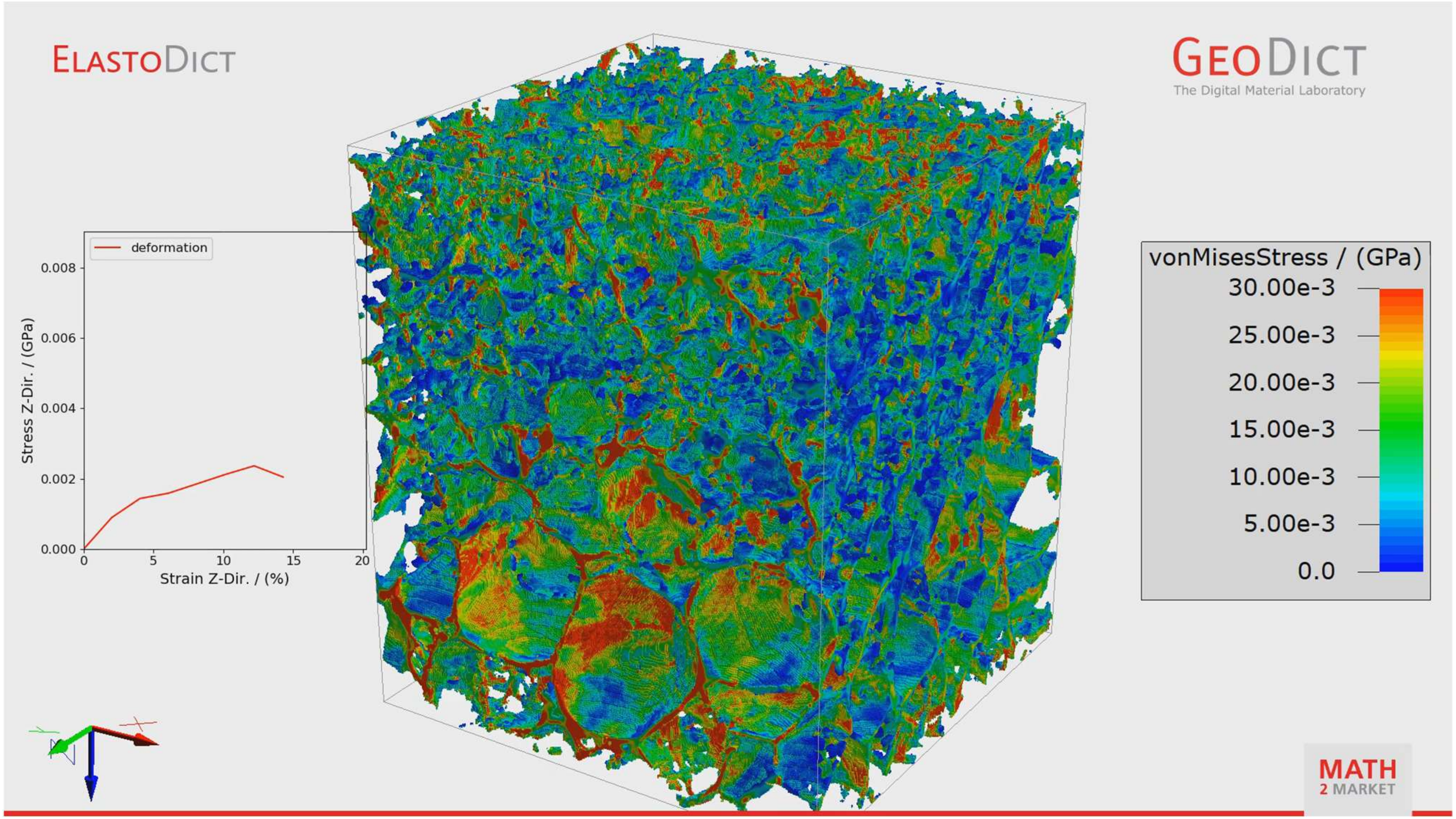
| Polypropylene particle foam | Compression of a single bead |
|---|---|





# FOAM AND STRESSES UNDER ELONGATION

GEODICT



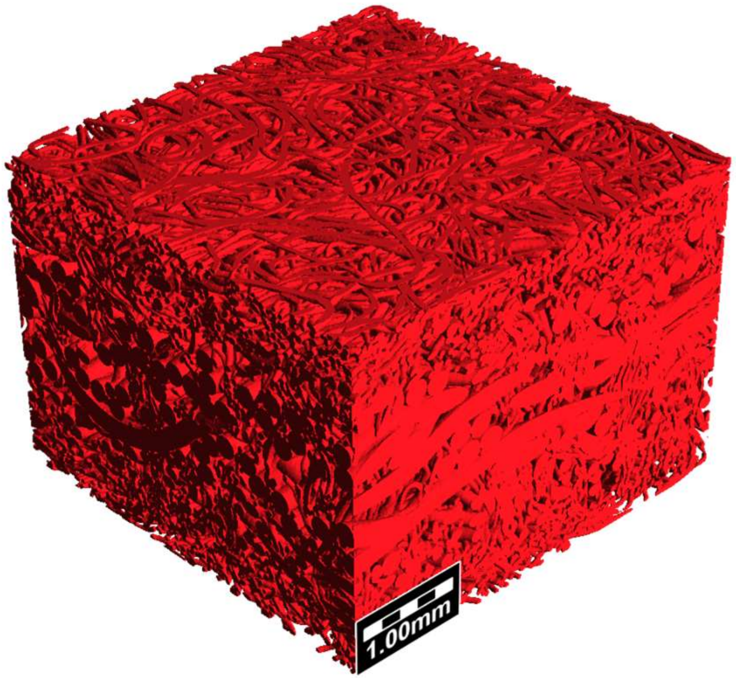


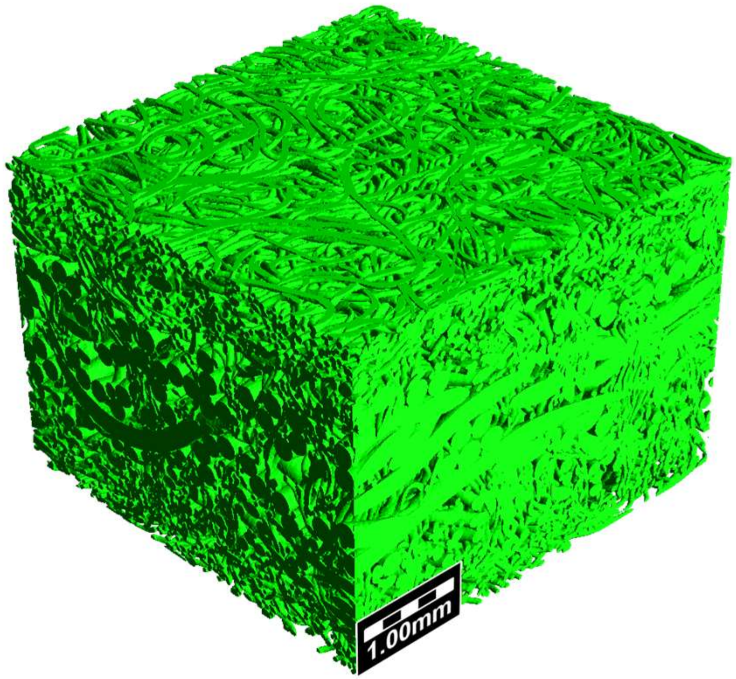



MATH 2 MARKET

## Compression Simulation of a Drainage Felt

# Compression @ 0.1 MPa

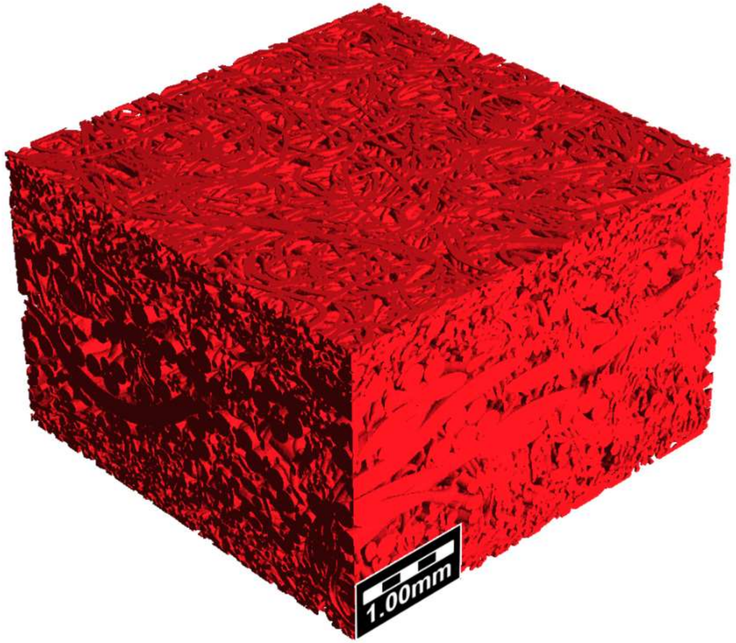


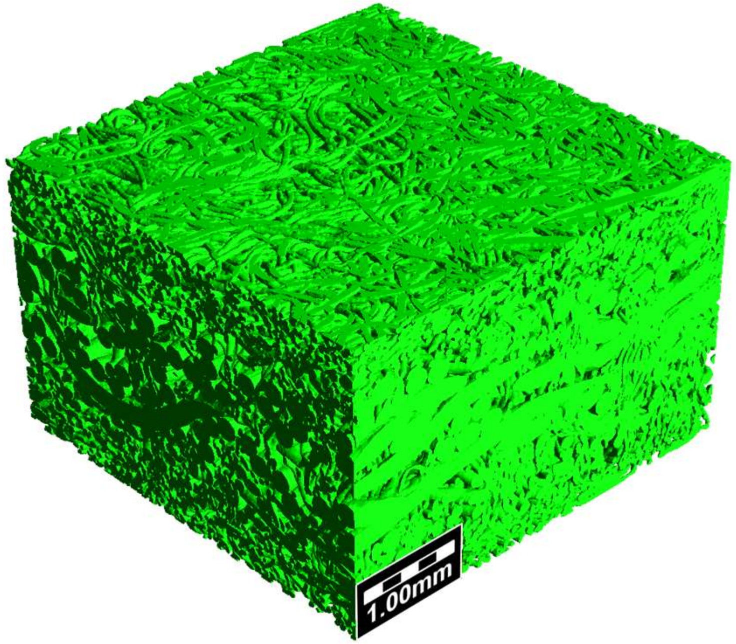




| Scan | ElastoDict |
|---|---|
| 547 x 546 x 410 Voxel<br>0% Deformation | 547 x 546 x 410 Voxel<br>0% Deformation |

GEODICT

# COMPRESSION @ 1.0 MPa




| Scan | ElastoDict |
|---|---|
| 547 x 546 x 358 Voxel | 547 x 546 x 358 Voxel |
| -12.68% Deformation | -12.68% Deformation |

VOITH



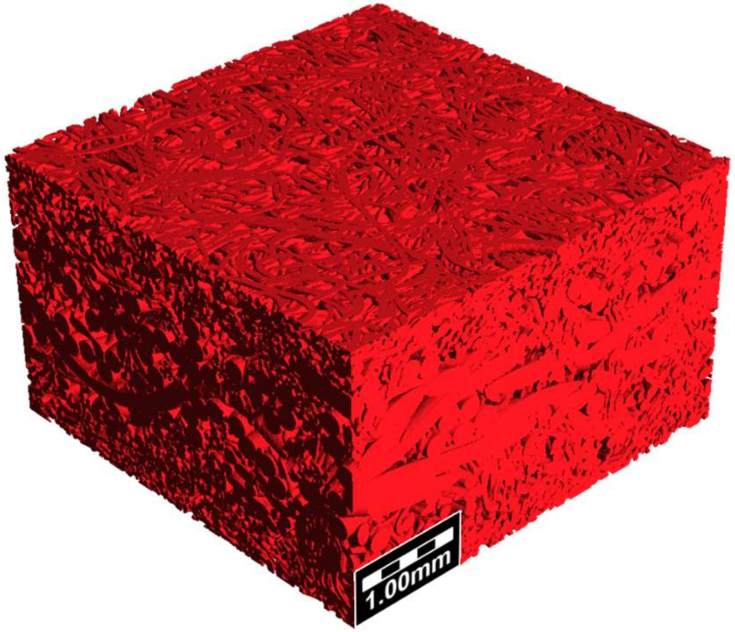


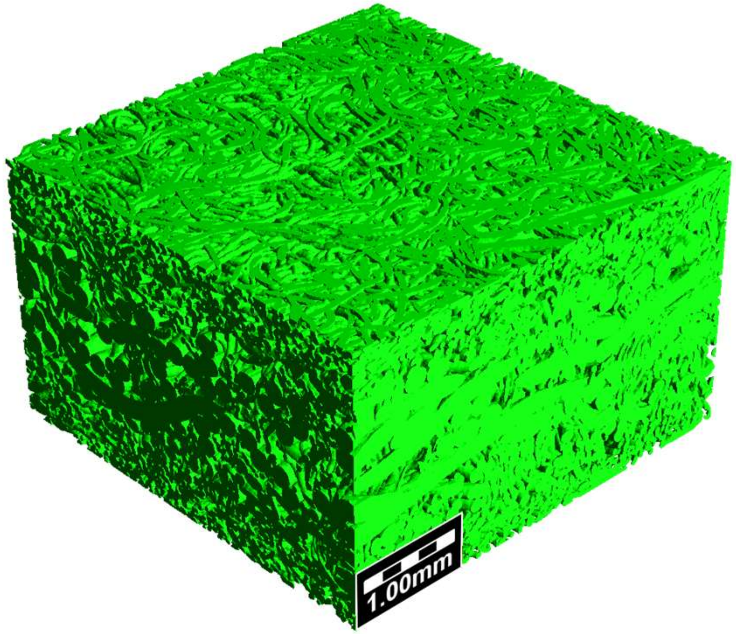
MATH 2 MARKET

## Compression Simulation of a Drainage Felt

GeoDict

# Compression @ 2.0 MPa




| Scan | ElastoDict |
| --- | --- |
| 547 x 546 x 341 Voxel | 547 x 546 x 341 Voxel |
| -4.75% Deformation | -4.75% Deformation |

VOITH



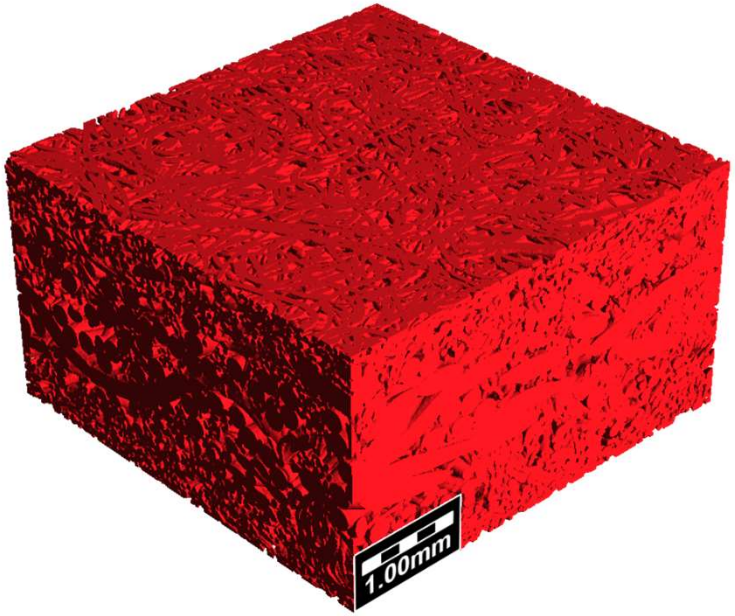


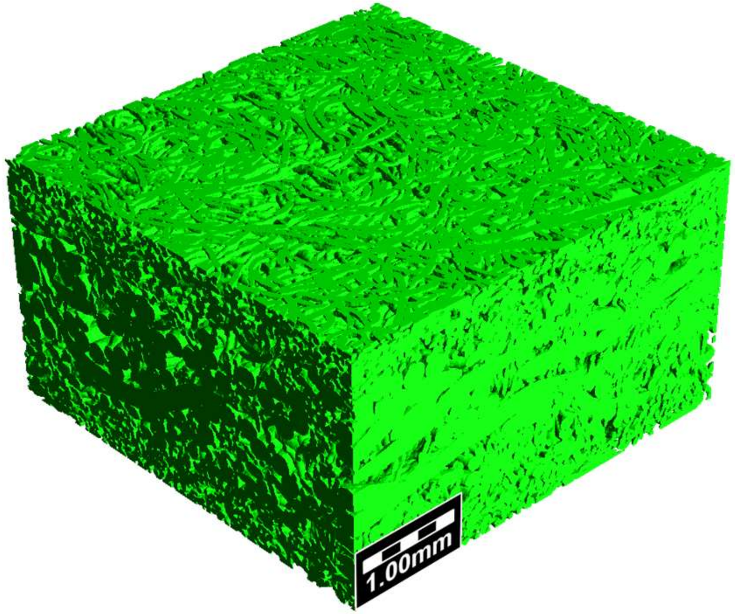
MATH 2 MARKET

# Compression Simulation of a Drainage Felt

## Compression @ 4.0 MPa

GeoDict




| Scan | ElastoDict |
| --- | --- |
| 547 x 544 x 314 Voxel | 547 x 544 x 314 Voxel |
| -7.92% Deformation | -7.92% Deformation |

VOITH



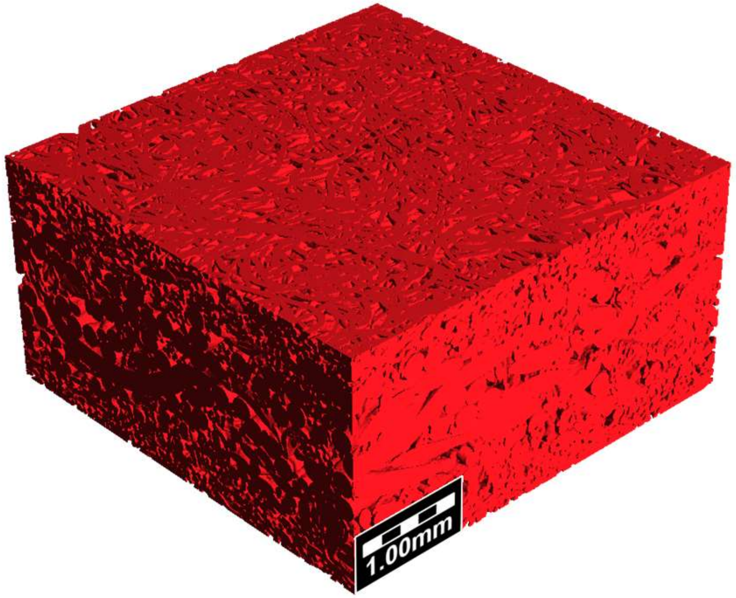


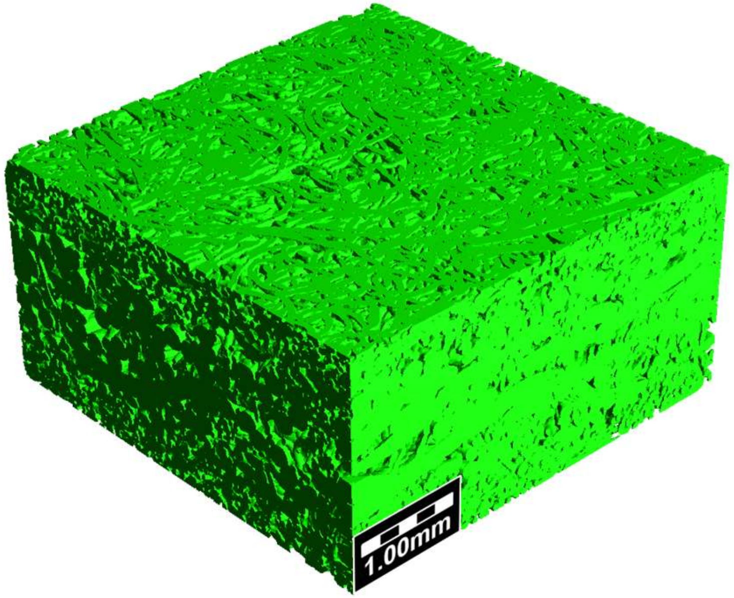
MATH 2 MARKET

Compression Simulation of a Drainage Felt

# Compression @ 6.0 MPa

GeoDict




| Scan | ElastoDict |
|---|---|
| 547 x 544 x 290 Voxel<br>-7.46% Deformation | 547 x 544 x 290 Voxel<br>-7.46% Deformation |

VOITH





MATH 2 MARKET

# OVERLAP-ANALYSIS @ 1.0 MPa

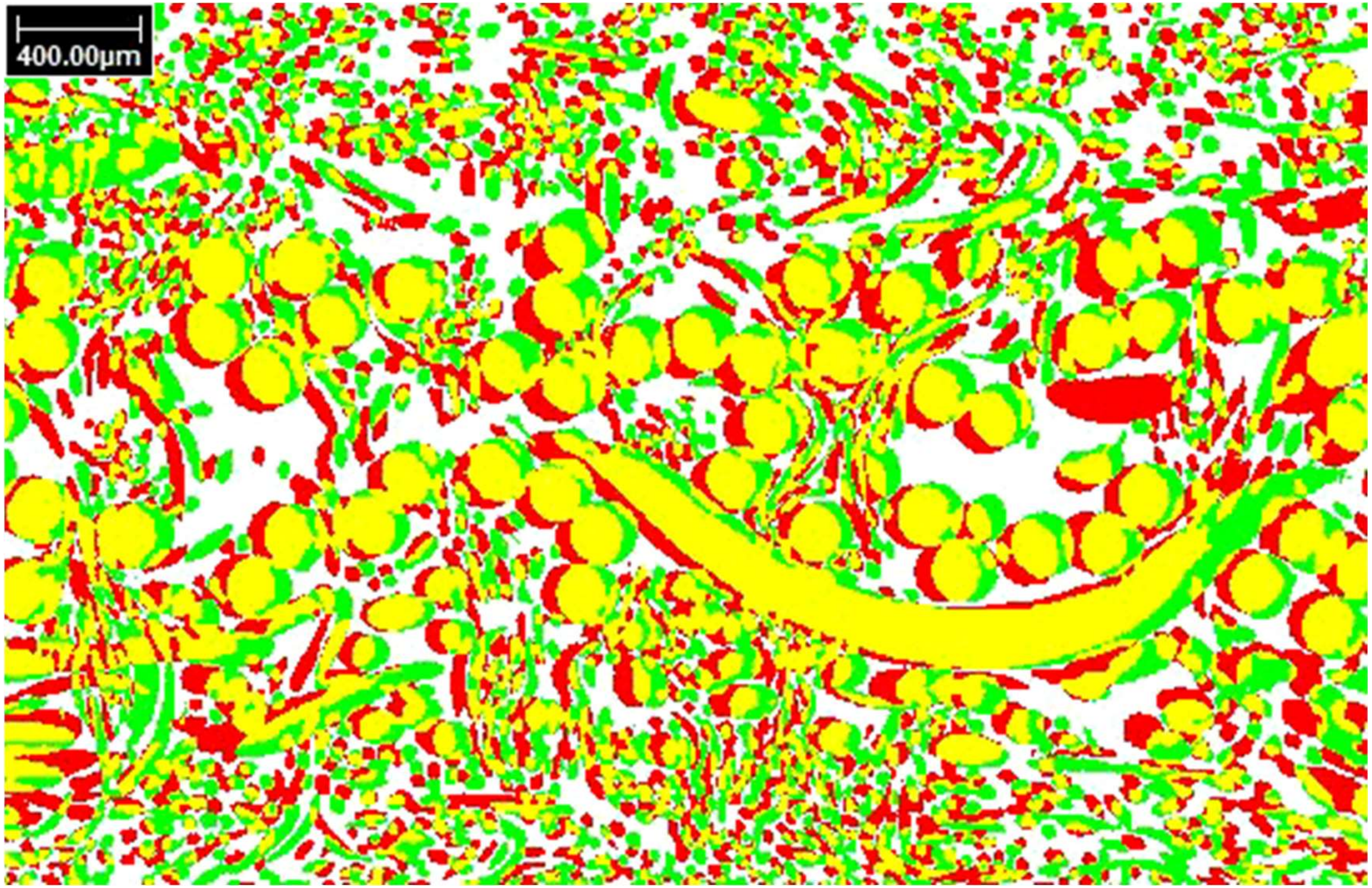
GEODICT

Scan

Simulation

Overlap

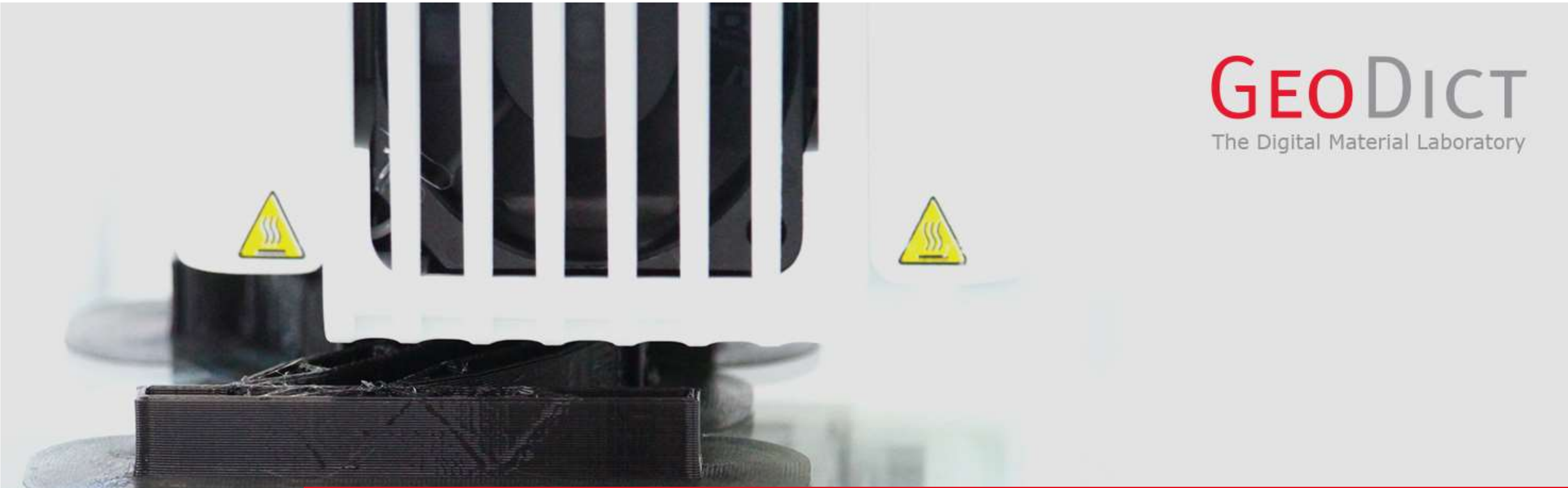
Pore








MATH 2 MARKET




# Simulating Effects of Printing Process in Additive Manufacturing

Janna Krummenacker (IVW), Franz Schreiber (ITWM),
Dr. Constantin Bauer (M2M), Andreas Grießer (M2M),
Andreas Wiegmann PhD (M2M).

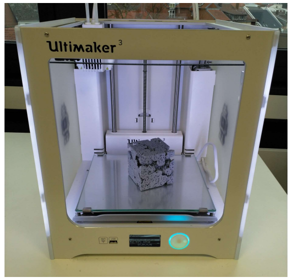


MATH 2 MARKET

# CONTRIBUTIONS

This work requires 3D printing, 3D imaging, mechanical testing, CAD, simulation of the printing process and simulation of the mechanical properties.

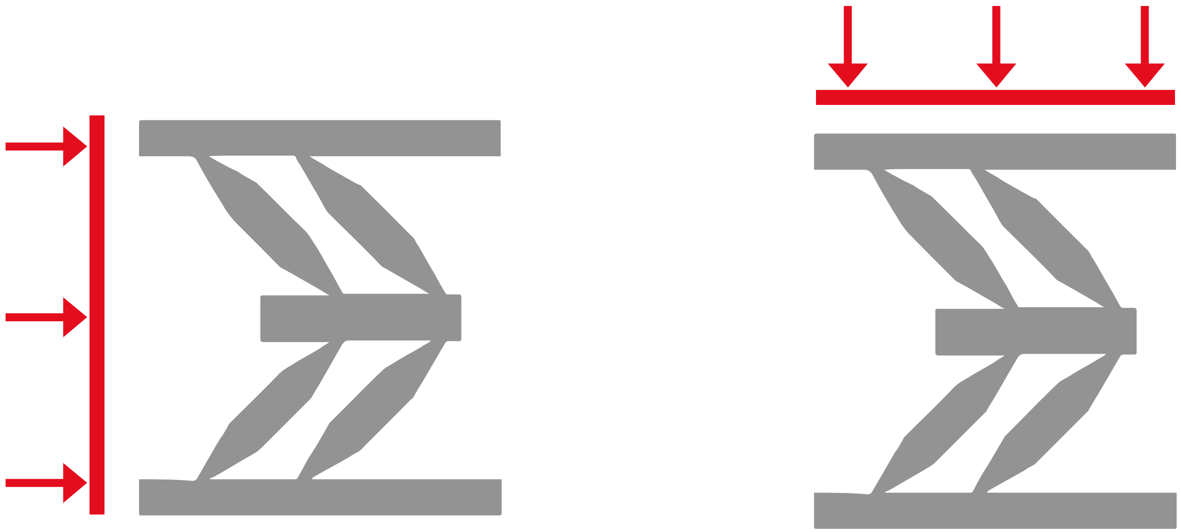
- 3D printing by Math2Market GmbH, Kaiserslautern, Germany, using a commercial Ultimaker 3 printer
- Mechanical Testing by Institute for Composite Materials, IVW, Kaiserslautern
- 3D µCT imaging by Fraunhofer Institute for Industrial Mathematics, ITWM, Kaiserslautern
- CAD design of the meta material, simulation of the printing process and simulation of the mechanical properties by Math2Market GmbH, using GeoDict and Fraunhofer ITWM's FeelMath



# What is special about this mechanical Metamaterial?

In the **horizontal direction**, the material is rather stiff.

In the **other direction**, this material is initially very soft before turning into a very stiff material.

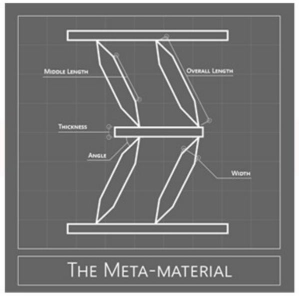


# Simulation on Digital Model

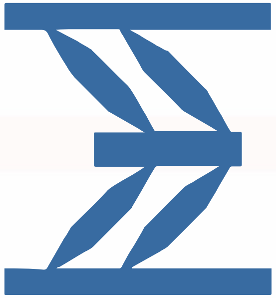
GeoDict

Meta-Material designed for Additive Manufacturing

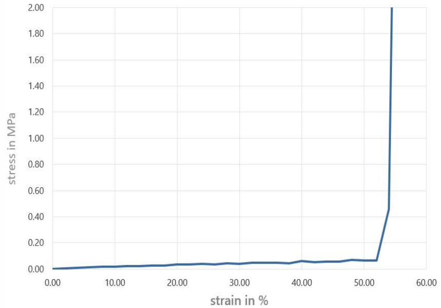
Digital Material




Model



Stiffness





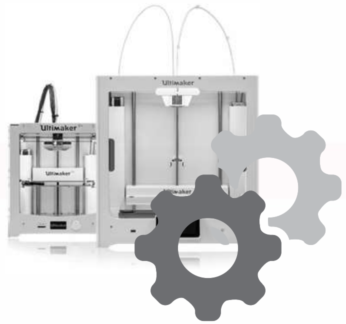
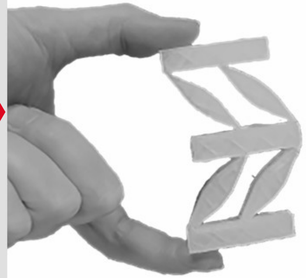



MATH 2 MARKET

# 3D Part by Fused Filament Fabrication

GeoDict

## Prototype manufactured by Additive Manufacturing

| STL-export | Print Parameters | 3D Printer | Physical part |
| --- | --- | --- | --- |
|  with ExportGeo-CAD |  for Slicer Software |  |  |

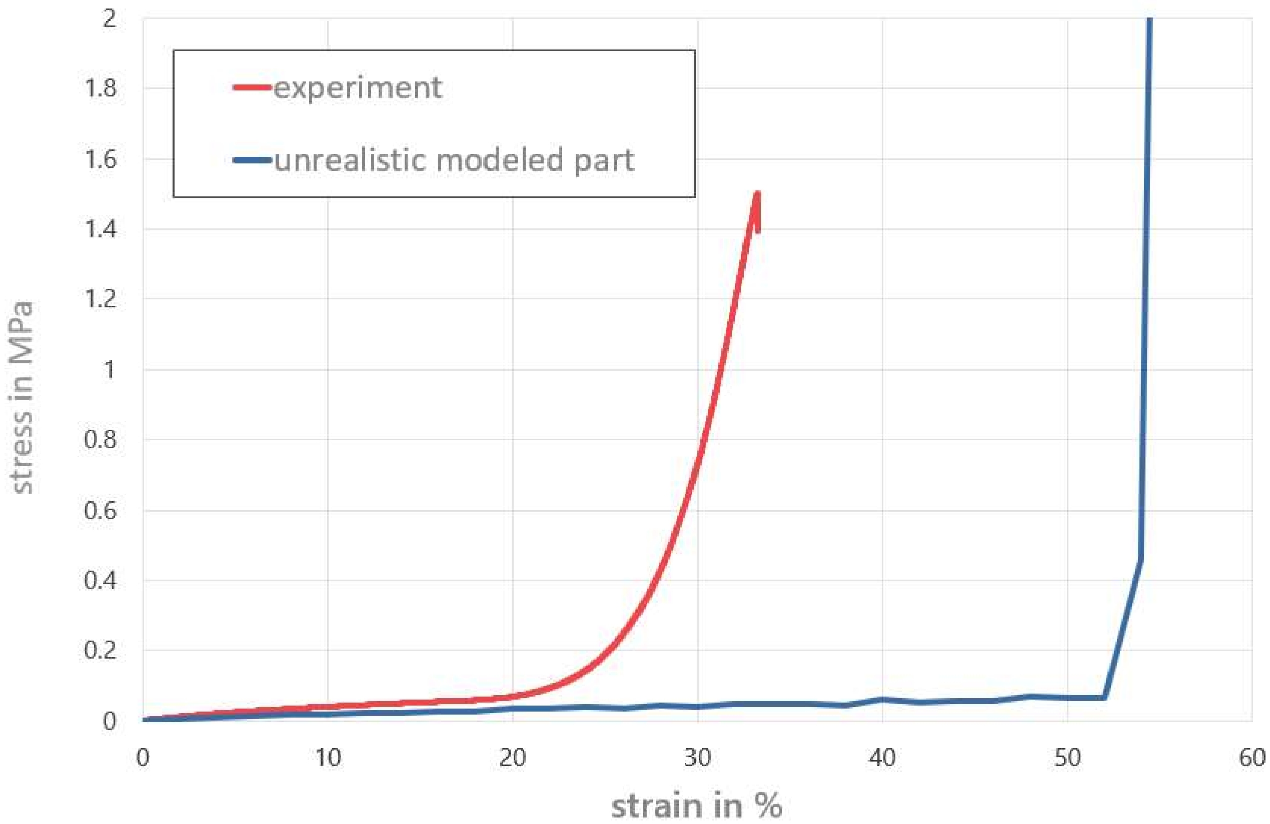




MATH 2 MARKET

# PROBLEM: STANDARD APPROACH TO STIFFNESS PREDICTION IS INSUFFICIENT

GEODICT




Simulated behavior **does not** agree with experiments

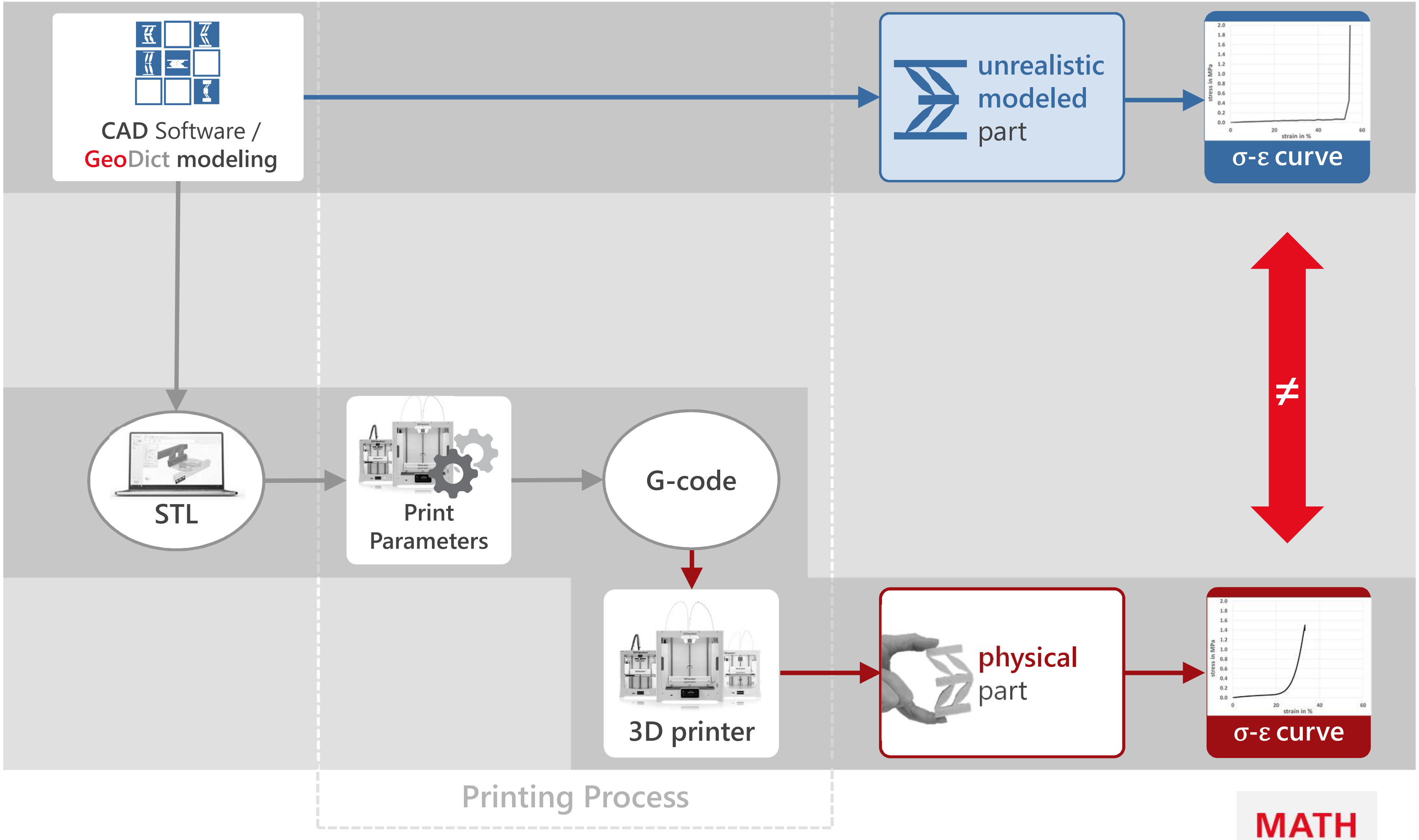




MATH 2 MARKET

# SIMULATION DOES NOT MATCH EXPERIMENT
# PRINTING PROCESS IS NOT MODELLED

GEODICT








MATH 2 MARKET

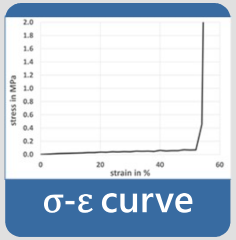
# SIMULATION DOESN'T MATCH EXPERIMENT BECAUSE PRINTING PROCESS IS NOT MODELLED

GeoDict

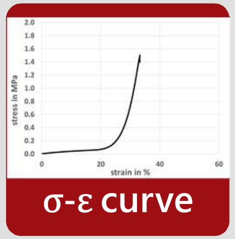
## Questions

- Where does the discrepancy between the curves come from?
- Is it due to not modelling the printing process?
- Is it due to  errors in the mechanics solver?
- Or even both?

?




≠






MATH 2 MARKET

GEODICT

# 1. µCT-SCAN AND IMPORT IN GEODICT

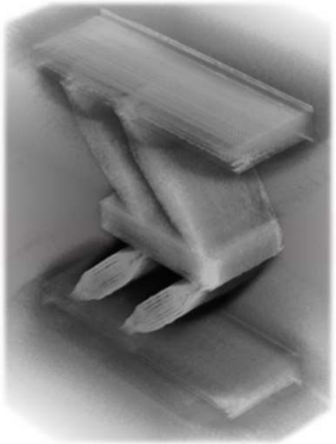
**Printed Part**

in µCT-scanner

**µCT-scanner**

at Fraunhofer ITWM

**CT-data import**



into GeoDict

**Segmented data**

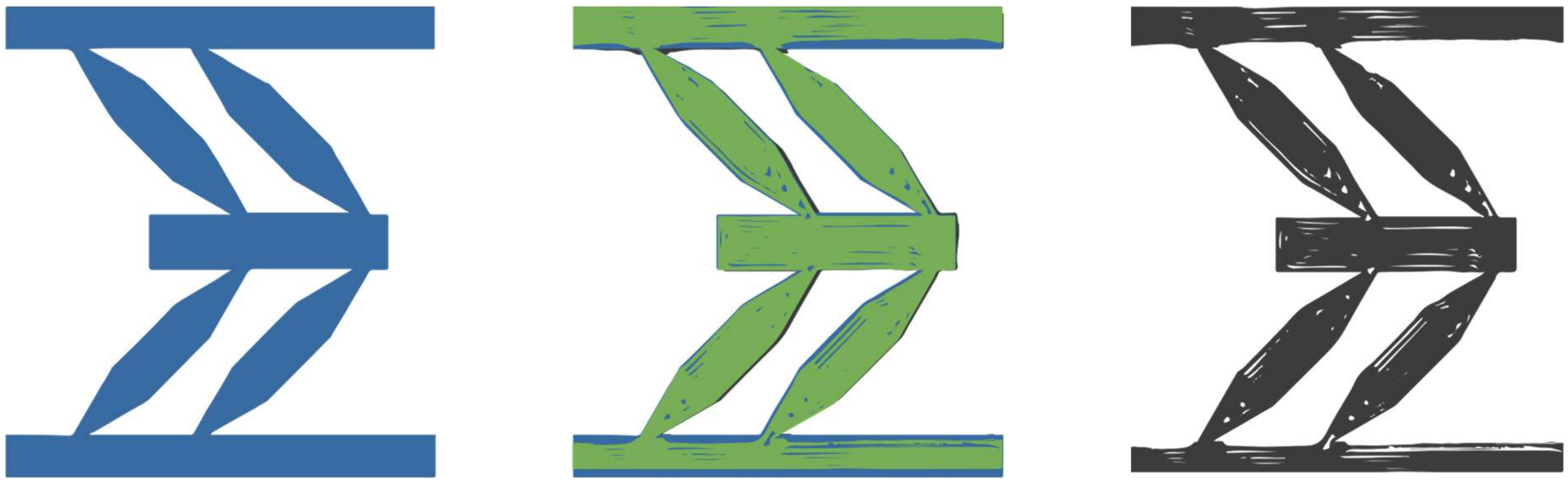




MATH 2 MARKET

# 2. COMPARISON OF UNREALISTIC MODELED AND µCT SCANNED PART



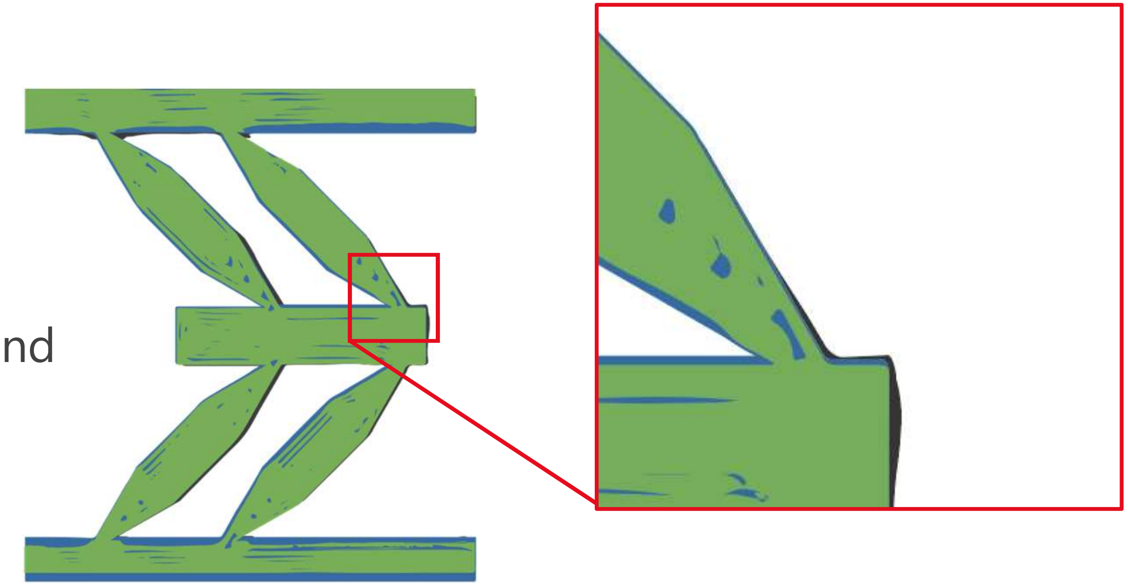


unrealistic modeled part | overlap | µCT scanned part

**Geometrical Validation**

# 3. COMPARISON OF CORNER DETAIL

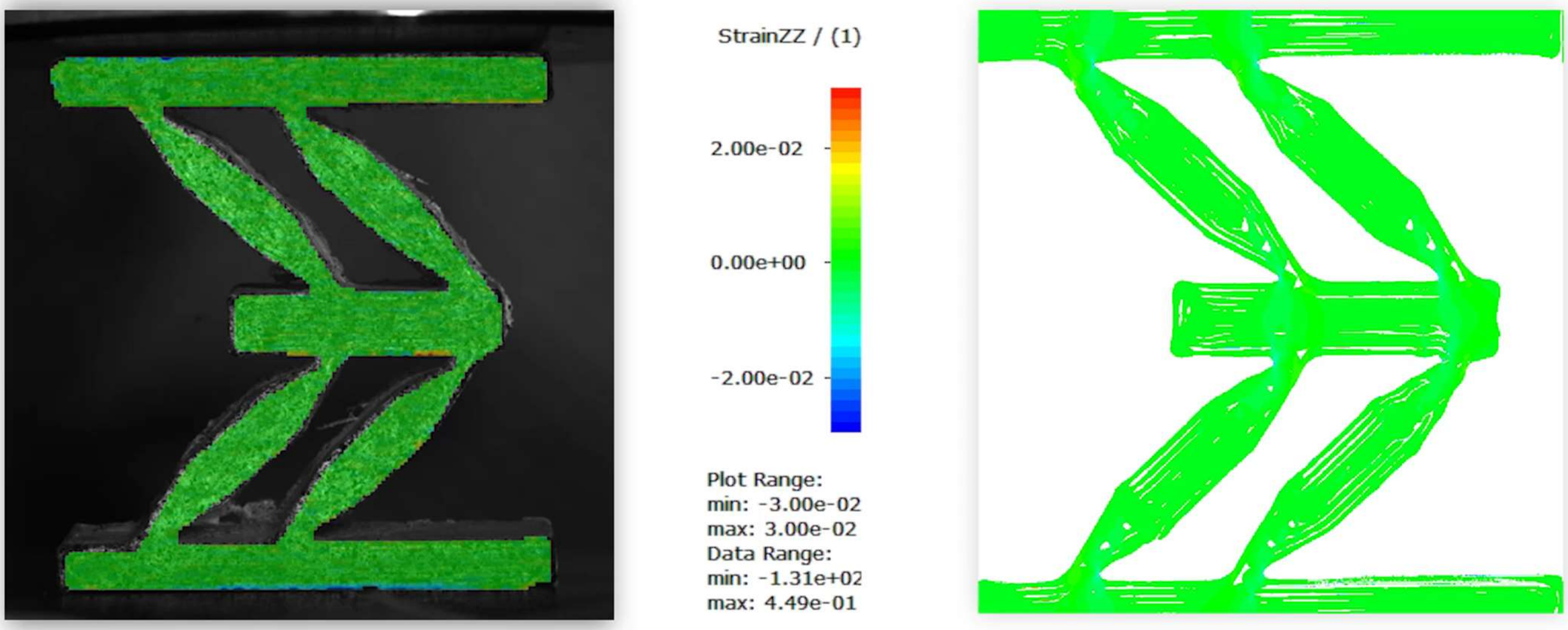
Overlap of
Unrealistic modeled and
CT scanned part



Geometrical Validation

# 4. COMPARISON OF EXPERIMENT WITH SIMULATION

GEODICT




Digital Image Correlation,
Compression experiment

ElastoDict simulation on µCT-scan

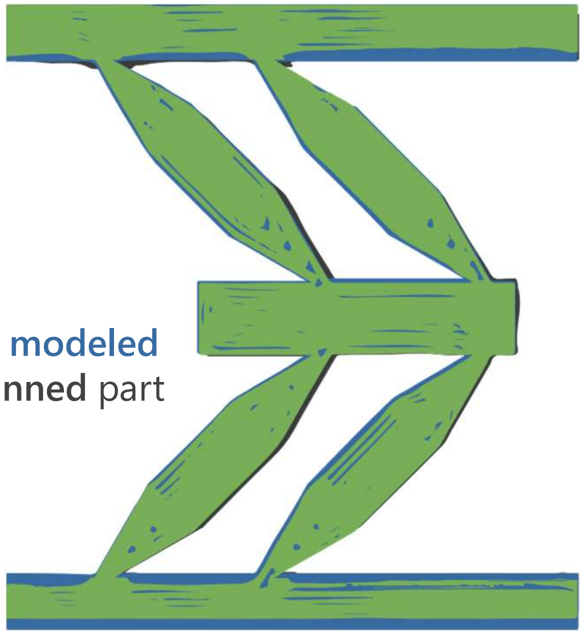




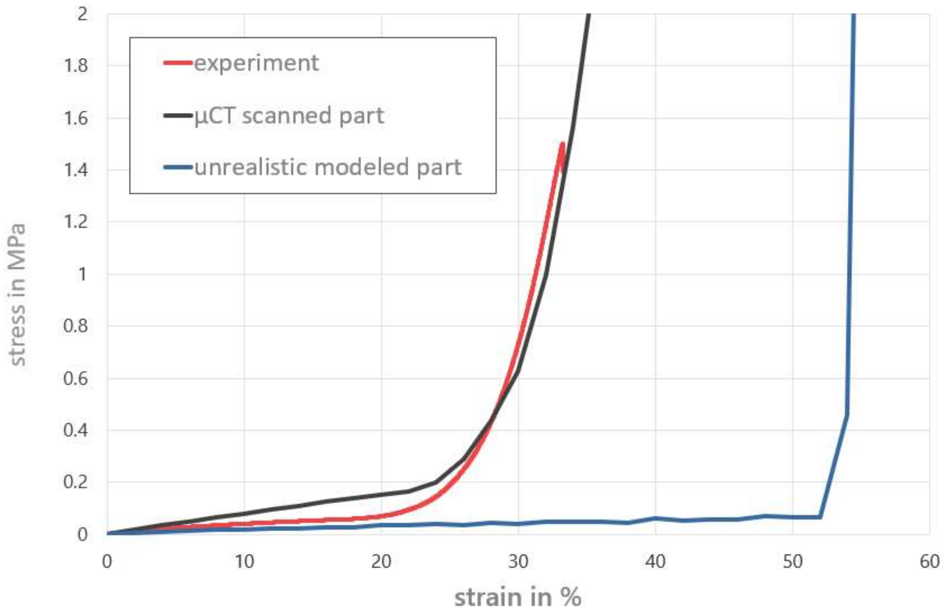
MATH 2 MARKET

# Mechanics simulation agrees with experiment when applied to µCT scan

GeoDict



Overlap of
Unrealistic modeled
and **CT scanned** part




Geometrical Validation

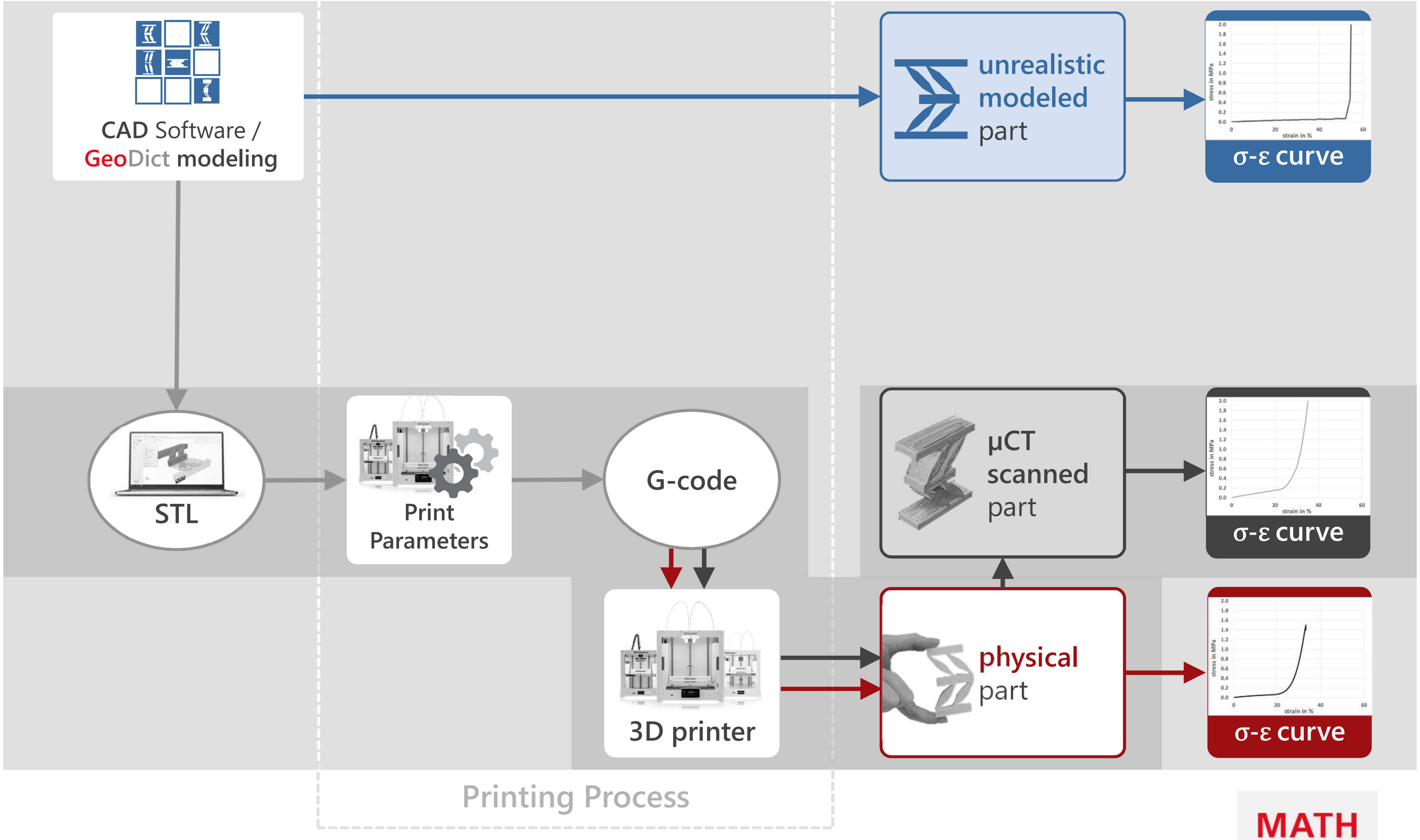
Property Validation





MATH 2 MARKET

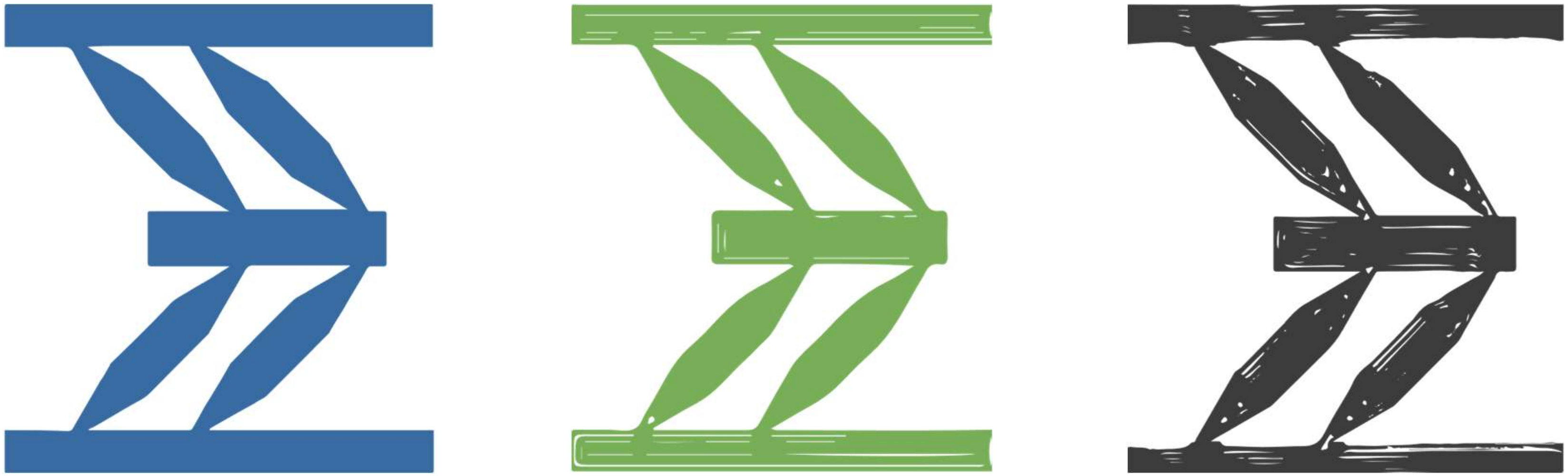
# PROBLEM WOULD BE SOLVED IF OUR MODEL WERE MORE SIMILAR TO THE µCT SCAN



## And here, magic happens…

# Introducing ImportGeo-AM

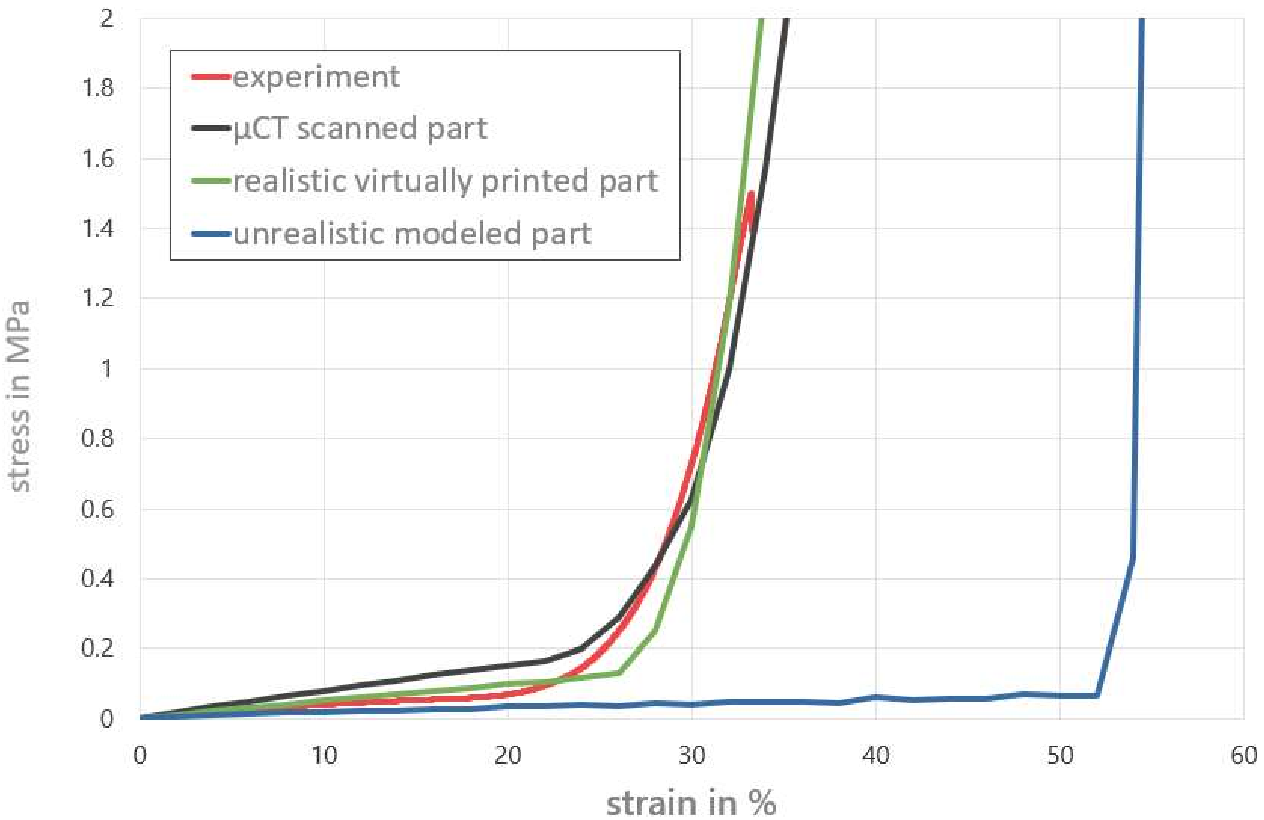
Take output of printer software and create 3D model that takes into account the printing process



unrealistic part | realistic virtually printed part | µCT scan of part

**Geometrical Validation**

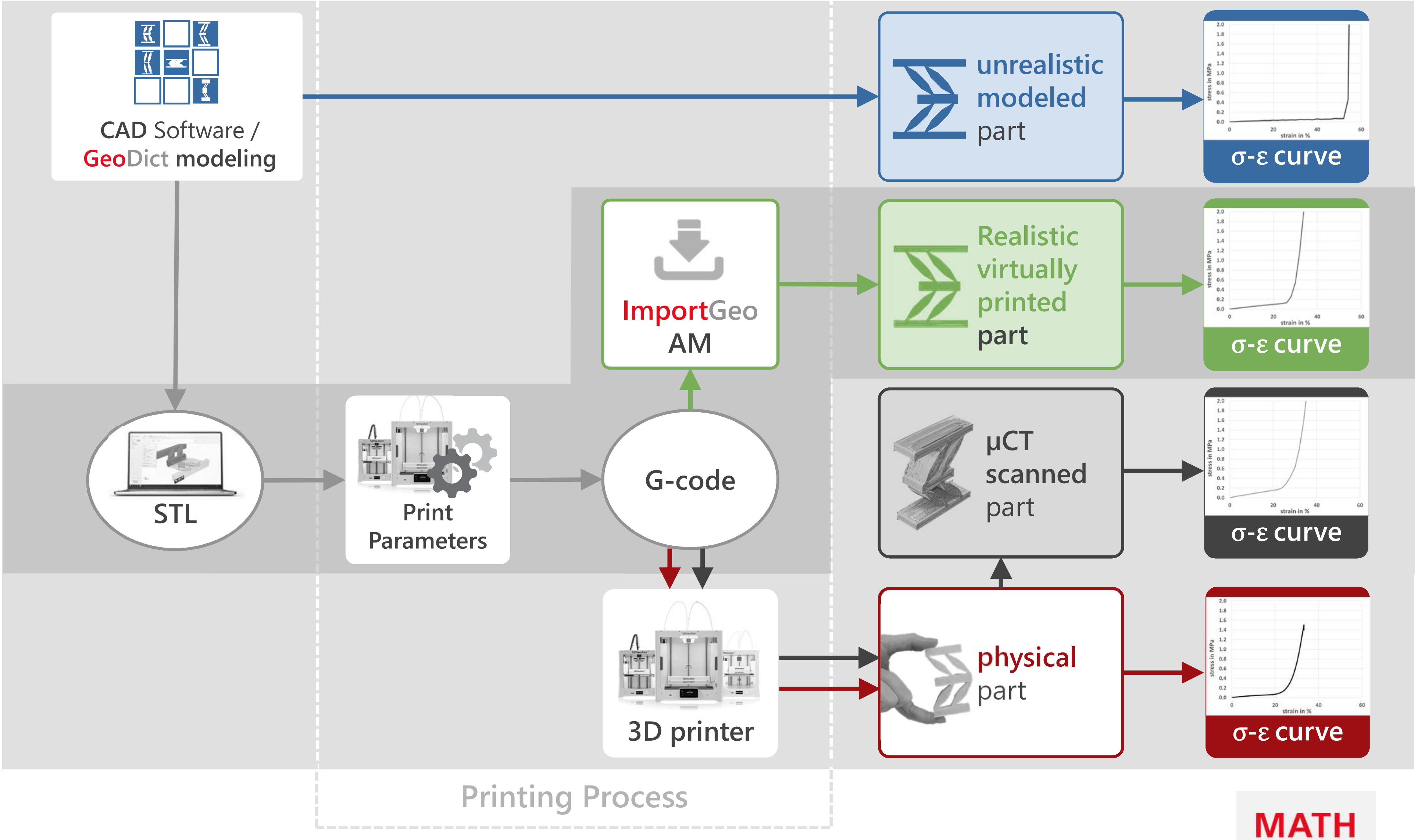
# SOLUTION: GEODICT ENHANCED APPROACH TO STRESS-STRAIN PREDICTION MATCHES EXPERIMENT




Simulation of the printing process is necessary for correct prediction of the stress-strain curve.

# Simulating the printing process leads to agreement of simulated and experimental curves

GeoDict



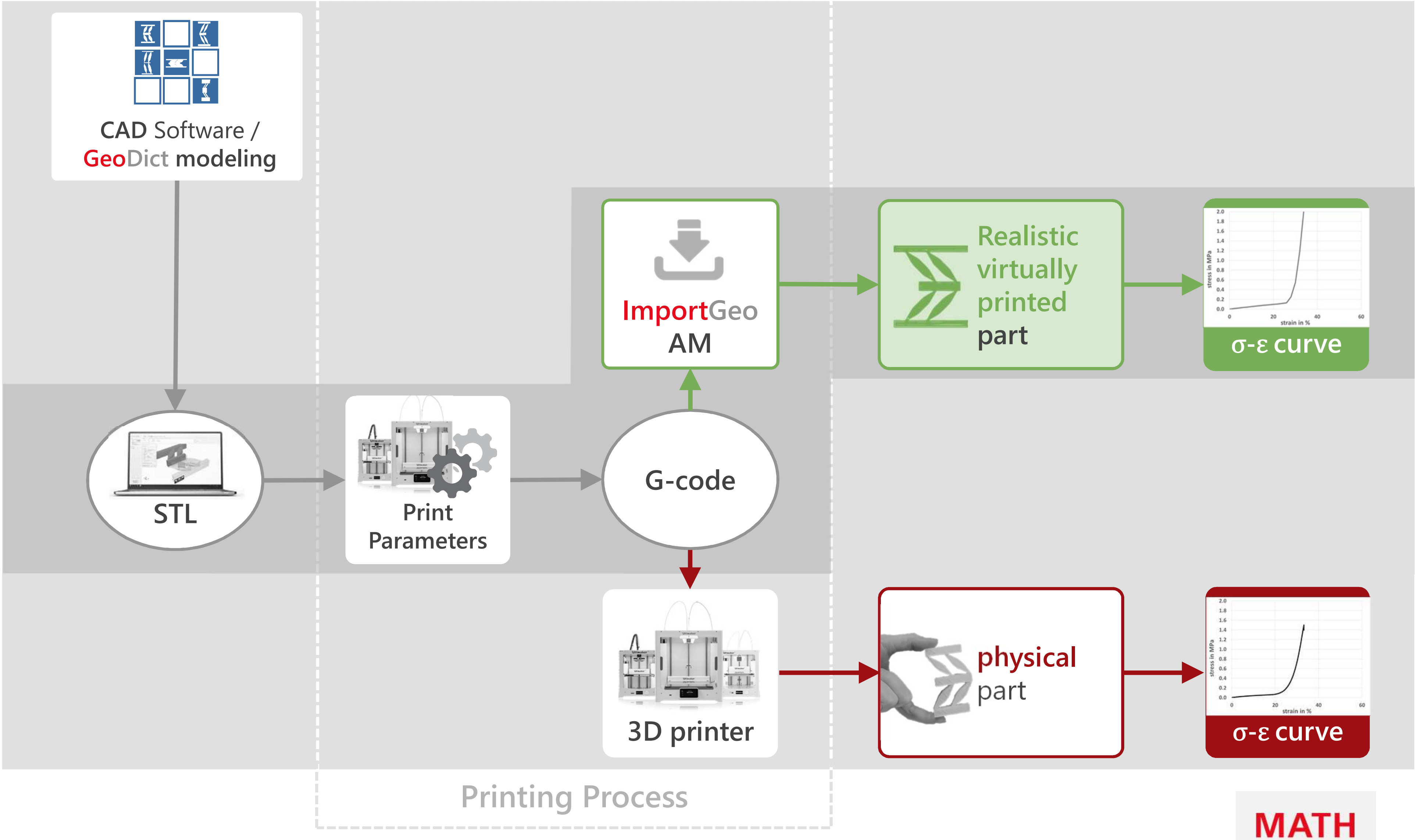





MATH 2 MARKET

# Modelling the printing process leads to agreement of stress-strain curves

GeoDict








MATH
2 MARKET

GEODICT
The Digital Material Laboratory

# CATALYTIC CONVERTERS, GPF AND DPF

Image source: https://www.thermofisher.com/blog/metals/new-reduced-platinum-catalyst-for-catalytic-converters/

**Andreas Wiegmann, Anja Streit, Andreas Weber, Liping Cheng, Mehdi Azimian, Erik Glatt & Jürgen Becker**

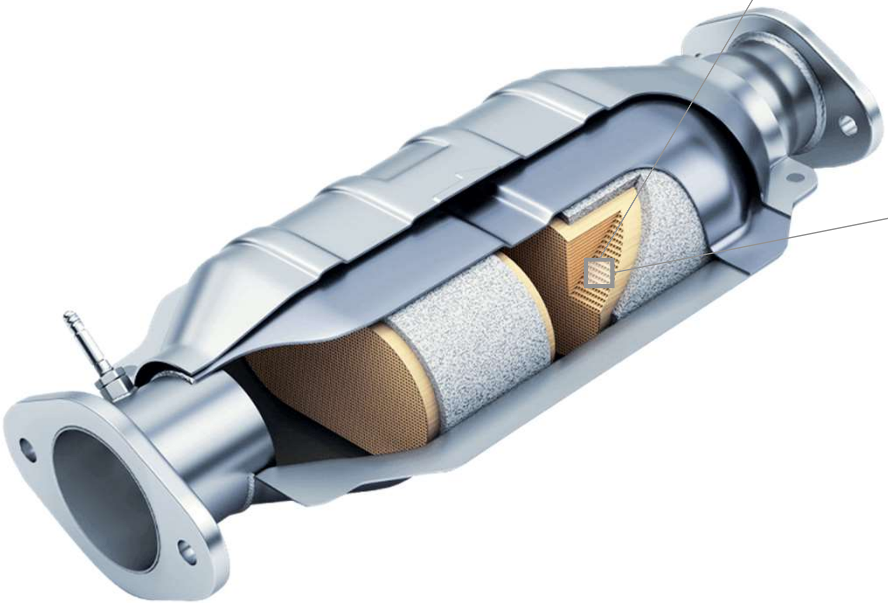
MATH 2 MARKET

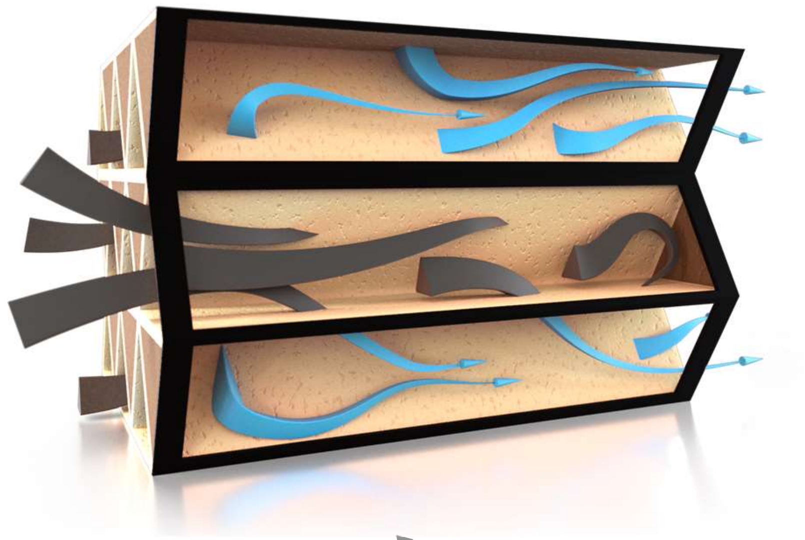
# Modeling aftertreatment using residence times

GeoDict

Reactive flow simulation with
AddiDict residence time tracking

For example in a car exhaust catalyst / DPF:
Reduction of Nox, HC and CO
Removal of soot







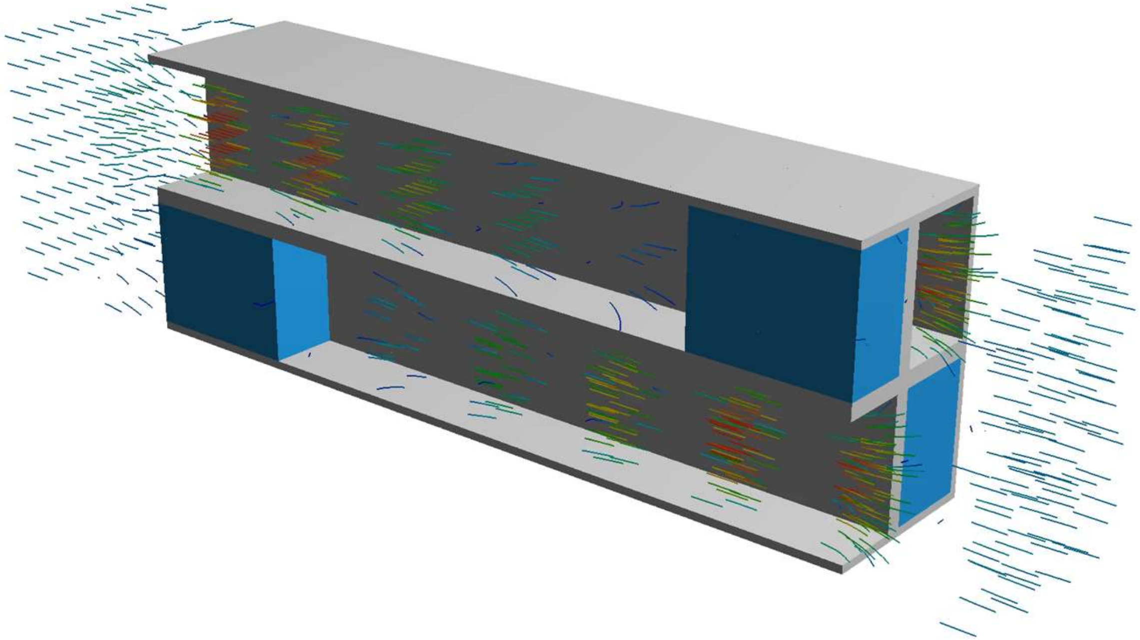


MATH 2 MARKET

# Flow Through Particulate Filter (plugged)

GeoDict

- Flow simulation through channels and walls (porous catalyst).
- Walls are modelled as porous material. Effective properties are computed from simulation on fully resolved scale.







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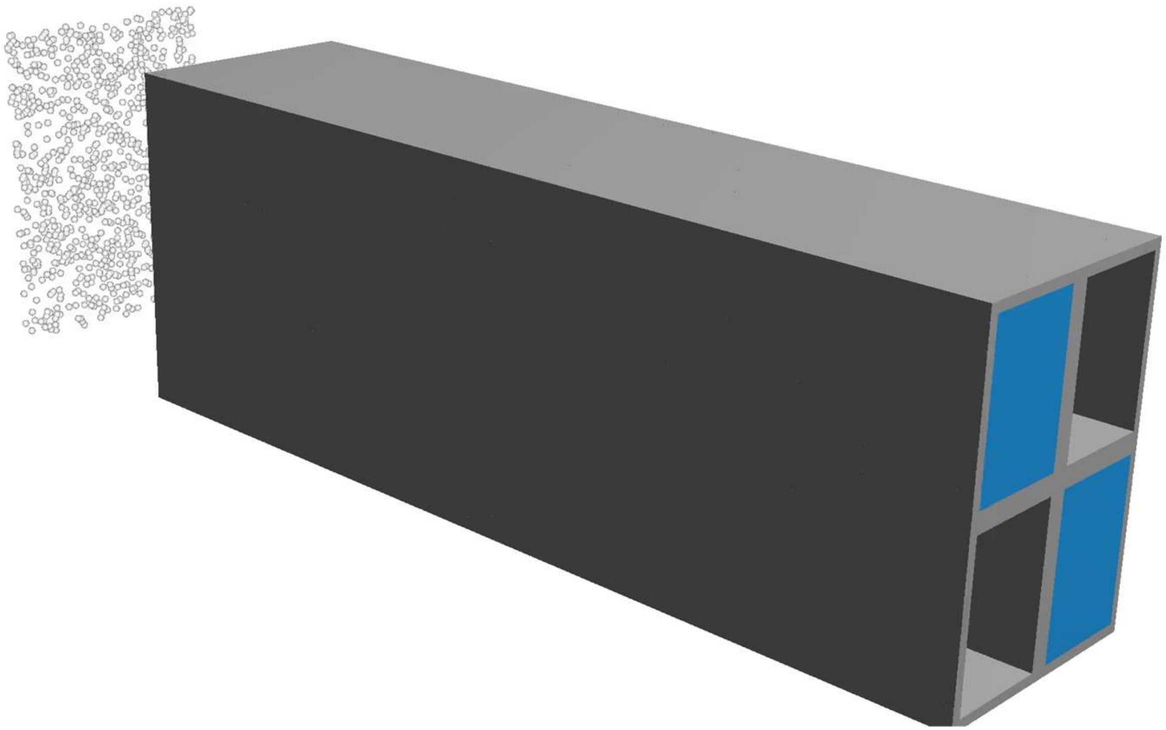
# Molecule Motion in particulate filter (plugged)

GeoDict

- Simulate molecule motion in flow field and due to diffusion.
- Bounces of the molecules at the interface between channel and the porous walls are available in GeoDict 2020.







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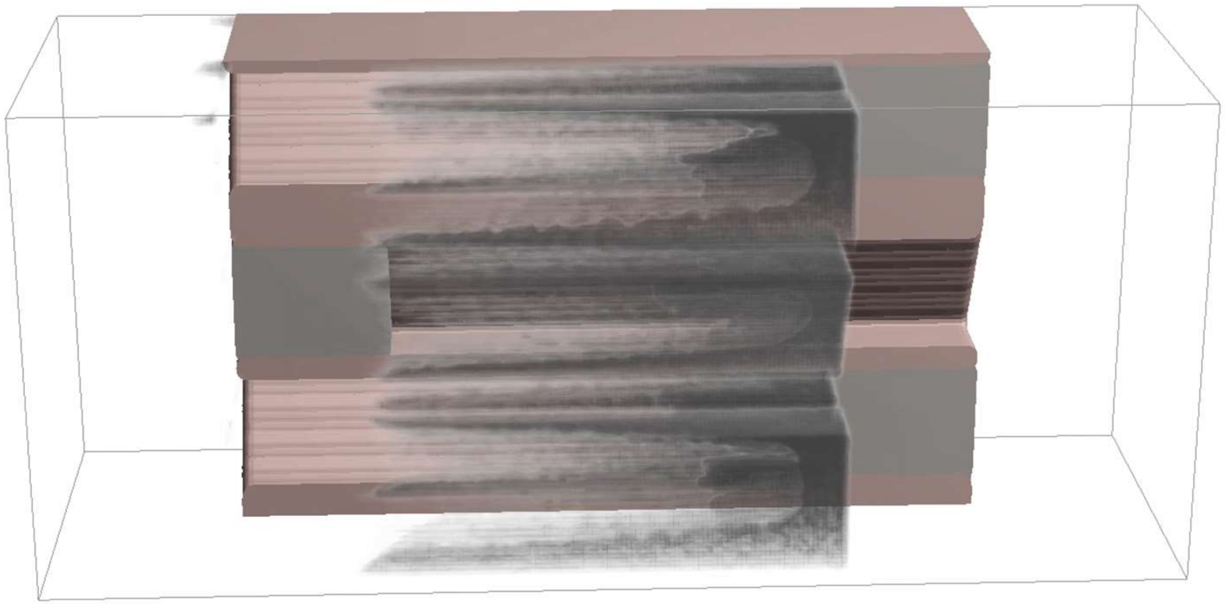
# SOOT DEPOSITION IN A HONEYCOMB

GeoDict







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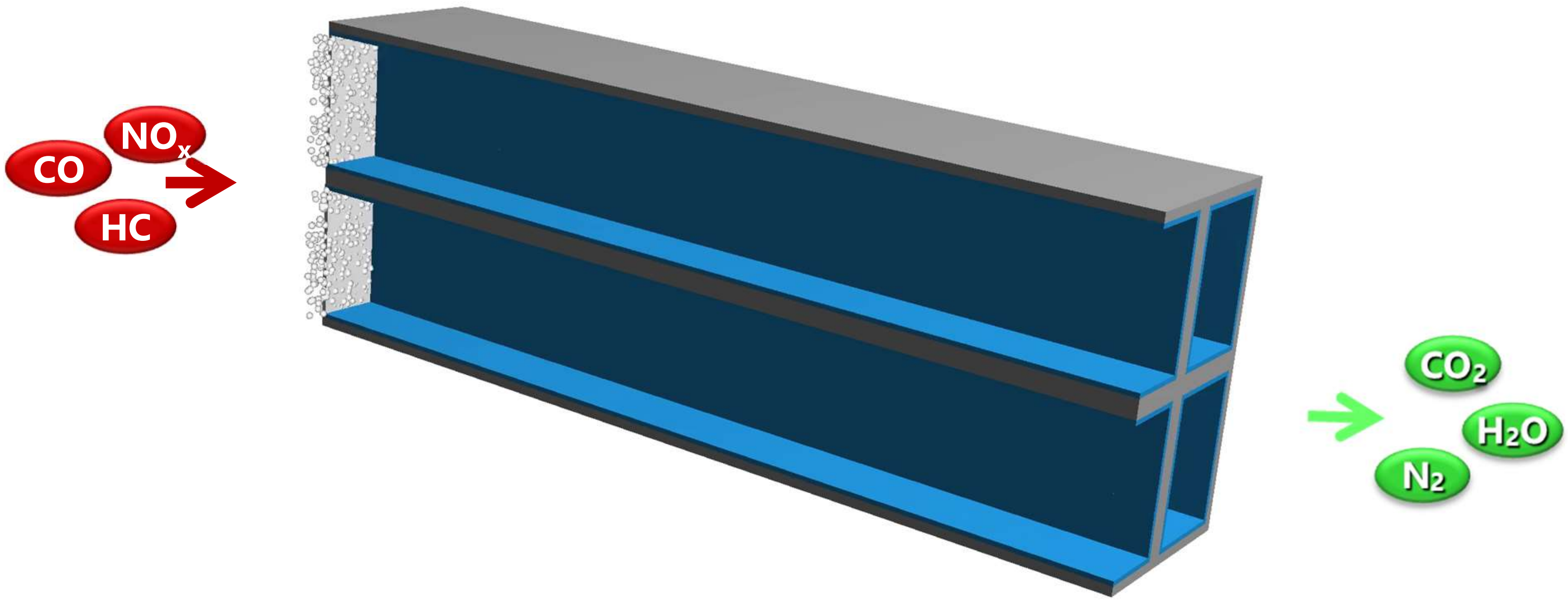
# MOLECULE MOTION IN CATALYST (NO PLUGS)

GEODICT

Flow simulation through channels, porous walls (dark gray) and reaction layer (blue). Used periodic boundary conditions to simulate much larger channel geometry. Use new feature of placing particles in specifiable locations (light gray area in the inlet)





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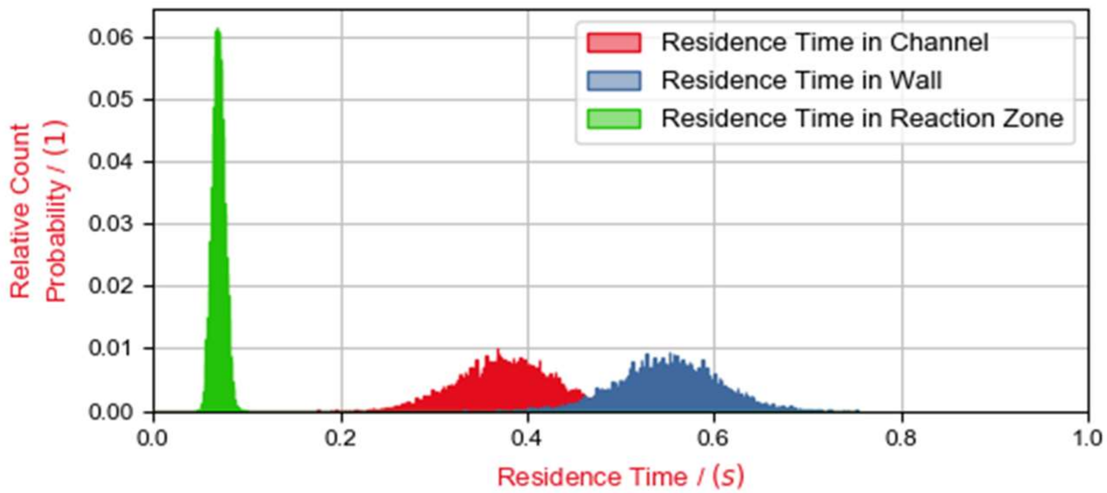
# Residence Times in Catalyst

GeoDict

- Track the residence times in channel, walls and reaction layer in GeoDict.
- Export the residence times for all molecules for postprocessing , for example for deriving reaction rates.




Total simulation time: 1s

Particles spend between 40% and 70% of the time in the wall. An around 7% of the time in the reaction layer.



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# TWO SOURCES OF PRESSURE LOSS IN DPF

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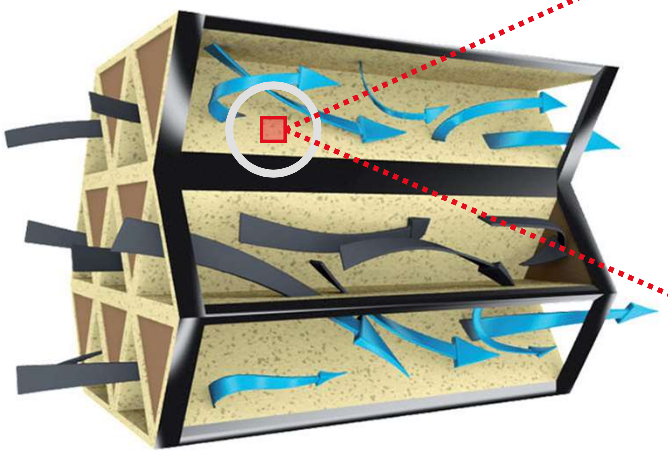
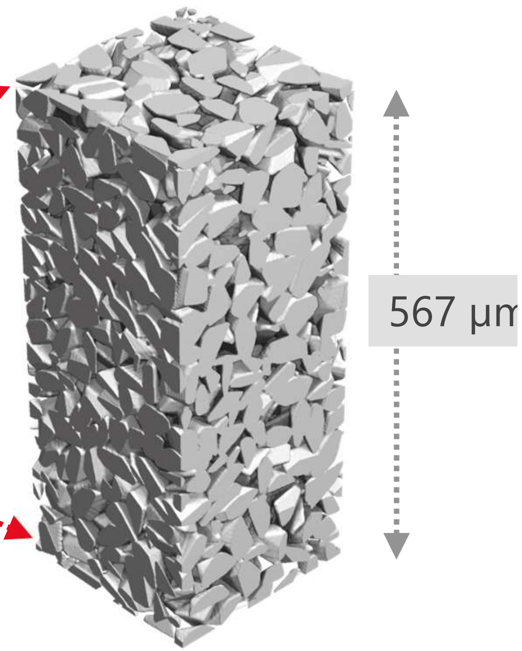
1. Across the ceramic micro structure
2. Along the channels due to capillary forces






2.

1.

- We simulate them separately.
- In both cases, we simulate the loading of an initially clean filter.

# Binarized PMS images

## FROM POLISHED MICROGRAPH SECTIONS AND MODELED SINTERED CERAMICS

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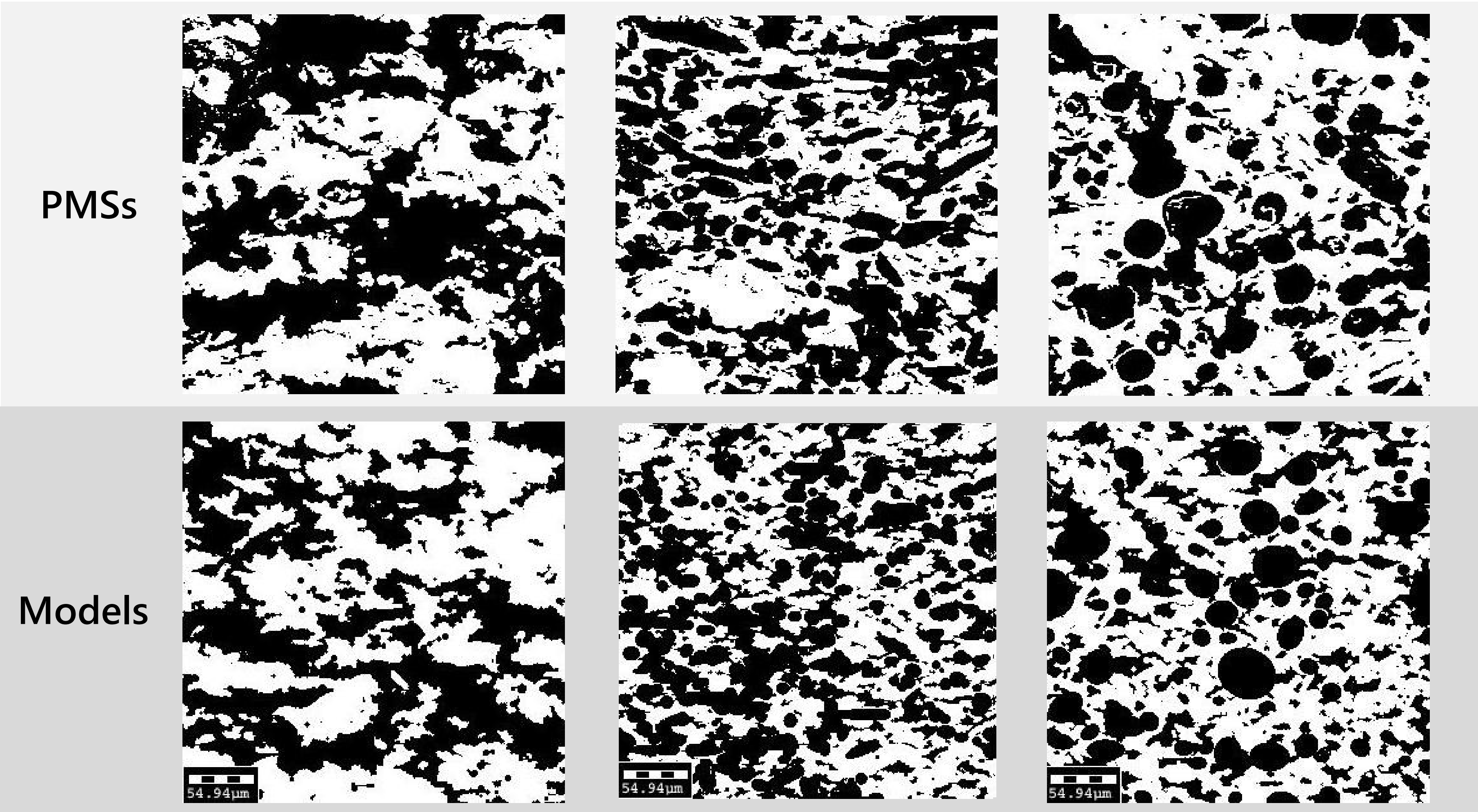

# Measured porosities & permeabilities

## of real ceramics vs modeled porosities & simulated permeabilities on modeled ceramics

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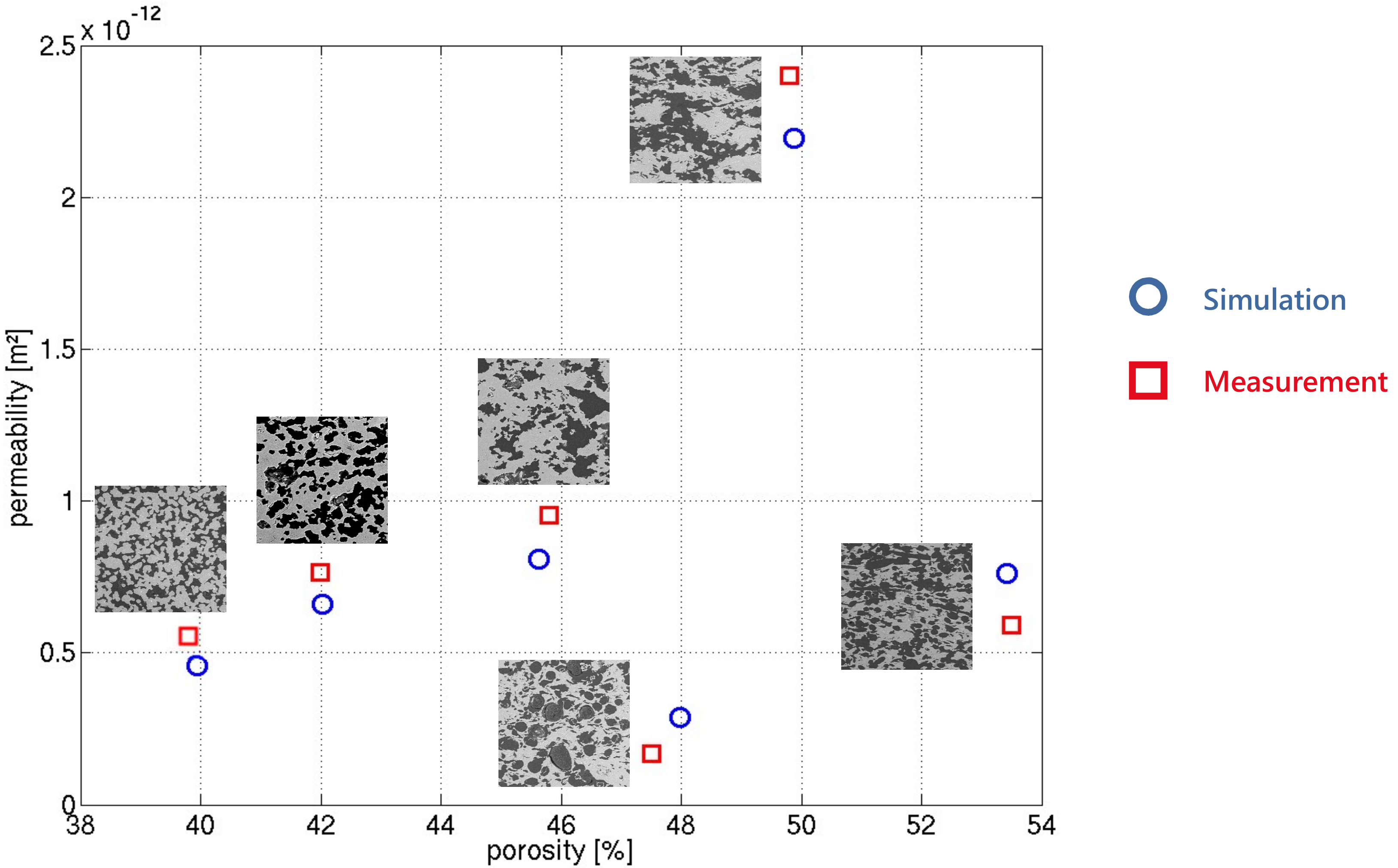

# SPATIAL PARTICLES DEPOSITION OVER TIME

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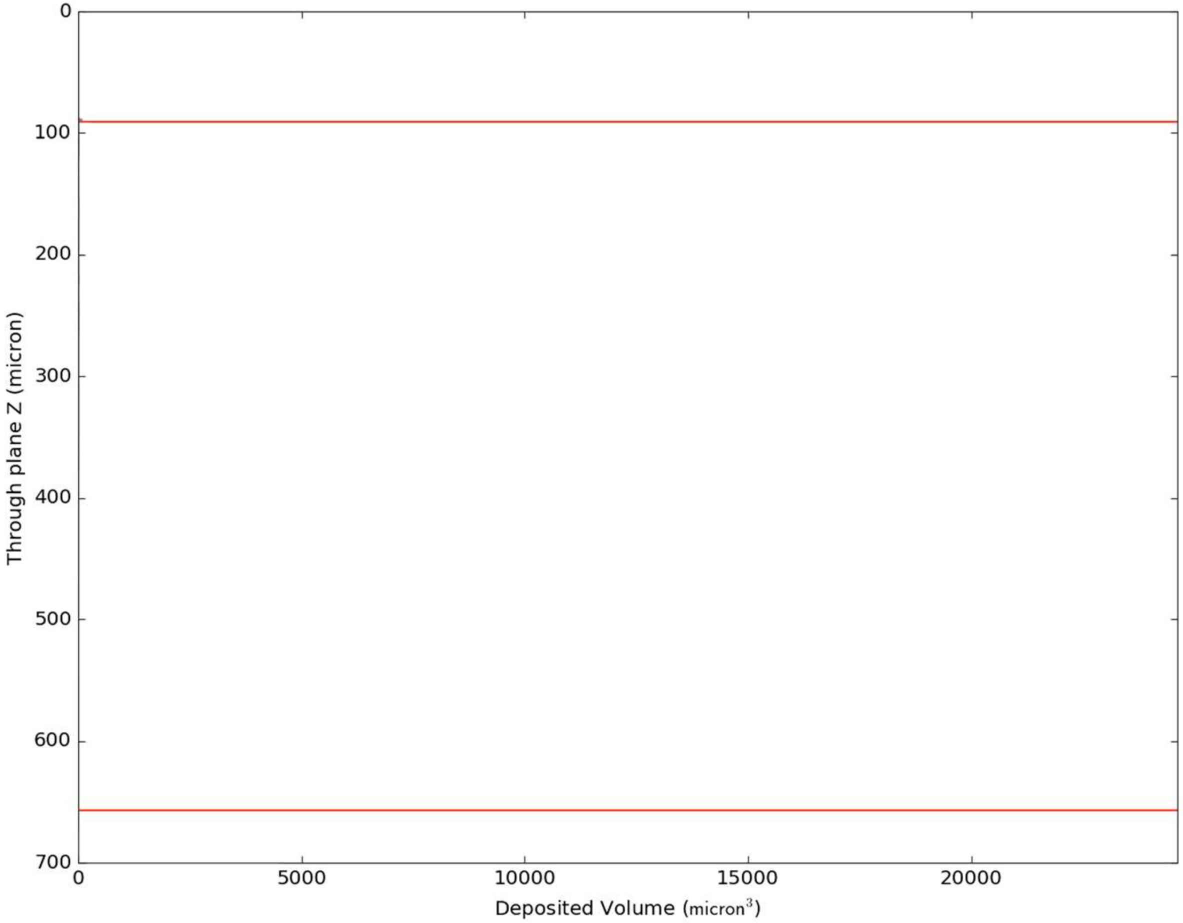


# REDUCED PRESSURE DROP OVER TIME

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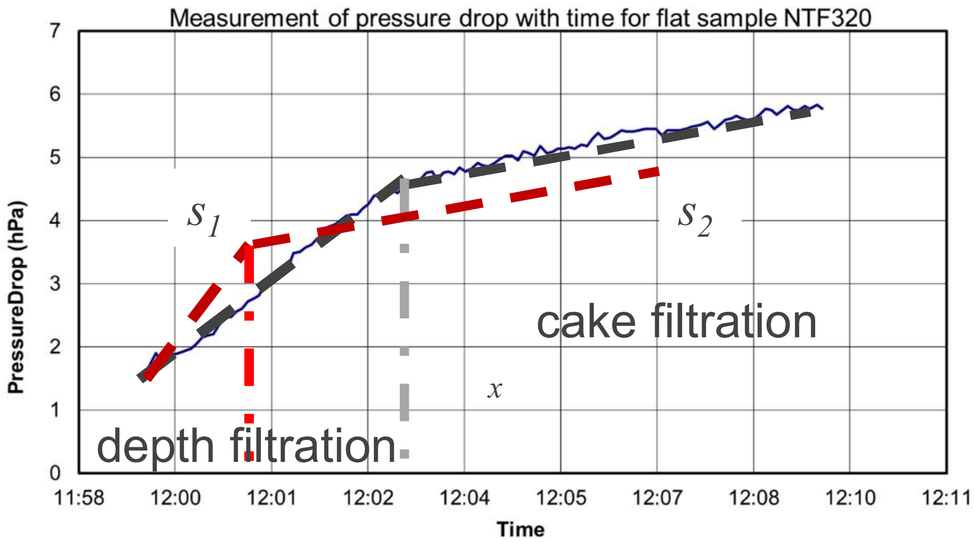
After fast initial pressure drop increase (slope s1, depth filtration phase)
follows long slower pressure drop increase (slope s2, cake filtration phase)

- Matched experiment with simulations

Fraunhofer IKTS

- **Shortened depth phase to lower pressure drop during cake phase**

- Fraunhofer IKTS manufactured ceramic, experiment matched simulations, and patent was granted: *Particulate filter, No. DE102012220181 A1*



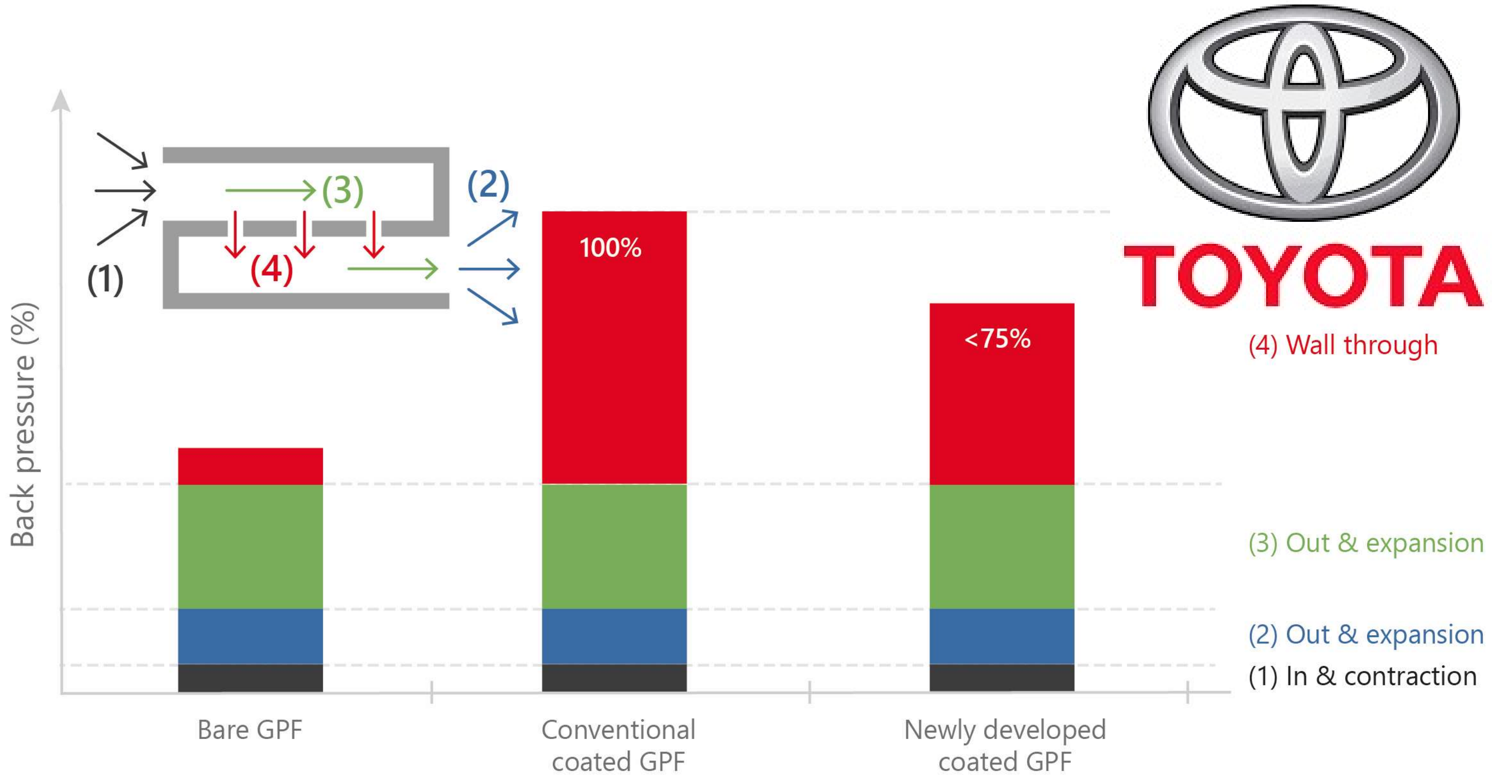

# FINDING A NEW GPF MATERIAL WITH GEODICT

GEODICT

At World Congress Experience 2018, **Toyota Motor Company** presented „Development of Low Pressure and High Performance GPF Catalyst".
https://www.sae.org/publications/technical-papers/content/2018-01-1261/

GeoDict software helps to reduce back pressure in Gasoline Particulate Filters by 25%.

microstructure of wash coats analyzed, understood and improved with GeoDict



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# Rendering of Materials and Simulation Results

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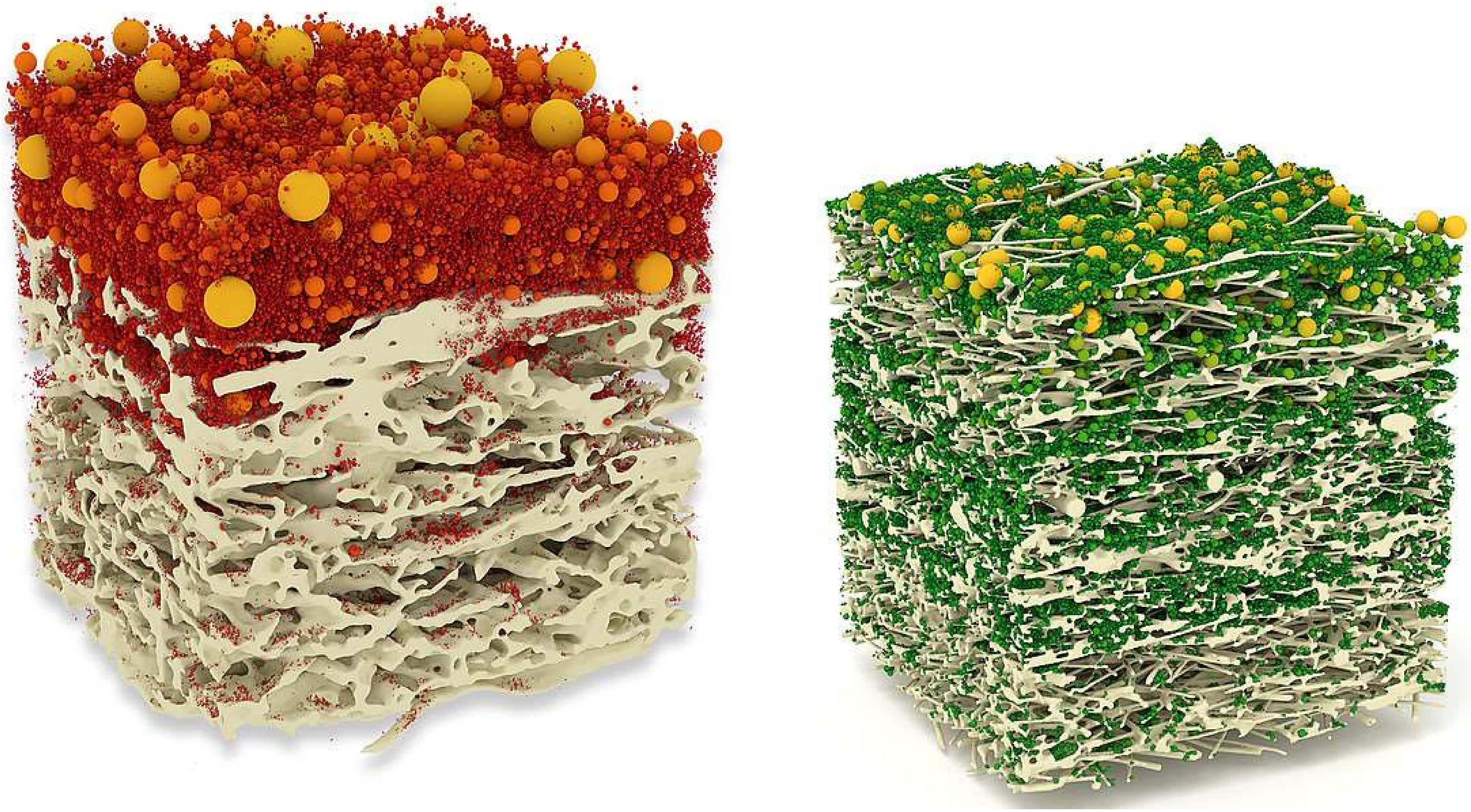

Source: **MANN+HUMMEL**

# GEODICT CAN ALSO BE USED TO EXPORT MODELS FOR 3-D PRINTING

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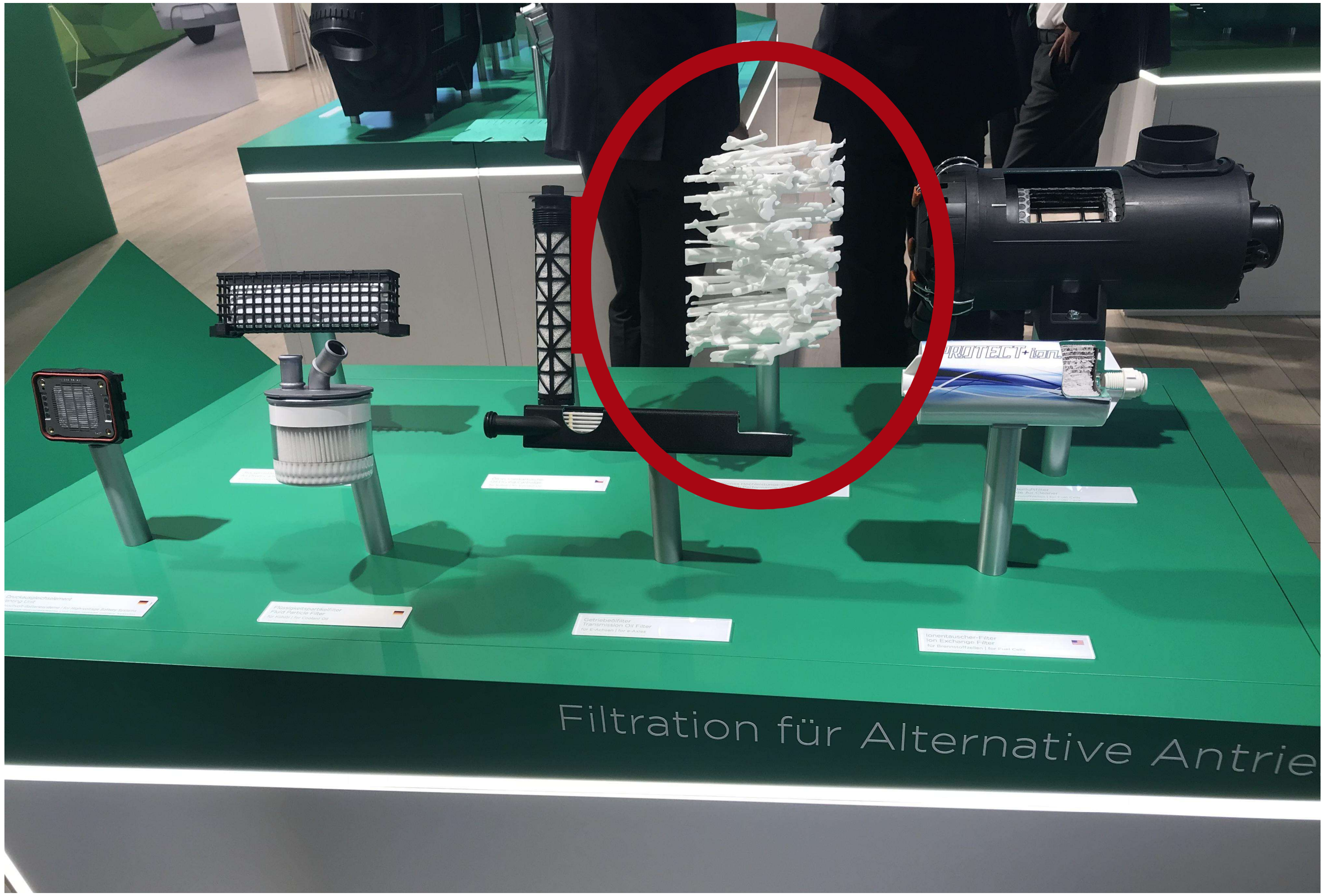
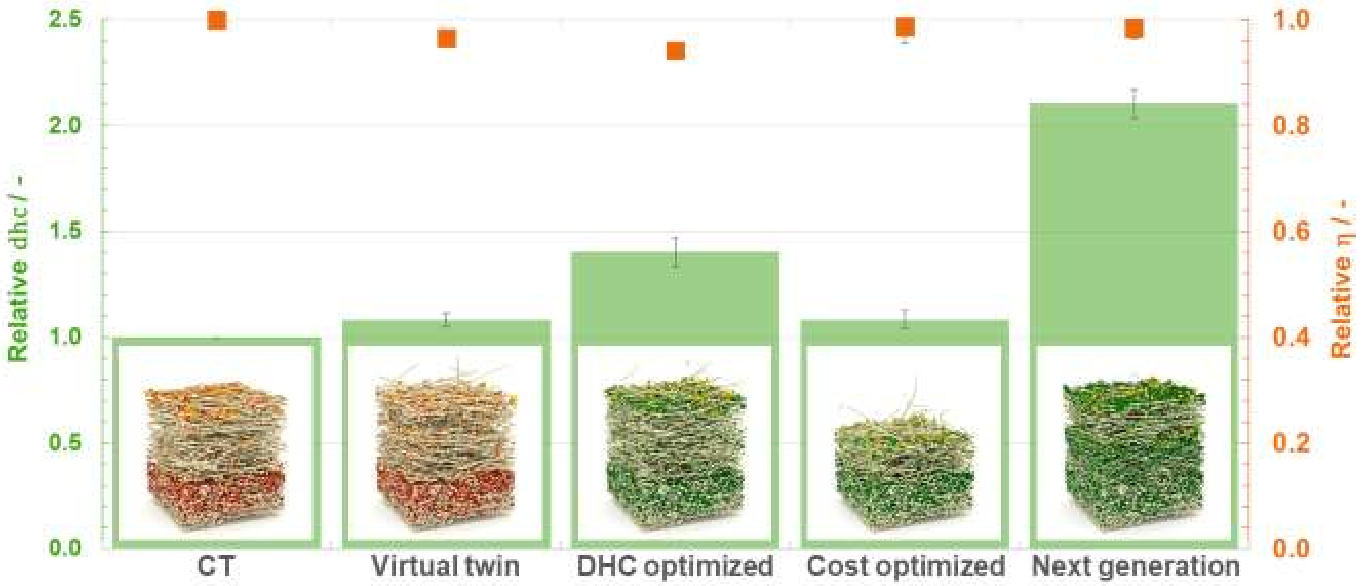



Source: **MANN+HUMMEL** on LinkedIn

MATH 2 MARKET

## Optimization of a virtual filter media prototype
## Pushing the limits 2.0 – next generation




11 | Kaiserslautern, September 27th, 2017
Simulation-driven development and optimization of virtual filter media prototypes

MANN+HUMMEL

Source: **MANN+HUMMEL**

## Simulation process automation with GeoPython
## There is no free lunch – what did it take?

| | Number of variations |
|---|---|
| ▪ **Fiber characteristics** | |
| ▪ Fiber type | |
| ▪ Fiber diameter $d$ | |
| ▪ Fiber shape $a\,b^{-1}$ | |
| ▪ Fiber orientation | |
| ▪ **Fiber structure** | |
| ▪ Number of layers $n$ | → 1 |
| ▪ Fiber mix $\varphi$ | → 5 |
| ▪ Grammage $G$ | |
| ▪ Thickness $t$ | → 4 |
| ▪ Packing density $1\text{-}\varepsilon$ | → 3 |
| Stochasticity → multiple samples per design | 3 x 60 |
| Total samples: | 180 |

Size of one domain: $1024\ x\ 1024\ x\ 2048$ voxels!

Computation time per simulation: ~2.5 weeks / ~420 hours

→ **~75 k hours**

→ managable only by high degree of automation
→ extensive use of GeoDict's macro features

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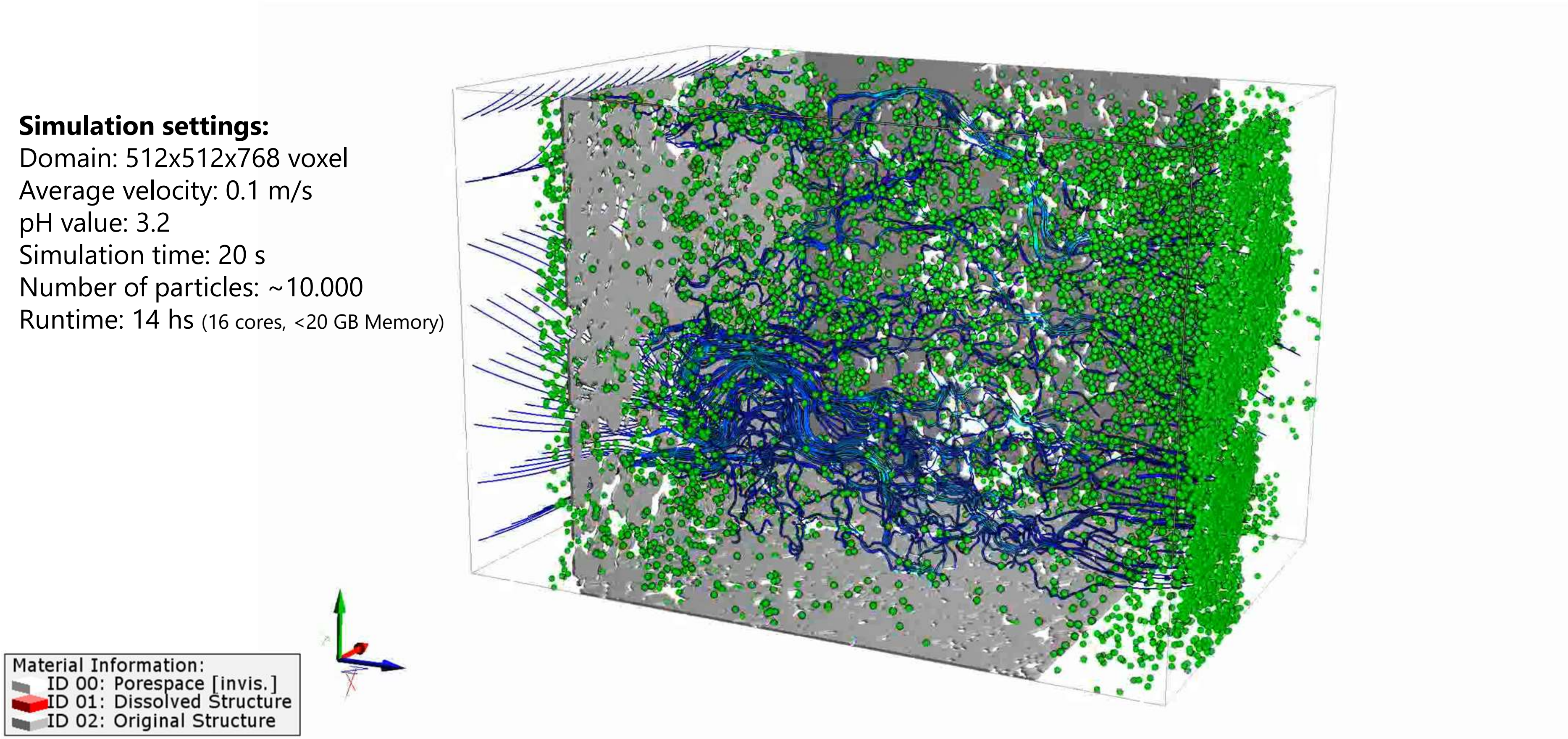
Simulation-driven development and optimization of virtual filter media prototypes

MANN+HUMMEL

Source: **MANN+HUMMEL**

# „LARGE“ SIMULATION

**Simulation settings:**
Domain: 512x512x768 voxel
Average velocity: 0.1 m/s
pH value: 3.2
Simulation time: 20 s
Number of particles: ~10.000
Runtime: 14 hs (16 cores, <20 GB Memory)



# CONCLUSION

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- For fuel cells, batteries and aftertreatment catalysts, the material's microstructure has a great influence on the performance
- The microstructure can be accessed by µCT, FIB-SEM & 3D image processing software
- The microstructure can be modelled by structure generators
- Material characterization can be done on images just as by experiments
  - Transport, Diffusion, Conduction
  - Stiffness, Deformation
- The development of next generation materials can be accelerated by screening designs digitally, first.
- You can do all this yourself with our easy-to-use, highly efficient and well-documented software

# NEXT GENERATION MATERIALS WITH GEODICT®

GEODICT

The materials of the future are within reach
and **we help you find them faster**.






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