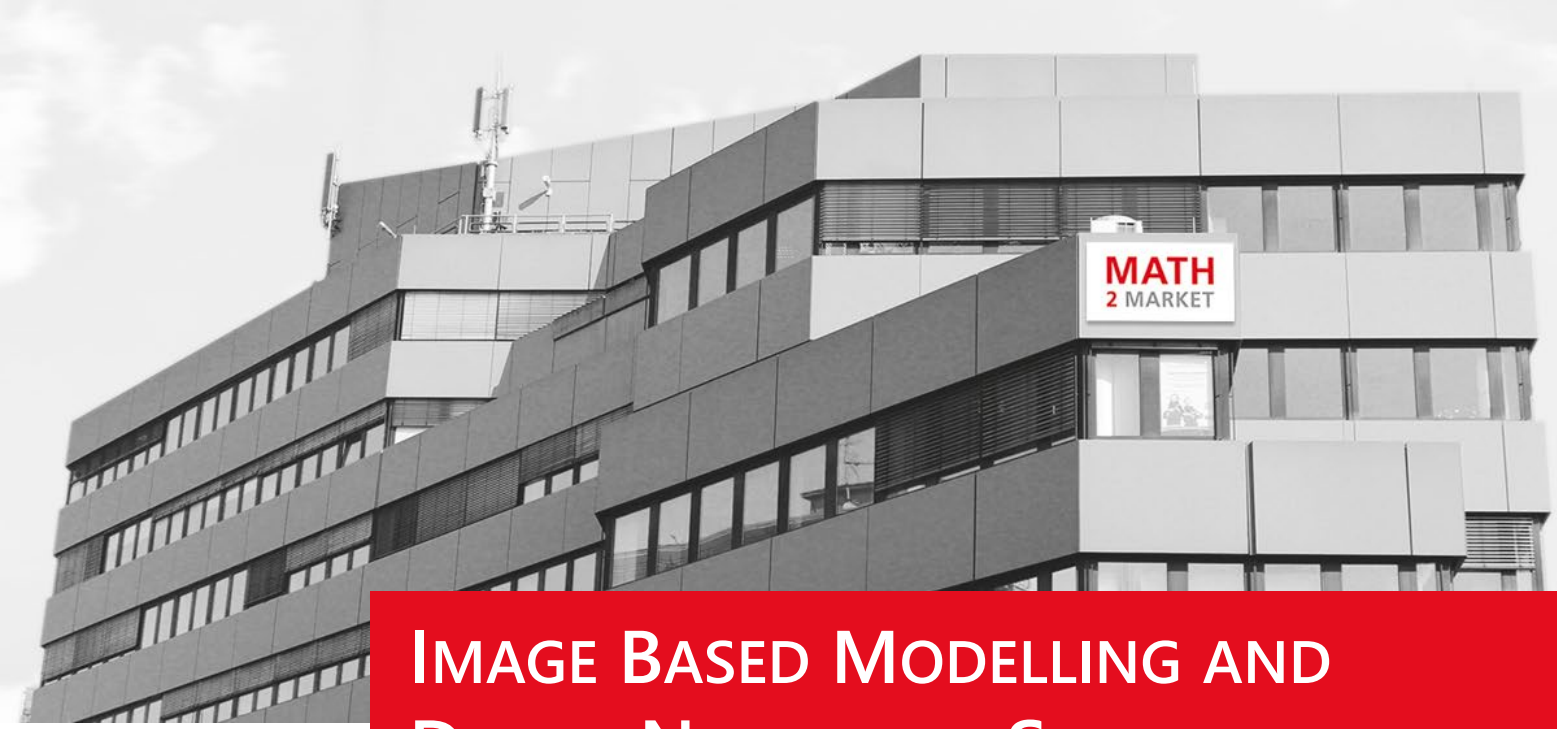


MATH
2 MARKET

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

IBFEM-4i

Swansea, September 12th, 2019

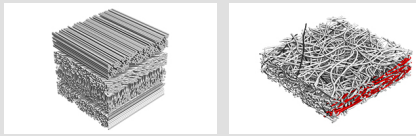
Andreas Wiegmann

GeoDict® Module Overview

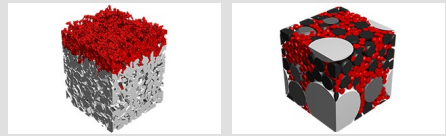
MATH 2 MARKET

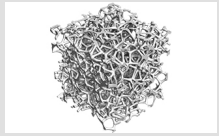

ImportGeo

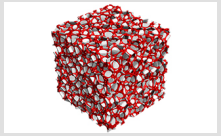

FiberGeo

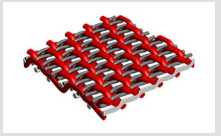


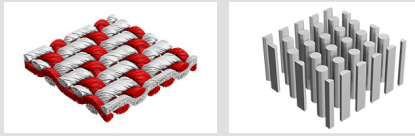

PaperGeo


GrainGeo

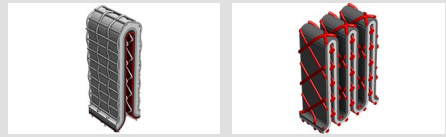

FoamGeo

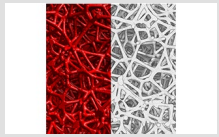


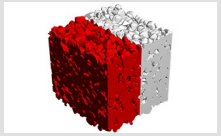

WeaveGeo

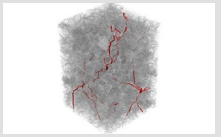



GridGeo

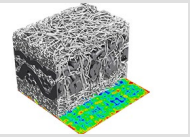

PleatGeo


MeshGeo

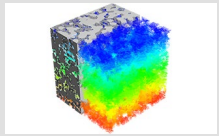

ExportGeo

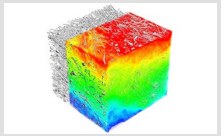

PoroDict

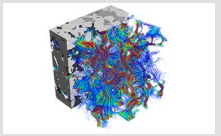
This is Innovation through Simulation

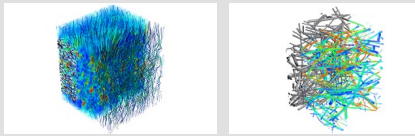

MatDict

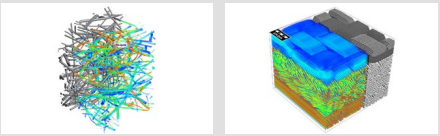

BatteryDict

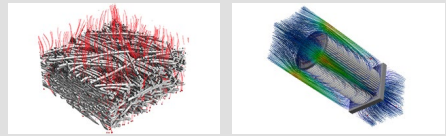

DiffuDict

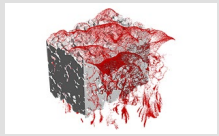

ConductoDict

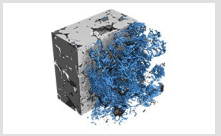

FlowDict

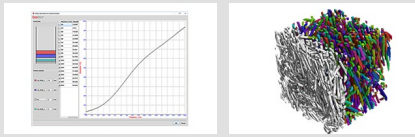


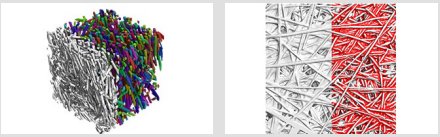

ElastoDict

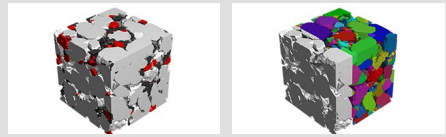

FilterDict Media & Element


AddiDict


SatuDict


AcoustoDict


FiberFind

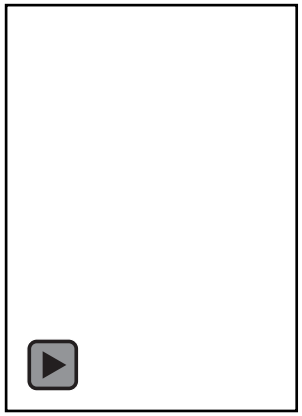

GrainFind

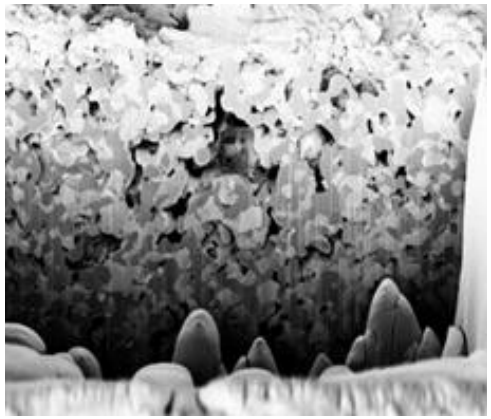
Selected Clients of a total of ~150 clients

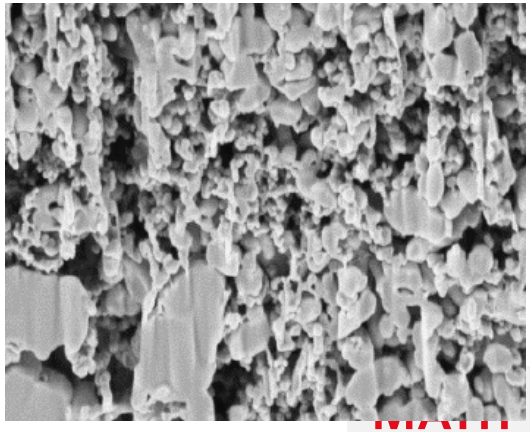
MATH 2 MARKET

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



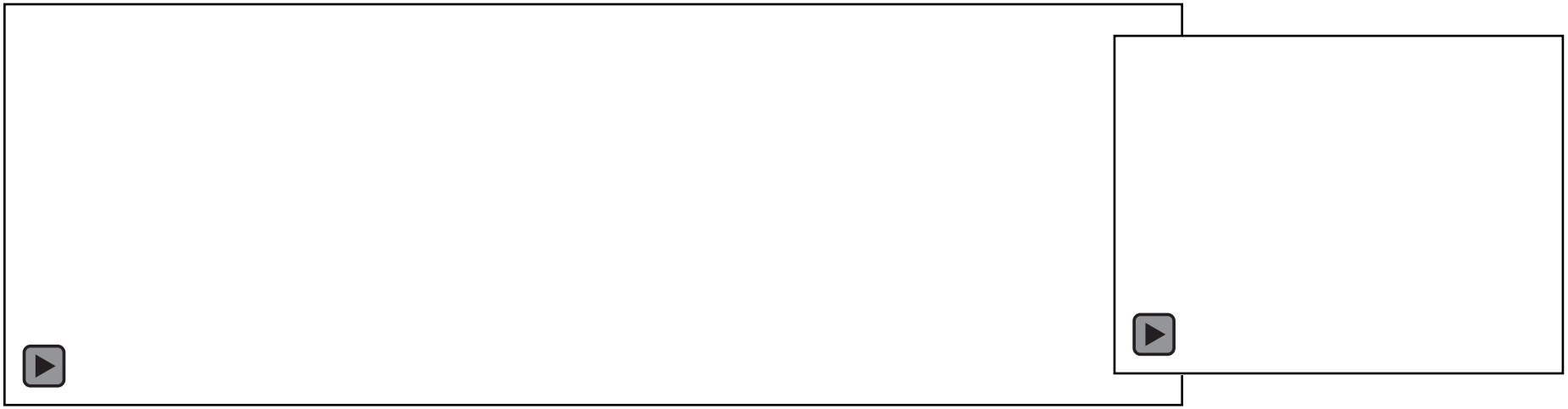




FIB-SEM IMAGE ALIGNMENT

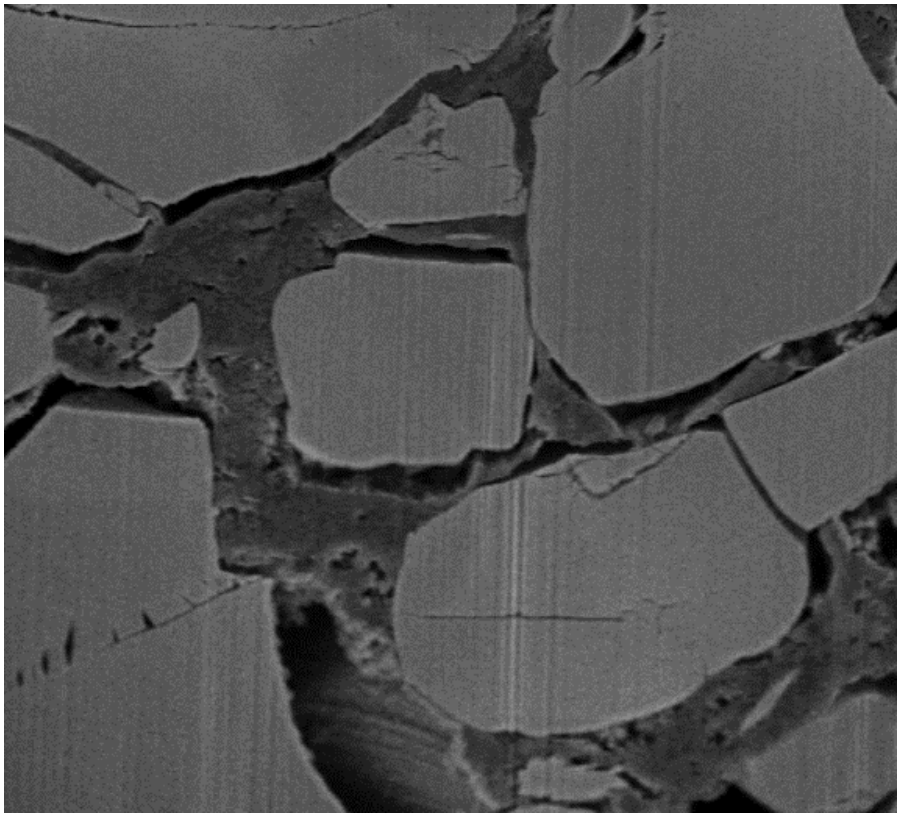
NANO-CT GRAY-VALUE CORRECTION

- 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

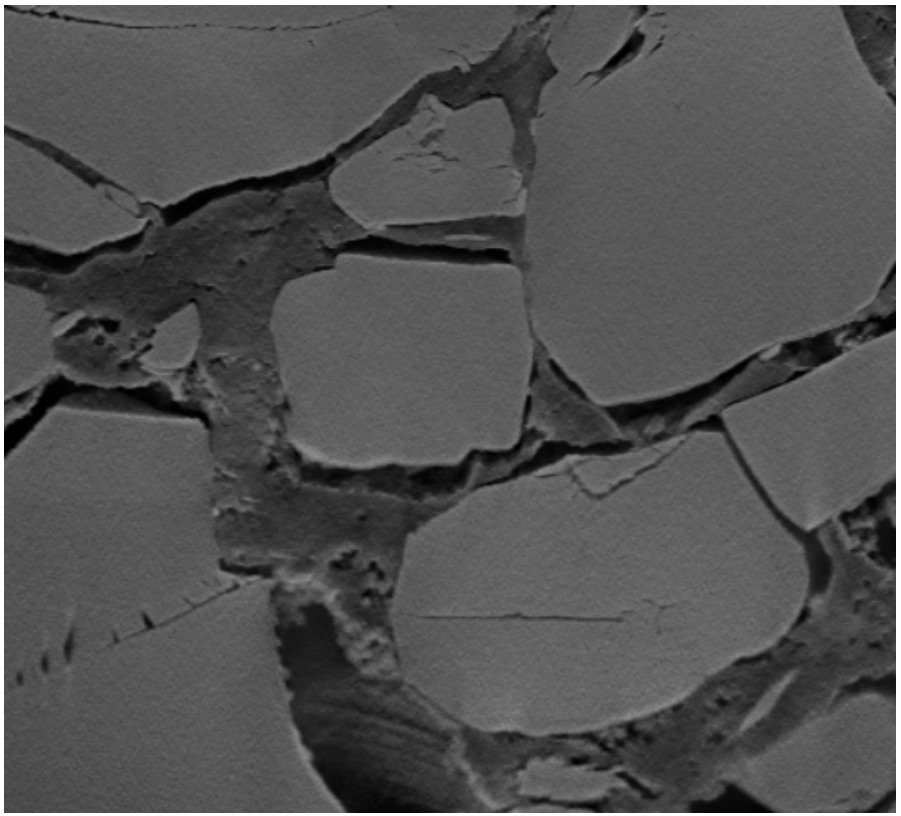


Curtain Filter

GeoDict



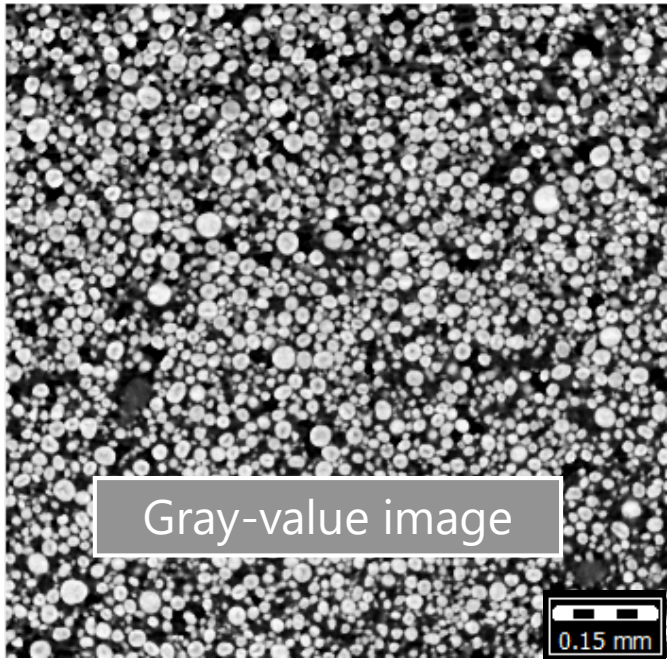
Original
SEM

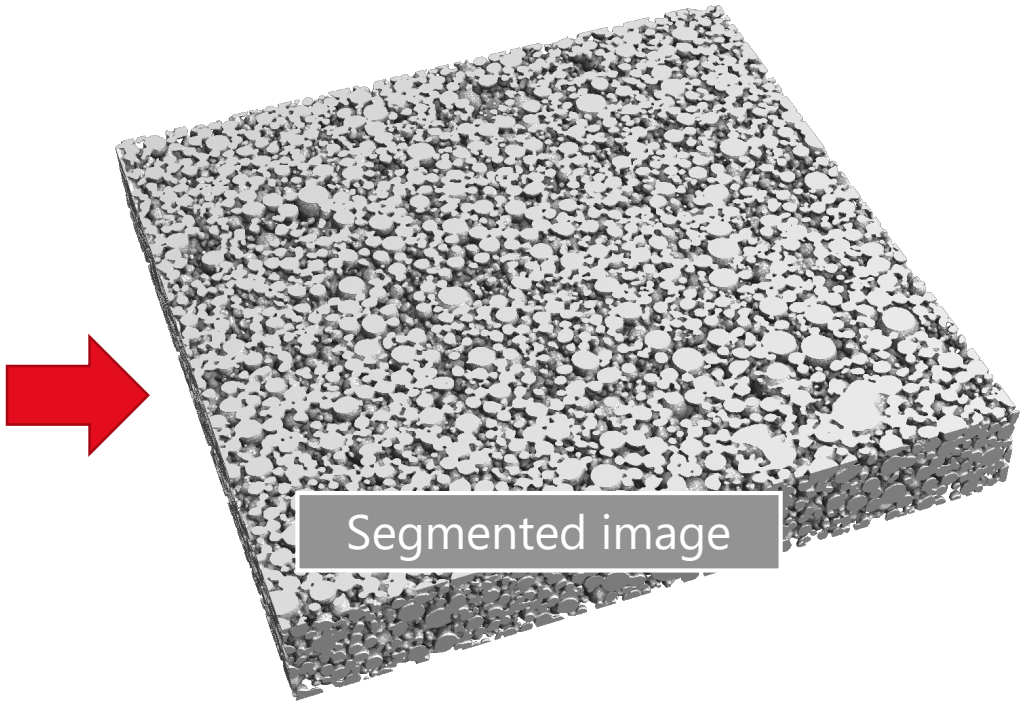


SEM
after applying the curtain filter

MATH 2 MARKET

IMPORTGEO

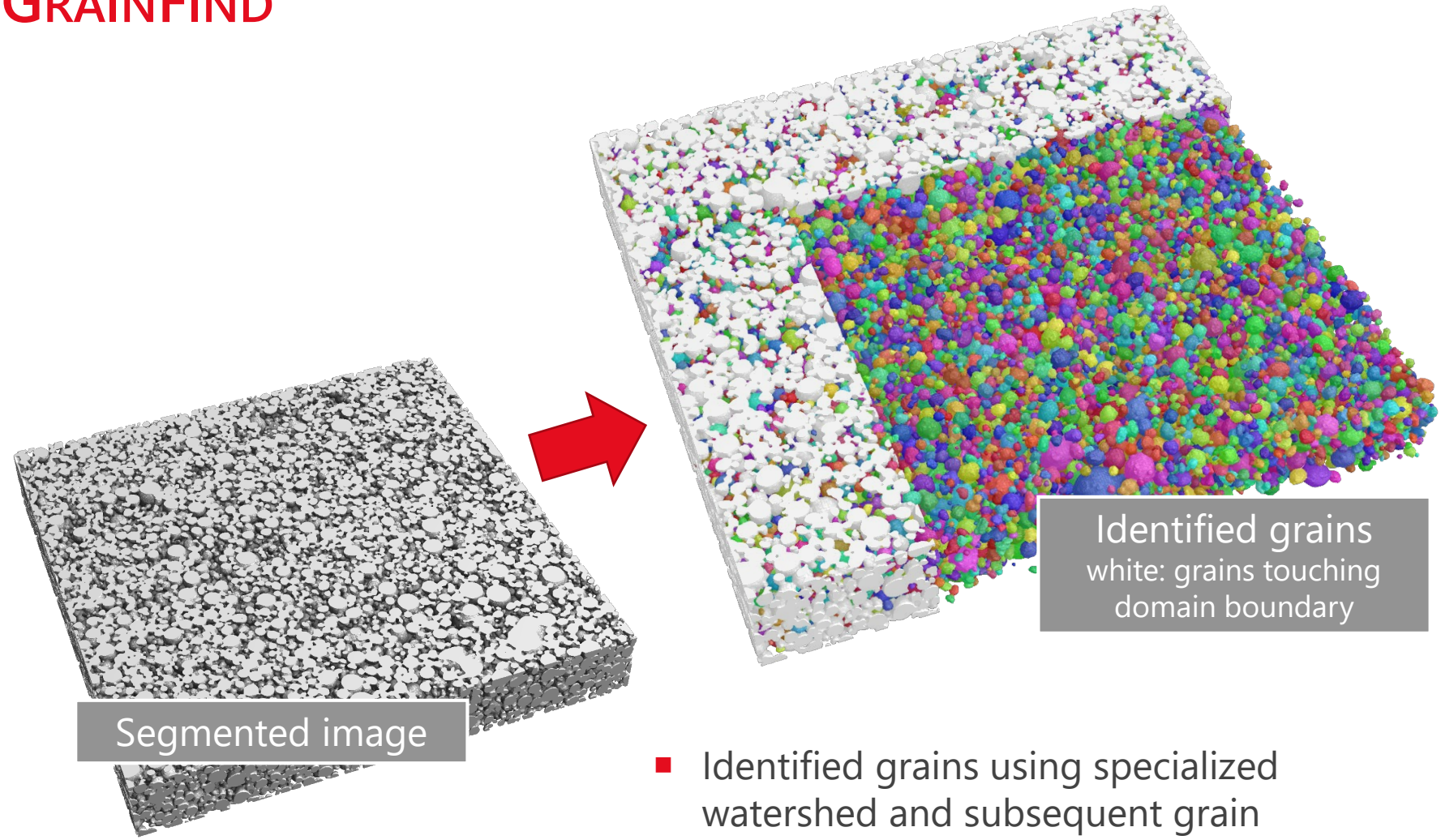




Applied Filters:

- Non-Local Means Filter
- Sharpen Filter

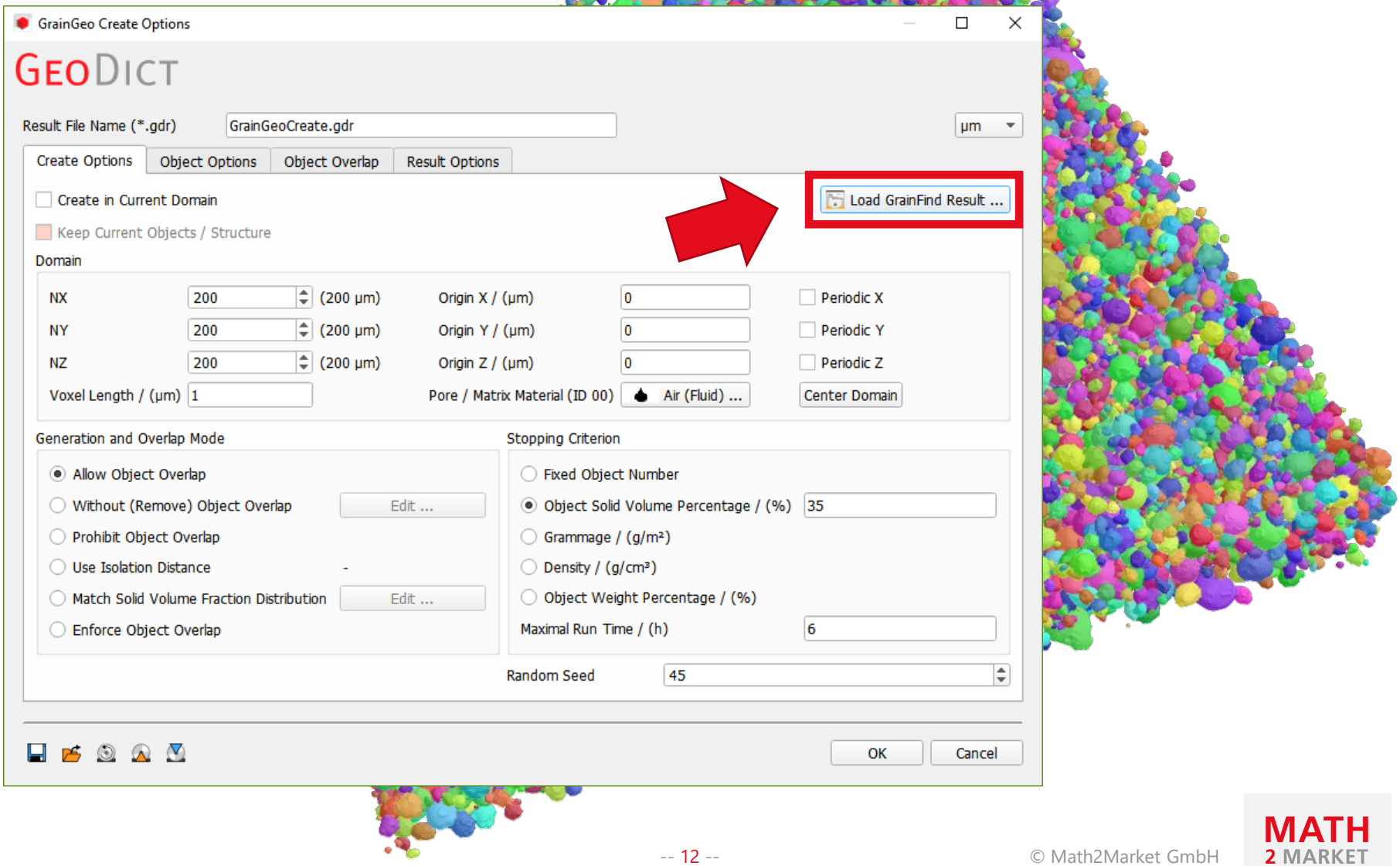
GRAINFIND



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

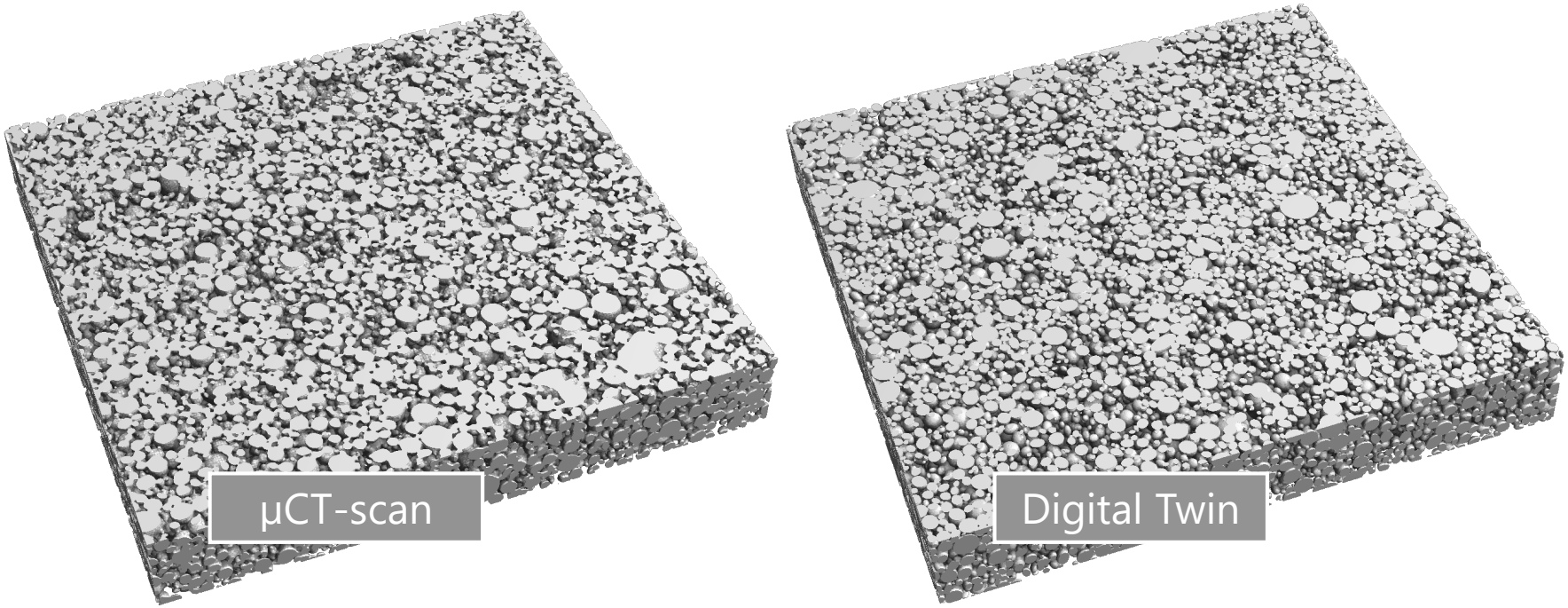
GEODICT

IMPORT GRAINFIND RESULTS INTO GRAINGEO



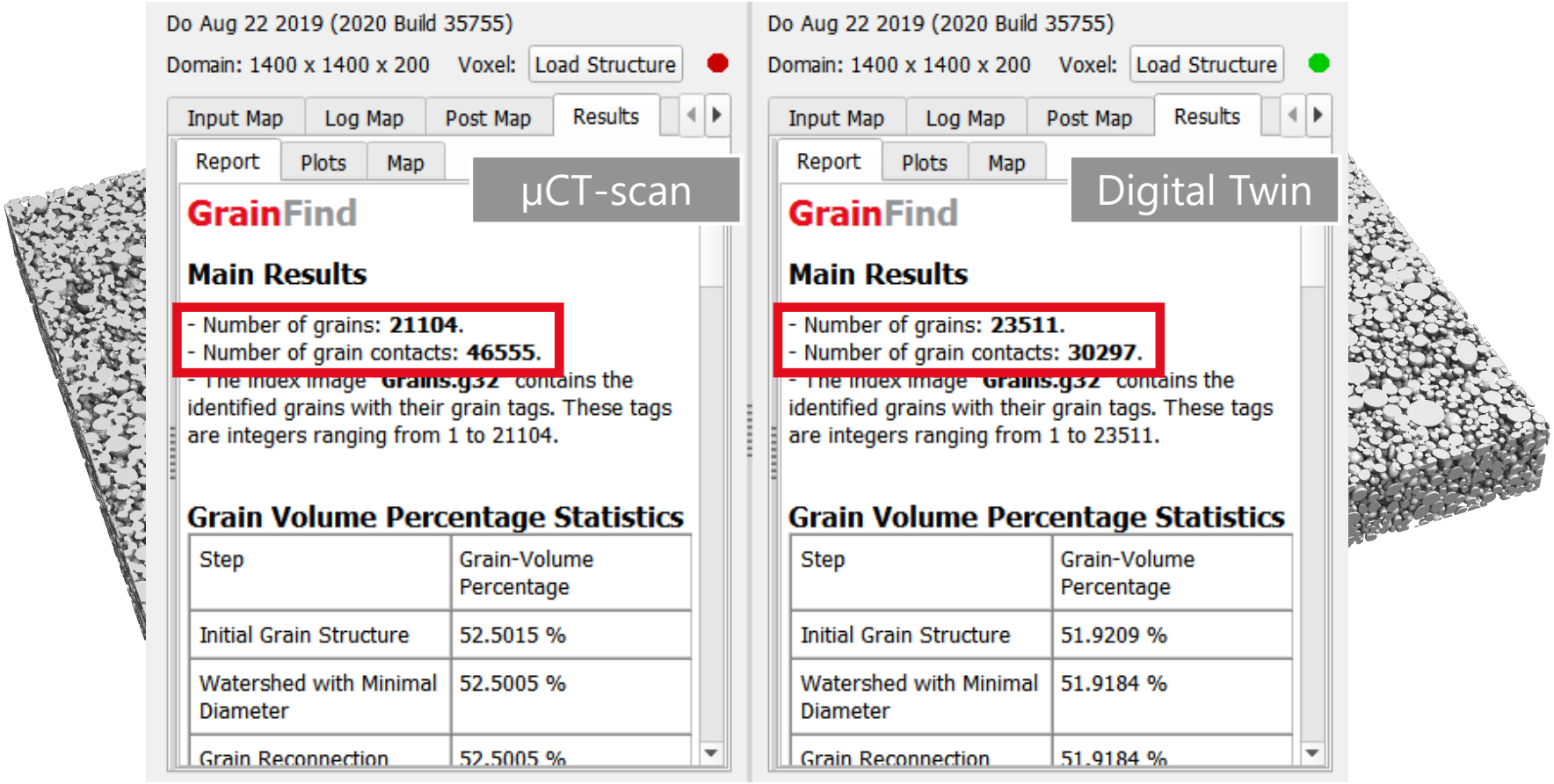
MATH 2 MARKET

GRAINGEO



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

COMPARISON OF STATISTICS



Do Aug 22 2019 (2020 Build 35755)

Domain: 1400 x 1400 x 200 Voxel: Load Structure

Input Map | Log Map | Post Map | Results

Report | Plots | Map

µCT-scan

GrainFind

Main Results

- Number of grains: **21104.**
- Number of grain contacts: **46555.**
- The index image **Grains.g32** contains the identified grains with their grain tags. These tags are integers ranging from 1 to 21104.

Grain Volume Percentage Statistics

Step	Grain-Volume Percentage
Initial Grain Structure	52.5015 %
Watershed with Minimal Diameter	52.5005 %
Grain Reconnection	52.5005 %

Do Aug 22 2019 (2020 Build 35755)

Domain: 1400 x 1400 x 200 Voxel: Load Structure

Input Map | Log Map | Post Map | Results

Report | Plots | Map

Digital Twin

GrainFind

Main Results

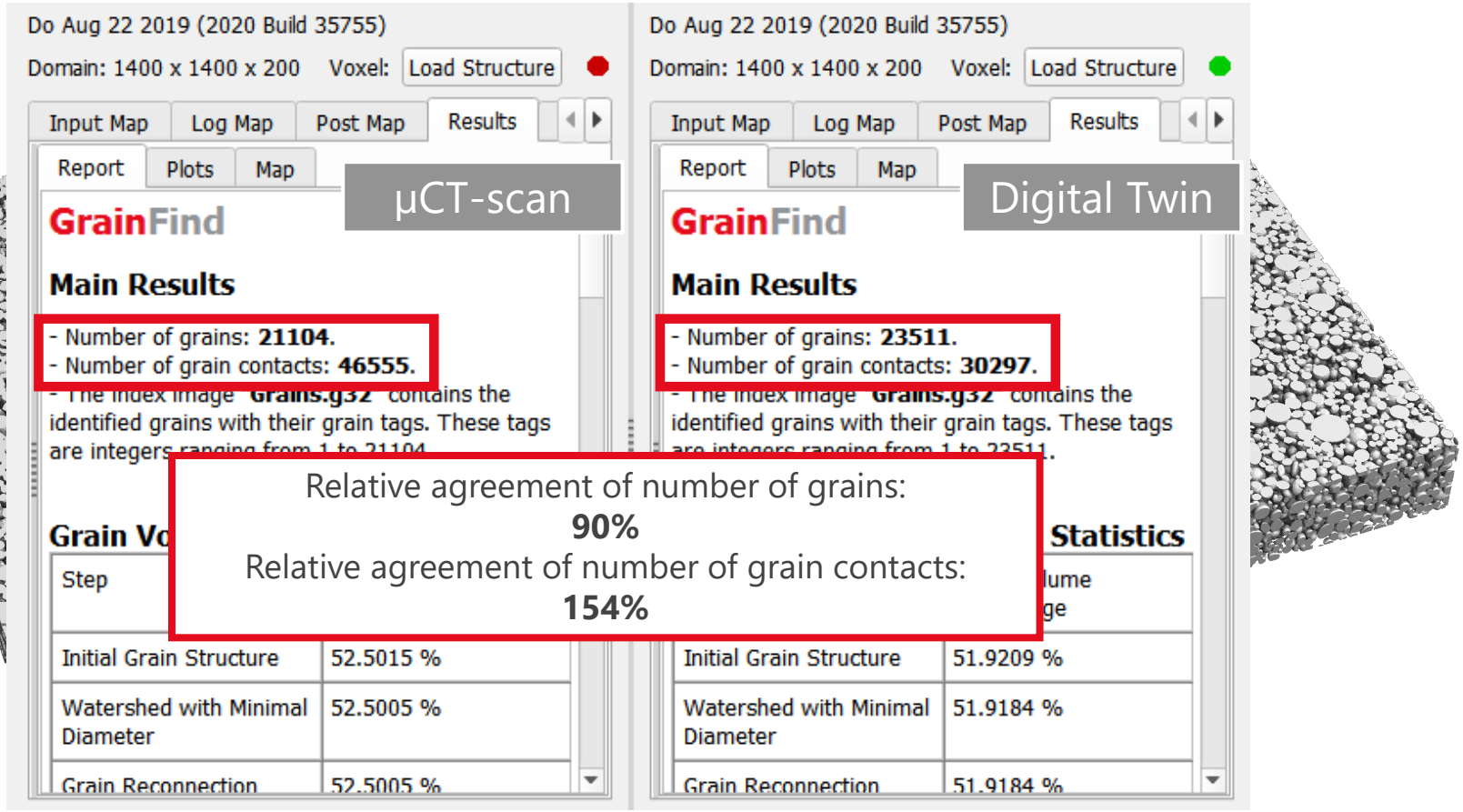
- Number of grains: **23511.**
- Number of grain contacts: **30297.**
- The index image **Grains.g32** contains the identified grains with their grain tags. These tags are integers ranging from 1 to 23511.

Grain Volume Percentage Statistics

Step	Grain-Volume Percentage
Initial Grain Structure	51.9209 %
Watershed with Minimal Diameter	51.9184 %
Grain Reconnection	51.9184 %

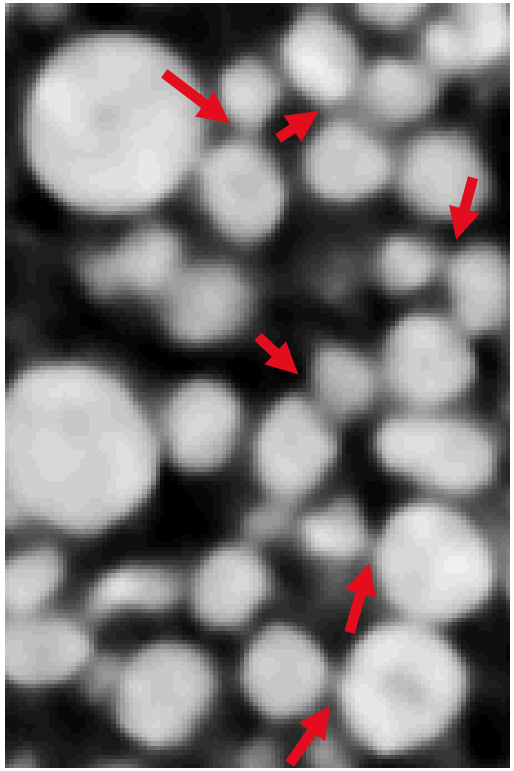
- Used GrainGeo's "Create Grains"
- Visual comparison is good
- However, statistics do not match perfectly

COMPARISON OF STATISTICS

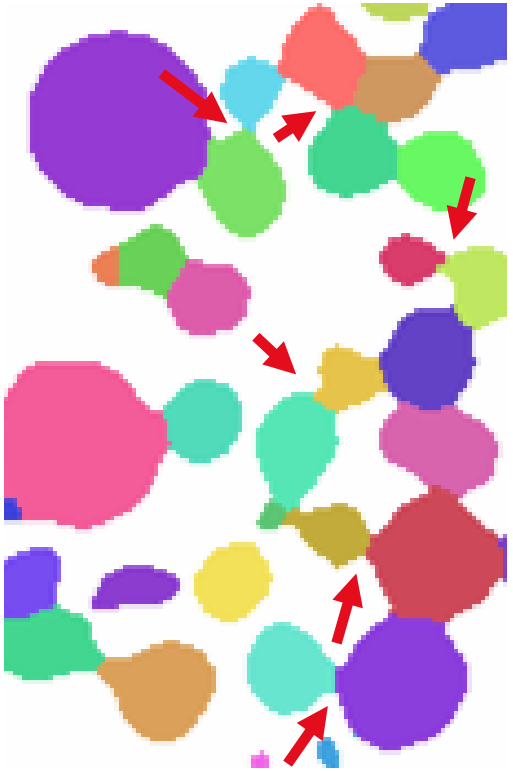


- Used GrainGeo's "Create Grains"
- Visual comparison is good
- However, statistics do not match perfectly

GRAINGEO: ADD BINDER!

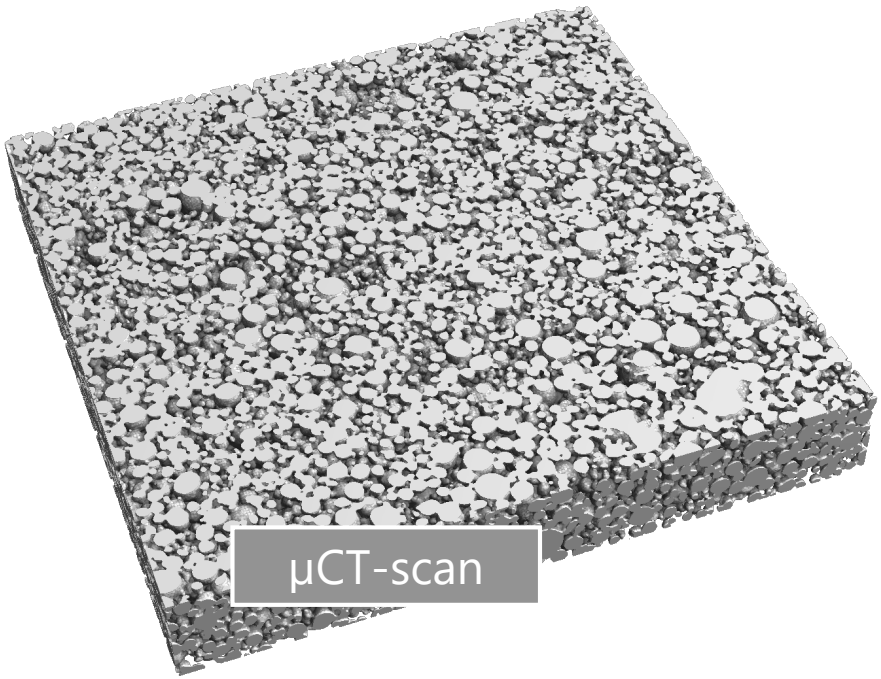


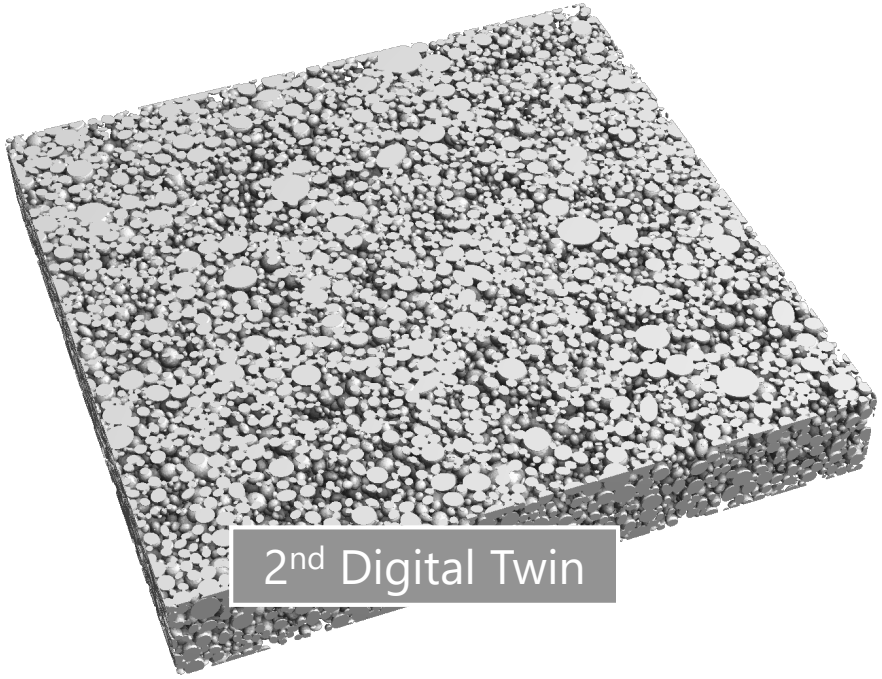
Slice from



Slice from Grain Identification

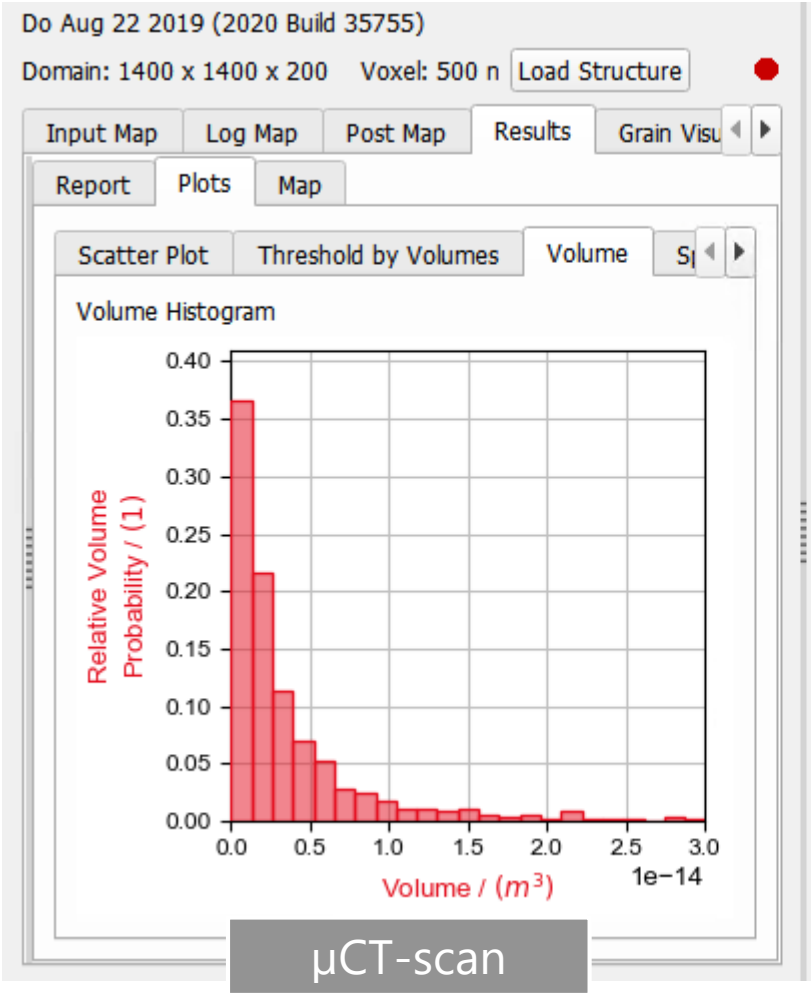
Visual Comparison



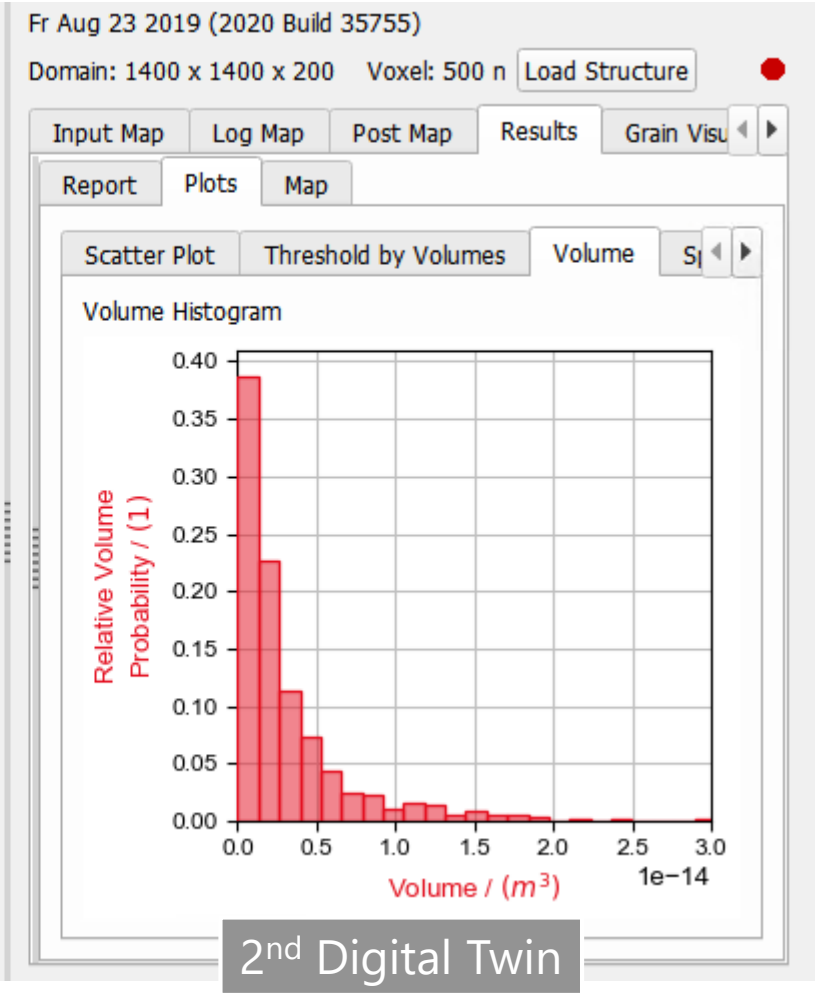


- Used GrainGeo's "Create Grains" and GrainGeo's "Add Binder"
- Visual comparison is good

COMPARISON PLOTS



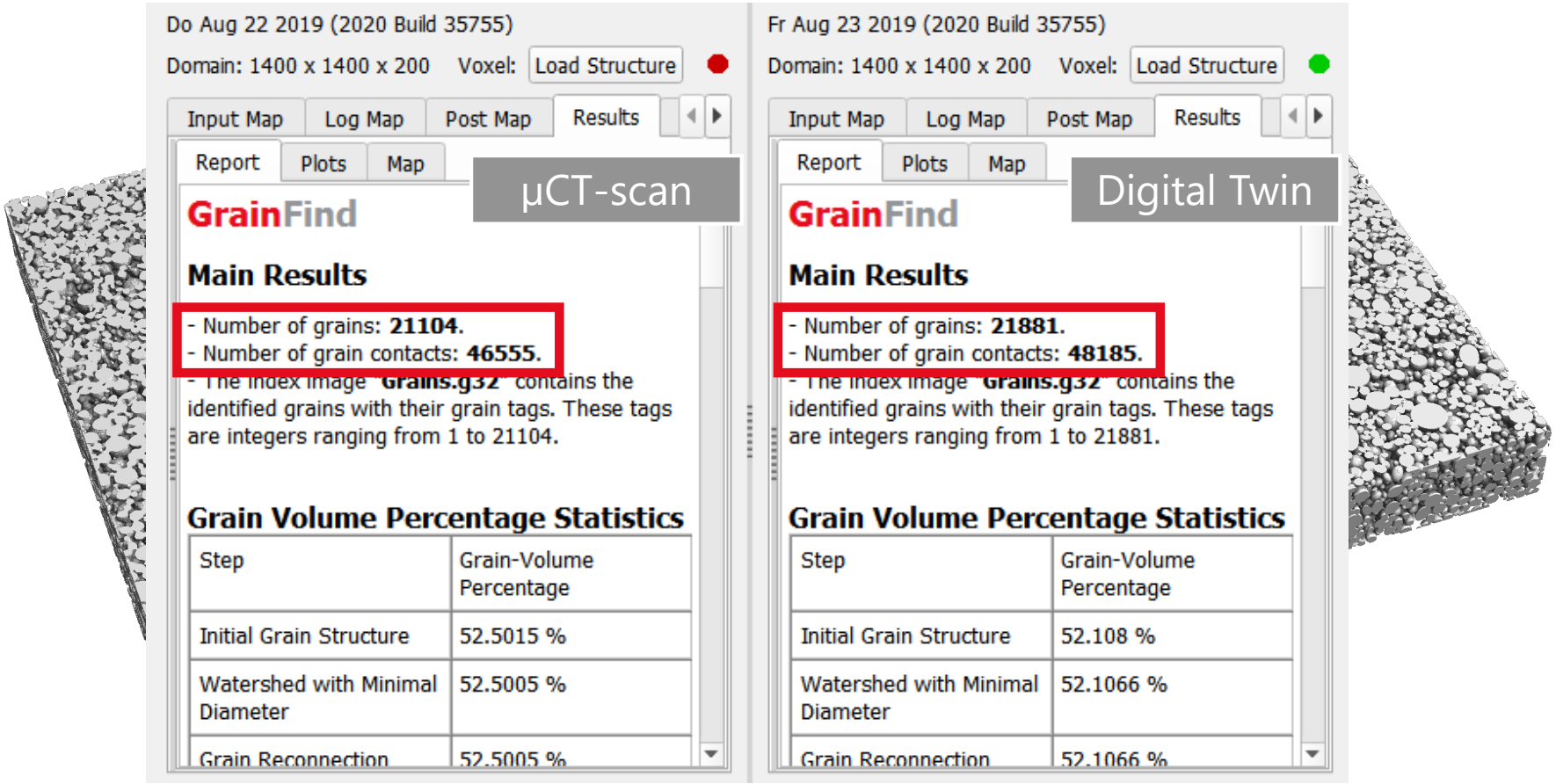
µCT-scan



2nd Digital Twin

GEODICT

VISUAL COMPARISON

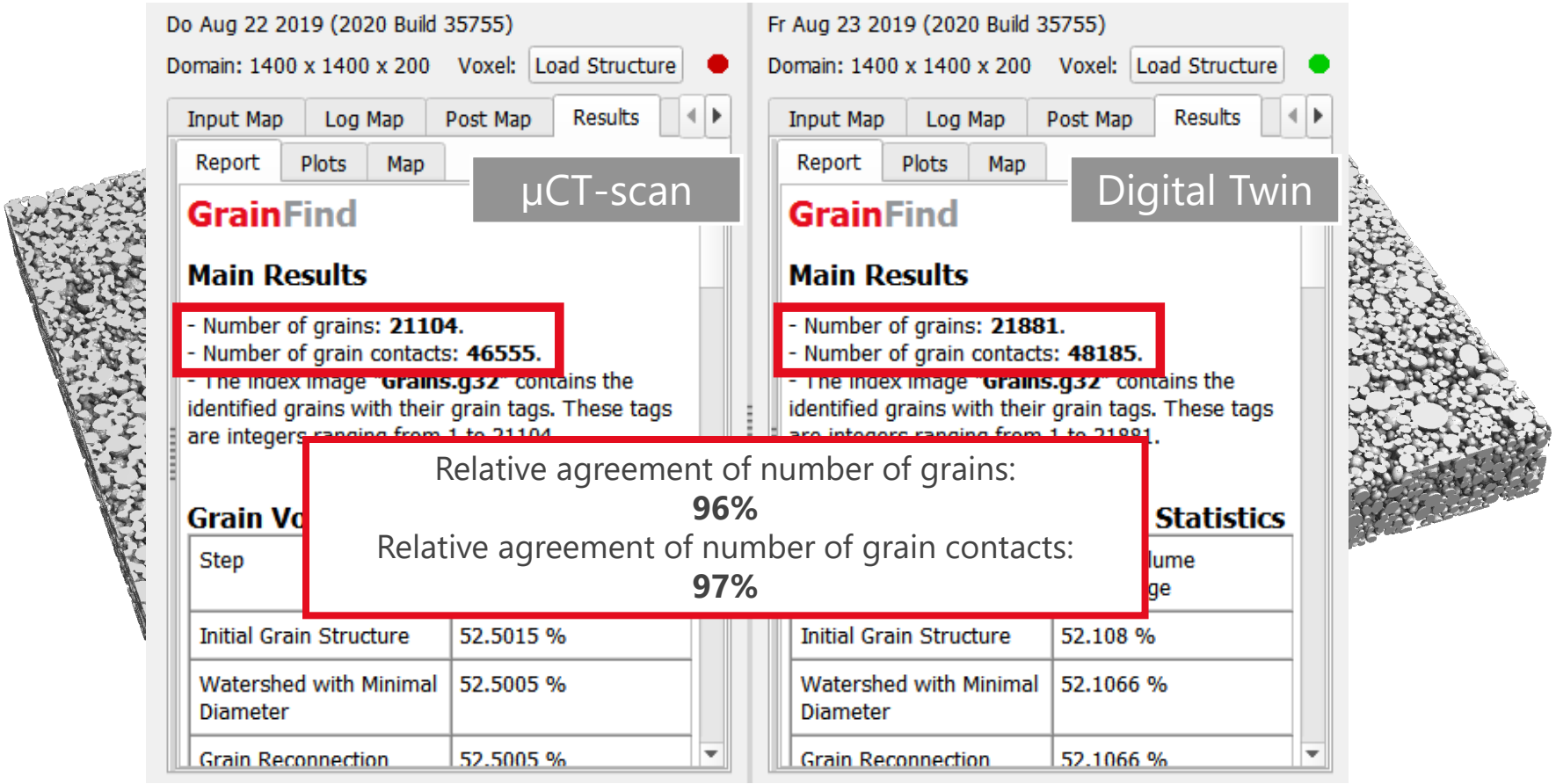


- Used GrainGeo's "Create Grains" and GrainGeo's "Add Binder"
- Visual comparison is good
- Statistics match nicely

MATH 2 MARKET

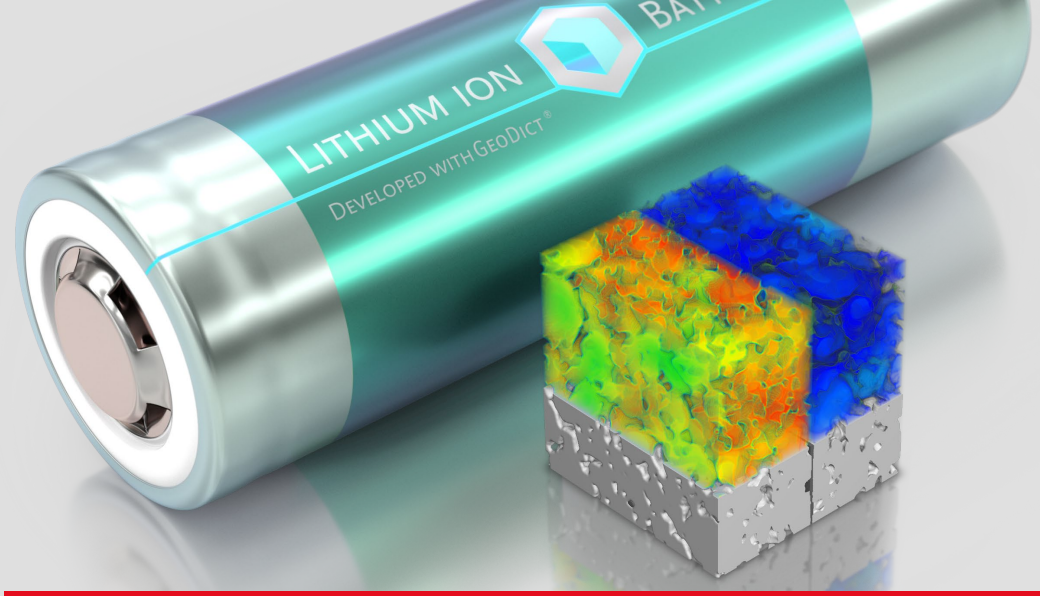
GEODICT

VISUAL COMPARISON



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

MATH 2 MARKET



GEODICT
The Digital Material Laboratory

DIGITAL BATTERY DEVELOPMENT

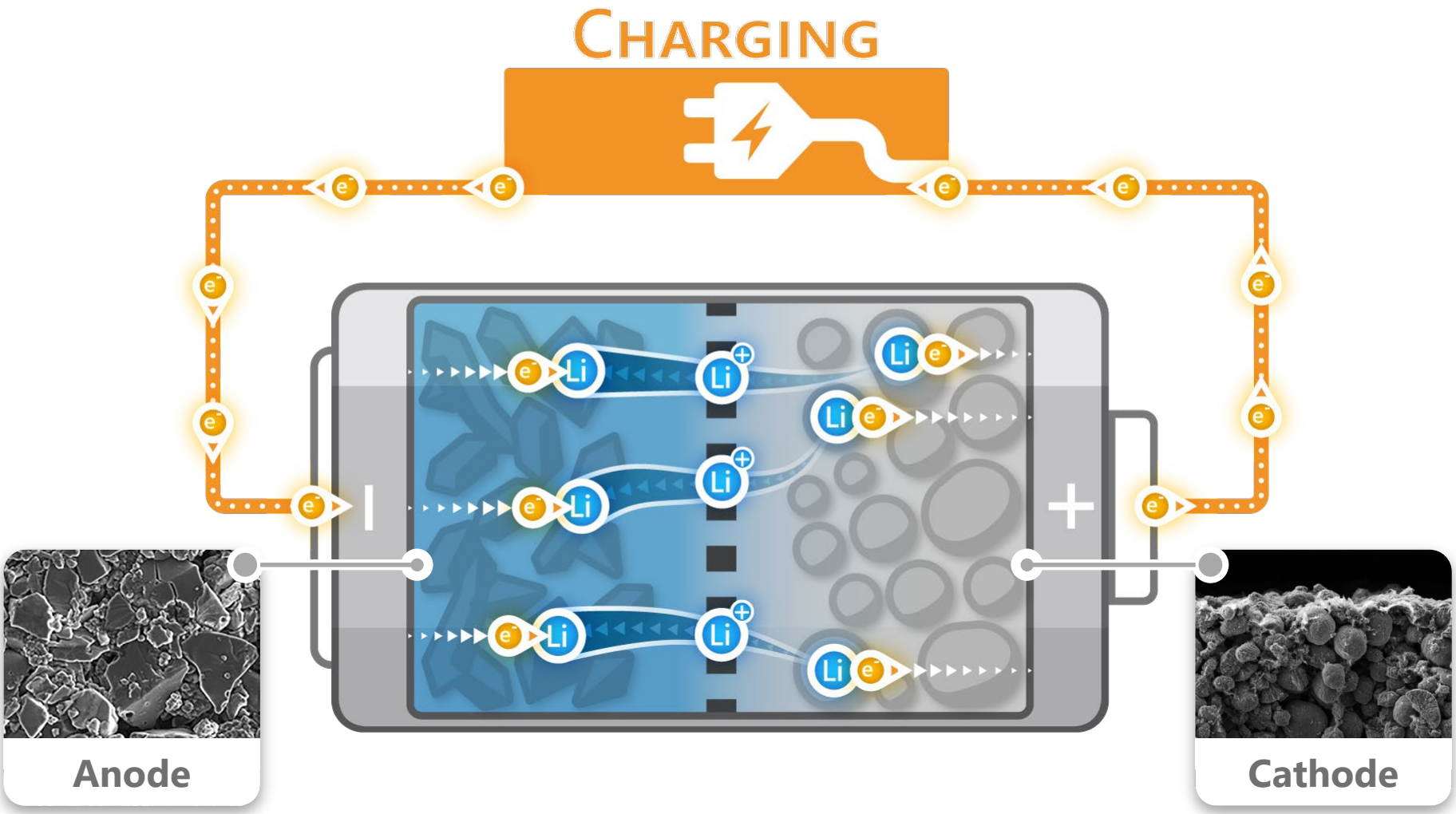
Solutions with **GeoDict®**

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



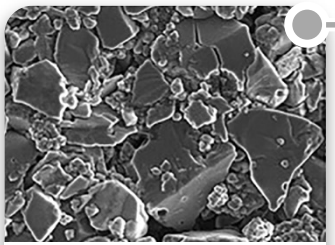
MATH 2 MARKET

Li-Ion Battery

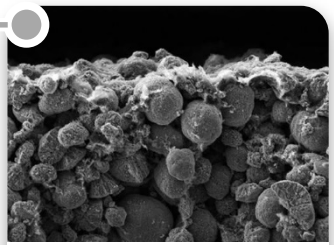
GeoDict

Challenges for Materials Design:

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



Anode



Cathode

MATH 2 MARKET

Microstructure of a Li-Ion – Cathode

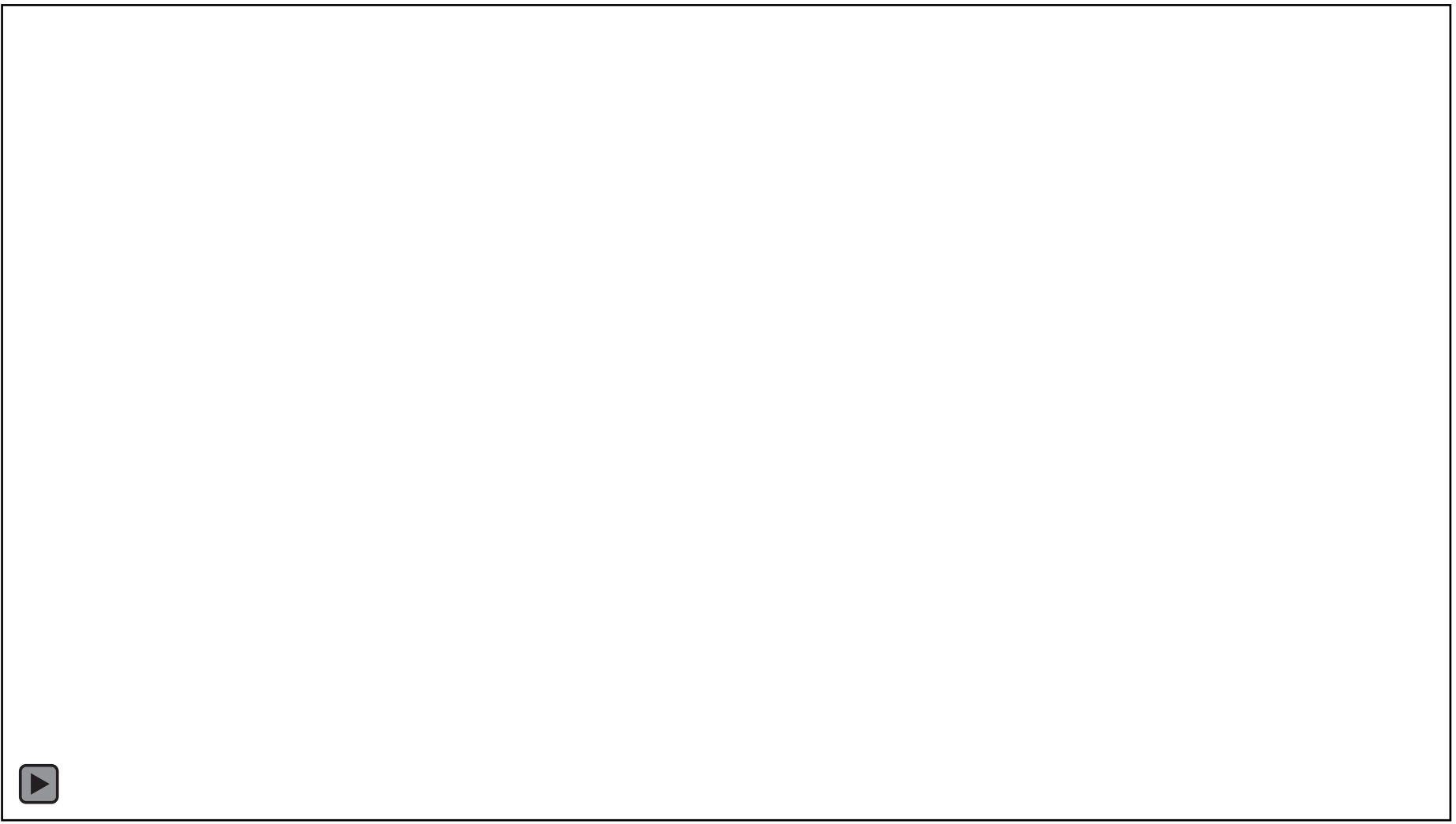
GeoDict

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

Microstructure of a Li-Ion – Cathode

GeoDict

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



MATH 2 MARKET

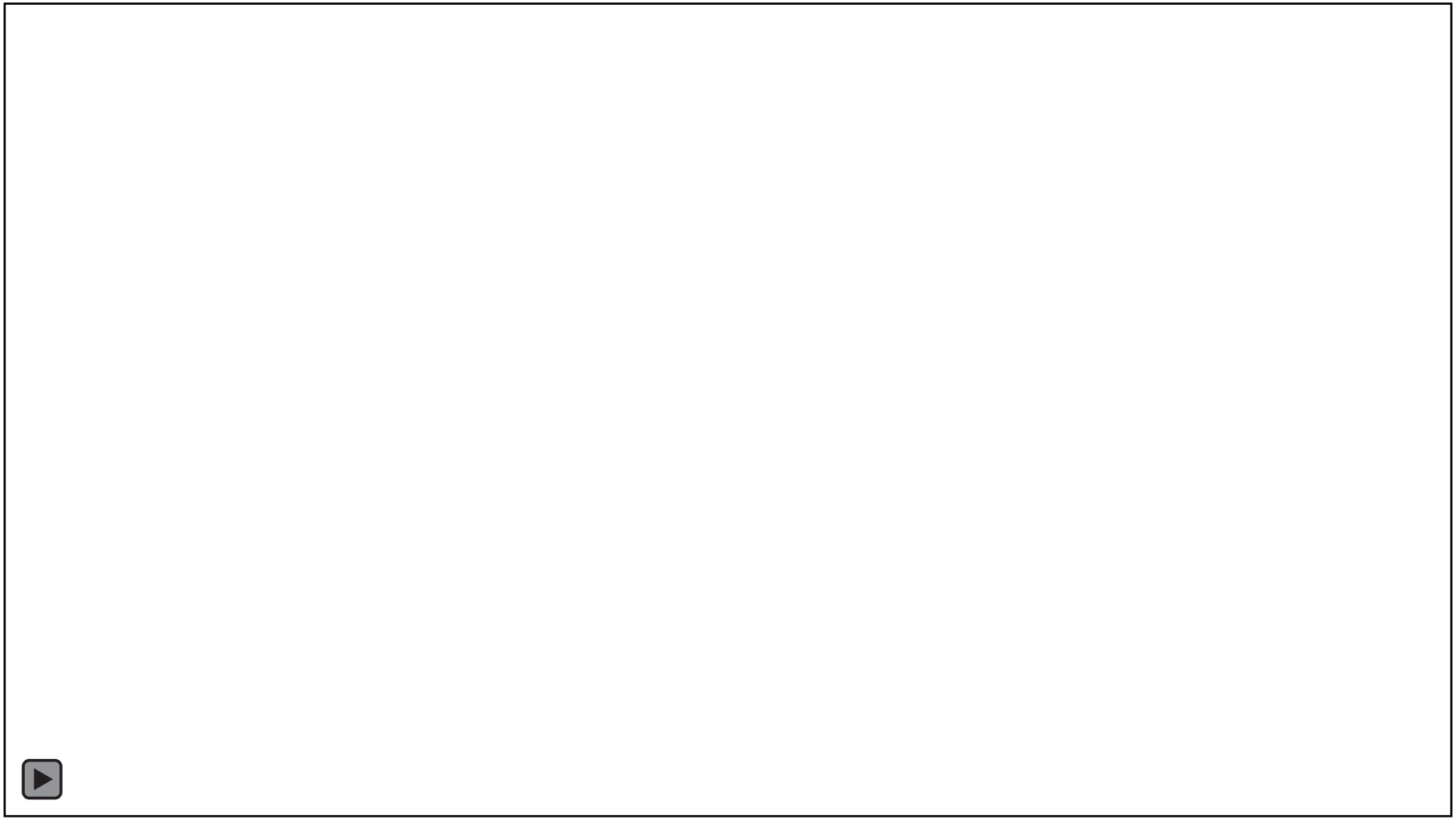
Particle Expansion due to Li-Intercalation

GeoDict FeelMath

MATH 2 MARKET

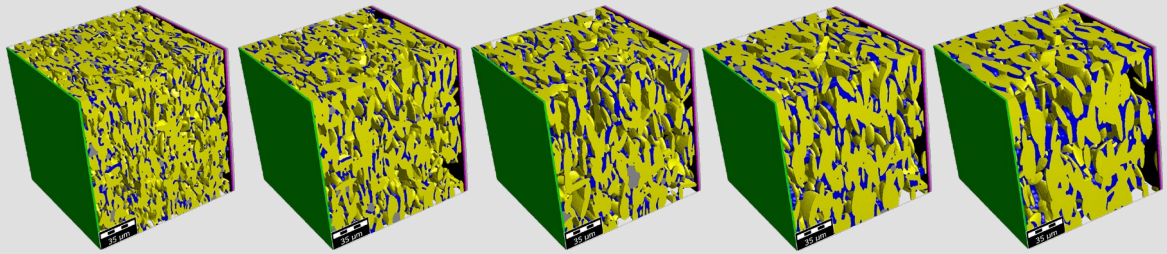
Particle Expansion due to Li-Intercalation

GeoDict FeelMath



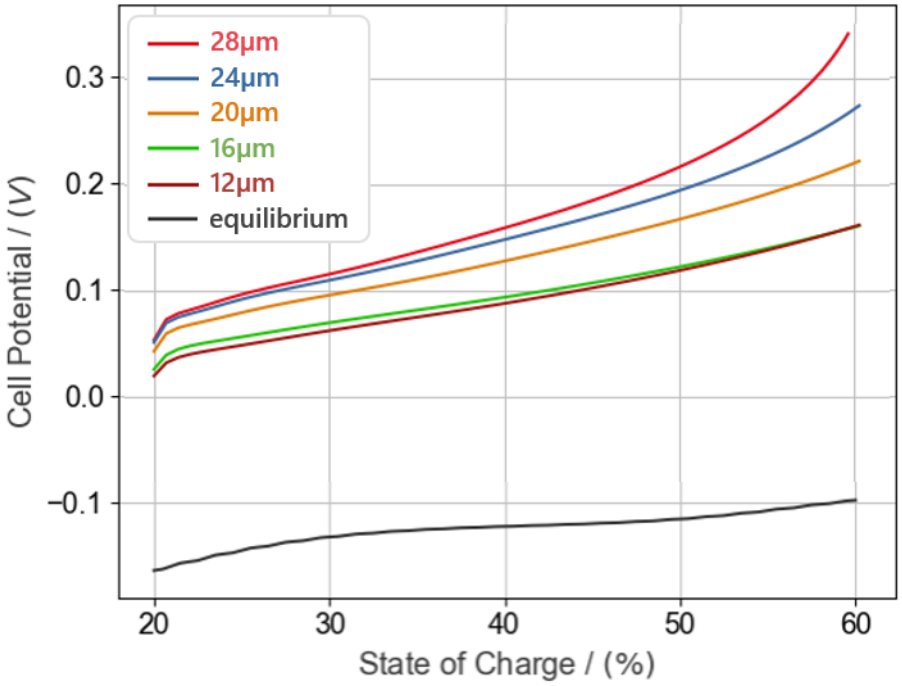
MATH 2 MARKET

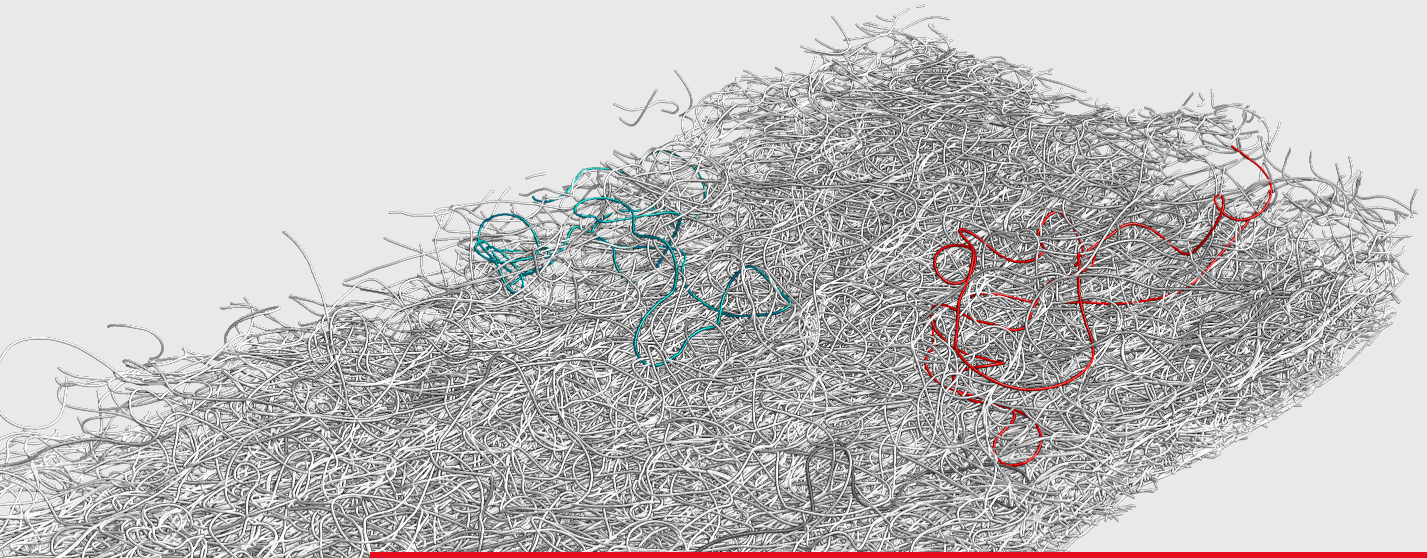
BATTERYDICT HALF-CELL SIMULATION



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

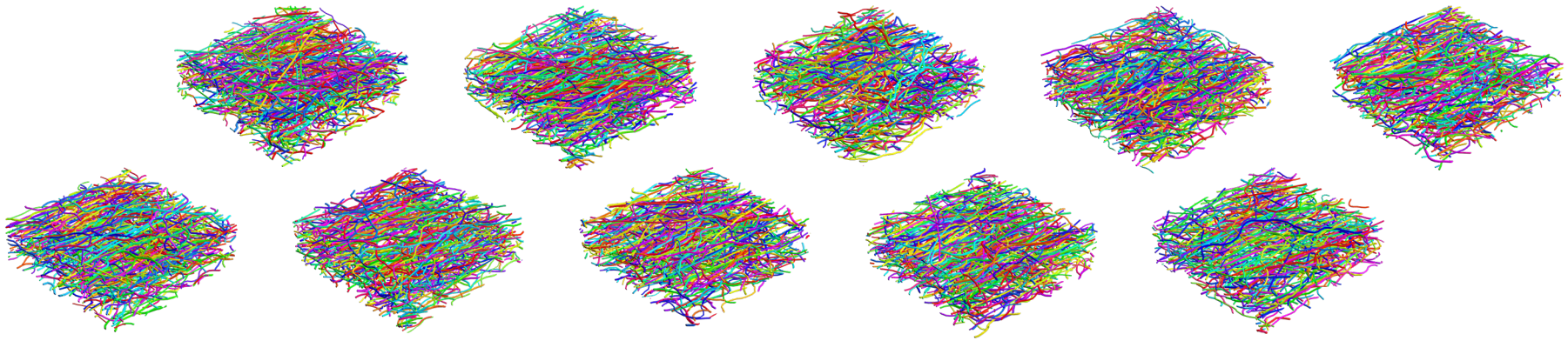
Andreas Grießer, Rolf Westerteiger, Steffen Schwichow, Andreas Wiegmann, Math2Market

Wesley DeBoever, Bruker µCT

MATH 2 MARKET

Digital Twins provide ground truth

GeoDict



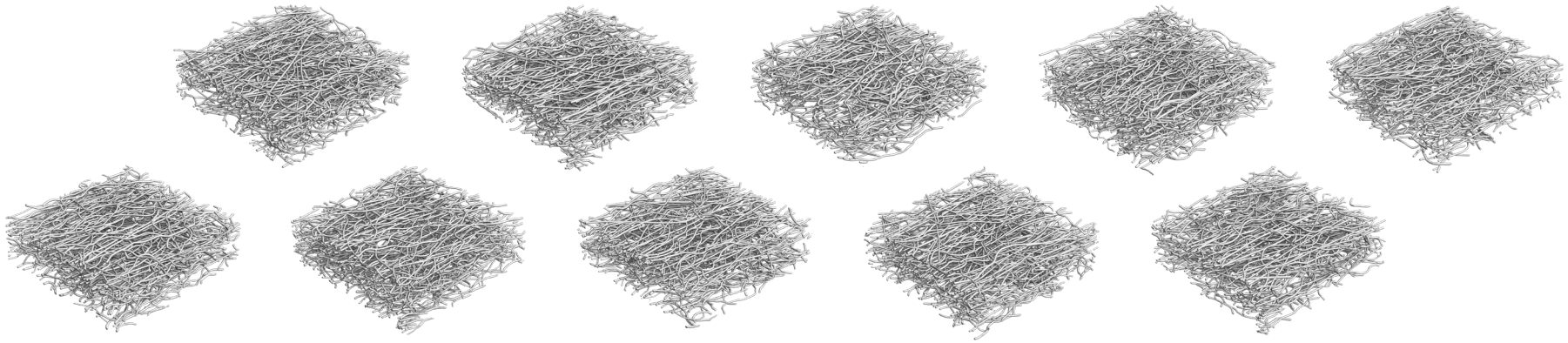
Training Data: Use GeoDict's unique fiber modelling capabilities:

- 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



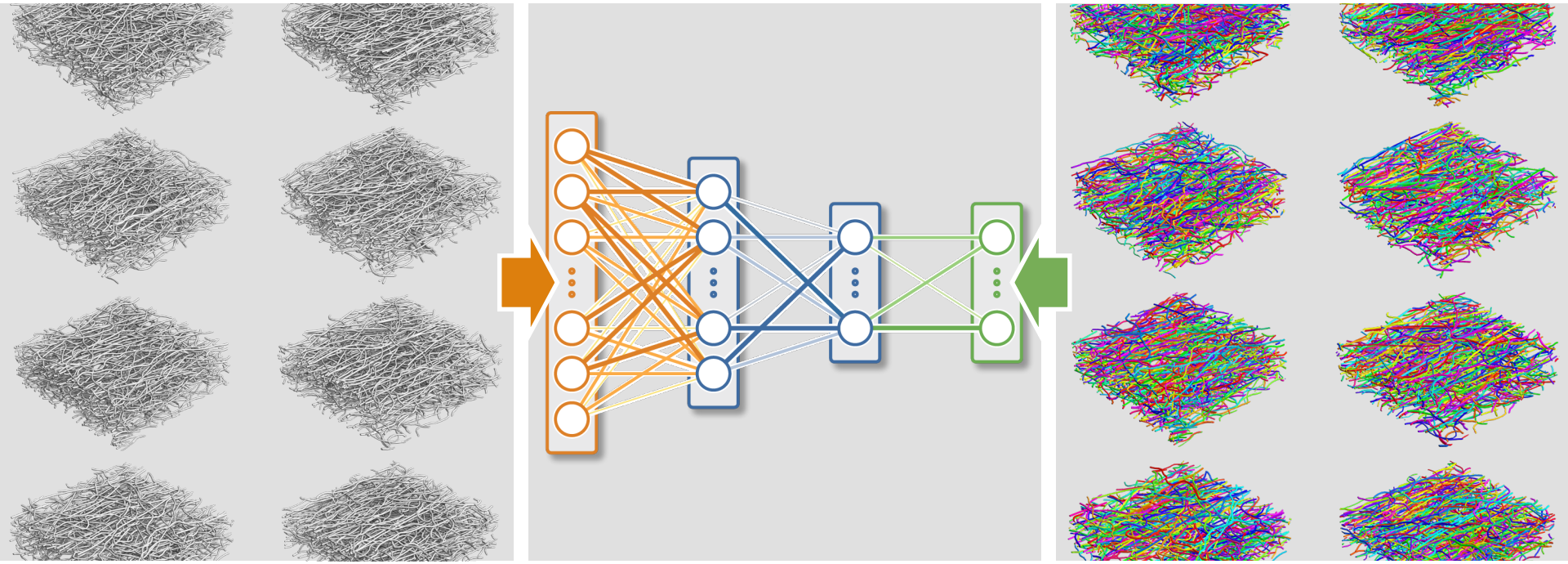
Training Data: Then make the models look like binarized scans!

- 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

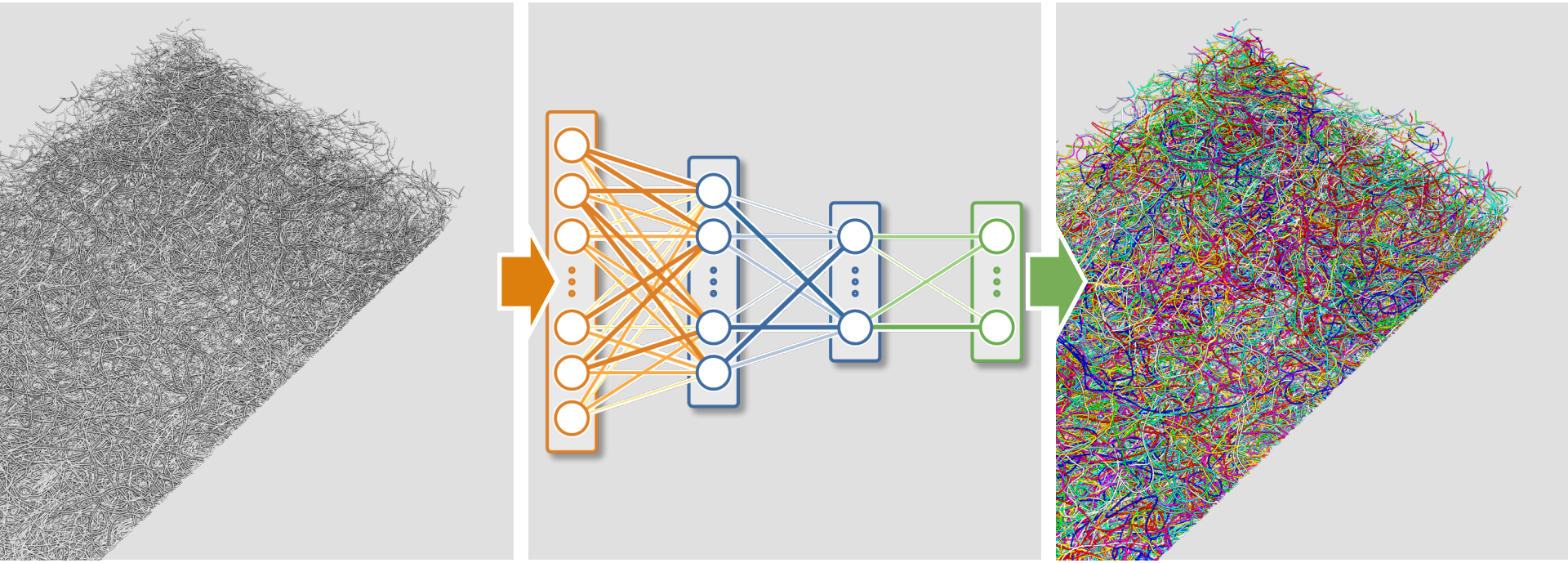
Neural Network learns weights for edges

Dozens of Original GeoDict models

MATH 2 MARKET

Usage Phase of NN

GeoDict



Segmented 3D scan

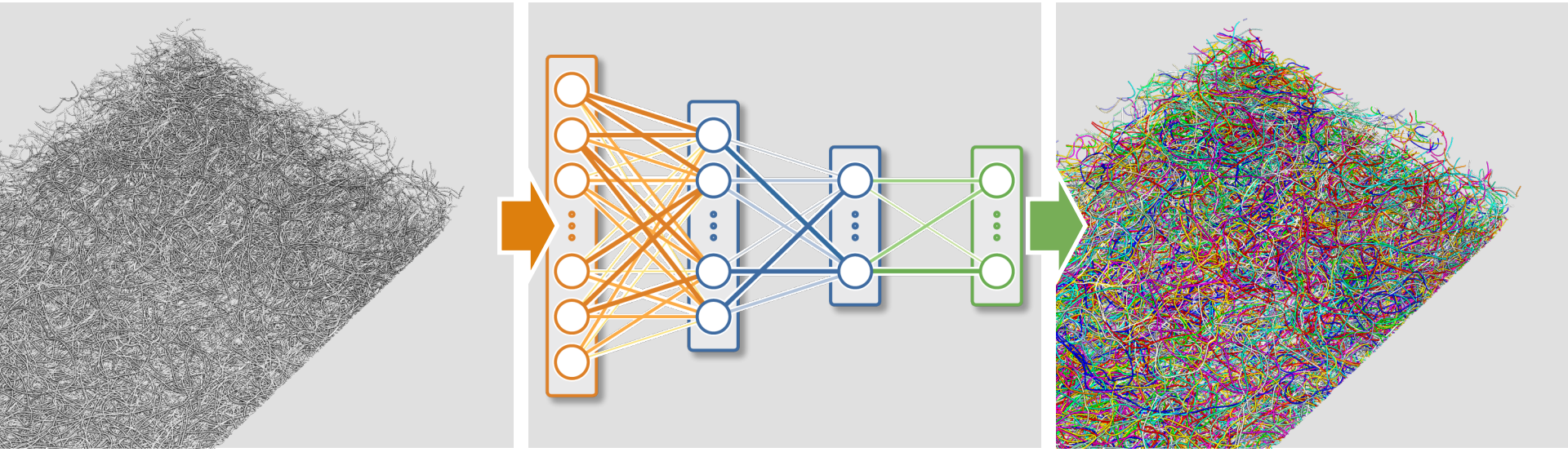
Neural Network with weights on edges

Labeled fibers for 3D scan

MATH 2 MARKET

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

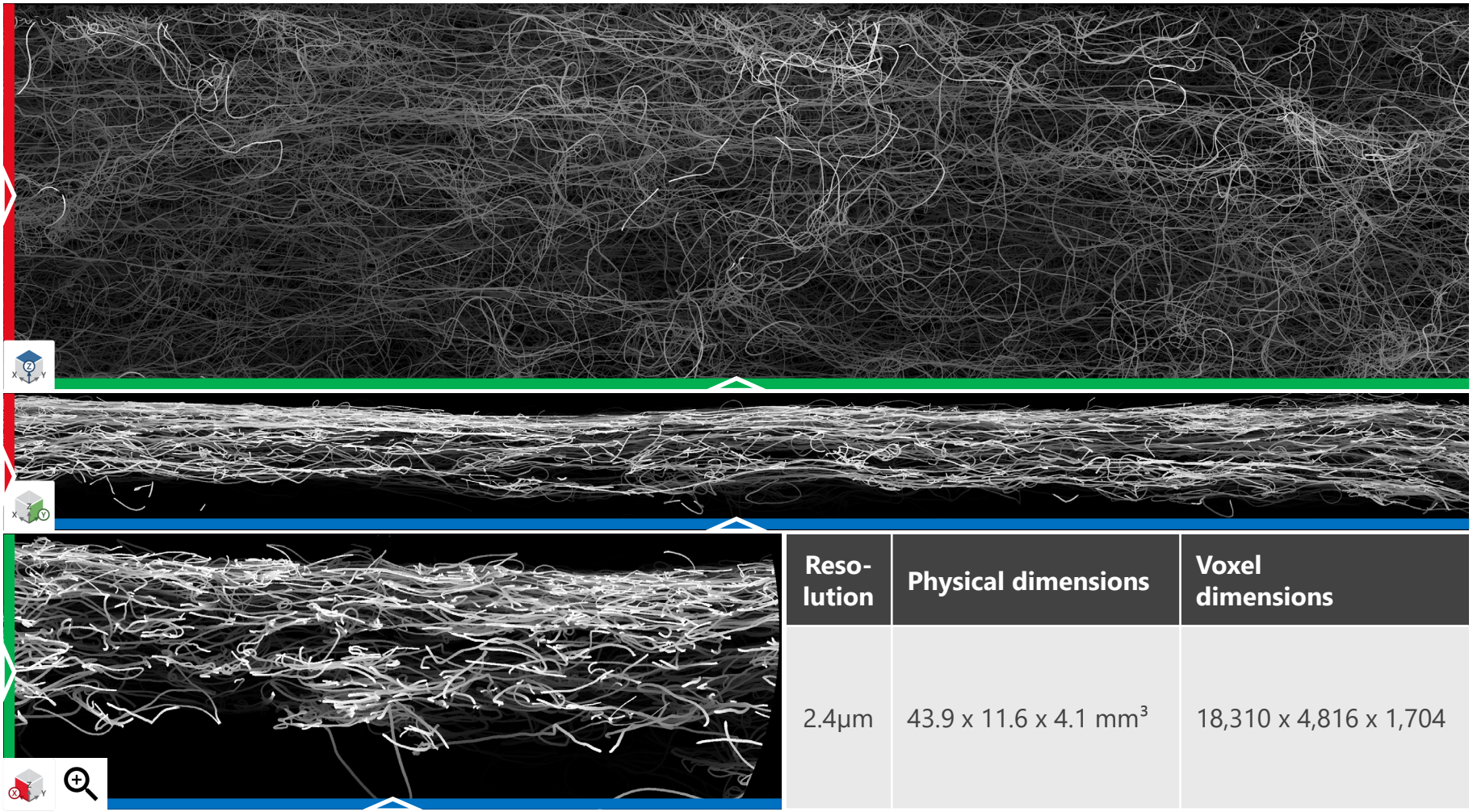
GeoDict

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

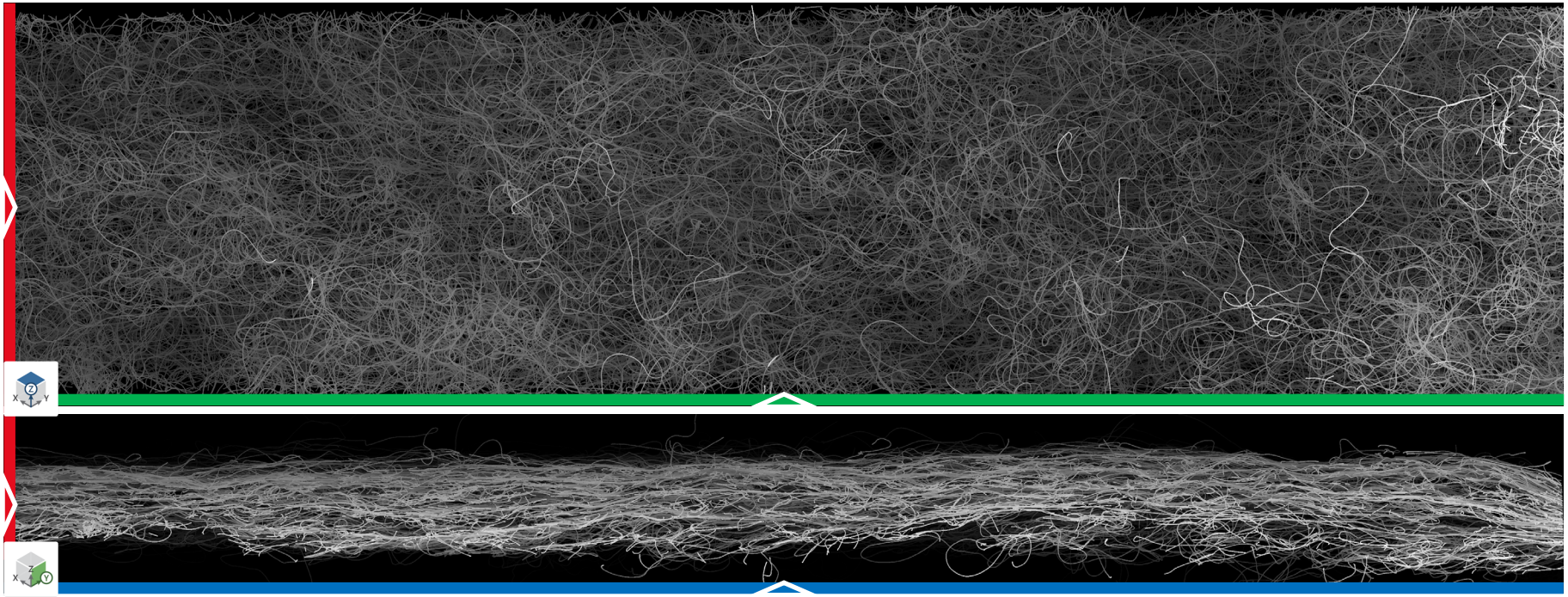


Reso-lution	Physical dimensions	Voxel dimensions
2.4µm	43.9 x 11.6 x 4.1 mm³	18,310 x 4,816 x 1,704

MATH 2 MARKET

Sample B – SEM view

GeoDict

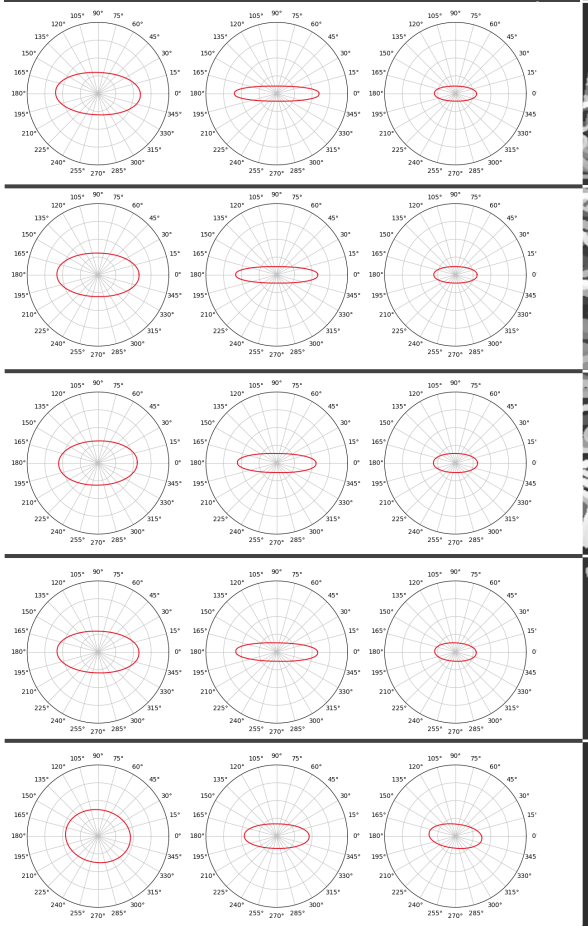


Resolution	Physical dimensions	Voxel dimensions
2.7µm	42.2 x 10.9 x 4.8 mm^3	15,619 x 4,032 x 1,796

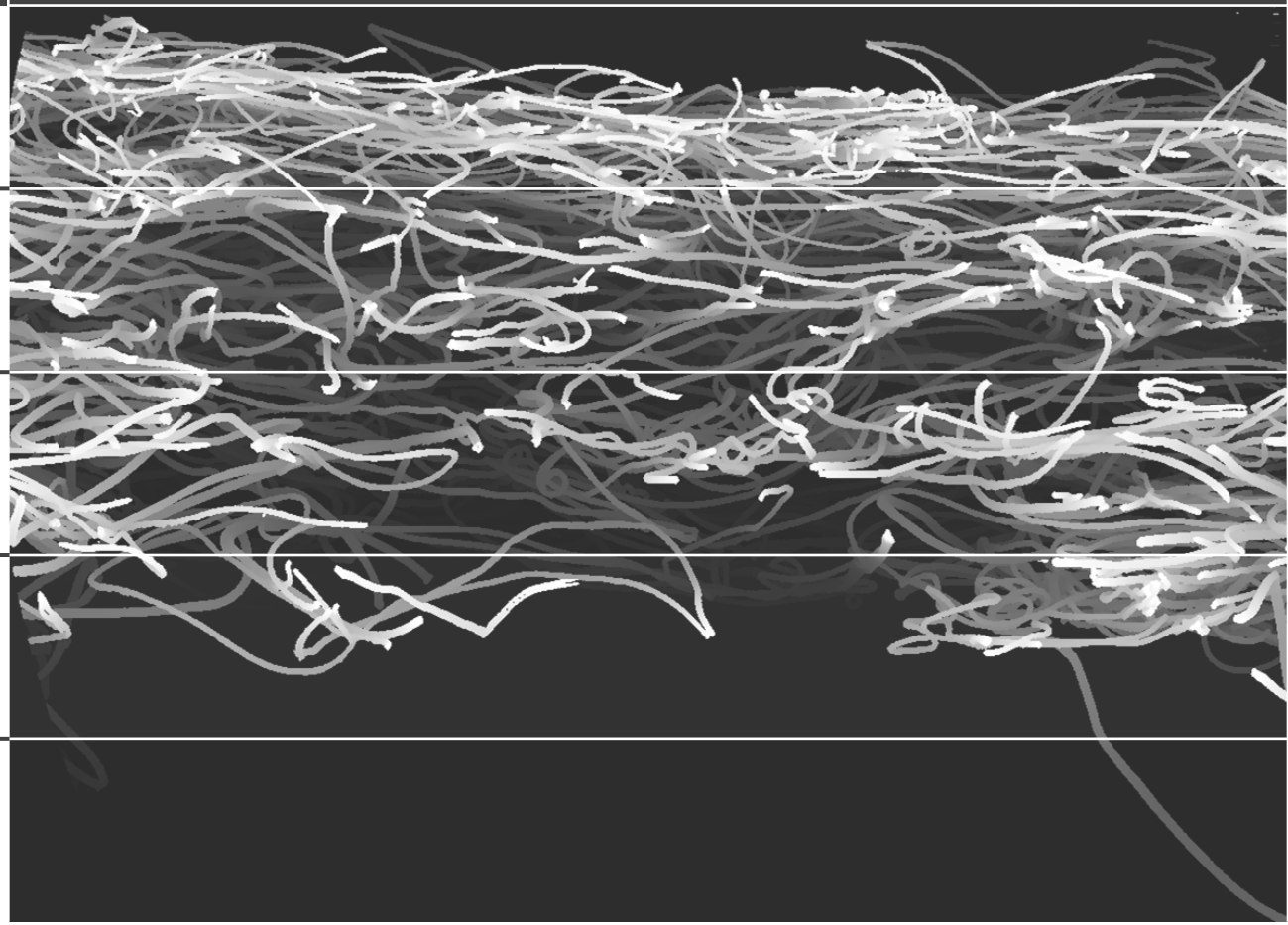
MATH 2 MARKET

Fiber orientations – sample A

GeoDict

XY	XZ	YZ
		

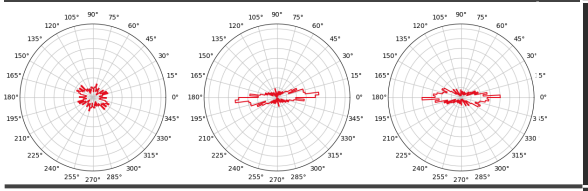
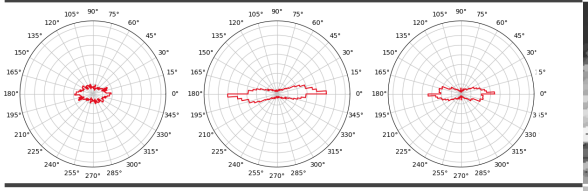
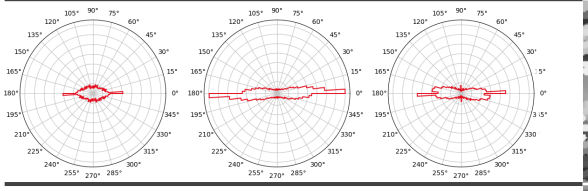
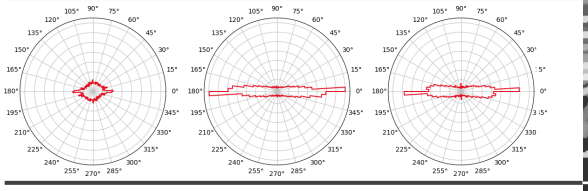
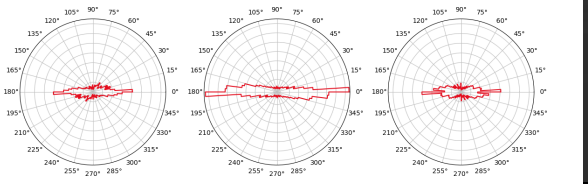
View of a section of the surface in the direction of the X axis.



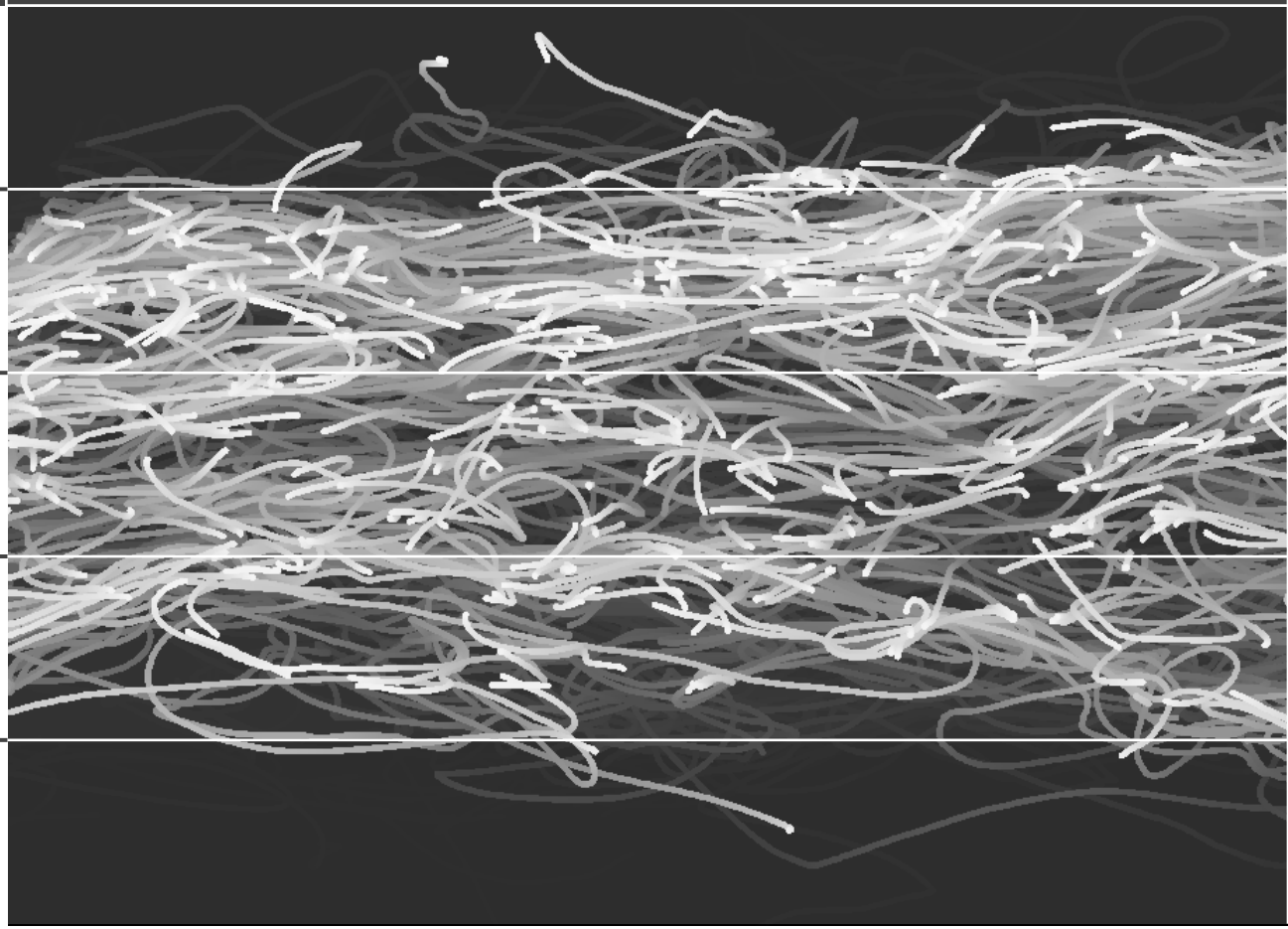
MATH 2 MARKET

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

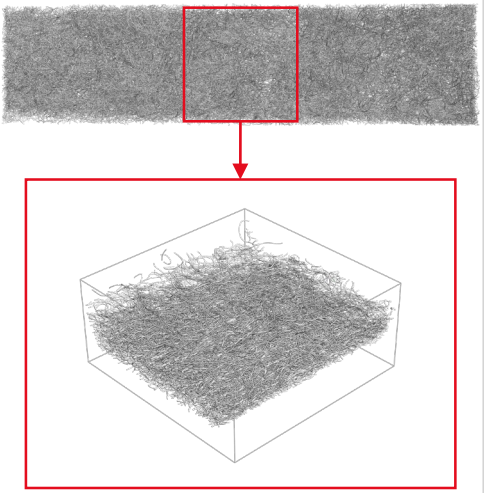
Fiber identification on Sample B

GeoDict

Sample B

FiberFind was used on the complete sample.

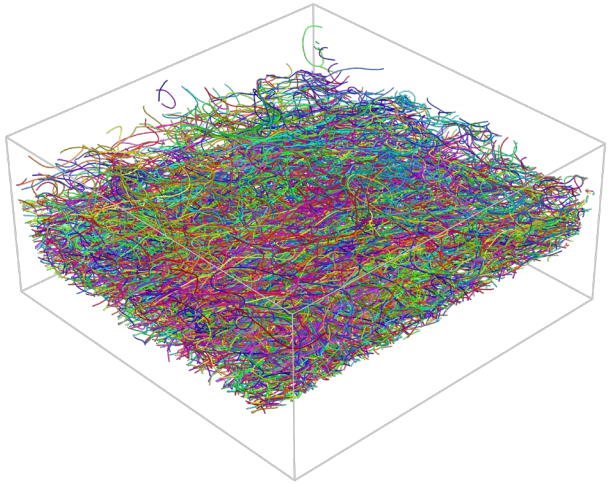
Process is explained on a smaller cutout



Labeling of fibers

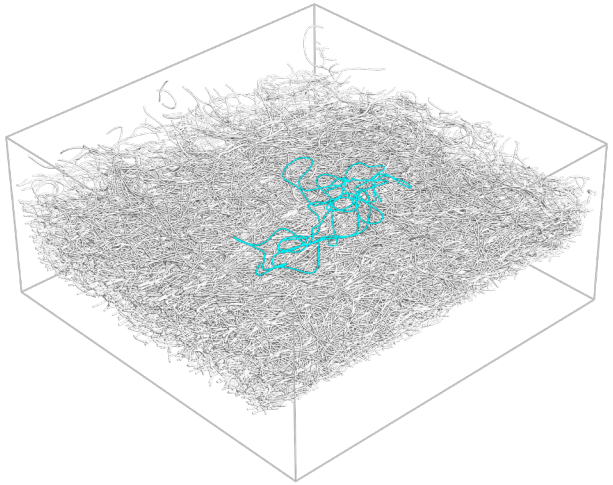
The artificial intelligence separates the solid voxels in the image data into individual fibers.

Each fiber becomes an independent, modifiable object which can be treated independently.

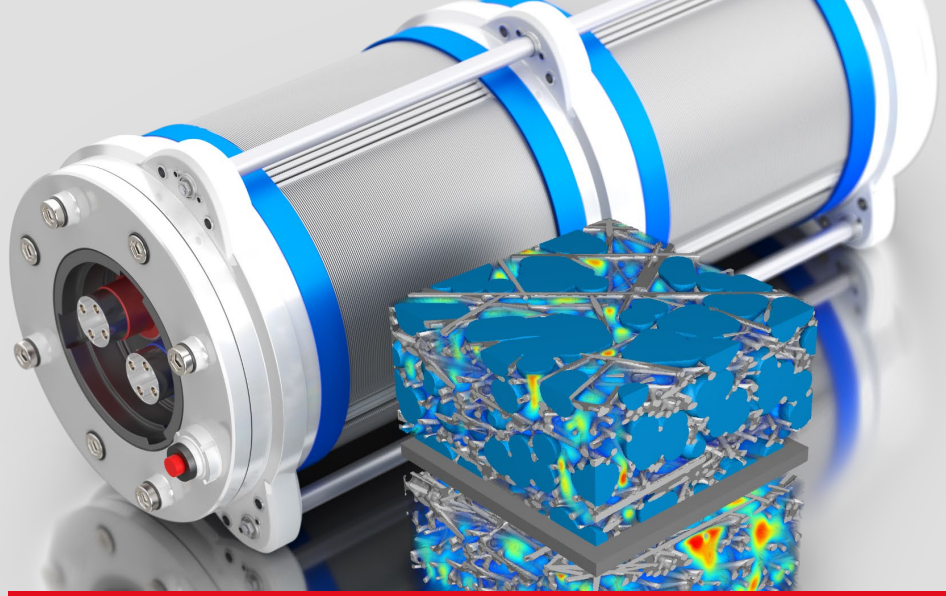


Data becomes information

Geometric information, such as fiber length, fiber segment orientation and fiber diameter, can be read directly from the object.



MATH 2 MARKET



GeoDict
The Digital Material Laboratory

Digital PEM Fuel Cell Development

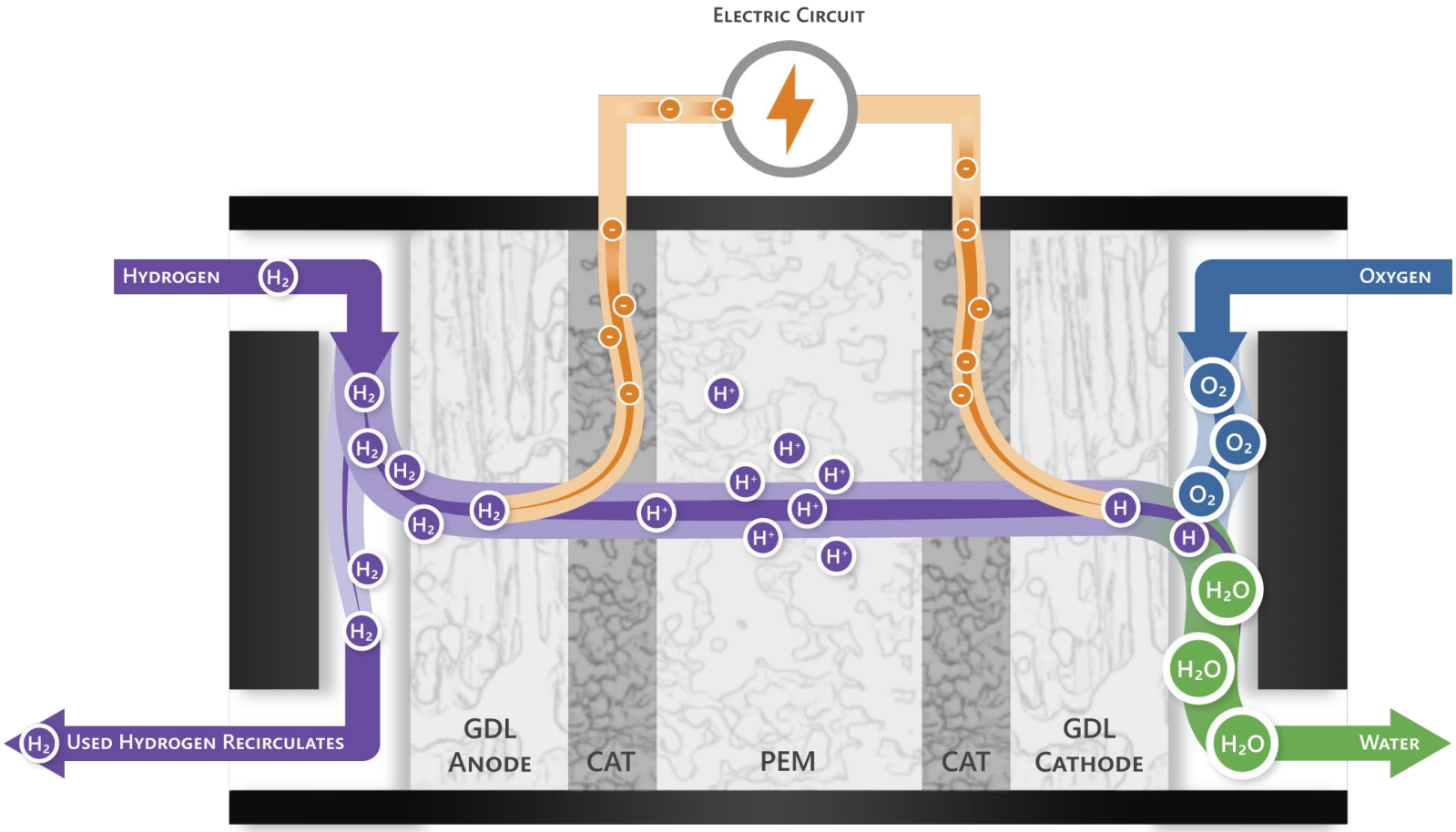
Solutions with **GeoDict**®

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

MATH 2 MARKET

PEM Fuel Cell

GeoDict



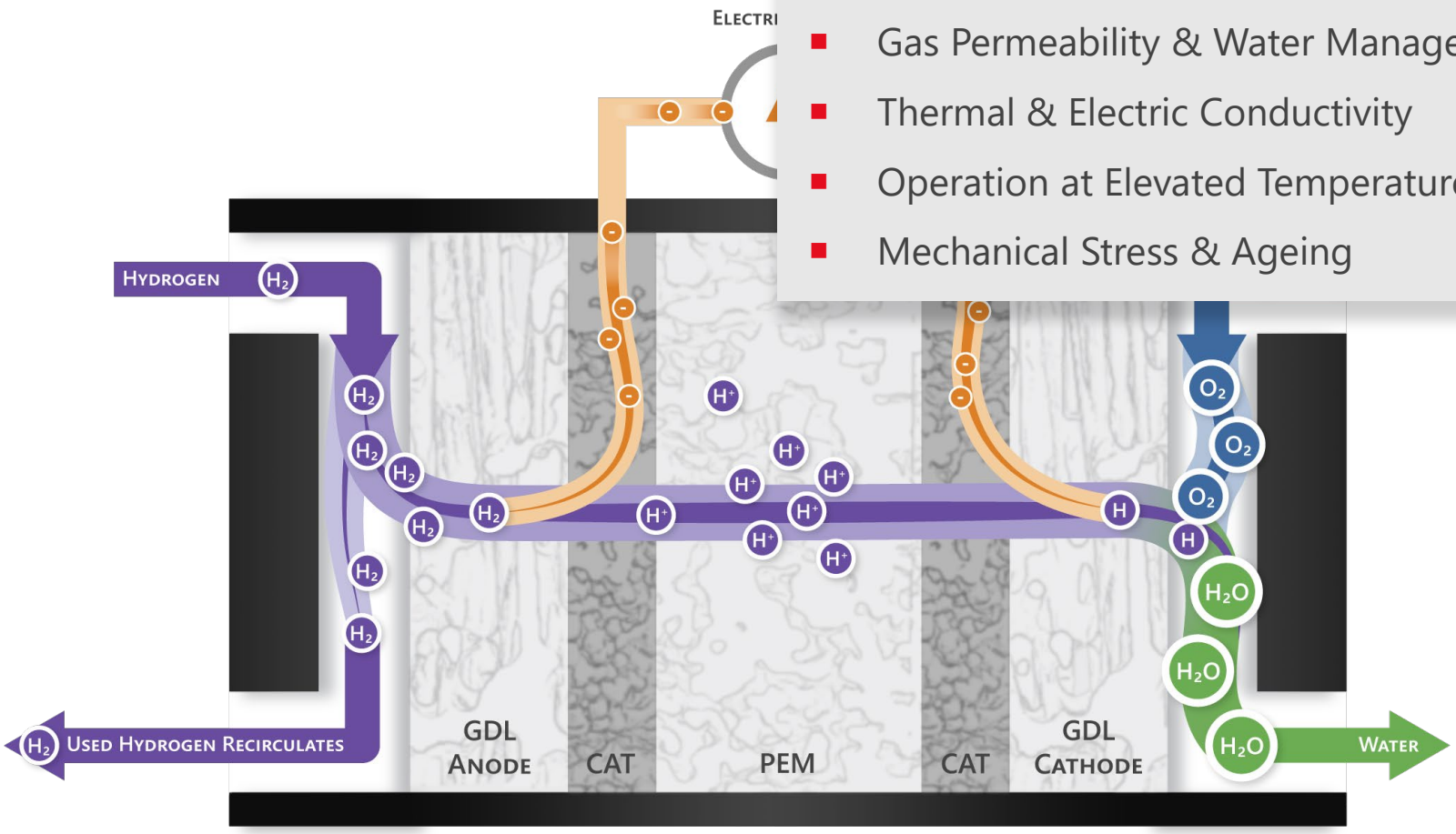
MATH 2 MARKET

PEM Fuel Cell

GeoDict

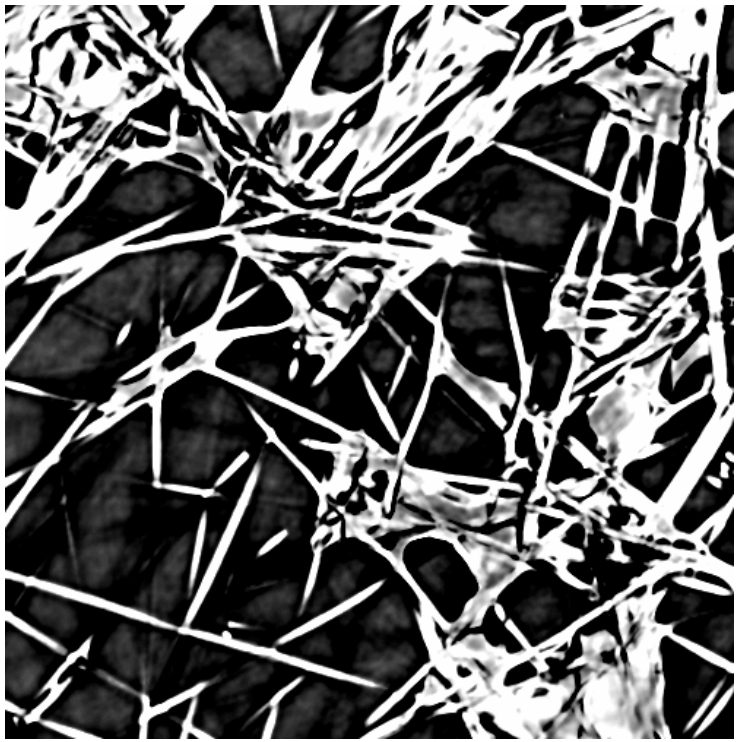
Challenges for Materials Design:

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



MATH 2 MARKET

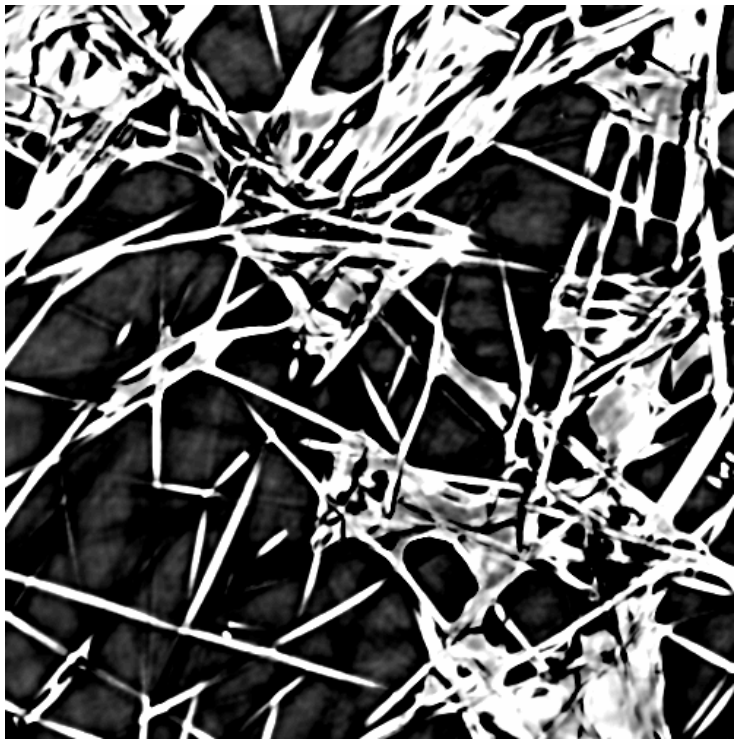
Import of a μCT Scan with GeoDict®



Data: μCT Scans of Toray TGP H 060, PSI Villingen (CH)

Segmentation with ImportGeo-Vol

Import of a μCT Scan with GeoDict®



Data: μCT Scans of Toray TGP H 060, PSI Villingen (CH)

Segmentation with ImportGeo-Vol

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

Segmentation of a GDL with FiberFind-AI*

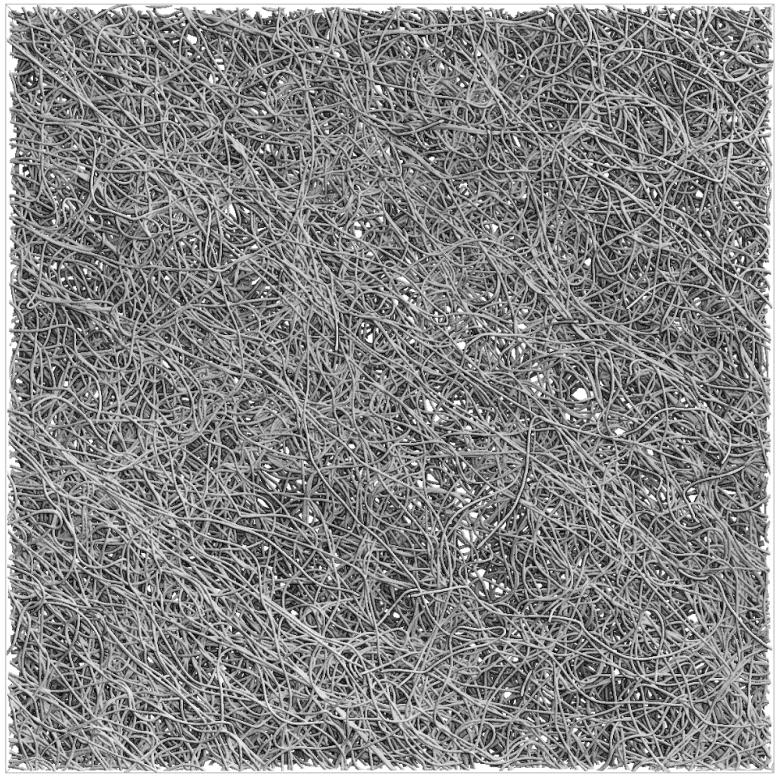
GeoDict

1. Imp

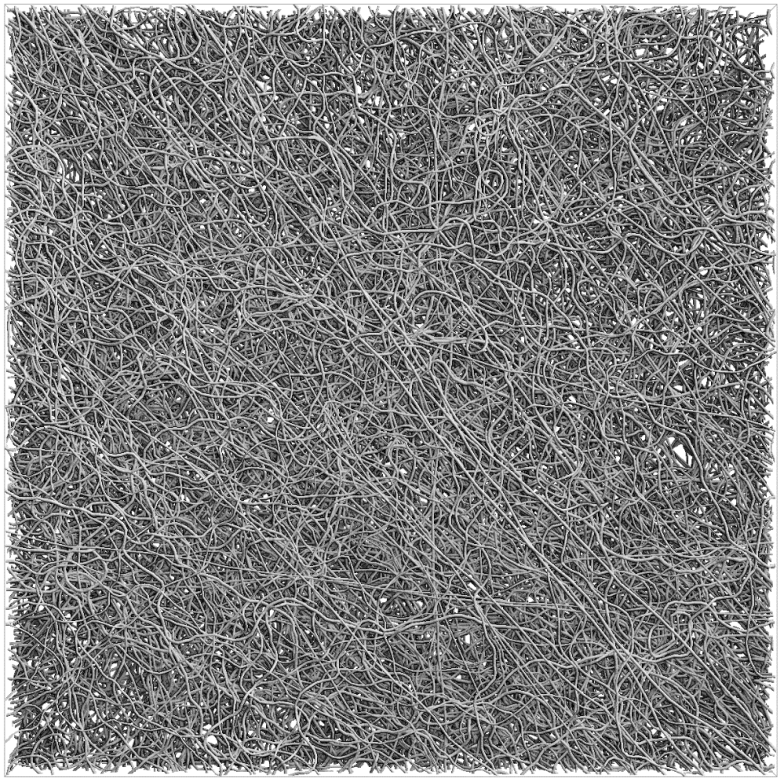
The neural network in FiberFind-AI, can distinguished fiber and binder of a Toray Paper

MATH 2 MARKET

CT-scan vs Digital Twin generated in GeoDict®



µCT-scan



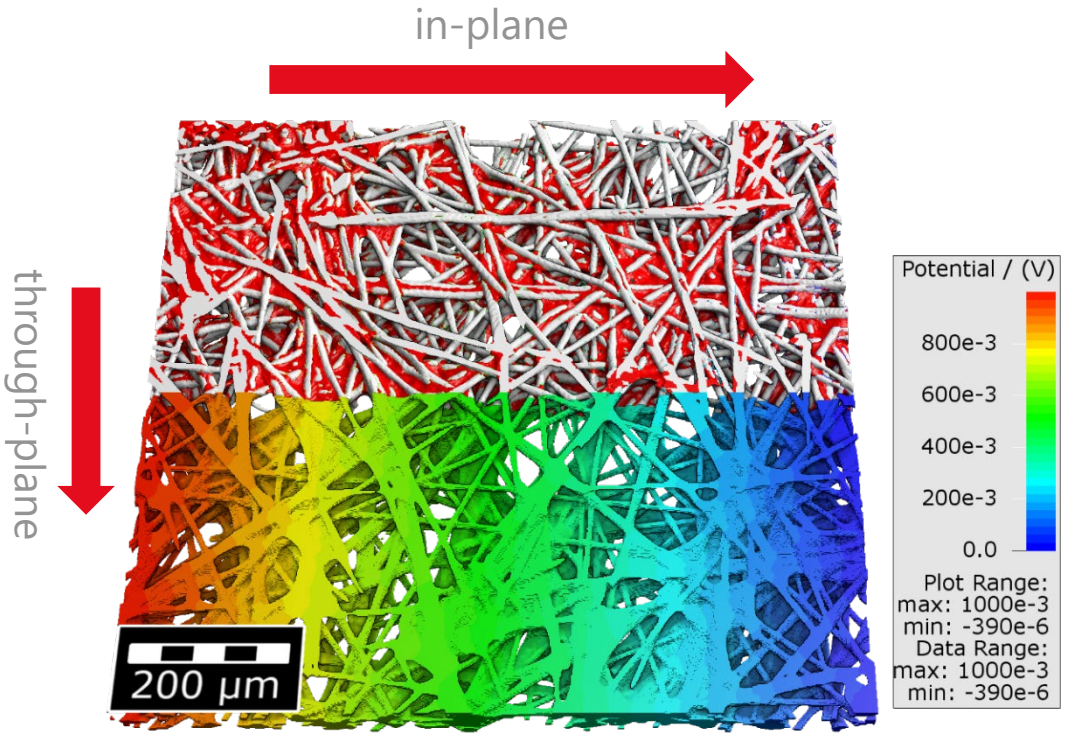
Digital Twin

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

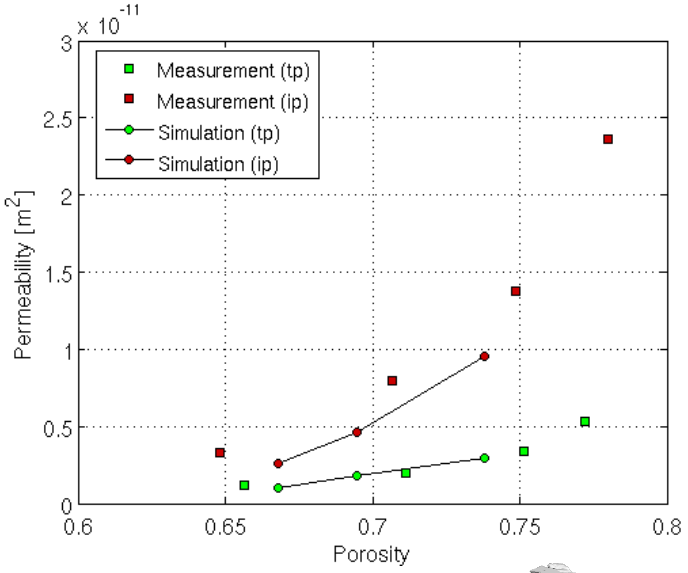
Transport Properties at Different Compression Levels

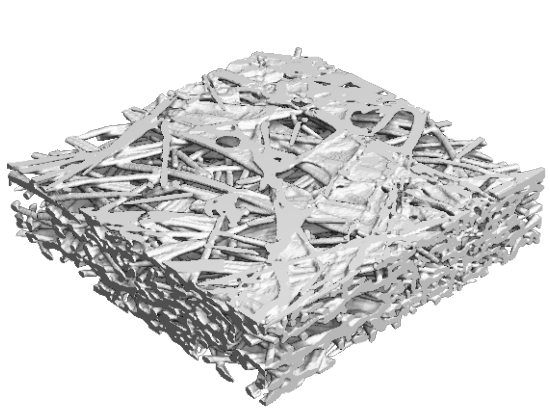
GeoDict

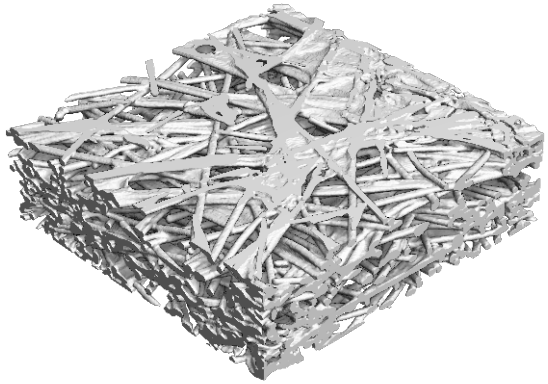
1. 2. Analyze » 3. Model » 4. Design »

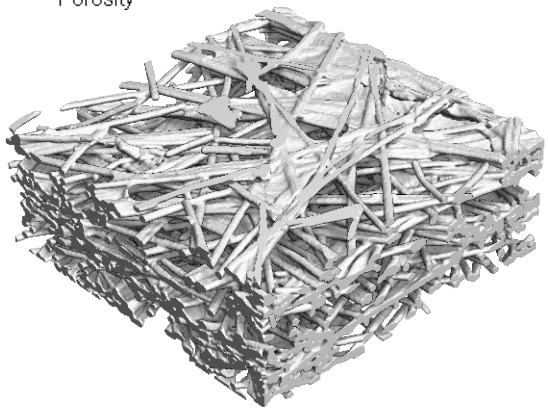
GeoDict simulations with PoroDict & DiffuDict:

- 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

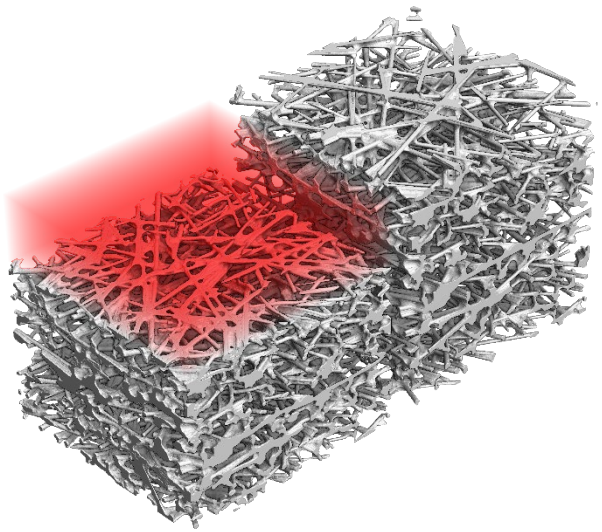
Water Saturation of a GDL simulated with SatuDict

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®*

Motivated by Jens Eller, Paul Scherrer Institut

Optimize Water Management with GeoDict®*

Motivated by Jens Eller, Paul Scherrer Institut

GeoDict
The Digital Material Laboratory

Compression of Porous Media with GeoDict

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

VOITH

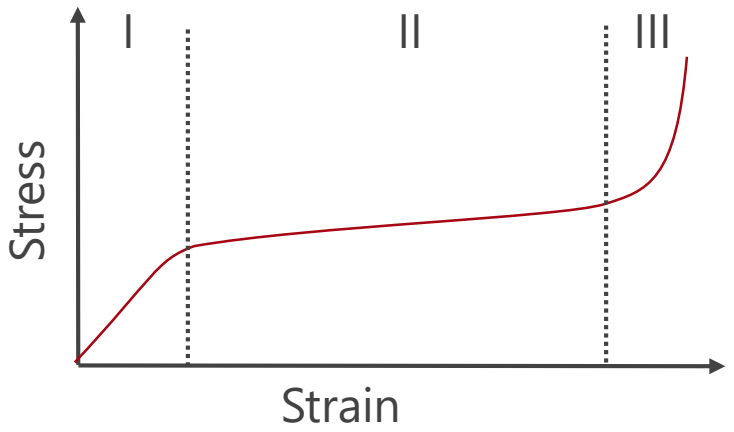
MATH 2 MARKET

Compression of Generated Foams

GeoDict

Stress-strain curve calculated with GeoDict

Theoretical stress strain curve



I. Linear elasticity,
II. Plateau
III. Densification

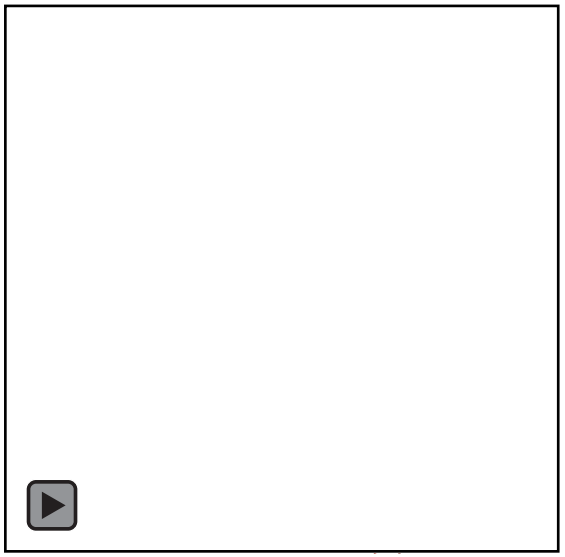
- Foam generated with FoamGeo
- 80 % compression (on deformed geometry)
- Buckling of cell walls can be observed
- Characteristical stress strain curve
- Constant positive pore pressure

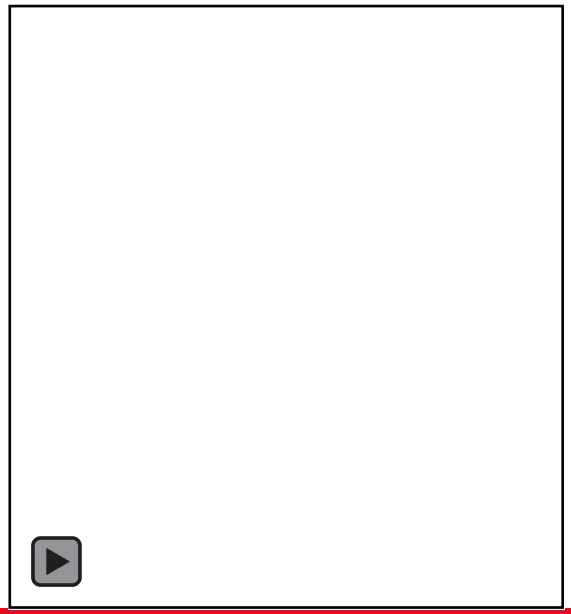
MATH 2 MARKET

Compression of Generated Foams

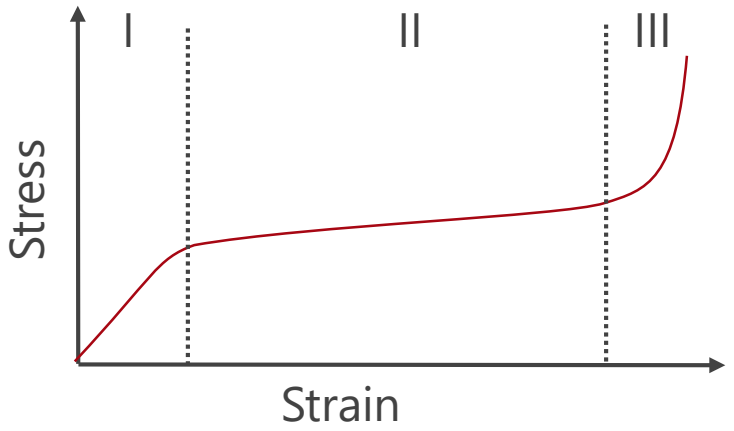
GeoDict

Stress-strain curve calculated with GeoDict





Theoretical stress strain curve



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MATH 2 MARKET

Compression of Generated Foams

GeoDict

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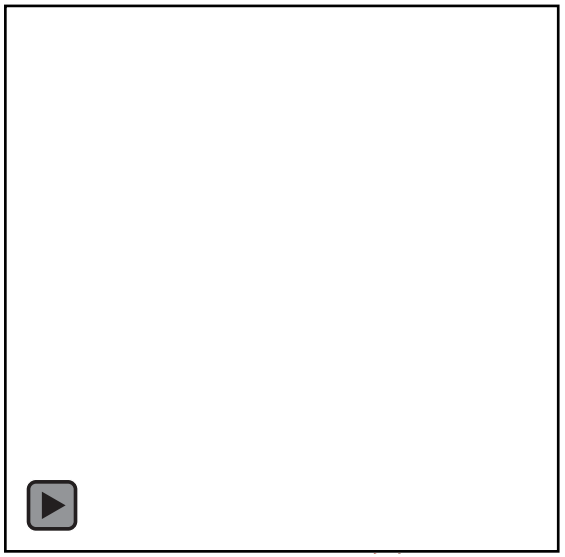
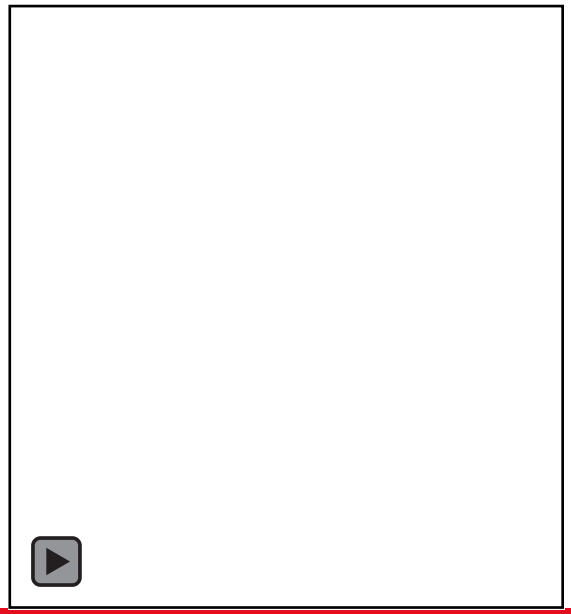
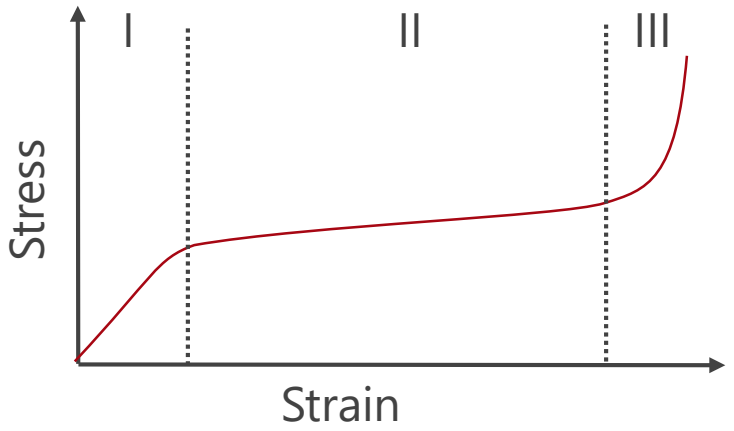




Theoretical stress strain curve



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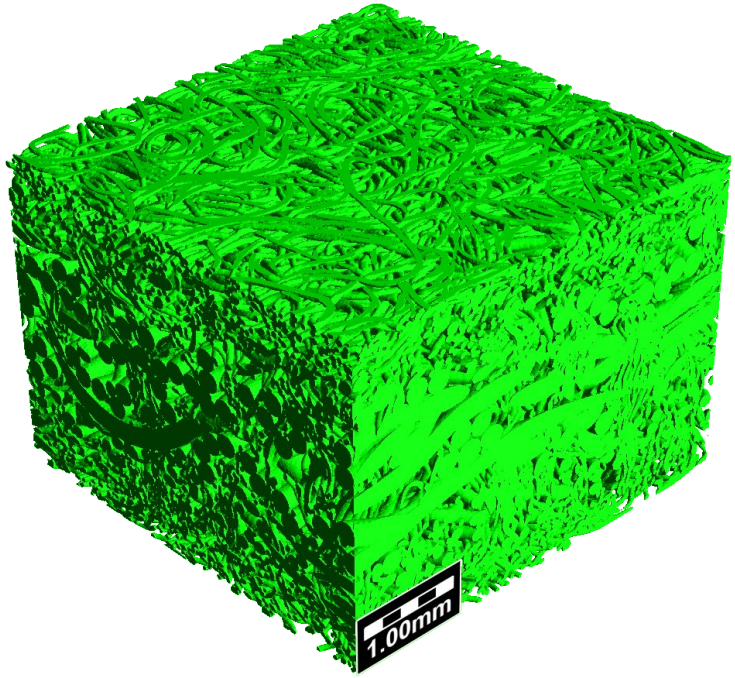
- Buckling of cell walls can be observed
- Characteristical stress strain curve
- Constant positive pore pressure

MATH 2 MARKET

GeoDict

Compression @ 0.1 MPa



Scan

547 x 546 x 410 Voxel
0% Deformation

ElastoDict

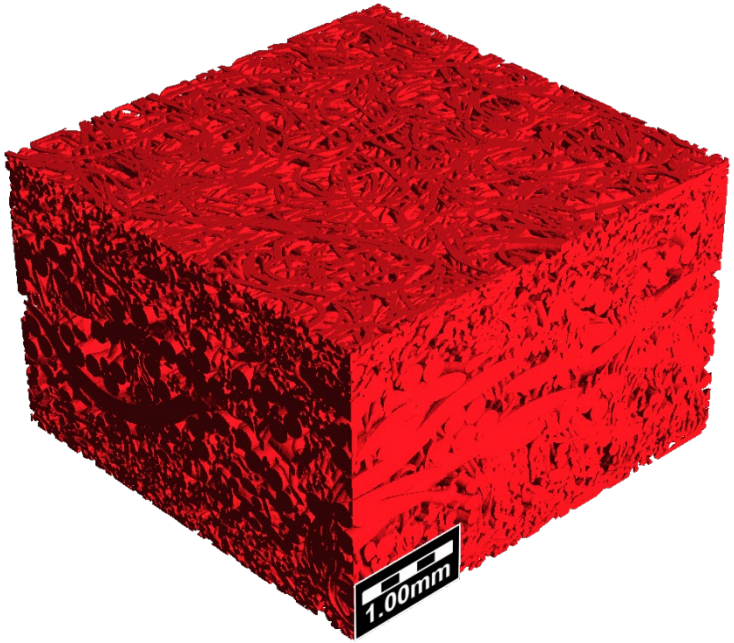
547 x 546 x 410 Voxel
0% Deformation

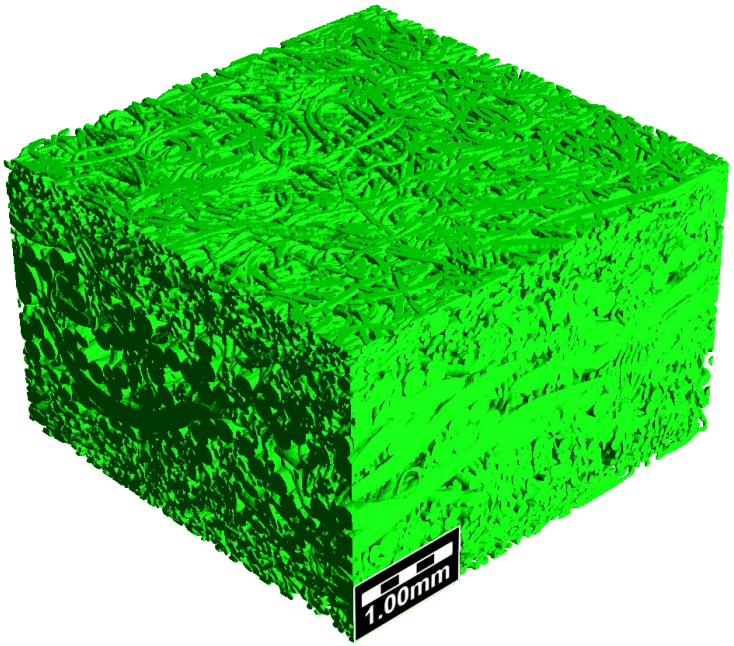
VOITH

MATH 2 MARKET

GeoDict

Compression @ 1.0 MPa





Scan

547 x 546 x 358 Voxel
-12.68% Deformation

ElastoDict

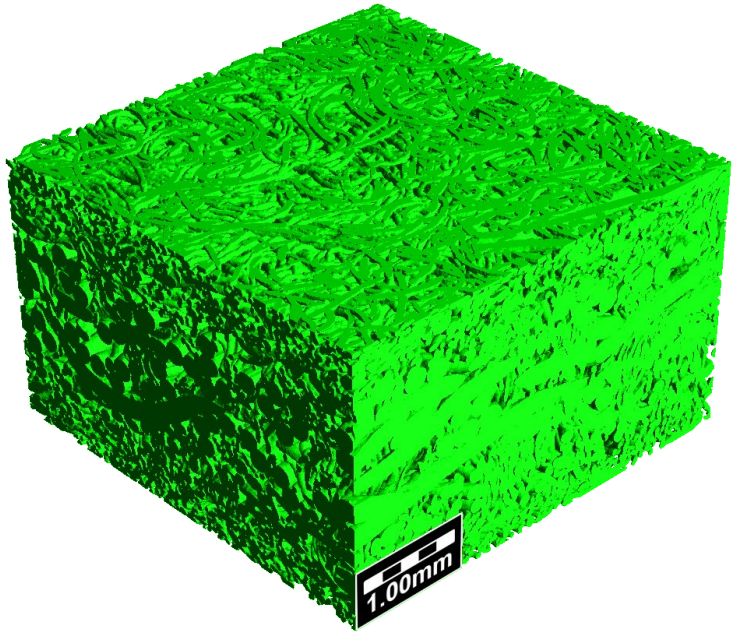
547 x 546 x 358 Voxel
-12.68% Deformation

VOITH

MATH 2 MARKET

GeoDict

Compression @ 2.0 MPa



Scan

547 x 546 x 341 Voxel
-4.75% Deformation

ElastoDict

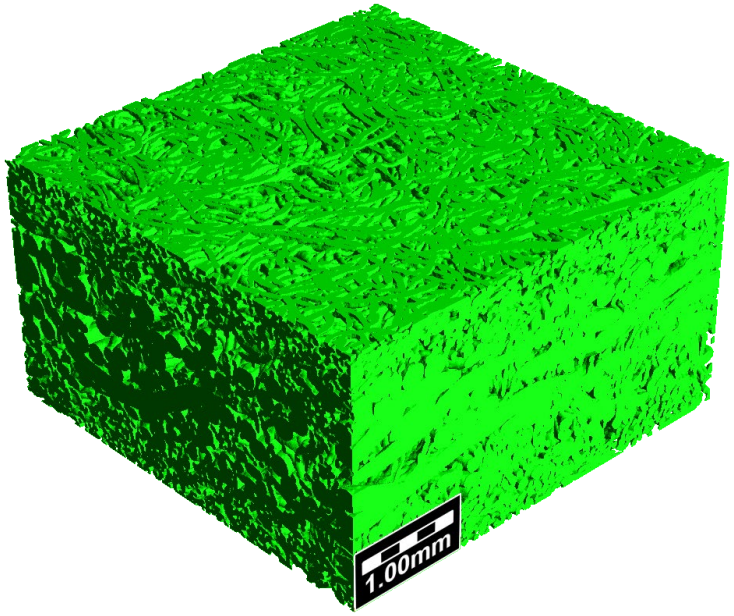
547 x 546 x 341 Voxel
-4.75% Deformation

VOITH

MATH 2 MARKET

GeoDict

Compression @ 4.0 MPa



Scan

547 x 544 x 314 Voxel
-7.92% Deformation

ElastoDict

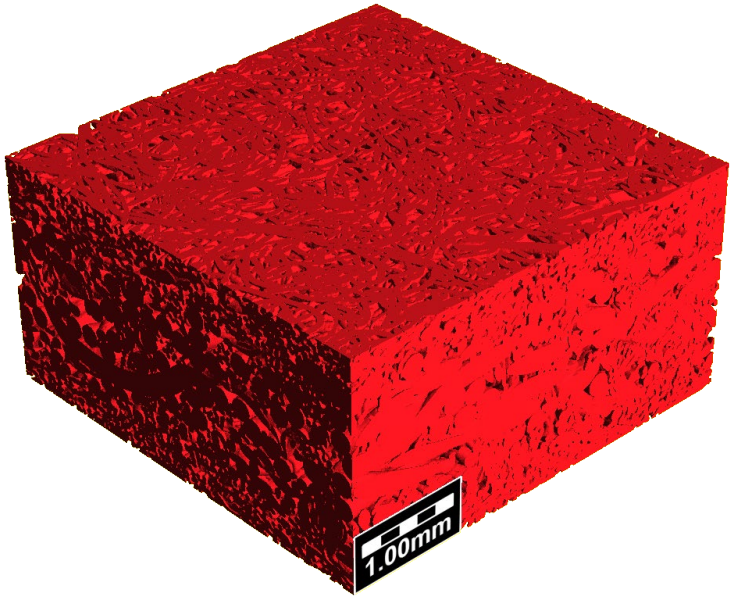
547 x 544 x 314 Voxel
-7.92% Deformation

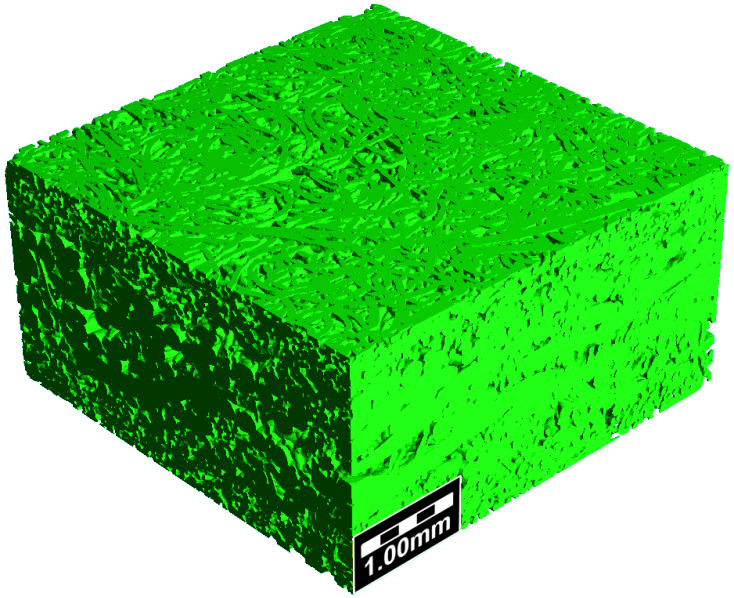
VOITH

MATH 2 MARKET

GeoDict

Compression @ 6.0 MPa





Scan

547 x 544 x 290 Voxel
-7.46% Deformation

ElastoDict

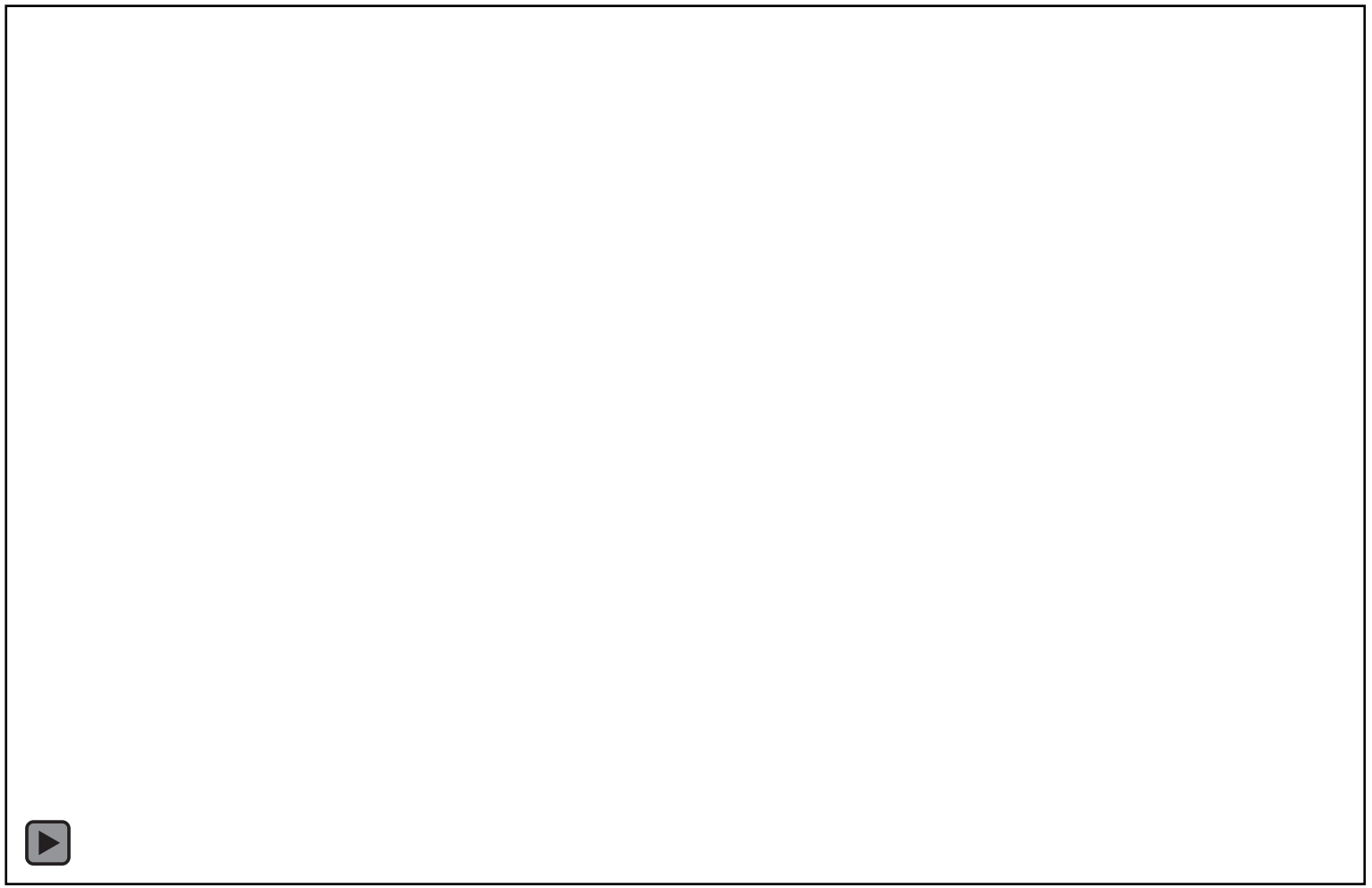
547 x 544 x 290 Voxel
-7.46% Deformation

VOITH

MATH 2 MARKET

GEODICT

OVERLAP-ANALYSIS @ 1.0 MPa



Scan

Simulation

Overlap

Pore

MATH 2 MARKET

GeoDict
The Digital Material Laboratory

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).

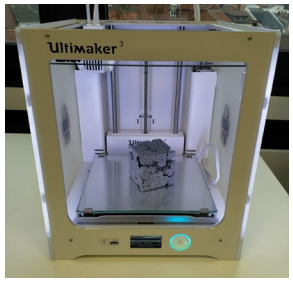
MATH 2 MARKET

CONTRIBUTIONS

GEODICT

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



Institut für Verbundwerkstoffe

Fraunhofer ITWM

MATH 2 MARKET

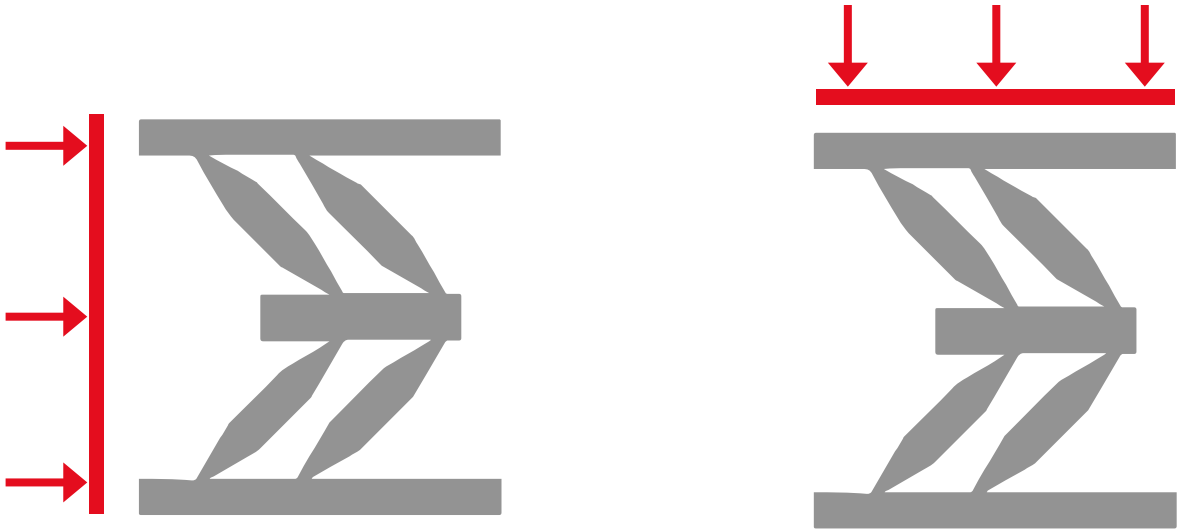
FeelMath

What is special about this mechanical Metamaterial?

GeoDict

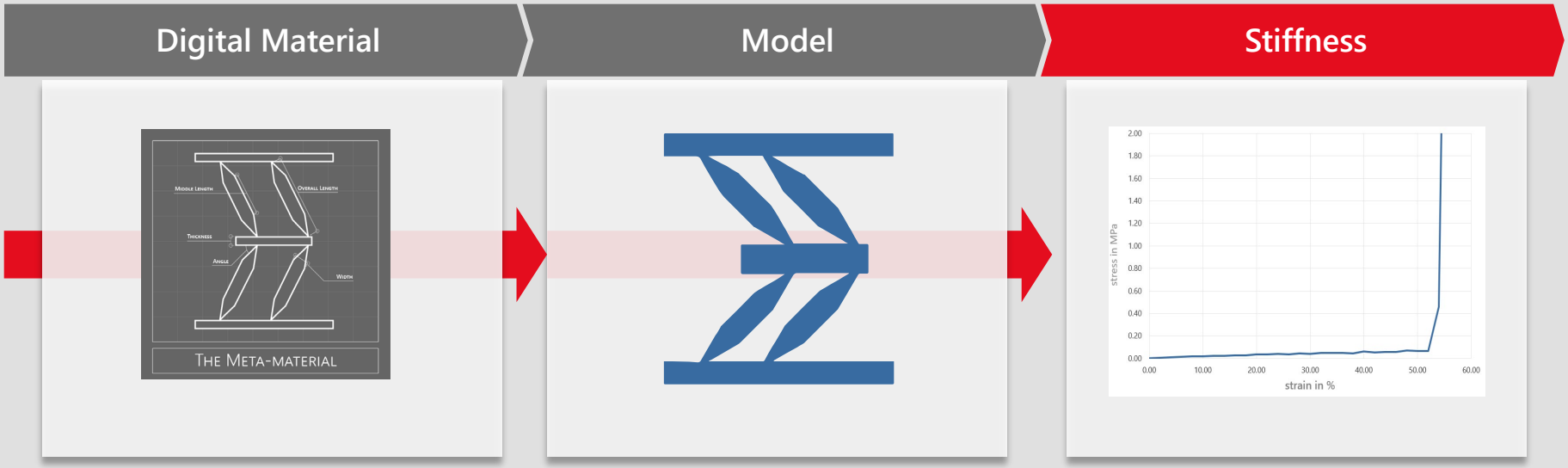
In the **horizontal direction**, the material is rather stiff.

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



SIMULATION ON DIGITAL MODEL

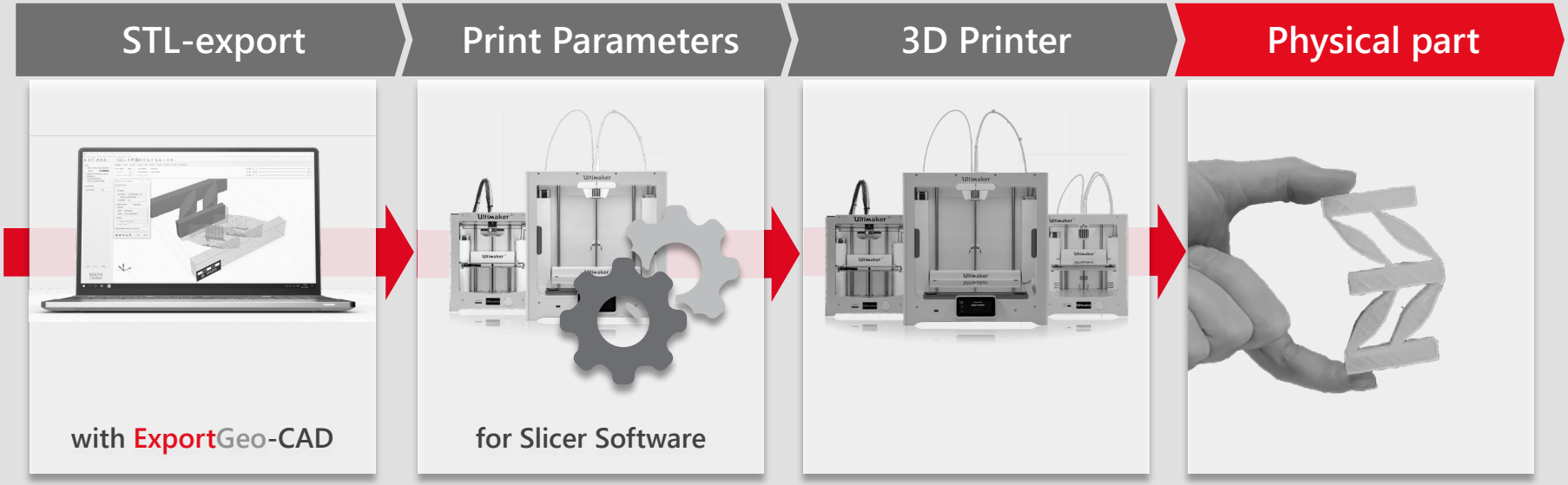
Meta-Material designed for Additive Manufacturing



3D Part by Fused Filament Fabrication

GeoDict

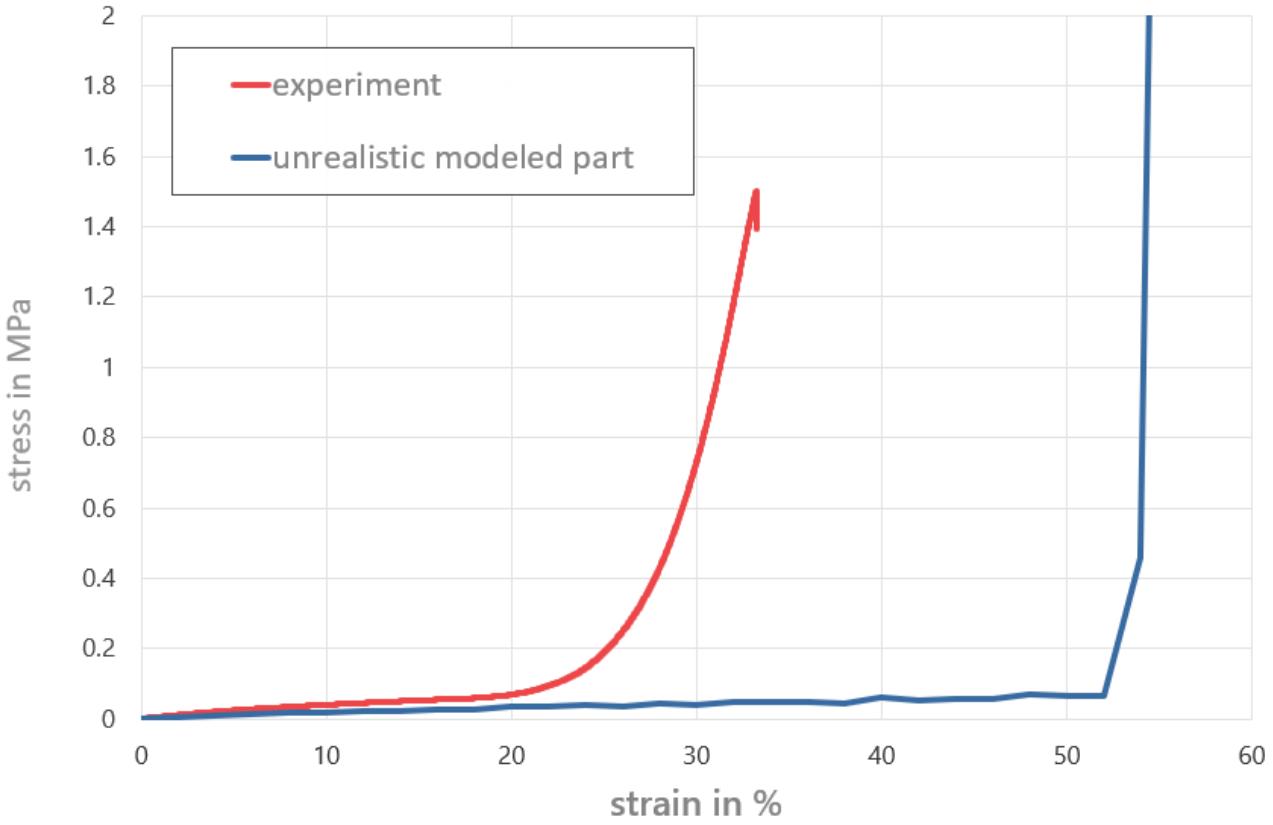
Prototype manufactured by Additive Manufacturing



MATH 2 MARKET

Problem: Standard Approach to stiffness prediction is insufficient

GeoDict



MATH 2 MARKET

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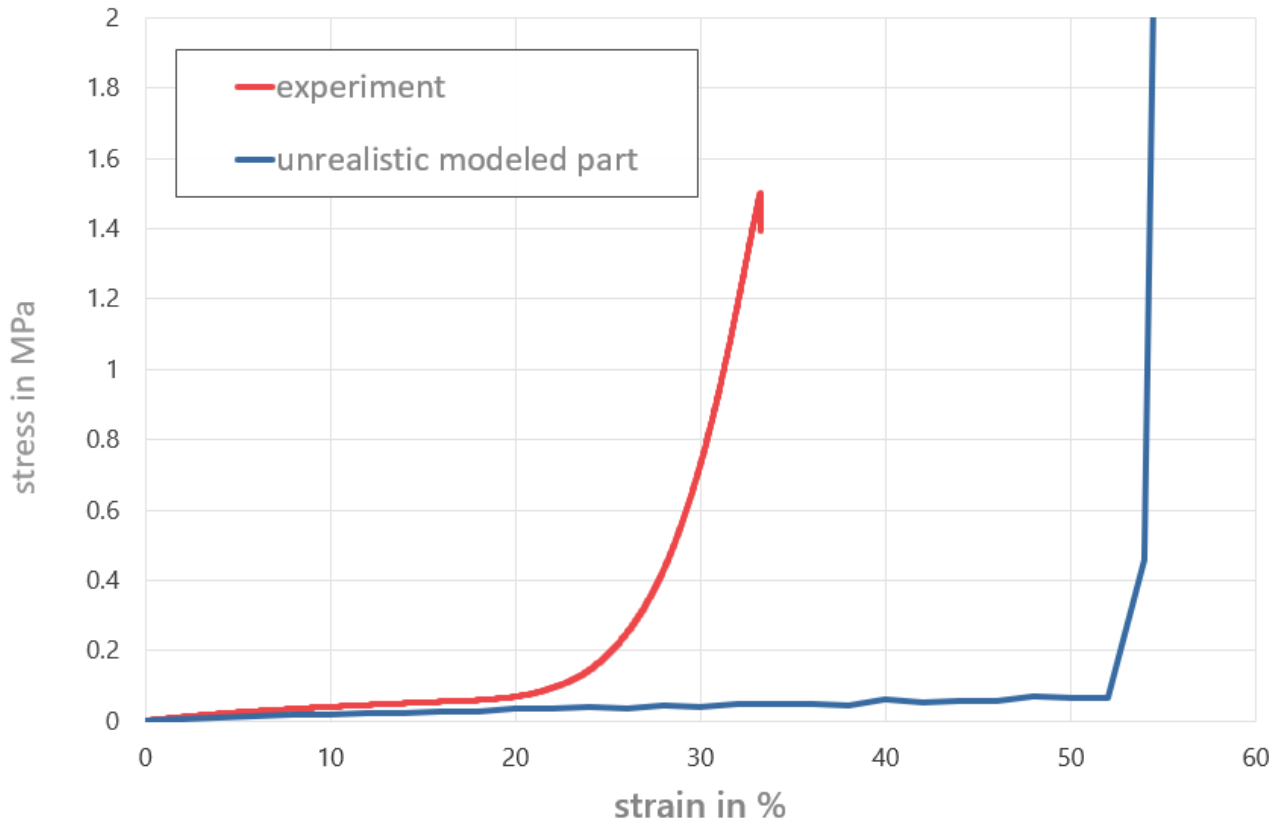
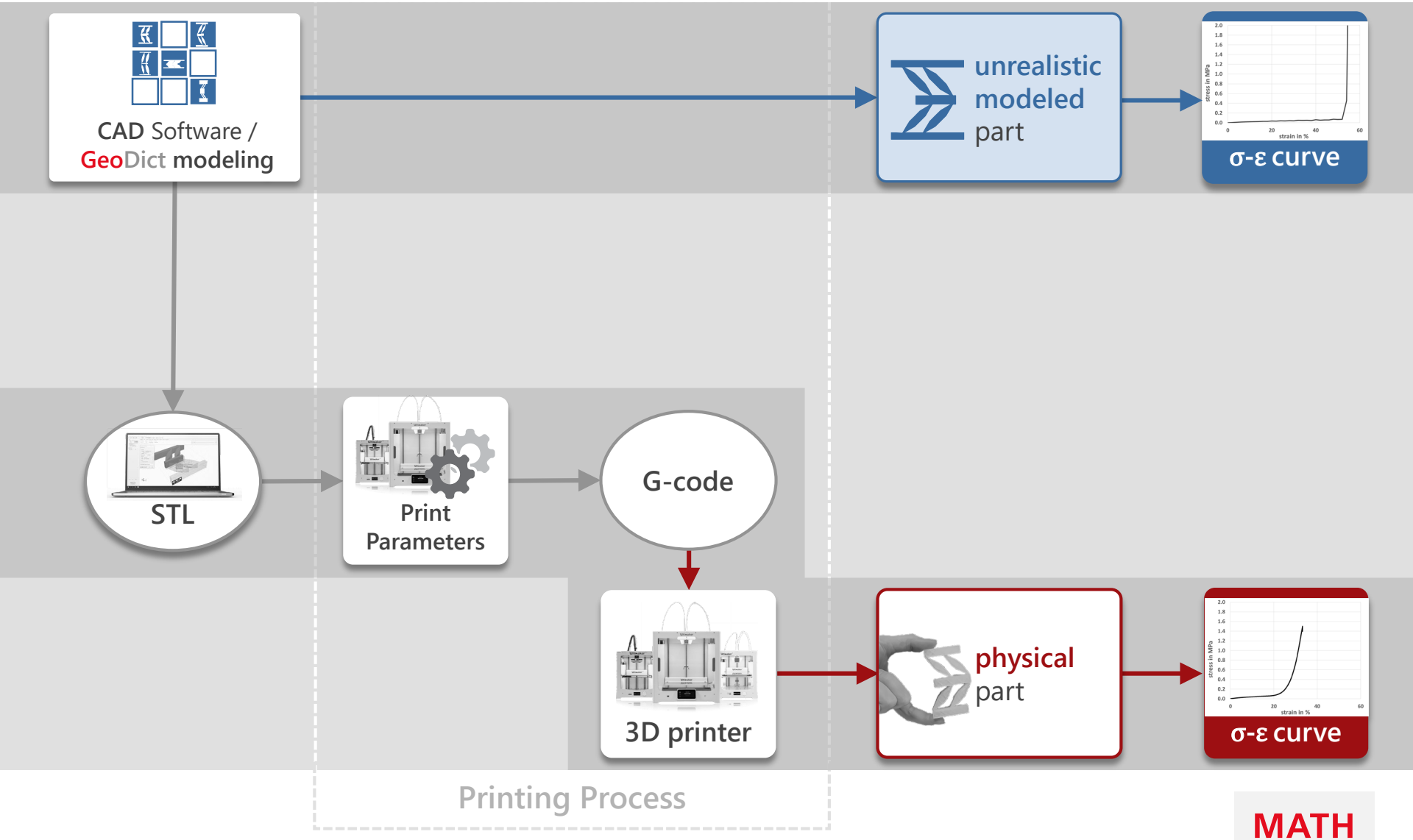


Simulated behavior does not agree with experiments

MATH 2 MARKET

Simulation does not match Experiment
printing process is not modelled

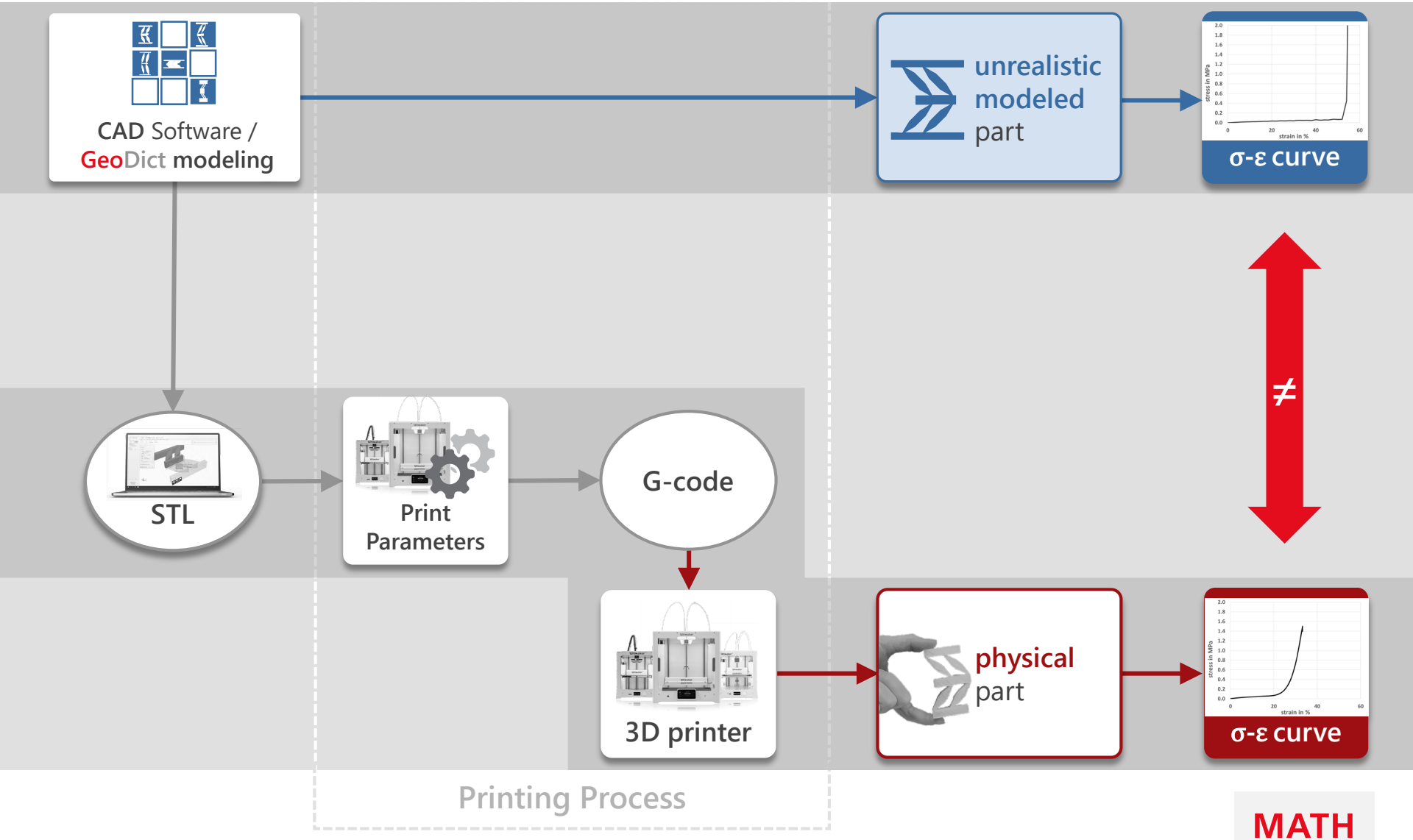
GeoDict



MATH 2 MARKET

Simulation does not match Experiment
printing process is not modelled

GeoDict



MATH 2 MARKET

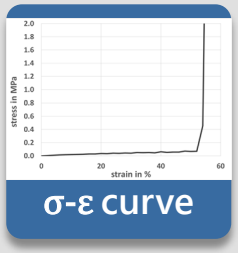
Simulation doesn't match Experiment because printing process is not modelled

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?

?



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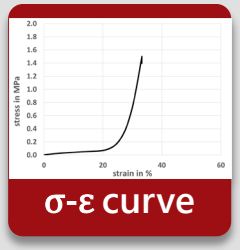
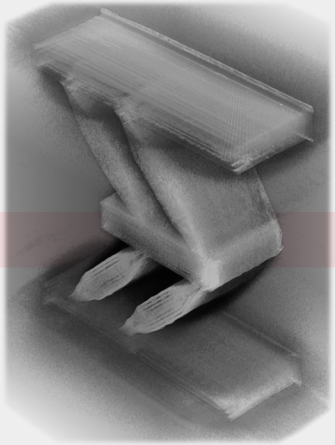
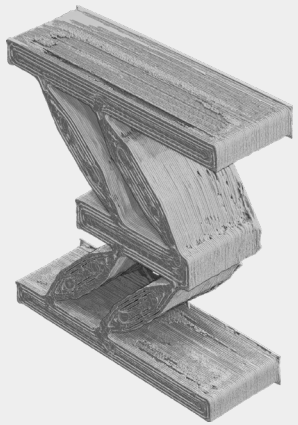


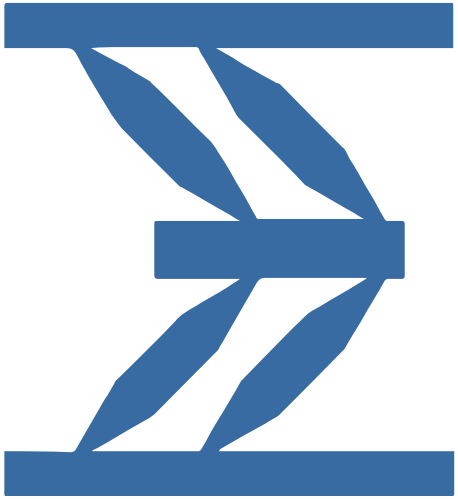
MATH 2 MARKET

1. µCT-SCAN AND IMPORT IN GEODICT

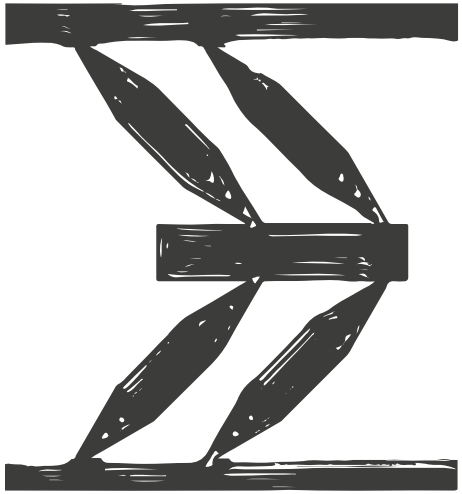
Printed Part	µCT-scanner	CT-data import	Segmented data
			
in µCT-scanner	at Fraunhofer ITWM	into GeoDict	

GEODICT

2. COMPARISON OF UNREALISTIC MODELED AND µCT SCANNED PART



unrealistic modeled part



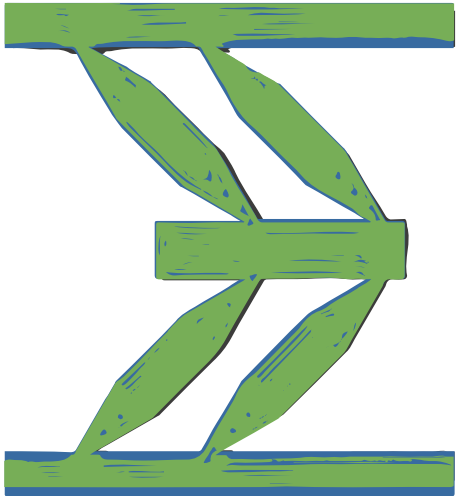
µCT scanned part

Geometrical Validation

MATH 2 MARKET

GEODICT

2. COMPARISON OF UNREALISTIC MODELED AND µCT SCANNED PART



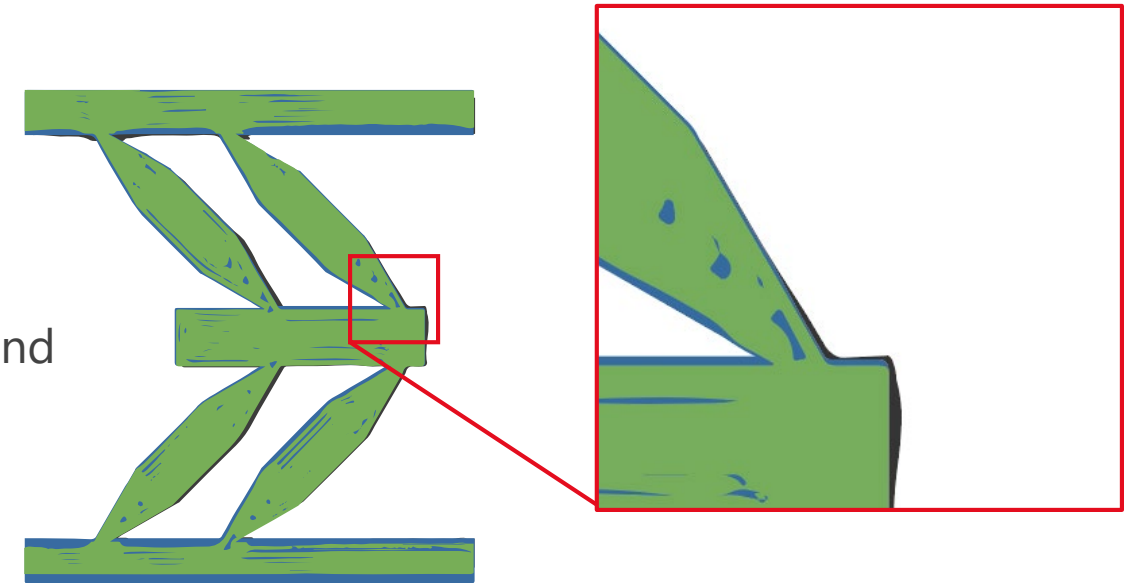
overlap

Geometrical Validation

MATH 2 MARKET

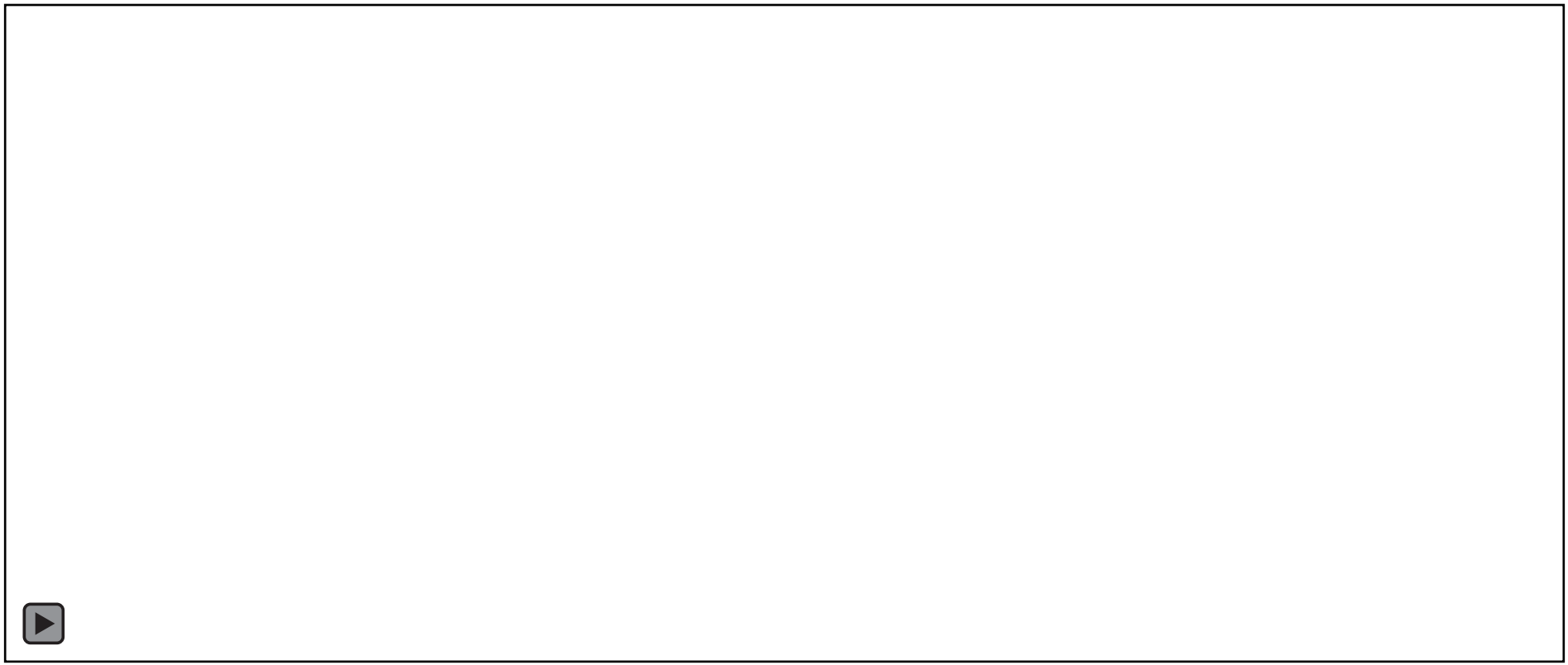
3. COMPARISON OF CORNER DETAIL

Overlap of
Unrealistic modeled and
CT scanned part



Geometrical Validation

4. COMPARISON OF EXPERIMENT WITH SIMULATION

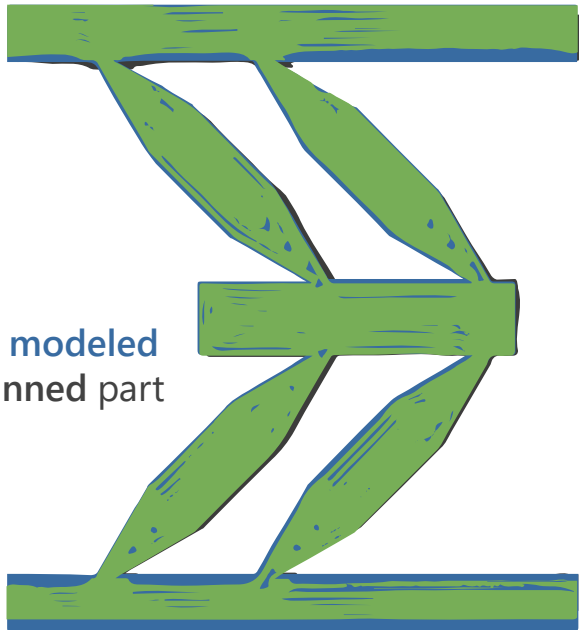


Digital Image Correlation,
Compression experiment

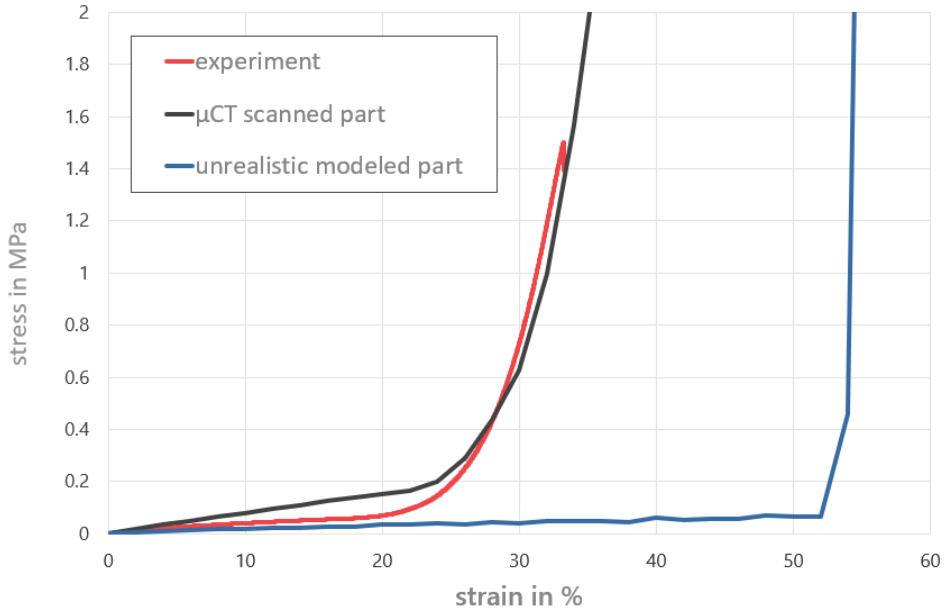
ElastoDict simulation on µCT-scan

Mechanics simulation agrees with experiment when applied to µCT scan

GeoDict



Overlap of
Unrealistic modeled
and CT scanned part



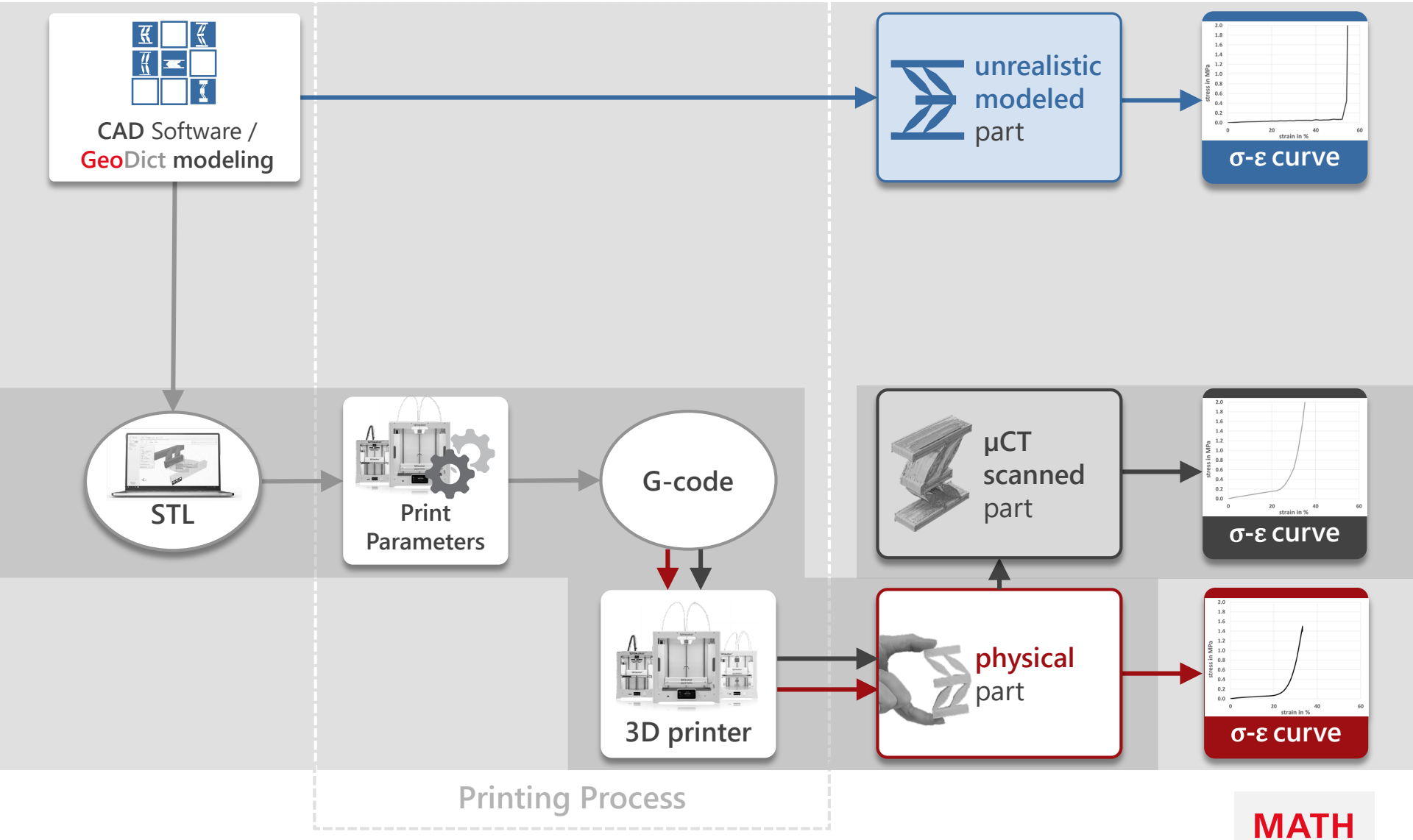
Geometrical Validation

Property Validation

MATH 2 MARKET

Problem would be solved if our model were more similar to the µCT scan

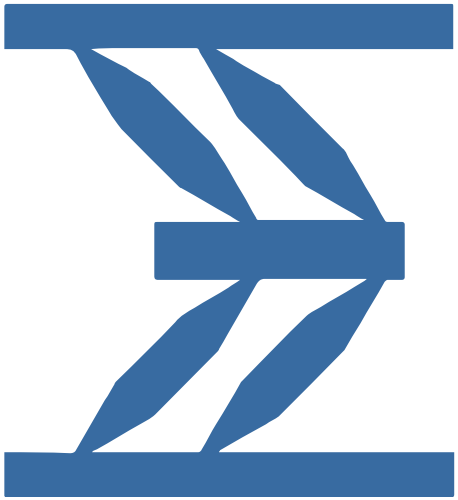
GeoDict



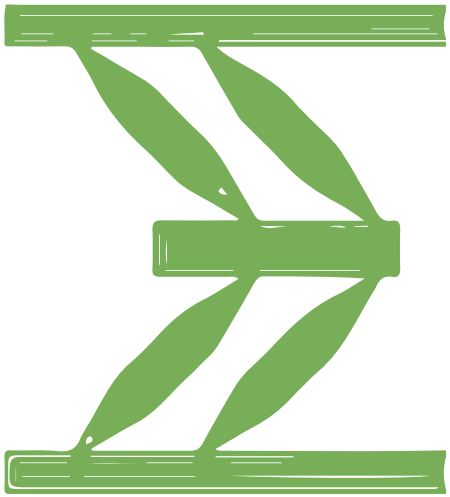
MATH 2 MARKET

INTRODUCING IMPORTGEO-AM

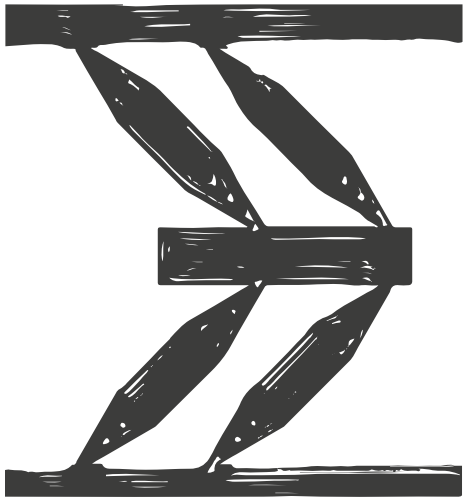
Take output of printer software and create 3D model that takes into account the printing process



unrealistic part



realistic virtually printed part

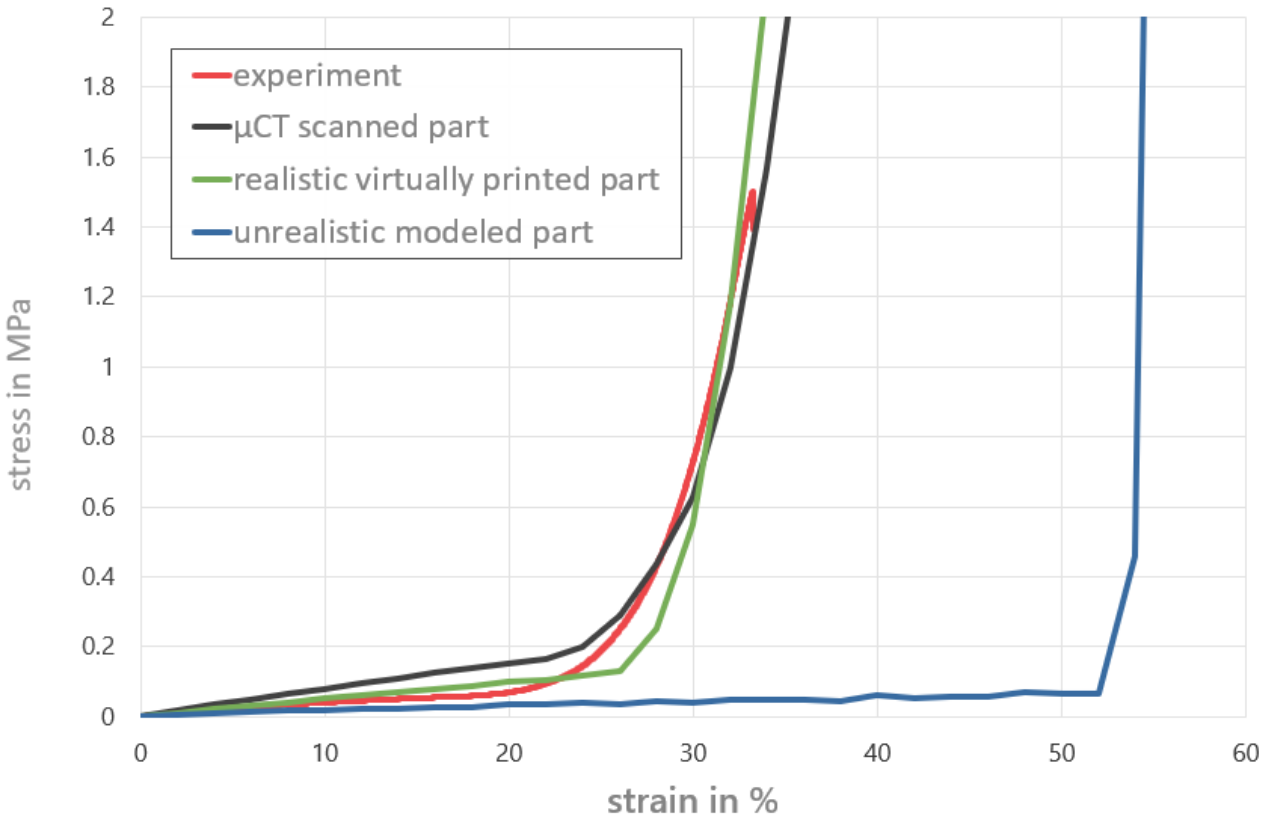


µCT scan of part

Geometrical Validation

Solution: GeoDict enhanced approach to stress-strain prediction matches experiment

GeoDict



MATH 2 MARKET

Solution: GeoDict enhanced approach to stress-strain prediction matches experiment

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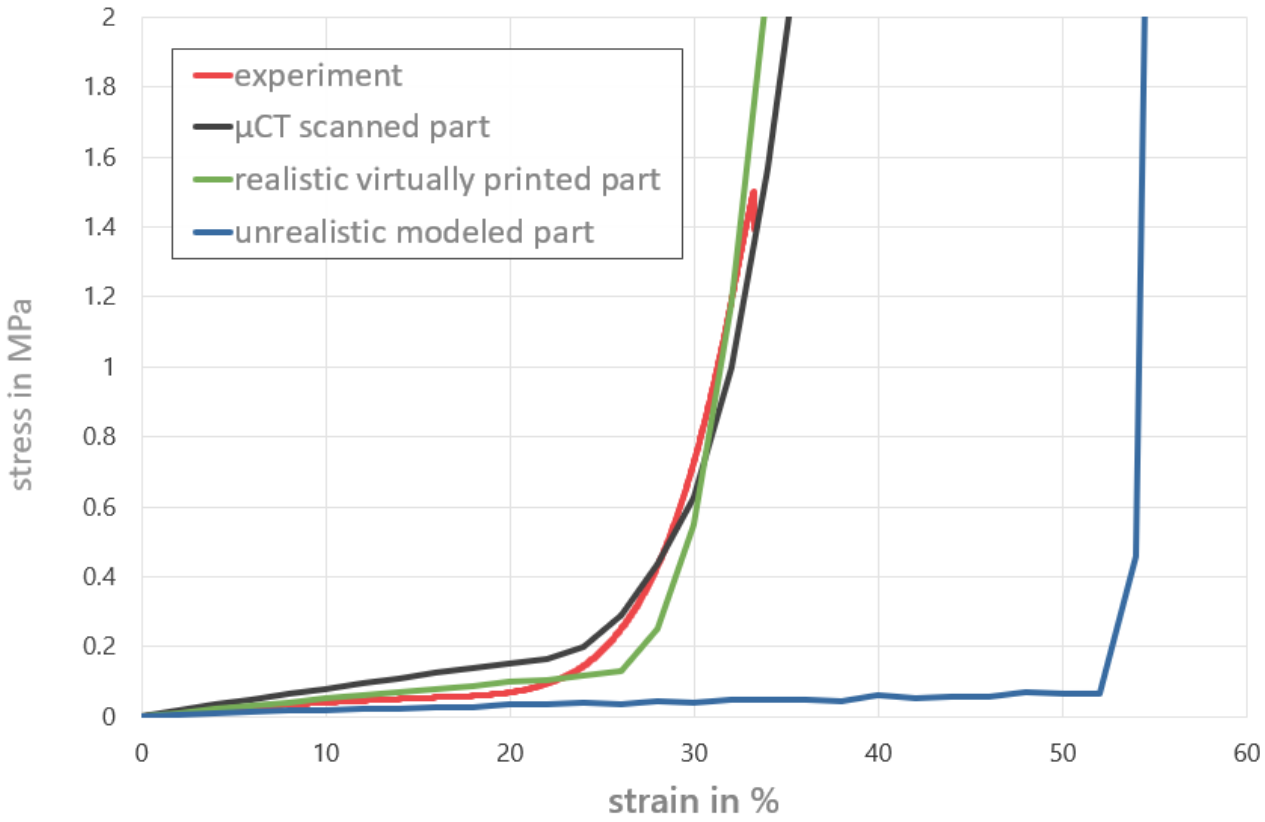
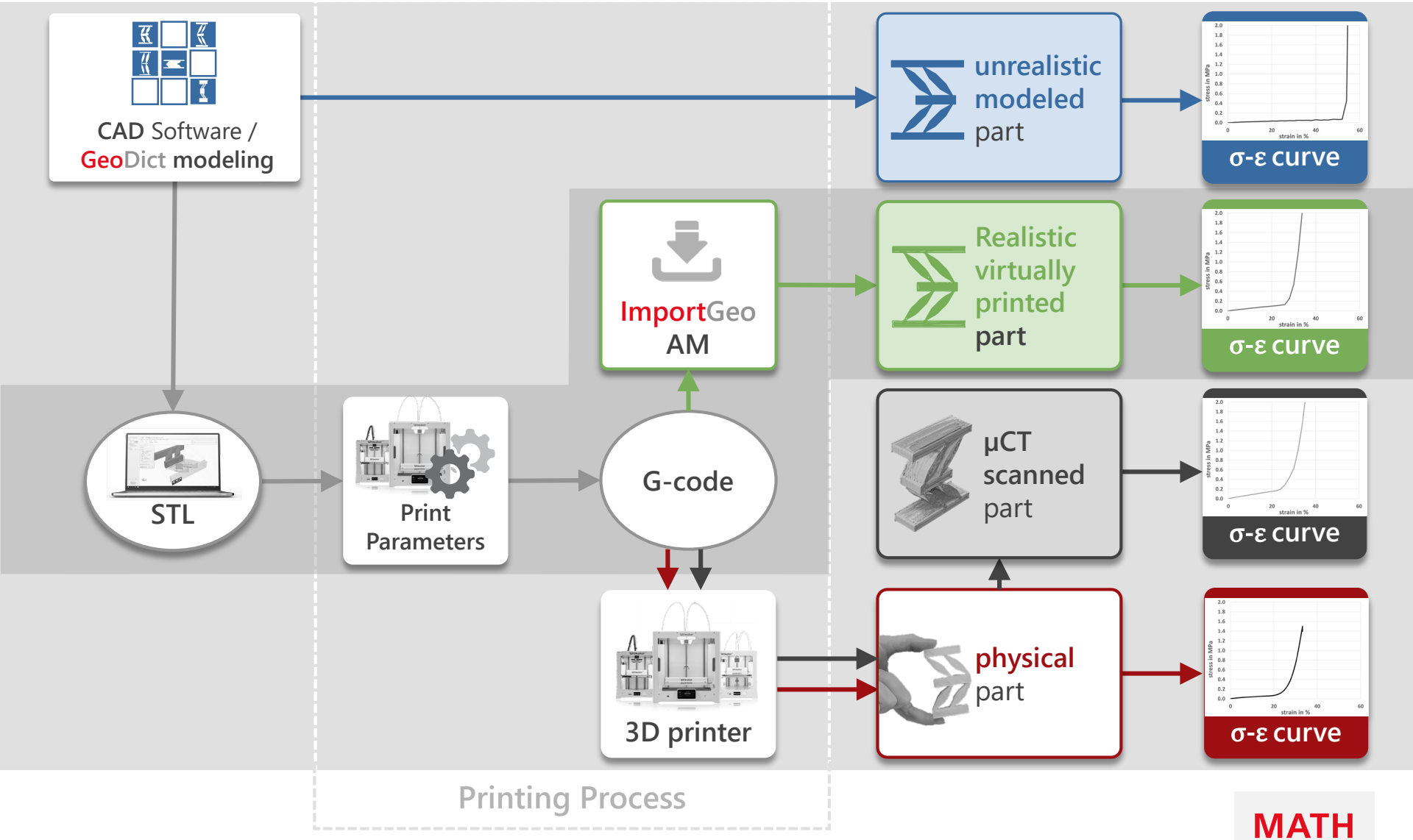


Simulation of the printing process is necessary for correct prediction of the stress-strain curve.

MATH 2 MARKET

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

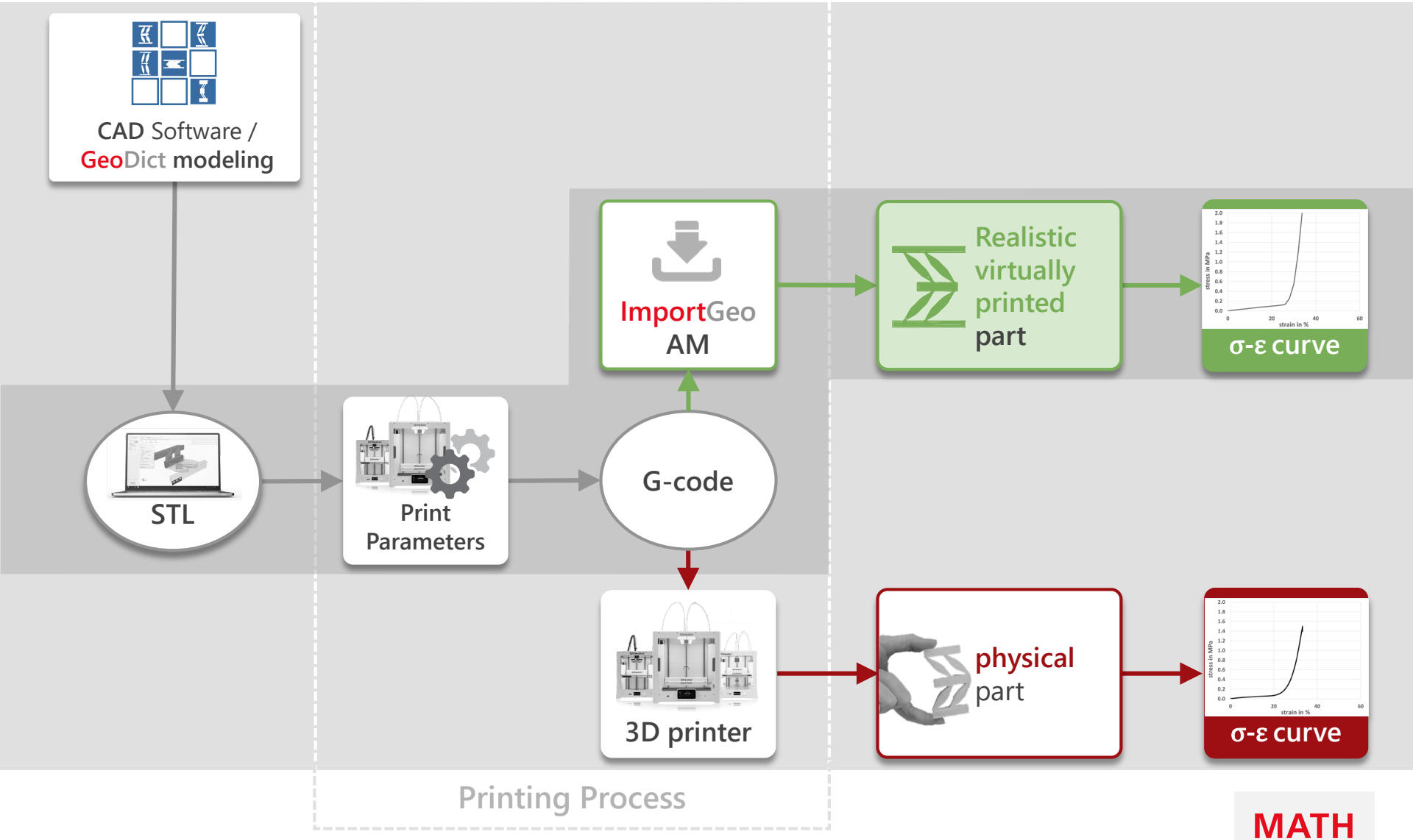
GeoDict



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/

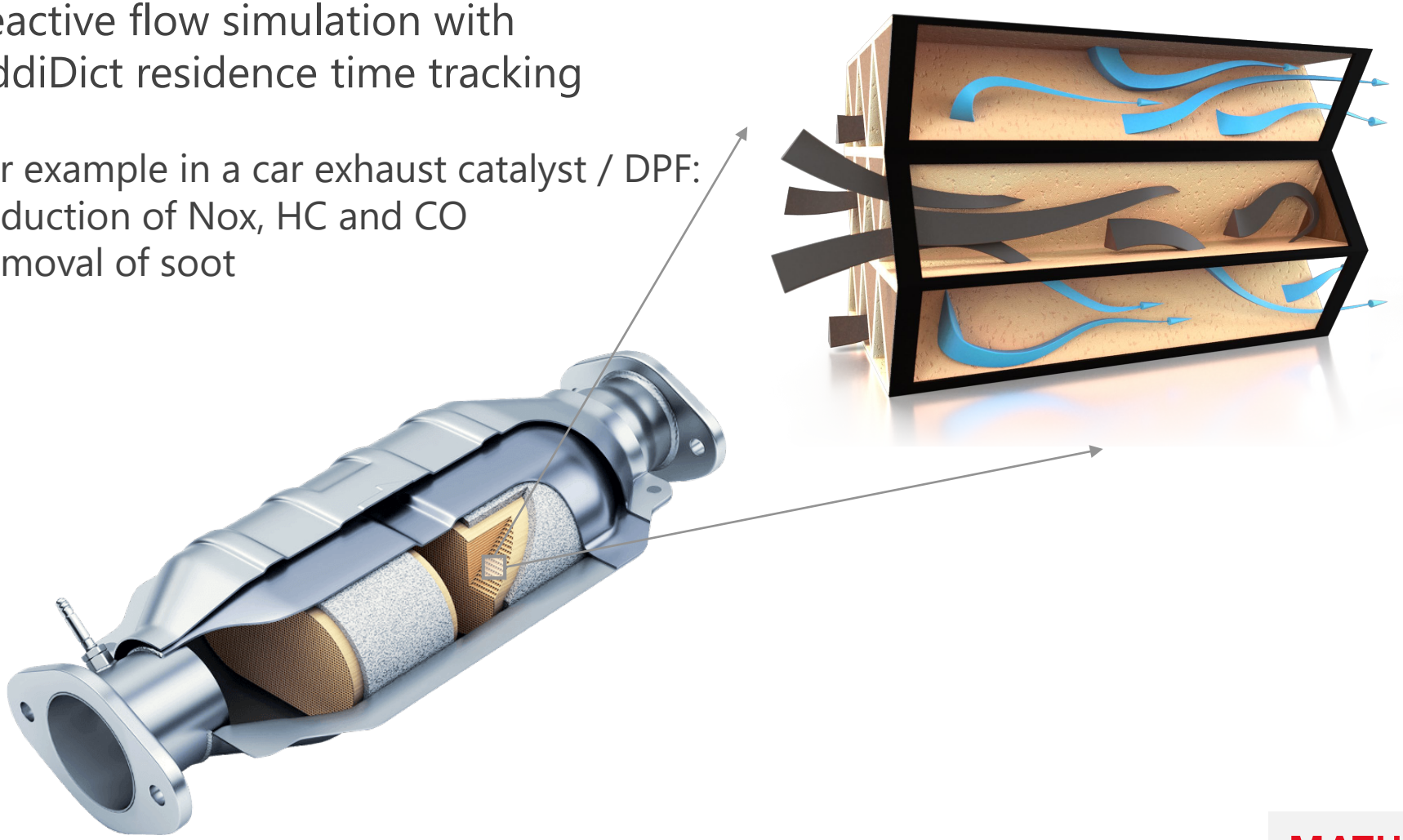
Andreas Wiegmann, Anja Streit, Andreas Weber, Liping Cheng, Mehdi Azimian, Erik Glatt & Jürgen Becker

MATH 2 MARKET

Modeling aftertreatment using residence times

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



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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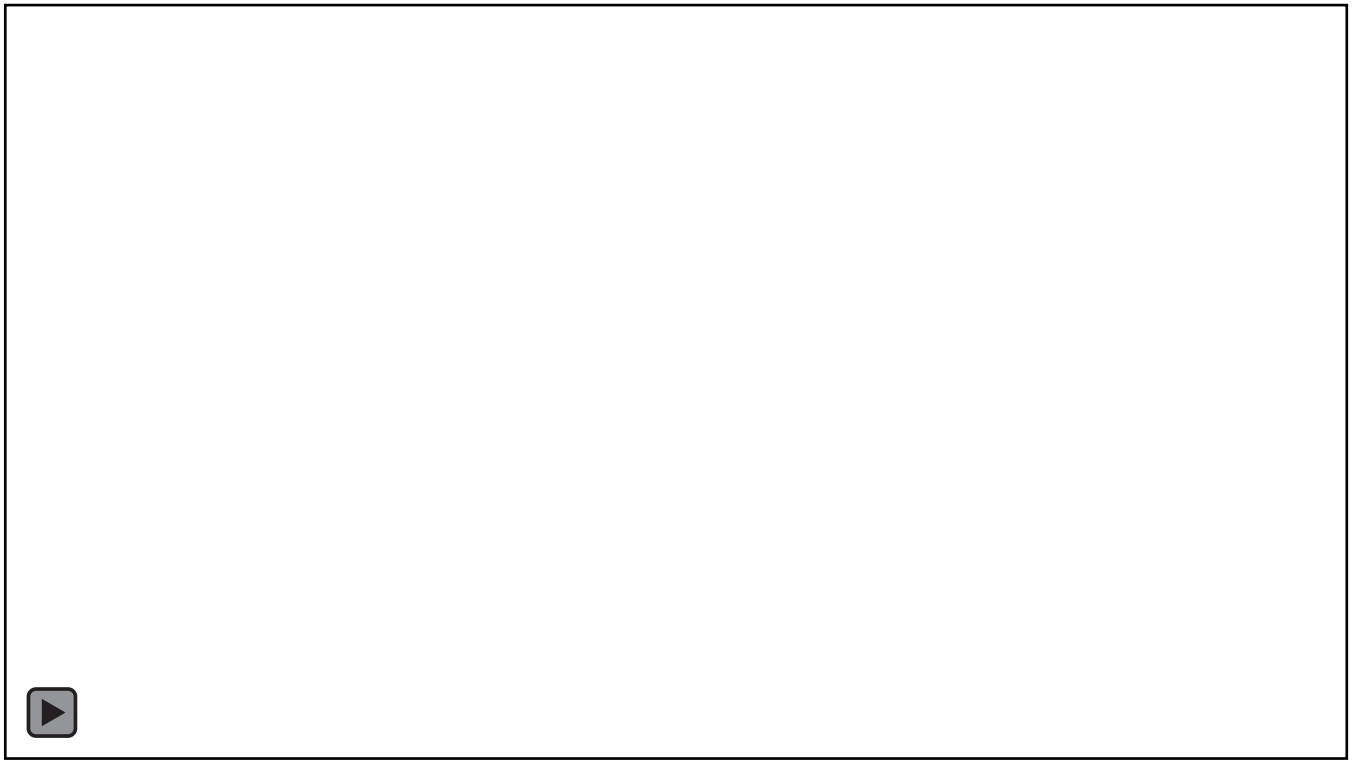

MATH 2 MARKET

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.

Molecule Motion in particulate filter (plugged)

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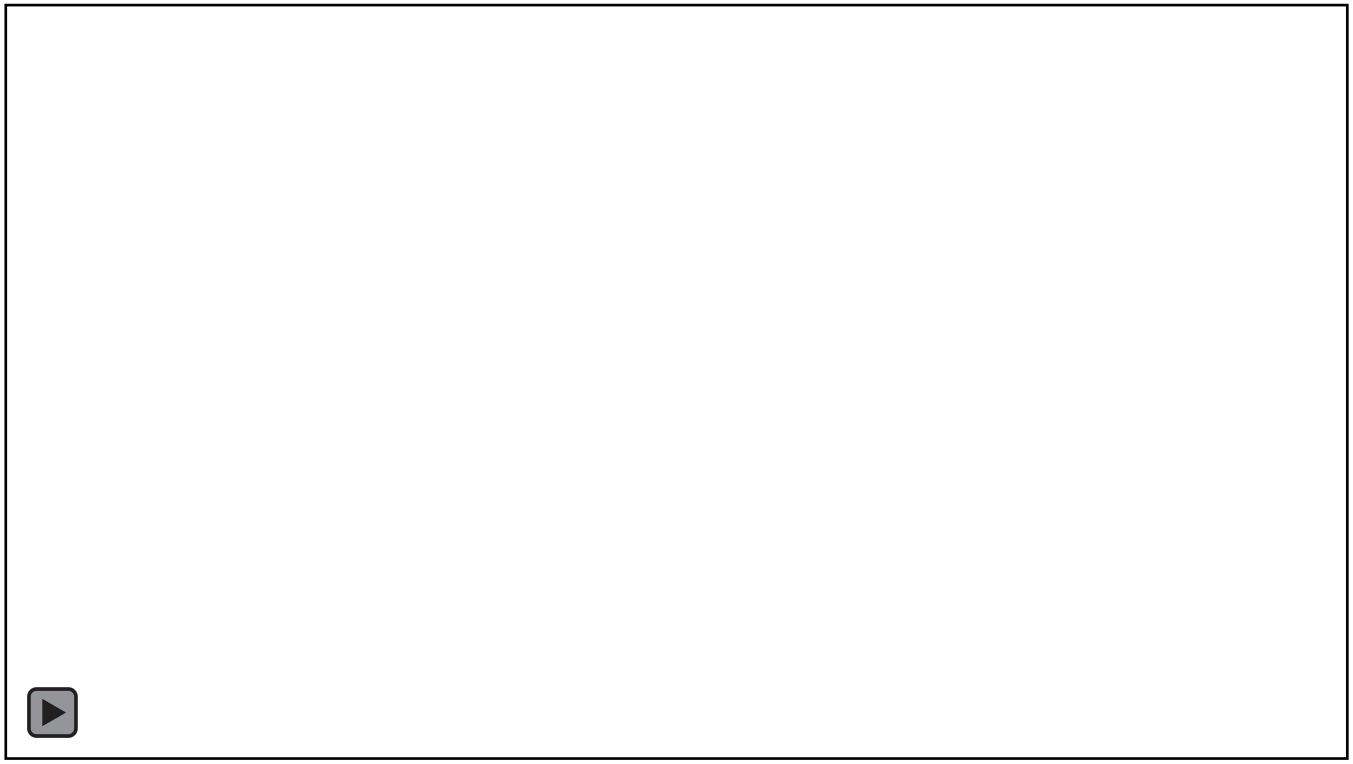
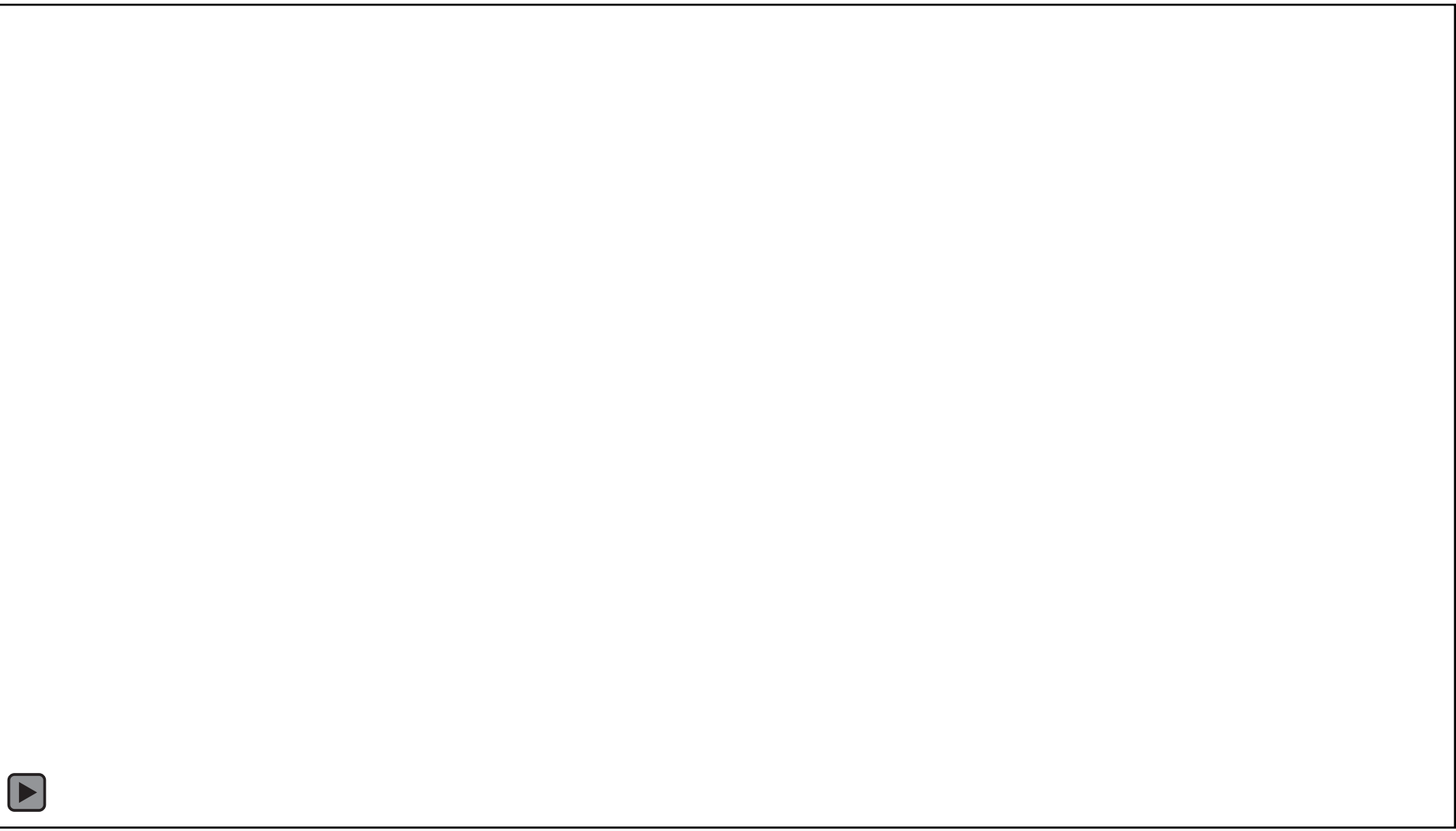


MATH 2 MARKET

Soot deposition in a honeycomb

Soot deposition in a honeycomb

GeoDict

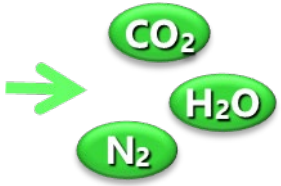


MATH 2 MARKET

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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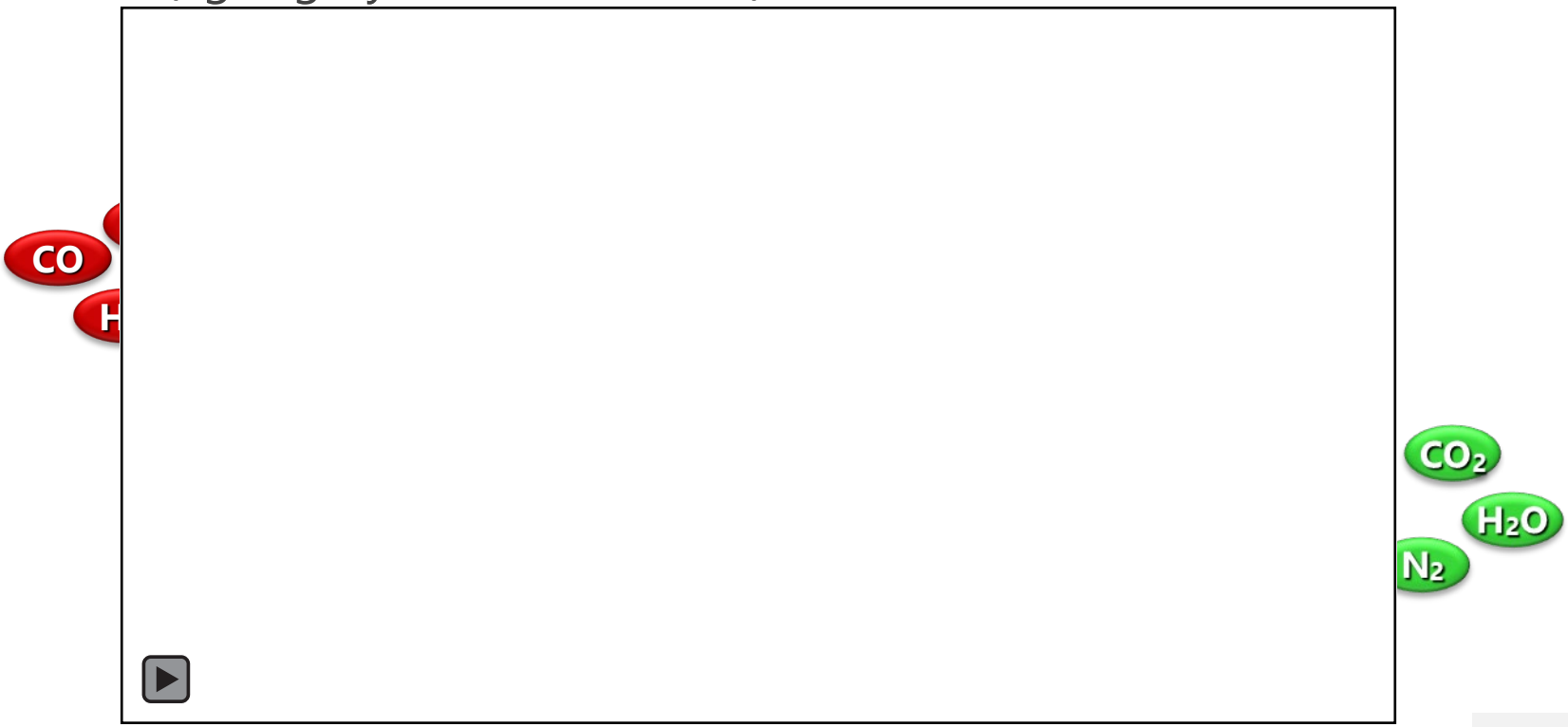
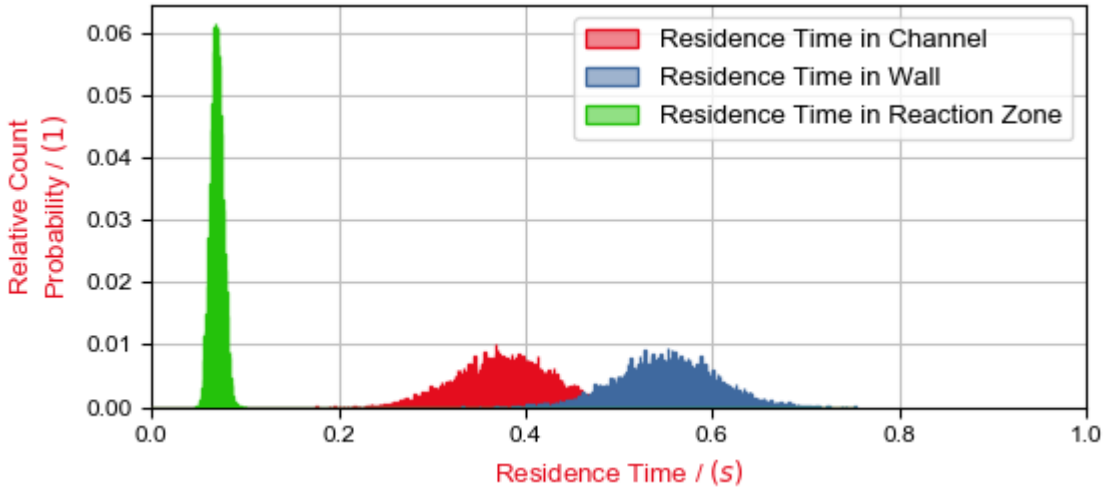


MATH 2 MARKET

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

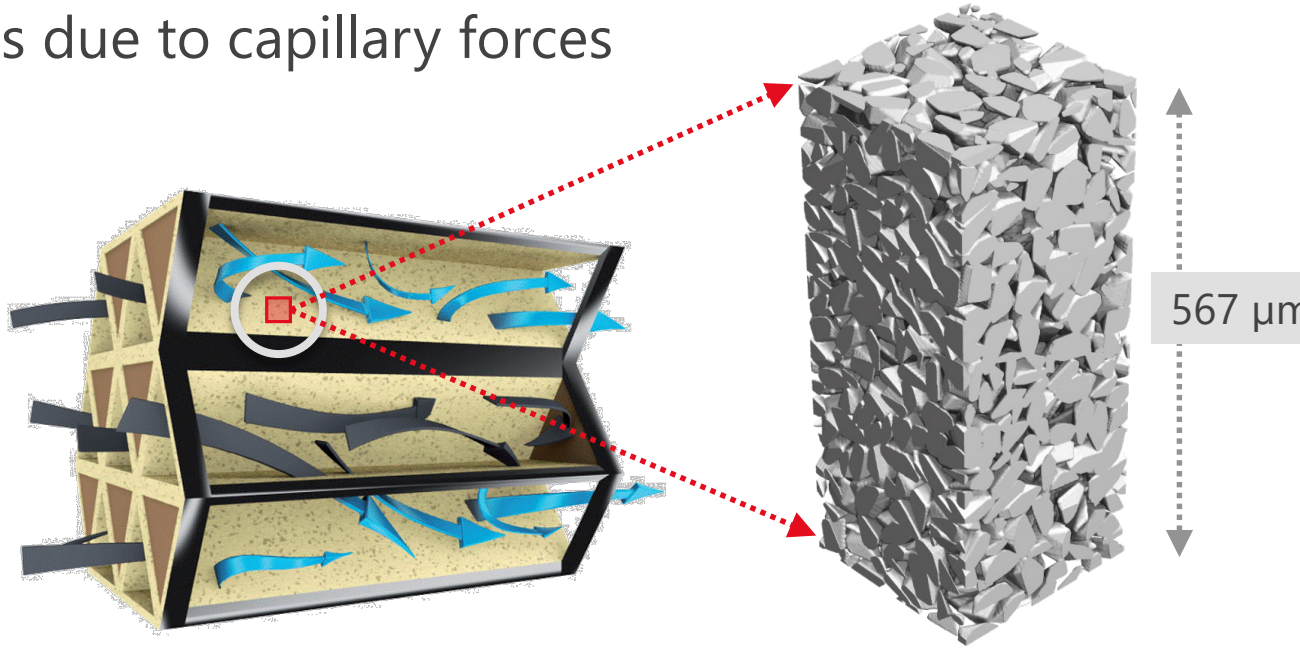
Particles spend between 40% and 70% of the time in the wall. An around 7% of the time in the reaction layer.

MATH 2 MARKET

Two sources of pressure loss in DPF

MATH
2 MARKET

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



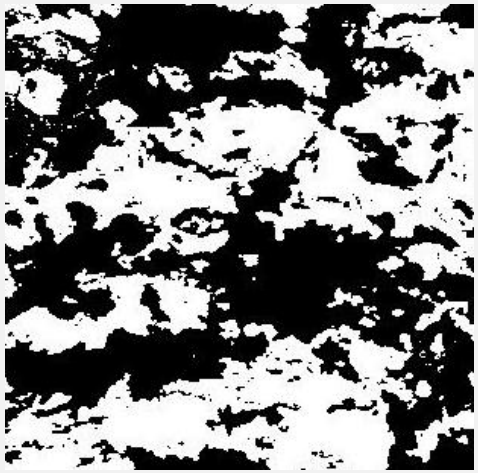
- We simulate them separately.
- In both cases, we simulate the loading of an initially clean filter.

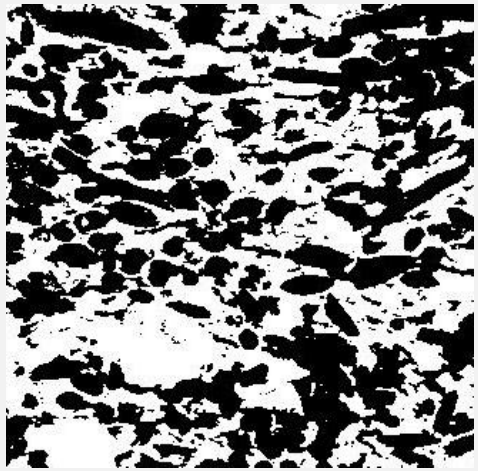
Binarized PMS images

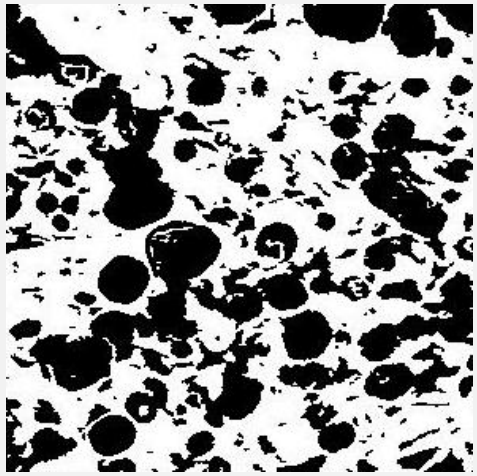
from polished micrograph sections and modeled sintered ceramics

MATH
2 MARKET

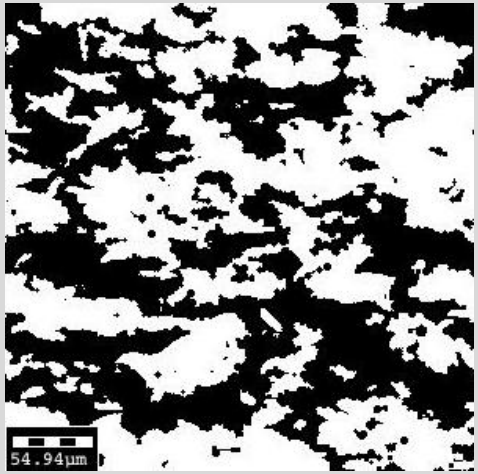
PMSs

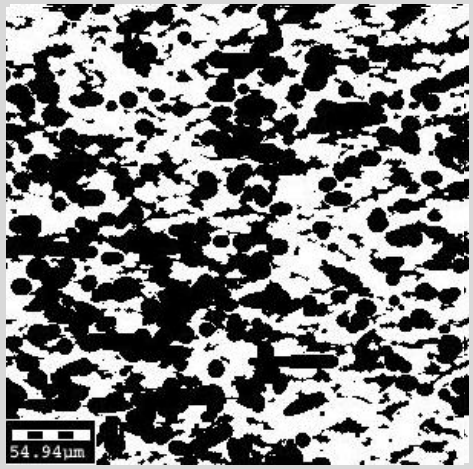


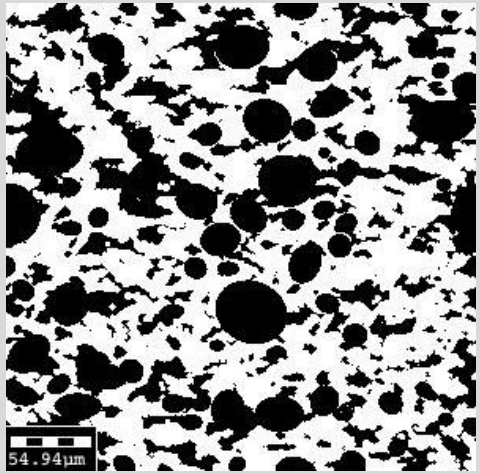




Models



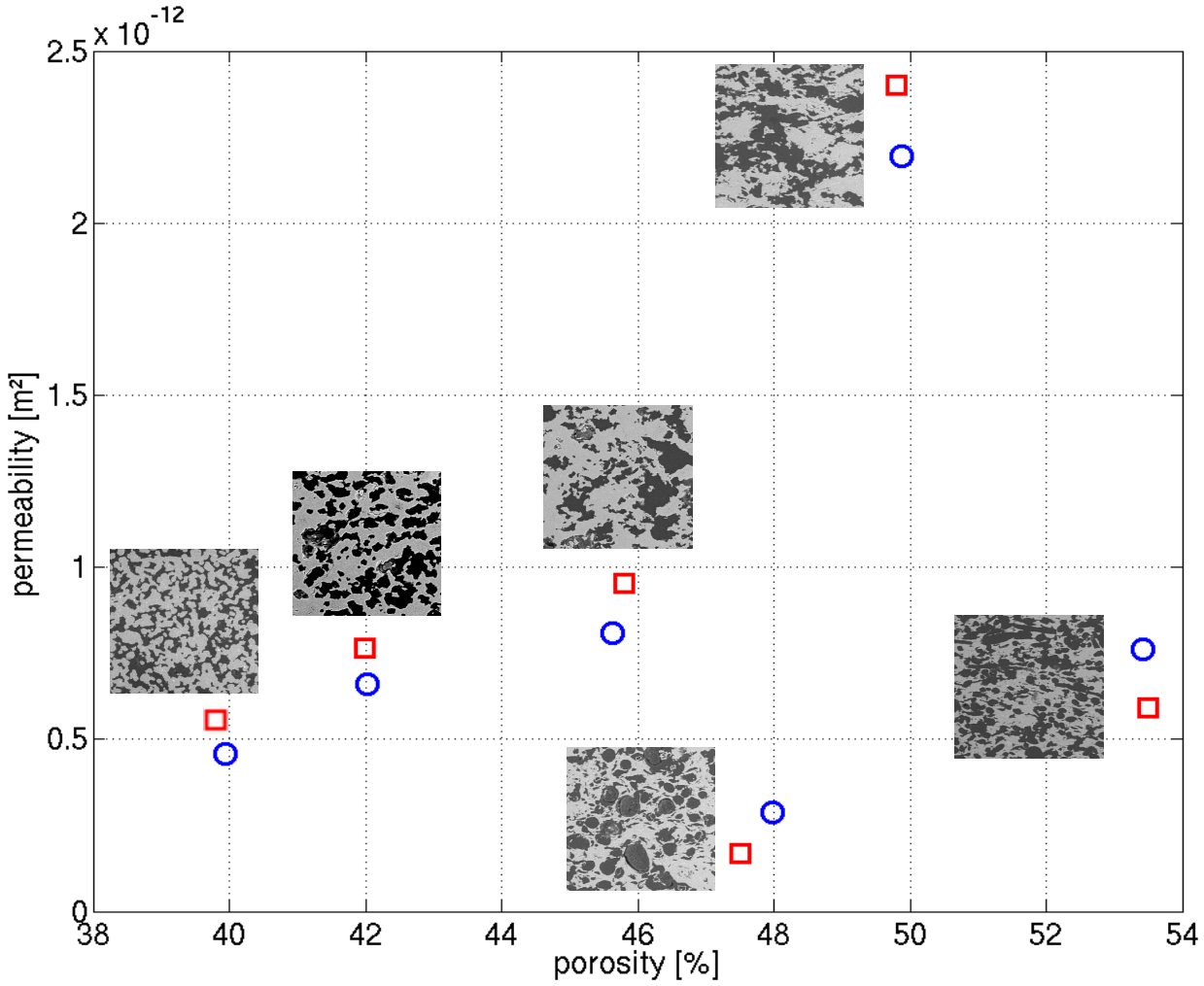




Measured porosities & permeabilities

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

MATH
2 MARKET



Simulation

Measurement

Spatial particles deposition over time

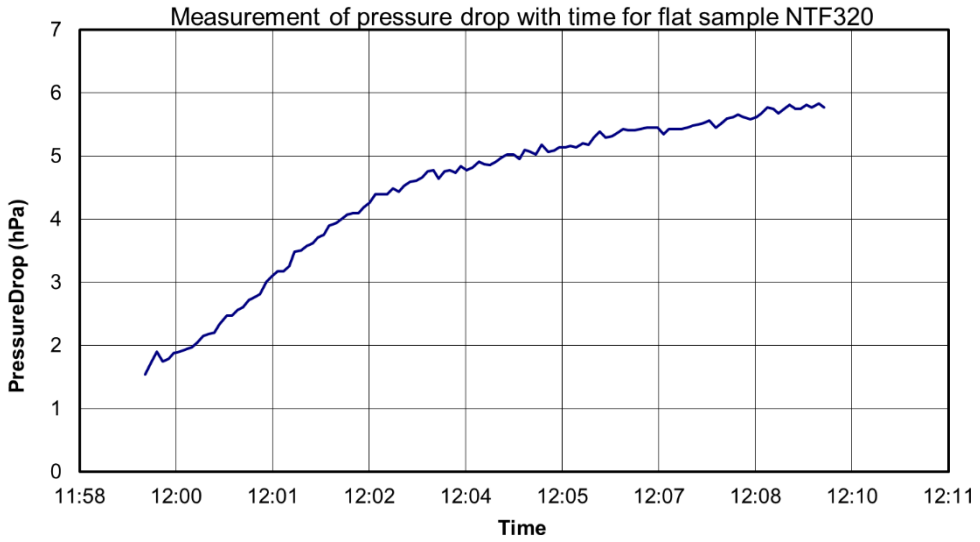
MATH
2 MARKET

Reduced pressure drop over time

MATH 2 MARKET

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

Fraunhofer IKTS



Reduced pressure drop over time

MATH 2 MARKET

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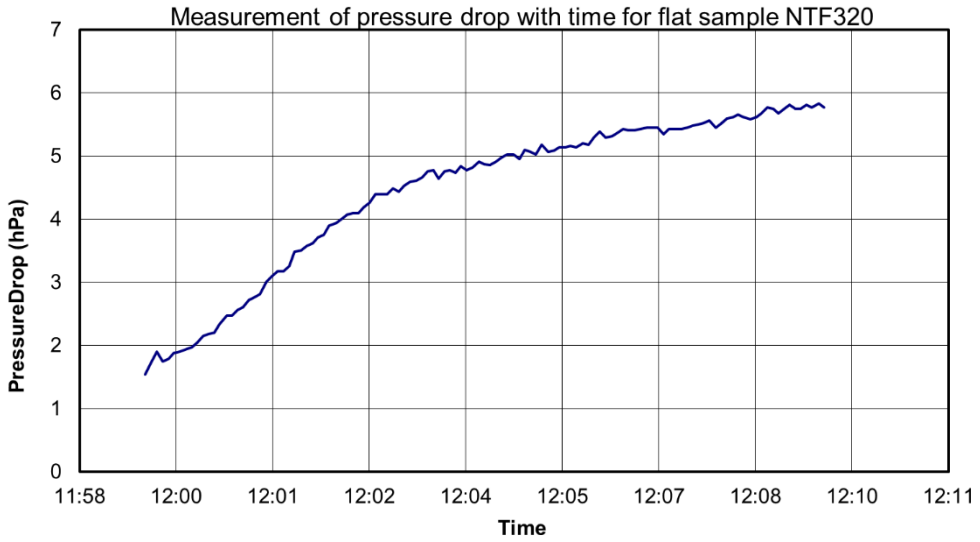
follows long slower pressure drop increase (slope s2, cake filtration phase)

Fraunhofer IKTS

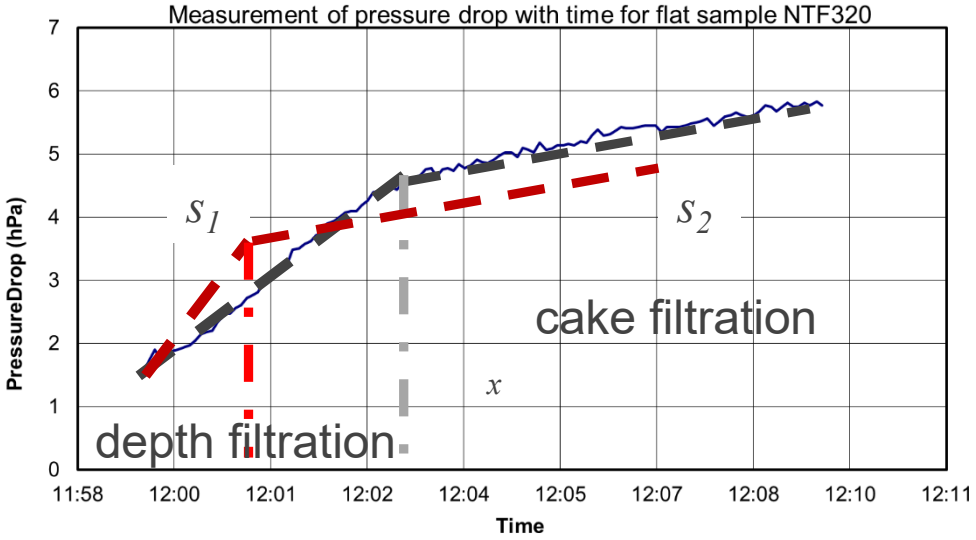


Reduced pressure drop over time

MATH 2 MARKET

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
- **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*



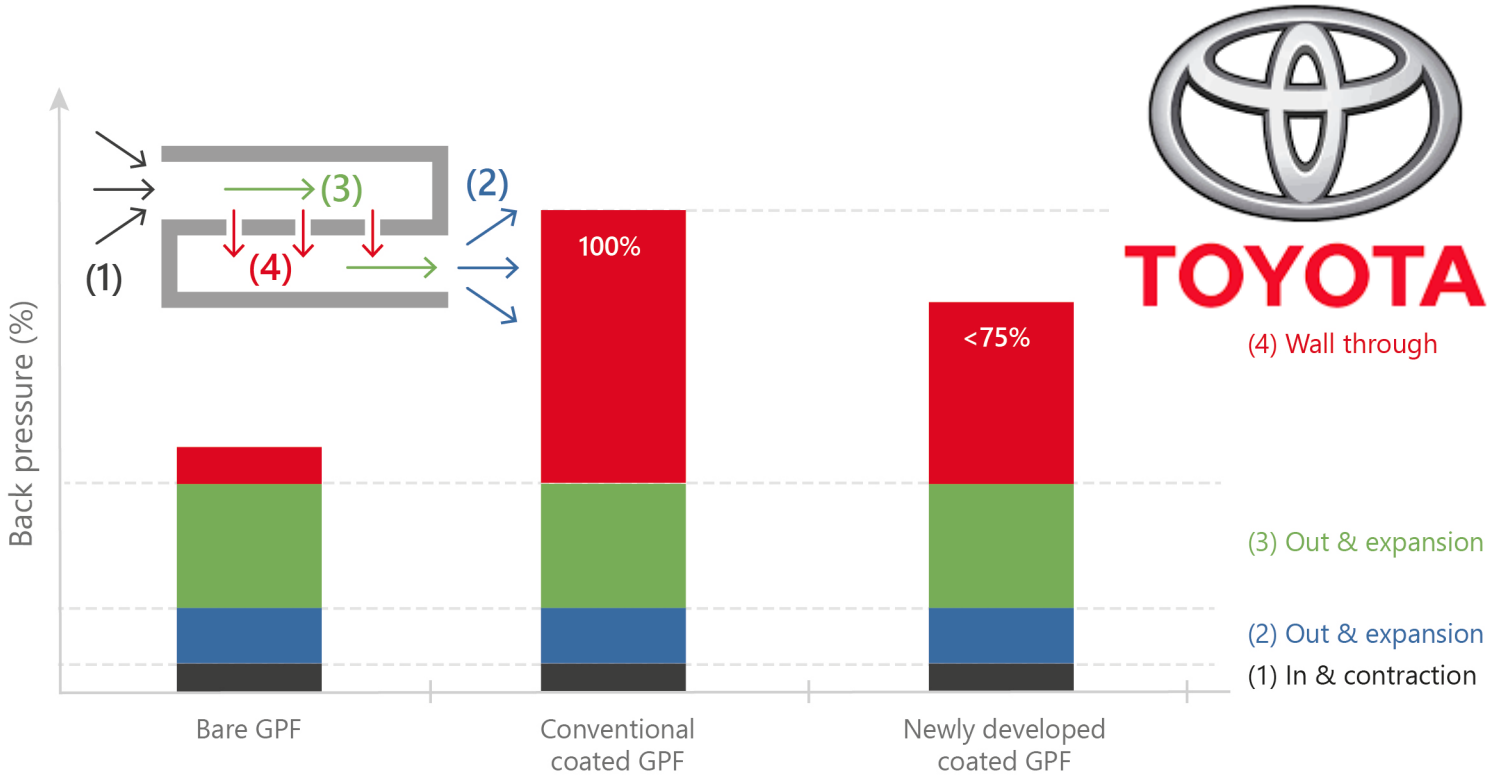
Finding a new GPF Material with GeoDict

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/

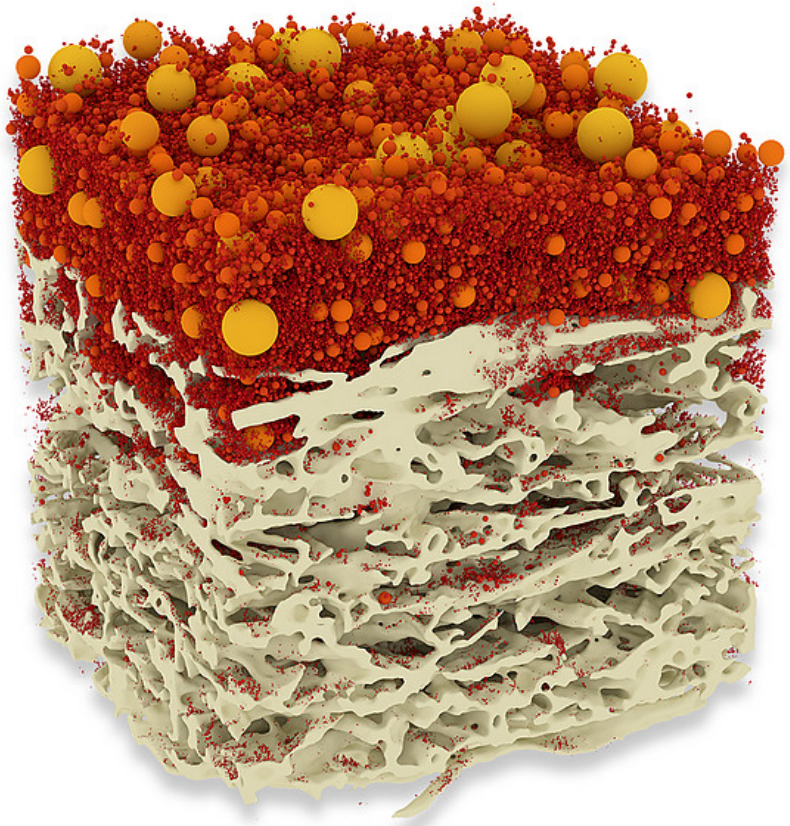
GeoDict software helps to reduce back pressure in Gasoline Particulate Filters by 25%.

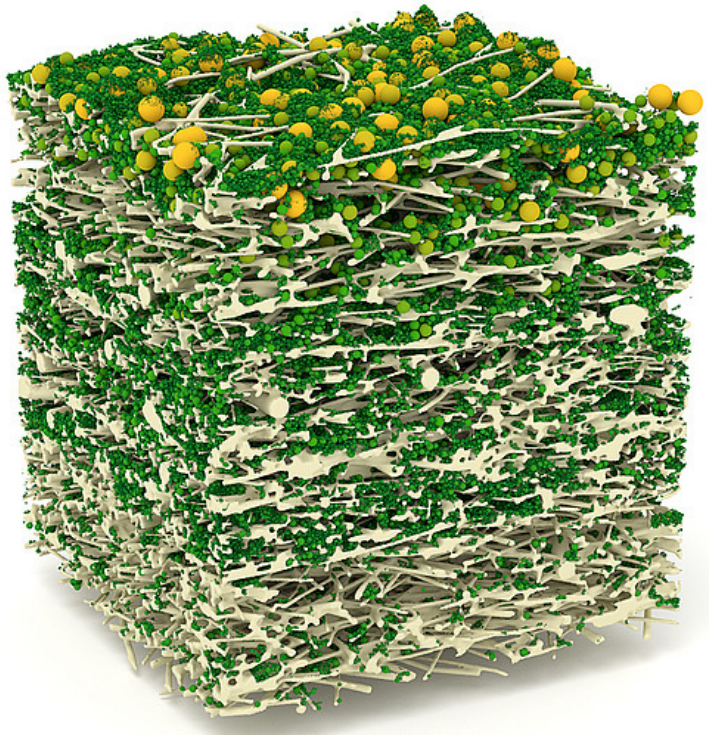
microstructure of wash coats analyzed, understood and improved with GeoDict



MATH 2 MARKET

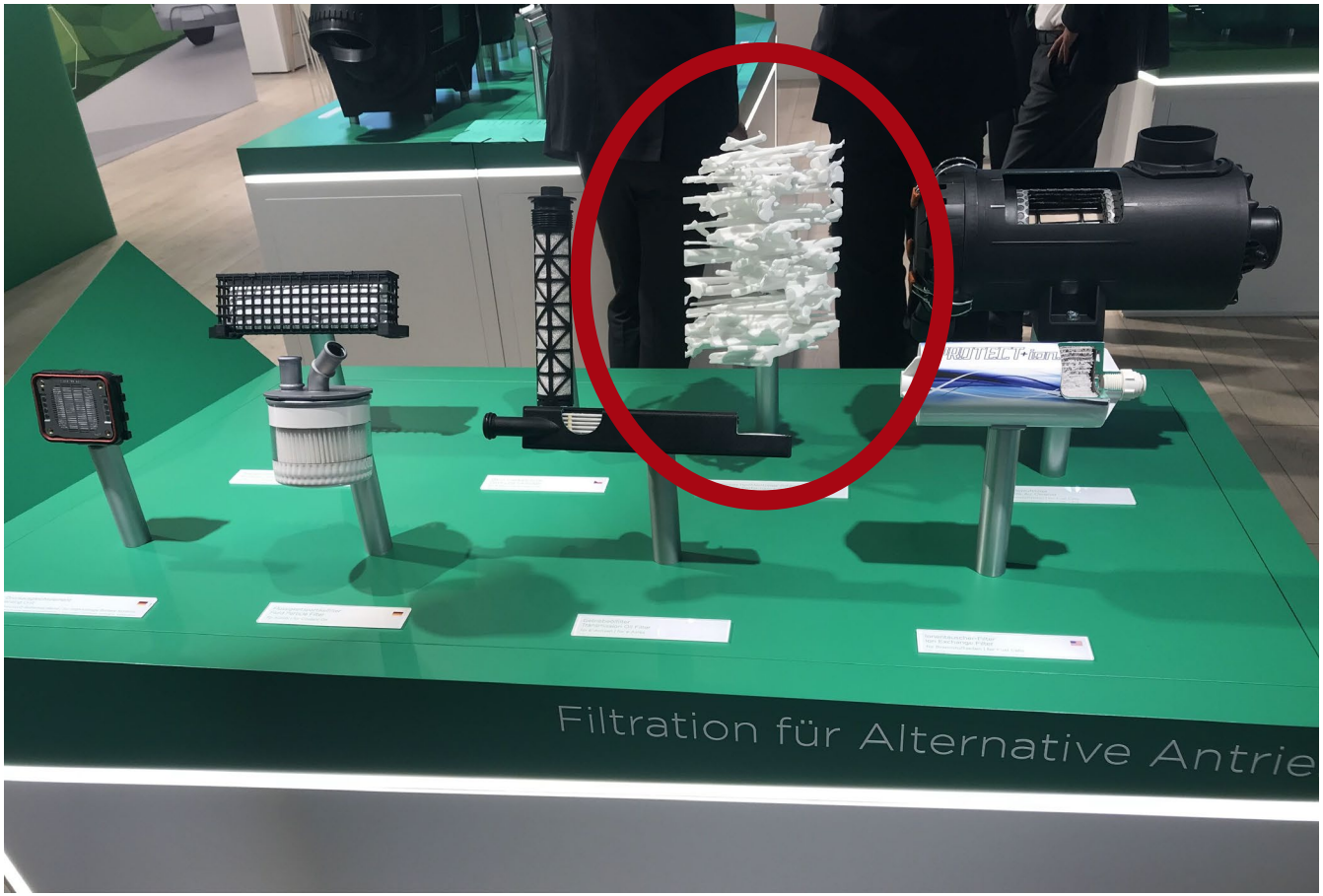
Rendering of Materials and Simulation Results





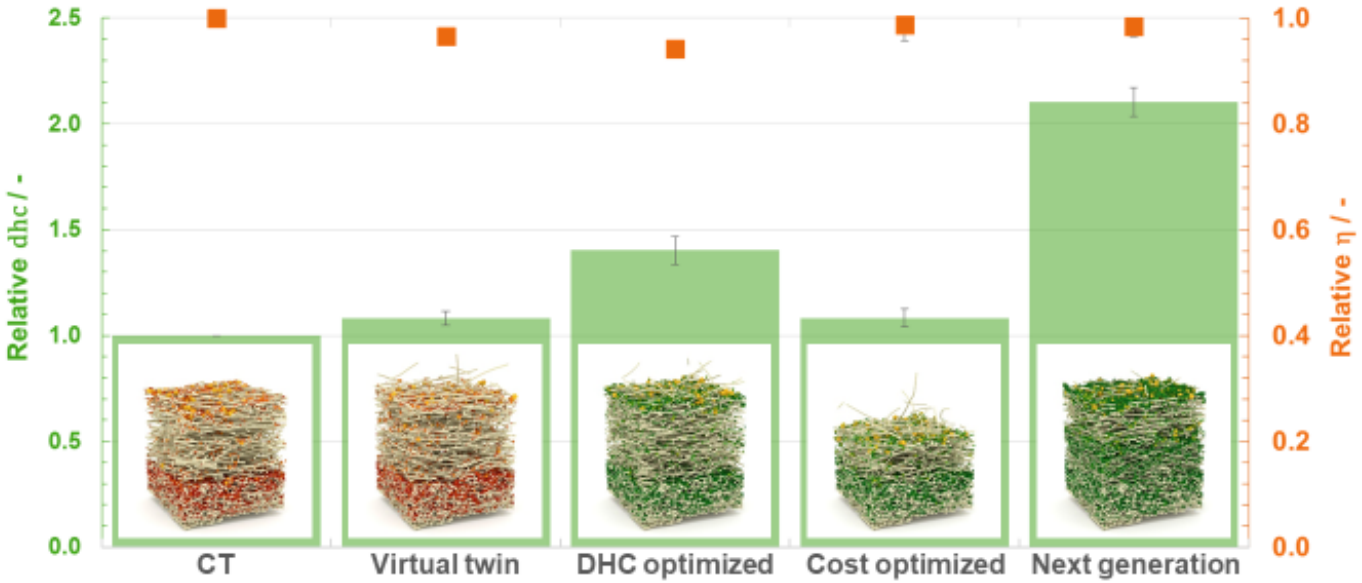
Source: MANN+HUMMEL

GeoDict can also be used to export models for 3-D printing



Source: **MANN+HUMMEL** on LinkedIn

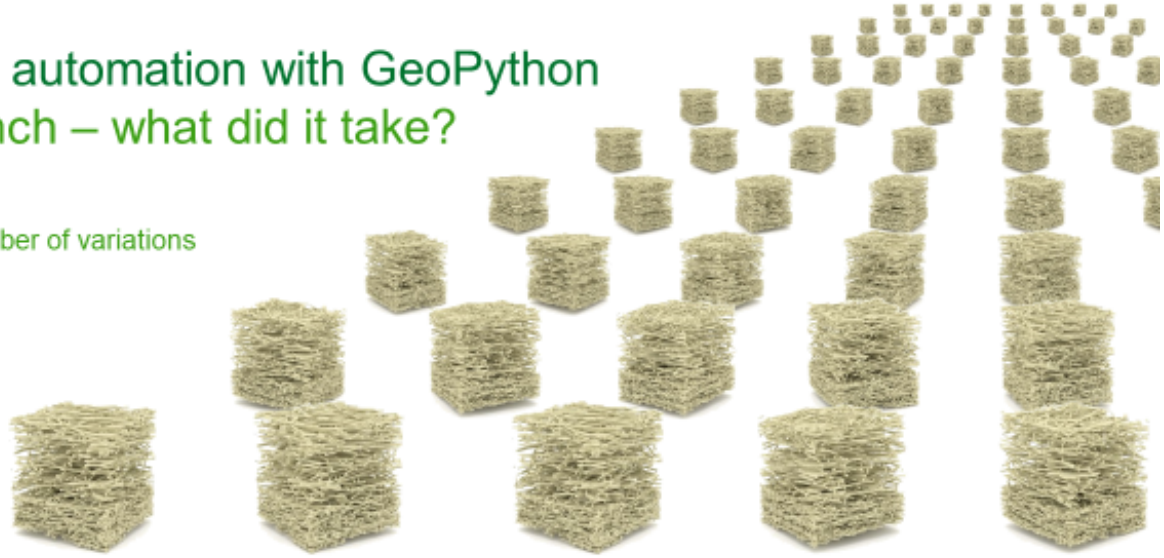
Optimization of a virtual filter media prototype
Pushing the limits 2.0 – next generation



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 φ	→ 5
▪ Grammage G	
▪ Thickness t	→ 4
▪ Packing density $1-\varepsilon$	→ 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

MANN+HUMMEL

Source: **MANN+HUMMEL**

„LARGE“ SIMULATION

MATH
2 MARKET

Simulation settings
Domain: 512x512x76
Average velocity: 0.1
pH value: 3.2
Simulation time: 20 s
Number of particles:
Runtime: 14 hs (16 co

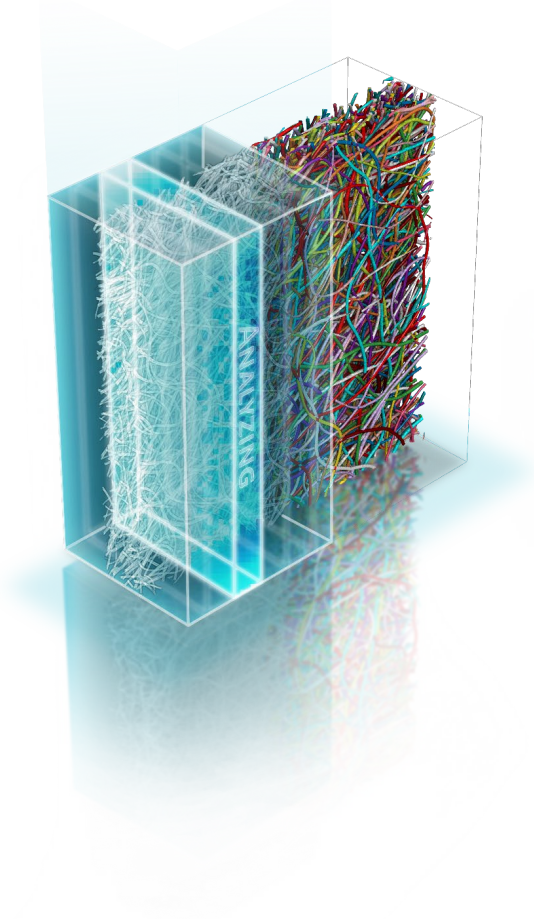
Conclusion

MATH
2 MARKET

- 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®

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



This is **Innovation**
through **Simulation**