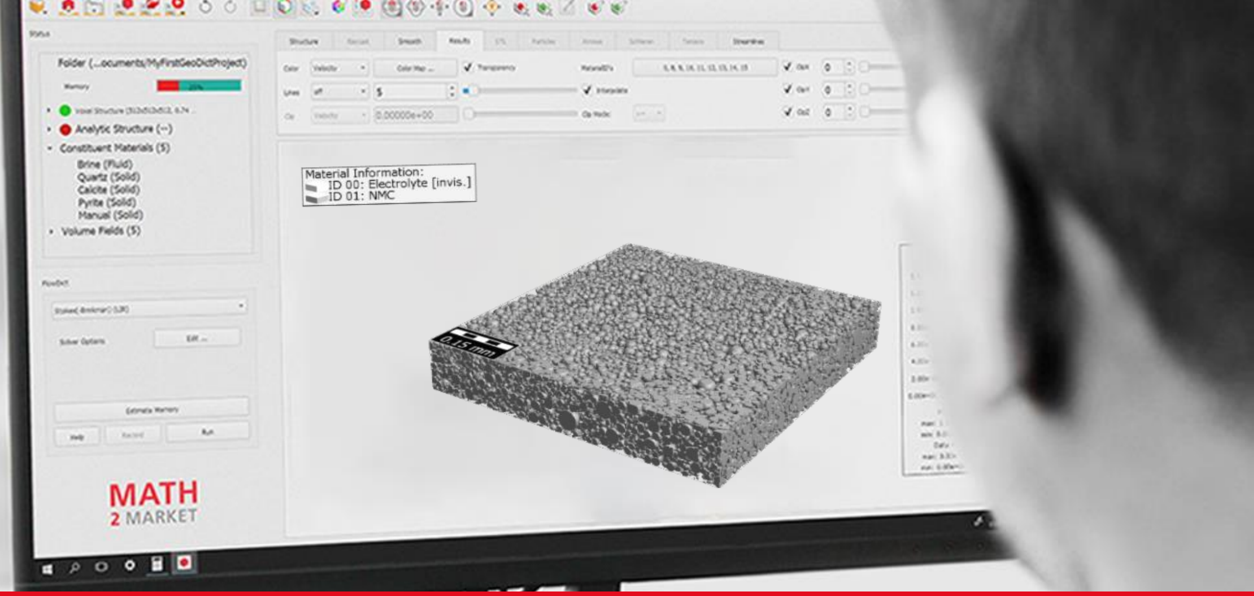
GeoDict
The Digital Material Laboratory



Digital 3D reconstruction from 2D scan of a Li-Ion Cathode

WOST 2019
Weimar, 07.06.2019

Aaron Widera, Ilona Glatt, Fabian Biebl, Erik Glatt

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AGENDA

GeoDict

1 What is GeoDict and Data for this talk

2 Motivation

3 Step 1: NMC cathode recreation using GeoDict only

4 Step 2: NMC cathode recreation using GeoDict and optiSLang

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Agenda

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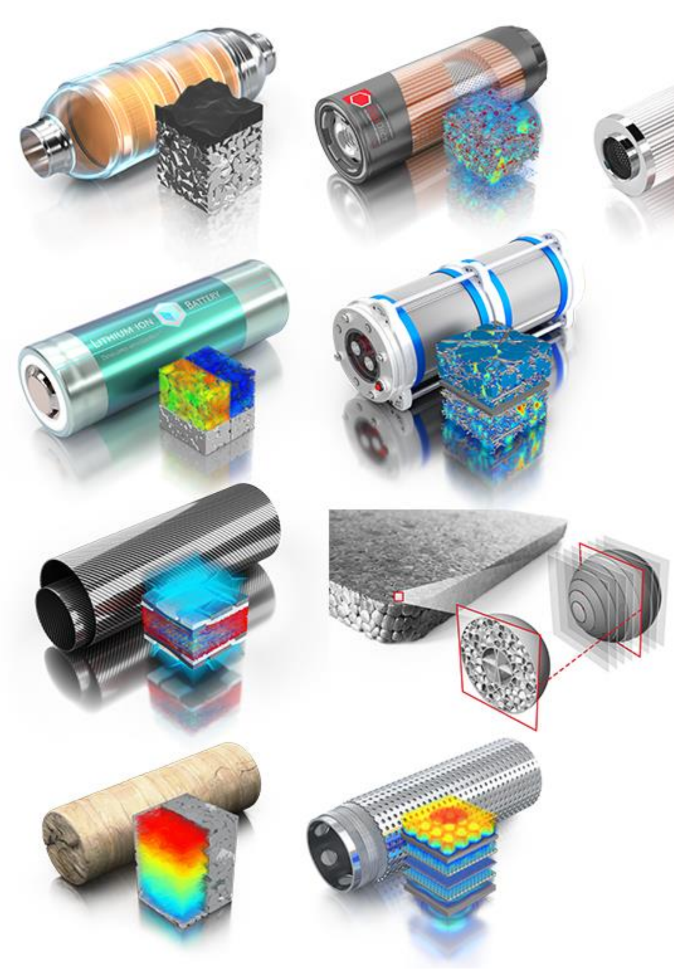
Core capabilities of GeoDict®

- Model & Design Materials
- Analyze & Simulate Material Properties
- Explore the Behavior of Materials
- Develop Novel Materials
- Optimize Processes

GeoDict® Solutions for ...

GeoDict

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



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Typical Workflow with GeoDict®

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

Import of 3d images captured by µCT or FIB/SEM techniques

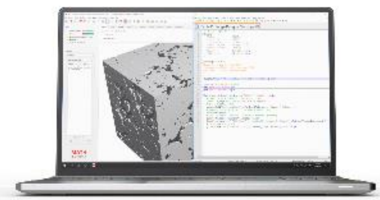
Digital Material

In-depth digital analysis and evaluation of material properties

Quantification of geometrical, structural, and physical **material properties**

Digital material design based on the statistical material properties

Digital Twin



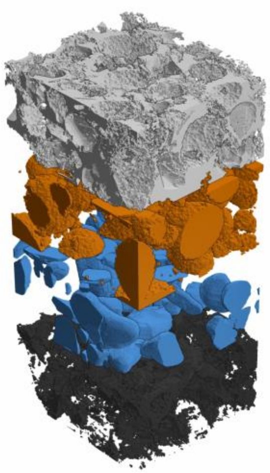
Design by varying the statistics of the geometry that govern the material properties

Digital Prototypes

Analysis with GeoDict®

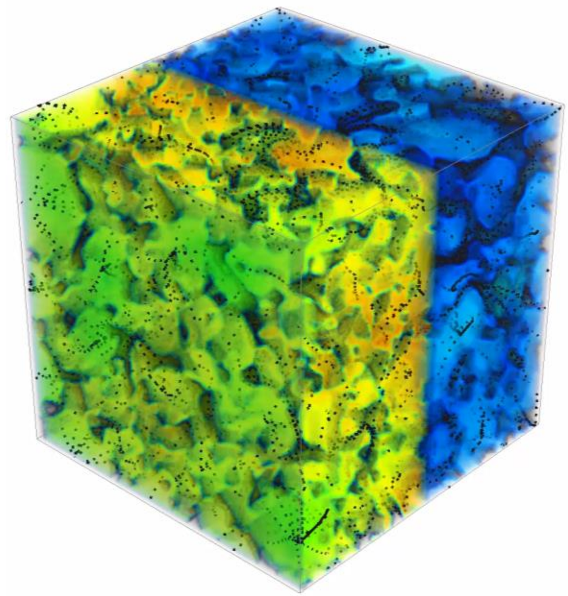
GeoDict

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



NCA-LCO-CATHODE

- 26% Electrolyte
- 35% NCA
- 24% LCO
- 15% Carbon + Binder



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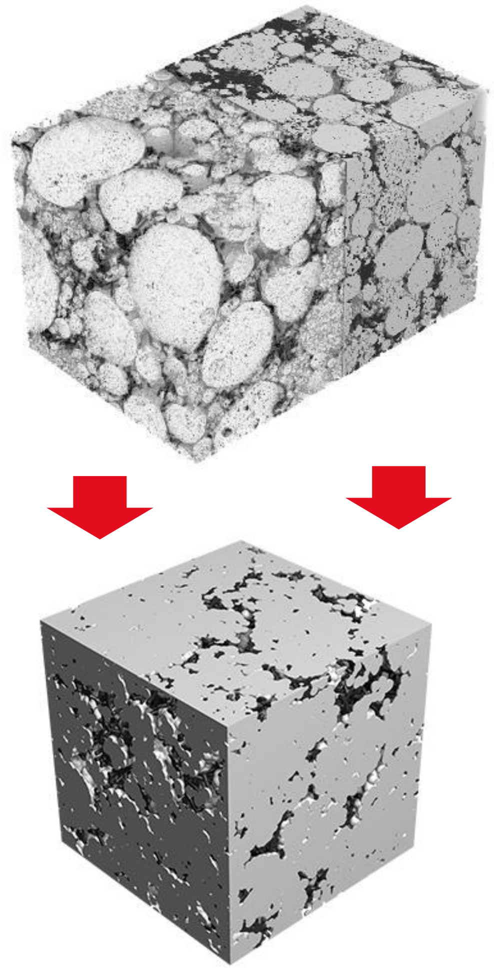
MODELLING WITH GEODICT®

GEODICT

1. | 2. | 3. MODEL | 4. DESIGN



The structural statistical information output of **GrainFind** is the input for **GrainGeo** and **FiberGeo**, the GeoDict® modules for the generation digital twins of the material.

GrainGeo

- Creates models of granular materials
- Here, it is used to model the structure of the active material

FiberGeo

- Creates models of fibrous materials
- Here, it is used to model the fibrous binder

> **Result:** Digital Twin

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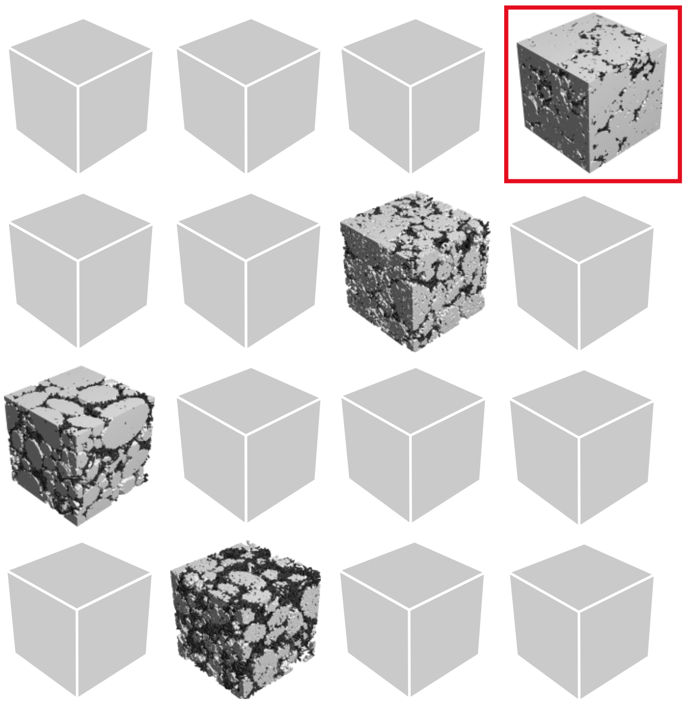
Material design with GeoDict®

GeoDict

1. 2. 3. 4. Design



Digital prototypes

Digital prototypes are quickly designed by varying the statistics of the geometry that govern the material properties.

Many digital prototypes of the cathode are swiftly and directly analyzed on the computer.

Result: Selection of digital prototypes with different volume fractions

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GeoDict modules and simulations used

GeoDict

- **ImportGeo** to process the image data
- **GrainGeo** to generate artificial cathode structures
- **GrainFind** to analyze granular structures for its geometrical properties
- **DiffuDict** to predict diffusivity and tortuosity

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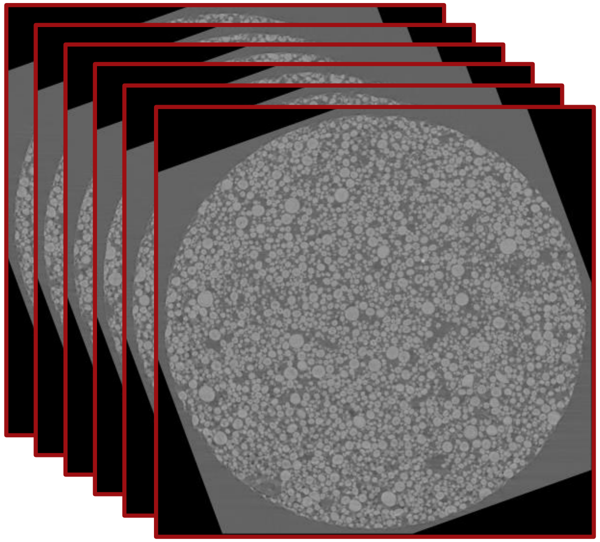
ImportGeo and Data sample used

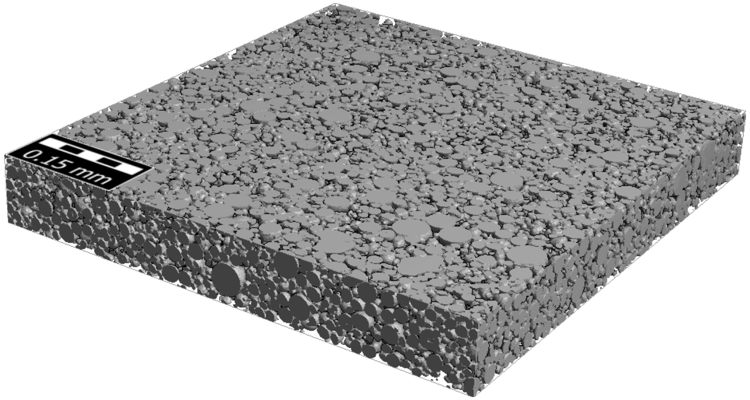
GeoDict

For this talk we use a data set kindly provided by:

KIT (Karlsruher Institute of Technology)



FIB-SEM image stack



Nickel Cobalt Manganese (NMC)cathode

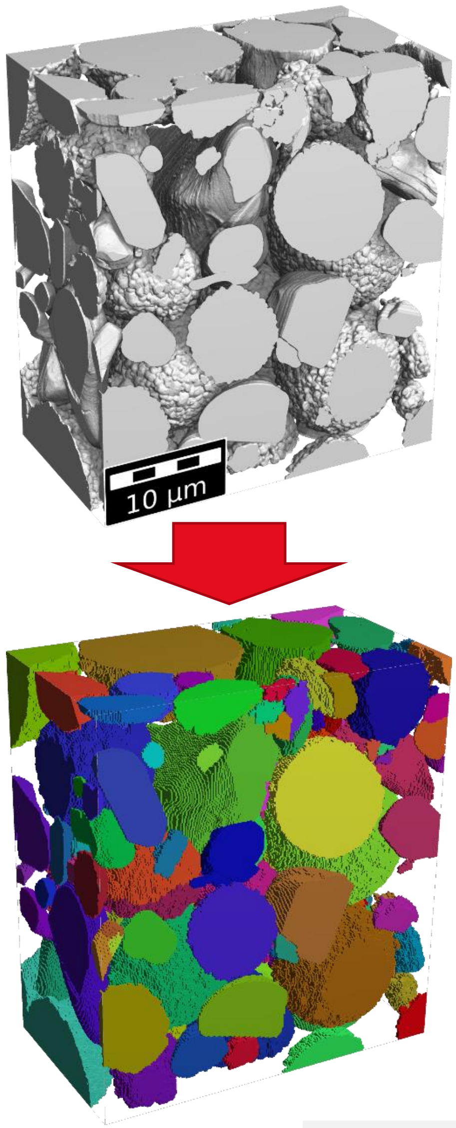
These data and further information such as tortuosity values can be found

in *Tortuosity Anisotropy in Lithium-Ion Battery Electrodes*[1],

[1] Tortuosity Anisotropy in Lithium-Ion Battery Electrodes: Martin Ebner, Ding-Wen Chung, R. Edwin García and Vanessa Wood

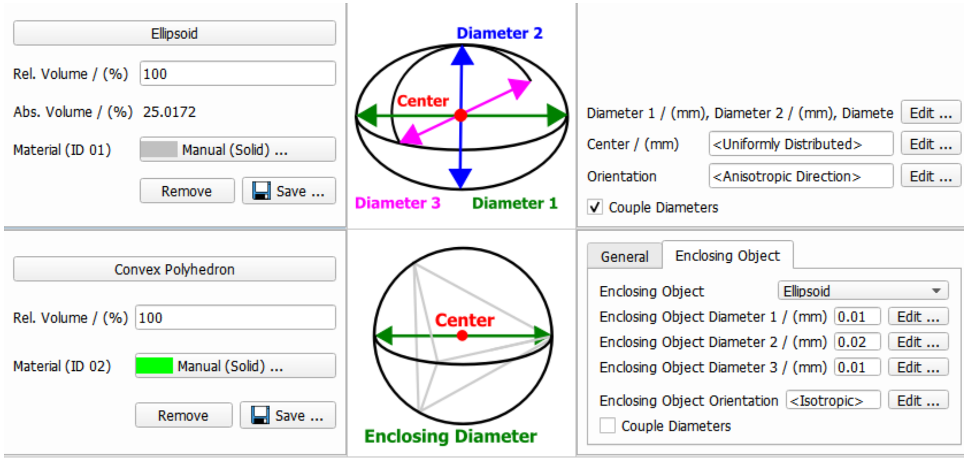
Geometric analysis tool GrainFind

- Some of the results per grain:
  - Volumes and diameters of volume-equivalent sphere
  - Diameters of inscribed spheres
  - Sheppard sphericities and Krumbein sphericities
  - Fit shape’s diameters, direction, and orientation
- Statistics about grains
  - Volume statistics
  - Diameter statistics
  - Sphericity statistics
  - Fit-shape direction statistics
- Classification of grain shapes

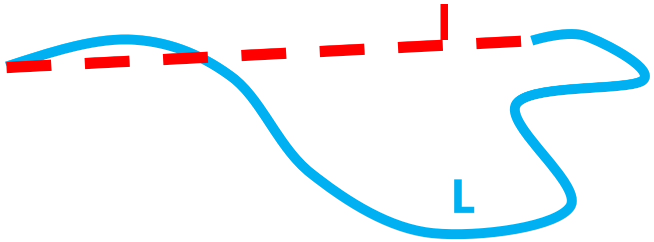


CATHODE CREATION TOOL GRAINGEO

- GrainGeo generates granular structures
- Different kind of grains can be generated:
  - Spheres and ellipsoids (described by their diameters)
  - Convex polyhedrons (described by diameters of enclosing ellipsoid)
  - Many others
- Objects can be randomly created
- Overlapping objects can be created
- Or overlap can be removed



DiffuDict simulates diffusion experiments of Bulk and Knudsen diffusion:



- Effective diffusivity
- Tortuosity:
  - For a curve (blue) in space, the tortuosity of this curve is the quotient between the length of the curve L and the length of the straight line l between the curve’s endpoints (red), $\tau = \frac{L}{l}$

AGENDA

GEODICT

1 What is GeoDict and Data for this talk

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MOTIVATION FOR DIGITAL EXPERIMENTS

GEODICT

- To reduce time and costs in cathode development processes:
  - Experiments can be performed digitally
  - Testing digital prototypes allows to only produce the most promising
- Use digital twin of cathode to understand real cathode better
  - Use this twin to see how changes to this cathode alter the performance
  - Develop the next generation cathode based on real cathode

→ But therefore we need the digital twin

- Obtain it by importing 3d FIB-SEM image stack
- Or use single 2d SEM image

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Motivation for using SEM

GeoDict

For digital experiments reliable digital representatives of the cathode material is needed:

- Import sample from FIB-SEMs
  - \+ This yields exact digital representative
  - – More expensive
  - – Sample is destroyed in the process
- Import sample from single SEM image
  - \+ Sample is not destroyed
  - \+ Cheaper than 3d scans
  - – No 3d representation

→ Develop methododology to create 3d digital twin from a single SEM image with optiSLang and GeoDict.

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3D RECONSTRUCTION FROM 2D SCAN

GeoDict

CHALLENGES

Main Problem is that **Information is missing!**

Where to get information for reliable 3d reconstruction?

- Knowledge from similar cathodes
- Knowledge from manufacturers
- Experimental Input:
  - Porosimetry by mercury intrusion
  - Porosity
  - Tortuosity
  - Permeabilities

→ Obtain geometric information of 2d scan by GeoDict and combine with external inputs

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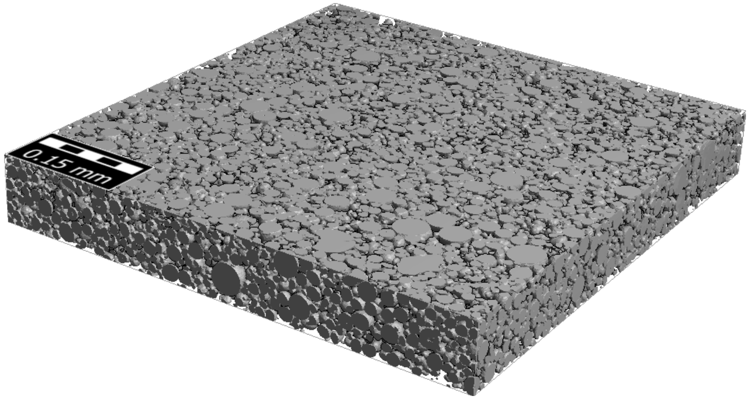
3D reconstruction from 2D scan
Methodology validation

1. Use 3d scan of NMC cathode
2. Take 2d slice as “SEM scan”
3. Reconstruct 3d digital cathode
4. Validate results with 3d scan from 1.



AGENDA

GEODICT

1	What is GeoDict and Data for this talk
2	Motivation and methodology
3	Step 1: NMC cathode recreation using GeoDict only
4	Step 2: NMC cathode recreation using GeoDict and optiSLang

Step 1: NMC recreation tools and prerequisites

GeoDict

For the NMC cathode in *Tortuosity Anisotropy in Lithium-Ion Battery Electrodes*[1], **tortuosity** values are given.

Workflow:

1. Use GrainFind on 2d scan
2. Recreate 3d cathode with 2d GrainFind information
   - Use GrainGeo for creation of artificial cathodes
3. Compare cathodes for their **tortuosities** from *[1]* and **porosity**

[1] Tortuosity Anisotropy in Lithium-Ion Battery Electrodes: Martin Ebner, Ding-Wen Chung, R. Edwin García and Vanessa Wood

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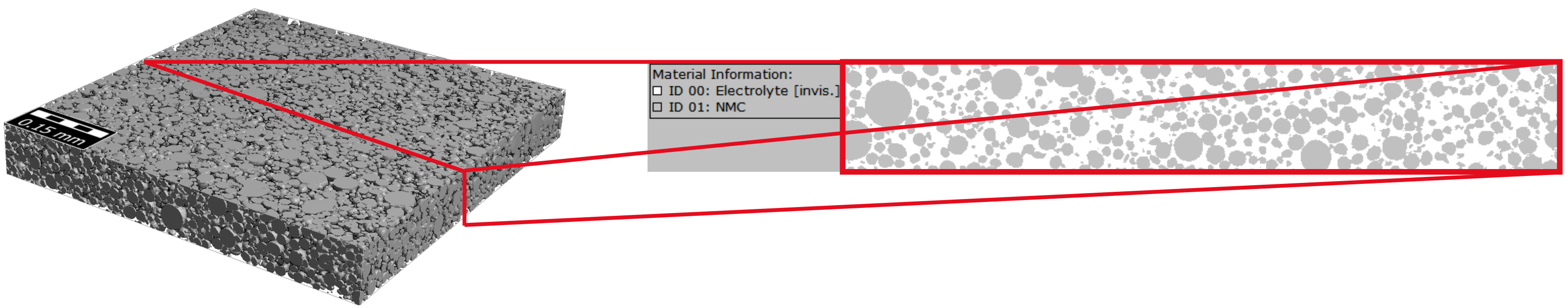
STEP 1: NMC RECREATION WITH GRAINFIND

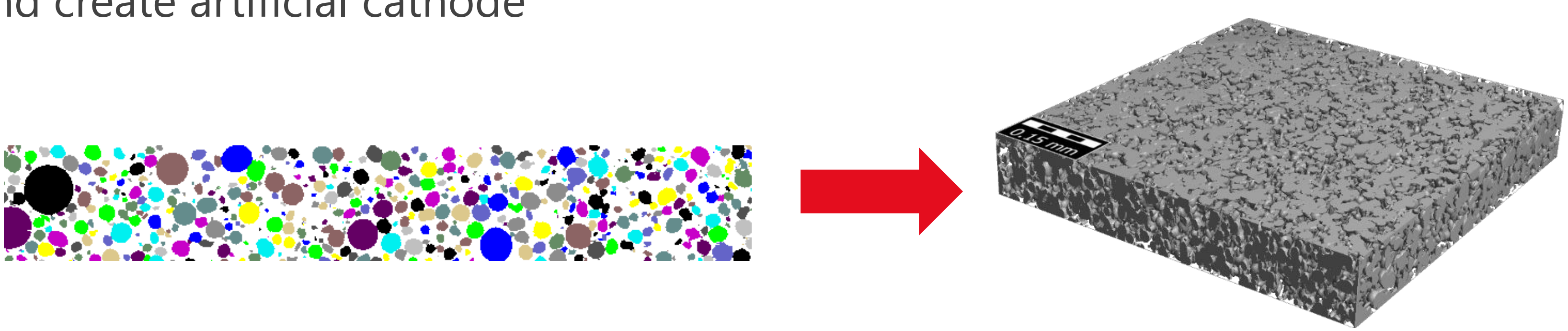
GEODICT

Take 2d slice of NMC scan



Use GrainFind to identify grains and obtain statistics

And create artificial cathode



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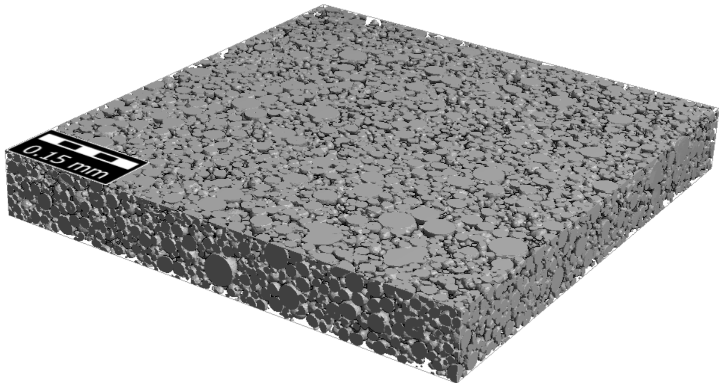
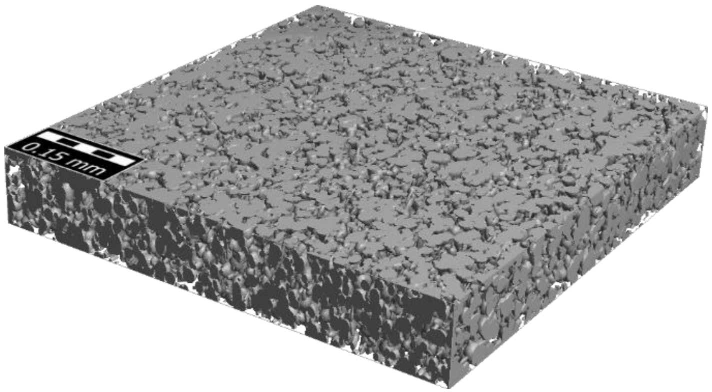
Step 1: NMC validation of 3D representation

GeoDict

3d scan



Digital cathode



Compute:
porosity and tortuosity

1.212	Tortuosity x	1.38
1.22	Tortuosity y	1.21
1.24	Tortuosity z	1.22
49.97 %	Porosity	49.79%

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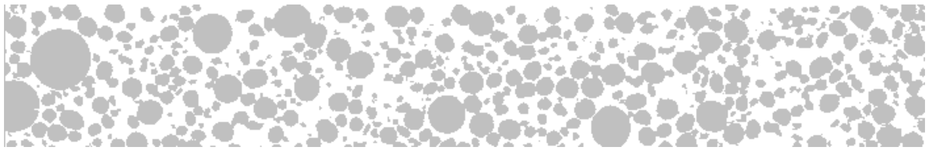
STEP 1: NMC VALIDATION OF 3D REPRESENTATION

GEODICT

Take 2d slice of 3d scan

Take 2d slice of digital cathode



Compute:
geometry statistics

4.98 µm	Mean of shortest Diameter	7.42 µm
6.52 µm	Mean of intermediate Diameter	10.64 µm
12.94 µm	Mean of longest Diameter	15.47 µm

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Step 1: NMC recreation with GrainFind Validation Results

GeoDict

Comparison of computed calibration parameters

	Sample	Reconstruction	Relative Error /(%)
Mean of shortest Diameter	4.98 µm	7.42 µm	49
Mean of intermediate Diameter	6.52 µm	10.64 µm	63
Mean of longest Diameter	12.94 µm	15.47 µm	20
Tortuosity x	1.212	1.38	12
Tortuosity y	1.22	1.21	0.2
Tortuosity z	1.24	1.22	2
Porosity	49.97 %	49.79%	0.3

→ Physical properties almost good, geometric properties not sufficiently accurate

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Step 2: NMC recreation GeoDict extended by optiSLang

GeoDict

GeoDict Workflow is basis for Sensitivity analysis:

Input parameters for Sensitivity analysis:

- Porosity
- Grain diameters in x, y and z direction (Assume 3 different kind of grains)
- Grain orientations

As responses use geometric and physical properties.

- **Tortuosity** and **porosity** (physical properties)
- **GrainFind** results (geometric properties)

Later apply optimization routine on the obtained MOP

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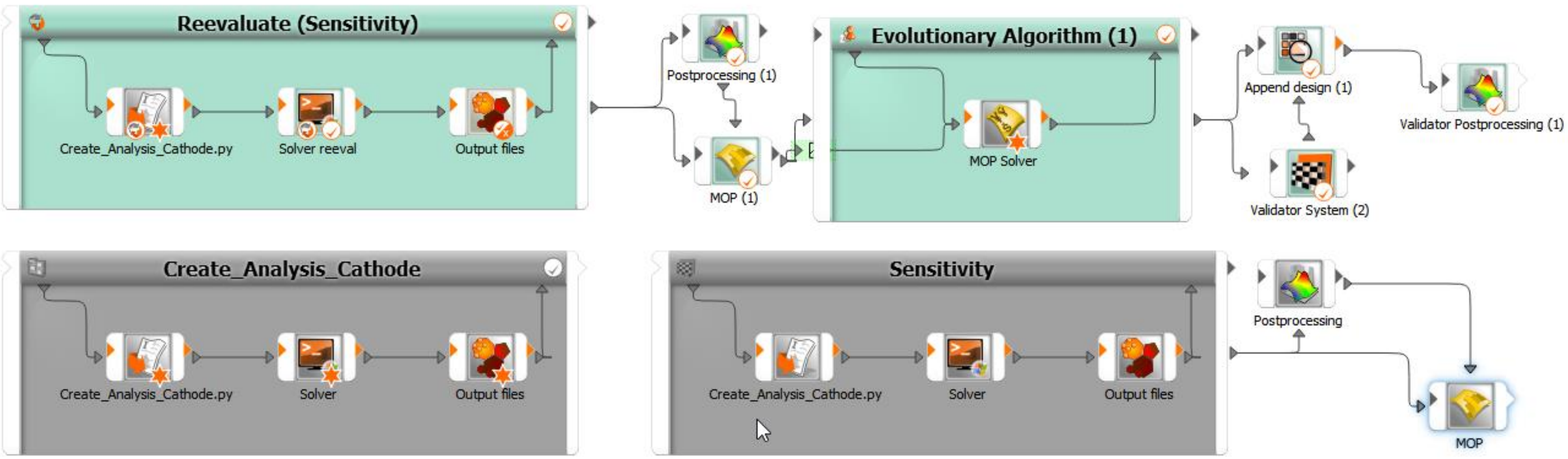
STEP 2: NMC RECREATION GEODICT OPTISLANG WORKFLOW

GEODICT

optiSLang workflow is simple and does not need large complexity:

150 designs calculated +1 validator system



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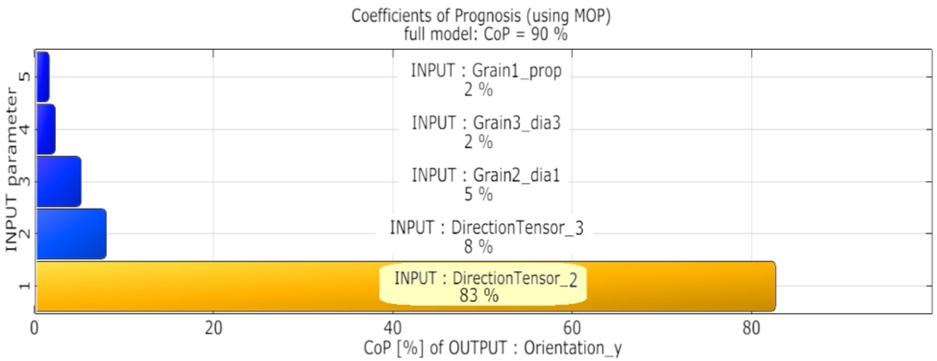
Step 2: NMC analysis by optiSLang: Sensitivity

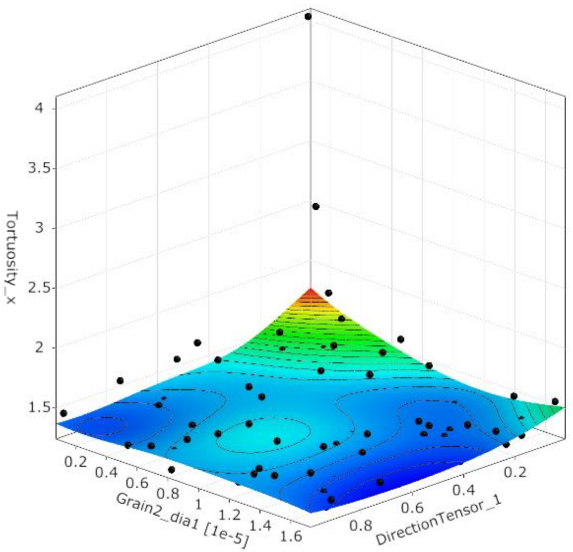
GeoDict



Orientation in y direction is dependend on:

- Input orientation in y direction
- Input orientation in z direction

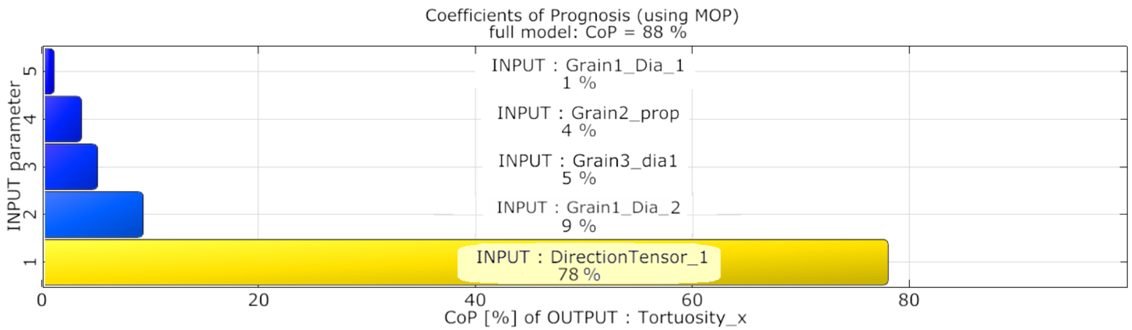
→ Expected and necessary criterion!



Tortuosity in x direction:

- Orientation in x direction
- Acceptable coefficient of prognosis

→ For later studies more designs should be calculated



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Step 2: NMC analysis by optiSLang: optimization on MOP

GeoDict

Knowledge from Step 1:

	Sample	Reconstruction	Relative Error /(%)
Mean of shortest Diameter	4.98 µm	7.42 µm	49
Mean of intermediate Diameter	6.52 µm	10.64 µm	63
Mean of longest Diameter	12.94 µm	15.47 µm	20
Tortuosity x	1.212	1.38	12
Tortuosity y	1.22	1.21	0.2
Tortuosity z	1.24	1.22	2
Porosity	49.97 %	49.79%	0.3

$\leq$ 20%

$\leq$ 10%

Improve the Diameter results → set those as constrains: rel. error ≤ 20%

Improve the physical results:

- Already pretty good so set constrained with rel. error ≤ 10%
- Tortuosity in x direction as optimization variable

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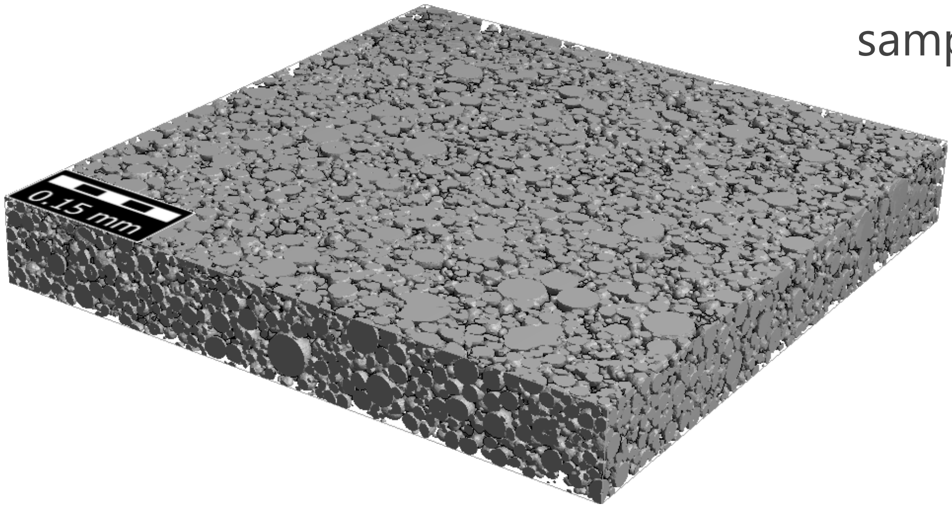
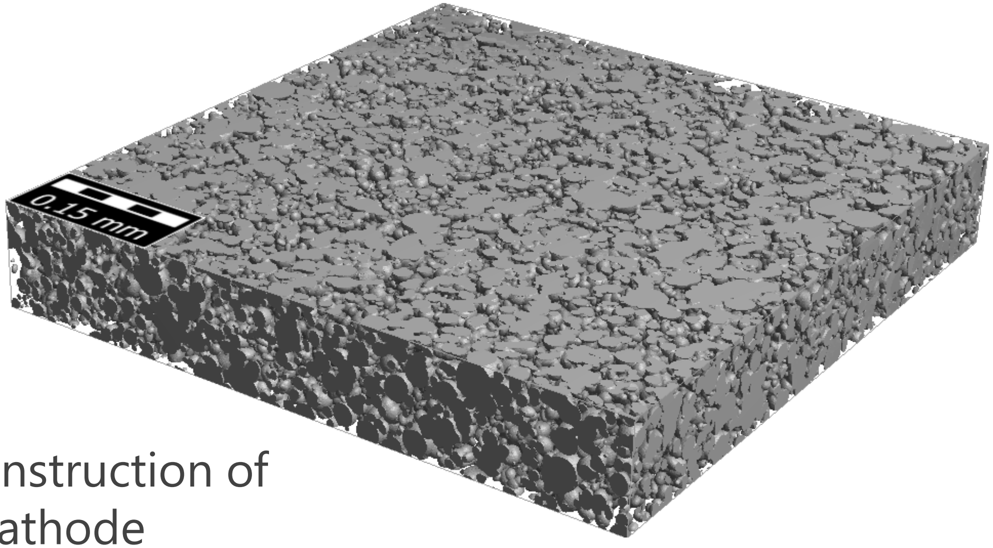
STEP 2: NMC ANALYSIS BY OPTISLANG: RESULTING CATHODE

GEODICT



sample of NMC cathode



artificial reconstruction of NMC cathode

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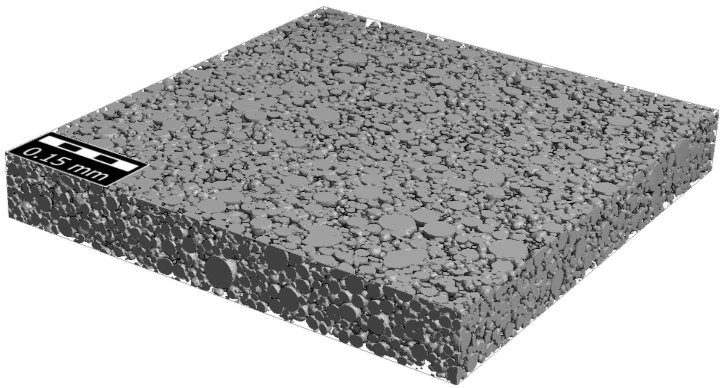
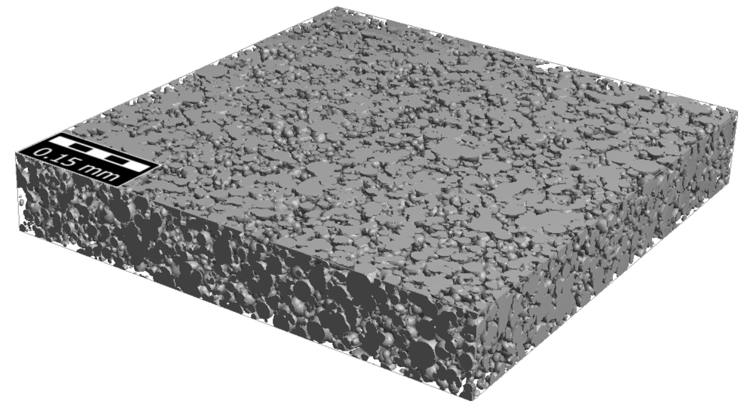
Step 2: NMC validation of 3D representation

GeoDict

3D scan



Digital Cathode



Compute:
Porosity and tortuosity

1.212	Tortuosity x	1.25
1.22	Tortuosity y	1.28
1.24	Tortuosity z	1.30
49.97 %	Porosity	47.06%

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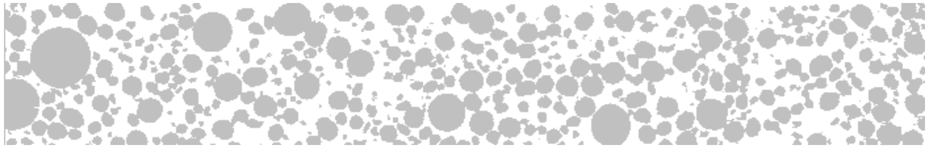
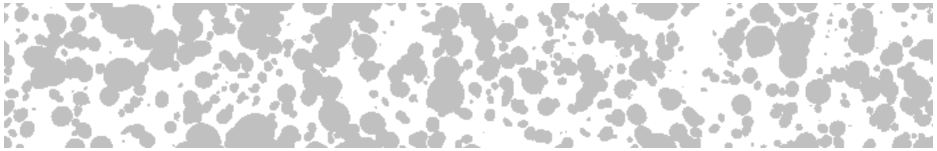
STEP 2: NMC VALIDATION OF 3D REPRESENTATION

GEODICT

Take 2d slice of 3d scan



Take 2d slice of digital cathode



Compute:
geometry statistics

4.98 µm	Mean of shortest Diameter	4.23 µm
6.52 µm	Mean of intermediate Diameter	5.30 µm
12.94 µm	Mean of longest Diameter	13.27 µm

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STEP 2: NMC ANALYSIS BY OPTISLANG: OPTIMIZATION RESULTS

GEODICT

As criteria we use results from Step 1:

	Sample	Reconstruction	Relative Error /(%)
Mean of shortest Diameter	4.98 µm	4.23 µm	15
Mean of intermediate Diameter	6.52 µm	5.30 µm	19
Mean of longest Diameter	12.94 µm	13.27 µm	3
Tortuosity x	1.212	1.25	3
Tortuosity y	1.22	1.28	5
Tortuosity z	1.24	1.30	5
Porosity	49.97 %	47.06%	6

All constraints and optimization variables are within bounds!

Some are at their limit, but did not exceed it

→ This artificial cathode is a digital twin for tortuosity and diffusivity

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CONCLUSION AND OUTLOOK

GEODICT

- Recreating an artificial cathode with standalone GrainFind and GrainGeo tools already yields good results
- But in combination with optiSLang results are improved
  - More designs for Sensitivity should be considered
- This methodology is applicable to homogenous cathodes very good

But:

- For inhomogeneous cathode this methodology can work but:
  - Needs more inputs
  - Needs to be extended and validated

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THANK YOU FOR YOUR ATTENTION!