The Digital Twin – A comparative study of material simulation on µCT-scanned and modelled microstructures

Constantin Bauer
Math2Market GmbH
What is GeoDict?

**IMPORT**
Diverse ways to import materials for modeling

**MODEL**
Detailed material models created in 3D

**ANALYZE**
Extensive analysis and evaluation of structural material properties

**PREDICT**
In-depth analysis and prediction of material behavior

**EXPORT**
GeoDict models made available for standard workflows
GeoDict Module Overview
What material are we looking at?

- **PA6GF50**
  - Polyamide 6 matrix
  - short glass fiber reinforcement
  - 50 % fibers by weight

- produced by injection molding

- used in mass production for structural components (e.g. engine bearer)
6 Steps to the Digital Twin

1. Import, process and segment the µCT-scan
2. Calculate the mechanical properties directly on the µCT-scan
3. Determine the geometrical properties of the material
   (fiber diameter, fiber orientation, fiber length)
4. Model the digital twin
5. Calculate the mechanical properties of the digital twin
6. Comparison of the results
used GeoDict Modules
Import and Segmentation

- Import a stack of 2d images
- Image processing to improve quality for segmentation (e.g. noise reduction, edge sharpening)

Applying a Non-Local Means Filter for noise reduction
Import and Segmentation

• automated thresholding using OTSU\(^1\) algorithm

Import and Segmentation

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Import and Segmentation

- automated thresholding using OTSU\(^1\) algorithm

Mechanical Analysis - µCT scan

• linear elastic simulation of 6 different load cases
  – 3 uniaxial experiments
  – 3 shear experiments

• used material properties
  – PA6: \( E=2.8 \) GPa / \( v=0.39 \)
  – Glass: \( E=72 \) GPa / \( v=0.22 \)

• computation time: 589 s
  – 4 CPUs
  – 0.5 GB memory
Mechanical Analysis - µCT scan

- calculated engineering parameters and stiffness tensor

<table>
<thead>
<tr>
<th>Orthotropic Approximation</th>
<th>Strain Equivalence</th>
<th>Energy Equivalence</th>
<th>Mean Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus $E_1$ (GPa)</td>
<td>7.1211</td>
<td>7.1213</td>
<td>7.1212 ± 0.0001</td>
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<tr>
<td>Young’s Modulus $E_2$ (GPa)</td>
<td>7.9283</td>
<td>7.9285</td>
<td>7.9284 ± 0.0001</td>
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<td>Young’s Modulus $E_3$ (GPa)</td>
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<td>11.3852</td>
<td>11.3852 ± 0.0000</td>
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<tr>
<td>Poisson Ratio $v_{23}$</td>
<td>0.3547</td>
<td>0.3547</td>
<td>0.3547 ± 0.0000</td>
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<tr>
<td>Poisson Ratio $v_{31}$</td>
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<td>Poisson Ratio $v_{13}$</td>
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<tr>
<td>Poisson Ratio $v_{12}$</td>
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<tr>
<td>Shear Modulus $G_{12}$ (GPa)</td>
<td>2.7558</td>
<td>2.7557</td>
<td>2.7558 ± 0.0001</td>
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<tr>
<td>Shear Modulus $G_{13}$ (GPa)</td>
<td>3.0113</td>
<td>3.0111</td>
<td>3.0112 ± 0.0001</td>
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<td>Shear Modulus $G_{23}$ (GPa)</td>
<td>3.8636</td>
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<th>Anisotropic Elasticity Tensor</th>
<th>(GPa)</th>
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<tr>
<td>$10.232$</td>
<td>5.4243</td>
</tr>
<tr>
<td>$5.4948$</td>
<td>0.025524</td>
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<tr>
<td>$6.0651$</td>
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<td>$0.1212$</td>
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<td>$-0.17072$</td>
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<td>$2.7558$</td>
<td>0.14133</td>
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</tbody>
</table>
Mechanical Analysis - μCT scan

- visualization of the von-Mises stress
Modeling the Digital Twin
Digital Twin – Geometrical Analysis of µCT-Scan

- fiber diameter distribution

Average fiber diameter: 9.38167e-06 m
Standard deviation: 1.95088e-06 m
Digital Twin – Geometrical Analysis of µCT-Scan

• fiber orientation analysis
  – using Star Length Distribution Algorithm
  – works on a per-voxel basis
  – analyzes the chord lengths through the voxel for a pre-defined set of directions
  – the relative length of the cords gives the per-voxel orientation tensor
  – tensors are averaged
Digital Twin – Geometrical Analysis of μCT-Scan

- fiber orientation analysis
  - homogenized orientation tensor for the entire scan
  - visualization of the main orientation
- calculation of the fiber volume fraction

$$\text{Block 0,0,0: Solid Volume Fraction} = 30.9137\%$$

<table>
<thead>
<tr>
<th></th>
<th>0.165335</th>
<th>-0.0166808</th>
<th>-0.0524757</th>
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<tr>
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<tr>
<td>-</td>
<td>-</td>
<td>0.545357</td>
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</tr>
</tbody>
</table>
Digital Twin – Modelling

- use all collected geometrical properties of the material for modelling the digital twin in FiberGeo
Digital Twin – Modelling

- visual comparison of the twin and the µCT-scan

µCT-Scan

Digital Twin
Digital Twin – Mechanical Analysis

• comparison of the stiffness tensor

--- Anisotropic Elasticity Tensor ---

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<thead>
<tr>
<th>Stiffness Formulation for Strain Equivalence / (GPa)</th>
<th>μCT-Scan</th>
<th>Digital Twin</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.232 5.4243 5.4948 0.025524 -0.010267 0.14141</td>
<td>10.757 5.4859 5.5878 0.053966 0.06989 0.16679</td>
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<tr>
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<tr>
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<tr>
<td>0.14133 0.12119 -0.12859 -0.17072 0.091522 2.7558</td>
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<td></td>
</tr>
</tbody>
</table>

→ very good agreement between μCT-scan and digital twin
Digital Twin – Some Examples
Digital Twin – Polysulfone micromembrane

• used for seawater desalination

[Shi et al., Water flow prediction for Membranes using 3D simulations with detailed morphology, 2015, Journal of Membrane Science]
Digital Twin – Sintered Ceramic

• used for soot particle filters

[Schmidt and Becker, Generating Validated 3D Models of Microporous Ceramics, 2013, Advanced Engineering Materials]
Digital Twin – Sintered Ceramic

[Schmidt and Becker, Generating Validated 3D Models of Microporous Ceramics, 2013, Advanced Engineering Materials]
Digital Twin – Gas Diffusion Layer

- used in fuel cells
Digital Twin – Gas Diffusion Layer

In the original CT Scan binder and fiber can not be separated

It is necessary to differentiate fibers from binder based on the shape
Digital Twin – Gas Diffusion Layer

Identifying binder with Machine Learning
Digital Twin – Gas Diffusion Layer

μCT-Scan

segmented image

Fibers: 16.2%
Binder: 13.2%
Thank You!

Dr.-Ing. Constantin Bauer
Math2Market GmbH
+49 631 205 605 – 28
constantin.bauer@math2market.de
www.geodict.com