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

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What are Math2Market & GeoDict?

Research Project “Math2Composites”

Flow Simulations on Large Structures
Math2Market GmbH

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

GeoDict® - The Digital Material Laboratory

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

<table>
<thead>
<tr>
<th><strong>Filtration</strong></th>
<th>Mostly automotive, filter media &amp; filters for water, sludge, oil, air and fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Electrochemistry</strong></td>
<td>Fuel cell media &amp; battery materials, catalyst materials</td>
</tr>
<tr>
<td><strong>Composites, Ceramics &amp; Metals</strong></td>
<td>CFRP, GFRP, mostly automotive, lightweight materials</td>
</tr>
<tr>
<td><strong>Digital Rock Physics</strong></td>
<td>Digital rock physics, digital sand control</td>
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</table>
The idea is the beginning. Design a material from scratch or import images from an existing material to create a digital model.

Discover the geometric properties and compute the physical properties of the material. This is the start of creating a Digital Twin.

A Digital Twin is the statistical representation of the material in the digital world. Here begins the design process.

Digital prototypes are easily and rapidly created. Simulate and evaluate in a loop to find the material with the desired properties.

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

This is innovation through simulation.
GeoDict® Module Overview

This is Innovation through Simulation

**ImportGeo**  **FiberGeo**  **PaperGeo**  **GrainGeo**
**FoamGeo**  **WeaveGeo**  **GridGeo**  **PleatGeo**
**MeshGeo**  **ExportGeo**  **PoroDict**  **MatDict**  **BatteryDict**
**DiffuDict**  **ConductoDict**  **FlowDict**  **ElastoDict**  **FilterDict Media & Element**
**AddiDict**  **SatuDict**  **AcoustoDict**  **FiberFind**  **GrainFind**
01 What are Math2Market & GeoDict?
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03 Flow Simulations on Large Structures
OUR DREAMS IN SHORT

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

- In the Math2Composites project, there is a twist:
  1. First make sure 3-D imaging + property computation agrees with *easy / cheap* experiments
  2. Infer that property computation is also correct for *difficult / expensive* experiments
**Research Project “Math2Composites”**

Large amount of experiments for the determination of material properties

<table>
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<tr>
<th>Test 1</th>
<th>Test 2</th>
<th>Test 4</th>
<th>Test 6</th>
<th>Test 8</th>
<th>Test 10</th>
</tr>
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Novel simulative-experimental approach for the determination of material properties

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<th>Test 1</th>
<th>Test 2</th>
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Replace a large amount of experiments by validated simulations
Structure of the non-crimped fabric Hacotech G300U-1270mm

- 0° glass fiber roving (80% of fiber volume fraction)
- 90° glass fiber roving (20% of fiber volume fraction)
- PET stitching

2 mm
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Novel simulative-experimental approach for the determination of material properties

µCT-Scan

Simulation

Model

Predicted validated simulation calibration of the simulation
Results of the permeability calculation 2017
Results of the permeability calculation 2017

![Bar chart showing permeability in m² for different samples and methods: Experiment, µCT-Scan, Model 2017. The chart includes data points for K1, K2, and K3 in each method, with values ranging from 1,00E-13 to 1,00E-09.]
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Novel simulative-experimental approach for the determination of material properties

μCT-Scan

- Good simulation results
- Huge experimental effort can’t be reduced

Model

- Low experimental effort
- Deviation from simulation and experiment too high

Digital Twin

- Can be reduced by improved modeling techniques

© Math2Market GmbH
- Structure of the non-crimped fabric Hacotech G300U-1270mm
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- modeling with WeaveGeo

Model 2017

µCT-Scan
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- modeling with WeaveGeo

3rd cousin

μCT-Scan
Implementation of roving undulation
modeling the PET stitching (yellow)
Compaction of the modeled structure with ElastoDict-LD
Calculation of the permeability with FlowDict

**next step:** using anisotropic permeabilities for the roving material
Calculated permeabilities by flow simulation on µCT-scan show very good agreement with experiments.

Elevated effort to obtain µCT-scan.

Modeled structures for permeability calculation must take material imperfections into account
- fiber undulation
- PET stitching
- roving deformation through compaction

Flow simulations on the new modeled structure with material imperfections show only small deviations from experiment.
Acknowledgement

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03 Flow Simulations on Large Structures
FLOW COMPUTATION WITH LIR SOLVER

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

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

![Runtime vs. Number of Processes](chart.png)

- GeoDict 2018
- Ideal
FILTER SIMULATION WITH GeoDict

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

- Transient filtration simulation

2650 s  →  8733 s  →  11340 s
FILTER SIMULATION WITH GEODict

- Transient filtration simulation
DISSOLUTION PATTERN – FACE DISSOLUTION

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

Material Information:
- ID 00: Porespace [Invis.]
- ID 01: Dissolved Structure
- ID 02: Original Structure
COMPARISON FACE DISSOLUTION PATTERN

GeoDict simulation

Maheshwari et al. 2013
COMPARISON CONICAL WORMHOLE PATTERN

GeoDict simulation

Maheshwari et al. 2013
COMPARISON WORMHOLE PATTERN

GeoDict simulation

Maheshwari et al. 2013
COMPARISON UNIFORM DISSOLUTION PATTERN

GeoDict simulation

Maheshwari et al. 2013
Machine Learning-based Binder Identification

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

- **Application phase**:
  - network transforms segmented µCT data into labeled output image
SYNTHEtic TRAINING DATA GENERATION

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

Cross-section in X-Direction:
**Binder Distribution in Through (Z) Direction (MatDict)**

- In production, binder is applied to the top of the paper and, then, intrudes into deeper layers.

- After labelling binder voxels, we can compute the distribution of binder in through direction (right).