The Virtual Material Laboratory

Designing integrated software for porous media characterization and engineering

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Computational Materials at your fingertips…
Where is M2M located, who are we?
The Virtual Material Lab lets you ...

- Import materials
- Model materials
- Characterize materials
- Characterize properties
I. GeoDict, InterPore and ITWM

GeoDict was developed at Fraunhofer Institute for Industrial Mathematics in Kaiserslautern since 2001. ITWM, about 400 employees, is one of 60 institutes in the Fraunhofer Society, the largest Applied Research Agency in Europe with 14,000 staff.

In 2011, the three main developers of GeoDict spun off Math2Market GmbH, Kaiserslautern, with full support from ITWM. M2M today has 6 full time and 6 part time staff, 3 of them off-site.

Math2Market and ITWM continue to closely collaborate with joint projects and joint personnel.

The connection with InterPore has been fruitful for GeoDict regarding requirements, publications, sales and project work ever since the inaugural meeting at Fraunhofer in Kaiserslautern in 2009.
FLOW AND MATERIAL SIMULATION

"The migration of our research and technology into commercial software used to take ten or more years."

“Together with M2M, this transfer happens much faster !”

Dr. Konrad Steiner, Head of department, Fraunhofer ITWM
II. The concept of Virtual Material Characterization & Engineering

Recent vailability of

- sub-micron resolution 3d images (µCT, FIB-SEM, …)
- affordable computers (1TB memory, 64 cores, 2GB graphics …)
- stochastic geometric models and highly efficient numerics

allows to

- model materials geometrically as 3d images
- characterize material properties *No meshing required!*
- engineer optimized materials for dedicated purposes
- in an integrated tool
Material Characterization & Engineering

**Lab**
- Porous media or Composite material
- measure
- Properties

**Computer**
- Model
  - generate
  - Voxel Mesh
  - compute
  - Properties

Properties include:
- pore size distribution
- pressure drop, permeability
- effective stiffness
- filter efficiency, capacity
- Pressure-saturation curve
- Relative permeability

manufacture next material; try next fluid

try next set of parameters
Validation - Step 1: Characterization

Porous media or Composite material

measure

Properties

image

CT Image

filter & segment

Voxel Mesh

compute

Properties

compare

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Validation - Step 2: Engineering

To achieve synergies for computations, CT images and models are converted to voxel meshes.
Material Characterization & Engineering

Lab

Real Media

image

CT Image

measure

Properties

Tomograph

Model

Voxel Mesh

filter & segment

generate

compute

Properties

GEO DICT
Computer Aided Material Engineering with GeoDict

**Geometry**
- 3d Image (µCT, FIB, …)
- Fibrous Model
- Sintered Model
- Woven Model
- Periodic Model
- …

**Voxel Mesh**

**+ Visualization**
**+ Scripting Language**
**+ Matlab Interface**
**+ Excel Interface**

**Pre-Definitions**
- Pressure Drop
- (relative) Permeability
- Filter Efficiency
- Filter Capacity
- Pore-Solid Analysis
- Pressure-Saturation

**Fluid parameters**
**Surface properties**
**Process parameters**
Integrative benefit of voxel meshes

- Integration via voxel mesh means any CT or FIB-SEM and any model is compatible with any material characterization and any property computation.

- Voxel meshes are the integrator, a lowest common denominator for volume representations like STL for surface representations.

- Voxel meshes allow highly efficient algorithms, most notably Fast Fourier Transform based PDE-solvers.

- Simple basis allows complex yet easy-to-use software
III Material Models

- nonwovens
- fiber reinforced composites
- papers
- ceramic materials
- rocks
- dense (sphere) packings
- woven materials
- closed cell foams
- open cell foams
- regular materials
Simulations performed on 3d structures composed of little cubes

Advantages: Straight forward
- automatic grid generation for computed tomography
- virtual structure generation
- solver implementation
- parallel implementation

Disadvantages: resolving features
- requires many grid cells
- requires very large scale computations
Analytic, surface and volume representation

<Object1>
  Color 1
  Type ShortCircularFiber
  Point1 6.6e-5,2.5e-5,4.8e-5
  Point2 8.9e-5,-2.04e-5,5.3e-5
  FiberEndType1 0
  FiberEndType2 0
  Diameter 1.2e-05
</Object1>
Glass fiber nonwoven

SEM visualization of 8 volume percent 5 micron fibers

anisotropy 100

anisotropy 7
Curled & inhomogeneous nonwoven

homogeneous model  
tomogram  
inhomogeneous model
Binarized SEM (top) and virtual sintered ceramics (bottom)
Virtual woven: multiple weft layers

weave.gmc
Virtual felt: woven, nonwoven & needling
Gas Diffusion Layer Model

Created with a stochastic process

Input:
- Porosity
- Fiber diameter and type
- Anisotropy
- (Fiber crimp)
- (Weight% binder)
3D Models: Catalyst Layer (CL)

Model example:

Porosity 33.3 %
Carbon/Pt  50.1 vol%
Electrolyte 16.6 vol%

Size: (800 nm)³, voxel length 1 nm
IV Material properties & processes

Effective thermal conductivity

Effective diffusivity (Knudsen < 1, > 1, ~ 1); tortuosity

Permeability (flow resistivity, pressure drop)

Effective stiffness

Particle filtration (efficiency / beta ratio, capacity / life time)

Advection & diffusion (break through curves, effective surface)

2-phase flow (pressure-saturation, relative effective properties)

Pore & Solids analysis (Porosimetry, bubble point, cloudiness, ...)

Large deformations

Scripting language for automation and optimization

Matlab Interface for pre- & post processing, Excel for post-proc.
Cloudiness analysis

• For a thin nonwoven, the mass in through-direction is added up and shown in colors.

• Red means much mass, blue little mass.

• It is another way to compare real and virtual nonwoven and evaluate the quality of material models.
Compression

Aim: how does a GDL change due to clamping pressure?

Current development together with Fraunhofer

- transverse isotropic elastic modulus for fibers
- isotropic elastic modulus for binder
- 30% compression

10 min on Laptop
13.5 mio grid points

See talk by V. Schulz, Thursday 17:55
Filtration Simulation: Pressure drop and Filter Efficiency

Basic idea:
1. Filter model
2. Determine flow field (pressure drop)
3. Track particles (filtered or not?)

Randomness:
- Starting positions
- Brownian motion

Result:
- Percentage of filtered particles
Filtration Simulation: Filter Life Time

1. Filter Model
2. Flow Field
3. Track Particles
4. Deposit Particles
5. Flow Field
6. Repeat ...
Sieving resolved particles

Cake with higher density & Lower permeability
The Multipass Test (ISO 4548)
Fractional Filtration Efficiency

See poster by Hahn et al.
Sub-voxel soot particles form a filter cake that is modeled as porous media with locally varying permeability.

These soot particles do most of the work to filter more particles.

A new ceramic was designed based on simulations, a joint patent with Fraunhofer IKTS is on its way.
Pressure drop from media & capillary

Wide outflow channel looses 1 bar over filter media

Narrow outflow channel looses 2 bars over filter media and channel

Pressure at 0.01 m/s
The optimized filter element ...

A new design for hydraulic filter pleat support structures was found based on simulations and a patent granted to Argo-Hytos in 2009.

**Extended service intervals**

Higher electrostatic capacity and improved flow fatigue stability are of particular importance in achieving extended service intervals.

**Higher operational reliability**

When used in existing machinery with fixed service intervals, EXARO®MAX 2 filter elements bring greater operational reliability, ensuring the reliability of machine components as well as reducing downtime causing by loss or contamination and improving maintenance work.

**Positive identification of elements**

The plastic rings used in the EXARO®MAX 2 filter elements can be printed as required. This substantially improves positive identification and ensures important components including oil and filter service and maintenance.

**Reduced operating and maintenance costs**

These innovations work together to further optimize and maintain machines, ensuring an improvement in the productivity and economical efficiency.
Drainage

- Hilpert / Miller 2001
- Guarantees connectivity of NWP to reservoir
- Idea: push spheres
  - Start: wet
  - Start: large radius (i.e. small $p_c$)
  - Steps: $<$ radius (higher $p_c$)
- No residual water

Non-wetting phase (air) reservoir

Wetting phase (water) reservoir
Drainage (+)

- Ahrenholz et al. 2008
- Additionally: WP must be connected to reservoir
- Residual water (orange)
Drainage - Sandstone Sample

- Slice of the 3D result
- Residual water: 8.6 %
- black: air
- red: residual water
- white: matrix material
Relative Permeability (Sandstone)

- Solids (white)
- Water (yellow)
- Stokes solver for relative oil permeability in remaining pores

See poster by L. Cheng et al.
Rock models for Fluent

• In a gas production operation, the flow of gas through piles of rocks must be simulated with Fluent.

• A model of the rocks is created and exported to Fluent from the analytic description of the position and shapes of the rocks.

Structure as Parasolid for further processing.
Bricks design for electric arc furnace

• In an electric arc furnace (blue and red), bricks of two materials (white and black) must be piled.

• The brick shapes can be designed and determine the performance of the furnace via packing density, contact areas, pile permeability, triple lines etc. etc.
V The GMC Scripting Language

- Every operation can be “recorded” and “played”
- Every operation consists of a command name and a list of parameters
- There exist variables and loops
- The variables enter in the parameter lists
- The loops provide value lists to enter into the parameters
- They can be used to provide input to multiple operations in a single, user-defined GUI
- They can be used to define long-running parameter studies
GeoDict Modules – 2012R2 edition


- **ImportGeo** e.g. CT, .stl / CAD import
- **ProcessGeo** 3d image processing
- **LayerGeo** layered media
- **ExportGeo** e.g. Fluent, Abaqus
- **FlowDict** single phase flow properties
- **ElastoDict** effective elastic properties
- **ConductoDict** effective conductivity
- **DiffuDict** effective diffusivity
- **PleatDict** porous media flow
- **FilterDict** delta P, efficiency, capacity
- **SatuDict** two phase flow properties
- **PoroDict** pore analysis
- **MatDict** solids analysis
- **AcoustoDict** acoustic absorption
- **AddiDict** advection, diffusion, adsorption
- **GMC** scripting language
- **Matlab** pre- and post processing
- **GeoDexcel** post processing
Technology & application areas

- Complete set of geometric material models as gad / stl / gdt
- From Fast Solvers for simple equations in complex structures to Fast Solvers for complex equations in complex structures for:
  - Filter Media and Hygiene materials
  - Composites (damage & delamination; modelling)
  - Batteries & Fuel Cells (electro-chemistry)
  - Oil & Gas industries
- Simple formulas (like DigiMat)
- Strong parallel performance & client server architecture
Thank You – and please come see more at our booth…

The Virtual Material Laboratory

www.geodict.com