The Virtual Material Laboratory

Designing integrated software for porous media characterization and engineering

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CEO

Math2Market GmbH

Computational Materials at your fingertips…

Where is M2M located, who are we?

Barbara Andreas Christian Jürgen Erik* Cornelia Liping* Vita Sven*

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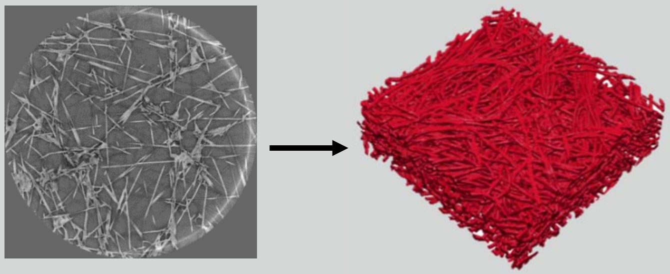
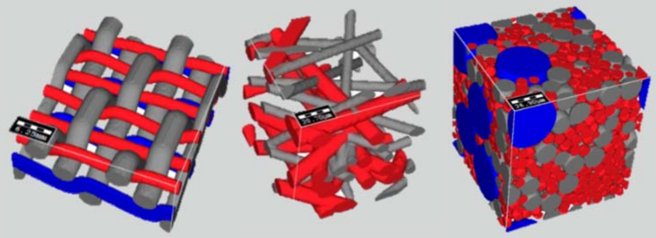
GeoDict

The Virtual Material Lab lets you ...

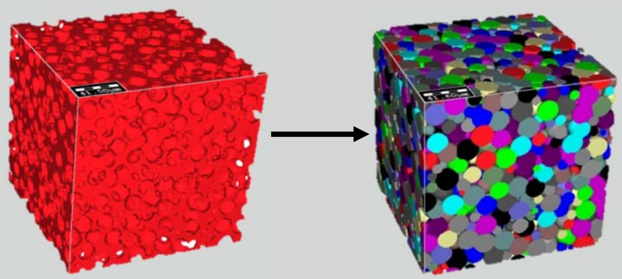
import materials



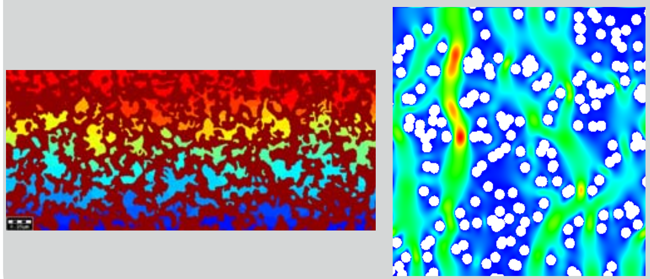
model materials



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.

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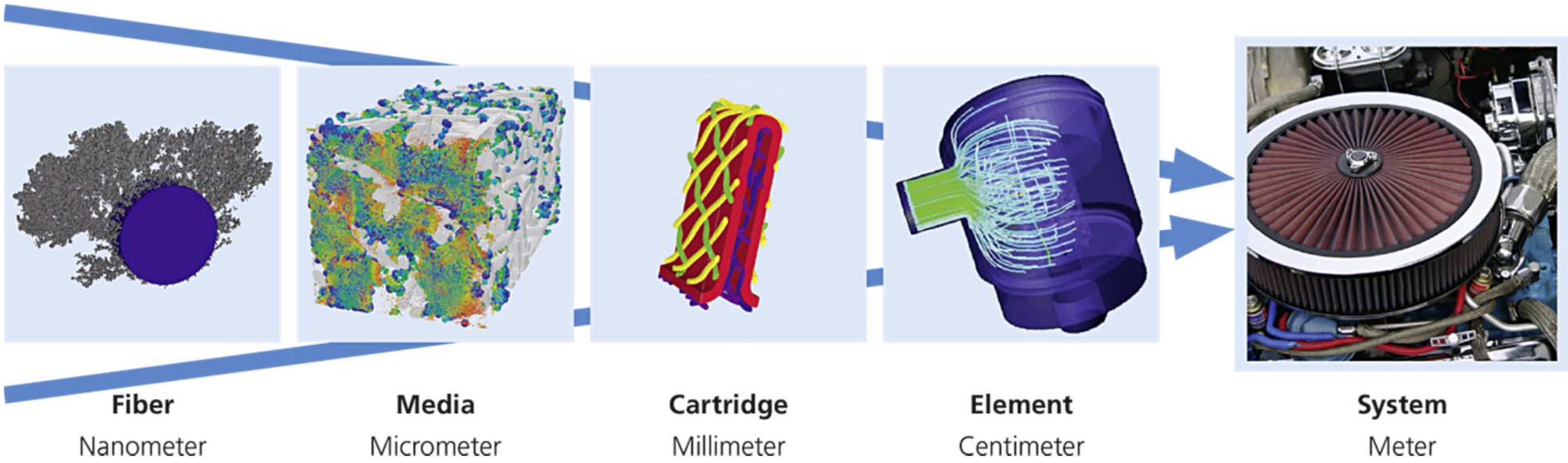
FLOW AND MATERIAL SIMULATION

”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



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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

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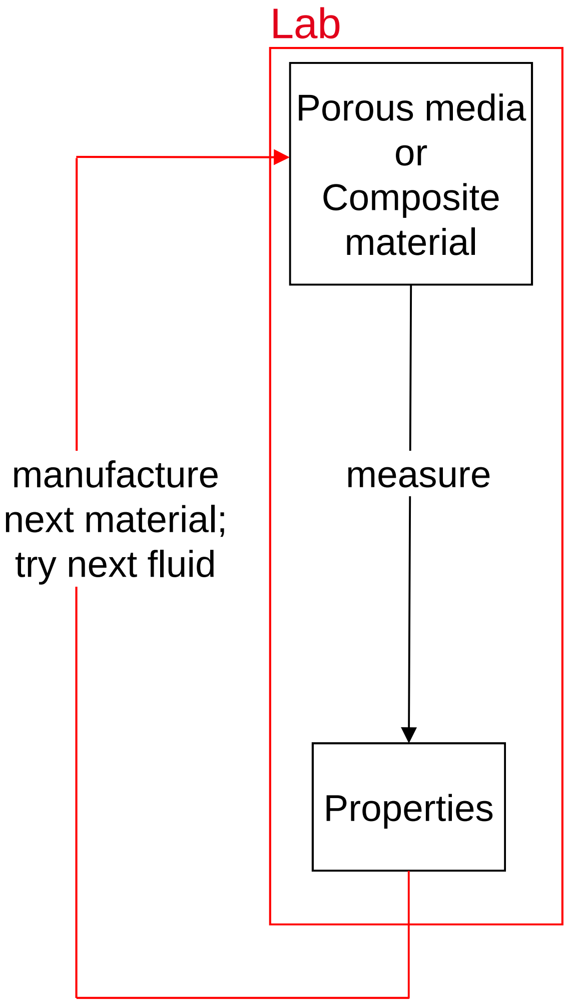
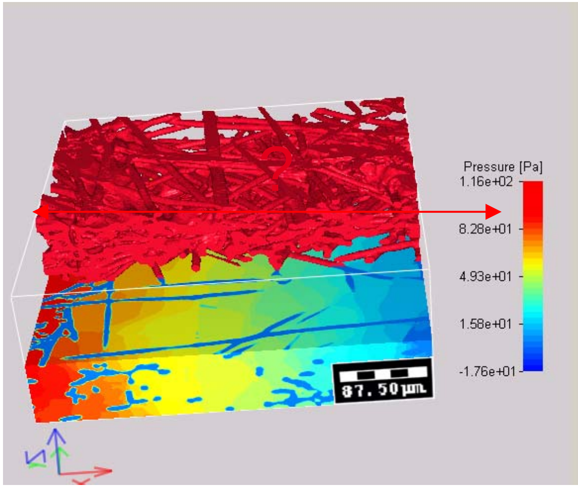
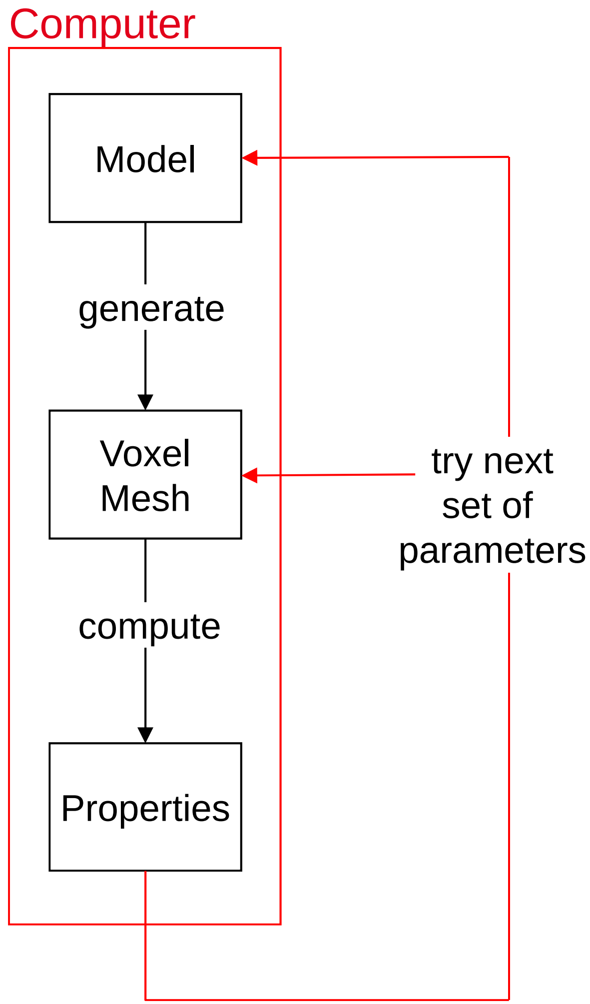
Material Characterization & Engineering

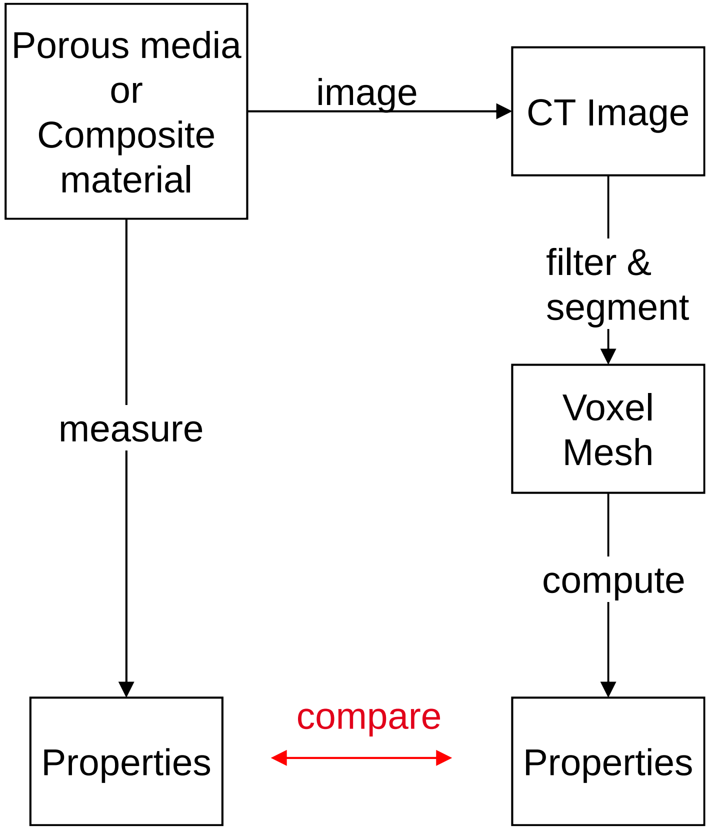


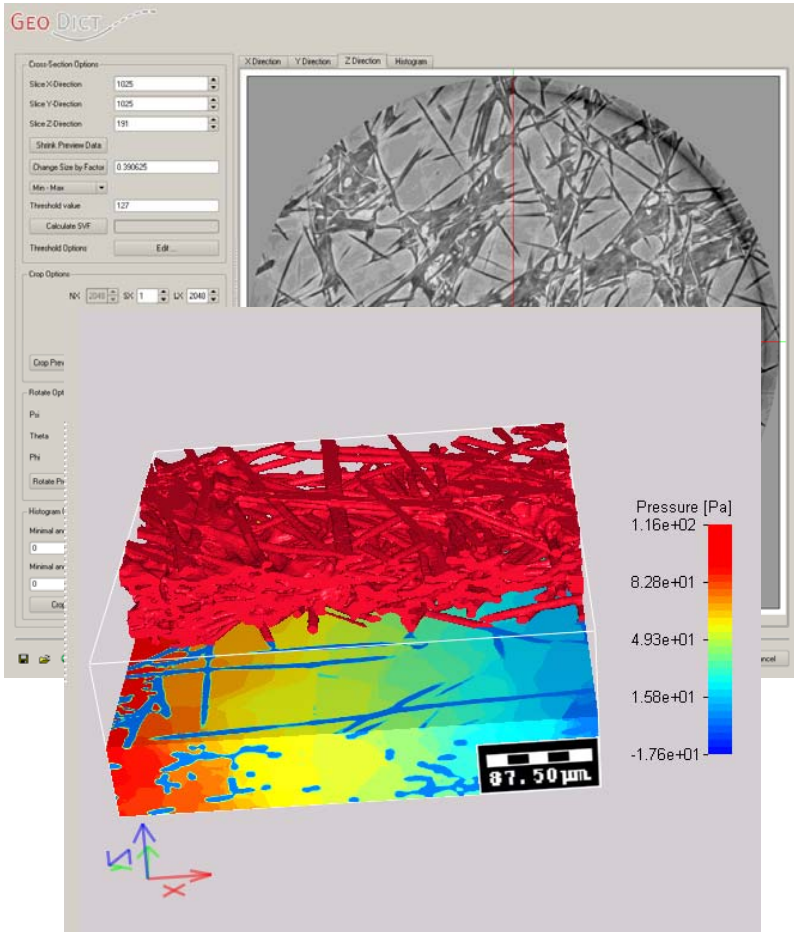




Properties include:
- pore size distribution
- pressure drop, permeability
- effective stiffness
- filter efficiency, capacity
- Pressure-saturation curve
- Relative permeability

Validation - Step 1: Characterization





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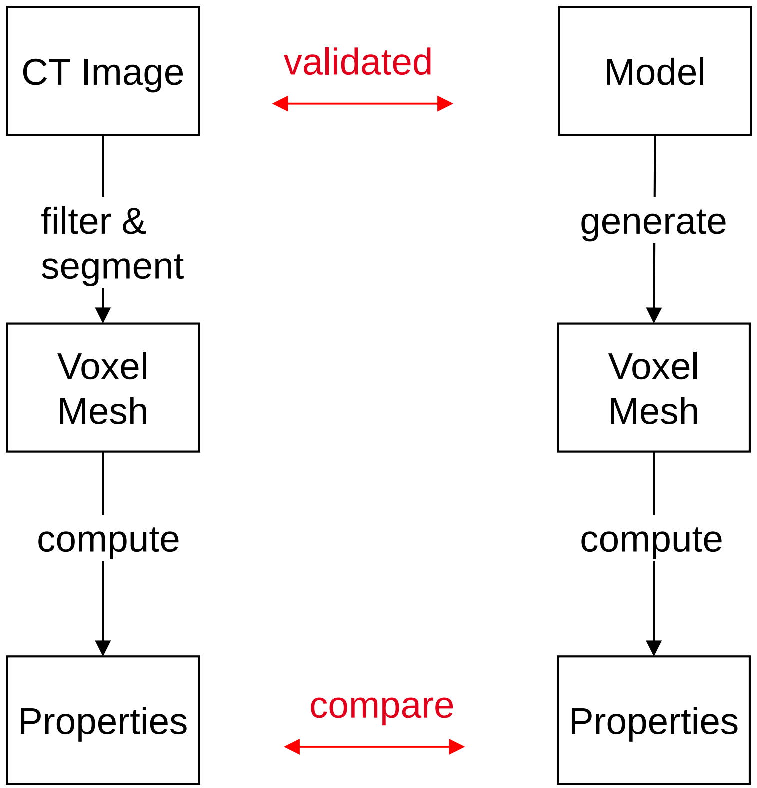
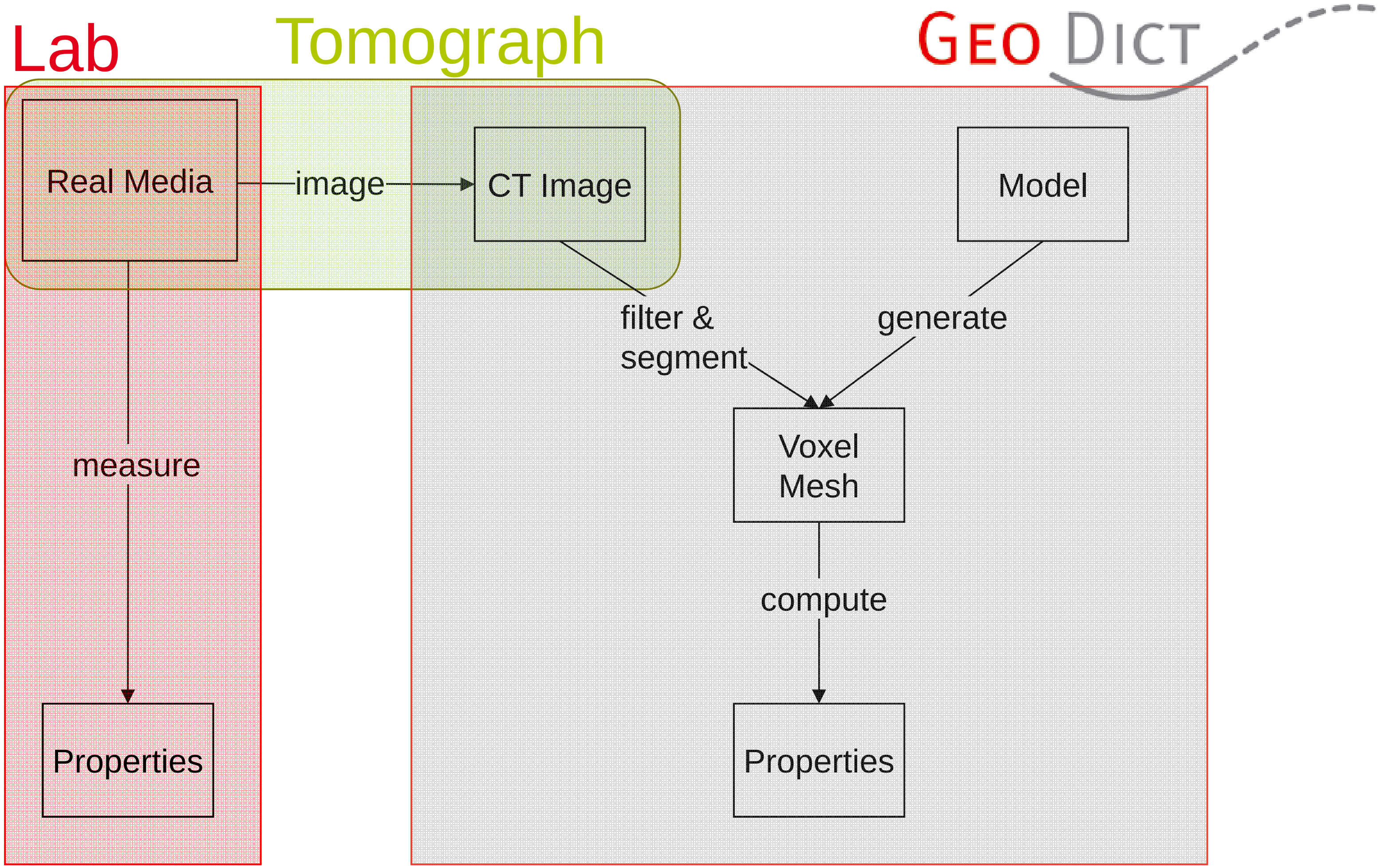
Validation - Step 2: Engineering

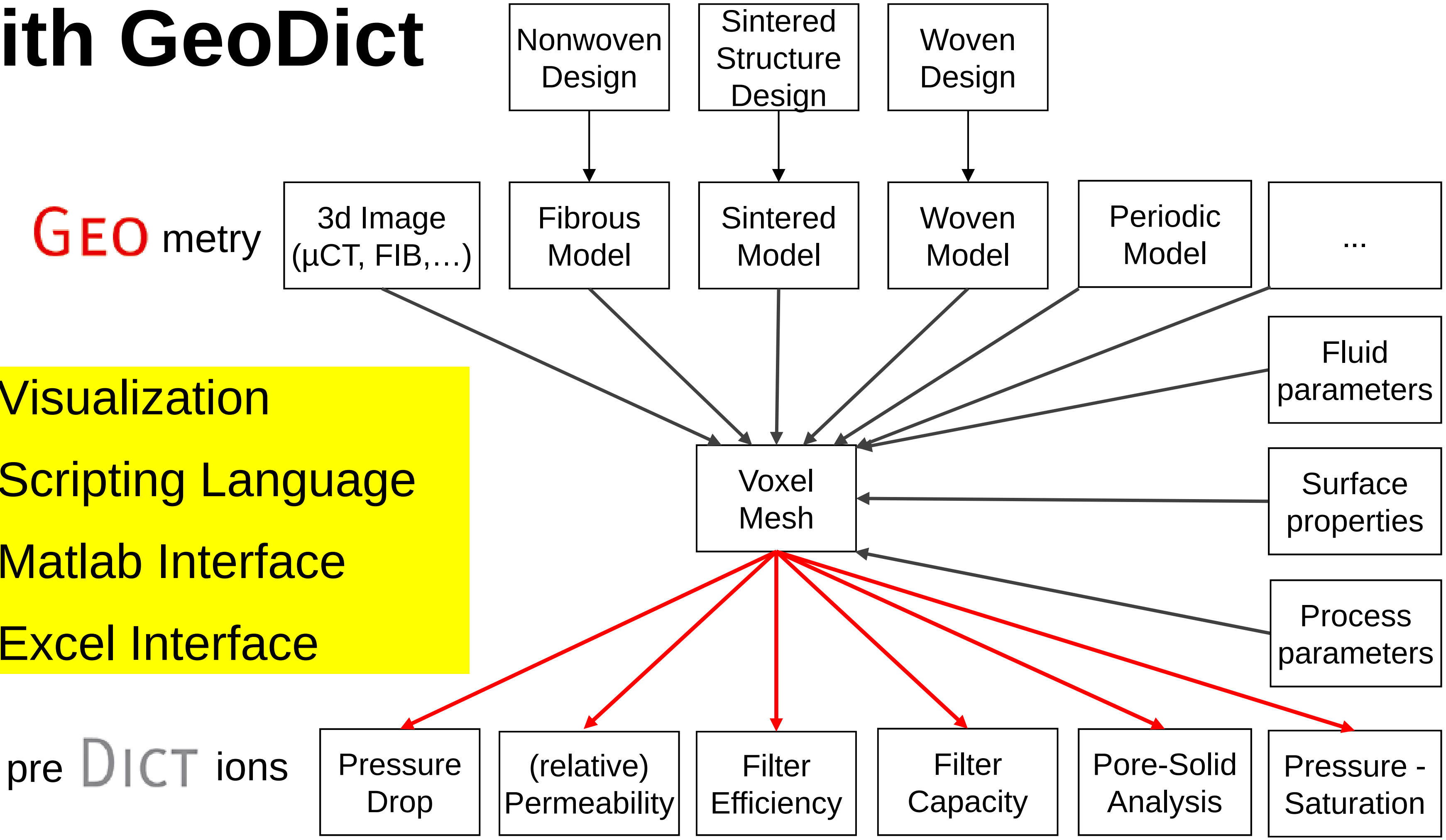
To achieve synergies for computations, CT images and models are converted to voxel meshes



Material Characterization & Engineering



Computer Aided Material Engineering with GeoDict



+ Visualization
+ Scripting Language
+ Matlab Interface
+ Excel Interface

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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

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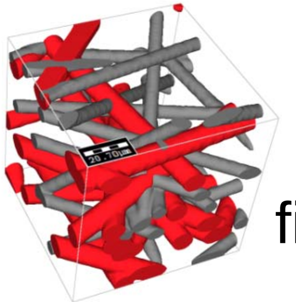
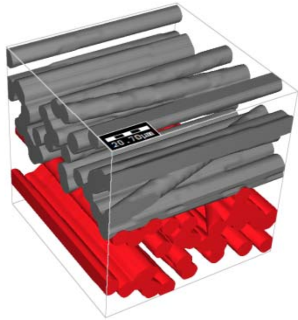
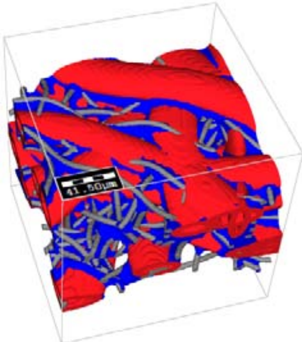
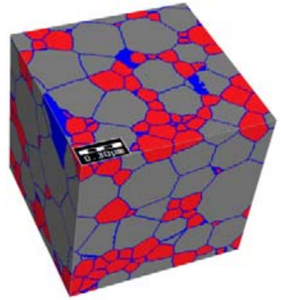
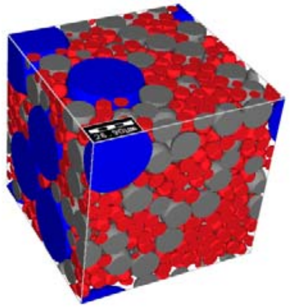
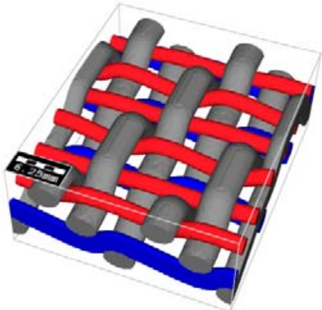
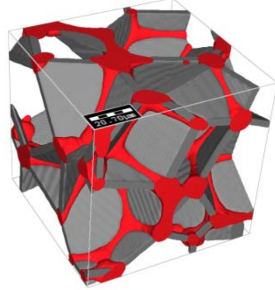
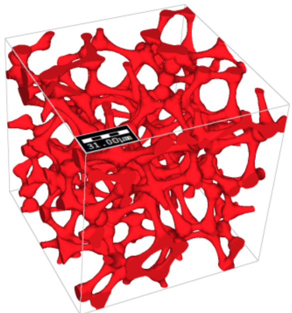
III Material Models


nonwovens

fiber reinforced composites

papers

ceramic materials

rocks

dense (sphere) packings

woven materials

closed cell foams

open cell foams

regular materials

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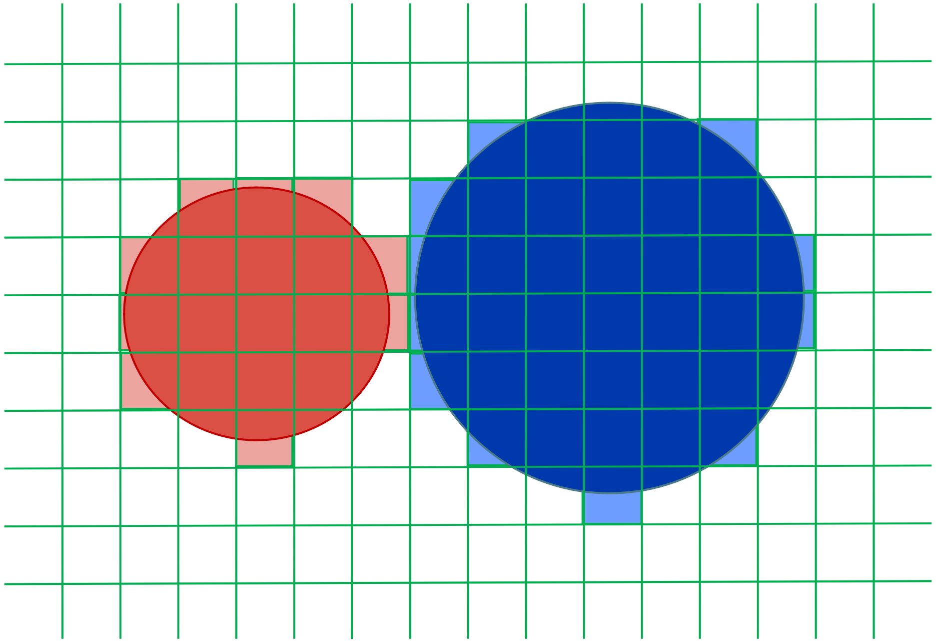
Simulations performed on 3d structures composed of little cubes



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

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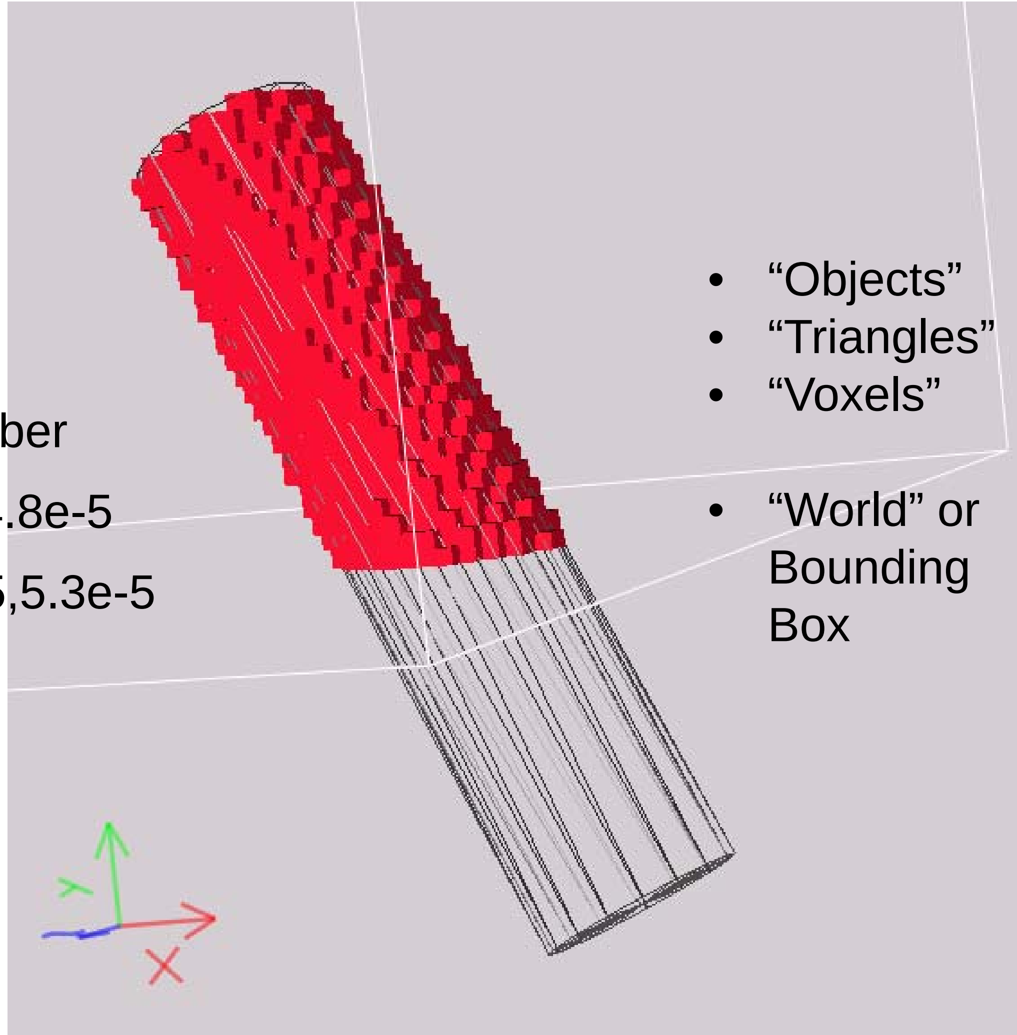
Analytic, surface and volume representation

<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>

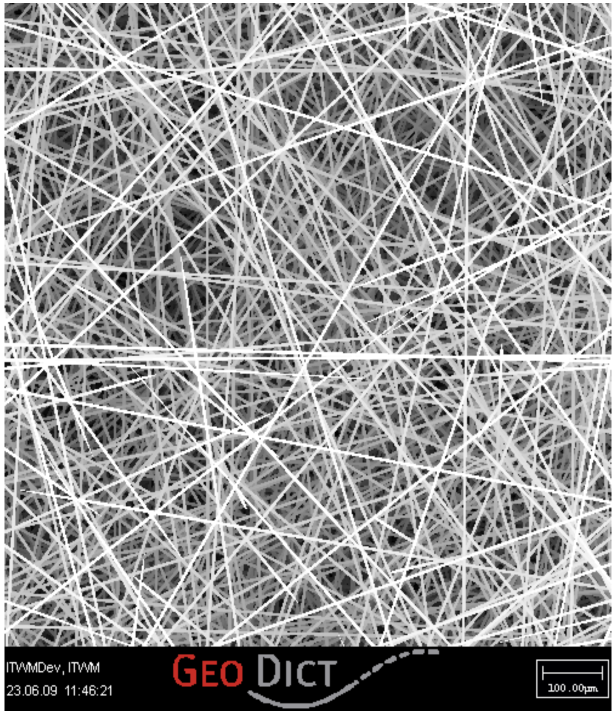


- “Objects”
- “Triangles”
- “Voxels”

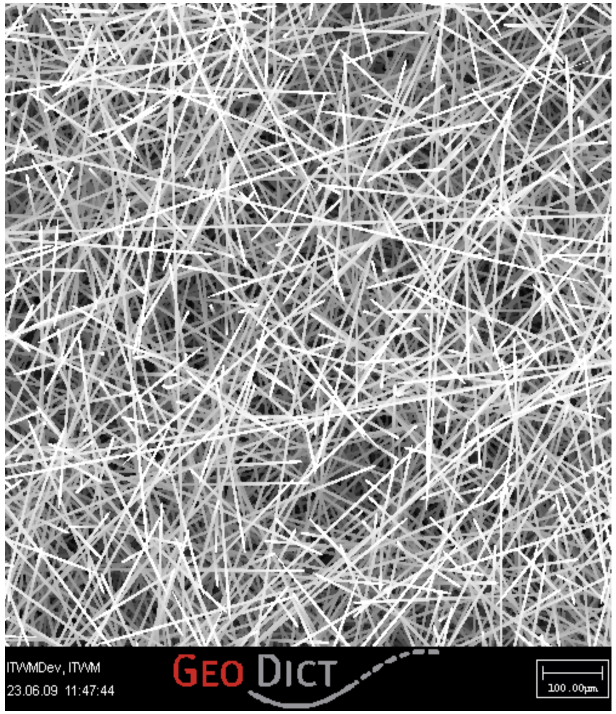
- “World” or Bounding Box

Glass fiber nonwoven

SEM visualization of 8 volume percent 5 micron fibers

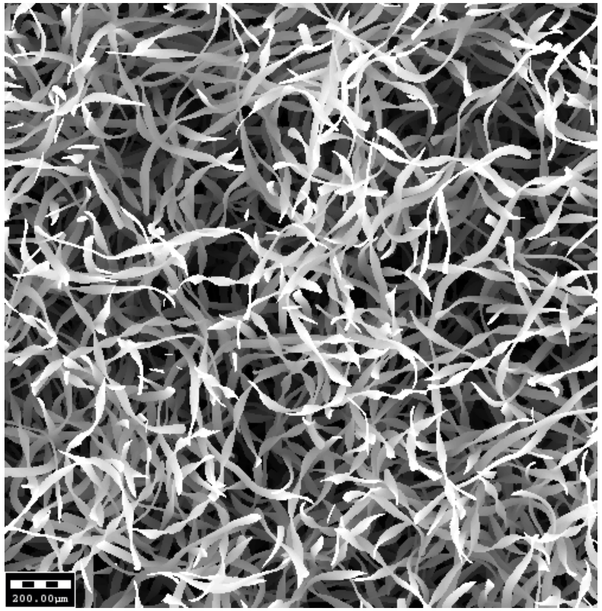


anisotropy 100

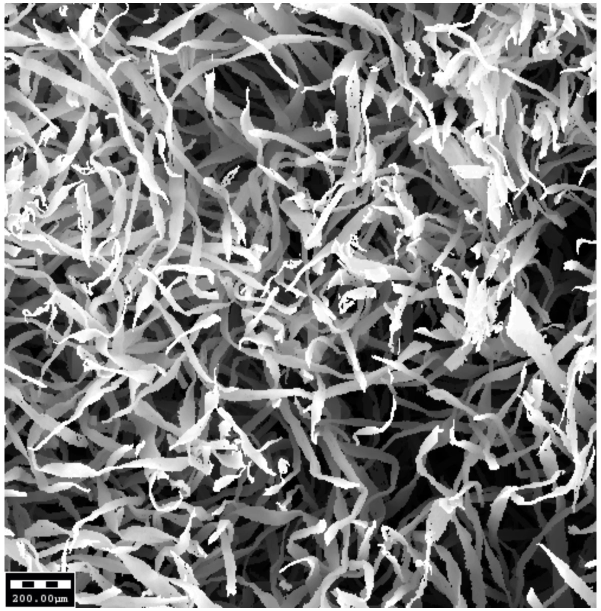


anisotropy 7

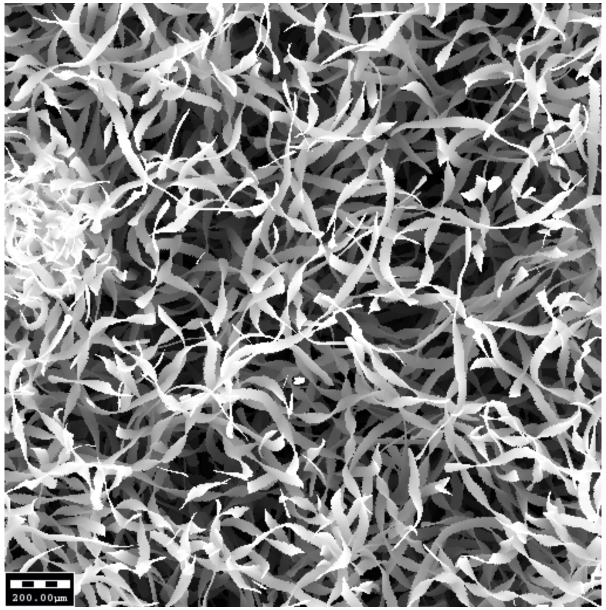
Curled & inhomogeneous nonwoven



homogeneous model

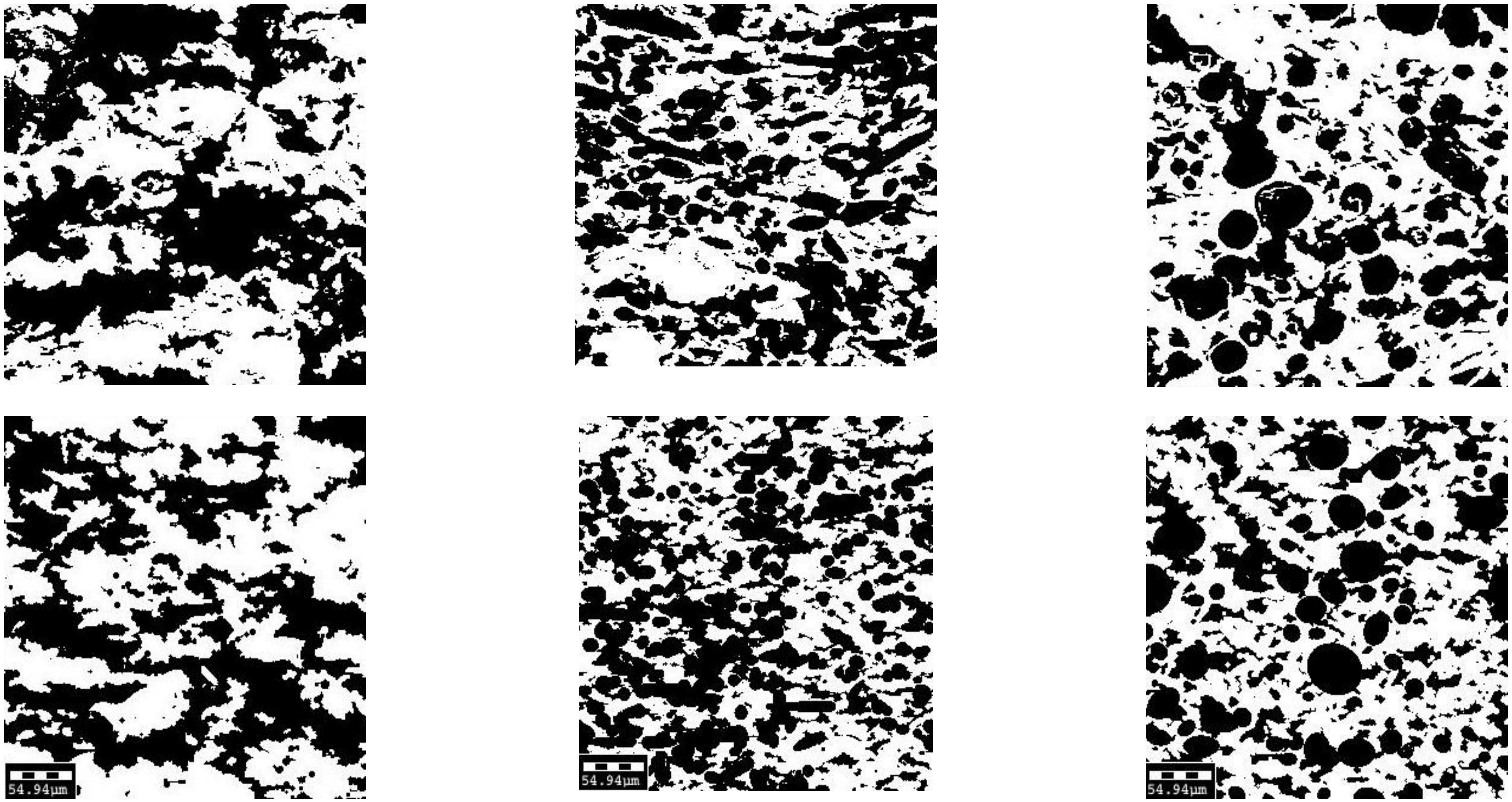


tomogram



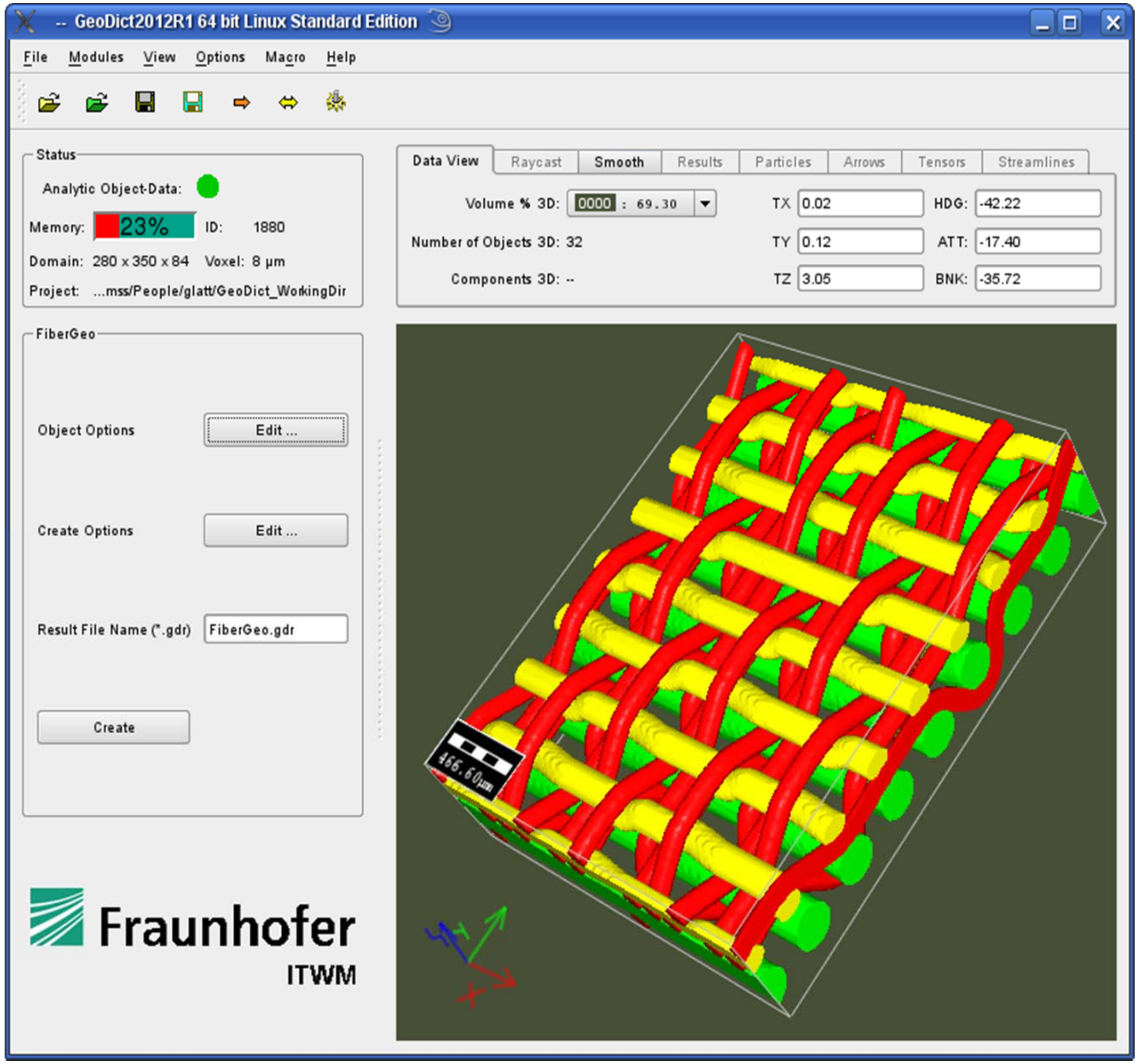
inhomogeneous model

Binarized SEM (top) and virtual sintered ceramics (bottom)

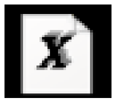


Virtual woven: multiple weft layers

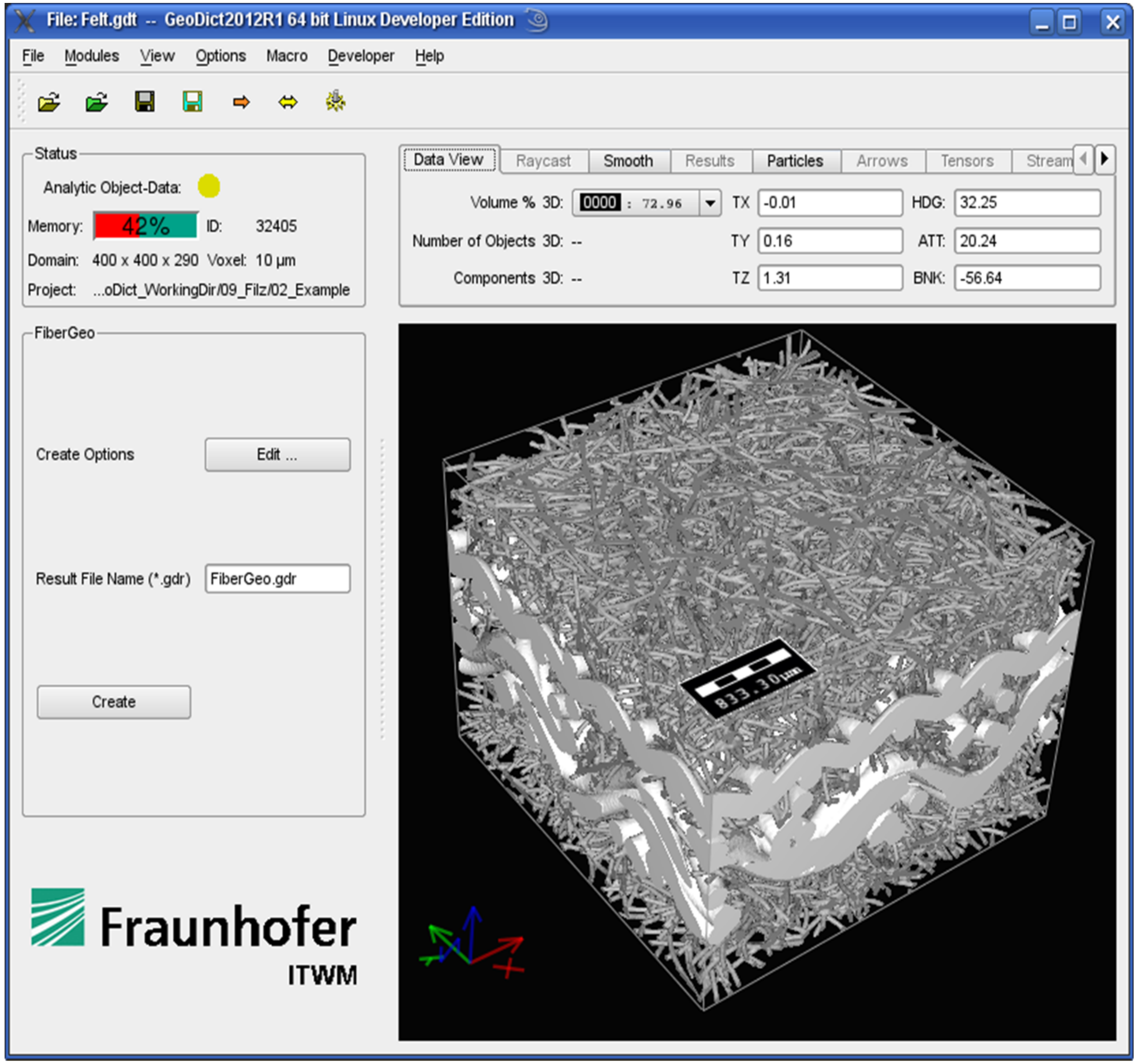
weave.gmc



Virtual felt: woven, nonwoven & needling



felt.gmc



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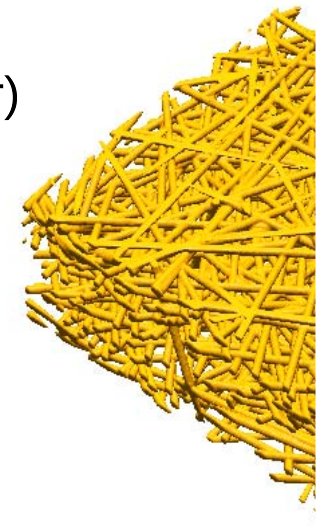
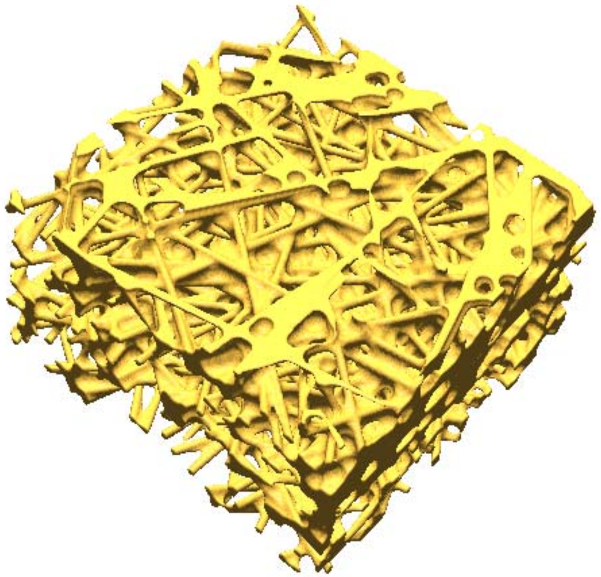
Gas Diffusion Layer Model

Created with a stochastic process

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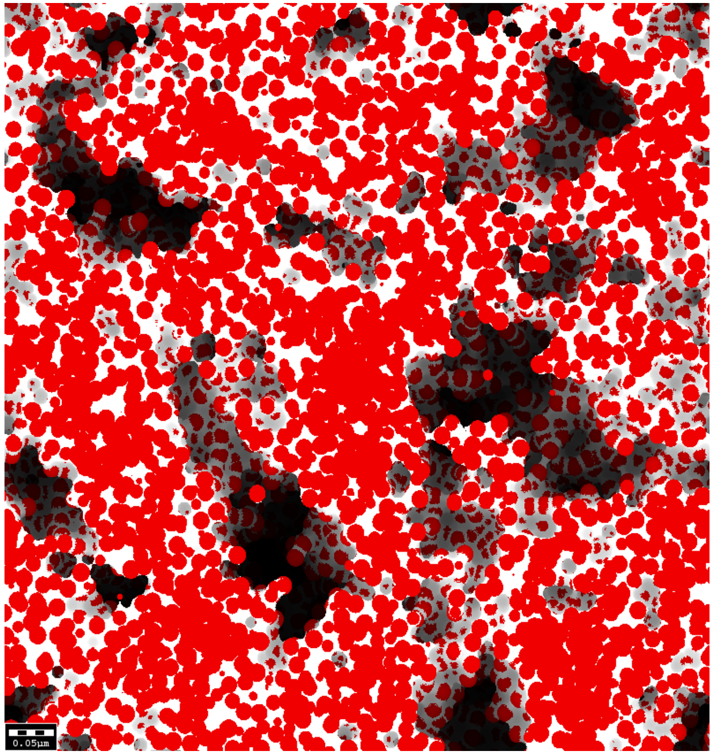
3D Models: Catalyst Layer (CL)

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)

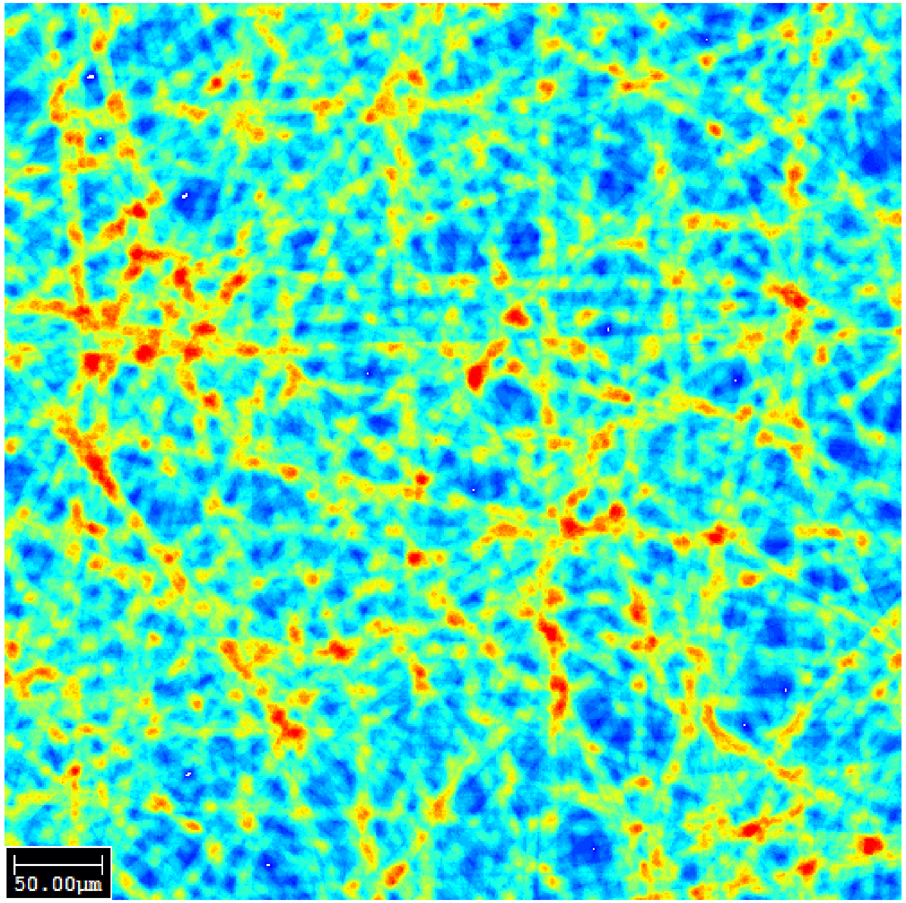
Pore & Solids analysis (Porosimetry, bubble point, cloudiness,…)

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.

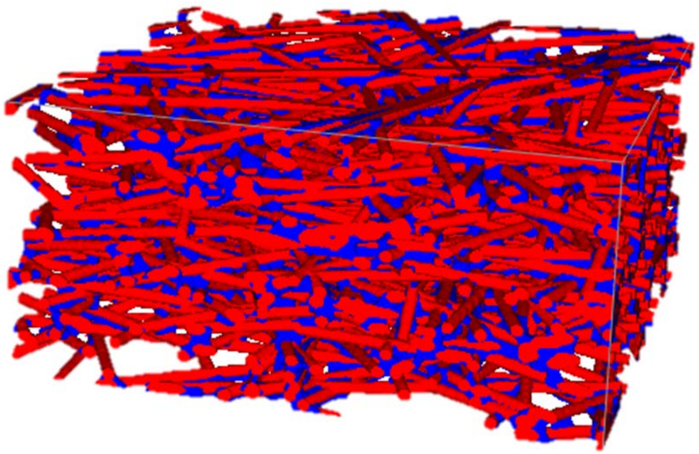
Compression

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

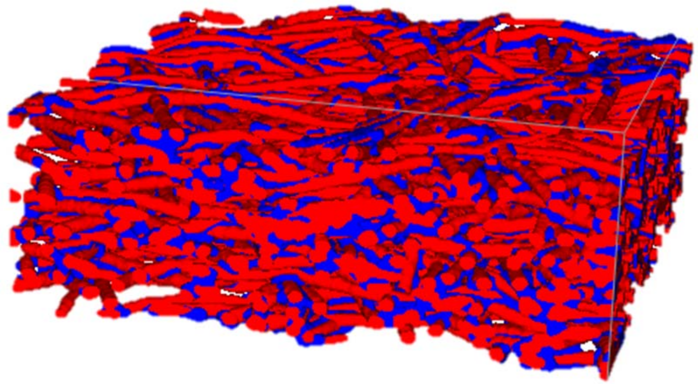
Current development together with Fraunhofer

FeelMath
Fraunhofer
ITWM

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



10 min on Laptop
13.5 mio grid points



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See talk by V. Schulz, Thursday 17:55

Filtration Simulation: Pressure drop and Filter Efficiency

Basic idea:

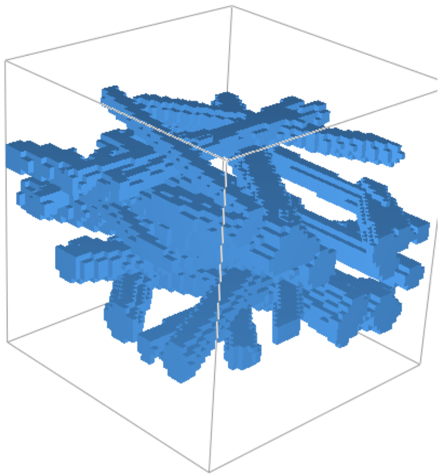
1. Filter model
2. Determine flow field (pressure drop)
3. Track particles (filtered or not?)

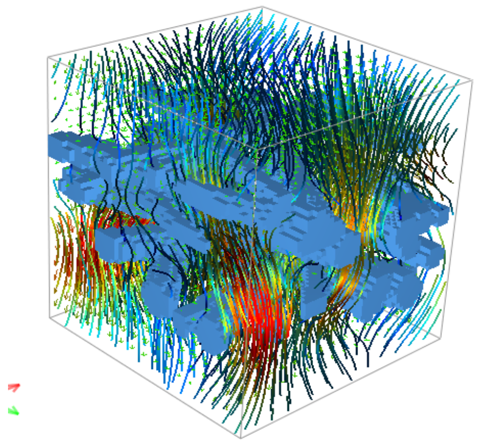
Randomness:

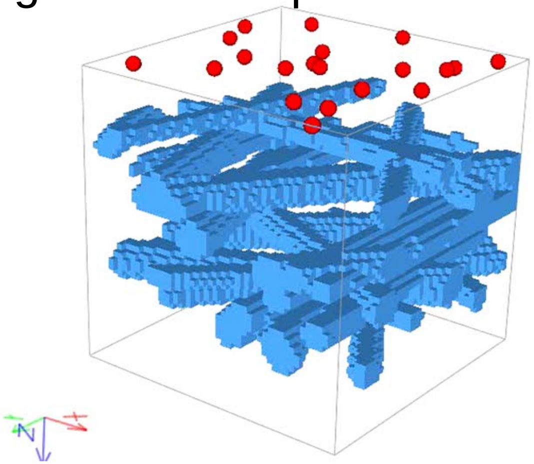
- Starting positions
- Brownian motion

Result:

- Percentage of filtered particles







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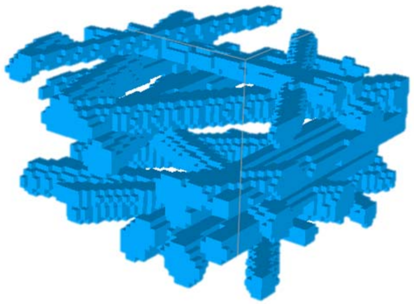
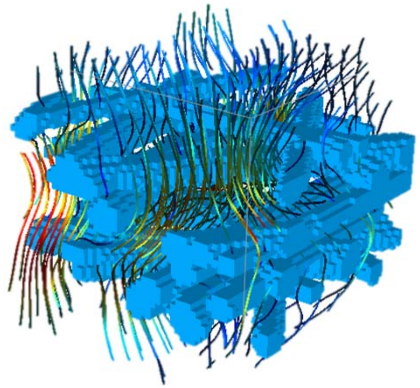
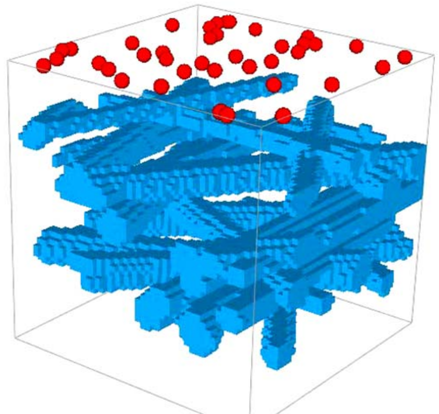
Filtration Simulation: Filter Life Time



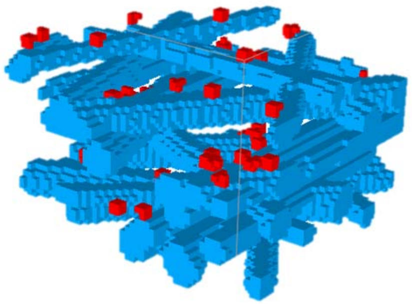
1. Filter Model



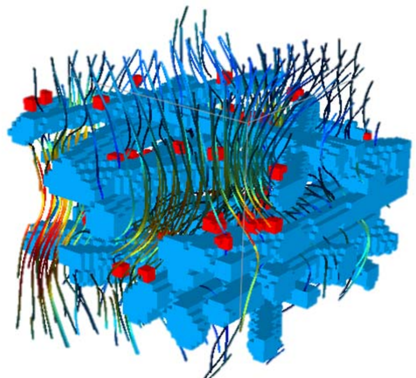
2. Flow Field



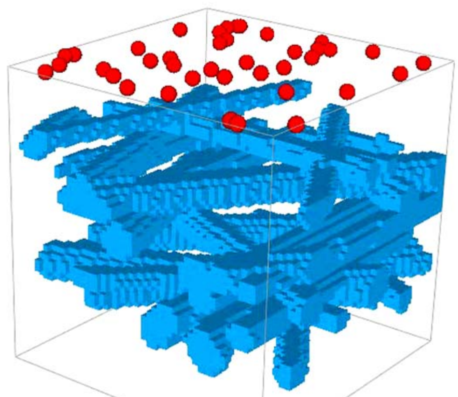
3. Track Particles



4. Deposit Particles



5. Flow Field



6. Repeat ...

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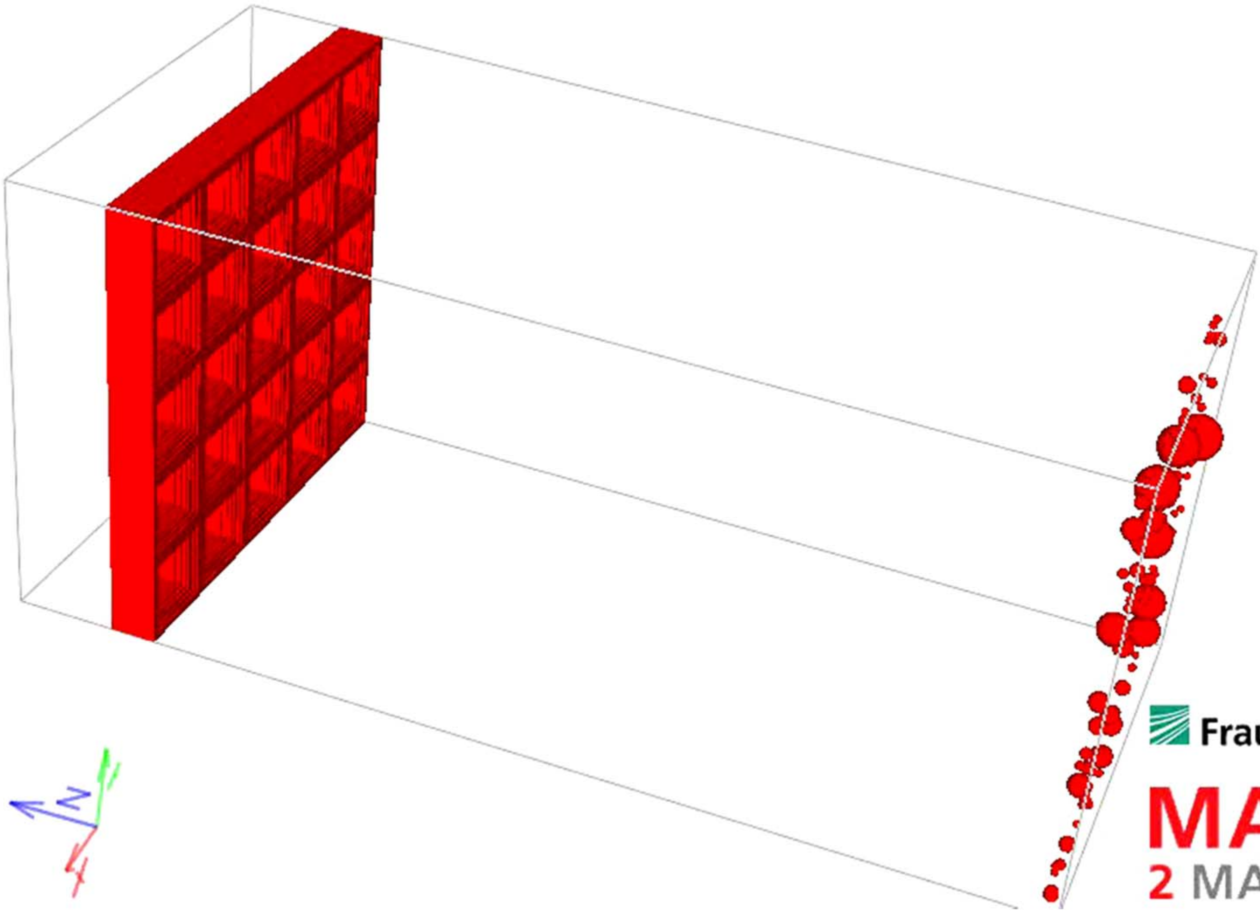
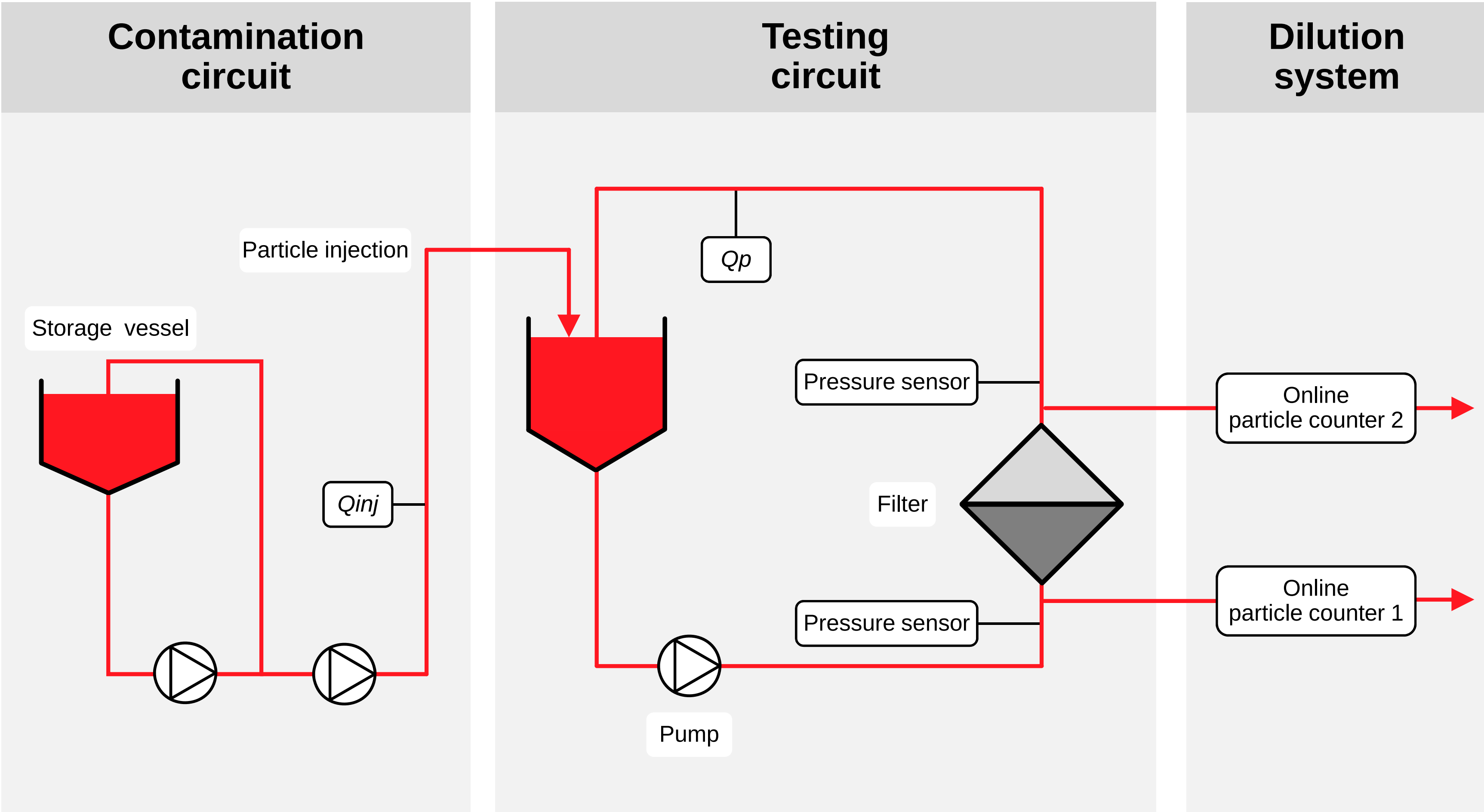
Sieving resolved particles

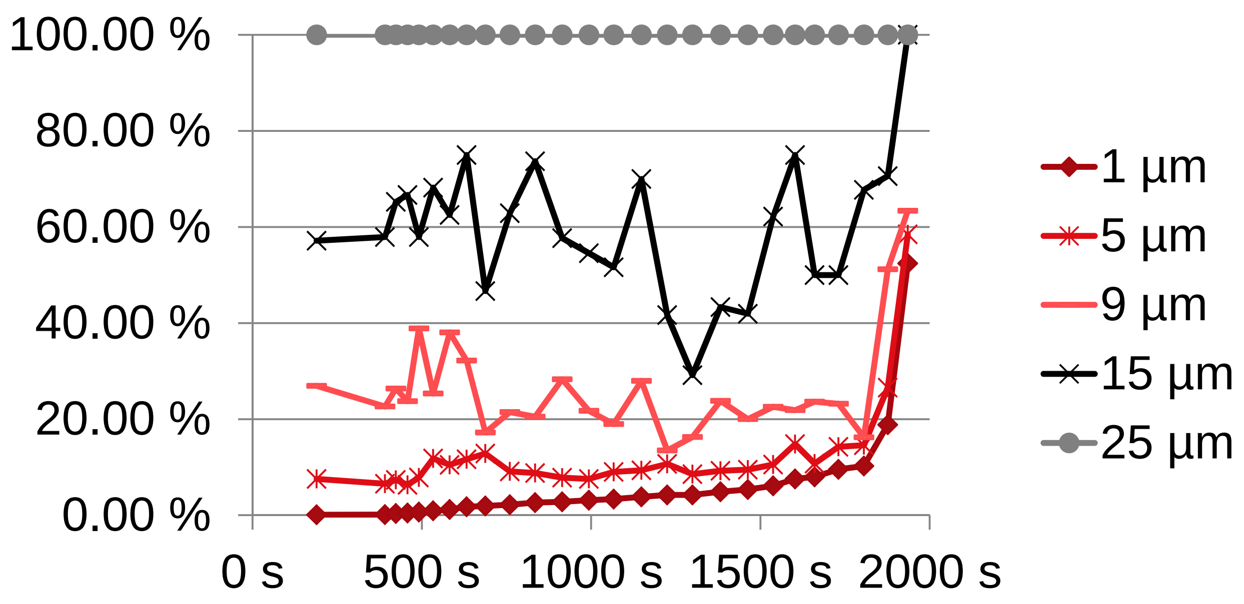


Cake with higher density & Lower permeability

The Multipass Test (ISO 4548)

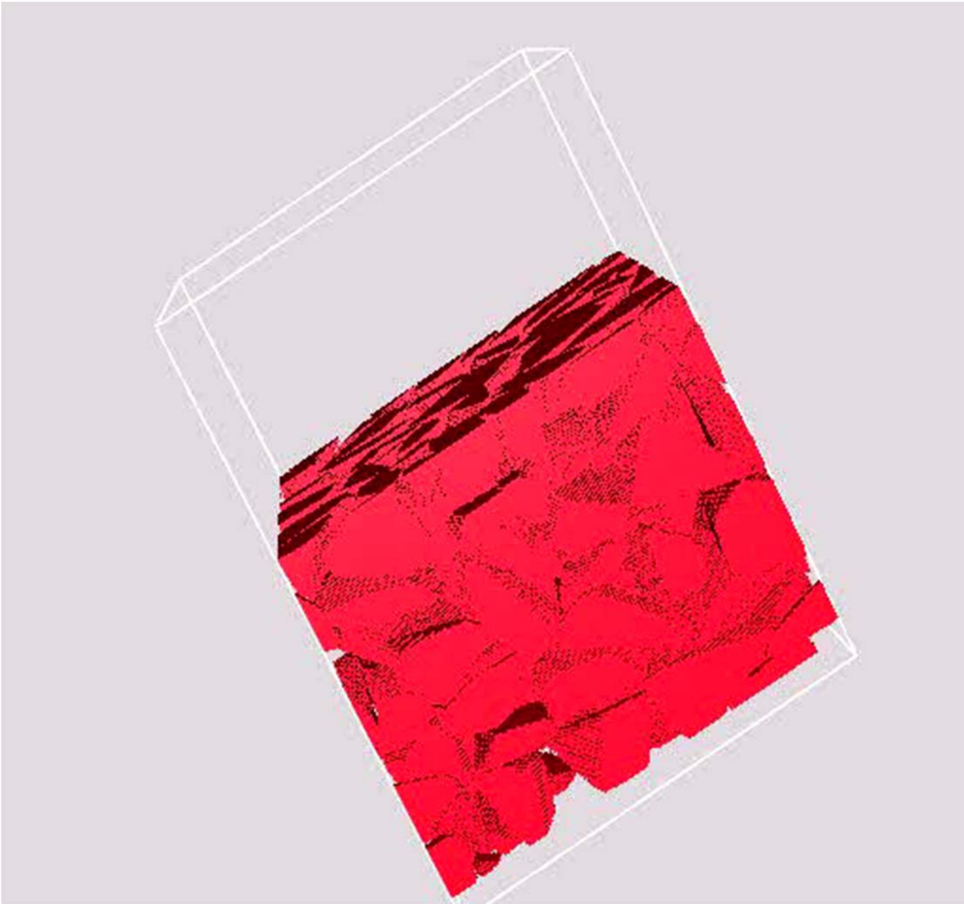


Fractional Filtration Efficiency



See poster by Hahn et al.

DPF ceramic and soot filtration



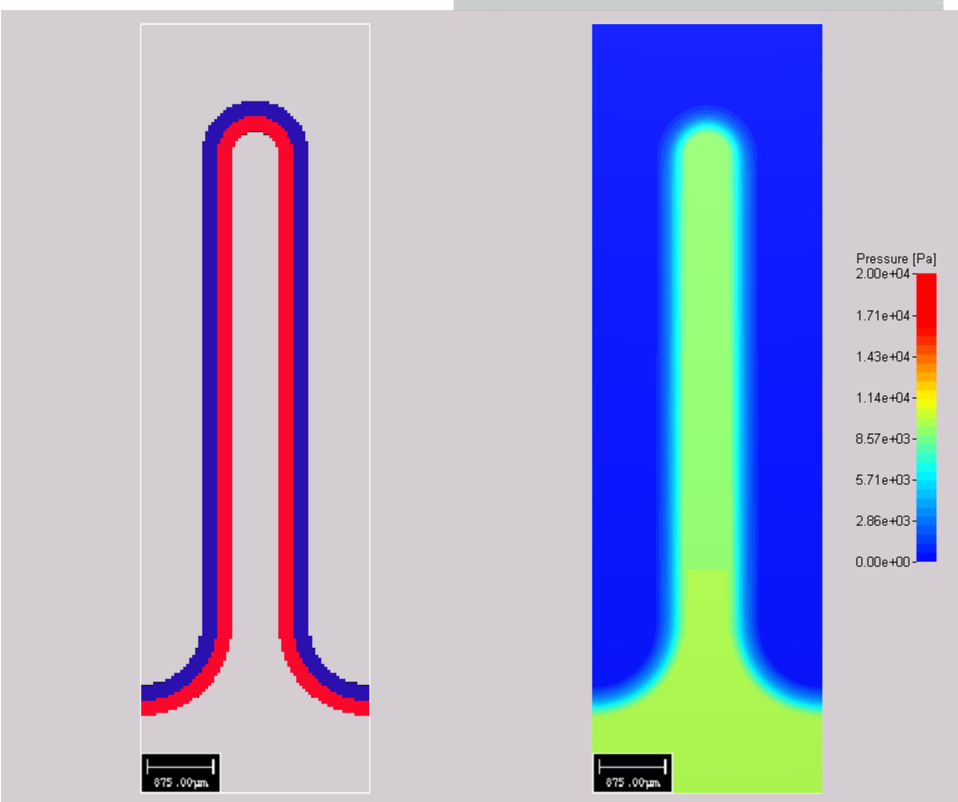
Sub-voxel soot particles form a filter cake that is modeled as porous media with locally varying permeability.

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

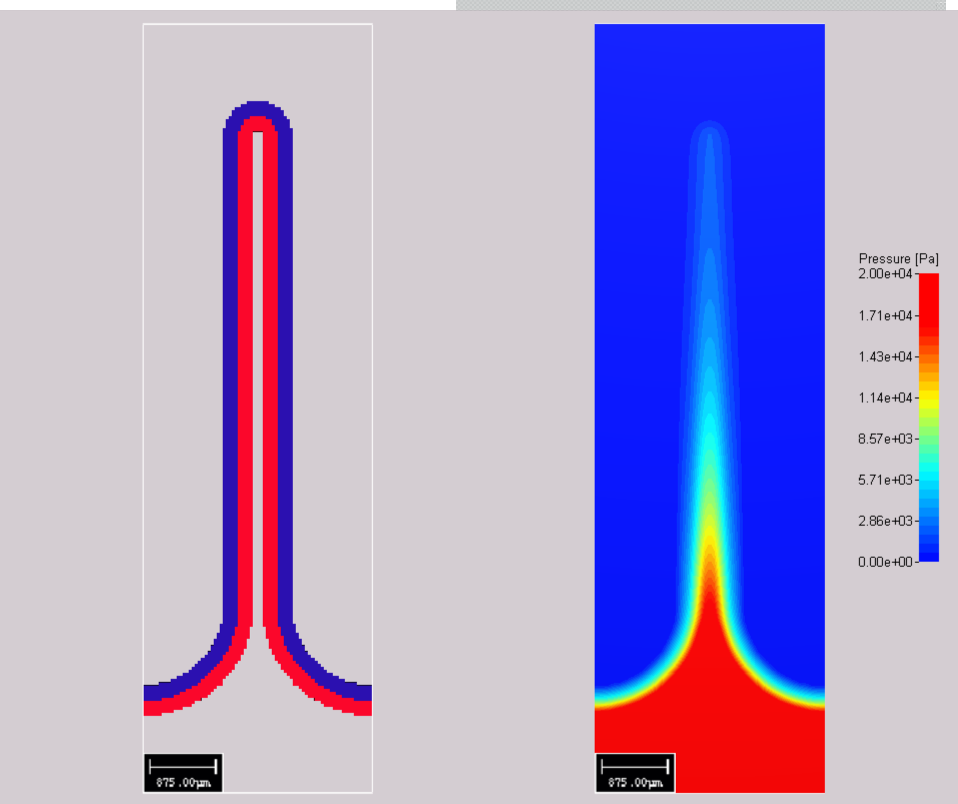
A new ceramic was designed based on simulations, a joint ***patent*** with Fraunhofer IKTS is on its way.

Pressure drop from media & capillary

Pressure at 0.01 m/s



Pressure at 0.01 m/s



Wide outflow channel looses 1 bar over filter media

Narrow outflow channel looses 2 bars over filter media and channel

The optimized filter element …

Innovation in filtration

Focus on user benefits

ARGO-HYTOS sets the standard with the introduction of EXAPOR®MAX 2

Higher machine availability, longer service intervals and lower operating costs. These were the development goals for the new generation of filter elements.

With the introduction of **EXAPOR®MAX 2**, ARGO-HYTOS is opening a new chapter in filtration for hydraulic and lubrication systems.

The structure of the specially developed 3-layer filter material was designed for optimum performance, using glass and polyester fibers of different finenesses combined with an improved hybrid support fabric (patent pending) made of stainless steel and polyester. This sets the standard for:

- **Pressure loss**
- **Dirt holding capacity**
- **Flow fatigue stability**

The plastic sleeve used on the **EXAPOR®MAX 2** for the fi… the following benefits:

- **Custom label**
- **Protection from damage**
- **Improvement of flow fatigue stability**

For the user, these improvements bring:

- **Extended service intervals**
- **Higher operational reliability**
- **Improved oil cleanliness**
- **Increased performance**
- **Positive element identification**
- **Reduced operating and maintenance costs**

Extended service intervals

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

The new performance-oriented structure of the filter material makes a substantial contribution to improving dirt holding capacity, reducing pressure losses and improving the differential pressure stability. The improved hybrid support fabric (patent pending) dissipates electrostatic charge completely, gives the best possible flexural strength while reducing pressure losses. The plastic sleeve shrunk onto the filter bellows ensures that it tightly fits the edges of the hole, which has a positive effect on flow fatigue stability. These improvements make a substantial contribution to increasing the life of the filter elements.

Higher operational reliability

When used on existing machinery with fixed service intervals, **EXAPOR®MAX 2** filter elements bring greater operational reliability, minimizing the risk of sudden machine downtimes as well as reducing downtime caused by time-consuming and expensive maintenance work.

…ive effect on both the life of components and that of the hydraulic … the new generation of filter elements the filter fineness has been … m(c) previously. The **EXAPOR®MAX 2** filter elements are available … 16 µm(c).

higher. The substantial reduction in pressure losses allied to an improved dirt holding capacity leads to an increase in power density, so that, depending on the application, smaller filters could be used.

Positive identification of elements

The plastic sleeve used on the **EXAPOR®MAX 2** filter elements can be printed as required. This substantially improves positive identification and is an important feature for building up and securing a strategic spare part business.

Reduced operating and maintenance costs

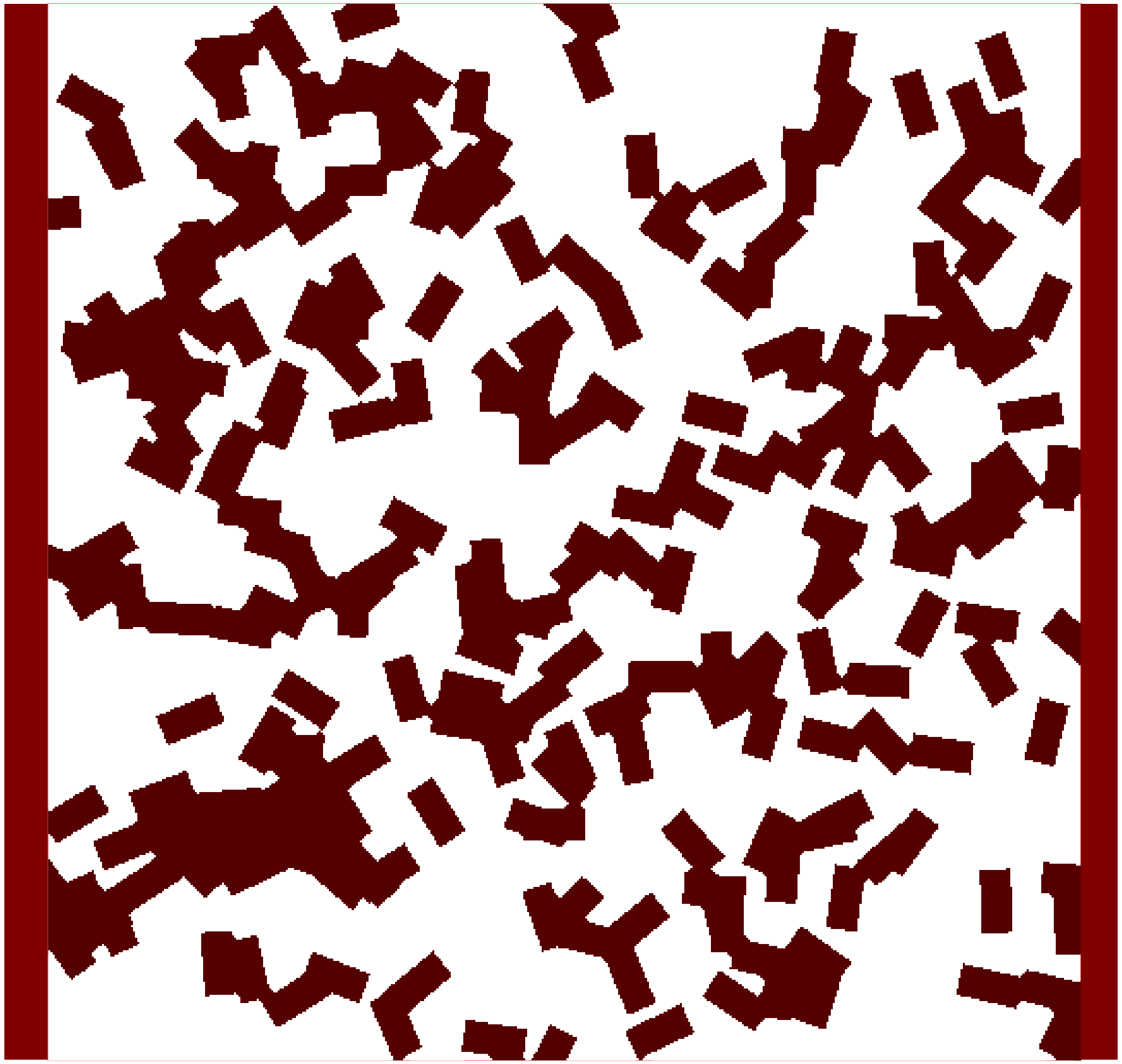
These innovations work together to reduce operating and maintenance costs and bring about an improvement in the productivity and economy of machinery and plant.

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

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

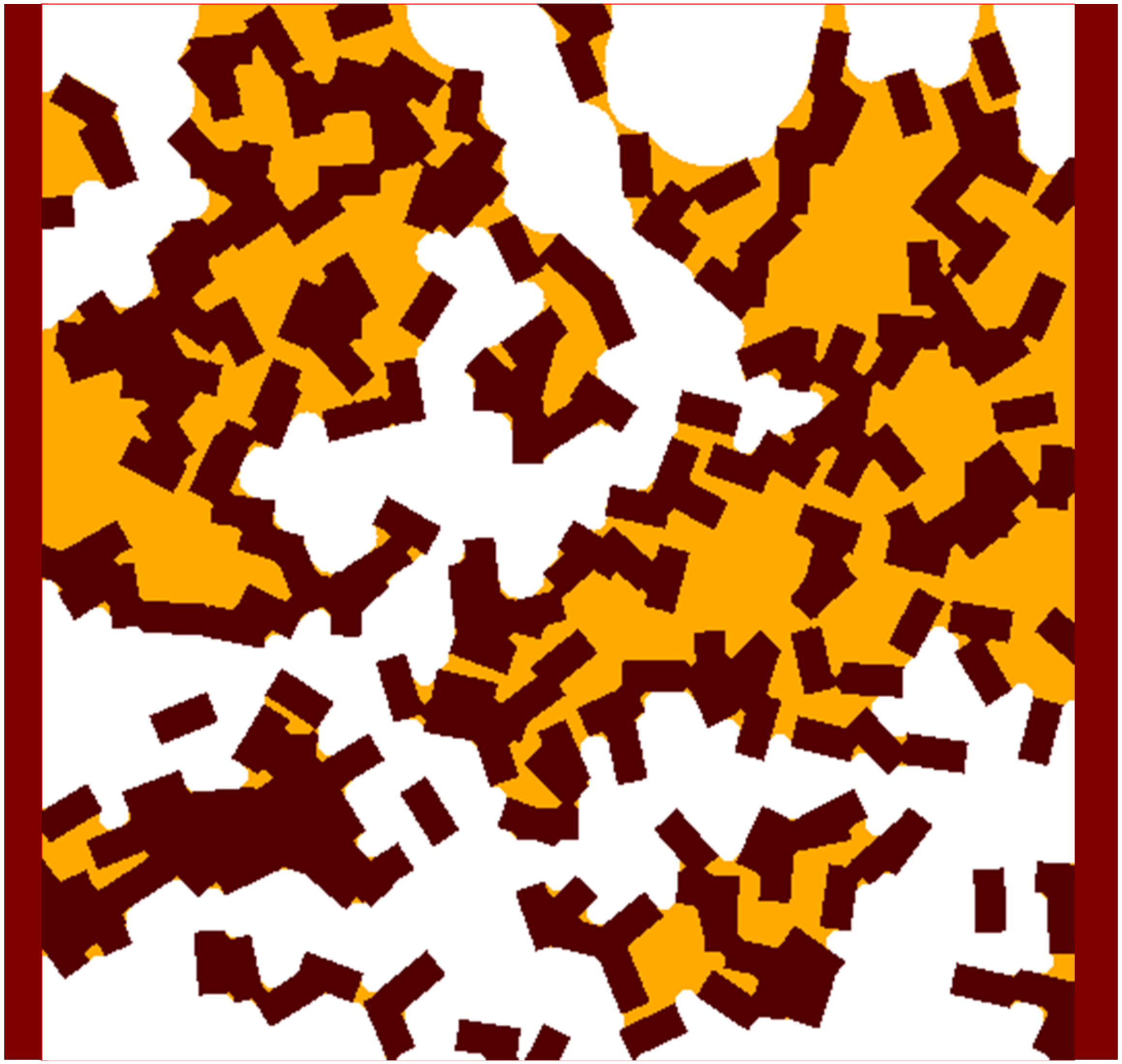


Wetting phase (water) reservoir

Drainage (+)

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

Non-wetting phase (air) reservoir

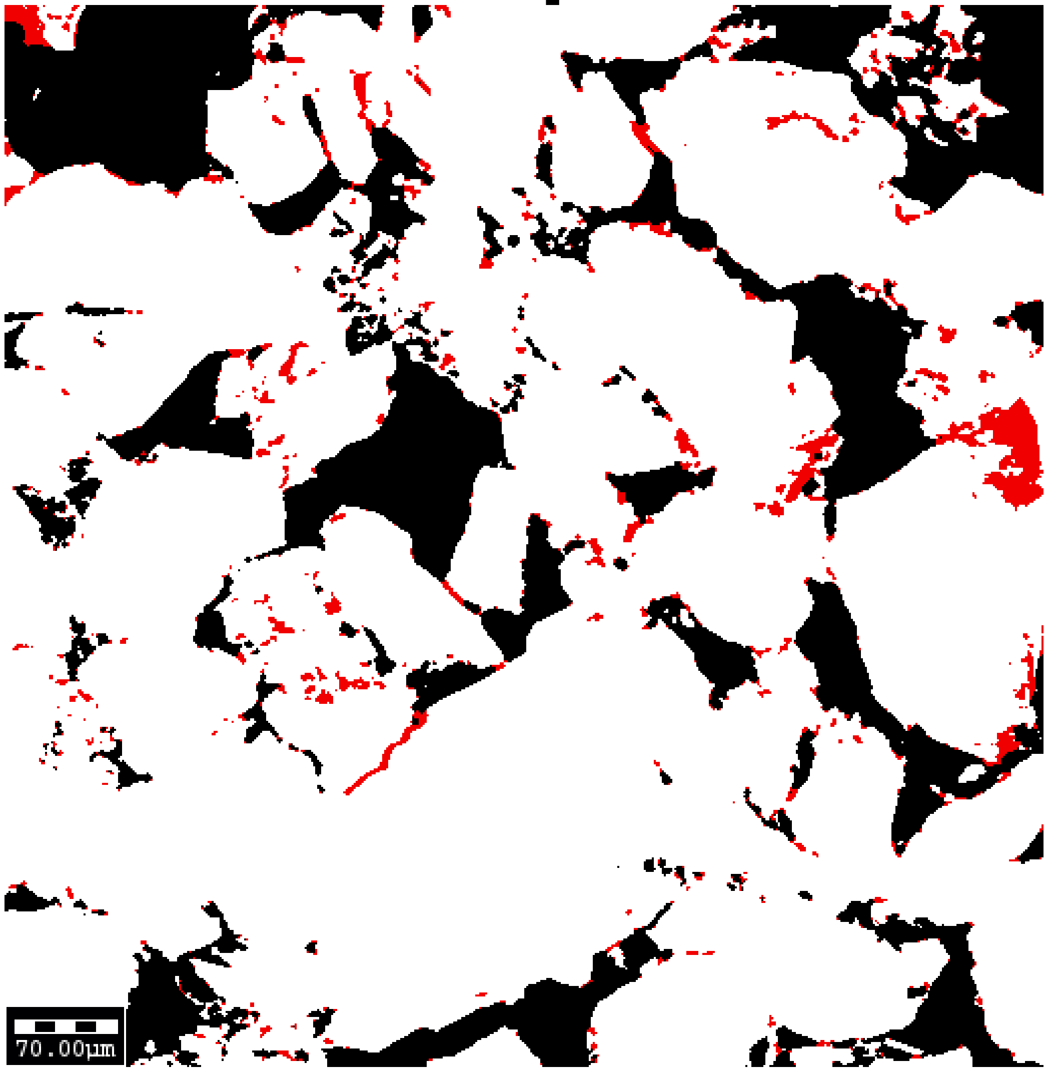


Wetting phase (water) reservoir

Drainage - Sandstone Sample

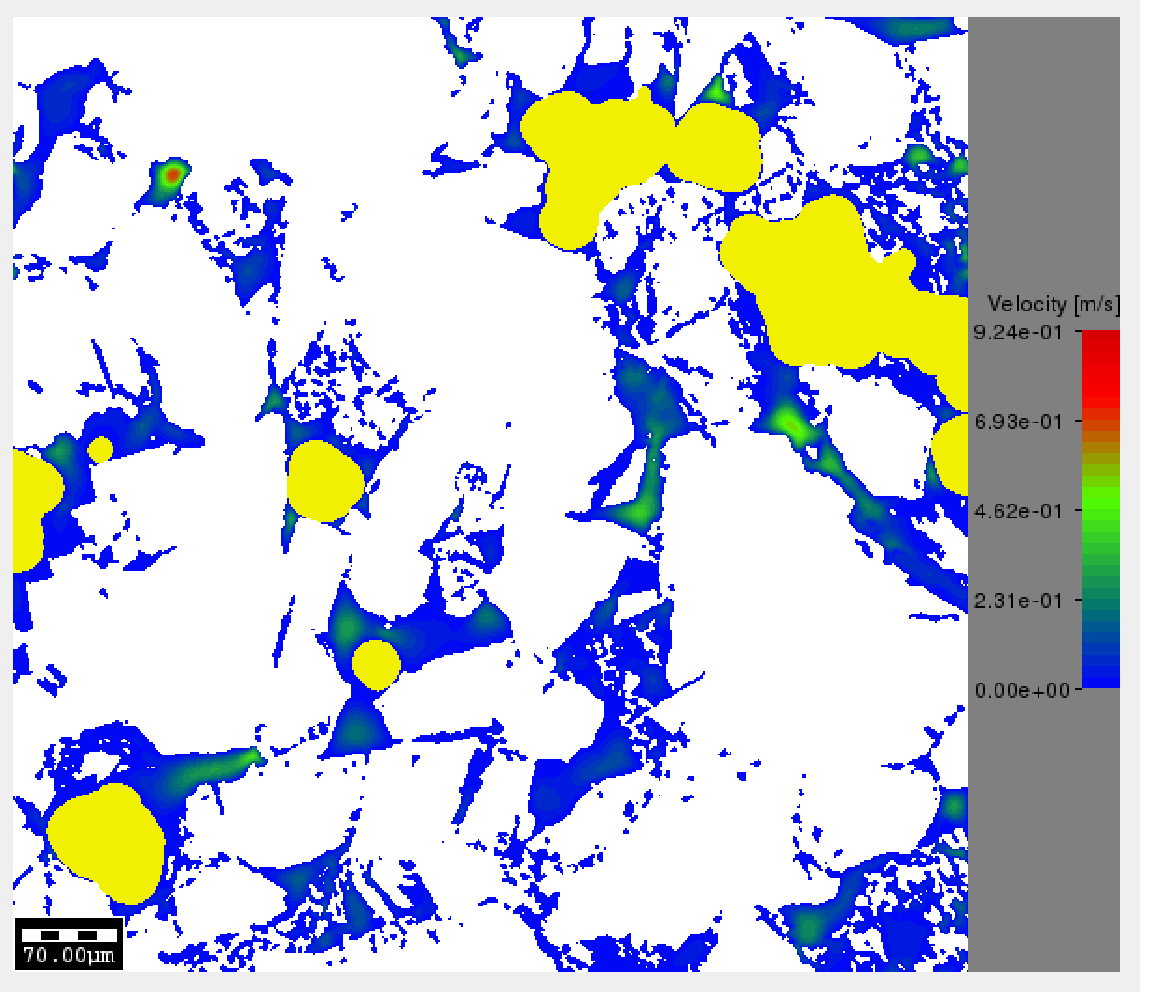
- Slice of the 3D result
- Residual water: 8.6 %

- black: air
- red: residual water
- white: matrix material



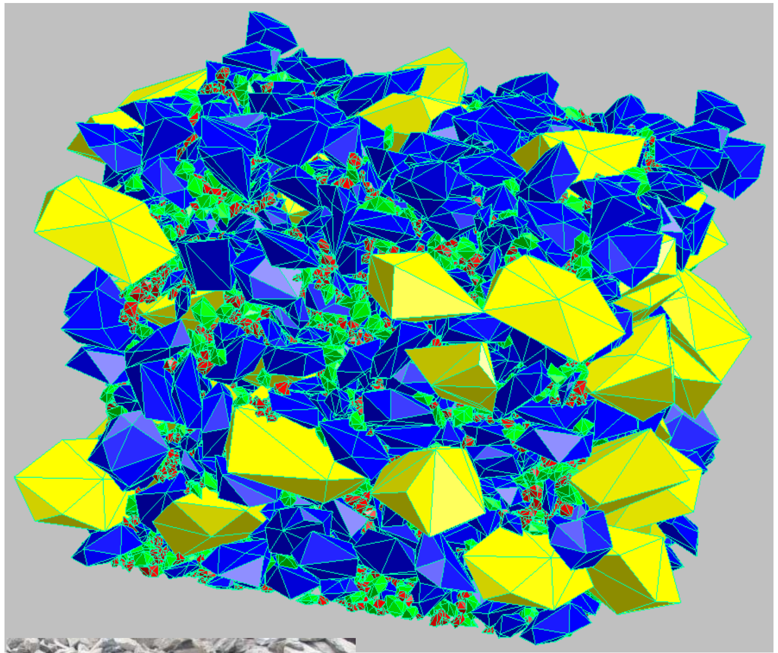
Relative Permeability (Sandstone)

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



See poster by L. Cheng et al.

Rock models for Fluent

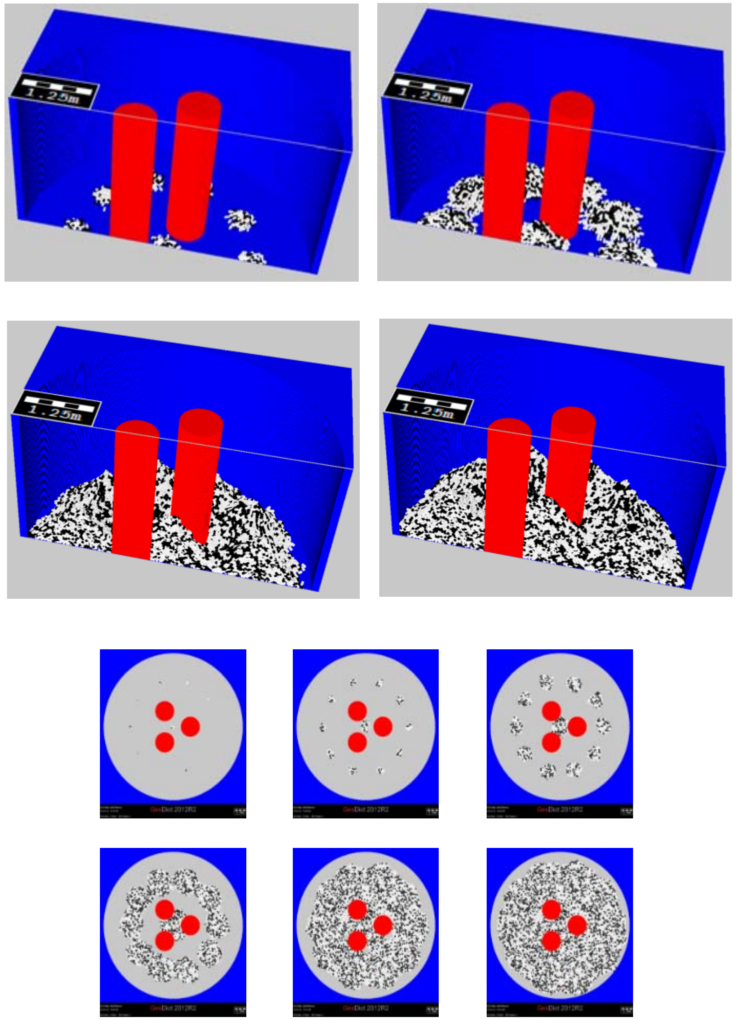


Structure as Parasolid for further processing.

- 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.

MATH 2 MARKET

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

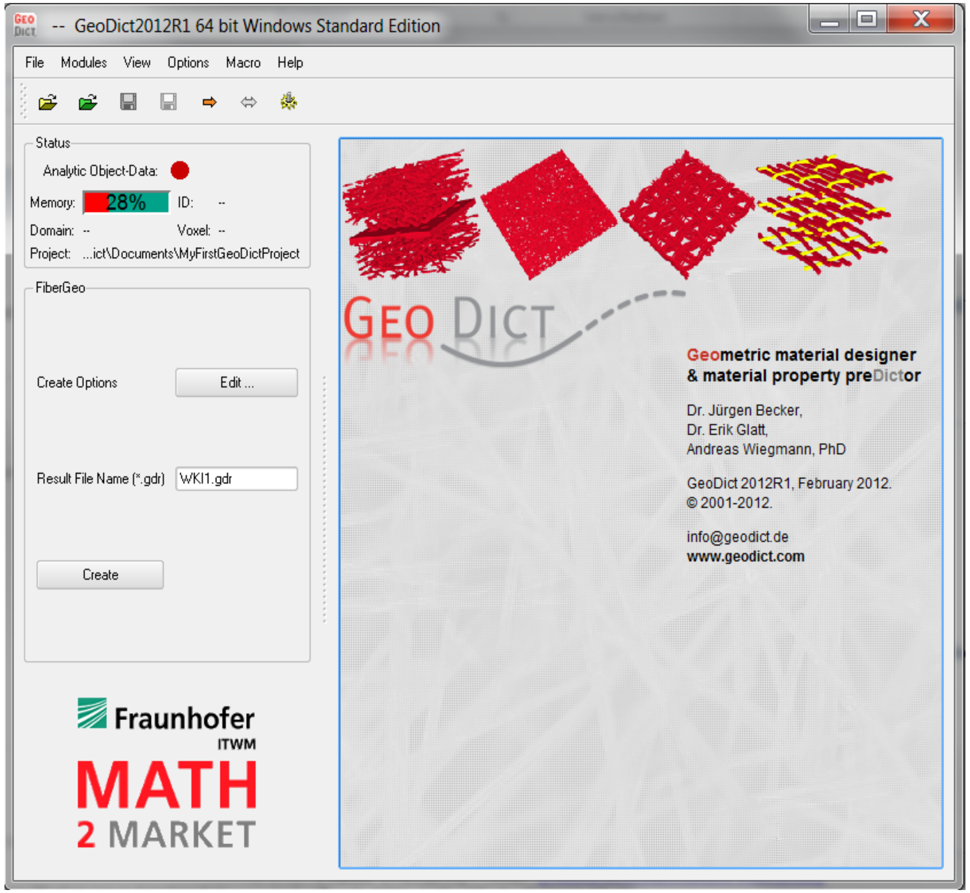
- ***Every*** operation can be “recorded” and “played”
- Every operation consists of a command name and a list of parameters
- There exist variables and loops
- The variables enter in the parameter lists
- The loops provide value lists to enter into the parameters
- They can be used to provide input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

MATH
2 MARKET

GeoDict Modules – 2012R2 edition

FiberGeo , PaperGeo, SinterGeo, WeaveGeo, GridGeo, PackGeo, PleatGeo: structure generators

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…

GeoDict

The Virtual Material Laboratory

www.geodict.com

MATH 2 MARKET