The Virtual Material Laboratory

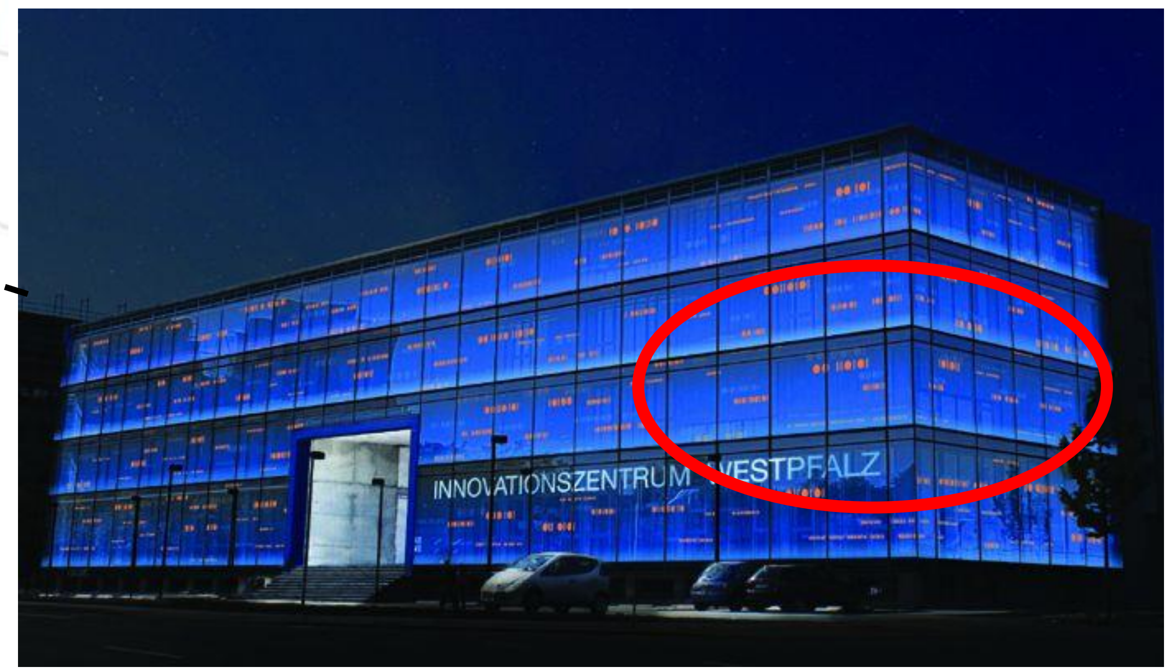
Dr. Erik Glatt

Math2Market GmbH

11th European Congress of Stereology and Image Analysis 2013

Where is M2M located, who are we?

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



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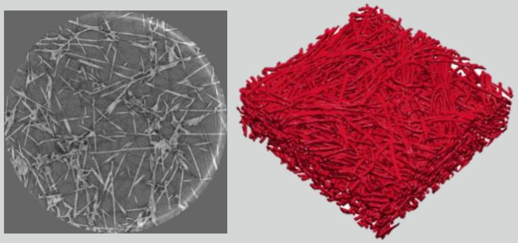
Outline

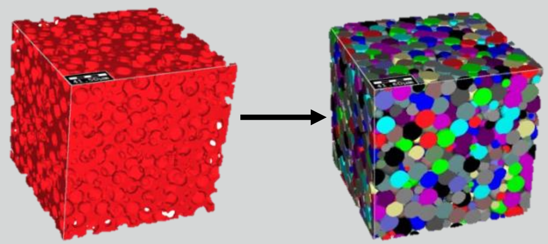
1. The Virtual Material Lab GeoDict
2. Fiberglass by Injection Molding
3. Digital Rock Physics
4. Summary and Conclusion

1. The Virtual Material Lab GeoDict

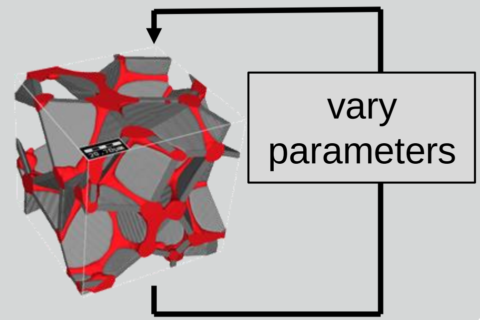
import materials



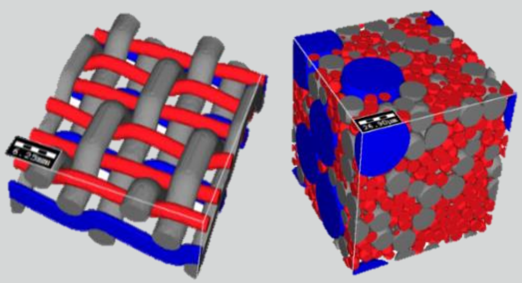
characterize materials



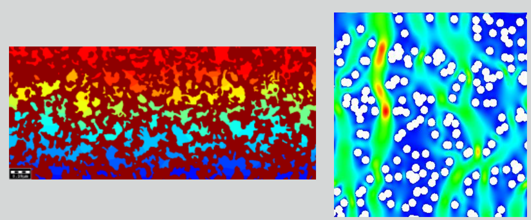
optimize materials



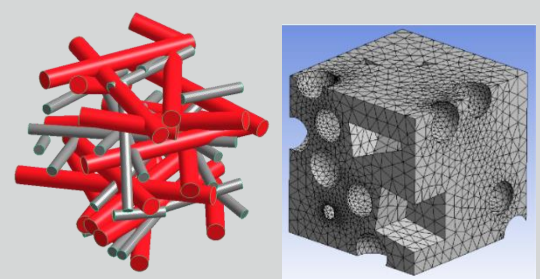
model materials



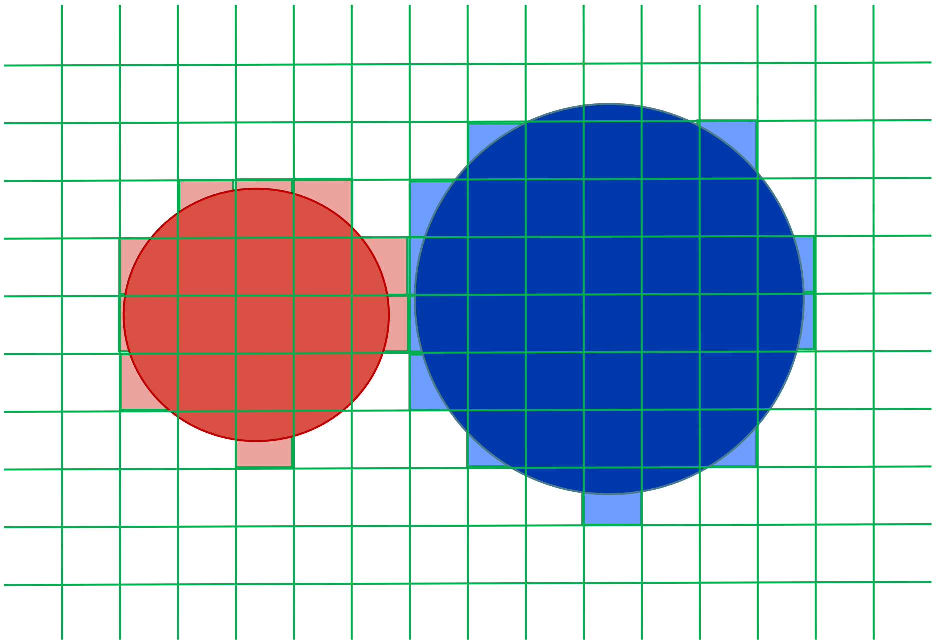
characterize properties



export materials



Simulations performed on 3d structures composed of little cubes (voxels)



Advantages: Straight forward

- automatic grid generation for computed tomography
- virtual structure generation
- solver implementation
- parallel implementation
- memory efficient

Disadvantages: resolving features

- requires many grid cells

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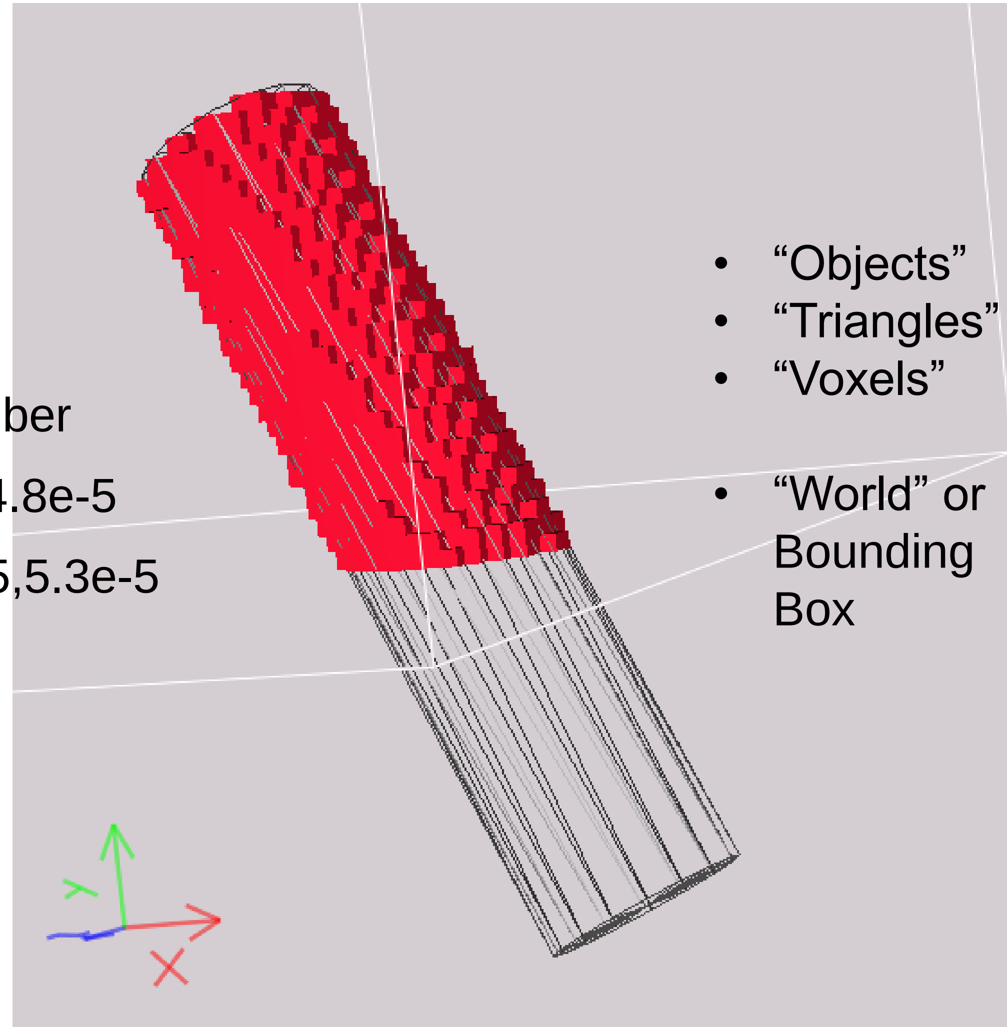
Analytic, surface and volume representation

<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

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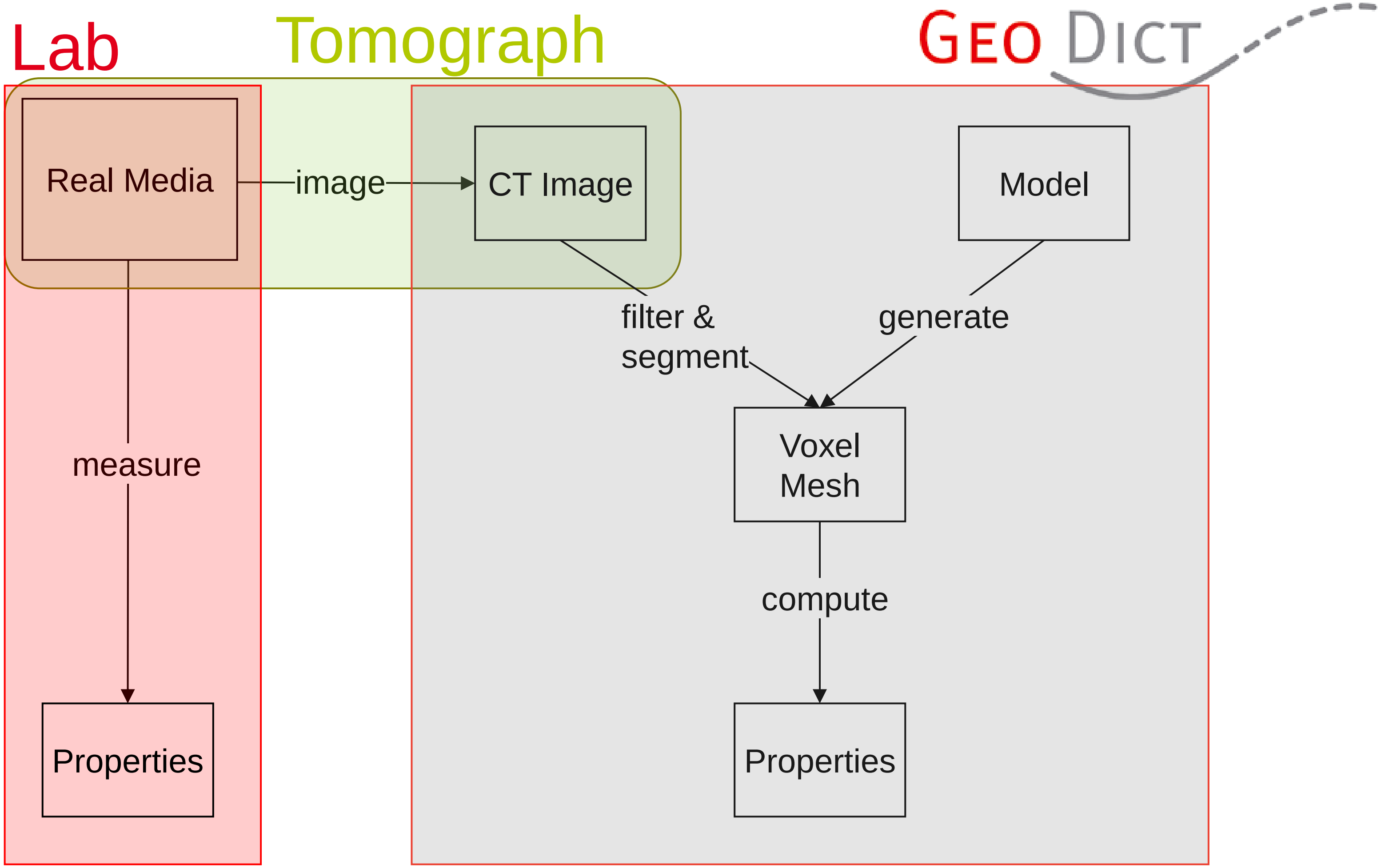
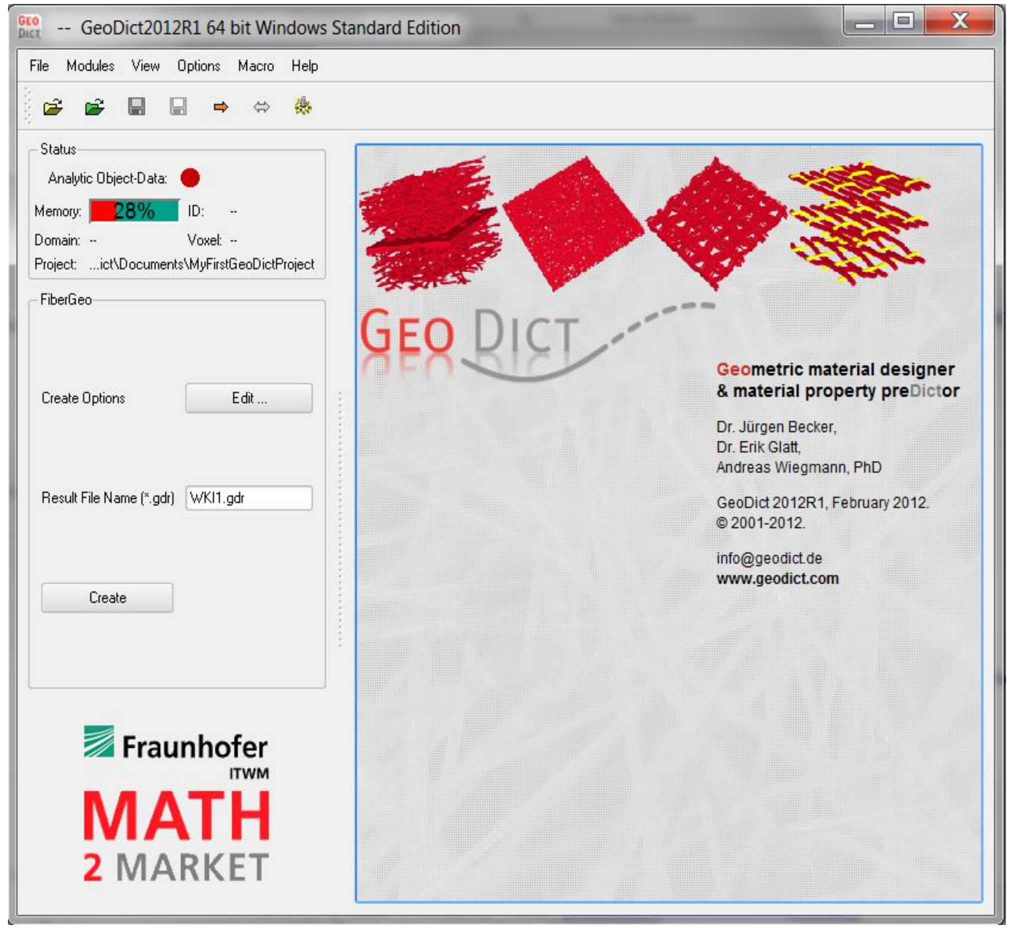
Material Characterization & Engineering



GeoDict Modules

FiberGeo, PaperGeo, SinterGeo, WeaveGeo, FoamGeo, 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)



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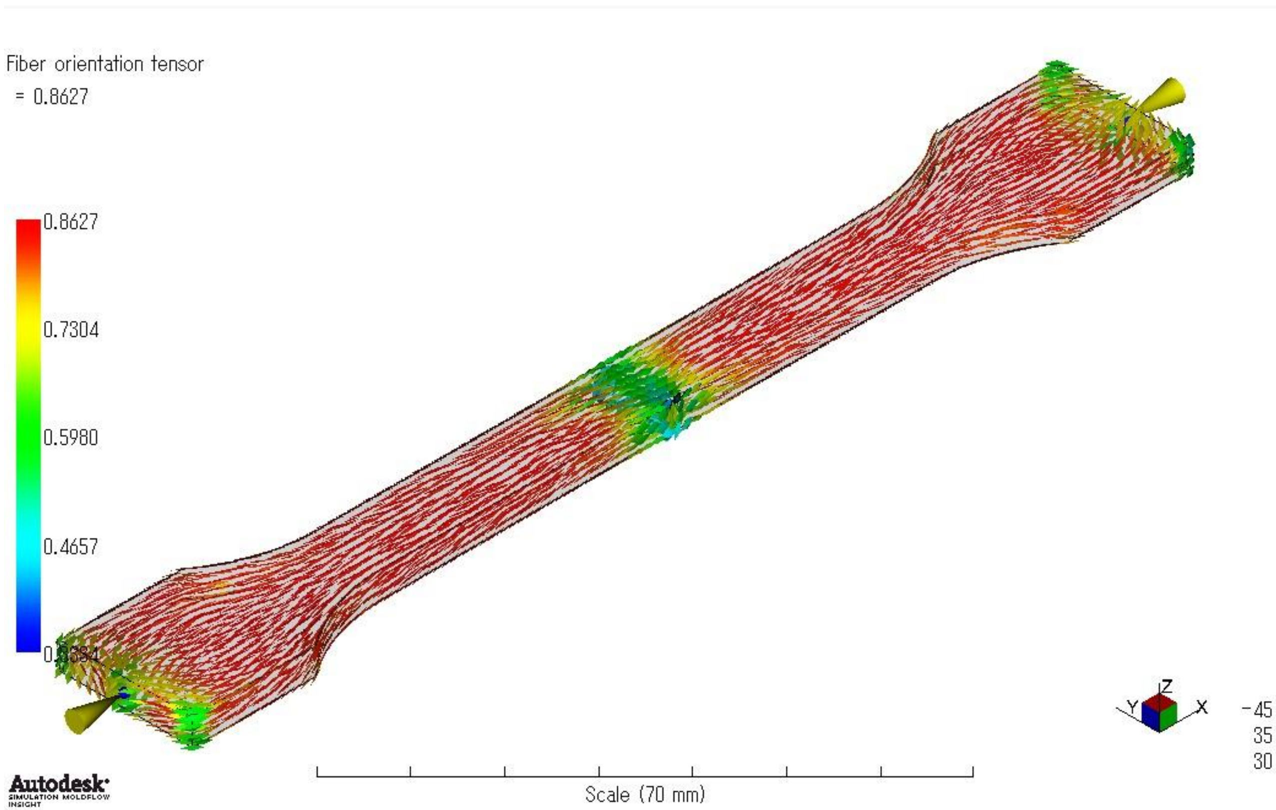
2. Fiberglass by Injection Molding

how does the microstructure influence the elastic properties:
glass fibers in epoxy
fiber diameter 8 µm, length 300 µm, weight 25%, Moldflow orientation simulation



Effective Elastic Properties

Hooke's Law:

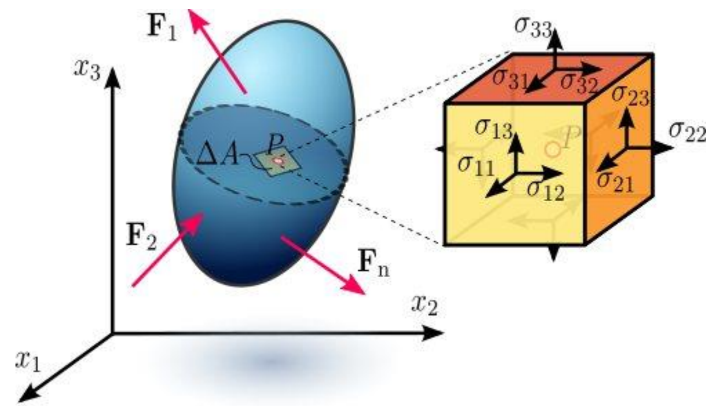
$$\sigma_{ij} = \sum_{r,s=1}^{3} c_{ijrs}\varepsilon_{rs} \; ; \quad i,j \in \{1,2,3\}$$

σ_{ij} : *stress tensor*

c_{ijrs} : *elasticity tensor*

ε_{rs} : *strain tensor*

Cauchy stress tensor:



Strain tensor:

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

u : *displacement*

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Effective Elasticity Tensor

- material parameters for microstructure
- solve six load cases on microstructure => effective elasticity tensor

$$c_{isotrop} = \begin{pmatrix} c_{xxxx} & c_{xxyy} & c_{xxyy} & 0 & 0 & 0 \\ c_{xxyy} & c_{xxxx} & c_{xxyy} & 0 & 0 & 0 \\ c_{xxyy} & c_{xxyy} & c_{xxxx} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{c_{xxxx}-c_{xxyy}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{c_{xxxx}-c_{xxyy}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{c_{xxxx}-c_{xxyy}}{2} \end{pmatrix}$$

Lame parameters:

$$\mu = (c_{xxxx} - c_{xxyy})/2$$
$$\lambda = c_{xxyy}$$

Young's modulus and Poisson's ration:

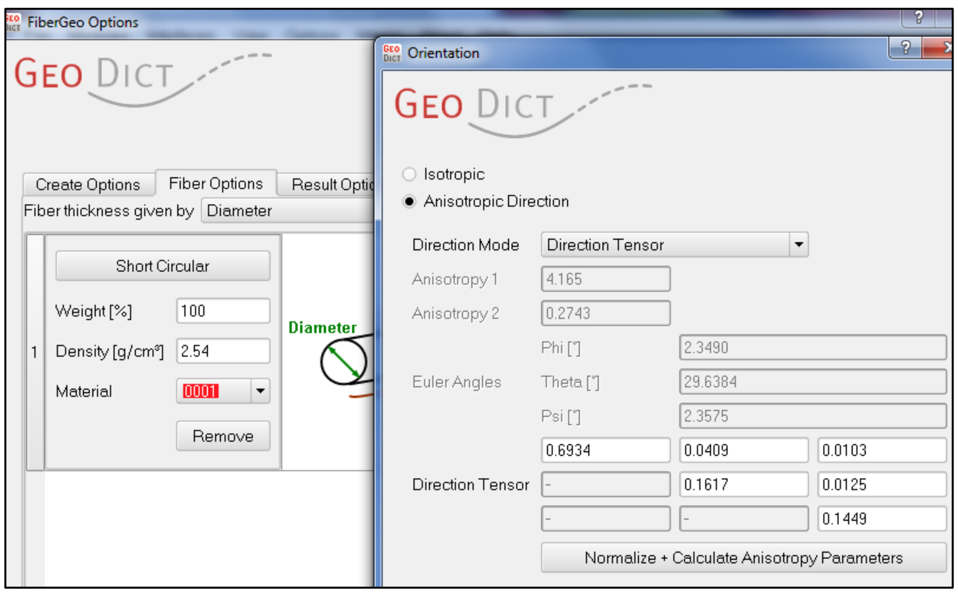
$$E = \mu(2\mu + 3\lambda)/(\mu + \lambda)$$
$$\nu = \frac{\lambda}{2}(\mu + \lambda)$$

FiberGeo: Fiberglass Microstructure

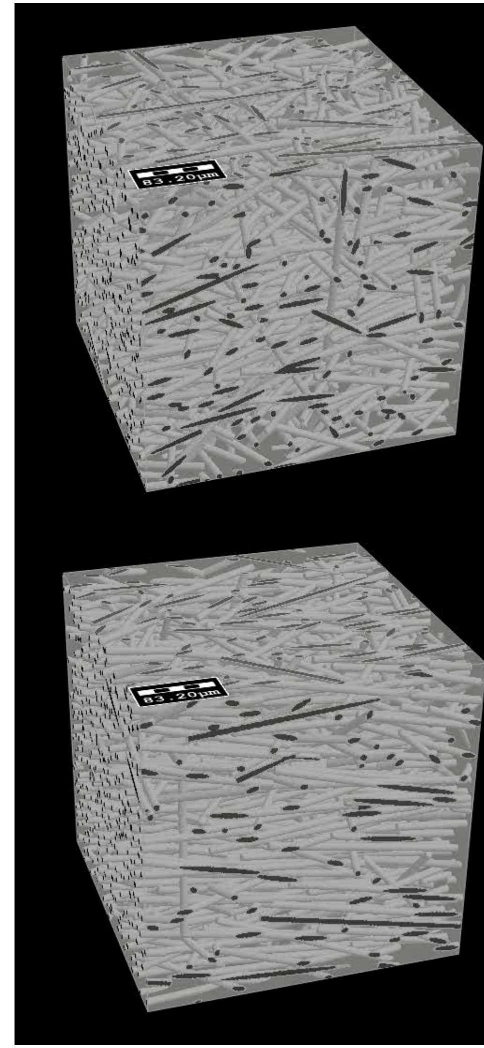

```
<ElementData ID="5423">
  <DeptValues>     6.9340e-001    1.6167e-001    1.4493e-001    4.0924e-002    1.0321e-002    1.2470e-002
</ElementData>
```

```
<ElementData ID="9330">
  <DeptValues>     8.3008e-001    7.4930e-002    9.4990e-002   -7.8231e-002   -6.5528e-002   -1.2559e-002
</ElementData>
```


enter parameters into FiberGeo



create microstructure



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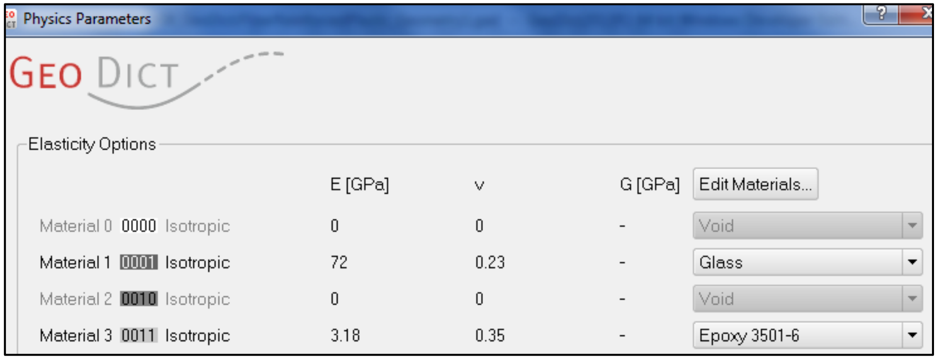
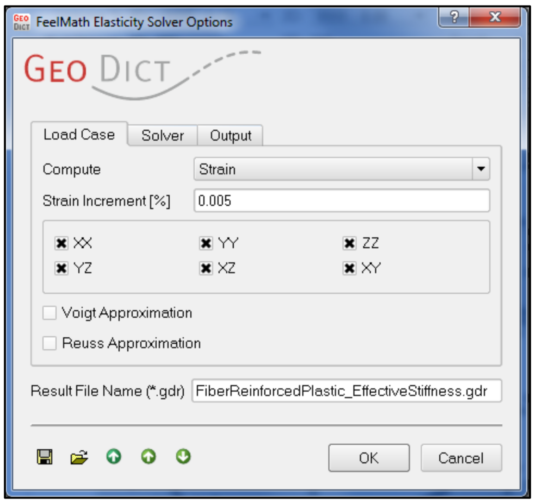
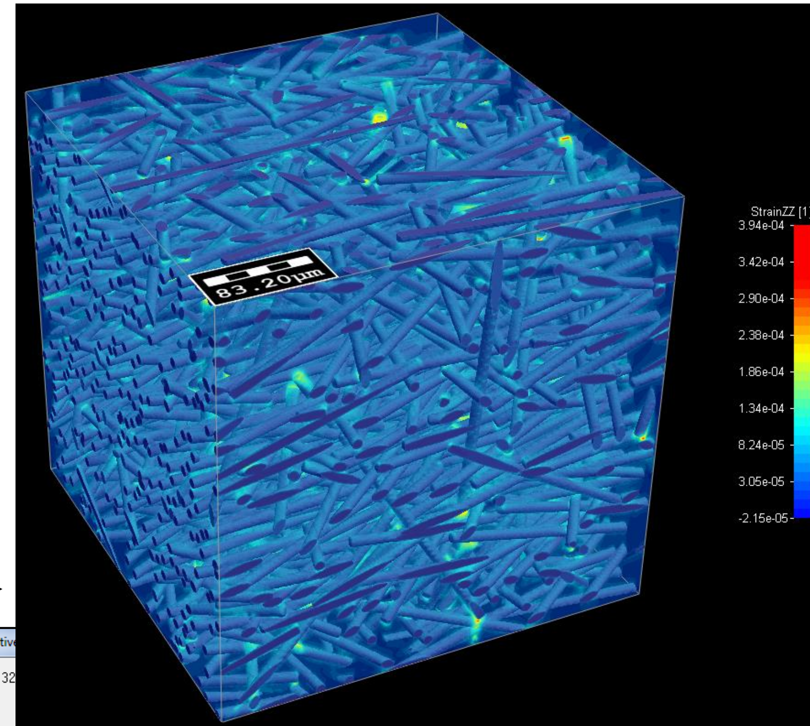
ElastoDict: Elastic Properties of Fiberglass

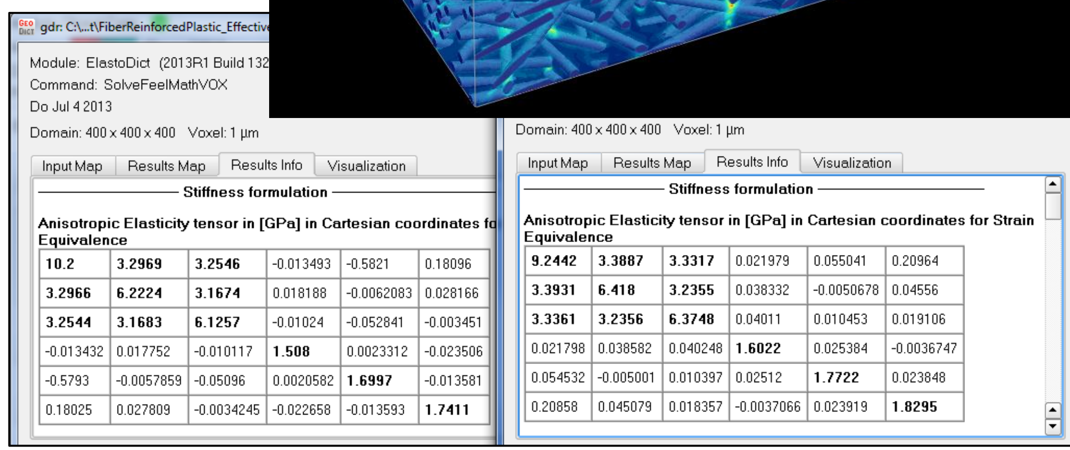




compute elastic properties

enter parameters into ElastoDict





10.2	**3.2969**	**3.2546**	-0.013493	-0.5821	0.18096
3.2966	**6.2224**	**3.1674**	0.018188	-0.0062083	0.028166
3.2544	**3.1683**	**6.1257**	-0.01024	-0.052841	-0.003451
-0.013432	0.017752	-0.010117	**1.508**	0.0023312	-0.023506
-0.5793	-0.0057859	-0.05096	0.0020582	**1.6997**	-0.013581
0.18025	0.027809	-0.0034245	-0.022658	-0.013593	**1.7411**

9.2442	**3.3887**	**3.3317**	0.021979	0.055041	0.20964
3.3931	**6.418**	**3.2355**	0.038332	-0.0050678	0.04556
3.3361	**3.2356**	**6.3748**	0.04011	0.010453	0.019106
0.021798	0.038582	0.040248	**1.6022**	0.025384	-0.0036747
0.054532	-0.005001	0.010397	0.02512	**1.7722**	0.023848
0.20858	0.045079	0.018357	-0.0037066	0.023919	**1.8295**

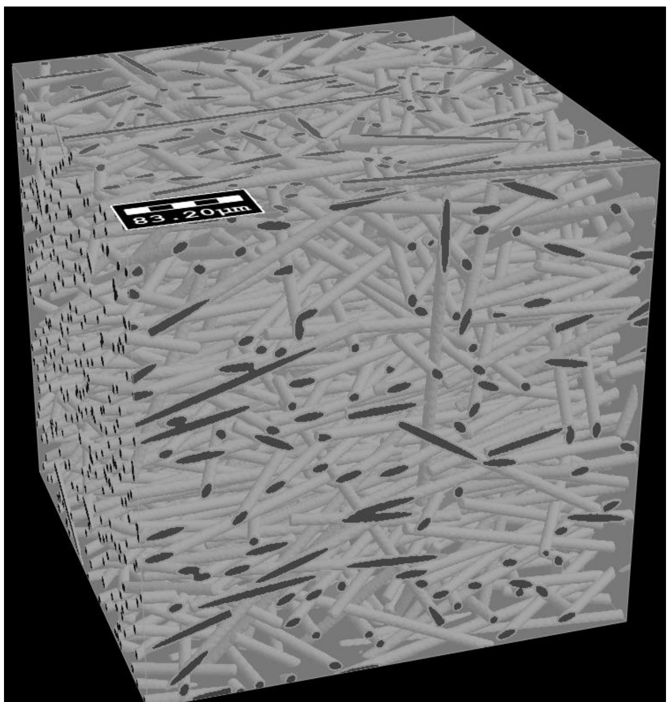
ElastoDict: Large Deformation

aim: how does the fiberglass microstructure deform for a given stress / strain?

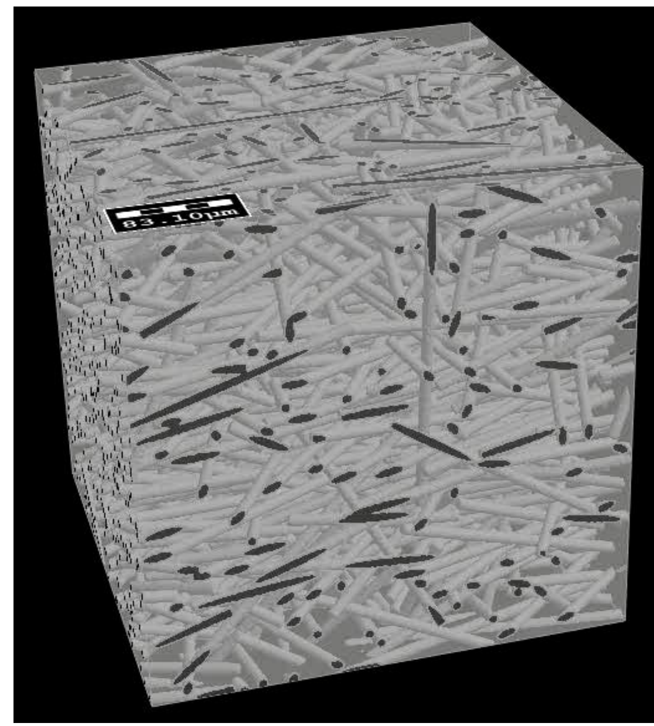
current development together with Fraunhofer,

large deformations, nonlinear material behavior

FeelMath
Fraunhofer ITWM

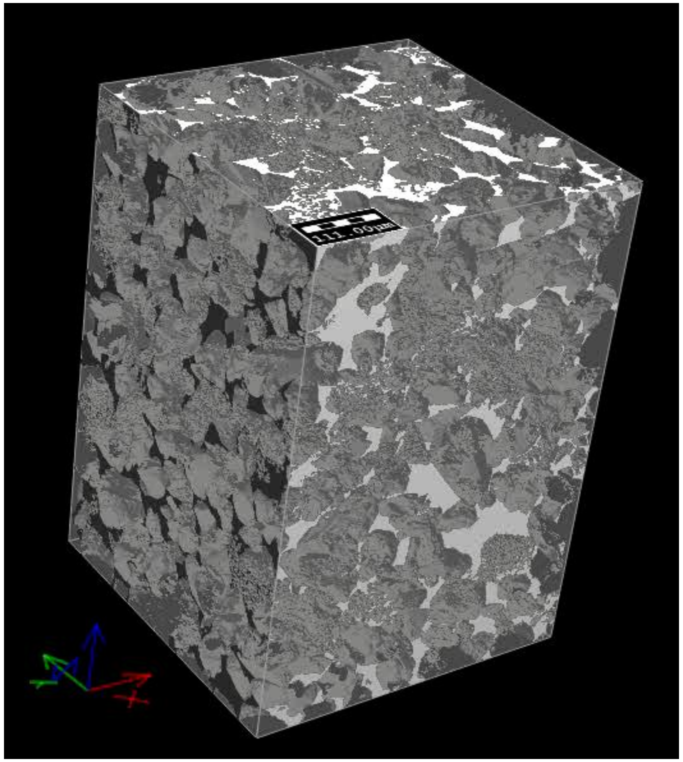


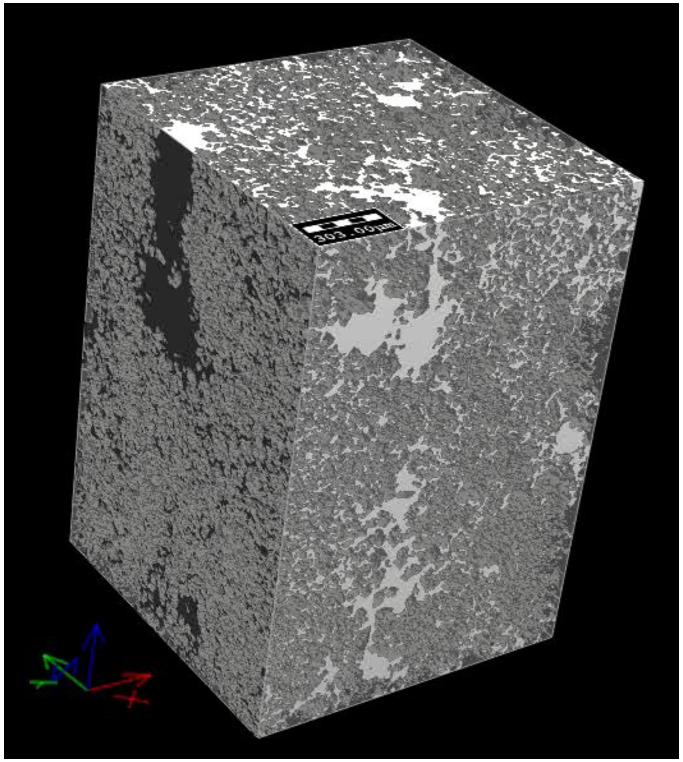
64 million grid points
12 GB memory
8 processes, 6 min



3. Digital Rock Physics

from computed tomograms to accurate reservoir simulations:
(left): pore space of Berea sandstone; (right): pore space of carbonate





Digital Rock Physics Benchmarks – Part I: Imaging and segmentation
Digital Rock Physics Benchmarks – Part II: Computing effective properties

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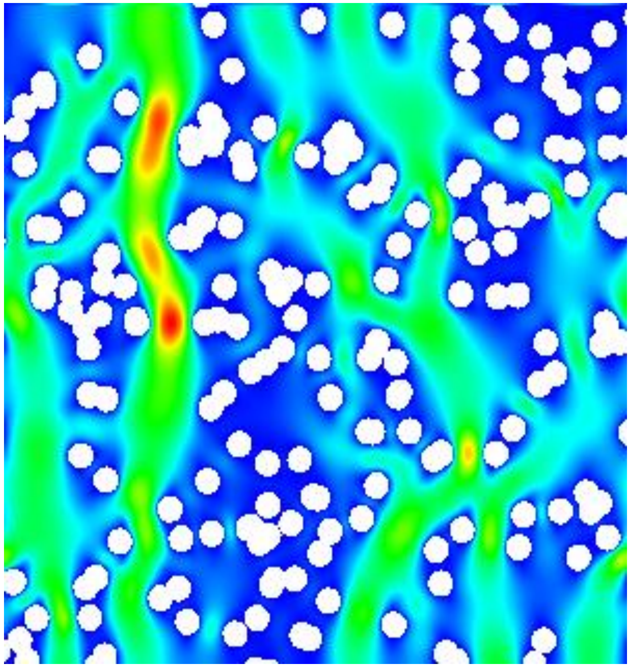
Permeability Computation

Macroscopic description
(homogenized porous media model)

Darcy's law : $$u = -\frac{1}{\mu}\kappa\nabla p$$

u : average flow velocity
κ : permeability tensor ***unknown***
μ : viscosity
p : pressure



Microscopic description
(pore structure model)

Stokes equation: $$-\mu\Delta u + \nabla p = 0$$

Boundary conditions: no-slip on fibre surface, pressure drop
κ can be determined from the solution!

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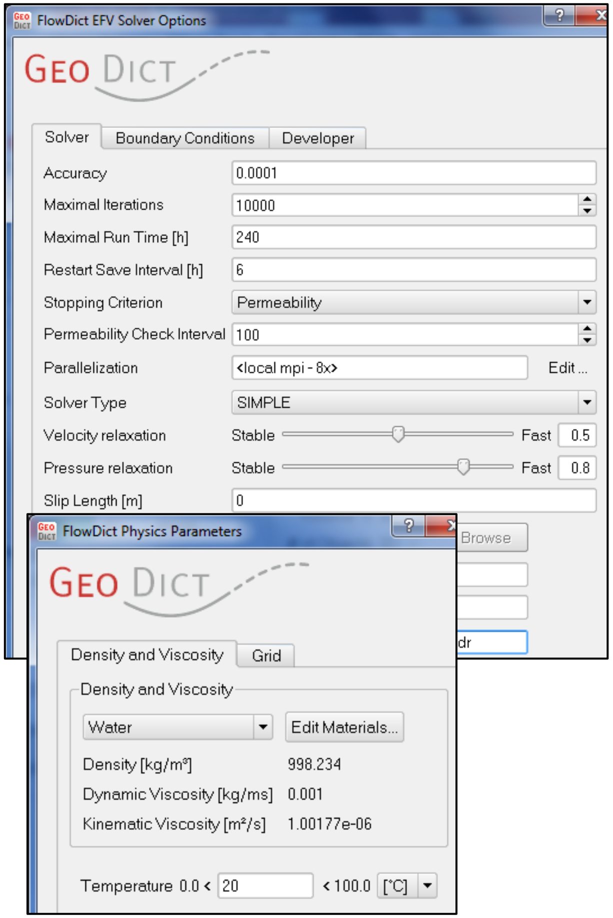
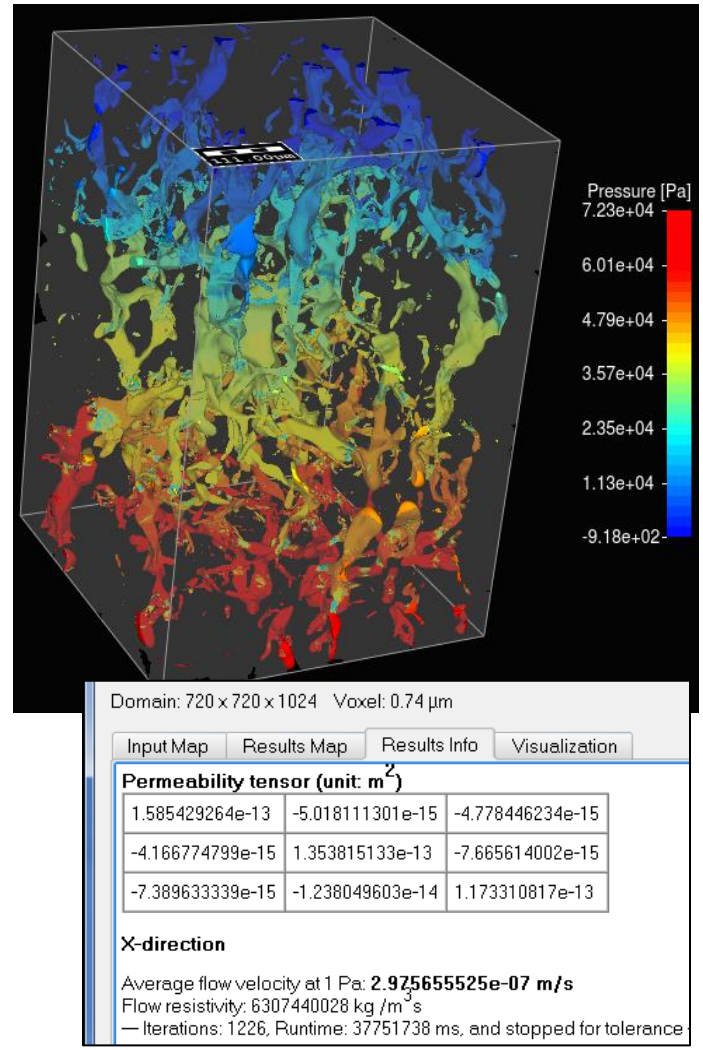
FlowDict: Rock Permeability Computation



compute flow properties

720x720x1024 voxel
46GB, 8 processes,
one direction 10 h



enter parameters into FlowDict

4. Summary and Conclusion

GEO DICT virtual material characterization & engineering

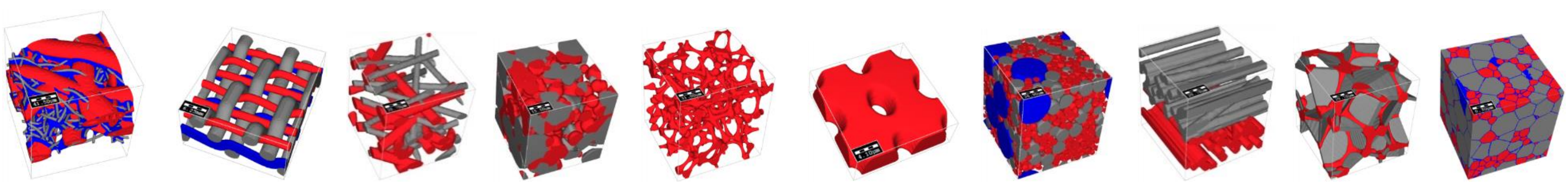
- property simulation on tomograms
- property simulation on material models
  - given parameters
  - change parameters to optimize microstructures
- use homogenized results from the micro-scale for macro-scale simulations
  - injection molding
  - digital rock

Thank You !

GEO DICT

The Virtual Material Laboratory

www.geodict.com



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