Modelling and Simulation of Filtration Processes
- a practitioners overview -

Andreas Wiegmann

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WFC 11
11th WORLD FILTRATION CONGRESS
APRIL 16 – 20, 2012 · GRAZ – AUSTRIA

Fraunhofer ITWM

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Thanks to collaborators at Fraunhofer ITWM

Currently at ITWM:

- Heiko Andrä, Jürgen Becker, Liping Cheng, Oleg Iliev, Mathias Kabel, Peter Klein, Zarah Lakdawala, Arnulf Latz, Sven Linden, Barbara Planas, Vita Rutka, Katja Schladitz, Konrad Steiner, Aivars Zemitis.

Currently ITWM *and Presenters at WFC 11*:

- Erik Glatt, Ralf Kirsch, Stefan Rief.

Formerly at ITWM:

- *Donatas Elvikis*, *Irina Ginzburg*, *Dirk Kehrwald*, *Joachim Ohser*, *Doris Reinel-Bitzer*, *Kilian Schmidt*, *Christian Wagner, Ashok Kumar Vaikuntam, Rolf Westerteiger*, *Qing Zhang*.

What about Math2Market GmbH & Fraunhofer ITWM / SMS?

Math2Market GmbH is a spin-off that markets and further develops the GeoDict software

M2M incorporated Sept. 2011, 4 core team members phase from SMS to M2M in 2012.

Andreas Wiegmann, PhD (the speaker), is

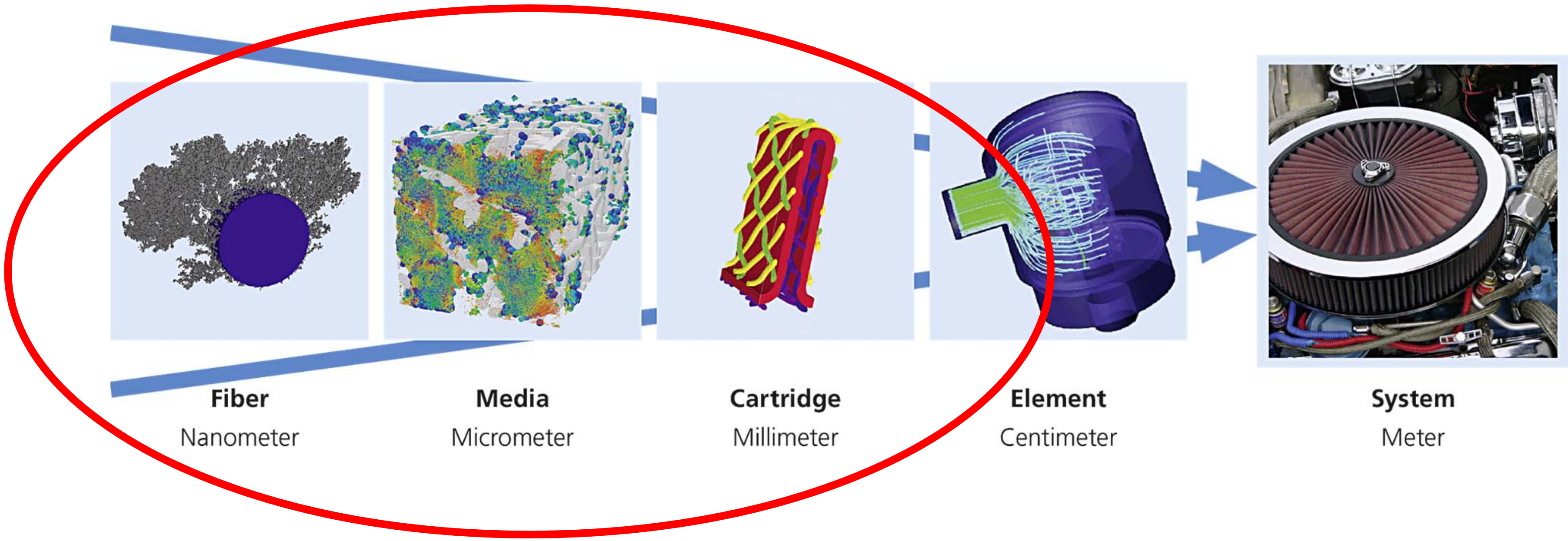
- Chief Executive Officer at Math2Market GmbH (50% now, 100% from July 2012)
- Deputy head of department SMS at Fraunhofer ITWM (50% now, 0% from July 2012)

M2M provides

- licenses,
- software support,
- consulting regarding modelling,
- simulation-based engineering services ,
- commercial-strength software engineering &
- close ties to Fraunhofer ITWM when mathematical research is required

Why Computer Aided Filter Media Engineering?

- "Left" effects govern behavior on the right
- Understand to improve
- New Insights through tomography
- Today's PCs are supercomputers



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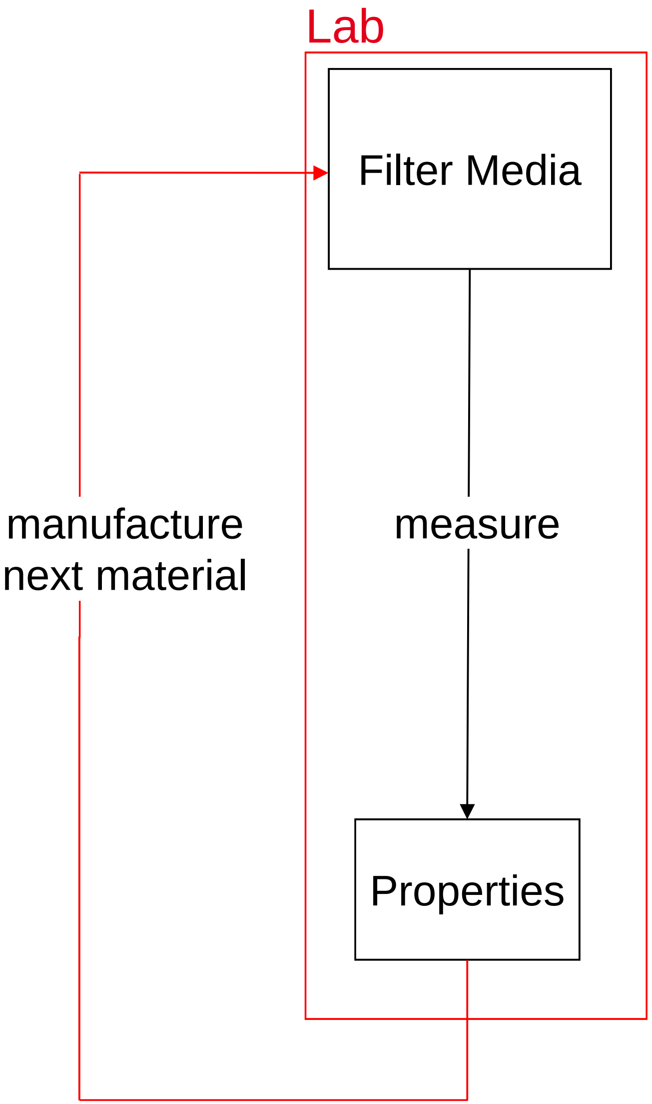
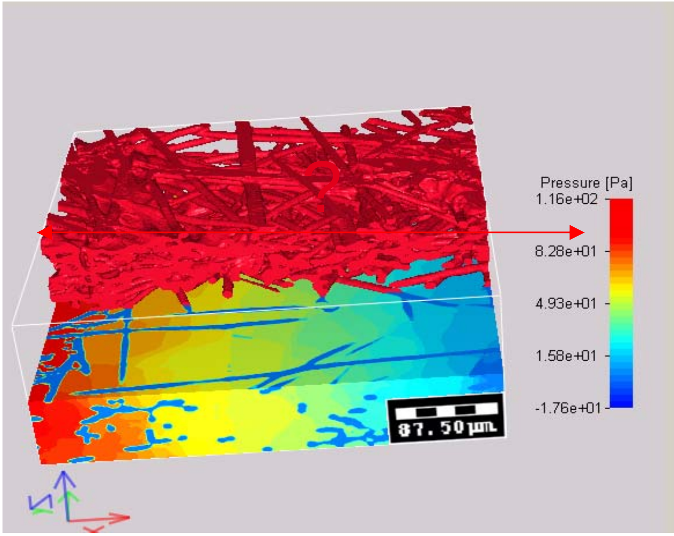
How does (direct numerical) filtration simulation work, anyway?

1. *Have a geometric model of the filter media or filter element*
2. *Have process conditions such as flow velocity, particle size and mass distributions, etc.*
3. *Know chemistry such as adhesion between particles and obstacles*
4. Compute liquid or gas flow: **get initial pressure drop**
5. Compute motion and deposition of (first batch of) particles: **get initial filter efficiency**
6. Update geometric model by deposited particles
7. Update liquid or gas flow: **get pressure drop over deposited mass**
8. Compute motion and deposition of (next batch of) particles: **get clogging and life time**
9. Go back to 6

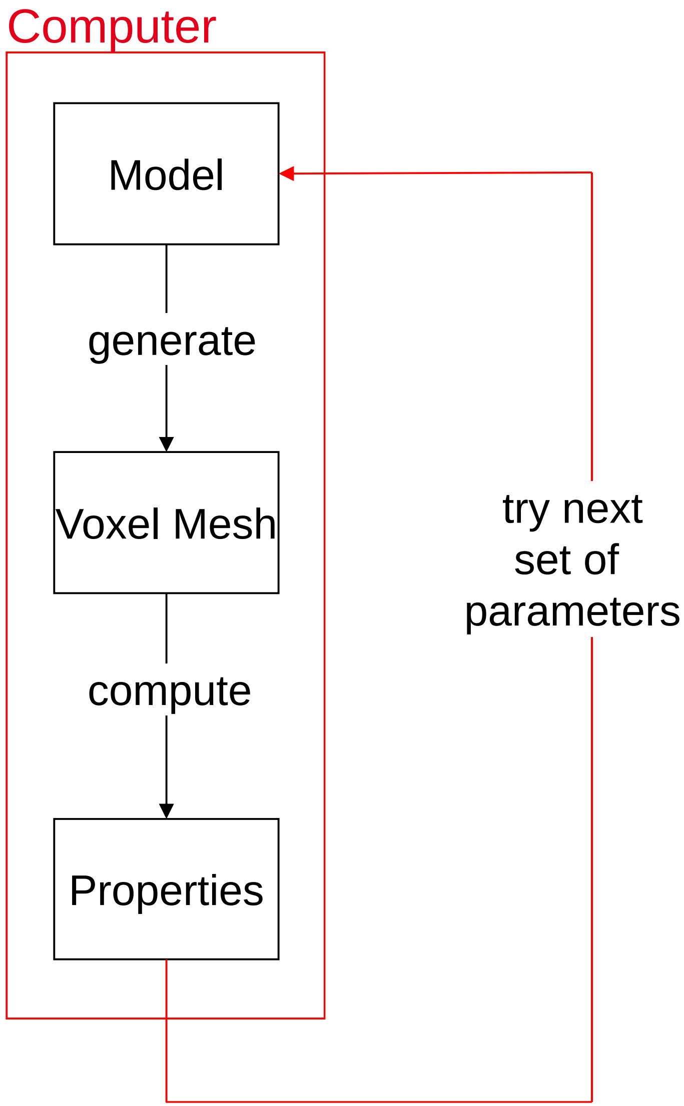
Computer Aided Filter Media Engineering



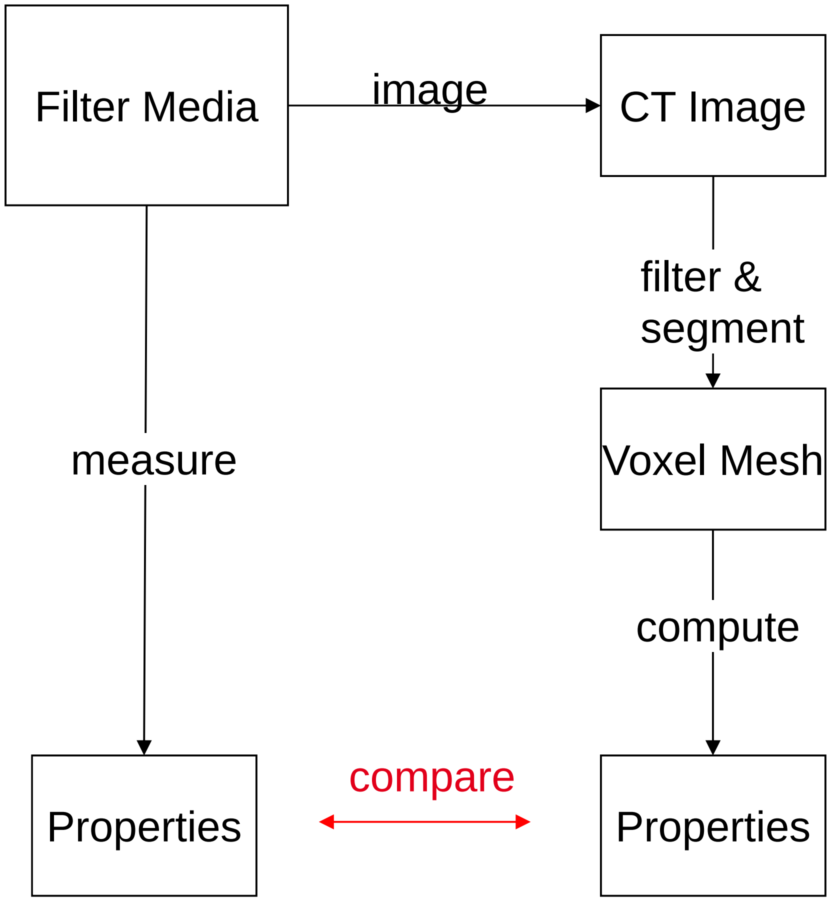


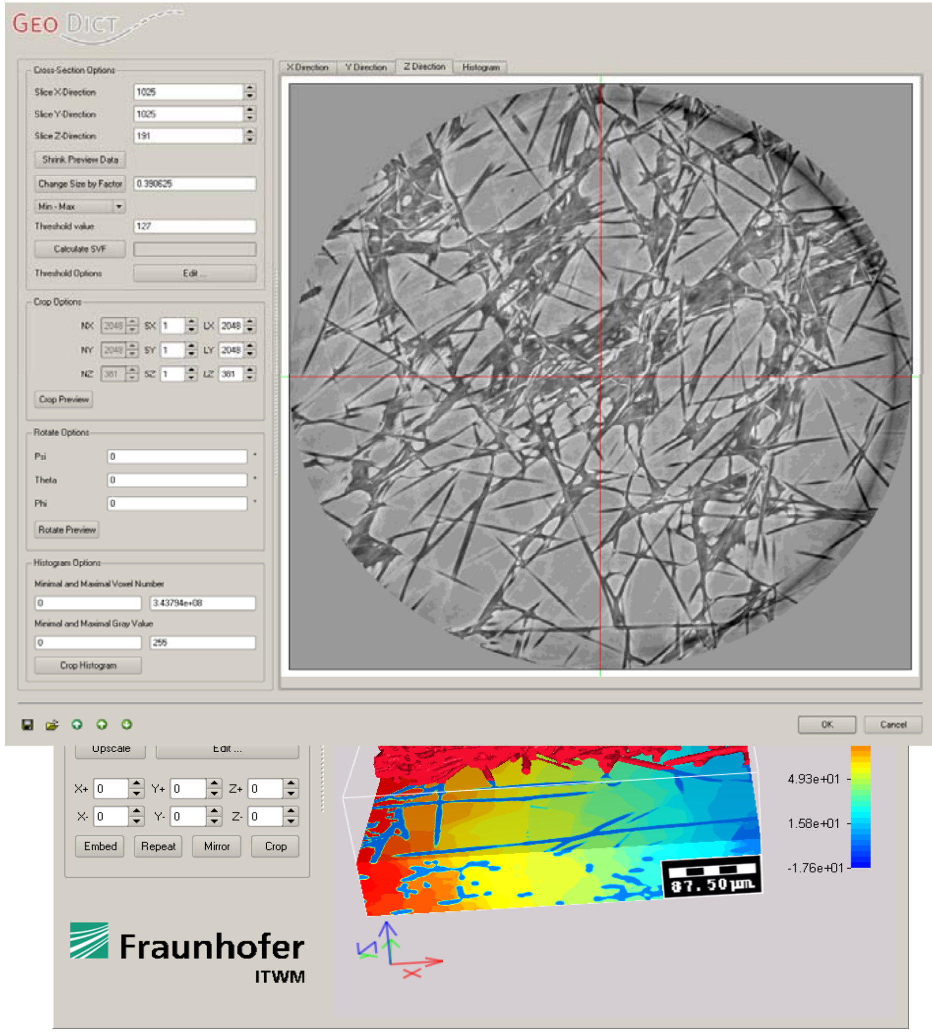
Properties include:

- pore size distribution
- pressure drop
- separation curve
- filter efficiency
- filter capacity
- filter cake formation

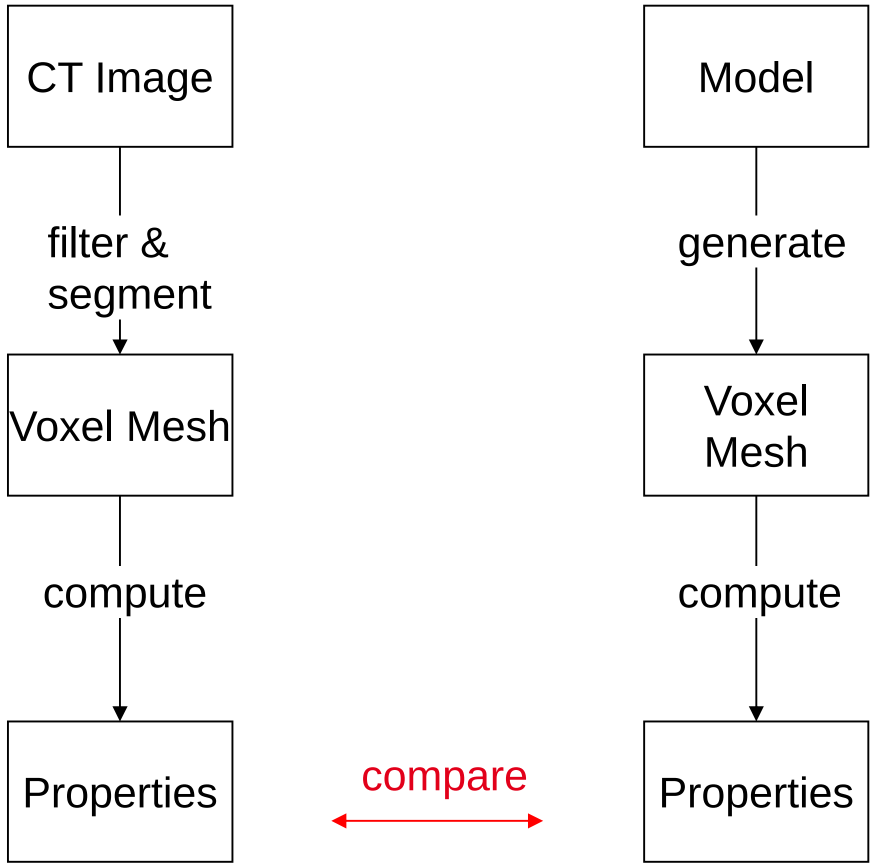


Validation - Step 1: Property Computations

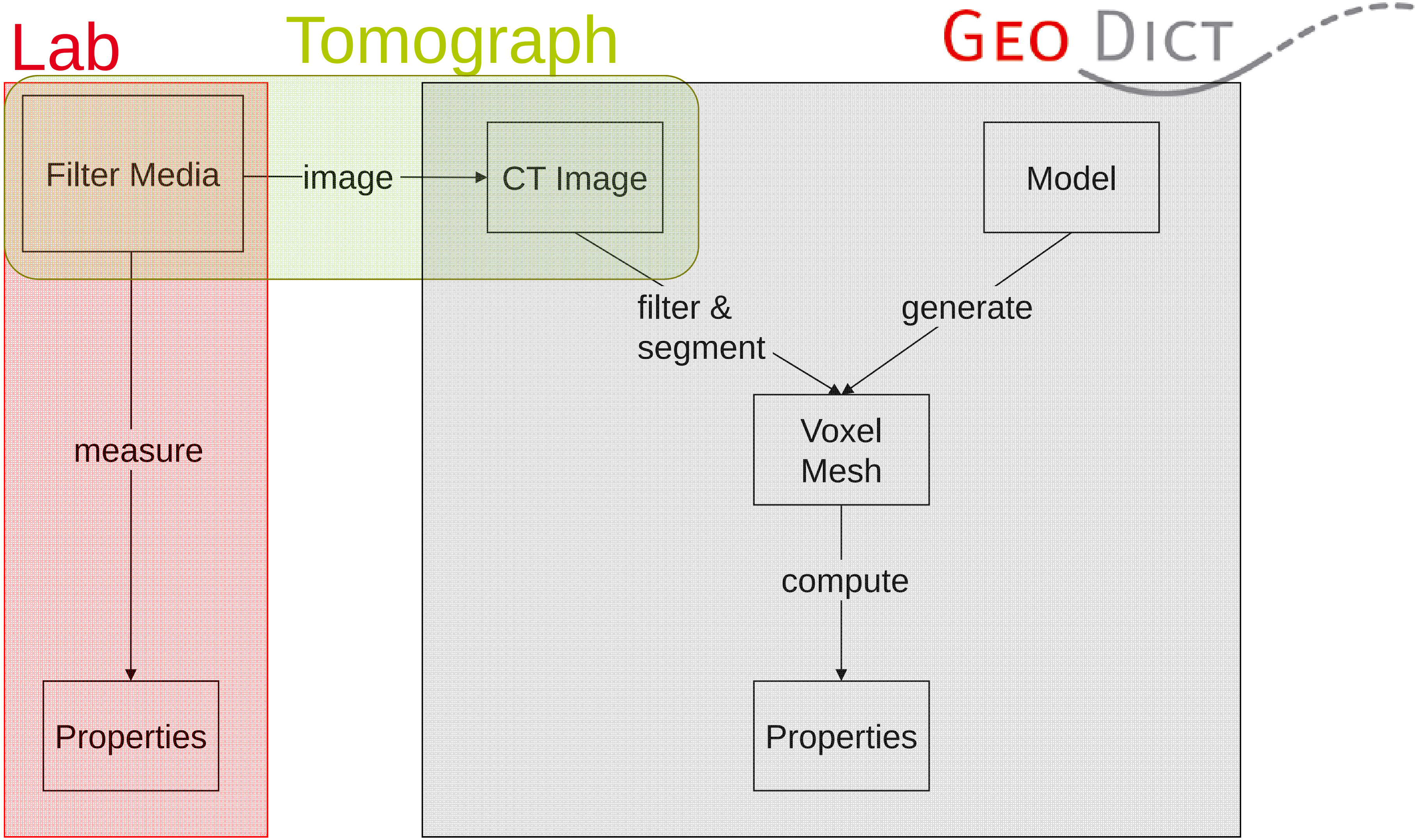




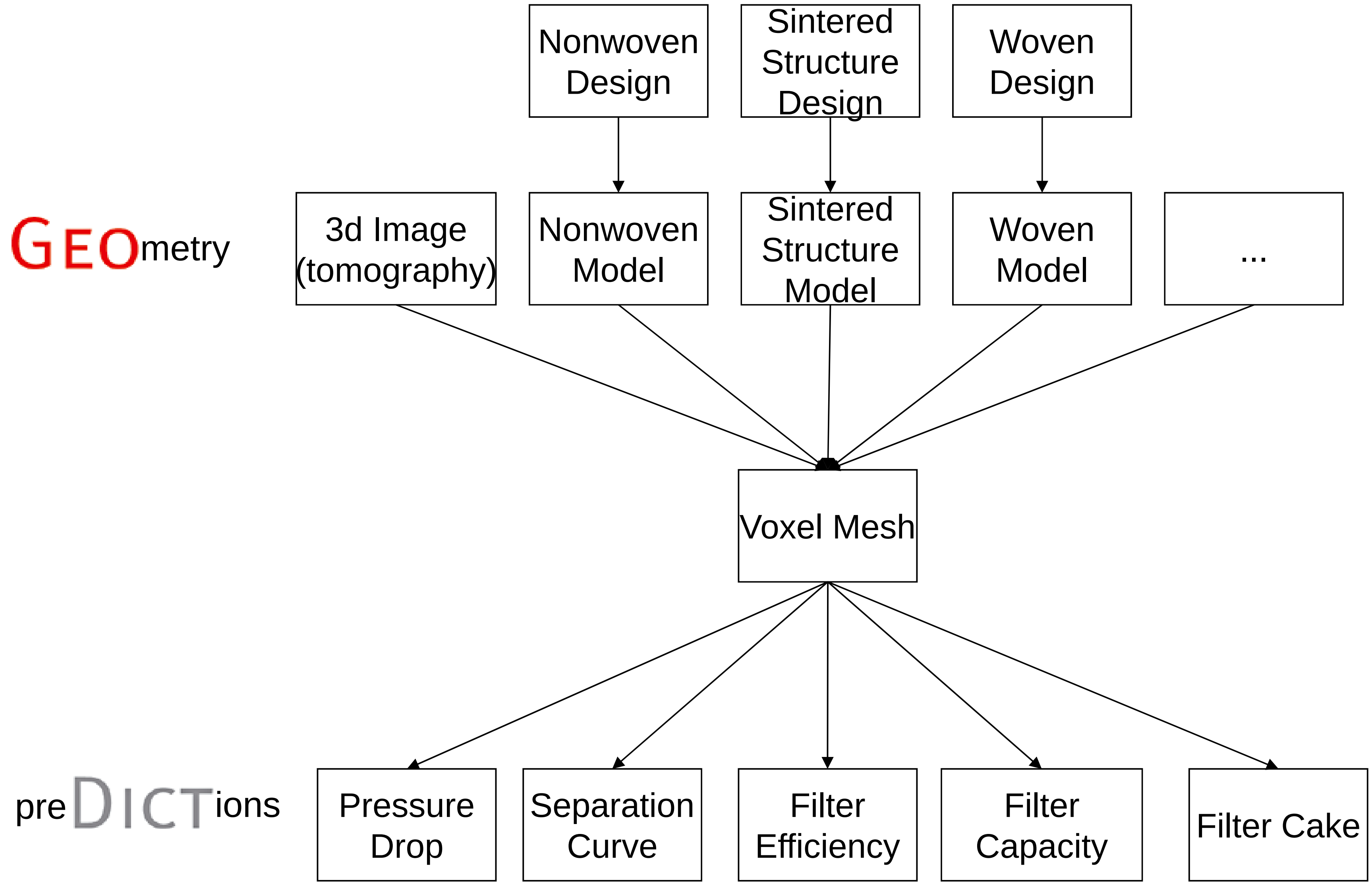
Validation - Step 2: Material Models



Computer Aided Filter Media Engineering



Computer Aided Filter Media Engineering



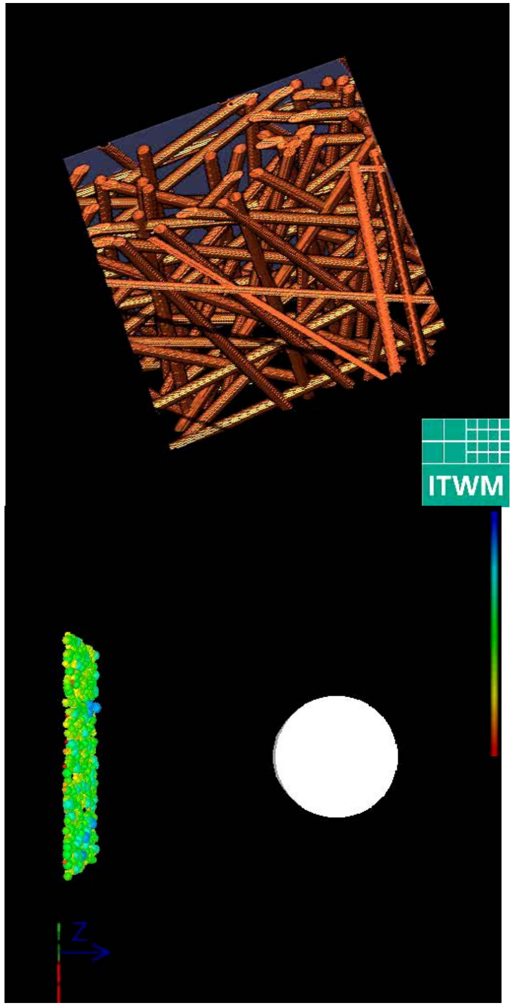
Virtual design cycle of filter media

Flow

1. Choose initial structural parameters
2. Generate / modify structure
3. Solve CFD problem
4. Compute particle transport and deposition
5. Compute filtration efficiency and pressure drop
6. Choose new structural parameters

OPTIMIZATION

LIFETIME



Single Fiber Simulation

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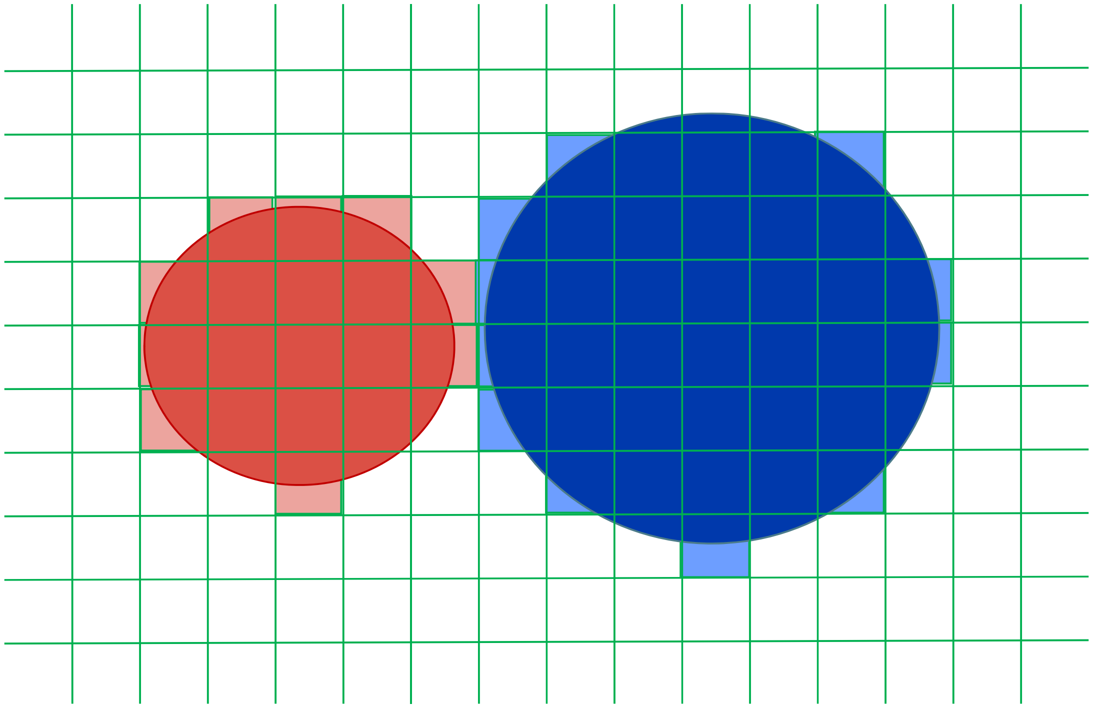
All simulations done are based on structures of little cubes



Advantages

- Saves grid generation times
- Compatible with computer tomography
- Straight forward structure generation
- Straight forward solver implementation
- Straight forward parallel computations

Disadvantages

- Resolved features require many grid cells
- Leads to very large scale computations

Analytic, surface and volume representation

<Object1>

Color 1

Type ShortCircularFiber

Point1 6.64451173e-05,25.77604784e-

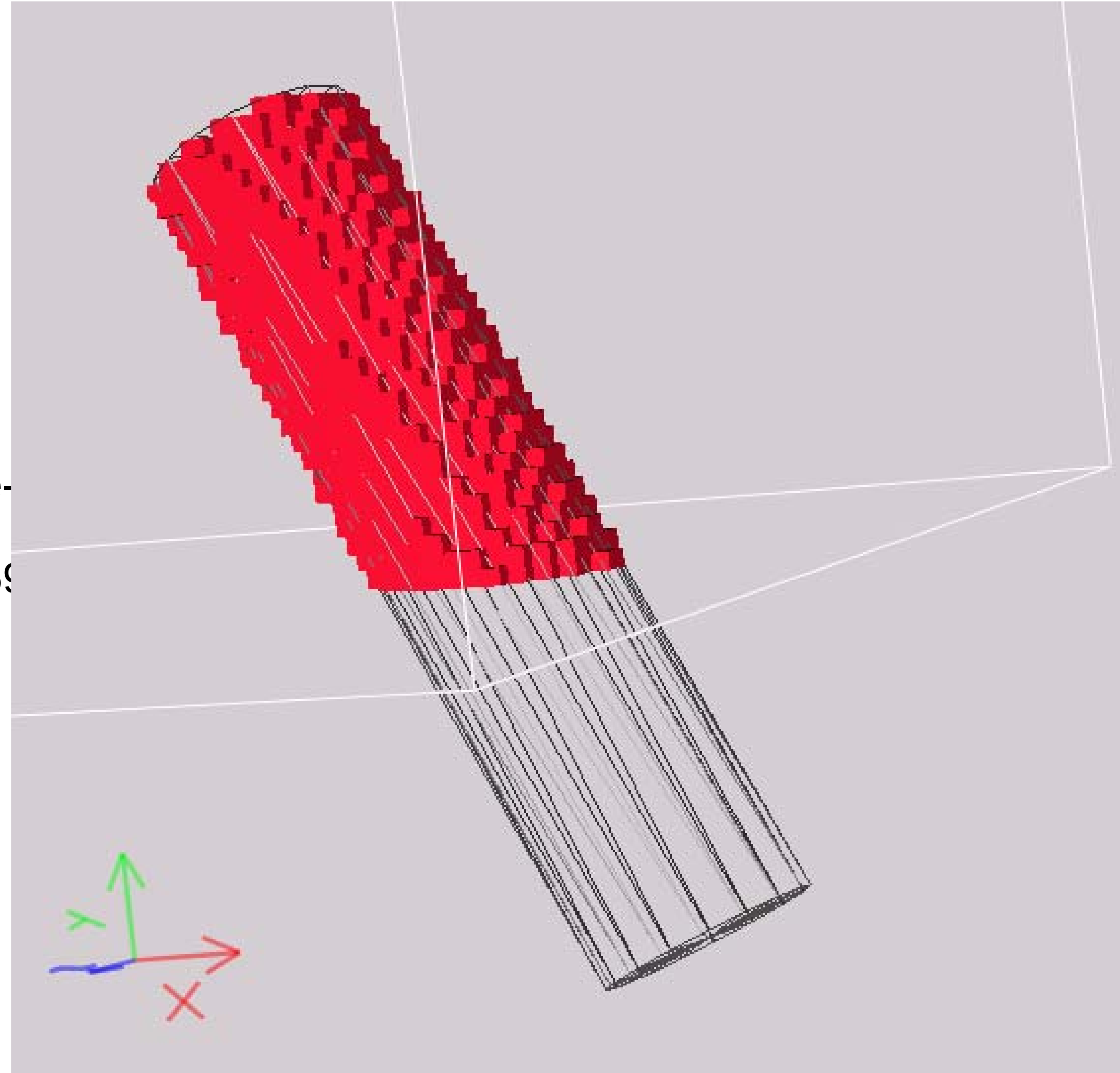
Point2 0.0000894540812,-2.040133859

FiberEndType1 0

FiberEndType2 0

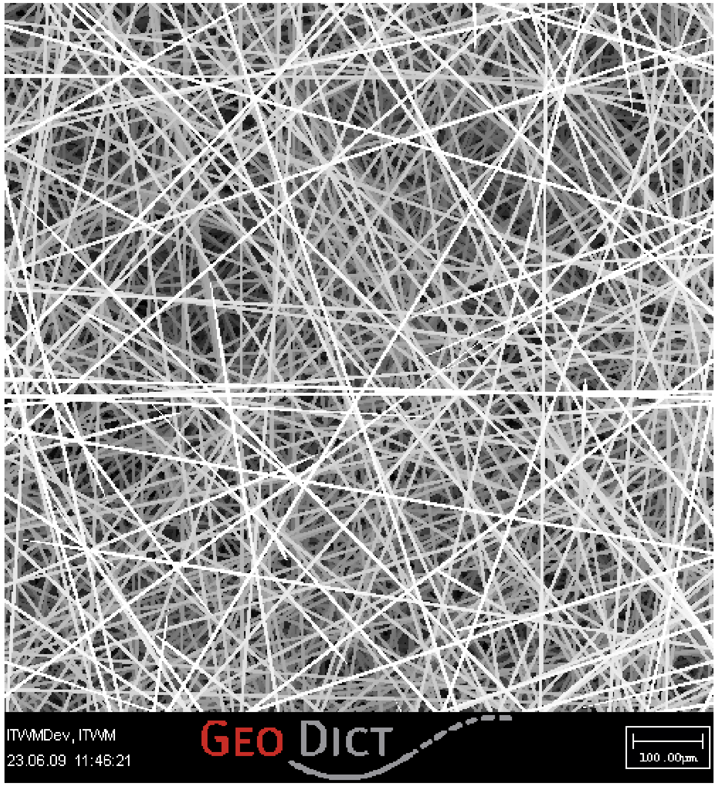
Diameter 1.2e-05

</Object1>

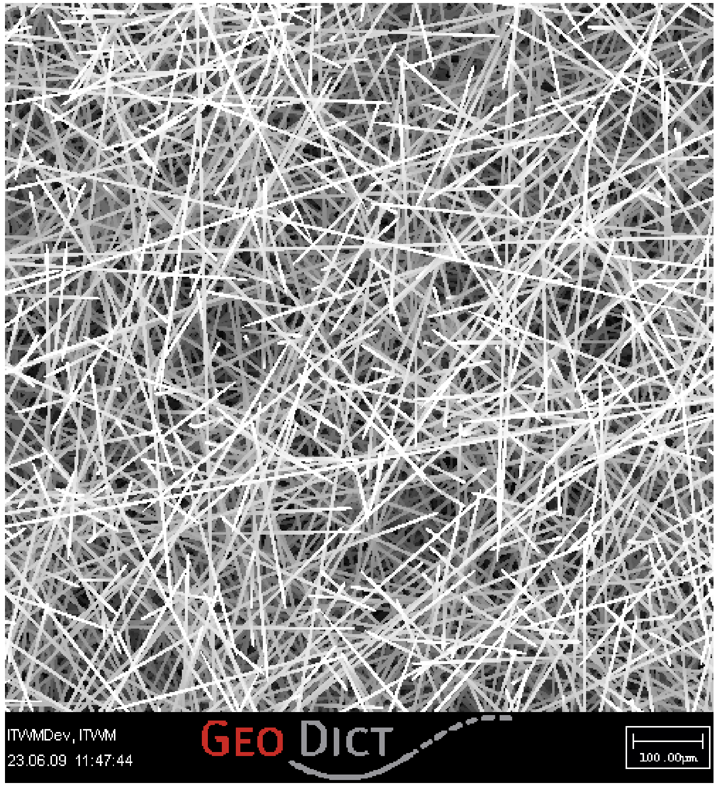


Nonwoven

SEM visualization of 8 volume percent 5 micron fibers

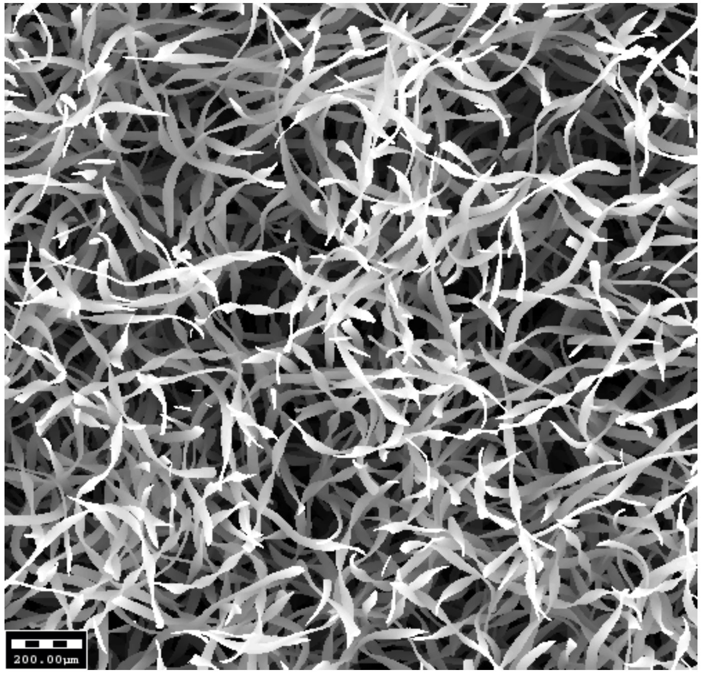


anisotropy 100

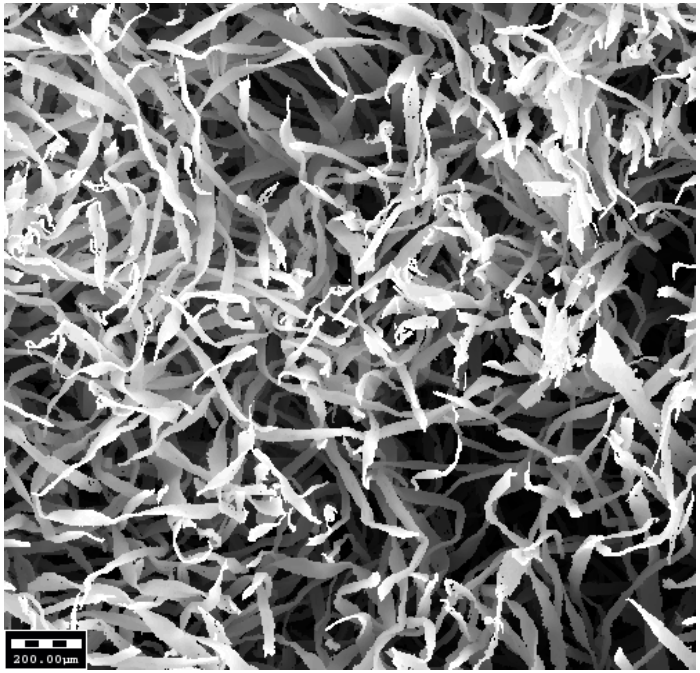


anisotropy 7

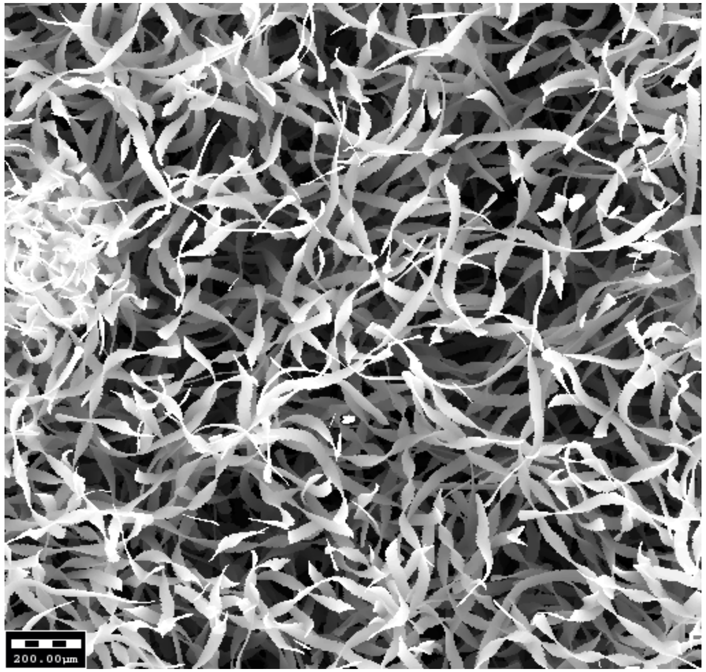
Curled and inhomogeneous nonwoven



homogeneous

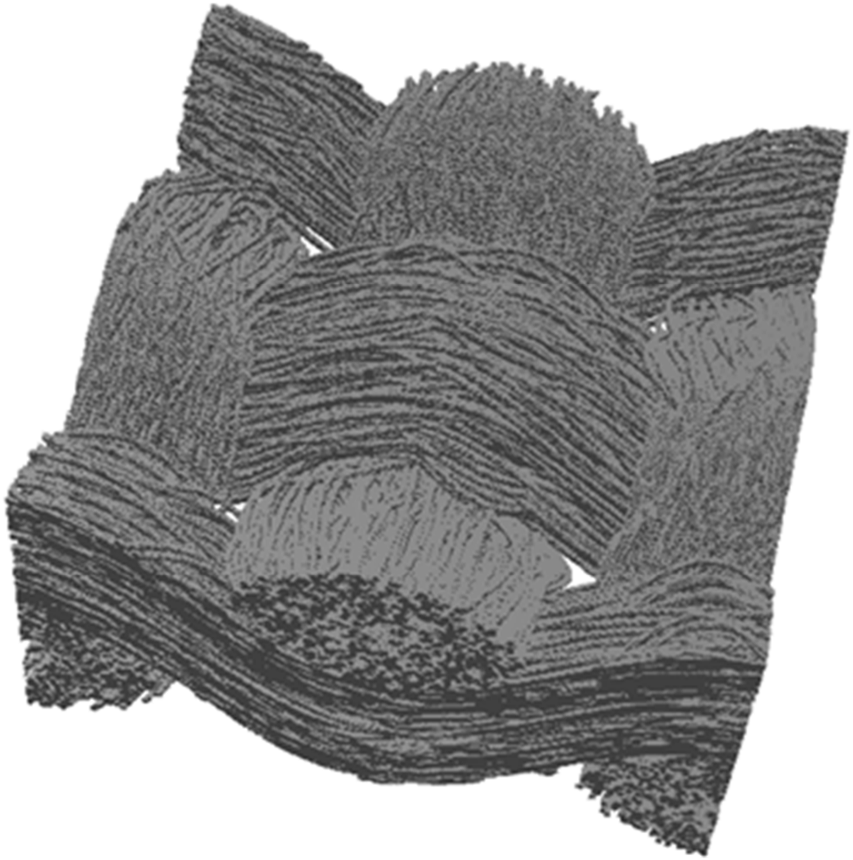


tomogram



inhomogeneous

Carbon fiber multi-filament woven

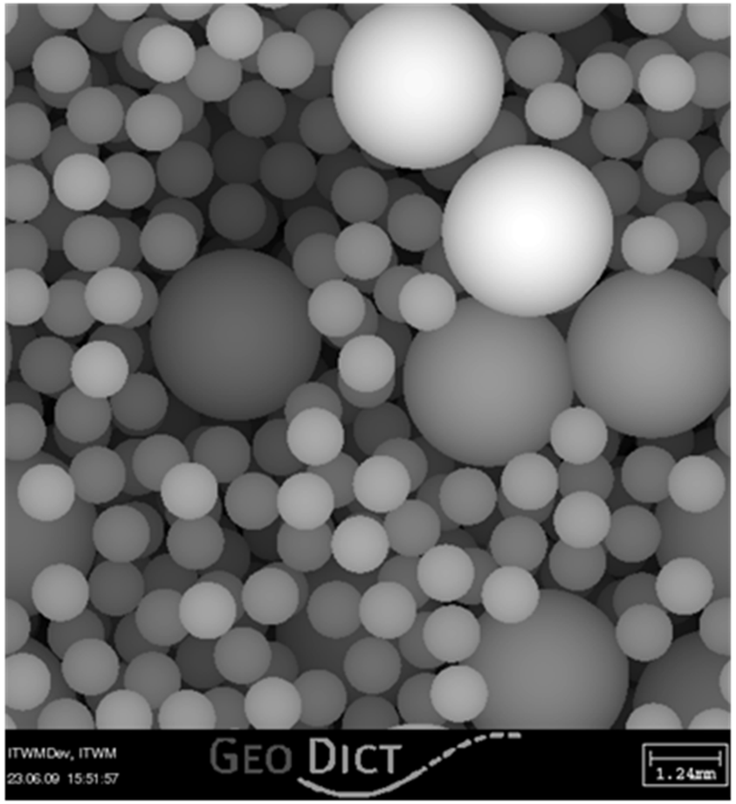


3D Visualization (generated)

SEM (real)

(SEM courtesy of Jeff Gostick, Univ. of Waterloo)

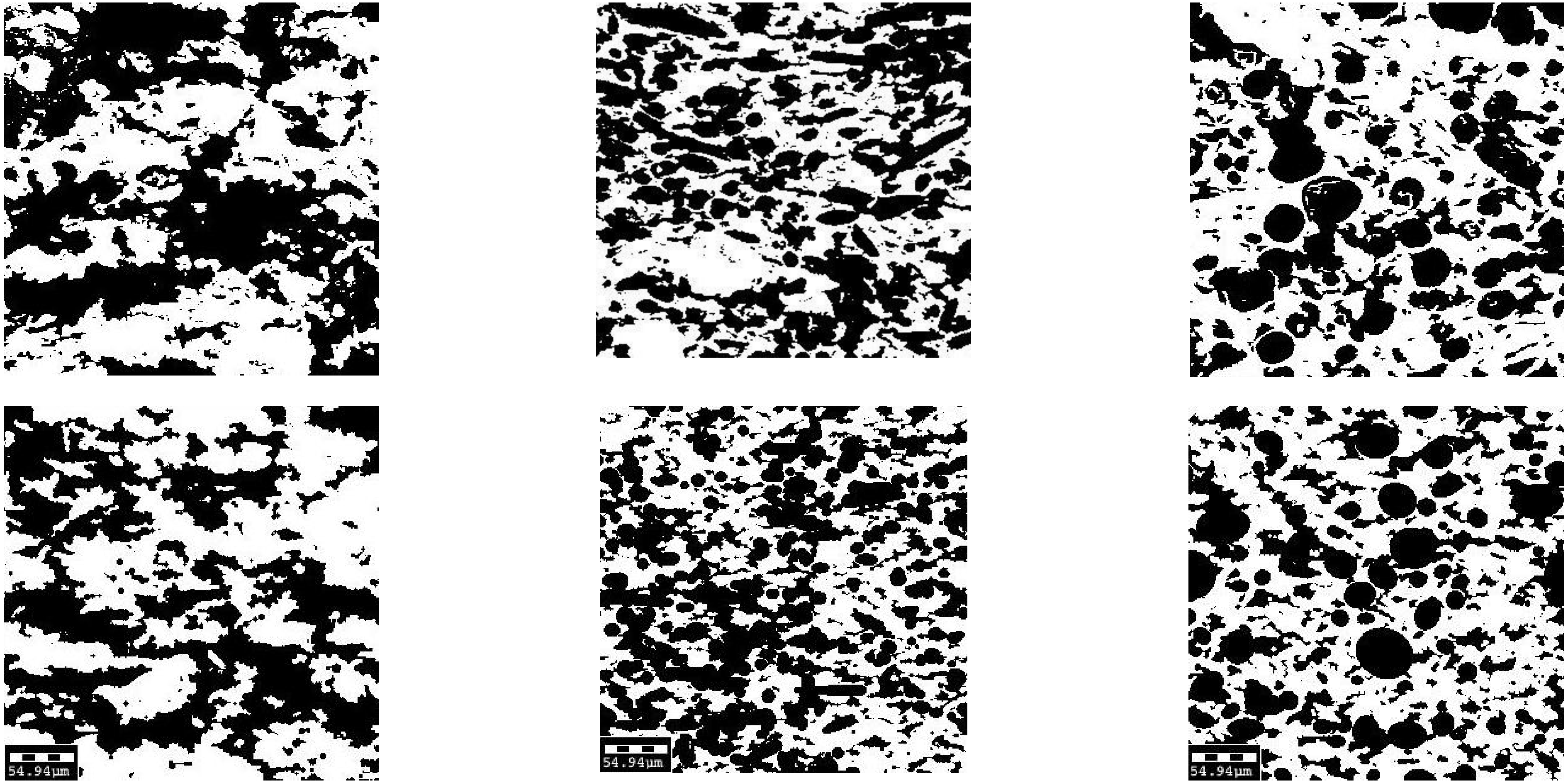
Packed bed of spheres and floating spheres



svf 0.64

svf 0.30

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



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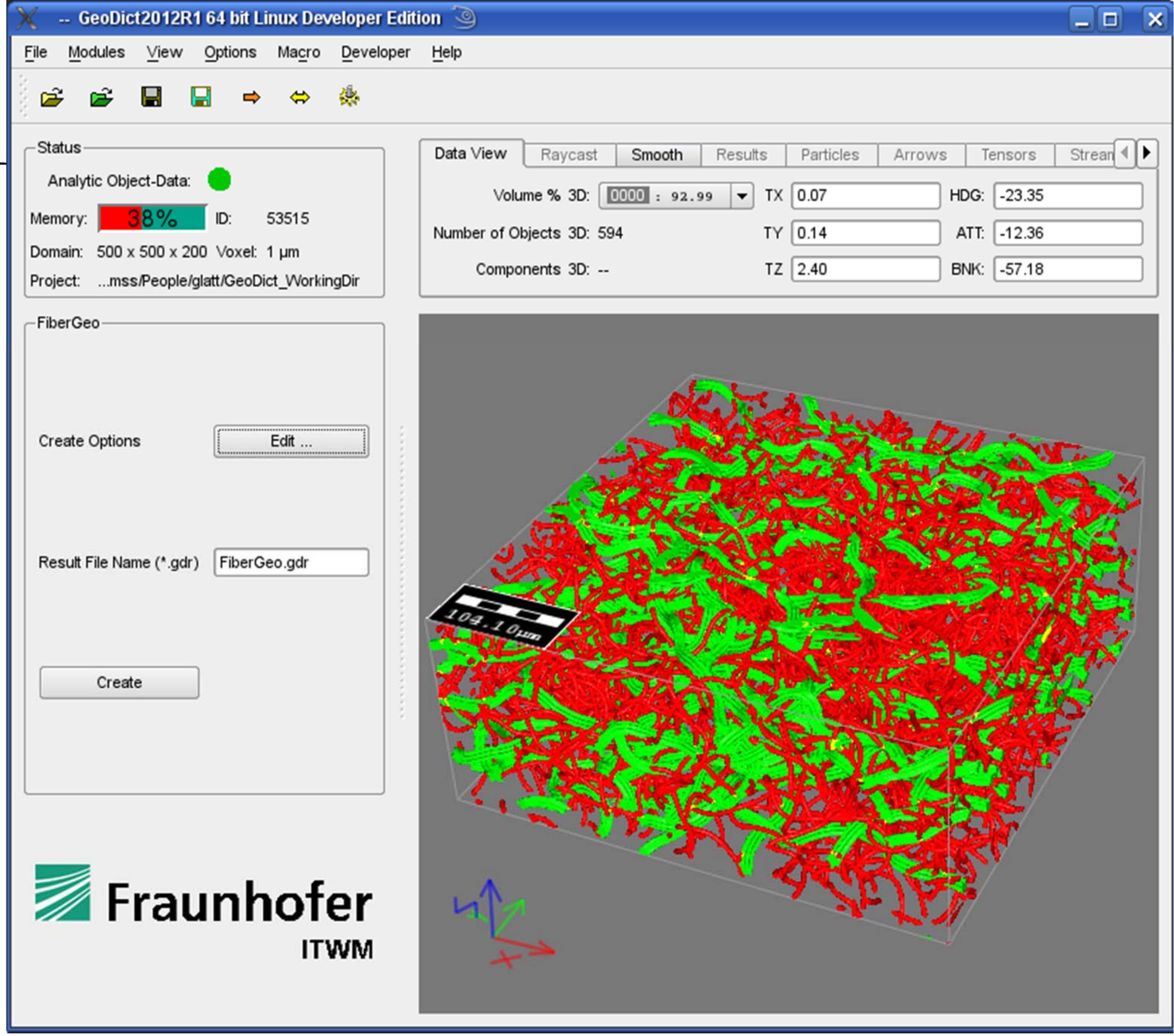
Virtual paper: cellulose fibers & fines

paper.gmc

paper.gad

paper.leS



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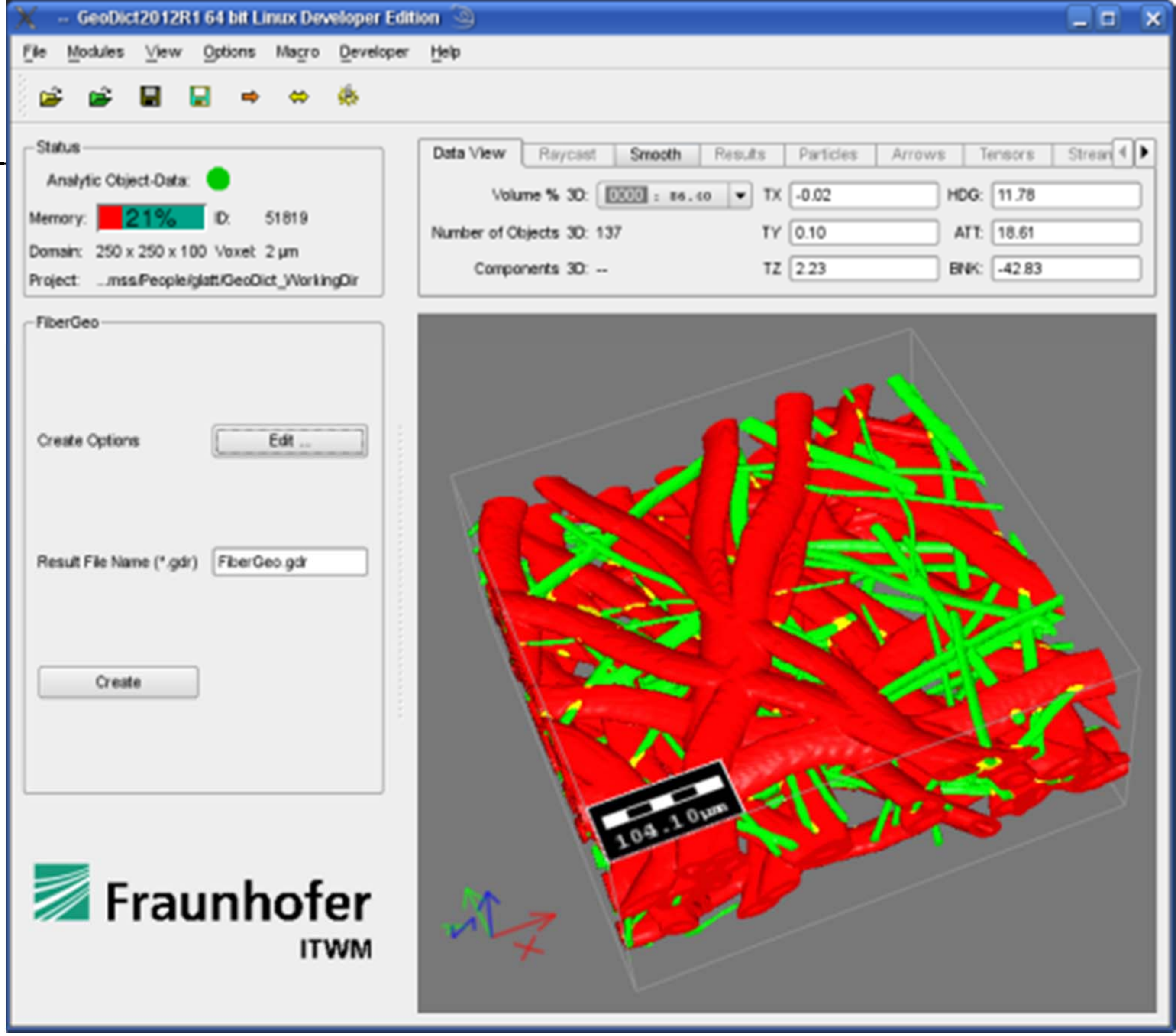
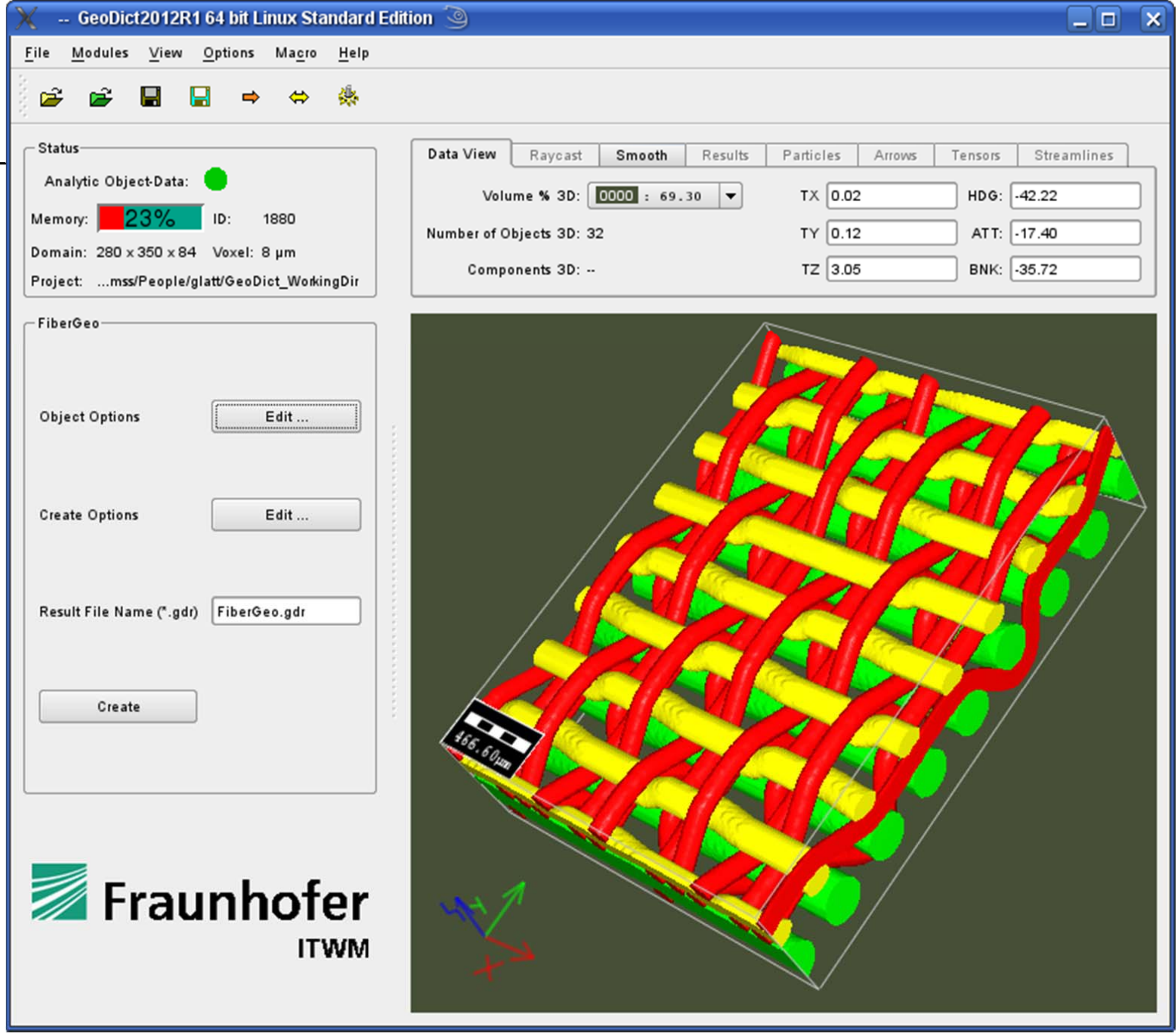
Virtual meltblown: curved fibers

meltblown.gmc



Virtual woven: multiple weft layers

weave.gmc



Virtual felt: woven, nonwoven & needling

felt.gmc

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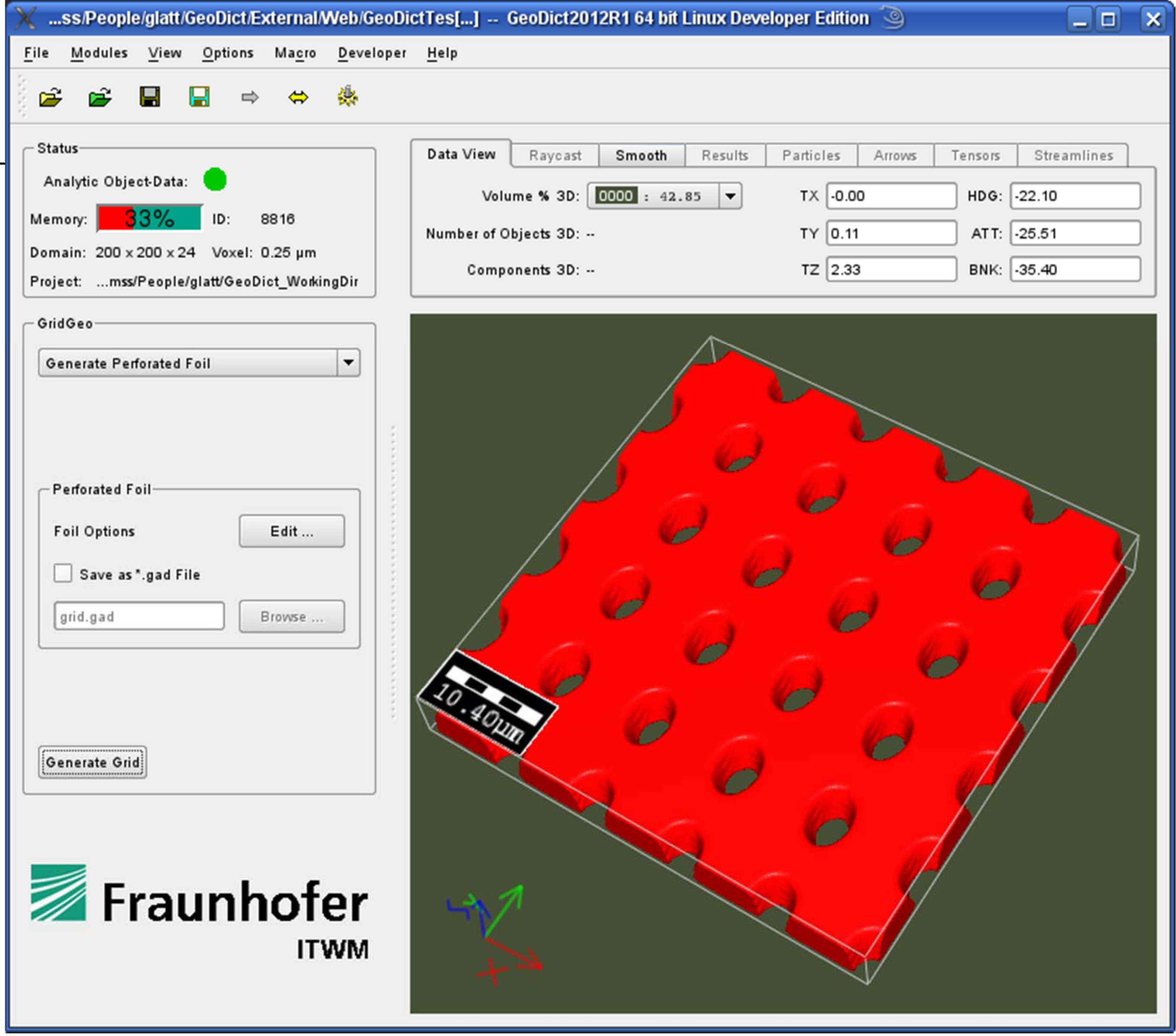
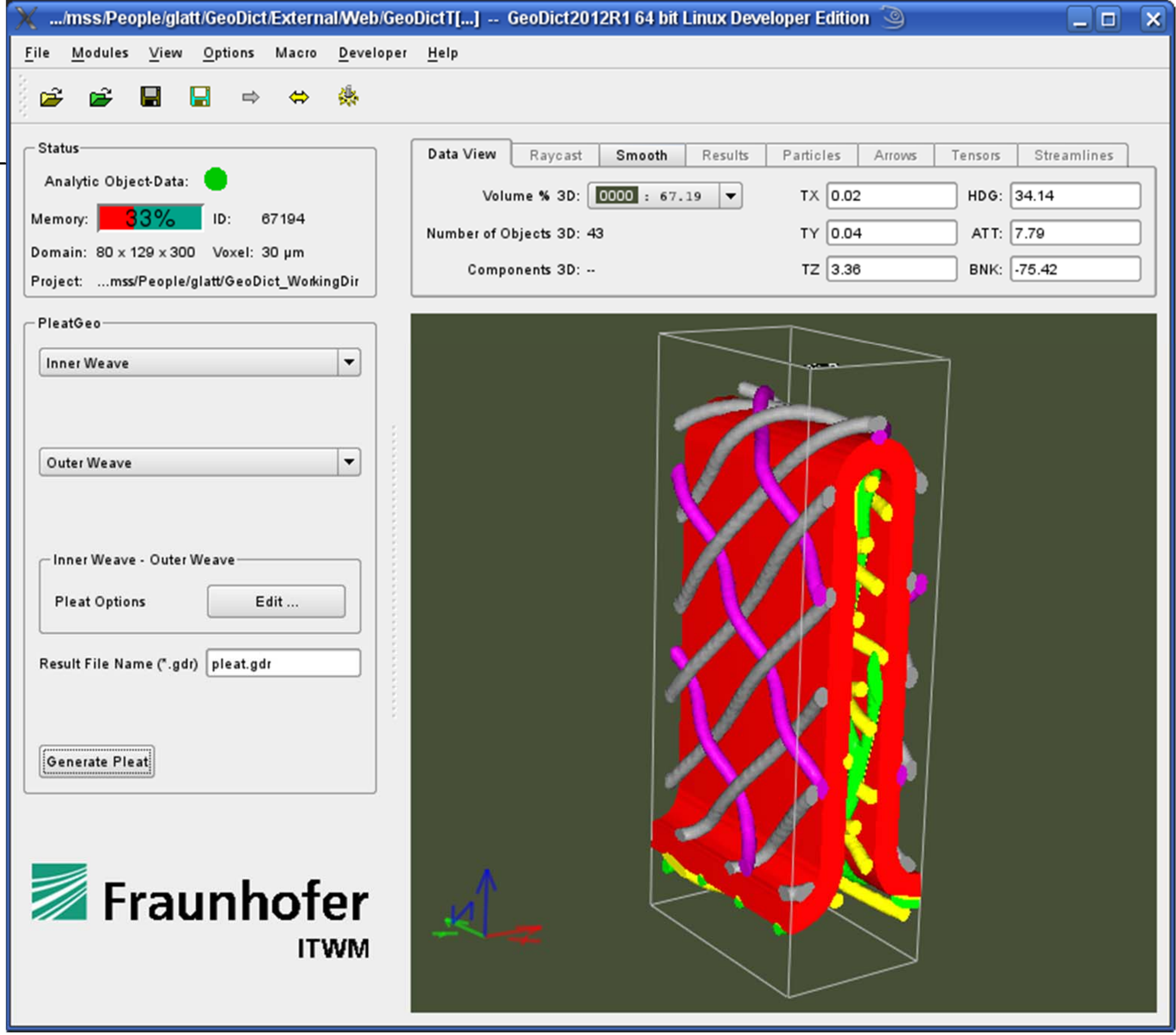
Virtual foil: oval & conical holes in arbitrary patterns

foil.gmc



Virtual pleat:
filter media +
interior and exterior
support structures

pleat.gmc



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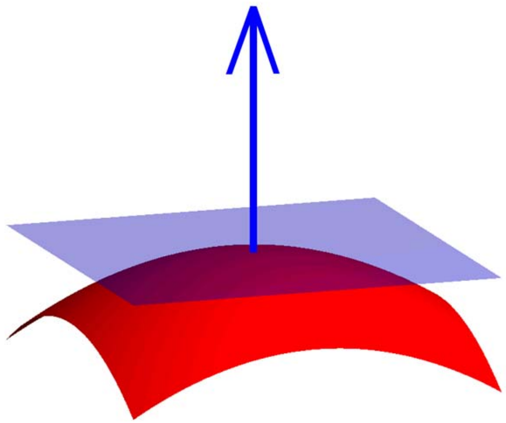
Stationary Stokes flow with no slip vs fractional slip

$$\begin{aligned} -\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\ \nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\ \vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)} \\ P_{in} &= P_{out} + c \text{ (pressure drop is given)} \end{aligned}$$



μ : fluid viscosity,

$\vec{u}$: velocity, periodic,

p : pressure, periodic up to pressure drop in flow direction.

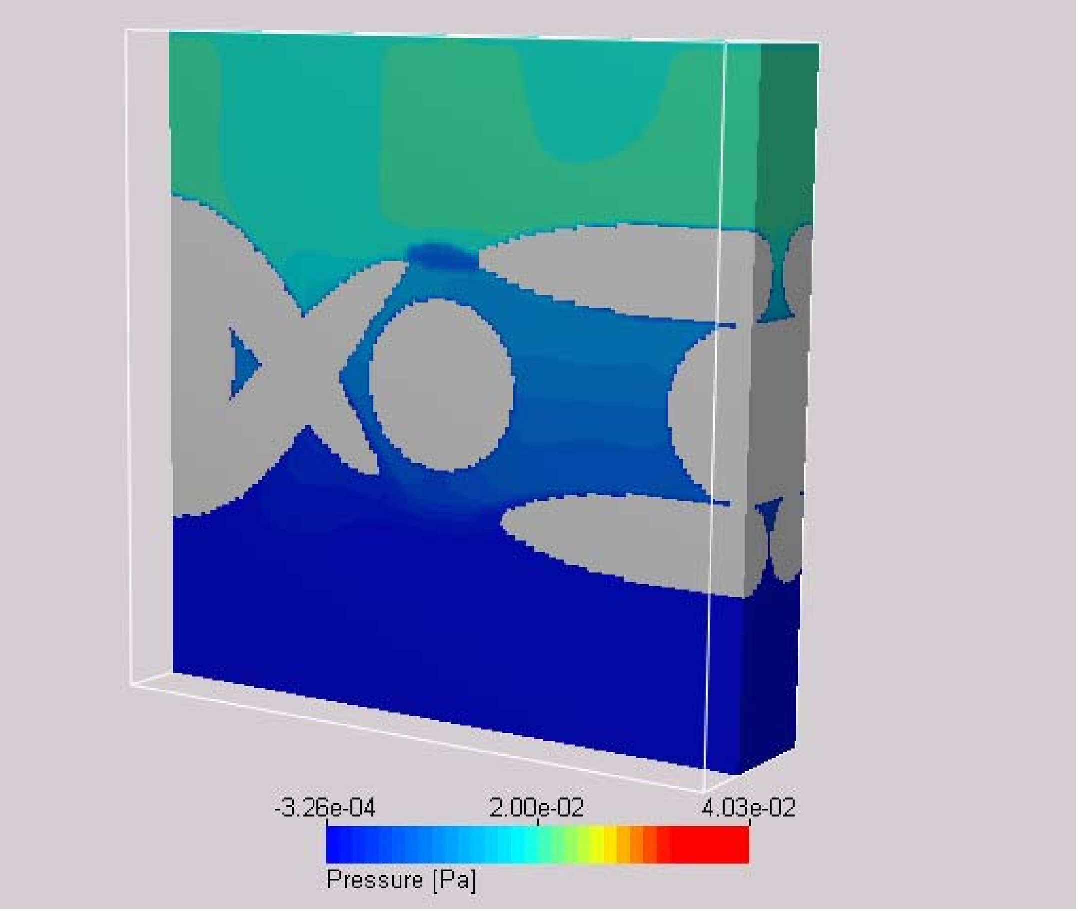
$$\begin{aligned} -\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\ \nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\ \vec{n}\cdot\vec{u} &= 0 \text{ on } \Gamma \text{ (no flow into fibers)} \\ \vec{t}\cdot\vec{u} &= -\lambda\vec{n}\cdot\nabla\left(\vec{u}\cdot\vec{t}\right) \text{ on } \Gamma \text{ (slip flow along fibers)} \\ P_{in} &= P_{out} + c \text{ (pressure drop is given)} \end{aligned}$$

$\vec{n}$: normal direction to the fiber surface,

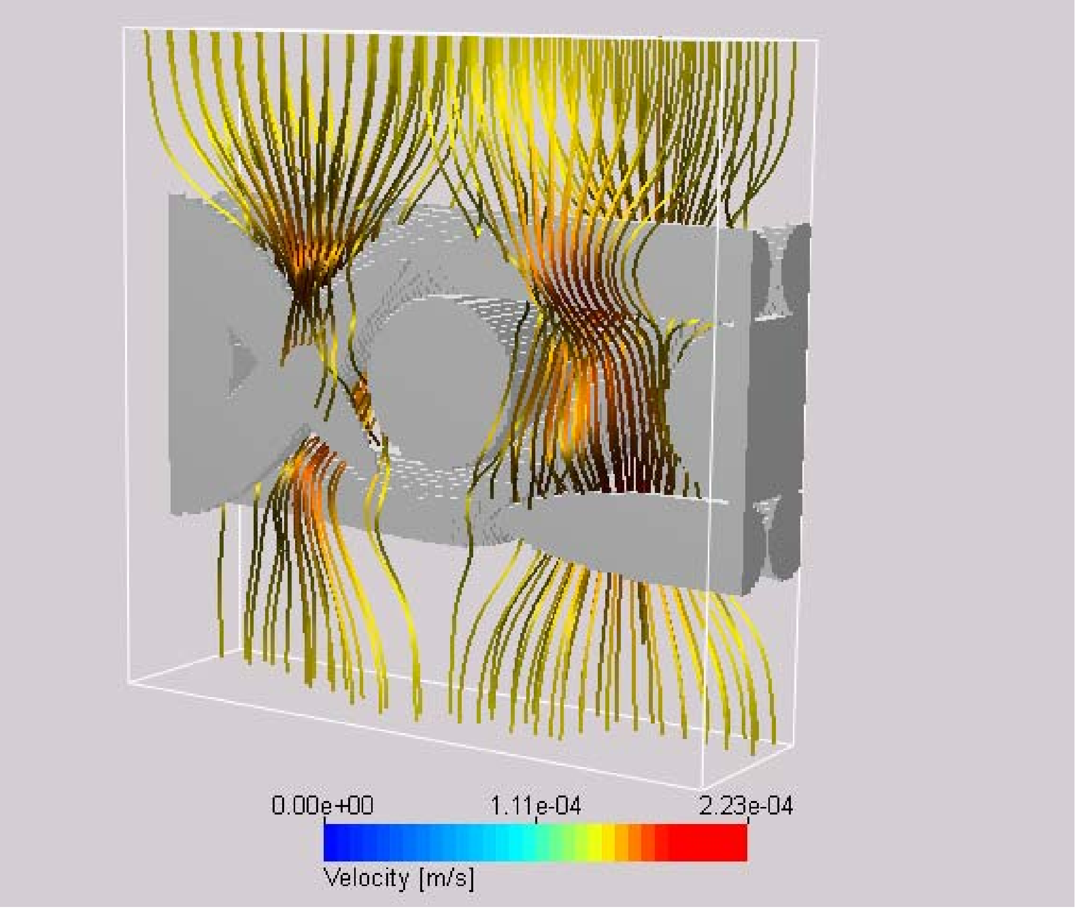
λ : slip length,

$\vec{t}$: any tangential direction with $\vec{t}\cdot\vec{n} = 0$.

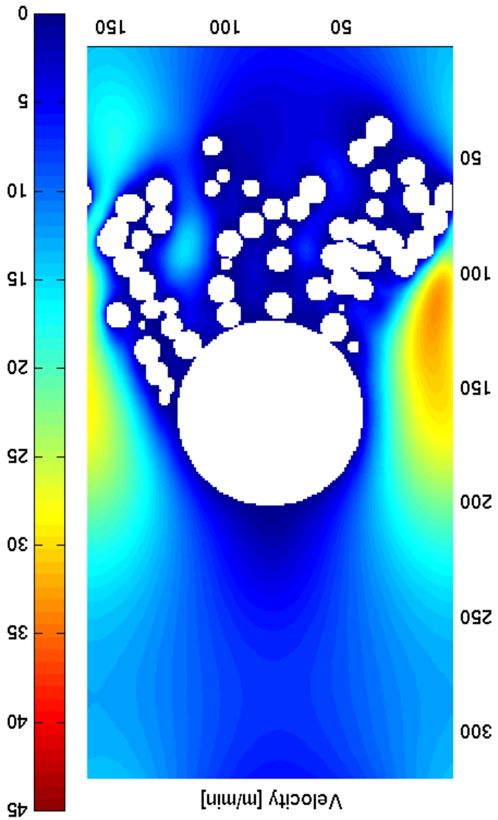
Pressure Drop Visualization

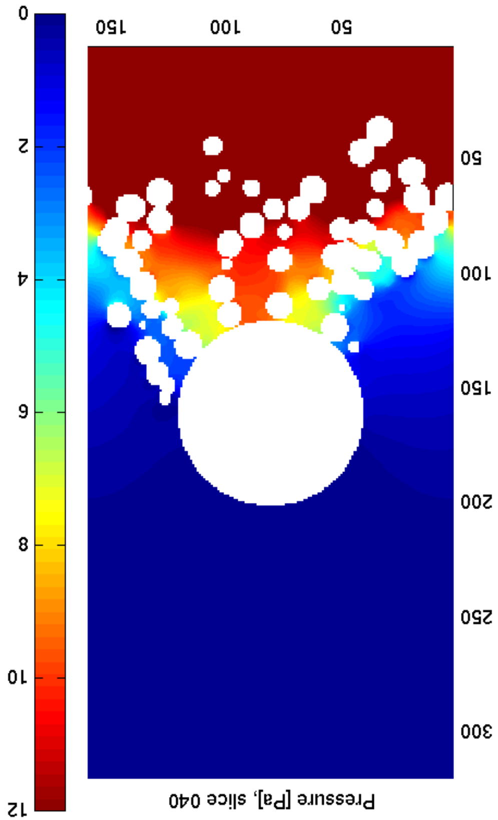


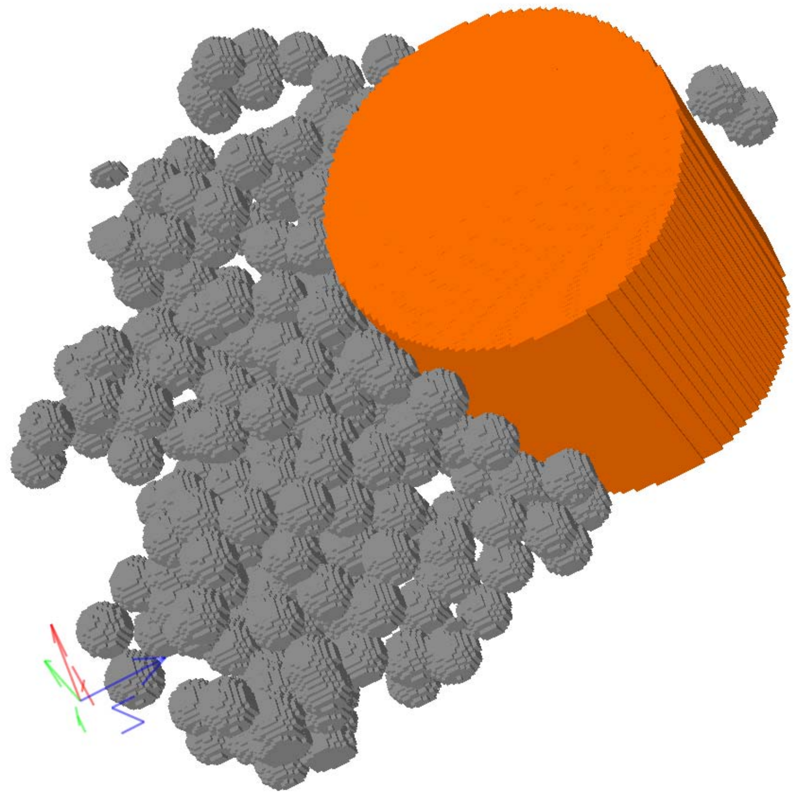
Flow Field Visualization (streamlines)



Pressure and Velocity in Clogging Simulation







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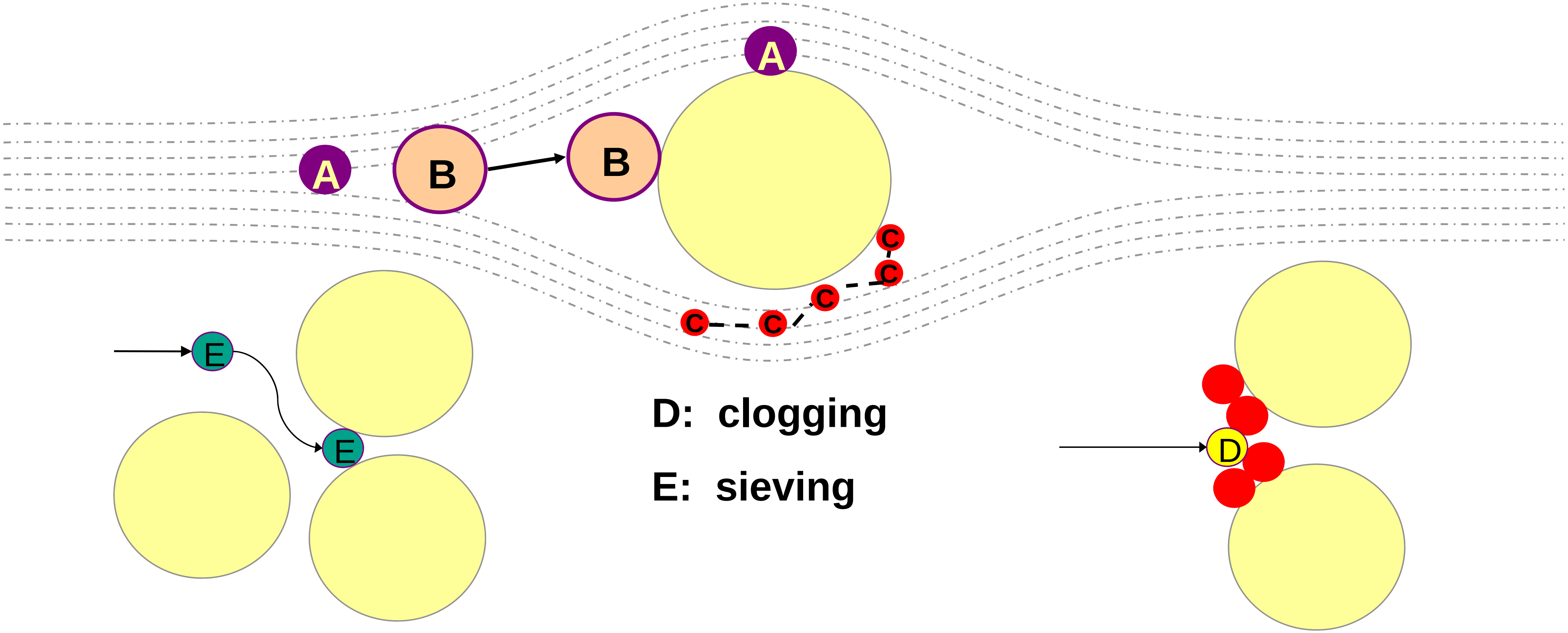
Filtration Effects I

A: direct interception

B: inertial impaction

C: diffusional deposition

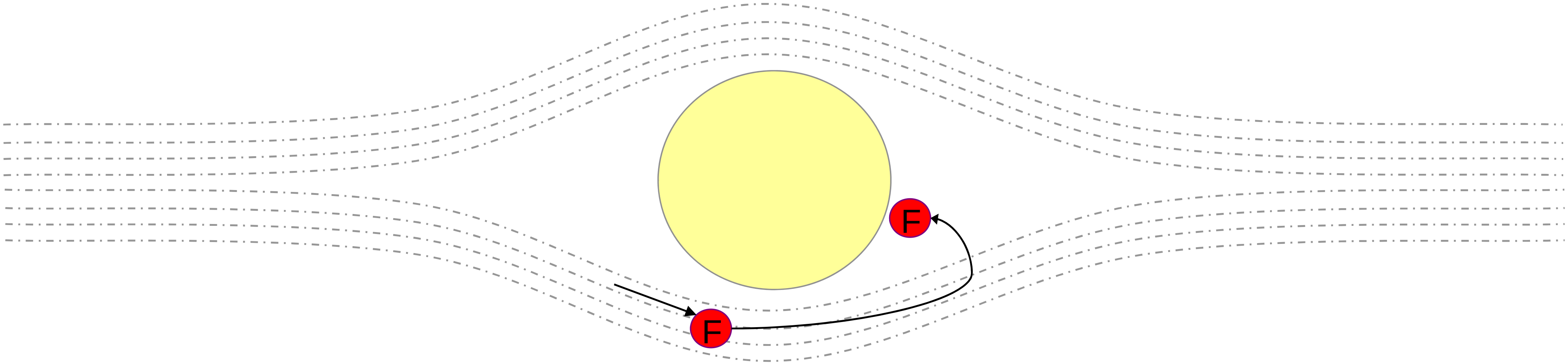


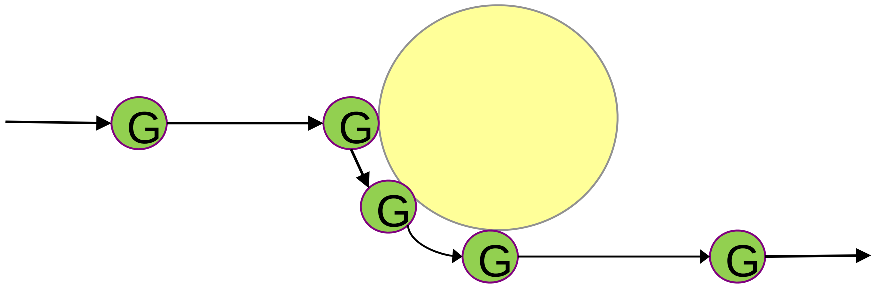
D: clogging

E: sieving

Filtration Effects II and modes of particle motion

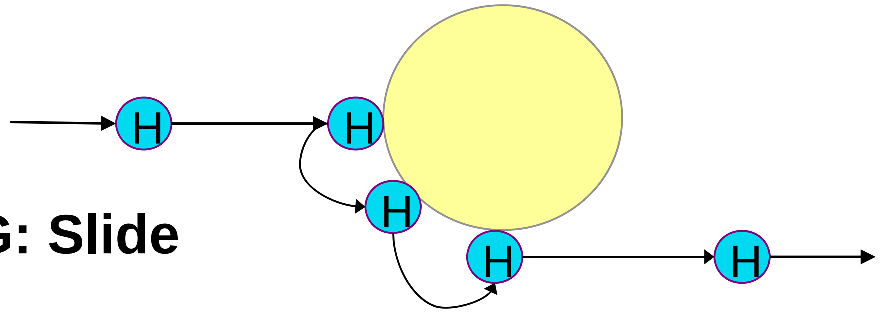
F: electrostatic attraction





G: Slide

H: Bounce



Description of particle motion

Friction with fluid Electric attraction Diffusive motion

$$d\vec{x} = \vec{v}\, dt,$$

$$d\vec{v} = -\gamma \times (\vec{v}(\vec{x}) - \vec{v}_\circ(\vec{x}))\, dt + \frac{Q\vec{E}_\circ(\vec{x})}{m} dt + \sigma \times d\vec{W}(t),$$

$$C_c = 1 + Kn \left(1.142 + 0.558 e^{-0.999/Kn}\right),$$

$$\gamma = 6\pi\rho\mu \frac{R}{C_c m},$$

$$\sigma^2 = \frac{2k_B T \gamma}{m},$$

$$\left\langle dW_i(t), dW_j(t) \right\rangle = \delta_{ij} dt,$$

$$Kn = \frac{\lambda}{R},$$

$$\lambda = \frac{k_B T}{\sqrt{32}\pi R^2 P}$$

t:	time
$\vec{x}$:	particle position
$\vec{v}$:	particle velocity
R:	particle radius
m:	particle mass
q:	particle charge
T:	ambient temperature
P:	total pressure
$d\vec{W}(t)$:	3d probability (Wiener) measure
γ:	friction coefficient
k_B:	Boltzmann constant
$\vec{E}_\circ$:	electric field
$\vec{v}_\circ$:	fluid velocity
ρ:	fluid density
μ:	fluid viscosity

A. Latz and A. Wiegmann, *Simulation of fluid particle separation in realistic three dimensional fiber structures*, Filtech, Düsseldorf, October 2003.

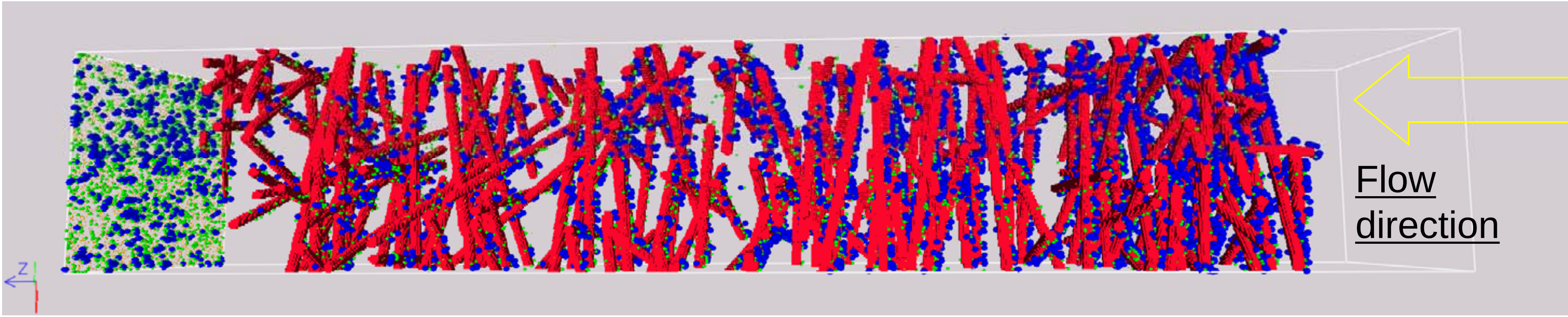
Deposition effects

$\alpha = 0.05$,

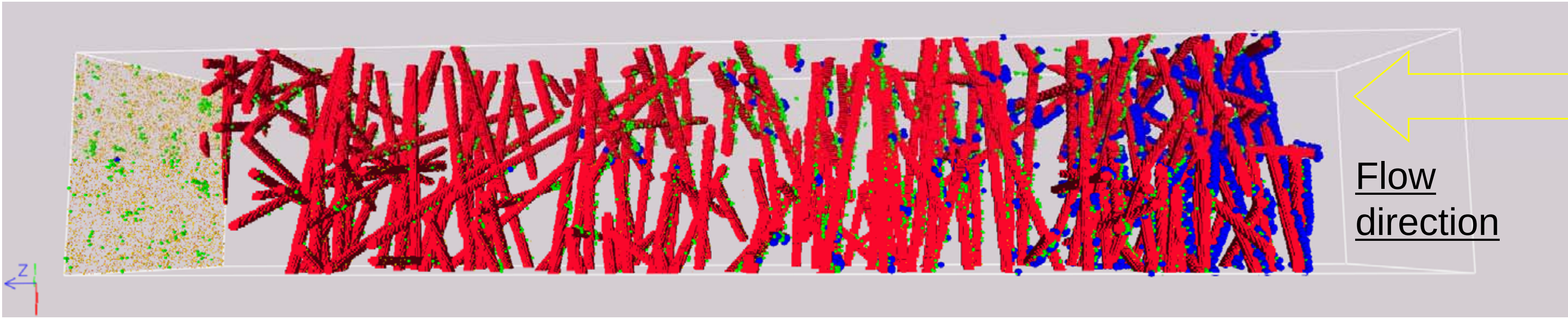
$d_F = 14$,

$v = 0.1 m/s$

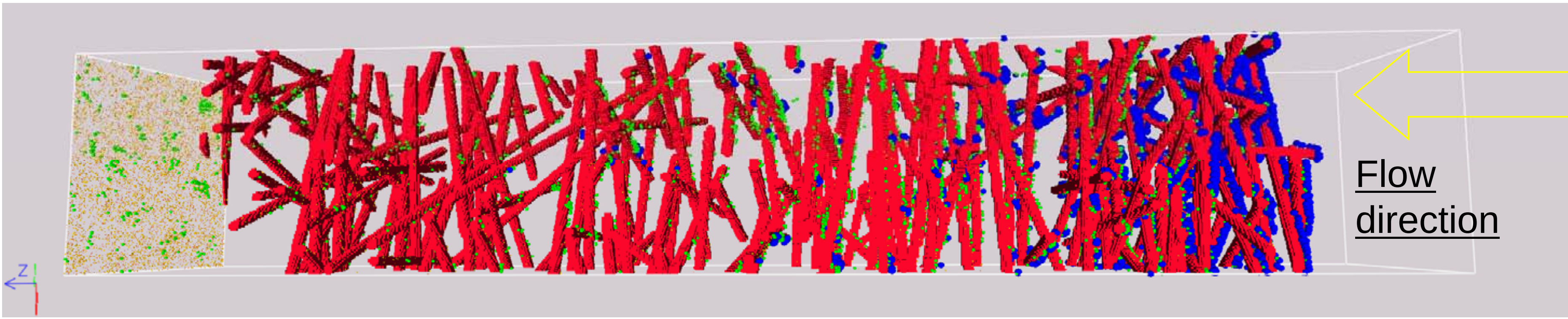
Interception



Interception
+ Impaction



Interception
+ Impaction
+ Diffusion



Velocity Effects

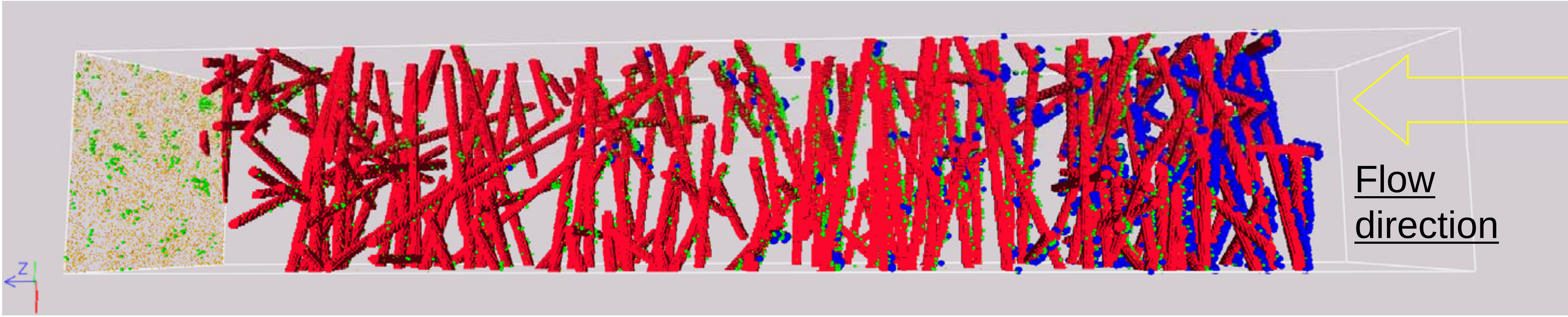
$\alpha = 0.05$,

dF = 14,

Interception + Impaction + Diffusion

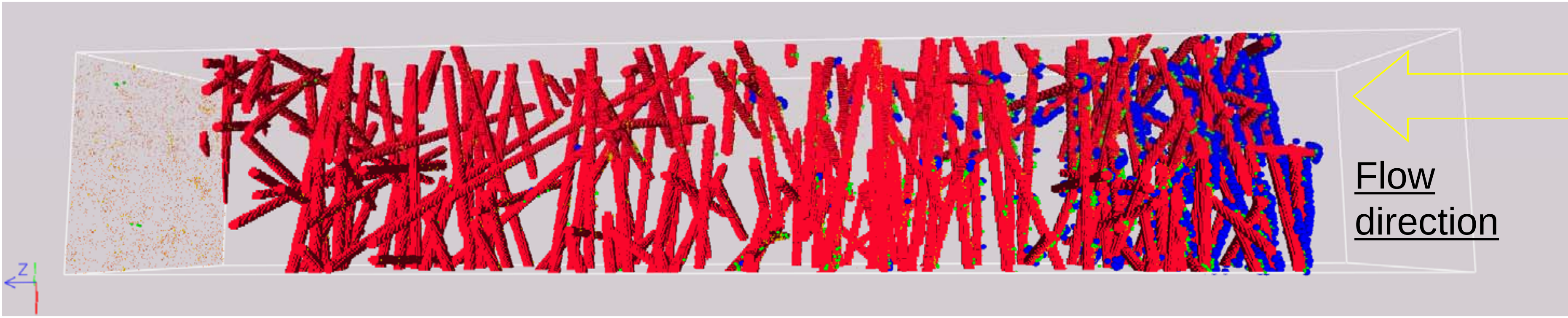
Velocity

v = 0.1 m/s



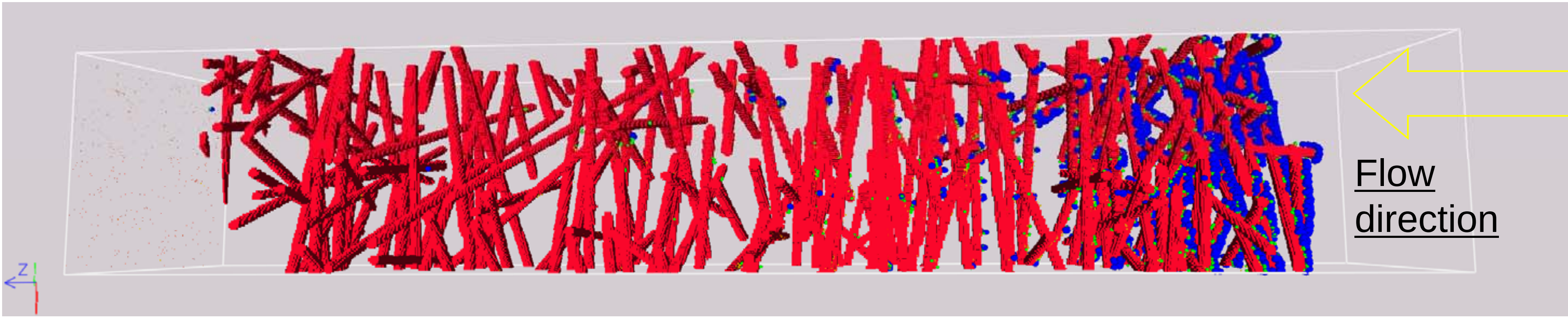
Velocity

v = 1 m/s



Velocity

v= 10 m/s



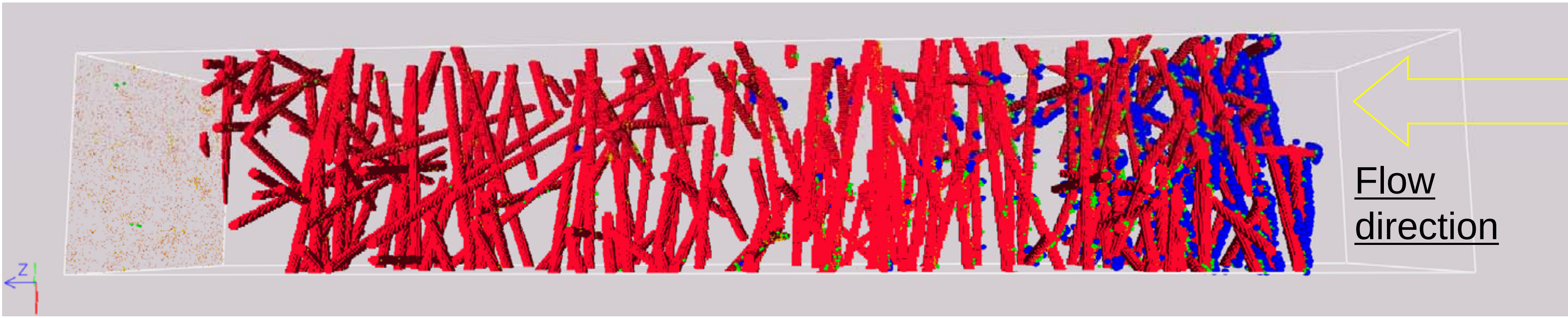
Effect of grammage (here: SVF)

dF = 14,

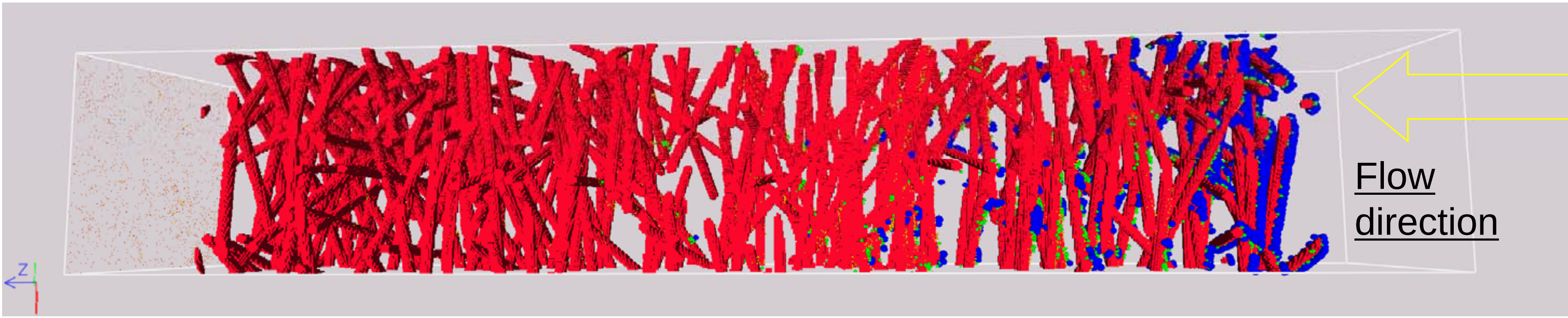
v = 1 m/s,

Interception + Impaction + Diffusion

SVF α=0.05

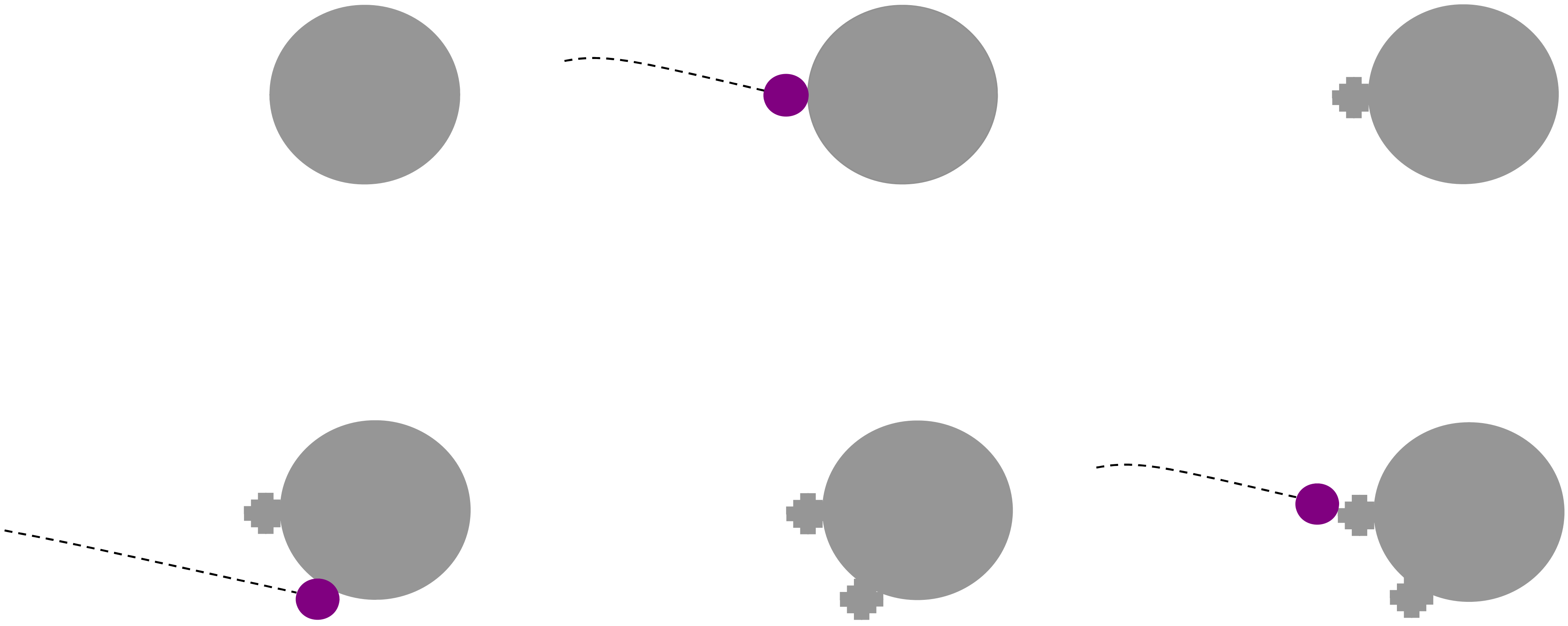


SVF α=0.07



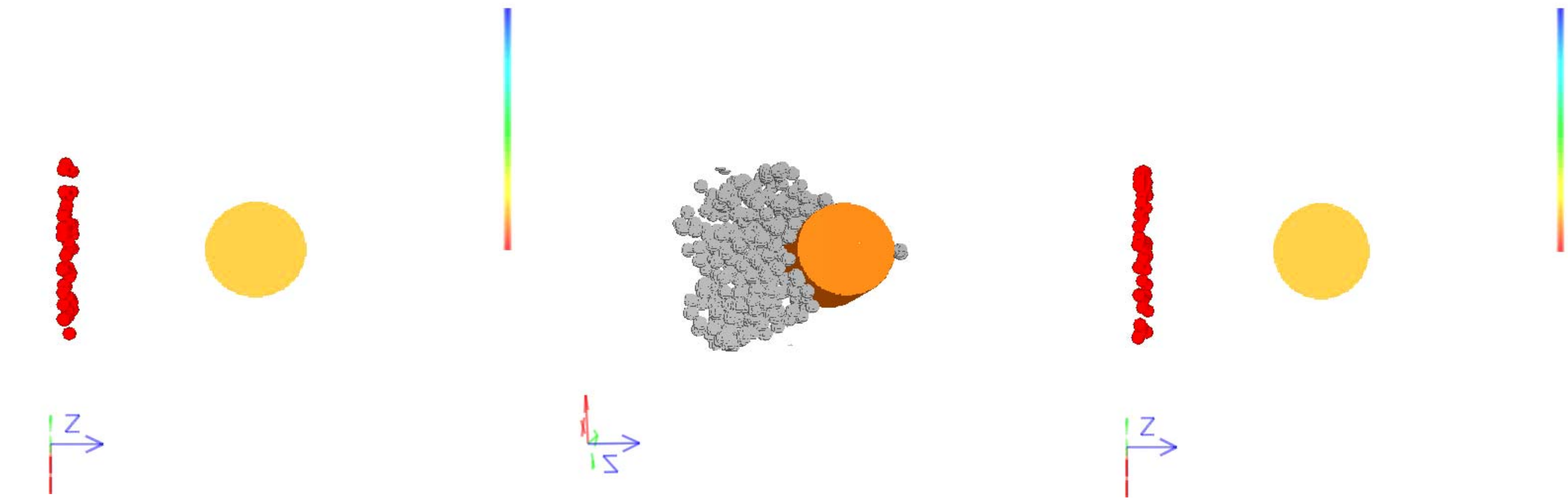
SVF α=0.1

Nano-Modus

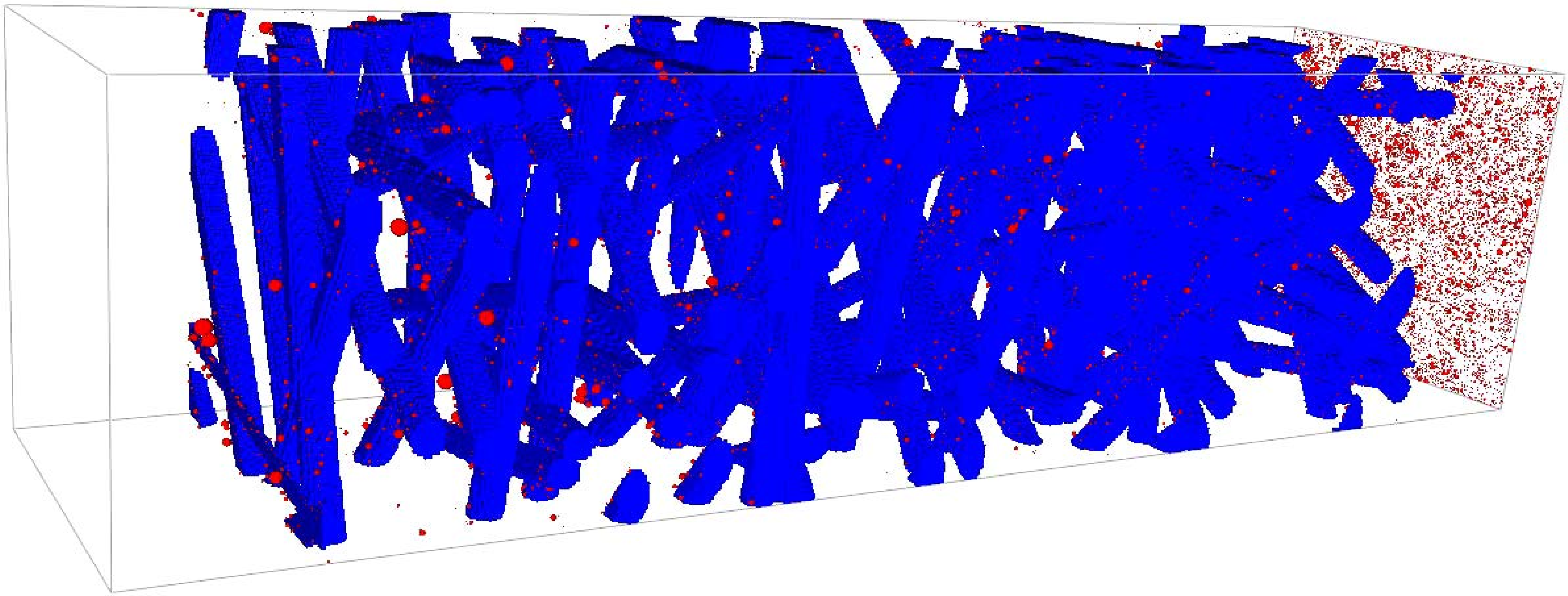


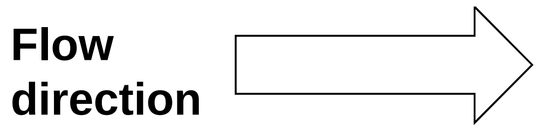
Influence of electric charge (air filtration)

No charges | Low charges | High charges



Transition from depth filtration to cake filtration in a single simulation

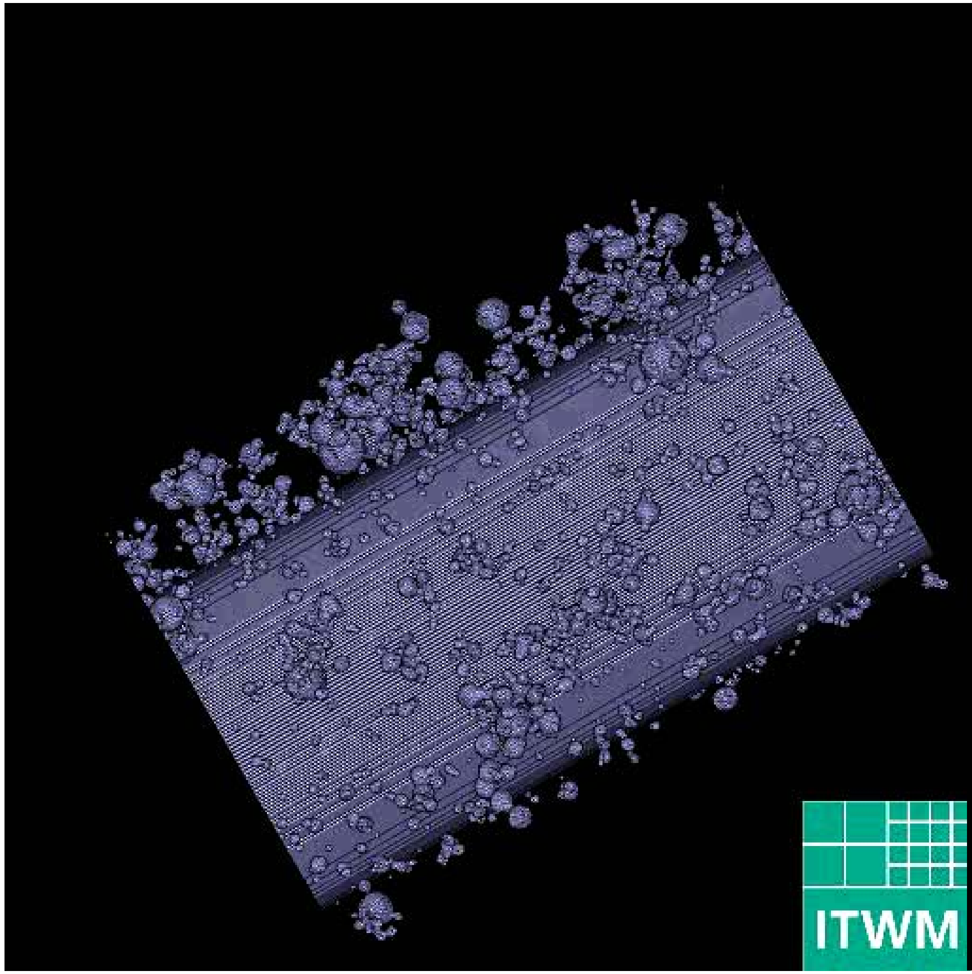




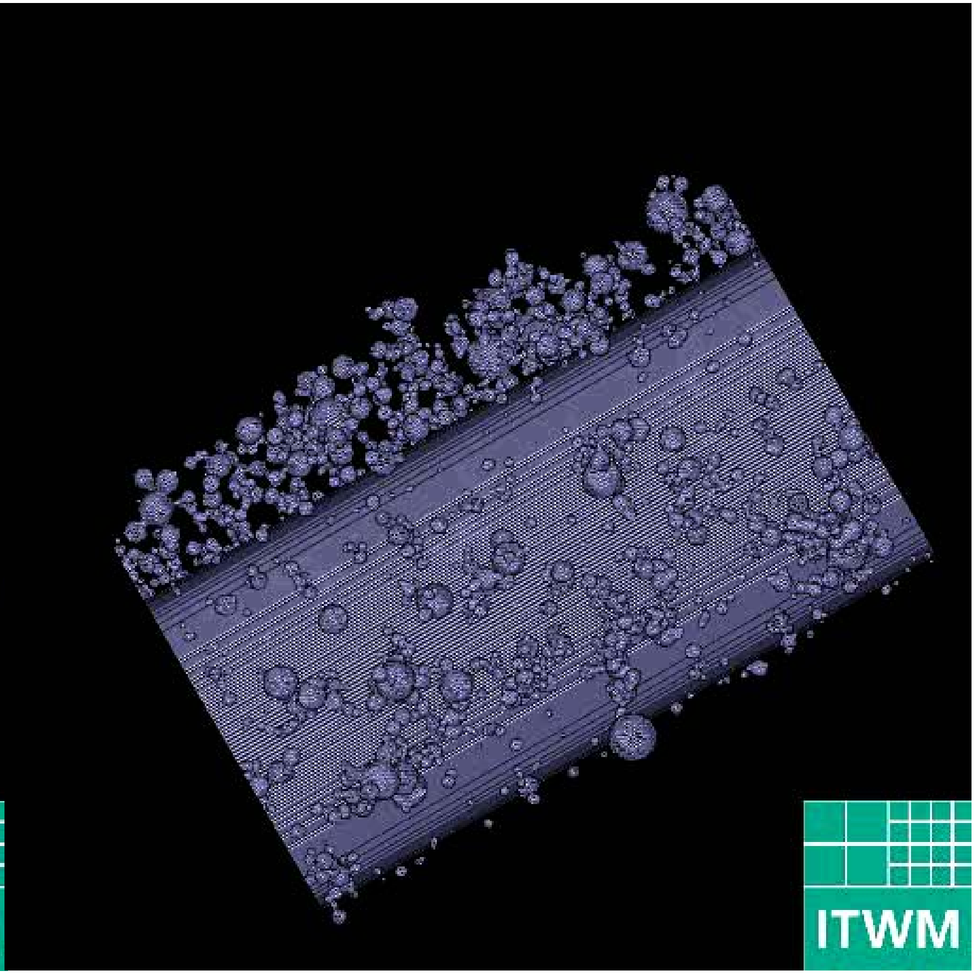
- Particles resolved by the cubes
- Filtration by “caught on first touch”
- Recompute flow after “batch” of particles
- Clogging in depth and cake filtration

Nano Simulations

1.67cm/sec



10.0cm/sec



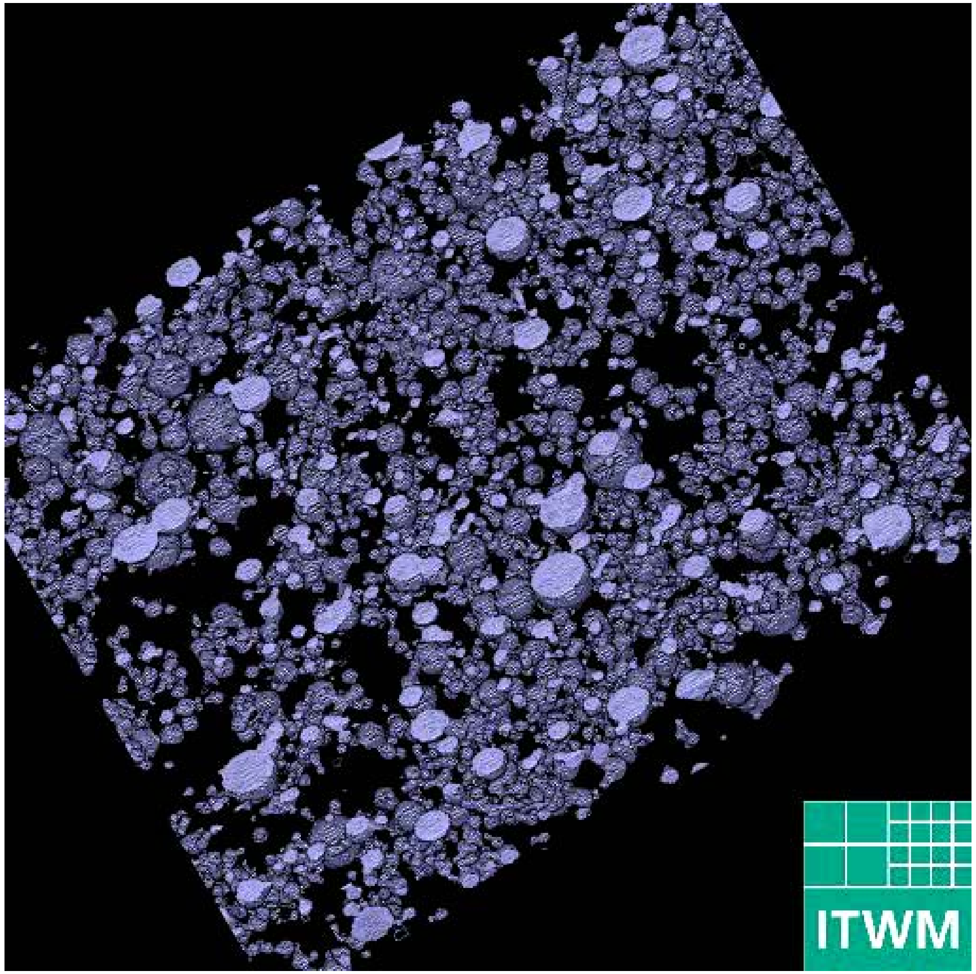
Nano Simulations

- **Deposition patterns and porosity depend on far field velocity, particle size distribution, etc.**

Result:

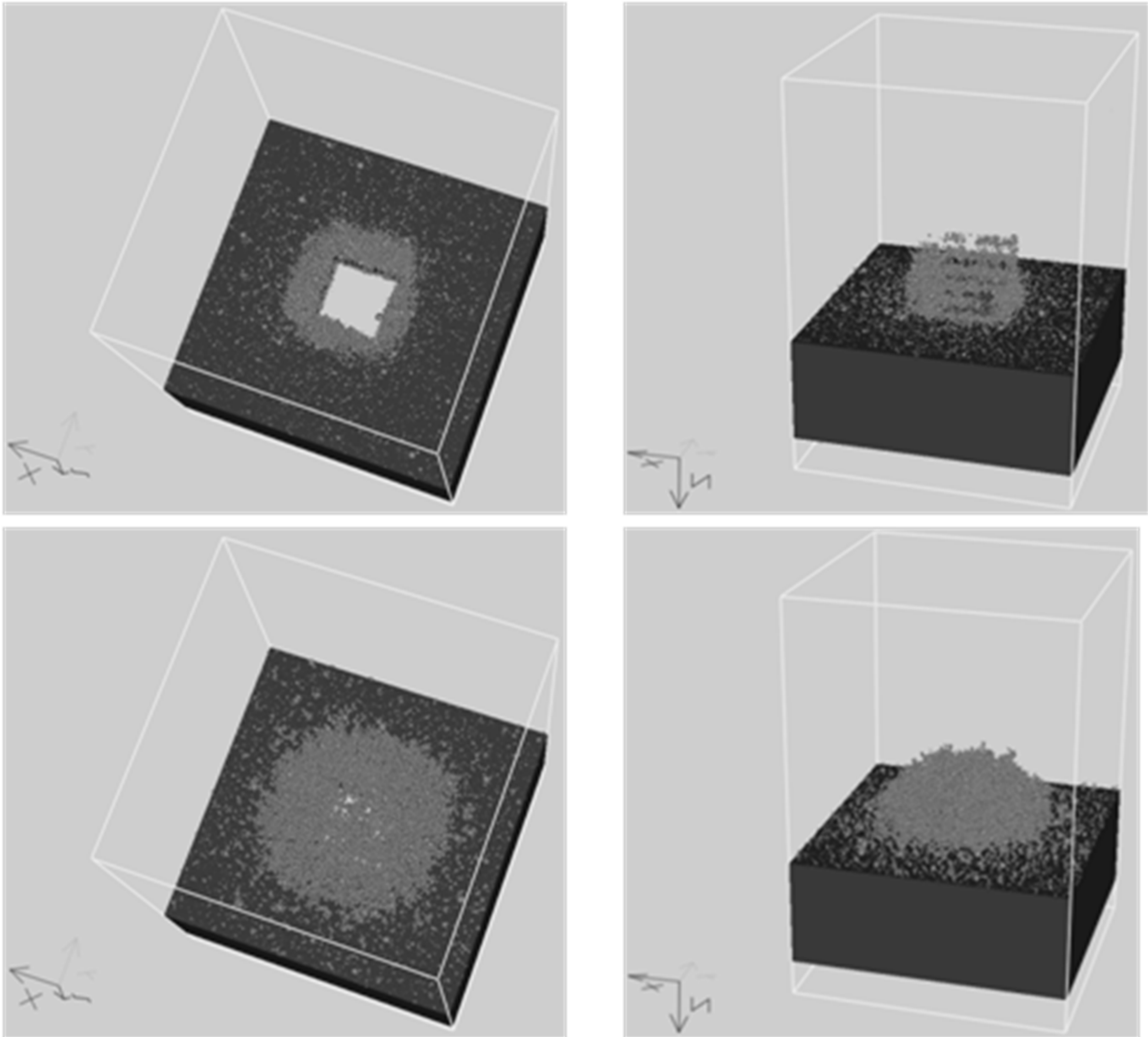
- **Find minimal porosity and permeability of the soot layers, s_{max} and κ_{min}**
- **Derivation by layers from single fiber highly resolved simulations**

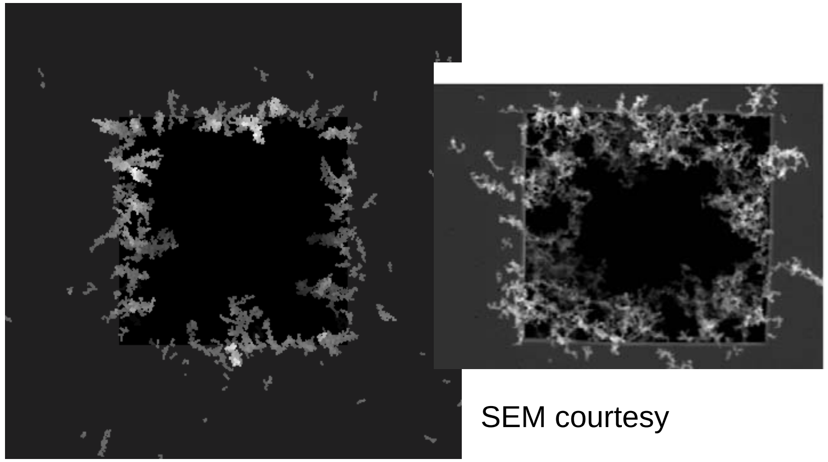
Soot Layer Cut-Out



S. Rief, D. Kehrwald, A. Latz, K. Schmidt and A. Wiegmann, *Virtual Diesel Particulate Filters: Simulation of the Structure, Exhaust Gas Flow and Particle Deposition*, Filtration, No. 4, Vol. 9, 2009, pp 315-320.

3d view, virtual SEM and real SEM (with FIB) of soot on micro sieve

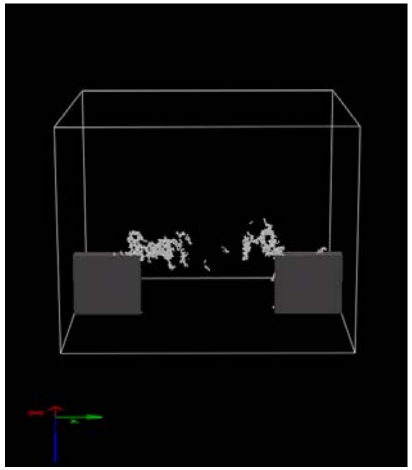


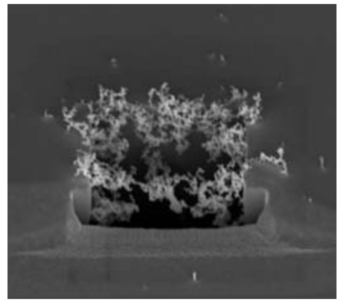


SEM courtesy

H. Schomburg,

Robert Bosch GmbH





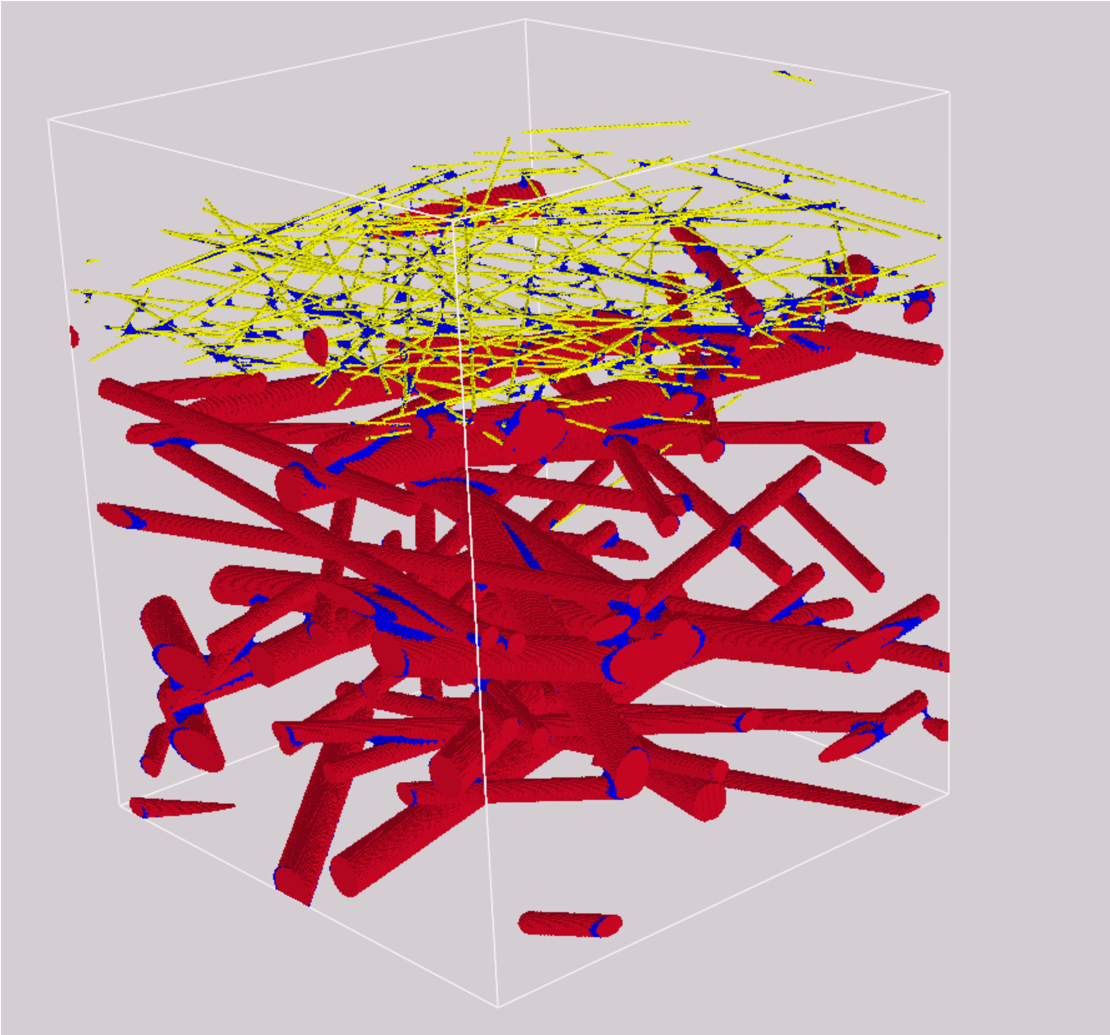
FIB & SEM courtesy

H. Schomburg,

Robert Bosch GmbH

Dissertation Kilian Schmidt, Kaiserslautern Technical University, 2011.

Nonwoven with binder and layer of nano fibers



5.0 µm fibers (red)

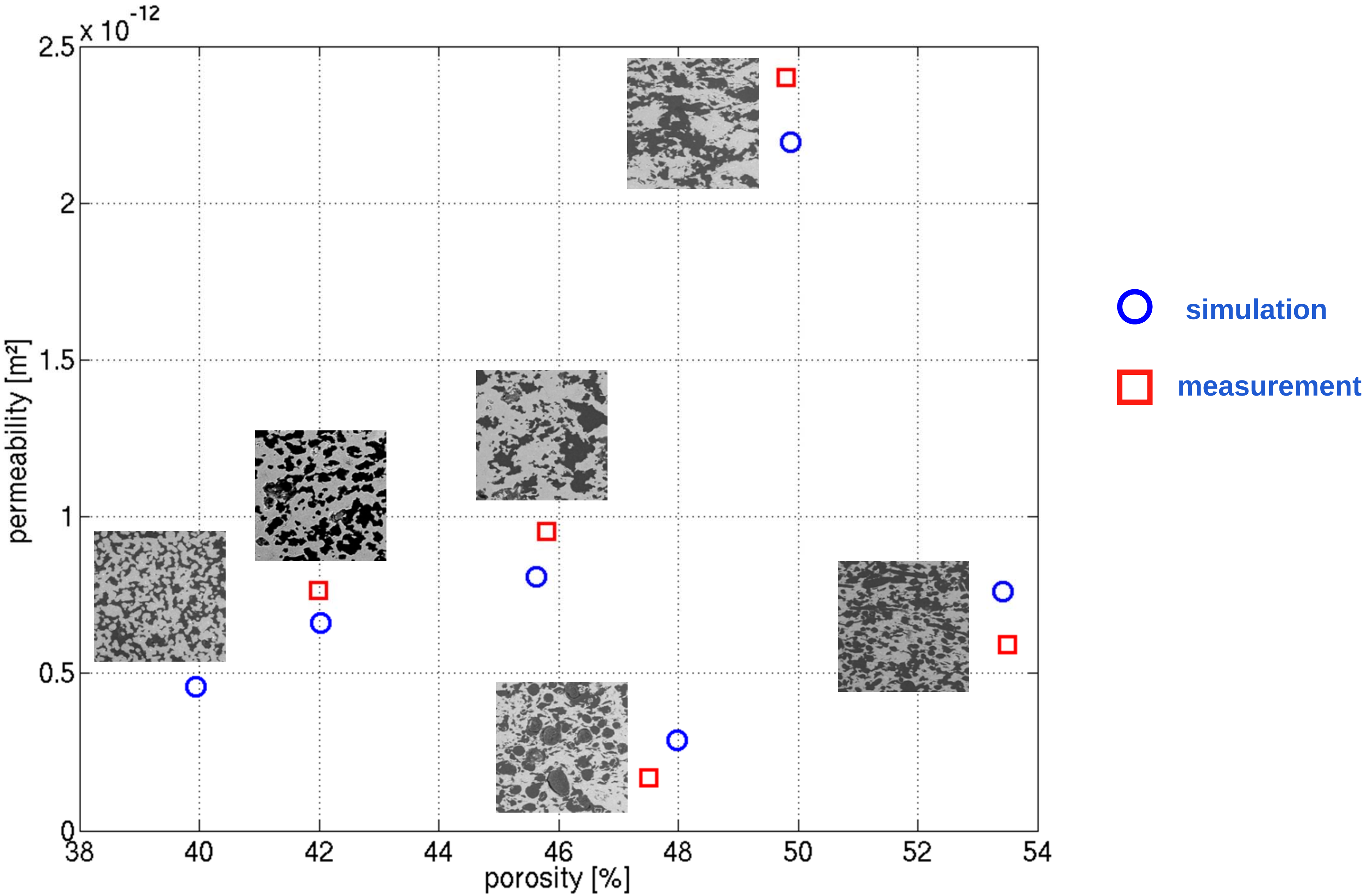
2.5 µm fibers (red)

0.3 µm fibers (yellow)

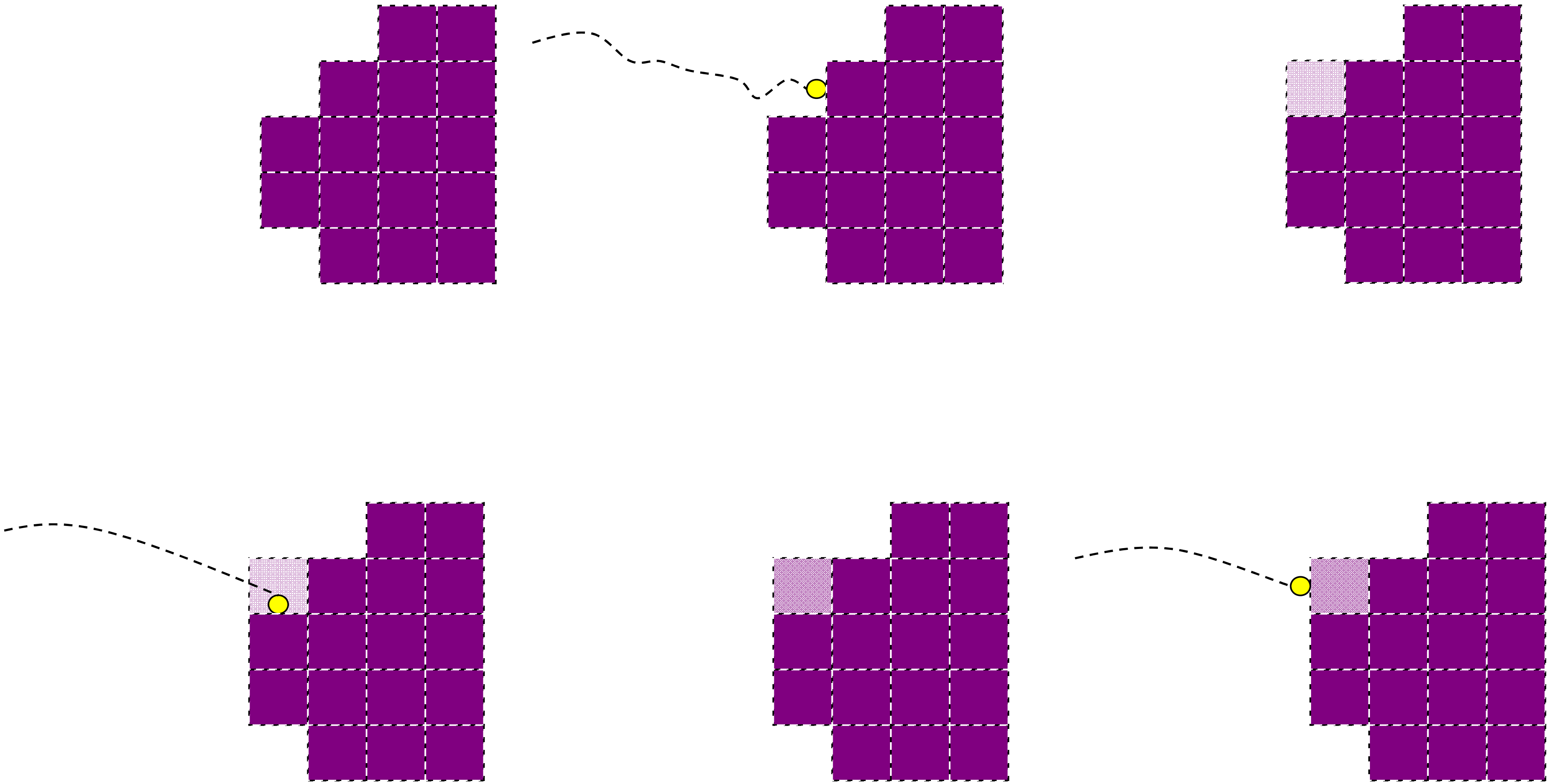
2 vol % binder (blue)

L. Cheng et al., Filtech 2009.

Computed and measured porosities and permeabilities of real & generated structures (from polished micrograph sections)



Mikro-Modus



Andreas Wiegmann

Stationary Flow with unresolved particles: Stokes-Brinkmann eqs

$$-\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \nabla p + \kappa^{-1}\vec{u} = \vec{\mathbf{f}} \text{ (momentum balance)}$$
$$\nabla\cdot\vec{u} = 0 \text{ (mass conservation)}$$
$$\vec{u} = 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)}$$

$\vec{\mathbf{f}} = (0, 0, f)$: force in flow(z)-direction,

$\kappa = \kappa_{min} \max\{1, s_{max}/s\}$: porous voxel permeability,

s : solid volume fraction in a voxel

$\vec{u}$: velocity,

μ : fluid viscosity,

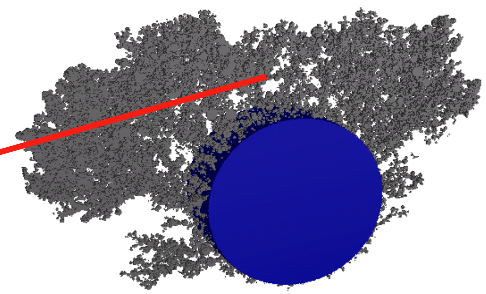
p : pressure and

Γ : fiber or deposited particle surfaces.

Solid volume fraction in voxel is increased until s_{max} is reached. Voxel becomes “collision-solid”. Neighbor voxels svf starts increasing upon particle arrival

O. Iliev, V. Laptev: *On Numerical Simulation of Flow through Oil Filters*, J. Computers and Visualization in Science, vol. 6, 2004.139-146.

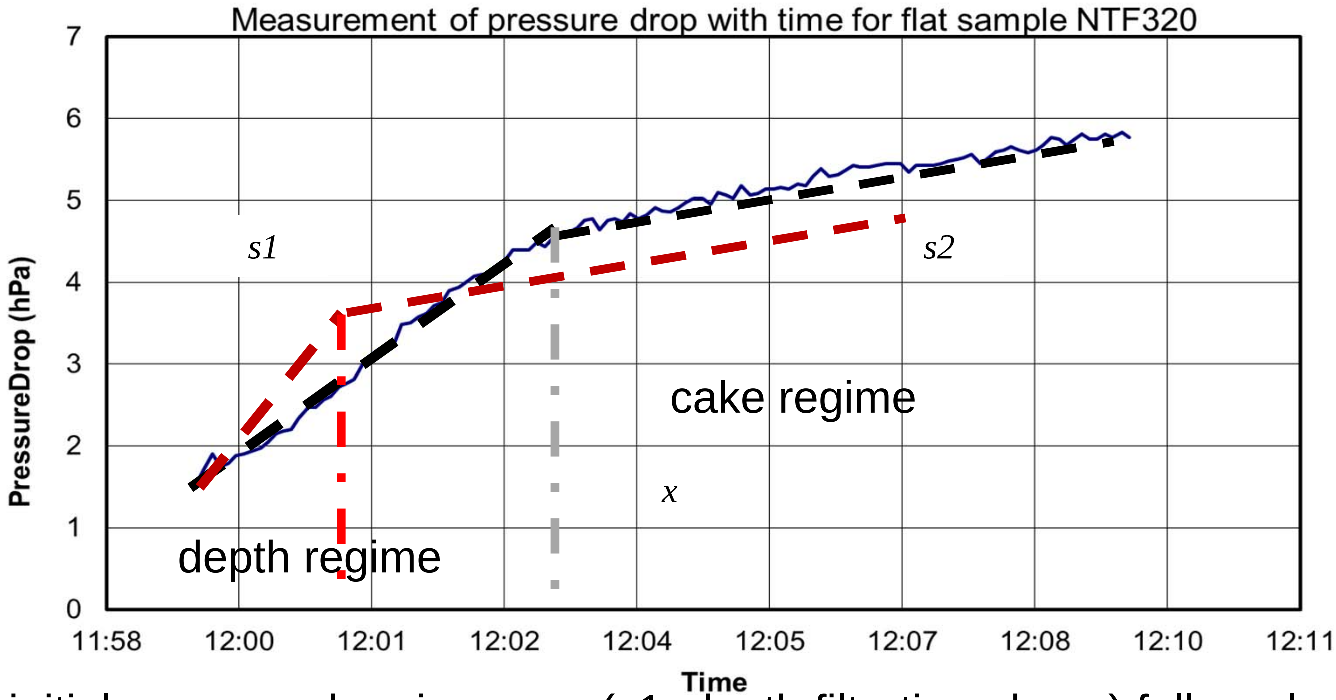
Particle Filtration Tasks: Multi-scale approach



Soot deposited on a single fiber
- resolved soot simulation -
identifies maximum packing density
and corresponding flow resistivity

Soot deposited in ceramic DPF
 - soot as porous media simulation –
requires maximum soot packing density
and corresponding flow resistivity

Depth vs cake filtration regime for DPF simulations



After fast initial pressure drop increase (s1, depth filtration phase) follows long slower pressure drop increase (s2, cake filtration phase)

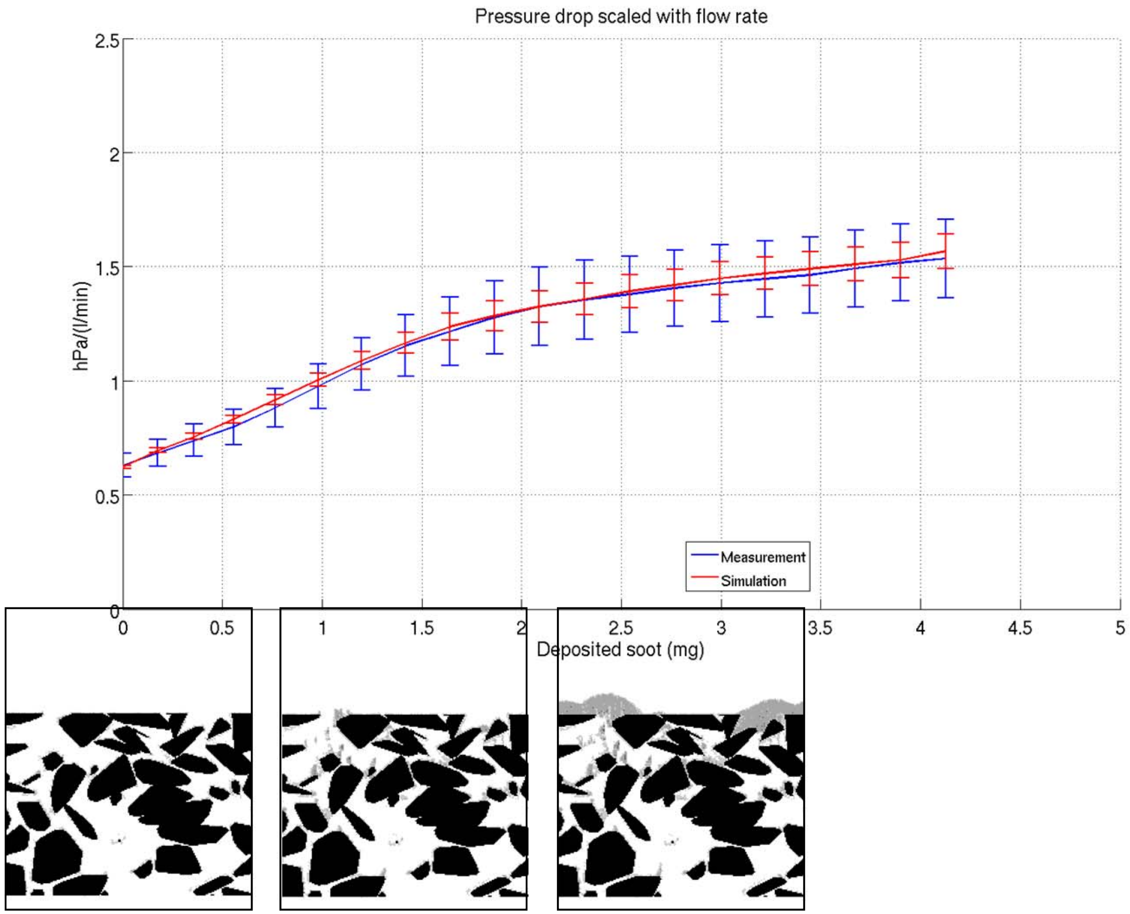
Objectives:

A. Match this behavior in simulations

B. Reduce depth filtration phase to lower overall pressure drop

C. Check that flat sample results are significant also for honeycombs (Fraunhofer IKTS)

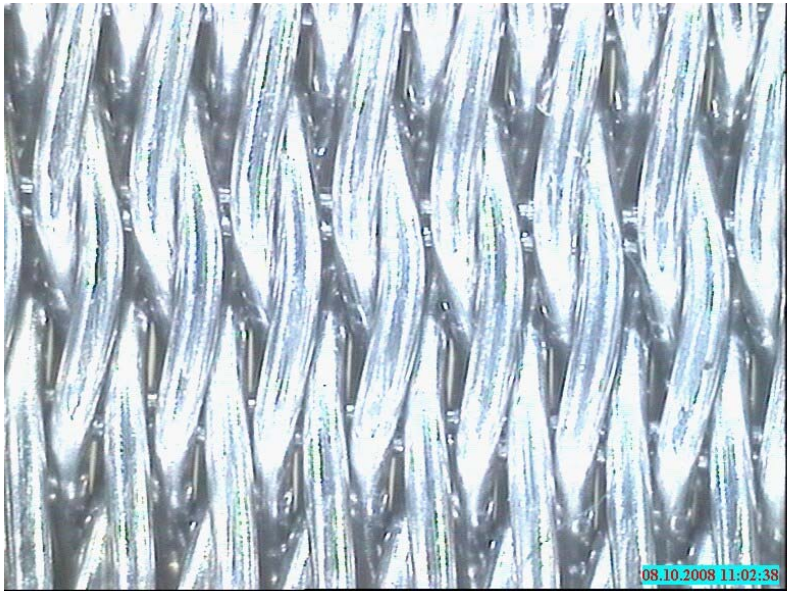
Horizonal layers

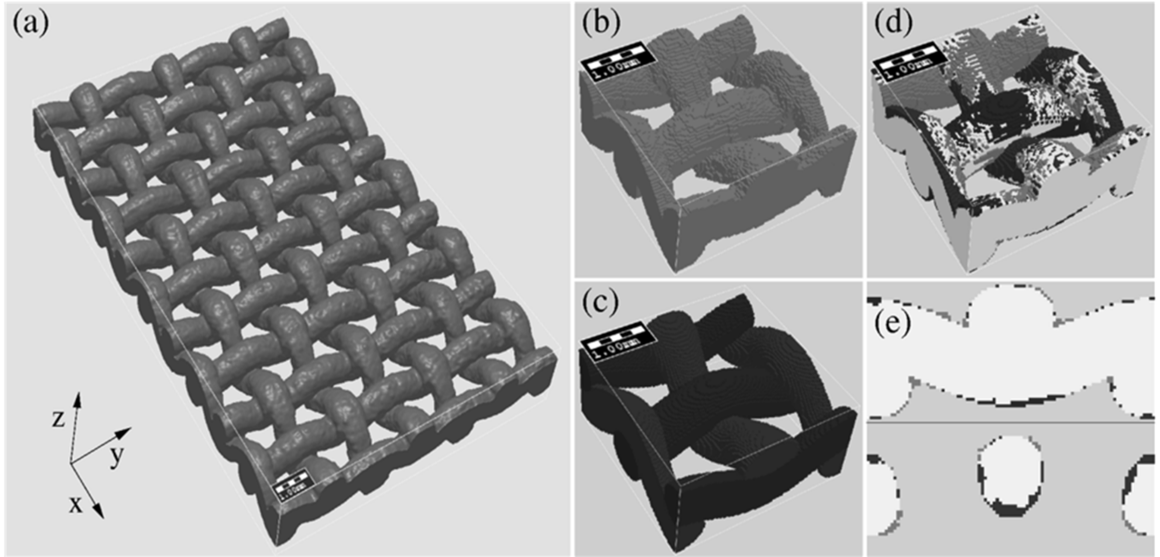


- Experimental and simulated pressure drop evolution with error bars induced by 5 measurements and 5 different realizations of the virtual structure.
- Match achieved by introducing different Brinkman parameters for depth and cake filtration.

L. Cheng et al., WFC 11, 2012.

Reconstruction of Woven

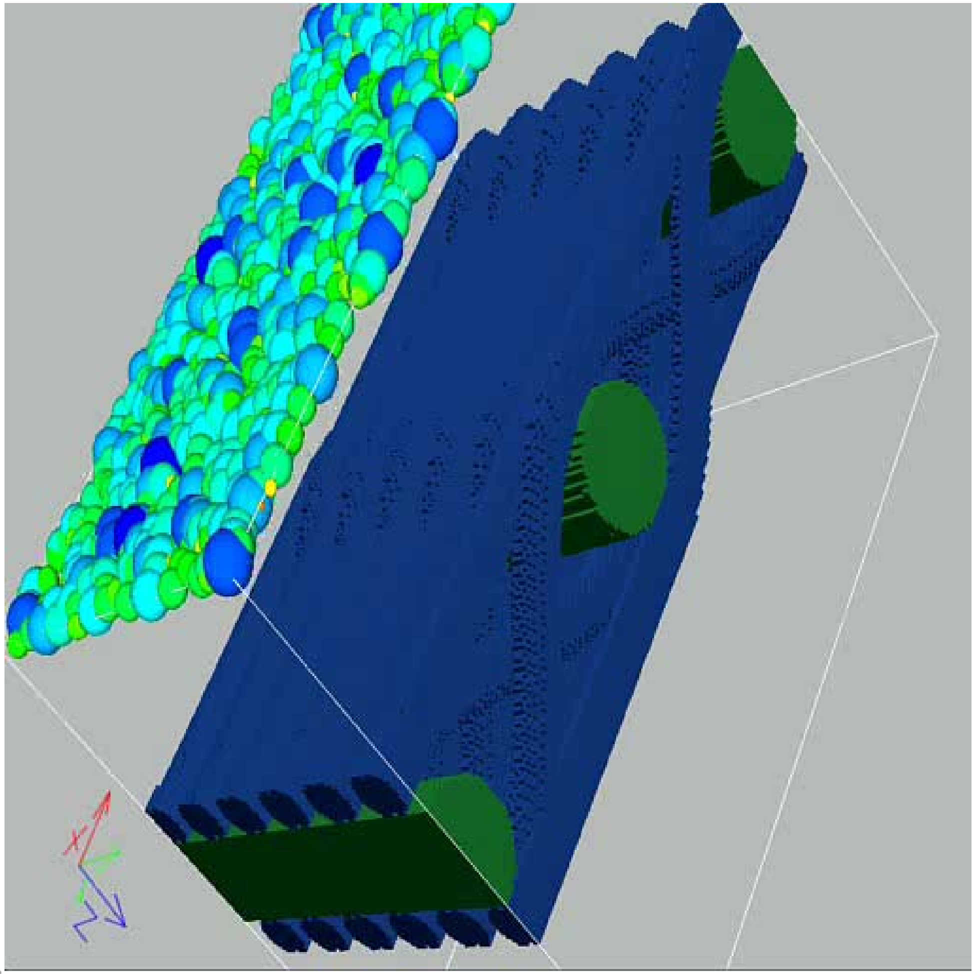




E. Glatt, S. Rief, A. Wiegmann, M. Knefel and E. Wegenke, *Structure and pressure drop of real and virtual metal wire meshes*, Bericht des Fraunhofer ITWM, Nr. 157, 2009.

Surface filtration in metal wire cloth

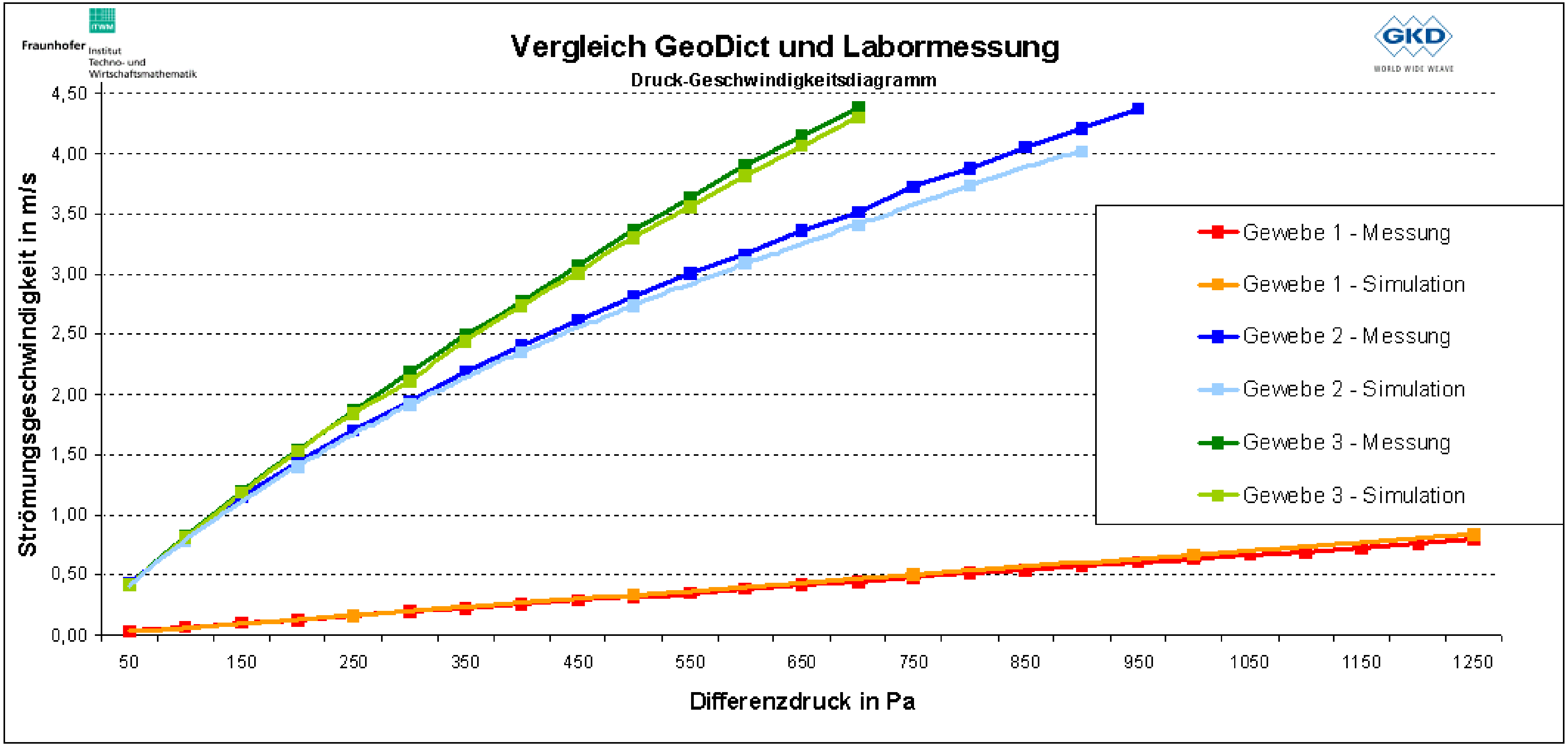
- Filtration by “sieving”
- Recompute flow after “batch” of particles
- Cake formation in surface filtration
- Filter Cake more efficient filter than metal wire mesh
- Pressure drop increase also available



Computed & animated with GEO DICT

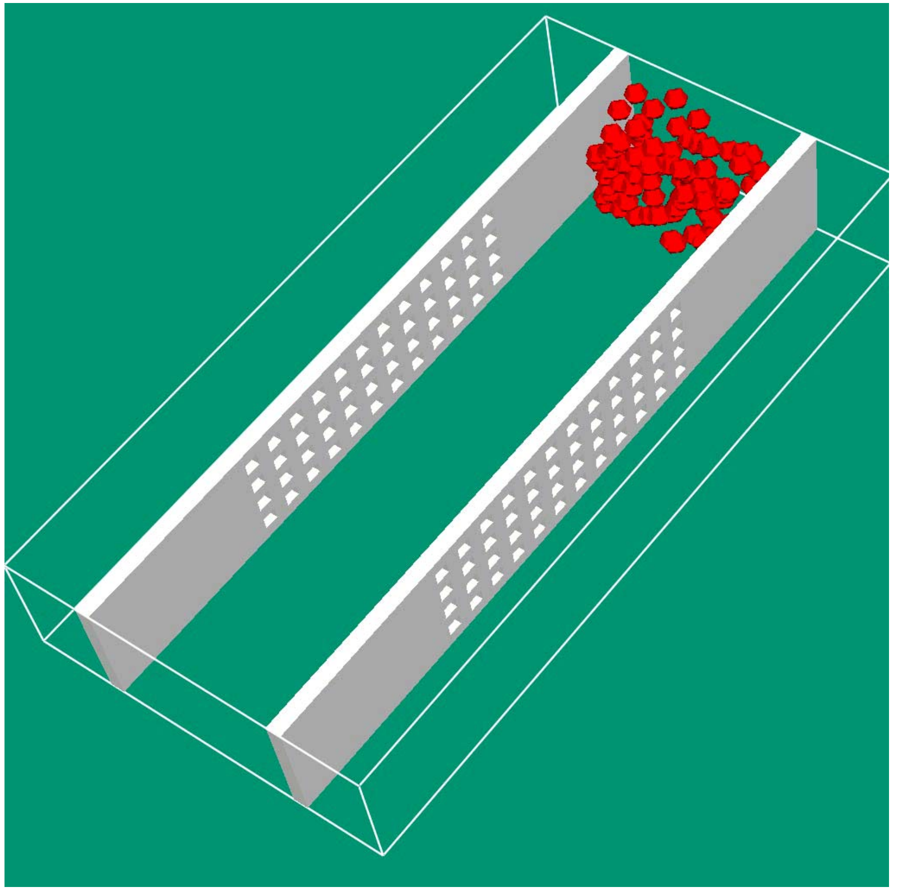
Courtesy M. Knefel, Gebr. Kufferath AG.

Measured vs Simulated pressure drop for GKD meshes

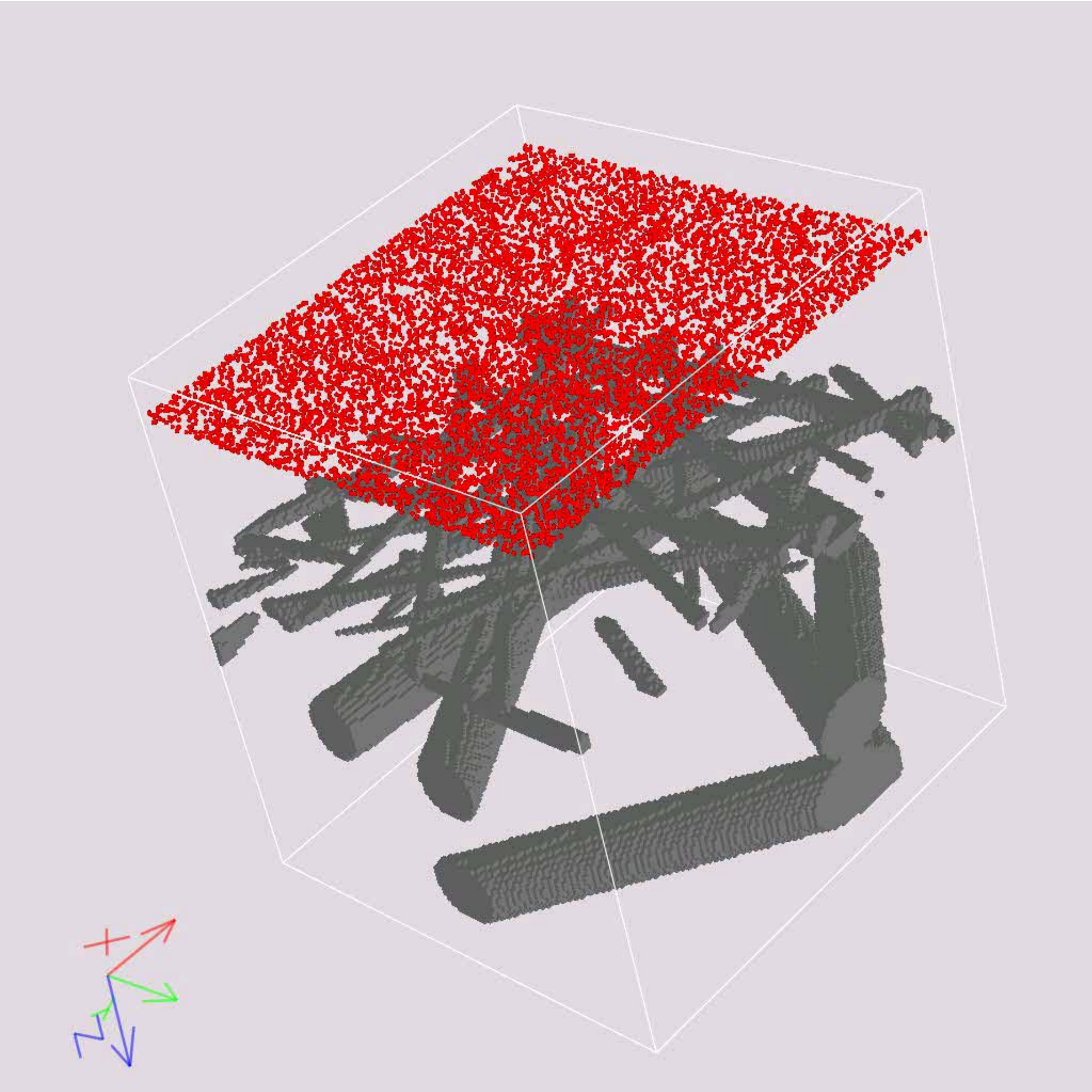


E. Glatt, S. Rief, A. Wiegmann, M. Knefel and E. Wegenke, *Structure and pressure drop of real and virtual metal wire meshes*, Bericht des Fraunhofer ITWM, Nr. 157, 2009.

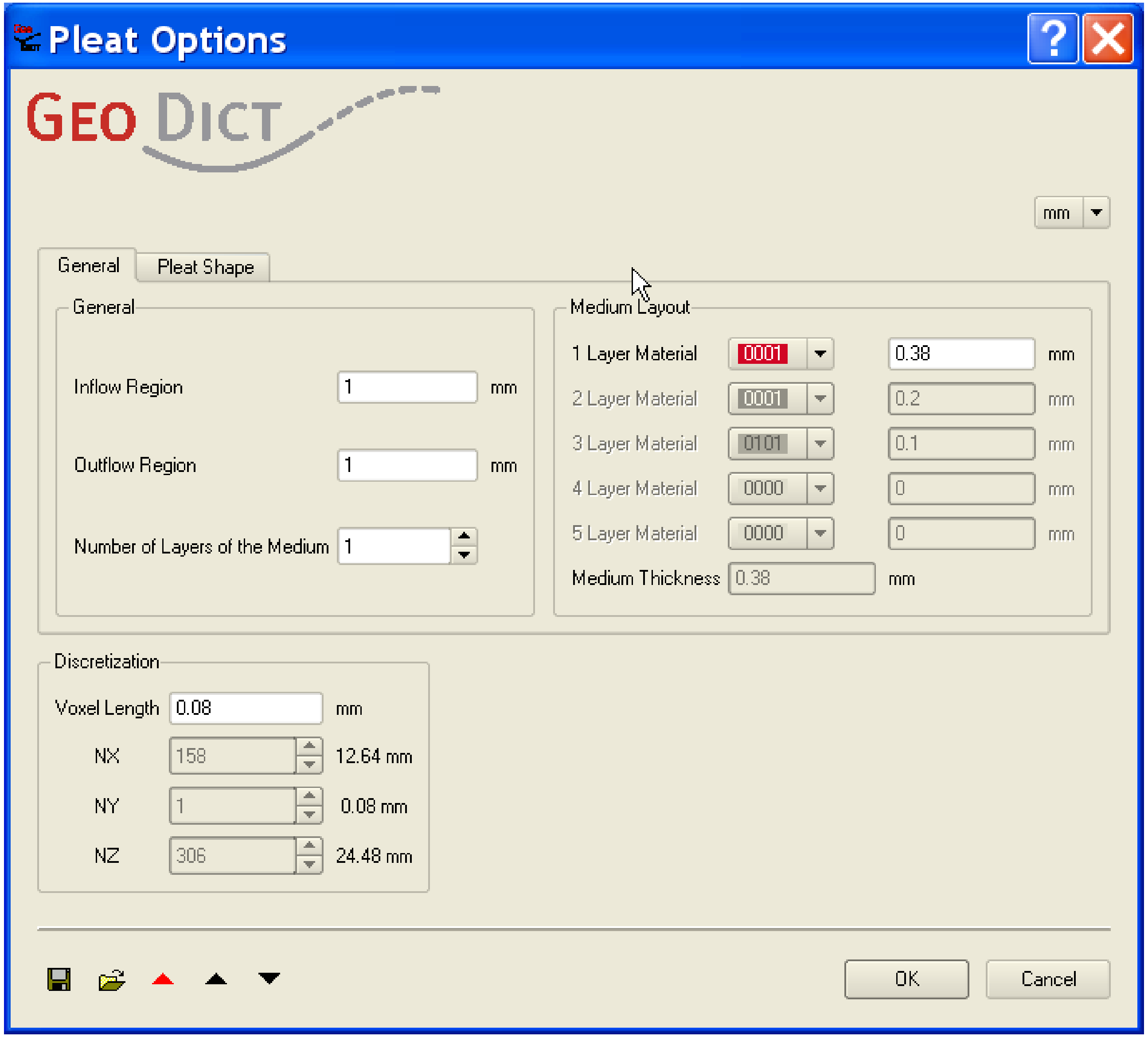
Cross Flow Filtration

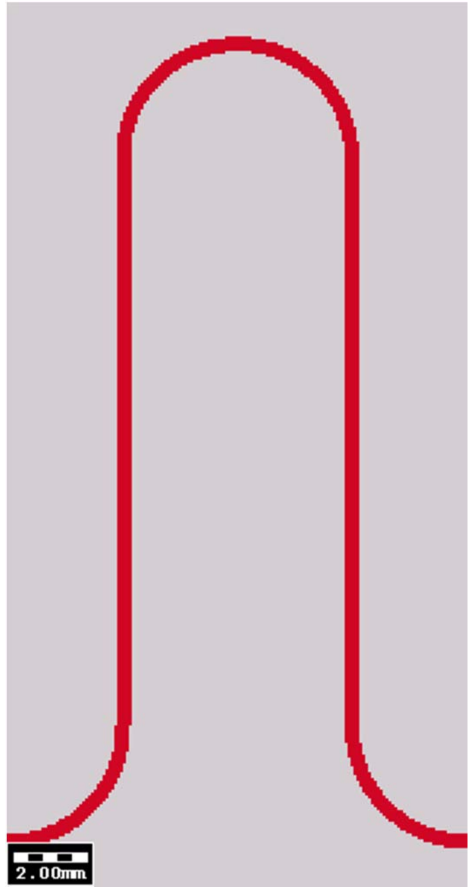


Pulse cleaning

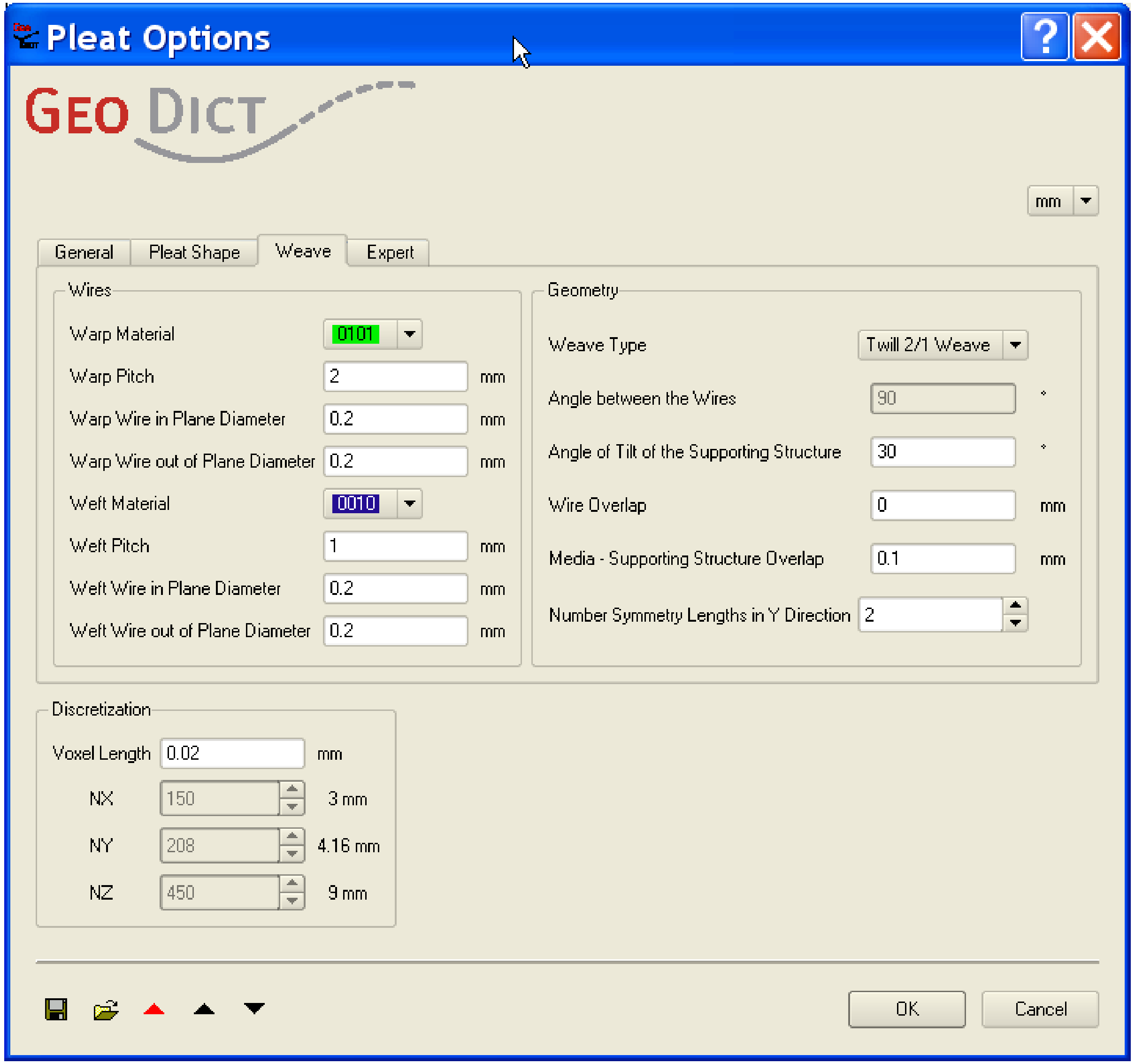


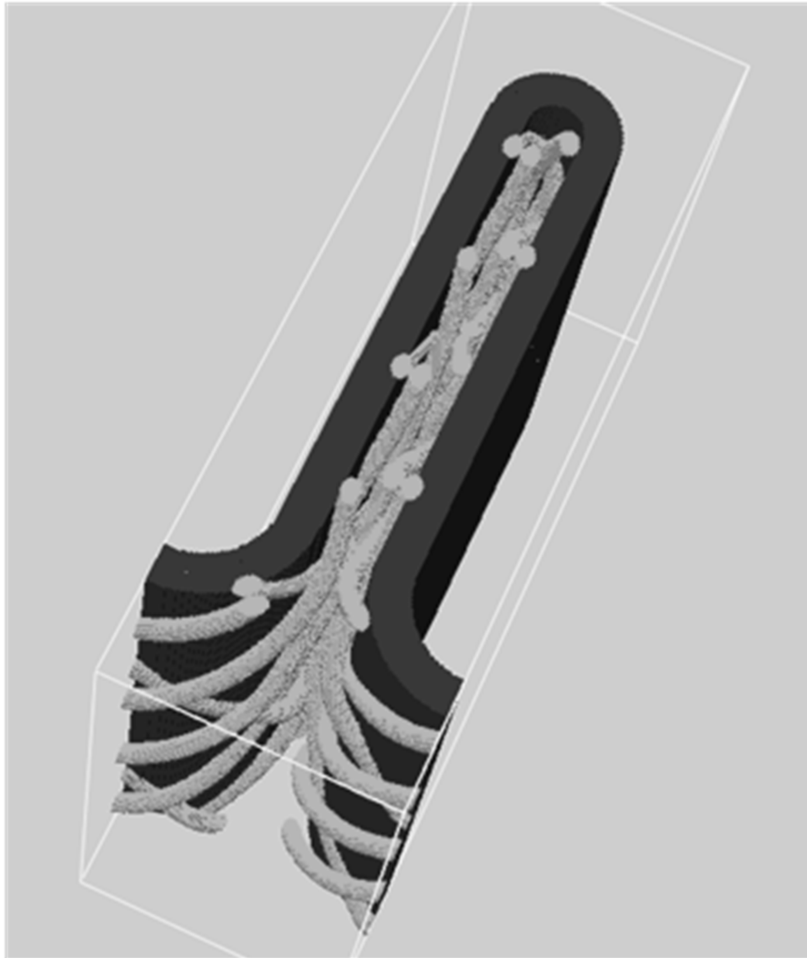
General Pleat Options





Weave Pleat Options





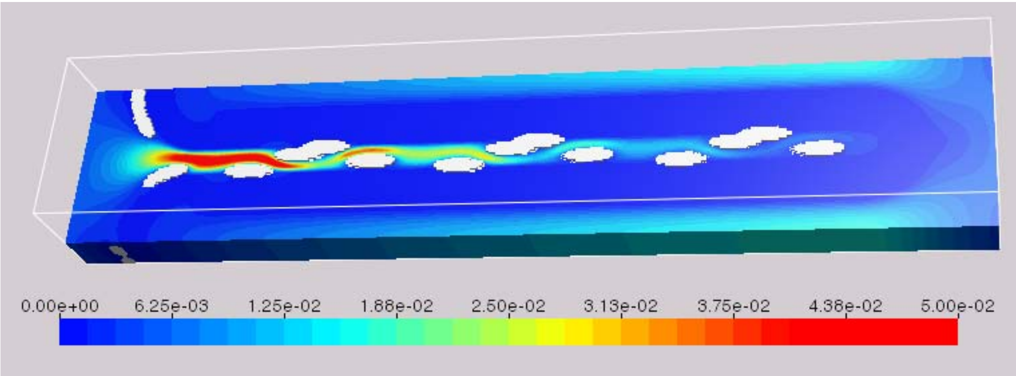
MATH 2 MARKET

Fraunhofer ITWM

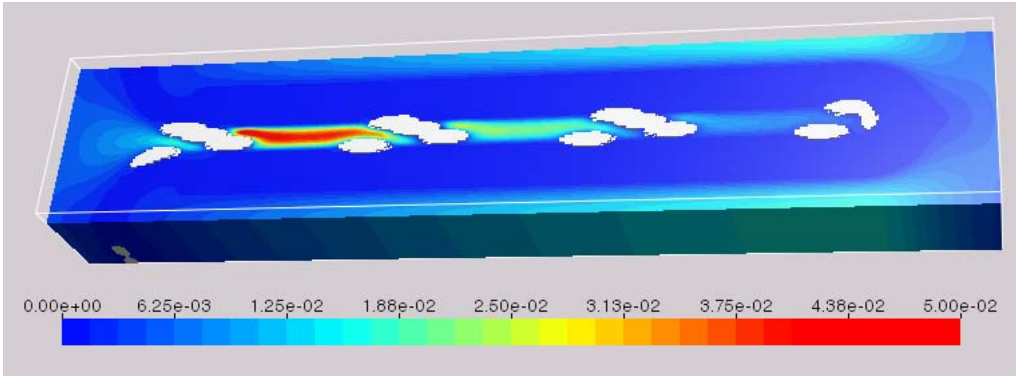
Andreas Wiegmann

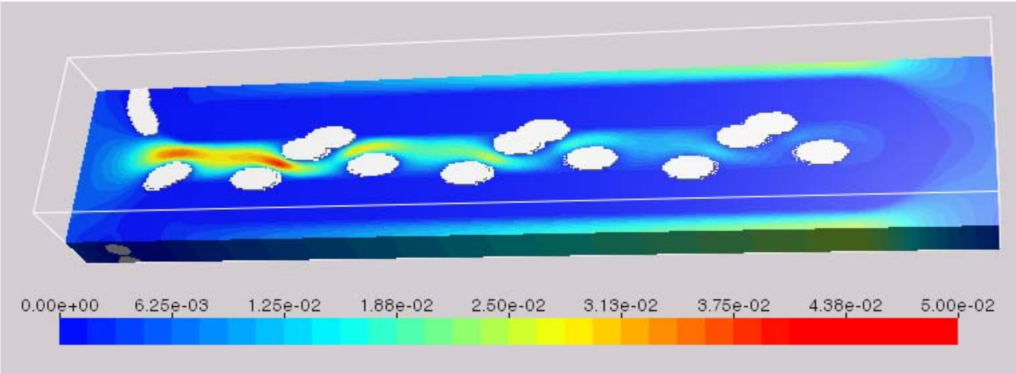
Oil flow in pleats with support structure: velocity

- Velocity: 0.15 m/s
- Oil: density 850 kg/m³ viscosity 0.17 m²/s
- Same pleat count
- Different in- and outflow channel widths
- Grid resolution 40 µm
- 50 x 70 x 380 cells

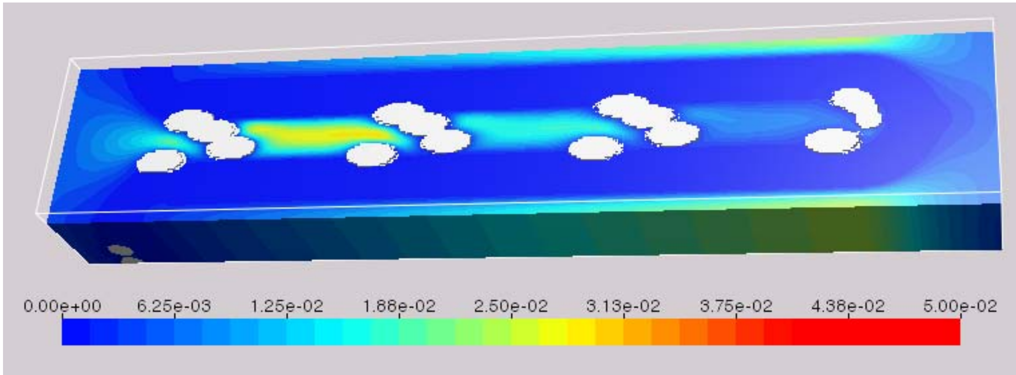


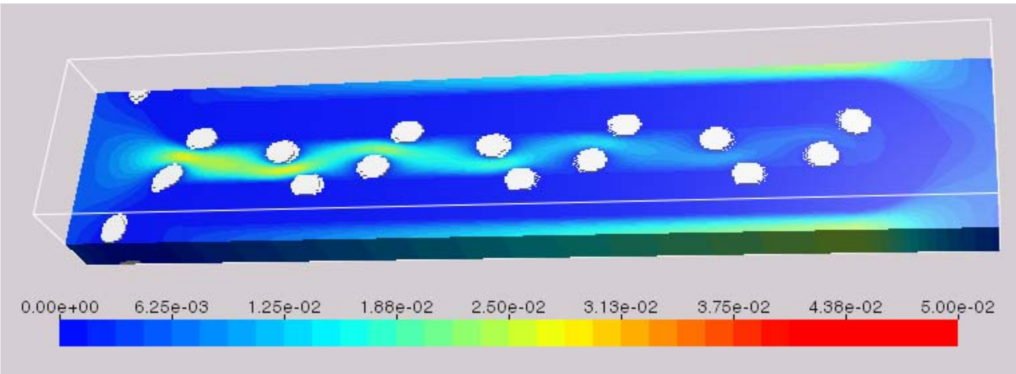
Narrow Channel



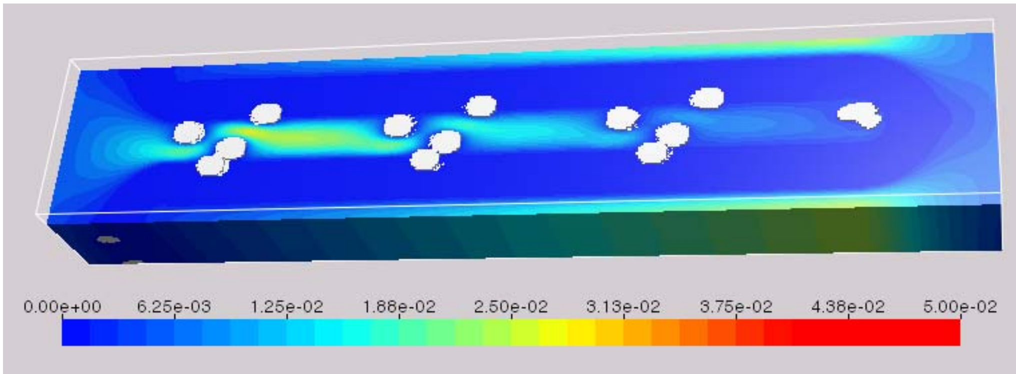


Thick Wire



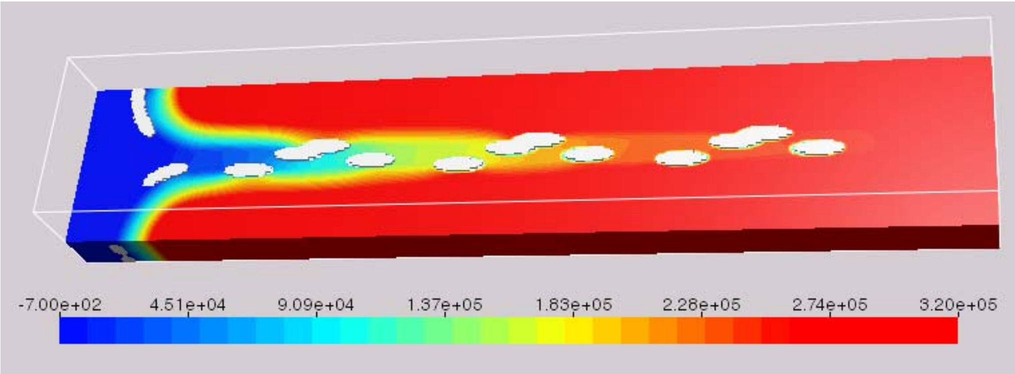


Thin Wire



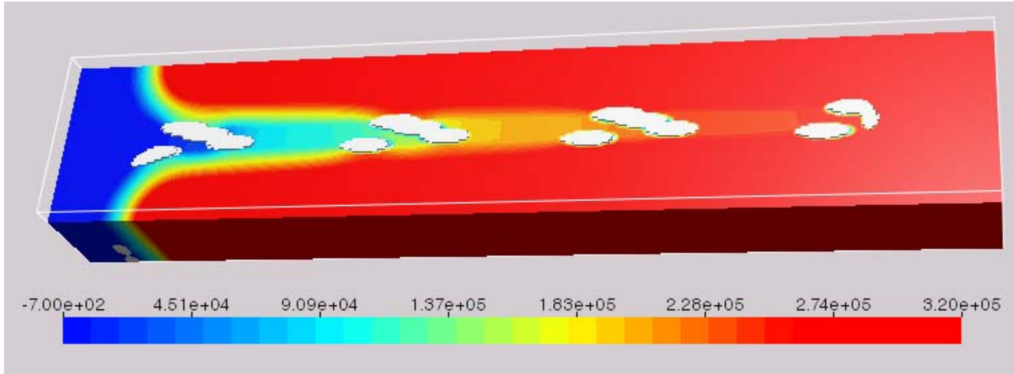
Oil flow in pleats with support structure: pressure

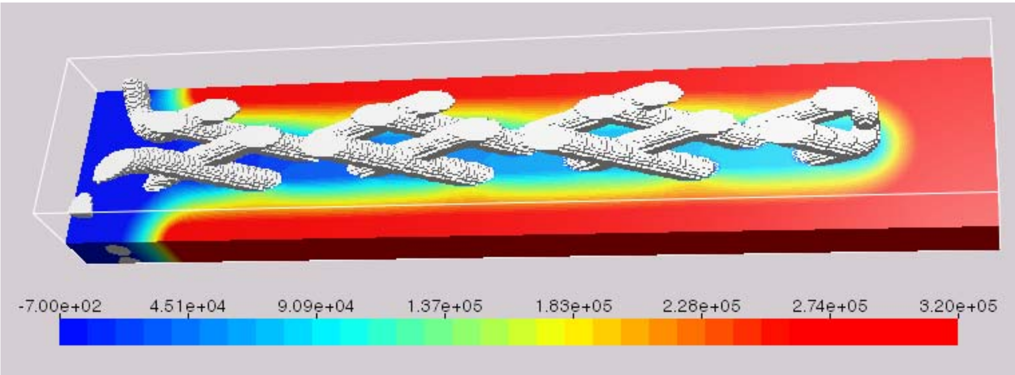
- Pressure in Pascal
- Oil: density 850 kg/m³ viscosity 0.17 m²/s
- Same pleat count
- Different in- and outflow channel widths
- Grid resolution 40 µm
- 50 x 70 x 380 cells



Narrow Channel:

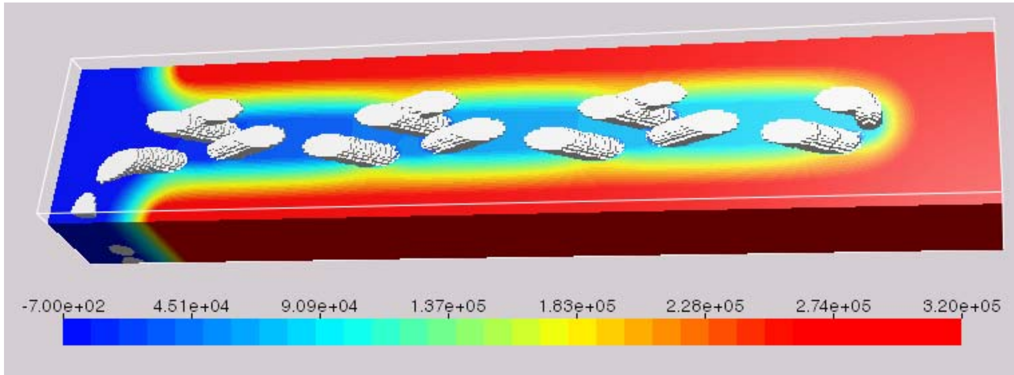
4 bar

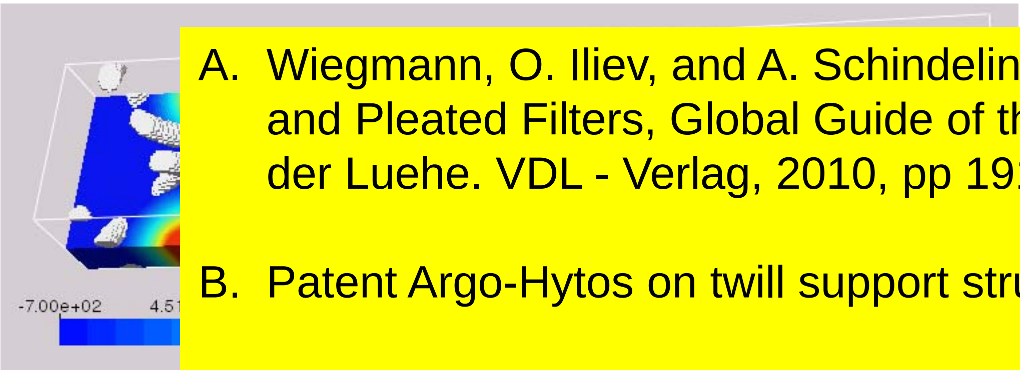


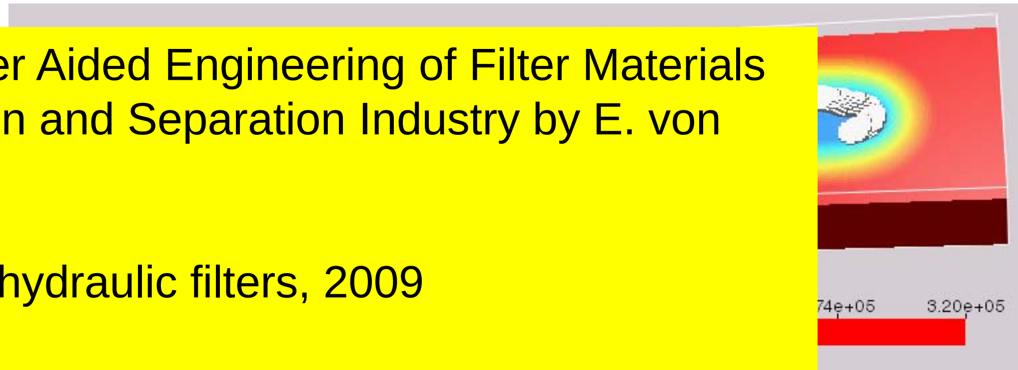


Thick Wire:

3.1 bar



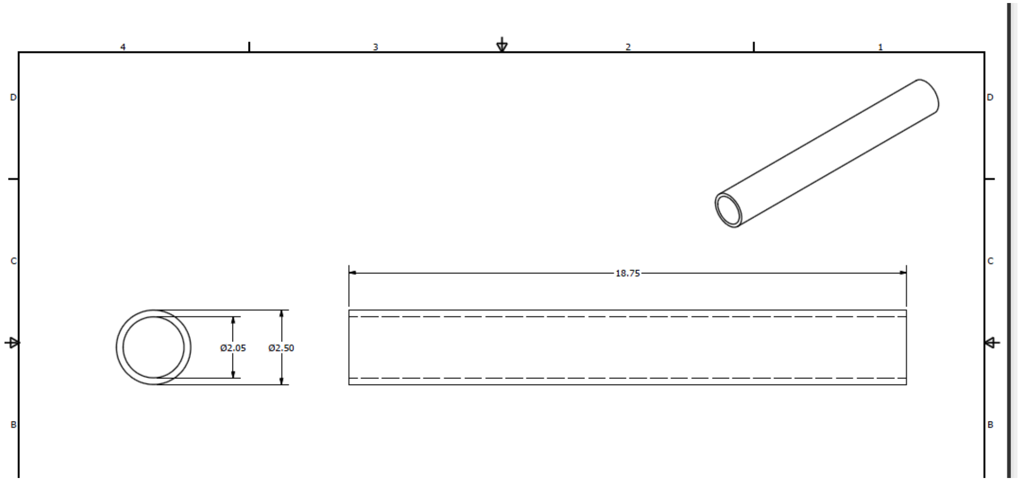


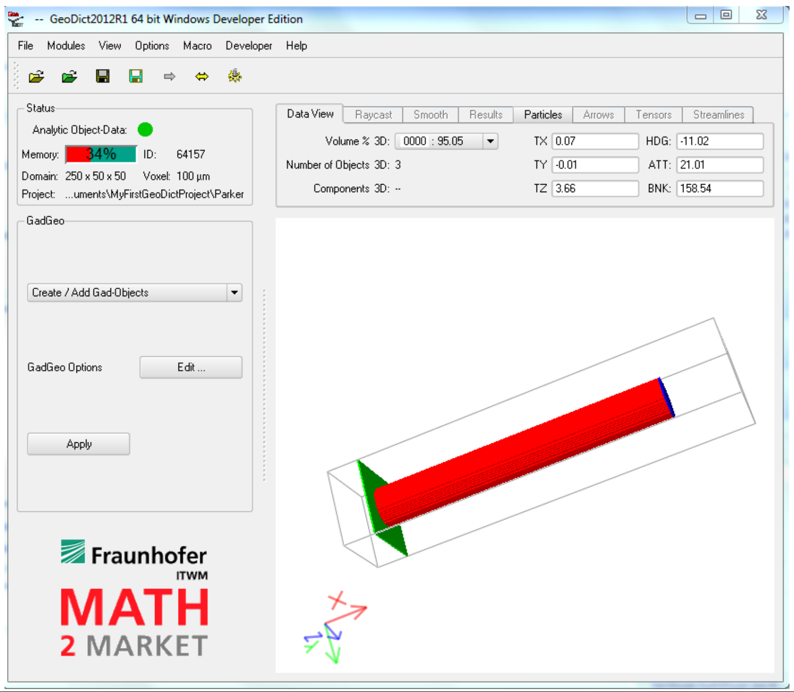


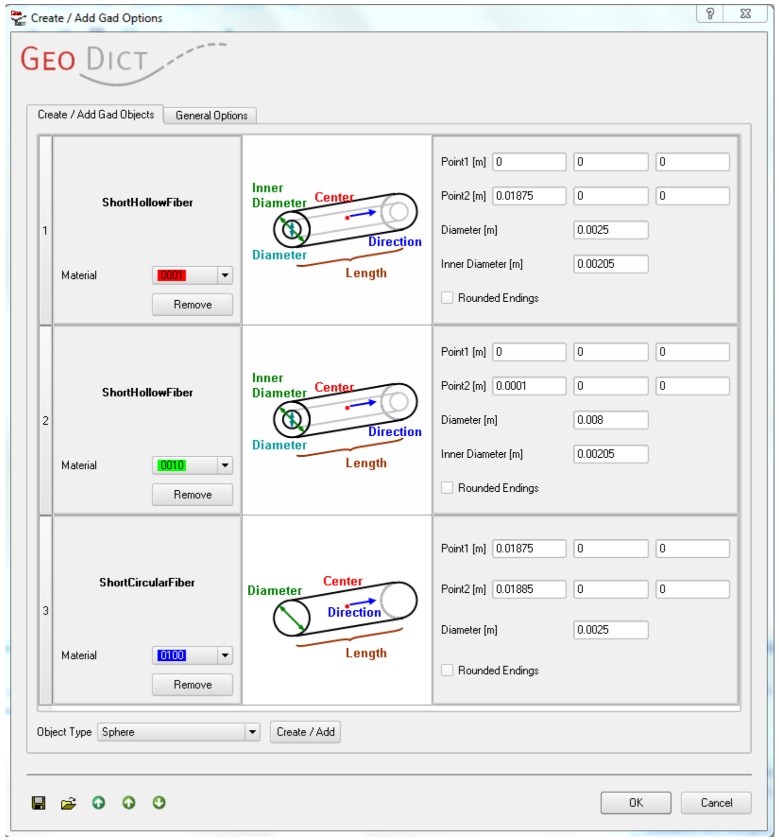
A. Wiegmann, O. Iliev, and A. Schindelin, Computer Aided Engineering of Filter Materials and Pleated Filters, Global Guide of the Filtration and Separation Industry by E. von der Luehe. VDL - Verlag, 2010, pp 191-198.

B. Patent Argo-Hytos on twill support structure for hydraulic filters, 2009

Pressure drop of Filter tube, Geometry







MATH 2 MARKET

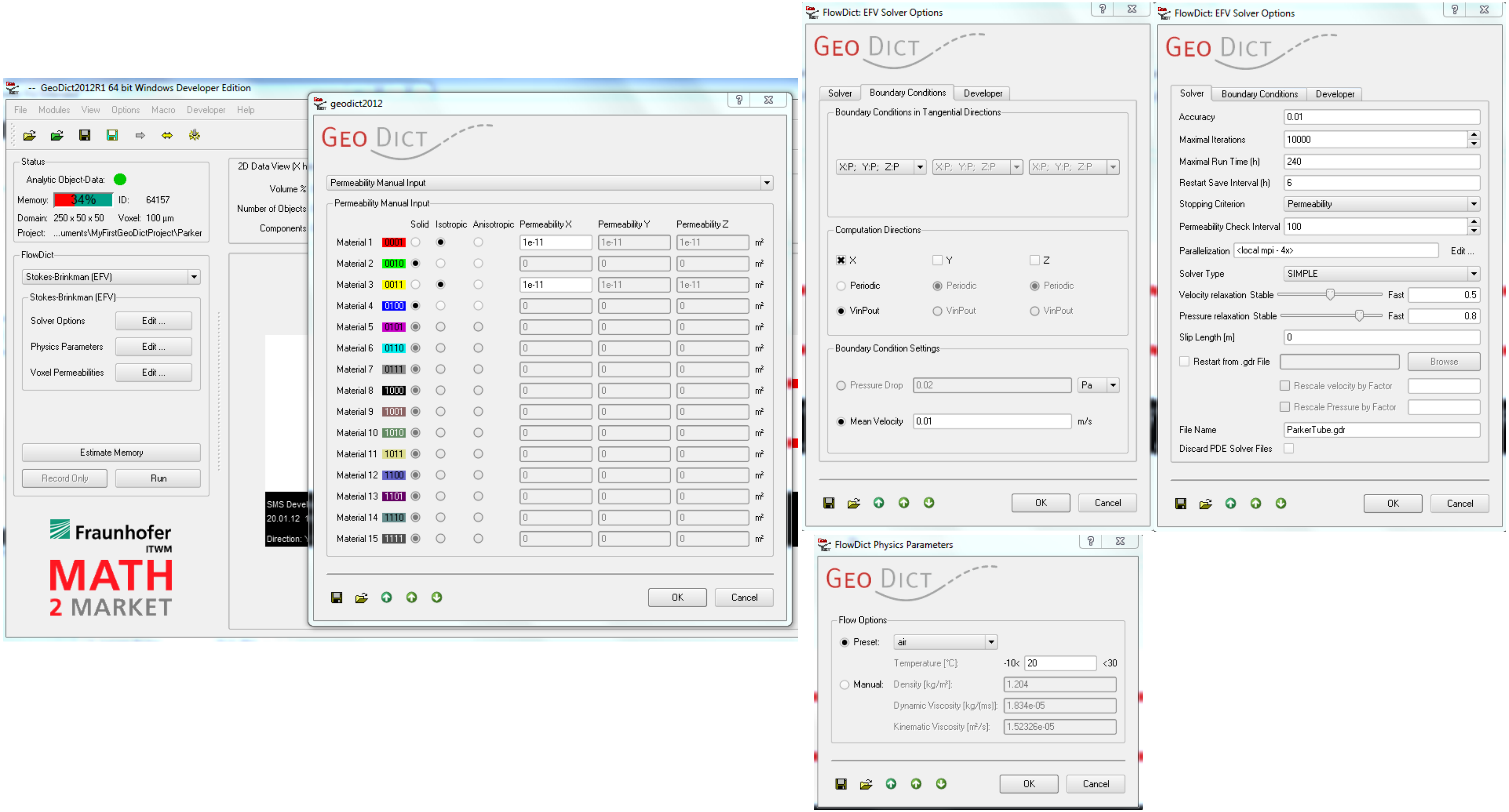
Fraunhofer ITWM

Andreas Wiegmann

WFC 11, Graz

19 April 2012

Pressure drop of Filter tube 1, parameters



MATH 2 MARKET

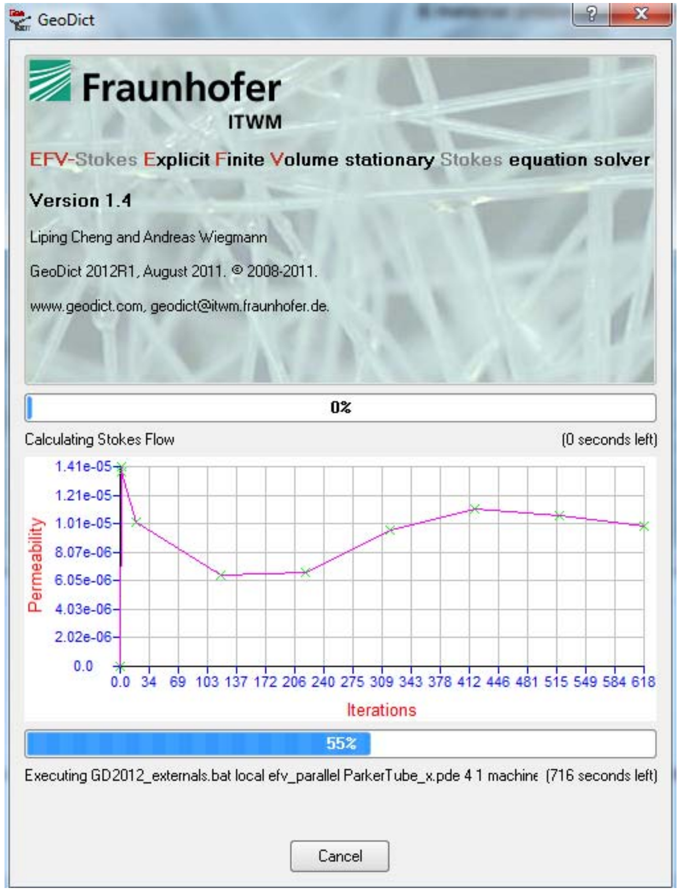
Fraunhofer ITWM

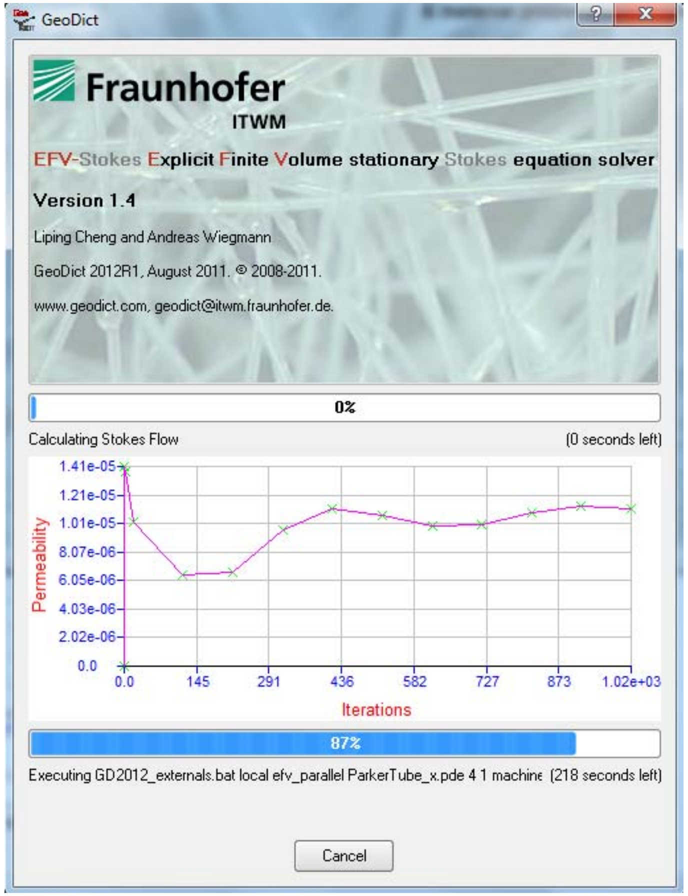
Andreas Wiegmann

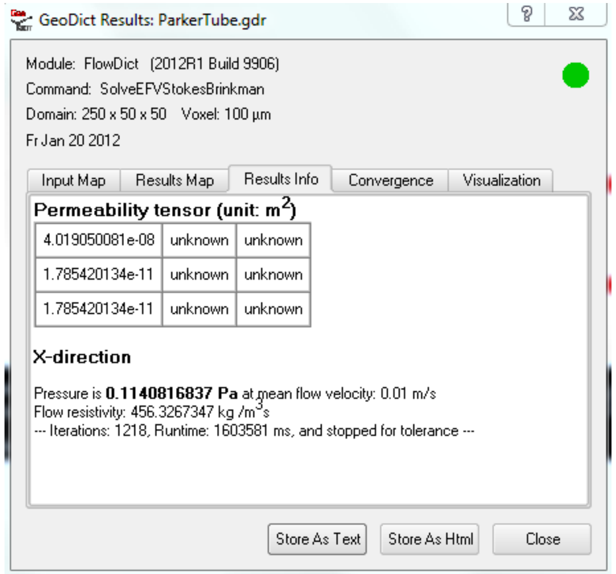
WFC 11, Graz

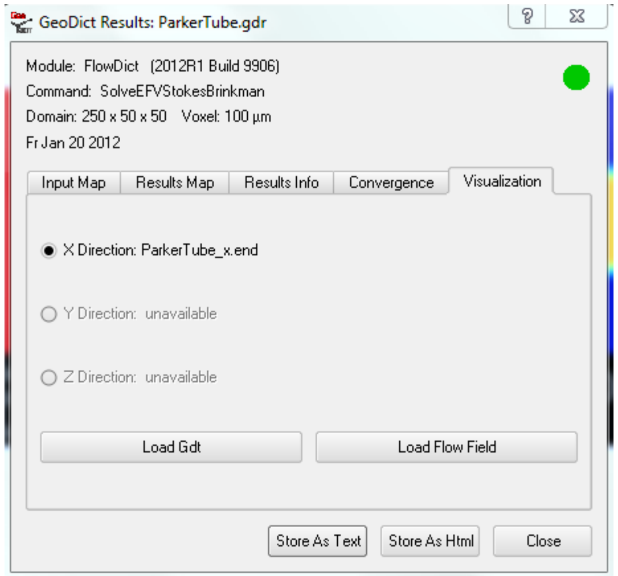
19 April 2012

Pressure drop of Filter tube, solve

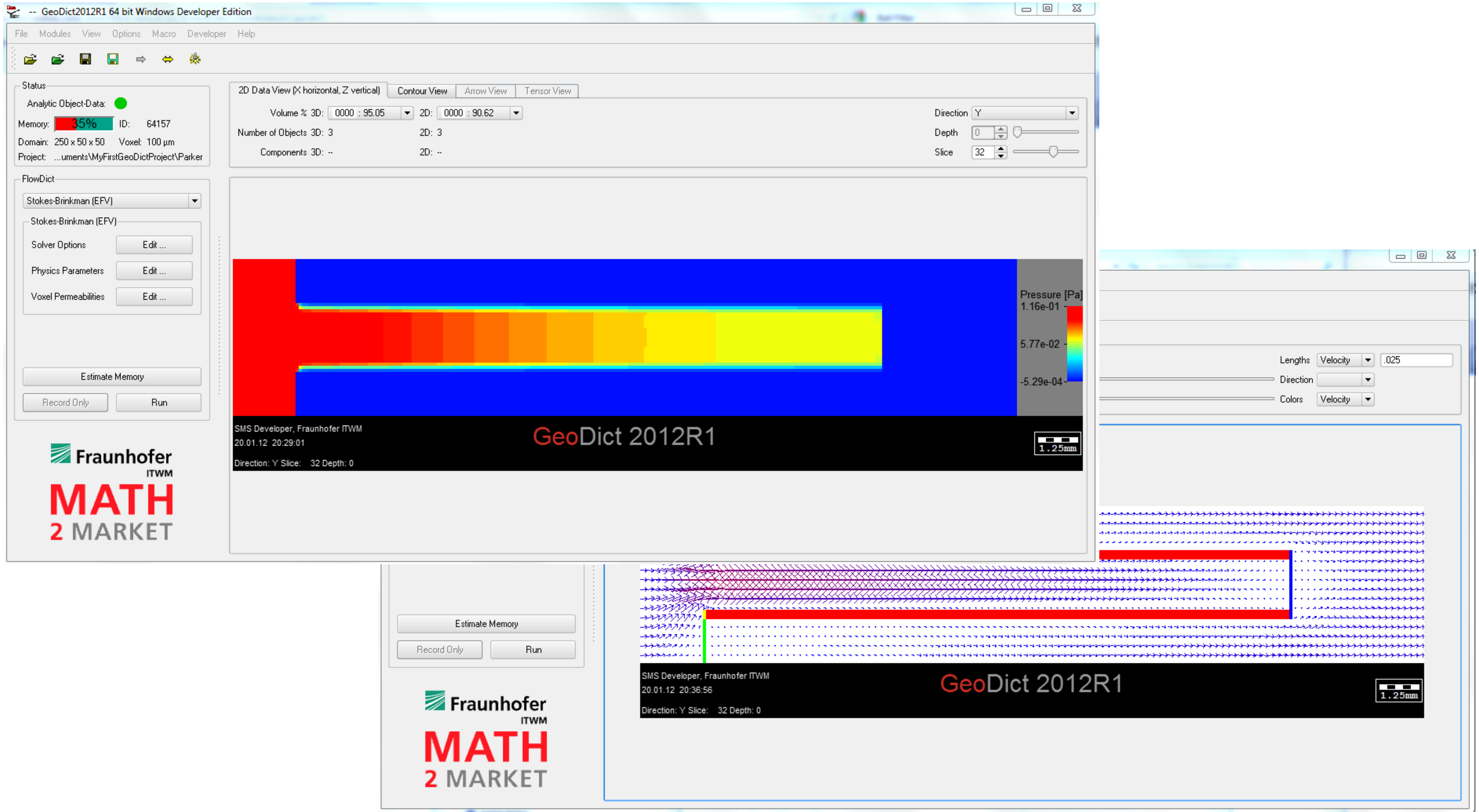






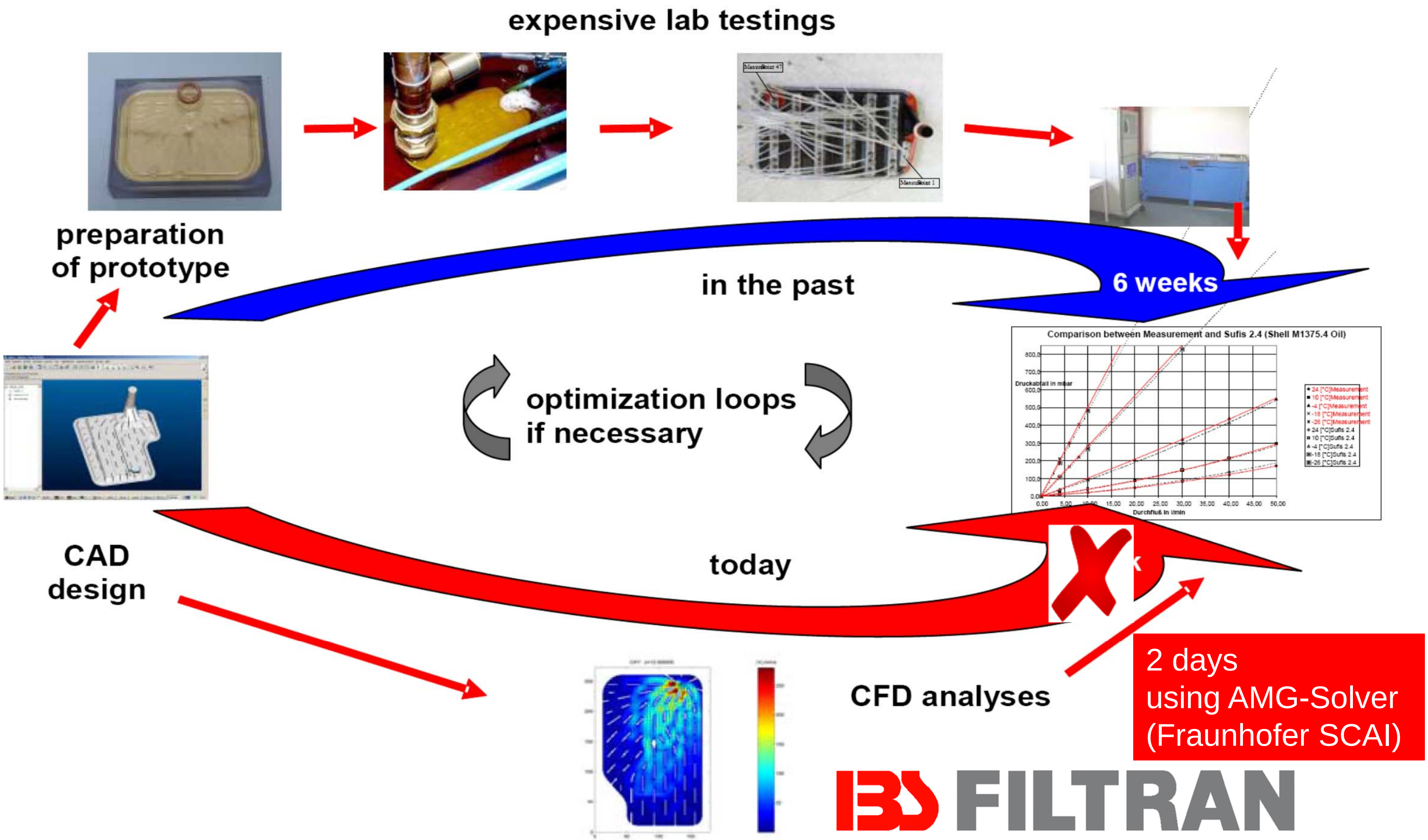


Pressure drop of Filter tube, results



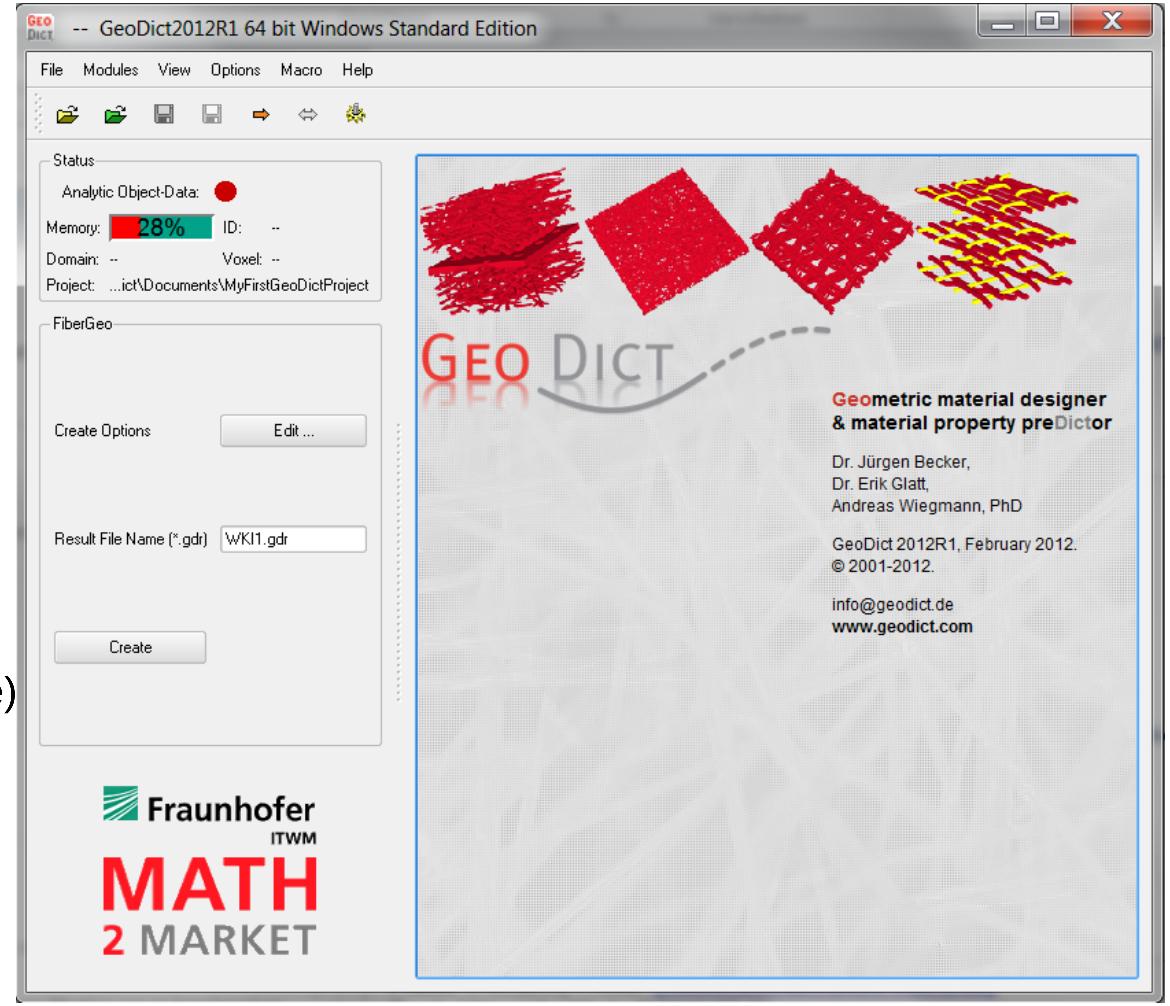
MATH 2 MARKET Fraunhofer ITWM

Benefits of SUFIS simulations



Modules of the GeoDict Software for GAD and GAE of Materials

- **FiberGeo**, **SinterGeo**, **WeaveGeo**, **GridGeo**, **PackGeo**, **PleatGeo**, **PaperGeo** (structure generators)
- **ProcessGeo** (3d image processing)
- **LayerGeo** (layered media)
- **ImportGeo** (e.g. tomographie, .stl)
- **ExportGeo** (e.g. Fluent, Abaqus)
- **FlowDict** (single phase flow properties)
- **PleatDict** (porous media flow)
- **ElastoDict** (effective elastic properties)
- **ThermoDict** (effective conductivity)
- **DiffuDict** (effective diffusivity)
- **FilterDict** (pressure drop, efficiency, life time)
- **SatuDict** (two phase flow properties)
- **PoroDict** (pore size measures)
- **AcoustoDict** (acoustic absorption)
- **AddiDict** (advection diffusion adsorption)



GeoDict contributors: 2001 - 2012

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Matthias Groß
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Rolf Westerteiger

PaperGeo
Erik Glatt

Conclusion: all issues and scales can be covered by simulation

- Filter media & pleat representation; solid particle representation
- Flow computation
- Particle tracking
- Collision & adhesion handling
- Solid & porous media update
  - e.g. cake formation
  - e.g. particle re-entrainment & back wash
- Postprocessing as data and visualizations

Outlook: aspects of all issues and scales still need to be addressed

(1) Filter media representation:

- Parameter identification for ceramics, cellular & meltblown *models*
- Image denoising and limited resolution for *tomography*

(2) Sheer domain sizes; parallel computing:

- Tomography data go towards 4000 x 4000 x 4000 cells
- nano fibers require resolution of 20nm
- Flow computations must be carried out with state-of-the-art algorithms on state-of-the-art computers

(3) Flow computations

- Slip modeling inconvenient on voxels
- Fast flows are not stationary

Outlook: aspects of all issues and scales still need to be addressed

(4) Range of particle sizes usually requires Stokes-Brinkman

- Solvers converge slower
- Finding parameters is inconvenient (detailed work)
- Dropping the small particles leads to wrong cake resistivity

(5) Cake formation

- Control of number of particles 2d/3d (overlap)
- Solver convergence for „stiffening“ problem

(6) Particle adhesion and restitution forces

- Determination of 2 material-dependent parameters
  - Sieving; Caught on first touch; Hamaker; Collision count; [Probability based]
- Re-entrainment under changing flow conditions
  - pressure build-up; impulse cleaning

Challenges

Inter-disciplinary nature

- Process engineering
- Textile engineering
- Software engineering
- Chemistry
- Physics
- Knowledge of testing equipment & validity
- Visualization
- High performance computing
- Numerical algorithms
- GUI-design
- ...

Continuity

- Software development needs are specific to filtration, hard to build into non-specific commercial CFD codes
- Software development needs are too large for a single customer project or single dissertation
- Filtration has little visibility for public funding agencies (compared to nuclear physics, energy, transportation and similar topics)

Despite the obstacles:

- **Filtration and separation simulation is an irreversible trend in Academic and Industrial R&D**

Visit Fraunhofer ITWM & Math2Market at Booth F8 if you like

Thank you for your kind attention