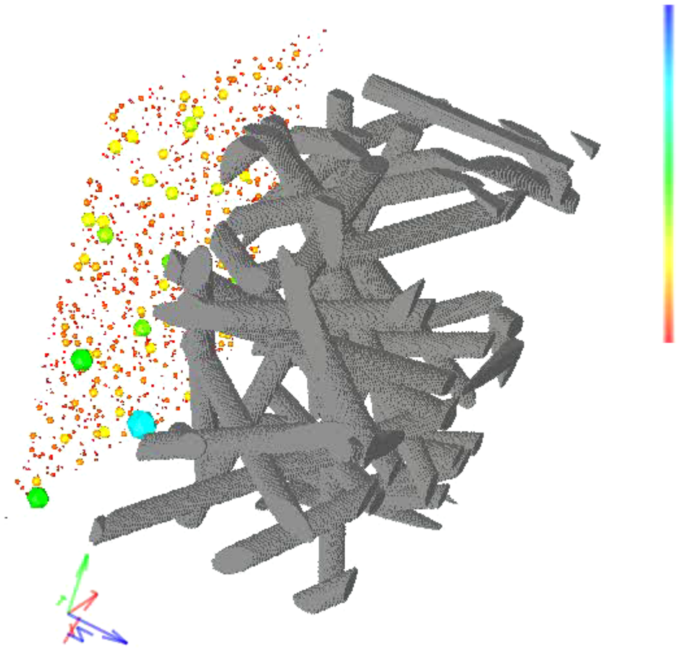
Toward predicting Filtration and Separation: Challenges & Progress



Andreas Wiegmann

Filtech 2009

13th October, 2009

Fraunhofer ITWM

= Fraunhofer Institute for Industrial Mathematics, Kaiserslautern

Thanks to collaborators at Fraunhofer ITWM

Currently at ITWM:

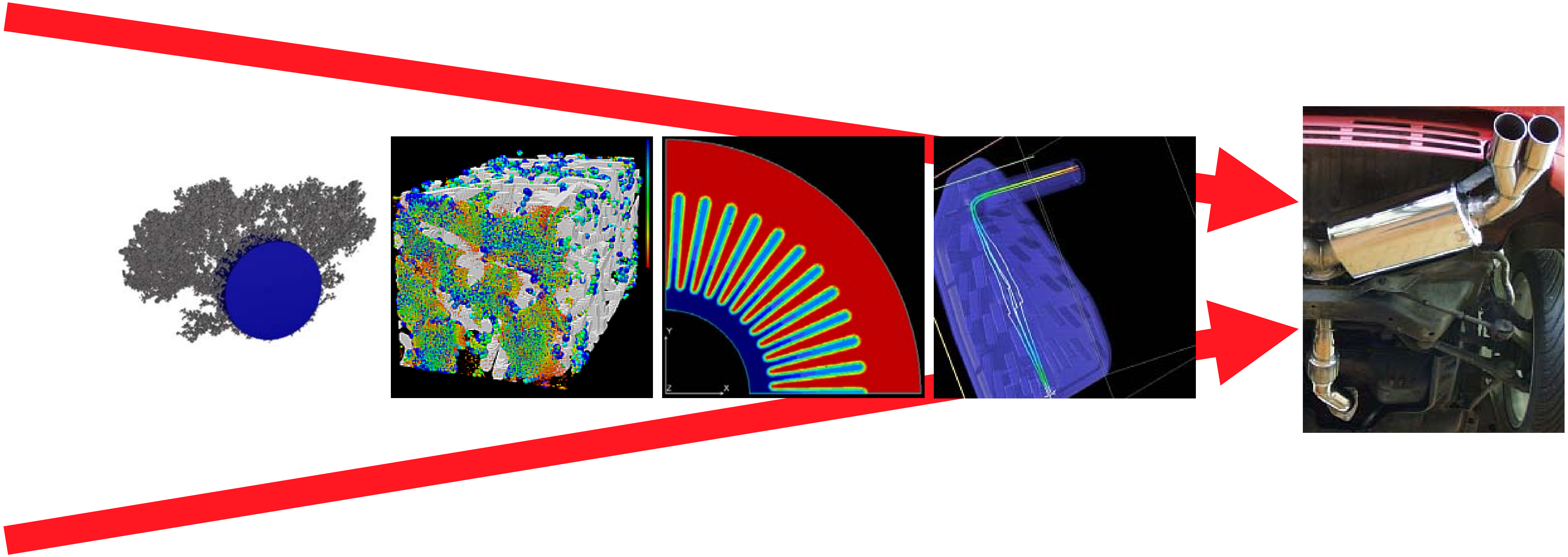
- Heiko Andrä, Jürgen Becker, Peter Klein, Arnulf Latz, Sven Linden, Barbara Planas, Stefan Rief, Katja Schladitz, Konrad Steiner, Aivars Zemitis.
- Presenters at Filtech 2009:
  - Liping Cheng, Erik Glatt, Oleg Iliev, Mathias Kabel, Zarah Lakdawala, Kilian Schmidt.

Formerly at ITWM:

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

Filtration and simulation occur on multiple scales

Single Fiber	Media	Cartridge	Element	Exhaust system
Nanometer	Micrometer	Millimeter	Centimeter	Meter



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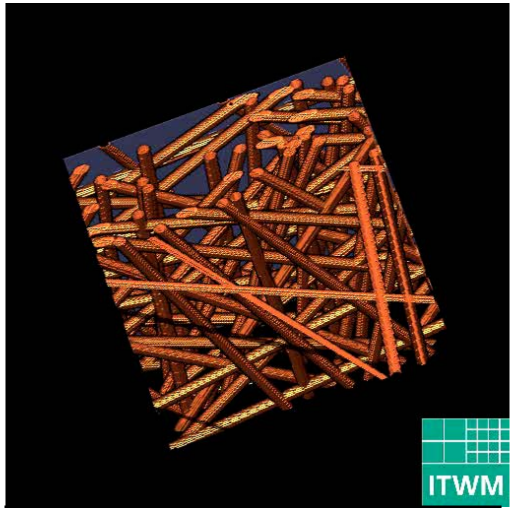
How does (direct numerical) filtration simulation work, anyway?

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

Virtual design cycle of filter media

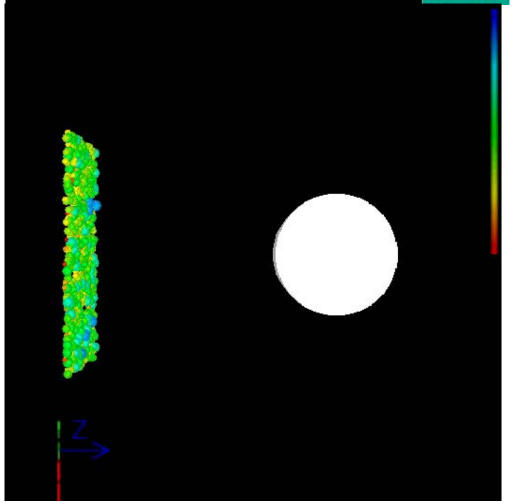
Flow



OPTIMIZATION

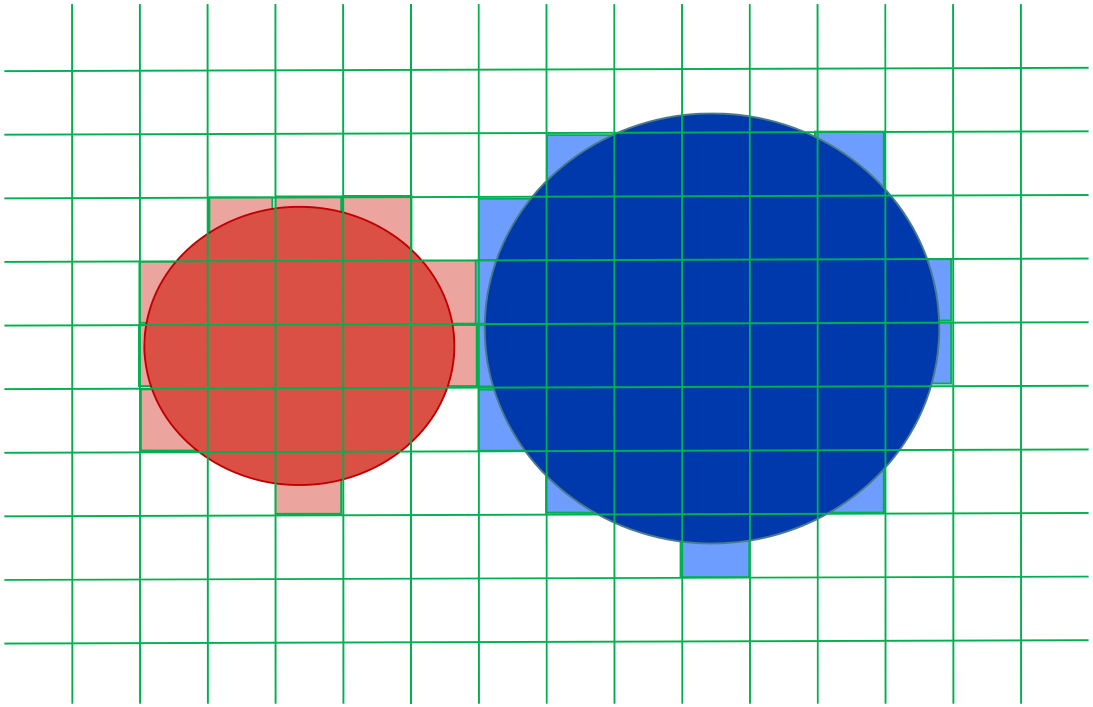
1. Choose initial structural parameters
2. Generate / modify structure
3. Solve CFD problem
4. Compute particle transport and deposition
5. Compute filtration efficiency and pressure drop
6. Choose new structural parameters

LIFETIME



Single Fiber Simulation

All simulations done are based on structures of little cubes



Advantages

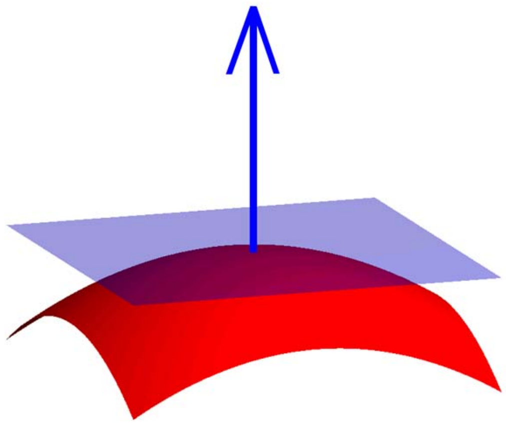
- Saves grid generation times
- Compatible with computer tomography
- Straight forward structure generation
- Straight forward solver implementation
- Straight forward parallel computations

Disadvantages

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

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.

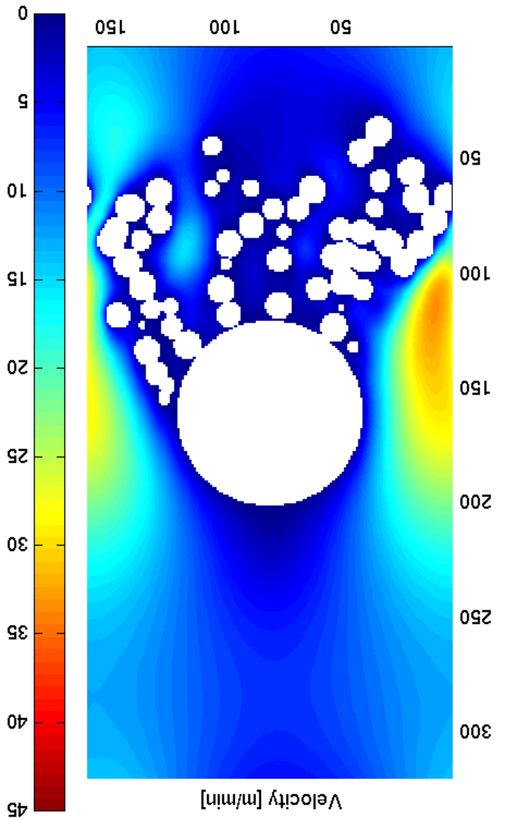
$$
\begin{aligned}
-\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\
\nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\
\vec{n}\cdot\vec{u} &= 0 \text{ on } \Gamma \text{ (no flow into fibers)} \\
\vec{t}\cdot\vec{u} &= -\lambda\vec{n}\cdot\nabla\left(\vec{u}\cdot\vec{t}\right) \text{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

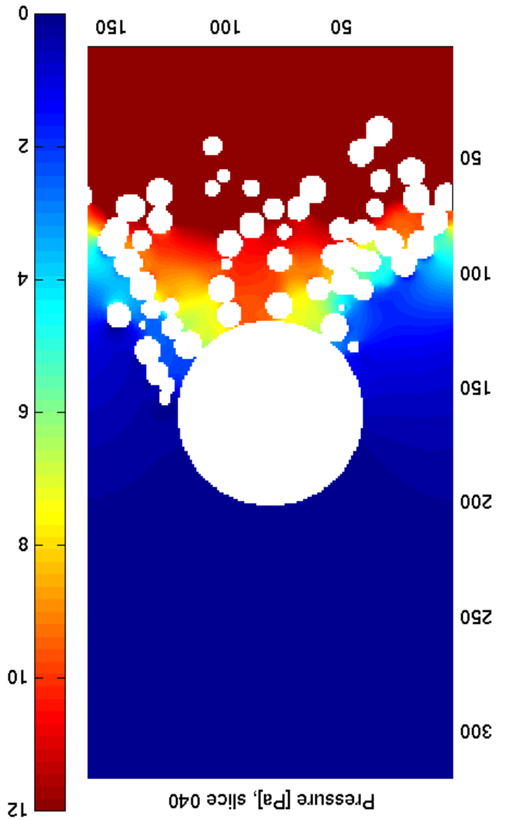
$\vec{n}$: normal direction to the fiber surface,

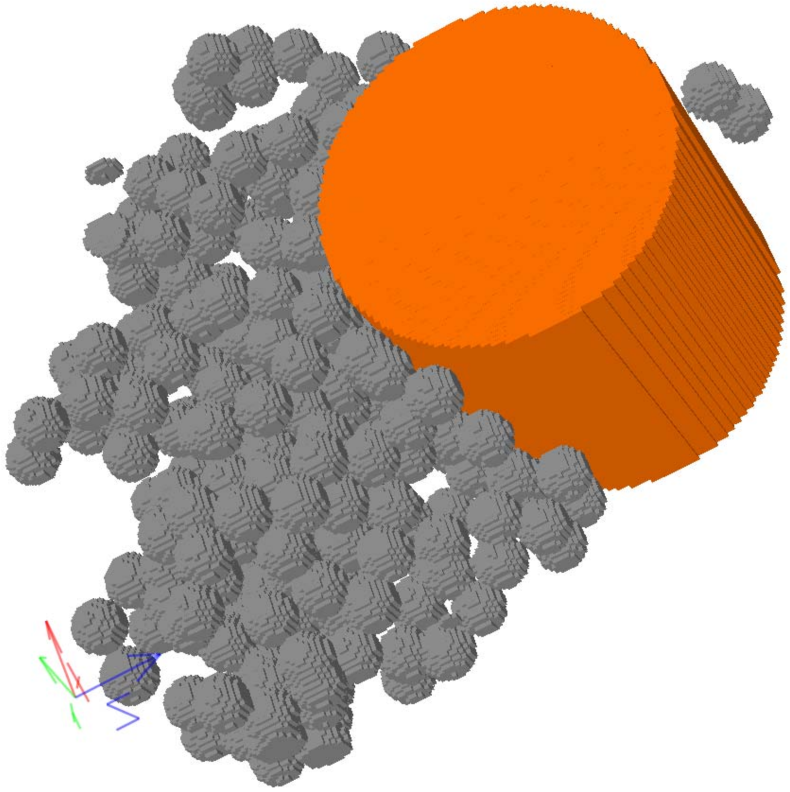
λ : slip length,

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

Pressure and Velocity in Clogging Simulation







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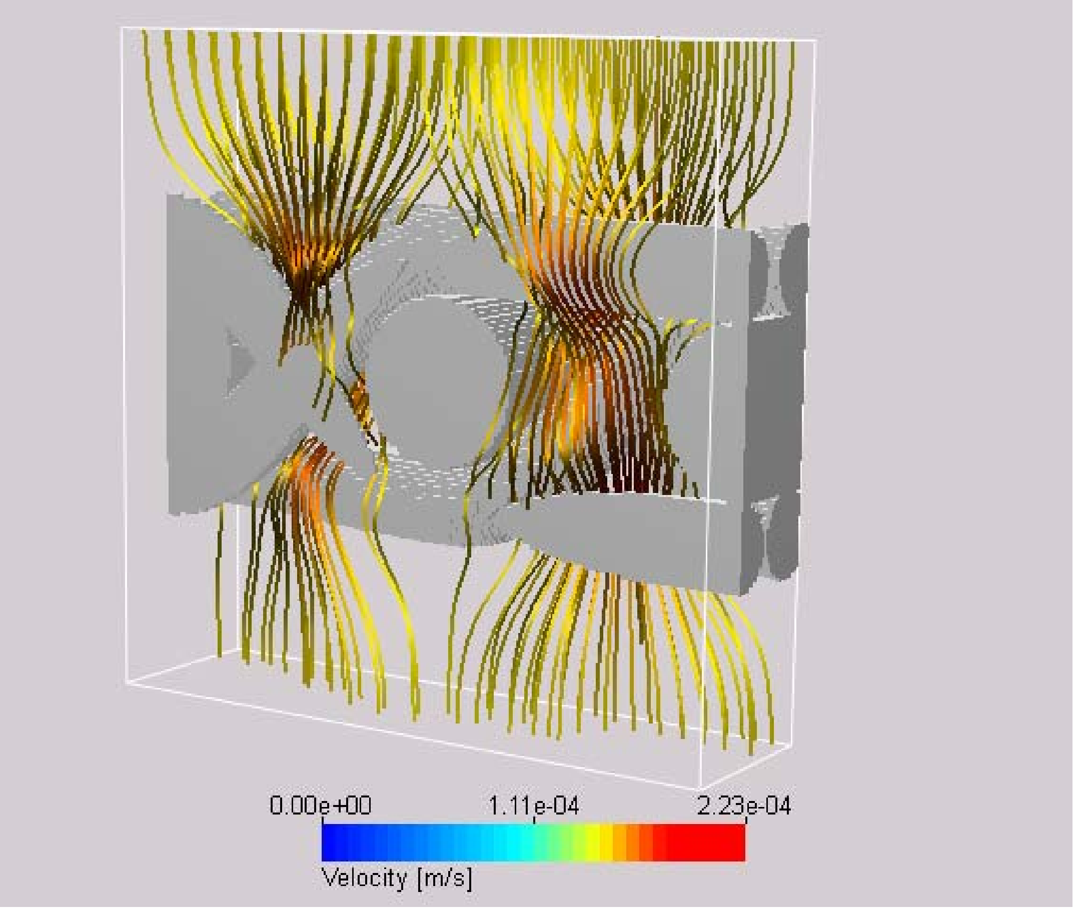
Flow Field Visualization



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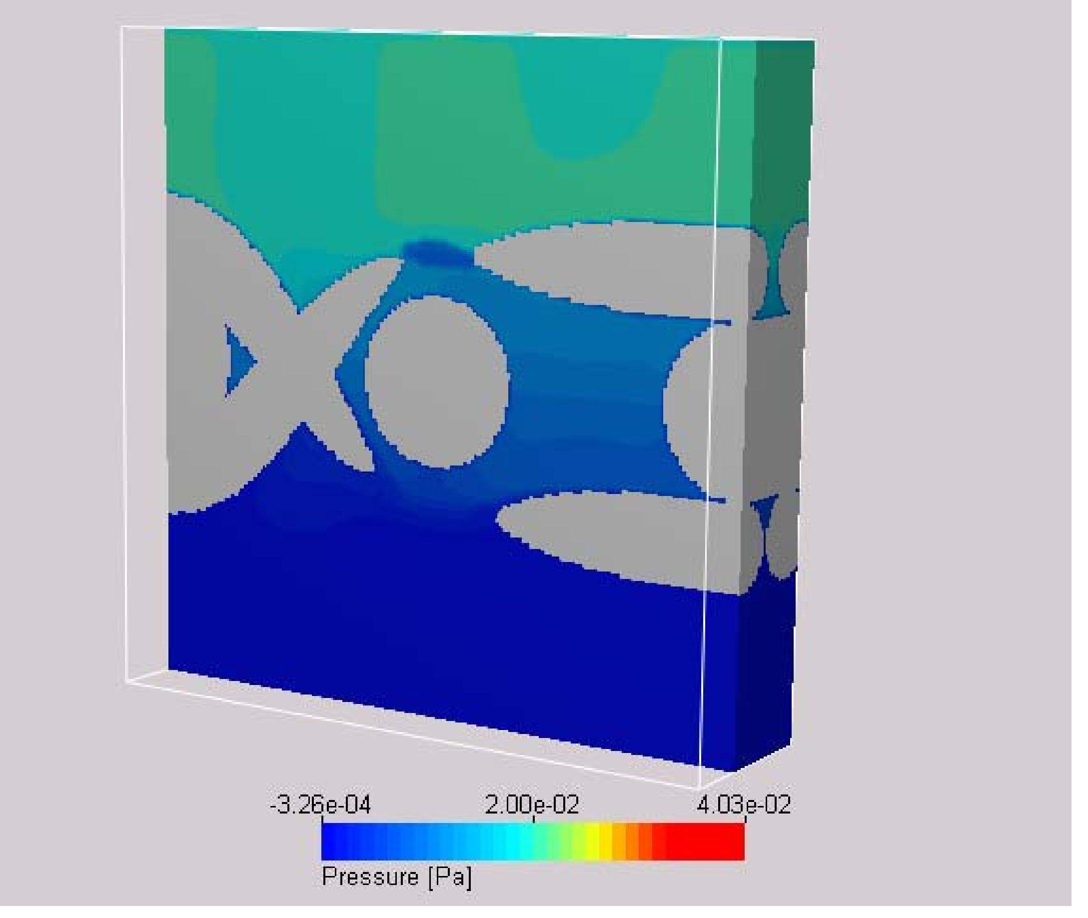
Pressure Drop Visualization



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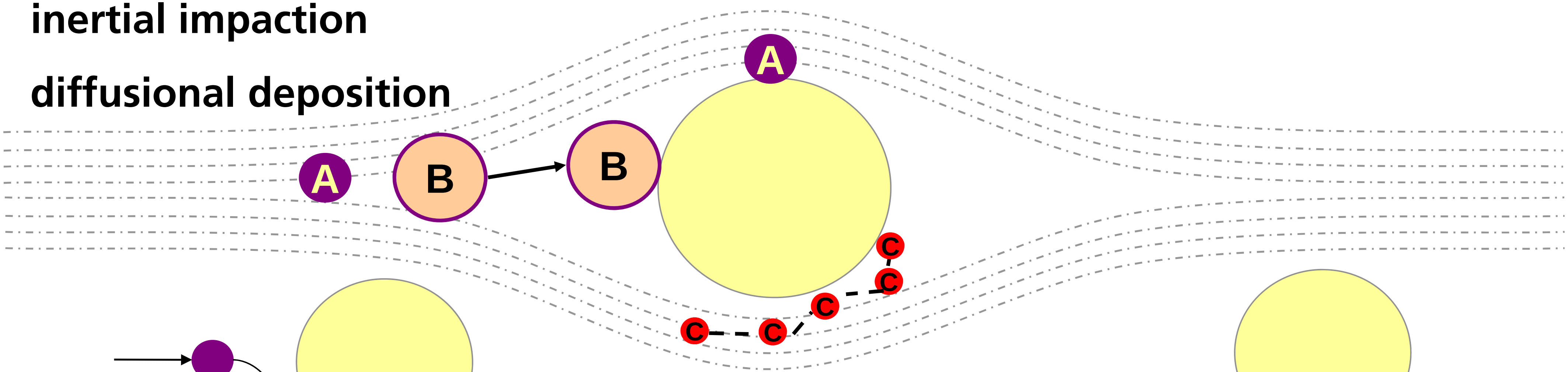
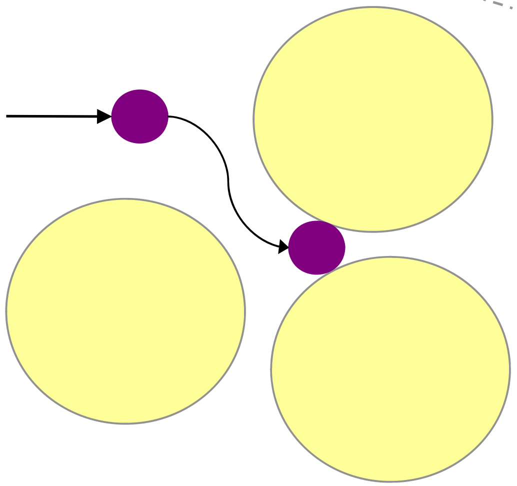
Filtration Effects I

A: direct interception

B: inertial impaction

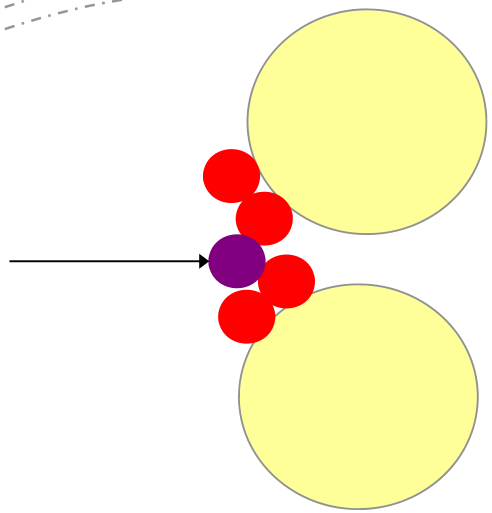
C: diffusional deposition





E: sieving

F: clogging



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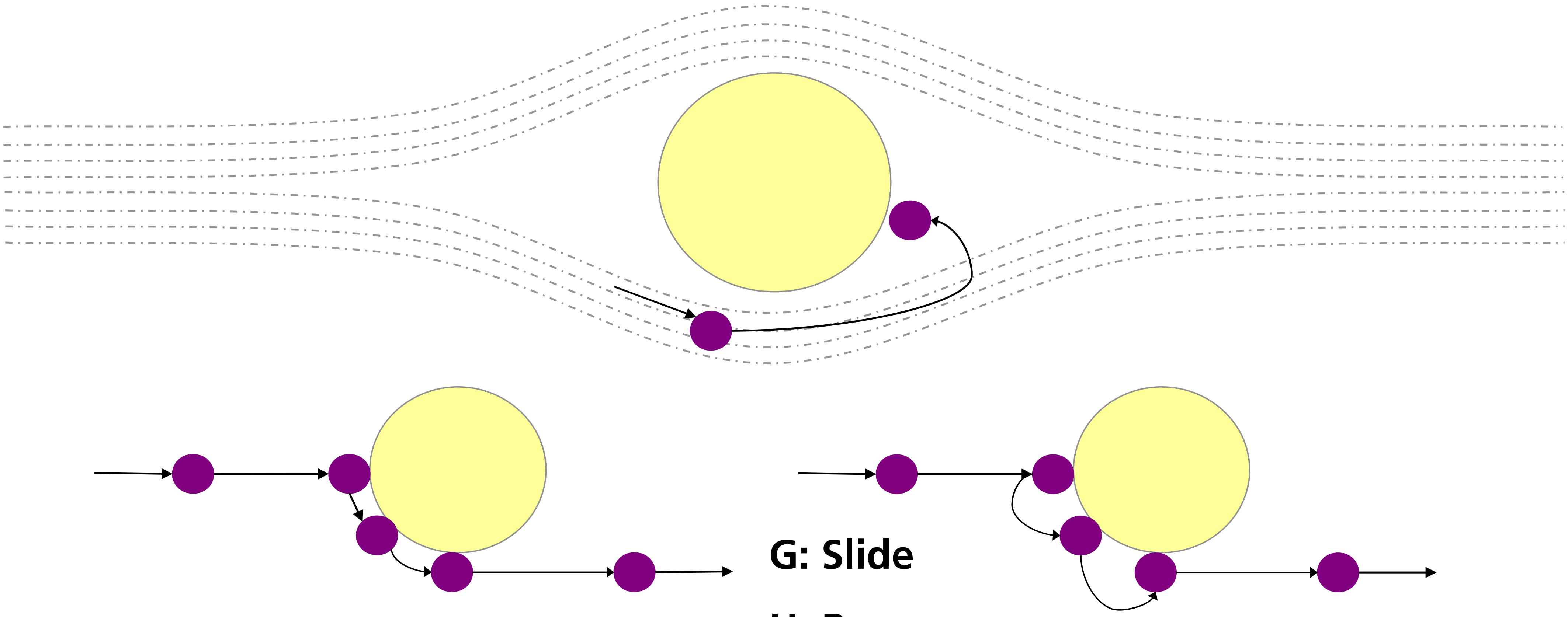
Filtration Effects II and modes of particle motion

D: electrostatic attraction



G: Slide

H: Bounce

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Description of particle motion

Friction with fluid — Electric attraction — Diffusive motion

$$
\begin{aligned}
d\vec{x} &= \vec{v}\, dt, \\
d\vec{v} &= -\gamma \times (\vec{v}(\vec{x}) - \vec{v}_\circ(\vec{x}))\, dt + \frac{Q\vec{E}_\circ(\vec{x})}{m} dt + \sigma \times d\vec{W}(t), \\
C_c &= 1 + Kn\left(1.142 + 0.558 e^{-0.999/Kn}\right), \\
\gamma &= 6\pi\rho\mu \frac{R}{C_c m}, \\
\sigma^2 &= \frac{2k_B T\gamma}{m}, \\
\left\langle dW_i(t), dW_j(t)\right\rangle &= \delta_{ij} dt, \\
Kn &= \frac{\lambda}{R}, \\
\lambda &= \frac{k_B T}{\sqrt{32}\pi R^2 P}
\end{aligned}
$$

- 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

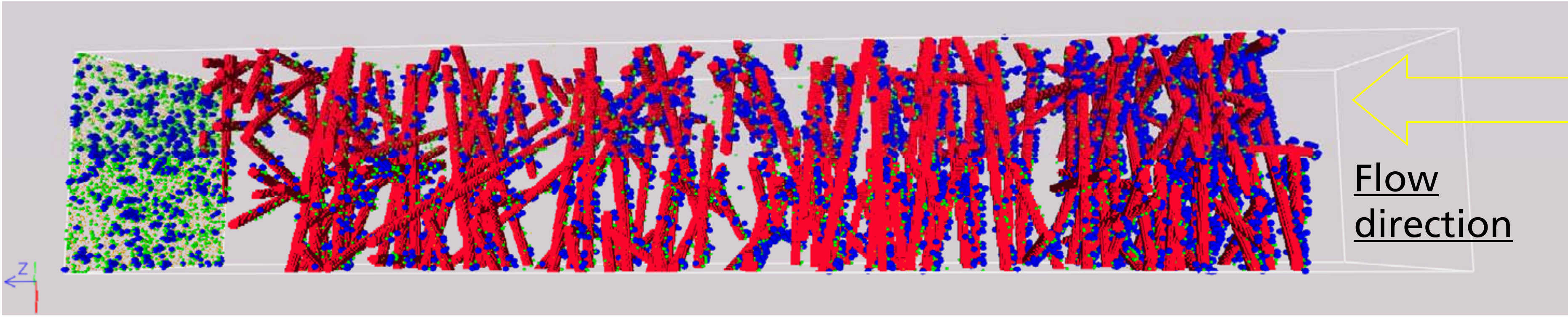
Deposition effects

$\alpha = 0.05$,

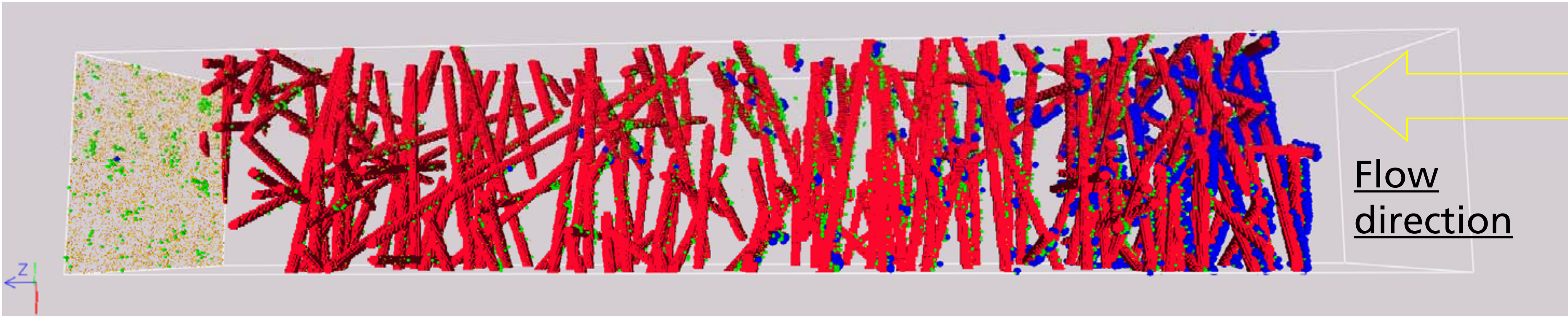
$d_F = 14$,

$v = 0.1 m/s$

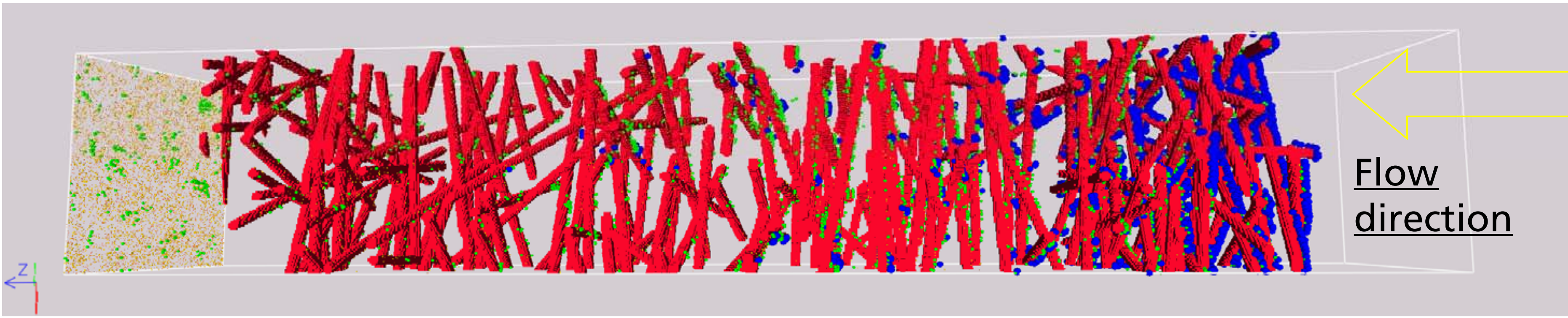
Interception



Interception
+ Impaction



Interception
+ Impaction
+ Diffusion



Velocity Effects

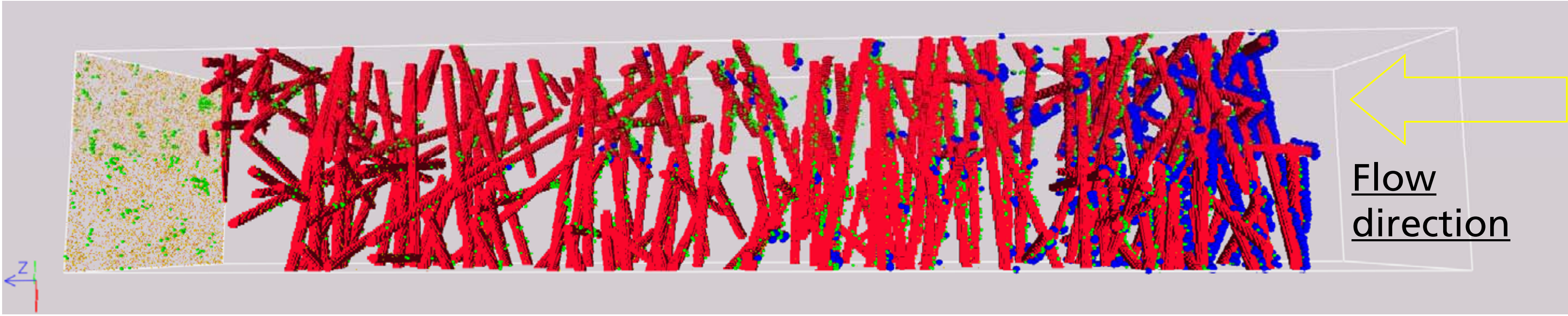
α = 0.05,

dF = 14,

Interception + Impaction + Diffusion

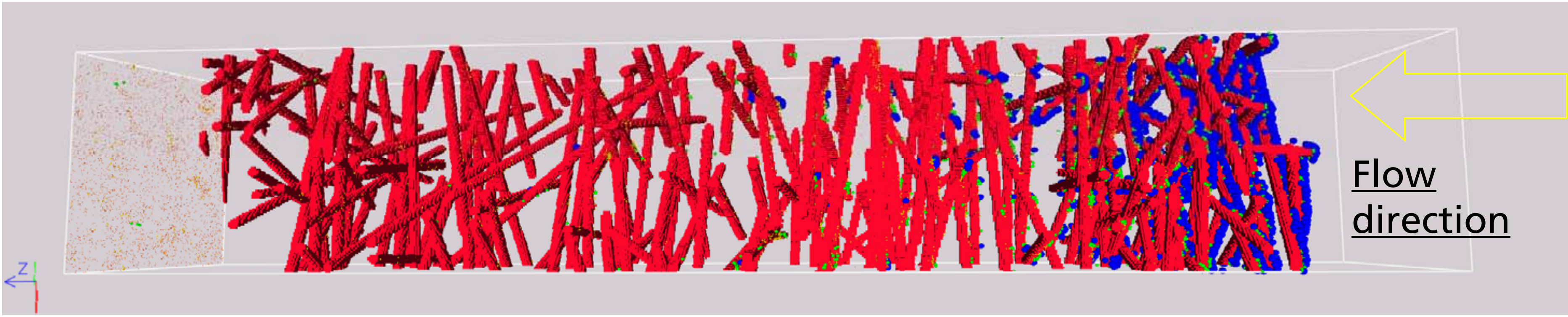
Velocity

v = 0.1 m/s



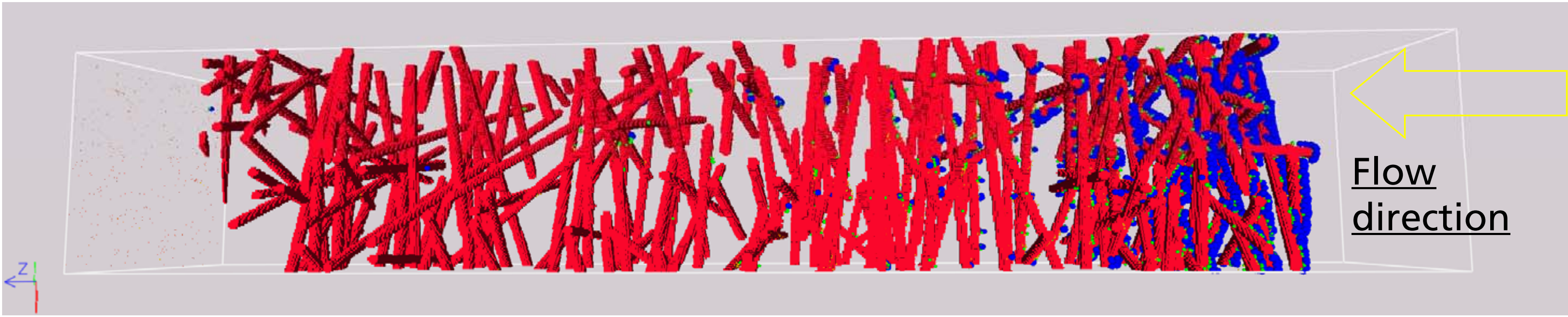
Velocity

v = 1 m/s



Velocity

v= 10 m/s



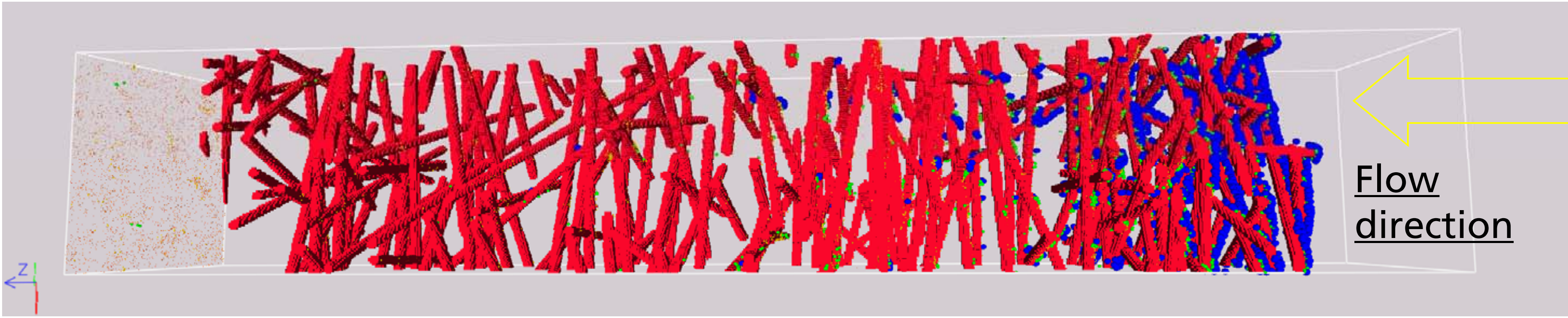
Effect of grammage (here: SVF)

dF = 14,

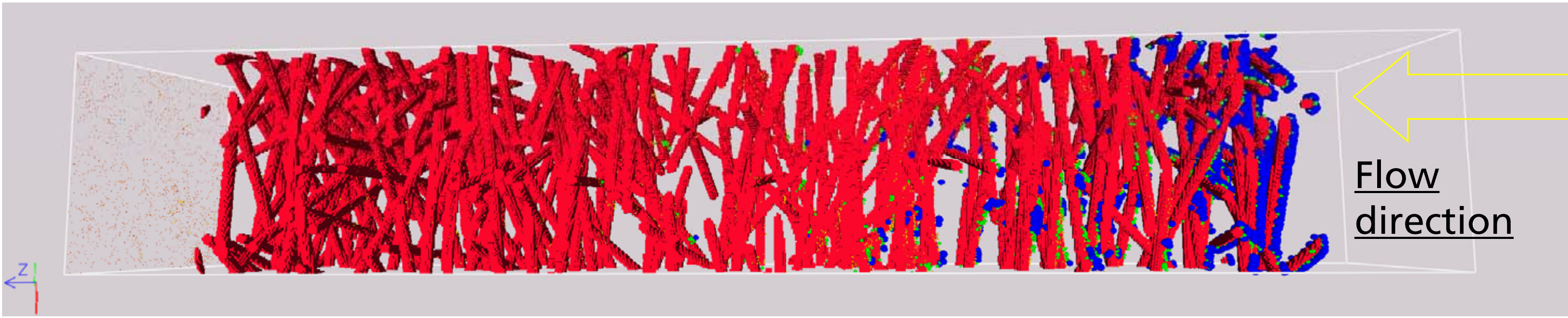
v = 1 m/s,

Interception + Impaction + Diffusion

SVF α=0.05

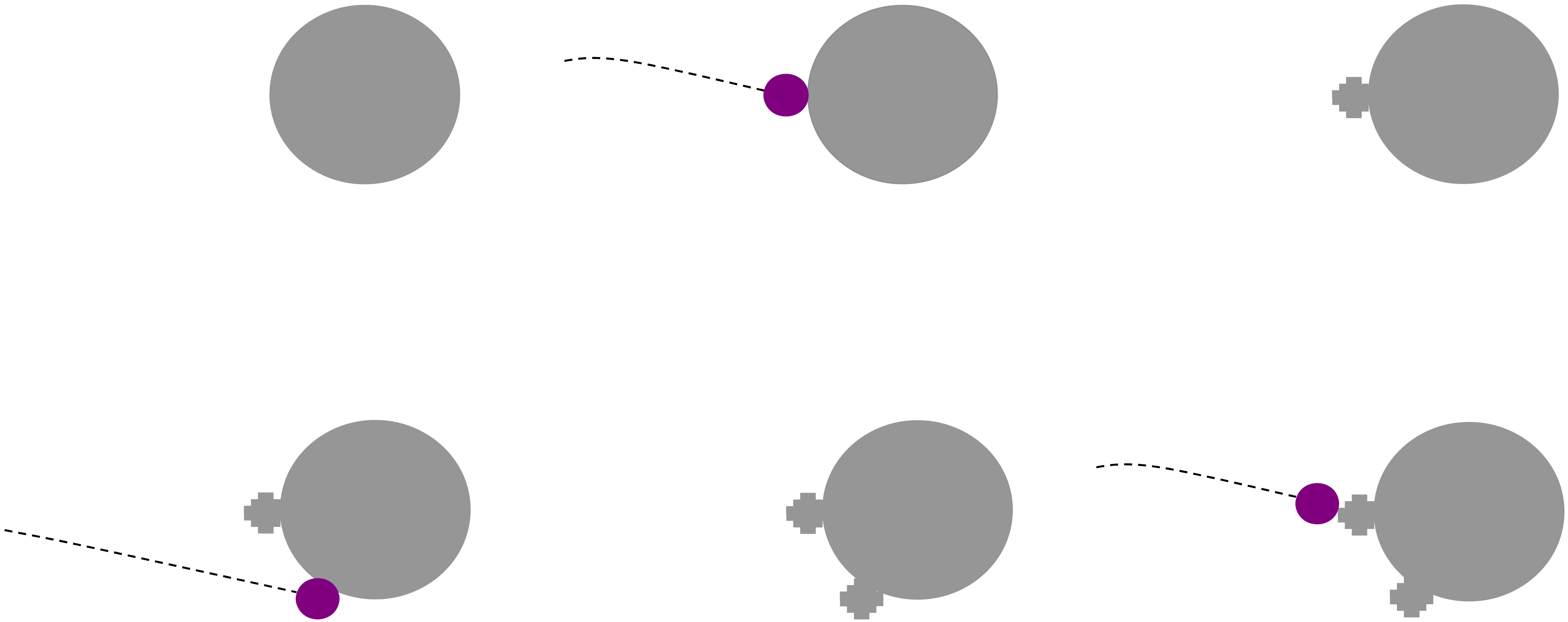


SVF α=0.07



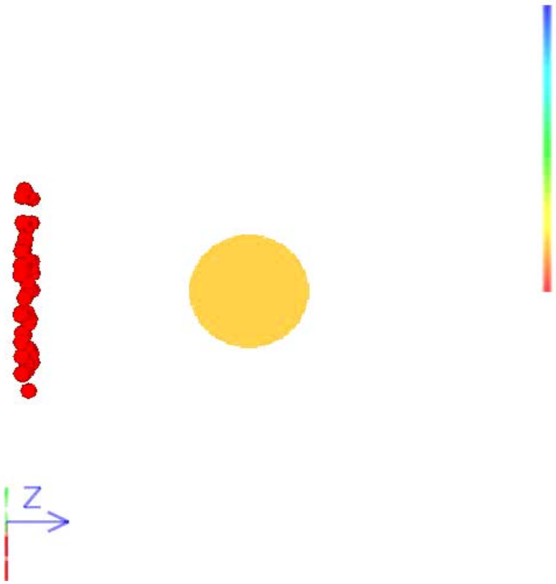
SVF α=0.1

Nano-Modus

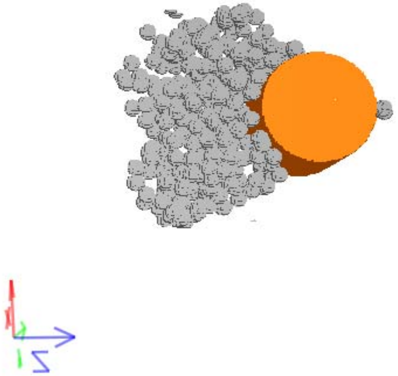


Influence of electric charge (air filtration)

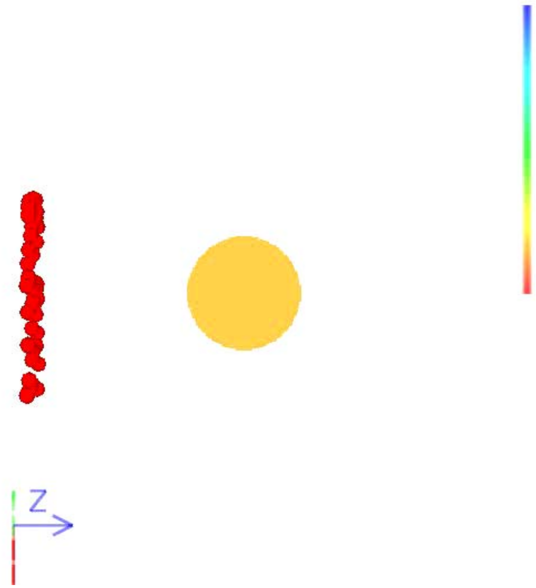
No charges



Low charges



High charges



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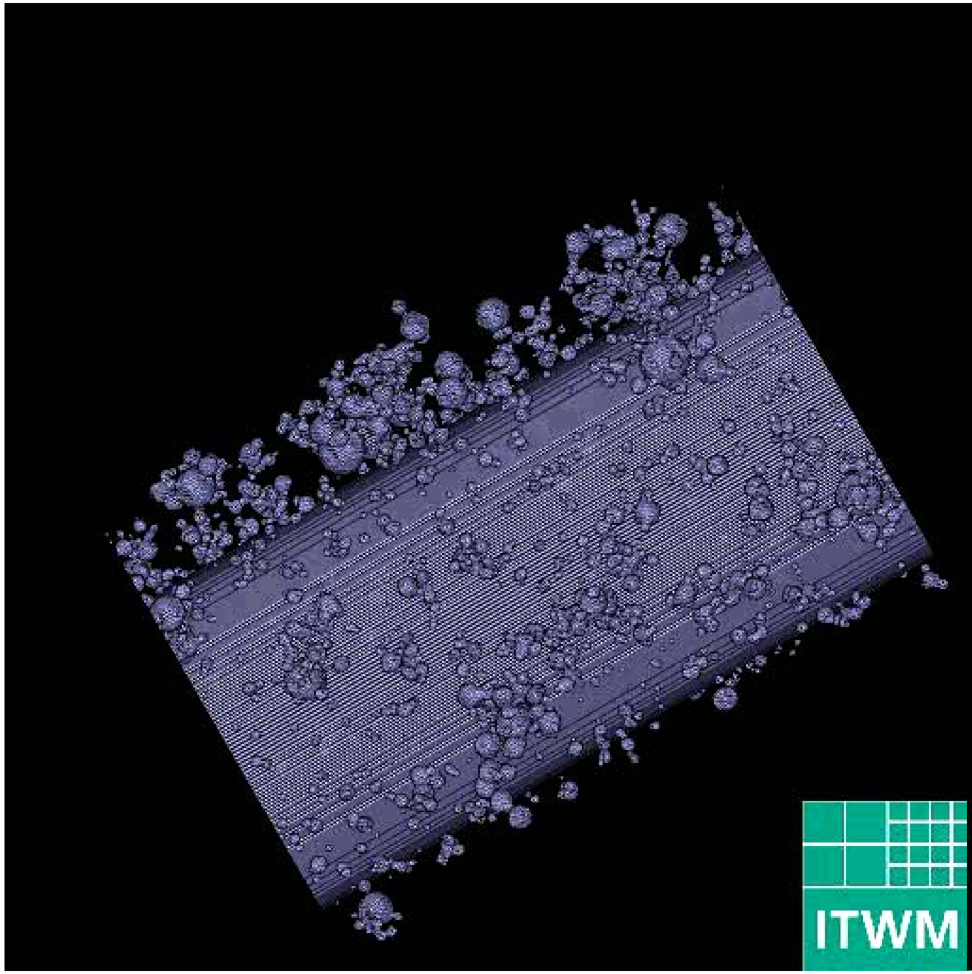
13 October 2009

Deposition of resolved particles

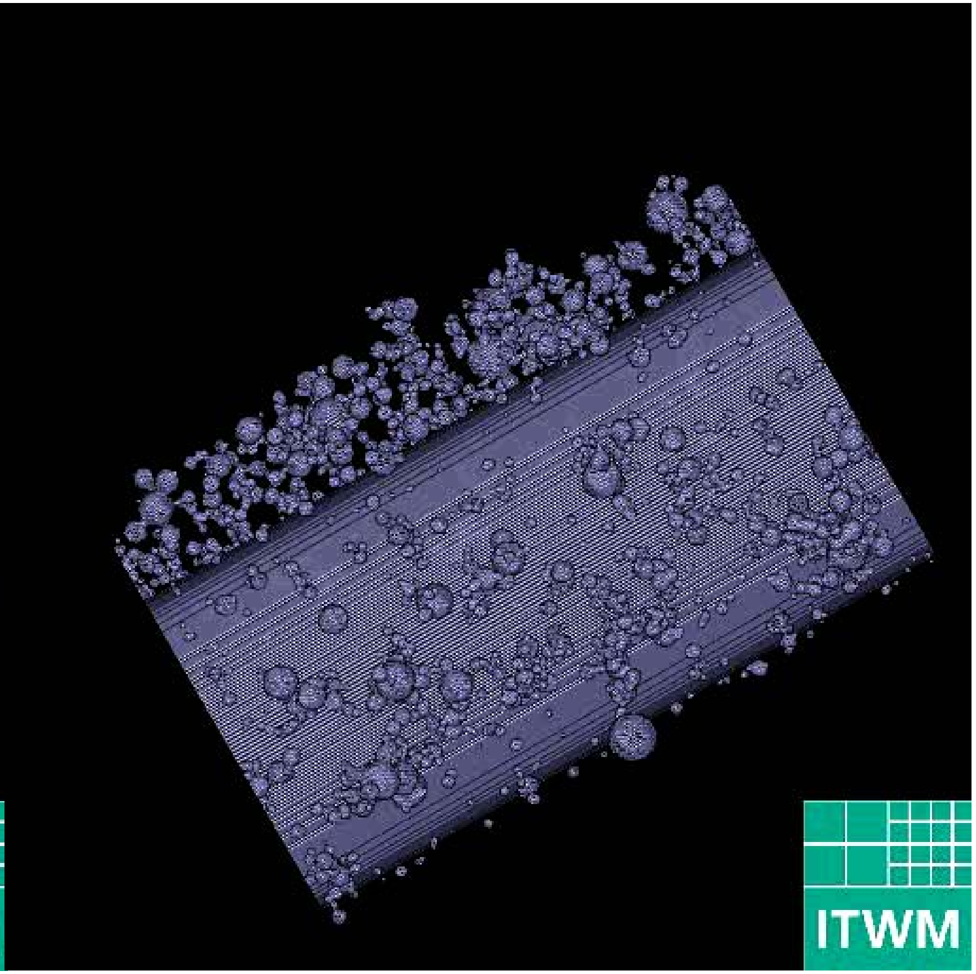
- Particles resolved by the cubes
- Filtration by “caught on first touch”
- Recompute flow after “batch” of particles
- Clogging in depth filtration

Nano Simulations

1.67cm/sec



10.0cm/sec



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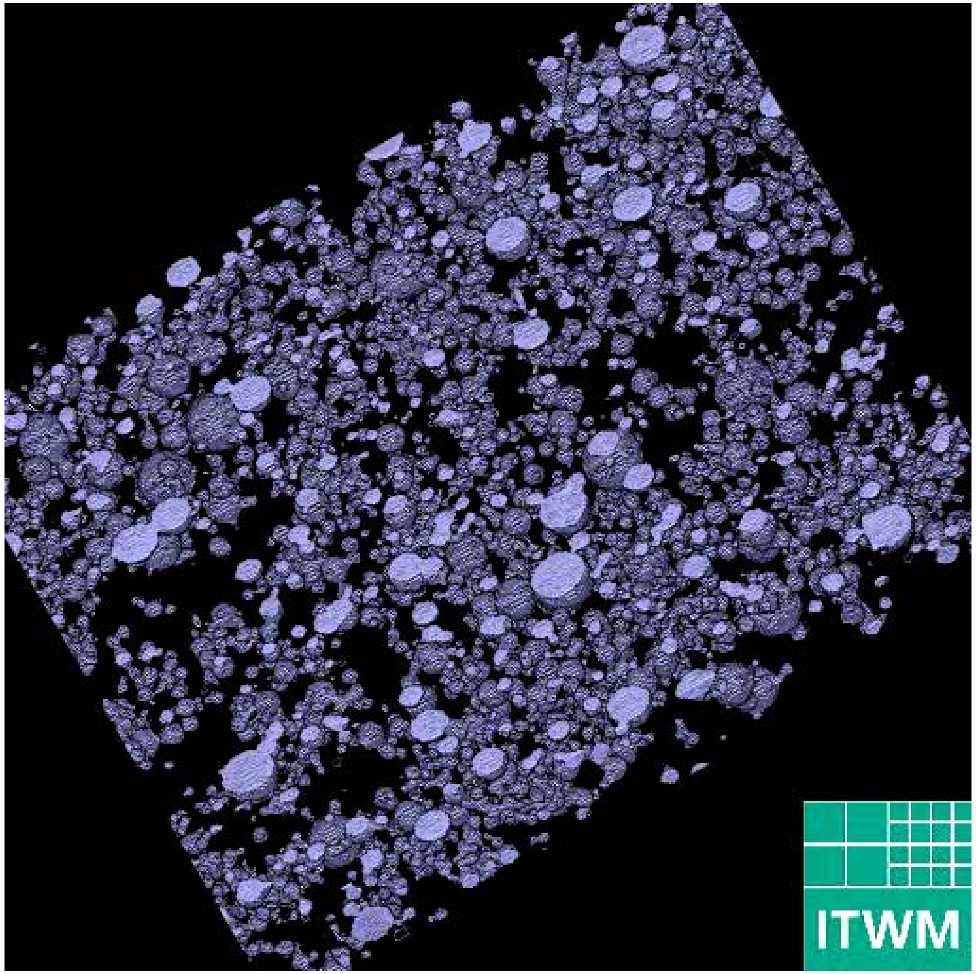
Nano Simulations

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

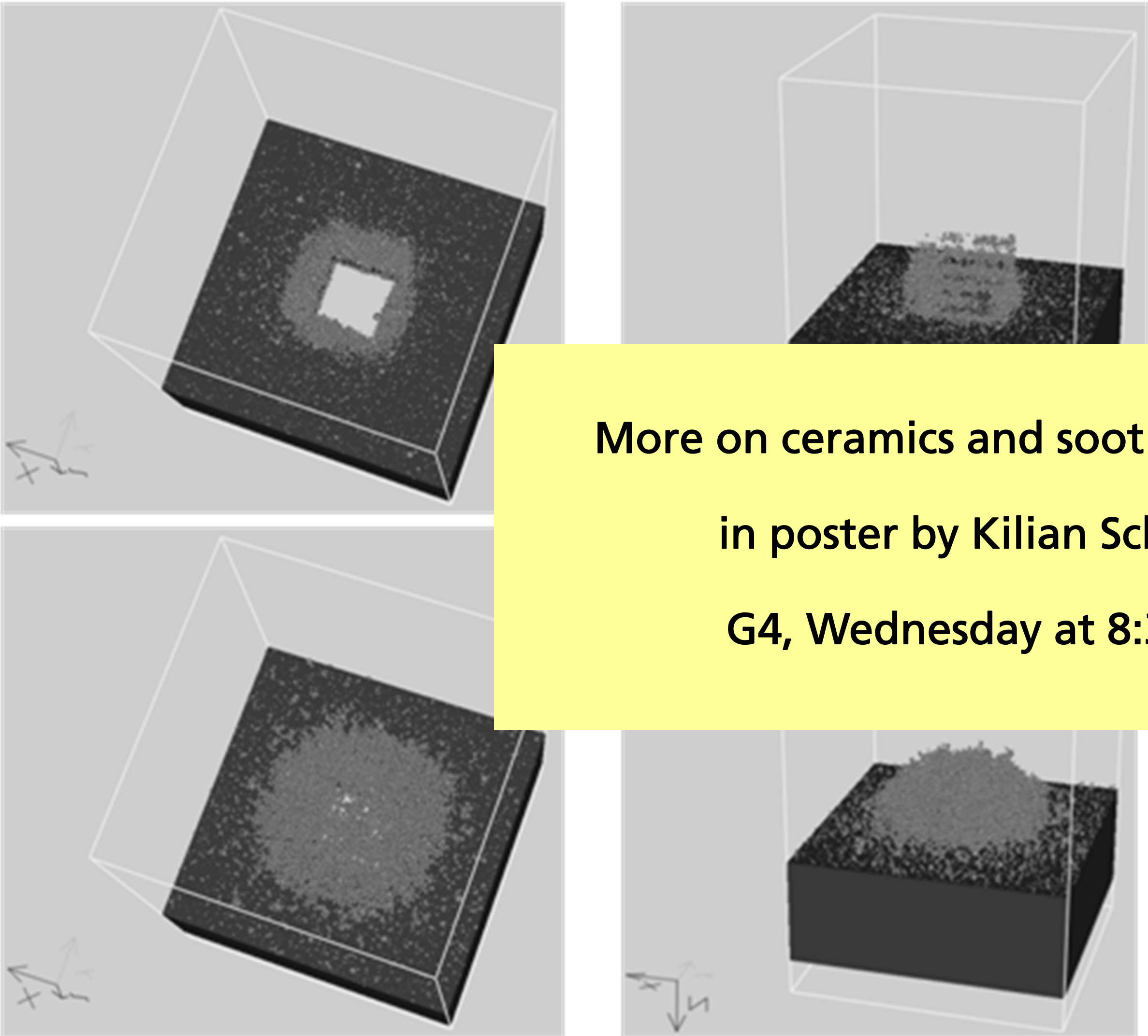
Result:

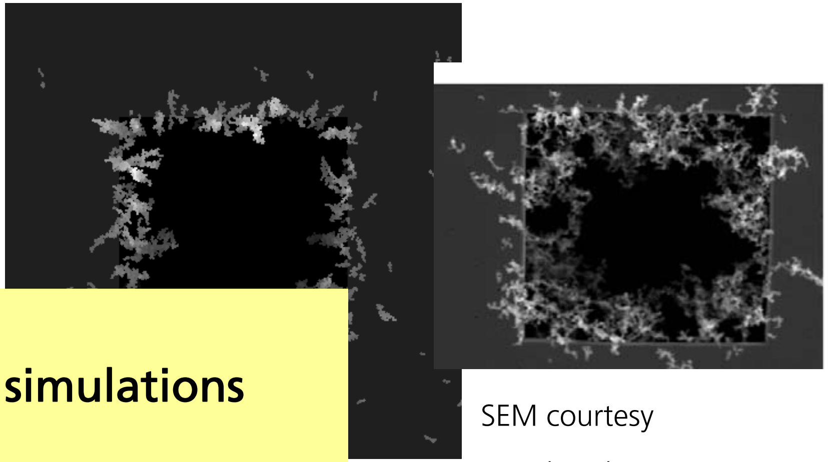
- Find minimal porosity and permeability of the soot layers, s_{max} and κ_{min}
- Derivation by layers from single fiber highly resolved simulations

Soot Layer Cut-Out



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





More on ceramics and soot simulations

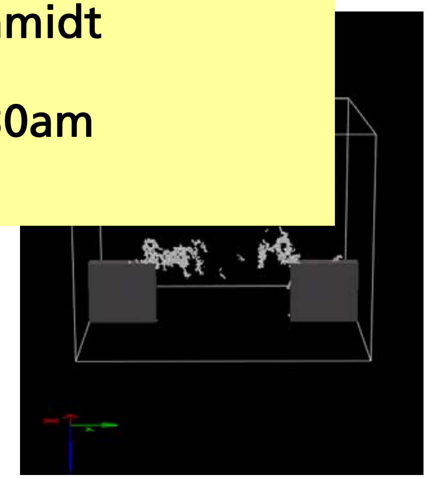
in poster by Kilian Schmidt

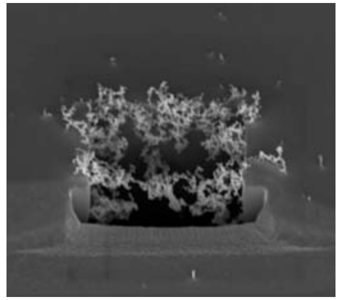
G4, Wednesday at 8:30am

SEM courtesy

H. Schomburg,

Robert Bosch GmbH



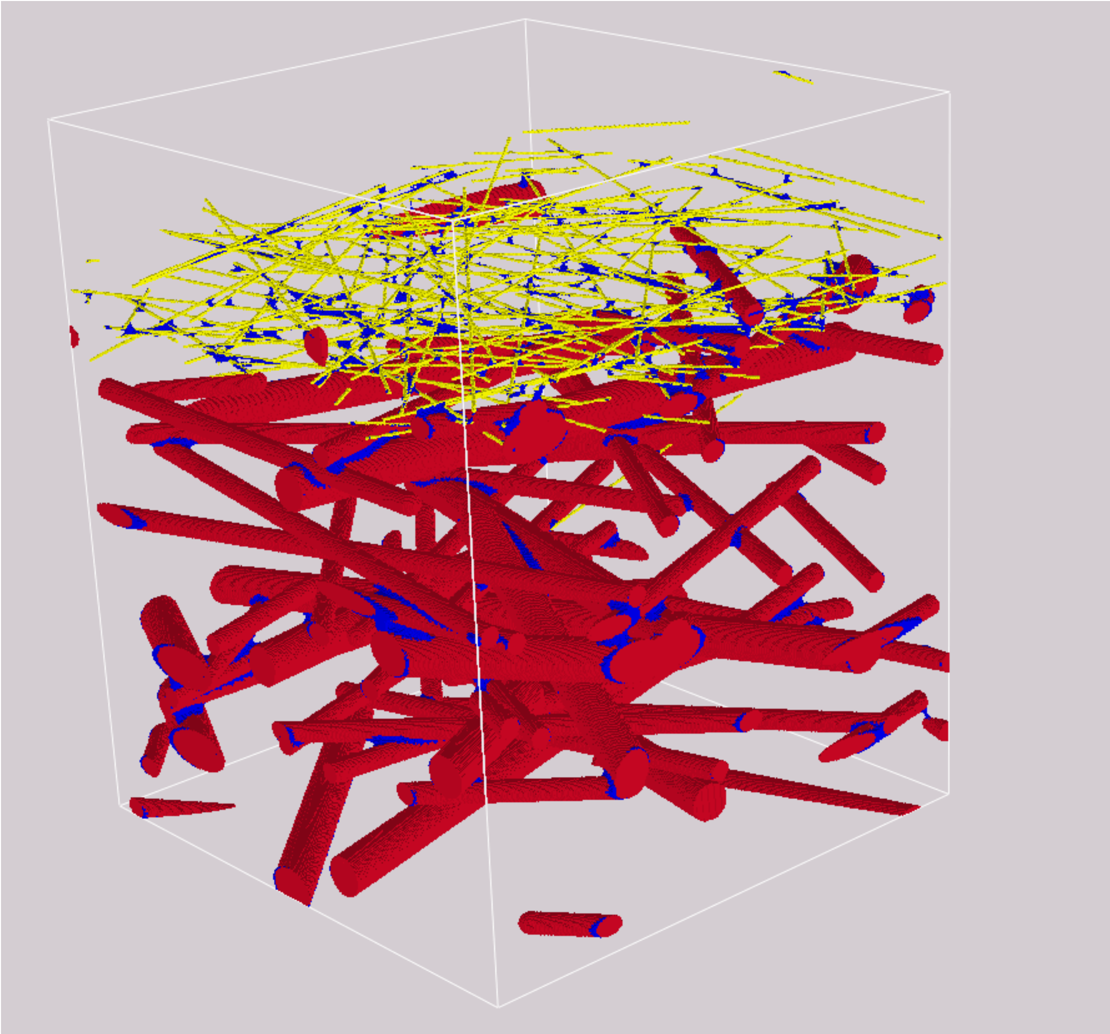


FIB & SEM courtesy

H. Schomburg,

Robert Bosch GmbH

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)

More on nano filtration media

in talk by Liping Cheng

G15, Thursday at 3:00pm

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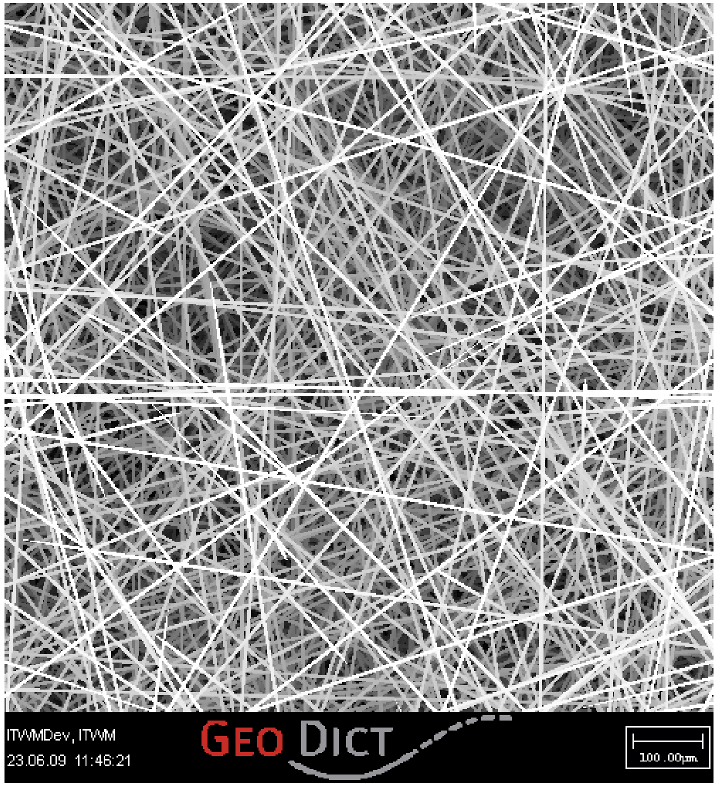
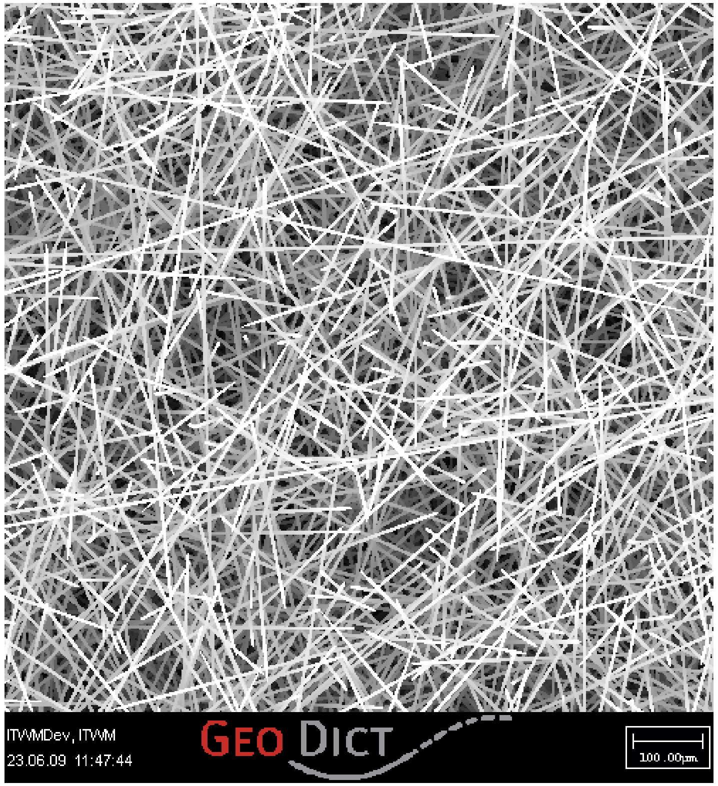
Nonwoven

SEM visualization of 8 volume percent 5 micron fibers

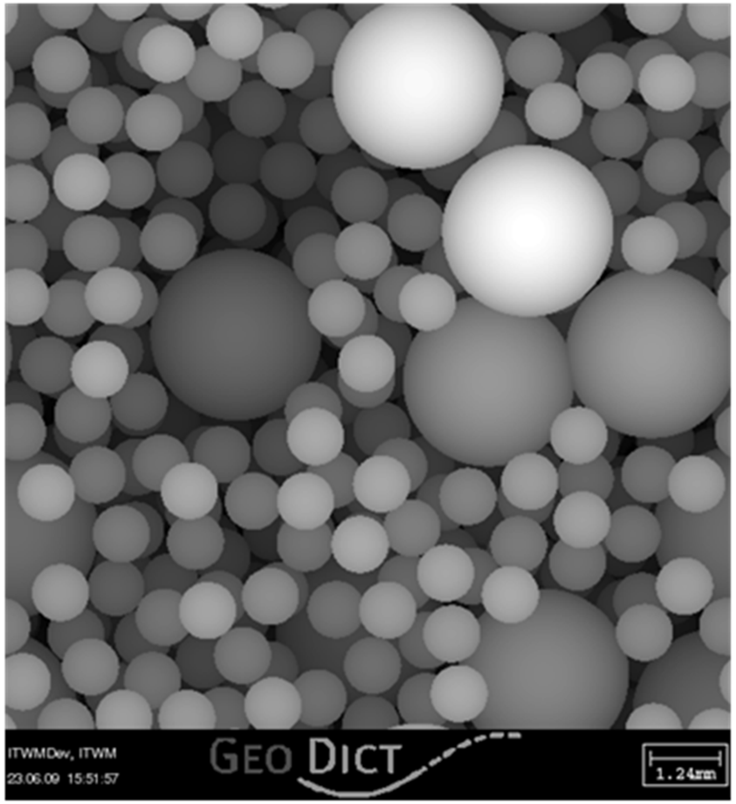


anisotropy 100



anisotropy 7

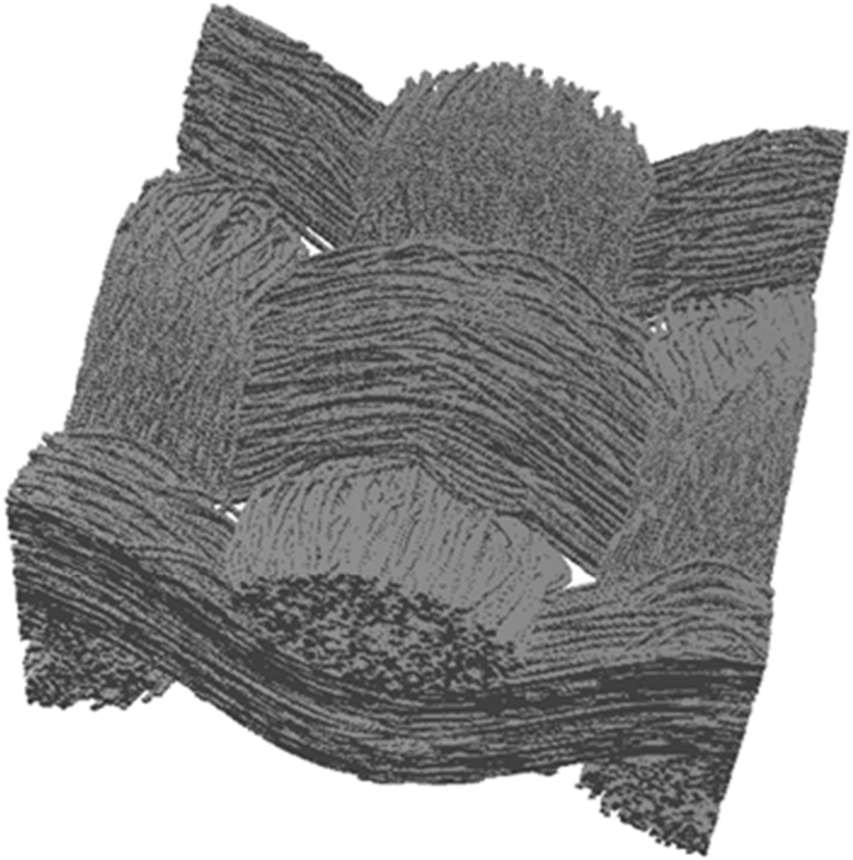
Packed bed of spheres and floating spheres



svf 0.64

svf 0.30

Carbon fiber multi-filament woven



3D Visualization (generated)

SEM (real)

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

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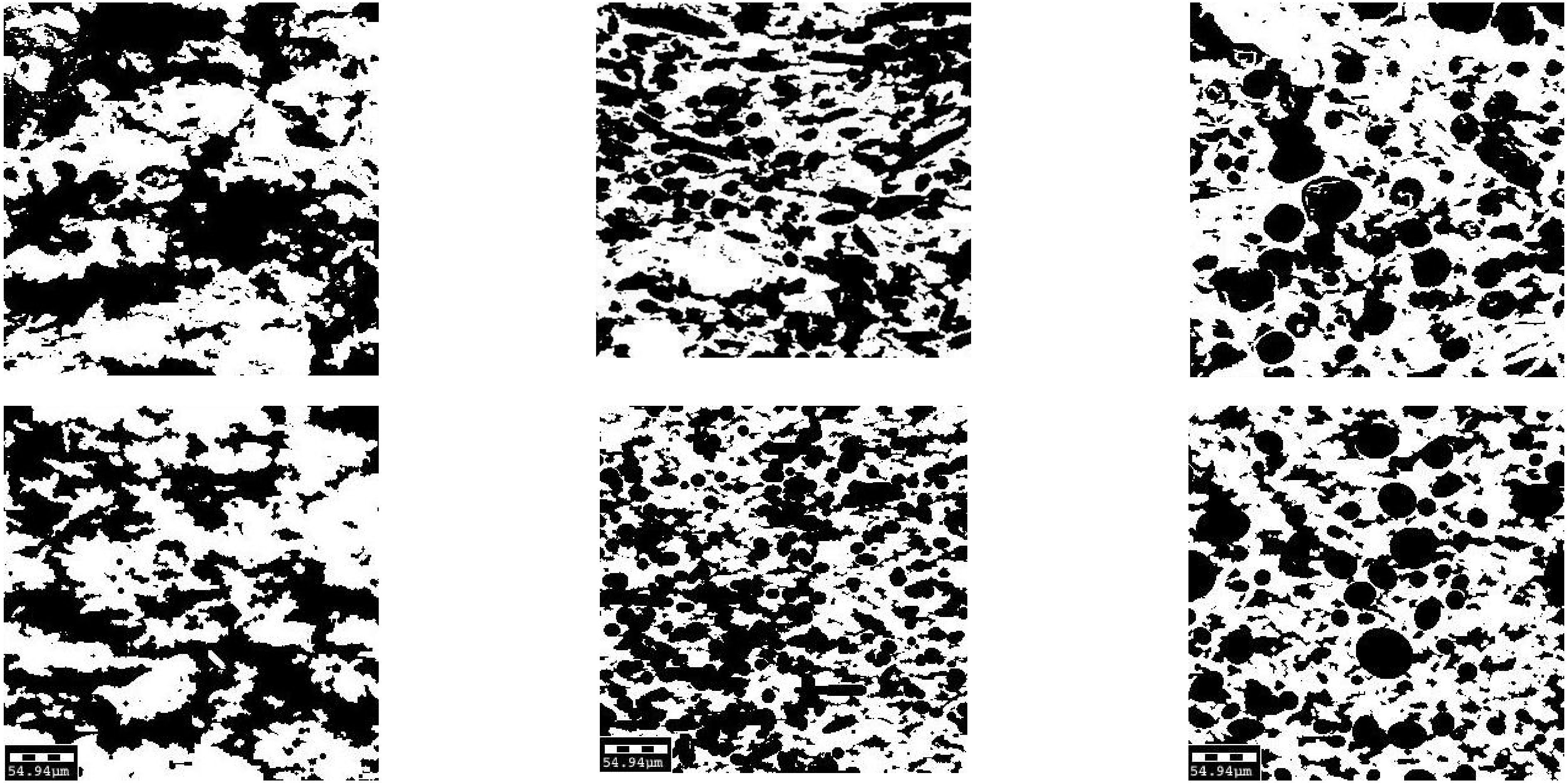
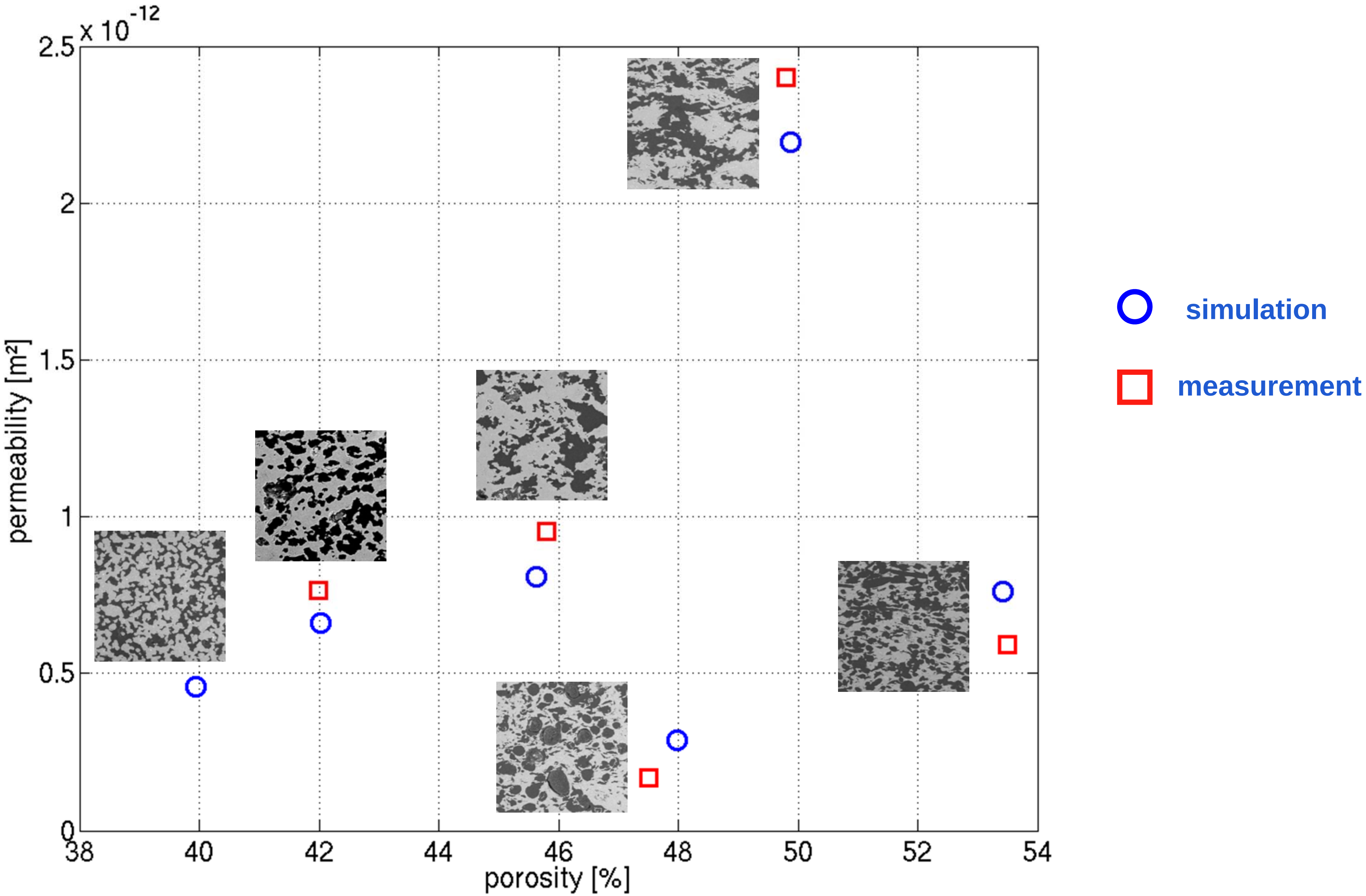
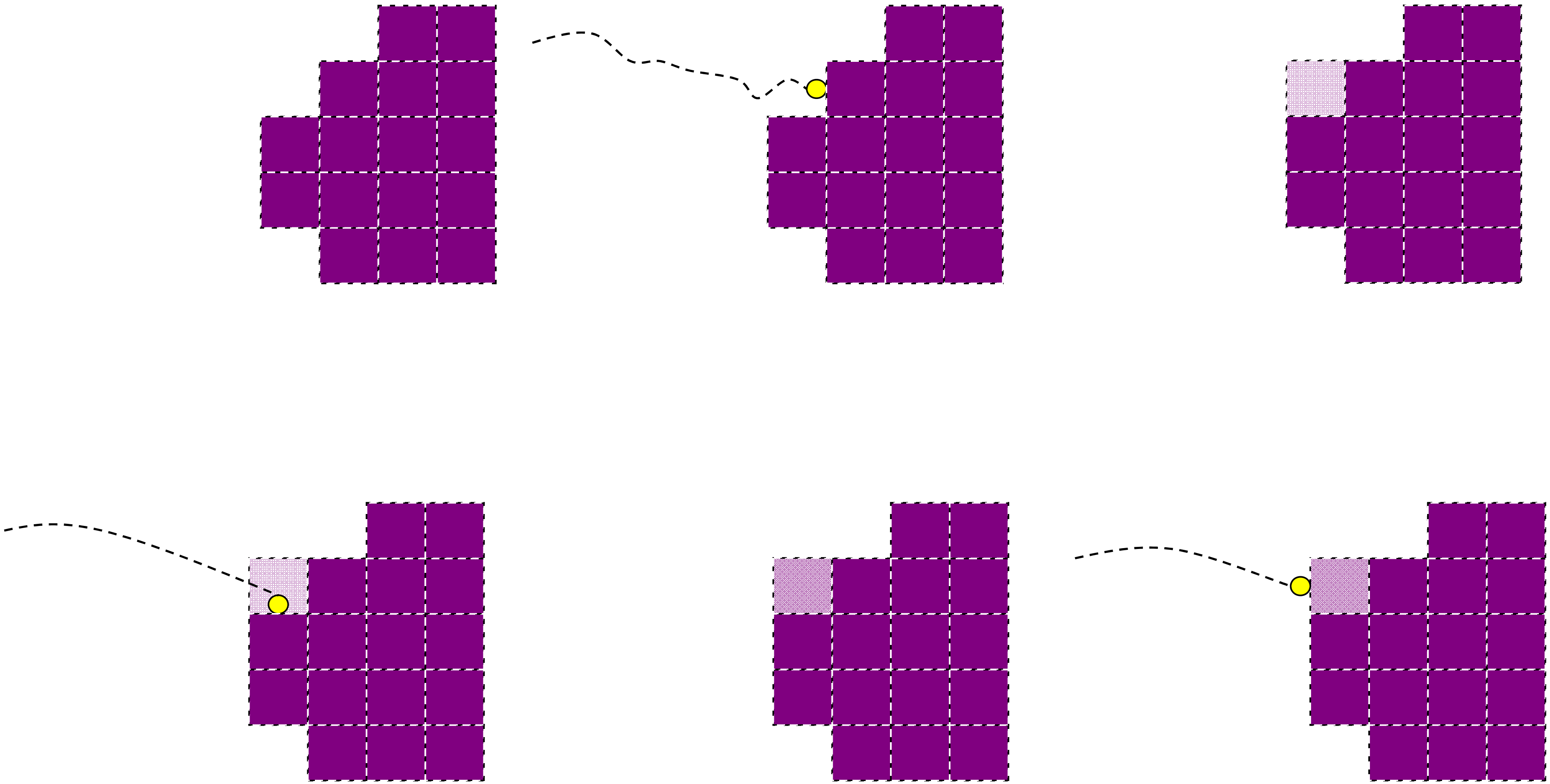
Binarized SEM (top) and virtual sintered ceramics (bottom)



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



Mikro-Modus



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Stationary Flow with unresolved particles: Stokes-Brinkmann eqs

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

$\vec{\mathbf{f}} = (0, 0, f)$: 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,

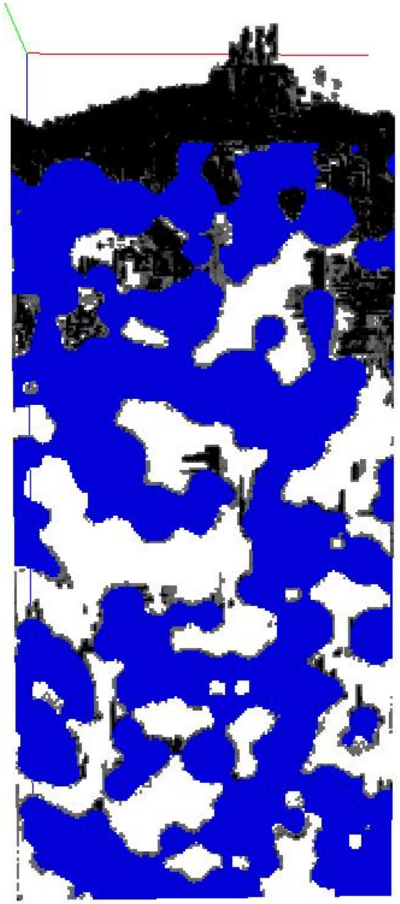
p : pressure and

Γ : fiber or deposited particle surfaces.

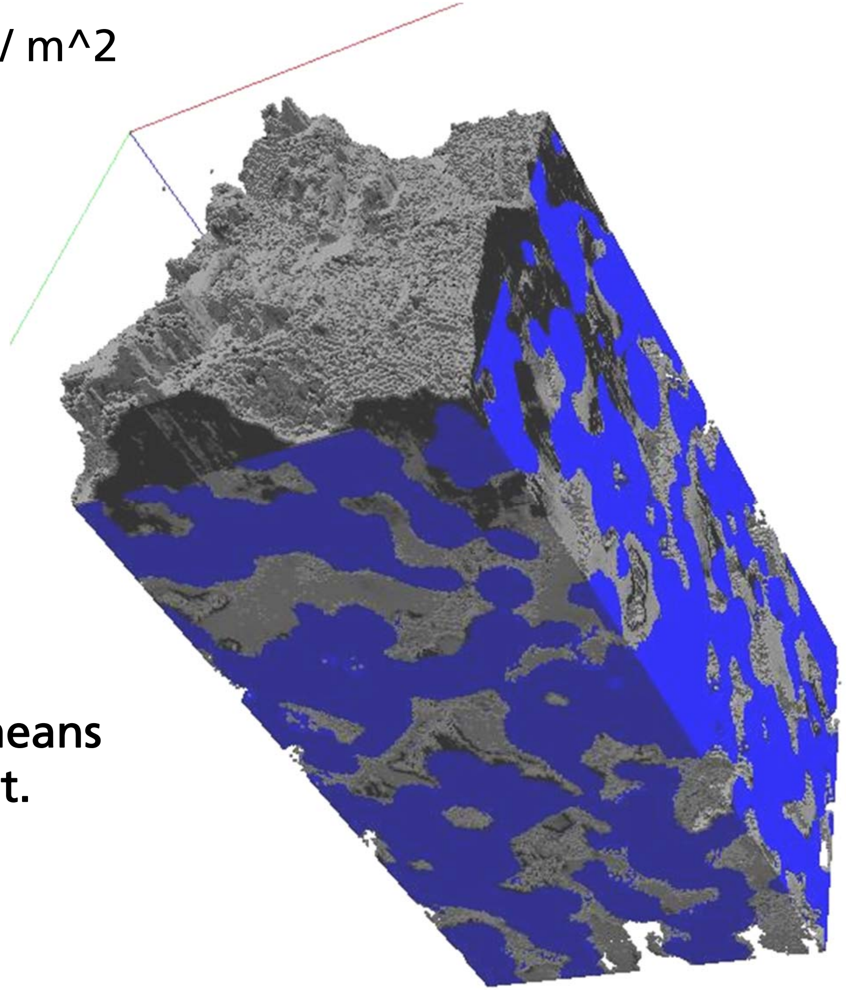
Solid volume fraction in voxel is increased until s_{max} is reached. Voxel becomes "collision-solid". Neighbor voxels svf starts increasing upon particle arrival

Micro Simulations

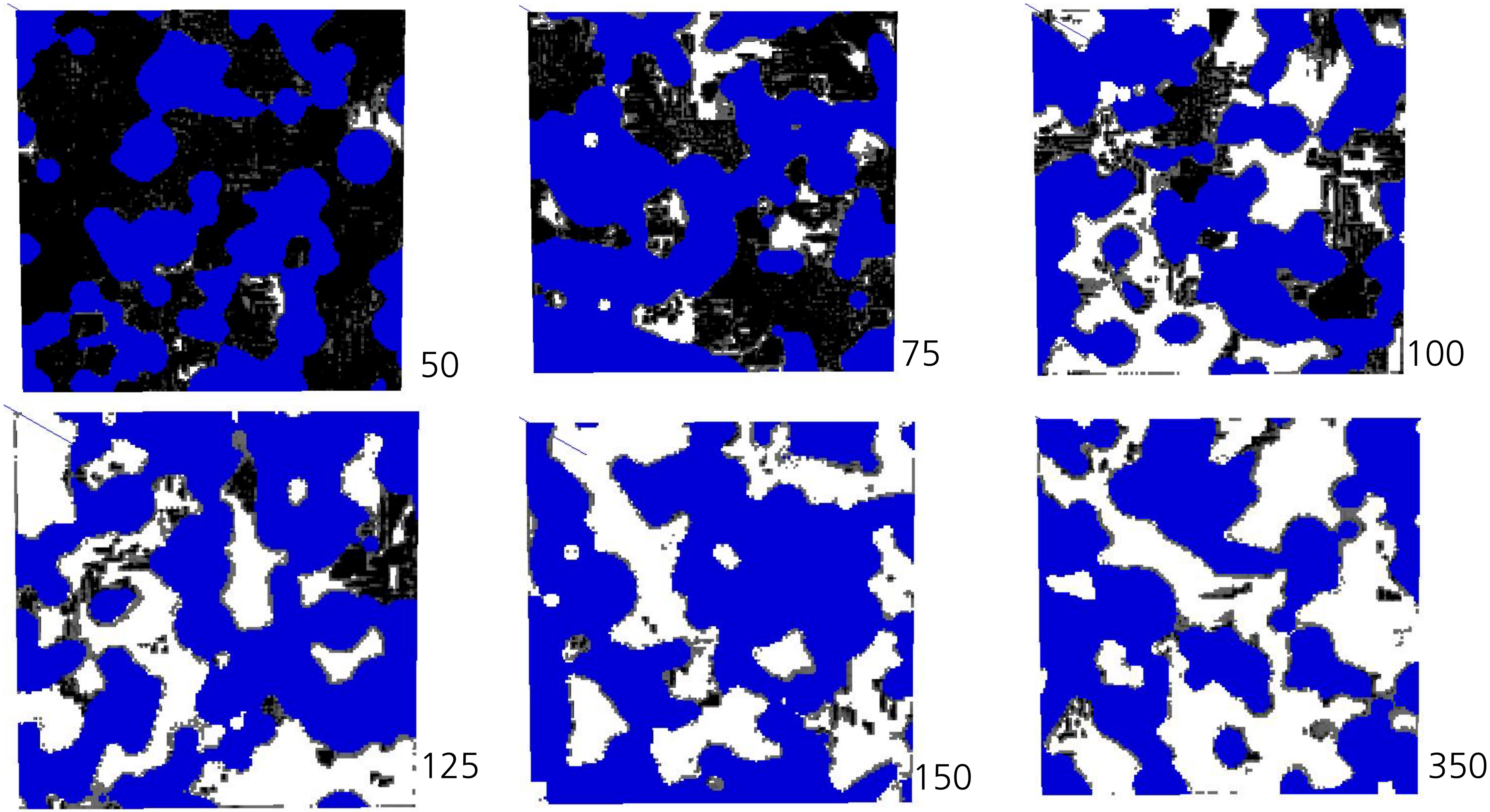
Final state at 5.1 g / m^2



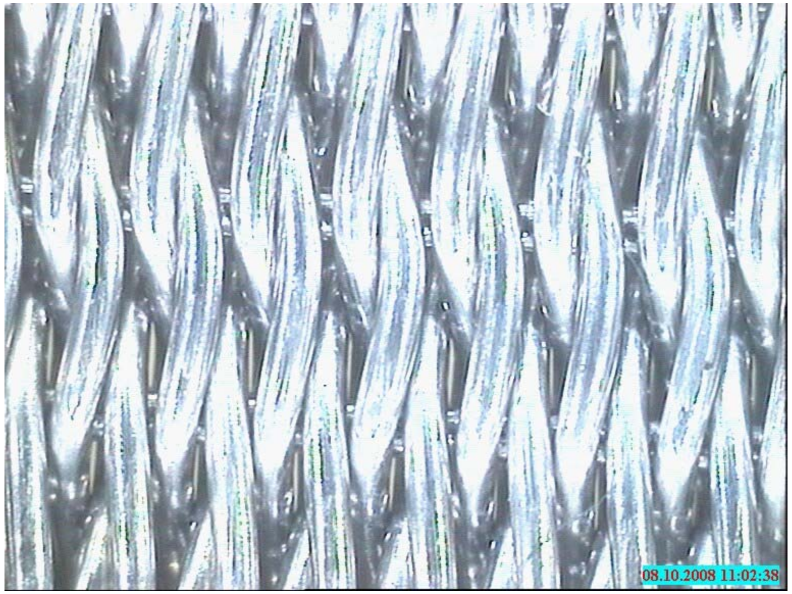
Darker gray means denser soot.

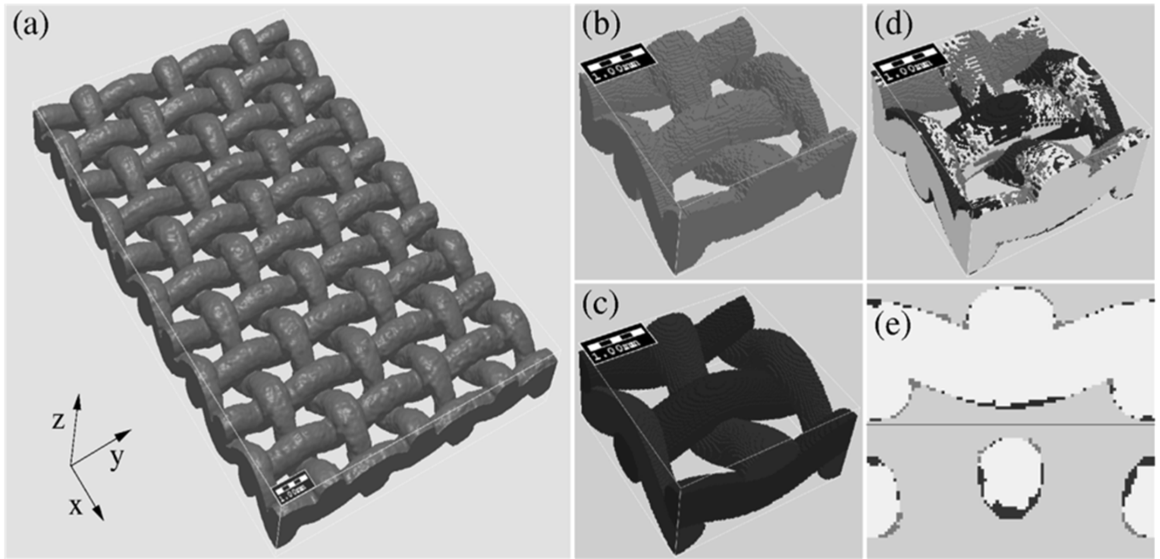


Horizonal layers



Reconstruction of Woven





Microscopy Courtesy M. Knefel, Gebr. Kufferath AG.

More on woven simulations

in talk by Erik Glatt

L6, Wednesday at 11:50am

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 GeoDict

Courtesy M. Knefel, Gebr. Kufferath AG.

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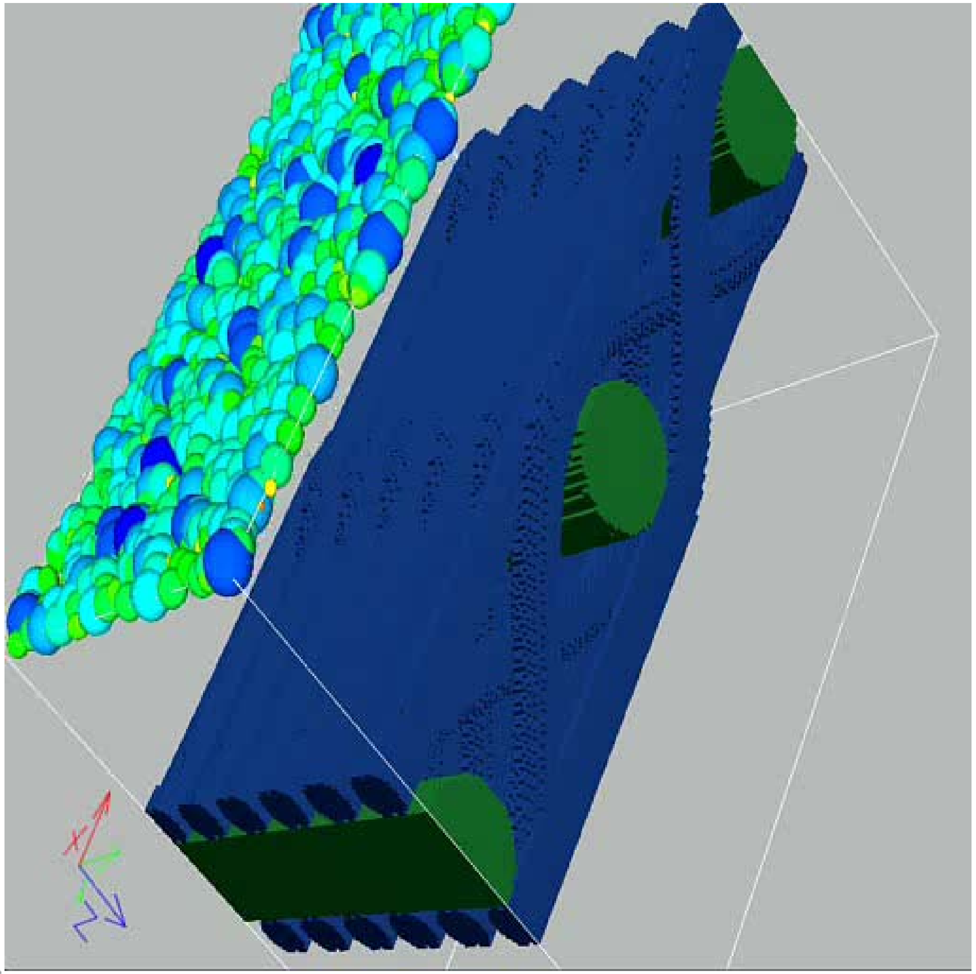

Computed & animated with GEO DICT

Courtesy M. Knefel, Gebr. Kufferath AG.

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Courtesy M. Knefel, Gebr. Kufferath AG.

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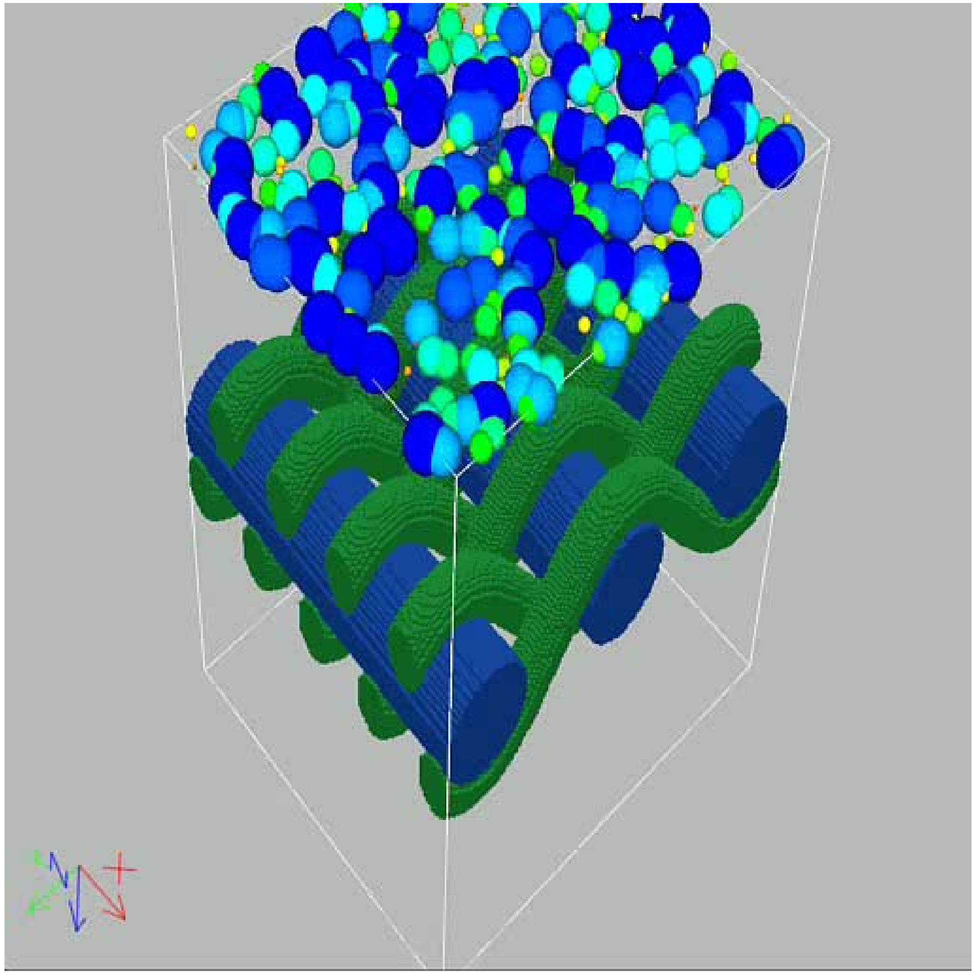
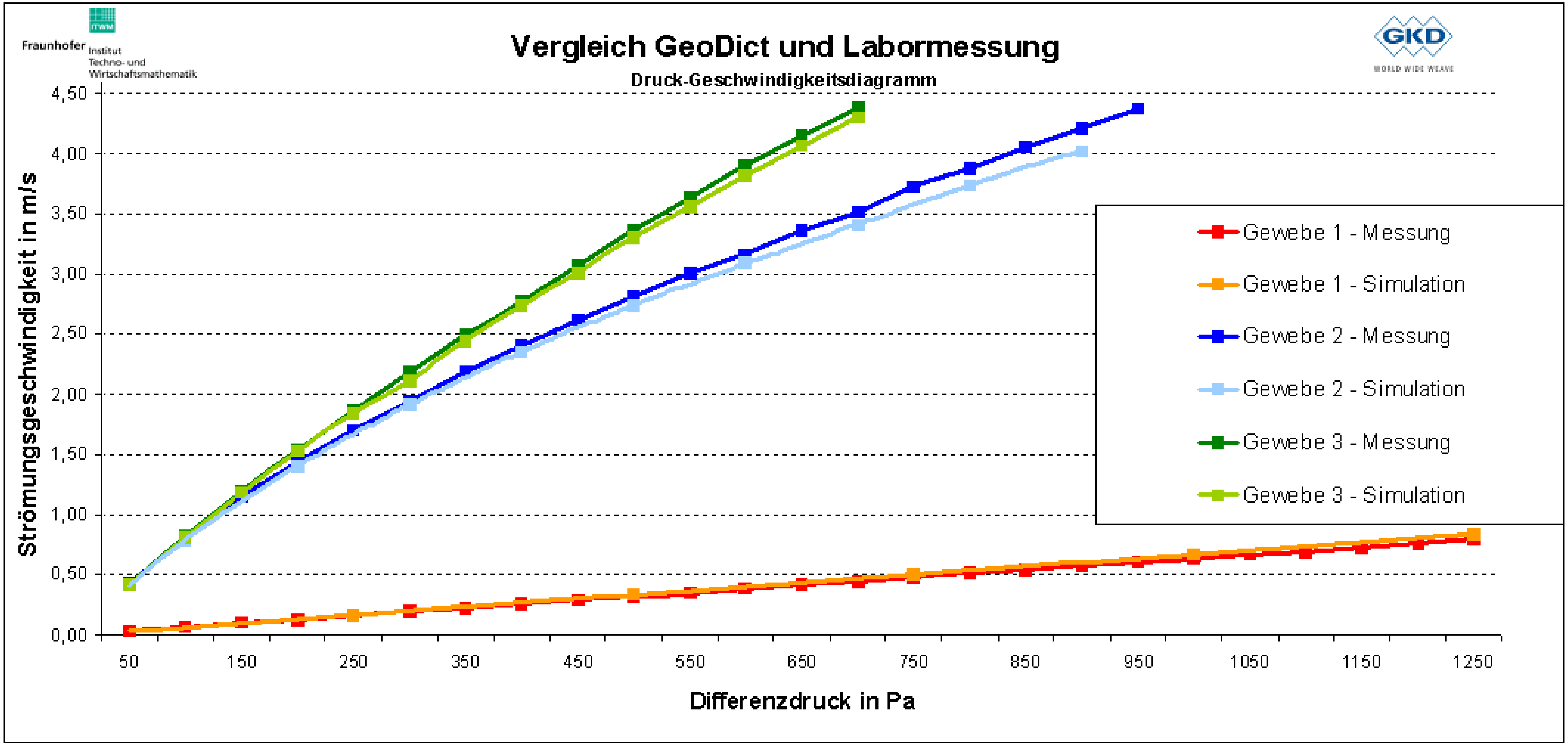
- Filter Cake more efficient filter than metal wire mesh
- Pressure drop increase also available



Computed & animated with GEO DICT

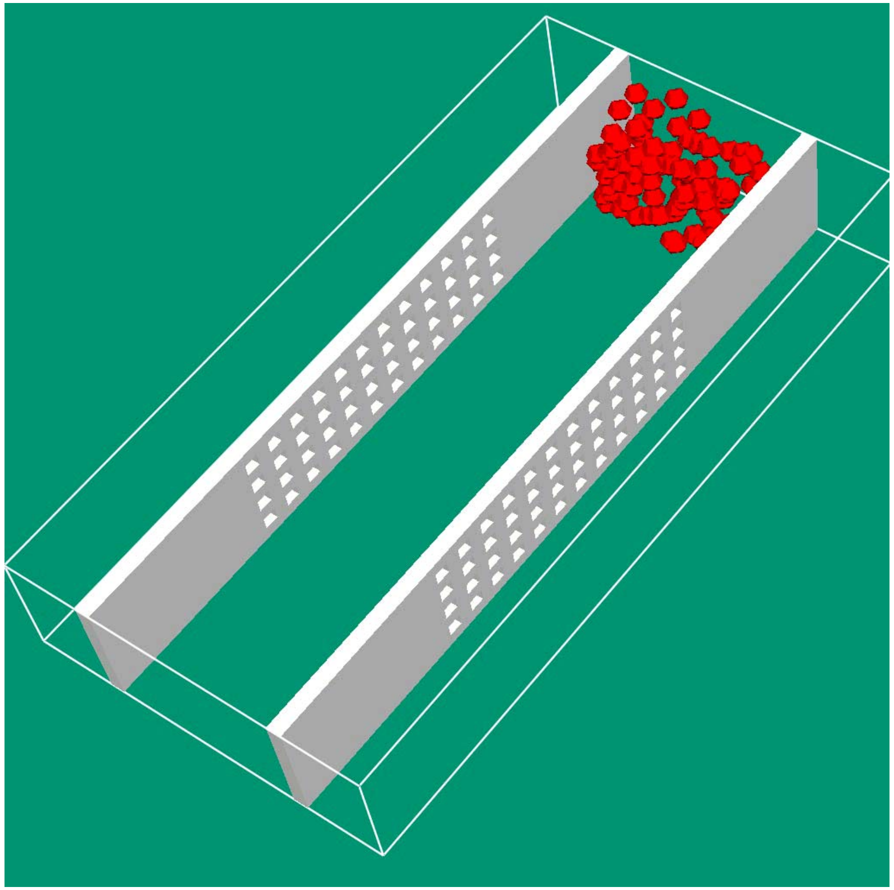
Courtesy M. Knefel, Gebr. Kufferath AG.

Measured vs Simulated pressure drop for GKD meshes



Courtesy M. Knefel & E. Wegenke, Gebr. Kufferath AG.

Cross Flow Filtration



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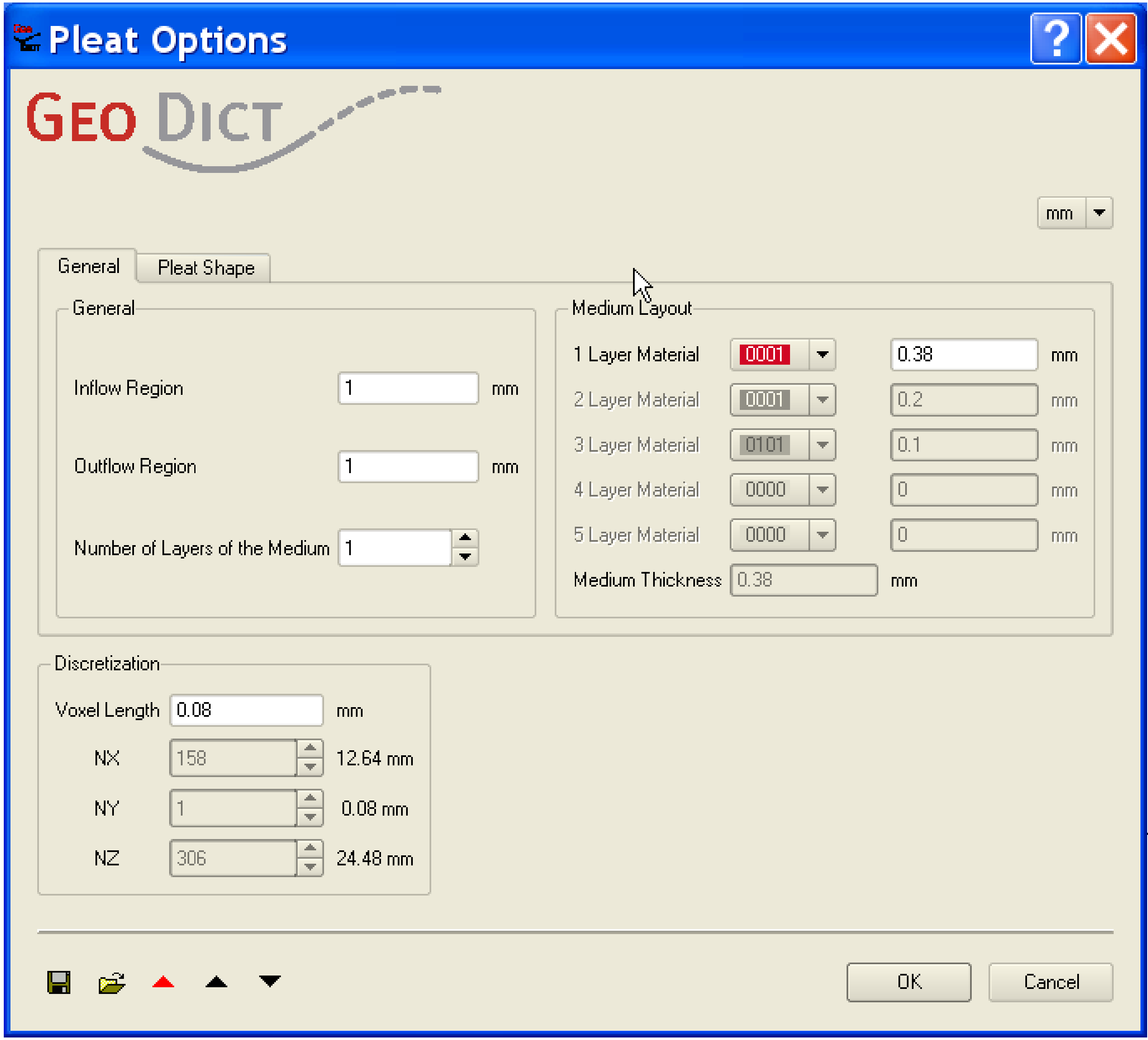
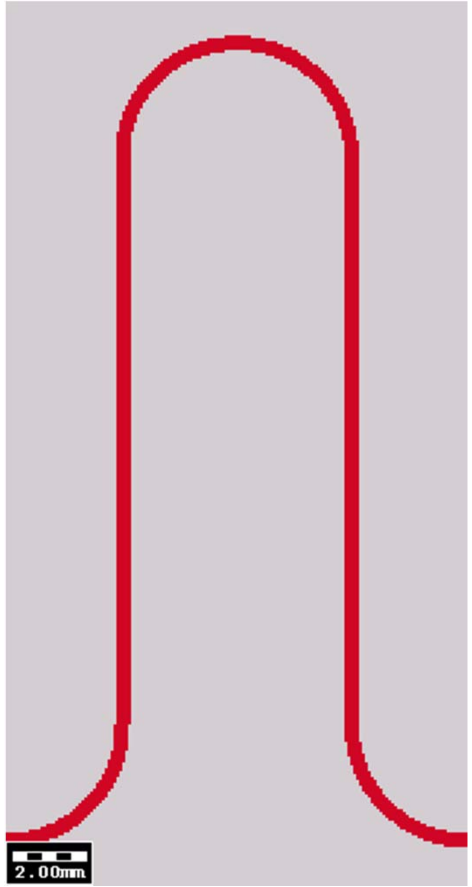
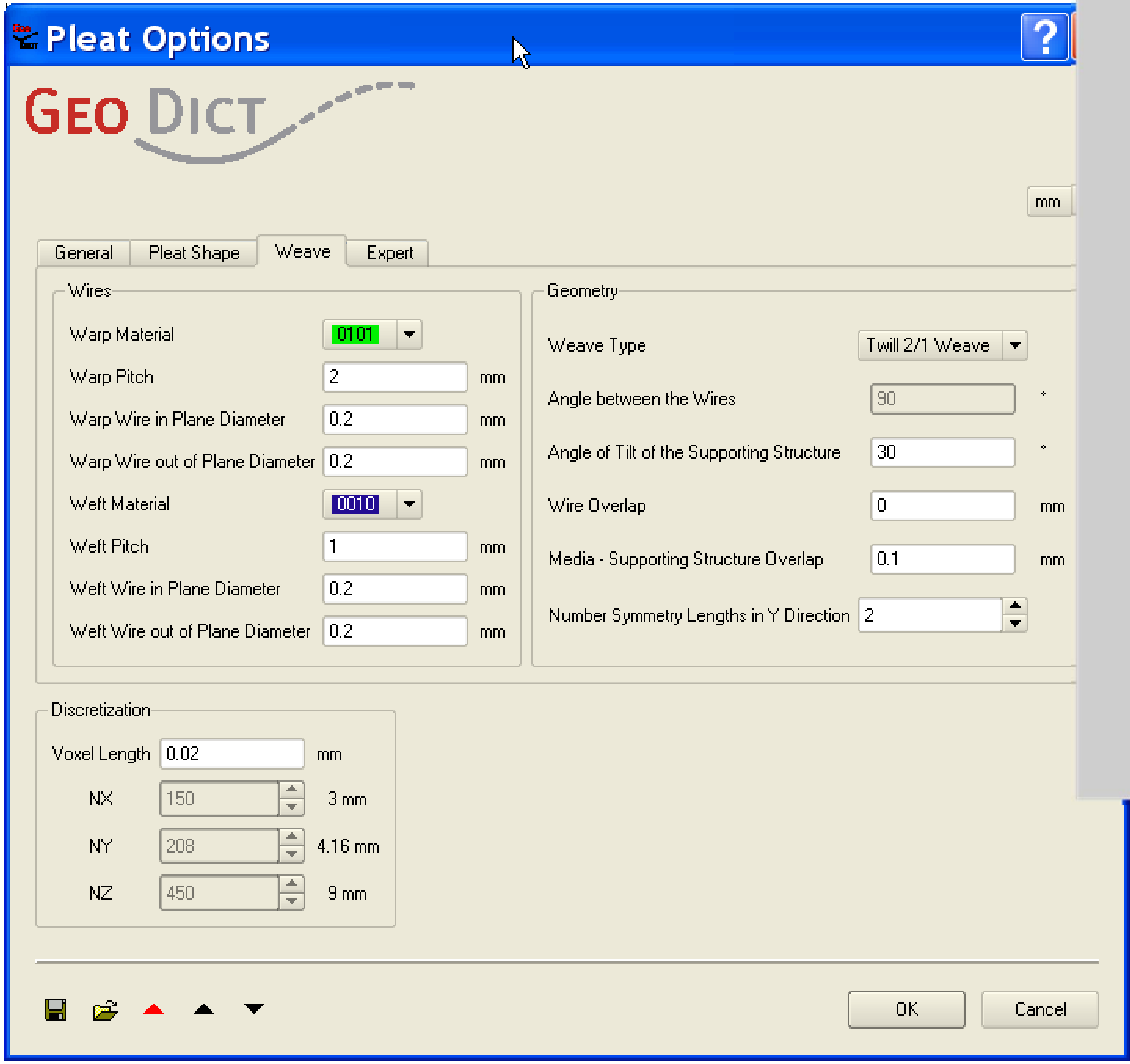
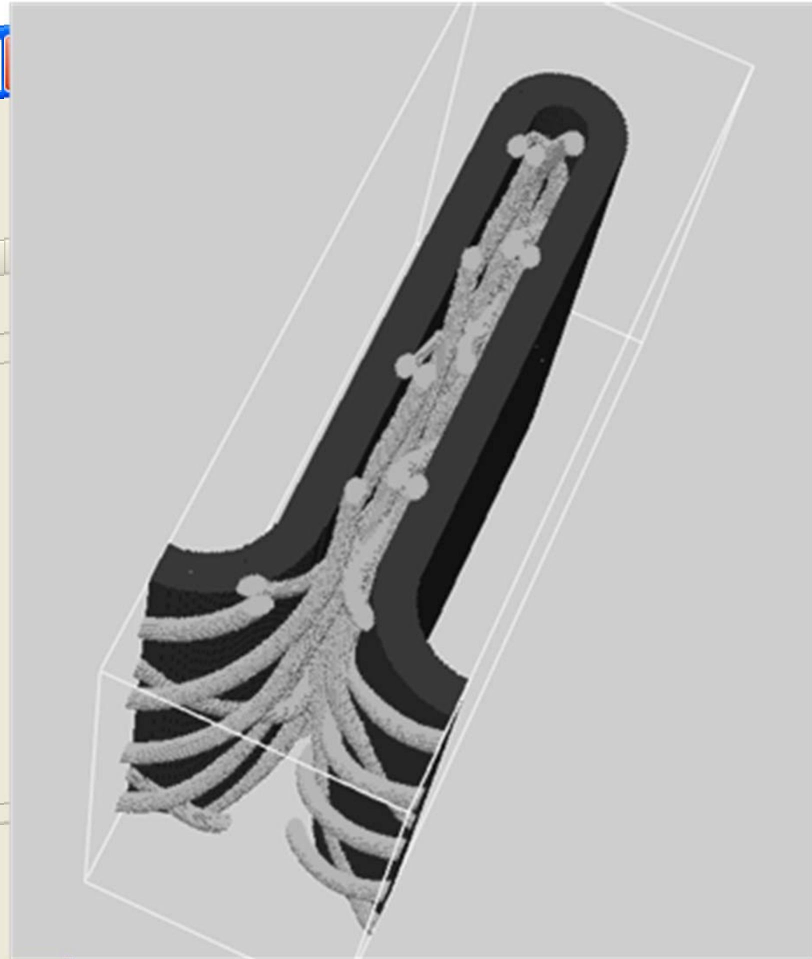
General Pleat Options





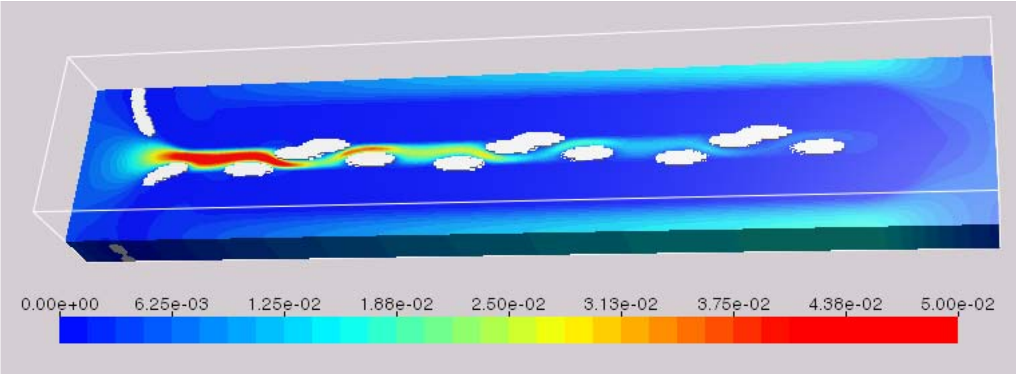
Weave Pleat Options



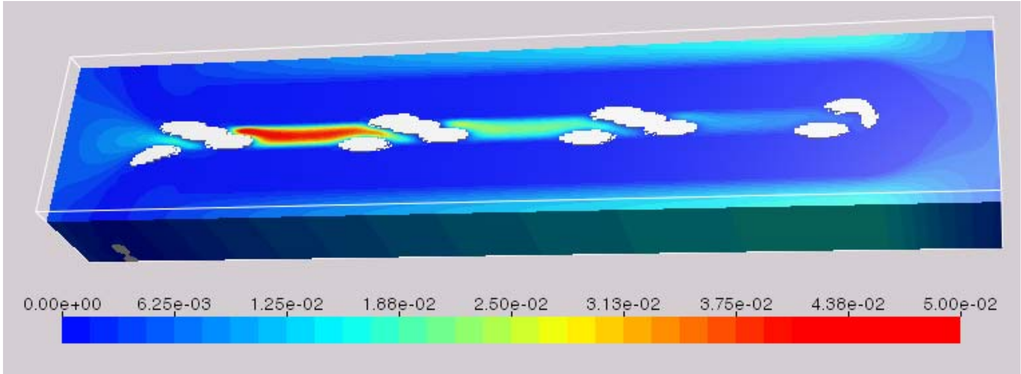


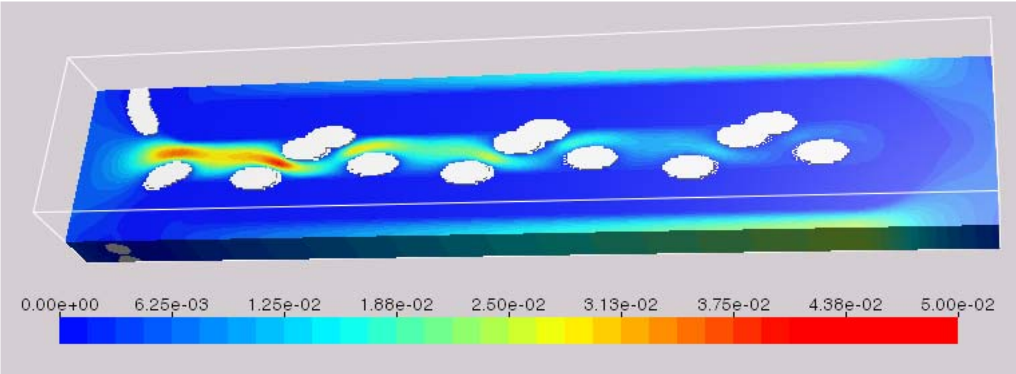
Oil flow in pleats with support structure: velocity

- 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

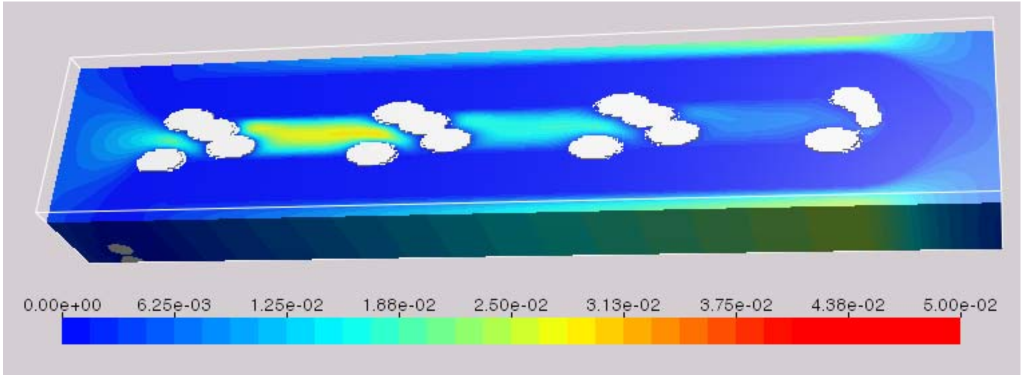


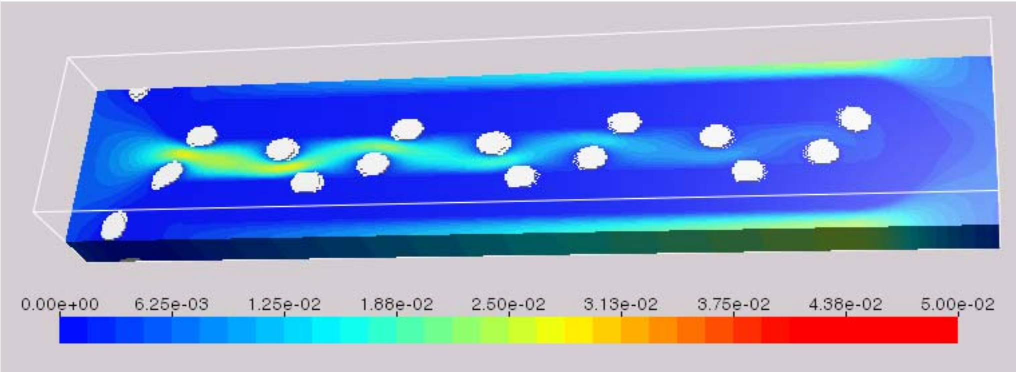
Narrow Channel



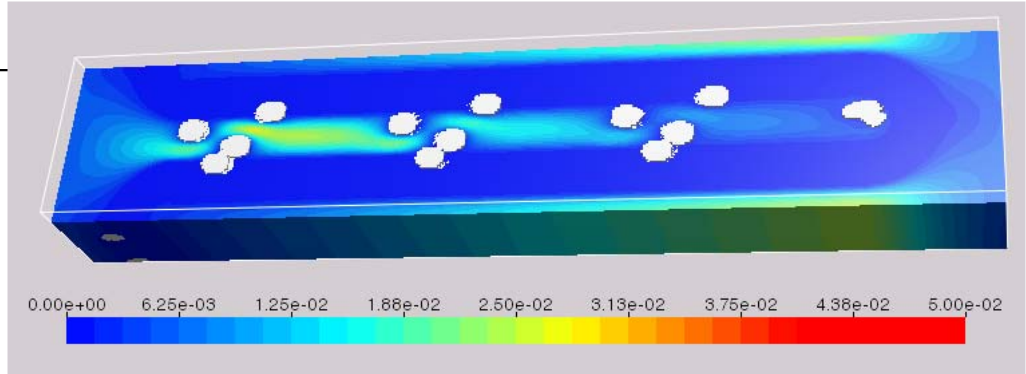


Thick Wire



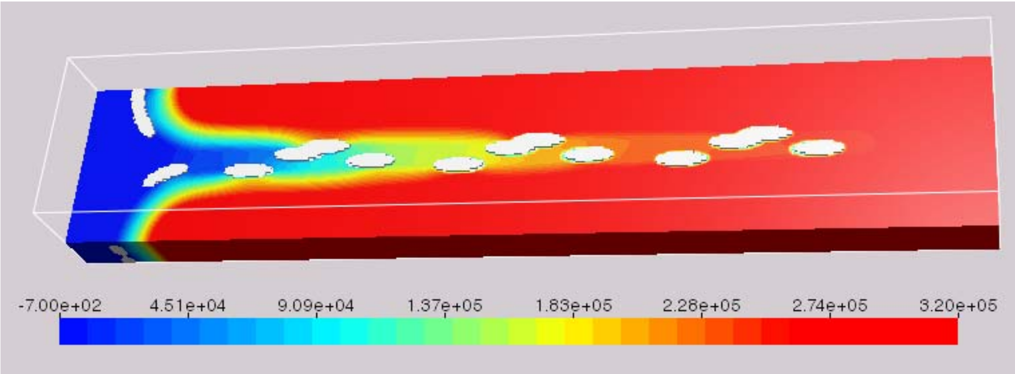


Thin Wire



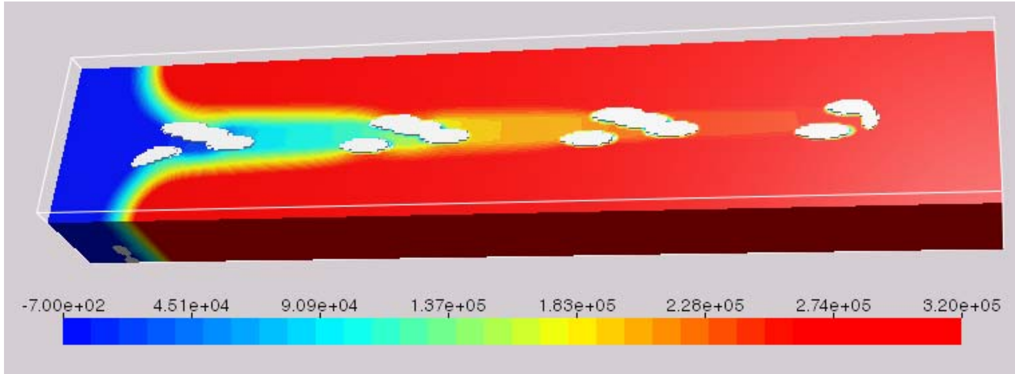
Oil flow in pleats with support structure: pressure

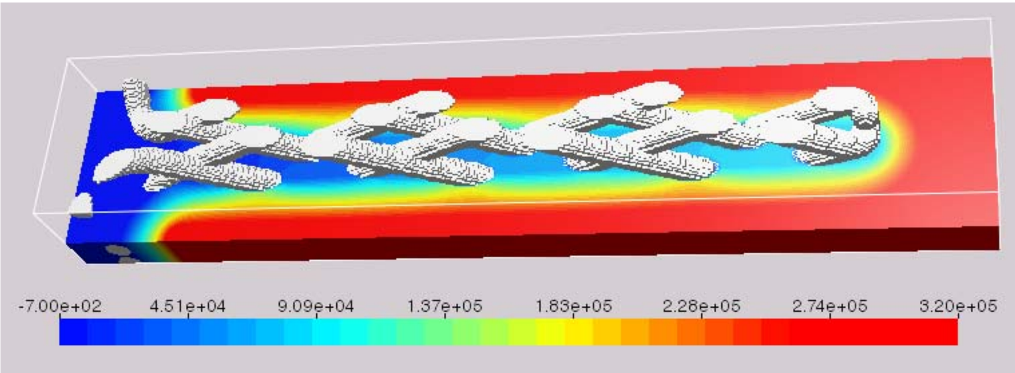
- Pressure in Pascal
- Oil: density 850 kg/m³ viscosity 0.17 m²/s
- Same pleat count
- Different in- and outflow channel widths
- Grid resolution 40 µm
- 50 x 70 x 380 cells



Narrow Channel:

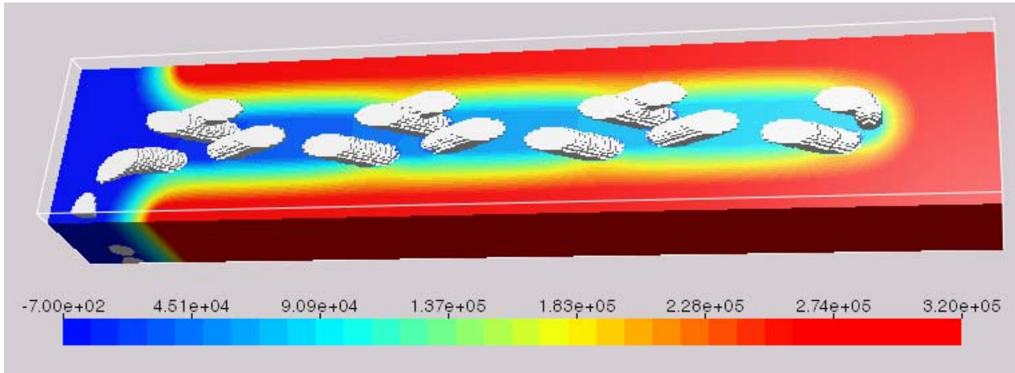
4 bar

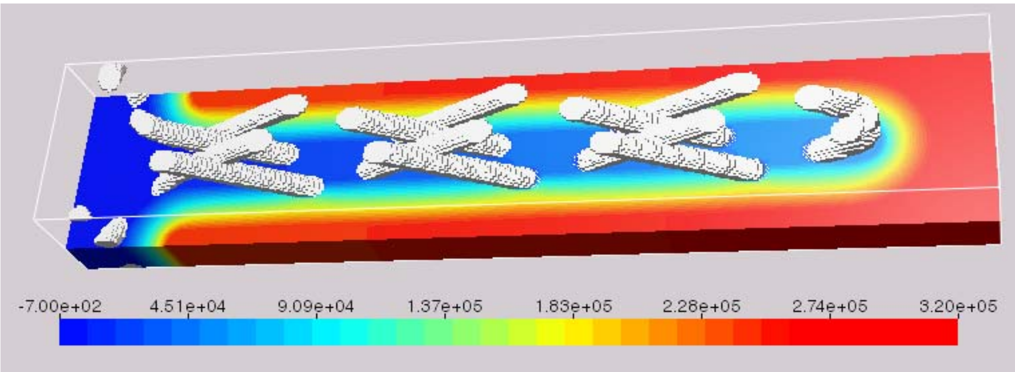




Thick Wire:

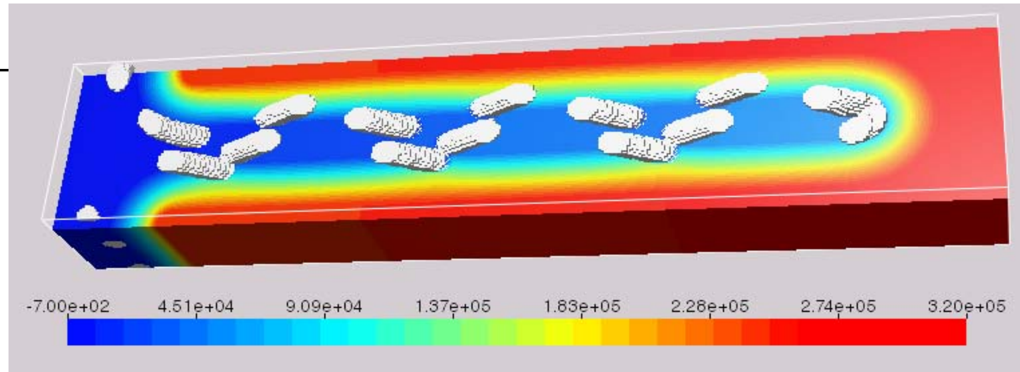
3.1 bar



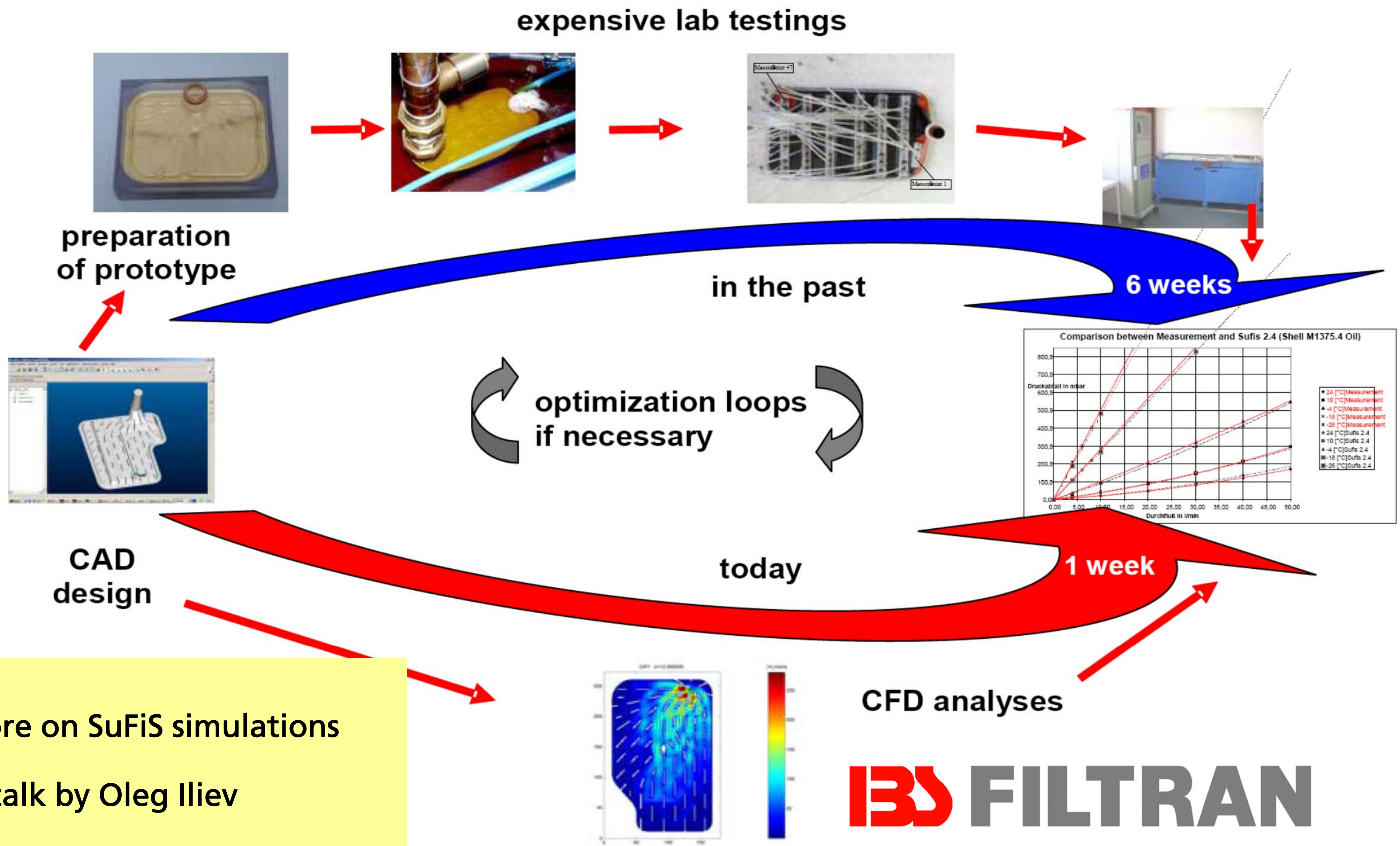


Thin Wire:

2.7 bar



Benefits of SUFIS simulations



More on SuFiS simulations

in talk by Oleg Iliev

L15, Thursday at 11:25am

Selected project partners and customers

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ITWM

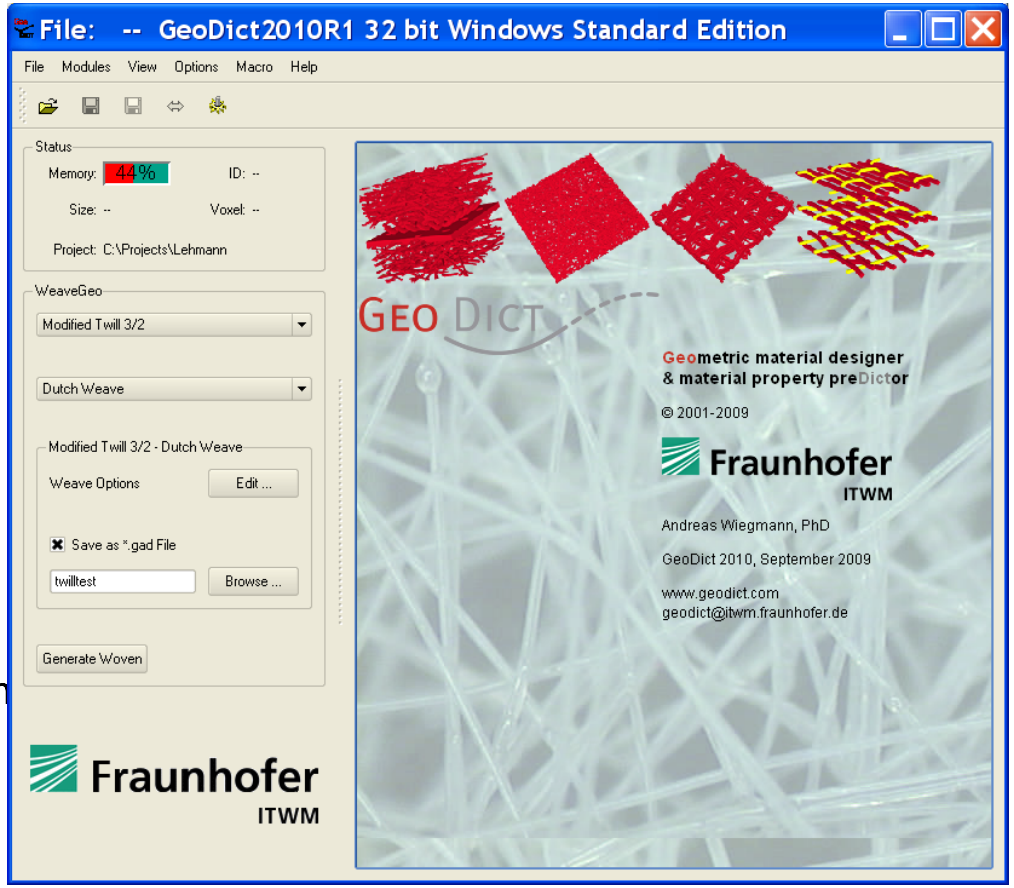
Andreas Wiegmann

Filtech, Wiesbaden

13 October 2009

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 tim
- SatuDict (two phase flow properties)
- PoroDict (pore size measures)
- AcoustoDict (acoustic absorption)



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13 October 2009

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Conclusions

Challenges

- Measurements
- deposition location
- electric charges
- Requirements: cost, material, space, energy
- Computing power
- Geometric resolution
- Geometry uncertain
- Analytic expressions to be derived

Progress

- 3d media and element models
- Navier-Stokes-Brinkman for gas and liquid
- Fast & low memory solvers
- Prediction of pressure drop for Re < 100
- Low concentration particle transport
- Predicition of filter efficiency
- Cake and porous media build-up
- Prediction of clogging and life time
- **Filtration and separation simulation spread in Academic and Industrial R&D**

Exhibit and talks at Filtech 2009 also by Fraunhofer ITWM

Visit us at Booth I A 12

Simulation of pleat deflection in talk by Matthias Kabel,	G1, Tuesday 1:40pm
More on ceramics and soot simulations in poster by Kilian Schmidt,	G4, Wednesday at 8:30am
More on woven simulations in talk by Erik Glatt,	6, Wednesday at 11:50am
Coupled particle and filter element level in talk by Zarah Lakdawala,	L10 Wednesday at 5:30pm
More on SuFiS simulations in talk by Oleg Iliev,	L15, Thursday at 11:25pm
More on nano filtration media in talk by Liping Cheng,	G15, Thursday at 3:00pm

Thank you for your attention

Fraunhofer ITWM