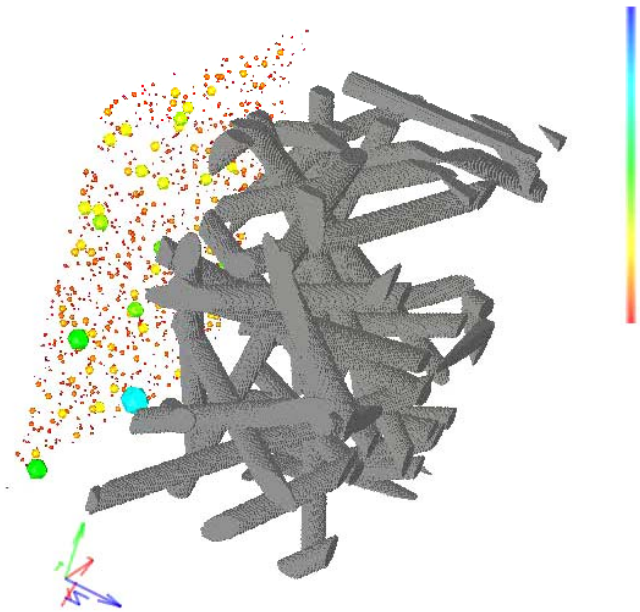
Progress & Challenges predicting Filtration and Separation



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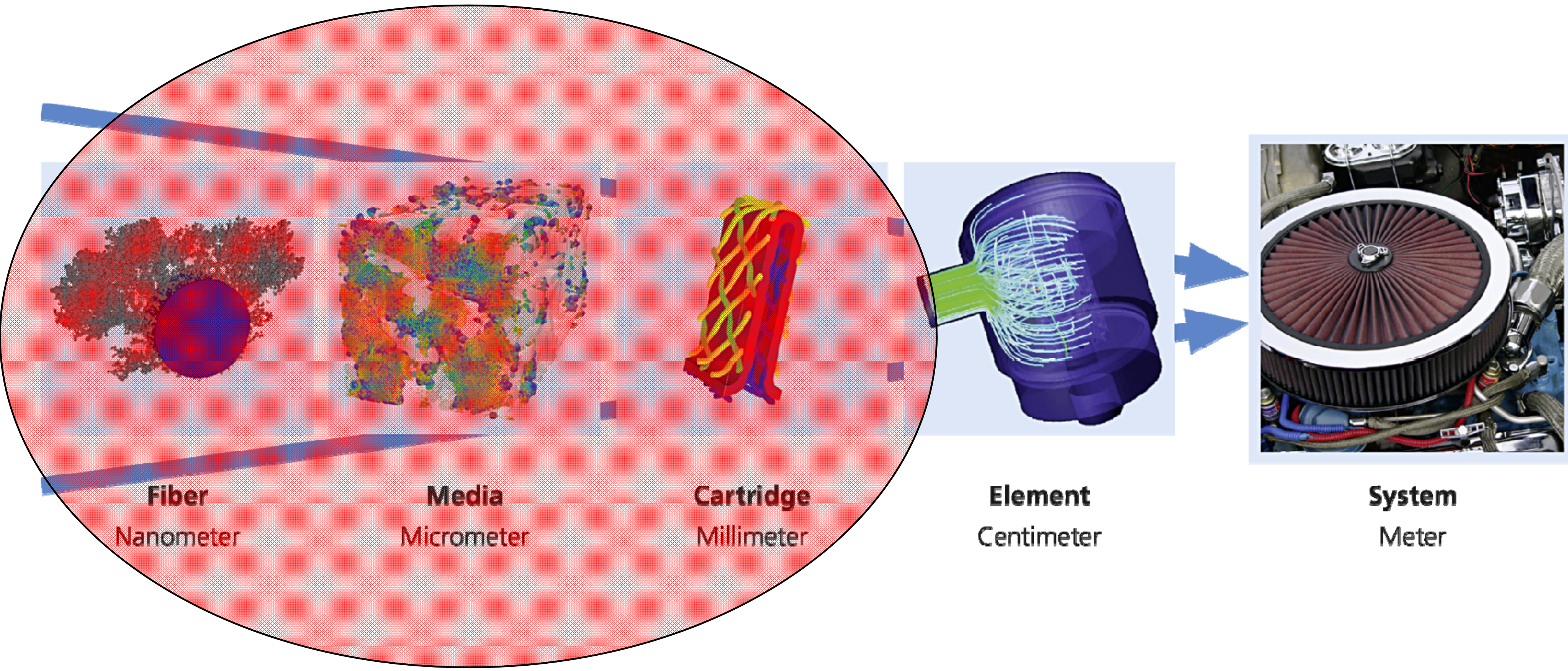
= Fraunhofer Institute for Industrial Mathematics, Kaiserslautern

AFS 2011
Louisville, KY, USA
10th May, 2011

Filtration and simulation occur on multiple scales



Virtual design cycle of filter media

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

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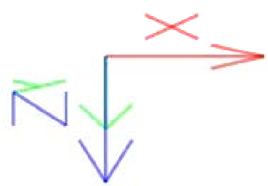
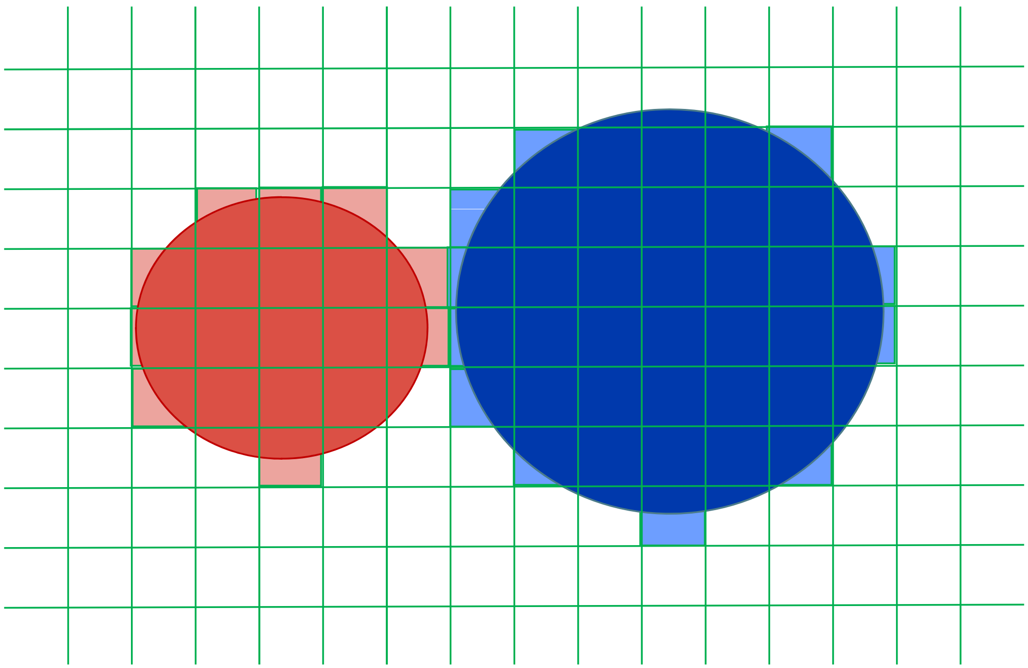


Our simulations are all based on structures of little cubes



Advantages

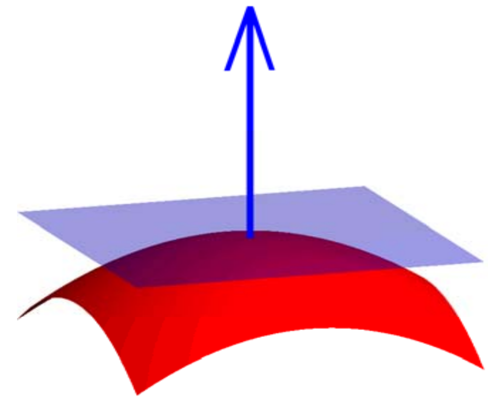
- Saves grid generation times
- Compatible with computer tomography
- Straight forward structure generation
- Straight forward solver implementation
- Straight forward parallel computations

Disadvantages

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

Description of fluid motion: Stationary Stokes flow w/wo 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.

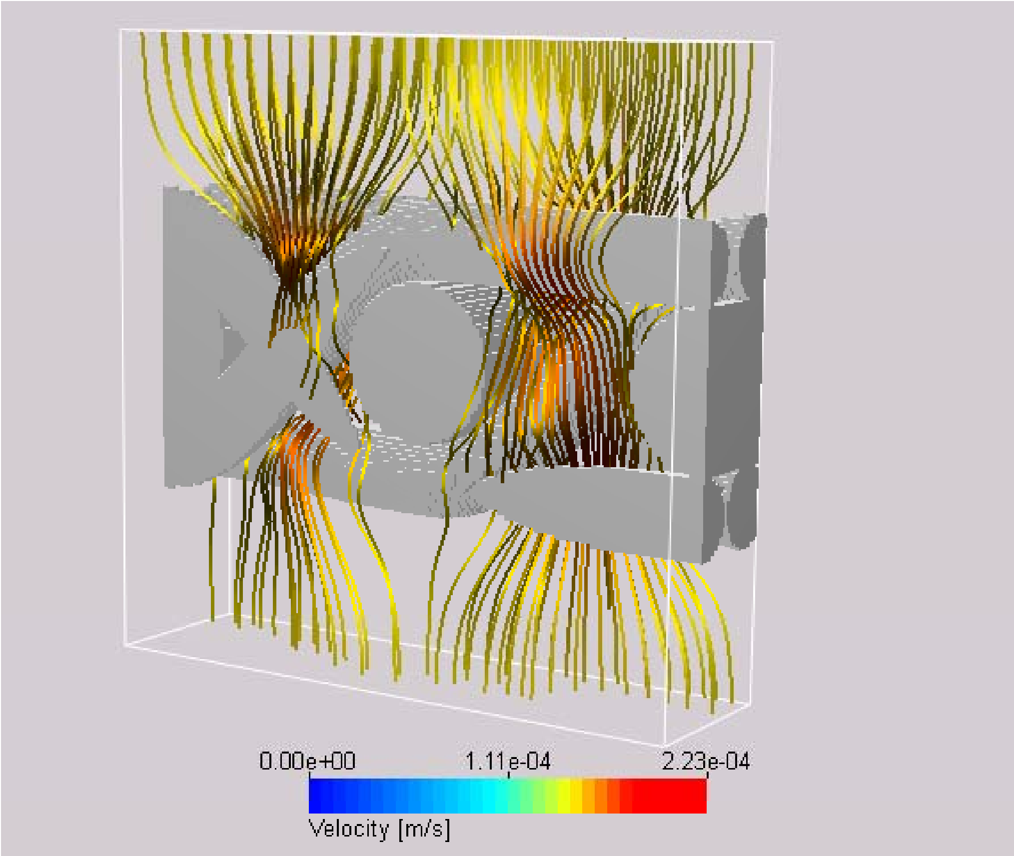
$$
\begin{aligned}
-\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)}\\
\nabla\cdot\vec{u} &= 0 \text{ (mass conservation)}\\
\vec{n}\cdot\vec{u} &= 0 \text{ on } \Gamma \text{ (no flow into fibers)}\\
\vec{t}\cdot\vec{u} &= -\lambda\vec{n}\cdot\nabla\left(\vec{u}\cdot\vec{t}\right) \text{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

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

λ : slip length,

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

Flow Field Visualization



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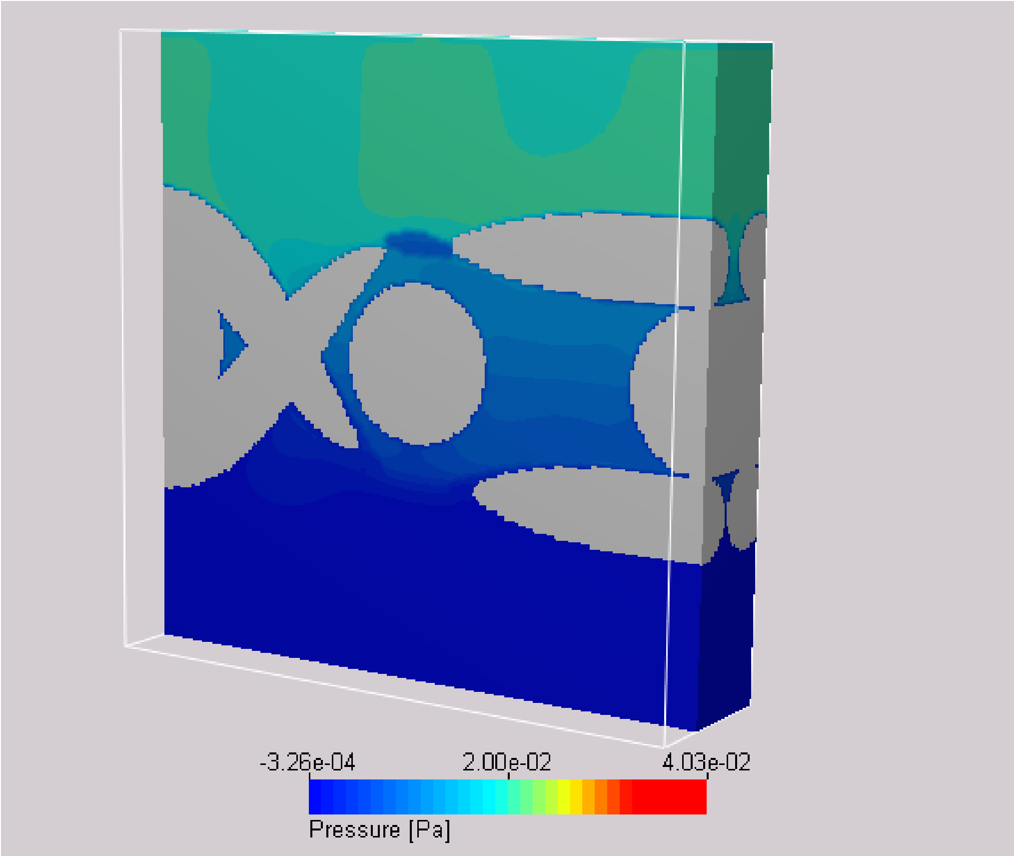
Pressure Drop Visualization



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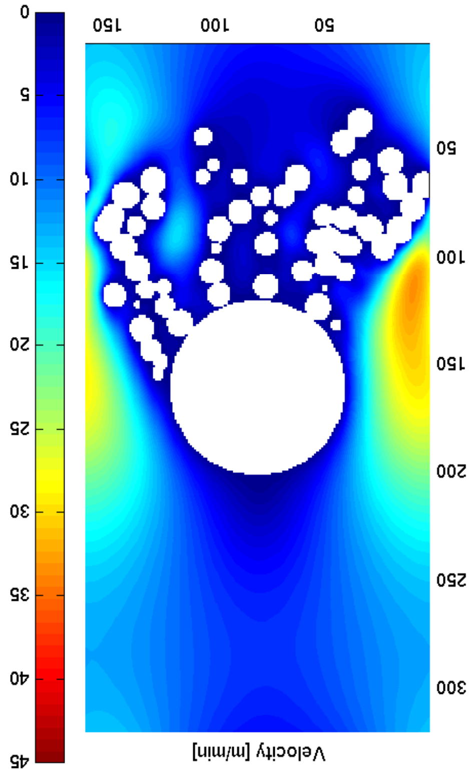
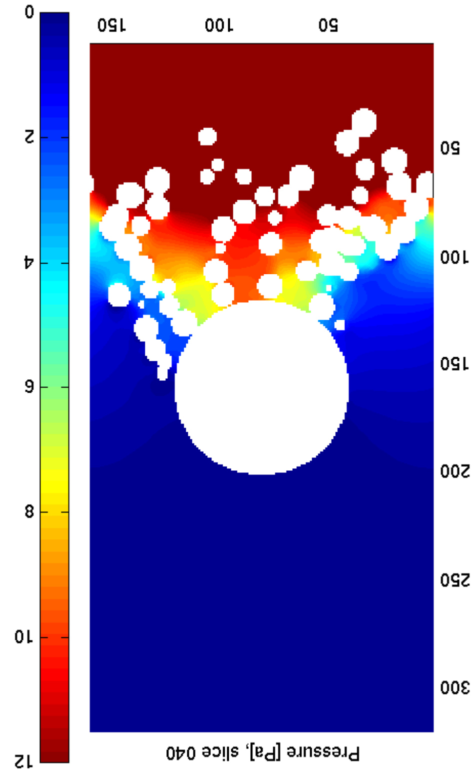
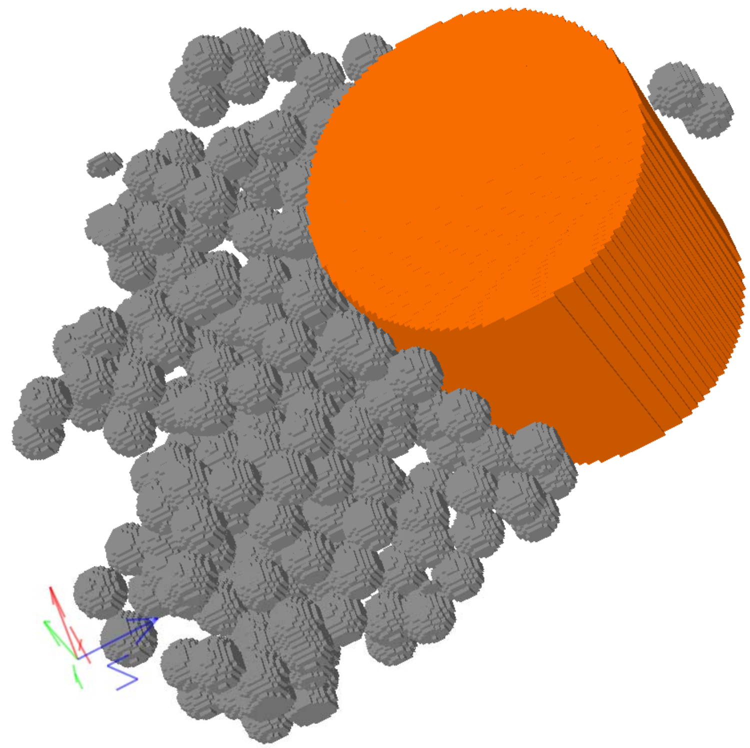
Pressure and Velocity in Clogging Simulation







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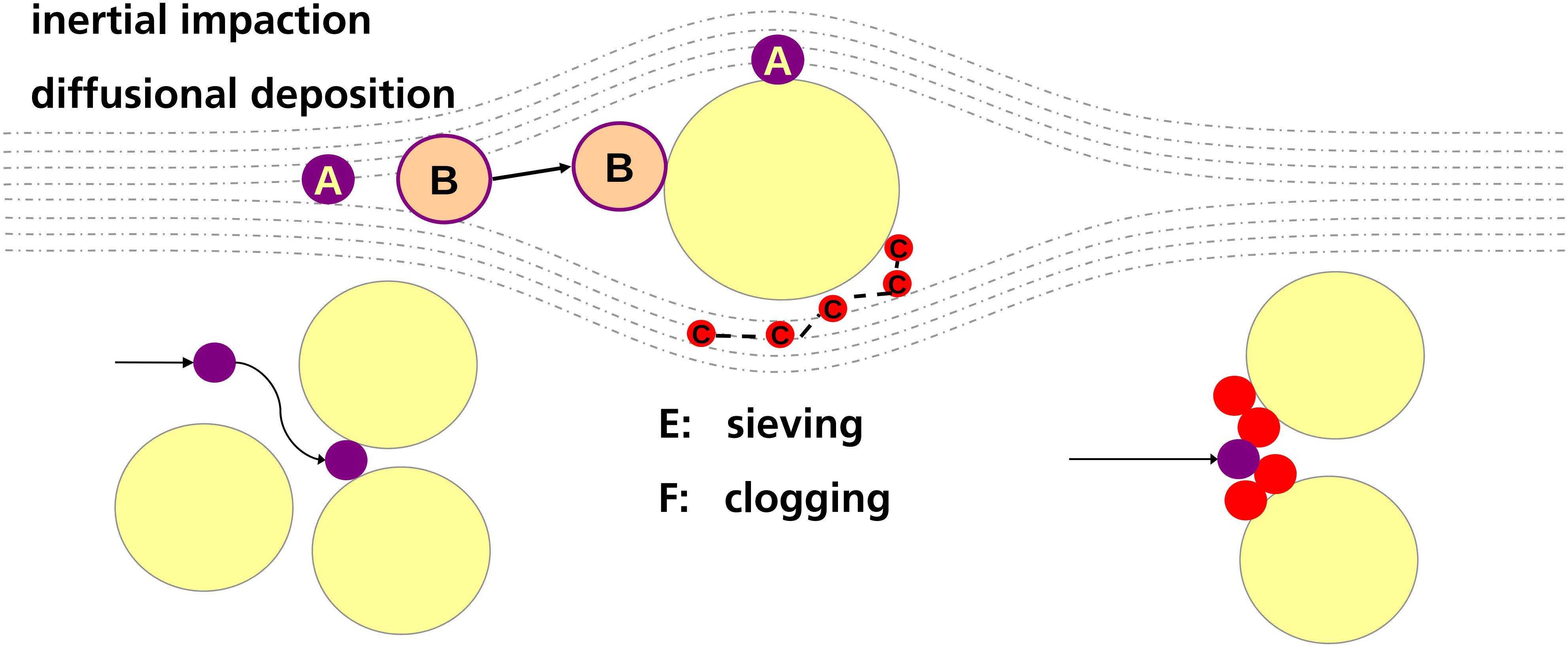
Filtration Effects I

A: direct interception

B: inertial impaction

C: diffusional deposition



E: sieving

F: clogging

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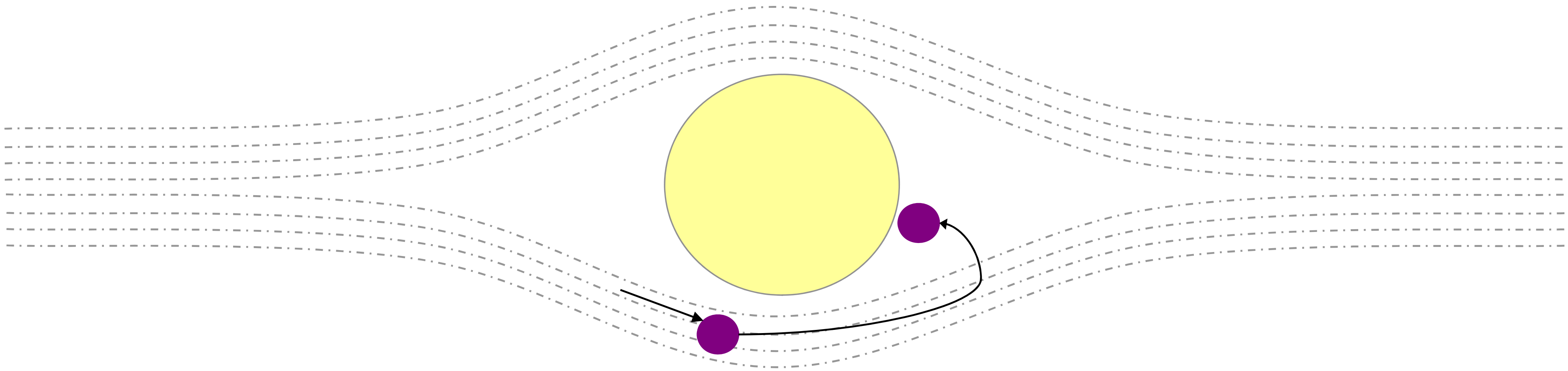
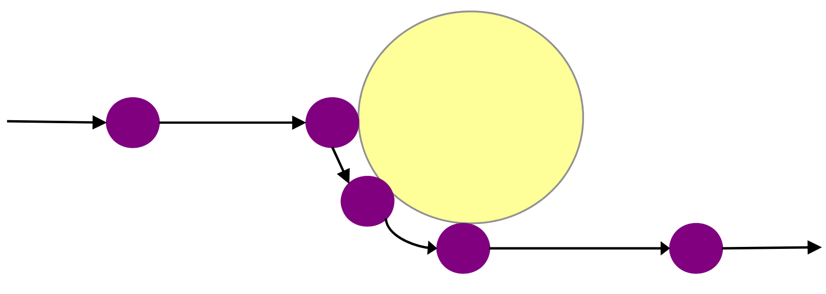
Filtration Effects II and modes of particle motion

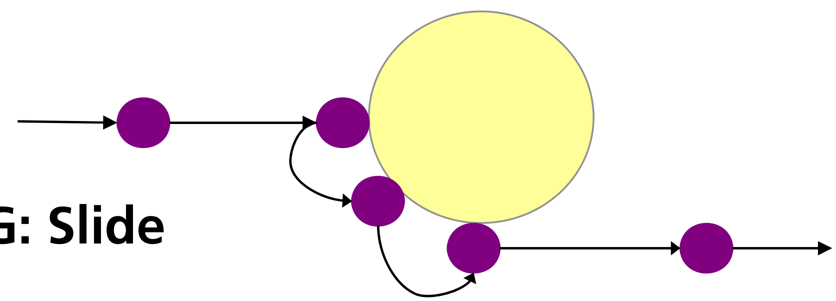
D: electrostatic attraction





G: Slide

H: Bounce



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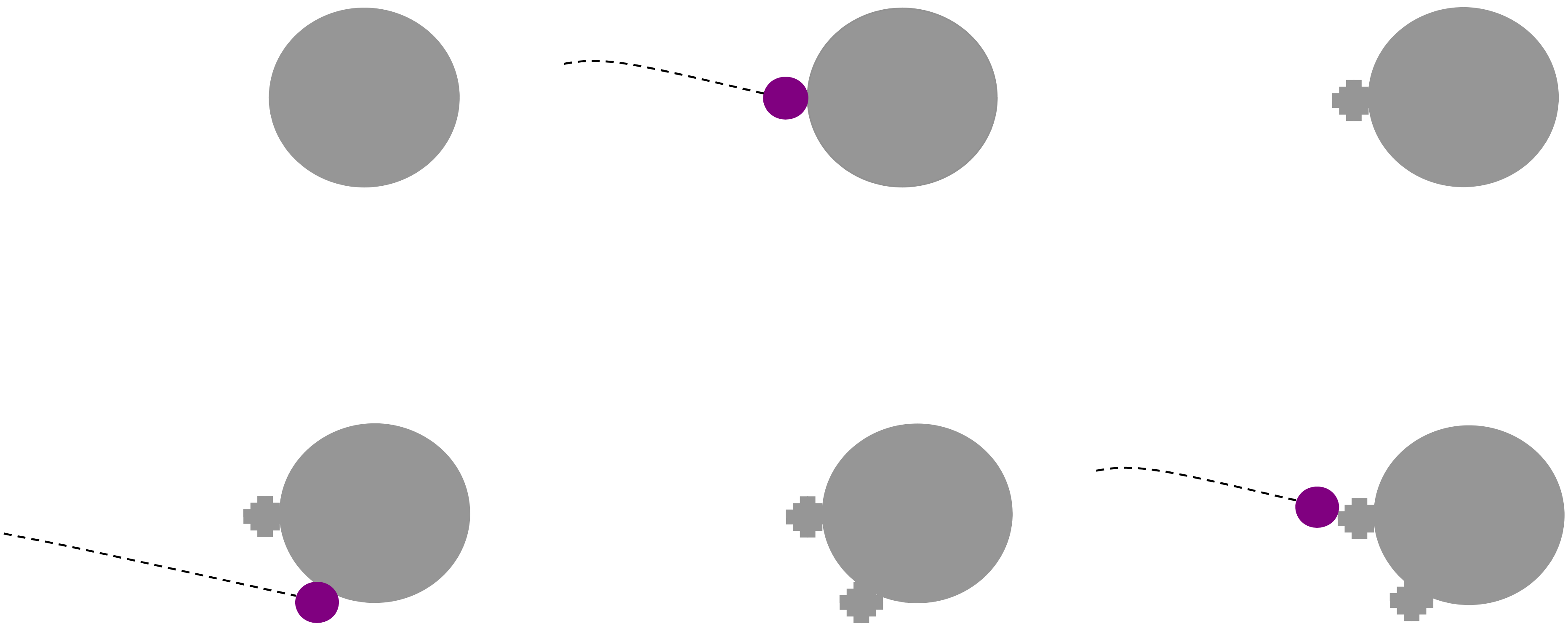
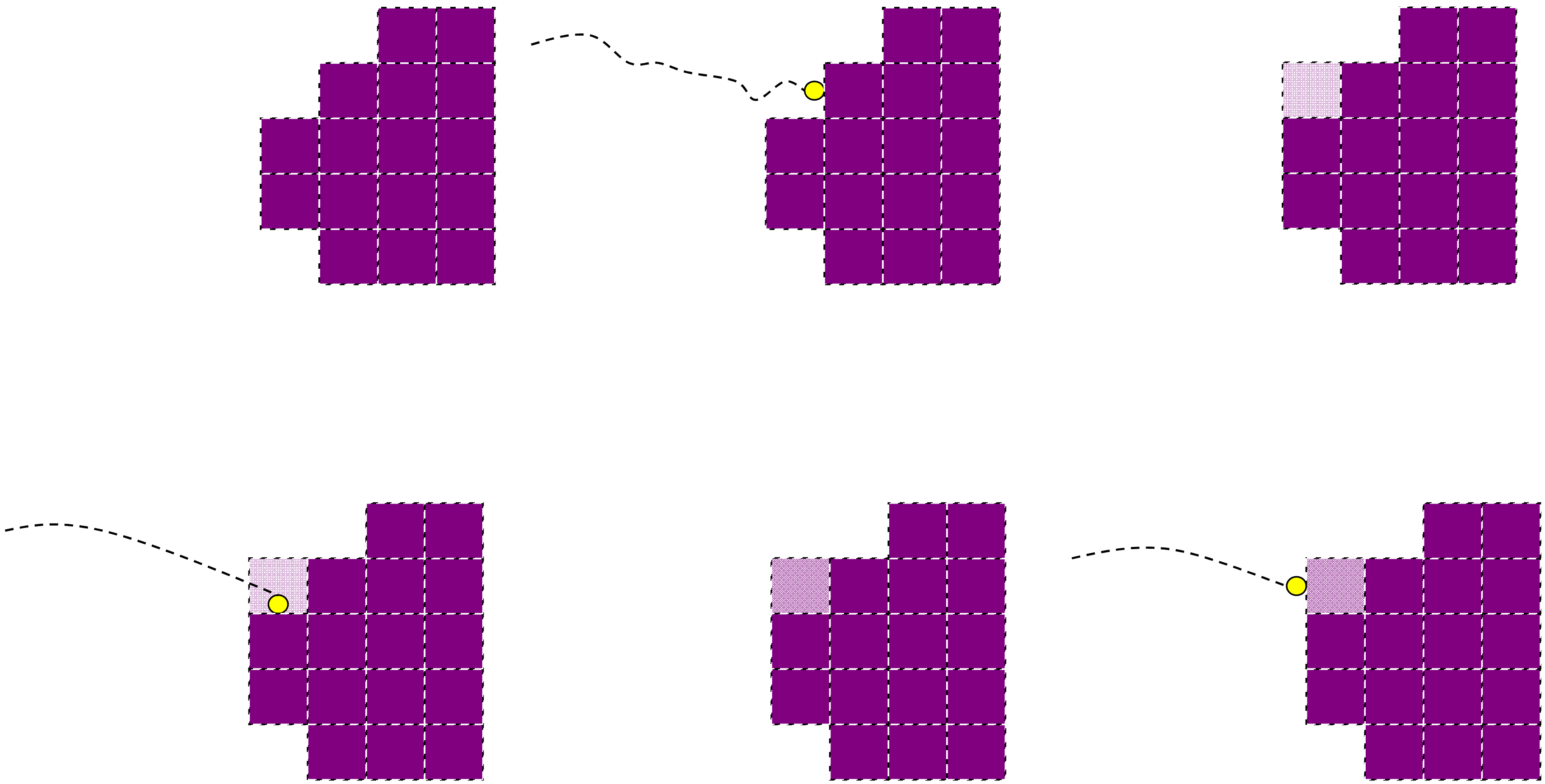
When particles are larger than the grid cells



When particles are smaller than the grid cells



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Description of particle motion

Friction with fluid — Electric attraction — Diffusive motion

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

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

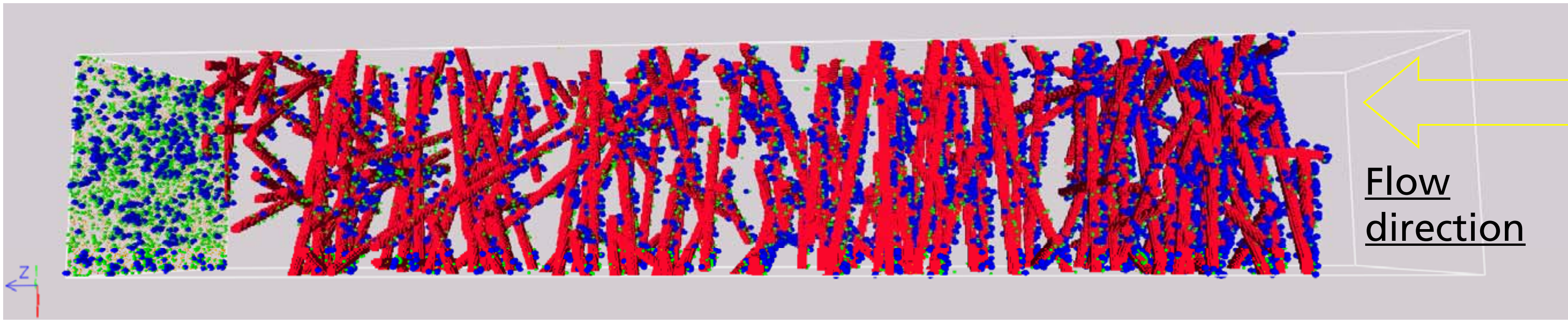
Deposition effects

α = 0.05,

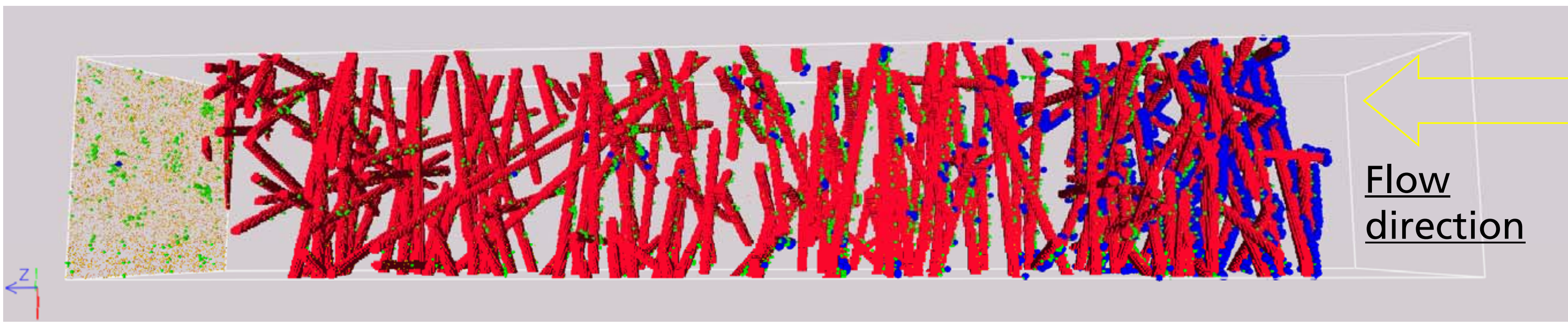
d_F = 14,

v = 0.1m/s

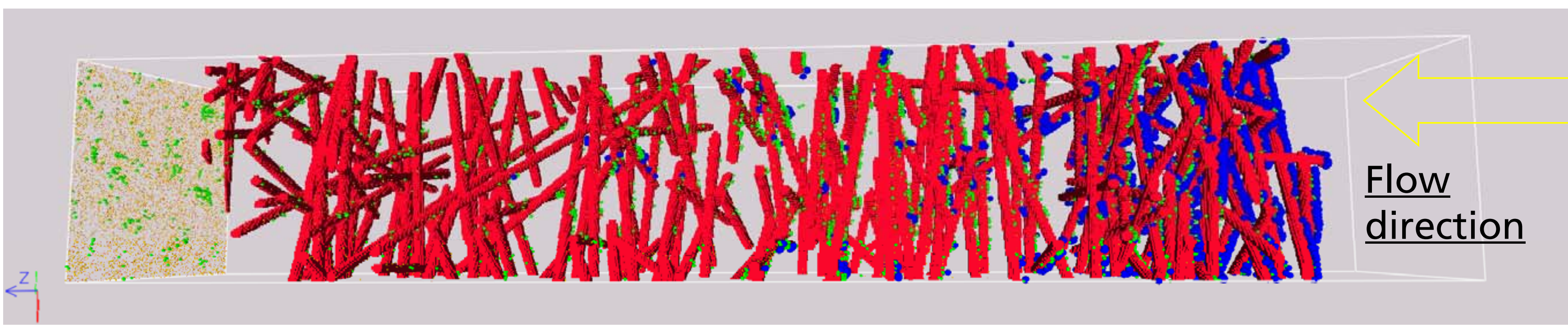
Interception



Interception
+ Impaction

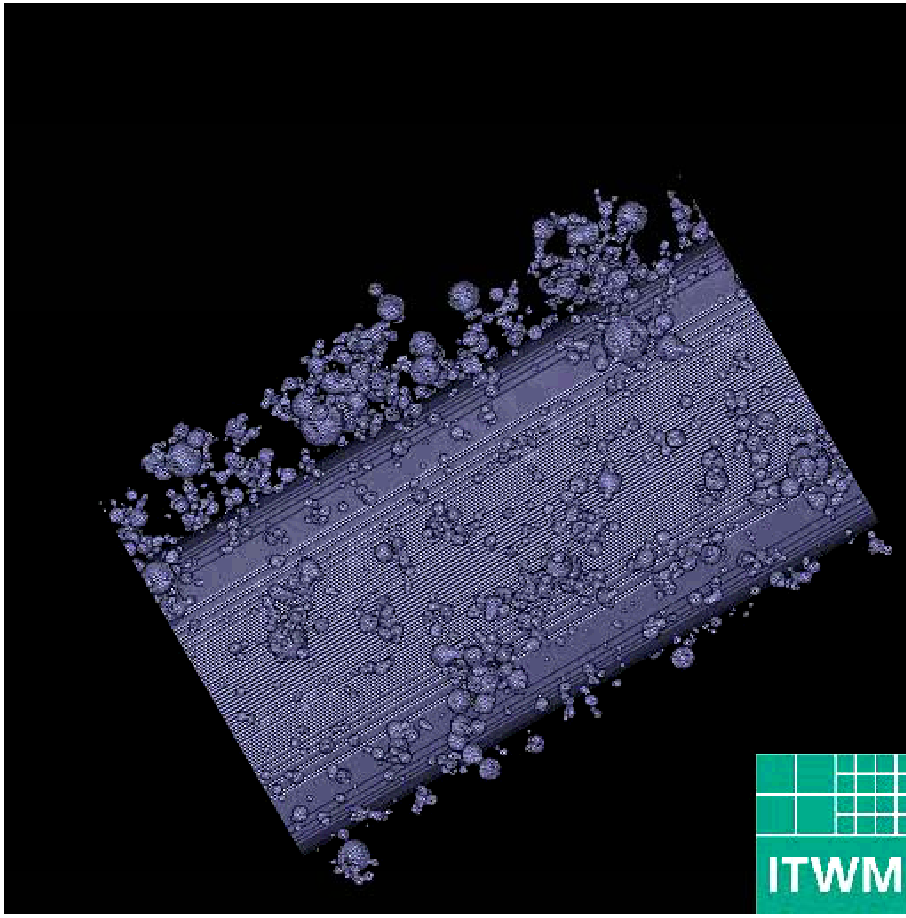


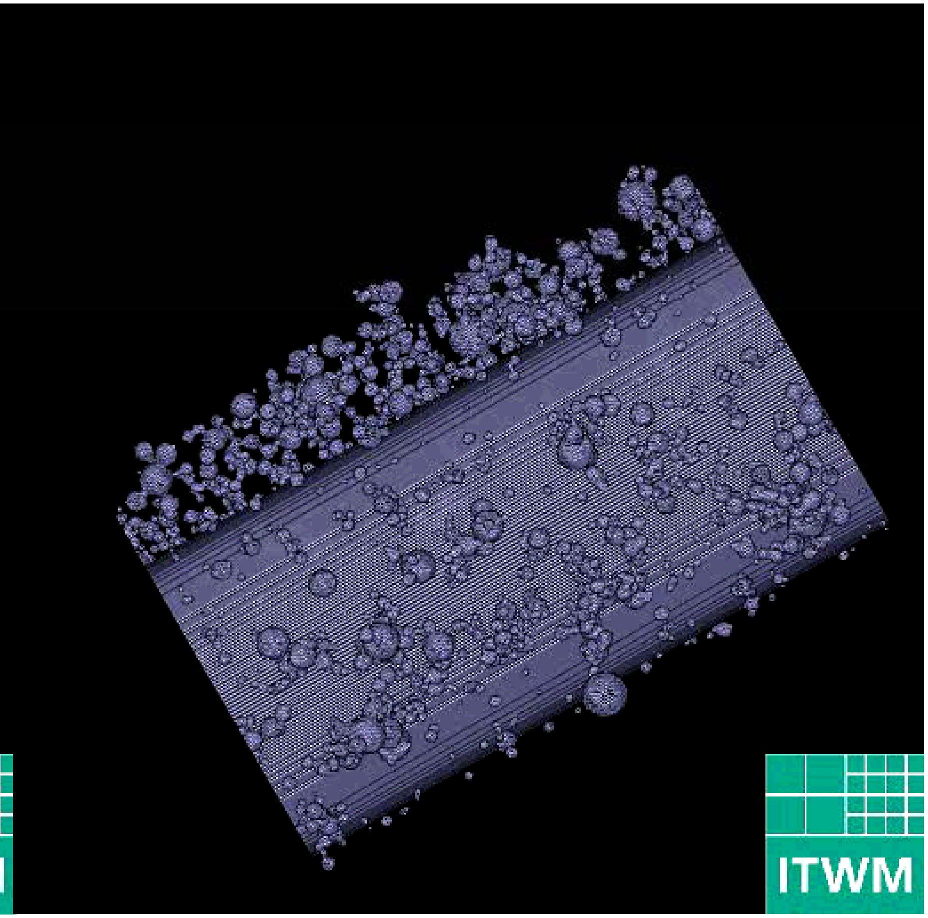
Interception
+ Impaction
+ Diffusion



Nano Simulations

1.67cm/sec | **10.0cm/sec**





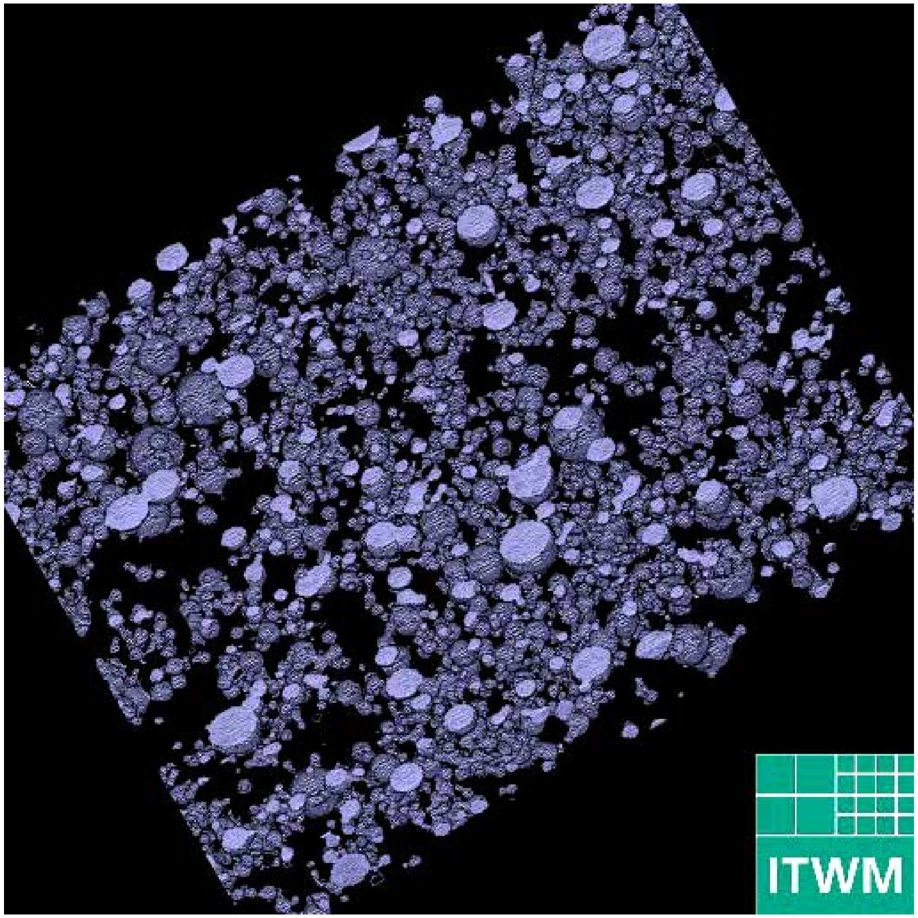
Nano Simulations

- 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



Stationary Flow with unresolved particles: Stokes-Brinkmann eqs

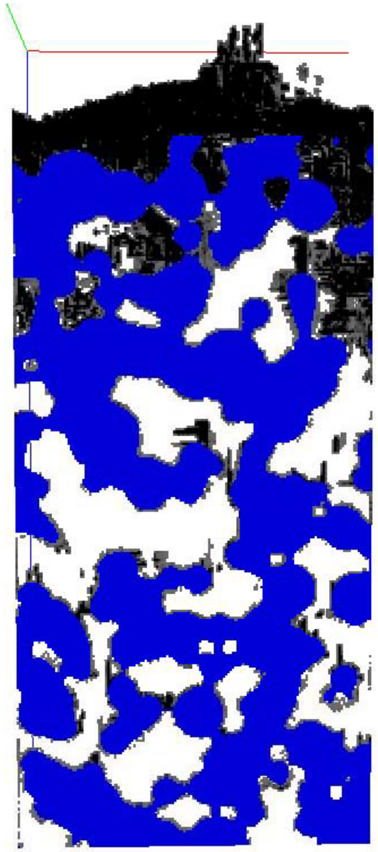
$$
\begin{aligned}
-\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \nabla p + \kappa^{-1}\vec{u} &= \vec{\mathrm{f}} \text{ (momentum balance)} \\
\nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\
\vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)}
\end{aligned}
$$

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

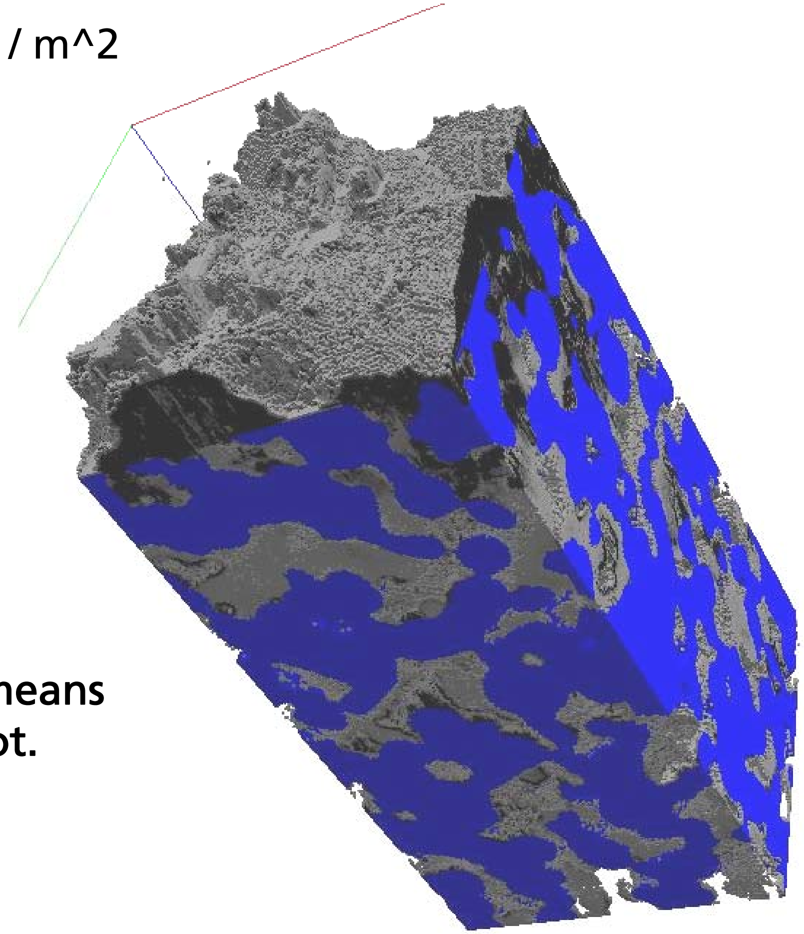
Solid volume fraction in voxel is increased until s_{max} is reached. Voxel becomes "collision-solid". Neighbor voxels svf starts increasing upon particle arrival

Micro Simulations

Final state at 5.1 g / m^2

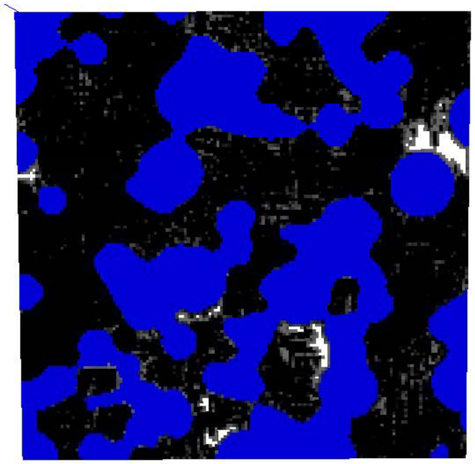


Darker gray means
denser soot.



Filtration_Animation.mpg

Horizonal layers



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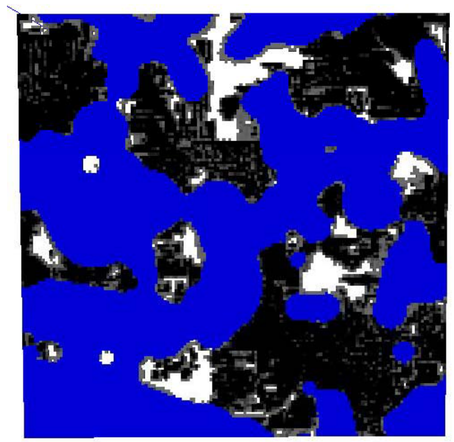

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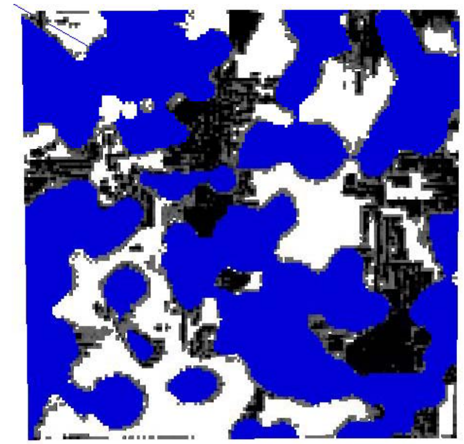
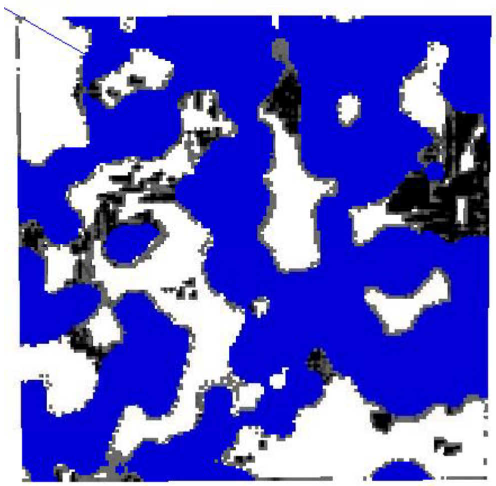
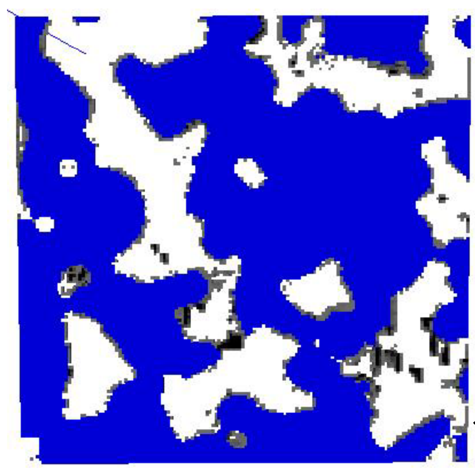


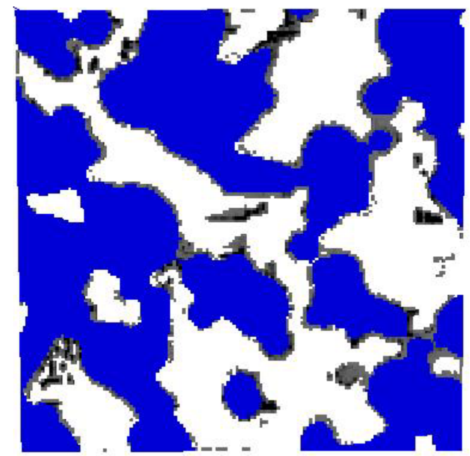
100



125

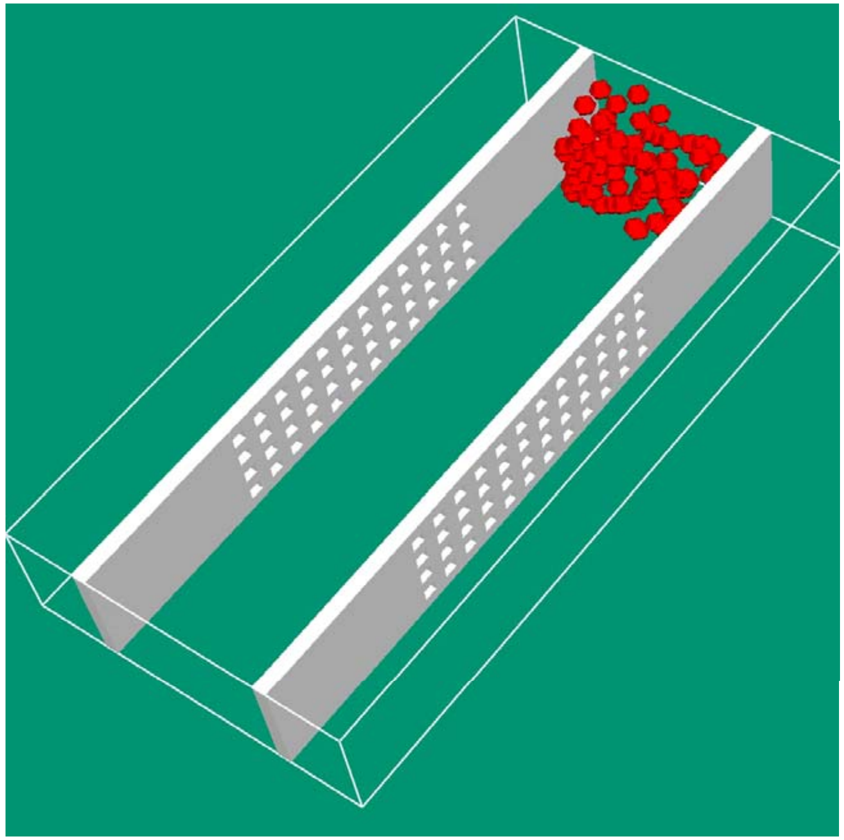


150



350

Cross Flow Filtration



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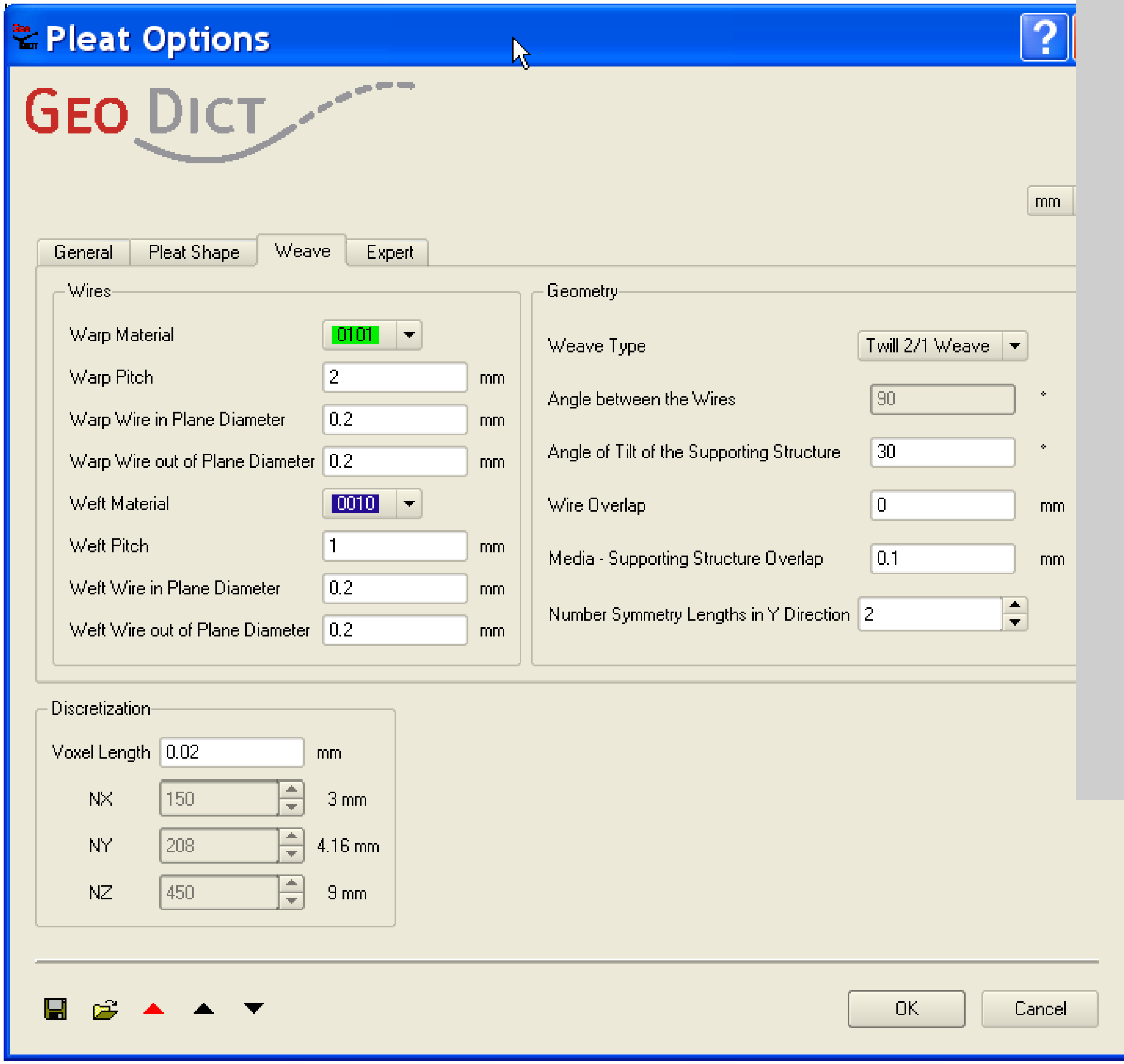
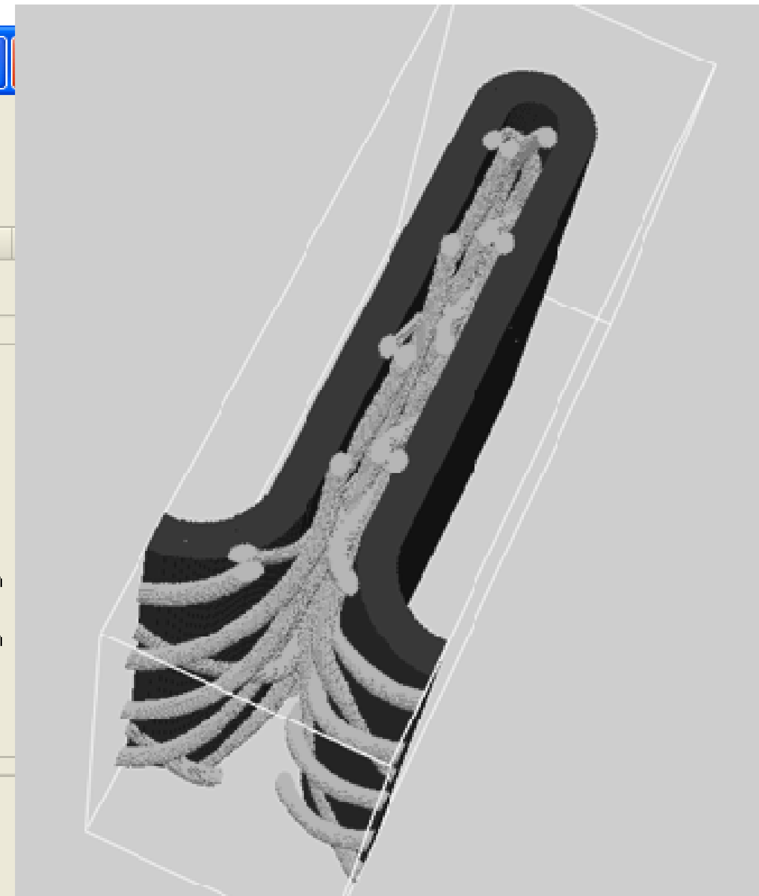
Weave Pleat Options





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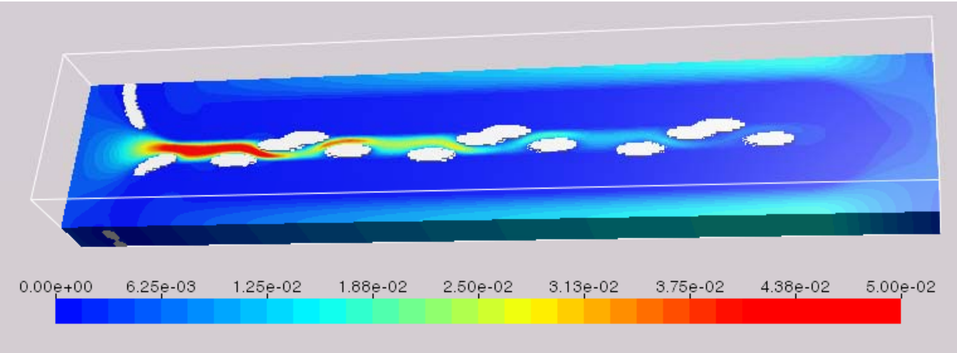
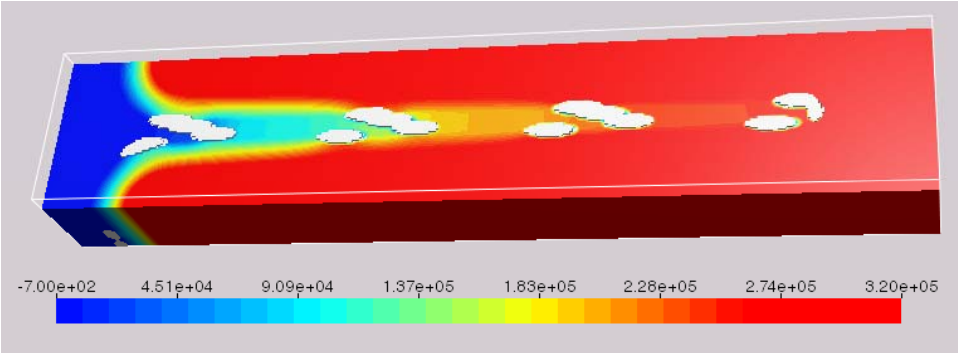
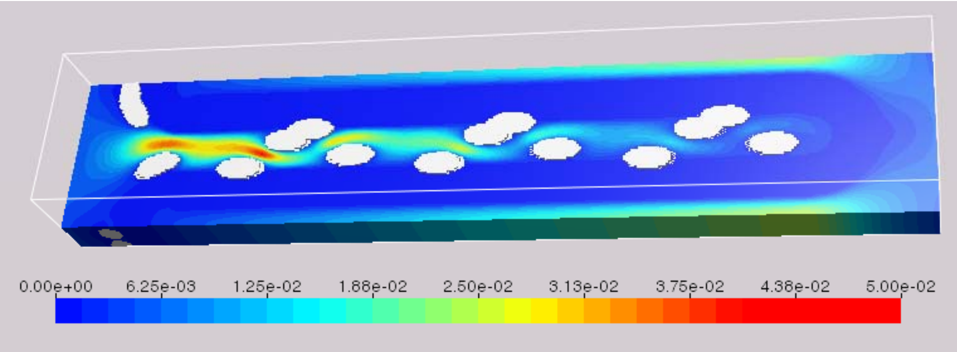
Oil flow in pleats with support structure: velocity & pressure

- 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

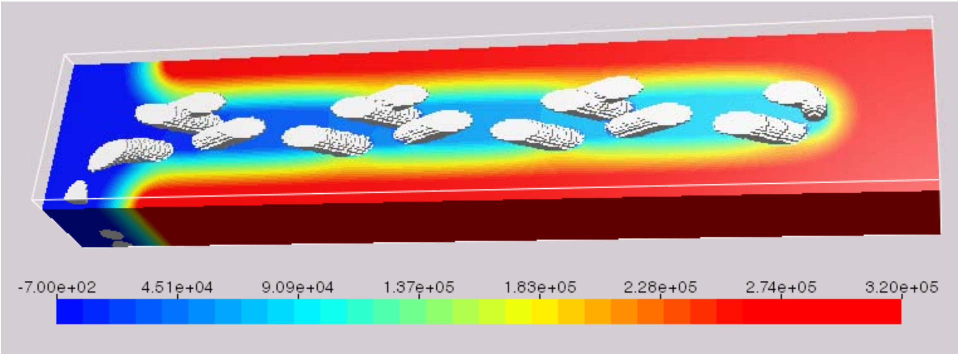


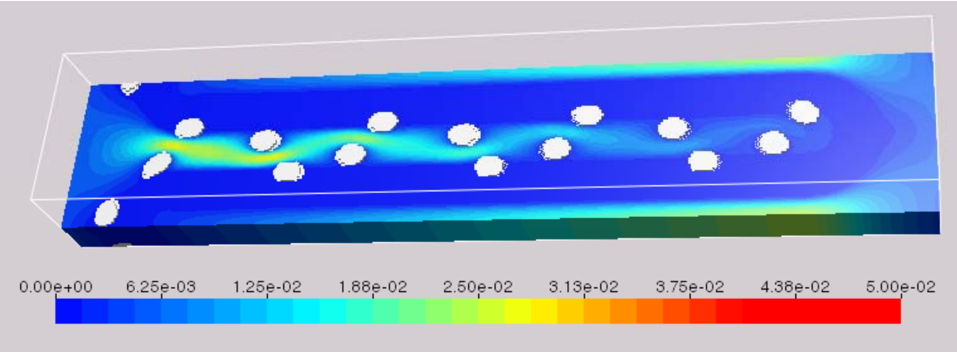
Narrow Channel



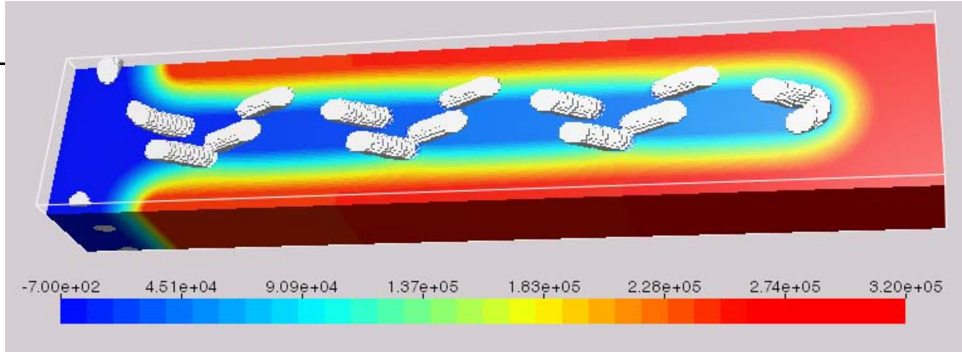


Thick Wire





Thin Wire



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**

Current "Hot" Simulation Topics:

- Multipass time step control (see my talk tomorrow)
- Re-entrainment of particles, pulse cleaning
- Coalescence
- Filtration in pleats and DPF honeycomb structures
- Nanofibers
- Electric charges
- Two phase flows in filters, rocks, diapers and fuel cells