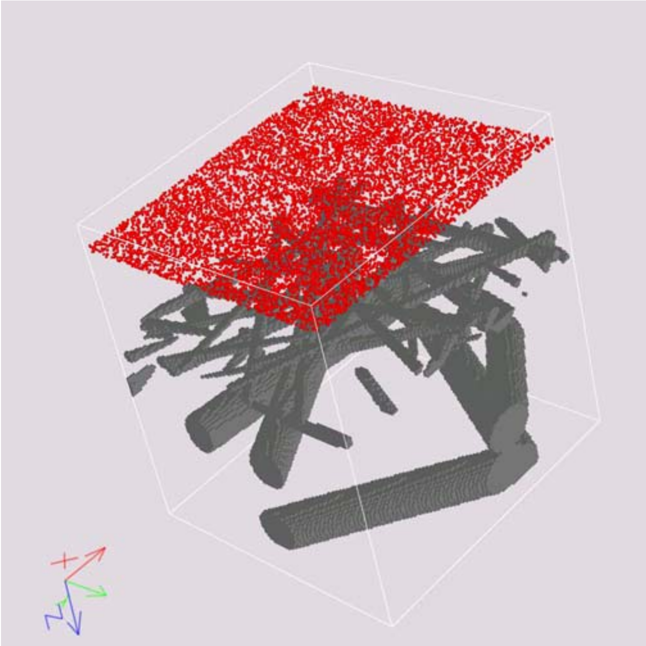


# Filtration simulation on the nano scale –the influence of slip flow

Liping Cheng, Andreas Wiegmann & Stefan Rief

FPS 2010
EUROPEAN CONFERENCE ON FLUID-PARTICLE SEPARATION

Fraunhofer ITWM

5 - 7 october 2010, Lyon - FRANCE

Sponsored by the German ministry for education and research (BMBF)

## Introduction

➢ Nanofiber filter media simulation: what and why?

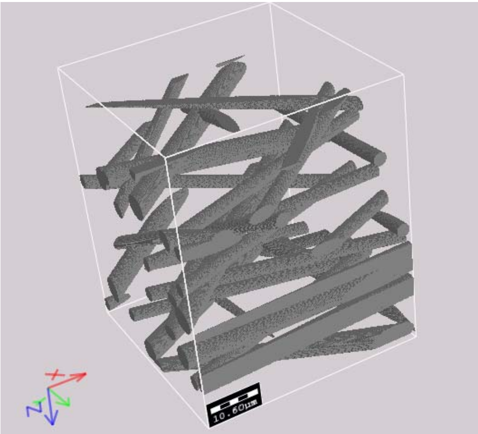
- Industry: nanofibers have a diameter < 1 µm
- Marked increase in filter efficiency; small increase of pressure drop
- Longer life and more dust holding capacity than conventional media
- Balance between advantages and cost

- Physics: Fluid flow
- Physics: Particle adhesion
- Physics: Particle deposition
- Simulation challenge: Resolution demands run-time & memory
- Modeling challenge: Slip instead of no-slip boundary condition

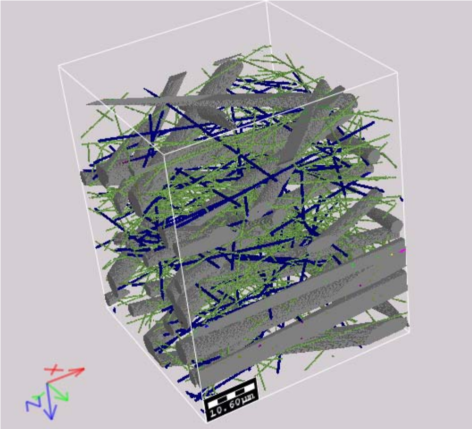
## Micro fibers vs. embedded nano fibers vs nano fiber layers

Medium 1: 3 and 5 µm fibers ; SVF10%
Medium 2: + 0.3 µm,0.5µm fibers (SVF +1%)
Medium 3: with 5 µm nano fiber layer
Medium 4: with 10 µm nano fiber layer

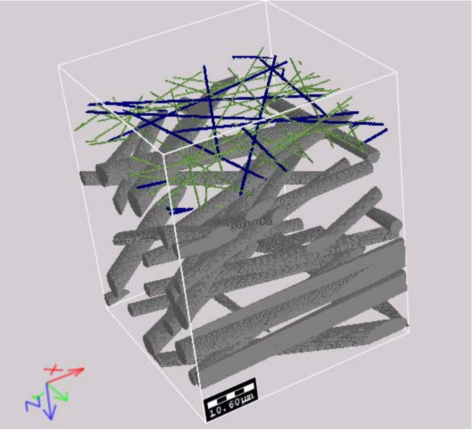
Voxel length: 100nm
Medium size: 512 x 512 x 512



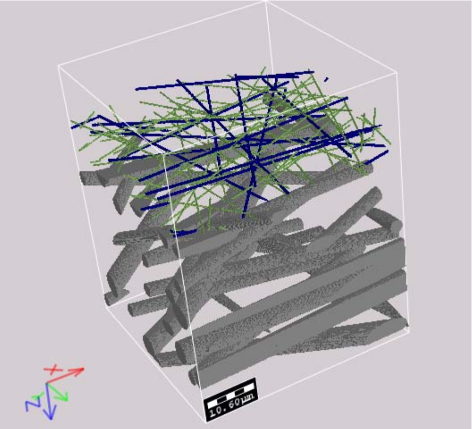
Medium 1



Medium 2



Medium 3



Medium 4

# Method

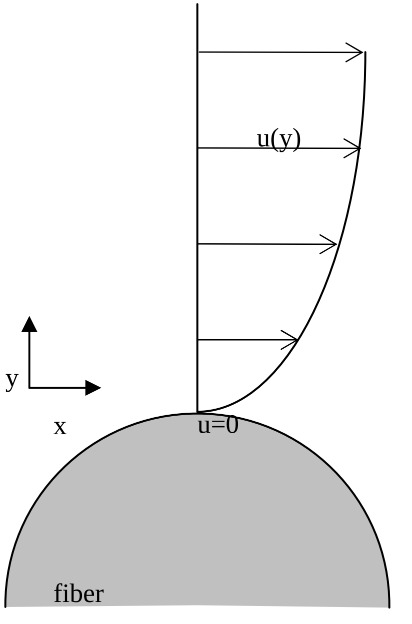
- **Eulerian Description of Stationary Stokes Flow**
  **No-Slip boundary condition**

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

$\mu$ : fluid viscosity,

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

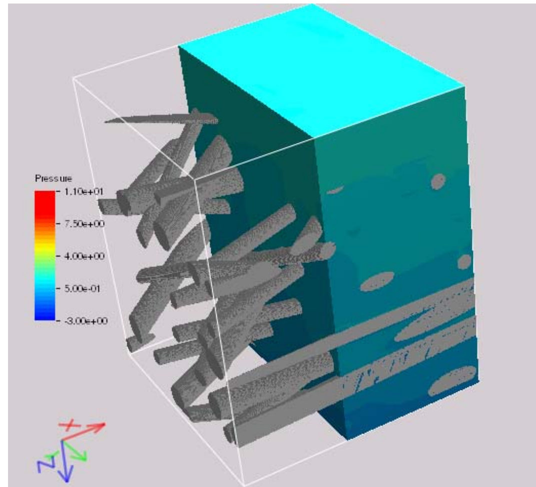
$p$ : pressure, periodic up to pressure drop in flow direction.

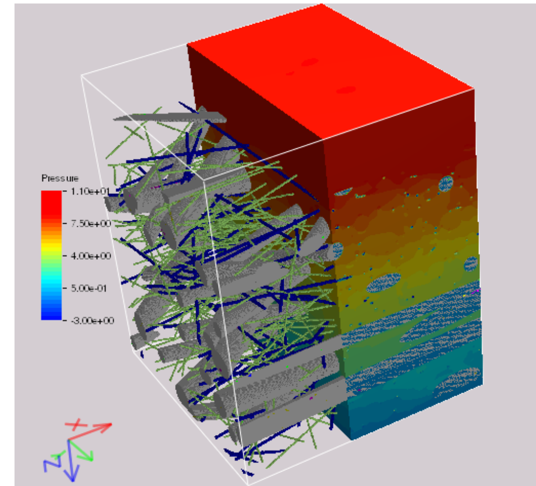


## Micro fibers vs. Micro+Nano fibers (no-slip boundary condition)

Medium 1 | Medium 2

Pressure



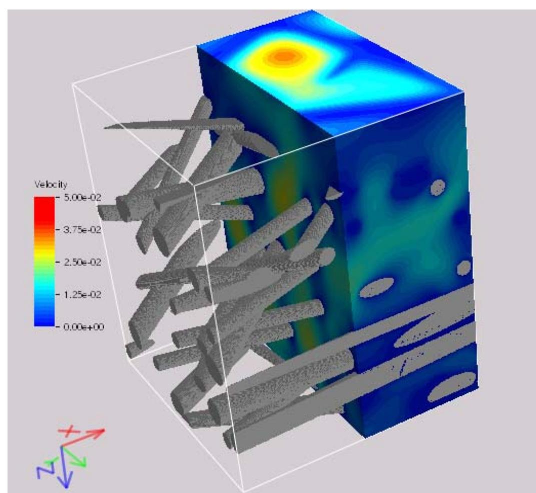



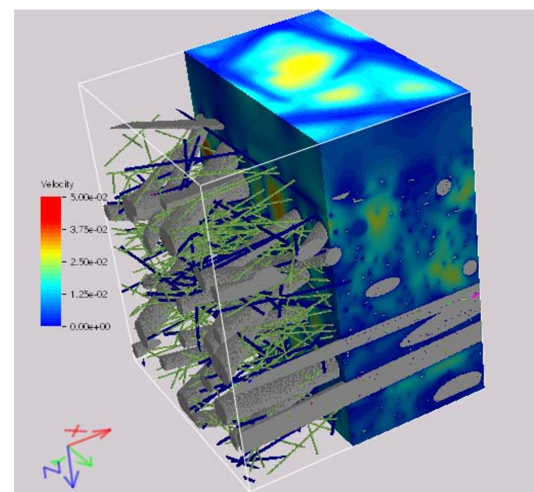

at mean velocity 0.01m/s

ΔP= 1.45 Pa

ΔP= 8.25Pa

Velocity



## ➢Particle Motion

$$d\vec{v} = -\gamma \times \left(\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))\right)dt + \sigma \times d\vec{W}(t),$$

$$d\vec{x} = \vec{v}(\vec{x}(t))dt,$$

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

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

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

$\vec{u}$ : fluid velocity

$\vec{v}$ : particle velocity

$t$ : time

$T$ : temperature

$\gamma$ : friction coefficient

$R$ : particle radius

$\rho$ : fluid density

$\mu$ : fluid viscosity

$\vec{W}$ : Wiener Measure (3d)

$k_b$ : Boltzmann constant

$m$ : particle mass

$Kn$ : Knudsen number

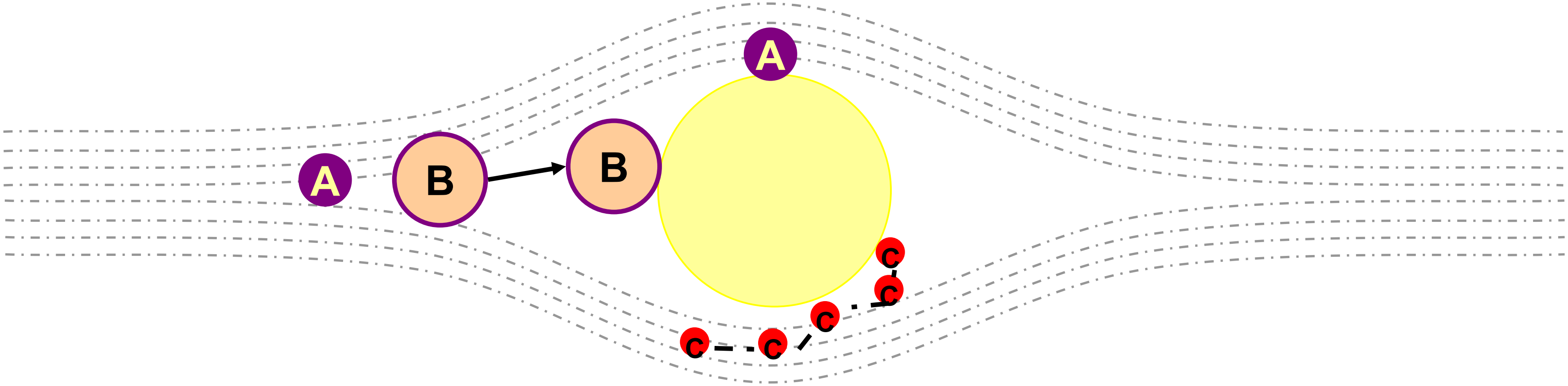
A. Latz and A. Wiegmann, *Simulation of fluid particle separation in realistic three dimensional fiber structures*, Filtech, Düsseldorf, October 2003.

## ➢Filtration Effects I

A: direct interception

B: inertial impaction

C: diffusional deposition

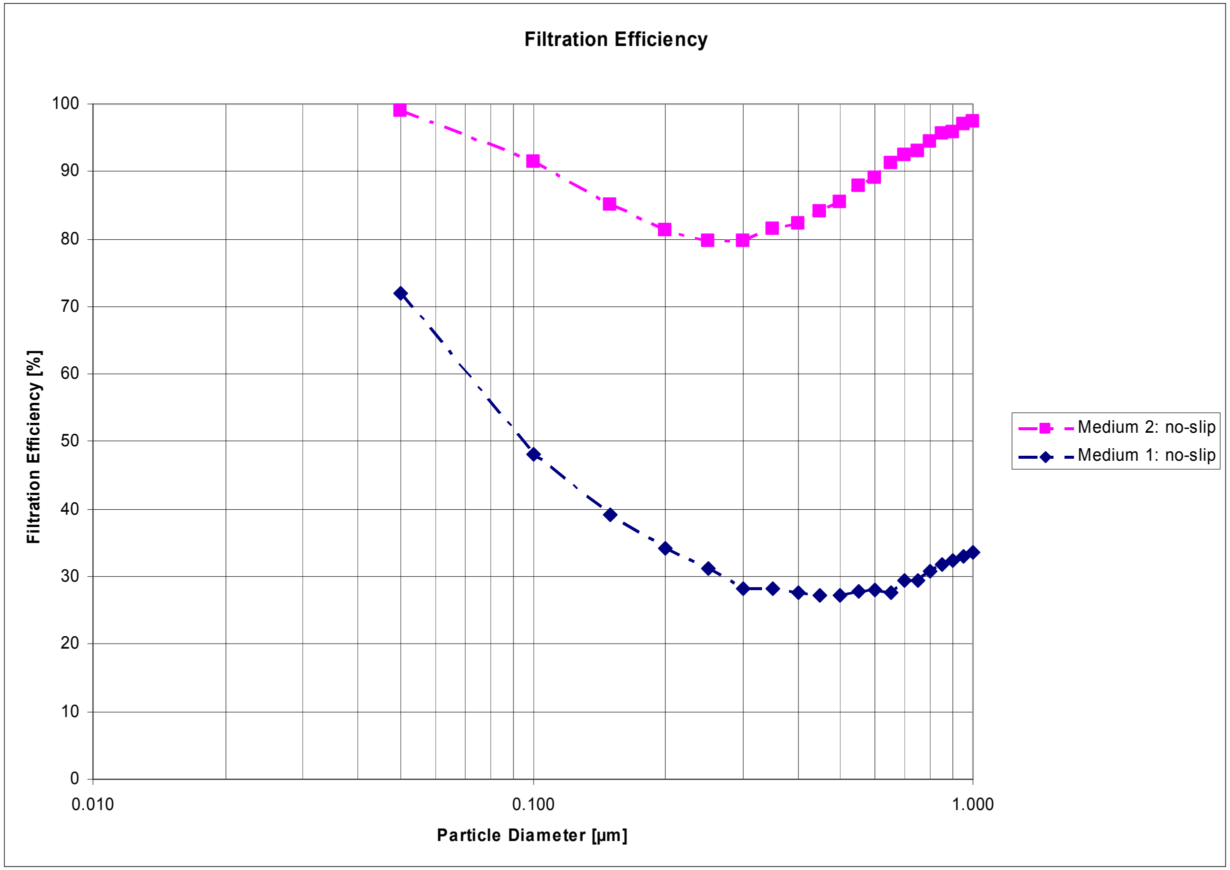


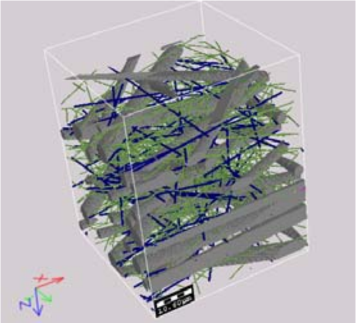
# Result

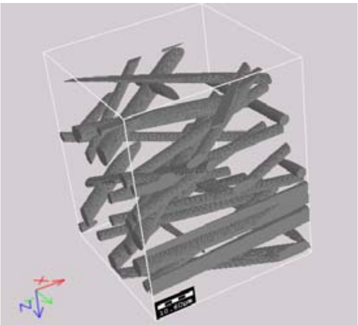
## Micro fibers vs. Micro + Nano fibers

- Air at 20°C
- NaCl, $d_p$ 50 to 1000 nm; 1 cm/s

| Media | 1 | 2 |
|---|---|---|
| **ΔP** | 1.45 | 8.25 |



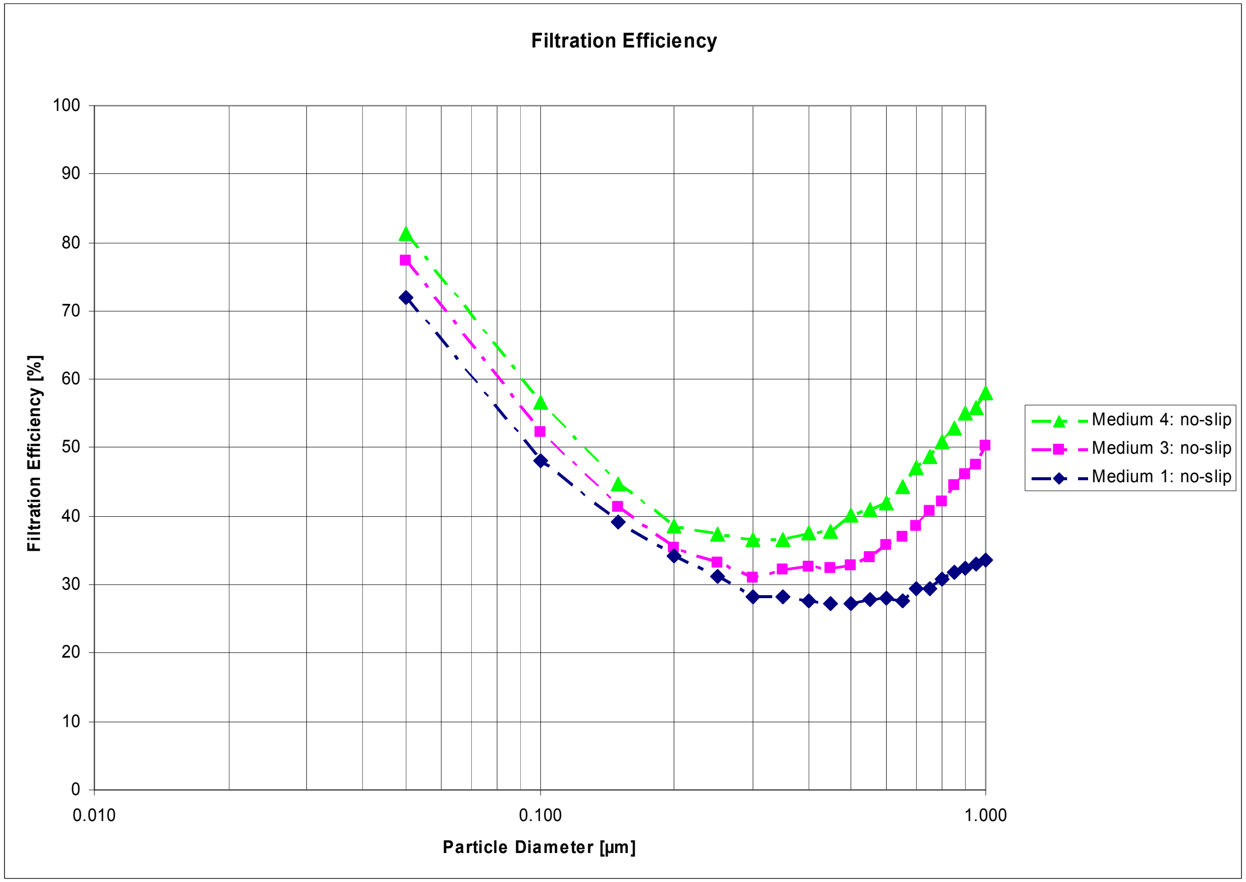



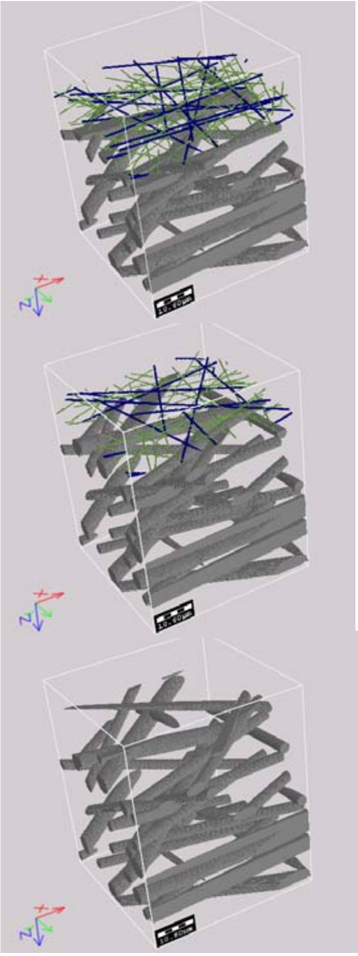


## Micro fibers vs. Nano fiber layer

| Media | 1 | 3 | 4 |
|---|---|---|---|
| ΔP | 1.45 | 1.99 | 2.16 |

- Air at 20°C
- NaCl, $d_p$ 50 to 1000 nm; 1 cm/s

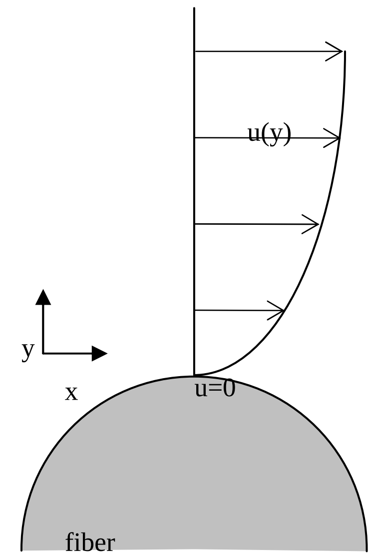


# Method

➢ **Eulerian Description of Stationary Stokes Flow**
**No slip vs fractional slip boundary condition**

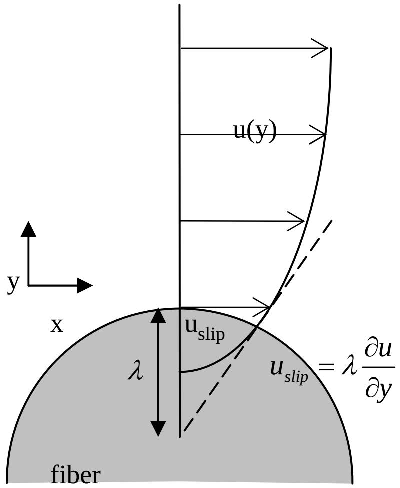
$$
\begin{aligned}
-\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\
\nabla \cdot \vec{u} &= 0 \text{ (mass conservation)} \\
\vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)} \\
P_{in} &= P_{out} + c \text{ (pressure drop is given)}
\end{aligned}
$$




$\mu$ : 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,

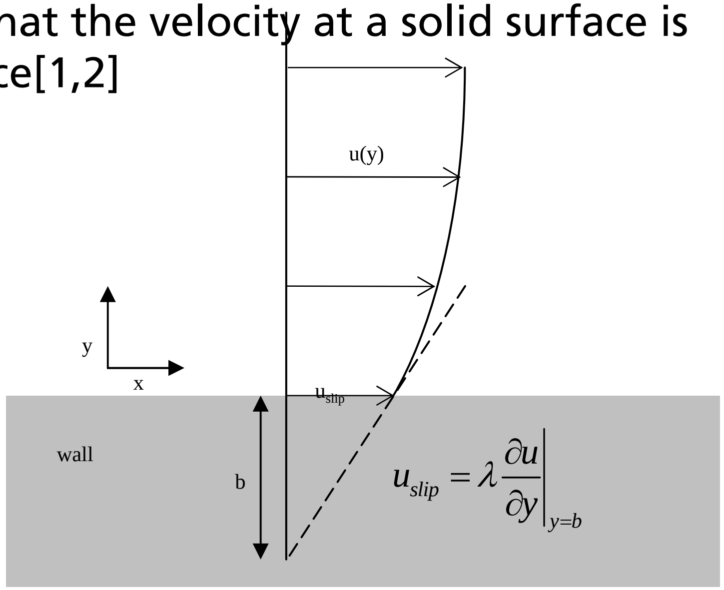
$\lambda$ : slip length,

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

## Slip boundary condition

- For slip boundary conditions, it is assumed that the velocity at a solid surface is proportional to the shear stress at the surface[1,2]

$$u = \lambda \frac{\partial u}{\partial y}$$

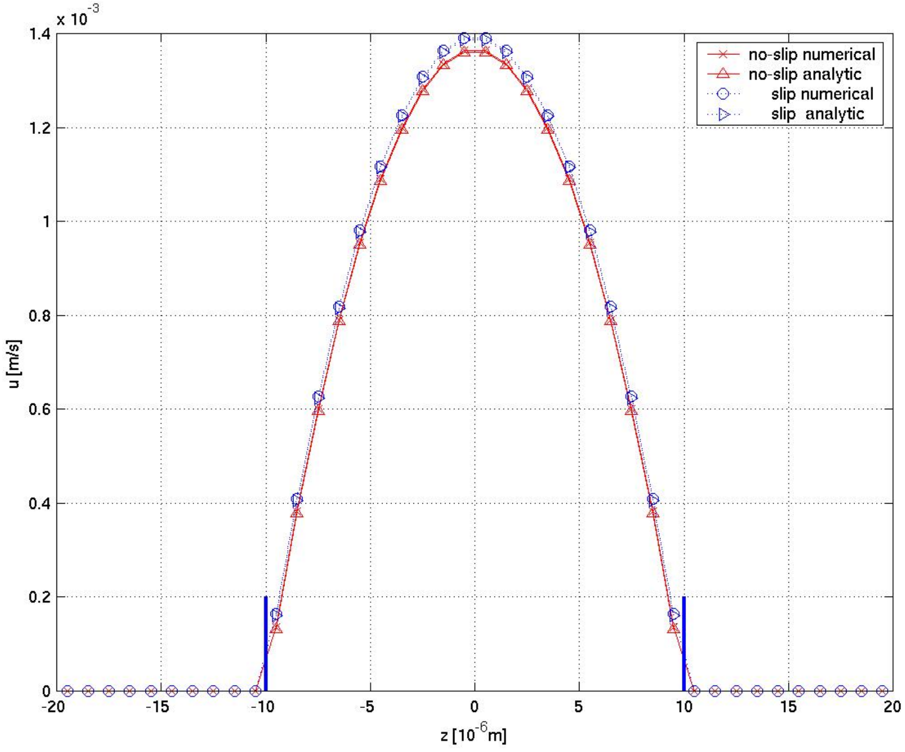



where $\lambda$ is the slip length or slip coefficient.


[1] C. L. M. H. Navier, Mem. Acad. R. Sci. Inst. France 1, 414 (1823).

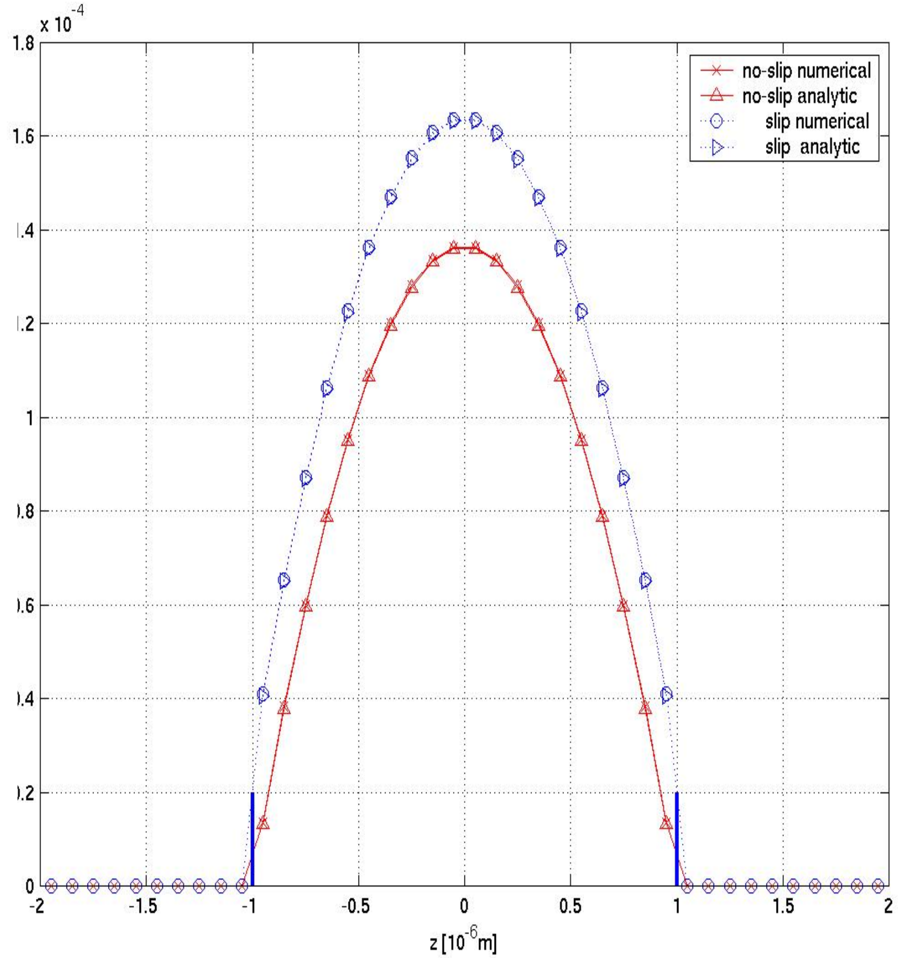
[2] S. Goldstein, Modern Developments in Fluid Dynamics (Dover, New York, 1965), vol. 2, p. 676

## Benchmark 1: parabola-shaped Poiseuille profile (flow between two infinite and parallel plates)




Distance between plates = 20µm;

$\lambda$ = 100 nm; dp/L = 5000Pa/m;




Distance between plates 2µm;

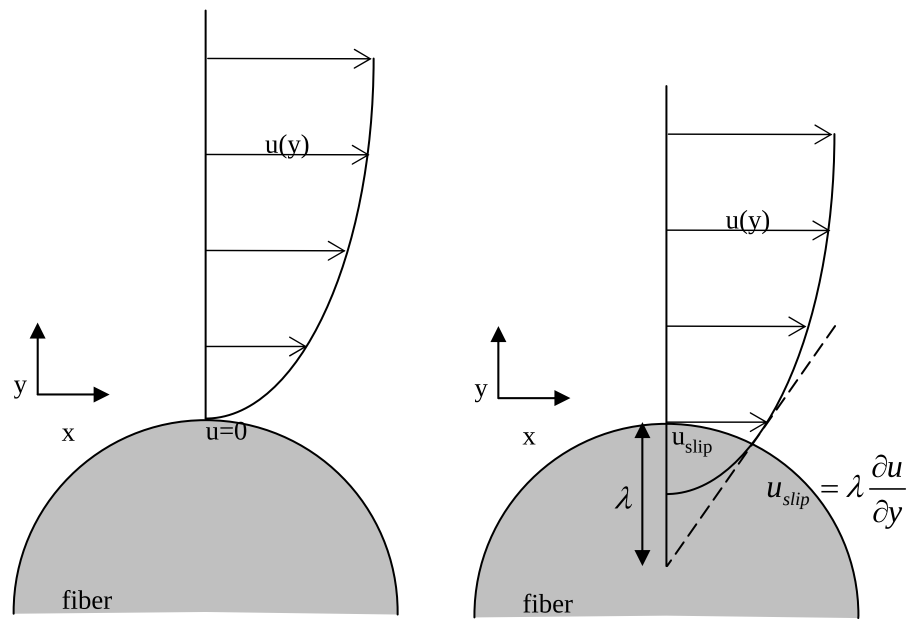
$\lambda$ = 100 nm; dp/L = 5000Pa/m;

## Slip boundary condition

Slip models the tangential velocity as proportional to the shear stress [1,2]

$$u = \lambda \frac{\partial u}{\partial y}$$

$\lambda$ , the slip length



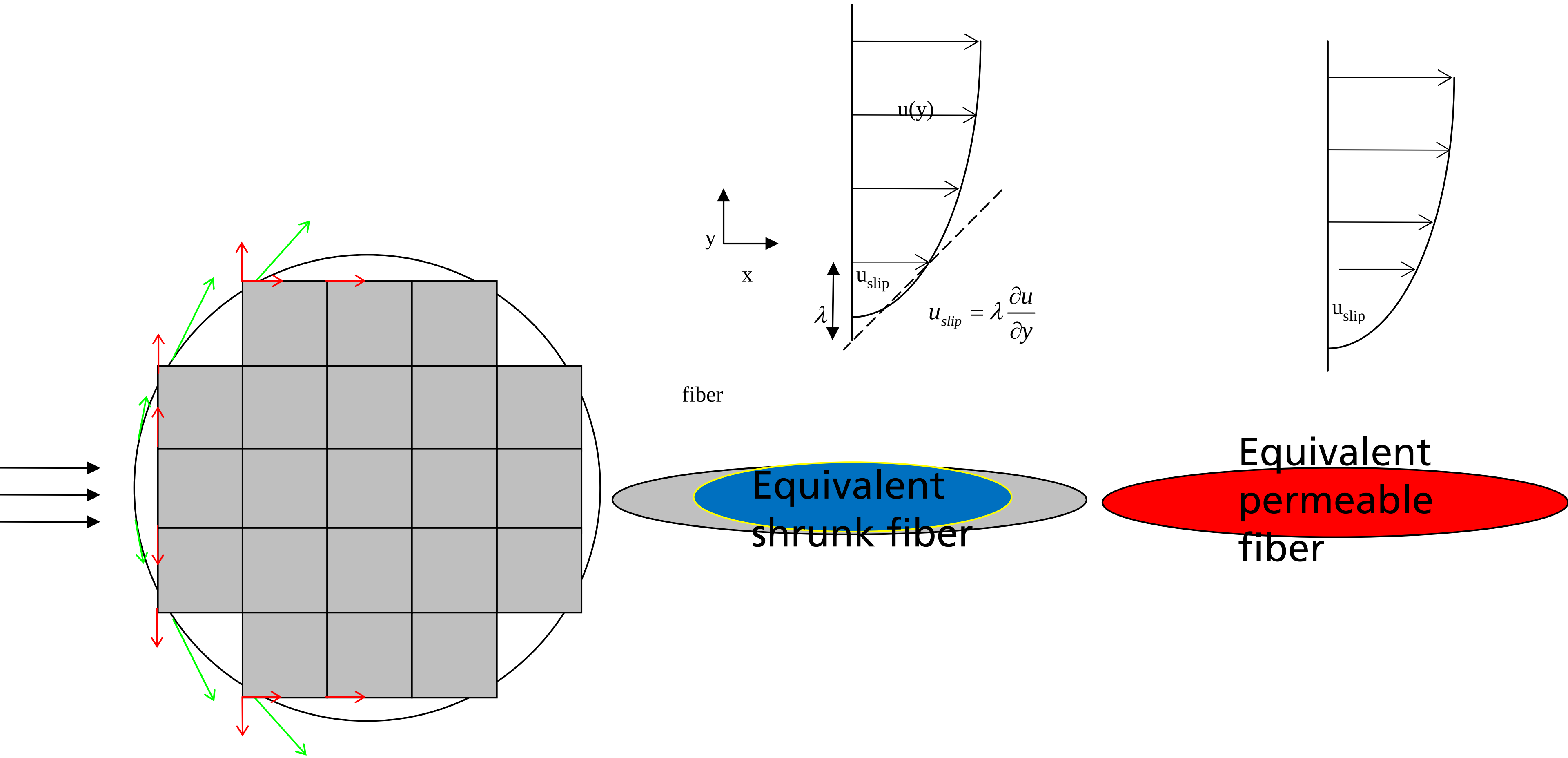

No-Slip boundary condition

Slip boundary condition

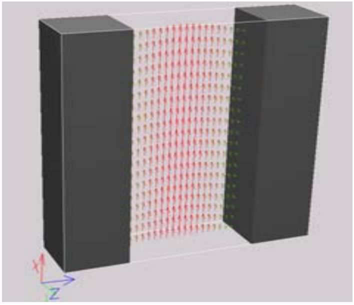

[1] C. L. M. H. Navier, Mem. Acad. R. Sci. Inst. France 1, 414 (1823).

[2] S. Goldstein, Modern Developments in Fluid Dynamics (Dover, New York, 1965), vol. 2, p. 676

## Explicit-Jump Flow solver on Voxelized fiber
## Equivalent shrunk fibers with no-slip and
## Equivalent permeable fibers (replace b.c. by NS-Brinkman equ.)



Benchmark 1: parabola-shaped Poiseuille profile
(flow between two infinite and parallel plates)

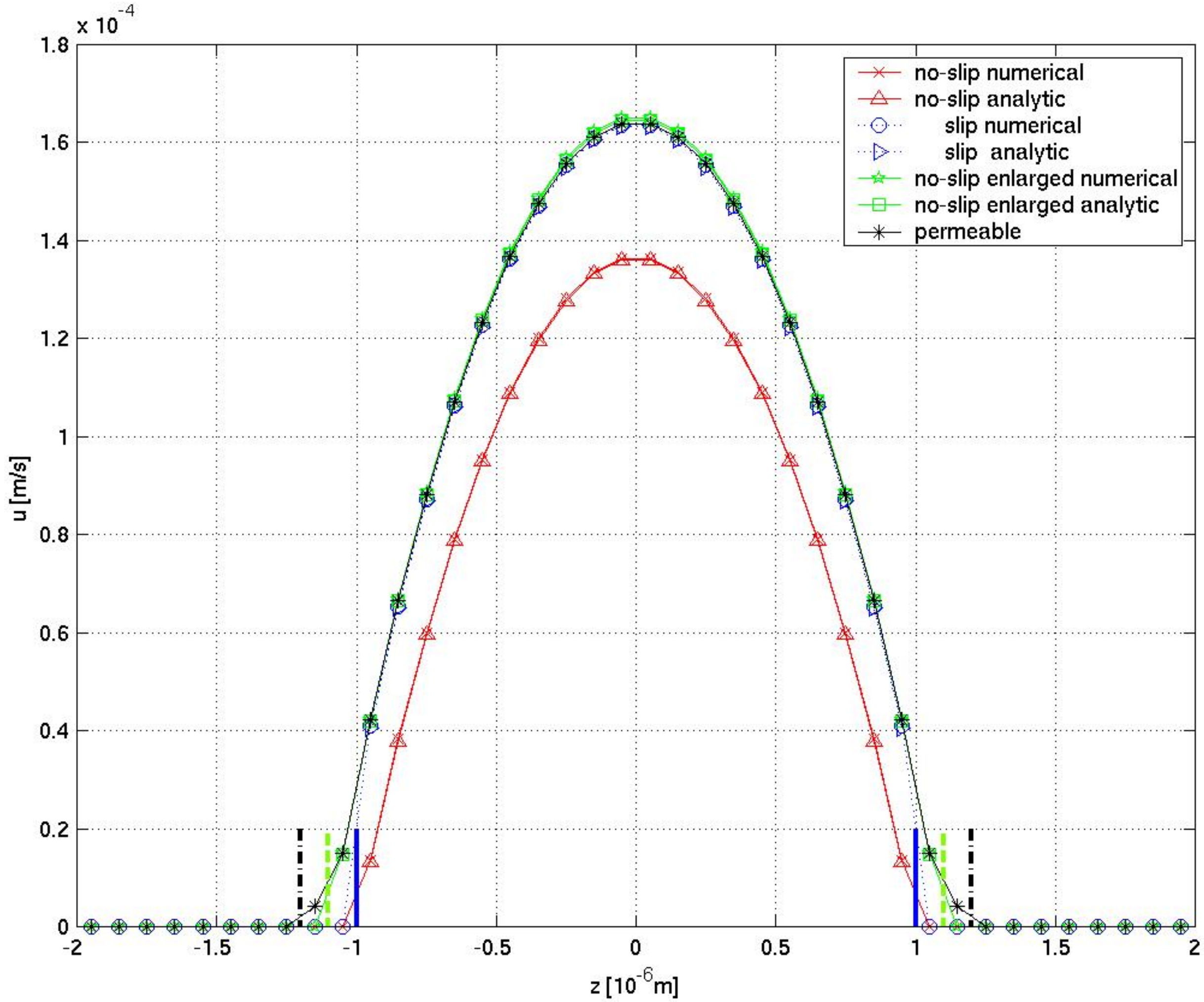


Distance between plates

2 µm

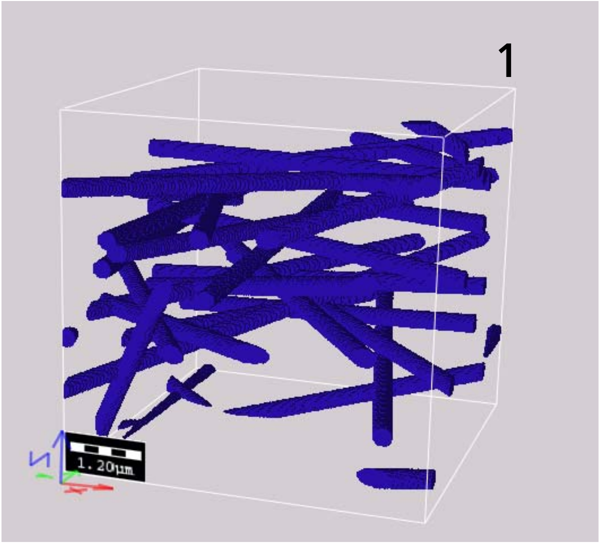
$\lambda$ = 100 nm

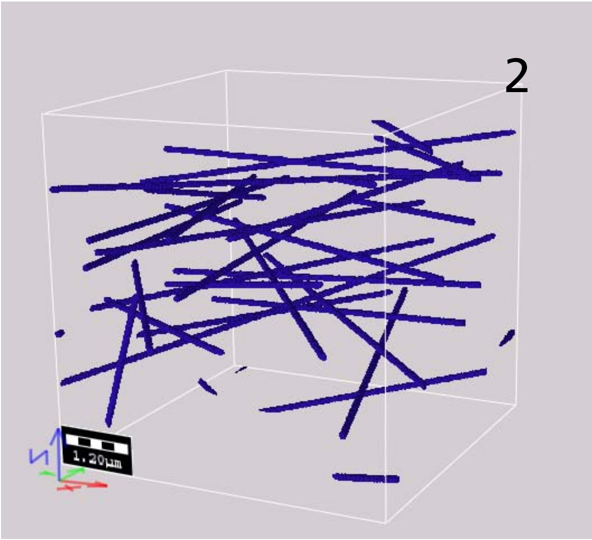
dp/L = 5000Pa/m



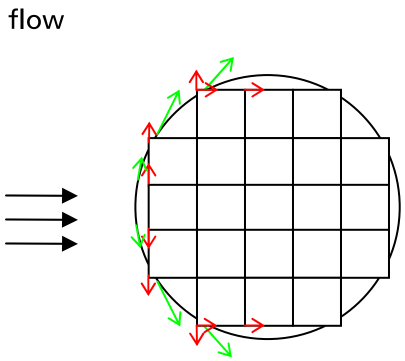

Permeable zones (blue – black), equivalent permeability is found by getting the same mean velocity as equivalent shrunk fiber

## 3 ways to simulate slip flow



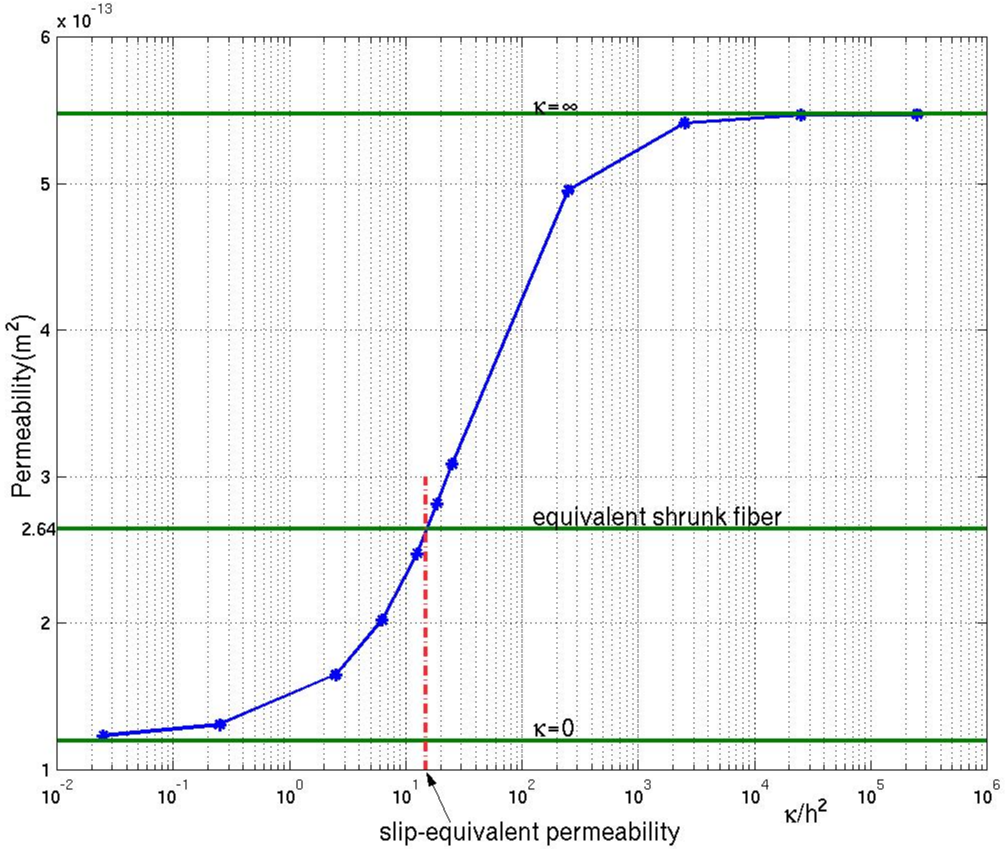


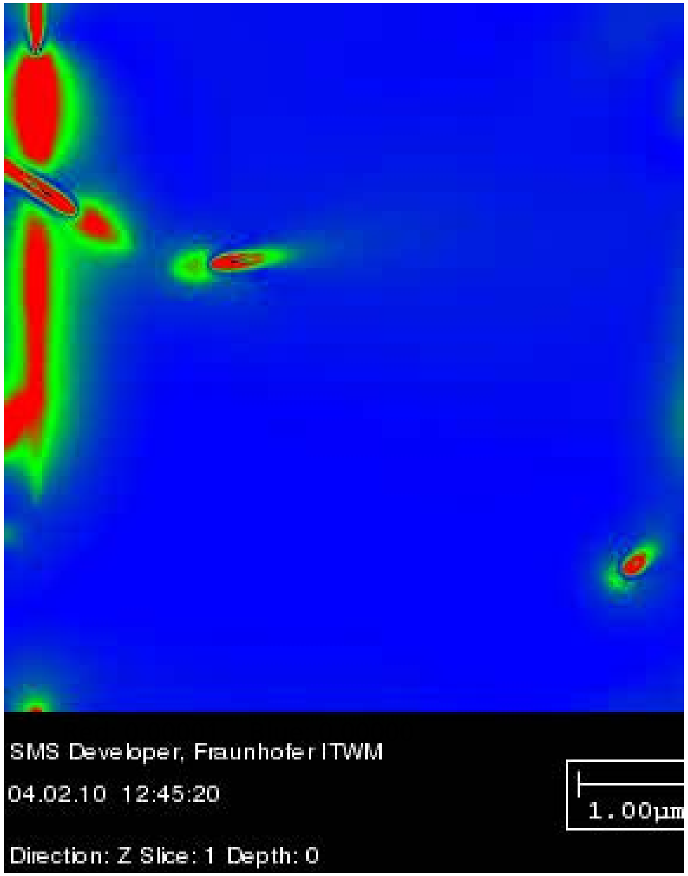



- Equivalent shrunk fibers with no-slip
- Fast
- Requires 1 for collisions

- Equivalent permeable fibers
- Slower
- Can be used for collisions

# Permeability of equivalent permeable fibers



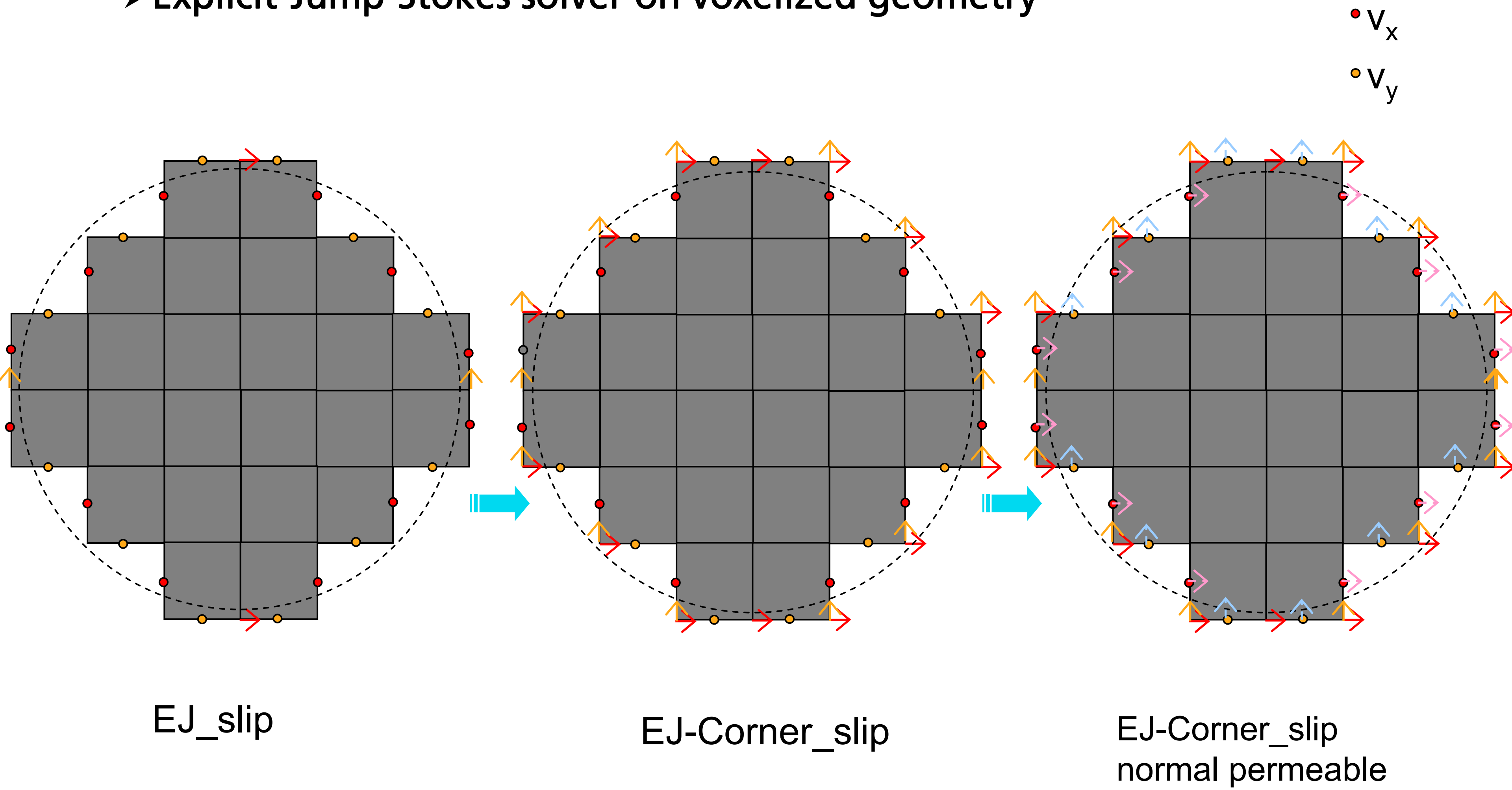

Voxel length: 20nm
Size: 300 x 300 x 300

Difference between flow fields from equivalent permeable fibers and equivalent shrunk fibers

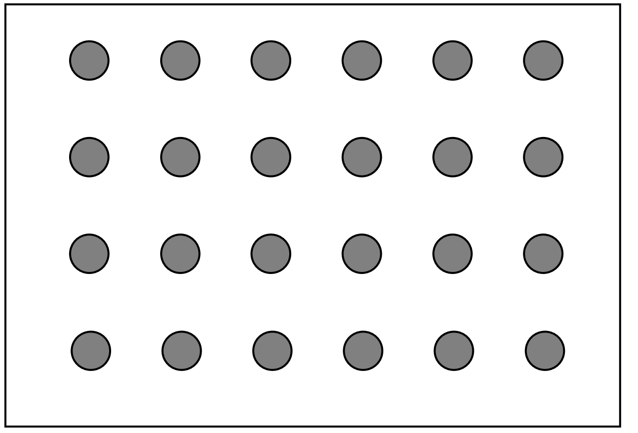
## Limitations

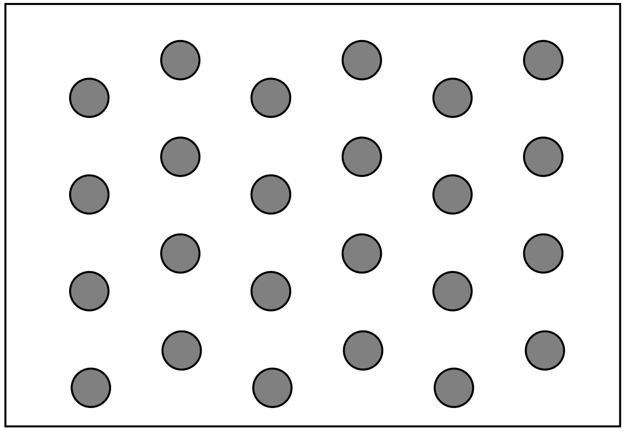
- Equivalent shrunk fiber
  - Not applicable when radius of fiber less than slip length
  - Can not be used for collision
- Equivalent permeable fiber
  - Finding slip-equivalent permeability

## ➢Explicit-Jump-Stokes solver on voxelized geometry



## Benchmark 2: Kuwabara's cell model





$$\Delta p = \frac{4\eta chU\left(1+1.996Kn\right)}{R^2\left[-\frac{1}{2}\ln(c)-0.75+c-\frac{c^2}{4}+1.996Kn\left(-\frac{1}{2}\ln(c)-0.25+\frac{c^2}{4}\right)\right]}$$

where $\eta$ is coefficient of viscosity, c is the packing fraction, h is the filter thickness, U is macroscopic air velocity, *Kn* is Knudsen number. R is the fiber radius.

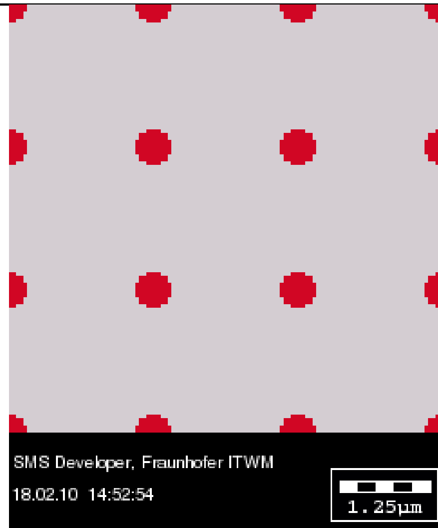
# Examples

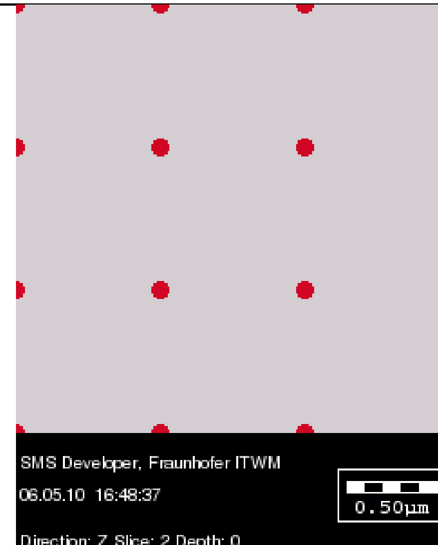
500nm-structure 1

Diameter : 500nm

Spacing in X: 2µm

Spacing in y: 2µm




100nm-structure 1

Diameter : 100nm

Spacing in X: 0.8µm

Spacing in y: 0.8µm

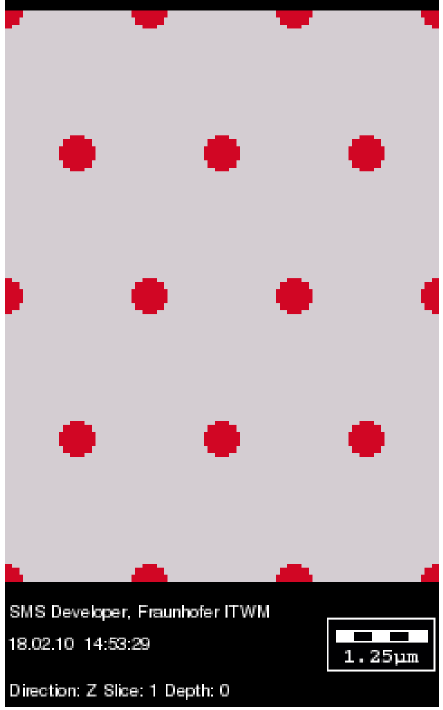
500nm-structure 2

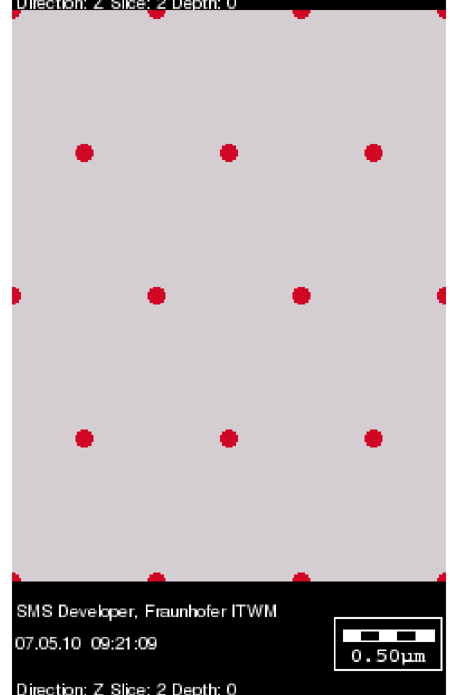
Diameter : 500nm

Spacing in X: 2µm

Spacing in y: 2µm

Raw shift : 1µm




100nm-structure 2

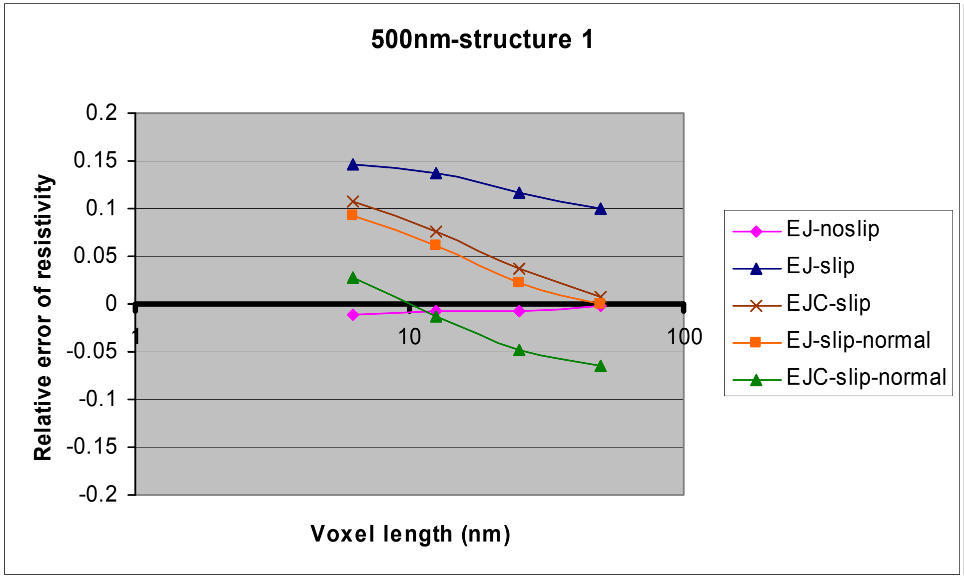
Diameter : 100nm

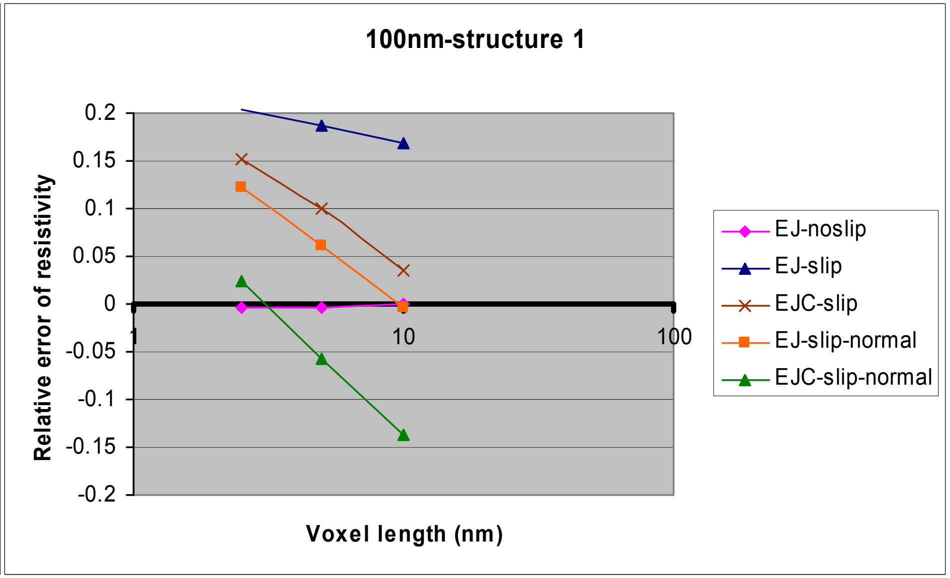
Spacing in X: 0.8µm

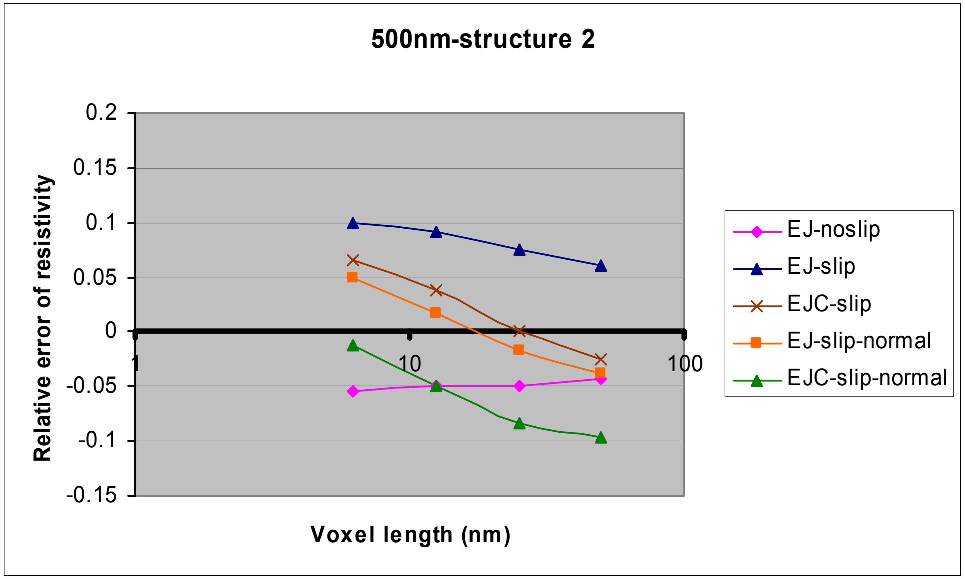
Spacing in y: 0.8µm

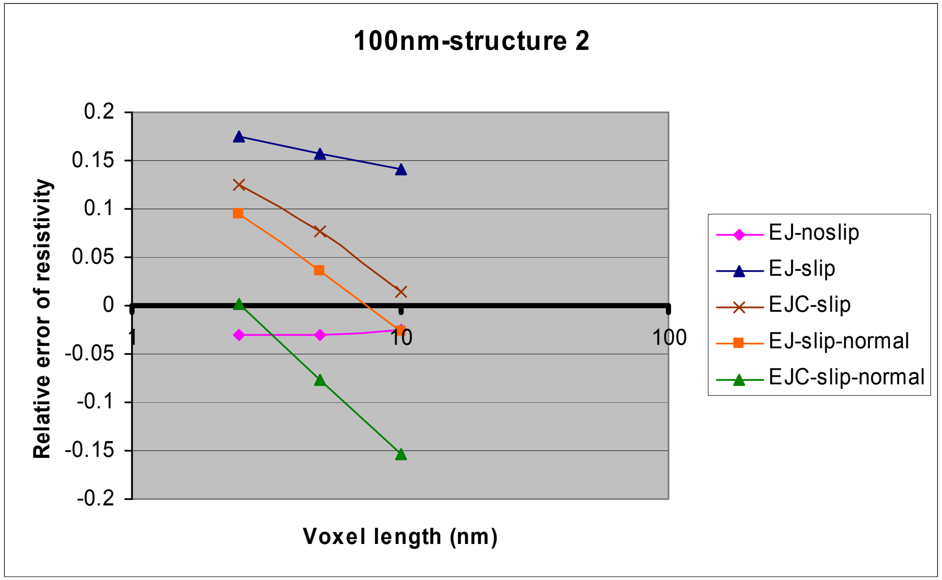
Raw shift : 0.4µm

# The comparison of EJs results and Kuwabara's analytic solutions



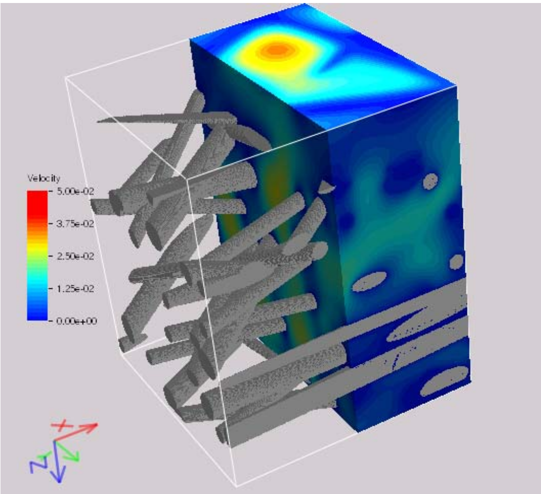



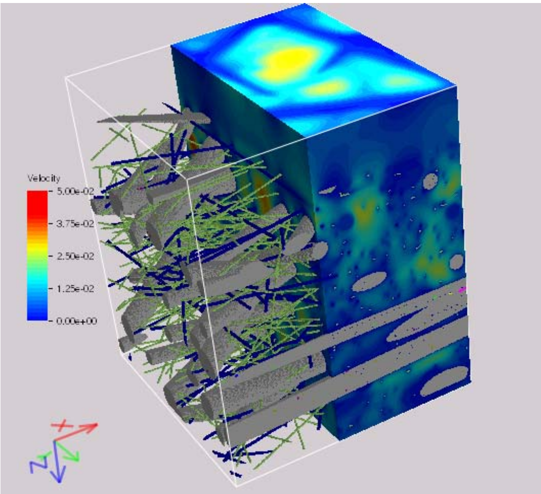



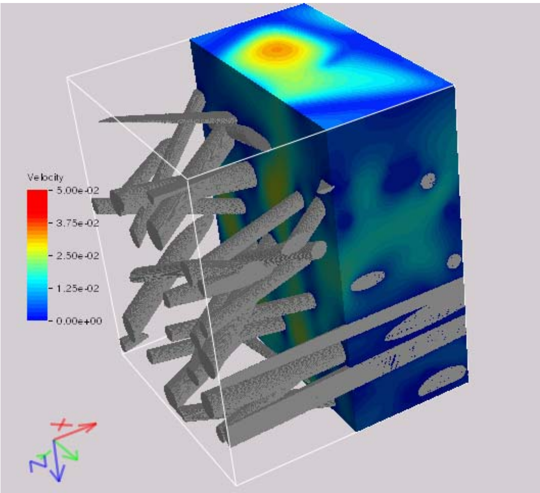
# Local Velocity: no-slip vs slip flow

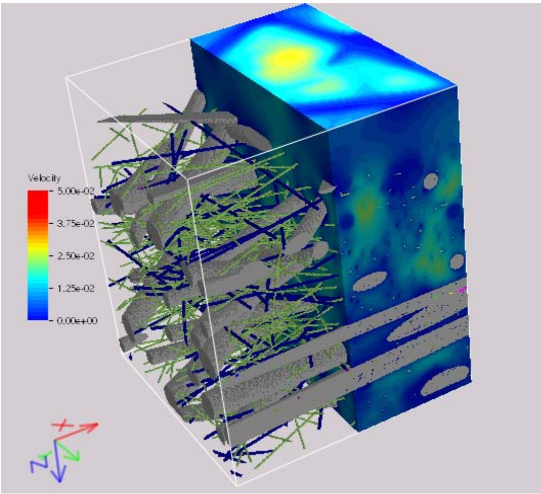
No_slip




Slip



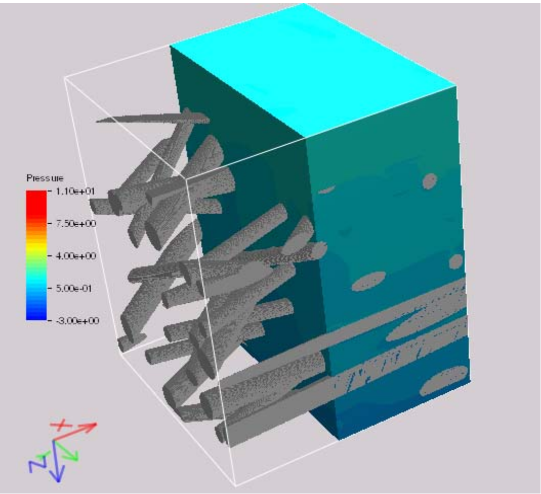

Medium 1

Medium 2

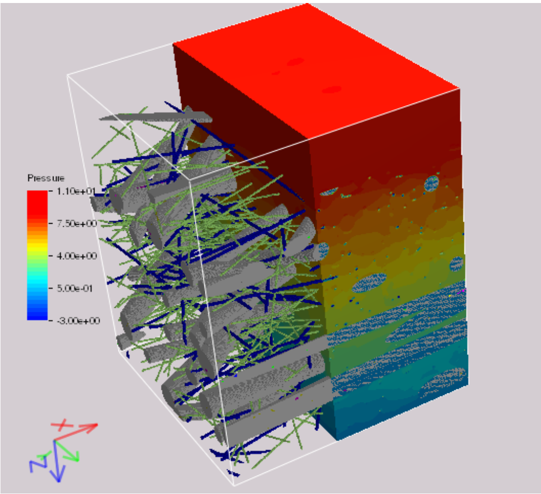
Mean velocity 0.01m/s

# Local pressure: no-slip vs slip flow

No_slip

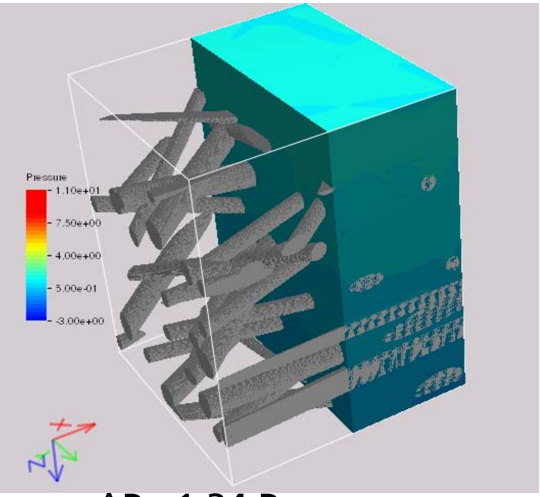



ΔP=1.45 Pa

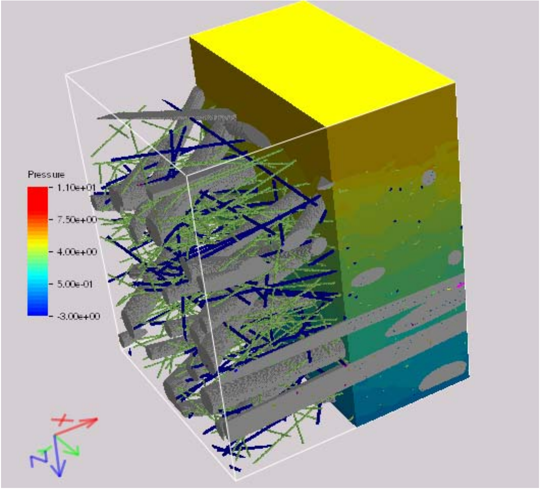



ΔP=8.25 Pa

Slip




ΔP= 1.34 Pa




ΔP= 5.44 Pa

Medium 1: diff 7.6%

Medium 2: diff 34%

Mean velocity 0.01m/s

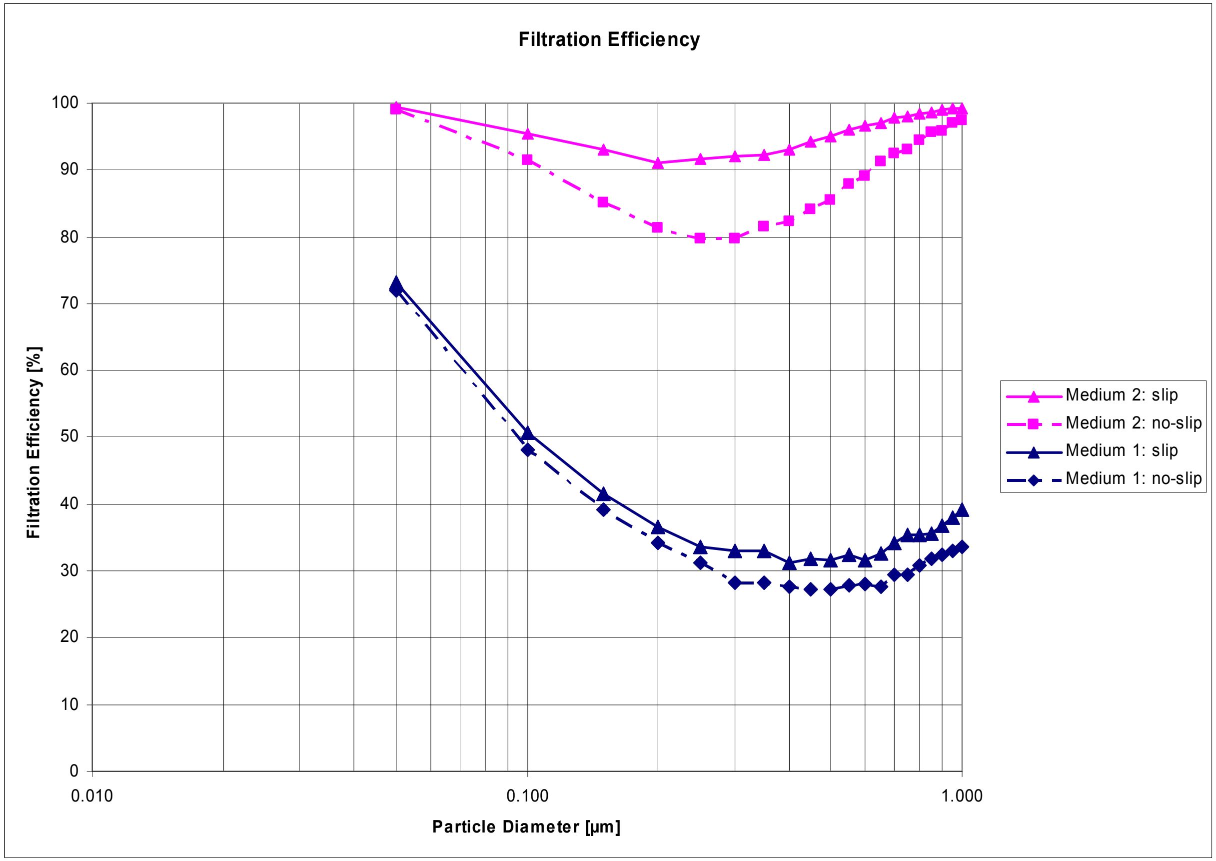
# Result: Micro fibers vs. Nano fibers

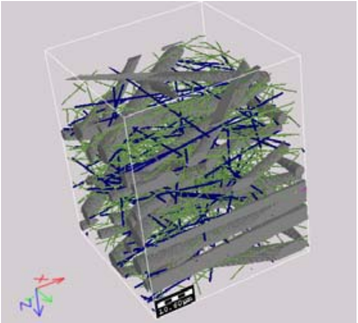
- Pressure drop

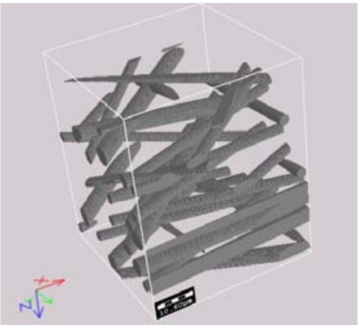
at 1cm/s

| Media | 1 | 2 |
|---|---|---|
| ΔP (no-slip) | 1.45 | 8.25 |
| ΔP (slip) | 1.34 | 5.44 |

- Filter efficiency





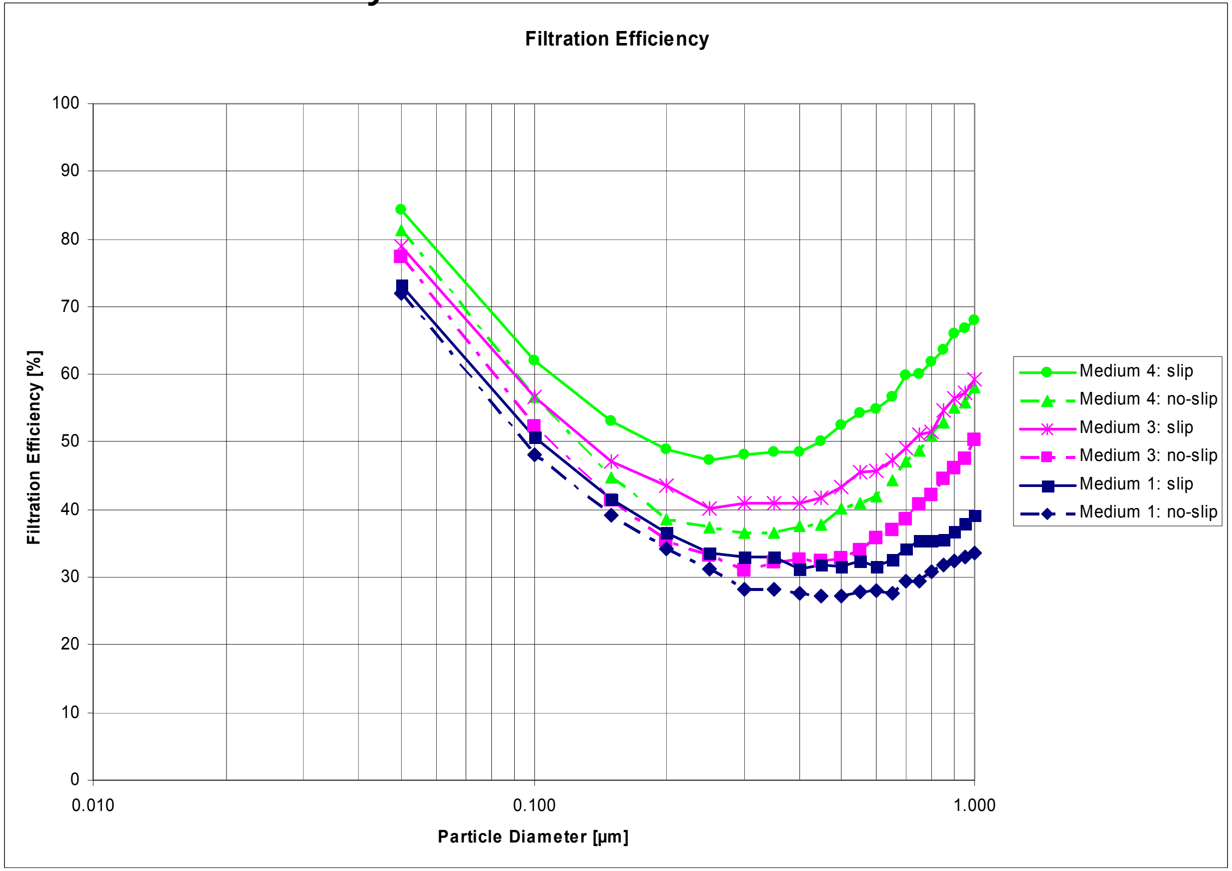
# Micro fibers vs. Nano fiber layer

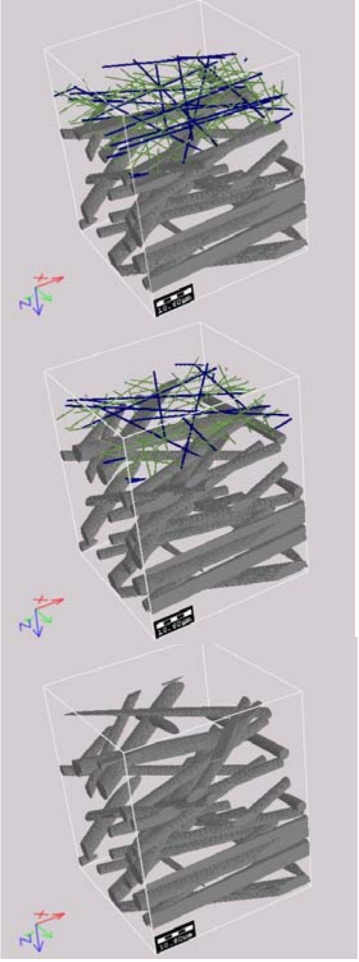
- Pressure drop

at 1cm/s

| Media | 1 | 3 | 4 |
|---|---|---|---|
| ΔP(no-slip) | 1.45 | 1.99 | 2.16 |
| ΔP(slip) | 1.34 | 1.63 | 1.68 |

- Filter efficiency



# Summary

- Simulation of pressure drop and filter efficiency
- Models for nano fibers „in depth“ and „on the surface“
- Nano fibers improve filter efficiency, increase pressure drop
- Slip flow via equivalent shrunk fibers and equivalent permeable fibers
- Explicit-jump solver: corner slip and/or penetrating in normal direction
- Slip flow further increases filter efficiency AND lowers pressure drop

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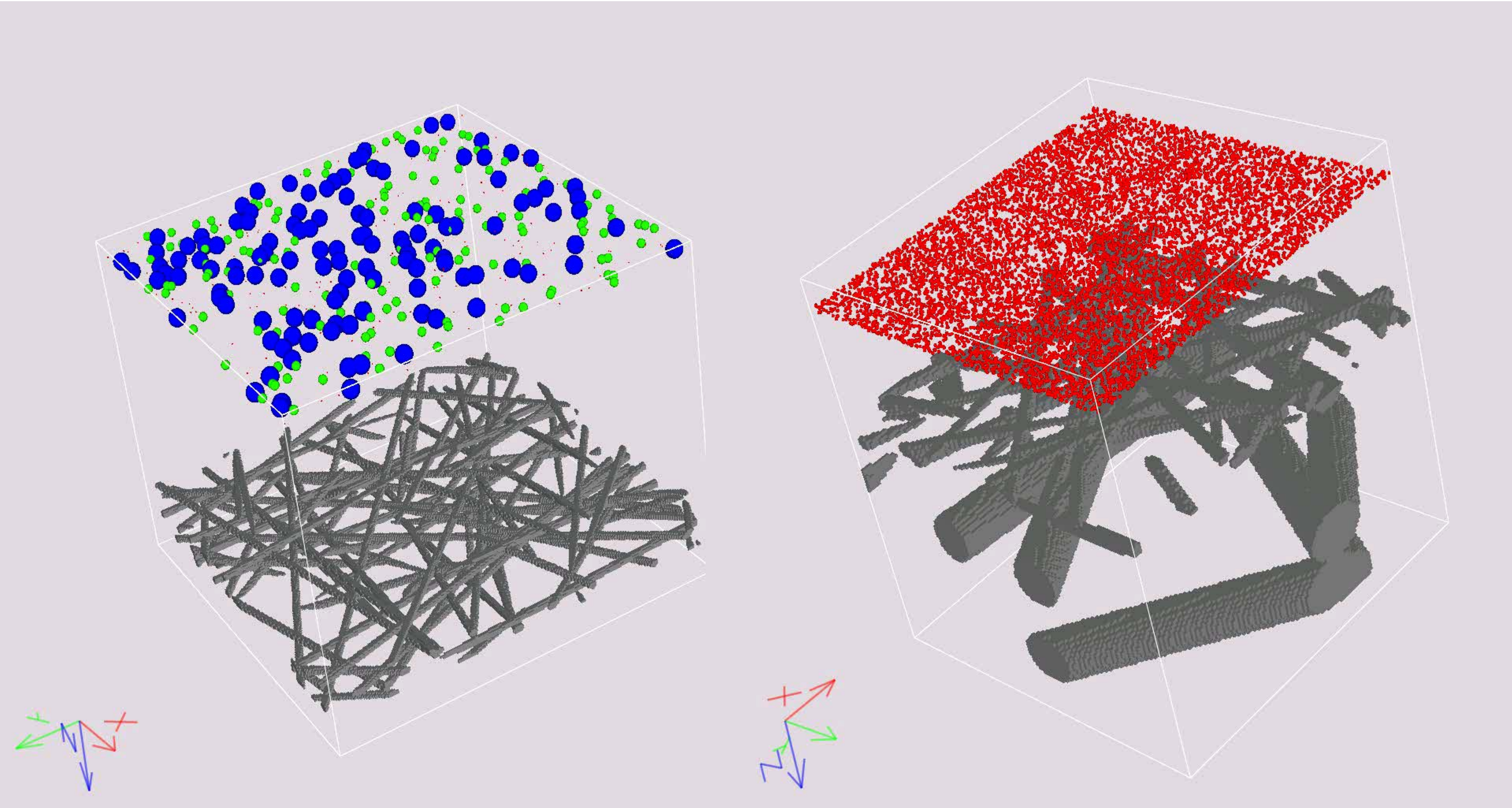
We thank the German ministry for education and research (BMBF) for support under FKZ 13N9861, in the project

Nano-Meltblown-Fibers for Filter media (NaBlo) - subproject: Modeling, Simulation and Optimization of Meltblown processes and  nano fiber filter media.



# …and thank you for your attention