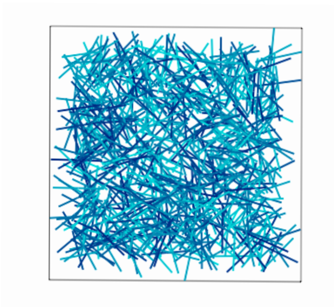
Large scale simulations of gravity induced sedimentation of slender fibers



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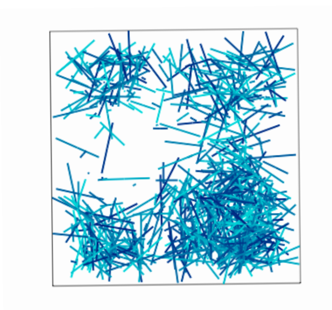
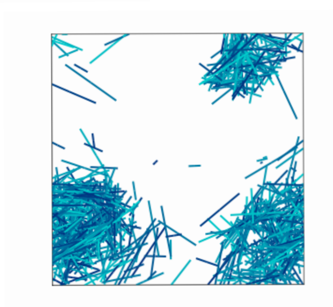
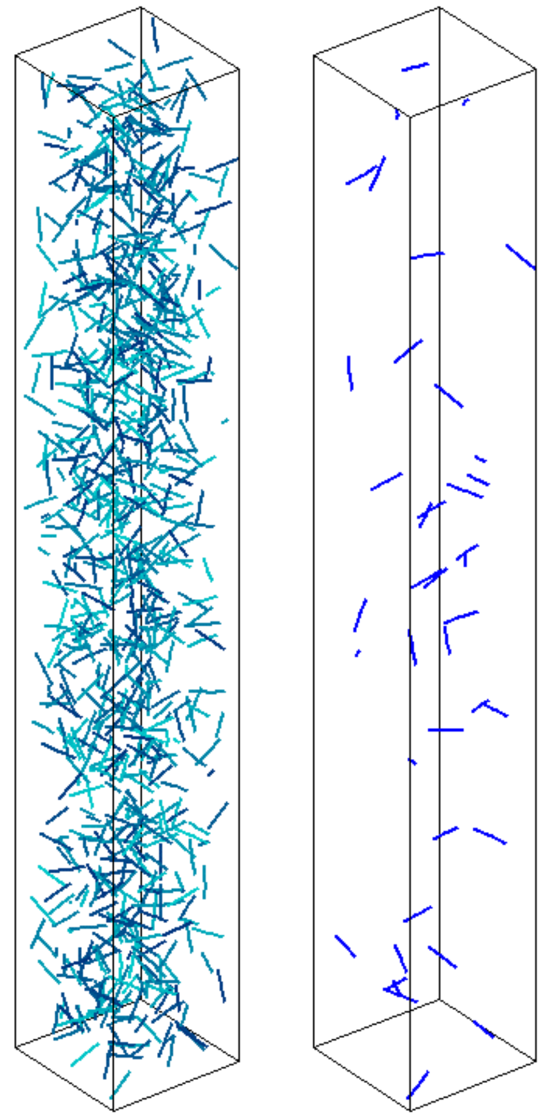




Simulations of rigid fibers
"Fibers in Waterland"

800 fibers sedimenting due to gravity (initial random distribution).

Right plot: showing 40 of these.



- Rigid fibers sedimenting due to gravity.
- Model of paper pulp.
- Two things that determine the quality of the paper
    - Orientation of the fibers - strength.
    - Distribution of fibers.
- Fibers align in direction of gravity
    - Weakens the paper in the other direction.
- "Clusters" or "flocs" of fibers form.
    - Creates uneven thickness and roughness.

Outline

- Part 1: Mathematical model
  - Mathematical modeling
  - Stokes equations
  - Boundary integral formulation
  - Boundary integral equations
  - Mathematical model for fiber suspensions:
    - Non-local slender body approximation
- Part 2: Numerical simulations of fiber suspensions
  - Introduction to fiber suspensions
  - Numerical methods and algorithms
  - Numerical experiments with parallel code
  - Ongoing and future work
- Work is done in cooperation with:
  - Prof. Anna-Karin Tornberg
  - PhD-student Jennifer Grünig
  - PhD-student Oana Marin

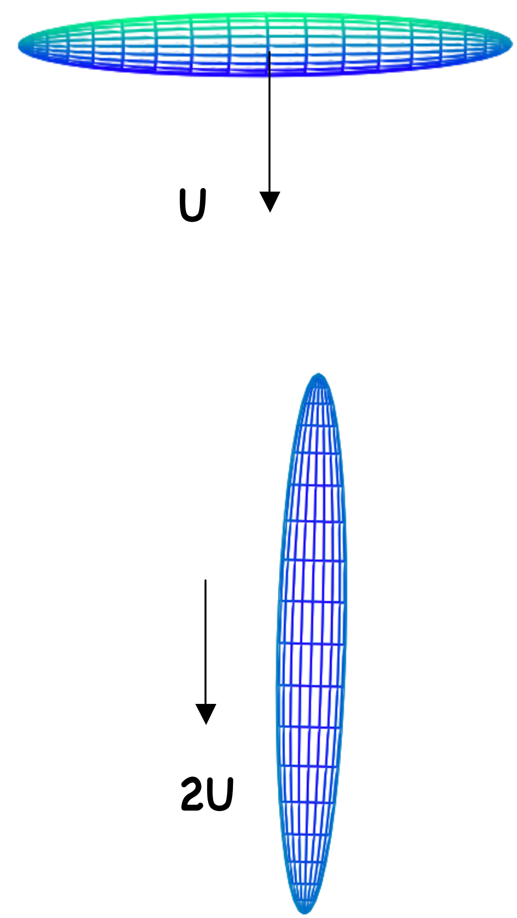
Mathematical modeling

- Idea – what do we want to investigate ?
- Physical model – what physical laws describe our problem ?
- Mathematical model – can we do any simplifications ?
- Numerical model – fast and accurate algorithms.
- Simulations and post-processing of computed data.
- Accuracy assessment – results are compared to experimental data.

We want to model and numerically simulate the flow around several objects – fibers.

Physical model

- The objects are immersed in a viscous fluid of viscosity μ .
- The objects are rigid bodies.
- External forces on the objects are given by gravity.
- The objects are heavier than the fluid but the difference is small.
- The objects will sediment "slowly" in the direction of gravity.
- The velocity of the objects depend on their orientation.
- Viscous fluid – objects will "drag" the fluid along.
- If more than one object they will interact only through the fluid.



Objects in a fluid – Navier-Stokes equations!

Mathematical model

- Flow around an object in a fluid can be described by the Navier-Stokes equations

$$\underbrace{\rho\left(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}\right)}_{\text{Convective term}} = -\nabla p + \underbrace{\mu\nabla^2\mathbf{u}}_{\text{Viscous term}} + \mathbf{f}$$

$$\nabla\cdot\mathbf{u} = 0$$

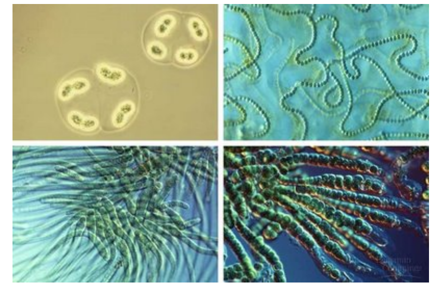
$\mathbf{u}$	velocity
p	pressure
$\mathbf{f}$	force
ρ	density
μ	viscosity

- They arise from applying Newton's second law to a fluid element.
- Time dependent and non-linear.
- Can we do any simplifications ?
- In our case: small velocity and large viscosity.
- Reynolds number $\mathrm{Re} = \dfrac{\rho U L}{\mu} \ll 1$
- Neglect convective terms.

Reynolds number: relation between convective and viscous terms

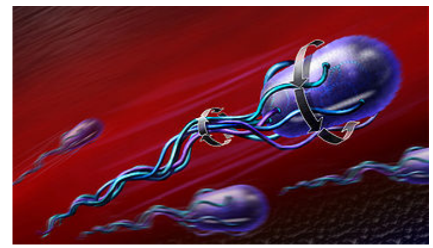
Stokes equations

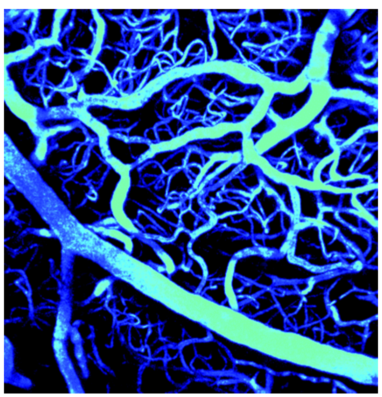
Stokes equations can describe a large variety of flows

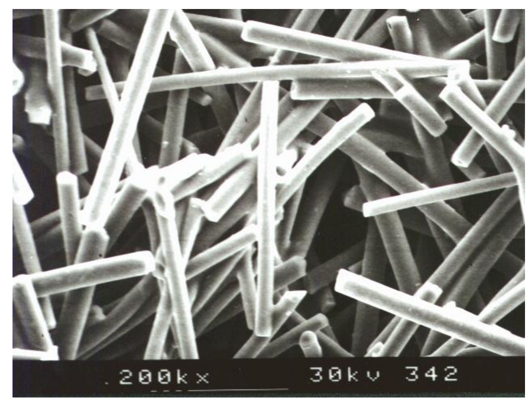


Few examples:

- Motion of microorganisms
  - Cilia, Flagella.
- Blood flow in capillaries.
- Drops and bubbles.
- Liquid-particle suspensions
  - Fiber suspensions.







http://www.liquidsculpture.com/

Stokes equations and…

- Stokes equations:

$$\nabla p - \mu\Delta\mathbf{u} = \mathbf{f}, \quad \nabla\cdot\mathbf{u} = 0$$

- and boundary conditions:

$$\mathbf{u} = \mathbf{u}_{\partial\Omega} \text{ on } \partial\Omega, \quad \mathbf{u} \to \mathbf{0} \text{ for } \mathbf{x} \to \infty$$

- No explicit time-dependence in equation. Time-dependent system due to motion of immersed objects.
- No intertia. In equilibrium in each instant in time.
- Linear PDE. Possible to reformulate as a boundary integral equation.

Boundary conditions:

- The fluid velocity at the boundary of the object equals the velocity of the object (no-slip).
- The fluid velocity far from the object is not affected by its presence.

...the Stokeslet

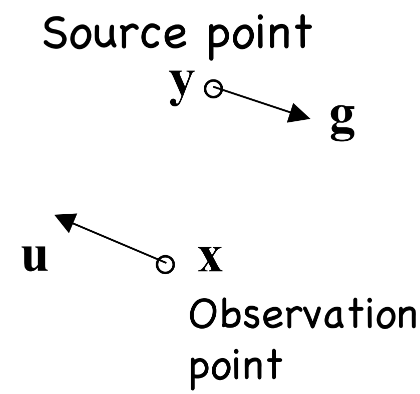
- The singularily forced Stokes equation

$$\nabla p - \mu \Delta \mathbf{u} = \mathbf{g}\delta(\mathbf{x}-\mathbf{y})$$

has the solution

$$u_i(\mathbf{x}) = \frac{1}{8\pi\mu} S_{ij}(\mathbf{x},\mathbf{y}) g_j$$

$$(S_{ij} g_j = S_{i1} g_1 + S_{i2} g_2 + S_{i3} g_3)$$



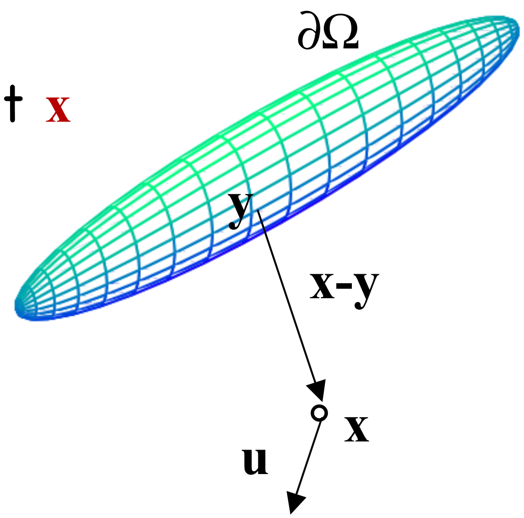
where

$$S_{ij}(\mathbf{x},\mathbf{y}) = \frac{\delta_{ij}}{|\mathbf{x}-\mathbf{y}|} + \frac{(x_i - y_i)(x_j - y_j)}{|\mathbf{x}-\mathbf{y}|^3}, \qquad i,j = 1,2,3.$$

S_{ij} is called the Stokeslet and is the fundamental solution or the free-space Green's function for the Stokes equations.

Immersed object in Stokes flow

- Let **y** be a point at the surface of the object.
- Let **f** be a force distribution on the surface of the object.
- Then the velocity, **u**, at the observation point **x** is given by



$$u_i(\mathbf{x}) = \frac{1}{8\pi\mu} \int_{\partial\Omega} S_{ij}(\mathbf{x},\mathbf{y}) f_j(\mathbf{y})\, dS_{\mathbf{y}}, \quad i = 1,2,3$$

Boundary integral formulation

- If **f** is known we can directly compute the velocity field at any point **x** **(at the boundary or outside the object).**
- **If** **u** is known at the boundary of the object we have to solve a boundary integral equation for **f**.

Boundary integral equation, BIE

- A general form: $u(s) = \int_C K(s,t) f(t)\ dt,\ s,t$ on C
- K(s,t) is called a kernel.

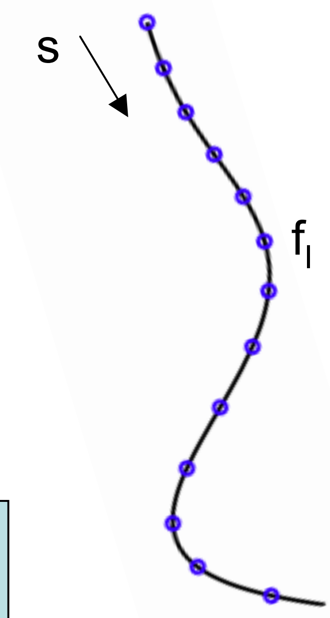
- Assume we know u along the curve C.
- We want to find f along the curve C.
- Discretize the integral with a quadrature rule defined by the weights w_l.

$$u_k = \sum_{l=1}^{N} w_l K(s_k, t_l) f_l,\ k = 1,2,\ldots,N$$

$$u_1 = w_1 K(s_1,t_1) f_1 + w_2 K(s_1,t_2) f_2 + \ldots w_N K(s_1,t_N) f_N$$

$$u_2 = w_1 K(s_2,t_1) f_1 + w_2 K(s_2,t_2) f_2 + \ldots w_N K(s_2,t_N) f_N$$

$$\vdots$$



This will yield a linear system of equations (NxN) to be solved for f

$$\mathbf{Af} = \mathbf{u}$$

Boundary integral equations, cont.

- For Stokes equation we have that

$$K_{ij}(\mathbf{x},\mathbf{y}) = S_{ij}(\mathbf{x},\mathbf{y}) = \frac{\delta_{ij}}{|\mathbf{x}-\mathbf{y}|} + \frac{(x_i - y_i)(x_j - y_j)}{|\mathbf{x}-\mathbf{y}|^3}$$

  so when both x and y are at the boundary the kernel will be singular! (But still integrable.)
- Different techniques to handle the singularity
  - Singularity subtraction.
  - Construct special quadrature rule to handle the singularity.

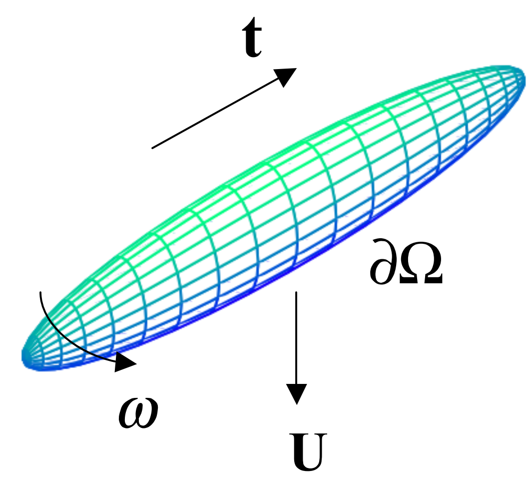
No details about this will be given in this talk…

Immersed *solid* object in Stokes flow,

- What if both f and u at the boundary are unkown ?
- We know the externally applied force (gravity).
- The object is centered at $\mathbf{x}_c$ with an associated orthonormal basis $\mathbf{t}$ and surface $\partial\Omega$.
- Rigid body motion and no-slip, i.e for $\mathbf{x} \in \partial\Omega$,

  $$\mathbf{u}(\mathbf{x}) = \mathbf{U} + \omega \times (\mathbf{x} - \mathbf{x}_c)$$

  with translational velocity $\mathbf{U}$
  and angular velocity ω.
- Integrated force over the object must be equal to externally applied force. Same for the torque.



Boundary integral formulation

- For the object we have the equation relating the forces on the surface to the velocity of the object:

$$\mathbf{U}_i + (\omega \times (\mathbf{x} - \mathbf{x}_c))_i = \frac{1}{8\pi\mu} \int_{\partial\Omega} S_{ij}(\mathbf{x},\mathbf{y}) f_j(\mathbf{y})\ dS_{\mathbf{y}}, \quad i = 1,2,3 \quad (1)$$

together with the constraints

$$\mathbf{F}_{body} = \int_{\partial\Omega} \mathbf{f}(\mathbf{y})\ dS_{\mathbf{y}} \qquad \mathbf{T}_{body} = \int_{\partial\Omega} (\mathbf{x} - \mathbf{x}_c) \times \mathbf{f}\ (\mathbf{y})\ dS_{\mathbf{y}}. \quad (2)$$

Unknowns:

f_1, f_2, f_3

U_1, U_2, U_3

$\omega_1,\ \omega_2,\ \omega_3$

- Solve the system of BIE, (1)-(2), for $\mathbf{f}(\mathbf{x})$, $\mathbf{U}$ and ω
- Update the position of the bodies by

$$\frac{d}{dt}\mathbf{x}_c = \mathbf{U}, \qquad \frac{d}{dt}\mathbf{t} = \mathbf{t} \times \omega$$

- The velocity field can be computed in any point $\mathbf{x}$ by

$$u_i(\mathbf{x}) = \frac{1}{8\pi\mu} \int_{\partial\Omega} S_{ij}(\mathbf{x},\mathbf{y}) f_j(\mathbf{y})\ dS_{\mathbf{y}}$$

(as a post-processing step)

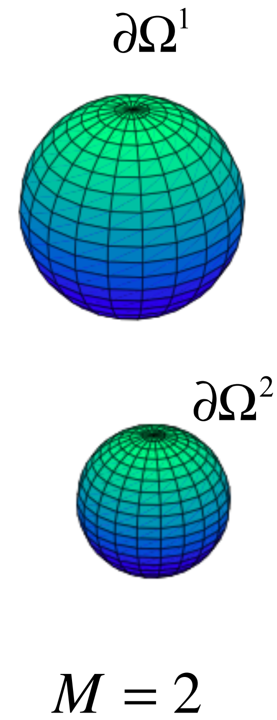
Many immersed objects in Stokes flow

- M immersed solid objects.
- Body m, $m = 1, \ldots M$ centered at $\mathbf{x}_c^m$ with an associated orthonormal basis $\mathbf{t}^m$ and surface $\partial\Omega^m$.
- As before, rigid body motion and no-slip, i.e for $\mathbf{x} \in \partial\Omega^m$

  $$\mathbf{u}(\mathbf{x}) = \mathbf{U}^m + \omega^m \times (\mathbf{x} - \mathbf{x}_c^m)$$

  with translational velocity $\mathbf{U}^m$

  and angular velocity ω^m.
- Integrated force over each body must be equal to externally applied force. Same for the torque.



Stokes equations are linear so we can use the superposition principle.

Boundary integral formulation

- For body no m, we now have

Sum over all objects

$$U_i^m + (\omega^m \times (\mathbf{x}-\mathbf{x}_c^m))_i = \frac{1}{8\pi\mu}\sum_{l=1}^{M}\int_{\partial\Omega_l} S_{ij}(\mathbf{x},\mathbf{y}) f_j^l(\mathbf{y})\ dS_{\mathbf{y}}, \quad (1)$$

together with the constraints

$$\mathbf{F}_{body}^m = \int_{\partial\Omega_m} \mathbf{f}^m(\mathbf{y})\ dS_{\mathbf{y}} \qquad \mathbf{T}_{body}^m = \int_{\partial\Omega_m} (\mathbf{x}-\mathbf{x}_c^m)\times \mathbf{f}^m(\mathbf{y})\ dS_{\mathbf{y}}. \quad (2)$$

- As before, solve (1)-(2) for $\mathbf{f}^m(\mathbf{x})$, $\mathbf{U}^m$ and ω^m, $m=1,\ldots,M$ and update the position of the bodies by

$$\frac{d}{dt}\mathbf{x}_c^m = \mathbf{U}^m, \qquad \frac{d}{dt}\mathbf{t}^m = \mathbf{t}^m \times \omega^m$$

- The velocity field can be computed in any point $\mathbf{x}$ by

$$u_i(\mathbf{x}) = \frac{1}{8\pi\mu}\sum_{l=1}^{M}\int_{\partial\Omega_l} S_{ij}(\mathbf{x},\mathbf{y}) f_j^l(\mathbf{y})\ dS_{\mathbf{y}}$$

(as a post-processing stage)

Unknowns:

$f^m{}_1, f^m{}_2, f^m{}_3$

$U^m{}_1, U^m{}_2, U^m{}_3$

$\omega_1^m, \omega_2^m, \omega_3^m$

$m=1:M$

Why use boundary integrals?

- We only need to consider the actual objects when solving the problem.
- If we want information about the flow in the fluid we can compute it as a post-processing.
- Reduction in dimensionality: we go from a partial differential equation (3D) to a boundary integral over a surface (2D).
- Still expensive to solve for many objects.
- N/many-body problem - all objects interact.

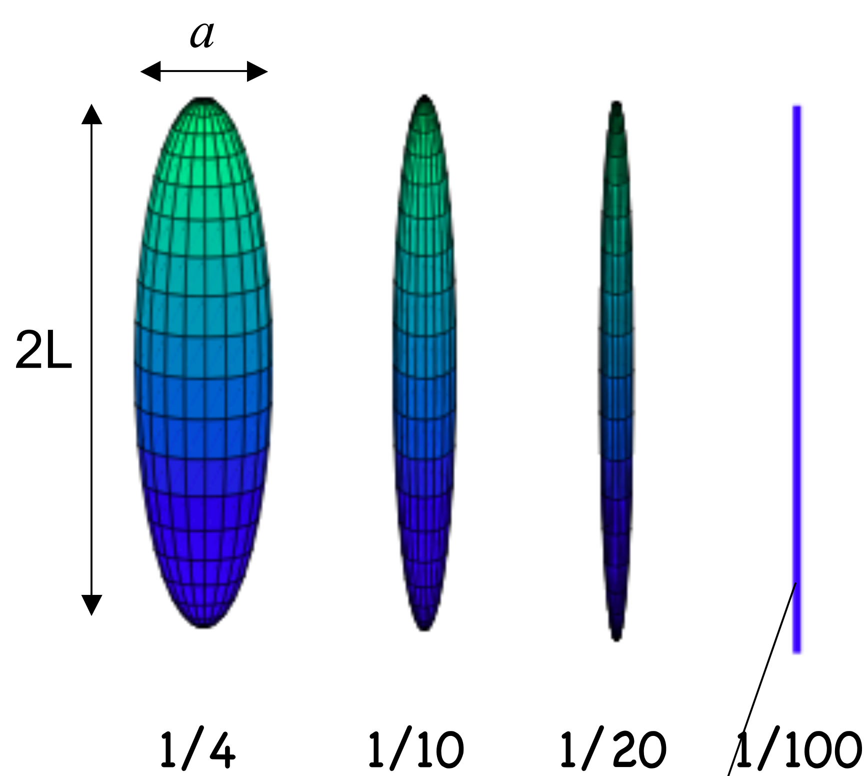
What about the fibers ?
We want many of them in our simulations!

Slender fibers in Stokes flow

- We are concerned with many and very slender fibers.
- Slenderness defined by a parameter.

$$\varepsilon = a / 2L << 1$$

- To expensive to discretize and solve numerically for slender fibers.
- Do an asymptotic expansions in the slenderness parameter.

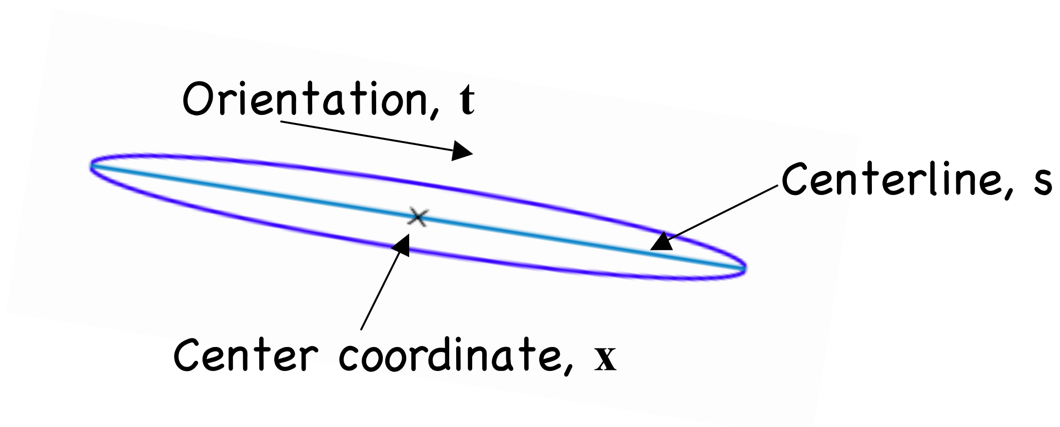


Slender body equations

Slender body approximation

Integral equations are solved along fiber centerlines – 1D!

- Fundamental solutions (Stokeslets and dipoles) are placed on fiber centerline (parametrized by s).
- For multiple fibers: Accurate to $O(\varepsilon)$.
- Formulation closed by enforcing no-slip condition on fiber surface, no angular variation in fiber velocity.



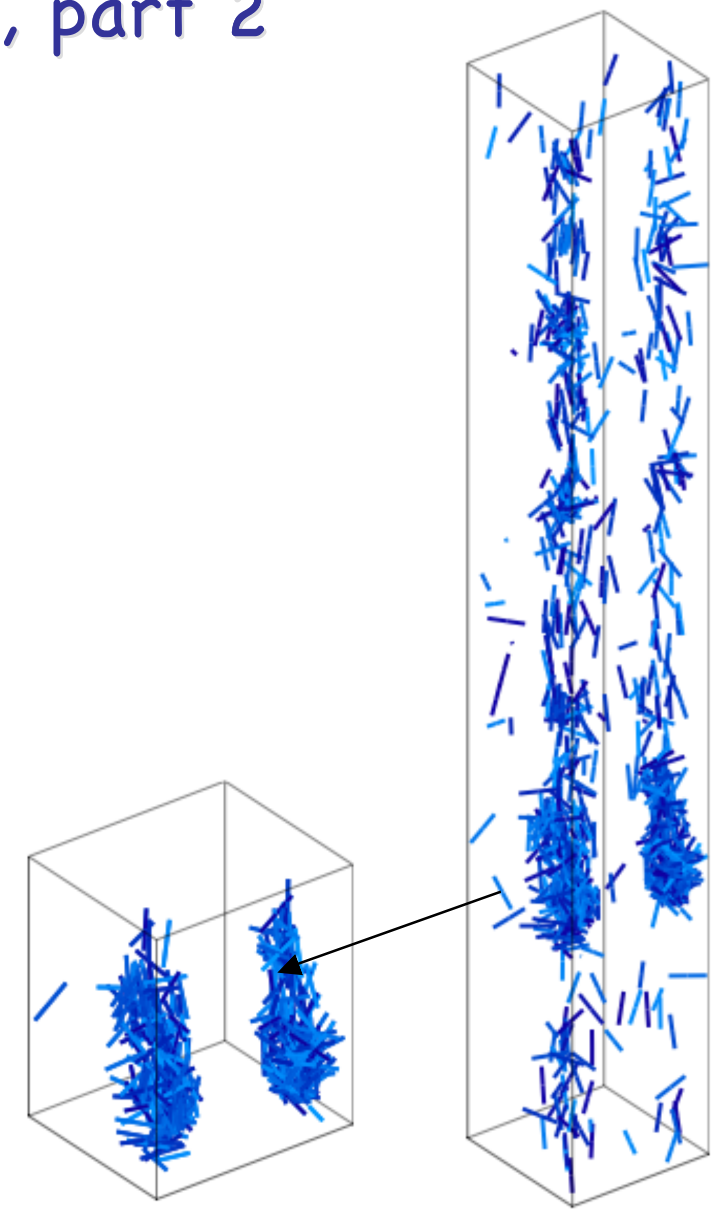
A fiber is defined by its center coordinate and orientation vector.

Part 2.

- Part 2: Numerical simulations of fiber suspensions
  - Introduction to fiber suspensions.
  - Summary from yesterday.
  - Mathematical model for many slender fibers.
  - Numerical methods and algorithms.
  - Numerical experiments with parallel.
  - Ongoing and future work.

Introduction, part 2

- Gravity induced sedimentation of rigid slender fibers in a viscous fluid.
- Microscopic description - track every fiber.
- Low Reynolds number flow - Stokes flow.
- Long range interactions and many body character yield a very complex behavior of the fibers.
- Collective dynamics of the suspension is given by the coupling between hydrodynamic interactions and the micro-arrangement of the fibers.
- Study micro-structure and its influences on averaged quantities.



Summary from yesterday

- Simulate many rigid and slender fibers in a viscous fluid.
- Slow motion - Stokes equations.
- Boundary integral formulation together with slender body approximation.
- Reduction in dimensionality from a PDE in 3D to a 1D integral equation.

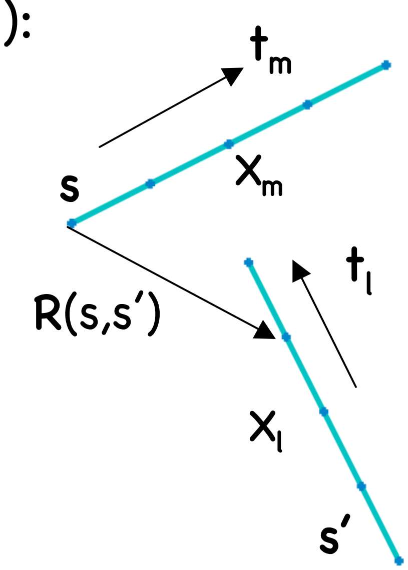
Slender body formulation for many fibers

- Velocity of fiber m is given by (rigid body motion):

$$\underbrace{\dot{\mathbf{x}}_{\mathrm{m}} + s\dot{\mathbf{t}}_{\mathrm{m}}}_{\text{Velocity of fiber m}} = \underbrace{\mathbf{L}(\mathbf{t}_{\mathrm{m}})\ \mathbf{f}_{\mathrm{m}}(s)}_{\text{Local contribution}} + \underbrace{(\mathbf{I} + \mathbf{t}_{\mathrm{m}}\mathbf{t}_{\mathrm{m}})\bar{\mathbf{K}}\left[\mathbf{f}_{\mathrm{m}}\right](s)}_{\text{Global contribution}}$$

$$+ \underbrace{\sum_{\substack{\mathrm{l}=1 \\ \mathrm{l}\neq \mathrm{m}}}^{M} \int_{-1}^{1} \mathbf{G}(\mathbf{R}(s,s'))\mathbf{f}_{\mathrm{l}}(s')\ ds'.}_{\text{Contribution from other fibers}} \qquad (1)$$

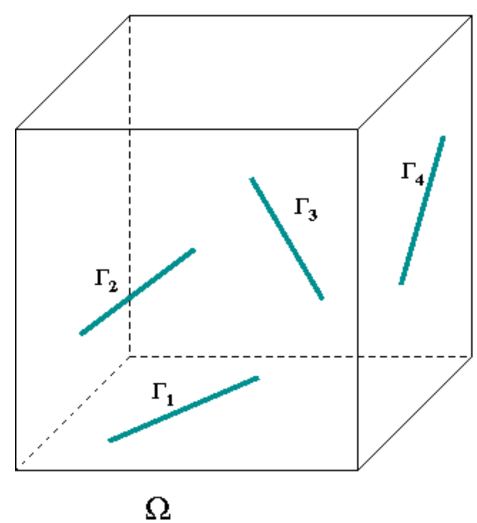
$$\mathbf{R}(s,s') = \mathbf{x}_{\mathrm{m}} + s\mathbf{t}_{\mathrm{m}} - (\mathbf{x}_{\mathrm{l}} + s'\mathbf{t}_{\mathrm{l}})$$



- G is a linear combination of two fundamental solutions:

$$\mathbf{G}(\mathbf{R}) = \mathbf{S}(\mathbf{R}) + \varepsilon^2\mathbf{D}(\mathbf{R})$$

- D(R) is called a Stokes doublet



3 unknowns but only one equation!

Two additional conditions

- Unknowns:
  - Forces acting on the fibers
  - Velocity of the fibers (translational and rotational)
- We have only one equation, need two additional conditions:
  - Total force on a fiber is given by gravity (external force)
  - No external torque

$$\mathbf{F}_m = \int_{-1}^{1} \mathbf{f}_m(s)\ ds = \mathbf{F}_g, \qquad \mathbf{M}_m = \int_{-1}^{1} s\ (\mathbf{t}_m \times \mathbf{f}_m(s))\ ds = 0 \qquad (2), (3)$$

total force on fiber m — total torque on fiber m

System closed. Equations (1)-(3) solves our problem!

Summary of mathematical model

- Velocity of fiber m given by:

$$\underbrace{\dot{\mathbf{x}}_{\mathrm{m}} + s\dot{\mathbf{t}}_{\mathrm{m}}}_{\text{Velocity of fiber m}} = \underbrace{\mathbf{L}(\mathbf{t}_{\mathrm{m}})\ \mathbf{f}_{\mathrm{m}}(s)}_{\text{Local contribution}} + \underbrace{(\mathbf{I} + \mathbf{t}_{\mathrm{m}}\mathbf{t}_{\mathrm{m}})\bar{\mathbf{K}}\left[\mathbf{f}_{\mathrm{m}}\right](s)}_{\text{Global contribution}} + \underbrace{\sum_{\substack{\mathrm{l}=1 \\ \mathrm{l}\neq\mathrm{m}}}^{M} \int_{-1}^{1} \mathbf{G}(\mathbf{R}(s,s'))\mathbf{f}_{\mathrm{l}}(s')\ ds'}_{\text{Contribution from other fibers}}. \qquad (1)$$

$$\mathbf{R}(s,s') = \mathbf{x}_{\mathrm{m}} + s\mathbf{t}_{\mathrm{m}} - (\mathbf{x}_{\mathrm{l}} + s'\mathbf{t}_{\mathrm{l}})$$

- Two extra conditions for fiber m:

$$\mathbf{F}_{\mathrm{m}} = \int_{-1}^{1} \mathbf{f}_{\mathrm{m}}(s)\ ds = \mathbf{F}_{g}, \qquad \mathbf{M}_{\mathrm{m}} = \int_{-1}^{1} s\ (\mathbf{t}_{\mathrm{m}} \times \mathbf{f}_{\mathrm{m}}(s))\ ds = 0 \qquad (2), (3)$$

Equations (1)-(3) for m=1, 2, …, M.
3M unknowns: $\dot{\mathbf{x}}_{\mathrm{m}},\ \dot{\mathbf{t}}_{\mathrm{m}},\ \mathbf{f}_{\mathrm{m}}$
How do we solve these equations ?

Numerical discretization

- Manipulations of equations (1)-(3) leads to a closed system for the forces $\mathbf{f}_{\mathrm{m}}$ (without $\dot{\mathbf{x}}_{\mathrm{m}}$ and $\dot{\mathbf{t}}_{\mathrm{m}}$) and two separate equations for $\dot{\mathbf{x}}_{\mathrm{m}}$ and $\dot{\mathbf{t}}_{\mathrm{m}}$.
- Force on each fiber expanded as a sum of Legendre polynomials:

$$\mathbf{f}_{\mathrm{m}} = \frac{1}{2}\mathbf{F}_{\mathrm{g}} + \sum_{n=1}^{N} \mathbf{a}_{\mathrm{m}}^{n} P_n(s)$$

where the coefficients $\mathbf{a}_{\mathrm{m}}^{n}$ are vectors with three components.

- N will be a parameter in our numerical algorithm.
- System of equations for the $\mathbf{f}_{\mathrm{m}}$'s yields a closed linear system of equations for the coefficients $\mathbf{a}_{\mathrm{m}}^{n}$, $n=1,\ldots,N$, $\mathrm{m}=1,\ldots,M$.
- The linear system is of size $3MN \times 3MN$.

System matrix for the force coefficients

- Let us write the system as $\mathbf{A}\bar{\mathbf{a}} = \bar{\mathbf{b}}$, where $\mathbf{A}$ and $\bar{\mathbf{b}}$ depends on all of $(\mathbf{x}_\mathrm{m}, \mathbf{t}_\mathrm{m}), \quad \mathrm{m} = 1, \ldots, M.$

$$\mathbf{A} = \begin{bmatrix} \mathbf{I} & \bar{\mathbf{A}}_{12} & \cdots & \bar{\mathbf{A}}_{1\mathrm{M}} \\ \bar{\mathbf{A}}_{21} & \mathbf{I} & \cdots & \bar{\mathbf{A}}_{2\mathrm{M}} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{\mathbf{A}}_{\mathrm{M}1} & \bar{\mathbf{A}}_{\mathrm{M}2} & \cdots & \mathbf{I} \end{bmatrix}$$

$\bar{\mathbf{A}}_{\mathrm{ml}}$ is the matrix $(3N \times 3N)$ for the contribution **to** the force coefficients for fiber m, **from** the force coefficients on fiber l.

- For each $\bar{\mathbf{A}}_{\mathrm{ml}}$ we need to compute N^2 3×3 matrices

$$\Theta_{\mathrm{lm}}^{kn} = \int_{-1}^{1} \left[\int_{-1}^{1} \mathbf{G}(\mathbf{R}(s,s')) \; P_k(s') \; ds' \right] P_n(s) \; ds, \; k,n = 1,2,\ldots N$$

- Inner integral evaluated analytically.
- Outer integral evaluated numerically with a Gauss quadrature.
- Similar for the right hand side.

Many-body problem! Time consuming!
Parallelization!

Parallelization and solving the system

- The code has been parallelized using MPI.
- Natural partitioning: A number of fibers assigned to each processor.
- For assembly of matrix and right hand side:

  Broadcast $\mathbf{x}_m$ and $\mathbf{t}_m$, $m = 1,\ldots,M$

  (6 degrees of freedom per fiber).
- All integrals

$$\Theta_{lm}^{kn} = \int_{-1}^{1}\left[\int_{-1}^{1}\mathbf{G}(\mathbf{R}(s,s'))\ P_k(s')\ \ ds'\right]P_n(s)\ \ ds$$

  can then be evaluated, for the fibers assigned.
- At end of assembly, subblocks of the matrix is communicated and collected on one processor.
- System solved with GMRES. Usually converges in 2-4 iterations.
- After solve, force coefficients are distributed ($3N$ degrees of freedom per fiber), and the velocities of the fibers are computed and their positions updated.

Fiber velocities and update of position

- Once the forces $\mathbf{f}_m$ are known:

  Determine translational and rotational velocities by evaluating

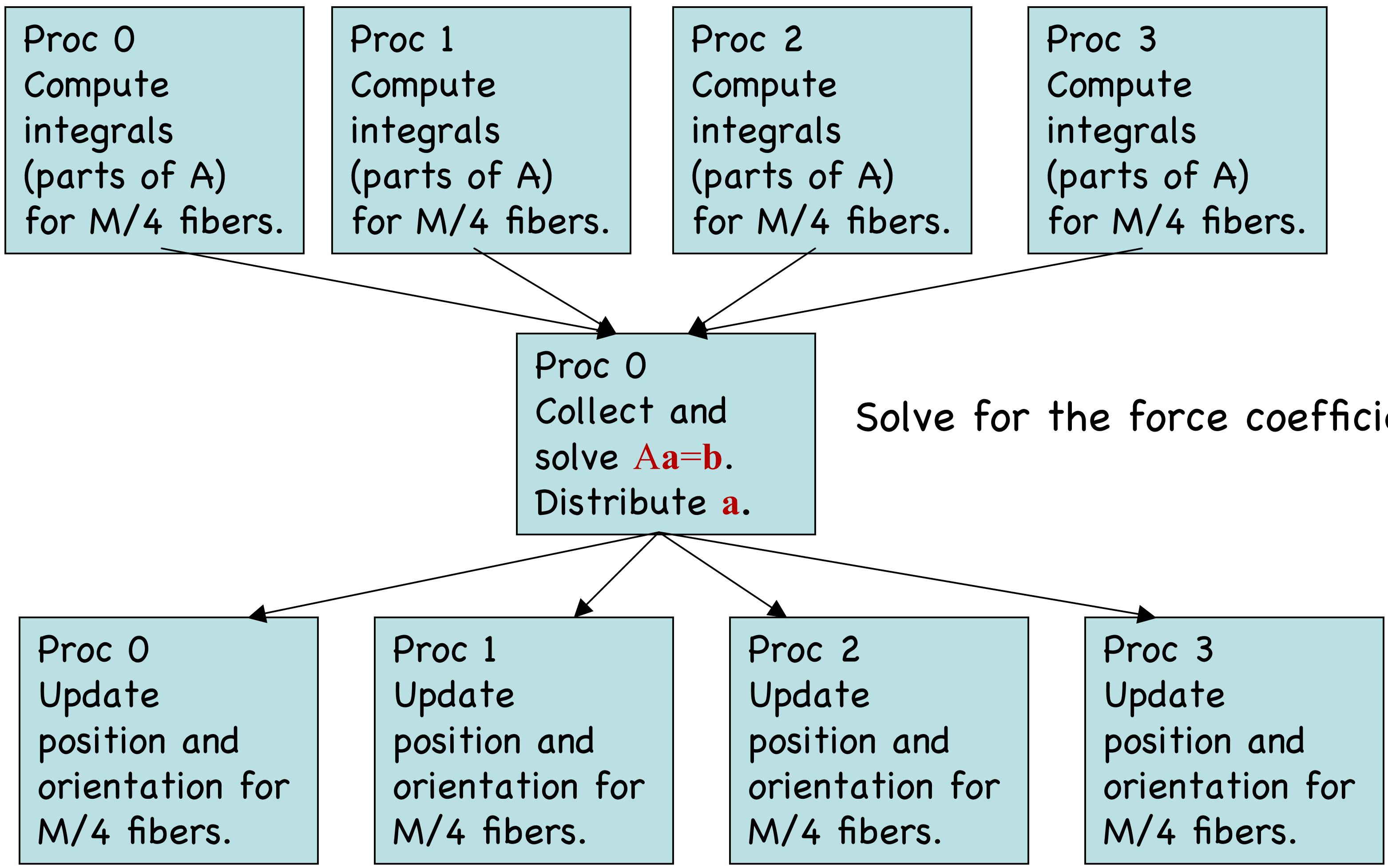
$$\dot{\mathbf{x}}_m = \frac{1}{2d}[d(\mathbf{I}+\mathbf{t}_m\mathbf{t}_m)+2(\mathbf{I}-\mathbf{t}_m\mathbf{t}_m)]\ \mathbf{F}_g + \frac{1}{d}\sum_{\substack{l=1,\\ l\neq m}}^{M}\int_{-1}^{1}\left[\int_{-1}^{1}\mathbf{G}(\mathbf{R}(s,s'))\ \mathbf{f}_l(s')\ \ ds'\right] ds$$

$$\dot{\mathbf{t}}_m = \frac{1}{d}\sum_{\substack{l=1\\ l\neq m}}^{M}\int_{-1}^{1}\left[\int_{-1}^{1}\mathbf{G}(\mathbf{R}(s,s'))\ \mathbf{f}_l(s')\ \ ds'\right] s\ \ ds$$

- ODEs for $\mathbf{x}_m$ and $\mathbf{t}_m$ discretized by second order multistep method.

Summary of algorithm

time step k $\mathbf{x}_m^k \quad \mathbf{t}_m^k \quad m = 1, 2, \ldots, M$



Solve for the force coefficients.

time step k+1 $\mathbf{x}_m^{k+1} \quad \mathbf{t}_m^{k+1} \quad m = 1, 2, \ldots, M$

Numerical experiments

- How can we analyze the results ?
- Accuracy assessment.
- Qualitative: Study the fibers/suspension as it proceeds in time – does it behave as expected ? (Compare in "eye-norm").
- Quantitative: Look at averaged quantities such as mean velocity, concentration and average orientation. (Compare numbers and trends.)
- Compare to available experimental findings.

Gustavsson & Tornberg, JCP 2006, PoF 2010

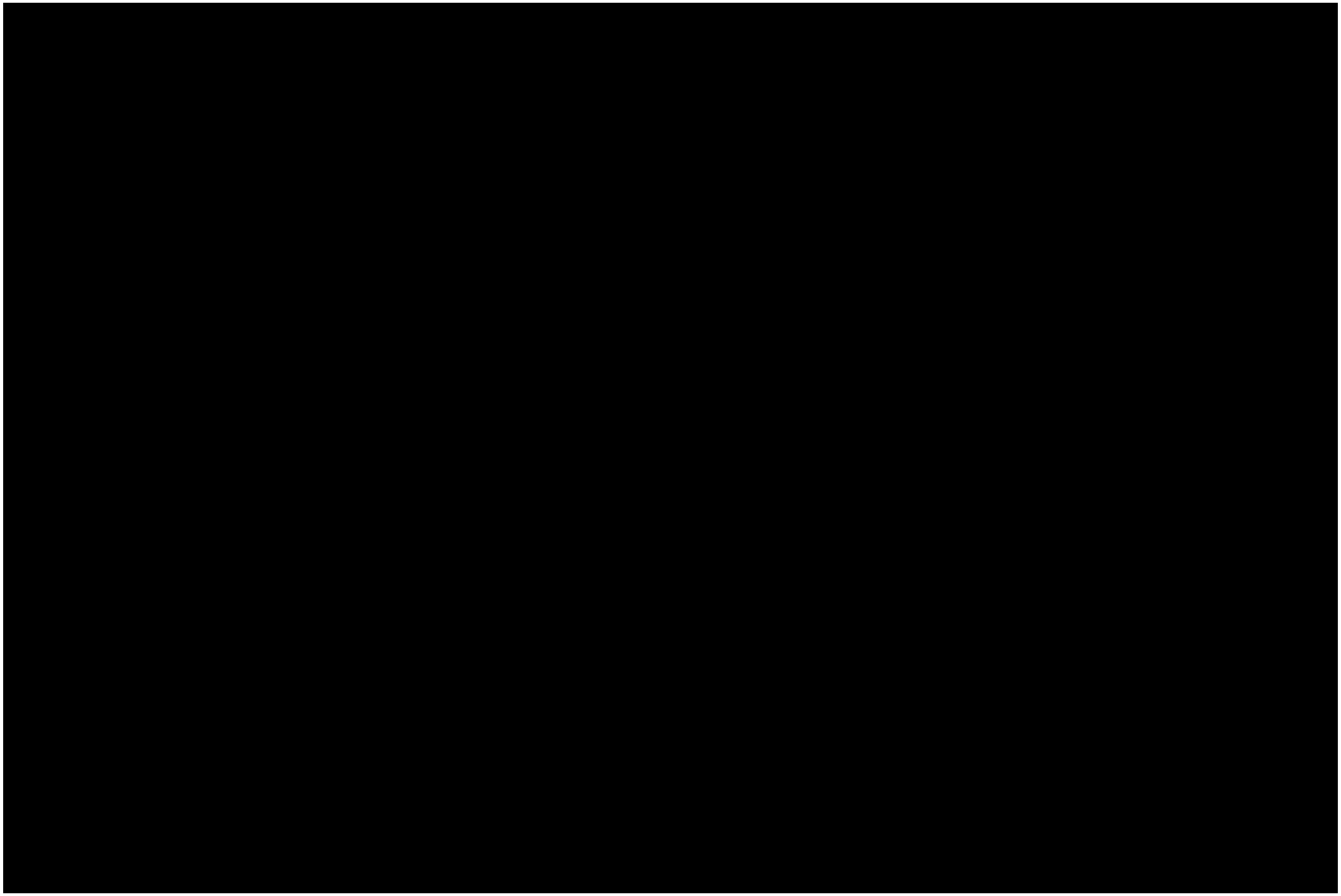
Numerical parameters

- Slenderness parameter: $\varepsilon = 0.01$
- Number of terms in force expansion: $N = 5$
- Number of quadrature points: $Nq = 24 \rightarrow 96$ (depends on distance between fibers).
- Timestep: $\Delta t = 0.05$
- Number of timesteps: 10 000 (typically)
- 800 fibers took approx. 1600 cpu-hours. (Run on 40 processors - 40 h)

Known from physical experiments

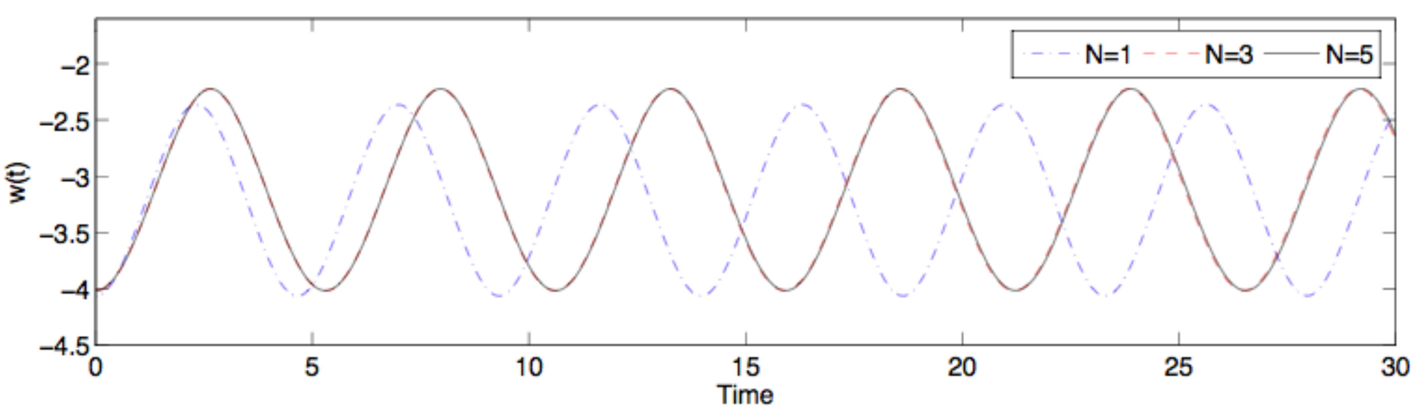
- Few or single fibers:
  - A vertically aligned fiber has twice the velocity of a horizontal fiber.
  - Tumbling orbits (repetitive cycles).
- Suspension of fibers:
  - Fibers form clusters (many fibers close to each other).
  - The clusters sediment faster than single fibers.
  - The mean sedimentation velocity is larger than the velocity of a single vertically aligned fiber (w=1).
  - Mean sedimentation velocity increases with concentration of fibers.
  - The fibers tend to align with gravity.

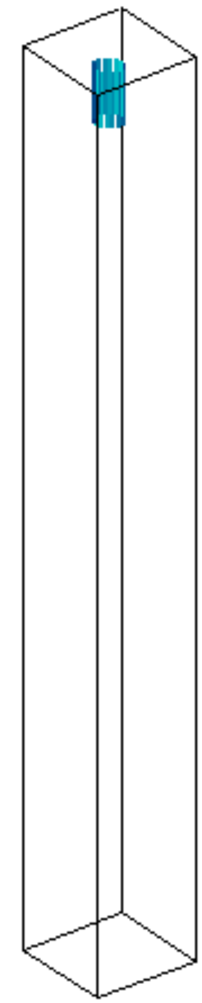
Tumbling orbits - the movie 1



Tumbling orbits – the movie 2

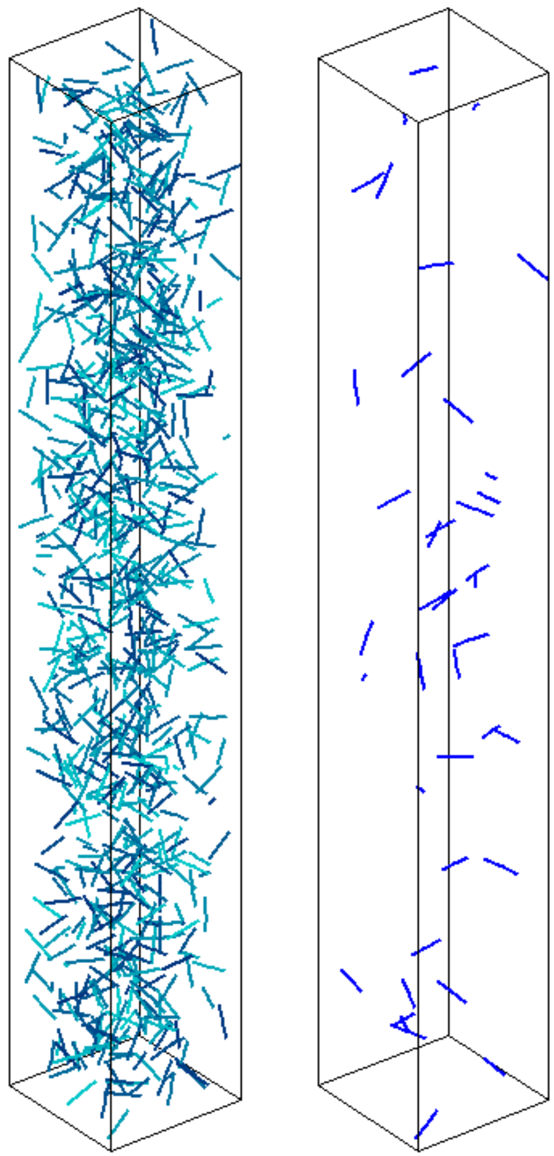
- 16 fibers arranged in a symmetric pattern
- Perform a repetitive tumbling orbit
- $|w_{max}|$ when fibers are vertically aligned
- $|w_{min}|$ when fibers are horizontal
- Solution depend on N (number of terms in force expansion)





Sedimenting suspension

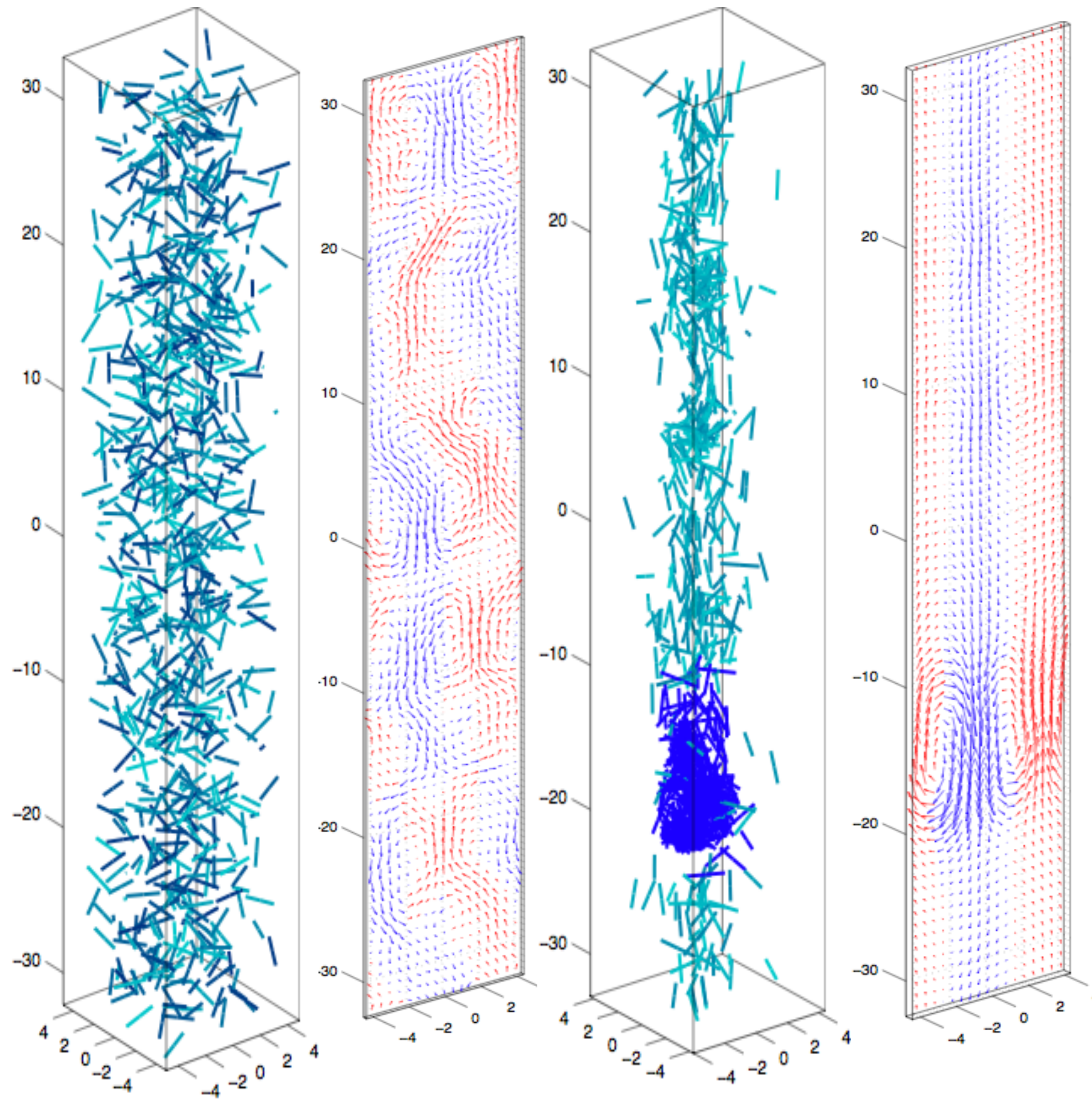
- Sedimentation of 800 fibers in a box of size $4L_f \times 4L_f \times 32L_f$ (L_f length of fibers).
- Gravity in negative z-direction.
- Periodic boundary conditions.
- Initial random distribution of fibers.
- Experimental findings *:
  - Fibers form streamers of fiber dense domains
  - Fibers form clusters
  - Fibers continuously entering and leaving clusters
  - Cluster sediments faster than single fibers
  - Fibers align with gravity
  - Cluster creates a backflow in the fluid - single fibers move upwards
  - Mean sedimentation velocity can exceed the velocity of a single vertically aligned fiber (w=1)



* Herzhaft et al. (1999), Metzger et al. (2007)

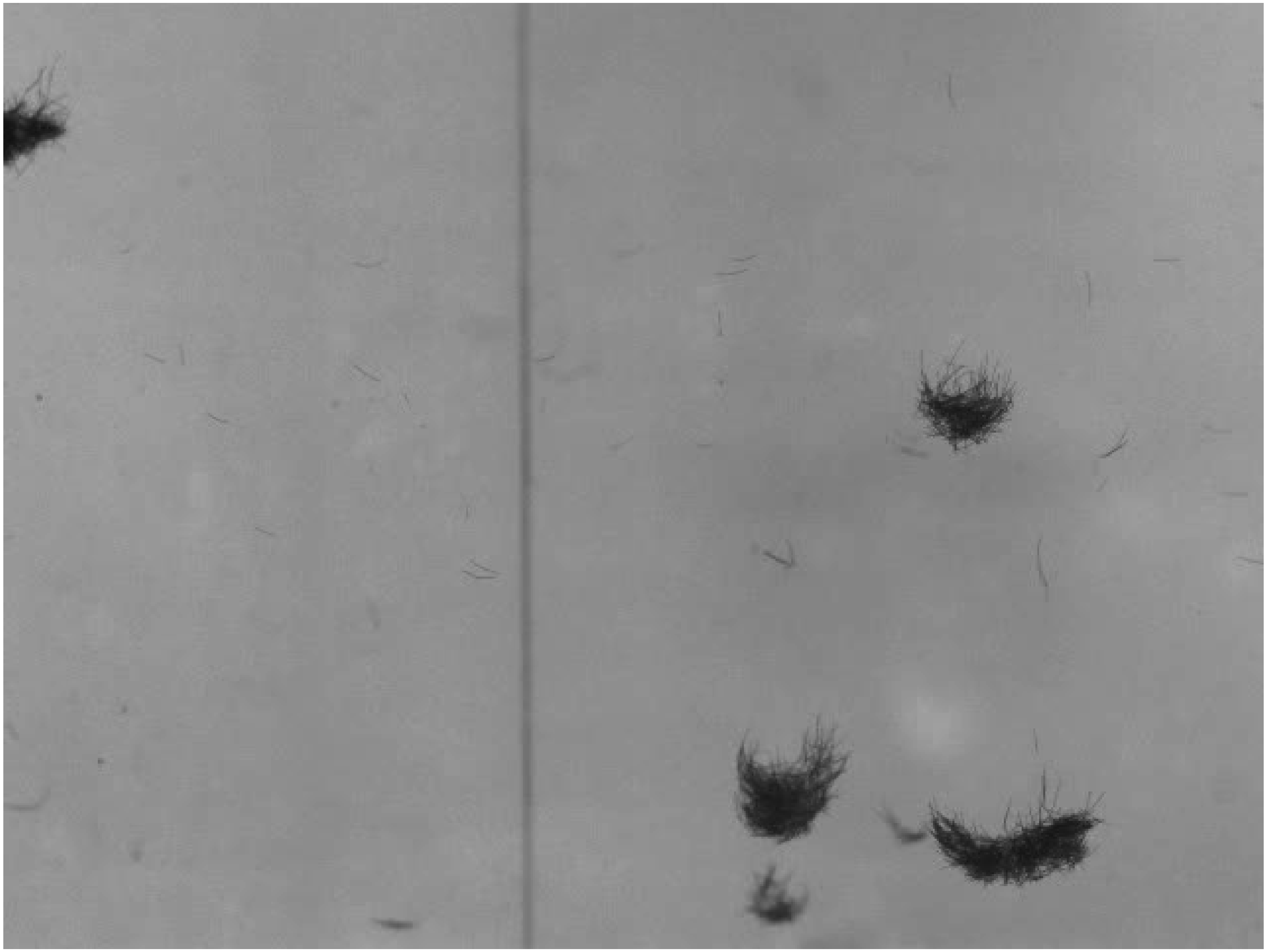
Fluid velocity

- Fluid velocity can be obtained by post processing
- At initial time: Up and downward flow with small recirculation zones
- At later time: Strong backflow in region with clear fluid and larger recirculation zone



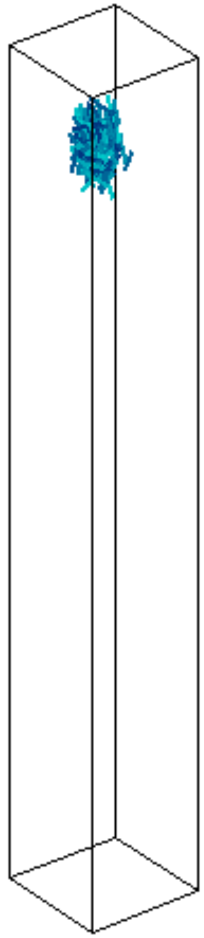
Note: different scaling of arrows

Clusters - the movie 1

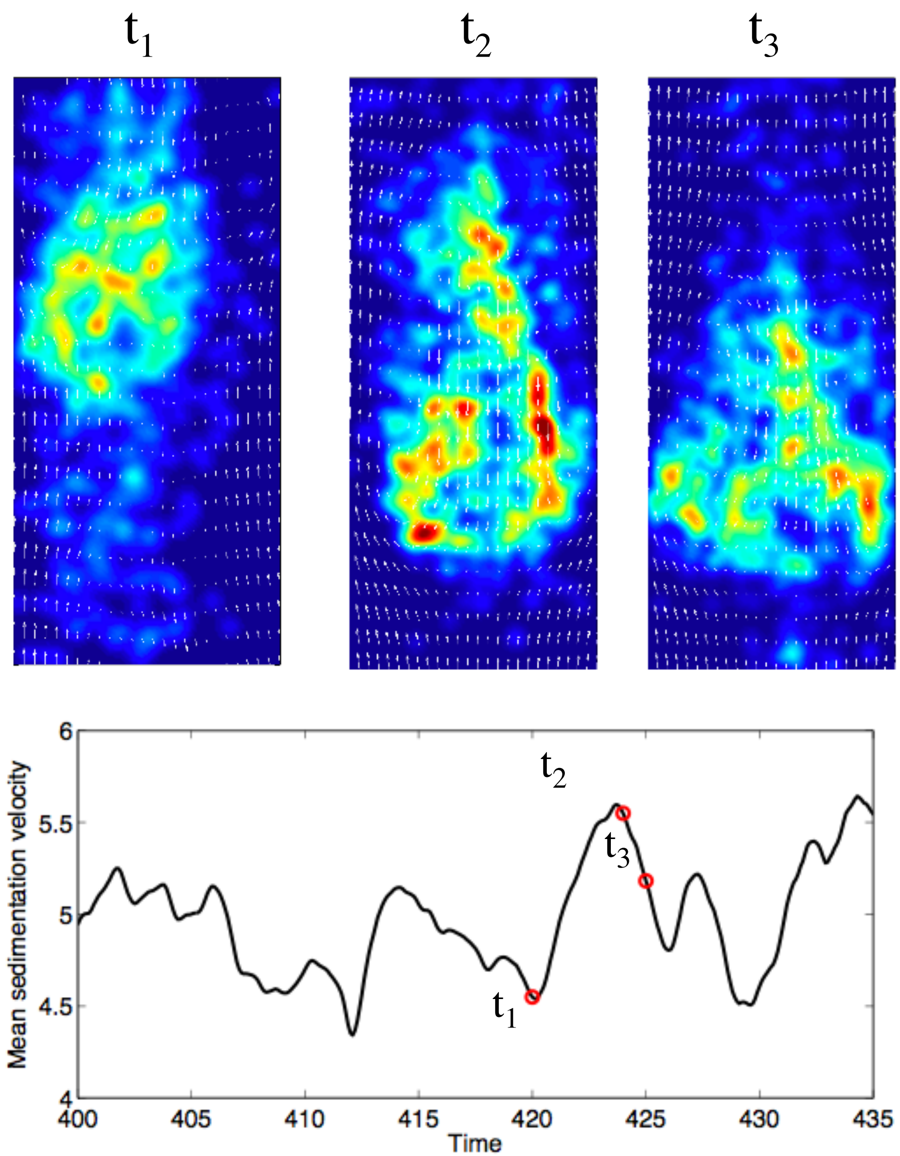


Clusters - the movie 2

- Visualization of a cluster (155/800 fibers)
- Fibers are leaving and entering the cluster
- Fibers in the rear end of the cluster are vertically aligned
- Fibers in outer region of the cluster will detach due to strong backflow in the fluid (recirculation zones)



Repetitive cycle of a cluster



- Repetitive cycle
- Densification phase (t1->t2)

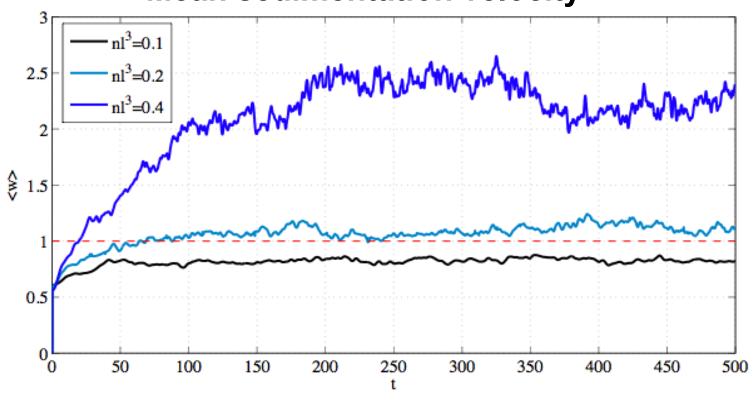
  Fiber "collecting". Cluster density and mean sedimentation velocity increases.
- Coarsening phase (t2->t3)

  Cluster expands and fibers detach. Cluster density and sedimentation velocity decreases.
- Correlation to mean velocity fluctuations

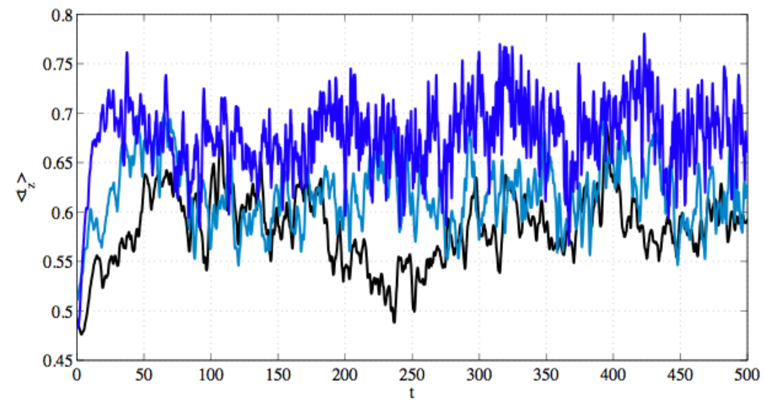
Sedimentation velocity

- Sedimentation velocity and mean vertical orientation depend on concentration
- Time to steady state depend on concentration

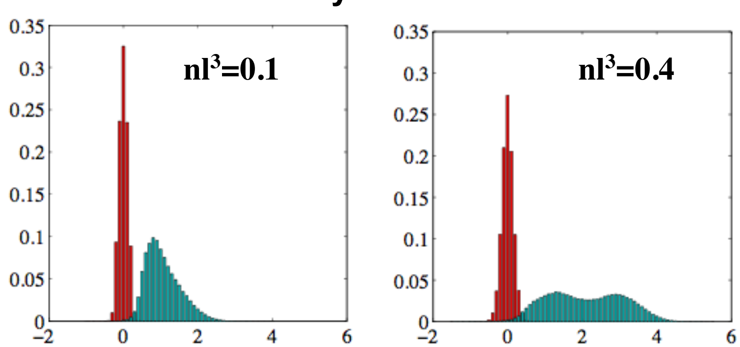
Mean sedimentation velocity



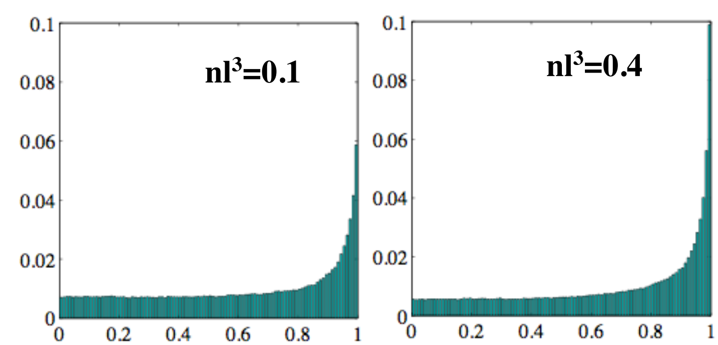
Mean vertical orientation



Velocity distribution

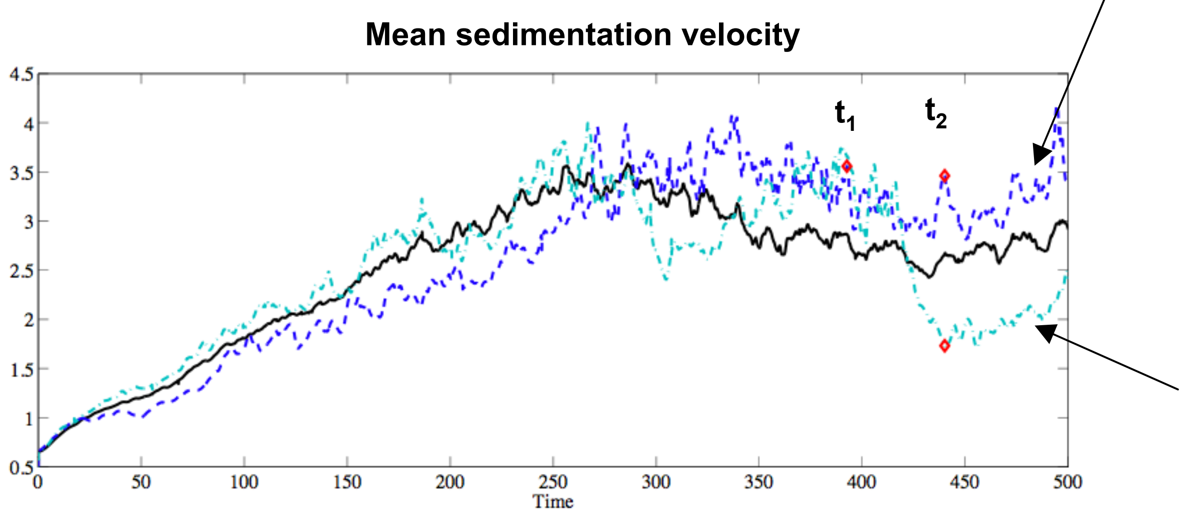


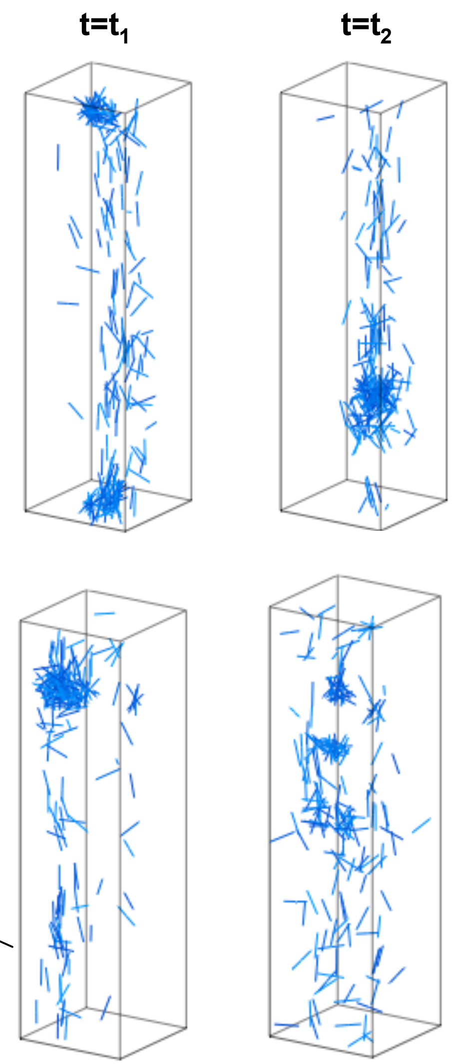
Vertical orientation distribution



Local vs. global effects

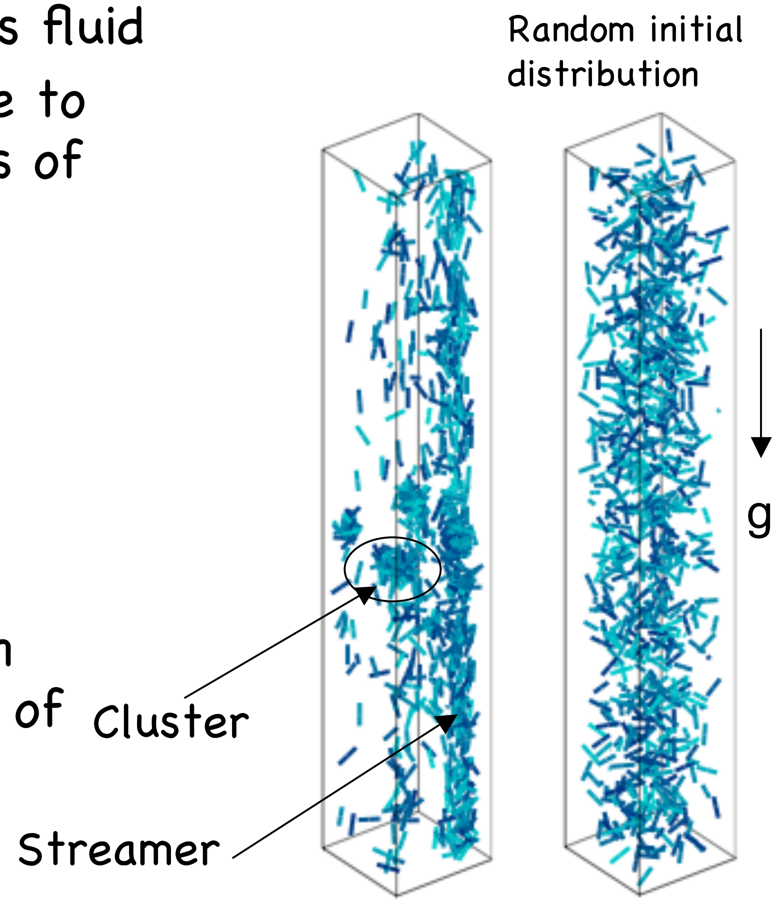
- Same macroscopic properties:
  - Same number of fibers
  - Same size of box
- Different initial random distribution
- Large differences in dynamical behavior on local scale
- Reflected in global quantities





Summary

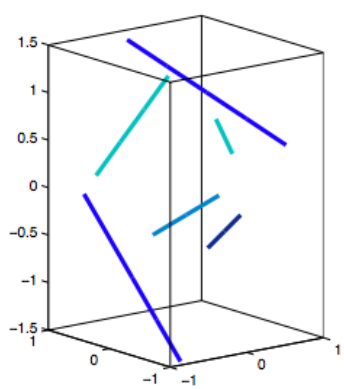
- We have used boundary integrals and the slender body approximation to compute the sedimentation of rigid fibers in a viscous fluid
- Using numerical simulations we are able to reproduce many characteristic features of sedimenting fibers/fiber suspension
  - Velocity depend on fiber orientation
  - Creation of clusters
  - Strong backflow in the fluid
  - Sedimentation velocity depend on concentration
  - Global quantities (e.g. sedimentation velocity) depend on local properties of the suspension

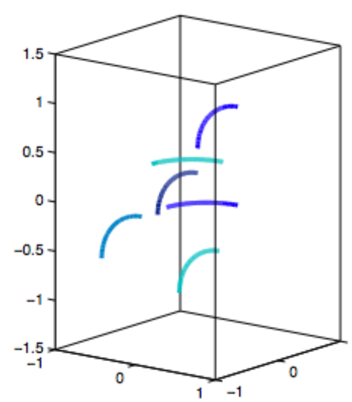


Simulations show good agreement to experimental data both on local and global levels

Future and ongoing work

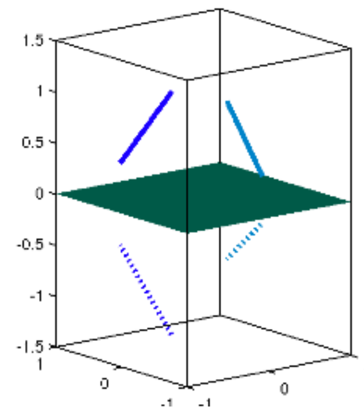
- Today all fibers are straight and of same length.
- Extend model and numerical algorithm to (w. Jennifer Grünig, PhD stud.):
  - Multi-disperse fiber suspensions.
  - Non-straight rigid fiber suspension.
- Motivation
  - Fibers in paper pulp.
  - Other kind of suspensions: micro organisms, bacteria.

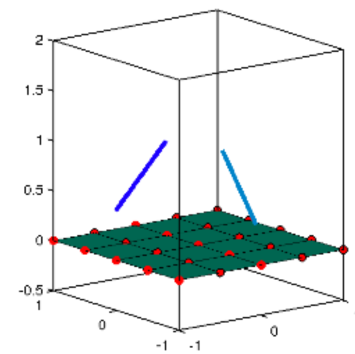


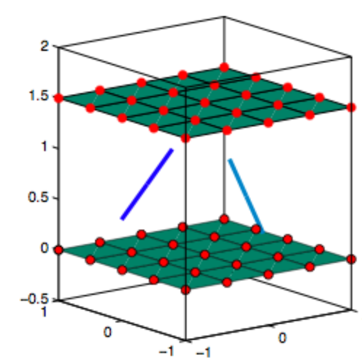


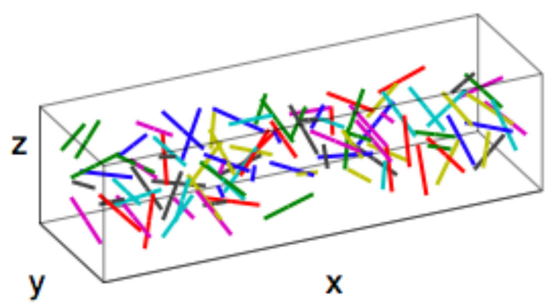
Future and ongoing work

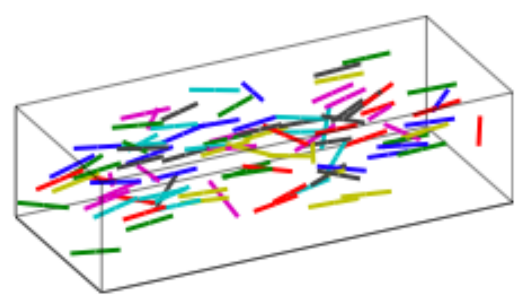
- Investigate different ideas/methods for handling wall boundary conditions in a boundary integral setting (w. Oana Marin, PhD stud.)
  - Method of images/reflextions
  - Direct discretization using a distribution of point forces
  - Combine boundary integral methods with grid based methods (future)
- Motivation
  - Wall bounded sedimentation yield more realistic simulations (compared to experimental set-up)
  - Particle - wall interactions
  - Suspensions in shear flow











Future and necessary work

- In order to include more (in the order of 10 times more) we need faster
  - Methods (fast multipole)
  - Algorithms (better parallelization)