Large scale simulations of gravity induced sedimentation of slender fibers

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Simulations of rigid fibers
“Fibers in Waterland”

- 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
  - Weaken the paper in the other direction.
- “Clusters” or “flocs” of fibers form.
  - Creates uneven thickness and roughness.

800 fibers sedimenting due to gravity (initial random distribution).
Right plot: showing 40 of these.
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 $\mu$.
- 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

\[ \rho \left( u_t + (u \cdot \nabla)u \right) = -\nabla p + \mu \nabla^2 u + f \]

Convective term
Viscous term

\[ \nabla \cdot u = 0 \]

• 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

\[ \text{Re} = \frac{\rho UL}{\mu} \ll 1 \]

• Neglect convective terms.

Stokes equations

Reynolds number: relation between convective and viscous terms

velocity
pressure
force
density
viscosity
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:
  \[ \mathbf{u} = \mathbf{u}_{\partial \Omega} \text{ on } \partial \Omega, \quad \mathbf{u} \to 0 \text{ for } x \to \infty \]
- No explicit time-dependence in equation. Time-dependent system due to motion of immersed objects.
- No inertia. 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 singularly forced Stokes equation
\[ \nabla p - \mu \Delta u = g \delta(x - y) \]
has the solution
\[ u_i(x) = \frac{1}{8\pi \mu} S_{ij}(x,y)g_j \]
\[ (S_{ij}g_j = S_{i1}g_1 + S_{i2}g_2 + S_{i3}g_3) \]
where
\[ S_{ij}(x,y) = \frac{\delta_{ij}}{|x - y|} + \frac{(x - y_i)(x - y_j)}{|x - y|^3}, \quad i, j = 1, 2, 3. \]

\( S_{ij} \) 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

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

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 $f$. 
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 \( w_i \).

\[
\begin{align*}
  u_k &= \sum_{i=1}^{N} w_i K(s_k, t_i) f_i, \quad k = 1, 2, \ldots, N \\
  u_1 &= w_1 K(s_1, t_1) f_1 + w_2 K(s_1, t_2) f_2 + \cdots + w_N K(s_1, t_N) f_N \\
  u_2 &= w_1 K(s_2, t_1) f_1 + w_2 K(s_2, t_2) f_2 + \cdots + w_N K(s_2, t_N) f_N \\
  \vdots \\
  u_N &= w_1 K(s_N, t_1) f_1 + w_2 K(s_N, t_2) f_2 + \cdots + w_N K(s_N, t_N) f_N 
\end{align*}
\]

This will yield a linear system of equations (N\times N) to be solved for \( f \)

\[ Af = u \]
Boundary integral equations, cont.

- For Stokes equation we have that

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

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 unknown?
- We know the externally applied force (gravity).
- The object is centered at $x_c$ with an associated orthonormal basis $t$ and surface $\partial \Omega$.
- Rigid body motion and no-slip, i.e., for $x \in \partial \Omega$, 
  $$u(x) = U + \omega \times (x - x_c)$$
  with translational velocity $U$ and angular velocity $\omega$.
- 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:

\[
U_i + (\omega \times (x - x_c))_i = \frac{1}{8\pi \mu} \int_{\partial \Omega} S_{ij}(x, y) f_j(y) \ dS_y, \quad i = 1, 2, 3 \quad (1)
\]

together with the constraints

\[
\mathbf{F}_{\text{body}} = \int_{\partial \Omega} f(y) \ dS_y, \quad \mathbf{T}_{\text{body}} = \int_{\partial \Omega} (x - x_c) \times f(y) \ dS_y. \quad (2)
\]

• Solve the system of BIE, (1)-(2), for \(f(x), U\) and \(\omega\)

• Update the position of the bodies by

\[
\frac{d}{dt} x_c = U, \quad \frac{d}{dt} t = t \times \omega
\]

• The velocity field can be computed in any point \(x\) by

\[
u_i(x) = \frac{1}{8\pi \mu} \int_{\partial \Omega} S_{ij}(x, y) f_j(y) \ dS_y
\]

(as a post-processing step)
Many immersed objects in Stokes flow

- $M$ immersed solid objects.
- Body $m, \ m = 1, \ldots \ M$ centered at $x^m_c$ with an associated orthonormal basis $t^m$ and surface $\partial \Omega^m$.
- As before, rigid body motion and no-slip, i.e. for $x \in \partial \Omega^m$
  
  $u(x) = U^m + \omega^m \times (x - x^m_c)$

  with translational velocity $U^m$
  and angular velocity $\omega^m$.
- 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

\[
U^m_i + (\omega^m \times (x - x^m_c))_i = \frac{1}{8\pi\mu} \sum_{l=1}^{M} \int_{\partial\Omega_i} S_{ij}(x,y)f^l_j(y) \, dS_y, \tag{1}
\]

together with the constraints

\[
F^m_{\text{body}} = \int_{\partial\Omega_m} f^m(y) \, dS_y \quad T^m_{\text{body}} = \int_{\partial\Omega_m} (x - x^m_c) \times f^m(y) \, dS_y. \tag{2}
\]

As before, solve (1)–(2) for \(f^m(x), \ U^m\) and \(\omega^m\), \(m = 1, \ldots, M\) and update the position of the bodies by

\[
\frac{d}{dt} x^m = U^m, \quad \frac{d}{dt} t^m = t^m \times \omega^m
\]

The velocity field can be computed in any point \(x\) by

\[
u_i(x) = \frac{1}{8\pi\mu} \sum_{l=1}^{M} \int_{\partial\Omega_i} S_{ij}(x,y)f^l_j(y) \, dS_y
\]

(as a post-processing stage)
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.
  \[ \varepsilon = \frac{a}{2L} << 1 \]
- To expensive to discretize and solve numerically for slender fibers.
- Do an asymptotic expansions in the slenderness parameter.

Slender body equations
Slender body approximation

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):

\[
\dot{x}_m + st_m = L(t_m) f_m(s) + (I + t_m t_m) \bar{K} f_m(s)
\]

(1)

- Velocity of fiber m

- Local contribution

- Global contribution

- Contribution from other fibers

\[
R(s,s') = x_m + st_m - (x_l + s't_l)
\]

- G is a linear combination of two fundamental solutions:

\[
G(R) = S(R) + \varepsilon^2 D(R)
\]

- 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

\[
\begin{align*}
F_m &= \int_{-1}^{1} f_m(s) \, ds = F_g, \\
M_m &= \int_{-1}^{1} s \left( t_m \times f_m(s) \right) \, ds = 0
\end{align*}
\]

(2), (3)

System closed. Equations (1)-(3) solves our problem!
Summary of mathematical model

- Velocity of fiber $m$ given by:

\[
\dot{x}_m + s \dot{t}_m = L(t_m) f_m(s) + (I + t_m t_m) \bar{K} \left[ f_m \right](s) + \sum_{l=1}^{M} \int_{s'}^{1} G(R(s,s')) f_l(s') \, ds'.
\]  

(1)

\[
R(s,s') = x_m + s t_m - (x_l + s' t_l)
\]

- Two extra conditions for fiber $m$:

\[
F_m = \int_{-1}^{1} f_m(s) \, ds = F_g, \quad M_m = \int_{-1}^{1} s (t_m \times f_m(s)) \, ds = 0
\]

(2), (3)

Equations (1)-(3) for $m=1, 2, \ldots, M$.

3M unknowns: $\dot{x}_m, \dot{t}_m, f_m$

How do we solve these equations?
Numerical discretization

- Manipulations of equations (1)-(3) leads to a closed system for the forces \( f_m \) (without \( \dot{x}_m \) and \( \dot{t}_m \)) and two separate equations for \( \ddot{x}_m \) and \( \ddot{t}_m \).
- Force on each fiber expanded as a sum of Legendre polynomials:
  \[
  f_m = \frac{1}{2} F_g + \sum_{n=1}^{N} a_m^n P_n(s)
  \]
  where the coefficients \( a_m^n \) are vectors with three components.
- \( N \) will be a parameter in our numerical algorithm.
- System of equations for the \( f_m \)'s yields a closed linear system of equations for the coefficients \( a_m^n, \ n=1,\ldots,N, \ m=1,\ldots,M \).
- The linear system is of size \( 3MN \times 3MN \).
System matrix for the force coefficients

• Let us write the system as $A\bar{a} = \bar{b}$, where $A$ and $\bar{b}$ depends on all of $(x_m, t_m)$, $m = 1, \ldots, M$.

$$A = \begin{bmatrix}
I & \bar{A}_{12} & \ldots & \bar{A}_{1M} \\
\bar{A}_{21} & I & \ldots & \bar{A}_{2M} \\
\vdots & \vdots & \ddots & \vdots \\
\bar{A}_{M1} & \bar{A}_{M2} & \ldots & I
\end{bmatrix}$$

$A_{ml}$ 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 $A_{ml}$ we need to compute $N^2$ $3 \times 3$ matrices

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

• 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 $x_m$ and $t_m$, $m = 1, \ldots, M$
  - (6 degrees of freedom per fiber).
- All integrals
  \[
  \Theta_{\text{im}}^{kn} = \int_{-1}^{1} \int_{-1}^{1} G(R(s,s')) P_k(s') \, ds' \int_{-1}^{1} P_n(s) \, ds
  \]
  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 $f_m$ are known:
  
  Determine translational and rotational velocities by evaluating

  $\dot{x}_m = \frac{1}{2d} \left[ d(I + t_m t_m) + 2(I - t_m t_m) \right] F_g + \frac{1}{d} \sum_{l=1, l \neq m}^{M} \int_{-1}^{1} \int_{-1}^{1} G(R(s,s')) f_l(s') \, ds' \, ds$

  $\dot{t}_m = \frac{1}{d} \sum_{l=1}^{M} \int_{-1}^{1} \int_{-1}^{1} G(R(s,s')) f_l(s') \, ds' \, ds$

- ODEs for $x_m$ and $t_m$ discretized by second order multistep method.
Summary of algorithm

time step $k$

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

Proc 0
Compute integrals (parts of A) for $M/4$ fibers.

Proc 1
Compute integrals (parts of A) for $M/4$ fibers.

Proc 2
Compute integrals (parts of A) for $M/4$ fibers.

Proc 3
Compute integrals (parts of A) for $M/4$ fibers.

Proc 0
Collect and solve $\mathbf{Aa} = \mathbf{b}$. Distribute $\mathbf{a}$.

Solve for the force coefficients.

Proc 0
Update position and orientation for $M/4$ fibers.

Proc 1
Update position and orientation for $M/4$ fibers.

Proc 2
Update position and orientation for $M/4$ fibers.

Proc 3
Update position and orientation for $M/4$ fibers.

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
- $|w_{\text{max}}|$ when fibers are vertically aligned
- $|w_{\text{min}}|$ 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 ($t_1 \rightarrow t_2$)
  Fiber “collecting”. Cluster density and mean sedimentation velocity increases.
- Coarsening phase ($t_2 \rightarrow t_3$)
  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](image)

![Mean vertical orientation](image)

![Velocity distribution](image)

![Vertical orientation distribution](image)
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

Mean sedimentation velocity

\[ t = t_1 \]

\[ t = t_2 \]
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/reflections
  • 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)