

# Immersed boundary simulations of gravitational settling

**John Stockie**

Department of Mathematics  
Simon Fraser University  
Burnaby, British Columbia, Canada

<http://www.math.sfu.ca/~stockie>

MIT Conference on Computational Fluid and Solid Mechanics

June 12, 2013

# Acknowledgments

Sudeshna Ghosh



Funding



Natural Sciences and Engineering  
Research Council of Canada

# Outline

- 1 Gravitational settling
  - Analytical solutions
  - Experimental results
  - Numerical simulations
- 2 Immersed boundaries with mass
  - Mathematical formulation
  - Immersed boundary method
- 3 Simulations of settling cylinders
  - Single particle
  - Two particles and draft–kiss–tumble dynamics
- 4 Conclusions

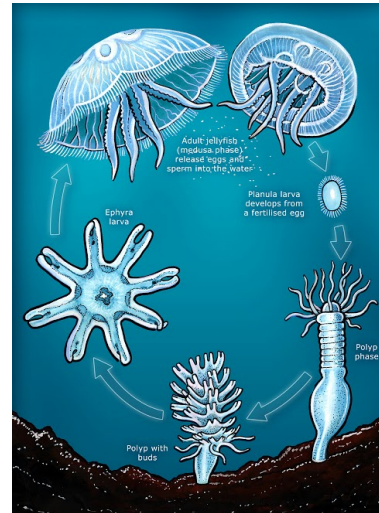
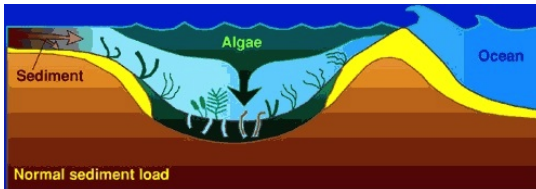
# Outline

- 1 Gravitational settling
  - Analytical solutions
  - Experimental results
  - Numerical simulations
- 2 Immersed boundaries with mass
  - Mathematical formulation
  - Immersed boundary method
- 3 Simulations of settling cylinders
  - Single particle
  - Two particles and draft–kiss–tumble dynamics
- 4 Conclusions

# Motivation: Sedimentation in applications

**Sedimentation** is the settling of particles under the influence of gravity:

- Biofilm dynamics.
- Marine organisms: algae, jellyfish.
- Industrial processes: wood pulp fibers, crystal precipitation, mine tailings.
- Natural phenomena: hailstorms, sediment transport in rivers and lakes.
- Tea leaves in a teacup.



# Previous work on sedimentation

Gravitational settling of particle suspensions has been studied **extensively** in the literature using

- mathematical analysis,
- experiments,
- numerical simulations.

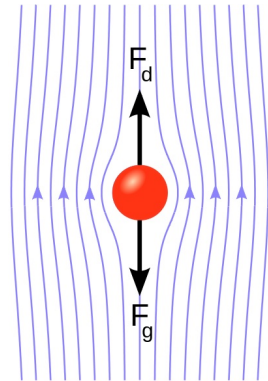
# Analytical solutions

- **Stokes' law (1851)**: in a creeping flow of infinite extent, balancing gravity and drag forces yields settling velocity for a sphere in 3D:

$$V_s = \frac{gD^2(\rho_p - \rho_f)}{18\mu}$$

where  $D$  = diameter,  $\mu$  = viscosity.

- Analogous result can be derived for a 2D circular particle (infinite cylinder)  $\implies$  a nonlinear equation in  $V_s$ .
- An overview of more recent analytical results can be found in **Guazzelli & Morris (2012)**.



Source: Wikipedia.

# Experimental results

- An enormous experimental literature exists owing to the importance of sedimentation in industrial and other applications.  
[Davis & Acrivos, 1985]
- Of particular interest to us are estimates of **wall-corrected settling velocity** for a particle in a channel of width  $W$ :

$$\tilde{V}_s = \frac{V_s}{\lambda(k)} \quad \text{where} \quad k = \frac{D}{W}$$

and  $\lambda(k)$  is a fitted correction factor.

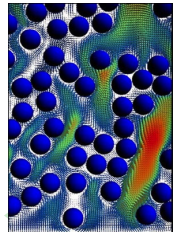
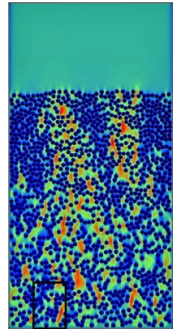
- For example, Faxén's (1946) experiments yield

$$\lambda(k) \approx \frac{-4\pi}{0.9157 + \ln(k) - 1.724k^2 + 1.730k^4 - 2.406k^6 + 4.591k^8}$$



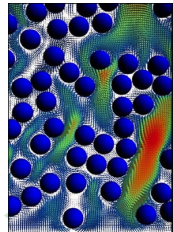
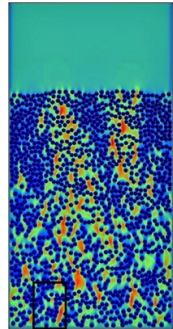
# Numerical simulations

- Many authors have simulated 2D and 3D suspension flows numerically using:
  - finite element method,
  - lattice-Boltzmann method,
  - boundary element method,
  - ...
- IB method has been applied to gravitational settling of
  - rigid fibers [Wang & Layton, 2009]
  - suspensions of swimming algal cells [Hopkins & Fauci, 2002]
- Direct-forcing IB approach has also been applied to sedimentation [Uhlmann, 2005] [Wang, Fan & Luo, 2008] [Breugem, 2012]
- However, there has not yet been an extensive validation of the IB method for particulate flows **with settling**.



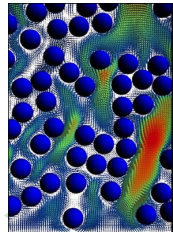
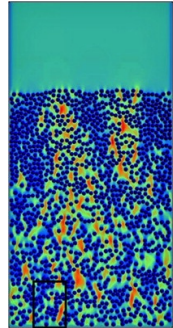
# Numerical simulations

- Many authors have simulated 2D and 3D suspension flows numerically using:
  - finite element method,
  - lattice-Boltzmann method,
  - boundary element method,
  - ...
- IB method has been applied to gravitational settling of
  - rigid fibers [Wang & Layton, 2009]
  - suspensions of swimming algal cells [Hopkins & Fauci, 2002]
- Direct-forcing IB approach has also been applied to sedimentation [Uhlmann, 2005] [Wang, Fan & Luo, 2008] [Breugem, 2012]
- However, there has not yet been an extensive validation of the IB method for particulate flows **with settling**.



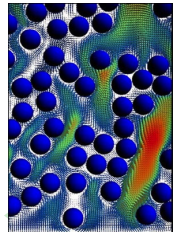
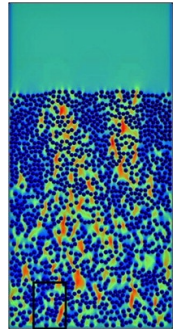
# Numerical simulations

- Many authors have simulated 2D and 3D suspension flows numerically using:
  - finite element method,
  - lattice-Boltzmann method,
  - boundary element method,
  - ...
- IB method has been applied to gravitational settling of
  - rigid fibers [Wang & Layton, 2009]
  - suspensions of swimming algal cells [Hopkins & Fauci, 2002]
- Direct-forcing IB approach has also been applied to sedimentation [Uhlmann, 2005] [Wang, Fan & Luo, 2008] [Breugem, 2012]
- However, there has not yet been an extensive validation of the IB method for particulate flows **with settling**.



# Numerical simulations

- Many authors have simulated 2D and 3D suspension flows numerically using:
  - finite element method,
  - lattice-Boltzmann method,
  - boundary element method,
  - ...
- IB method has been applied to gravitational settling of
  - rigid fibers [Wang & Layton, 2009]
  - suspensions of swimming algal cells [Hopkins & Fauci, 2002] ← basis for our approach!
- Direct-forcing IB approach has also been applied to sedimentation [Uhlmann, 2005] [Wang, Fan & Luo, 2008] [Breugem, 2012]
- However, there has not yet been an extensive validation of the IB method for particulate flows **with settling**.



# Aims of this study

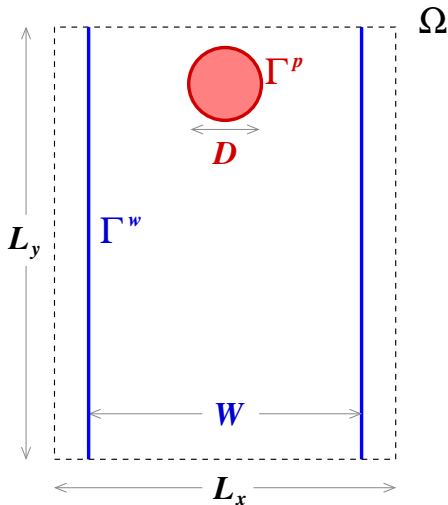
- Sedimentation is very well-studied for rigid particles such as spheres, ellipsoids, fibers, . . .
- For simplicity, we consider spherical particles that are only slightly heavier than the suspending fluid:  $\frac{\rho_p - \rho_f}{\rho_f} \ll 1$ .
- We develop a very general numerical approach and validate it using results for rigid particles.
- Our long-term aim is to simulate sedimentation of both rigid and **deformable** particles. Hence, the need for the IB method!

# Outline

- 1 Gravitational settling
  - Analytical solutions
  - Experimental results
  - Numerical simulations
- 2 Immersed boundaries with mass
  - Mathematical formulation
  - Immersed boundary method
- 3 Simulations of settling cylinders
  - Single particle
  - Two particles and draft–kiss–tumble dynamics
- 4 Conclusions

# Problem geometry

- $\Gamma^p$ : Particle, diameter  $D$   
 $\Gamma^w$ : Walls, separated by  $W$   
 $\Omega$ : Fluid domain, size  $L_x \times L_y$   
Periodic boundary conditions



# Governing equations

**Variables:**  $\mathbf{u}(\mathbf{x}, t)$  = velocity,  $p(\mathbf{x}, t)$  = pressure,  $\mathbf{X}(s, t)$  = IB position

**Parameters:**  $\rho_f$  = fluid density,  $\rho_p$  = particle density,  $\mu$  = viscosity

**Incompressible Navier-Stokes equations:** (Boussinesq approximation,  $\rho_p \gtrsim \rho_f$ )

$$\rho_f \frac{\partial \mathbf{u}}{\partial t} + \rho_f \mathbf{u} \cdot \nabla \mathbf{u} = \mu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f}_{IB} + \mathbf{f}_G$$

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

**IB evolution equation:**

$$\frac{\partial \mathbf{X}}{\partial t} = \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) d\mathbf{x}$$

**IB elastic force:**

$$\mathbf{f}_{IB}(\mathbf{x}, t) = \int_{\Gamma^{w,p}} \mathbf{F}_{IB}(s, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) ds$$

(specify discrete  $\mathbf{F}_{IB}$  later)

**Gravitational settling term:**

$$\mathbf{f}_G(\mathbf{x}, t) = - \begin{bmatrix} 0 \\ \mathbf{g} \end{bmatrix} \int_{\Gamma^p} (\rho_p - \rho_f) \delta(\mathbf{x} - \mathbf{X}(s, t)) ds$$



# Immersed boundary method

We apply a straightforward discretization of the IB problem using:

- centered finite differences in space,
- cosine approximation for delta function,
- ADI for diffusion and advection terms,
- explicit treatment of IB force and settling terms,
- split-step projection scheme, with an FFT solve for the pressure Poisson equation.

Details are in [Ghosh & JS \[arxiv:1304.0804, 2013\]](#).

# Discrete IB force for the walls

- The stationary walls are divided into  $N_w$  equally-spaced **tether points** with fixed locations

$$\mathbf{Y}_\ell^w = \left[ (L_x \pm W)/2, \ell L_y / N_w \right] \quad \text{for } \ell = 1, 2, \dots, N_w$$

- Each wall IB point  $\mathbf{X}_\ell(t)$  is connected to the corresponding tether point by a stiff spring with force density

$$\mathbf{F}_\ell^w(t) = \sigma_w (\mathbf{Y}_\ell^w - \mathbf{X}_\ell(t))$$

- The force integral approximation involves a **length scaling factor**:

$$\mathbf{f}_{i,j} = \sum_{\ell=1}^{N_w} \mathbf{F}_\ell^w \delta_h(\mathbf{x}_{i,j} - \mathbf{X}_\ell) \frac{L_y}{N_w}$$

# Discrete IB force for the particle

- “Uniform” triangulation of particle with nodes  $\mathbf{X}_\ell(t)$  for  $\ell = 1, 2, \dots, N_p$ .
- Following Alpkvist & Klapper (2007), edges generate spring forces with

$$\mathbf{F}_\ell^p = \sigma_p \sum_{\substack{m=1 \\ \mathbb{I}_{\ell,m} \neq 0}}^{N_p} \mathbb{I}_{\ell,m} \frac{\mathbf{d}_{\ell,m}}{d_{\ell,m}} (d_{\ell,m}(0) - d_{\ell,m})$$

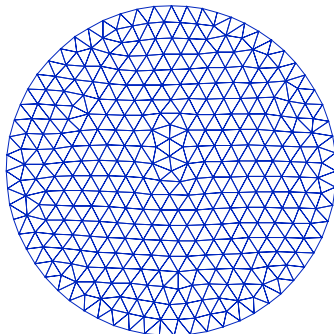
$$\mathbf{d}_{\ell,m}(t) = \mathbf{X}_\ell(t) - \mathbf{X}_m(t)$$

$$d_{\ell,m} = |\mathbf{d}_{\ell,m}|$$

$$\mathbb{I}_{\ell,m} = [0/1 \text{ incidence matrix}]$$

- Force integral is scaled by an area factor:

$$\mathbf{f}_{i,j} = \sum_{\ell=1}^{N_p} \mathbf{F}_\ell^p \delta_h(\mathbf{x}_{i,j} - \mathbf{X}_\ell) \underbrace{\frac{\pi D^2}{4N_p}}_{\triangle \text{ area}}$$



Particle triangulation  
with  $N_p = 2015$  nodes.

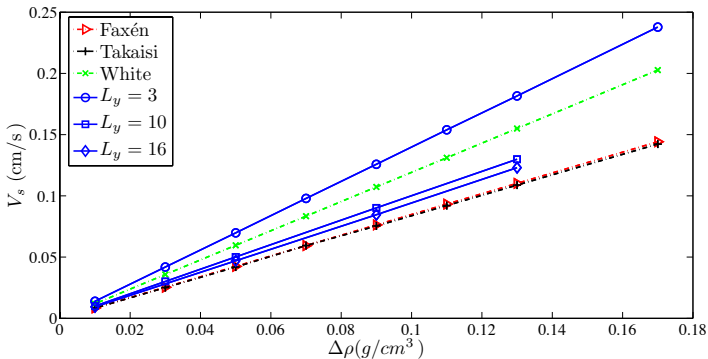
[Hopkins & Fauci, 2002]

# Outline

- 1 Gravitational settling
  - Analytical solutions
  - Experimental results
  - Numerical simulations
- 2 Immersed boundaries with mass
  - Mathematical formulation
  - Immersed boundary method
- 3 Simulations of settling cylinders
  - Single particle
  - Two particles and draft–kiss–tumble dynamics
- 4 Conclusions

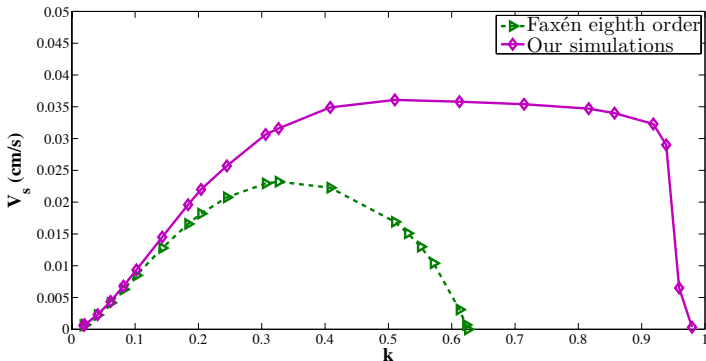
Single particle: Comparison to wall-corrected  $\tilde{V}_s$ 

For small  $\Delta\rho = \rho_p - \rho_f$ , the settling velocity  $V_s$  approaches Faxén's (1946) result as the channel length  $L_y$  increases:



# Single particle: Varying particle size

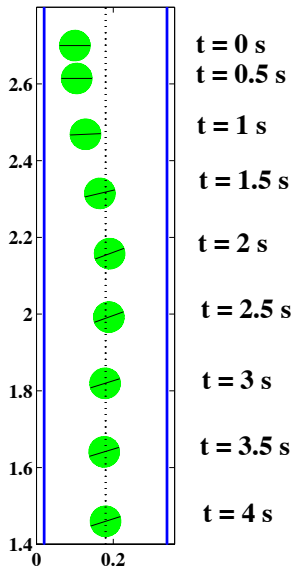
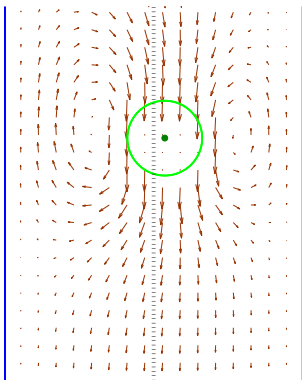
Wall-corrected  $\tilde{V}_s$  formulas are only valid for small  $k = W/D$ .



Our simulations demonstrate physically reasonable behaviour as  $k \rightarrow 1$ .

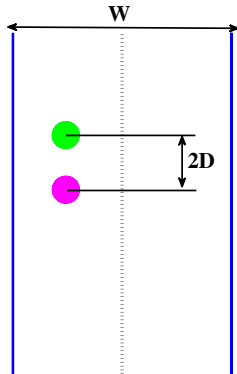
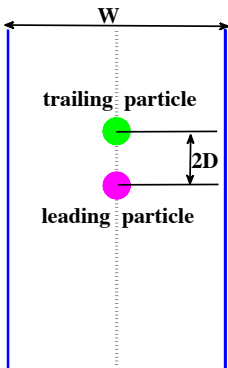
# Single particle: Released off-center

- At Reynolds number  $Re = 4.9$ , a single particle released off-center migrates toward the centerline.
- Hydrodynamic forces between the particle and the walls are in balance.



# Simulations of two particles

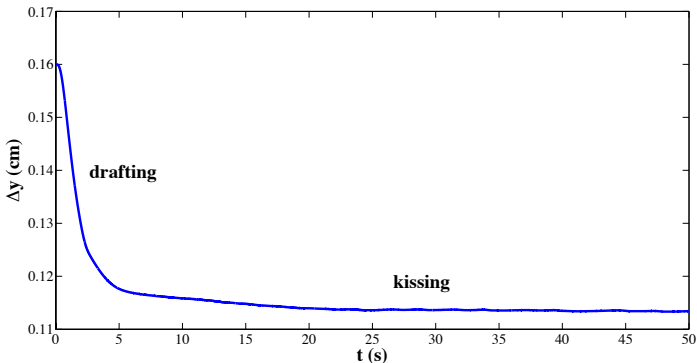
Consider two initial configurations, centered and off-center, with particles separated by a distance  $2D$ :





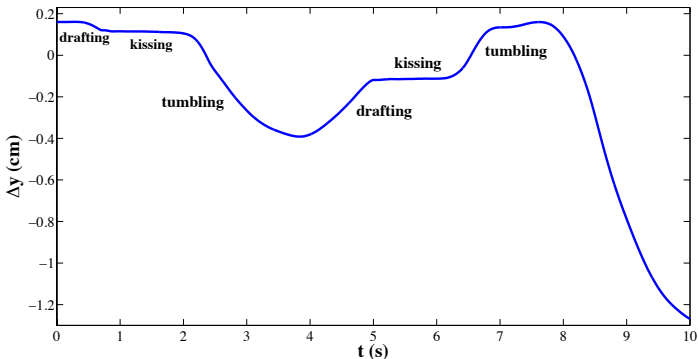
# Two particles at low Re: Drafting and kissing

At low Reynolds number ( $Re = 3$ ), the particles approach each other (**draft**) and nearly touch (**kiss**):

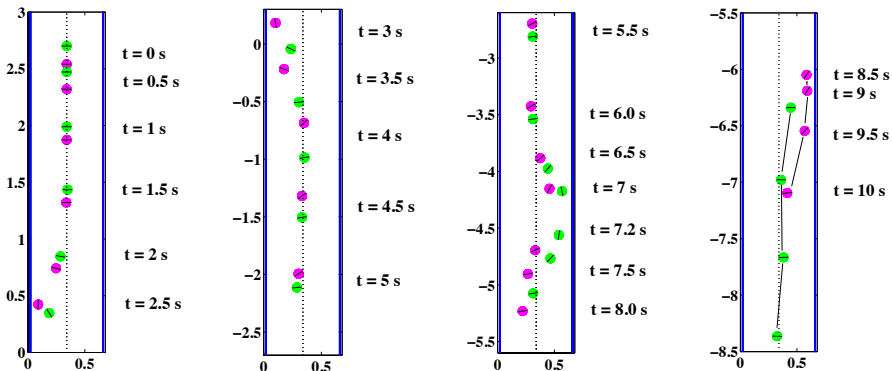


# Two particles at $Re = 80$ : DKT behaviour

At higher Reynolds number ( $Re = 80$ ), the particles undergo a **tumbling** motion after drafting and kissing:



# Two particles at $Re = 80$ : DKT behaviour (cont'd)

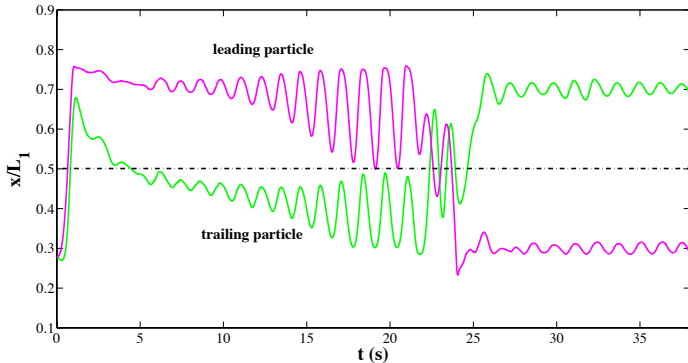


Results match qualitatively with FEM simulations of [Feng, Hu & Joseph \(1994\)](#).

[Video]

# Two particles at $Re = 47$ , off-center

More interesting behaviour arises at an intermediate Reynolds number ( $Re = 47$ ) for two particles released off-center:



[Video]

# Outline

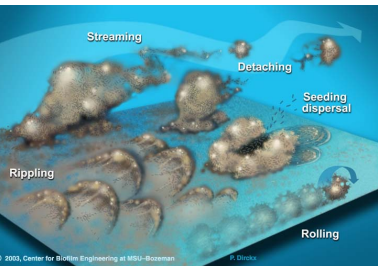
- 1 Gravitational settling
  - Analytical solutions
  - Experimental results
  - Numerical simulations
- 2 Immersed boundaries with mass
  - Mathematical formulation
  - Immersed boundary method
- 3 Simulations of settling cylinders
  - Single particle
  - Two particles and draft–kiss–tumble dynamics
- 4 Conclusions

# Closing remarks

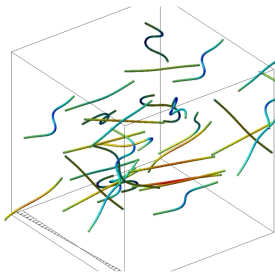
- We developed a 2D immersed boundary method that handles gravitational settling in the presence of walls.
- Computed settling velocities match with experiments.
- More complicated two-particle dynamics are consistent with simulations of [Feng, Hu & Joseph \(1994\)](#).

# Current and future work

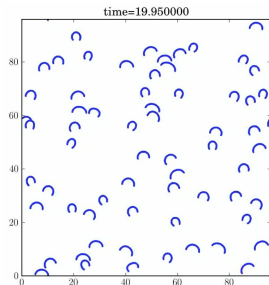
- Study settling of deformable, non-spherical particles.
- Investigate applications to:
  - biofilm floc deformation,
  - flexible fiber suspensions,
  - jellyfish swimming dynamics.
- Simulate large numbers of particles using Wiens' parallel IB algorithm.  
[Wiens & JS, submitted to *J. Comput. Phys.*, arXiv:1305.3976, 2013]



Biofilms  
(MSU Bozeman)



Flexible fibers  
(M. Shelley, NYU, 2004)



Jellyfish in 2D  
(Jeff Wiens, 3:00 Wed)

# Thank-you!

<http://www.math.sfu.ca/~stockie>



# References I

- ▶ **Erik Alpkvist and Isaac Klapper.**  
Description of mechanical response including detachment using a novel particle model of biofilm/flow interaction.  
*Water Science and Technology*, 55:265–273, 2007.
- ▶ **Wim-Paul Breugem.**  
A second-order accurate immersed boundary method for fully resolved simulations of particle-laden flows.  
*Journal of Computational Physics*, 231(13):4469–4498, 2012.
- ▶ **Robert H. Davis and Andreas Acrivos.**  
Sedimentation of noncolloidal particles at low Reynolds numbers.  
*Annual Review of Fluid Mechanics*, 17:91–118, 1985.
- ▶ **Olov Hilding Faxén.**  
Forces exerted on a rigid cylinder in a viscous fluid between two parallel fixed planes.  
*Proceedings of the Royal Swedish Academy of Sciences*, 187:1–13, 1946.
- ▶ **James Feng, Howard H. Hu, and Daniel D. Joseph.**  
Direct simulation of initial value problems for the motion of solid bodies in a Newtonian fluid. Part 1. Sedimentation.  
*Journal of Fluid Mechanics*, 261:95–134, 1994.

# References II

- ▶ **Sudeshna Ghosh and John M. Stockie.**  
Numerical simulations of particle sedimentation using the immersed boundary method.  
*Journal of Computational Physics*, May 2013.  
submitted, arXiv:1304.0804.
- ▶ **Élisabeth Guazzelli and Jeffrey F. Morris.**  
*A Physical Introduction to Suspension Dynamics.*  
Cambridge Texts in Applied Mathematics. Cambridge University Press, 2012.
- ▶ **Matthew M. Hopkins and Lisa J. Fauci.**  
A computational model of the collective fluid dynamics of motile microorganisms.  
*Journal of Fluid Mechanics*, 455:149–174, 2002.
- ▶ **Markus Uhlmann.**  
An immersed boundary method with direct forcing for the simulation of particulate flows.  
*Journal of Computational Physics*, 209:448–476, 2005.
- ▶ **Jin Wang and Anita Layton.**  
Numerical simulations of fiber sedimentation in Navier-Stokes flow.  
*Communications in Computational Physics*, 5(1):61–83, 2009.
- ▶ **Zeli Wang, Jianren Fan, and Kun Luo.**  
Combined multi-direct forcing and immersed boundary method for simulating flows with moving particles.  
*International Journal of Multiphase Flow*, 34:283–302, 2008.

# References III

- ▶ Jeffrey K. Wiens and John M. Stockie.  
An efficient parallel immersed boundary algorithm using a pseudo-compressible fluid solver.  
*Journal of Computational Physics*, May 2013.  
submitted, arXiv:1305.3976.