Fluid dynamics at small scales

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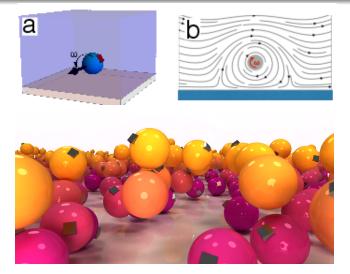
Modeling and Simulation Group Sept 17th 2020 Masters Sachin Natesh (now Ph.D. at Colorado Boulder) Ph.D. students Ondrej Maxian, Zhe Chen, Raul Perez (Madrid Spain) Postdocs Brennan Sprinkle, Sophie Marbach, Zecheng Gan (NYUSH)

I lead our NSF-funded Research and Training Group (RTG) in **Modeling and Simulation**, together with Miranda Cerfon-Holmes, Leif Ristroph, Charles Peskin, and Esteban Tabak.

I co-lead the Interdisciplinary Research Group on Active Matter (Soft Condensed Matter Physics) in the NYU Materials Research Center.

- The primary focus of my research is fluid dynamics at small scales (100nm- $10\mu m)$, where **thermal fluctuations / Brownian motion** play an important role.
- A key approach I use and try to understand is **fluctuating hydrodynamics** (stochastic partial differential equations).
- Tools: fast methods, fast algorithms, computational fluid dynamics, applied stochastic analysis.
- Physical systems of current interest: suspensions of **colloids** (soft matter, Chem E) and **fibers** (comp bio), **electrolytes** (ionic solutions).

Microrollers



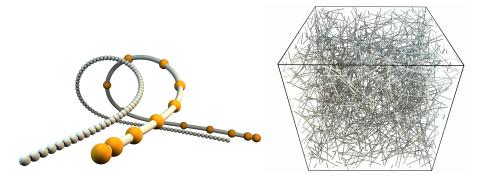
B. Sprinkle, E. B. van der Wee and Y. Luo and M. Driscoll, and A. Donev, *Driven dynamics in dense suspensions of microrollers*, **ArXiv:2005.06002**

A. Donev (CIMS)

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Fibers

Very **slender semi-flexible fibers** abound in the cell cytoskelleton (actin, microtubules) and cell mechanics in general (flagella).



O. Maxian, A. Mogilner and A. Donev, **ArXiv:2007.11728** An integral-based spectral method for inextensible slender fibers in Stokes flow [2]

Fibers in Stokes flow

- Fiber centerline **X** (s) where the arc length $0 \le s \le L$.
- The tangent vector is $\tau = \partial \mathbf{X} / \partial s = \mathbf{X}_s$, and the fibers are inextensible, $\tau(s, t) \cdot \tau(s, t) = 1$ for all s and t.
- Hydrodynamics relates the fluid velocity $\mathbf{v}(\mathbf{r}, t)$ to the force density $\mathbf{f}(s, t)$ along the fiber centerlines. For (unsteady) Stokes flow, $\nabla \cdot \mathbf{v} = \mathbf{0}$ and

$$\partial_t \mathbf{v} + \nabla \pi = \eta \nabla^2 \mathbf{v} + \int_0^L ds \, \mathbf{f}(s,t) \delta_s (\mathbf{X}(s,t) - \mathbf{r}) + \nabla \cdot \left(\sqrt{2\eta k_B T} \, \mathcal{W}\right),$$

where δ_a is a regularized delta function whose width is proportional to the radius of the fiber *a*.

• For an inextensible semi-flexible fiber

$$\mathbf{f} = -\kappa_b \mathbf{X}_{ssss} + \boldsymbol{\lambda},$$

where $\lambda(s, t)$ is a Lagrange multiplier for inextensibility.

Fluctuating hydrodynamics

Dynamics of the fiber

$$\begin{split} \mathbf{J}(s,t) &= \partial_t \mathbf{X}(s,t) = \int d\mathbf{r} \, \mathbf{v}(\mathbf{r},t) \, \delta_a \left(\mathbf{X}(s,t) - \mathbf{r} \right) . \\ &= \overline{\mathbf{U}}(t) + \int_0^s ds' \, \left(\mathbf{\Omega}^{\perp} \left(s',t \right) \times \boldsymbol{\tau} \left(s',t \right) \right) \end{split}$$

- The **thermal fluctuations** (Brownian motion of fiber) are driven by a white-noise **stochastic stress tensor** $\mathcal{W}(\mathbf{r}, t)$.
- Open mathematical question: What is the **overdamped** limit $\eta/\rho \rightarrow \infty$ (steady Stokes).
- How to **efficiently simulate** the dynamics of a suspension of many (fluctuating) fibers of different slenderness?

References



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Brennan Sprinkle, Ernest B. van der Wee, Yixiang Luo, Michelle Driscoll, and Aleksandar Donev.

Driven dynamics in dense suspensions of microrollers. *Soft Matter*, 16:7982 – 8001, 2020.

Ondrej Maxian, Alex Mogilner, and Aleksandar Donev.

An integral-based spectral method for inextensible slender fibers in Stokes flow. Submitted to Phys. Rev. F, ArXiv preprint 2007.11728, 2020.