Modeling, Simulation, and Optimization of Rigid Particles in Stokes Fluid

Keywords
Modeling, simulation, Stokes equations, fluid-structure interactions

General Context

Particle-laden flows, where solid particles are transported and interact within a fluid, are ubiquitous in both natural and industrial systems. They play a crucial role in phenomena such as sediment transport in rivers, resuspension of microplastics or pollutants in aquatic systems, dispersion of aerosols and pollens in the atmosphere, and in many industrial processes including surface cleaning and additive manufacturing.

The dynamics of these flows are governed by complex multiscale and nonlinear phenomena such as hydrodynamic forces, particle–wall interactions, lubrication effects, collisions, adhesion, and turbulence. Developing predictive models and control strategies for such systems is challenging due to their strong spatial and temporal variability.

The main objective of this project is to describe and simulate the dynamics of one or several rigid particles moving in a fluid. Solving these dynamics requires coupling the **Stokes equations** for the fluid flow with the **Newton equations** governing particle motion. The work will consist of developing numerical simulations of this coupled system using a hierarchy of modeling approaches:

- **Asymptotic models:** In this simplified framework, only asymptotic hydrodynamic effects are retained. The dynamics reduce to solving a system of ordinary differential equations (ODEs), enabling fast numerical experiments.
- **High-fidelity simulations:** The complete Stokes problem will be solved using two complementary numerical strategies:
  1. The *Arbitrary Lagrangian–Eulerian (ALE)* finite element method implemented in the `Feel++` library (see [2]),
  2. The *Boundary Element Method (BEM)* based on Green's functions, implemented with `Gypsilab` (see [1]).

If sufficient progress is achieved, this modeling and simulation work may lead to the integration of **artificial intelligence techniques** (e.g., reinforcement learning for optimization [3,4]) to design strategies for controlling and optimizing the trajectories of rigid particles in complex flows.

Scientific Objectives

The primary objective of this project is to develop a rigorous understanding of the dynamics of one or several rigid particles immersed in a viscous fluid at low Reynolds numbers. This requires coupling the **Stokes equations** describing the fluid motion with the **Newton equations** governing the translation and rotation of rigid bodies. The specific goals are:

- Formulate and implement a hierarchy of mathematical models, from simplified asymptotic descriptions to high-fidelity simulations, to capture particle–fluid interactions at different levels of accuracy.
- Compare and validate numerical methods to solve the coupled particle–fluid system, focusing on efficiency, scalability, and accuracy.
- Perform numerical experiments to explore how geometry, boundary conditions, and hydrodynamic interactions influence particle dynamics.
- Provide a framework that can later be extended to optimization and control of particle trajectories, possibly using reinforcement learning or other machine learning techniques.

This project is intended to train students in advanced modeling, numerical simulation, and computational fluid dynamics techniques, while laying the groundwork for further research in optimization and control of particle motion.

Numerical Methods

To address the modeling challenges, we propose a hierarchy of numerical approaches:

1. **Asymptotic Models and ODE Solvers.** In the simplest approach, hydrodynamic interactions are approximated using asymptotic expansions. The motion of particles is governed by a reduced system of ordinary differential equations (ODEs), enabling rapid simulations over a large parameter space. These models are ideal for sensitivity studies and preliminary exploration.
2. **Finite Element Method (FEM) with Arbitrary Lagrangian–Eulerian (ALE) Formulation.** For higher accuracy, the full Stokes equations will be solved using an ALE formulation that allows the computational mesh to deform with particle motion. This method, implemented in the `Feel++` library, enables precise representation of fluid-particle interactions and boundary effects.
3. **Boundary Element Method (BEM) with Green's Functions.** Alternatively, the Stokes problem can be reformulated using boundary integral equations. By exploiting analytical Green's functions for the Stokes operator, the dimensionality of the problem is reduced and computational efficiency improved. This approach will be implemented using the `Gypsilab` library.

These different modeling strategies will be combined in a **multi-fidelity framework** to balance accuracy and computational cost. Low-fidelity models will serve as a tool for exploring parameter spaces and identifying promising configurations, while high-fidelity simulations will provide detailed validation and insight. This hierarchical approach will also create a strong foundation for future optimization and control studies, where techniques such as reinforcement learning could be used to design strategies for particle trajectory manipulation.

Supervision

This project will be supervised Laetitia Giraldi, a researcher at Inria Sophia-Antipolis within the CALISTO team. The supervisor will closely follow the students' progress through weekly remote meetings (video calls) and will provide additional support sessions if needed. The aim is to ensure strong scientific and technical guidance while encouraging autonomy and initiative.

Depending on the students' progress and interests, this project may lead to a **Ph.D. opportunity**, allowing further development of the numerical methods, modeling approaches, and optimization strategies introduced in this work.

References

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