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Internship on lubrication forces between objects near contact in a fluid

Keywords	Modeling, Theory, Numerical simulation, Data analysis, Dispersed two-phase flow
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Hosting Team	Team CaliSto 🗹, Inria Center at Université Côte d'Azur 🗹

Context

Particles are omnipresent in our daily lives and the environment. To name a few examples, particles are present in atmospheric sciences (dispersion of pollutants, aerosols and/or pollens in the air) or in marine sciences (plastic contamination in rivers or oceans) or in medical applications (microswimmers in blood for drug delivery). These particles can be either passive (i.e. transported by the underlying flow) or active (i.e. with their own self-motility).

When two objects are immersed in a fluid, specific forces arise as these objects come close to each other. These specific interactions govern the way particles interact with each other, possibly leading to the formation of aggregates or clusters. This implies that accurate models are key to properly predict the formation of aggregates/clusters.

The aim of this internship is to propose and validate a numerical scheme based on solvation forces, well-known in the field of chemistry for nanoscale molecules, to compute inter-particle interactions in the framework of continuum fluid mechanics, called lubrication forces.

Objectives

The dynamics of objects immersed in a fluid flow is described using Newton's second law of motion:

$$\frac{d\mathbf{X}_p}{dt} = \mathbf{U}_p \tag{1}$$

$$m_p \frac{d\mathbf{U}_p}{dt} = \sum \mathbf{F} \tag{2}$$

$$I_p \frac{d\mathbf{\Omega}_p}{dt} = \sum \mathbf{T}_F \tag{3}$$

with \mathbf{X}_p the object's position, \mathbf{U}_p its translational velocity, $\mathbf{\Omega}_p$ its rotational velocity, m_p its mass, I_p its moment of inertia and \mathbf{F} (resp. \mathbf{T}_F) the forces acting on the object (resp. the torques). Yet, behind this apparent simplicity lies complex modeling issues. As displayed in Figure 1, when two objects approach each other, various forces arise [4]:

- The lubrication forces, which result from the viscous forces generated when the fluid is squeezed out of the gap between the objects [1,2,3].
- The contact forces, which result from the collision between the two objects in contact.

In the fluid mechanics community, lubrication forces can be approximated numerically by solving the fluid flow around each individual object. This implies that the grid size used to compute the fluid flow has to be smaller than the grid between the objects. Yet, close to the contact point, the separation distance eventually becomes smaller than the grid size, implying that lubrication forces have to be modeled. Since these lubrication forces usually diverge when the separation distance nears 0, cut-off distances are introduced to obtain a finite value of the lubrication at contact [4].

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Figure 1: Sketch of the resolved and modeled lubrication forces depending on the separation distance (taken from [4]).

Alternatively, in the field of interface chemistry, solvation forces are the equivalent of lubrication forces, except that they designate forces acting within the nanometre scale. Models for solvation force are thus derived from descriptions at the molecular level, i.e. from the motion of each water molecules squeezed between the two objects. Such models thus apply to scales at which the continuum level of description used for fluid mechanics breaks down [5].

The aim of this internship is to develop more advanced lubrication models that bridge the gap between theories developed in the two communities (namely fluid mechanics and interface chemistry). Depending on the student preferences, a number of topics are foreseen, among which:

- i. a detailed review of the literature on lubrication and solvation forces;
- ii. the development of a theoretical model that combines ideas coming from fluid mechanics (lubrication forces) and interface chemistry (solvation forces);
- iii. the implementation of a new model in a solver for the dynamics of particles in suspension;
- iv. the assessment of the model performance and its accuracy, as well as a detailed evaluation of the sensitivity of the model to the input parameters.

The student will be encouraged to write a publication in an international journal at the end of the internship. Motivated students will be encouraged to pursue their work on this topic with a PhD thesis.

Candidate profile

We are looking for candidates with a strong background in applied mathematics (Numerical methods, Numerical simulations, Statistics), physics (Statistical Physics, Fluid dynamics, Modelling) or mechanical engineering (Chemical Engineering).

Candidates should be fluent in English, have a good experience in programming and in data analysis.

We will appreciate candidates with the following skills (optional):

- Knowledge in fluid dynamics
- Knowledge in statistical physics
- · Rigorous, autonomous and creative thinking
- · Interest in environmental/medical applications

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Duration and period

The internship will cover a period of 5-6 months, between February and September 2025. The exact starting/end dates are quite flexible and can be adapted to the constraints of the student.

Host institution

The internship will take place within Team CaliSto \Box , located in Inria Centre at Université Côte d'Azur \Box . The student will be in contact with researchers that collaborate with the team members on this topic across both France (in particular Strasbourg, Paris and Marseille) and Europe (mostly in Germany).

To apply

Interested candidates are required to send a cover letter, a CV, a transcript of their grades from their Master studies and at least one recommendation letter to laetitia.giraldi@inria.fr and christophe.henry@inria.fr

References

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