# Coupling fictitious domains / discrete elements applied to the simulation of a dense suspension of polyhedral grains

## Context:

The proposed PhD work falls within the general framework of numerical simulation of the duct-flow of a dense assembly of non-colloidal particles suspended in a fluid at low Reynolds number. This field of research has a wide application scope directly connected to the concept of sustainable cities, insofar as they face rainwater and sewage clogging issues potentially leading to pipes overflow (worsen by climate change), or building materials pumping issues to mention just a few. Simulating such a flow requires accounting for fluid-grain coupling, with grains motion obeying Newton's laws and fluid motion being governed by the conservation laws of continuum mechanics (Navier-Stokes equations for a Newtonian fluid). The main difficulties then lie in the calculation of interaction forces between fluid and grains (lubrication and long-range forces) but also between grains when the particles are close to each other. These difficulties increase further with the presence of non-spherical particles, very common in the previously mentioned applications, since the shape of particles plays a significant role in flow behavior that shall be accounted for.

From a methodological viewpoint, fluid-grains coupling may be simulated using various numerical strategies (e.g. Stokesian dynamics [1], CFD/DEM coupling [2], LBM/DEM coupling [3]). A common limit is often the calculation costs, in particular related to the treatment of the variety of timescales characterizing the phenomena but also to the integration of a non-Newtonian rheology for the suspending fluid, which is an active field of research. In addition, DEM-based coupling methods rely on existing DEM codes capable of well simulating dense granular flows of dry grains, however these codes are mostly dedicated to sphere assemblies for which contact detection is quick and easy. For non-spherical grains, contact characterization is much more challenging and calculation-intensive, which is another active field of research.

The GPEM laboratory has just developed a parallelized DEM simulation code to model the behaviour of dense assemblies of polyhedra [4]. Likewise the laboratory has developed a code for the numerical simulation of viscoplastic fluid flow under complex agitation, using fictitious domain methods with both boundary and distributed multipliers. The coupling of these tools is therefore part of a research perspective combining two, or even three crucial aspects of the subject: grain shape and fine management of the local dynamics, even non-Newtonian suspending rheology.

In addition, the GPEM laboratory will continue the development of the LBM code initiated during the master2 internships of A. Bisoulier (2021) and L. Chaillou (2023) and couple it with the DEM code, which will eventually make it possible to compare the mixed CFD/DEM and LBM/DEM approaches.

**Goals:**

First, the main objective of the thesis lies in the coupling of the two 3D codes of the laboratory, the CFD code and the DEM code, by seeking a compromise between precision and calculation time. In the coupling process, the DEM code transmits to the CFD code the contact forces between polyhedra, while the CFD code provides the DEM code with the update of the position and orientation of the grains in suspension.

Then, the final code will be implemented to simulate the low Reynolds number flow of a dense suspension in elementary pipe network configurations (typically: "L", "T" or "+" shapes ), for which the behavior of the flow is not known, with perspective resolution strategies in realistic geometries of complex networks. Particular attention will be paid to the influence of the shape of the grains. Finally, the results of one or more previous elementary configurations will be compared with those of the first simulations carried out using the LBM/DEM coupling developed by the laboratory.

**Scientific obstacles and chalenges:**

— Accuracy of fluid/grain and intergrain force calculations

— Calculation time due to the high number of particles (1cm3 may contain 10^6 grains of diameter 0.1mm), difficulty increased by the non-spherical shape of the grains

— Unified temporal discretization strategy integrating different time scales between fluid and grains with local variations

**Main steps:**

— Bibliographic study: fluid/grain coupling, numerical or instrumented experimental results (NMR, etc.), calculation acceleration techniques

— Getting started and pairing the two home-made codes

— Tests in straight pipe with 1 single then 2 close grains - benchmarking with experimental and numerical results from the literature

— Simulations in straight and annular pipes for a dense suspension - benchmarking with experimental and numerical results from the literature

— Simulation of dense flows in elementary network patterns using the CFD/DEM approach

— Comparison with the LBM/DEM approach under development in the laboratory, to compensate for the lack of literature dealing with the simulation of these configurations

**Originality of the subject:**

— Polyhedral grains not necessarily convex in suspension in a Newtonian fluid or not

— Analysis of the flow of such suspensions in elementary patterns of pipe networks

**Candidate profile:**

Applicants are expected to fulfill the following requirements in the domain of mechanics, applied mathematics and scientific computing:

— Master 2 with cursus in continuous or discrete numerical modeling
— scientific programming experience
— wide scientific curiosity and pronounced interest in the rheology of suspensions

In addition, knowledge in the following areas will be particularly appreciated:

— continuum media mechanics, rheology
— numerical methods for fluid mechanics and non-smooth mechanics
— modern Fortran (2008 standard at least)

Excellent writing skills, especially in English, are also expected.

**References:**

[1] J. F. Brady and G. Bossis, “Stokesian dynamics,” Annual Review of Fluid Mechanics, vol. 20, no. 1, pp. 111–157, 1988.
[2] C. Selcuk, A. Ghigo, S. Popinet, and A. Wachs, “A fictitious domain method with distributed lagrange multipliers on adaptive quad/octrees for the direct numerical simulation of particle-laden flows,” Journal of Computational Physics, vol. 430, 10 2020.
[3] N. J. Di Vaira, L. Laniewski-Wollk, R. L. Johnson Jr., S. M. Aminossadati, and C. R. Leonardi, “Influence of particle polydispersity on bulk migration and size segregation in channel flows,” J. Fluid Mech., vol. 939, p. A30, 2022.
[4] Y. Descantes, “A new discrete element modelling approach to simulate the behaviour of dense assemblies of true polyhedra,” Powder Technology, vol. 401, p. 117295, 2022.