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Particulate flows with the subspace projection method

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ABSTRACT

A novel finite element method for the 3d simulation of (many) particles in a Newtonian carrier liquid is presented. The methods features the celebrated one domain approach, a *subspace projection method* to account for the rigid body motion within the particles and operator splitting. Combined with local mesh refinement the method results in a fast and accurate, though conceptually simple to implement algorithm.
Validation is achieved using the sedimentation of one particle and comparing the resulting drag coefficient with theoretical and experimental results. Furthermore, a viscometer is considered, where the effective viscosity of a particle laden fluid is compared with analytic results.

1. Introduction

Particulate flow, i.e. the flow of a carrier fluid loaded with particles, is central to many technical applications. Let us just mention reactors, fluidized beds, production of nano particles and many more. There exists a hierarchy of models how to describe the particulate phase and how to describe the interaction between particles and fluid. For certain applications it is mandatory to describe the fluid–particle interaction and also a possible particle–particle interaction in full detail without simplified parametrizations. Computational methods based on such full models are called *direct numerical simulations*.

There are two main distinguishing features for finite element methods approximating detailed particulate flows. The first one is how to computationally represent the particles' geometry, while the second one is how to enforce the constraint of rigid body motion within the particles. Both questions are intimately linked.

In turn there are two main classes of finite element methods. The first one uses body fitted meshes. Here, the nodes on the particles' boundary move along with the particle. The grid in the fluid domain then has to be smoothed by, for instance, a Laplace equation. An interesting variant of a mesh-moving method is presented in [1]. There the mesh smoothing is also used as an *r*-adaptive method to concentrate degrees of freedom close to the particles. The mesh moving is accounted for by a mesh velocity added to the convective terms. This is the technique of *Arbitrary Lagrangian–Eulerian* (ALE) coordinates. It has the advantage of very accurately representing the geometry, while the drawback here is that remeshing is needed, when the distortion of the mesh becomes to severe. This may happen rather frequently in certain physical situation. While remeshing is relatively easily achieved in 2d, this issue might be a major problem in 3d, in particular when simulating many particles, and heavily relies on the availability of high quality mesh generators. We refer to [2–6,1] regarding this approach.

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The second approach is based on the method of *fictitious domains*. The constraint of particle motion within the particles' domain is here usually achieved by a Lagrangian multiplier approach. Let us mention the articles [7–11] as representative work in this direction. In [12] the use of Lagrangian multipliers could be avoided by resolving the interaction forces through an integral equation (explicit or implicit) for the end-of-step velocity.

Closely related to the aforementioned fictitious domain technique is the immersed boundary method (IB), originally introduced in [13] for the simulation of the human heart. Here, the interaction forces are modeled by singular forces attached to Lagrangian points moving with the particles, see for instance [14–17] for more details.

Further differences among the diverse methods arise from how the set of equations are coupled/decoupled. While only few authors suggest to solve a fully coupled system [18], most methods are based on decoupling strategies. Besides their more convenient computational structure, the reason why decoupled schemes can be more efficient lies in the fact that for simulating particulate flows small time steps are needed anyway in order to capture the dynamics of the problem.

An alternative to the above described methods that are all continuum-based, discretizing the system of partial differential equations by finite element (or finite differences, finite volumes) is the lattice Boltzmann method (LBM). This approach is particularly suited for dense particle suspension. In essence, the LBM solves for a particle distribution function (representing an ensemble average of particles) at grid nodes, analogous to the continuous, microscopic density function of the Boltzmann equation. Since this approach is rather disjoint from the above cited articles we just refer to [19–22] for more details about LBM applied to the simulation of particulate flow.

Analytical results regarding existence, uniqueness and qualitative behavior of solutions can be found for instance in Galdi and Serre [23,24].

The approach presented in this article is based on the *one domain approach* by [24,7], but does not fit into one of the two classes of methods mentioned above. It differs from the articles cited above in several aspects, since it

- does not require an explicit meshing of the particles' domain;
- does not need an explicit evaluation of forces;
- uses a *subspace projection method* to account for the constraint of rigid body motion within the particles, thus avoiding a saddle point problem for this constraint;
- uses time dependent adaptively refined meshes to provide the necessary geometric resolution;
- an error estimate for the most important sub-problem can be shown.

It turns out that this novel method is therefore easy to implement (only few modules have to be added to an existing standard software) and rather efficient.

The rest of this paper is organized as follows.

The mathematical model and its dimensionless formulation as well as the weak formulation of the *one domain approach* are presented in Section 2.

In Section 3 the numerical method is explained in detail. Each of its subsections addresses the necessary steps of the overall procedure: the time splitting, the Navier–Stokes solver, the subspace projection method (SPM), adaptivity in space, preconditioning and the particle–particle interaction. Moreover, an error estimate for the core subproblem of the SPM is given.

Section 4 discusses two computational experiments for validating the code and its underlying methods: the sedimentation of a single particle as well as the rheological behavior of particle laden fluids are studied. As a qualitative benchmark we additionally included the well known drafting–kissing–tumbling experiment.

In the last section we give a short conclusion and outlook.

2. Mathematical formulation

2.1. Model

In this section we introduce the mathematical model for particulate flows. For the ease of presentation this will be done for the $3d$-case with only one particle. The extension to more particles is straightforward, simply by adding an index. The model also holds for the $2d$-case, one just has to adapt the definition of the cross-product involved in the equations.

Denote by $\Omega(t) \subset \mathbb{R}^3$ the time-dependent domain occupied by an incompressible, Newtonian fluid with velocity $\mathbf{u}$ and pressure p. Its motion is described by the incompressible Navier–Stokes-equation. A homogeneous no-slip condition is prescribed on the outer boundary Γ_D.

$P(t) \subset \mathbb{R}^3$ is the time-dependent domain of a rigid particle, with its center of mass given by $X = \frac{1}{|P(t)|}\int_{P(t)} \mathbf{x}\, d\mathbf{x}$, while $\mathbf{r} = \mathbf{x} - X$ is its relative coordinate. The particle's motion, being a rigid body motion, is governed by Newton's law, describing values for the translational and angular velocities $\mathbf{U}$, $\boldsymbol{\omega}$, respectively, and the position $\mathbf{X}$. Furthermore, let $\boldsymbol{\Theta} = [\Theta_1\ \Theta_2\ \Theta_3]$, $\Theta_i \in \mathbb{R}^3$, denote a coordinate system attached to the particle describing its orientation in space. Since the particle is impermeable, we assume $\Omega(t) \cap P(t) = \emptyset$ for all times $t > 0$. Finally we assume (for simplicity) that the whole volume $\Omega_c = \Omega(t) \cup P(t) \cup \partial P(t)$ is time independent. See also Fig. 1 for a sketch of the situation.

The motions of fluid and particle are coupled on one hand by the *no-slip-condition* on the particle boundary equation (4) below and on the other hand by the stress and pressure forces of the fluid acting on the particle (in the right hand sides of