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Lattice Boltzmann simulation of dense rigid spherical particle suspensions using immersed boundary method

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ABSTRACT

We present a lattice Boltzmann model designed for the simulation of dilute and dense finite-sized rigid particle suspensions under applied shear.

We use a bottom-up approach and fully resolve the mechanical interaction between fluid and particles. Our model consists in coupling a lattice Boltzmann scheme for Newtonian and incompressible fluid flows with an immersed boundary scheme to simulate two-ways fluid-particles interaction. We introduce a simple yet robust contact model that includes repulsive elastic collision between particles, and neglects lubrication corrections. We apply this model to simple sheared flow with rigid spherical particles and we provide results for the relative apparent viscosity of the particle suspension as a function of the particle volume fraction and strain rate of the flow.

We show that, using the proposed approach, there is no need for a lubrication model in the Newtonian regime, provided that an elastic contact model is included. Our algorithm, therefore, can be based only on physically sound and simple rules, a feature that we think to be fundamental for aiming at resolving polydispersed and arbitrarily shaped particle suspensions.

Comparing our results with Krieger–Dougherty semi-empirical law, we confirm that the simulations are not sensitive to the particle Reynolds number for $Re_p \ll 1$ in the Newtonian regime. We show that the proposed model is sufficient to obtain a correct description of the rheology of particle suspension up to volume fraction equal to 0.55 (approaching the critical random packing fraction for monodispersed spheres), which goes beyond the state of the art.

1. Introduction

The fundamental investigation of dense particle suspensions finds its application in several fields of applied science and engineering as, amongst others, blood rheology [1], food technology [2,3], concrete and mortar properties [4]. A great challenge in this field of research is to improve the understanding of the rheological properties of such suspensions in increasing complex physical scenarios. An important example of that is magma flow.

Magma is a multicomponent mixture of silicate melt and crystals (*i.e.* crystals bearing magma) that, while evolving (changes in pressure and temperature), can also experience the exsolution of volatiles and form a three phase suspensions (*i.e.* crystals and bubbles bearing magma). The rheology of magmas has been extensively investigated experimentally and it has been found that magma exhibits non-Newtonian behavior at both high particle volume fraction ϕ and/or strain rate $\dot{\gamma}$ (see [5,6]). Experimental investigations focused on determining the rheology of bubbles and crystals bearing magmas also exists (refer to Mader et al. [6] for instance). However the complex non-linear interaction between the three coexisting phases substantially increases the complexity of magma rheology characterization. In this context, numerical modeling of increasingly complex magma-like suspensions may reveal fundamental to improve our understanding of magma rheology.

As a first step to build such a tool, a two-phase (fluid and particles) scenario is considered in this article. In particular, to validate our approach, it is crucial that the rheological behavior of the simulated particle suspension follows the Krieger–Dougherty law [7], that relates the relative apparent viscosity μ_r of the suspension to the particle volume fraction ϕ as:

$$\mu_r = \left(1 - \frac{\phi}{\phi_M}\right)^{-B\phi_M}, \quad (1)$$

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with ϕ_M the maximum packing fraction. Throughout all this study, we used $B = 2.5$, which is a common value for rigid spheres [8–11]. Eq. (1) is widely used and proves to be in good correlation with experimental data [6,8,12].

Moreover, as a first step to model particle suspensions that mimic a magmatic environment, one should reproduce as much as possible a viscous (particle Reynolds number, $Re_p \ll 10^{-3}$), strongly coupled (Stokes number, $St \ll 1$) regime [6]. The particle Reynolds number of a suspension Re_p is defined as $Re_p = \rho_f r^2 \dot{\gamma}/\mu_0$, where ρ_f is the density of the suspending fluid phase, r is the particle radius, $\dot{\gamma}$ is the strain rate and μ_0 the viscosity of the pure fluid phase. Similarly, using the density ρ_s of the solid phase (particles), the Stokes number of the flow reads $St = \rho_s r^2 \dot{\gamma}/\mu_0$ and characterizes the coupling between solid and fluid phases.

Particle suspension dynamics is often simulated including rheological parametrization for non-Newtonian fluids into Navier–Stokes equations (see [13–15]). Our goal here is to develop a more fundamental model, in which the non-Newtonian viscosity of the suspension emerges naturally from the interaction between a Newtonian fluid (*i.e.* the melt) and the particles it contains (*i.e.* the crystals). LB is a well suited technique for reaching such a goal due to its capability to deal with complex physics and geometry (see [16,17] for instance). Indeed, our choice of LB method is dictated by our desire to eventually develop a three phase magma model, for instance two immiscible fluids (where LB is known to excel [18]) interacting with moving solid particles.

To the best of authors' knowledge, LB works targeted to model particle suspension under magmatic flows conditions do no exist. However, many LB works aiming at achieving direct numerical simulation of particles suspensions have been published and several are the methods proposed to simulate moving solid boundaries. In [19–21], a generalization of the bounce-back rules for moving boundaries is developed. The immersed boundary (IB) method [22,23], based on a Lagrangian point of view, is an alternative that is increasing in popularity [24,25]. In the present paper, we focus on a multi-direct forcing approach of IB which has recently been adapted to the field of LB methods [26] and that we think particularly well suited to the case where multiphase fluid phases may interact with each other and the solid particles.

In the LB literature for particle suspensions, excellent agreement with theory has been reported in [11] for $\phi < 0.5$. In [27], the authors investigate particle suspension up to $\phi < 0.2$. On the same line, Kulkarni and Morris [28] simulate suspensions with $\phi \leq 0.3$. While the aforesaid works all use rigid spheres as suspended particles, [29], coupling LB to a finite-element method for particle deformation, simulate deformable spheres as well as blood platelets and obtain good results for $\phi < 0.5$. In [30], a wide range of particle shapes are simulated and shows good agreement with other authors, and different lubrication models are compared. Whilst the aforementionned authors incorporate lubrication correction to their numerical models over a wide range of flow parameters, it should be mentioned that Shakib-Manesh et al. [10] provide good results with no lubrication model. It is thus a priori unclear if a lubrication correction should be used in the type of flow targeted by the present study.

Probably due to its less straightforward implementation, the IB method has been used more sporadically in this field. In [1] good results using IB method for spherical and deformable platelets particles are presented, while Bogner [31] apply it to a large number of spherical particles, yielding correct results for $\phi < 0.4$.

Some of the aforementioned LB studies obtain good agreement with the experimental data. However, for what concerns the relative apparent viscosity μ_r as a function of ϕ, it seems still difficult to properly model the case of very high particle concentrations, where ϕ is approaching the maximum packing fraction ϕ_M ($\phi_M \approx 0.64$ in the case of spheres). In particular, no work reports convincing results for $\phi > 0.5$. The investigation of such relationship is one of the main goals of this work.

Finally, in [8], it is stressed that slight differences in the hypotheses on which the contact and/or lubrication model are based result in substantially different outputs. A similar observation is done in [32], where the authors remark how, at high particle volume fraction, models results are extremely sensitive to nonhydrodynamic interparticle forces. The authors conclude, therefore, that the most crucial point for a successful particle suspension simulation is to employ a proper contact model. This point of view is supported by several works studying the impact of interparticle interaction on suspensions rheology. Therefore, it seems to be critical to us to be able to achieve realistic simulations using a minimum number of modeled ingredients.

2. Method

In this work we resolve the Navier-Stokes equations for an incompressible fluid using a Bhatnagar-Gross-Krook (BGK) single relaxation time collision model [33] with a D3Q19 topology. We used the Palabos open-source library [34] for all the simulations presented.

Many physical properties of magma are difficult to simulate: in the context of this work, the most extreme one is the high viscosity of the silicate melt (from 10^{-1} Pa·s to 10^6 Pa·s approximately, depending on the melt composition [35]) that makes the flow Reynolds number Re extremely low. Indeed, for $Re \ll 1$ and for fixed lattice spacing Δx and relaxation time τ, the lattice time step Δt has to be kept very small because τ is directly related to the viscosity. Discussions on the scaling of Δt for low Re can be found in [1,36]. In this study, we kept the value $\tau = 1$ and adapted Δt consequently (see Section 2.4 for a detailed description of the parameters).

2.1. Fluid-Solid coupling

Here we represent particles as rigid bodies whose motion, in absence of particle-particle interaction, follows the classical laws of mechanics as determined solely by the interaction between the fluid and a solid body. We model that by using the multi-direct forcing IB scheme [37], following the implementation presented in [26].

As a benchmark for our implementation, we used Jeffery's solution for the angular velocity $\dot{\varphi}$ of an ellipsoid with aspect ratio r_e in a shear flow with strain rate $\dot{\gamma}$ [38]:

$$\dot{\varphi} = \frac{\dot{\gamma}}{r_e^2 + 1}\left(r_e^2 \cos^2 \varphi + \sin^2 \varphi\right), \tag{2}$$

and the period T of the ellipsoid reads $T = 2\pi (r_e + 1/r_e)/\dot{\gamma}$.

In Fig. 1, we show the normalized angular velocity $\dot{\varphi}T/2\pi$ about the vorticity vector for several different ellipsoids simulated with our IB implementation against the reference solution.

2.2. Contact model

A common approach (see [11,30,32,39] for instance) to the modeling of particle-particle interaction makes use of two steps: 1) a lubrication model, which is a sub-grid model accounting for the non-resolved pure hydrodynamic effect of increasing repulsive force, that a particle experience while it approaches another solid boundary [40], and 2) an additional contact model for very close particles, supplying the lubrication model, which fails for very small gap between boundaries [8,11,30]. In some cases a third, non-physical model for extremely close or interpenetrating particles is also used [11].