NUMERICAL SIMULATIONS OF DENSE SUSPENSIONS RHEOLOGY USING A DEM-FLUID COUPLED MODEL

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Abstract. The understanding of dense suspensions rheology is of great practical interest for both industrial and geophysical applications and has led to a large amount of publications over the past decades. This problem is especially difficult as it is a two-phase media in which particle-particle interactions as well as fluid-particle interactions are significant. In this contribution, the plane shear flow of a dense fluid-grain mixture is studied using the DEM-PFV coupled model. We further improve the original model: including the deviatoric part of the stress tensor on the basis of the lubrication theory, and extending the solver to periodic boundary conditions. Simulations of a granular media saturated by an incompressible fluid and subjected to a plane shear at imposed vertical stress are presented. The shear stress is decomposed in different contributions which can be examined separately: contact forces, lubrication forces and drag forces associated to the poromechanical couplings.

1 INTRODUCTION

The rheology of grain-fluid mixtures is subject of practical interest for both industrial and geophysical applications. When the solid fraction of such mixture is high enough, i.e. in *dense* suspensions, the bulk behavior is affected by intricated phenomena combining the viscosity of the fluid phase as well as the interactions between the solid particles through solid contacts. Moreover, the contact interactions may be modified by the presence of the fluid, as described by lubrication theories. Additionaly, in transient situations,

poromechanical couplings may develop long range interactions by coupling the local rate of volume change to the pore pressure field.

Direct particle-scale modeling of this problem is a promising way to better evaluate the interactions between phases and to link the microscale properties and phenomena to the quantities measured for the bulk material, as it needs much less simplifications than former analytical developements (such as [6, 11, 1]). This modeling can be based on lubrication models [9], or more elaborated methods to reflect the fluid viscosity through pair interactions between particles [14]. This is advantageous as it does not need to actually solve Navier-Stokes (NS) equations in the fluid phase. The price to pay is that long range interactions due to poromechanical couplings are difficult to reflect. An alternative is to really solve NS in the fluid phase using a CFD solver, or to use a lattice-Boltzman model [7]. It is to be noted that direct resolution of NS does not eliminate the need for a proper modeling of the lubrication forces, due to mesh size dependencies [8]. The main difficulty associated to this approach is the high computational cost, so that following large deformations of thousands of immersed particles in 3D remains a challenging task.

A new method to simulate fluid-particle interactions has been developed recently and may be of some help to tackle the computational challenge [3]. In this method, the solid phase is modelized with the discrete element method (DEM), and the fluid flow is solved using a pore-scale finite volume method (PFV). The key aspects of this DEM-PFV coupling are recalled in the first part of this paper. It was implemented in the open source code Yade-DEM [12]. Extensions of this method in order to study dense suspensions are being undertaken by the first author. Namely, the original model lacks a coupling term to link the fluid forces to the deviatoric strain, as explained in section 2.2. We also generalized the boundary conditions in order to allow very large deformations of the suspension in simple shear. Typical results of the preliminary enhanced model are presented in the last part.

2   NUMERICAL MODEL

2.1   Original DEM-PFV Coupled Model

Our DEM approach defines the mechanical properties of the interaction between grains whose shape is assumed to be spherical. Following Newton's laws, the positions of particles are updated and calculated at each time-step of the DEM simulation. As introduced in [4], the PFV formulation is based on a simplified discretisation of the pore space as a network of regular triangulation and its dual Voronoi graph (1).

This network simplifies the formulation and resolution of the flow problem. The continuity equation is expressed for each pore, linking the rate of volume change of one tetrahedral element $\dot{V}_i^f$ to the fluxes q_{ij} through each facet. Each flux can be related to
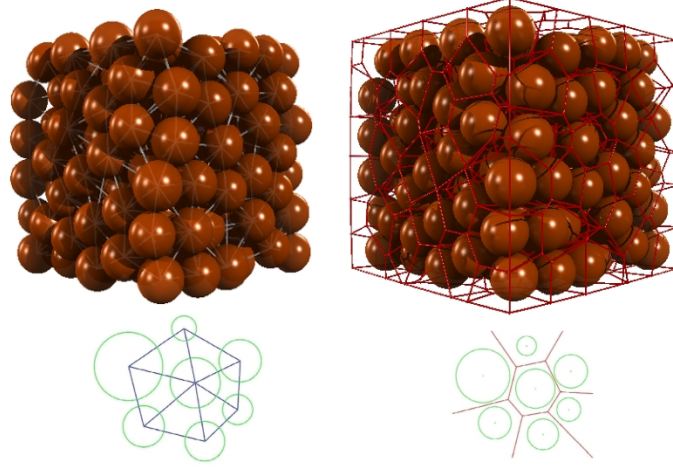
Figure 1: Regular triangulation (left) and Voronoi graph (right).

the pressure jump between to elements via a generalised Poiseuille's law, so that

$$\dot{V}_i^f = \sum_{j=j_1}^{j_4} q_{ij} = K_{ij}(p_i - p_j) \tag{1}$$

couples the particles velocity to the fluid pressure field. The expression of conductivity K_{ij} has been validated recently by comparisons with glass beads experiments [10].

The total force exerted by the fluid on particle k can then be defined as [5]:

$$
\begin{aligned}
F^k &= \int_{\partial \Gamma_k} \rho_k \Phi(x) nds + \int_{\partial \Gamma_k} pnds + \int_{\partial \Gamma_k} \tau nds \tag{2} \\
&= F^{k,buoyancy} + F^{k,pressure} + F^{k,viscous} \tag{3}
\end{aligned}
$$

2.2 Lubrication Forces

As classical poromechanics, the original DEM-PFV model takes into account the isotropic part of the stress and strain tensors (pressure and divergence of solid phase velocity) in the coupling (eq. 1 in our case). The contribution of the fluid to the bulk shear stress is de facto neglected. It is worth noting that the shear part of the coupling is similarly lacking in discrete models inspired by the coupling equations of poromechanics, such as the continuum-discrete methods [15, 16].

In order to deal with sheared suspensions, another viscous contribution has to be introduced for modeling the shear stress. Various ways may be used for this purpose such as viscous forces obtained in the framework of the lubrication theory developed by Van Den Brule [11]. The shear lubrication force defined by equations 4 seems to be in concordance with the formulation obtained by the Finite Element Method (the Stokes solver of Comsol is used for this purpose). Results of this comparaison performed on a

simple configuration of a sphere rotating at a given angular velocity in a regular assembly of identical particles, are shown in figure (2).
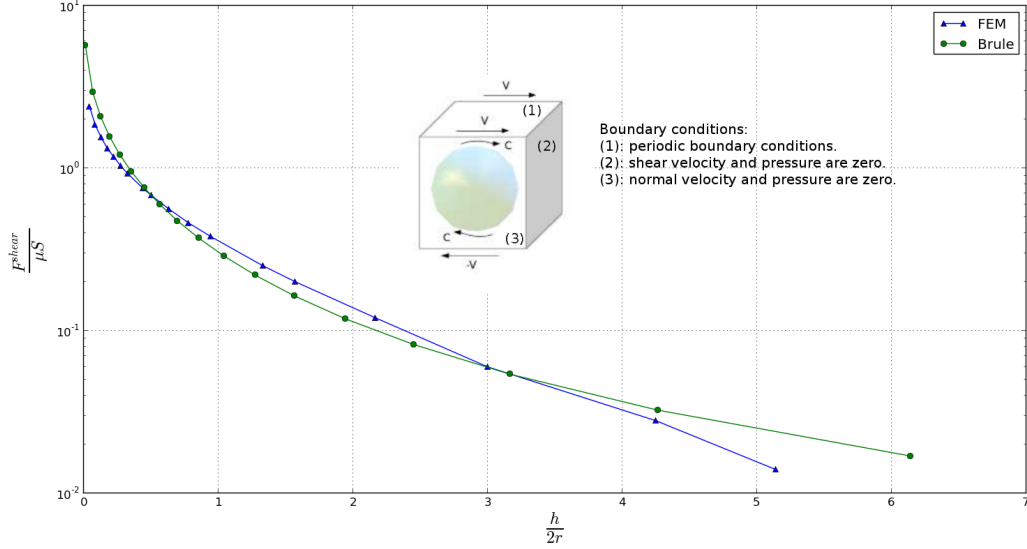

Figure 2: Comparaison of viscous shear forces for the case of rotating sphere in a regular assembly of particles. h is the surface-to-surface distance and r is the particles radius.

$$F_{shear}^{lub} = \frac{\pi\mu}{2}(-2r + qln(\frac{q}{h}))v_t \qquad and \qquad F_{normal}^{lub} = \frac{3}{2}\pi\mu\frac{r^2}{h}v_n \qquad (4)$$

μ is the fluid viscosity, r the particle's radius, q the distance between particles,h is the surface-to-surface distance and v_t and v_n are respectively the shear and normal velocity of the particle.

The normal interaction between two elastic-like particles in a viscous fluid is described by the Maxwell visco-elastic scheme (figure 3) which combines a spring of stiffness k in series with a pad of viscosity η. This combination between the lubrication and the elasticity is close to that adopted by Rognon [9]. The force generated from this model is then: $F = ku_e = \nu\dot{u}_v$ where k is the model's stiffness, u_e is the elastic displacement, u_v is the viscous displacement ($u = u_e + u_v$ is the total displacement) and ν is the instantanious viscosity of the model defined, using the equation 4 as:

$$\nu = \frac{\frac{3}{2}\pi r^2 \mu}{u_v}.$$

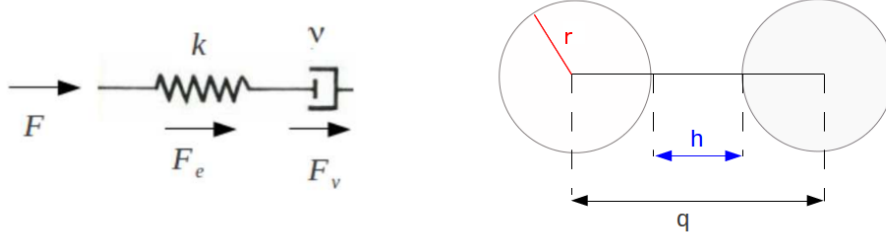By equalizing the elastic force and the viscous force, we have:

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Figure 3: Visco-elastic scheme.

$$
\begin{aligned}
ku_e &= \frac{\frac{3}{2}\pi r^2 \mu}{u_v}\dot{u}_v \\
&= \frac{3}{2}\pi r^2 \mu \frac{(\dot{u} - \dot{u}_e)}{u - u_e} \\
&= \frac{3}{2}\pi r^2 \mu \frac{(\dot{u} - \frac{\dot{F}}{k})}{u - \frac{F}{k}}
\end{aligned}
\tag{5}
$$

Using the finite difference method, F can be written as $F = (F^+ - F^-)/\Delta t$ ($F^+ = F(t + dt)$ and $F^- = F(t)$). By substituting this relation into equation 5, we obtain:

$$
F^+ = \frac{3}{2}\pi r^2 \mu \frac{(\dot{u} - \frac{F^+ - F^-}{k\Delta t})}{u - \frac{F^-}{k}}
\tag{6}
$$

When we express F^+ as a function of F^-, the normal lubrication force is:

$$
F = F^+ = \frac{\nu(\dot{u} + \frac{F^-}{k\Delta t})}{1 + \frac{\nu}{k\Delta t}}
\tag{7}
$$

2.3 Periodic Boundary Conditions

As the system is considered infinite in the flow direction, some problems can arise from the boundary effects in the numerical simulation. In order to avoid such problems, periodic boundary conditions are implemented in the PFV model (figure 4) (the periodicity for the DEM part was developped independently [13]). Denoting by $\mathbf{S} = [s_1, s_2, s_3]$ (figure 4)

the period size in the three dimensions and by $\mathbf{i} \in \mathbb{N}^3$ is the distance between one point of coordinates $\mathbf{r}$ and its periodic image $\mathbf{r'} = \mathbf{r} + \mathbf{S} \cdot \mathbf{i}$ in an adjacent period, then the pore pressure is expressed as follow:

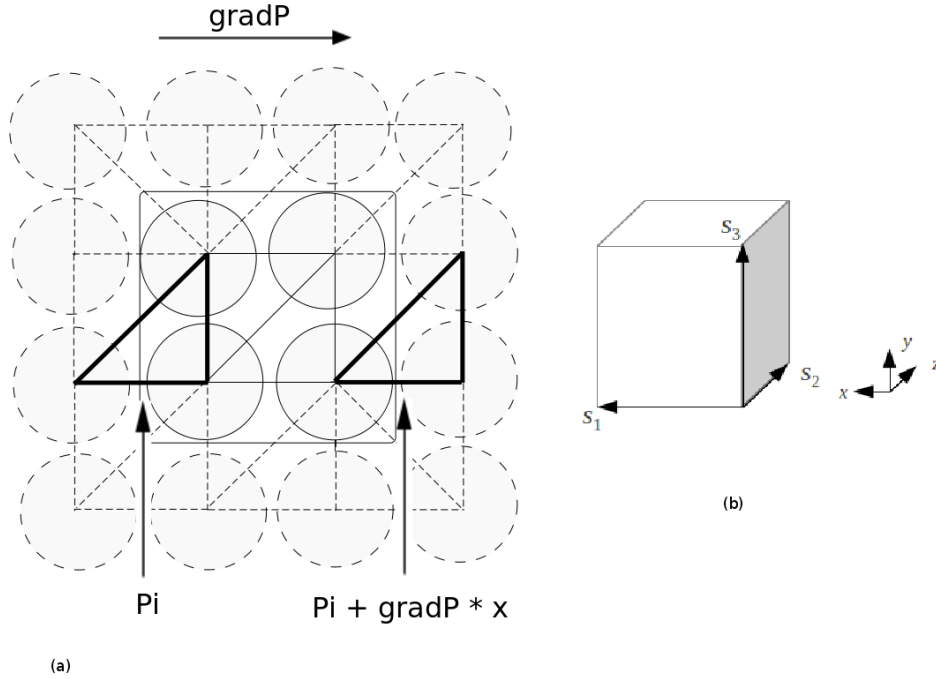$$p' = p + \bigtriangledown p \cdot \mathbf{S} * \mathbf{i} \tag{8}$$

Figure 4: 2D periodic cell

3   NUMERICAL RESULTS

We generate an assembly of N=500 frictional grains of average diameter $d = 0.14 \pm 0.03$, density $\rho = 2500$ and friction angle $\Phi = 30$. The assembly (Figure 5) is H=13d high, L=9d large and l=9d wide. The granular material is first confined under a constant pressure P, then sheared without gravity, between two parallel walls distant from H and moving at a velocity $\pm V/2$ respectively. In order to satisfy a quasi-static regime, V is chosen to be small so that the inertial number $I = d\dot{\gamma}\sqrt{\rho/P}$ is less than 10^{-3}.
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Simulations of such an assembly saturated of an incompressible fluid of viscosity μ and submitted to a simple shear with shear rate $\dot{\gamma} = \frac{dV}{dH}$ at imposed vertical pressure P
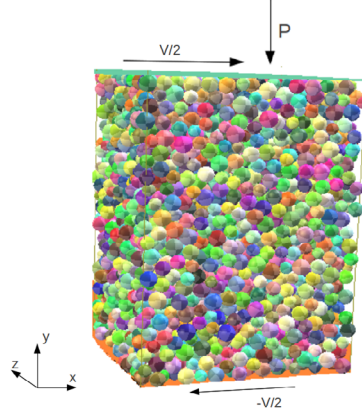
Figure 5: Simulation cell. The boundary conditions are: $u_x = V/2$, $\sigma_{yy'} = P$, $u_z = 0$ and fluid pressure is zero. Periodic boundary conditions are applied in the x and y directions.

are presented. The viscous stress is decomposed in different contributions which can be examined separately: contact forces, lubrication forces and drag forces associated to the poromechanical coupling.

Figure 6 shows the different contributions of each force applied on the granular media. Contrary to what is sometimes postulated in the litterature, our numerical results show that tangential lubrication forces are significant compared with the normal ones. The total shear stress applied on the material, being dry in the first stage, increases twice when the normal lubrication force is applied. The shear lubrication force, added after, is not negligeable; it participates with around 80% of the normal contribution. This result is interesting as tangential lubrication forces usually neglected compared with the normal ones (e.g. Rognon et al [9])

4   CONCLUSIONS

In this contribution, we presented a new hydromechanical coupled model able to describe the behavior of dense granular materials subjected to a shear flow under constant pressure. Contrary to what is sometimes postulated in the literature, the tangential lubrication forces are significant compared with the normal ones. The proposed numerical model is able to describe the behavior of dense suspensions; the friction and dilatancy laws $\mu(I_v)$ et $\Phi(I_v)$, respectively, will be compared to experiments and rheological model from the litterature [2] in future work.
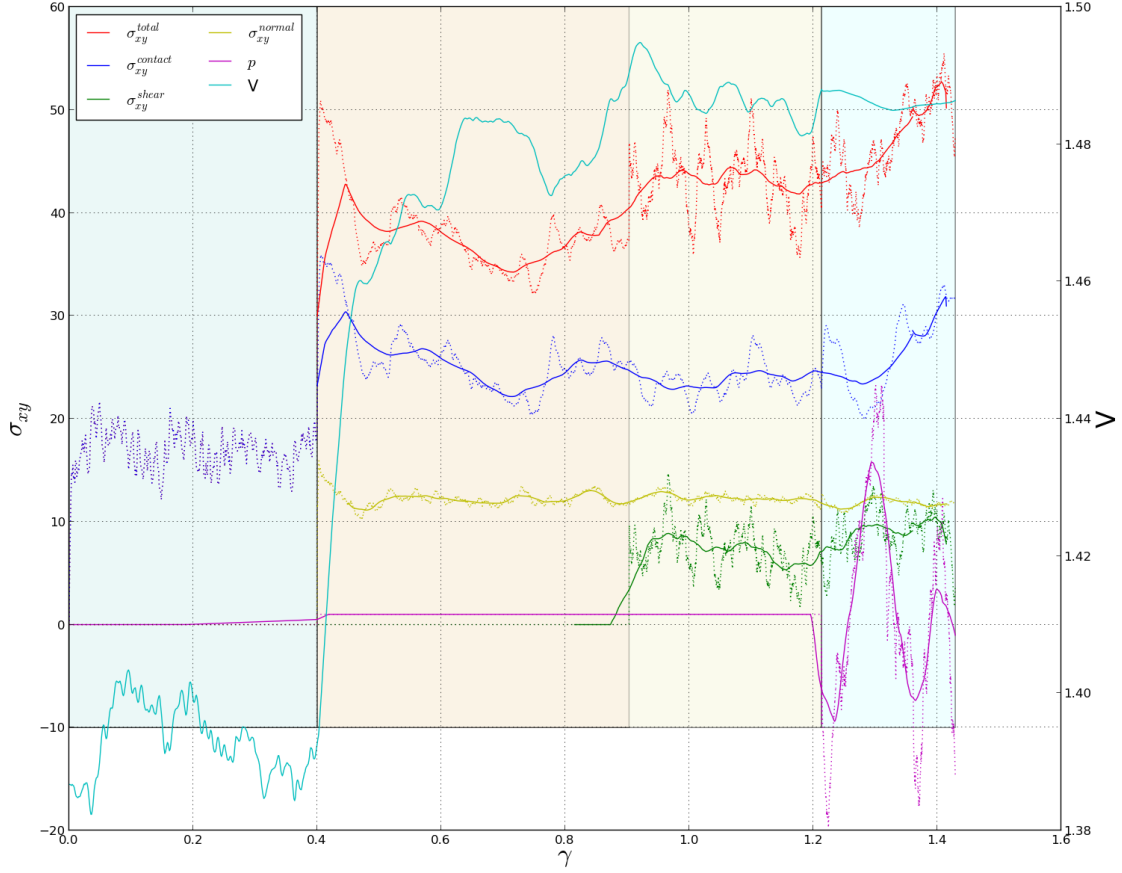
Figure 6: Shear stress applied on the granular media function of the shear rate. In a first stage we generate a dry material. Normal lubrication forces are added when 40% of skeleton's deformation are reached. Shear lubrication forces are applied then. Finally, pressure forces associated to the poromechanical coupling are applied.

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