

Numerical methods for flows of immersed grain clusters

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²Mouais, à voir.

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CHAPTER 1

Introduction

ἔν οἶδα ὅτι οὐδέν οἶδα
I know that I know nothing.

— Σωκράτης - Socrates.

Whether the reader knows it or not, immersed granular flows are actually implied in many aspects of their everyday life. As it turns out, in terms of number of metric tons, granular matter is the second most manipulated type of material in the world, the first being water (de Gennes (1999)), and in many cases this granular matter is mixed with a fluid phase. Some examples are trivial, such as the bowl of cereals with milk in the morning or the cooking of macaroni in boiling water for supper, but some others are not. In the mining industry, the processes to refine the raw ores of copper, iron or lithium often include an immersion in a liquid (Myburgh (2010)). These materials are in turn used in our phones, cars, computers and various appliances we use every day. In the construction sector, the recycling of concrete involves crushing for reuse as aggregate. In order to improve the physical properties of the obtained fragments, a hot gas rich in carbon dioxide is passed through them to absorb it (Harifidy et al. (2022)). In many chemical reactors, the reactants are in a fluid form and go through a bed made of solid grains that serve as catalysts to increase the performance of the reaction (Luo et al. (2016)). It is with these kind of processes that the drugs we use to cure our illnesses are produced.

The fermentation process for the brewing of the beer we might enjoy on a Friday night requires the mixing of solid yeast grains with liquid water (Klembt et al. (2021)). To some extent, even blood circulation can be a relevant example, with the solid platelets flowing in the liquid plasma (Yamaguchi et al. (2010)). At an even larger scale, immersed granular flows are implied in some of the disasters that can wreak havoc on entire cities and have terrible consequences in terms of economic costs and human lives. Indeed, avalanches, landslides and debris flows are common natural phenomena all around the globe, often caused by heavy rain or earthquakes (Conte and Troncone (2012)). One of the deadliest volcanic hazard occurs when ashes suspended in hot gas flow downhill at the tremendous speed of 30 m/s in what is called a pyroclastic flow (Auker et al. (2013)). As can be seen, immersed granular flows can be found at a wide range of scales and in many different high-stakes applications.

But what exactly are immersed granular flows? Obviously, they imply a granular material and a fluid phase. A granular material can be defined as a large collection of interacting particles, called the grains, whose sizes range from $1\mu\text{m}$, so that they are athermal (i.e. not sensitive to thermal motion), to several meters in the rings of Saturne and asteroid belts. Such a granular material is said to be immersed when it interacts with a surrounding fluid phase, which can be gaseous or liquid, in a way that significantly modifies its behaviour compared to the dry case. As it may often happen, behind such a simple definition is a very complex matter that was the subject of many studies mobilising thousands of researchers across decades (Radjai et al. (2017)). As a matter of fact, dry granular materials are in themselves quite peculiar, being able to flow like a liquid and resist shear like a solid. In the immersed case, the interactions between the grains and the fluid can be very diverse in nature and further complexify the behaviour of the material.

In view of this, the tremendous rise in the use of numerical methods to try and understand and model them does not come as a surprise. Numerical methods indeed present several crucial advantages over real life experiments. They allow the study of large size systems at a much reduced cost since available space is not a limiting factor. Moreover, they offer a complete control of all the physical parameters relevant to the system, such as boundary conditions, grain size and polydispersity, friction coefficients and so on. They also provide a total reproducibility of the results as the initial position of each grain can be set precisely. Finally, they give a unique insight on properties and details that are difficult to observe: the fluid flow can be determined to track the transport of a reactant, or the forces between each pair of grains in contact can be computed to obtain the contact network and the stress state inside the grains. Although numerical methods can be very powerful tools, they still require some calibration, or at least a validation to ensure the results they yield can be trusted. Therefore, a generally good investigation strategy would be to

calibrate a numerical model with a small-scale experiment, and then use it to study the considered system in the conditions of interest.

In front of the complexity of the subject and of the wide span of the dedicated research, it seems very difficult to accurately present a complete state of the art. However, it is the avowed objective of this introduction chapter to try and give a sufficient glimpse on the matter so that the reader has in mind a global picture of the subject in which this thesis takes its place. To do so, the current chapter will start by presenting the main features of dry granular materials. As will be seen, the discrete nature of this kind of media gives rise to a wide range of peculiar behaviours, in which friction and grain shape often play a major role. Afterwards, the influence of a surrounding fluid on the already complex granular media will be explored. Focus will be set on the effects of the fluid on individual grains and on the special behaviours of granular suspensions. Next, the principal numerical modelling approaches will be presented, with their strengths and weaknesses, and the model used in this thesis will be highlighted. Lastly, a brief overview of the objectives of the thesis is presented.

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1.1 Many brains for many grains

Since granular materials are ubiquitous, they have been used and manipulated by humankind for centuries and even millenia, for example in construction in ancient Egypt (Chaabane et al. (2022)). One of the first scientific publications regarding granular matter was made by Coulomb, who wanted to model the behaviour and failure properties of granular assemblies at rest (Coulomb (1773)). Ever since, the interest of the scientific community for the subject kept growing, especially in the late second half of the twentieth century with the rise of appropriate numerical tools. To this day, the field of granular materials has expanded in many different directions whose links between them are not always clearly determined, a unified approach still being difficult to establish (Radjai et al. (2017)). The goal of this section is to introduce the reader to some of the most important features of granular materials among the many peculiar ones they exhibit. At first, granular materials in dry conditions are considered, so that the features that are intrinsic to them are pointed out. Then, the effects of a surrounding fluid on the grains and the interactions between both phases are highlighted.

1.1.1 Dry conditions

One of the most striking features of granular materials is that they can behave similarly to the three most common states of matter found on Earth, i.e. gaseous, liquid and solid, and yet with significant differences from their classical counterparts. Their so-called state mainly depends on the shear rate they are subjected to and on the nature of the contacts between the grains (Goddard (2014); Forterre and Pouliquen (2008)). Sometimes, all three states can be observed in the same application, as in an hourglass for example (see Fig. 1.1).

In a granular gas, the grains are dilute and rapid and interact via instantaneous, binary collisions. This state is shown in the middle row of the right part of Fig. 1.1. The main difference with classical gases is that since the collisions are inelastic and dissipate energy, a constant supply of energy (for example in the form of vibrations) is necessary to sustain it. Otherwise, grain clustering and inelastic collapse – an infinite number of collisions in a finite time – take place (Jaeger et al. (1996); McNamara and Young (1994)) and the material transitions to a liquid or even solid-like state. At lower shear rates, the grains are denser and start to interact via frictional contacts as well, and a fluctuant contact network appears. This is the liquid-like state, or inertial regime, depicted in the top right part of Fig. 1.1. In this state, the material behaves like a non-newtonian fluid (Pouliquen et al. (2006)). As the shear rate further decreases, the grains now almost only interact via lasting frictional contacts, and the contact network is persistent. This is the solid-like state, or quasi-static regime (Roux and Combe (2002)). It is shown in the bottom right of Fig. 1.1.

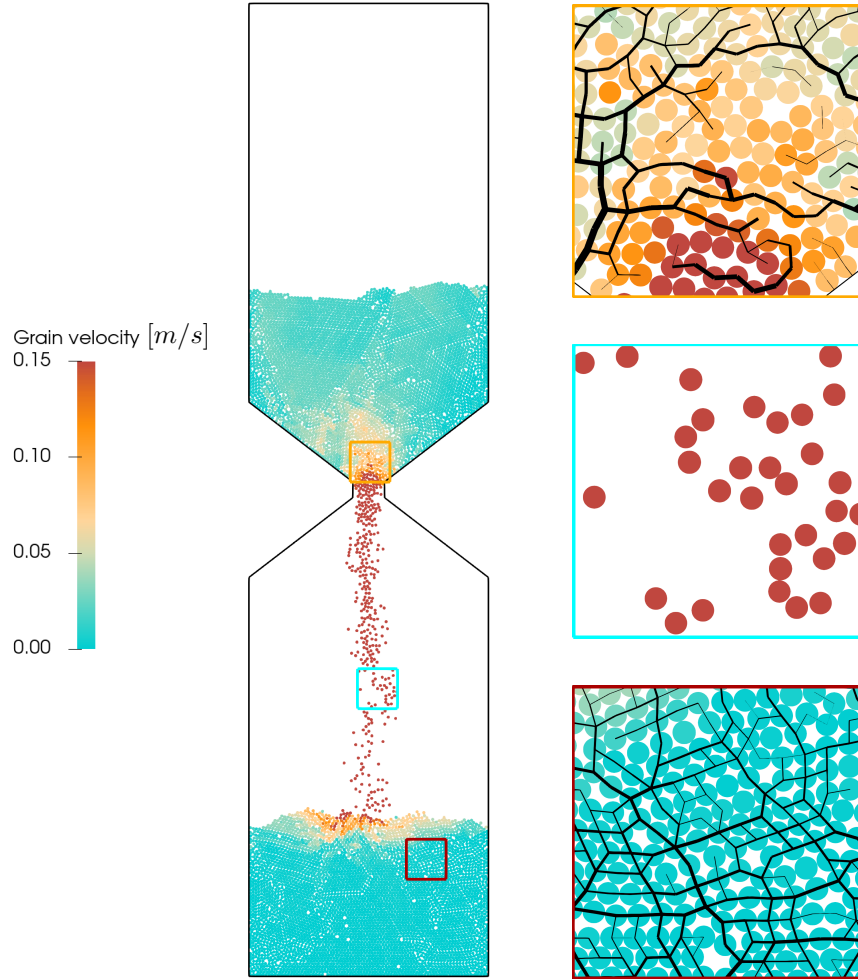


Fig. 1.1: Left: dry granular flow in an hourglass. Top – right: enlargement showing the granular liquid state. Top – middle: enlargement showing the granular gaseous state. Top – down: enlargement showing the granular solid state. The contact network is shown in black. The wider the line, the larger the contact force between two grains.

In what follows, the focus is set on the last two states, i.e. liquid-like and solid-like. The divided nature of granular media implies that the stress state and force transmission inside them is dependent on their microstructure, and vice-versa. When subject to external constraints, the forces inside the granular material are transmitted through a contact network which is heterogeneous and changes much on a scale close to the particle scale. This network can be seen as the sum of two different contributions : a strong network and a weak network. The strong network comprises the forces that are larger than the average contact force, while the weak network concerns the forces that are lower. Although the majority of the grains belong the latter, which carries the average pressure and dissipates energy through sliding contacts, it is the former that carries the majority of the load with nonsliding contacts (Radjai et al. (1998)). The strong network also tends to be more anisotropic than the weak one, and to align with the direction of the principal compressive stress (Peters et al. (2005)). The number of contact forces larger than the mean exhibits an exponential decay, while the contact forces lower than the mean decrease as a power law (Radjai et al. (1996)). The shape of the grains has a strong influence on the mechanical properties of the material. As it departs from spherical, the anisotropy of the force tensor increases, and so does the mobilisation of friction, which leads to an increase in the shear strength of the material (Azéma and Radjaï (2009, 2010)). It is to note that the force and fabric tensors are most of the time different. The former concerns the orientation of the contact forces, while the latter involves the center-to-center vectors, also called the branch vectors. It is only for frictionless spherical grains that both are equivalent.

In general, the contact network and the microstructure are history dependent, because of the frictional nature of the contacts between the grains. Indeed, according to the type of loading the grains were subjected to, the distribution of the normal forces and the correlation length of the contacts can be different (Majmudar and Behringer (2005)). However, if the external load is sustained for a sufficiently long time, the material reaches a state where its past history is completely irrelevant (Roscoe et al. (1958)), even if this can be localised for example in specific shear bands (Radjai et al. (2017)). This state, labeled the critical state, is usually described by two variables that correspond to a stress ratio and a packing fraction (Schofield and Wroth (1968)). The grain shape has a significant influence on the critical values of the aforementioned variables corresponding to the critical state. For example, the more irregular the grains, the less compact their critical state is at a given stress ratio (Jerves et al. (2016); Nie et al. (2021)). The behaviour of the material can then be characterised based on the distance between its current state and its critical state (Radjai et al. (2017)). First observed by Reynolds, dilatancy is a good illustration of this feature (Reynolds (1885)). This property typical to granular media implies that under shearing at constant pressure they will expand if they

are denser than their critical state for the corresponding stress or contract if they are looser.

Upon adequate conditions, a granular material can undergo jamming. Jamming consists in an abrupt transition from a liquid-like state to a disordered solid-like one that is out of thermodynamic equilibrium. Although often seen as a phenomenon with negative consequences, it can actually be caused by design for applications such as soft robotics and architecture (Jaeger (2015)). But what are adequate conditions? The onset of jamming depends, in athermal systems such as granular assemblies, on the applied shear stress and on the packing fraction ϕ_g . Intuitively, if no shear stress is applied, the material will not deform and is hence considered as jammed. Conversely, there exists a given packing fraction ϕ_{gm} above which the material inevitably jams, no matter the applied shear stress (Liu and Nagel (1998)). This point has been shown to depend on the history of the material and the intergrain friction (Chaudhuri et al. (2010)). As jamming also results from steric exclusion, the shape of the grains can change the critical packing fraction or cause jamming anisotropy (Börzsönyi and Stannarius (2013)). In between the two extremes, a given amount of stress that depends on the packing fraction must be applied to overcome the jamming of the grains. Phase diagrams have therefore been established in the plane $1/\phi_g, \tau$ with τ the applied shear stress (Behringer and Chakraborty (2018)). It should be noted that, although shearing will tend to unjam the material, it can also have the opposite effect. Because of the dilatancy, shearing at constant volume can cause a jamming of the material since it is prevented from expanding as it would normally do to reach its critical state. This shear-jamming occurs at packing fractions lower than the critical packing fraction (Bi et al. (2011)).

A typical example of a jammed granular material is a sand pile. The ability to form such heaps and resist the shear from gravity is one of the most obvious properties of granular matter. The stability and shape of those heaps is directly related to the so-called angle of repose of a given granular media, which corresponds to the angle of the steepest stable slope of the free surface of the material that can be formed when it is at rest. This property is of interest in various fields such as geotechnical engineering or numerical model calibration (Al-Hashemi and Al-Amoudi (2018)), and even entomology for the behavioural study of antlions which hunt ants by luring them into sand pits (Botz et al. (2003)). Many different methods exist to measure this property, that are somewhat linked to the application in which it is to be used. In general, both a static and a dynamic angle of repose can be defined. They can be distinguished as the angle at which the material starts to flow and the one at which the flow stops (Kleinhans et al. (2011)). The angle of repose is influenced by many parameters, such as the grain shape, the particle size or the inter-grain friction. It increases with greater irregularity in shape, smaller grain size, and higher friction. It is important to note that the angle of repose

is linked, but not equivalent to the angle of internal friction, which corresponds to the angle between the normal and the resultant force at failure upon shearing of the material, and to the interface friction angle, which corresponds to the arctangent of the friction coefficient between two grains (Al-Hashemi and Al-Amoudi (2018)).

To summarise, dry granular matter on its own exhibits many behaviours that are at the boundary of several states of matter, with their own specificities that sometimes defy common intuition. Their properties notably depend on their density, their past deformation history, the grain shape, and the intergrain friction to name a few. Although the rough approximation of frictionless spherical grains is able to reproduce some of the behaviours of granular materials (Roux (2000); Peyneau and Roux (2008)), those last two features thus appear to be of significant importance when building a model from the microscopic, grain-scale point of view.

1.1.2 Influence of a surrounding fluid

Oftentimes, granular materials happen to be mixed with a certain amount of fluid. Sometimes by chance, because of the rain or even because of the condensation of water from the relative humidity of the air (Bocquet et al. (1998)). Sometimes on purpose, as in industrial granulation, a process where a binding fluid is added to a granular material to form clusters (Iveson et al. (2001)). Most times the surrounding fluid is a liquid, but it can also be a gas, for example in fluidised bed reactors (Deen et al. (2007a)).

The effects of an interstitial fluid on a granular medium mainly has two different origins: the change in the contact interface between the grains and the forces that the fluid phase applies on each grain individually. Concerning the change at the contact interface, cohesion and lubrication are the main phenomena involved. While lubrication can appear for both liquids and gases, cohesion is due to capillary forces and hence only concerns liquids. In general, lubrication tends to fluidise the granular phase and reduce the contacts between the grains. The occurrence of cohesion depends on the fluid content, from which four different states can be distinguished (Newitt (1958)):

- At low liquid contents, the granular material is in the pendular state, where liquid bridges form between the grains.
- At intermediate liquid contents, the material is in the funicular state, where some of the pores are entirely filled with liquid.
- At high liquid contents, the material is in the capillary state, where all the spaces between the grains are filled with liquid whose pressure is below the one of the air and whose surface forms menisci.

- Further increasing the liquid content leads to a fully immersed granular material, where all capillary effects disappear.

Because of cohesion, the angle of repose of the granular material linearly increases with the liquid content, and can sometimes exceed 90° which enables the construction of sandcastles on the beach (Hornbaker et al. (1997); Halsey and Levine (1998)). However, the cohesion ends up saturating (Richefeu et al. (2006)), and with it the angle of repose. As cohesion first increases and then saturates with the liquid content, the critical density for the jamming of wet grains is first reduced and then increased, implying an optimal liquid content for jamming (Mitarai and Nori (2006)).

When immersed in a fluid flow, a grain can undergo various hydrodynamic forces that originate from a relative velocity or acceleration or from pressure gradients, for example. Most often, the expressions of these forces are quite complicated and strongly depend on the flow characteristics, and analytic expressions are rarely obtained, except in some simplified cases. Those forces on a single grain can be listed as follows (Crowe et al. (2011)):

- The drag force: it comes from the relative velocity between the grain and the fluid, and acts in the opposite direction so as to ultimately cancel it. At Reynolds number smaller than 1, the analytical solution of the flow past a spherical grain was derived by Stokes (Stokes et al. (1851)), implying a linear dependency on the relative velocity. When the Reynolds number increases, inertial terms cannot be neglected, and a square dependency appears. The main difficulty consists in modelling the proportionality coefficient between the square of the relative velocity and the drag force. It strongly depends on the flow characteristics, including turbulent effects and grain shape.
- The pressure gradient force: this force originates from a difference in pressure along the boundary of the grain. Assuming the pressure gradient is constant on the scale of the grain, the magnitude of the related force is obtained as the product of the grain volume and the pressure gradient. If the considered pressure is only hydrostatic, this term corresponds to buoyancy. This force does not depend on the shape of the grain.
- The Saffman force: it comes from a velocity gradient around the grain giving rise to pressure differences, as a faster fluid exhibits a lower pressure (Saffman (1965)). This results in a lift force in the direction of increasing flow velocity. It is proportional to the relative velocity between the grain and the fluid and to the size of the grain.
- The Magnus force: it comes from the rotation of the grain that, combined with the flow velocity, creates a difference in velocity at the opposite points of the boundary of the grain and hence a pressure difference

(Magnus (1853)). It is proportional to the size of the grain, its angular velocity and the relative velocity between the fluid and the grain.

- The added mass force: it comes from a relative acceleration between the fluid and the grain, since in order to accelerate the grain has to accelerate the surrounding fluid. It is called that way because mathematically it results in adding a term to the mass of the grain that is proportional to the volume of displaced fluid. This force is hence relevant if the grain density is not too large compared to the fluid density.
- The Basset force: it results from a delay between the establishment of the flow in the boundary layer at the surface of the grain because of viscous effects (Basset (1888)), and is therefore also called the history term. It is proportional to the square root of the fluid density and dynamic viscosity and to the integral over time of the change in the relative velocity between the grain and the fluid.

In an immersed granular assembly, those hydrodynamic forces compete with grain inertia and contact forces. Depending on the type of problem and on the physical properties of both the grains and the fluid, the relative importance of these forces change, so that some of them may not be significant (this point will be further discussed in the next chapter when the model for the fluid-grain interaction force is explained). For example, the collapse dynamics of immersed grain columns can be characterised by the Stokes number and the density ratio $r = \sqrt{\rho_g/\rho_f}$, with ρ_g and ρ_f the grain and fluid density, respectively. The Stokes number $St = \rho_g \dot{\gamma} d^2 / \eta$ is the ratio between particle inertia and fluid viscous effects, with d the grain diameter, $\dot{\gamma}$ the shear rate to which it is submitted (for a column collapse it can be estimated as $\dot{\gamma} = \sqrt{g|\rho_g - \rho_f|/2d\rho_g}$) and η the fluid dynamic viscosity. When $St \gg 1$ and $r \gg 1$, the fluid phase almost has no effect on the granular phase, and the column collapses as in dry conditions in the so-called free-fall regime. When $St \gg 1$ and $r \ll 1$, the fluid phase dominates the flow in the so-called inertial regime. When $St \ll 1$, both the grains and the fluid influence the flow in the so-called viscous regime.

Just as the fluid phase acts on the grains, the grains act on the fluid phase. The immersed grains, because of the perturbations they induce in the flow of the fluid, modify the effective viscosity of the latter. At low grain packing fraction ($\phi_g < 0.1$), i.e. when the interactions between the grains play a minor role, models were established that predict a dependency of the effective viscosity as a quadratic function of the packing fraction (Einstein (1905); Batchelor and Green (1972)):

$$\eta_e = \eta(1 + 2.5\phi_g + 7.6\phi_g^2).$$

At high densities however, the interactions between the grains cannot be neglected anymore. Moreover, above a given packing fraction the granular phase becomes jammed and the effective viscosity diverges to infinity. One of the

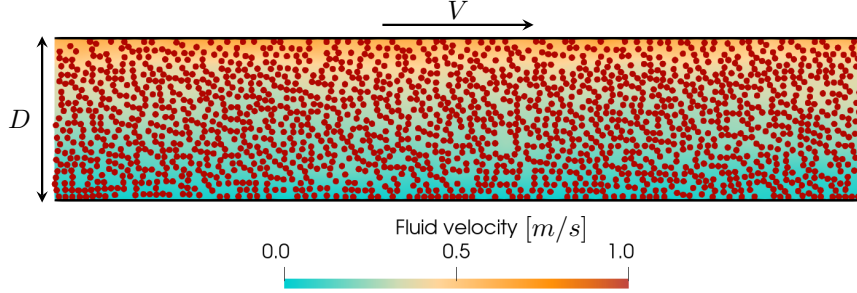


Fig. 1.2: Shear of a granular suspension at constant volume fraction $\phi_g = 0.45$ and shear rate $\dot{\gamma} = V/D = 10$.

most used models to account for this is the Krieger-Dougherty law (Krieger and Dougherty (1959)):

$$\eta_e = \eta(1 - \phi_g/\phi_{gm})^{-n}.$$

In general, the maximum packing fraction ϕ_{gm} and the exponent n are fitting parameters than can be tuned to recover the Batchelor law at low ϕ_g (Ovarlez et al. (2006)). Besides jamming, other typical granular behaviours can influence the fluid phase. For example, the pore pressure feedback mechanism results from the dilatancy of granular materials (Rondon et al. (2011); Iverson et al. (2000)). If the grains are in a dense state, they will expand so that they reach their critical state defined in the previous section. This creates a negative pore pressure between the grains that sucks fluid in, pushing the grains against each other and enhancing frictional interactions between them. If the grains are in a loose state, they will contract, resulting in a positive pore pressure that squeezes fluid out, lubricating the contacts between the grains.

As such, the interactions between both solid and fluid phases can give rise to complex macroscopic behaviours. Dense granular suspensions can behave as a non-Newtonian fluid, even if the surrounding fluid is newtonian. When sheared at a controlled granular pressure, the suspension can undergo shear-thinning, i.e. a reduction in its viscosity with the shear rate, because of the dilatancy of the granular phase that reduces its volume fraction and hence the effective viscosity of the fluid (Boyer et al. (2011)). When sheared at a constant volume fraction (see Fig. 1.2), it exhibits shear thickening, i.e. an increase in the effective viscosity with the shear rate (Trulsson et al. (2012)). In this configuration, the distinction between the newtonian regime and the shear thickening one can be made on the basis of the interactions between the grains (Fernandez et al. (2013)). At low shear rates, the contact between particles are lubricated and the energy dissipation is essentially due to viscous processes in

the fluid, leading to a newtonian behaviour. At high shear rates, the contacts are mostly frictional and the energy dissipation is mainly due to the contacts between the grains, leading to a shear thickening behaviour. Depending on ϕ_g , this shear thickening can be either continuous (i.e. smooth) or discontinuous (i.e. steep). When ϕ_g is below the maximum volume fraction for the frictional contact regime ϕ_{gm}^f which is in turn lower than the maximum volume fraction for frictionless spheres ϕ_{gm} , a smooth, continuous shear thickening takes place as energy is dissipated by the contacts. When $\phi_{gm}^f < \phi_g < \phi_{gm}$, no inertial regime can take place and the systems undergoes a steep discontinuous shear thickening as shear jamming occurs (Seto et al. (2013)).

Although already complex by themselves, granular materials become even more difficult to study and describe when they are mixed with a fluid because of the many different interactions they exhibit. These interactions and the challenge they represent are often key to the development of adequate models, that require a careful balance between including relevant ones and ruling out insignificant ones for the considered application.

1.2 All models are wrong, but some are useful

Generally attributed to the British statistician Georges Box (1919-2013), the above sentence is a very good illustration of why many different modelling approaches have been developed concerning immersed granular materials. Given their vast complexity and the different scales of the phenomena from which this complexity arises, a single unified theory that fully and accurately describes immersed granular flows is yet to be found. However, by considering a judicious balance between the required level of detail and the available computational resources, it is possible to obtain a satisfying model that focuses on a given type of problems.

Three kinds of models can be distinguished when it comes to immersed granular flows: two fluids models, direct numerical simulation models, and multiscale models.

Two fluids models consider the granular phase as a continuous one, smoothing out the details from the grain scale (see Fig. 1.3 top). The resulting low computational cost explains their dominant use in large scale geophysical applications, such as landslides (Li et al. (2020)), submarine avalanches (Si et al. (2018)) or volcanic eruptions (Neri et al. (2022)). This continuous approach requires constitutive laws for the granular phase, which can be obtained with various methods and assumptions (Gidaspow (1994); Papalexandris (2004); Montellà et al. (2021)).

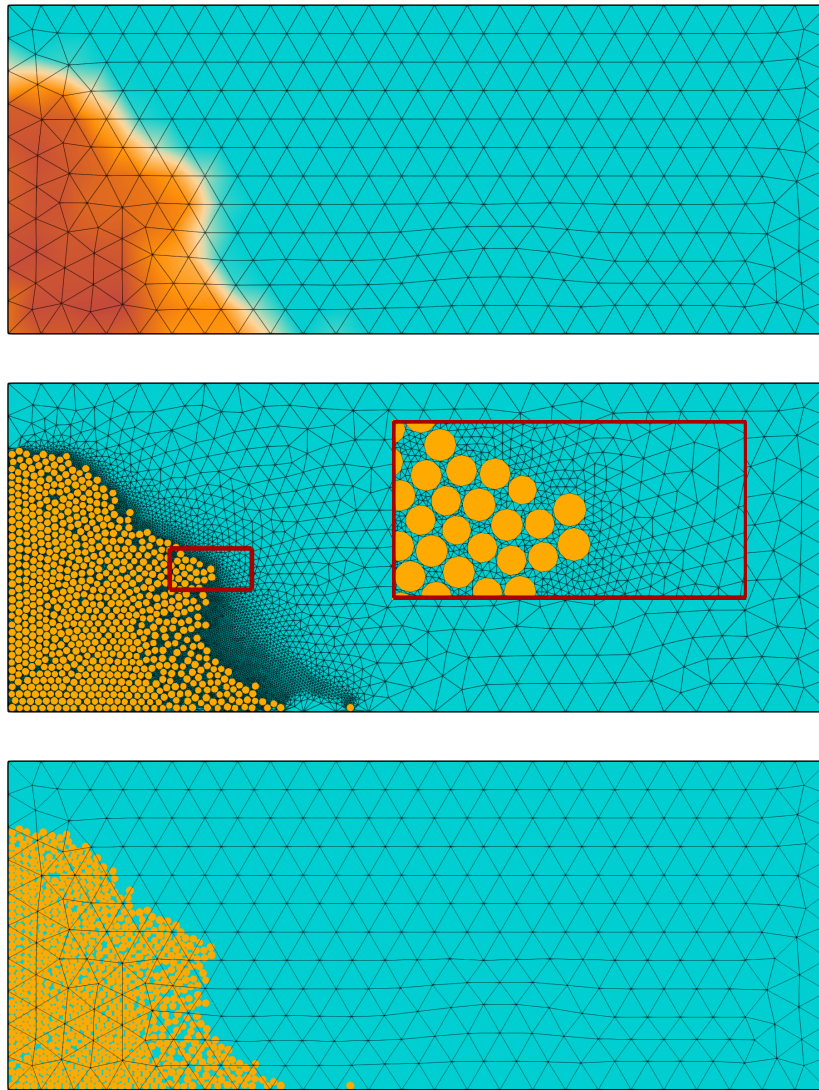


Fig. 1.3: Illustration of the three main possibilities for numerical models of immersed granular flows. Top: two-fluids model. Intermediate: direct numerical simulation. The inset is an enlargement showing details of the mesh. Bottom: multi-scale model.

As far as quasi-static or inertial flows are concerned, the so-called $\mu(I)$ rheology has emerged over the past two decades as the dominant approach (Pouliquen et al. (2006); Pouliquen and Forterre (2009)). This approach links the macroscopic friction coefficient of the granular phase μ , defined as the ratio between the shear stress τ and the confining pressure P inside the grains, to an inertial number $I = d\dot{\gamma}\sqrt{\rho_g/P}$ constructed by considering the relevant stresses at stake. First developed for dry, cohesionless grains, it has since been extended to immersed and cohesive flows (Boyer et al. (2011); Trung Vo et al. (2020)). Recent developments also allow to take the grain shape and orientation into account by adding an orientational tensor in the constitutive law, but it is restricted to ellipsoidal grains (Nadler (2021)).

In some applications, the physical processes at the grain scale cannot be ignored. This is the case in fluidized bed chemical reactors for example, where the gaz-particle interactions are key for the reaction follow-up (Luo et al. (2016)). Direct numerical simulation (DNS) techniques use a Lagrangian method to solve the granular phase. By tracking the positions and velocities of each particle and solving the contacts between them, high precision can be achieved in terms of grain physics. The interactions with the fluid phase are computed directly as the fluid flow is explicitly resolved around each grain (Hu et al. (1992); Zhang et al. (1999); Peskin (2002)). The high accuracy of these methods comes with a high computational cost that can be prohibitive. Indeed, the typical cell size of the fluid domain has to be smaller than the grains (see Fig. 1.3 middle). Moreover, when the positions of the grains are updated, the whole fluid computational domain has to be rebuilt, though non boundary-conforming mesh methods can avoid this at the cost of adding a parametrisation for the definition of the grain surface. For these reasons, DNS is used in small scales applications, or to calibrate coarser models (Municchi and Radl (2017)).

To circumvent the high computation cost issues of DNS, hybrid, multi-scale methods combine the Lagrangian approach for the granular phase with a coarse representation of the fluid on a larger scale than the grains (Tsuji et al. (1993); Deen et al. (2007b), see Fig. 1.3 bottom). The Navier-Stokes equations are volume averaged based on the fluid volume fraction in the computational cell. These methods prove advantageous for the simulation of mesoscale granular assemblies in a surrounding fluid, although they sacrifice precise fluid-grain interactions. The main drawback is that for these interactions, empirical parametrised formulas have to be used. Because of the turbulent nature of the flow around a grain, many different models exist concerning the drag coefficient.

It is possible to further reduce the computational cost of multi-scale models by reducing the accuracy on the granular phase. This approach, called coarse graining, consists in considering grains that are a few times larger than the original ones (Sakai and Koshizuka (2009); Sakai et al. (2014)). Each larger grain then represents a group of smaller ones. Its position and velocity correspond to the averages of the ones of the original grains it represents. If the

coarse grain is k times larger, the forces acting on it (from the contacts, the fluid phase or gravity) are assumed to be k^3 larger than the ones acting on a single original grain (k^2 in two dimensions). This allows the same physical parameters to be used as for small grains. The loss of accuracy is limited and quantified, but not yet in complex geometries and highly heterogeneous flows (Di Renzo et al. (2021)).

The MigFlow software falls within the category of hybrid, multi-scale numerical models. MigFlow¹, which stands for Model for Immersed Granular Flows, is an open-source software resulting from a collaboration between the Université Catholique de Louvain (UCLouvain) in Louvain-la-Neuve, Belgium, and the Laboratoire de Mécanique et de Génie Civil (LMGC) from the Université de Montpellier in Montpellier, France. It was first developed by Jonathan Lambrechts (Lambrechts et al. (2015)), and extended to the version presented in chapter 2 by Matthieu Constant during his thesis (Constant (2020)). Its purpose is to model immersed granular materials at various solid volume fractions and grain size distributions, with a representation of the grain physics while keeping the computational cost reasonable. To do so, the numerical method for the granular phase was chosen carefully for the considered applications and its implementation optimised, while the fluid phase is not resolved at the grain scale. It was successfully used in the study of Stokes clouds made of grains falling in a viscous fluid, air injection in an immersed granular bed, and the density sorting of grains using water jigging. To this end, a relevant fluid-interaction force model and multi-phase flow equations were implemented, as well as a stable numerical scheme that couples the granular and fluid solvers.

1.3 Drops in the ocean... but which ones?

The resulting numerical model was the starting point of the current thesis, whose objectives are to extend the model to frictional interactions between the grains and to grain shapes more complex than a simple sphere. Since these two aspects are implied in many key behaviours of granular materials, it should significantly enlarge the field of application of MigFlow, making it a relevant and functional tool for the study of immersed granular flows in various conditions and situations at an affordable computational cost. To illustrate this, two different physical applications will be investigated. In each of them, one of the implemented features plays a key role.

The first step is the extension of the granular solver to frictional contacts. This will be done by implementing an existing method (Jean (1999)). This aspect is essential in many industrial applications. Consider a rotating mill for example (see Fig. 1.4). The mill rotates and, under the effect of friction, sets the grains in motion. This type of device is widely used in the

¹www.migflow.be

mining industry for the grinding of ores (Golpayegani and Rezai (2022)) or in the chemical industry for the pyrolysis of materials (Sanginés et al. (2015)). The grains can undergo different flowing regimes, depending on various parameters such as the filling degree or the friction coefficients, but mainly on the Froude number $Fr = \omega^2 r / g$, with ω the angular velocity of the mill, r its radius and g the acceleration due to gravity (Mellmann (2001)), see Fig. 1.4.

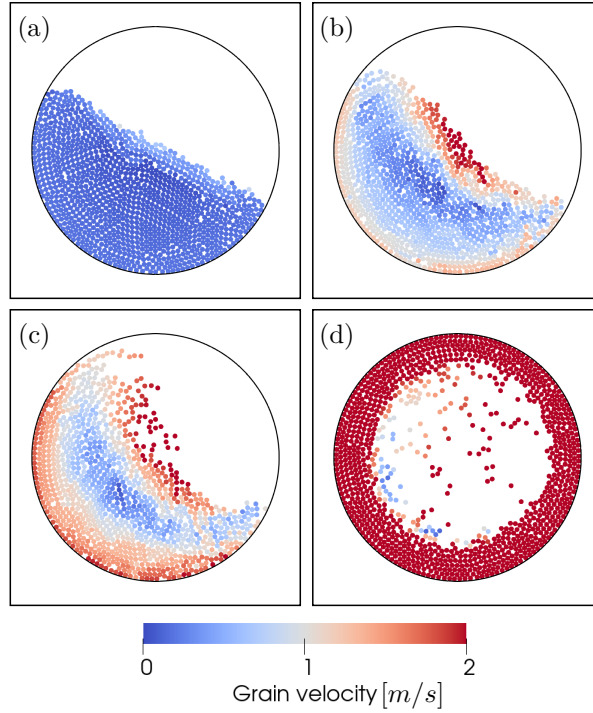


Fig. 1.4: Different flowing regimes for dry grains in a rotating mill. (a): rolling at $Fr = 0.008$. (b): cascading at $Fr = 0.4$. (c): cataracting at $Fr = 0.9$. (d): centrifuging at $Fr = 2.5$.

The next goal is to study the drag force exerted on a rigid body in dry and immersed granular flows. Since the contact network between the grains is highly fluctuating in nature, so is the drag force (see Fig. 1.5). Previous research established that, for flowing velocities below a given threshold, this force did not depend on the flowing velocity but rather on the stresses inside the granular phase (Faug (2015)). Moreover, it was shown that a fluid phase reduces at first the drag force by changing the apparent weight of the grains, but leads to a lower threshold for the velocity dependence of the drag (Costantino

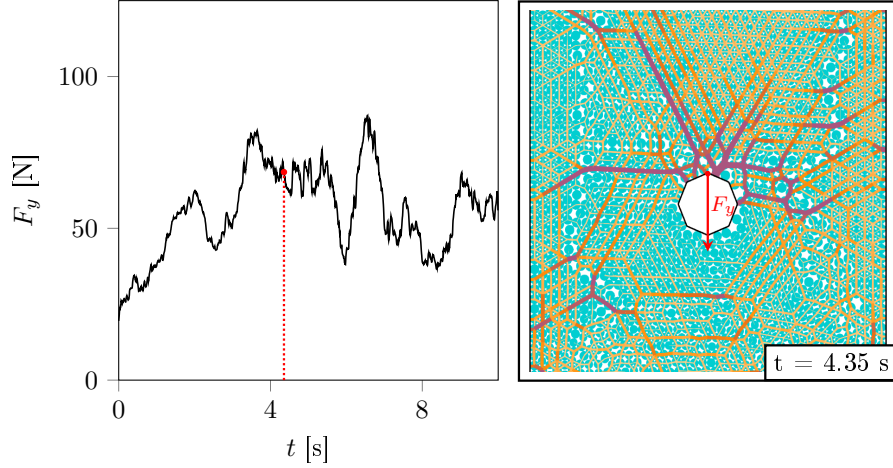


Fig. 1.5: Left: drag force exerted on a discretised cylinder by a moving granular media as a function of time. Right: snapshot of the grains and contact network at time $t = 4.35$ s. The more purple and the wider the line, the larger the contact force between the grains.

et al. (2011); Allen and Kudrolli (2019); Panaitescu et al. (2017)). The objective is to characterise the flow structure and stress states in different flowing regimes, and to investigate of the influence of the friction coefficients.

The following objective is to consider grains with arbitrary shapes.

The two main difficulties associated with arbitrary shapes concern the contact resolution and the computation of the fluid-grain interaction force. The shape of the grain can indeed strongly influence its dynamics in a fluid. For example, when free-falling in a fluid, a rod may undergo different types of motion that are essentially two-dimensional (Willmarth et al. (1964)). The type of motion depends mainly on the initial inclination (Lau et al. (2018)), the aspect ratio, the dimensionless moment of inertia $I^* = \rho_g w / \rho_f l$ (with w and l the width and length of the rod, respectively) and the Reynolds number (Andersen et al. (2005)). One of these possible types of motion is called fluttering: the rod oscillates from left to right and leaves vortices behind (Belmonte et al. (1998)), as depicted in Fig. 1.6.

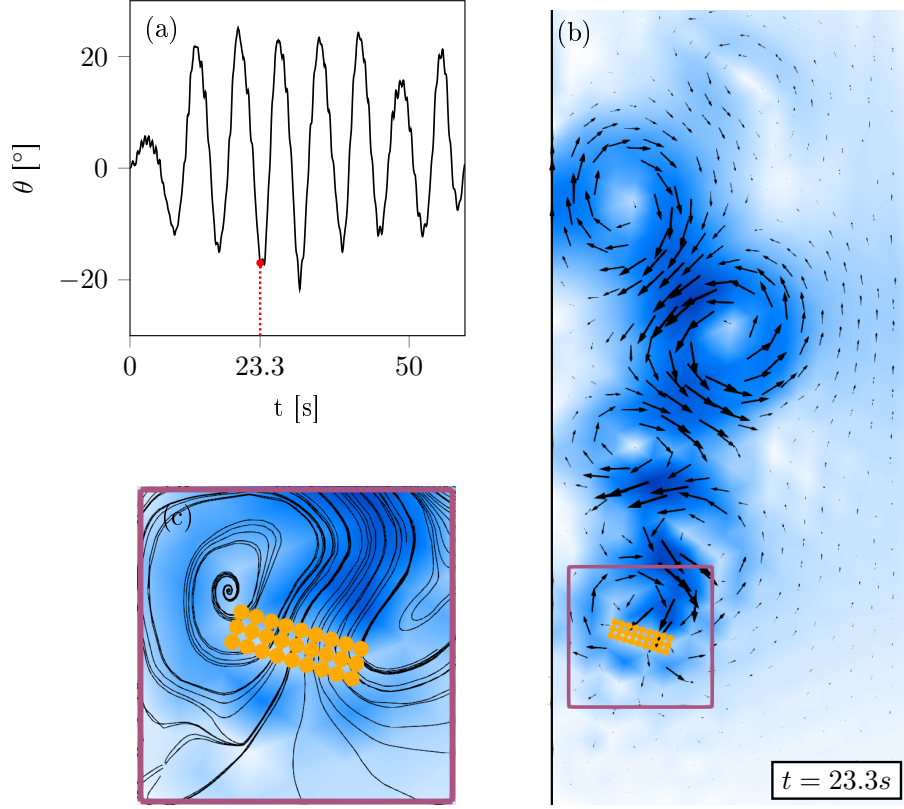


Fig. 1.6: Fluttering of a rod-like grain made of disks falling in water. (a): Euler angle θ of the grain as a function of time. (b): Snapshot of the simulation at time $t = 23.3$ s. The arrows show the orientation and magnitude of the fluid velocity, while the color indicates its magnitude. (c): Zoom of (b) showing the streamlines of the fluid around the grain.

The last goal is to investigate the collapse dynamics of dry and immersed columns made of elongated grains in two dimensions. Widely studied and recognised as a benchmark case to examine the behaviour of granular material, the column collapse consists in releasing a column of grains and let it flow under its own weight on a flat surface (Pinzon and Cabrera (2019)). The focus is generally put on the collapse dynamics and the final runout, which corresponds to the distance travelled by the grains after the collapse. In general, it can be determined from the contact network as the position of the farthest grain that is still in contact with the main mass (see the inset of Fig. 1.7).

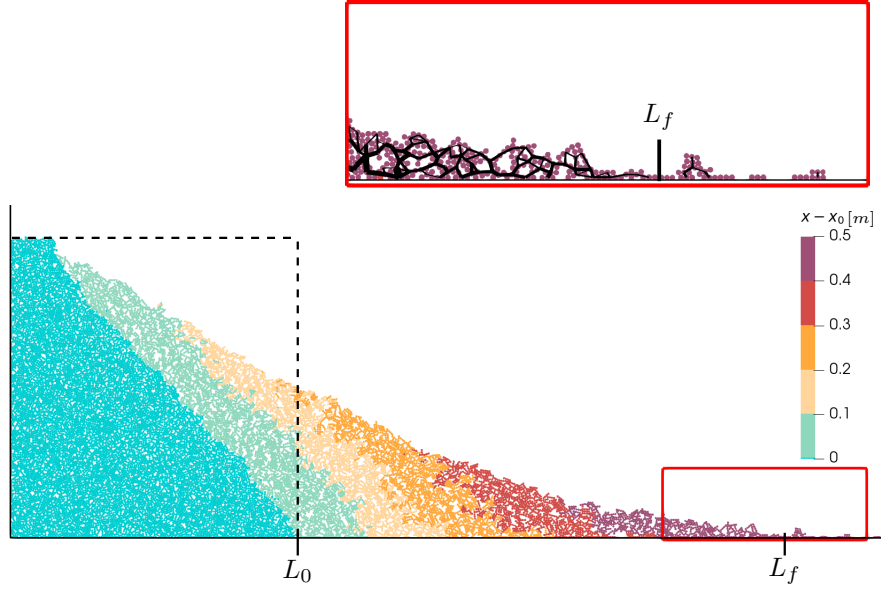


Fig. 1.7: Final state of a collapsed column with aspect ratio $H_0/L_0 = 1$ of elongated grains in dry conditions. The dashed lines indicate the initial shape of the column. The grains are coloured according to their displacement. The inset is an enlargement of the area in the red rectangle and shows the contact network between the grains.

Yet, as of today, few results exist concerning columns made of elongated grains in the immersed case, although the dry case has already been explored (Trepanier and Franklin (2010); Tapia-McClung and Zenit (2012)). For spherical or roughly spherical grains, the collapse dynamics and final runout have been shown to depend on the column aspect ratio and the properties of the surrounding fluid (Lajeunesse et al. (2004); Lacaze et al. (2021)). The objective is to study the influence of the grain orientation on the runout and the collapse dynamics, as well as its evolution during the collapse.

The present work is organised as follows. In the second chapter, the numerical model that is used in MigFlow – without the contributions from this thesis – is presented. After an introduction about the numerical methods used for hybrid models, the equations for both the fluid and granular phase are presented, and the coupling between the two phases explained. The focus of the third chapter is twofold: friction and the granular drag. First, the physical phenomenon of friction and the classical laws used to model it are shortly summarised. After that, the implementation of friction and the changes it implies in the numerical method are detailed. Next, the main results on the granular

drag force are highlighted. In the fourth chapter, before presenting the results about the collapse dynamics of dry and immersed columns of elongated grains, the extension of the numerical method for the granular phase to grains with non-spherical shapes is explained. In the final chapter, the contributions of this thesis are contextualised. Afterwards, some perspectives and the associated challenges are explored.

1.4 Supporting publications

- **Coppin, N.**, Henry, M., Cabrera, M., Azéma, E., Dubois, F., Legat, V., Lambrechts, J., (2023).
Collapse dynamics of two-dimensional dry and immersed granular columns of elongated grains .
Physical Review Fluids (under review).
- **Coppin, N.**, Constant, M., Lambrechts, J., Dubois, F., Legat, V. (2022).
Numerical analysis of the drag on a rigid body in an immersed granular flow.
Computational Particle Mechanics 9, 393-406.
- Constant, M., **Coppin, N.**, Dubois, F., Artoni, R., Lambrechts, J., Legat, V. (2021).
Numerical investigation of the density sorting of grains using water jiggling.
Powder Technology 393, 705-721.
- Constant, M., **Coppin, N.**, Dubois, F., Vidal, V., Legat, V., Lambrechts, J. (2021).
Simulation of air invasion in immersed granular beds with an unresolved FEM-DEM model.
Computational Particle Mechanics 8, 535-560.

1.5 Conference talks

- **Coppin, N.**, Henry, M., Cabrera, M., Azéma, E., Dubois, F., Legat, V., Lambrechts, J., (2022).
Numerical simulation of immersed avalanches of elongated grains.
Avalanches 2022, Debrecen, Hungary.
- **Coppin, N.**, Lambrechts, J., Cabrera, M., Azéma, E., Dubois, F., Legat, V. (2022).
Simulation numérique d'avalanches de grains allongés.
CSMA2022, Presqu'île de Giens, France.

- **Coppin, N.**, Constant, M., Lambrechts, J., Dubois, F., Legat, V. (2021).
Numerical analysis of the drag on a rigid body in an immersed granular flow.
Particles 2021, Hamburg, Germany.
- **Coppin, N.**, Dubois, F., Lambrechts, J., Legat, V. (2019).
Numerical study of the drag in fluid-grain medium with the MigFlow software.
Particles 2019, Barcelona, Spain.
- **Coppin, N.**, Constant, M., Lambrechts, J., Dubois, F., Legat, V. (2019).
Validation du frottement dans un modèle multi-échelles d'écoulements granulaires immergés en vue de l'étude numérique de la traînée.
CSMA2019, Presqu'île de Giens, France.

CHAPTER 2

A model for immersed granular flows

Πάντα ρεῖ - Everything flows.

— Ἡράκλειτος - Heraclitus.

As already explained, there exist several approaches concerning the numerical simulation of immersed granular flows, depending on the scale and the level of detail that is required. At large scales, two-fluids models are used in order to limit the computational cost. At small scales, direct numerical simulations offer a high precision but at a high cost. For problems of intermediate size, hybrid models are used. They still use a Lagrangian method for the granular phase, but relieve the precision on the fluid phase. This is the approach used in MigFlow.

Several kinds of methods can be used to solve the equations associated to the fluid phase. Structured grid methods often offer a simplicity of implementation and parallelisation, which can be key to the large scale deployment of the numerical simulations. These include Lattice-Boltzmann (Amarsid et al. (2017)) and Finite Differences (Luo et al. (2016)) or Finite Volumes (Deen et al. (2007b)). However, rendering complex geometries on structured grids can prove computationally difficult. This issue can be tackled with adaptive grid refinement (Berger and Oliger (1984)), but complex geometries can be more easily represented with Finite Elements. Although they present a higher implementation difficulty, they also provide an easier adaptive refining of the

grid, implying a higher level of precision in the areas of interest without additional cost in the other areas of the domain. Finite Elements are the chosen method for the resolution of the fluid phase in MigFlow.

Concerning the Lagrangian resolution of the granular phase, it was made possible by the ability of computers to perform arithmetical and logical operations repetitively and on a scale unrivaled by the human brain. The first Lagrangian approaches focused on Molecular Dynamics (MD), modelling the interactions between molecules with potentials (Walton (1984)). It was later applied to systems of macroscopic particles, such as granular materials. Being dissipative in nature, on the contrary to molecular interactions, the collisions between the grains are treated with simpler force models rather than potentials.

Smooth methods were the first to be developed, notably by the pioneering work of Cundall and Strack in the 1970's (Cundall and Strack (1979)). These methods explicitly relate the contact reaction to the relative interpenetration of the grains, regularising the steep laws of frictional contacts. Different contact laws can be adopted, from the simple linear Hook law to the nonlinear Hertz contact theory (Mishra (2003)). Other features such as friction and cohesion can also be taken into account (Anand et al. (2009)). These methods are easy to implement but nonetheless have inherent weaknesses. First, the regularisation of the contact problem yields stiff differential equations, requiring small time steps to avoid instabilities. Second, it is necessary to add global damping on the particle motion to avoid persistent vibrations. Finally, the calibration of the parameters for the complex contact laws can be difficult because they influence the macroscopic response and the dynamical properties as well as the contact condition (Dubois et al. (2018)).

On the other hand, nonsmooth methods neglect the contact physics and consider instantaneous, unilateral contacts. This implies a discontinuity in the velocities of the particles and prevents the particles from overlapping. The event-driven method (ED) assumes binary contacts happening at distinct times. Once a contact between two particles is solved, the solver jumps to the time of the next contact, updating the positions of the particles. This method is adaptative by nature: the value of the time step adapts to the time to the next contact. Although computationally convenient, it is only suitable for granular gases where the time between two contacts is well defined (Bizon et al. (1999); Alam and Luding (2002)). For dense systems, this time vanishes and a so-called inelastic collapse occurs. The Nonsmooth Contact Dynamics (NSCD) deals with the discontinuity of velocities with an implicit formulation of the contact laws, which amounts to a balance of momentum, coupled to a Coulomb law for dry friction. This event-capturing scheme has a constant time step, over which all contacts are solved at once. It is done by using an iterative procedure like Non Linear Gauss Seidel iterations (Jean (1999)). This implicit time-stepping resolution has several advantages: it avoids inelastic collapse when the time between collisions vanishes, it allows to use a larger time step than

explicit methods, and it eliminates the need for global damping in smooth methods to reach an equilibrium state. For the above reasons, Nonsmooth Contact Dynamics is the chosen Lagrangian method for the granular phase in MigFlow. Although static and dynamic situations are accurately rendered, the method still faces problems, such as hyperstaticity or the impossibility to reach exactitude both in position and velocity (Acary (2013)).

This chapter first describes the volume-averaged fluid equations, how they are obtained and how they are solved. Afterwards, the focus is put on the basic model for the granular phase, considering only frictionless spherical grains. Lastly, the interactions between the grains and the fluid are detailed, as well as the coupling issues between both solvers and the solutions employed in MigFlow.

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2.1 Fluid phase dynamics

Although modelled on a coarser scale, many of the problems that could lead to the failure of the simulations originate from the fluid phase equations. Therefore, a consistent resolution of the fluid phase is of high importance. To this end, a stabilised P1-P1 finite element method is used in MigFlow, so that regions of interest can be adaptatively refined and complex geometries better captured. This section first highlights the volume averaging procedure and the resulting Navier-Stokes equations. Afterwards, the FEM and its features are presented. Finally, the equations to solve a secondary fluid phase are shown.

2.1.1 Volume averaged equations

Initially interested in the description of fluidized beds, Anderson and Jackson (1967) developed a volume averaged approach of the fluid equations to smooth the discontinuities from the grains. At the heart of the method is the hypothesis that the variations of the fluid fields are the sum of two contributions: one at the entire system scale, and one at the grain spacing scale. The local mean value of a fluid field can then be computed as a weighted average of the point fields based on a given kernel function δ with the following properties:

- $\delta(r)$ is a strictly positive function decreasing with r , the distance to a given point in space.
- δ is normalised so that $\int_{\Omega} \delta d\Omega = 1$, with Ω indicating the whole domain.
- δ has derivatives of all orders for every value of r , and these derivatives are integrable on Ω .

From δ , the fluid volume fraction or porosity ϕ can be defined as:

$$\phi(\mathbf{x}, t) = \int_{\Omega_f(t)} \delta(\|\mathbf{x} - \mathbf{y}\|) d\Omega_y, \quad (2.1)$$

with $\Omega_f(t)$ the volume of all points $\mathbf{y}$ occupied by the fluid phase and $d\Omega_y$ a small element of volume around point $\mathbf{y}$. The average value $a(\mathbf{x}, t)$ of a fluid point property $a'(\mathbf{x}, t)$ can then be computed as:

$$a(\mathbf{x}, t) \phi(\mathbf{x}, t) = \int_{\Omega_f} a'(\mathbf{y}, t) \delta(\|\mathbf{x} - \mathbf{y}\|) d\Omega_y. \quad (2.2)$$

In agreement with the underlying hypothesis of the two scales contributions to a fluid property, this definition of an average value will be insensitive to the radius or detailed form of δ provided that this radius is of intermediate

size between the two considered scales. With this formalism, the Navier-Stokes equations for an incompressible flow become:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{v} = 0, \quad (2.3)$$

$$\frac{\partial \rho_f \mathbf{v}}{\partial t} + \nabla \cdot \frac{\rho_f \mathbf{v} \mathbf{v}}{\phi} = \nabla \cdot \left(2\eta \phi \mathbf{d} \left(\frac{\mathbf{v}}{\phi} \right) - p \mathbf{I} \right) + \mathbf{f} + \phi \rho_f \mathbf{g}, \quad (2.4)$$

where $\mathbf{v}$ is the volume-averaged fluid velocity, ρ_f its density, η its dynamic viscosity, $\mathbf{d}$ the deformation rate tensor, p the pressure, $\mathbf{I}$ the identity tensor, $\mathbf{f}$ the fluid-grain interaction force, and $\mathbf{g}$ the acceleration due to gravity.

2.1.2 Finite Element solver

The principle of the Finite Elements method is to approximate the fluid fields by discretising them over a finite space $\hat{V}, \hat{P}$ so that:

$$\begin{aligned} \mathbf{v} \approx \mathbf{v}^h &= \sum_{i=1}^N \mathbf{V}_i \tau_i, & \mathbf{v}^h \in \hat{V}, \\ p \approx p^h &= \sum_{i=1}^N P_i \tau_i, & p^h \in \hat{P}, \end{aligned}$$

with τ_i interpolation functions, $\mathbf{V}_i$ and P_i the nodal values of $\mathbf{v}$ and p , respectively, and N the number of nodes.

The weak form of the problem consists in finding $(\mathbf{v}^h, p^h) \in (V^h, \times P^h)$ such that $\forall (\hat{\mathbf{v}}^h, \hat{p}^h) \in (\hat{V}^h, \hat{P}^h)$:

$$\left\langle \frac{\partial \phi}{\partial t}, \hat{p}^h \right\rangle - \left\langle \mathbf{v}^h, \nabla \hat{p}^h \right\rangle + \left\langle \mathbf{v}^h, \hat{p}^h \mathbf{n} \right\rangle = 0 \quad (2.5)$$

$$\begin{aligned} \left\langle \frac{\partial \rho_f \mathbf{v}^h}{\partial t}, \hat{\mathbf{v}}^h \right\rangle + \left\langle \nabla \cdot \left(\frac{\rho_f \mathbf{v}^h \mathbf{v}^h}{\phi} + p^h \mathbf{I} \right), \hat{\mathbf{v}}^h \right\rangle &= \left\langle 2\eta \phi \mathbf{d}^h, \nabla \cdot \hat{\mathbf{v}}^h \right\rangle \\ &\quad - \left\langle 2\eta \phi \mathbf{d}^h, \hat{\mathbf{v}}^h \cdot \mathbf{n} \right\rangle \\ &\quad + \left\langle \mathbf{f}^h + \phi \rho_f \mathbf{g}, \hat{\mathbf{v}}^h \right\rangle, \end{aligned} \quad (2.6)$$

with the notations $\langle \cdot, \cdot \rangle$ and $\langle \langle \cdot, \cdot \rangle \rangle$ corresponding to the scalar products on the domain and its boundary, respectively.

For computational convenience, the interpolation functions are chosen as linear, implying $P1 - P1$ finite elements. This choice is consistent with the coarse representation of the fluid phase. However, it makes the numerical resolution unstable. Unwanted pressure oscillations are introduced into the solution (Tezduyar et al. (1992)), leading to the failure of the simulations. This is because the Brezzi-Babuska condition is not respected, implying a singular

discrete matrix (Babuška (1973); Brezzi and Pitkäranta (1984)). In order to cope with that issue, a Pressure-Stabilizing/Petrov-Galerkin (PSPG) term is added in the continuity equation.

Oscillations can also occur in the velocity field because of the non positive-definite matrix corresponding to the convective terms (Brooks and Hughes (1982)). These can be balanced by adding a numerical diffusion term called Streamline Upwind/Petrov-Galerkin (SUPG) in the momentum equation. However, the addition of the PSPG term in the continuity equation threatens the incompressibility properties of the flow. To minimize this issue, a final penalty term is added in the momentum equation, the Least-Square on Incompressibility Constraint (LSIC) term. In order to obtain convergent methods, the PSPG, SUPG and LSIC terms are computed on the basis of the residuals of the momentum and continuity equations, respectively. It is to note that the stabilisation terms are parametrized with coefficients computed on the basis of element matrices and vectors (Tezduyar and Osawa (2000)).

The interpolation functions are used as the averaging kernel when computing the nodal values of the porosity:

$$\phi_i = 1 - \frac{1}{\int_{\Omega} \tau_i(\mathbf{x}) d\mathbf{x}} \sum_{k=1}^{N_g} V_k \tau_i(\mathbf{x}_k), \quad (2.7)$$

with N_g the number of grains and V_k and $\mathbf{x}_k$ the volume and position of grain k . This links the kernel to the mesh size and implies that to avoid a null porosity the element size should be larger than the grain size. However, in highly polydisperse materials, it would be desirable to be able to have grains larger than the mesh size so that the accuracy on the fluid phase remains relevant for the smallest grains. This can be achieved by smoothing the kernel and adding a diffusion step in the averaging process (Capecelatro and Desjardins (2013)). Nonetheless, this diffusion process is itself limited by the size of the domain and grains much larger than the mesh size cannot be considered. For these ones, methods such as the Immersed Boundary Method (IBM) can be employed (Peskin (1977); Uhlmann (2005)). With the IBM, the solid boundaries corresponding to the grains are not explicitly defined in the fluid phase, suppressing the need to remesh the domain each time the grains are moved. Their influence on the fluid phase is replaced by a force density so that the fluid that coincides with the grains has the corresponding velocity. The interactions are then explicitly computed from the fluid fields at the grain boundaries. Nonetheless, a significant number of elements is necessary to correctly capture the grain boundary.

For the sake of stability and large time steps, the fluid solver uses an implicit Euler time stepping scheme. Inevitably, this results in more time consuming iterations. However, because the fluid is solved on a coarser scale, the main computational effort comes from the granular phase.

Thus, this implicit scheme should not significantly affect the computational performance of MigFlow, while making it more robust.

The time discretisation of the fluid problem is the following:

$$\frac{\phi^i - \phi^{i-1}}{\Delta t} + \nabla \cdot \mathbf{v}^{i+1} = 0 \quad (2.8)$$

$$\begin{aligned} \rho_f \left(\frac{\mathbf{v}^{i+1} - \mathbf{v}^i}{\Delta t} + \nabla \cdot \frac{\mathbf{v}^{i+1} \mathbf{v}^i}{\phi^i} \right) &= \nabla \cdot 2\eta \phi^i \mathbf{d}^{i+1} - \phi^i \nabla p^{i+1} \\ &\quad + (\mathbf{f}^{i+1} + V_p \nabla p^{i+1}|_{\mathbf{x}^{i+1}}) \\ &\quad + \phi^i \rho_f \mathbf{g} \end{aligned} \quad (2.9)$$

2.1.3 A word about two-fluids flows

In many problems, granular materials may be subject to the influence of more than one fluid. A typical example is the fluidisation of an immersed granular bed. This can notably happen in submarine thermal vents (Newman et al. (2008)) or in environmental applications such as soil contaminant cleaning (Semer et al. (1998)). To cope with this, the MigFlow software includes the possibility to simulate two immiscible fluid phases. This is done by introducing a phase indicator function a , with value 1 for the first fluid and 0 for the second one. This phase indicator is subject to the following equation:

$$\frac{\partial a \phi}{\partial t} + \nabla \cdot (a \mathbf{v}) = 0. \quad (2.10)$$

To avoid a too inaccurate representation of the interface between the two fluid phases, this equation is solved with a discontinuous Galerkin procedure. In order to take this phase indicator into account in the fluid equations, the fluid properties are averaged on its basis as follows:

$$\rho_f = a \rho_{f_1} + (1 - a) \rho_{f_2} \quad (2.11)$$

$$\eta = \left(a \frac{\eta_1}{\rho_{f_1}} + (1 - a) \frac{\eta_2}{\rho_{f_2}} \right). \quad (2.12)$$

In order to render physical effects such as phase separation, the surface tension has to be taken into account. Since it is impossible to directly apply a force at the interface as it is not precisely defined, a volume force is chosen instead as developed by Brackbill et al. (1992). This force is significant where the concentration gradient is high and vanishes where it is low, and is proportional to the curvature of the interface $\kappa = (-\nabla a / \|\nabla a\|)$:

$$\mathbf{T} = \sigma \nabla \cdot \left(- \frac{\nabla a}{\|\nabla a\|} \right) \nabla a, \quad (2.13)$$

with σ the surface tension coefficient.

However, special care has to be given to the fact that with such a volume force representation of the surface tension, spurious currents can appear at the interface. If the time scale of these currents is significant with respect to the one of the simulation, stabilizing strategies can be implemented (Lafaurie et al. (1994); Popinet and Zaleski (1999); Jamet et al. (2002)). Equation 2.10 is solved with the following time discretisation:

$$a^{i+1} = a^i - \Delta t \frac{\mathbf{v}^{i+1}}{\phi^i} \cdot \nabla a^i. \quad (2.14)$$

2.2 Granular phase dynamics

The grains influence the fluid phase dynamics through the porosity and the fluid-grain interaction force. It has already been stated that to avoid numerical issues due to a null porosity, the elements of the mesh should be larger in size than the grains. This condition is sufficient provided that the grains do not interpenetrate. The non-interpenetration requirement is more strongly ensured by nonsmooth methods. Moreover, it should be interesting to use an implicit method for the granular phase so that large time steps can be used, on a comparable scale with the one used for the fluid phase. For these reasons, the DEM used in MigFlow corresponds to Nonsmooth Contact Dynamics. The NSCD was developed on the basis of convex analysis by Moreau (Moreau (1988)) and Jean (Jean (1999)) and implemented in the open-source software LMG90 by Dubois and Jean (Dubois and Jean (2013)). Its ability to cope with different body shapes, time integration schemes and contact laws made it a useful tool in many applications: granular materials (Saussine et al. (2006)), masonry structures (Chetouane et al. (2005)), crack propagation (Perales et al. (2010)), or even deep drawing (Jourdan et al. (1998)).

The goal of this section is to present the general theoretical framework of NSCD and its features for frictionless spherical bodies. The extensions to contacts implying friction and clusters of spheres are presented in the next two chapters. In a second time, strategies used to reduce the computational cost of some steps of the process such as contact detection will also be explained. Finally, the time discretisation of the problem is addressed.

2.2.1 Global and local equations

In a classical Lagrangian way, the positions $\mathbf{x}$ and velocities $\mathbf{u}$ of the grains are tracked through time with Newton's second law of motion:

$$\mathbf{M} \frac{d\mathbf{u}}{dt} = \mathbf{M}\mathbf{g} + \mathbf{f} + \mathbf{r} \quad (2.15)$$

$$\mathbf{x}(t) = \mathbf{x}(t=0) + \int_0^t \mathbf{u}(\tau) d\tau, \quad (2.16)$$

with $\mathbf{M}$ the masses of the grains and $\mathbf{r}$ the contact forces. The main challenge resides in finding those contact forces. This consists in first detecting the potential contacts between pairs of grains and then solving them iteratively until convergence is reached. This iterative process is necessary because each time a contact is solved, the resulting velocity corrections on the corresponding grains can affect the state of the other contacts in which those grains are involved. The resolution of a contact is made based on local contact laws. This means that it is necessary to switch to a local frame with corresponding local variables proper to the contact. Once the local reaction force is determined, the switch can be performed backwards to obtain the global reaction force and modify the velocities of the grains accordingly.

Let the vector $\mathbf{n}^\alpha$ constitute the local frame (see Fig. 2.1) of a contact α . Usually, a tangential vector (two in three dimensions) is part of the local frame. However, as the tangential part of the contacts is irrelevant in the case of frictionless spheres, it shall be ignored in this section. In the following, the variables are specific to each contact, but the subscript α will be omitted for the sake of simplicity. The normal vector $\mathbf{n}$ is constructed so that it connects the forecast contact points on the two grains. When it comes to spherical grains, the direction of $\mathbf{n}$ coincides with the one of the vector connecting the two centers of the grains. For other shapes, especially polygons, this is not true anymore and the choice of the projected contact points and the normal vector is not obvious (Jean (2010)). Then, the relative velocity $\mathbf{U}$ between the projected contact points can be defined with the following transformation:

$$\mathbf{U} = \mathbf{H} \cdot (\mathbf{u}_i, \mathbf{u}_j). \quad (2.17)$$

Since $\mathbf{H}$ depends on the local frame, it is specific to each contact. From an equality of power, it can be shown that the transformation from the local frame to the global one is simply the transpose of $\mathbf{H}$, so that the global contact reaction force is obtained as follows:

$$\mathbf{r} = \mathbf{H}^T \mathbf{R}, \quad (2.18)$$

with $\mathbf{R}$ the local contact reaction force. Again, the subscript α denoting the specific contact was omitted. As for frictionless spherical bodies the tangential part of the relative velocity plays no role in the contact resolution, it will be omitted for now. The normal component of the relative velocity is thus obtained as $U_n = (\mathbf{u}_j - \mathbf{u}_i) \cdot \mathbf{n}$.

In the way the contacts are considered, discontinuities in velocities are inevitable. To treat with these, it is necessary to consider the relative velocity as a bounded variation function. This means that for every instant t , it has a left limit $\mathbf{U}^-$ (the velocity just before the contact) and a right limit $\mathbf{U}^+$ (the velocity just after the contact). Consequently, the reaction force R is to be seen as a density of impulse with respect to a Lebesgue measure (Jean (2010)).

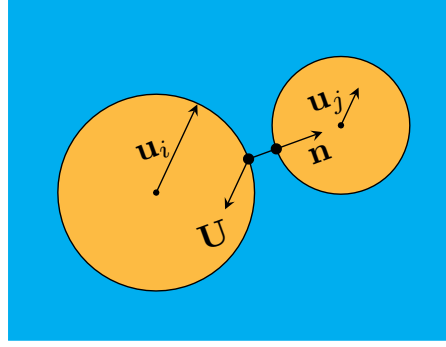


Fig. 2.1: A potential contact between two grains i and j , with the local frame ($\mathbf{n}$) and the relative velocity $\mathbf{U}$.

As they prevent the grains from interpenetrating, nonsmooth methods are sometimes called hard-sphere methods. To ensure this non-interpenetrability, the distance between the contact points is set to be non-negative, $d \geq 0$. It can be shown that this condition is implied by the following:

$$\text{If } d_0 \geq 0, \quad (2.19)$$

$$\text{Then } d \leq 0 \implies U_n^+ \geq 0, \quad (2.20)$$

with d_0 the value of the distance between the contact points at some initial time t_0 . Additionally, whenever a contact reaction occurs, the normal component of the relative velocity should be zero, $R_n \geq 0 \implies U_n^+ = 0$. Finally, although adhesive contacts can be considered (Pérales et al. (2006)), they are ignored in the current framework, implying $R_n \geq 0$. These constraints can be summed up as the velocity Signorini condition, or the inelastic shock law:

$$\text{If } d > 0 \text{ then } R_n = 0, \quad (2.21)$$

$$\text{If } d \leq 0 \text{ then } R_n \geq 0, U_n^+ \geq 0, R_n U_n^+ = 0. \quad (2.22)$$

This law implies perfectly inelastic collisions between the grains, which proves useful to dissipate energy and avoid damping to reach a static equilibrium in dense assemblies.

2.2.2 Time discretisation

When discretising time, the question of the integration scheme arises. Because of the many expected shocks that result in velocity discontinuities, the latter is expected to be nondifferentiable, as is stated in the very nature of nonsmooth methods. Therefore, first order schemes are preferred over higher order ones (Jean (1999)), as for example the θ scheme. Here, a forward Euler scheme ($\theta = 0$) is used for the integral of the force due to gravity while a backward Euler scheme ($\theta = 1$) is used to update velocities and compute the contact reactions. The case of the fluid-grain interaction force is a bit more complex. It is known at the beginning of the time step and treated as constant from the point of view of the granular solver, but it should not be considered as entirely explicit as it is part from a predictor-corrector scheme described in section 2.3. As the precise time at which a contact happen is ill defined, the value of the reaction force is to be understood as the mean of an impulse $\mathbf{p}^{i+1}$ over the time step. The numerical problem to be solved for the dynamical equation is then:

$$\mathbf{u}^{i+1} = \mathbf{u}^i + \Delta t \mathbf{M}^{-1} \left(\mathbf{M} \mathbf{g} + \mathbf{f}^i + \frac{\mathbf{p}^{i+1}}{\Delta t} \right) \quad (2.23)$$

$$\mathbf{x}^{i+1} = \mathbf{x}^i + \Delta t \mathbf{u}^{i+1}. \quad (2.24)$$

During the contact resolution at the local scale, the values of U^- and U^+ correspond to U_n^i and U_n^{i+1} , respectively. It is to note that, as the transformation used to compute the local variables depends on the positions of the two grains, its value is not constant along the time step. However, if the change in position of the two grains over the time step is small with respect to the curvature of the grains, a constant approximation for $\mathbf{H}$ proves sufficiently accurate. In general, given the values of the time step and the radii of the grains, this condition is fulfilled.

A particular discretized form of the inelastic shock law is used:

$$\frac{\max(\mathbf{d}^i, 0)}{\Delta t} + U_n^{i+1} \geq 0, \quad (2.25)$$

$$R_n^{i+1} \geq 0, \quad (2.26)$$

$$\left(\frac{\max(\mathbf{d}^i, 0)}{\Delta t} + U_n^{i+1} \right) R_n^{i+1} = 0. \quad (2.27)$$

This law means that a contact will occur in two separate time steps. During the first one, a reaction will be found so that the two grains come in contact. During the second one, a reaction will be found so that their relative velocity is zero. The use of the positive part of the distance, $\max(\mathbf{d}^i, 0)$, ensures that if some interpenetration due to previous numerical errors is present, no repulsion will take place. Note that the distance $\mathbf{d}^i$ is computed at the beginning of the time step. This choice respects the consistency of the gap approximation with

unilateral condition which requires that if $\mathbf{d}^i = 0 = \mathbf{d}^{i+1}$, then $U_n^{i+1} = 0$ (Jean (1999)).

2.2.3 Solver optimisation

Over the past decades, available computational resources have grown exponentially. Even in these circumstances, numerical optimisation has been a key factor to get finer results on larger domains. In the near future, the exponential growth will probably come to an end (Waldrop (2016)) although parallel computing with GPU units seems promising to tackle this growth slow down (Leiserson et al. (2020)). Nevertheless, MigFlow is not yet parallelised, and optimisation plays a crucial role in its ability to yield attractive computational performances. For the granular solver, the two major optimisations concern the contact detection as well as the iterative procedure management.

Contact detection is a preliminary process that takes place at the beginning of every time step. In smooth methods, whose explicit nature results in a large amount of time steps, this process can represent a large part of the computational effort (Huang et al. (2020)). In the case of NSCD, its computational cost accounts for less than 10% of the total in dense problems but can significantly increase for gaseous states (Renouf et al. (2004)). In general, pair-wise tests between every grains are avoided because they result in a high computational cost, the number of required operations being proportional to the square of the number of grains. Most contact detection algorithms consist of two phases: a broad-phase that determines which pairs should be tested, and a narrow-phase which actually tests the preselected pairs of grains (Kockara et al. (2007)). The narrow phase is straightforward for spherical grains, but can be more tricky for more complicated shapes (Lubbe et al. (2020)). Since MigFlow deals with spheres, the optimisation of the contact detection phase focuses on the broad-phase.

The principle is to use an Octree, which has proven useful for problems with polydisperse grains (Raschdorf and Kolonko (2009)). In this type of tree, each node is associated to a region of space and either has eight (four in 2D) or no children. A node without children is called a leaf, and each leaf can contain at most eighty grains. The broad phase, i.e. the construction of the tree, and the narrow phase are conducted concurrently. At the start, the tree consists of a single leaf. Then, the grains are inserted one after another. A grain is inserted in the leaf whose associated space intersects its bounding box, the smallest cube (square in 2D) that can contain the grain. If the maximum number of grains in a leaf is reached, the leaf becomes a node and is split into eight new leaves. The grains are then reassigned to the corresponding leaves. After the insertion, the narrow phase takes place: contacts with all the other grains from the same leaf are checked. A contact is considered active if the distance between the two grains is inferior to a given value that corresponds

to the maximum distance that can be covered in a single time step by two grains going towards each other. Note that in practice, the time step of the granular solver is adapted so that it prevents grains from moving by a larger distance than the value used in the contact detection. When all grains have been inserted, the tree is complete and all contacts have been detected.

Because of its implicit nature, the NSCD method requires an iterative procedure. Indeed, when solving a contact, the velocity changes resulting from the reactions of yet unsolved contacts are unknown. Moreover, the resolution of one contact may affect a previously solved contact. To deal with these issues, most implementations iterate over the whole contact set until convergence is reached. Several approaches exist such as the Non-Linear Gauss-Seidel (NLGS) process and variants (Jean (1999); Anitescu and Tasora (2010)), or the Conjugate Gradients method (Renouf and Alart (2005)). To accelerate these processes, it is possible to use the velocity corrections from the last time step as a first guess for the current one. Since in static situations, contacts are persistent and grain velocities do not change much, this results in a significant speed-up with equivalent accuracy (Alart (2014)).

These approaches reconsider every contact at each iteration of the process. In order to reduce the computational cost, MigFlow uses a queue structure that allows considering only a specific part of the contacts. Additionally, velocity corrections from the last time step are used as a first guess. First, all contacts are inserted in the queue upon detection. Then, each contact is solved in turn. When a contact is solved, it is removed from the queue. It is considered converged if the difference in the contact reaction between two successive iterations δR_n is below a given geometrical threshold:

$$\delta R_n \frac{m_i + m_j}{m_i m_j} \Delta t^2 < \zeta, \quad (2.28)$$

with Δt the time step and m_i and m_j the masses of grain i and j , respectively. If the contact is not converged, then the contacts implying either of the corresponding grains are put back in the queue, if they are not already. Convergence is reached when the queue is empty.

However, convergence is not guaranteed, except in special cases (Jean (1999)) for different reasons. One of them is that the kinematic constraints due to the constant approximation of the local frame of reference can be too large (Jean (2010)). To tackle this precise reason, a recursive adaptative strategy on the time step was implemented. When convergence cannot be reached, the current time-step is split in two sub time-steps that are solved with half the geometrical tolerance, to preserve accuracy. To avoid infinite splitting when the non-convergence is due to another reason, a maximum number of splits is specified. When convergence is reached for all sub time-steps, the computation can go on to the next time step.

2.3 Fluid-grain interactions

The link between the two phases resides in the fluid-grain interaction forces. Since the fluid phase is solved on a coarser scale than the granular one, the integration of the exact interaction around the grain boundary is irrelevant. Instead, empirical laws for the momentum transfer are used. Although computationally convenient, they require calibration involving different parameters. The more parameters, the more difficult it is to tune the laws so that on the one hand the physics of the problem are reproduced, and on the other hand the problem is numerically solvable. With that in mind, only the drag and the pressure gradient contributions are taken into account in the MigFlow model, neglecting the Magnus, added mass, Basset and Saffman forces.

The ratio between the Magnus force and the drag force exerted on a rotating grain with velocity u in a fluid at rest is given by:

$$\frac{f_{Magnus}}{f_d} = \frac{\omega d}{u}, \quad (2.29)$$

with ω the angular velocity of the grain and d its diameter. This indicates that the Magnus force can become significant for large grains with a large angular velocity and a small linear velocity. The value of ω is difficult to predict, as it strongly depends on the type of application studied. In cases where the grains are densely packed, it should be small, while when they are loosely packed, it can be either small or large. Additionally, no interaction between grain rotation and fluid vorticity is currently implemented in the model. In consequence, this effect is neglected in MigFlow, although it could be included in further refinements.

The so-called added mass force requires the knowledge of the added mass coefficient C_{am} for its computation, whose value is close to 0.5 for isolated spheres (Simcik et al. (2008)). When the grains are in a suspension and interacting with each other, the computation of this term is non-trivial and analytical solutions are most of the time out of reach, although numerical investigation led to some progress in the case of gas bubbles in a liquid (Simcik et al. (2008)). The influence of this force is limited to transient dynamics and to applications where the grain density is lower than or similar to the one of the fluid, which, in addition to the difficulty of establishing a valid expression, leads many models to neglect it (Delannay et al. (2017); Schmeeckle (2014)), as is done here.

As far as the Basset history force is concerned, a general expression valid in different flowing regimes is difficult to obtain because of the integral over the full history of the grain it implies. It is hence often neglected in numerical models of grain suspensions although some numerical and experimental evidence shows it should not always be the case (Haller (2019)). Recently, a new approach based on the diffusion equation was developed, allowing an easier analytical treatment of this force (Prasath et al. (2019)). Nonetheless, only the transient

dynamics of the suspension are significantly influenced and not its statistical properties (Jaganathan et al. (2023)). Moreover, the presence of many grains in the vicinity of each grain should erase the historical effects from the velocity of the considered grain (Anderson and Jackson (1967)). The Basset history term is therefore neglected in the current model, although it could be included as an interesting refinement in some particular applications in a dilute regime.

As for the Saffman lift force, its value decreases quickly to very small values for Reynolds numbers larger than one (McLaughlin (1991)), and it should then not influence the global behaviour of the grains.

The drag force on a single spherical grain i is given by:

$$\mathbf{f}_{d,i} = \gamma_i \left(\mathbf{u}_i - \frac{\mathbf{v}}{\phi} |_{\mathbf{x}_i} \right) = C_d \frac{\pi d^2}{4} \left\| \mathbf{u}_i - \frac{\mathbf{v}}{\phi} |_{\mathbf{x}_i} \right\| \left(\mathbf{u}_i - \frac{\mathbf{v}}{\phi} |_{\mathbf{x}_i} \right), \quad (2.30)$$

with C_d the drag coefficient. Dallavalle and Klemin (1943) gave a formula for this drag coefficient that is valid for the whole practical range of grain Reynolds numbers Re_i :

$$Re_i = \frac{d \rho_f \phi |_{\mathbf{x}_i}}{\eta} \left\| \mathbf{u}_i - \frac{\mathbf{v}}{\phi} |_{\mathbf{x}_i} \right\| \quad (2.31)$$

$$C_d = \left(0.63 + \frac{4.8}{\sqrt{Re_i}} \right)^2. \quad (2.32)$$

In order to take into account the influence of the neighbouring grains, this drag force for an isolated grain has to be multiplied by a function of the porosity which is of the form:

$$g(\phi) = \phi^\beta. \quad (2.33)$$

In MigFlow, the value of the exponent β is taken as -1.8 , as showed suitable for low and high Reynolds regimes by Wen and Yu (1966). More detailed expressions have been developed (Di Felice (1994); Li and Kuipers (2003)) but have not been retained for the sake of computational convenience. The fluid-grain interaction force is then computed as:

$$\mathbf{f}_i = \underbrace{-V_i \nabla p |_{\mathbf{x}}}_{\text{pressure gradient}} - \underbrace{\gamma_i \left(\mathbf{u}_i - \frac{\mathbf{v}}{\phi} |_{\mathbf{x}_i} \right)}_{\text{drag}}, \quad (2.34)$$

where V_i is the volume of grain i . This interaction force was validated in the MigFlow software for Stokes clouds of glass beads falling in a viscous fluid (Constant et al. (2019)).

From the fluid point of view, the grains are considered as point particles. Hence, the interaction forces correspond to dirac functions associated to the position of each grain. Since the fluid phase is solved with finite elements, it is

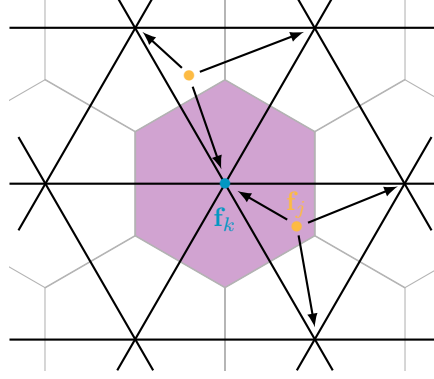


Fig. 2.2: Computation of the fluid grain interaction force on a given node.

necessary to redistribute these dirac functions on the mesh nodes. This is done on the basis of the form functions. The force resulting from the interaction with the grains on a node k can be computed as:

$$\mathbf{f}_k = \frac{1}{V_k} \sum_{i=1}^N \sum_{j=1}^{N_g} \mathbf{f}_j \tau_i(\mathbf{x}_j), \quad (2.35)$$

with V_k the volume associated to node k . This computation is illustrated in Fig. 2.2

For the sake of computational convenience, the fluid and the granular solvers are explicitly coupled. Remember that the granular solver time step is limited so that grains cannot move by a distance larger to the contact detection alert distance with their current velocities. This implies that the granular solver may perform sub time steps with respect to the fluid solver. During these sub time steps, the fluid interaction force is considered constant. If the number of sub time steps is not too high, this assumption does not have a significant influence on the behaviour of the granular phase.

However, with such an explicit coupling, the term corresponding to $\mathbf{f}$ can become large. This would strongly reduce the critical size of the time step at the expense of computational cost. In order to circumvent this problem, $\mathbf{f}$ is computed with a semi-implicit scheme (Patankar (1980)).

Instead of using $\mathbf{u}^i$, a prediction is made based on external forces at time $i+1$ and contact forces at time i :

$$\frac{\mathbf{u}_i^* - \mathbf{u}_i^i}{\Delta t} = \mathbf{g} + \frac{1}{m_i} \left(\mathbf{r}^i + m\mathbf{g} - V_i \nabla p - \gamma^i \left(\mathbf{u}_i^* - \frac{\mathbf{v}^{i+1}}{\phi^i} \middle| \mathbf{x}_i^i \right) \right). \quad (2.36)$$

This leads to:

$$\mathbf{u}_i^* = \frac{\Delta t}{m + \gamma^i \Delta t} \left(\frac{m}{\Delta t} \mathbf{u}_i^i + m \mathbf{g} + \mathbf{r}_i - V_i \nabla p + \gamma^i \frac{\mathbf{v}^{i+1}}{\phi^i} \Big|_{\mathbf{x}_i^i} \right) \quad (2.37)$$

$$\mathbf{f}_i^{i+1} = \gamma^i \left(\mathbf{u}_i^* - \frac{\mathbf{v}^{i+1}}{\phi^i} \Big|_{\mathbf{x}_i^i} \right). \quad (2.38)$$

Please note that the superscript i , indicating the time step i , should not be confounded with the subscript i , indicating a grain i , as they are independent from one another. To further increase the stability of the explicit coupling, a predictor-corrector scheme is used. This scheme is presented in Fig. 2.3.

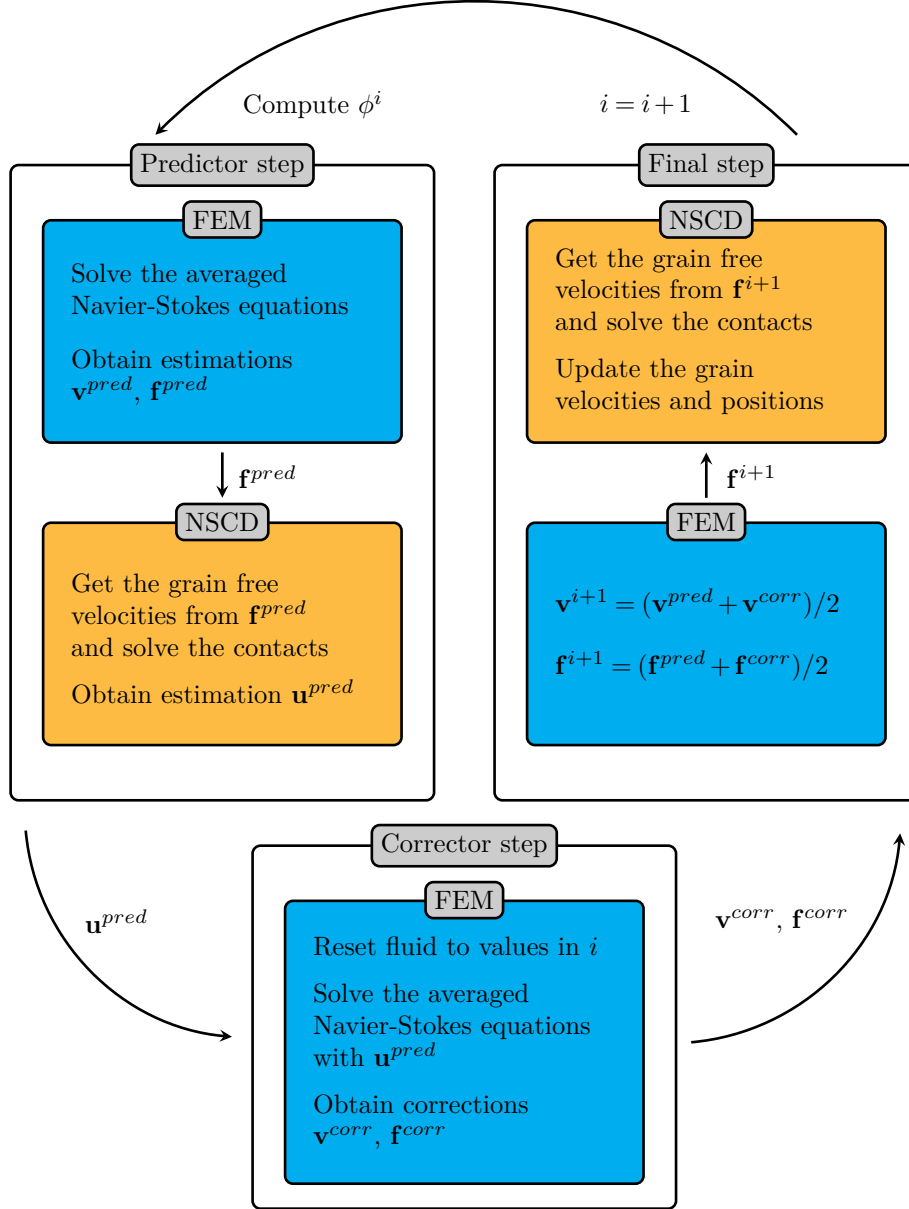


Fig. 2.3: Predictor-corrector scheme used for the coupling of the fluid and grain solvers

CHAPTER 3

Friction and the drag force

In some applications, grains are in a loose state and the external forces play a more important role than the contact forces. In such cases, what matters the most is that grains do not interpenetrate: frictional interactions are not crucial. This is the case for example when studying the dynamics of Stokes clouds of grains falling in a viscous fluid (Constant et al. (2019)). However, in denser situations, it appears that dry friction is at the origin of many specific behaviours of granular materials (Radjai et al. (2017)). This does not come as a surprise, as for example frictional grains can roll on each other instead of gliding, converting a part of their kinetic energy to rotational energy and changing their relative motion. Two somehow counter intuitive examples of those behaviours that are specific to granular materials and due to friction will be seen in this chapter. First, the Janssen effect that consists of a saturation of the static pressure in the grains with depth in a silo. Second, the drag force exerted on an object immersed in a granular flow, that is independent of the flow velocity when the latter is low enough (Wieghardt (1975)). However, difficulties arise with the inclusion of friction in the resolution of the contacts between the grains.

The macroscopic models of friction are discontinuous in nature, although their simplicity is in striking contrast with the complexity of the physics at the microscale. Moreover, when considering frictional rigid bodies, indeterminacy and inconsistency in the equations of motion can appear, leading to the so-called Painlevé paradox (Painlevé (1895, 1905a,b)) with the contact forces

growing unbounded. From a numerical point of view, these kinds of problems will tend to make the convergence of the problem for large collections of grains slower. Lastly, friction is involved in the tangential part of the contact: the corresponding component of the relative velocity becomes important and the angular velocity of the grains can no longer be overlooked.

This chapter concerns the implementation of friction in MigFlow and the simulation and investigation of the drag force exerted on a rigid body in an immersed granular flow. First, an outlay of friction as a phenomenon and how it is modelled is presented. Then, the details of the implementation of this feature in MigFlow are explained. Finally, the resulting extended numerical model is validated and used in the study of the drag force. The content of the present chapter led to the following publication:

Coppin, N., Constant, M., Lambrechts, J., Dubois, F., Legat, V., 2022. Numerical analysis of the drag on a rigid body in an immersed granular flow. *Computational Particle Mechanics* 9(3), 393-406.

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3.1 Complex, you said?

Broadly speaking, the phenomenon of friction is defined as the resistance to the relative motion between two material elements. Depending on the nature of these elements, i.e. solid, liquid or gaseous, the resulting macroscopic behaviour is significantly different. The case within the scope of the present chapter corresponds to friction between two solid surfaces, also called dry friction.

It is sometimes considered a nuisance. In wind turbines for instance, friction between the rotating shaft and the rotor not only causes them to wear out, but also results in a loss of a part of the mechanical energy that is converted to heat. Nonetheless, it can prove crucial in some applications. For example, in land transport both power transmission from the engine to the wheels and braking rely on friction. Moreover, the wheels of the vehicle can roll without sliding thanks to friction between them and the ground. Although already discussed during the Antiquity (Sambursky (2014)), the main empirical observations about dry friction date back to the 17th and 18th centuries with Amontons and Coulomb (Popova and Popov (2015)):

- The friction force F_t is directly proportional to the normal force F_n between the two surfaces in contact.
- The coefficient of proportionality between F_t and F_n is different when the surfaces are sticking or sliding.
- The friction force is *mostly* independent from the sliding velocity.
- The friction force is *mostly* independent from the contact area.

Those observations are translated into the so-called Coulomb model:

$$F_t \leq \mu_s F_n \text{ while sticking,} \quad (3.1)$$

$$F_t = \mu_k F_n \text{ while sliding.} \quad (3.2)$$

with F_t the friction force, F_n the normal force, and μ_s and μ_k the static and kinetic coefficients of friction, respectively. It is to note that, as observed by Coulomb himself (Coulomb (1821)), this is an oversimplification, hence the terms *mostly* in the above observations. Indeed, dry friction results of a combination of complex physical interactions. Both geometrical interactions between asperities and chemical bonds between molecules of the surfaces play a significant role in the apparition of friction (Filippov et al. (2004); Müser et al. (2001); Hanaor et al. (2016)). However, the dependencies on the sliding velocity or the contact area happen to be weak, so that for most applications a fine understanding of the phenomena is not necessary and the simple Coulomb model can be successfully adopted.

Concerning granular materials, a distinction has to be made between microscopic grain-grain friction μ and the macroscopic friction coefficient μ^* that relates the shear stress τ of the bulk material to its normal stress σ and prescribes its response to external constraints:

$$\tau = \underbrace{\tan(\varphi)}_{\mu^*} \sigma, \quad (3.3)$$

with φ being called the angle of internal friction. This concept is useful for granular flows in the quasi-static and inertial regimes but starts to be irrelevant for granular gases where kinetic theories are more suitable. Note that it is not necessarily a constant property across the material (Campbell (2006)). It is a key component of constitutive laws used in continuous models (Jaeger et al. (1990); Pouliquen et al. (2006); Pouliquen and Forterre (2009); Boyer et al. (2011); Trung Vo et al. (2020)). Astonishingly, it results more from structural effects than from grain-to-grain friction. Indeed, frictionless spheres exhibit a macroscopic friction coefficient that is nonzero (Peyneau and Roux (2008)). Hence, the macroscopic friction coefficient is not a simple function of the microscopic one, but is also influenced by the fabric anisotropy of the grains and the normal force chains (Radjai et al. (2017))

3.2 Let there be friction

As seen in the previous section, friction results from complex interactions but can be satisfyingly modelled with simple equations that are nonetheless discontinuous in nature. Although intergrain friction is not the only factor influencing the macroscopic response of the granular material to external shear or stress, it still plays a crucial role in many key features of granular materials and is hence worth including in the present numerical model.

Since Nonsmooth Contact Dynamics is implicit and discontinuous by essence, the inclusion of friction in its equations comes as a natural feature that was actually present since its foundation. Friction being involved in the tangential components of a contact between rigid bodies, the corresponding component of the relative velocity has to be described correctly. To this end, it is now necessary to consider the rotation of the grains, defining new variables $\boldsymbol{\theta}$ and $\boldsymbol{\omega}$ the Euler angles and angular velocities of the grains. It is important to note that in three dimensions, $\boldsymbol{\omega}$ is not the time derivative of $\boldsymbol{\theta}$, contrary to $\mathbf{u}$ with $\mathbf{x}$. If it is necessary to obtain the orientation of the grain as a function of time, special care has to be given to the conversion between $\boldsymbol{\omega}$ and $d\boldsymbol{\theta}/dt$. However, since only spherical grains are considered here, only their angular velocities are relevant and not their orientation. Therefore, the latter will be discarded in what follows.

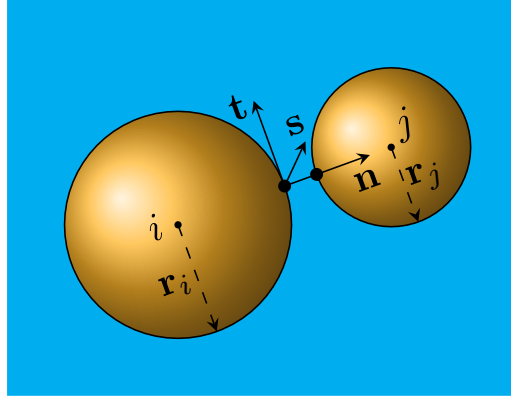


Fig. 3.1: A potential contact between two grains i and j with radii $\mathbf{r}_i$ and $\mathbf{r}_j$, with the local frame $(\mathbf{n}, \mathbf{t}, \mathbf{s})$.

Again, let us consider a pair of spherical bodies i and j in a potential contact. This time, the local frame also consists of two orthonormal vectors (one in 2D) $\mathbf{t}$ and $\mathbf{s}$, in addition to the normal vector $\mathbf{n}$ (see Fig. 3.1). The components of the relative velocity at the contact point, $\mathbf{U}$, can be obtained with the following transformation:

$$\mathbf{U} = \begin{pmatrix} U_n \\ U_t \\ U_s \end{pmatrix} = \mathbf{H} \cdot (\mathbf{u}_i, \boldsymbol{\omega}_i, \mathbf{u}_j, \boldsymbol{\omega}_j) = \begin{pmatrix} (\mathbf{u}_i + \boldsymbol{\omega}_i \times \mathbf{r}_i - \mathbf{u}_j - \boldsymbol{\omega}_j \times \mathbf{r}_j) \cdot \mathbf{n} \\ (\mathbf{u}_i + \boldsymbol{\omega}_i \times \mathbf{r}_i - \mathbf{u}_j - \boldsymbol{\omega}_j \times \mathbf{r}_j) \cdot \mathbf{t} \\ (\mathbf{u}_i + \boldsymbol{\omega}_i \times \mathbf{r}_i - \mathbf{u}_j - \boldsymbol{\omega}_j \times \mathbf{r}_j) \cdot \mathbf{s} \end{pmatrix}. \quad (3.4)$$

The equation of dynamics at the contact level can be written as:

$$\mathbf{U}^+ = \mathbf{U}^- + \overbrace{\mathbf{H} \mathbf{M}^{-1} \mathbf{H}^T}^{\mathbf{W}} \mathbf{P}, \quad (3.5)$$

with $\mathbf{U}^+$ and $\mathbf{U}^-$ the relative velocity just before and just after the contact, $\mathbf{M}^{-1}$ the inverse of the mass matrix, $\mathbf{W}$ the so-called Delassus operator and $\mathbf{P}$ the contact impulse due to the integral of the contact reaction force $\mathbf{R}$ over the

contact duration. Since this duration is undetermined, it is more convenient to use $\mathbf{P}$ than $\mathbf{R}$. This matrix is diagonal, which comes from the symmetric nature of the spherical grains. This diagonal matrix implies that the normal and tangential parts of this equation are uncoupled and can be solved one after another. The following set of uncoupled equations for the contact is then to be solved:

$$\begin{cases} U_n^+ = U_n^- + W_{nn}P_n \\ W_{nn} = m_j^{-1} + m_i^{-1} \end{cases} \quad (3.6)$$

$$\begin{cases} \mathbf{U}_t^+ = \mathbf{U}_t^- + \mathbf{W}_{tt}\mathbf{P}_t \\ \mathbf{W}_{tt} = \text{diag}(W_{nn} + r_i^2 I_i^{-1} + r_j^2 I_j^{-1}) \end{cases} \quad (3.7)$$

with I_k the inertia of grain k .

To do so, contact laws have to be formulated. In addition to the inelastic shock law, a classical Coulomb model is adopted for friction. This yields the following:

$$\text{If } d > 0 \text{ then } P_n = 0, \quad (3.8)$$

$$\text{If } d \leq 0 \text{ then } P_n \geq 0, U_n^+ \geq 0, P_n U_n^+ = 0, \quad (3.9)$$

$$\|\mathbf{P}_t\| \leq \mu P_n, \quad \|\mathbf{U}_t^+\| \neq 0 \Rightarrow \mathbf{P}_t = -\mu P_n \frac{\mathbf{U}_t^+}{\|\mathbf{U}_t^+\|}, \quad (3.10)$$

with d the distance between the two grains and μ the static coefficient of friction. The relation 4.4 means that the tangential impulse will take a value that cancels the tangential component of the relative velocity just after the contact, unless that value is larger than a threshold corresponding to the normal impulse multiplied by the friction coefficient. In that case, the two grains are slipping on each other since $\mathbf{U}_t^+$ is not zero, and the tangential impulse takes the threshold value prescribed by the normal impulse. It is to note that as such, the static and kinetic friction coefficients are considered equivalent. In most problems, this is satisfactory, but it is quite straightforward to implement a contact law with different values.

The perfectly inelastic shock law and the coulomb friction yield:

$$P_n = -\frac{U_n^-}{W_{nn}} \quad (3.11)$$

$$\mathbf{P}_t = \min(\mu P_n, \|\mathbf{P}^{\text{stick}}\|) \frac{\mathbf{P}^{\text{stick}}}{\|\mathbf{P}^{\text{stick}}\|}, \quad (3.12)$$

with $\mathbf{P}^{\text{stick}} = -\mathbf{W}_{tt}^{-1}\mathbf{U}_t^-$ the impulse that cancels the tangential relative velocity.

As already explained in Chapter 2, a first order backward Euler scheme is used to integrate the equations of motion of the grains. The dynamic equation at the contact scale becomes:

$$\mathbf{U}^{i+1} = \mathbf{U}_{free} + \Delta t \mathbf{W} \mathbf{R}^{i+1}, \quad (3.13)$$

where $\mathbf{U}_{free}$ is the free relative velocity of the grains, i.e. the relative velocity they would have because of the external forces without solving the contact. Note that the contact is supposed to occur over the whole time-step, with $\mathbf{U}^{i+1}$ and $\mathbf{U}_{free}$ corresponding to $\mathbf{U}^+$ and $\mathbf{U}^-$, respectively, and with $\Delta t \mathbf{R}^{i+1}$ the mean impulse due to the contact forces over the time step. Finally, the solution to the discretised form of the frictional contact problem becomes:

$$P_n^{i+1} = -U_{nfree}/W_{nn} \quad (3.14)$$

$$\mathbf{P}_t^{i+1} = \min(\mu P_n^{i+1}, \|\mathbf{P}^{stick}\|) \frac{\mathbf{P}^{stick}}{\|\mathbf{P}^{stick}\|}. \quad (3.15)$$

The resolution of the contacts between the entire collection of grains follows the same iterative procedure described in chapter 2. However, because the contact forces now have a tangential component, it is necessary to update the criterion convergence to take that into account:

$$\delta R_n W_{nn} \Delta t^2 < \zeta \text{ and } \delta R_t W_{tt} \Delta t^2 < \zeta \text{ and } \delta R_s W_{ss} \Delta t^2 < \zeta. \quad (3.16)$$

As such, the convergence becomes more difficult to achieve. Moreover, the problem can become undetermined or even inconsistent, leading to unavoidable failures of the convergence of the iterative process. In order to tackle a part of such issues, it is possible to use a Coulomb-Orowan model for friction, which sets a maximum threshold for the tangential component of the contact force (Alart and Renouf (2018)). Other techniques such as relaxation can also be considered.

3.3 The drag force on a rigid body in an immersed granular flow

This section is devoted to the force exerted on an object that is intruding a granular material, which is involved in many practical and industrial problems such as the design of mixing and plowing devices (Wiegardt (1975)), or anti-avalanche protections (Sovilla et al. (2010)). It should not be confused with the drag force exerted on a body or grain in motion in a viscous fluid, although such a fluid can oftentimes significantly modify the dynamic or static behaviour of the granular phase, hence influencing the first one.

In the dry case, experiments on the granular drag begun in the early 1970's with Wiegardt's work. He noticed that the drag did not mainly depend on

the flow velocity, but rather on the shape and size of the intruder (Wieghardt (1975)). Further experiments established that at moderate velocities, the velocity had no impact on the drag force. The latter mostly depends on the object shape and size and on gravitational stress inside the material (Faug (2015); Albert et al. (1999); Chehata et al. (2003); Zhou et al. (2004)). This is because the motion of the intruder implies a reorganisation of the spatial structure of the grains, which in turn depends on geometrical parameters and on the gravitational stress that maintain the grains together. Hence, the flow can be characterised with the Froude number $Fr = V/\sqrt{gL}$ with V the flow velocity, g the acceleration due to gravity and L a characteristic length – e.g. the intruder diameter, the hydraulic radius of the channel or the intruder’s penetration depth in the granular bed, depending on the geometry of the problem. At Froude number greater than 10, the granular material becomes fluidized. Then, the transfer of momentum between the grains and the object dominates over the grain network reorganisation in the drag force, yielding a square velocity dependence (Takehara and Okumura (2014); Faug (2015); Wassgren et al. (2003)).

Several experiments were led in the presence of an interstitial fluid. When the material is not saturated, the velocity dependence on the drag force is similar to the dry case, although mechanisms such as cohesion and contact lubrication have an influence (Artoni et al. (2019)). On the other hand, when the grains are fully immersed, the buoyancy due to the fluid decreases the apparent weight of the grains. This decreases the value of the drag force (Costantino et al. (2011)) and the Froude number, leading to an earlier fluidisation. The ratio between the drag force and the average weight of the grains on the object was observed to vary as a power law of a so-called viscous number $J = \eta\dot{\gamma}/P$ with η the viscosity of the fluid, $\dot{\gamma}$ the shear rate and P the pressure in the granular material (Panaitescu et al. (2017); Allen and Kudrolli (2019)).

To validate the ability of the grain solver to study applications concerning the drag force, it is confronted to a physical experiment performed by Chehata et al. (2003). They measured the drag force exerted on a cylinder inside a gravity-driven granular flow, and observed that it did not depend on the flow velocity. The experimental apparatus, depicted in Fig. 3.2 left, consists of a vertical hopper through which a cylinder of diameter $D = 38.1$ mm is placed at a position $\mathbf{x}_c$. The top of the hopper is connected to a grain tank, while an aperture of variable size at its bottom controls the flow. The system is filled with glass grains with radius $r = 3$ mm and density $\rho_g = 2500$ kg/m³. In the simulations, a small polydispersity based on a uniform distribution in the range $0.95r - 1.05r$ was introduced to prevent crystallisation effects. The coefficients of friction are μ_g between the grains and μ_w between the grains and the walls. For the sake of simplicity, the coefficient of friction between the grains and the cylinder is also μ_w . To be convenient with the finite element method used to solve the presence of a fluid in further simulations, the cylinder

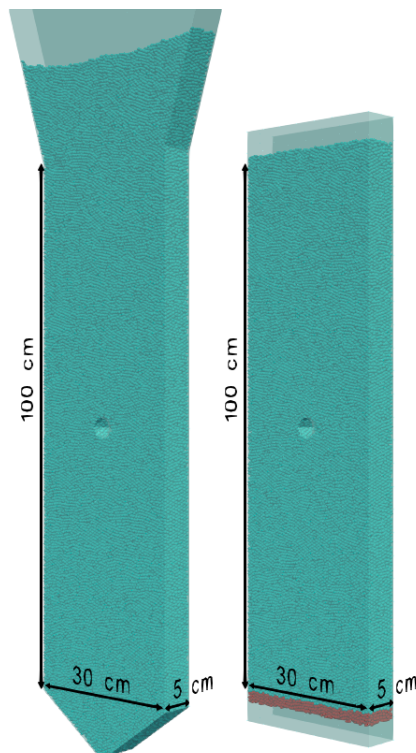


Fig. 3.2: Left: hopper geometry. Right: channel geometry.

is discretised as an octagonal prism. Instead of a large reservoir, grains are regularly injected when the level of the grains goes below a given limit, reducing the computational cost. The injection of the grains is carefully processed so that its impact on the force measured on the cylinder is negligible. Finally, a channel geometry depicted in Fig. 3.2 right is tested. In this case, the grains rest on a fixed bed of grains (represented in red in Fig. 3.2 right), in a similar way to what is done in Landry et al. (2003). In addition to be less CPU time consuming, this geometry allows a better control on the flow velocity, since it can be directly prescribed on the fixed bed. Furthermore, it is more suitable to the simulation of an interstitial fluid because the fluid flow is not disturbed by the change of directions of boundaries.

Although the experiment is quasi-2D, 2D simulations with MigFlow yield values of the drag force much higher than the experimental results. While they capture the velocity-independent behaviour, it is necessary to resort to 3D simulations for quantitative validation. These 3D simulations with 100000

grains for 40 s take approximately 40 hours on a SkyLake 2.3 GHz CPU. A sensitivity analysis on the convergence criterion showed that at value of 10^{-6} m for the geometrical tolerance allows good confidence in the value of the drag force. Fig. 3.3 shows a typical curve for the norm of the drag force versus time. This force is computed as the sum of all the contact impulses on the cylinder over the time step, divided by the time step:

$$\mathbf{F} = \frac{1}{\Delta t} \sum_{\beta} m_{\beta} (\delta U_n \mathbf{n} + \delta \mathbf{U}_t \cdot \mathbf{t}), \quad (3.17)$$

where β denotes the contacts in which the cylinder is implied and m_{β} the mass of the corresponding grains. Remember that the velocity corrections are with respect to the free velocities of the grains computed from the external forces. Hence, these are not zero in static situations. The grains are at rest for five seconds before the flow begins, either by opening the aperture in the hopper geometry, or by setting the grain bed in motion in the channel geometry. After a while, the reloading stops and the container empties. The value of the drag force is taken as the average value between the start of the flow and the stop of the grain injection. Fig. 3.4 shows a snapshot of the contact network in

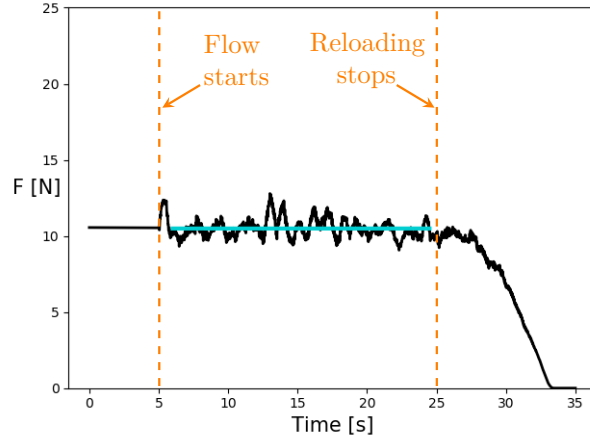


Fig. 3.3: Typical curve for the drag force, resulting from a moving average with span $t_{av} = 0.5$ s that only takes past data into account. The mean drag force is in blue. The flow velocity is $V = 64$ mm/s and the time step is .001 s.

2D between the grains when they are flowing. This network fluctuates quickly as contacts are continuously initiated and broken, which is reflected by the variability of the data in Fig. 3.3.

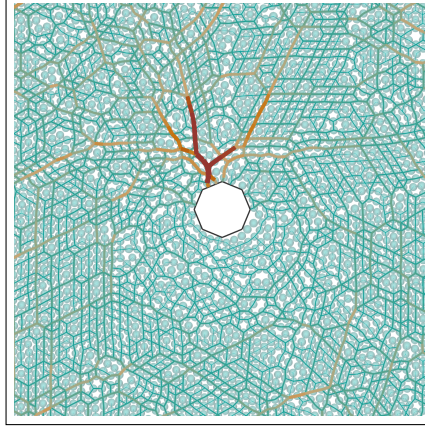


Fig. 3.4: Snapshot of the contact network in 2D between the grains when they are flowing. The redder and wider the line, the larger the contact force between the two grains.

3.3.1 Static stress state

The value of the static force before the flow begins is difficult to validate as such, because of the complex structure of the contact network. It varies from a simulation to another. Because of this, the focus is put on the static stress inside the granular material, which is linked to the drag force (Chehata et al. (2003); Faug (2015)). The discrete stress tensor can be computed at given grid points directly from the contact forces between the grains:

$$\sigma_{ij} = \frac{1}{V} \sum_{\beta \in V} f_i^\beta \cdot l_j^\beta, \quad (3.18)$$

where V is a given volume around the grid point, f_i^β is the i^{th} component of the contact force of contact β and l_j^β the j^{th} component of its centre to centre vector. The volume V is chosen as $8\pi d^3/6$ and the grid points are separated by a distance $2\sqrt{2}d$, with $d = 2r$ the grain diameter.

The vertical stress σ_{yy} has been shown to asymptote to a saturating value σ_0 as depth increases, unlike hydrostatic stress in newtonian fluids. Indeed, because of the frictional nature of the contacts, arches appear that deflect a part of the weight of the grains onto the side walls. This feature was first modelled by Janssen (1895). He supposed that the horizontal stress was uniform across a vertical section of the container, and that the contact forces of the grains with the walls were at the point of Coulomb failure, i.e. $f_t = \mu_w f_n$. He obtained

what follows:

$$\sigma_{yy}(y) = \sigma_0 \left(1 - \exp \left(- \frac{H-y}{y_0} \right) \right) \quad (3.19)$$

$$\sigma_0 = \phi_g \rho_g g y_0. \quad (3.20)$$

where g is the norm of the acceleration due to gravity, H the total height of the granular column and ϕ_g the packing fraction. In all simulations, ϕ_g was close to the maximum value for spheres in 3D $\phi_g \sim 0.64$. In rectangular containers, the value of y_0 is given by (Chehata et al. (2003)):

$$y_0 = \frac{1}{K \mu_w} \frac{(L-2r)(W-2r)}{2(L+W-4r)}, \quad (3.21)$$

with L and W the length and width of the container, respectively, and r the grain radius. The latter is used to take finite grain size effects into account. For the Janssen effect to be significant, the ratios H/W and H/L need to be large enough, which is the case in the considered experiment. The parameter K is called the coefficient of earth pressure. It represents the ratio between the horizontal stress and the vertical stress in a granular material. In a container filled by pouring, it can be assessed as (Mesri and Hayat (1993)):

$$K = \frac{1 - \sin(\psi)}{1 + \sin(\psi)}, \quad (3.22)$$

where ψ is the internal angle of friction of the material. Here, it is estimated as $\tan^{-1}(\mu_g)$.

If a stress load of magnitude Q_0 is applied at the top of the granular column, then the Janssen equation must be modified by adding a term $Q(y)$ that takes this load into account (Nedderman (1992)):

$$Q(y) = Q_0 \exp \left(- \frac{H-y}{y_0} \right). \quad (3.23)$$

This term is useful to compare stress curves in granular columns with different total heights. The same height bounds are taken for every column so that the relative position of the cylinder is the same, and the stress state above the upper bond is rendered as an applied load Q_0 . The stress profiles obtained with the simulations for the hopper, the channel, and the channel without cylinder are given in Fig. 3.5.

The curves corresponds to the model from Eq. 3.20, but with values of y_0 that are different from Eq. 3.21. Since L , W and r are purely geometrical, the differences should arise either from K or μ_w . The parameter K has a mean value between 0.7 and 0.8, which is close to the value of 0.74 predicted by Eq. 3.22. Although the hypothesis of uniform horizontal stress is wrong, the

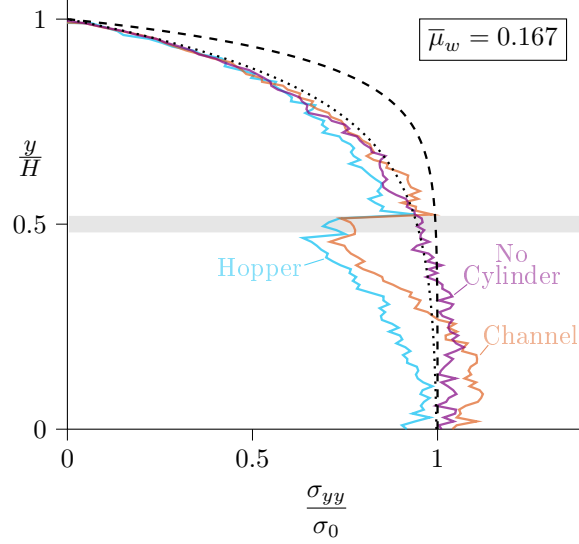


Fig. 3.5: Width and length averaged vertical stress as a function of height inside the grains before the flow starts. The grey zone indicates the position of the cylinder. Solid curves represent the simulation data. The dashed curve represents Eq. 3.20 with y_0 from Eq. 3.21. The dotted curve is Eq. 3.20 with $\mu_w = \bar{\mu}_w$ in Eq. 3.21.

differences between the estimated and the measured value of K are too small to explain the contrast in y_0 . This could actually be due to μ_w , because the contacts at the walls are not at the point of Coulomb failure. As the grains could slip on one another, the walls could not support tangential forces much higher than the one between the grains (Landry et al. (2003)). The fitted effective value of the wall friction coefficient $\bar{\mu}_w$ is given in Fig. 3.5. Such a lower value of effective friction is also observed in the dynamic case, because of the force network fluctuations (Artoni and Richard (2015)). As seen in Fig. 3.5 and Fig. 3.6, the cylinder significantly modifies the stress field inside the grains, and the hopper and channel geometries yield similar results.

In Fig. 3.6, the stress magnitude is lower in the top of the domain for the channel because the total height of grains above the cylinder is lower than with the hopper. However, the difference vanishes as depth increases and the saturating stress is reached before the cylinder. Just before the cylinder, the stress increases and suddenly drops afterwards. This is because the cylinder shields the grains directly below by deflecting the weight of the grains towards the walls. The drop is recovered over three to four cylinder diameters. The cylinder also gives the stress field a semi-circular orientation – indicated by

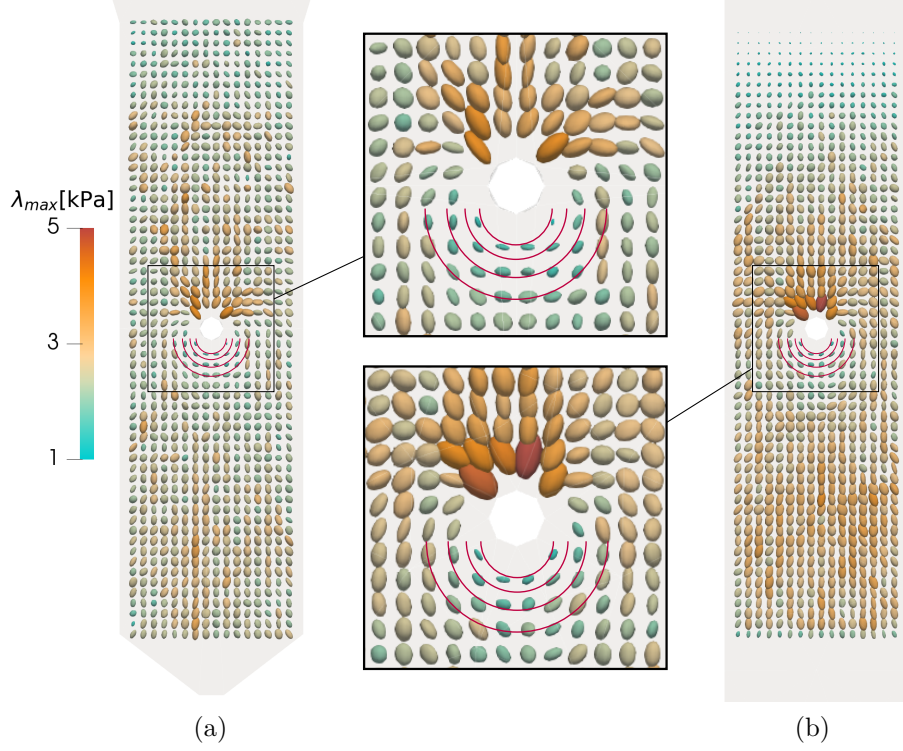


Fig. 3.6: Stress field inside the grains before the flow starts. (a): hopper geometry. (b): channel geometry. The ellipses' axes represent the principal stresses. Red lines underline the semi-circular orientation of the stress field.

the red lines in Fig. 3.6 – downstream, which persists for approximately two diameters.

3.3.2 Drag force

When the flow starts, the force exerted on the cylinder changes to reach the regime drag force. Results presented in Fig. 3.7 are the average over 4 runs, each with new random starting positions for the grains. Both geometries yield results matching the data from Chehata et al. (2003), although the channel seems to be slightly below the hopper. The drag force itself has a significant standard deviation but its mean value did not change much over the different runs, with mean standard deviations of 0.031 N and 0.059 N for the hopper and the channel respectively. The coefficients of friction were set to $\mu_g = 0.15$ between the grains and $\mu_w = 0.3$ between the grains and the walls to obtain

matching results. This difference should arise from the hypothesis of the same friction coefficient with the walls and with the cylinder. As detailed in section 3.3.3, the former tends to reduce the drag force and the latter tends to increase it. Hence, the higher value of μ_w compared to μ_g is a results from a competition between those two phenomena. Concerning the stress field, its norm evolves upon flowing of the grains but its orientation remains unchanged. Both norm and orientation do not significantly change with the flowing velocity. The orientation indicates that the drag is mainly due to compressive stress in front of the cylinder, i.e. in the stagnation zone, as supposed by Chehata et al. (2003). The semi-circular shape downstream supports the assumption of a circular zone of influence of the object (Faug (2015); Tordesillas et al. (2014)). The channel geometry yields results similar to the hopper geometry. Because

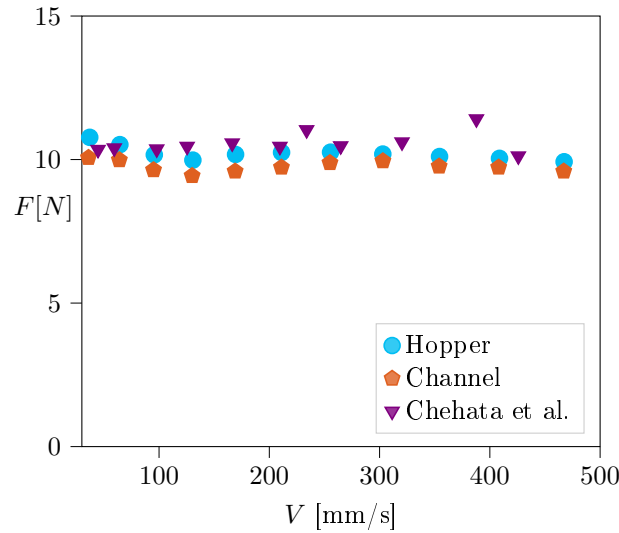


Fig. 3.7: Comparison of the drag force versus velocity from Chehata et al. with hopper and channel geometry simulations.

of its simplicity and its lower computational cost, it is used to study the influence of both friction and the interstitial fluid. Friction is at the origin of the velocity-independent behaviour of the drag. It also impacts the drag through the Janssen effect which determines the static stress in contained grains. Many applications of the granular drag – such as industrial mixing or avalanche protecting devices – feature an interstitial fluid. Its effects include drag reduction and fluidisation at lower velocities.

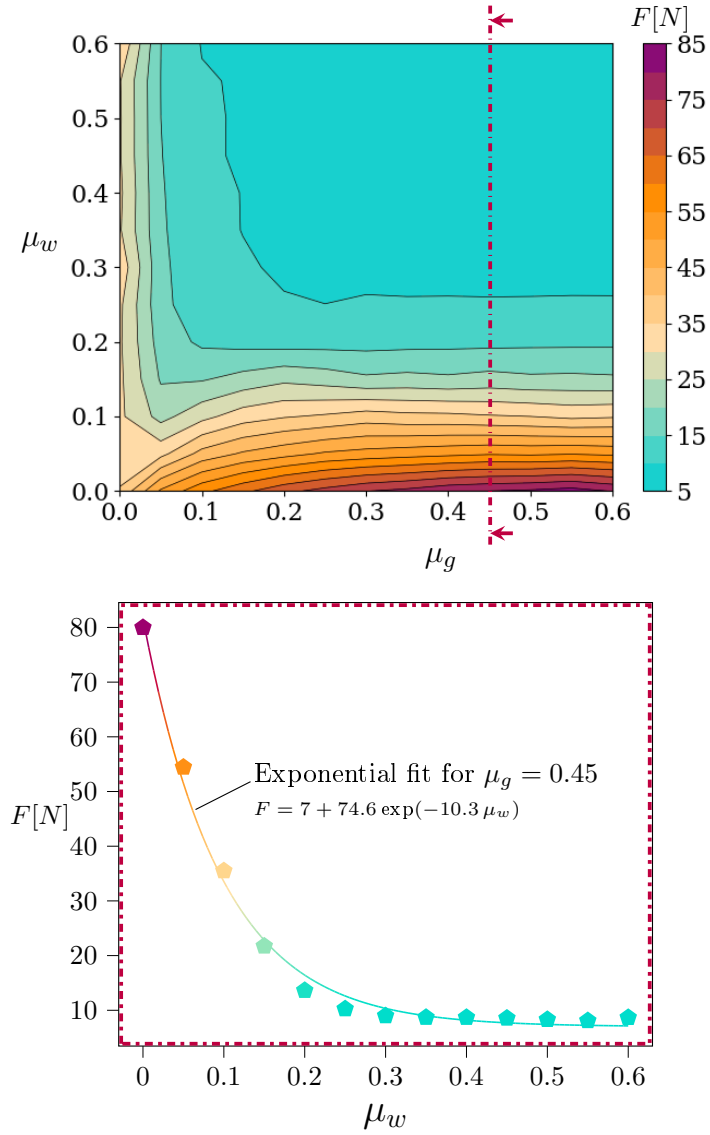


Fig. 3.8: Top: drag force as a function of the friction coefficients. Bottom: drag force as a function of μ_w for $\mu_g = 0.45$.

3.3.3 Impact of friction coefficients

Simulations were performed with a mean velocity of $V = 64$ mm/s with both friction coefficients ranging independently from 0 to 0.6 by steps of 0.05. The results are presented in Fig. 3.8. For a fixed grain friction coefficient $\mu_g > 0.1$, the drag decreases exponentially as the wall friction coefficient μ_w increases. At low $\mu_g < 0.1$, the exponential flattens and the drag becomes independent of μ_w . For a fixed $\mu_w > 0.1$, the drag decreases exponentially as μ_g increases. At low $\mu_w < 0.1$, the drag increases with μ_g . Other simulations show that when friction vanishes, inertial effects are predominant and the drag force exhibits a velocity dependent behaviour.

Those behaviours indicate that the drag F is linked to the saturating stress. The latter decreases with increasing friction, as the walls are able to support a larger part of the load. This Janssen effect should be taken into account in the choice of the dimensionless quantity F^* , sometimes referred to as the effective friction (Allen and Kudrolli (2019); Pouliquen and Forterre (2009)):

$$F^* = \frac{F}{PDW}, \quad (3.24)$$

with $P = \sigma_{yy}(\mathbf{x}_c)$ computed with Eq. 3.20. It is to note that the Janssen effect was shown to remain qualitatively valid in flowing conditions – at least for velocities up to 35 mm/s – but with an even stronger screening effect (Bertho et al. (2003)). The exact difference being difficult to compute, the formula for the static case is used. This should not affect the general behaviour of the data, but only its absolute value. F^* is plotted as a function of μ_w for different values of μ_g in Fig. 3.9.

Two regimes can be distinguished. From $\mu_w = 0.3$ on, F^* linearly increases with μ_w with a slope that decreases with increasing μ_g . It can be fitted with the following functional form:

$$F^* = \underbrace{A\mu_w}_{\text{Cylinder friction}} + B, \quad (3.25)$$

with A and B fitting parameters functions of μ_g . Fitting A for μ_g yields:

$$A(\mu_g) = \frac{2.6}{0.074 + \mu_g}. \quad (3.26)$$

This linear term is associated to the friction between the cylinder and the moving grains. It is directly proportional to μ_w , but as μ_g increases, the grain network reorganisation dominates. If the data for $\mu_g < 0.3$ is taken into account, the constant term in the model becomes a Gauss function:

$$F^* = \underbrace{A\mu_w}_{\text{Cylinder friction}} + B \exp(-C(\mu_w - D)^2), \quad (3.27)$$

with C and D fitting parameters also functions of μ_g .

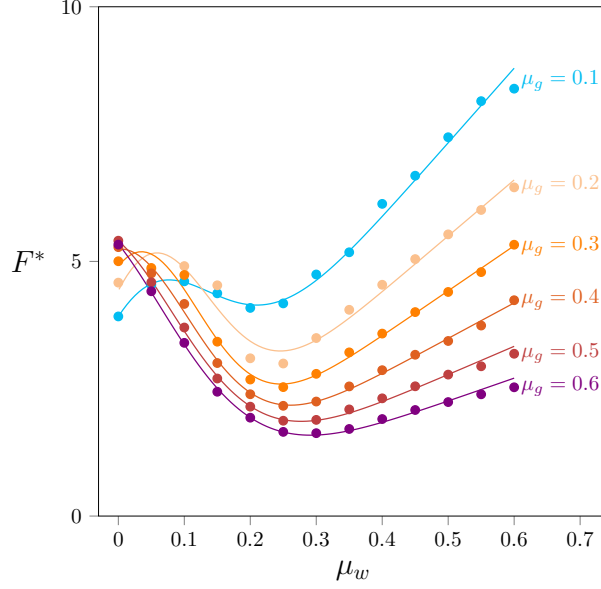


Fig. 3.9: F^* as a function of the friction coefficients for different values of μ_g . Each point is the average value over 4 simulations, each time with random positions for the grains. In all simulations, the packing fraction was close to $\phi_g \sim 0.64$. Solid lines are fits from Eq. 3.27. For clarity, some curves have been omitted.

3.3.4 Effect of an interstitial fluid

The steady flow of a uniform fluid-grain mixture injected under gravity through a channel with a given velocity is simulated. Such circumstances are met in civil engineering applications like raising the level of a building or stabilising its foundations by injecting sand mixed with water (Affeld et al. (2006)). The entrance and the exit of the channel are considered to be very far from the cylinder on which the drag force is measured. No-slip boundary conditions are prescribed on the walls and the cylinder. Results for the drag force are presented in Fig. 3.10. Although the force exerted on the cylinder by the fluid is negligible – 3 to 4 orders of magnitudes lower than the total drag – the presence of a fluid significantly decreases the drag force because it modifies the apparent weight of the grains and hence the gravity-induced stress (Costantino et al. (2011)). The same dimensionless quantity F^* is computed as in Eq. 3.24 but corrected for the apparent weight, collapsing the data for different fluid densities. The behaviour of the stress tensor indicated a Janssen stress saturation effect that was similar in all simulations. As seen in Fig. 3.10 (a), the

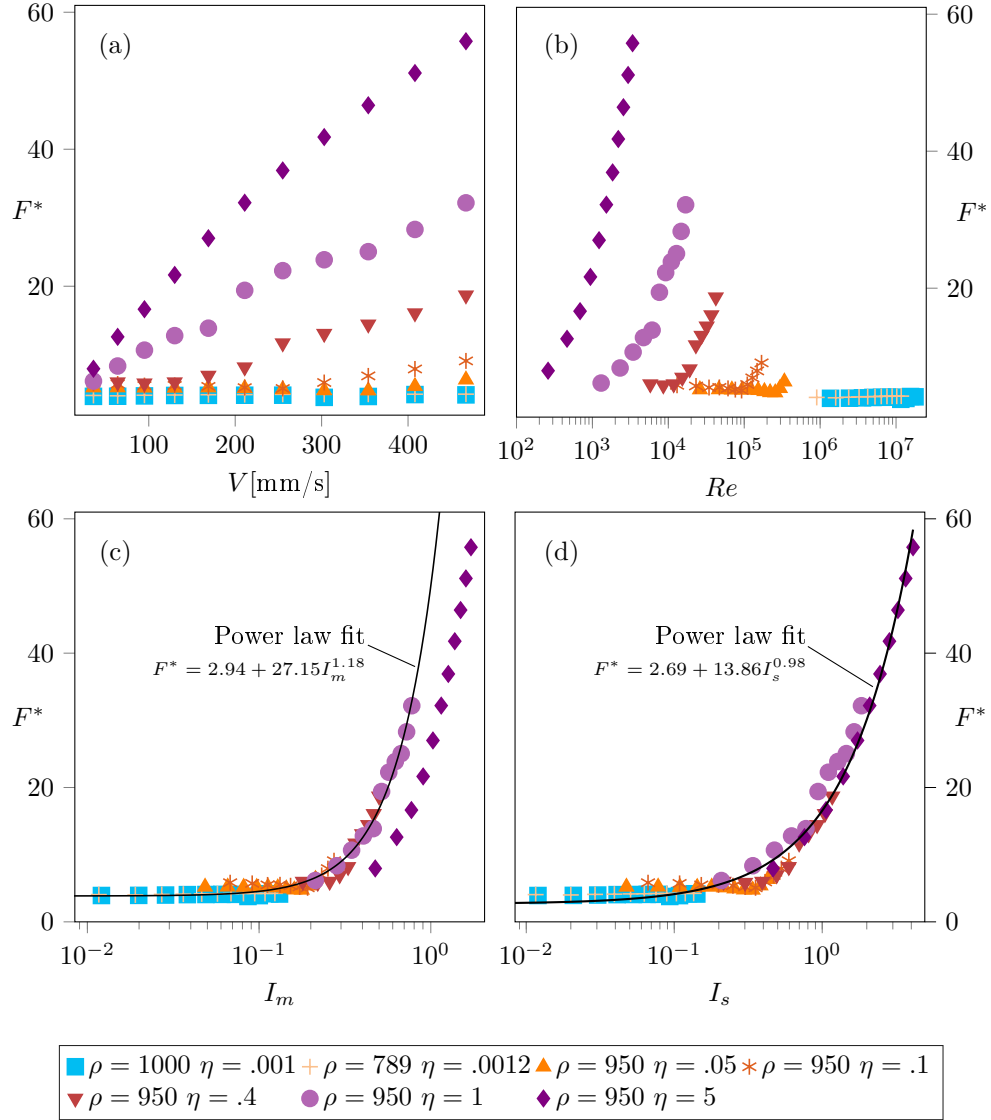


Fig. 3.10: Dimensionless drag force as a function of different parameters, (a): flow velocity, (b): Reynolds number, (c): modified inertial number, (d): modified viscous number. Densities are in kg/m^3 and viscosities in $\text{Pa}\cdot\text{s}$.

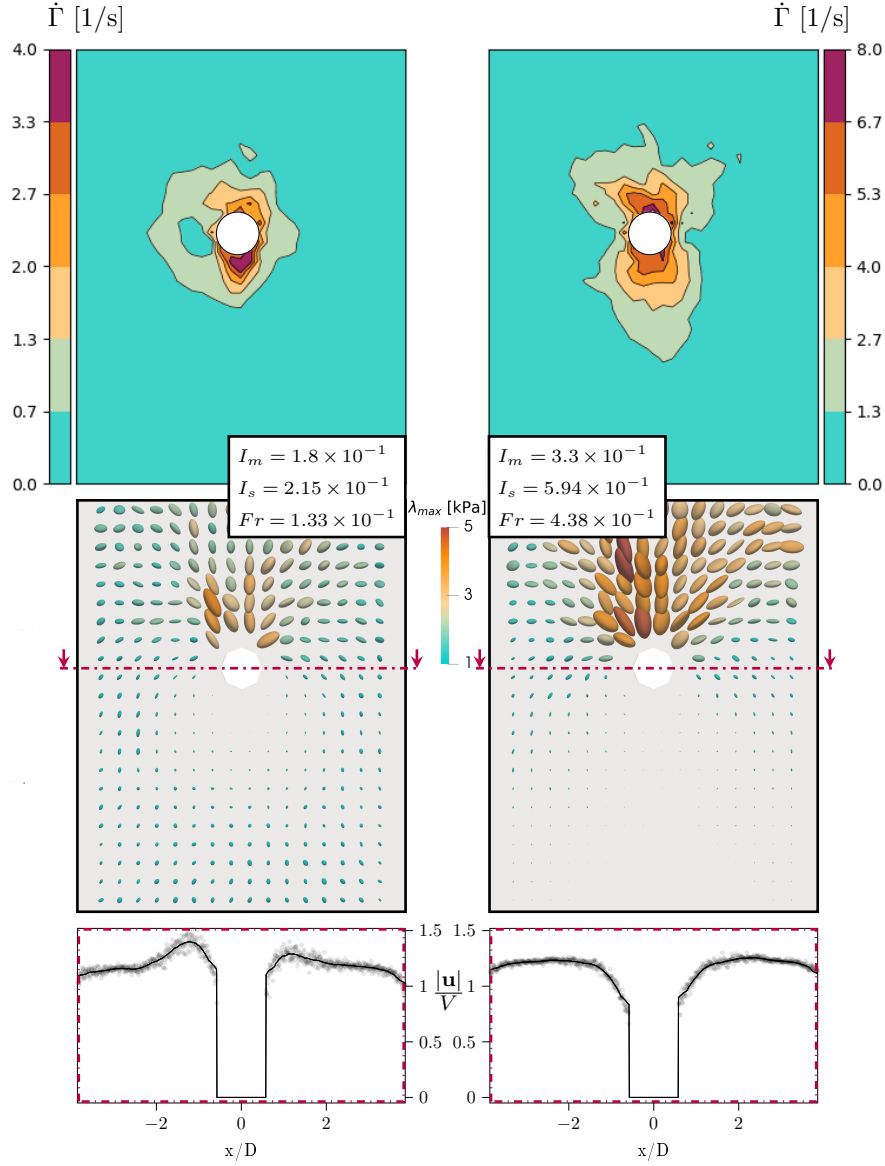


Fig. 3.11: Grain shear rates $\dot{\Gamma}$, stress fields and normalised velocity $|\mathbf{u}|/V$ profiles near the cylinder. Left: quasi-static regime. Right: fluidized regime. The average shear rate is computed with the same grid than the stress tensor. The grey dots in the velocity profiles are the average velocity at grid points. The grid stretches across the whole width of the channel horizontally, and one diameter above and below the cylinder vertically. The black line is the corresponding smoothed curve.

drag force becomes velocity dependent for a smaller velocity with increasing fluid viscosity. To fully describe the rheology of the fluid-grain mixture, a proper scaling implying both velocity and viscosity is necessary. Fig. 3.10 (b) shows that the Reynolds number $Re = \rho_f V D / \eta$ is not sufficient, because it lacks information about the granular part of the mixture. By considering the stresses at stake – inertial $\rho_g (d\dot{\gamma})^2$, viscous $\eta\dot{\gamma}$, and static P – it is possible to construct a dimensionless number that characterises the flow. The static stress P is computed with Eq. 3.20 adapted for the apparent weight. It should be noted that the visualisation of the stress tensor showed that the Janssen effect is still valid with a surrounding fluid. Actually, as the saturating stress is smaller because of buoyancy, the static stress and hence Janssen effect should decrease in importance relative to the inertial and viscous stresses.

The so-called modified viscoinertial number is taken as the square root of the ratio of a linear combination of the inertial and the viscous stresses to the static stress (Amarsid et al. (2017); Trung Vo et al. (2020)):

$$I_m = \sqrt{\frac{\rho_g (d\dot{\gamma})^2 + \beta \cdot \eta \dot{\gamma}}{P}}, \quad (3.28)$$

where $\dot{\gamma}$ is the shear rate and β is a fitting parameter that should depend on material properties such as grain shape and size distribution and friction coefficients (Trung Vo et al. (2020)). In granular flows, the shear rate may depend on both the cylinder diameter and the grain diameter when the ratio of the two is small (Seguin et al. (2013)). However, since the ratio D/d is around 6.35, the grain diameter is neglected in the shear rate which is chosen as $\dot{\gamma} = V/D$. Nonetheless, the grain diameter is already taken into account in I_m . The value of β that best fits the data is 39.9. As seen in Fig. 3.10 (c), this allows a collapse of all curves except the one with the highest viscosity. Ignoring the latter, the data is fitted by a single power law given in the figure. It is possible to collapse all the data by considering shear thickening, which has been observed for immersed granular flows (Fall et al. (2010)). In this case, the viscosity depends on the shear rate as follows:

$$\eta_s = H \dot{\gamma}^n, \quad (3.29)$$

with H a constant having appropriate units. The value of n that best collapses the data is $n = 0.7$. Replacing η by η_s to obtain a shear-thickening viscoinertial number:

$$I_s = \sqrt{\frac{\rho_g (d\dot{\gamma})^2 + \beta \cdot \eta_s \dot{\gamma}}{P}}, \quad (3.30)$$

yields Fig. 3.10 (d). Again, the data can be fitted with a single power law. Several physical mechanisms could explain the shear thickening of dense granular suspensions. Heussinger suggested that it is due to energy dissipation, notably through the formation of hydrodynamic clusters increasing viscous dissipation

(Heussinger (2013)). These clusters have a size linked to the viscosity of the surrounding fluid, which could explain why the data with the highest viscosity is the most affected by the consideration of shear thickening. Others suggested that it originates from constraints on grain rotation and relative sliding. These constraints can come from intergrain friction (Seto et al. (2013)) but also from hydrodynamic forces (Jamali and Brady (2019)). As hydrodynamic forces increase with viscosity, this could again explain the higher sensitivity of the high viscosity data set to shear thickening. However, it is still unclear how shear thickening manifests in the simulations and if I_s should be used, or if the highest viscosity data set is at the limit of the numerical model and I_m should be used.

The transition between the quasi-static – $F^* = \text{constant}$ – and the fluidized regimes occurs between $I_m = 0.15$ and $I_m = 0.4$ or between $I_s = 0.3$ and $I_s = 0.6$. The corresponding Froude numbers corrected for the apparent gravity due to buoyancy – $Fr = V/\sqrt{(1 - \rho_f/\rho_p)gD}$ – are below the threshold value of 10. This confirms that the fluid causes fluidisation at lower velocities. Fig. 3.11 shows the grain shear rate, the stress state and the velocity profiles in the quasi-static and the fluidized regimes close to the transition. The grain shear rate is computed as the Frobenius norm of the deformation rate tensor :

$$\dot{\Gamma} = \sqrt{\sum_i \sum_j \left(\frac{1}{2} \frac{\partial u_i}{\partial x_j} + \frac{1}{2} \frac{\partial u_j}{\partial x_i} \right)^2}. \quad (3.31)$$

The velocities are evaluated on a grid as the average of the velocities of the grains near the grid points. Their derivatives are computed with a first order central finite difference scheme. The grid is the same than the one used to compute the stress tensor. The shear zone size increases as expected with the flow velocity, but its shape changes from roughly circular in the quasi-static regime to an elongated shape aligned with the flow direction in the fluidized regime. Fluidisation decreases the stress field downstream of the cylinder, implying a reduction of the amount of intergrain contacts. In the quasi static regime, the increase in velocity occurs in the vicinity of the cylinder only: the flow slips in this region (Chehata et al. (2003)). In the inertial regime, the velocity increase is uniform across the channel and decays near the cylinder, which is characteristic of a viscous flow.

3.4 Conclusion

A simple model of Coulomb friction was successfully implemented in MigFlow. In order to validate it and illustrate the interest of such an implementation, the granular flow around a cylinder was simulated in both dry and immersed cases and the granular drag force was measured. The Janssen effect was captured

with an effective wall friction coefficient closer to the grain friction coefficient than to the prescribed wall friction coefficient. The independent behaviour of the drag force versus velocity was quantitatively recovered. A channel simulation geometry was validated in the dry case against physical experiments. Visualization of the stress field showed that the drag force is mainly due to compressive stress upstream of the cylinder. Its circular orientation downstream of the cylinder supports the hypothesis of a spherical zone of influence of the penetrating object.

The impact of the wall and grain friction coefficients was studied. The drag force was found to decrease exponentially with the friction coefficients, as the walls take a larger part of the gravitational load. A scaling for the drag force was then proposed based on the Janssen effect. It was found that the dimensionless drag force as a function of the wall friction coefficient follows two regimes. For high wall friction, the drag increases linearly with the wall friction coefficient, with a slope decreasing with increasing grain friction. For low wall friction, the drag follows a Gaussian function with parameters depending on grain friction. A more accurate study of the physical phenomenon of this contribution is required to fully characterise it.

In the immersed case, the contribution of the fluid on its own was found negligible compared to the one of the grains. Two dimensionless numbers were used to characterise the flow. The modified viscoinertial number I_m , based on a ratio of relevant stresses yielded a good collapse of the data except for the highest fluid viscosity. Considering shear thickening and using an adapted viscoinertial number I_s yielded a collapse of the whole data. Further investigation should be led to determine if I_m or I_s should be preferred. The transition between the quasi-static and the fluidized regime was accompanied by a reduction of the intergrain contacts downstream of the cylinder. The shear zone changes from circular to elongated in the direction of the flow. The velocity profile shifted from a slipping behaviour in the vicinity of the cylinder to a viscous one with a uniform velocity increase across the channel section and a decay close to the cylinder.

CHAPTER 4

Grain clusters and column collapse

So far, only spherical grains have been considered. This simplification has several advantages. First, the computational and implementational costs are decreased as spheres are more easily handled by numerical models. Second, the number of parameters to take into account is reduced as any shape parameter except the radius can be overlooked. Nonetheless, there is a wide range of grain shapes that modify the collective shear strength of granular assemblies by rate-dependent fabric and contact anisotropies (Pöschel and Buchholtz (1993); Azéma and Radjaï (2009, 2010); Hidalgo et al. (2009); Lu et al. (2015)). Grain shapes can vary from concave and elongated grains to convex grains, where interlocking and clustering is rapidly formed (Hidalgo et al. (2009)). For instance, elongated grains tend to form clusters more easily than spheres as they are subject to more important geometrical constraints, especially when interacting with boundary surfaces (Kudrolli et al. (2008)). Their length to width ratio is a key parameter, and they exhibit nonlinear behaviours in closed containers because of competing geometrical mechanisms (Lumay and Vandewalle (2004)). With that in mind, the ability to render those various shapes can prove very useful for a relevant numerical model. One of the simplest ways to render different grain shape is to use clusters of disks or spheres (Thomas and Bray (1999)), where the constituting particles are rigidly attached together with unbreakable bounds. The centres of mass and moments of inertia of the grains are computed a priori, and the contact topology and detection remain almost the same as for spheres. The main drawback is that the resulting grains have

rough surfaces whose rugosity depends on the radius of their constituting particles. To tackle this problem, the clusters can be made of overlapping spheres, but special care must be taken to adequately compute the inertia of the grains (Ferrellec and McDowell (2010)), or the porosity field in immersed cases. Intermediate approaches with other shapes such as spherocylinders (Pournin et al. (2005)), ellipses (Cleary and Sawley (2002)) or polyhedras (Azéma and Radjaï (2009)) offer a better capture of the grain shape. However, the computational cost is higher, notably the one associated to the contact detection as the contact point is not unique anymore and must be chosen adequately (Jean (2010)). Finally, the most accurate techniques to describe the surface of arbitrarily shaped grains rely on spherical harmonics (Garboczi (2002); Wang et al. (2021)). In general, the shapes of a real set of grains are obtained with a 3D scan, and the resulting coordinates are used to fit a spherical harmonics expansion. The real grain shapes can then be used, or even a set of shapes that shares statistically equivalent properties. However, more complicated shapes imply a much higher computational cost in term of contact detection and resolution.

The choice made in MigFlow is to use non-overlapping clusters of spherical particles in order to render more complex shapes. This allows to keep the computational cost reasonable, as is part of the objectives of the current model, while extending its relevancy range. In addition to keeping almost identical contact detection and resolution procedures, this choice also facilitates the computation of the fluid-grain interaction force. In the present chapter, the implementation of grains as disk clusters in MigFlow is detailed. Then, the resulting numerical model is applied to the study of granular assemblies made of elongated grains in dry and immersed conditions, more specifically to the column collapse experiment. A particular focus is set on the influence of the orientation of the grains.

The content of this chapter is largely inspired from the following paper:

Coppin, N., Henry, M., Cabrera, M., Azéma, E., Dubois, F., Legat, V., Lambrechts, J. 2023. Collapse dynamics of two-dimensional dry and immersed granular columns of elongated grains. *Physical Review Fluids* (under review).

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4.1 Clusters of disks

As already mentioned, irregularly shaped grains are modelled as rigid clusters of non-overlapping disks in MigFlow. The fact that the grains do not overlap avoids a possible null porosity when considering immersed problems. It also facilitates the computation of the mass and inertia of the grains, which is straightforward with the parallel axis theorem. The variables of interest are the positions $\mathbf{x}$ and velocities $\mathbf{u}$ of the centres of mass of the grains, as well as their Euler angles $\boldsymbol{\theta}$ and angular velocities $\boldsymbol{\omega}$. It is to note that now, the Euler angles cannot be overlooked as the grains may not have a symmetric shape. In three dimensions, as rotations are not commutative, this implies a careful treatment of the conversion between the angular velocities $\boldsymbol{\omega}$ and the time derivative of the Euler angles $d\boldsymbol{\theta}/dt$. So far, only two-dimensional clusters have been implemented in MigFlow. Therefore, the rest of the section focuses on the two-dimensional aspects of the Nonsmooth Contact Dynamics for grains made of disk clusters.

A contact frame is built at the contact point, with a normal vector $\mathbf{n}$ and a tangent vector $\mathbf{t}$, as well as the vectors $\mathbf{r}_i$ and $\mathbf{r}_j$ that link the contact point to the centres of mass of grain i and j , respectively (see Fig. 4.1).

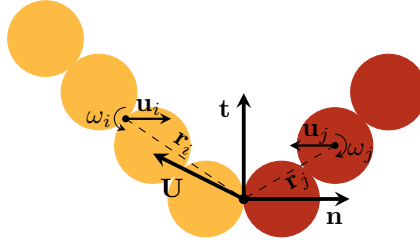


Fig. 4.1: A contact between two grains i and j formed as line clusters of disks, with the local frame $(\mathbf{n}, \mathbf{t})$, the radii $\mathbf{r}_i$ and $\mathbf{r}_j$, their velocities $\mathbf{u}_i$ and $\mathbf{u}_j$ and angular velocities ω_i and ω_j , and the resulting relative velocity $\mathbf{U}$.

The equation of dynamics in the contact frame is given by:

$$\mathbf{U}^+ = \mathbf{U}^- + \mathbf{W}\mathbf{P}, \quad (4.1)$$

with the $+$ and $-$ subscripts denoting the moments just after and just before the contact, $\mathbf{U}$ the relative velocity at the contact point, $\mathbf{W}$ the Delassus operator and $\mathbf{P}$ the impulse due to the integration of the contact reaction force over the duration of the contact. This equation is coupled to the following contact laws

that were already introduced in the previous chapters:

$$\text{If } d > 0 \text{ then } P_n = 0, \quad (4.2)$$

$$\text{If } d \leq 0 \text{ then } P_n \geq 0, \ U_n^+ \geq 0, \ P_n U_n^+ = 0, \quad (4.3)$$

$$\|\mathbf{P}_t\| \leq \mu P_n, \quad \|\mathbf{U}_t^+\| \neq 0 \Rightarrow \mathbf{P}_t = -\mu P_n \frac{\mathbf{U}_t^+}{\|\mathbf{U}_t^+\|}, \quad (4.4)$$

with d the distance between the two grains and μ the static coefficient of friction. In two dimensions, the solution of this contact problem can be discussed as follows:

$$\begin{aligned} &\text{if } P_t^{\text{stick}} + \mu P_n^{\text{stick}} < 0 : & (4.5) \\ &P_n = \frac{-U_n^-}{(1 - \mu \frac{W_{nt}}{W_{nn}})W_{nn}}, & P_t = -\mu P_n \\ &\text{if } P_t^{\text{stick}} - \mu P_n^{\text{stick}} > 0 : \\ &P_n = \frac{-U_n^-}{(1 + \mu \frac{W_{nt}}{W_{nn}})W_{nn}}, & P_t = \mu P_n \\ &\text{else} & : \\ &\mathbf{P} = \mathbf{P}^{\text{stick}}. \end{aligned}$$

with $\mathbf{P}^{\text{stick}} = -\mathbf{W}^{-1}\mathbf{U}^-$ the impulse that cancels the relative velocity. This solution is unique as long as the following condition is respected (Jean (1999)):

$$-1 < \mu \frac{W_{nt}}{W_{nn}} < 1, \quad (4.6)$$

meaning that the coupling between the normal and tangential components of the problem must be sufficiently low to avoid dynamical arching, i.e. unbounded reaction forces and the Painlevé paradox. In three dimensions, if the matrix $\mathbf{W}$ is not diagonal (i.e. the grains are not spherical), the solution of the frictional contact problem is not trivial and an iterative scheme must be employed, such as a Newton-Raphson for instance. The same iterative strategy described in the previous chapters is used to solve the contacts for the whole collection of grains. However, this time the contact frame $(\mathbf{n}, \mathbf{t})$ and radii $\mathbf{r}_i$ and $\mathbf{r}_j$ are recomputed at each iteration. Indeed, the predicted position of the contact point can significantly change between different iterations, notably because of the rotation of the grains. Moreover, contrary to the case of spherical grains, the position of the contact point now influences the matrix $\mathbf{W}$ through $\mathbf{r}_i$ and $\mathbf{r}_j$, which in turns influences the contact resolution.

4.1.1 Fluid-grain interactions

The interaction force is computed individually on each constituting disk. Afterwards, the fluid forces acting on each disk are added into the resulting net force and torque on the grain (see Fig. 4.2). This approach has already been used in several studies, notably to simulate sediment transport (Sun et al. (2017)) or fluidized beds of elongated grains (Jiang et al. (2021)). One of the main advantages of representing grains as clusters of disks is that the expression used to compute the drag force remains the same. Indeed, although many refined expressions exist for computing the drag force on nonspherical grains (Ma et al. (2022)), they often come at the cost of generality. Moreover, whereas most models using a modified drag coefficient to reckon with the grain shape ignore the hydrodynamic torque, it is explicitly computed here. Naturally, because of the spaces between the disks, the grains are porous and the fluid interactions are to some extent different than the ones for impermeable bodies. However, by carefully – i.e. avoiding a null porosity in the corresponding fluid cell – correcting the apparent surface of the grains for the fluid phase this difference can be reduced.

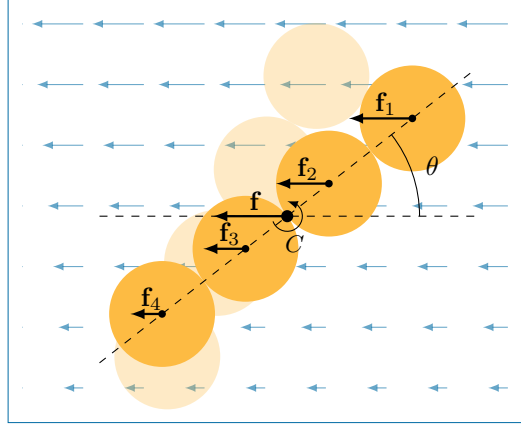


Fig. 4.2: Fluid forces exerted on disks in a shear flow and the resulting net force $\mathbf{f}$ and torque C on the corresponding elongated grain. The transparent drawing indicates the consequent motion of the grain. The blue arrows represent the fluid velocity.

The prediction of the velocity of the disks that is done in the Patankar scheme should take into account that the individual disks are now part of indivisible clusters and that their motion is hence constrained. To this end, the Patankar scheme is adapted by using a matrix $\mathbf{W}_d$ associated to disk d similar to the Delassus operator that takes into account the inertial and structural

information about the whole cluster:

$$\mathbf{W}_d = \begin{pmatrix} \frac{1}{m_{i(d)}} + \frac{r_{d,y}^2}{I_{i(d)}} & \frac{r_{d,x}r_{d,y}}{I_{i(d)}} \\ \frac{r_{d,x}r_{d,y}}{I_{i(d)}} & \frac{1}{m_{i(d)}} + \frac{r_{d,x}^2}{I_{i(d)}} \end{pmatrix} \quad (4.7)$$

$$\mathbf{r}_d = \mathbf{x}_d - \mathbf{x}_{i(d)}, \quad (4.8)$$

with $m_{i(d)}$, $I_{i(d)}$ and $\mathbf{x}_{i(d)}$ the mass, the inertia and the position of the centre of mass of the grain i to which the disk d belongs. It should be noted that this approach still ignores the effects of the fluid on the other disks of the cluster. For a very long elongated grain, the fluid fields may have significantly different values at the two opposite ends of the grain, which could eventually lead to instabilities because of the spatial coupling induced by the grain. Nonetheless, this should be mitigated by the predictor-corrector scheme presented in Chapter 1.

The prediction of the velocity of the disk at the next time step thus becomes:

$$\frac{\mathbf{u}_d^* - \mathbf{u}_d^i}{\Delta t} = \mathbf{W}_d \left(\mathbf{r}^i + m\mathbf{g} - V_d \nabla p - \gamma^i \left(\mathbf{u}_d^* - \frac{\mathbf{v}^{i+1}}{\phi^i} \Big|_{\mathbf{x}_d^i} \right) \right), \quad (4.9)$$

which leads to:

$$\mathbf{u}_d^* = \Delta t (\mathbf{I} + \mathbf{W}_d \gamma^i \Delta t)^{-1} \left(\frac{\mathbf{u}_d^i}{\Delta t} + \mathbf{g} + \mathbf{W}_d (\mathbf{r}^i - V_d \nabla p) + \gamma^i \mathbf{W}_d \frac{\mathbf{v}^{i+1}}{\phi^i} \Big|_{\mathbf{x}_d^i} \right) \quad (4.10)$$

$$\mathbf{f}_d^{i+1} = \gamma^i \left(\mathbf{u}_d^* - \frac{\mathbf{v}^{i+1}}{\phi^i} \Big|_{\mathbf{x}_d^i} \right). \quad (4.11)$$

4.2 Column collapse of elongated grains

A common simplified approach to study the behaviour of granular material is the collapse of a granular column (Lube et al. (2004); Lajeunesse et al. (2004)), recognised as a benchmark case in dry, saturated, and immersed conditions (Bougouin and Lacaze (2018); Pinzon and Cabrera (2019); Taylor-Noonan et al. (2021)). In this configuration, a column of initial height H_0 and initial width L_0 is released and collapses under self-weight over a horizontal surface. After release, part of the column's potential energy is converted into kinetic energy and is then dissipated until the column comes to rest and forms a deposit. The deposit runout L_f follows a piece-wise power law as a function of the column aspect ratio H_0/L_0 , allowing a differentiation between short and tall columns (Lube et al. (2004); Lajeunesse et al. (2004)). The fraction of dissipated energy increases with H_0/L_0 and is independent of surface or material parameters, like the grain size or the grain size distribution (Lube et al. (2004);

Lajeunesse et al. (2004); Cabrera and Estrada (2019, 2021)). In addition, granular flows are strongly affected by the dilatant or contractant behaviour defined by the system packing fraction, setting a clear distinction between initially dense and initially loose granular systems (Rondon et al. (2011); Lacaze et al. (2021); Polanía et al. (2022)). This dependency is unified in a simple scaling, requiring only the fluid-grain density ratio, proportional to the packing fraction, and the front kinetic energy for describing the system runout (Polanía et al. (2022)). However, grain shapes that depart from spheres may modify, to some extent, the dependency with H_0/L_0 and with the initial density ratio (Trepanier and Franklin (2010); Zhao et al. (2020); Karapiperis et al. (2022)). For example, elongated grains show orientational features associated with a collective entanglement, or interlocking, that might prevent the column from collapsing (Trepanier and Franklin (2010); Tapia-McClung and Zenit (2012)) and yet form relatively loose granular systems; or lead to the formation of ordered structures of aligned grains in the deposit that result in dense granular systems (Hidalgo et al. (2010); Tapia-McClung and Zenit (2012); Jara and Cabrera (2021); Lumay and Vandewalle (2006)). Nonetheless, for aspect ratios that are not sufficiently large to prevent the collapse, the influence of the grain shape on the collapse dynamics has been found to be small (Lube et al. (2005); Tapia-McClung and Zenit (2012)), except for particles with high blockiness which have a reduced runout (Hoang and Nguyen (2023)). In the immersed case, most studies on elongated grains concentrate on colloidal suspensions of rods, which have similarities to polymer solutions and exhibit shear-thinning due to orientational ordering (Solomon and Spicer (2010); Boek et al. (1997)). For larger grains, the features specific to elongated grains are further amplified when surrounded by a fluid (Jara and Cabrera (2021)), but the extent to which they affect the mobility of granular flows is yet poorly understood, especially in the immersed case. The latter is, for example, of great interest in understanding the jamming of driftwood debris (Schalko et al. (2020, 2021); Piton et al. (2023)) or in the stability of layered cliffs which can result from debris or pyroclastic flows (Major (1998); Zrelak et al. (2020)), where the collective orientation of its constituent grains plays a dominant role in the process.

In this section, the effects of grain orientation in dry and immersed granular flows are studied, comparing initially disordered (i.e. a random initial grain orientation) and initially ordered (i.e. an initial grain orientation aligned with a given direction) granular systems. To that end, the column collapse of two-dimensional elongated grains is explored. The two-dimensional column collapse allows the simplification of the orientation of grains into a single scalar θ , and hence helps in isolating its associated effect. Focus is set on the role of grain orientation and varying H_0/L_0 , while employing elongated grains that are far from interrupting the column collapse (Trepanier and Franklin (2010)). The studied collapses shed light on the distinct orientational features, at the scale of the grains, that are amplified by the ambient fluid, like grain-clustering or

grain re-orientation, and that could modify the collapse sequence and thus its runout. The effect of grain orientation is then generalised in the description of the mobility of granular flows, adding a viscous-like term to the simplified scaling proposed by Polanía et al. (2022). Finally, conclusions and further effects of grain orientation are discussed.

4.2.1 Simulation strategy

Elongated grains are simulated as a single-line cluster of disks, as in Tapia-McClung and Zenit (2012), computing the fluid-grain interaction forces at the disk level. Note that these simplified two-dimensional hydrodynamic interactions on an elongated grain are inevitably different than those for three-dimensional rods. Nevertheless, we assume that they are still relevant for capturing the interplay between grain orientation and fluid kinematics. We tested the current implementation of a line cluster of disks with the experimental observations of the free-fall kinematics of a single rod immersed in a fluid and within a planar setup (Jara and Cabrera (2021)). Remarkably, the fluid-rod-like interactions, like fluttering and settling, are recovered by the fluid-grain system. Further improvements can be achieved by adding multi-line clusters and by correcting the surface of the grain so that it matches the one of the rod. However, in a large collection of grains such a surface correction could lead to a null porosity in a fluid element. For this reason, and for computational convenience, the simplest representation of a single-line of disks was adopted for the study of grains orientation in a granular flow.

Taking inspiration from Jara and Cabrera (2021), the elongated grains are made of disks with a diameter $d = 2.15$ mm, with a density $\rho_g = 1840$ kg/m³, and have a variable length l . Hence, two collections of elongated grains are employed in this work, clustering 3 or 4 disks with the aim of obtaining an overall mean grain aspect ratio of $d/l = 3.21$. Moreover, a slight polydispersity of $1.05d$ on each grain was introduced for preventing crystallisation. The friction coefficients were calibrated to $\mu_w = 0.3$ between the grains and the wall, and $\mu_g = 0.9$ between grains, matching the results from Jara and Cabrera (2021) in terms of runout and deposit shape. In the immersed scenarios, the surrounding fluid is water with $\rho_f = 1000$ kg/m³ and $\eta = 10^{-3}$ Pa s. For computational reasons, the mesh was finer near the initial column position and coarser at the other end of the domain. The most refined elements were ≈ 4.7 times the size of an elongated grain.

The samples were generated by depositing artificial disks under gravity and within a rectangular container. The artificial disks have diameters that correspond to the elongated grains lengths. When the deposit comes to rest, the disks are replaced by the elongated grains with a desired orientation θ with respect to the horizontal. Their rotation is frozen, and the grains settle. Then, their rotation is freed and the grains settle again, forming a two-dimensional

axisymmetric column. To avoid grain size effects, the column's initial width is set to $L_0 = 0.29$ m, being slightly larger than 75 times the grains length (Cabrera and Estrada (2019)). The column is released by removing one of the container's lateral walls. For the sake of statistical significance, every configuration was simulated three times, resulting in 144 simulations. The maximum number of grains in a simulation was 89000. The studied dry column collapses are in the free-fall regime and the immersed columns are in the inertial regime according to Courrech du Pont et al. (2003). Therefore, the inertia of the grains is expected to control the flow.

The simulations are divided into two groups. The first group of simulations focuses on the general dynamics of a column collapse of initially disordered elongated grains (i.e., grains randomly oriented) in dry and immersed conditions. The initial disordered column is set as a random distribution of elongated grains with initial orientation within a full rotation ($0^\circ \leq \theta \leq 360^\circ$). The initial porosity for this stage is uniform across the column, with $\phi = 0.237 \pm 0.014$. The column aspect ratio was increased from $H_0/L_0 = 0.125$ to $H_0/L_0 = 16$, exploring the transition from short to tall columns. In the second group of simulations, a short and a tall column are studied ($H_0/L_0 \in [0.5; 8]$), exploring the effect of ordered grains (i.e., columns having all grains preferentially oriented in a given direction) with main initial orientations $\theta_0^* \in [-90^\circ; -60^\circ; -45^\circ; -30^\circ; 0^\circ; 30^\circ; 45^\circ; 60^\circ; 90^\circ]$. Note that columns with a main orientation of $\theta_0^* < 0^\circ$ have a tendency to lean on the left wall. In this stage, the resulting porosity range is $\phi = 0.207 \pm 0.017$. Therefore, it can be argued that dense columns are studied in both stages.

4.2.2 Randomly oriented grains

The column collapse of elongated grains shows a similar sequence as that of collapses involving spherical or nearly spherical grains (Bougouin and Lacaze (2018); Pinzon and Cabrera (2019); Taylor-Noonan et al. (2021)). This sequence initiates with an accelerating phase where the grains free-fall or move laterally (see Fig. 4.3 and Fig. 4.4 (b)), then transition to a predominant side-propagation phase (see Fig. 4.3 and Fig. 4.4(c)), and finally a decelerating phase until forming a deposit (see Fig. 4.3 and Fig. 4.4 (d)). Here, the collapse sequence duration is normalised by a reference dimensionless time $\tau = \sqrt{2H_0/g^*}$, accounting for the relative free-fall time of a grain from the initial height of the column H_0 and with $g^* = g(\rho_g - \rho_f)/\rho_g$ as the effective gravity correcting for buoyancy (Lajeunesse et al. (2005); Meruane et al. (2010)).

Interestingly, a clear distinction between dry and immersed column collapses is observed on the released volume at the initiation phase and the velocity at which it propagates. In dry columns almost all moving grains are in motion after initiation, while in immersed columns only a thin vertical layer, next to the release face, starts moving and propagates inwards during collapse.

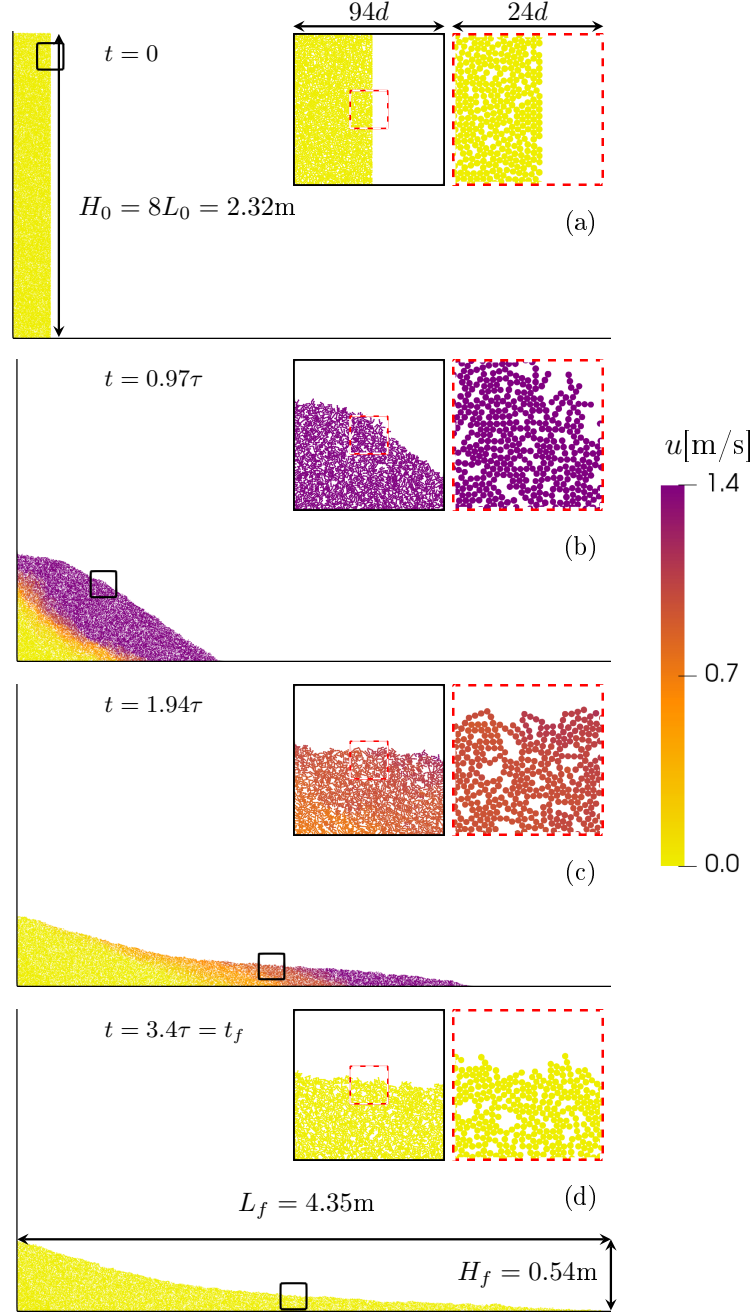


Fig. 4.3: Snapshots of a dry column collapse with initial aspect ratio $H_0/L_0 = 8$ and random initial grain orientation. The grains are coloured with their instantaneous velocity u . The insets correspond to zooms on the column region marked with the same border pattern.

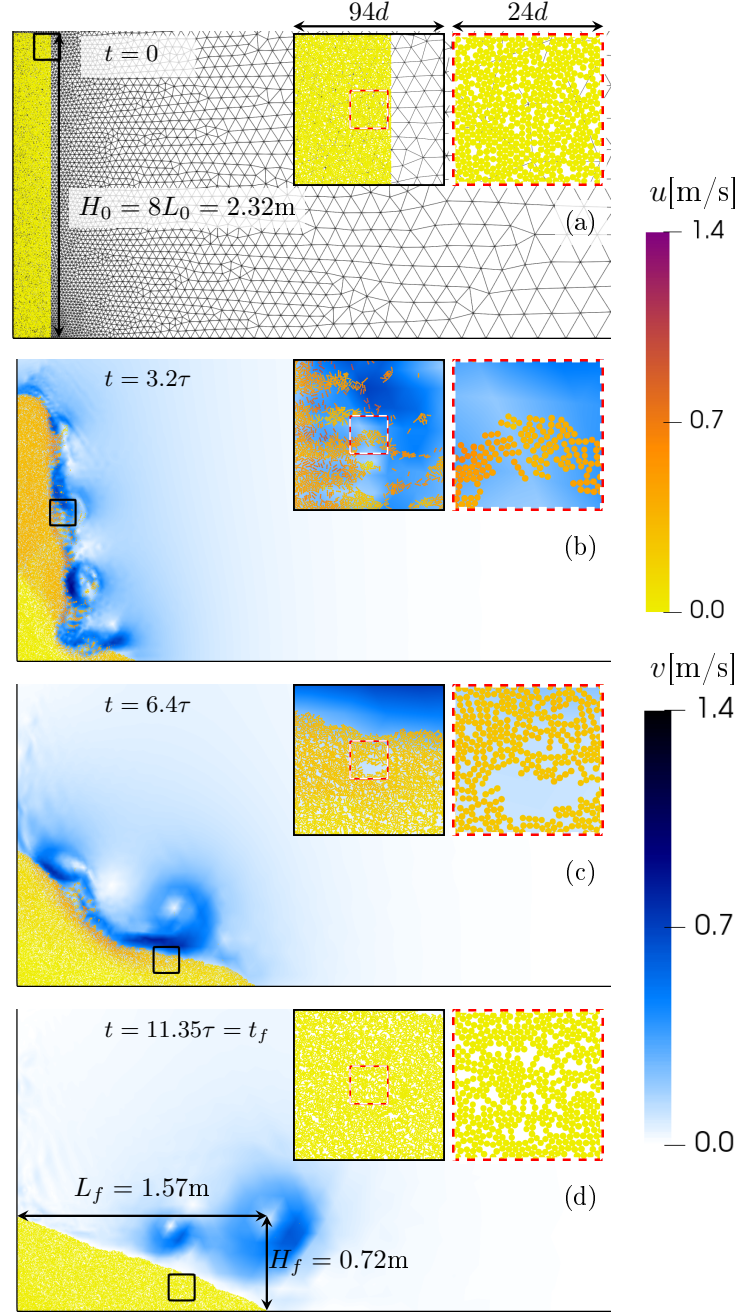


Fig. 4.4: Snapshots of an immersed column collapse with initial aspect ratio $H_0/L_0 = 8$ and random initial grain orientation. The grains and fluid elements are coloured with their instantaneous velocity u and v , respectively. The insets correspond to zooms on the column region marked with the same border pattern.

This localised mobilisation is not surprising, being observed in the collapse of dense columns (Rondon et al. (2011); Polanía et al. (2022)) and attributed to the competing action of the grains tendency to dilate and the fluid infiltration. This pore pressure effect (Iverson (2005)) is well captured by the current numerical model, as the pressure is lower inside the grains when the columns starts to collapse. As a result of the corresponding fluid motion, the observed contact forces between the grains are more important in the immersed case with respect to the apparent gravity. Moreover, in immersed columns, the grains near the free surface form finger-like structures perpendicular to the moving mass (see Fig. 4.4 (c,d)). As these structures accelerate, they cross each other and recirculate with the so-induced vortexes in the fluid. This dynamic is similar to the one of interacting Stokes clouds (Constant et al. (2019)). As they reach the bottom surface, they accumulate and form a concave surface behind the flow front. The concave surface deflects the flow upwards, similar to a hydraulic ski jump (Steiner et al. (2008)), and sets the grains to deposit halfway from L_0 . At the deceleration phase, the flow limits to a region near the free surface. Tall columns form a concave deposit shape in dry collapses and a roughly triangular shape in immersed collapses, as a result of the smoothing induced by the remaining vortexes in the fluid (see Fig. 4.5).

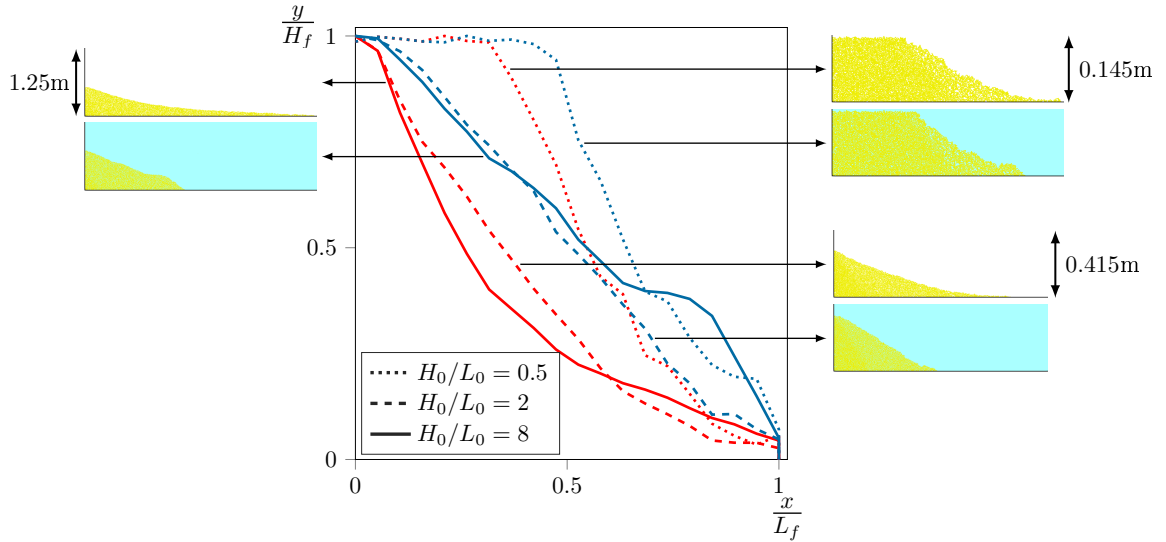


Fig. 4.5: Dimensionless deposit profiles for different column aspect ratios H_0/L_0 . The red and blue colours indicate dry and immersed collapses. The insets show snapshots of the corresponding profiles. The light blue backgrounds indicate the immersed cases.

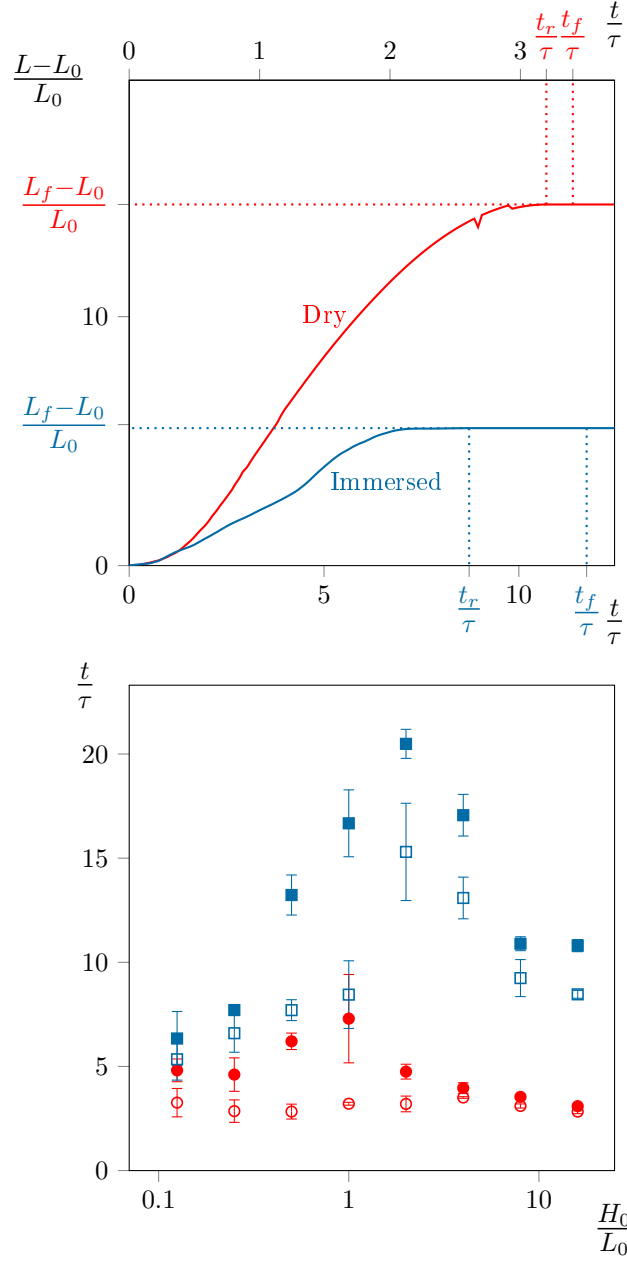


Fig. 4.6: Top: Temporal evolution of the normalised front position during the collapse for a column of aspect ratio $H_0/L_0 = 8$. The dotted lines indicate the dimensionless runout times t_r/τ and final t_f/τ times relative to the normalised runout $(L_f - L_0)/L_0$. Bottom: Dimensionless runout t_r/τ (empty symbols) and final times t_f/τ (solid symbols) as a function of H_0/L_0 . The red circles and the blue squares indicate dry and immersed collapses, respectively.

Note that some bumps due to the hydraulic ski jump behaviour can appear in the final deposit shape for immersed collapses. The differences between dry and immersed collapses vanish for short columns, as in that case the motion only takes place in a wedge in the upper right corner of the column. The collapse sequence can be captured by following the released mass front position L (see Fig. 4.6 top). It should be noted that avalanches are transient in nature and that a steady state in the side-propagation phase does not really occur, but rather an inflexion from acceleration to deceleration (Staron and Hinch (2007)). Nevertheless, the average velocity U^{fr} of the front position L can be defined as a characteristic of the side-propagation phase, averaging the slope of the curve in Fig. 4.6 between the times at which 30% and 70% of the final runout are reached. From this, the front kinetic energy can also be defined as $E_k^{fr} = MU^{fr^2}/2$, with M as the column total mass. Moreover, in the presence of a fluid, multiple collapse phases can be observed, as in (Lacaze et al. (2008)) for saturated columns, but their reproducibility between the simulations is low.

The runout time t_r and the final collapse time t_f are defined as the elapsed time until $L = L_f$ and as the elapsed time until the grains come to rest, respectively (see Fig. 4.6 top).

Both, t_r and t_f are found to vary with the ambient fluid and with the column initial aspect ratio H_0/L_0 , leading to longer collapses in the immersed cases (see Fig. 4.6 bottom). In dry columns, t_r/τ is nearly constant, indicating a free fall regime independent of H_0/L_0 . The value of t_f/τ first increases as more grains are available to flow on the free surface of the deposit without increasing the runout. After a maximum at $H_0/L_0 = 1$, indicating a transition from short to tall columns, t_f/τ gets closer to t_r/τ as the motion localises in a shallow flowing layer at the front. In the immersed case, both t_r/τ and t_f/τ increase with H_0/L_0 as the grain motion is hindered by the fluid phase. The difference between them also increases as the fluid motion is more important and is able to sustain grain motion at the free surface of the deposit for a longer time. As the columns get taller, the finger-like structures start to appear. These clusters of grains can have a larger settling velocity than isolated grains (Schneider et al. (2021)), which could explain the associated decrease of both t_r/τ and t_f/τ . This time, the difference between them decreases, as the fluid motion is even more important and is able to push the grains forward.

As mentioned above, a characteristic of the column collapse is the distinction between short and tall columns. These collapse types follow a piece-wise power law for the normalised runout $(L_f - L_0)/L_0$, increasing with H_0/L_0 and being steeper for the case of short columns. Here, the distinction between short and tall columns is also observed (Fig. 4.7 top), being independent to the employed grain shape ratios ($d/l \approx 3$). The transition between short and tall columns is not exactly identified but occurs for H_0/L_0 somewhere between 2 and 4 for the dry case, and between 1 and 2 for the immersed case.

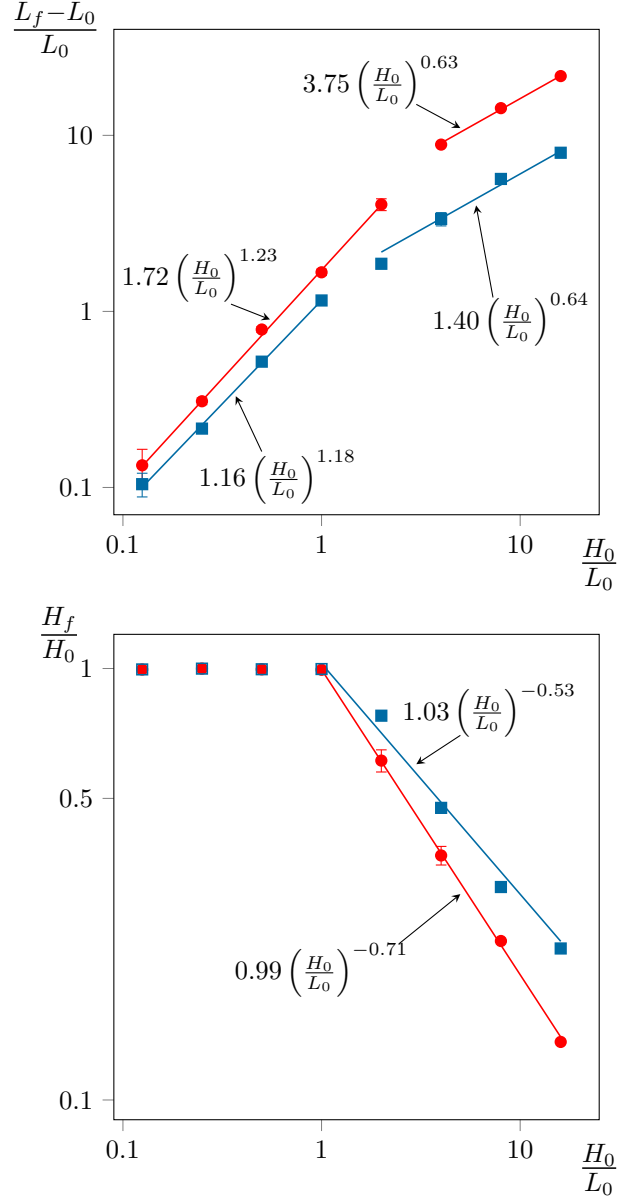


Fig. 4.7: Normalised runout (top) and normalised final height (bottom) for columns with randomly oriented grains as a function of the column aspect ratio H_0/L_0 . The red circles and the blue squares indicate dry and immersed collapses, respectively. Error bars correspond to one standard deviation. Note that some of the error bars are sufficiently small so that they cannot be distinguished.

Moreover, the normalised deposit final height H_f/H_0 also follows a piece-wise power law (see Fig. 4.7 bottom). The transition occurs at $H_0/L_0 = 1$ in both cases, resulting in a lower slope for the immersed case. This is due to the fluid preventing the grains from sliding too far, and hence, by mass conservation, leading to higher final heights.

The grain orientation is tracked during the collapse, focusing on the main orientation and corresponding anisotropy of the moving grains. Let $\mathbf{s}_n = (\cos(\theta_n), \sin(\theta_n))$ be the orientation vector of the grain n parallel to its longest dimension, with θ_n as the corresponding angle with respect to the horizontal. Since keeping track of the orientation of each grain is too complex and demanding, the focus is set on the probability density function $P(\theta) = N_\theta/\delta\theta$, such as N_θ is the number of grains with orientation between $[\theta - \delta\theta/2; \theta + \delta\theta/2]$ and $\theta \in [-90^\circ; 90^\circ]$. This periodic distribution can be approximated with the first two terms of its Fourier series expansion (Reddy et al. (2009)):

$$P(\theta) = \frac{1}{2\pi} (1 + a \cos(2(\theta - \theta^*))), \quad (4.12)$$

where θ^* is the main orientation and a describes the anisotropy of the distribution. Furthermore, the values θ^* and a are computed from a so-called fabric tensor (Azéma and Radjaï (2010); Botton et al. (2013)):

$$S_{ij} = \frac{1}{N} \sum_n s_n^i s_n^j, \quad (4.13)$$

with N as the total number of grains. The anisotropy a can then be obtained as $2(S_1 - S_2)$, with S_1 and S_2 the principal values of $\mathbf{S}$, and the main orientation θ^* as the orientation of the first principal direction of $\mathbf{L}$. For consistency, these quantities focus on the moving grains, excluding all grains that moved less than a distance d between $t \in [0 : t_f]$.

The time evolution of θ^* and a of a typical column collapse sequence is shown in Fig. 4.8. Here, the initial random orientation is slightly anisotropic and aligned along the horizontal, which comes from the sample generation process driven by gravity deposition (Börzsönyi and Stannarius (2013)). After the collapse starts, the grains align with the granular flow direction, changing from nearly -10° in dry flows and -20° in immersed flows, to then nearly horizontal orientations (instants II and III in Fig. 4.8).

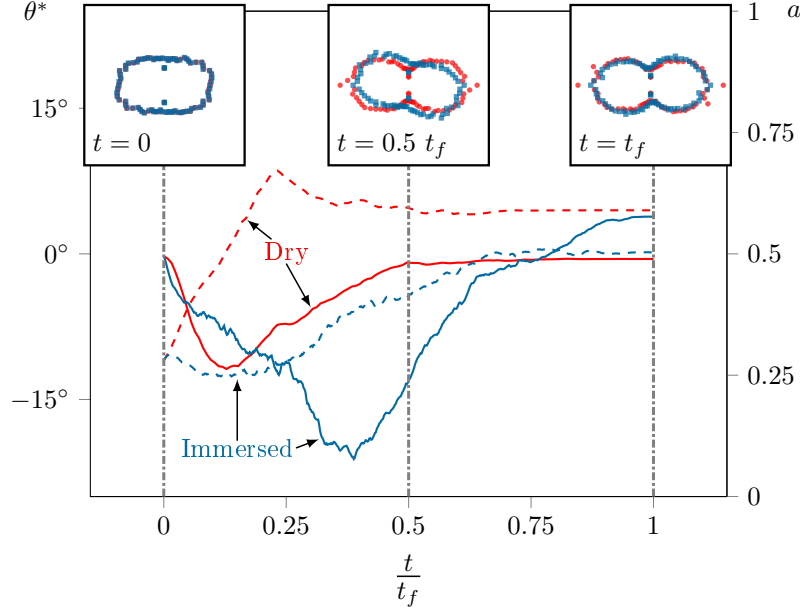


Fig. 4.8: Temporal evolution of the main orientation θ^* (solid) and anisotropy a (dashed) of the orientation distribution for a random initial orientation and $H_0/L_0 = 8$. The red and blue colours indicate dry and immersed collapses. The insets are polar plots of the orientation distribution showing the relative frequency of a given orientation.

Overall, the moving grains anisotropy increases with time, having a steeper increase in dry collapses. In dry columns, the orientation of the grains stagnates halfway the end of the flow, while in immersed columns, the grains orientation changes during the whole collapse duration. This is because in dry flows the grains motion localises more rapidly into a shallow flowing layer, while in immersed flows the fluid vortexes keep interacting with the grains even after the formation of the shallow flowing layer. Note that the final values of θ^* and a are similar for both cases, reaching a state often referred to as a nematic configuration (Hidalgo et al. (2010); Jara and Cabrera (2021)).

4.3 Columns with an initial grain orientation

This section focuses on exploring the effect of the initial main grain orientation ($\theta_0^* \in [-90^\circ : 90^\circ]$) in short and tall columns ($H_0/L_0 = [0.5, 8]$), respectively. The collapse dynamics, the runout and the evolution of θ^* are compared to the random case that was explored in the previous section.

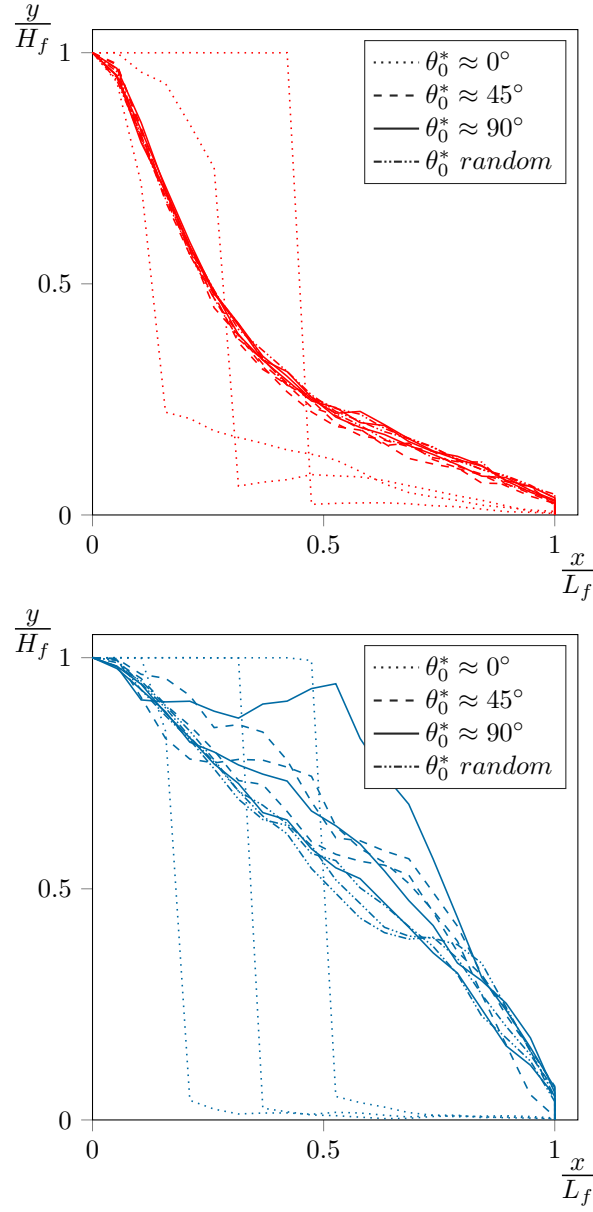


Fig. 4.9: Dimensionless deposit profiles for different initial grain main orientations θ_0^* in the dry (top, in red) and immersed (bottom, in blue) cases. The columns have an aspect ratio $H_0/L_0 = 8$.

Overall, when a column collapse takes place ($\theta_0^* \neq 0^\circ$), the initial grain orientation does not modify the collapse sequence described in Sec. 4.2.2. However, for the meta-stable case of $\theta_0^* = 0^\circ$, i.e. a “brick-wall” configuration, only a few grains are released from the column, forming a step-like deposit (see the dotted profiles in Fig. 4.9). In addition to this, in immersed tall column collapses, with $\theta_0^* \neq 0^\circ$, the bumps can be more important (see Fig. 4.9). Moreover, columns with main grain orientations $\theta_0^* \neq [0^\circ; 90^\circ]$ tend to slide in stacked clusters of grains, reaching a longer runout when the main grain orientation favours the slide at release ($\theta_0^* < 0$).

The collapse duration is also modified by θ_0^* , both when reaching the runout distance t_r and final deposit t_f (see Fig. 4.10). However, the effect of grain orientation is different in short and tall columns, leading to longer collapse durations in short columns when $\theta_0^* \neq [0^\circ; 90^\circ]$, and the opposite in tall columns, where collapses consistently last longer than in columns with an initially random grain orientation. The longer collapse times in tall columns is asymmetric, leading to longer collapses for $\theta_0^* = -30^\circ$. This behaviour is linked to the change in collapse dynamics mentioned above, with the release of stacks of grains sliding on each other. Overall, the variance of the data within collapse repetitions is large, indicating a strong dependency on the initial fabric tensor prior collapse.

Contrary to the collapse duration, the column runout is slightly affected by θ_0^* , with a marked difference when $\theta_0^* = 0^\circ$ and showing a similar trend for both short and tall columns (see Fig. 4.11). As expected, the observed trend is asymmetric, leading to longer runouts in initially unstable configurations ($\theta_0^* < 0^\circ$) for both dry and immersed collapses. In these configurations the stacked release of grains favours hydrodynamic interactions, propelling the grains further away. Note that for columns consisting of an arrangement of nearly vertically oriented grains ($\theta_0^* \approx 90^\circ$) the runout distance is almost that of columns with initially randomly oriented grains. This is found to be associated to rapid changes in the grains orientation, transitioning to a more uniform distribution and without forming grain stacks.

Tall and short columns share a similar trend in the variation of main grain orientation θ^* and anisotropy a during collapse. In these collapses, θ_0^* and the initial column anisotropy a_0 transition towards a main horizontal orientation and a more uniform fabric. This transition occurs earlier in the collapse in dry columns than in immersed columns, but the final distribution is nearly the same (see instants $0.5t_f$ and t_f in Fig. 4.12 bottom). Contrary to randomly oriented immersed columns, the grain main orientation saturates before t_f , reaching a nearly nematic configuration in most cases. The variation of a with θ_0^* shows a peak at $\theta_0^* = 0^\circ$ and then decays in a nearly symmetrical function and towards the fabric anisotropies observed in the initially random collapses (see Fig. 4.12 bottom). The peak at $\theta_0^* = 0^\circ$ is expected, since only very few grains collapse, while the attraction to the common value $a \in [0.54 : 0.62]$ indicates a behaviour independent of θ_0^* .

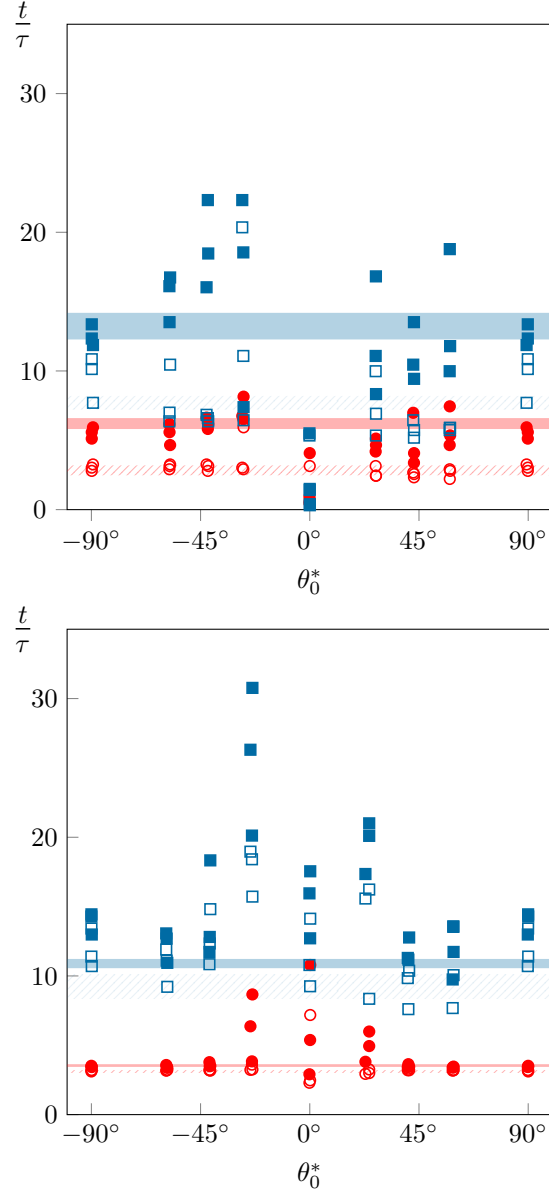


Fig. 4.10: Dimensionless runout times t_r (empty symbols) and final times t_f (solid symbols) as a function of the initial main grain orientation θ_0^* . Top: short columns ($H_0/L_0 = 0.5$). Bottom: tall columns ($H_0/L_0 = 8$). The hatched areas present the range of t_r and the uniform shaded areas indicate the range of t_f for the random initial orientations presented in Fig. 4.6, with their widths corresponding to two standard deviations. The red circles and blue squares indicate dry and immersed collapses, respectively.

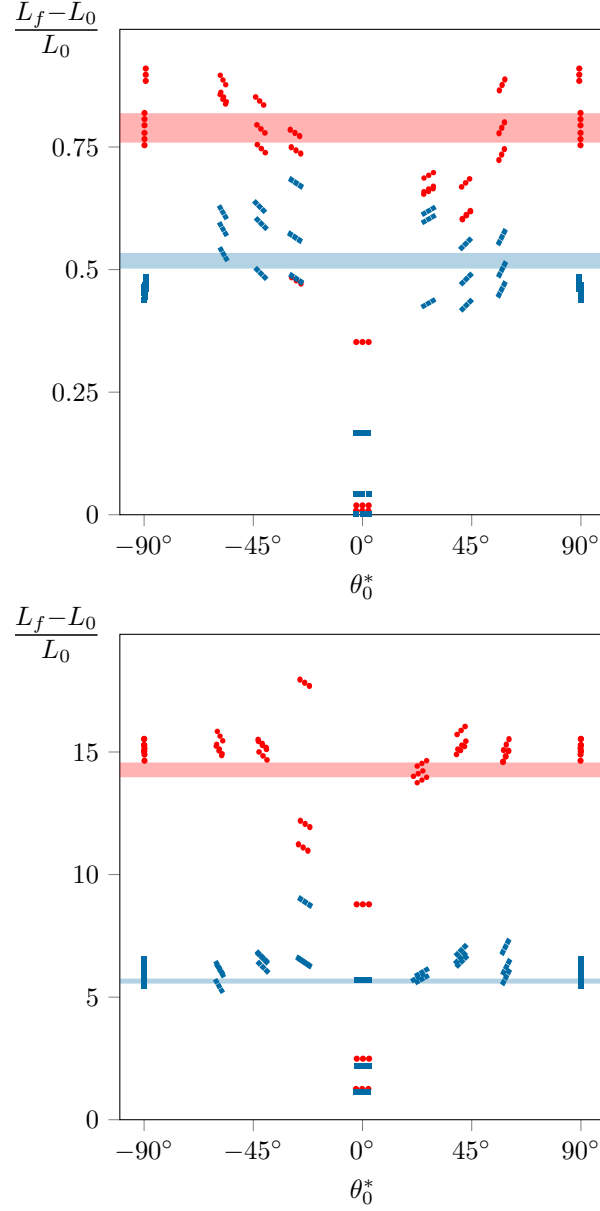


Fig. 4.11: Effect of initial main grain orientation θ_0^* in the column runout. Top: short columns ($H_0/L_0 = 0.5$). Bottom: tall columns ($H_0/L_0 = 8$). The shaded areas indicate the mean runout observed in columns with random initial orientations and their widths correspond to two standard deviations. The markers are grains aligned with the prescribed grain orientation. The red and blue colours indicate dry and immersed collapses.

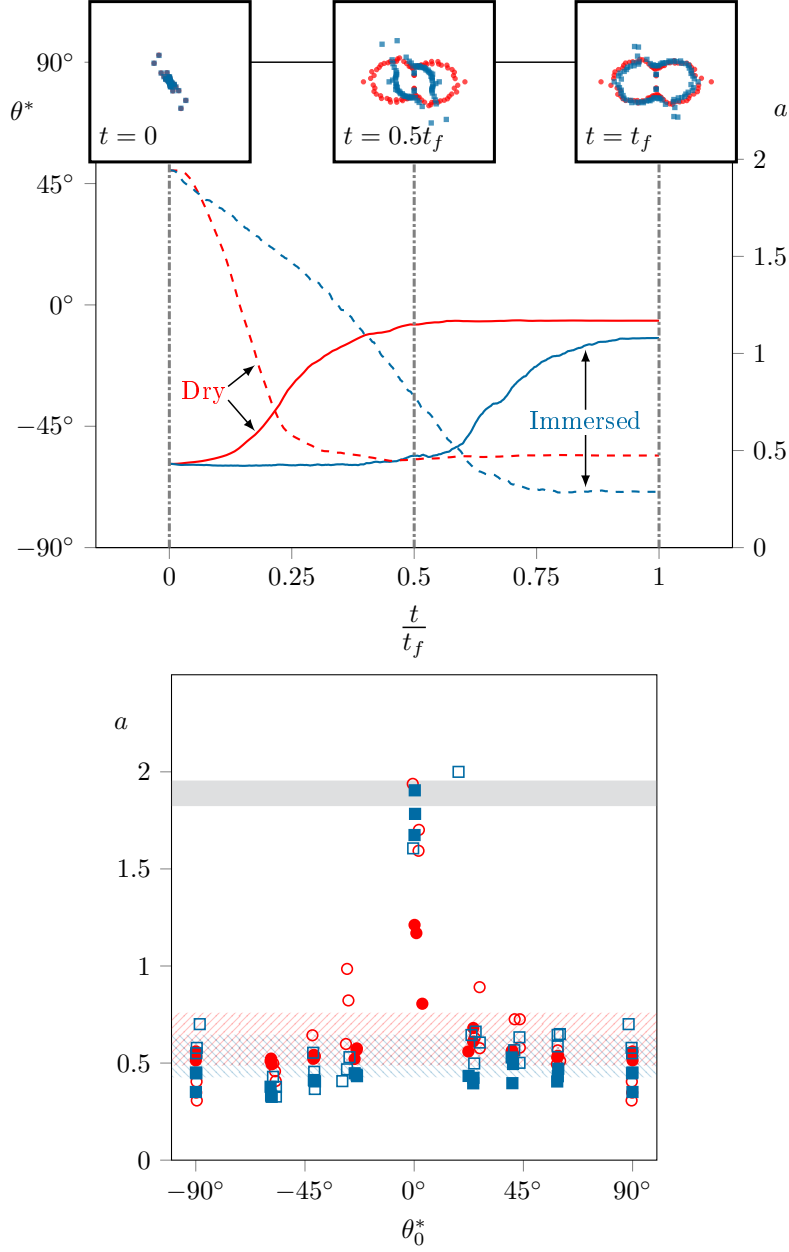


Fig. 4.12: Top: temporal evolution of the main orientation θ^* (solid) and anisotropy a (dashed) of the orientation distribution for a column with $H_0/L_0 = 8$ and initial grain orientation $\theta_0^* = -60^\circ$. The insets are polar plots of the orientation distribution showing the relative frequency of a given orientation. Bottom: final a as a function of θ_0^* . Full symbols indicate tall columns and empty ones short columns. The hatched areas indicate the mean value of a for random initial orientations and their widths correspond to two standard deviations. The red circles and blue squares indicate dry and immersed collapses, and the grey band corresponds to the mean initial value of $a \pm$ a standard deviation.

In summary, the initial main grain orientation θ_0^* does not have a significant influence on the collapse sequence, the final deposit shape, or the runout distance, but it slightly increases the collapse duration in tall columns. Only orientations close to the horizontal change the general behaviour of the column, because of their collective stability. This can be seen in the runout but also in the runout and final times, as well in the deposit shape.

4.4 Energy considerations

Previous works have used an energy approach for describing the column collapse sequence and link it with the common features of granular flows (Staron and Hinch (2005); Zenit (2005); Tapia-McClung and Zenit (2012); Topin et al. (2011); Jing et al. (2018, 2019); Polanía et al. (2022)). In a column collapse a part of the initial potential energy E_p transforms into kinetic energy E_k . These can be computed as:

$$E_p = \sum_{n=0}^N m_n g^* y_n \quad (4.14)$$

$$E_k = \underbrace{\frac{1}{2} \sum_{n=0}^N m_n u_{nx}^2}_{E_{kx}} + \underbrace{\frac{1}{2} \sum_{n=0}^N m_n u_{ny}^2}_{E_{ky}} + \underbrace{\frac{1}{2} \sum_{n=0}^N I_n \omega_n^2}_{E_{kr}}, \quad (4.15)$$

where y_n is the height of grain n , m_n and I_n are its mass and inertia, respectively, and u_n and ω_n are its translational and angular velocities, respectively. It is important to note that the rotational kinetic energy E_{kr} is negligible when compared to the translational components E_{kx} and E_{ky} , as observed in Utili et al. (2015) for spherical particles. Therefore E_{kr} is discarded. Moreover, in immersed cases, the fluid phase also gains kinetic energy E_{kf} in the form

$$E_{kf} = \frac{1}{2} \rho_f \sum_{n=0}^{N_n} v_n^2 V_n \phi_n, \quad (4.16)$$

where v_n and ϕ_n are the fluid velocity and porosity at node n , respectively, V_n is the volume associated to node n , and N_n is the total number of nodes. The kinetic energy is gradually either dissipated through friction and inelastic collisions in the granular phase, or through viscous dissipation in the fluid phase. Then, the total dissipated energy E_d is computed as:

$$E_d = E_p(t=0) - E_p - E_k - E_{kf}, \quad (4.17)$$

assuming that the change in the potential energy of the fluid phase is negligible. These quantities are computed for all columns and traced during collapse.

The temporal evolution of the kinetic energy components and the dissipated energy show a complementary view of the collapse sequence (see Fig. 4.13). This evolution is similar for initially disordered and ordered columns. Short columns dissipate a smaller fraction of their initial potential energy, as the mobilised material limits only to a lateral wedge. Also for short columns, the energy dissipation mainly occurs when the wedge collides with the base. On the contrary, tall columns dissipate a much larger part of their initial potential energy, initiating with a rapid increase in E_{ky} , in-line with a predominant free-fall motion, and then transitioning to E_{kx} rising when the grains enter the side-propagation phase. The proportion of dissipated energy is similar to the one for spherical grains (Jing et al. (2018)). In the immersed case, the energy evolution is less smooth, indicating a non-intuitive coupling between the grains and the fluid. In immersed collapses, the particles fall and transfer an equivalent quantity of energy to the fluid. Part of this energy is dissipated through viscous effects, maintaining the collective motion of grains (e.g., finger-like structures) and delaying the column motion, in comparison to its dry counterpart. This is because the fluid keeps the kinetic energy for much longer than the grains through a slower viscous dissipation, e.g., $E_{kf} > 0$ at $t = t_f$.

Based on similar observations with the energy approach, the column runout is suggested to depend on its ability to transform the initial potential energy into horizontal kinetic energy (Topin et al. (2011); Jing et al. (2019); Yang et al. (2021); Jing et al. (2018)). Recent findings on polydisperse column collapses of disks indicate that the runout might be simply controlled by just the front kinetic energy E_k^{fr} . In order to highlight the influence of E_k^{fr} on the column runout, a simple model simplifying the column as a rigid block with mass M and initial horizontal velocity U^{fr} is proposed (Polanía et al. (2022)). Note that E_k^{fr} is much higher than E_{kx} and E_{ky} , as in this simplification the whole column is assumed to move with the front velocity U^{fr} (see Sec. 4.2.2).

The block is subjected to a resistive force $-k\dot{x}$, with k a constant representing the effective viscosity of the granular material. Solving the block's equation of motion $M\ddot{x} = -k\dot{x}$ for an infinite time leads to:

$$\frac{L_f - L_0}{L_0} = \frac{\sqrt{2}}{kL_0} \sqrt{M^*} \sqrt{\frac{\rho_g}{\rho_g - \rho_f}} \sqrt{E_k^{fr}}, \quad (4.18)$$

where $M^* = M(\rho_g - \rho_f)/\rho_g$ is the column effective mass. From Equation 4.18, the following dependence for the runout is suggested (Polanía et al. (2022)):

$$\frac{L_f - L_0}{L_0} \propto \left(\frac{1}{L_0}\right)^\alpha M^{*\beta} \left(\frac{\rho_g}{\rho_g - \rho_f}\right)^\gamma E_k^{fr\delta}, \quad (4.19)$$

with $(\alpha, \beta, \gamma, \delta)$ the exponents controlling the influence of each factor.

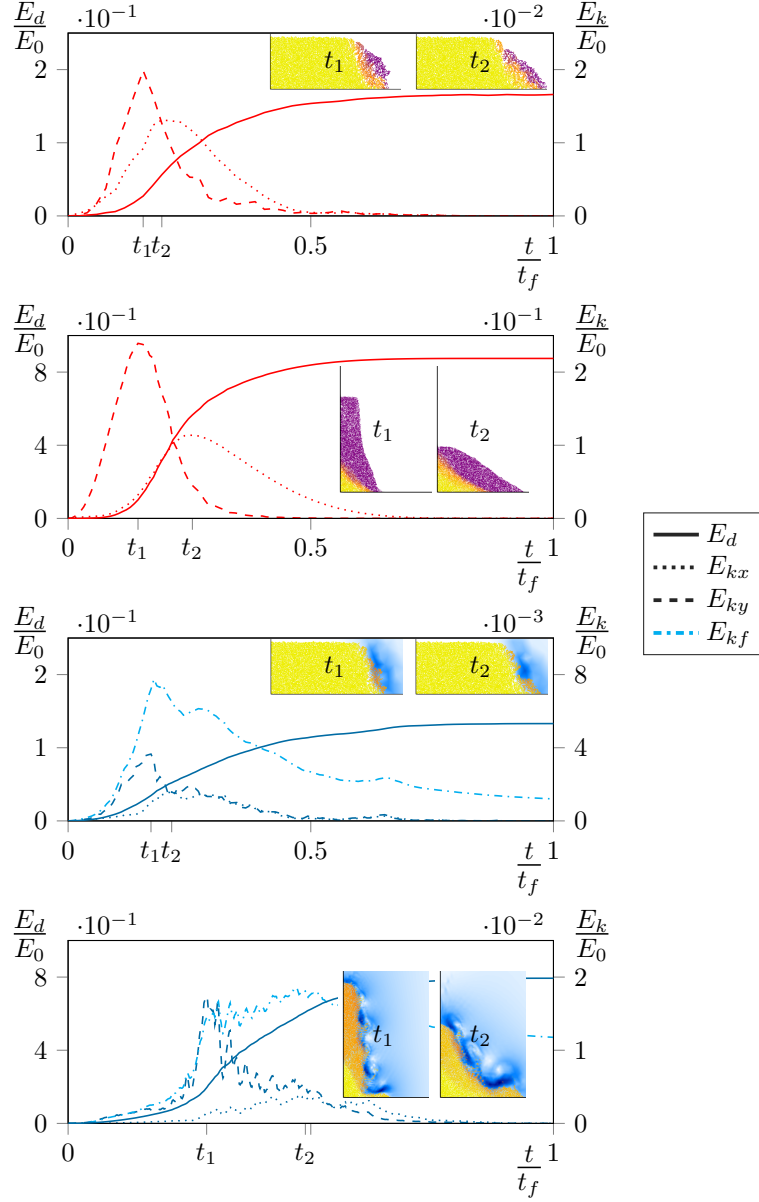


Fig. 4.13: Temporal evolution of the different forms of energy for initially disordered columns. Top two: for a short ($H_0/L_0 = 0.5$) column in the dry (top) and immersed (bottom) cases. Bottom two: for a tall ($H_0/L_0 = 8$) column in the dry (top) and immersed (bottom) cases. The red and blue colours indicate dry and immersed collapses, with cyan corresponding to the fluid phase. The insets show the grain velocity at times t_1 and t_2 . The inset colour bars are the same as in Fig. 4.4.

By a proper fitting of these exponents, they observed a collapse of all data on a single trend, regardless of the level of polydispersity, the column aspect ratio and the fluid (see the black circles in Fig. 4.14). The fitted values are $\alpha = 1$ (from the nondimensionalisation of the runout), $\beta = 0$ (neglecting the column mass), $\gamma = 1$ (indicating a stronger influence of the fluid), and $\delta = 0.5$.

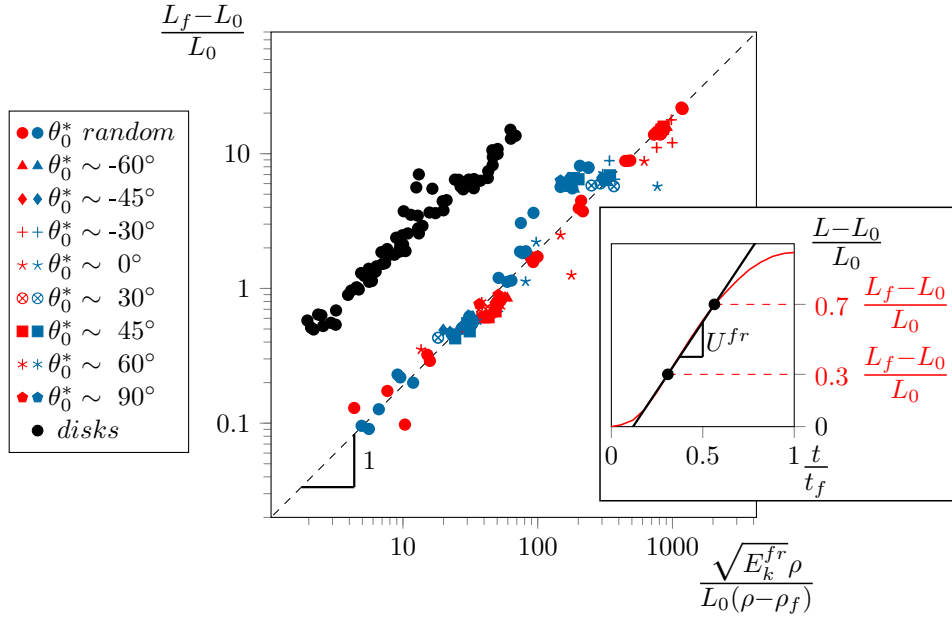


Fig. 4.14: Runout of the columns scaled with the kinematics of Eq. 4.19. Data points for short columns with $\theta_0^* = 0^\circ$ were removed as their runout was not relevant. The red and blue colours indicate dry and immersed collapses. Black circles correspond to the data from Polanía et al. (2022) for polydisperse disks. The dashed line is a guide to the eye. The inset illustrates the computation of U^{fr} used to obtain E_k^{fr} for a dry column with $H_0/L_0 = 8$.

The data for elongated grains collapses on a single trend for both dry and immersed cases, whatever the column aspect ratio or the initial main grain orientation when the exponents from Polanía et al. (2022) are used (see the coloured symbols in Fig 4.14). This trend has the same slope than the one for the polydisperse disks. Note that with these exponents, Eq.4.19 is not dimensionless. The main interest of Eq.4.19 is to highlight that this scaling collapses the data with a slope of 1. Nonetheless, it could be made dimensionless by adding a multiplying factor with dimensions of the square root of a typical mass, for example the one of a single grain. A downward vertical shift with

respect to the data for disks corresponding to dividing the data for elongated grains by a constant is observed. In other words, for an equal quantity of energy in the column, the runout is reduced for elongated grains. Since the proportion of dissipated energy is equivalent, we suggest that a part of the available energy is consumed by a change in the microstructure of the column, i.e. the orientational rearrangement of the grains. This rearrangement leads to a similar final state for all columns, regardless of the initial main orientation (see Sec. 4.3). Therefore, the importance of this process should be directly linked grain properties like grain shape and elongation, although only a weak dependence of the runout on the grain elongation was reported (Tapia-McClung and Zenit (2012)). With this in mind, the factor $\frac{1}{k}$ from Eq. 4.18, that was discarded in Eq. 4.19, should be taken into account. The scaling for the runout becomes:

$$\frac{L_f - L_0}{L_0} \propto \frac{1}{kL_0} \frac{\rho_g}{\rho_g - \rho_f} \sqrt{E_k^{fr}}. \quad (4.20)$$

The parameter k in the model is linked to the ability of the granular material to flow and reorganise its microstructure. We expect its value to depend on the grain shape, i.e. be more important for grains that have a larger inertia, or a better ability to interlock. In that sense, it would be interesting to vary the aspect ratio of the elongated grains. The influence of grain inertia is expected to be easier to determine than the one of their ability to interlock.

4.5 Conclusions

The column collapse of two-dimensional elongated grains was simulated with an unresolved FEM-DEM model both in dry and immersed conditions. The elongated grains were modelled as clusters of disks, facilitating the computation of the fluid-grain interactions in the immersed case. The focus was set on the effect of the column aspect ratio and the initial grain orientation on the collapse dynamics and runout, distinguishing columns with an initial grain orientation that is random or aligned with a given direction.

For randomly oriented grains, the collapse dynamics are found to be analogous to the ones for circular (spherical) grains. Classical power laws were recovered for the runout and final height, with the fluid phase reducing the runout. The grains align with the flow direction during the collapse, ending up in a nematic configuration.

Concerning columns with a given initial grain orientation, both short (with $H_0/L_0 = 0.5$) and tall (with $H_0/L_0 = 8$) columns were considered. In general, the collapse dynamics and the evolution of the grain orientation distribution are merely unaffected by the initial grain orientation (unless for the extreme cases where the grains are horizontally oriented). The runout is slightly affected, exhibiting an asymmetric increase that is more important for columns with

a negative initial grain orientation. Only the collapse duration is increased compared to the case where grains are randomly oriented. The grain orientation transitions to the same nematic state than for columns with randomly oriented grains.

Finally, the evolution of the different forms of energy during the collapse was described and found similar to the one for circular (spherical) grains, with an equivalent proportion of dissipated energy. A scaling of the runout based on the front kinetic energy was used. It collapses the data well on a single line regardless of the column size and initial orientation or the presence of an ambient fluid. When comparing with the data for disks, the runout for a given energy was found smaller for elongated grains. From this, the inclusion of an additional factor in the scaling was suggested in the form of a viscous-like parameter that should account for the grain properties.

Future work should concentrate on identifying the relationship between the additional factor of the front kinetic energy scaling and grain properties. Due to the importance of hydrodynamic interactions with the fluid phase, further efforts could be put in improving their modelling, notably by considering real rod-like grains. Lastly, an extension of the model to three-dimensional configurations should also be interesting.

CHAPTER 5

Conclusion

This is not the end. It is not even the beginning of the end. But it is, perhaps, the end of the beginning.

— Winston Churchill

Immersed granular flows are ubiquitous. Their involvement in many industrial or geophysical phenomena, from the small scale of blood flow (Yamaguchi et al. (2010)) to the large scale of volcanic eruptions (Bergantz et al. (2015)) makes their understanding a subject of high importance. Unfortunately, this understanding is made difficult by the high complexity of such immersed granular flows. Mechanisms at the grain scale that result from the divided nature of the underlying granular media give rise to peculiar behaviours that are at the boundary between the one of gases, liquids and solids. As it happens, many of those mechanisms are sensitive to or originate from intergrain friction and grain shape. The presence of the surrounding fluid further complexifies the behaviour of the mixture. On the one hand, the fluid influences the dynamics of the grains. Either by modifying the interactions between them, with cohesion or lubrication, either by applying various forces on the grains themselves, forces which sometimes also strongly depend on the grain shape. On the other hand, the grains influence the fluid phase by perturbing its normal flow, changing its effective viscosity. The overall combination of those interactions generates a

rich panel of particular behaviours. The shear thinning and thickening of dense granular suspensions are just examples among many.

In front of that, numerical methods have emerged as a credible solution to investigate the flow of fluid-grain mixtures. Indeed, they are generally cheaper and more reproducible than real-life experiments, and they offer a better control over physical parameters as well as an easier access to data of interest. Apart from stability issues, their main limitation is the available computational power. For large scale applications where the details of the grain scale interactions are irrelevant, such as landslides, two-fluids models are convenient. Nonetheless, they require adequate constitutive laws for the granular phase. In small scale problems such as blood flow, direct numerical simulations offer an unrivaled accuracy. They consider each grain individually in a Lagrangian way and explicitly compute the fluid flow on the boundary of the grains, allowing a high precision in the fluid grain interactions. In most industrial problems, though, the grain scale is relevant but the size of the problem results in prohibitive computational costs for direct numerical simulations. Multiscale models tackle this issue by taking the advantages of both aforementioned methods: grains are still solved with a Lagrangian approach, but the fluid flow is computed on a larger scale, strongly reducing the computational cost. Naturally, this comes at the cost of precision in the evaluation of fluid-grain interactions that has to be done with empirical relations. MigFlow makes use of this approach, which has proven successful in different applications (Constant et al. (2019, 2021b,a)). However, only frictionless spheres were considered, ruling out important aspects of the dynamics of immersed granular materials. The contributions of this thesis to MigFlow in terms of friction and grain shape and the numerical results obtained therewith in selected applications are highlighted in this concluding chapter. Finally, on the basis of the limitations of this work, perspectives for future improvements are drawn.

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5.1 Contributions of this work

The present thesis was led at UCLouvain in collaboration with the LMGC from Université de Montpellier. Its goal was to broaden the field of application of the numerical model used in MigFlow by including key aspects that influence granular dynamics (i.e. friction and grain shape), and to do so while maintaining a reasonable computation cost, which is at the heart of the approach. In order to have a good understanding of the numerical model, its bases were presented in chapter 2. The equations for both the fluid phase and the granular phase were described, as well as implementation details. The parametrisation of the fluid-grain interactions was addressed, and the explicit temporal coupling between the fluid and granular solvers was explained.

As a first step, **the solver for the granular phase was extended to frictional contacts**. This was done by implementing the corresponding feature of the Nonsmooth Contact Dynamics method, adapting MigFlow's own optimisations accordingly. The newly obtained contact solver was then used to study the drag force exerted on a rigid body in a granular flow, in both dry and immersed conditions. It successfully reproduced the Janssen effect (the saturation of pressure from a certain depth in grains stored in a container) and experimental values of the drag force, both qualitatively and quantitatively. The flowing regime was described with a dimensionless number based on the different stresses at stake, and the differences in the stress state, shear zones and velocity profiles near the obstacle were pointed out. Yet, it was necessary to consider shear-thickening to obtain a good collapse of the data based on the aforementioned dimensionless number. Whether this is a numerical artifact or not and how it manifests are still open questions.

In a second time, **the simulation of grains with arbitrary shapes was enabled**. The approach of disks clusters was selected for its simplicity and its efficiency, principles which are fundamental to MigFlow. An important advantage was that the parametrisation of the drag can remain unchanged, as the fluid forces on each constituting disk are summed to obtain the resultant force and torque on the grain. This makes the grains porous though, and hence changes the fluid-grain interaction compared to more accurate grain representations. Nonetheless, this interaction is still satisfactory, notably to reproduce the interplay between fluid forces and grain orientation. Concerning the contact resolution, the change in the Delassus operator that prescribes the mechanical response of the two grains to the contact impulse made the system to solve more complex. At the moment, only the two dimensional case is supported, as the solution of the system can then still be explicitly discussed. An extension is still required to solve the three dimensional case with an iterative solver.

Finally, **the two-dimensional collapse dynamics of columns of elongated grains in both dry and immersed conditions was studied.** The focus was set on the influence of the initial orientation of the grains and its evolution with the collapse. It was found that, regardless of the initial orientation, all samples converged towards a nematic horizontal state with a similar orientation distribution anisotropy. The fluid phase delays the transition to this nematic state and reduces the value of the final anisotropy. The runout (the furthest distance travelled by the grains still in contact with the main mass) shows a power law dependence on the aspect ratio of the column, as for spherical grains. The initial orientation of the grains slightly influences the runout, with more stable configurations resulting in a shorter runout. Regardless of the orientation of the grains, the aspect ratio of the column, or the presence of an ambient fluid, the runout was successfully predicted with the kinetic energy of the front of the column. Compared to polydisperse disks, columns of elongated grains with the same kinetic energy exhibit a shorter runout. This result shed light on the importance of the microstructure in the ability of the material to flow, as for elongated grains a part of the energy is consumed by the change in the orientation of the grains. This suggests the inclusion of a new, viscous-like parameter that depends on the microstructure in the scaling employed previously for the polydisperse disks, underlying the importance of the grain shape.

This ends the summary of the contributions that were brought into MigFlow during this thesis. The study of the two selected applications demonstrated the possibility to use the resulting version of MigFlow in cases where friction and grain shape are important. However, these cases also raised questions about the numerical method itself, suggesting the next challenges that should be taken on in the future. Those are explored in the next section.

5.2 Look beyond what you see

The past work on the numerical model used in MigFlow (Constant (2020)) raised several questions and challenges that were not addressed during this thesis. Although they are still relevant to this day, they will be set aside so that the focus is set on the perspectives that result from the present work. These perspectives include the extension of the arbitrary grain shape to three dimensions for a more accurate representation of some physical situations, the improvement of the fluid-grain interactions considering the arbitrary grain shapes, and the parallelisation of the code to increase the computational performance of MigFlow.

5.2.1 Another dimension

So far, only two-dimensional clusters were considered, for two main reasons. First, the selected application of the column collapse is particularly well suited to a two-dimensional set-up, due to its symmetry, and has been shown to yield qualitatively equivalent result as three dimensional axisymmetric cases (Lube et al. (2005); Balmforth and Kerswell (2005)). Second, solving the frictional contact problem in three dimensions for bodies of arbitrary shape is more complex because the Delassus operator $\mathbf{W}$ is not diagonal. This results in a set of nonlinear equations for the contact that have to be solved with an iterative procedure, such as a Newton-Raphson scheme for instance (Curnier and Alart (1988)).

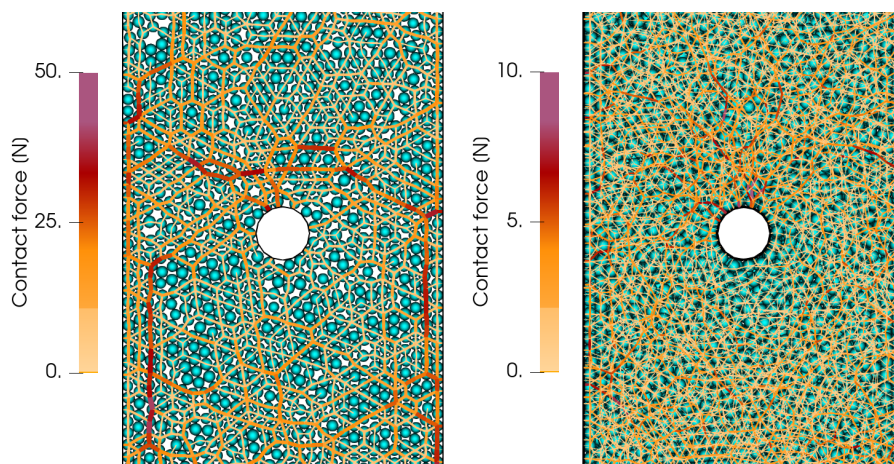


Fig. 5.1: Snapshot of the simulation of a dry granular flow around a cylinder in two (left) and three (right) dimensions showing the contact network. The wider and the redder the line, the larger the contact force between two grains. The physical parameters are equivalent for both cases.

However, three dimensional problems are in most cases more representative; not all applications can be simplified in a two-dimensional paradigm, at least without changing significant aspects of the physics at stake. As an example, consider the drag force exerted on a rigid body in an immersed granular flow that was studied in chapter 3. Its value is linked to the ability of the granular phase to reorganise its microstructure to circumvent the obstacle (Albert et al. (1999)). Because of the reduced number of degrees of freedom in the two dimensional case, this reorganisation is much more difficult, and the drag force undergone by the obstacle is considerably increased compared to the three-dimensional case (see Fig. 5.1). Therefore, two-dimensional configu-

rations are mostly qualitative and not quantitative. Moreover, it is not always clear if the grains are considered as spheres or cylinders, leading to uncertain parametrisations for the fluid-grain interactions. Lastly, even in cases where the two-dimensional simplification is relevant, a three dimensional approach could offer insights on phenomena that are less significant but that still should be investigated for a finer understanding of the problem.

For the above reasons, the extension of the current model to three dimensions seems necessary. Since this is only a matter of implementation, this aspect should be the less difficult improvement discussed in this section. It should be noted that the study of three dimensional applications will result in a strong increase of the computational cost. The equations to solve are more complex, the variables to store and update are more numerous, and the number of contacts for the granular phase or elements for the fluid phase is significantly higher. For these simulations to be feasible, this extension should be accompanied by a solution to decrease their time cost. This involves an efficient code optimisation as well as the implementation of parallel computing, which will be discussed later in this chapter.

5.2.2 Fluid-grain interactions

Fluid-grain interactions are at the core of the present numerical model, making the bridge between the fluid and granular phases. Although their empirical nature in unresolved models such as the one used here led to many discussions about the various parameters and refinements (Liu and Yu (2022)), they yield satisfying results for spheres. In the case of nonspherical bodies, this is not obvious. The complexification that arbitrary shapes bring to the interactions between the grains and the fluid, to the point that even analytical solutions are out of reach, resulted in various approaches (Ma et al. (2022)).

The approach selected in this work to model arbitrary shapes with non overlapping disk clusters proves efficient and convenient in terms of implementation, while allowing to take the hydrodynamic torque into account. Nonetheless, the induced porosity of the obtained grains might lead to an underestimation of the fluid-grain interactions, which can be partially corrected by changing the apparent volume of the grains. Moreover, the accuracy of the current approach depends just as much on the discretisation level of the considered grain as on the discretisation level of the fluid phase.

Since the latter needs to be larger than the diameter of a constituting disk or sphere (in practice, more or less three times larger), the refinement of the grain is limited by the fluid phase. Because the Finite Elements method uses P1 elements to represent the velocity, its precision is limited so that if the grain is much more refined than the fluid, the difference in velocity between two successive constituting disks or spheres may be so small that the refinement of the grain becomes irrelevant. To avoid this, it would be advantageous to

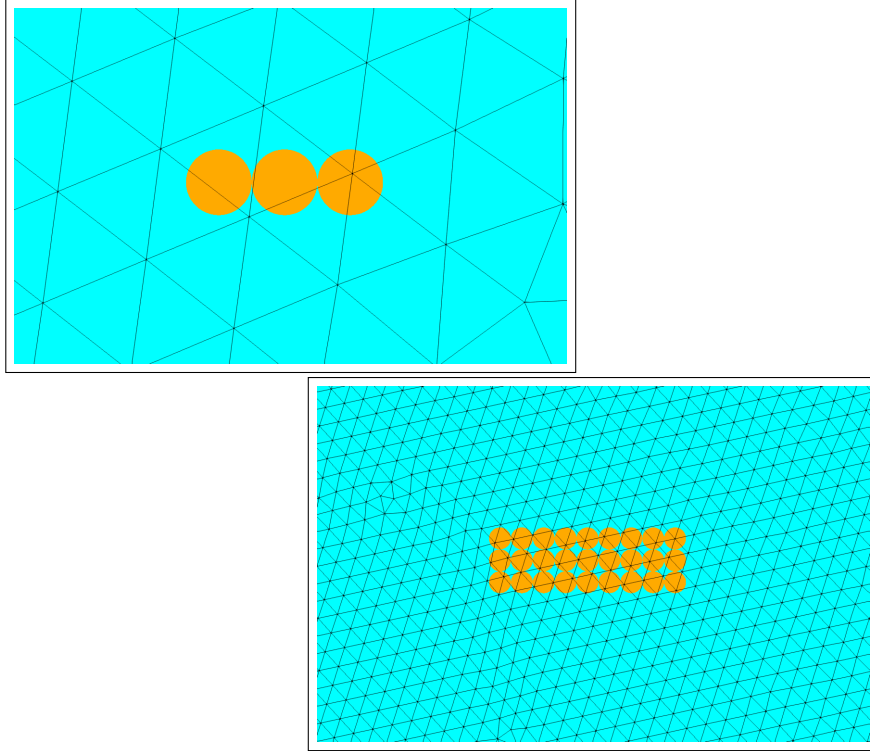


Fig. 5.2: Top: rod-like grain discretised as 3 disks, with a mesh size larger than the disks. Bottom: same rod-like grain discretised as 27 disks, with a mesh size smaller than the disks.

consider a mesh size that is smaller than the one of the constituting disks, see Fig. 5.2. Naturally, doing so with the current volume average technique would result in a null porosity and a crash of the simulations. Several techniques were developed to tackle this issue, all considering a given averaging kernel whose size is larger than a fluid mesh element (Capecelatro and Desjardins (2013); Wang et al. (2019)). In those cases the treatment of the domain boundaries are nevertheless nontrivial, as they result in a truncation of the averaging kernel (Chen et al. (1999)).

Such a refinement of the fluid mesh would, however, inevitably increase the computational cost of solving the fluid phase equations. Another approach would be to select a parametrisation of the drag force that is sensitive to the shape and orientation of the grain (Hölzer and Sommerfeld (2008); Haider and Levenspiel (1989); Leith (1987)). Unfortunately, this kind of parametrisa-

tion is very specific to a given shape, and often fails to include the hydrodynamic torque. It might be interesting to couple both approaches, i.e. a finer parametrisation and a discretisation of the grain into disks.

5.2.3 Divide and conquer

As already stated, one of the main limitations of numerical methods, apart from stability issues, is the CPU time they require for a given simulation. Realistic problems often imply millions or even billions of grains. These huge numbers result in prohibitive memory and computational costs. Reducing these costs is a crucial issue for the feasibility of numerical simulations. It would allow the study of systems that are larger in size, or more extensive and precise studies of small scale systems. It is precisely one of the objectives of the current numerical model to offer results in a convenient calculation time. In order to reduce this time, two strategies exist and can be employed simultaneously: reducing the computational cost of the method and employing more computational resources. Apart from code optimisation, the cost can be reduced by using coarse graining, which proved relevant for many applications (Di Renzo et al. (2021)). However, this approach is not well suited when the shape of the grains plays an important role. The second strategy concerns parallel computing, which consists in mobilising several computing units and sharing the work between them. The availability of large computing centres with computer clusters has strongly increased in the last decade, notably with the rise of GPU parallel computing. Therefore, several parallel solvers based on the GPU paradigm have been developed for granular materials, be they academic (Jajcevic et al. (2013); Govender et al. (2014)) or commercial^{1,2}. Parallel computing thus appears as a strategic feature of any program that aims at solving real scale problems for granular flows.

In general, a parallelisation algorithm will split the computational domain into partitions, which will in turn be assigned to the computing units so that they can solve the problem on their subdomain. The processors may communicate, depending on the chosen strategy. A shared memory approach reduces the communication between the processors but implies a careful treatment of the memory accesses to avoid race conditions. A distributed memory approach, where each processor stores the memory relative to its subdomain, avoids race conditions but requires communication between the processors. In addition to the communication and memory access costs, a key aspect is the load balance. To obtain an efficient speed-up, i.e. a speed-up that is directly proportional to the amount of processors used, the work load should be fairly distributed among the processors.

¹Anslys Rocky: <https://www.ansys.com/products/fluids/ansys-rocky>

²Altair EDEM: <https://altair.com/edem/>

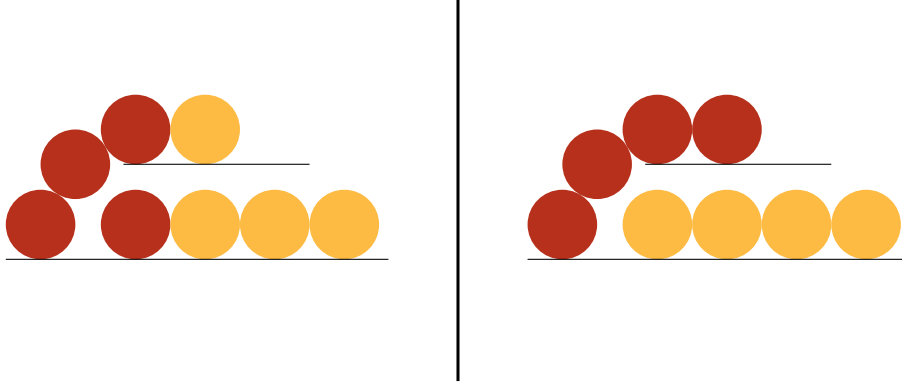


Fig. 5.3: Disks resting on flat frictional surfaces. The computational domain is decomposed into two partitions (red and orange) for the parallel resolution of the contacts. Left: geometrical decomposition according to the horizontal coordinates. Right: topological decomposition according to the contact network.

The adequate partition of the domain thus appears as an important step. Two approaches exist: geometrical decomposition, based on the positions of the objects that are considered, or topological decomposition, based on the interactions between them (see Fig. 5.3).

Obviously, both the fluid phase solver and the granular phase solver should be parallelised. As far as the fluid phase is concerned, a geometrical decomposition seems adequate, since the geometry of the domain will not evolve during the simulation (except in case of remeshing, which should not take place many times in most simulations). The work load is roughly equivalent between the elements, so that as long as each processor is assigned an equivalent number of elements the work load is well balanced.

This is not the case, nevertheless, for the granular solver. The positions of the grains can evolve in time, and the grains can be quite irregularly distributed inside the domain. Moreover, grains that are distant may interact because of their relative velocities, while grains that are close may not. For these reasons, topological domain decompositions are preferred for granular solvers. Here, this approach should also be preferred as the contact detection algorithm is not very costly. The Nonsmooth Contact Dynamics method was parallelised in both shared memory and distributed memory (Owen et al. (2000); Shojaaee et al. (2012)). Finally, another possibility is to parallelise the contact loop in the iterative procedure (Renouf et al. (2004)). This method is independent of any domain decomposition, and requires only a careful renumbering of the contacts that groups together contacts which influence each other. Whether or not the queue structure used in MigFlow would still be relevant in such a case

is an open question. Since this structure offers better performances than the classical non-linear Gauss-Seidel procedure, this should be worth investigating in future work.

5.3 This is the end, isn't it?

As this final chapter comes to an end, so does the work done during this thesis. The result is a numerical model that allows the study of immersed granular flows with frictional grains of arbitrary shape with an insight on the grain physics and at a convenient computational cost (see Fig. 5.4). Its use for the selected applications shed light on some particular aspects linked either to friction or grain shape, demonstrating the interest of including such features in the model. Furthermore, questions and perspectives for improvements were drawn, notably by taking inspiration from the limitations encountered in the studied applications. Since every answered research question rises several more, this project is not entirely over: this is not the end. But, perhaps, it can be said that this is at least the end of the beginning.



Fig. 5.4: Snapshot of the simulation of the two-dimensional collapse of a partially submerged column made of grains with shapes inspired from the Tetris game. The grains are coloured according to their moment of inertia. The fluid is coloured according to the corresponding phase: blue for water, white for air.

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