

Friction in granular flows

A numerical implementation

Dissertation presented by
Nathan COPPIN

for obtaining the Master's degree in
Physical Engineering

Supervisor(s)
Vincent LEGAT, Jonathan LAMBRECHTS

Reader(s)
Evelyne VAN RUYMBEKE, Matthieu CONSTANT

Academic year 2017-2018

Acknowledgements

First, I would like to thank my father for his time and help during the writing of this thesis. Then I would like to thank my mother, for her encouragements during the entrance exam. I would like to express my gratitude to my grand-parents, for all the exam periods over the years. Finally, I thank Matthieu, Vincent and Jonathan for their support, advice and availability over the whole year.

Contents

List of symbols	vi
1 Introduction	1
2 State of the Art	3
3 The Non-Smooth Contact Dynamics Method	7
3.1 The global problem	7
3.2 The local frame	8
3.3 From global to local and back again	10
3.4 The contact law	11
3.4.1 Contact with a wall	13
3.4.2 Validation	16
3.5 The friction law	16
3.5.1 Validation	18
4 Implementation	25
4.1 Contacts detection	25
4.2 Contacts management	28
4.3 Contacts resolution	29
5 Angle of repose	31
5.1 Static angle of repose	31
5.1.1 Experimental set-up	31
5.1.2 Results	32
5.2 Dynamic angle of repose	39
6 An application : mixing of particles	45
6.1 Experimental set-up	45
7 Conclusion	51
Bibliography	53

List of Symbols

Symbol	Definition	Units
q_i	Vector of the coordinates of the grain i	[m], [rad]
x_i	Horizontal coordinate of the grain i	[m]
y_i	Vertical coordinate of the grain i	[m]
θ_i	Angular coordinate of the grain i	[rad]
$\dot{q}_i$	Vector of the velocities i	[m/s], [rad/s]
u_i	Horizontal velocity of the grain i	[m/s]
v_i	Vertical velocity of the grain i	[m/s]
ω_i	Angular velocity of the grain i	[rad/s]
M_i	Vector of the mass and inertia of the grain i	[kg], [kg·m ²]
m_i	Mass of the grain i	[kg]
I_i	Inertia of the grain i	[kg·m ²]
F_i	Resultant of the forces acting on the grain i	[N]
N	Number of grains	[1]
q	Vector of the coordinates of all the grains	[m]
M	Matrix of the masses and inertias of all the grains	[kg], [kg·m ²]
F	Vector of the resultant of the forces acting on the grains	[N]
F_e	Vector of the external forces acting on the grains	[N]
r	Vector of the forces acting on the grains due to the contacts between them	[N]
Δt	time-step	[s]
p	Impulse on the grains due to the contacts between them	[kg·m/s]
α	Superscript designating a contact	[/]
$\mathbf{n}$	Normal vector to the point of contact between two grains	[1]
$\mathbf{t}$	Tangential vector to the point of contact between two grains	[1]
$\mathfrak{d}$	Distance between two grains	[m]
R_n	Normal component of the reaction force in the local frame	[N]
w	Vector of the relative velocities between two grains	[m/s]
w_n	Normal relative velocity between two grains	[m/s]
w_t	Tangential relative velocity between two grains	[m/s]
μ_k	Coefficient of kinetic friction	[1]
μ_s	Coefficient of static friction	[1]

Symbol	Definition	Units
P_n	Normal component of the impulse between two grains due to the contact	[1]kg·m/s
P_t	Tangential component of the impulse between two grains due to the contact	[kg·m/s]
$\mathbb{M}$	Total mass of two grains involved in a contact	[kg]
$\mathbf{H}$	Mapping between the local frame and the global frame	[/]
$\mathbf{H}^*$	Mapping between the global frame and the local frame	[/]
N_x	Horizontal component of the normal vector, $\mathbf{n}$	[1]
N_y	Tangential component of the normal vector, $\mathbf{n}$	[1]
T_x	Horizontal component of the normal vector, $\mathbf{t}$	[1]
T_y	Tangential component of the normal vector, $\mathbf{t}$	[1]
rad_i	Radius of the grain i	[m]
$\mathbb{C}$	Matrix of the coefficients of redistribution of the impulse between the grains involved in the contact	[1]
β	Angle by which the initial normal must be rotated in order to obtain the projected normal	[°]
γ	Angle between the initial normal and the relative velocity between the grain and the circular wall	[°]
$\mathfrak{r}$	Radius of the circular wall	[m]
β_0	Starting iterate for the Newton-Raphson method	[/]
N_l	Number of particles contained in a leaf of the quadtree	[1]
N_m	Maximal number of particles per leaf in the quadtree	[1]
N_{li}	Number of particles contained in the leaf associated to grain i	[1]
θ_r	Static angle of repose	[°]
ρ	Ratio of the radii of the grains between an experiment and the reference one	[1]
Fr	Froude number of the rotating mill	[1]
ϕ	Degree of filling of the rotating mill	[1]
μ_{kpw}^c	Critical sliding friction coefficient between the wall and the particles under which rolling does not take place 0.95	[s]
θ_d	Dynamic angle of repose	[°]
Fr_c	Critical value of the Froude number above which cascading occurs	[1]
d	Diameter of the grains	[m]
M	Mixing index	[1]
d_{min}	Minimum diameter of the grains	[m]
t_{mix}	Mixing time	[s]
$t_{0.95}$	Time at which the mixing index reaches 0.95	[s]

Chapter 1

Introduction

From its early ages, mankind has always tried to understand its environment, mainly with the goal to learn how to modify it at will. This formidable "machine to learn", through its individual and social abilities, has built over the ages a solid, yet incomplete, understanding of the surrounding phenomena in its everyday life. It is this same thirst for knowledge that drove the interest in granular flows, and how to efficiently model them. Indeed, this kind of phenomenon occurs not only at various scales, but also in very different frames, be it in natural events like avalanches or debris flows, or in pharmaceutical applications like the mixing of powders.

The particularity of these kinds of flows is that they involve a solid phase. Obviously, solids do not usually flow. However, granular materials make a formidable exception to this rule of thumb, but without behaving exactly like a fluid either. This complex behaviour is a source of challenges for the scientific community, and several approaches at different scales have been used to model it, like continuum mechanics or molecular dynamics.

A granular media consists of a large collection of particles, or grains, of various sizes and shapes. Although composed of solids, its divided nature allows the media to undergo a flow under some circumstances, showing properties similar to a Bingham fluid, which behaves as a solid at low stress and as a liquid at high stress (Jop et al., 2006). From the design of hourglasses to the industrial mixing of particles, their flowing ability is of high interest. Another characteristic property of such materials is the formation of heaps, which strongly differentiates them from Newtonian fluids. The slope of the heap depends on several parameters, such as the shape and size of the grains and the friction between them. This static behaviour is also an important matter of study, be it in the construction field for the design of retaining walls, or in the agribusiness for the design of silos.

When the granular material is wet, i.e. partially or totally immersed in a liquid, the contact forces between the particles are changed, due to lubrication or capillarity. Plus, the behaviour of each sole grain is influenced by the motion of the fluid around it, and inversely. These mesoscopic changes have macroscopic consequences, notably on the stability of a heap or in the flowing behaviour of the media. It is important to make the difference between immersed granular medias and colloids, where the grains are small enough to be influenced by the Brownian motion of the fluid particles, whose properties are different. Typically, a material can be considered to be a colloid if the size of the particles is below $1\mu m$.

Several industrial or phenomenological applications are at stake with the development of a model able to describe accurately the behaviour of a frictional granular material, be it dry or immersed. Regarding the industry, the classical example of concrete can be cited, but others exist, notably in the agribusiness, like the blending of cereals in the dry case, or the mixing of

flour with water or milk in the immersed case¹. In the metallurgic industry, rotary kilns are crucial devices. They consist of a rotating hollow cylinder, slightly inclined to the horizontal, in which granular materials such as iron ore are heated by the injection of hot gas. Finally, the debris flows down a mountain slope, avalanches, or lava flows are amongst the devastating natural phenomena that could be fitted with an accurate model. It is thus appearing that many fields, from mankind physical or food safety to industrial efficiency, can benefit from a model able to reproduce the behaviour of the considered system.

The method presented in this paper is set in the framework of the model developed by Jonathan Lambrechts, Matthieu Constant, Vincent Legat and Frédéric Dubois. It is a hybrid model, which combines a coarse scale continuum mechanics approach for the fluid and a small scale, multi-body dynamics, approach for the grains, hence the multi-scale name. The fluid is solved with a Finite Elements Method, that uses averaging equations to solve the fluid and take the solid phase into account, with the concept of porosity (the fraction of the total volume occupied by the fluid). In order for this approach to be valid, it is necessary that the size of the elements used in the FEM is quite larger than the one of the grains. The grains, in turn, are solved with a discrete elements method that treats them as distinct particles and follows their trajectories in the frame of a Lagrangian approach. First, the equations of the fluid are solved, taking into account the position of the grains through the porosity. Afterwards, the forces exerted on the grains by the fluid are extracted, and the velocity of the grains is computed. Finally, the possible contacts between the grains are solved, and their positions are updated. The momentum transfer between the solid and the fluid phases is based on empirical relationships, and has been developed and validated by Constant (Constant et al., 2017). The model was able to simulate accurately complex geometries and interactions, such as the fall of clouds of particles in a fluid and their interactions, with a good accuracy and a convenient computational cost. However, it still lacks the aspect of friction between the grains, which is significant in applications such as avalanches or the mixing of particles. This master thesis is focused on the granular phase. It aims to present an efficient method for the resolution of the contacts that takes friction into account, and validate it against experimental and literature results, with the prospect of adding the method to the multi-scale model for immersed flows.

First, a state of the art is presented, so that the reader has an idea of the scientific background on the matter of granular matter simulation and experiments. The various experiments on the static and dynamic behaviours of granular materials are summarised, with their empirical conclusions. Some theoretical approaches, based on strong hypotheses whose validity depends on the considered case, and their limitations are outlined, and numerical methods specific to granular matter are described, with their strengths and weaknesses. In Chapter 3, the working principles of the Non-Smooth Contact Dynamics (NSCD) method are presented, in a rigorous way at first and then in a more practical fashion, and the contacts with the walls are briefly discussed. This method is then validated for contacts with and without friction. Next, a section is devoted to the machine-implementation of the general contact algorithm as done in the existing model for immersed flows, detailing the tricks used to gain time on the costly step of contact detection, management, and resolution. Following this, the performances of the model are tested for the prediction of the static and dynamic angle of repose of glass beads. Some parameters such as friction and particle size in the static case or rotational speed in the dynamic one are investigated, and the results are compared with ones from literature. Finally, the model is used to simulate the mixing of two groups of particles in a rotating drum, and the problem of segregation due to differences in density is addressed.

¹Indeed, the size of the flour particles is above the micrometre, making them eligible for immersed granular flows.

Chapter 2

State of the Art

Granular and immersed granular flows exhibit complex behaviours, and have been the subject of many experimental, theoretical and numerical studies. While the experiments and the establishment of a predictive theoretical model began as early as the end of the 18th century with Coulomb, who studied the angle of repose of granular materials and derived a predictive model based on the friction coefficient between the particles (Coulomb, 1773), the development of numerical models truly began in the early 1970s, with various approaches and implementations.

The angle of repose, which is a characteristic property of the granular material, was experimentally studied in various conditions. Its definition does not make an overall consensus, and should be associated with the application it is related to, (Beakawi Al Hashemi and Baghabra Al-Amoudi, 2018), but two concepts can be highlighted : the static angle of repose, and the dynamic one.

There exist two aspects of the static angle of repose, that are somewhat conflated. The upper angle of repose is defined as the maximal angle of the slope at which a stable heap of the material can be formed (Mehta and Barker, 1994), while the lower angle of repose is defined as the angle of the slope that forms after an avalanche has occurred, (Cheng and Zhao, 2017). Various methods have been investigated to measure the static angle of repose, depending on the desired type (lower or upper), such as the hollow cylinder method, where a bottomless cylinder placed on a plate is filled with grains and moved up, or the fixed-funnel method where the grains go through a fixed, or slowly raising, funnel onto a surface with known roughness properties (Beakawi Al Hashemi and Baghabra Al-Amoudi, 2018), (Liu, 2008). It has been observed that the particle size and shape, as well as the friction coefficient between them, have an influence on the value of the static angle of repose, (Burkalow, 1945), (Carrigy, 1970). From these observations, Carstensen *et al.* derived an empirical relationship between the size of the particles and the angle of repose, (Carstensen and Chan, 1976).

As for the dynamic angle of repose, it is defined as the angle of the free surface of the material while it undergoes a flow. Its measurement is performed by placing the grains inside a hollow rotating cylinder, and measuring the angle of the slope they form during a continuous avalanche. Several flow regimes have been identified, depending on the size and rotation speed of the mill, of which the most appropriate one to measure the angle of repose is rolling, when the continuous flow shows a linear free surface, (Mellmann, 2001). It was found that this angle depends on the friction between the grains (Carrigy, 1970), and on the rotation speed of the cylinder, (Yang et al., 2003). Dury *et al.* have shown that the wall effect in the rotating drums was important, causing a difference of $\sim 5^\circ$, (Dury and Ristow, 1998).

Experiments have also been led in the flowing regime. Fowler *et al.* studied the flow of different granular materials, such as sand or sugar, through orifices of various shapes and sizes, and found an empirical expression for the flow velocity through the orifice depending on the shape, size and density of the particles, as well as geometric parameters, (Fowler and Glastonbury, 1959). The formation of arches during flow through an orifice was investigated by Vivanco *et al.*, who observed intermittent force networks between the grains, which was responsible for the fluctuations of the vertical velocity, whose magnitude depends on the opening size and inclination angle of the walls. Lube *et al.* carried out a study of the collapse of two-dimensional granular columns on a horizontal surface, and observed that a triangle-shaped region of the grains, with constant slope and a width equal to the one of the initial column, never moved. They also pointed out two different flow regimes for the collapse, delimited by a critical value for the aspect ratio (i.e. the ratio between the initial height and width of the column) which corresponds to the tangent of the slope of the triangular static region, (Lube et al., 2005). The flow of granular matter down an inclined plane was studied by Azanza *et al.*, who determined the range of inclination and particle flux for the flow to be stationary and uniform, and measured the velocity profile along the vertical direction, (Azanza et al., 1999). Goujon *et al.* explored the influence of the roughness of the inclined plane, by gluing one layer of grains on it, and discovered the existence of a maximum of friction, implying a maximal deposit and a minimal spreading, depending on the relative size of the flowing particles and the glued ones, but not on the angle of inclination, (Goujon et al., 2003).

The theoretical modelling of granular flows presents challenges due to the divided nature of the media, and the difficulty to take each single grain into account in the model. To overcome this difficulty, the kinetic theory assumes that granular flows behave like dense gases. The velocity of each grain is decomposed in two contributions : the mean velocity of the bulk mass, and an apparently random velocity that describes the difference of the motion of the particle with respect to the mean bulk velocity. This way, the mean value of this random velocity can be seen as an analogous concept to the one of temperature in gases, hence the name of *granular temperature*. It is also assumed that the collisions between the particles are the main mechanism for the transport of momentum and energy. The main difference between the kinetic theory of gases and the one for granular flows is that the collisions are assumed to be inelastic in the case of the granular media. This kind of model revealed to be able to reproduce the shear flows moderately well, (Lun et al., 1984), (Campbell, 1990).

The difficulty of multiple grains can also be overcome with a continuous hypothesis. Several assumptions are made, such as the incompressibility of the media, simple Coulomb-like behaviour for the internal friction (which means that the maximum shear stress to cause a brittle fracture of the material is linearly dependent on the normal stress, through a coefficient of internal friction, (Irgens, 2008)), and a Coulomb friction law for the basal friction. By an additional hypothesis of a small depth to length ratio, it was possible to use the mass and momentum balance equations, averaged over the depth of the bulk mass. Two similarity solutions were found, one in the form of a M-wave with vertical faces at the two extremities of the media, and the other one in the form of a parabolic cap, which revealed to be the solution towards which the system tends for large times. The model was able to give a description in qualitative and quantitative agreement with experiments, for rock slides and plastic particles, and is applicable to rockfalls, landslides and snow avalanches, if they are not consisting of powder snow, (Savage and Hutter, 1989), (Savage and Hutter, 1991).

This consideration of a continuous phase is also used in the case of immersed granular flows, and is at the base of the so-called two-phase models. The interactions between the two are of hydrodynamic origin, but their choice is up to empirical considerations (Pailha and Pouliquen,

2009). This kind of model leads to good phenomenological results, such as the rheology of wet granular media, debris flows or the evolution of underwater avalanches (Courrech du Pont et al., 2003), (Pudasaini, 2012), (Armanini, 2013). However, although sufficiently accurate for macro-scale applications, continuum approximations fail to give an insight on the physics of the grains.

In order to study the behaviour of a granular material by taking into account each grain, it is necessary to use numerical simulations, based on more or less accurate models, depending on the situation. A first idea is to use the so-called Molecular Dynamics, a time-stepping method which has been able to simulate microscopic systems with a large number of particles, be it atoms or molecules. In Molecular Dynamics, the trajectories of the particles are determined by integrating the Newton equations of motion. Those particles are treated as point masses that interact via chosen potentials, from which the forces are derived, (Rignanese et al., 2017), thus allowing them to overlap. This idea was adapted by Cundall and Strack in the 1970's to granular materials, who thereby introduced the Distinct Element Method (in opposition to Finite Element Methods, and also called Discrete Element Method), or DEM, whose name is sometimes confounded with the secular one of Molecular Dynamics. As for MD, the particles are followed individually in a Lagrangian approach, obeying the Newton laws of motion. When they come into contact, the particles are allowed to overlap (it should be noted that this overlap is small compared to the size of the particles) and the interaction force is computed from the magnitude of the overlap, (Cundall and Strack, 1979). The force is separated in two contributions, a normal one and a tangential one. The calculation of the normal force is performed by considering a damped spring elastic behaviour, using a normal stiffness and a damping term, so that dissipation can take place. The tangential one is computed in the same way, except that the spring extends as the two bodies slide on each other, and that this tangential force cannot be higher than a Coulomb threshold. Other, more complex force laws exist, notably following the Hertzian theory of contact, (Dubois and Radjai, 2010). The DEM has the advantage to be applicable for elements of various sizes and shapes, making it eligible for realistic simulations of many systems.

This method has been widely used in different applications, and allowed to draw conclusions on the behaviour of the considered systems. Regarding static applications, Zhou *et al.* and Li *et al.* were able to simulate the static angle of repose of glass beads with good agreement with experiments, and observed relationships between this angle and parameters such as friction or geometrical constraints, (Li et al., 2005), (Zhou et al., 2002). As for flowing cases, the flow of a bidisperse assembly of disks down an inclined plane was studied by Rognon et. al, who observed the segregation of the material in three layers and showed that the rheological behaviour can be described by a local friction law, (Rognon et al., 2007). Pöschel observed good agreement between the method and experimental results for the flow properties of monodisperse disks in the same situation, (Pöschel, 1993).

However, those methods considered overlapping, deformable grains. When the latter are considered as perfectly rigid, other methods exist. Since the grains cannot interpenetrate each other, a first approach is to use an event-driven scheme, or ED. In the ED methods, the collisions are considered to be instantaneous, and hence binary. At the beginning of each time-step, all the possible collisions are detected. The collision with the smallest time until occurrence is selected, and all the particles are updated towards the corresponding time. The unique collision taking place at that precise moment is solved, using a simple collision law with a chosen restitution coefficient, and the procedure goes on ; the time-step is thus not constant. Since this method offers a simpler solving of the contacts (because their resolution is straight forward, and does not imply a calculation of a force and its integration with the equations of motion), it is very useful in applications like granular gases, where collisions are well separated in time, (Dubois and

Radjai, 2010), which suits well with the kinetic theory described earlier. Bizon *et al.* observed a good match between the kinetic theory and ED computed shear viscosity, and a factor 2 overestimation of the thermal conductivity by ED, (Bizon et al., 1999). Alam and Luding studied the rheology of bidisperse granular material with ED and showed good agreement between their numerical results and the kinetic theory, as well as the role of the bidispersity on the increase of the non-Newtonian behaviour, (Alam and Luding, 2002). However, in systems when the number of particles is high, and the collisions frequent, this kind of method fails, because of the vanishing time between collisions.

In order to model granular systems with a high number of particles and collisions efficiently, the contact dynamics method, first introduced by Jean and Moreau in the 1990s is very suitable. It allows the treatment of frictional contacts without the need to compute a repulsion force explicitly, thanks to an iterative procedure and a balance of momentum. This kind of method, which is used here and detailed in the next chapter, is able to simulate accurately the behaviour of granular assemblies where friction plays an important role, from a Couette granular flow between cylinders to stones in masonry, and also for the continuous problem of deep drawing a steel plate, (Jean, 1999), (Radjai and Richefeu, 2009)

Chapter 3

The Non-Smooth Contact Dynamics Method

The Non-Smooth Contact Dynamics (NSCD) Method, which allows to accurately simulate granular materials, is presented in two dimensions. The grains are considered to be rigid spheres (disks in 2D), unable to deform, with varying radii. The laws for the resolution of the contacts without and then with friction are presented and validated.

3.1 The global problem

For the sake of simplicity, the following is focused on bi-dimensional representation, but can without problem be generalised to the three-dimensional case.

Let $q_i = \begin{bmatrix} x_i \\ y_i \\ \theta_i \end{bmatrix}$ and $\dot{q}_i = \begin{bmatrix} u_i \\ v_i \\ \omega_i \end{bmatrix}$ be the vectors that describe the coordinates and the velocities of a perfectly rigid grain i in the frame of reference associated with the system of interest, and $M_i = \begin{bmatrix} m_i \\ m_i \\ I_i \end{bmatrix}$ its mass and inertia vector. This grain i obeys the second Newton law of motion :

$$M_i \frac{d\dot{q}_i}{dt} = F_i, \quad (3.1)$$

with F_i the resultant of the forces acting on i . When the system consists of N particles, the following compact notation can be used :

$$q = \begin{bmatrix} q_1 \\ \vdots \\ q_N \end{bmatrix}$$

$$M = \text{diag}(M_1, \dots, M_N),$$

and 3.1 can be generalised as :

$$M \frac{d\dot{q}}{dt} = F.$$

It appears convenient to separate F into two contributions : F_e which represents the resultant of the external forces acting on the grains due to gravity or the fluids, and which can be computed at each time t , and r which represents the resultant of the forces due to the contacts between

the grains and which are not explicitly known (Dubois and Radjai, 2010). In a system with many grains that are close together, these contacts are expected to imply shocks. Due to our rigid bodies modelling, these shocks are characterised by instantaneous (and bounded) changes in velocity. Since for these events, the derivative of $\dot{q}$ is not defined anymore, because of the discontinuity, it is necessary to work with a weaker, integral form of the equations of motion, which is satisfied even for shocks :

$$M(\dot{q}^{t_2} - \dot{q}^{t_1}) = \int_{t_1}^{t_2} F_e ds + p. \quad (3.2)$$

Because the changes in velocity are bounded, (3.2) can be rewritten as a differential measure equation, Dubois and Renouf (2015) :

$$\begin{aligned} M d\dot{q} &= F_e dt + dp \\ q(t) &= q(t_0) + \int_{t_0}^t \dot{q}^t dt. \end{aligned}$$

Since the goal is to work with a time-stepping scheme, time has to be discretised in time-steps, noted Δt . If the time is denoted by the superscript i , integrating over one time-step yields :

$$\begin{aligned} M(\dot{q}^{i+1} - \dot{q}^i) &= \int_{t_i}^{t_{i+1}} F_e ds + \int_{t_i}^{t_{i+1}} \\ q^{i+1} &= q^i + \int_{t_i}^{t_{i+1}} \dot{q} ds. \end{aligned}$$

Using a backward Euler scheme finally gives :

$$M(\dot{q}^{i+1} - \dot{q}^i) = F_e^{i+1} \Delta t + p^{i+1} \quad (3.3)$$

$$q^{i+1} = q^i + \Delta t \dot{q}^{i+1}. \quad (3.4)$$

Since it is an implicit scheme, it is unconditionally stable, which is precisely the desired property, since the goal is to solve the system with a fixed time-step, whose value is dictated by a compromise between accuracy and computational convenience. However, these type of schemes imply, due to their very nature, the use of iterative procedures. Here, the iterative procedure focuses on the impulse term p^{i+1} , as will be seen. Finally, the external forces contribution is actually computed using the forces at time t_i instead of time t_{i+1} . In a model with a fluid, this requires indeed a stability condition on the time-step, because the forces between the grains and the fluid depend notably on the velocity of the grains. However, the only external force in dry granular flows is the one due to gravity¹, which is constant over time and does not depend on the velocity of the grains. Therefore, the method is always stable, for any time positive time-step.

3.2 The local frame

Now that the problem is stated, it is still necessary to find a resolution approach. This can be done by putting the focus on each contact in particular, i.e. at a local *scale*. Consider an upcoming contact between two spherical grains, i and j . In 2D, a local reference *frame* can be defined with a normal and a unique tangential vector, denoted by $\mathbf{n}$ and $\mathbf{t}$ respectively, starting from the contact point α (from now on, for the sake of simplicity, the superscript α denoting the contact is omitted) on the particle i , see Fig. 3.1. The orientation of the tangential vector can be chosen arbitrarily to be towards the left or towards the right; the choice is made to take it as going to the right.

¹Assuming the effect of the air can be neglected, which is done here and in the literature.

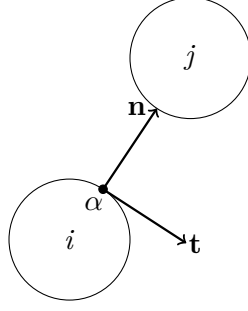


Figure 3.1: Local frame for two grains i and j candidate to a contact α

An important work hypothesis is the impenetrability of the grains, implying what is called unilateral contacts. This means that the distance between the grains, denoted $\mathfrak{d}$, is always positive. It is only when this gap is equal to zero that an interaction between the grains can take place. It is also important to note that no attraction or repulsion takes place between the grains, and that the normal component of reaction force R_n is never negative and vanishes when the two grains are not in contact. This can be stated as the so called Signorini condition (Jean, 1999) :

$$\begin{aligned}\mathfrak{d} &\geq 0 \\ R_n &\geq 0 \\ \mathfrak{d}R_n &= 0.\end{aligned}$$

Let $w = \begin{bmatrix} w_n \\ w_t \end{bmatrix}$ be the relative velocity of grain i with respect to grain j . It is interesting to note that the normal component of the relative velocity is also the time derivative of the distance . This will be useful to predict the gap at the next time-step, and thus detect the future contacts. The three variables can be linked with the following relationships (Radjai and Richefeu, 2009), Moreau (1994):

$$\begin{aligned}\mathfrak{d} > 0 &\implies R_n = 0 \\ \mathfrak{d} = 0 &\implies w_n \leq 0 \\ w_n \leq 0 &\implies R_n = 0.\end{aligned}$$

In other words, the first line means that when the distance between the particles is non-null, the reaction force is null, in agreement with the Signorini conditions. The second one states that when they are in contact, the relative velocity can only be null, and the contact is persistent, or negative, and the contact is vanishing. Finally, the third one explains that when the contact is persistent or vanishing, the reaction force is also null.

Now that relationships have been established for the normal components of the contact problem, the tangential one can be considered. This is where friction comes into action. The choice is made to model friction with the simple Coulomb law of dry friction :

$$\begin{aligned}w_t > 0 &\implies R_t = -\mu_k R_n \\ w_t < 0 &\implies R_t = \mu_k R_n \\ w_t = 0 &\implies R_t \leq \mu_s R_n,\end{aligned}$$

with μ_k the coefficient of kinetic friction and μ_s the coefficient of static friction. It is important to make the difference, since in most cases $\mu_k < \mu_s$. However, the Signorini-Coulomb relationships are not sufficient to describe the precise behaviour of the interaction between the grains during a collision. Therefore, it is necessary to add contact laws to the model, involving the normal and

tangential components of the relative velocity and the impulse.

$$\begin{aligned}\text{ContactLaw}(P_n, w_n, \mathfrak{d}) &= 0 \\ \text{FrictionLaw}(P_t, w_t) &= 0.\end{aligned}$$

They are chosen as balances of momentum, due to the instantaneous nature of the collisions, as explained earlier :

$$\text{ContactLaw} \equiv \frac{P_n}{\mathbb{M}} = w_n - \frac{\mathfrak{d}}{\Delta t}, \quad (3.5)$$

$$\text{FrictionLaw} \equiv w_t + \frac{P_t}{\mathbb{M}} = 0, \quad (3.6)$$

where $\mathbb{M} = m_i + m_j$ the total mass of the grains. Those relationships and their meaning are developed in the next two sections.

3.3 From global to local and back again

These laws allow the resolution of the contacts one by one only at the local *scale*, i.e. in the local *frame*. Since the goal is to solve the system with the global variables, q and $\dot{q}$, and for each contact, a link between the two frames needs to be done. This link is called a *mapping*, and will be noted $\mathbf{H}$: it will allow converting and redistributing the new value of the relative velocity obtained from the local contact laws to the global velocities of the two grains involved in the solved contact. Obviously, in order to be able to use the local laws and solve the contacts one by one, it also necessary to have an inverse mapping that will translate the variables the other way around. It can be shown, through an equality of powers in the local and global frame (Dubois and Renouf, 2015), that this inverse mapping is simply the transpose of $\mathbf{H}$, and is noted $\mathbf{H}^*$. The inverse mapping $\mathbf{H}^*$ simply consists in converting the velocities of the two grains into their relative velocity expressed in the normal-tangent frame. This is done by subtracting the velocity of the grain j to the one of the grain i , and performing the scalar product with the normal vector, for the normal component of w , w_n . For the tangential component, w_t , the same is done but the scalar product is performed with the tangential vector, and the result of the cross products of the angular velocities with their radii (along the normal) is added. This can be written as :

let $\mathbf{v} = \begin{bmatrix} \dot{q}_i \\ \dot{q}_j \end{bmatrix}$ be the vector of the velocities of the two grains involved in the contact, and let $\mathbf{w} = \begin{bmatrix} w_n \\ w_t \end{bmatrix}$ be the vector of the relative velocity between those two grains.

The link between the two is made by the mapping $\mathbf{H}^*$:

$$\begin{aligned}w^T &= \mathbf{v}^T \cdot \mathbf{H}^* \\ w^T &= \mathbf{v}^T \cdot \begin{bmatrix} N_x & T_x \\ N_y & T_y \\ 0 & rad_i \\ -N_x & -T_x \\ -N_y & -T_y \\ 0 & rad_j \end{bmatrix},\end{aligned}$$

where N_x, N_y , and T_x, T_y are the x and y components of the normal and the tangent, respectively, and rad_i, rad_j the radii of the grains.

When the contact laws have been activated and the local impulse computed, it is still necessary to redistribute this impulse to the two grains. This is done by using a matrix of coefficients :

$$\mathbb{C} = \begin{bmatrix} \frac{m_j}{\mathbb{M}} & & & & & \\ & \frac{m_j}{\mathbb{M}} & & & & \\ & & \frac{m_i - m_j}{I_i \mathbb{M}} & & & \\ & & & \frac{m_i}{\mathbb{M}} & & \\ & & & & \frac{m_i}{\mathbb{M}} & \\ & & & & & \frac{m_j - m_i}{I_j \mathbb{M}} \end{bmatrix}$$

The $\frac{m_k}{\mathbb{M}}$ coefficients are the crossed masses of the particles. This way, the heavier the grain, the less it feels the correction, which is in agreement with physics. The two other coefficients are related to the inertia of the grains, and are necessary to convert an impulse into angular velocity. The transformation of the local impulse to the global one can be written as :

Let $P = \begin{bmatrix} P_n \\ P_t \end{bmatrix}$ be the vector of the impulse on the grains because of the contact in the local frame, and let $s = \begin{bmatrix} p_i \\ p_j \end{bmatrix}$ be the vector of the impulse because of the contact in the global frame.

The link between the two is made by the mapping $\mathbf{H} = \mathbf{H}^{*T}$:

$$s^T = P^T \cdot \mathbf{H} \cdot \mathbb{C}$$

$$s^T = P^T \cdot \begin{bmatrix} N_x & N_y & 0 & -N_x & -N_y & 0 \\ T_x & T_y & rad_i & -T_x & -T_y & rad_j \end{bmatrix} \cdot \begin{bmatrix} \frac{m_j}{\mathbb{M}} & & & & & \\ & \frac{m_j}{\mathbb{M}} & & & & \\ & & \frac{m_i - m_j}{I_i \mathbb{M}} & & & \\ & & & \frac{m_i}{\mathbb{M}} & & \\ & & & & \frac{m_i}{\mathbb{M}} & \\ & & & & & \frac{m_j - m_i}{I_j \mathbb{M}} \end{bmatrix}$$

3.4 The contact law

The friction law is of high importance for two reasons. First because the convergence criterion of the algorithm is put on the sum of all the normal impulses, which have been computed accordingly, and secondly, because this is the value of the normal impulse that will determine the maximal value that the tangential one can take, as will be explained in the next section.

Remembering the contact law stated above :

$$\frac{P_n}{\mathbb{M}} = w_n - \frac{\mathfrak{d}}{\Delta t}$$

Suppose that a contact has been detected and that 3.5 has been activated. The physical meaning of this contact law is that, knowing the normal relative velocity w_n , it must be corrected by an amount $\frac{P_n}{\mathbb{M}}$ so that at the end of the time-step, the grains do not interpenetrate each other. This way, the two grains come into contact at the next time-step. However, their respective velocities have only been reduced so that they do not interpenetrate each other, and their relative velocity is then still greater than 0 when they touch. The contact law is activated again, and a new correction is computed and applied, which has for effect to cancel the relative velocity, and the two grains go on in the same direction with the same velocity : this is thus a perfectly inelastic choc law.

This choice of perfectly inelastic collisions between the grains can be discussed. Indeed, in applications, this is not always the case, and the collisions are located between the two ideal

types of perfectly elastic and perfectly inelastic collisions. The reason behind this choice is simple. Consider a bucket filled with tennis balls. When another tennis ball is dropped in the bucket, it experiences a more or less perfectly inelastic collision with the balls at the top and stops, while all the other balls stay still. This is due to the fact that the energy of the impacting ball is dissipated in heat and small deformations of all the other balls. However, in the model, the grains are considered as perfectly rigid and cannot deform so in order to dissipate the energy. If the choice of elastic collisions was made, the balls in the bucket would vibrate indefinitely. With the perfectly inelastic choice, it is not the case, and the behaviour of the system reflects more the reality.

All contacts are thus solved with 3.5 at each time-step. The number of these contacts can be high, and the resolution of a contact can affect the resolution of another one. This is why all contacts are solved at the same time, iteratively. First, all the possible contacts are listed, using the maximum velocity, $\max(\dot{q})$ to predict the intersections between the grains. From these possible contacts, only the active ones² are solved with the contact law during the first iteration, maybe activating other ones. When a contact is solved, the correction associated with it is stored, and at the end of each iteration, the sum of the corrections is computed. When this sum is inferior to a given threshold, the algorithm is considered to have converged. According to 3.3, the grains are then moved and the simulation can proceed to the next time-step.

Algorithm 1 Contact law

At each time-step :

From the previous velocities and the forces, compute the new free velocities

Detect all possible contacts for each grain from the maximum velocity

while $\sum_{\alpha} P_n^{\alpha} > \text{tol}$ **do** ▷ Until convergence is reached

for All possible contacts **do**

if $w_n > \frac{d}{\Delta t}$ **then** ▷ Check if the contact is active

$\frac{P_n^{\alpha}}{\mathbb{M}^{\alpha}} = w_n - \frac{d}{\Delta t}$ ▷ Find the correction

$u_i = u_i - N_x \cdot \frac{P_n^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$ ▷ Update the velocities

$u_j = u_j + N_x \cdot \frac{P_n^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$

$v_i = v_i - N_y \cdot \frac{P_n^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$

$v_j = v_j + N_y \cdot \frac{P_n^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$

else

$P_n^{\alpha} = 0$ ▷ Do nothing

end if

end for

end while

With the converged velocities, update the positions

²It is important to make the difference between possible and active contacts. Active contacts are the ones which will effectively take place during the next time-step, if things were to evolve unchanged. However, since the resolution of such contacts implies a change in the velocity of the corresponding grains, it is possible that a new, previously undetected contact arises. For this reason, it is necessary to use a list of all possible contacts over the next time-step, that is, the contacts that could occur, or not, depending on the other ones. This is done by using, in the prediction of the contacts, the overall maximum velocity, as in step 3 of Fig. 3.2.

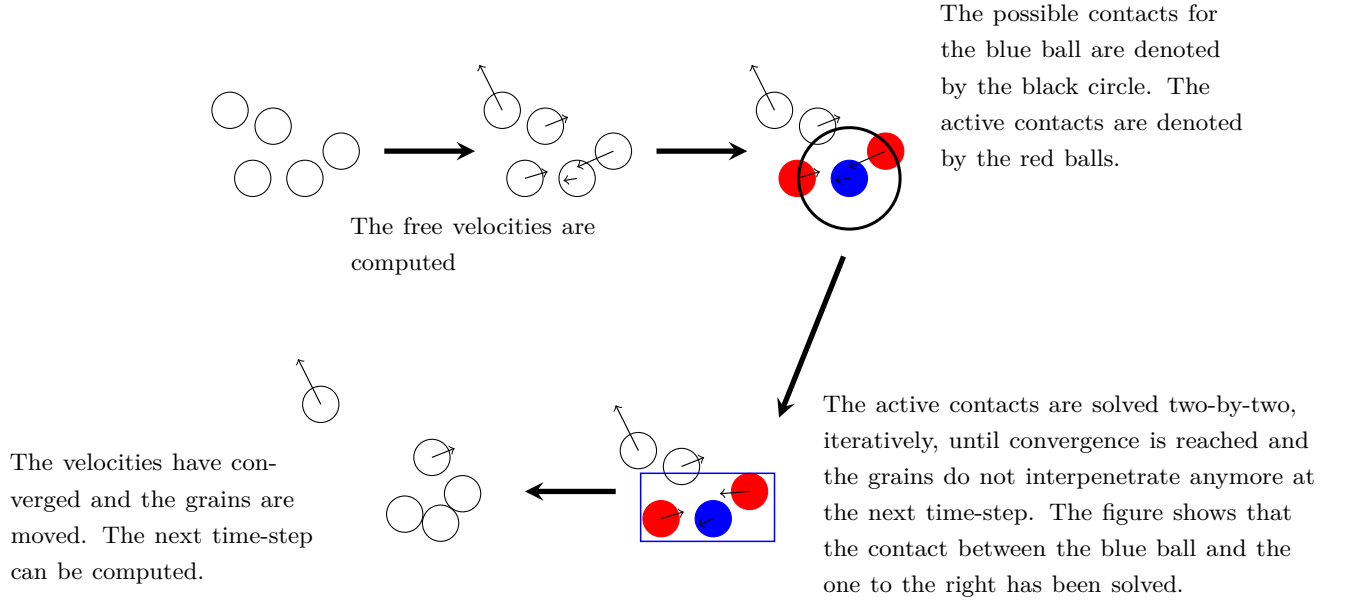


Figure 3.2: Steps for the resolution of contacts over one time-step.

3.4.1 Contact with a wall

The problem of a contact with a wall is a bit more tedious, since the computation of the distance and the normal is somewhat different. Indeed, the second object of the contact is no more consisting of a single point. First, the case of a grain in a square box is considered. When the grain comes into contact with a wall, the collision is treated just like the one between two grains, except that the wall is assumed to have infinite mass, and all the corrections are redistributed to the grain. Again, there are two possibilities : elastic or inelastic collisions. As can be seen on Fig. 3.3, the perfectly elastic choice creates energy : the ball jumps higher and higher from the wall under the influence of gravity. Plus, in a simulation with a larger number of grains, oscillations are generated. This is why the choice of perfectly inelastic collisions at the walls is made.

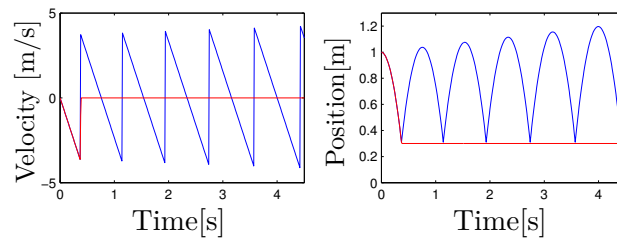


Figure 3.3: Left - Y velocity of the ball through time. Right - Y position of the ball through time. The perfectly inelastic case is presented in red while the perfectly elastic one is in blue.

Contact with a circular wall

For the more complicated case of a circular wall, a problem arises. Indeed, when the normal is computed, the naive projection is not valid anymore. This is because the grain, in addition to normal relative velocity, also has tangential relative velocity, that will shift it left or right from the position for which the correction has initially been calculated. For a linear wall, this is not a problem since the y position of the wall is the same for all x . However, for a circular wall, this y position has changed, and the computed correction is no more valid, since it implies

an interpenetration, as can be seen in Fig. 3.4. The proposed solution consists in calculating the normal to the projected point of contact, that is, the intersection between the line with the same orientation as the velocity of the grain and the circular wall. Further on, it is called the projected normal, in opposition to the classical one, called the initial normal. The correction is then computed based on this new normal. This way, the ball will neither interpenetrate the wall in the direction of the projected normal, nor in the direction of the initial one. The challenge is to compute the components of the projected normal. It amounts to rotate the initial normal by an angle β , as indicated in Fig. 3.4.

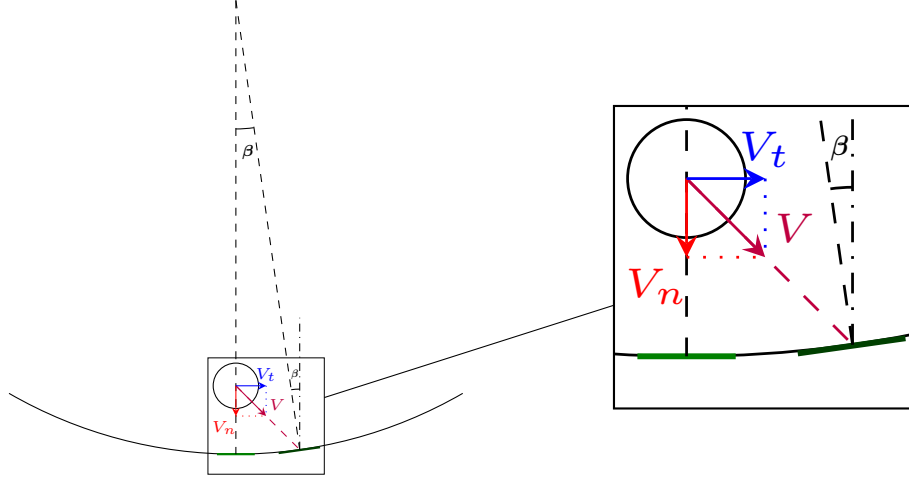


Figure 3.4: Contact of a grain with a circular wall. $\mathbf{w}$ is the relative velocity between the wall and the grain, w_n is the projection of $\mathbf{w}$ along the initial normal, and w_t is the associated tangential component. The contact is detected from the initial normal, but the associated correction is not sufficient, since it is only valid for a tangent line indicated in green. It is necessary to find the intersection of $\mathbf{w}$ with the circular wall and calculate the correction with a normal to the tangent in that point, indicated in dark green, so that the grain does not intersect the wall.

This problem can be solved with the help of geometry and trigonometry. First, the representation of the problem can be simplified to the one of Fig. 3.5.

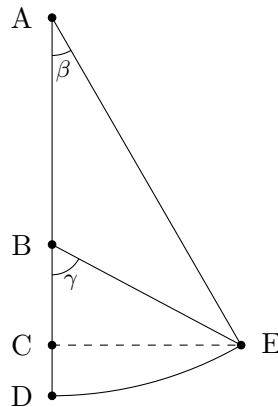


Figure 3.5: Simplified representation of the problem.

From the definition of the tangent, it can be found that :

$$\tan(\gamma)\overline{BC} = \overline{CE} \quad (3.7)$$

Since the triangle ACE is rectangle :

$$\overline{CE} = \overline{AE} \sin(\beta) = r \sin(\beta),$$

with r the radius of the circular wall. Obviously, the distance $\overline{BC}$ is equal to $\overline{BD}$, the distance d between the grain and the wall, minus $\overline{DC}$, which corresponds to the sagitta generated by an angle 2β :

$$\overline{DC} = r(1 - \cos(\beta))$$

These expressions injected in 3.7 yield :

$$\tan(\gamma)(d - r(1 - \cos(\beta))) = r \sin \beta,$$

which finally gives :

$$\sin(\beta) - \tan(\gamma) \cos(\beta) + \tan(\gamma) \frac{r-d}{r} = 0.$$

Since this equation is not linear, it needs to be solved with an iterative method. A simple, well-known method is the Newton-Raphson method which consists in finding the zero of a function $f(x)$ by the iterative process given below :

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)},$$

where f' represents the first derivative of f with respect to x . Here, $f = f(\beta) = \sin(\beta) - \tan(\gamma) \cos(\beta) + \tan(\gamma) \frac{r-d}{r}$ and $f' = f'(\beta) = \cos(\beta) + \tan(\gamma) \sin(\beta)$.

Although simple, it requires to choose a good first iterate that is "not too far" from the exact solution, otherwise the method will never reach convergence. In order to make a reasonable choice, it is necessary to further examine the problem. Since an upcoming contact has been detected, the relative velocity between the grain and the wall has to have some normal component. Therefore, the value of gamma is bounded as follows :

$$|\gamma| < \frac{\pi}{2}.$$

Obviously, when γ tends to zero, so should β . But what happens when γ tends to $\pm \frac{\pi}{2}$? When this is the case, it means that the normal component tends to be null, and thus, in order for the contact to be detected, the distance d also tends to zero. However, when γ tends to zero, the triangle ABE tends to be rectangle, and it appears that $\cos(\beta) = \frac{r-d}{r}$. Since d tends to zero, $\cos(\beta) = 1$ and $\beta = 0$. The first guess β_0 should thus respect the previous relationships : if γ is close to 0, so should β_0 , and if γ is close to $\pm \frac{\pi}{2}$, β_0 should also tend to 0. In the intermediate cases, β_0 should always be smaller than γ . The proposed formula for β_0 is thus :

$$\beta_0 = |\gamma| \cos(\gamma) \sin(\gamma).$$

However, when γ gets closer to $\frac{\pi}{2}$, $\tan(\gamma)$ strongly increases, and so does the value of the solution (which is not a real problem in itself, since this high value modulo 2π stays in the correct ball park for the rotation of the normal vector) making the starting iterate given by the formula above too far from the solution, and preventing the method from converging. Therefore, in such a case, the starting iterate will be taken as $\beta_0 = \tan(\gamma)$. Finally, a stopping criterion has to be specified. An arbitrary tolerance of 10^{-6} has been set on the result $f(\beta)$. However, a maximal number of iterations of the Newton-Raphson method is necessary so that, when convergence is not met, the program stops and the computational cost is not too high. When this maximum number of iterations is met, since there is no guarantee that the value of β is still close to the desired tolerance, the choice is made to return $\beta = 0$ so that no correction is applied. This maximum number of iterations is arbitrarily chosen to be 1000, so that the computations are not slowed down in a too significant manner.

3.4.2 Validation

Here, the method that was presented above is validated against an event driven code in 1D.

Contact between grains

What concerns the contact between grains, a numerical comparison between the presented time-stepping algorithm and an event driven scheme that uses exact classical physics formulas, has been led in a one-dimensional case, as can be seen in Fig. 3.6.

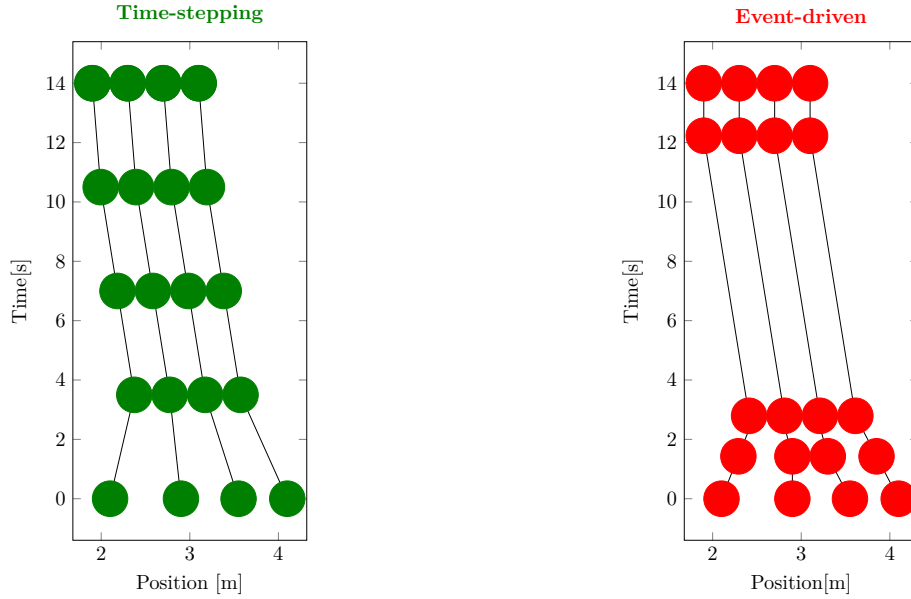


Figure 3.6: Positions of 4 balls with random initial velocities inside two walls, with perfectly inelastic collisions and in 1D, solved with the time-stepping dynamic algorithm on the left and an event-driven scheme on the right. The time-stepping scheme used time-steps of $3.5s$.

Over the first time-step, three collisions (one of them was not represented for the sake of simplicity) occurred. The event-driven algorithm thus made 3 jumps forward in time, each one of a different value so that the precise moment of impact is reached, whereas the time-stepping algorithm detected and solved all three contacts at once during one time-step. This behaviour is of high interest in applications with a large number of grains, since in that case the time between collisions vanishes and the number of jumps to be made by the event-driven scheme increases very strongly.

3.5 The friction law

Now that the contact law has been presented and that the contacts are solved regarding the point mechanics, friction can be introduced. This feature is especially important to correctly model the behaviour of the system, since it will involve static equilibria that were not possible before, such as arching and piling in heaps. Remembering the law that was stated in section 3 :

$$w_t + \frac{P_t}{\mathbb{M}} = 0.$$

Suppose that a contact has been detected and the contact law as well as the friction law have been activated. This friction law means that at the moment of contact, the tangential impulse is computed so that it cancels out the tangential relative velocity of the grains. Though, this

impulse cannot take an arbitrarily high value. This is why the friction law is combined with the Coulomb law of dry friction, meaning that the maximum value of the tangential impulse is given by the coefficient of static friction μ_s times the normal impulse P_n , and if the tangential impulse required to cancel the tangential relative velocity is higher, then its value is given by the normal impulse times the kinetic coefficient of friction, μ_k , because the grains slide on each other. It can be stated as :

$$0 = w_t + \frac{P_t}{M} \quad (3.8)$$

$$|P_t| \geq |\mu_s P_n| \implies |P_t| = |\mu_k P_n|. \quad (3.9)$$

The algorithm is presented in algorithm 2. The first thing to notice is that the friction law, in addition to modifying the angular velocities, also modifies the linear velocities : this is logical since the tangential impulse also acts on the centres of mass of the grains ; this is what allows arching or piling in heaps. Secondly, while the correction was applied positively to the j grain and negatively to the i grain, it is always negative what concerns the angular velocity. Why is it so? Consider two grains of equal mass and radius undergoing a collision, and consider that the contact law has been activated and that the normal impulse has been found, as in Fig. 3.7. Remains the tangential impulse and its effects. The tangential impulse is, according to 3.8, calculated so that it cancels out the tangential relative velocity. Then, it is redistributed between the grains. As in the contact law, the grain i receives a negative correction, and the grain j a positive one. However, their radii go in opposite directions. Therefore, when the cross-product is performed with the correction, the difference of sign cancels, and the two grains receive a negative correction for their angular velocities. The choice of the sign is due to the fact that rotation is taken to be positive when the grains rotate clockwise.

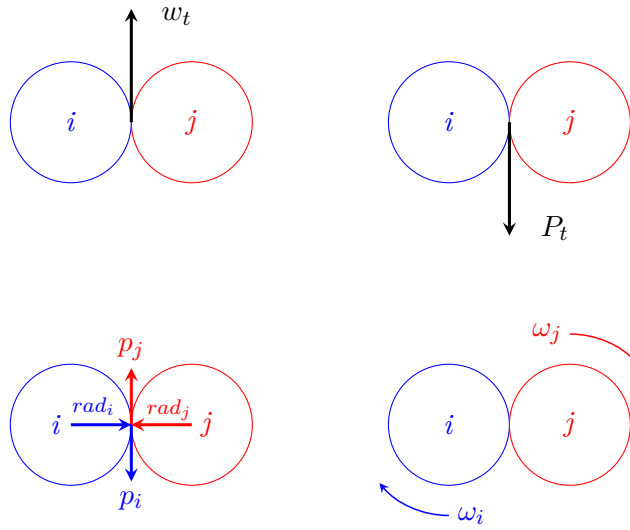


Figure 3.7: Friction law : treatment of the angular velocities.

Algorithm 2 Friction law

At each time-step :

From the previous velocities and the forces, compute the new free velocities

Detect all possible contacts for each grain from the maximum velocity

while $\sum_{\alpha} P_n^{\alpha} \geq tol$ **do** ▷ Until convergence is reached

for All possible contacts **do**

if $w_n > \frac{d}{\Delta t}$ **then** ▷ Check if the contact is active

 Use the contact law to get P_n^{α}

if $w_t \neq 0$ **then** ▷ Check if the tangential relative velocity is non-null

$$\frac{P_t^{\alpha}}{\mathbb{M}} = \max(\mu_s \frac{P_n^{\alpha}}{\mathbb{M}}, w_t)$$

if $P_t^{\alpha} = \mu_s P_n^{\alpha}$ **then** ▷ Check for sliding friction

$$P_t^{\alpha} = \mu_k P_n^{\alpha}$$

end if

$$u_i = u_i - T_x \cdot \frac{P_t^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}} \quad \text{▷ Update the velocities}$$

$$u_j = u_j + T_x \cdot \frac{P_t^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$$

$$v_i = v_i - T_y \cdot \frac{P_t^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$$

$$v_j = v_j + T_y \cdot \frac{P_t^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$$

$$\omega_i = \omega_i - \frac{m_i}{I_i} \cdot \frac{P_t^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$$

$$\omega_j = \omega_j - \frac{m_j}{I_j} \cdot \frac{P_t^{\alpha}}{\mathbb{M}^{\alpha}} \cdot \frac{m_j}{\mathbb{M}^{\alpha}}$$

end if

else

$$P_n^{\alpha} = 0 \quad \text{▷ Do nothing}$$

end if

end for

end while

With the converged velocities, update the positions

3.5.1 Validation

In order to validate the frictional algorithm, numerical experiments have been led with the help of Matlab. Since it was difficult to find a simple problem with an analytic solution for the frictional contact between two disks in the literature, the focus was put on the friction between the grains and the walls. The simple problem of a spherical grain rolling down an inclined plane is first analytically solved, and the results yielded by the algorithm are confronted with the ones predicted by theory.

Contact with a wall

Consider a ball initially at rest on a plane inclined at an angle α and subjected to earth gravity. Due to this gravity, the ball will start to go down the slope. Two cases are possible : either the ball rolls with or without slipping. The distinction between the two cases appears to depend on

the angle of the slope and on the friction coefficient between the ball and the slope, and this relationship will be detailed later.

First, the case of rolling without slipping is considered. In order to determine the speed along the slope (which corresponds to the speed in the x direction of the reference frame aligned with the slope), it is necessary to use the Newton equations of motion and list the forces acting on the ball :

$$ma = \sum F$$

$$I \frac{d\omega}{dt} = \sum \tau,$$

with m the mass of the ball, I its inertia, a its linear acceleration, ω its angular velocity, and F and τ the forces and torques acting on it, respectively. As can be seen in Fig. 3.8, several forces act on the ball : the force due to gravity, denoted F_g , the reaction force, denoted F_n and the frictional force, denoted F_f .

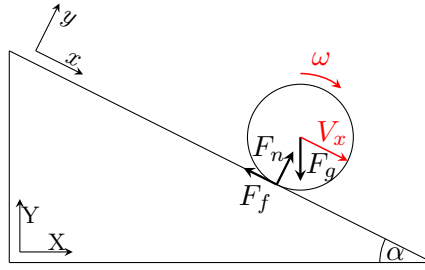


Figure 3.8: A ball rolling down an inclined plane without slipping

From trigonometry, one can find that F_g can be decomposed in the following x and y components :

$$F_{gx} = mg \sin \alpha$$

$$F_{gy} = -mg \cos \alpha.$$

From this, the value of the reaction force can be found, with the second law of Newton. Indeed, since the ball stays in contact with the slope, the sum of the forces in the y direction has to be null. This implies that :

$$F_n = mg \cos \alpha. \quad (3.10)$$

A balance of forces can also be made in the x direction :

$$ma_x = mg \sin \alpha - F_f$$

A balance of torques gives :

$$I \frac{d\omega}{dt} = r F_f,$$

with r the radius of the ball. At this point, a final relationship is necessary to close the system of equations above. This relationship is provided by the no-slip condition, which states that the speed of the contact point needs to be null. This means that :

$$\omega r = V_x.$$

differentiating the equation with respect to time gives :

$$a_x = \frac{d\omega}{dt} r.$$

Injecting in the balance of torques yields :

$$F_f = \frac{I a_x}{r^2}, \quad (3.11)$$

which can be injected in the balance of forces in x to give :

$$a_x \left(m + \frac{I}{r^2} \right) = mg \sin(\alpha).$$

Since for a spherical grain, the inertia is $I = \frac{2mr^2}{5}$, it finally gives :

$$a_x = \frac{5}{7} g \sin(\alpha) \quad (3.12)$$

By integrating with respect to time, one finally gets the expression for the velocity along the ramp :

$$V_x = V_x(t=0) + \frac{5}{7} \sin \alpha g t$$

It can be noticed that this velocity is smaller (due to the $\frac{5}{7}$ coefficient) than in the case where no friction occurs. This is because part of the potential energy is transformed into rotational kinetic energy, through the action of friction, whereas in the no-friction case all this potential energy is converted in linear kinetic energy. Now that an analytic expression has been found for the down slope velocity, the conditions on the angle of the slope in order to satisfy the no-slip conditions can be derived. For static friction to take place, the friction force needs to be inferior to $\mu_s F_n$. Injecting 3.12 into 3.11 and using 3.10, this yields :

$$\tan(\alpha) < \frac{7}{2} \mu_s. \quad (3.13)$$

Numerical experiments have been led for a ball of steel rolling down a steel ramp, with the following values for the friction coefficients³ :

$$\begin{aligned} \mu_s &= 0.78 \\ \mu_k &= 0.42, \end{aligned}$$

with a ramp inclined at 21.8° , which corresponds to a line with a slope coefficient of 0.4. The fall along the slope was simulated for $t_{end} = 5s$, with a time-step of $\Delta t = 0.01s$. The results are presented in Fig. 3.9

As can be seen in the top figure, the two solutions are so close that they are difficult to distinguish. On the magnified frame and on the bottom figure, it can be seen that the numerical solution oscillates around the analytic one. The oscillations are due to the nature of the algorithm : the correction is applied so that the ball does not intersect the wall, which, since the wall is inclined, gives the ball a positive velocity along this wall. At this moment, the calculated velocity is higher than the theoretical one, since it is only at the next time-step that the algorithm "sees" that the tangential relative velocity is non-null. The algorithm then applies a correction in order to make the ball rotate. However, since the ball acquired a speed that was too high during the first time-step, a larger correction is needed so that it rotates. Therefore, which will give a velocity slightly under the one it should have analytically. Surprisingly, the maximal no-slip angle was found to be determined by the kinetic coefficient of friction μ_k instead of the static one μ_s . This can be explained that, in practice, the actual maximal friction force that is felt by the ball is the one given by the product of μ_k and the normal force, since, due to the jumps up and down the analytic solution because of the nature of the algorithm, the ball is often in a sliding situation.

³Taken from http://www.roymech.co.uk/Useful_Tables/Tribology/co_of_frict.htm#method, accessed on 27/04/2018.

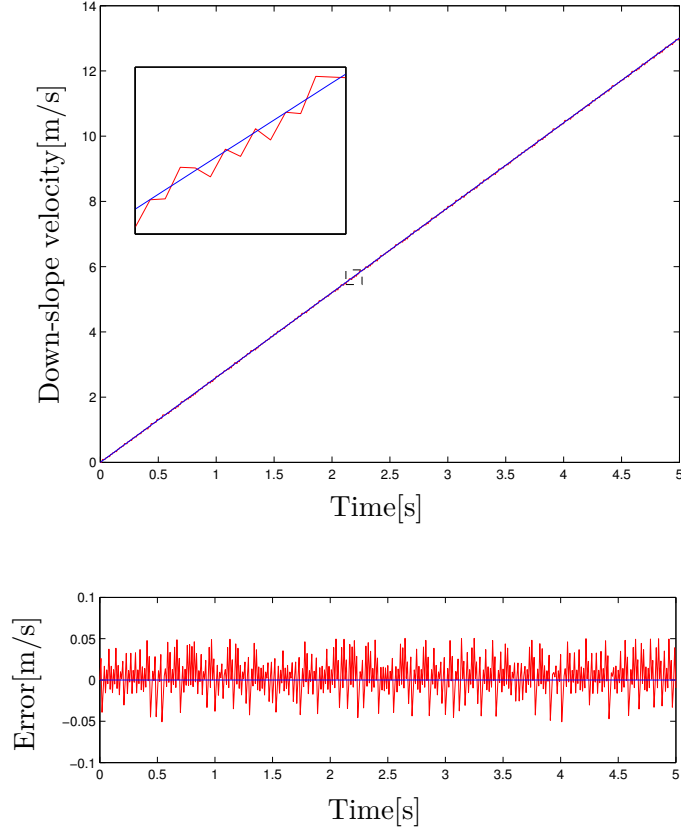


Figure 3.9: Top : comparison between the numerical results, in red, and the analytic solution, in blue, for the down slope velocity. The small frame is magnified 13 times. Bottom : error committed at each time-step.

It can also be seen that the error stays within a constant range of $[-0.05; 0.05]$, indicating that the algorithm is stable. The value of the error was further investigated. The convergence of the algorithm with the time-step was studied, with the two following norms :

$$L_{\infty} = \max_i(|e_i|)$$

$$L_2 = \sqrt{\Delta t \sum_i e_i^2},$$

with e_i the difference between the numerical solution and the analytic one. The convergence study was made for different simulation times, from $t_{end} = 1s$ to $t_{end} = 500s$. The results are presented in Fig. 3.10 and Fig. 3.11.

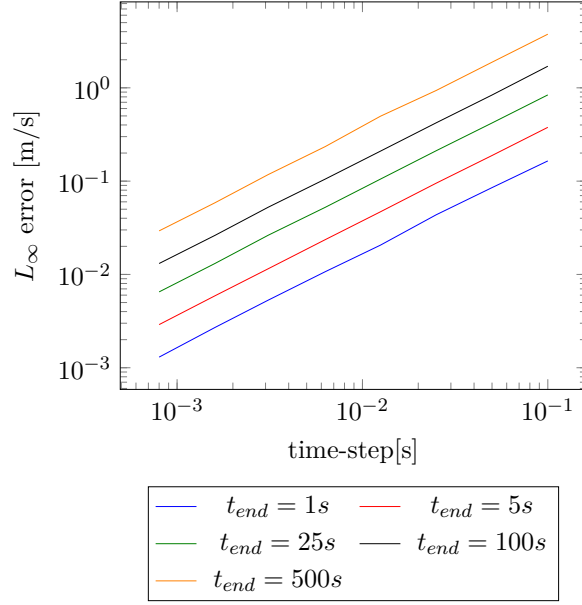


Figure 3.10: Log-Log plot of the L_2 error. It appears that the convergence rate is the same for all simulation times.

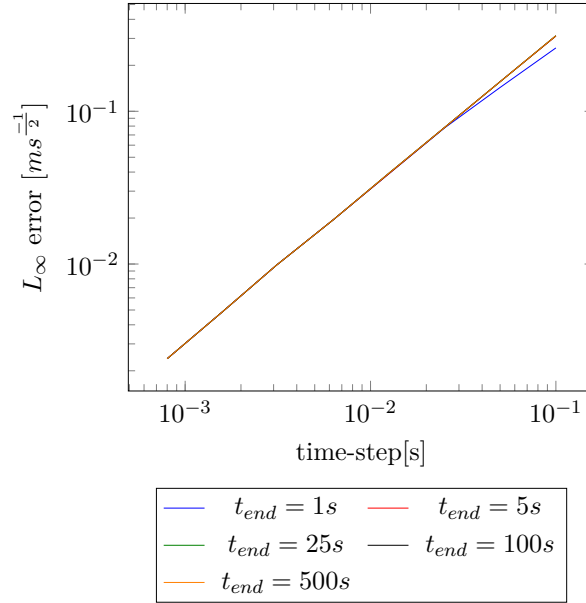


Figure 3.11: Log-Log plot of the L_∞ error. The error seems to be very similar for the different simulation times.

The difference of magnitude between the errors in the L_2 graph compared to the ones for the L_∞ graph are explained by the fact that the former norm L_2 implies a summation over all the elements of the error vector, and as the simulation time is higher, so is the number of elements of this vector. In the two graphs, the error converges linearly with the time-step. Based on this, the choice of a time-step of 0.005 seconds seems reasonable, in terms of accuracy and computational convenience.

The model presents valid results in simple test cases. For frictionless contacts, the method predicted the accurate behaviour for a one-dimensional case, even with a very long time-step. As for the frictional contacts, the method is stable, as was expected by the use of an implicit scheme, and the error converges linearly with decreasing time-steps. From these observations, comparison of the results for a larger number of grains with ones from literature, be it experimental or numerical, can be performed in order to evaluate the influence of this error ; this is done in chapter 5. Before that, a small summary of the computational tricks used in the immersed model is presented, so that the reader has in mind the way the algorithm is efficiently implemented, so that it can be used in large-scale simulations.

Chapter 4

Implementation

The working principle of an algorithm is one thing, but its implementation on a machine so that it yields results in a decent computational time is another one. This task presents many challenges, as it is necessary to find new, original ways to write down the method into the code so that time complexity is reduced, but without altering its basic properties so that the result is the same.

For the small test codes that were used for validation purpose in this paper, the naive implementation was good enough, due to the rather small (1~500) number of grains. In this simple implementation, the detection of the possible contact is done by going through the list of the grains, and for each one, checking the intersection with all the next ones (that is, the grains that have not been tested yet). This way,

$$\sum_{i=1}^{N-1} i = \frac{N(N-1)}{2}$$

operations are made, and the time complexity for the contact detection is in $O(n^2)$. The management of the possible contacts is made without taking into account the probabilities of the contacts to become active at the next iteration of the algorithm, and the computation of each correction is made again at each iteration, without taking the correction from the last iteration into account.

For applications with a high number of grains, however, this kind of code is too slow. It is necessary to find tricks so that the time-cost is reduced. In the complete model developed by Constant et al. (2017), several of these tricks are used. The optimisation concerns the detection of the contacts, their management, and their resolution.

4.1 Contacts detection

The detection of the contacts is a crucial problem. Compared to the naive method, several improvements can be found in the literature. Generally, efficient contact detection algorithms consist of two phases : the broad-phase, where the objects are distributed in broad groups which are tested for intersections and a list of possible contacts is made for the next phase, and the narrow-phase, where the possible contacts of the list made in the broad-phase are tested more precisely, (Kochara et al., 2007).

The optimisation is based on a tree data structure called a quadtree (or octree in 3D). This tree subdivides space into different regions. Each element of the tree has exactly 4 children, or none, in which case the element is called a leaf(Wikipedia contributors, 2018). Each region

represented by a leaf contains N_l particles, which cannot be more than a maximal number, N_m . If this number of particles is too high, the leaf becomes a branch and is split into four other elements, each one containing the particles located in the associated space. This quadtree is built incrementally with the detection of the contacts, as will be explained. The optimisation also rests on the concepts of bounding boxes. Those bounding boxes are squares, rectangles or disks, within which the particle is bound in the next time-step. They are calculated with the maximal velocity of the grains, $\max(\dot{q})$.

Now that the tools have been presented, the method can be described. The particles are placed one after another in the tree. Each time a particle is placed, its bounding box is calculated. The elements of the tree that intersect this bounding box are further traversed, and so on from parent to children until a leaf is reached. This is the broad-phase. Then, for each reached leaf, the contacts are checked with all the particles contained in the space associated with the leaf, which corresponds to the narrow-phase. As the particles are placed into the tree, new leaves are created, because the number of particles increases and locally surpasses the maximal number allowed for leaves, which thus split into four new ones. A graphical explanation can be found in Fig. 4.1 and Fig. 4.2.

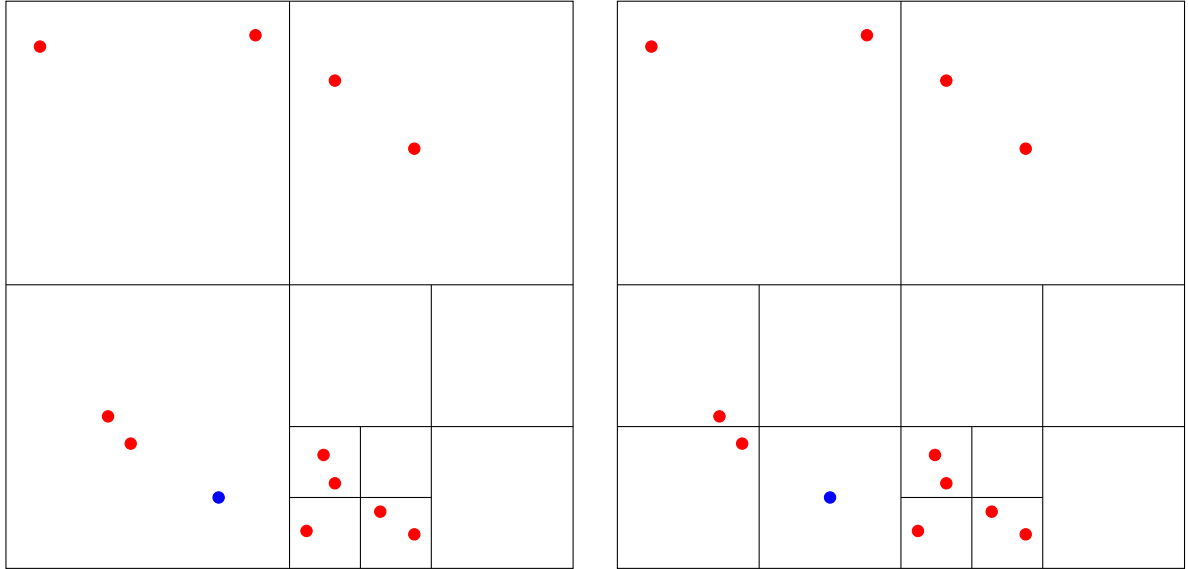


Figure 4.1: Consider a square spatial domain, which is already subdivided by a tree, that has been built incrementally with the placing of the particles. The maximal number of particles allowed per leaf is $N_m = 2$. The blue particle is added to the tree according to its position, as can be seen in the left figure. Since the number of particles contained in the corresponding leaf becomes equal to 3, the leaf is split in four children, as can be seen in the right figure.

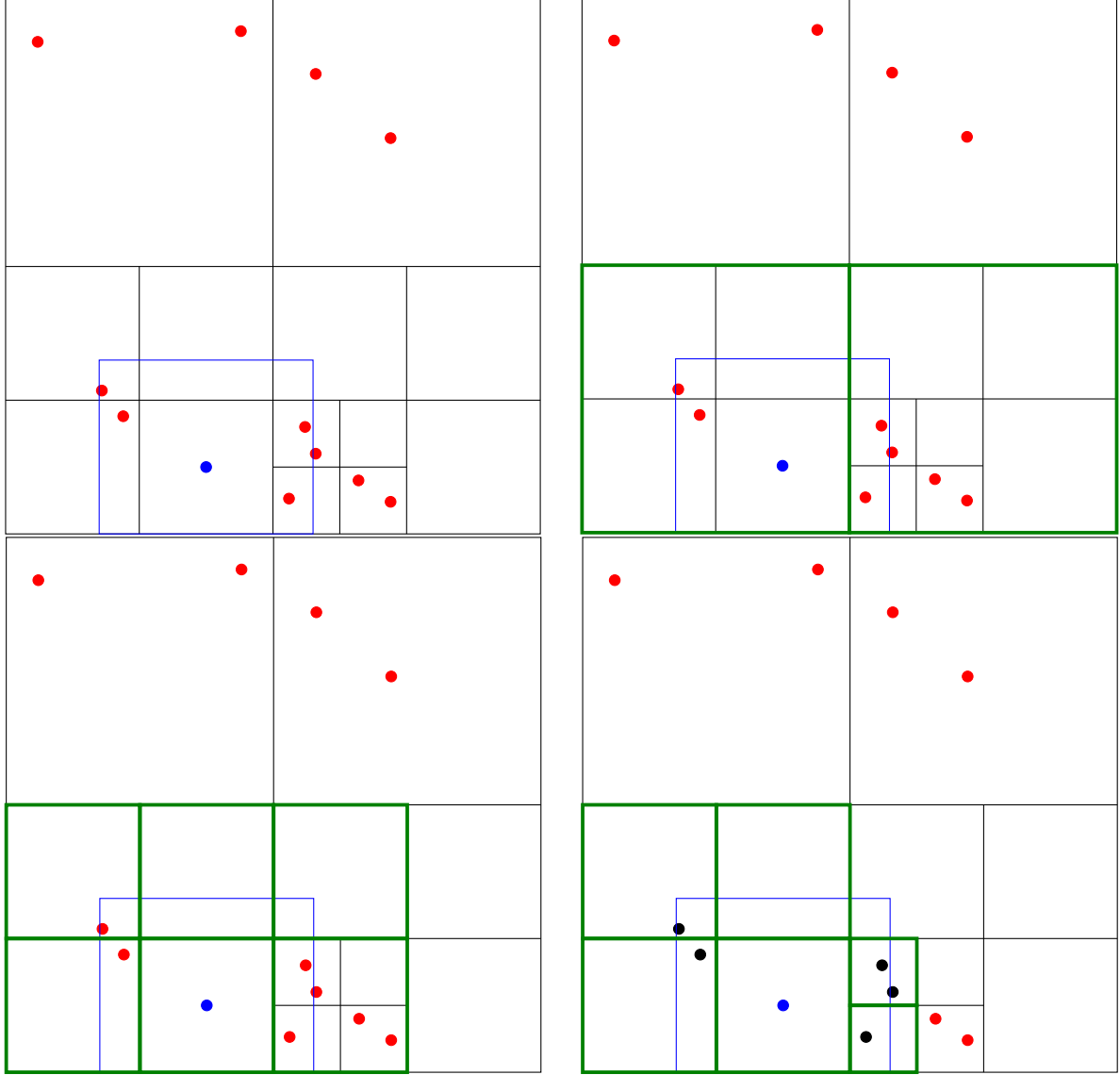


Figure 4.2: Once the leaf has been split and the tree expanded, the bounding box is calculated around the blue particle, which is represented by a blue rectangle, as is pictured in the top left figure. This rectangle is in fact a square, whose side length is equal to the maximum overall velocity, which was truncated because of the domain boundaries. Then, the elements of the tree that intersect this box are selected for further investigation. First, the two children represented in green are selected (top right figure). Then, since they are no leaf, their children which intersect the box are selected (bottom left figure). The same operation is done once again, until the remaining selected elements are all leaves. All the particles belonging to these leaves, represented in black, are then directly checked for an intersection with the blue particle (bottom right figure).

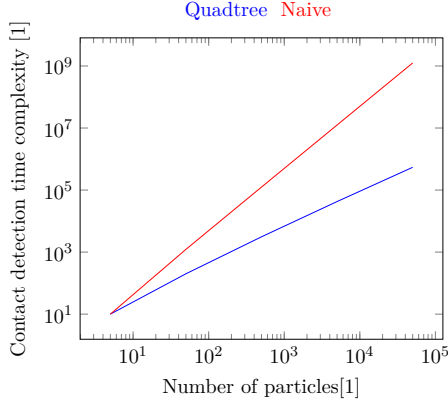


Figure 4.3

By placing the particles one after another, the computation of the contact detection between grain i and grain j is avoided, because the same calculus will be carried out between the grain j and the grain i , which allows another gain in time-cost. Each tree traversal, searching for the leaves that intersect the bounding box of a particle, has a time cost in $O(\log(N))$. Since this operation is repeated for each grain, the total time cost of the contact detection method is in $O(N \log(N))$, which represents a large gain, as can be seen in Fig. 4.3

4.2 Contacts management

Once those contacts are detected, it is still necessary to manage them efficiently. Instead of just going through a vector containing the possible contacts over and over again, a queue is used. This queue works with the First In First Out (FIFO) principle. It is initialised as a vector containing all the possible contacts. One after another, the contacts are popped out of the queue and solved. If its resolution necessitated a correction that is larger than the accepted tolerance for convergence, all the previously solved contacts in which the two grains of the present contact were involved are put back in the queue, on condition that they are not already in the queue. This operation is repeated until the queue is empty, which means convergence has been reached. An example can be found in Fig. 4.4

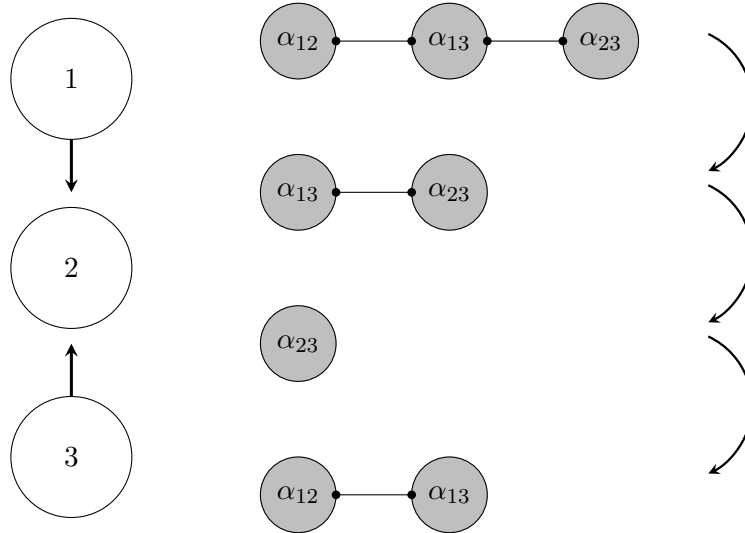


Figure 4.4: Consider that 3 possible contacts α_{ij} have been detected, between grains 1, 2 and 3. First, the contact between grain 1 and 2 is popped and solved. Since the contacts involving 1 and 2 are already in the queue, there is no insertion. Then the contact between 1 and 3 is popped and solved. Since the required correction is equal to $0 < tol$, there is again no insertion. When contact 23 is popped and solved, the contacts 12 and 13 are requeued. The process is repeated until the queue is empty and convergence is reached.

4.3 Contacts resolution

Additionally, the computation of the normal corrections is optimised. The value of the correction is stored in memory, and used as a first guess for the next iteration. In a dynamic situation, this is not very helpful, since the contacts are changing at a high rate. However, in a static situation, the value of the correction is the same for most grains, and it is so for each time-step as long as the situation does not change. The computation of the correction is thus instantaneous, and the time cost is improved.

Finally, a method to efficiently treat the contacts can be laid down : Now that the improve-

Algorithm 3 Efficient contact treatment

At each time-step :

Detect the contacts :

for Each grain i **do**

Place the grain into the leaves of the tree, according to its position

if $N_{li} > N_m$ **then**

Split $Leaf_i$ and reassign the grains accordingly.

end if

Build the bounding box with the overall maximum velocity.

Traverse down the elements of the tree that intersect the box, recursively.

Check the contacts with the grains of the leaves intersecting the box.

Add the contacts to the queue.

end for

Solve the contacts :

for Each contact α in the queue **do**

if First iteration **then**

Solve the contact with algorithm 2.

else

Solve the contact with 2, using the precedent correction as a first guess.

end if

if Correction > tolerance **then**

Insert the contacts involving the two grains in the queue if they are not already in

end if

end for

ments required for large-scale simulations have been presented, the method can be tested against experimental and numerical results found in the literature.

Chapter 5

Angle of repose

One of the characteristic variables describing a granular material is its angle of repose. Two aspects exist : the static angle of repose, when the material is at rest, and the dynamic one, when the material undergoes constant avalanche, for example in a rotating mill. In this chapter, both are investigated with the model, and results are checked with the ones from literature, numerical as well as experimental.

5.1 Static angle of repose

The static angle of repose is defined as the maximal angle of a stable slope formed by the material after being poured, or having undergone an avalanche. It is not to be confused with the angle of maximal stability of the material, which is the angle, between the slope of its free surface upon tilting and the horizontal, above which it begins to flow, (Albert et al., 1997). Sometimes, they are denoted as the lower angle of repose, and the upper angle of repose, (Liu et al., 2005)

In order to challenge the numerical model against theory and experiment, a numerical experiment was performed, according to the method presented by Li *et al.*, (Li et al., 2005). They use a 3D code to simulate a quasi-2D experiment, in which glass beads are put in a narrow box (hence the quasi-2D qualification), which presents an aperture at the bottom, and is slowly raised so that the beads flow down and accumulate to form a heap, whose static angle of repose is measured.

5.1.1 Experimental set-up

The experiment concerns the flow of glass beads with mean radius $rad_m = 6mm$ through an aperture of $5 \cdot rad_m = 3cm$. In the original experiment from Li *et al.*, the grains are placed in a first box, with an aperture and the centre of the bottom so that the grains can flow through, itself placed in a second box in order to collect the grains. In this experiment, the boxes are $49cm$ wide, see Fig. 5.1.

The important parameters of the simulations are given in Table 5.1.

Parameter	Value
Particle density	2456 [kg/m^3]
Particle-particle coefficient of static friction, μ_{spp}	0.3090 [1]
Particle-particle coefficient of sliding friction, μ_{kpp}	0.1545 [1]
Particle-wall coefficient of static friction, μ_{spw}	0.2666 [1]
Particle-wall coefficient of sliding friction, μ_{kpw}	0.1333 [1]
Time-step	0.005[s]

Table 5.1: Parameters used for the numerical experiment.



Figure 5.1: Dimensions of the boxes used for the numerical experiment

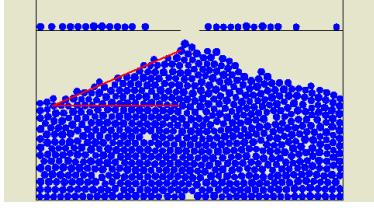


Figure 5.2: Measurement of the angle of repose.

Li *et al.* use a contact model based on Hertz theory of friction, which only implies the sliding coefficient of friction μ_k , (Li et al., 2005). It was then necessary to determine a value for μ_s . Due to the fact that the goal was to obtain similar results with a limited precision, the simple choice was made to use $\mu_s = 2\mu_k$, which is approximately often the case. In other applications, either more precise relationships can be found, either the two can be experimentally measured or found in the literature. The experiment was led with 750 beads, which are slightly poly-dispersed, in order to avoid crystal-like ordering which can have a significant effect in 2D, (Staron and Hinch, 2018) : approximately

one fourth have a radius of $5.5mm$, another fourth have a radius of $6.5mm$ and the other half have a radius of $6mm$. The balls are initially placed in a regular lattice at the top of the box with a random angular velocity, and then rain down towards the bottom of the box due to gravity, so that a well-mixed system is obtained. After 6s, the experiment starts : the inner box is raised at a rate of $0.005m/s$, and the grains start to flow through the aperture. In order to have statistically significant results, several initial and boundary conditions were tested. The angle of repose was measured as the angle between the horizontal and the steepest stable slope found in the results, with the help of the *ImageJ* image analysis software.

5.1.2 Results

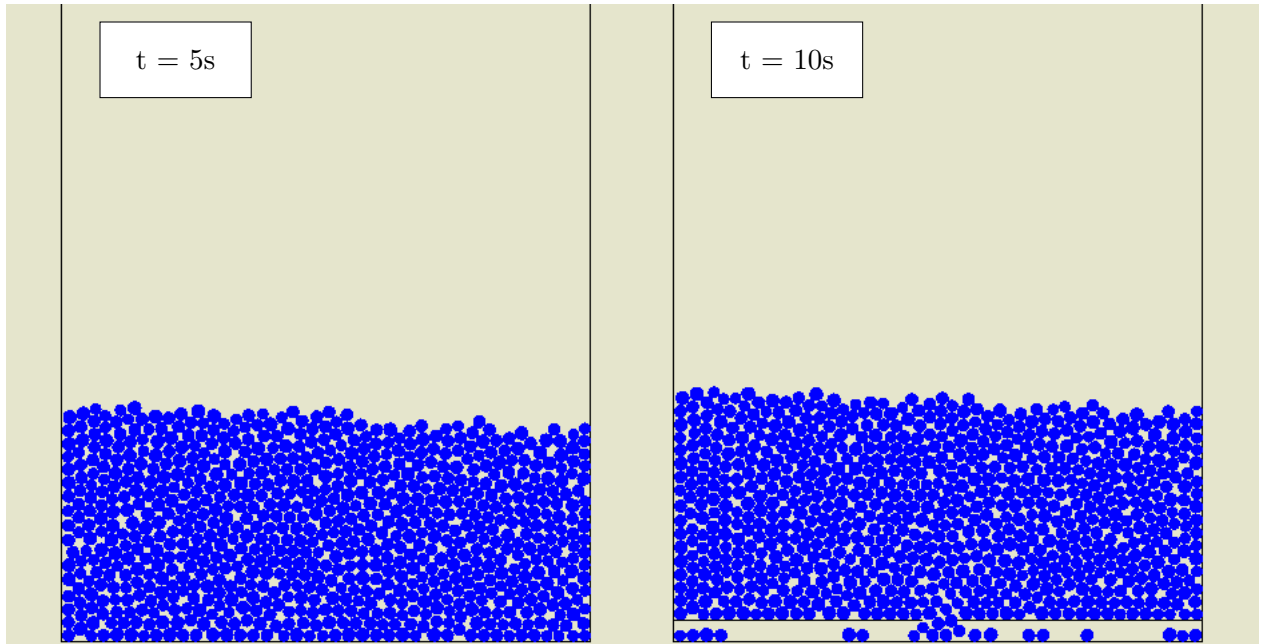


Figure 5.3: Snapshots of the simulation for times of 5s and 10s.

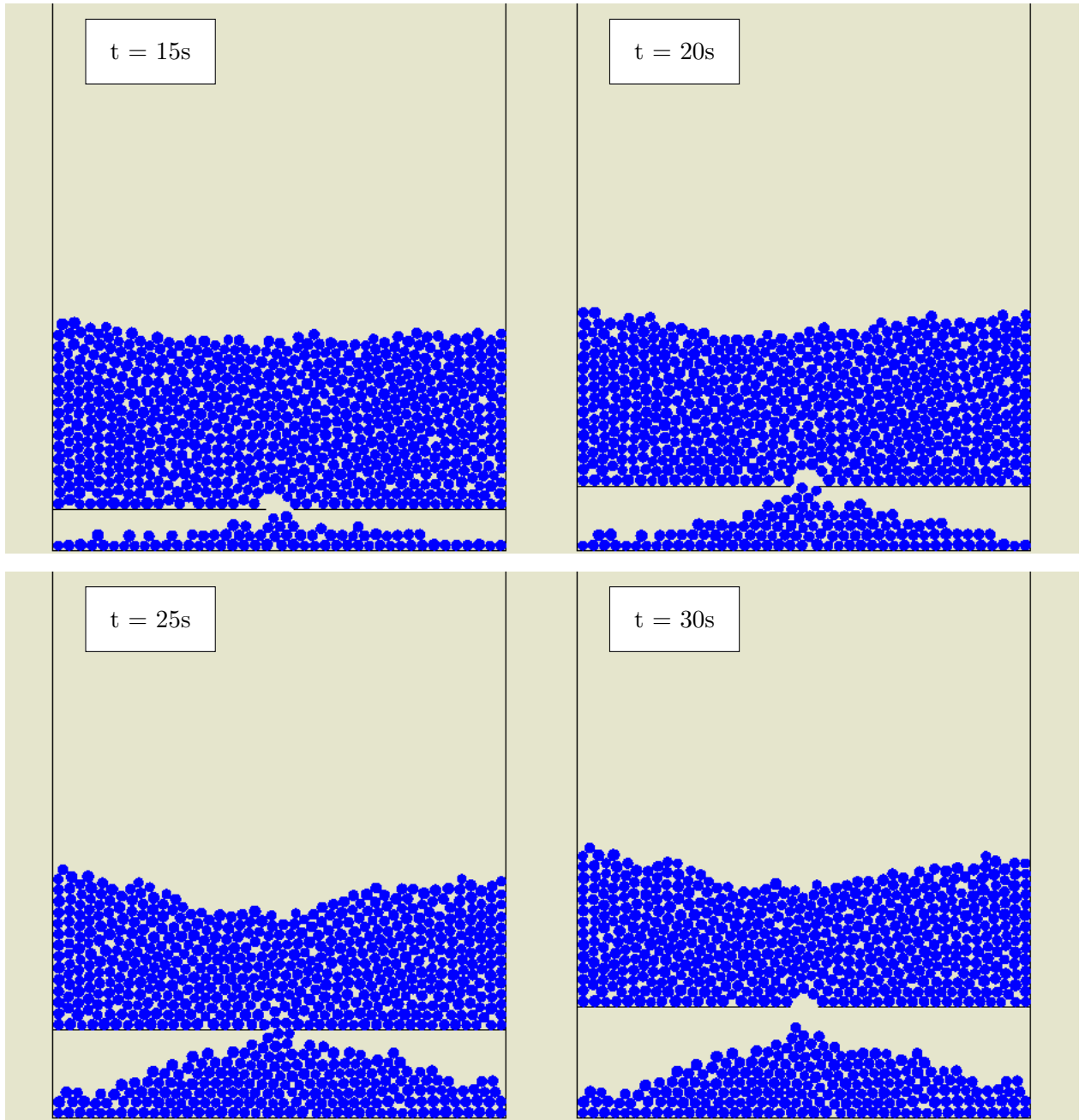


Figure 5.4: Snapshots of the simulation for times from 15s to 30s.

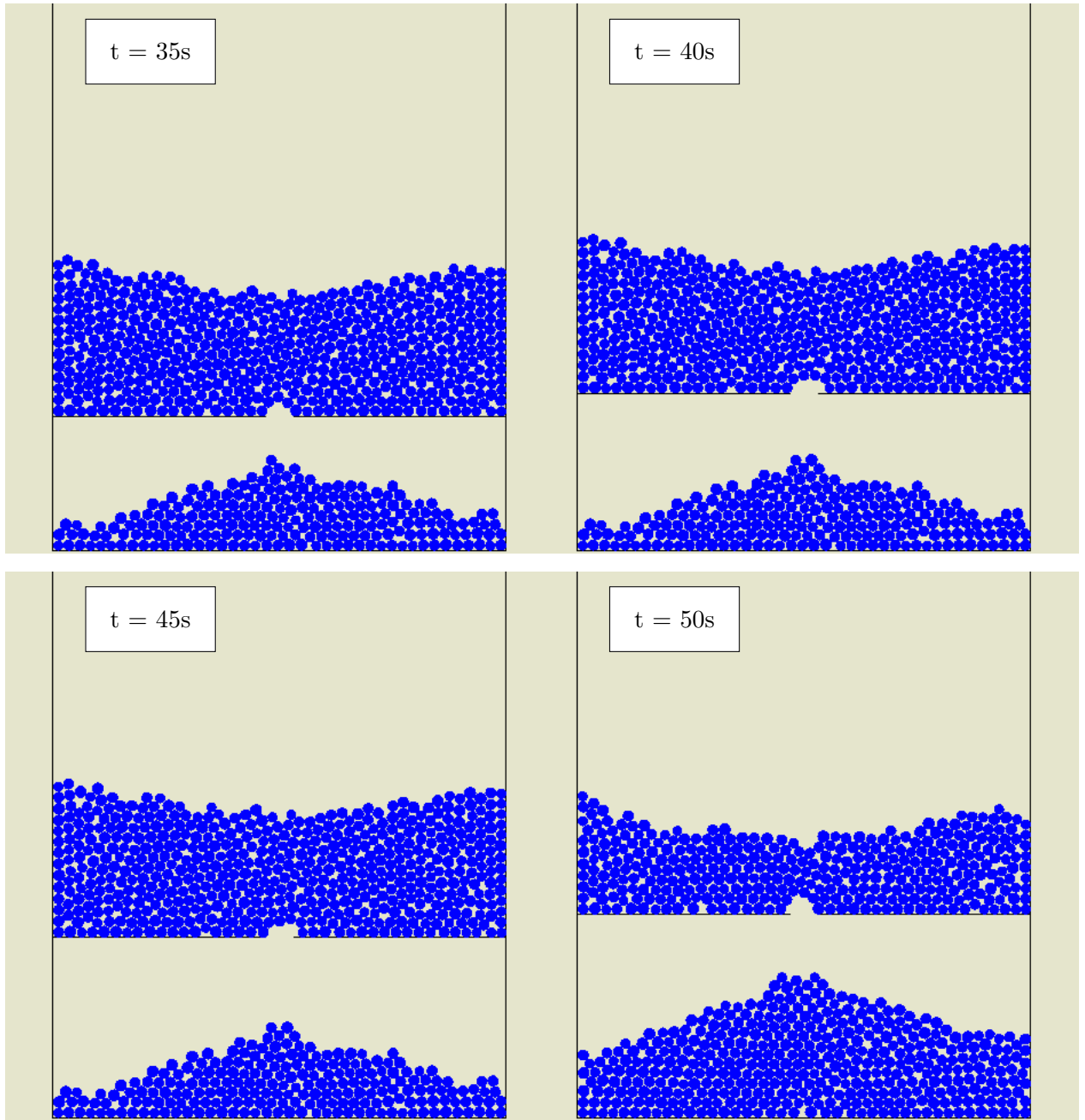


Figure 5.5: Snapshots of the simulation for times from 35 to 50s. It can be seen that an arching phenomenon is frequent, preventing the grains from flowing through.

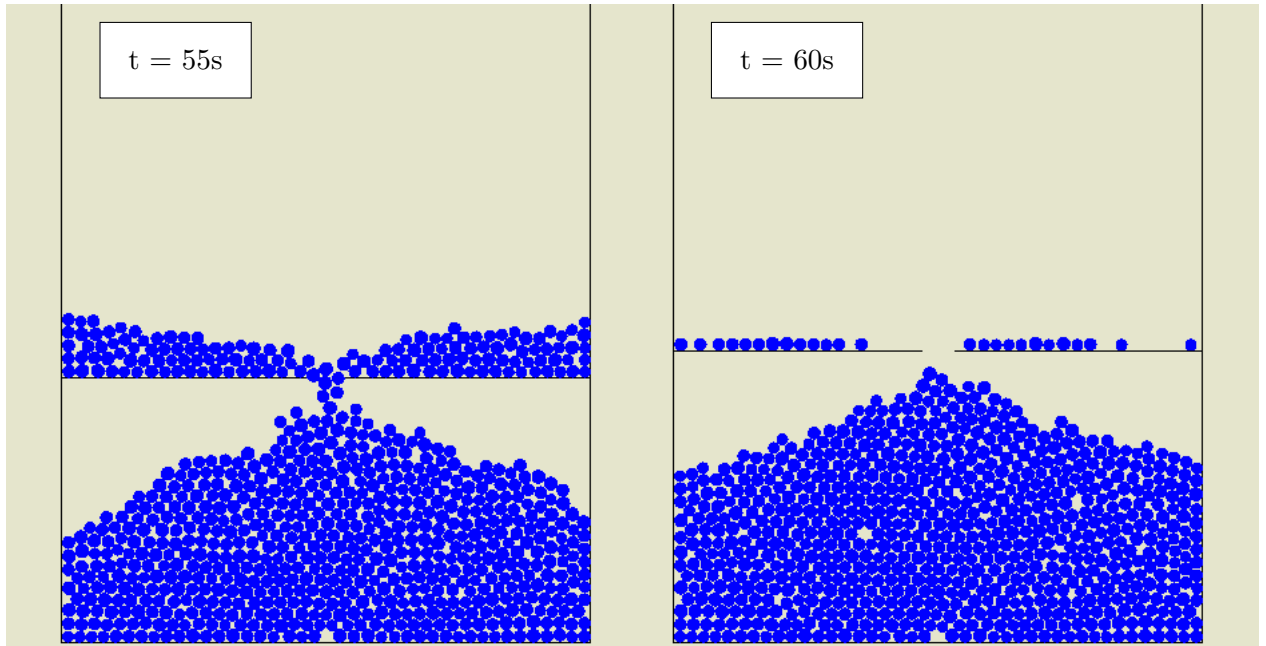


Figure 5.6: Snapshots of the simulation for times of 55s and 60s.

Experimental	Li <i>et al.</i>	Simulation
26.3°	26.9°	23.2°

Table 5.2: Comparison of the results for the angle of repose.

As can be seen in Table 5.2, the angle of repose resulting from the simulation, measured as indicated in Fig. 5.2, is quite lower from the ones found in the work of Li *et al.*, (Li et al., 2005). However, even if the configuration was quasi-2D, their simulation was 3D, implying some wall effects, which Zhou *et al.* have shown to be quite important, (Zhou et al., 2002). What is more, the angle of repose of smooth disks is found to be in the range of 23-25°, (Albert et al., 1997).

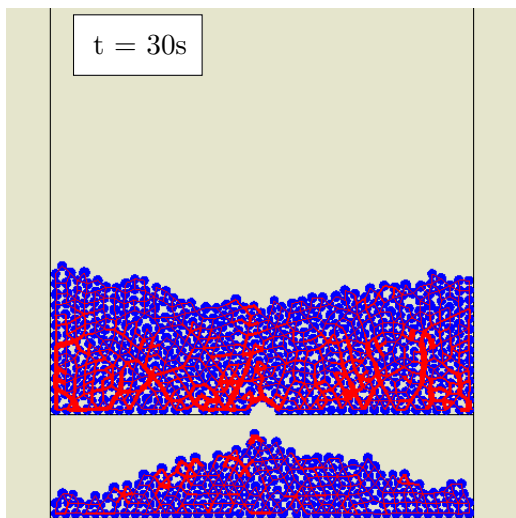


Figure 5.7: Network of the forces in the assembly of beads.

Arching

Throughout the simulation, the flow of the beads across the aperture was not constant. Indeed, *arching* occurred several times, completely blocking the flow. This can happen when the size of the aperture is smaller than the *critical outlet width*, which is the minimal length of the aperture so that the granular material can flow without obstruction. This phenomenon results from an equilibrium situation, and is due to friction, which is proportional to the normal force in the static case, which raises the interest for the forces network. Since the algorithm computes the normal impulse corrections, it is possible to store them and obtain a network of these corrections, as in Fig. 5.7, which is equivalent to the one of the forces scaled by a constant.

This force network can be put in contrast with the velocity field of the grains, as in Fig. 5.8.

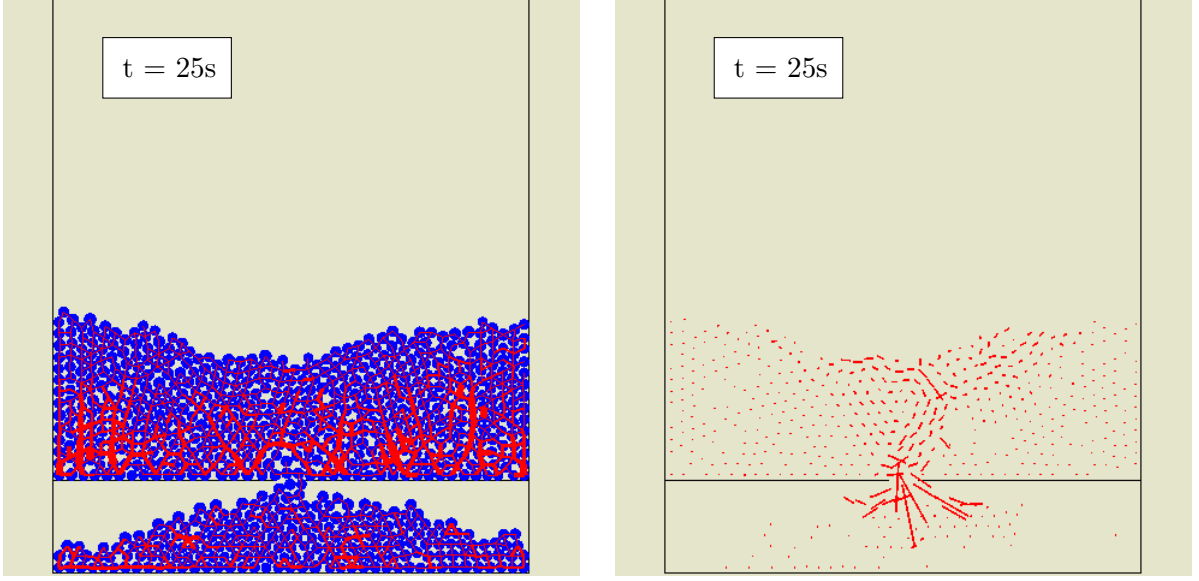


Figure 5.8: Comparison of the force network, where the thickness of the line is proportional to the magnitude of the force (left), with the velocity field of the grains, scaled by the ratio between the mean radius of the grains and the aperture's width (right). For convenience, the beads were not represented in the left figure.

As can be seen in Fig. 5.8 right, the intensity of the normal forces between the grains increases with the depth of the deposit, because of the accumulated weight of the above grains. However, close to the aperture, the forces are weak, which corresponds to high downward velocity, as seen in Fig. 5.8 right. Just above the aperture, the forces network indicates that a new arch formed, which correlates with the sudden decrease in the magnitude of the downward velocities. Finally, it is to note that the grains located near the walls are almost still, although more mobile than the ones that have already flown down and are piled up in a heap, whereas the ones at the centre have a higher velocity and participate more directly to the flow.

Parametric study

Reportedly, θ_r increases with increasing μ_s (thus also for increasing μ_k since we took μ_k as twice μ_s). Therefore, the experiment was repeated for increasing values of μ_k in order to check if this behaviour is reproduced by the algorithm. However, the initial and boundary conditions, as well as the number of grains, have been changed so that it was possible to see if the results were statistically significant. Regarding the boundary conditions and the number of beads, the size of one experiment was led with 500 beads and a 40cm wide box (set 1), three with 750 beads and a 49cm wide box (set 2 to 4), and one with 1000 beads and a 56.5cm wide box (set 5). In other words, the number of beads was multiplied by a constant, $\frac{2}{3}$ for the first one and $\frac{4}{3}$ for the last one, and the edges of the box were multiplied by the square root of this constant so that the area is multiplied by the same constant as the number of beads. As for the initial conditions, they were varied for the three experiments with the base-sized boxes. In the first case, the balls just rained down as in the experiment shown above (set 2). In the second one, the box was shaken after 4s so that the beads have a positive velocity in the y direction of 2, and then came back down due to gravity (set 3). Finally, the beads were given an initial velocity towards the bottom-right corner before they rain down (set 4). The results are presented in Fig. 5.9.

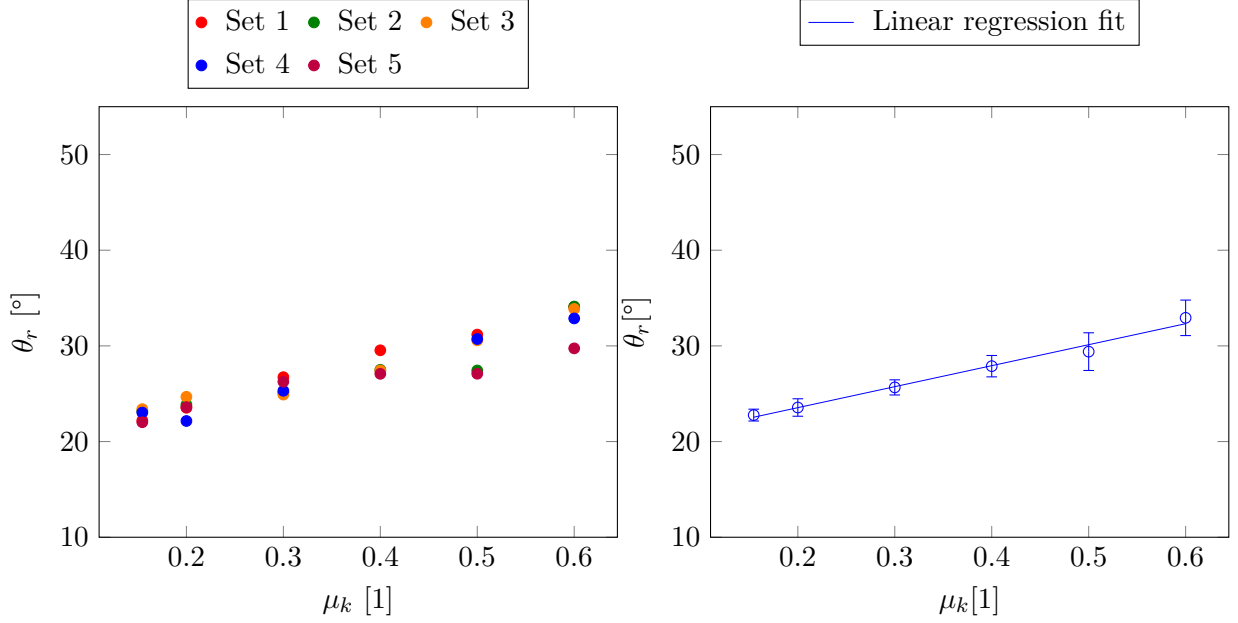


Figure 5.9: Left : results for the angle of repose versus the kinetic coefficient of friction for the different simulation sets. Right : corresponding error bars, fitted by linear regression.

One can see on Fig. 5.9 left that the initial and boundary conditions do not imply drastic differences in the results, although the difference between the sets seems to be increasing with increasing μ_k . This could be explained by the fact that increasing friction means an increase in the probability of arching. These arching phenomena cause the flow to be discontinuous, and are a source of irregularity in the measures, because when the grains are suddenly released from an arch, they go down and crash onto the heap with a higher velocity than they would have if they had flown continuously through the aperture. As expected, θ_r increases with increasing friction.

Generally reported parameters influencing the angle of repose, apart from friction, are the size of the particles, and their shape. Notably, the roundness¹ of the grains has been shown to influence θ_r : the more round the grains are, the lower θ_r is (Riley et al., 1978). Additionally, it might be expected that heterogeneous particles have a higher angle of repose, because the number of configurations is higher. The consideration of various shapes would imply serious modifications of the contact algorithm. Indeed, when the particles are polyhedral, the contact point is not unique anymore, and the definition of the normal is ambiguous, (Dubois and Renouf, 2015). Therefore, the investigation on the heterogeneity will be focused on the relative sizes of the particles, which corresponds to the polydispersity, i.e. the statistical distribution of the radii of the particles.

Particle size Let $\rho = \frac{rad_i}{rad_1}$ with $rad_1 = 0.006mm$ the mean radius of the beads in the first series of experiments. New ones were conducted with $\rho = 0.2$ and $\rho = 2.0$ in order to compare the results and determine the significance of a size effect. For each of those two new values of ρ , five simulation sets were used, with different initial conditions. In set 1, the beads were placed on a regular lattice before raining down as usual. In set 2 and 3, the beads were given an additional initial velocity towards the left and the right corner of the bow, respectively. In set 4 and 5, the bow was shaken after respectively 1 and 2 seconds, so that the grains have an upward velocity. The size of the box and of the aperture were rescaled to better match the one of the beads. The results are presented in Fig.5.10.

¹The roundness of a particle describes its resemblance to a circular shape. It is defined as the ratio between the radius of the maximum inscribed circle and the radius of the minimum circumscribed circle in the 1101 ISO norm.

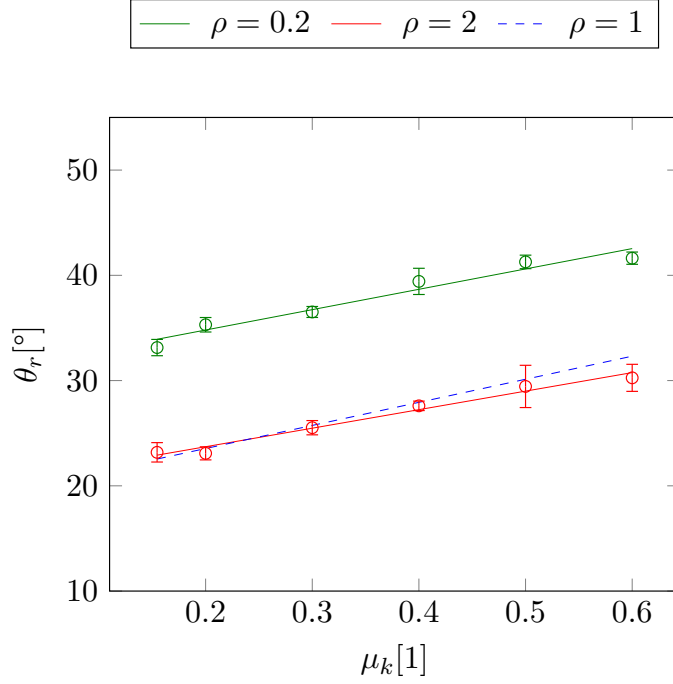


Figure 5.10: Angle of repose in function of the sliding coefficient for different particle sizes.

It can be seen that θ_r has strongly increased when the size of the particles was reduced, while the slope of the linear fit stays approximately the same. On the other hand, the decrease of θ_r with the increase of the size was very small, and the slope of the fit stayed again approximately equal. This feature has already been observed (Burkalow, 1945), (Carrigy, 1970), and empirically described (Carstensen and Chan, 1976). The results are in agreement with the results of Zhou *et al.* who studied the angle of repose of mono-sized coarse glass spheres with a similar experimental set-up. They also observed that the angle of repose decreased with increasing particle size, and that this decrease was bounded, θ_r tending towards a stationary value, (Zhou et al., 2002). Finally, it can be noticed that, although θ_r increased with μ_k , the slope of the fit was more or less unchanged, indicating that there is little to no interaction effect between friction and size.

Polydispersity In order to investigate the effect of polydispersity on the angle of repose, 3 series of experiments were led, with samples of different radius distribution, with different standard deviations, $\sigma_1 = 0.1mm$, $\sigma_2 = 0.5mm$ and $\sigma_3 = 1mm$. Since the mass scales with the radius to the third power, the common mean for the samples was chosen to be $\mu = 4mm$, so that for the samples with $\sigma = 0.001$ 97.5% of the grains have a radius equal or inferior to 0.007, which is equivalent to $\rho \sim 1.16$. This way, the presence of too large grains that could significantly influence the results is avoided. Each of these distributions were simulated with 5 different sets of initial conditions, identical to the ones used for the experiments on the particle size. The results are presented in Fig. 5.11.

First, it can be noticed that the samples with $\sigma = 0.0001$ yield strongly varying values ; in this case the angle of repose does not seem to significantly depend on friction. This is because of the quasi-monodispersity of the grains. In 2D, such a radius distribution can lead to crystal-like ordering, as explained by Staron and Hinch, (Staron and Hinch, 2018). The grains just pile up according to a regular pattern, which is more or less respected due to the initial velocity of the grains when they come into contact with the heap. It can also be seen that the samples with $\sigma = 0.0005$ are rather well fitted by a linear regression, just as in the cases studied above. However, increasing the polydispersity, i.e. increasing σ , to an even higher value does not yield

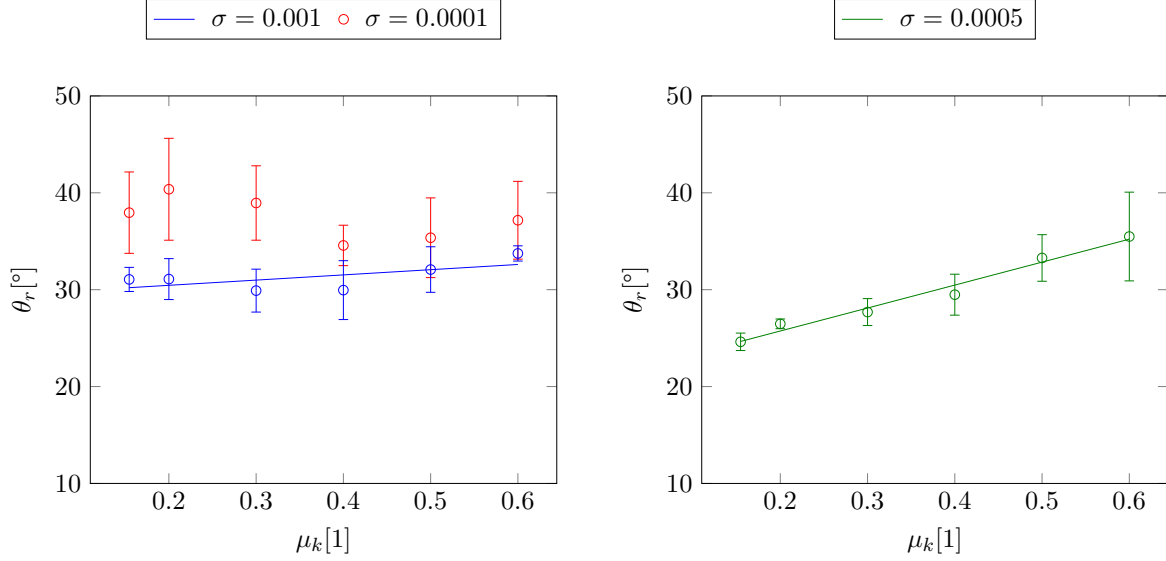


Figure 5.11: Angle of repose in function of the sliding coefficient for different radius distributions.

the expected increase in θ_r . Instead, θ_r seems to tend to a constant behaviour. Therefore, it appears that the principal feature of the heterogeneity hypothesis is the heterogeneity of shapes, not sizes.

5.2 Dynamic angle of repose

The dynamic angle of repose is the angle of the slope that is formed when the granular material is continuously avalanching, be it along an inclined plane or inside a rotating mill. It can also be defined as the minimum slope for a particle to slide down the heap. A simple experimental method to measure consists in placing particles inside a rotating mill, and rotate it so that the grains undergo a flow. The grains can undergo several flowing regimes, divided into three categories for increasing rotation speed : sliding, when the grains only slide on the circular wall, cascading, when avalanches occur, and cataracting, when the grains are projected from the bed in the free space of the cylinder, (Henein et al., 1983). From the definition of the dynamic angle of repose, the regime of interest is the cascading one, which can itself be divided into three categories :

- **Slumping** : occurring at relatively low rotation speeds that are still sufficient to avoid a sliding regime, the slumping regime is characterised by a discrete succession of avalanches. Due to static friction, the grains follow the rotation of the cylinder, until the maximal angle of stability is reached, and an avalanche occurs, sending the grains back to the bottom of the cylinder so that equilibrium is restored, and the same process is repeated.
- **Rolling** : at slightly higher speeds, the grains first start to follow the rotation of the drum, and then undergo a continuous avalanching regime, with a well-defined free flowing surface that follows a straight line.
- **Cascading** : at even higher speeds, but not sufficient to observe a cataracting motion, the continuous avalanche regime is maintained, but the free surface becomes S shaped.

From the definitions above, the best regime to measure the dynamic angle of repose is the rolling regime. The distinction between those regimes has been shown to depend on the adimensional Froude number (Mellmann, 2001), which is defined as :

$$Fr = \frac{\omega^2 R}{g},$$

where ω is the angular velocity of the mill, R its radius, and g the acceleration due to gravity. This Froude number characterises the importance of the kinetic energy with respect to the potential energy ; in our case, it represents the ratio between the centripetal force and the gravitational force. In order to observe a rolling regime, it is generally necessary that $10^{-4} < Fr < 10^{-2}$. Mellmann also noted that the flowing regime depends on the sliding friction coefficient between the wall and the particles, (Mellmann, 2001). Precisely, the existence of a critical particle-wall sliding friction coefficient so that the flowing regime is in the cascading family was reported. This critical coefficient of friction depends mainly on the degree of filling ϕ , but also on the Froude number and the dynamic angle of repose :

$$\mu_{kpw}^c = f(\phi, Fr, \theta_d)$$

The dynamical angle of repose θ_d is not known a priori, but can be coarsely estimated with θ_r to $\sim 23^\circ$ when $\mu_k = 0.1545$. Fixing the filling degree to 0.5, the results of Mellmann show that a safe choice is $\mu_{kpw} = 0.5$. After some calibration, it was observed that a Froude number of $Fr = 0.002$ yielded a stable rolling regime. The parameters of the simulation are given in table 5.3.

Parameter	Value
Particle density	2456 [kg/m ³]
Particle-particle coefficient of static friction, μ_{spp}	0.3090 [1]
Particle-particle coefficient of sliding friction, μ_{kpp}	0.1545 [1]
Particle-wall coefficient of static friction, μ_{spw}	1.0 [1]
Particle-wall coefficient of sliding friction, μ_{kpw}	0.5 [1]
Time-step	0.005[s]
Cylinder diameter	0.5 [m]
Fr	0.002 [1]

Table 5.3: Parameters used for the numerical experiment on the dynamic angle of repose.

Again, a slightly poly-dispersed sample was used, as described in section 5.1.1. As for the initial conditions, the grains were again placed in a regular lattice with a random initial angular velocity, and rained down. After 1s, the cylinder started to rotate. θ_d was taken as the average of measures at different times in the rolling regime. The results are presented in Fig. 5.12.

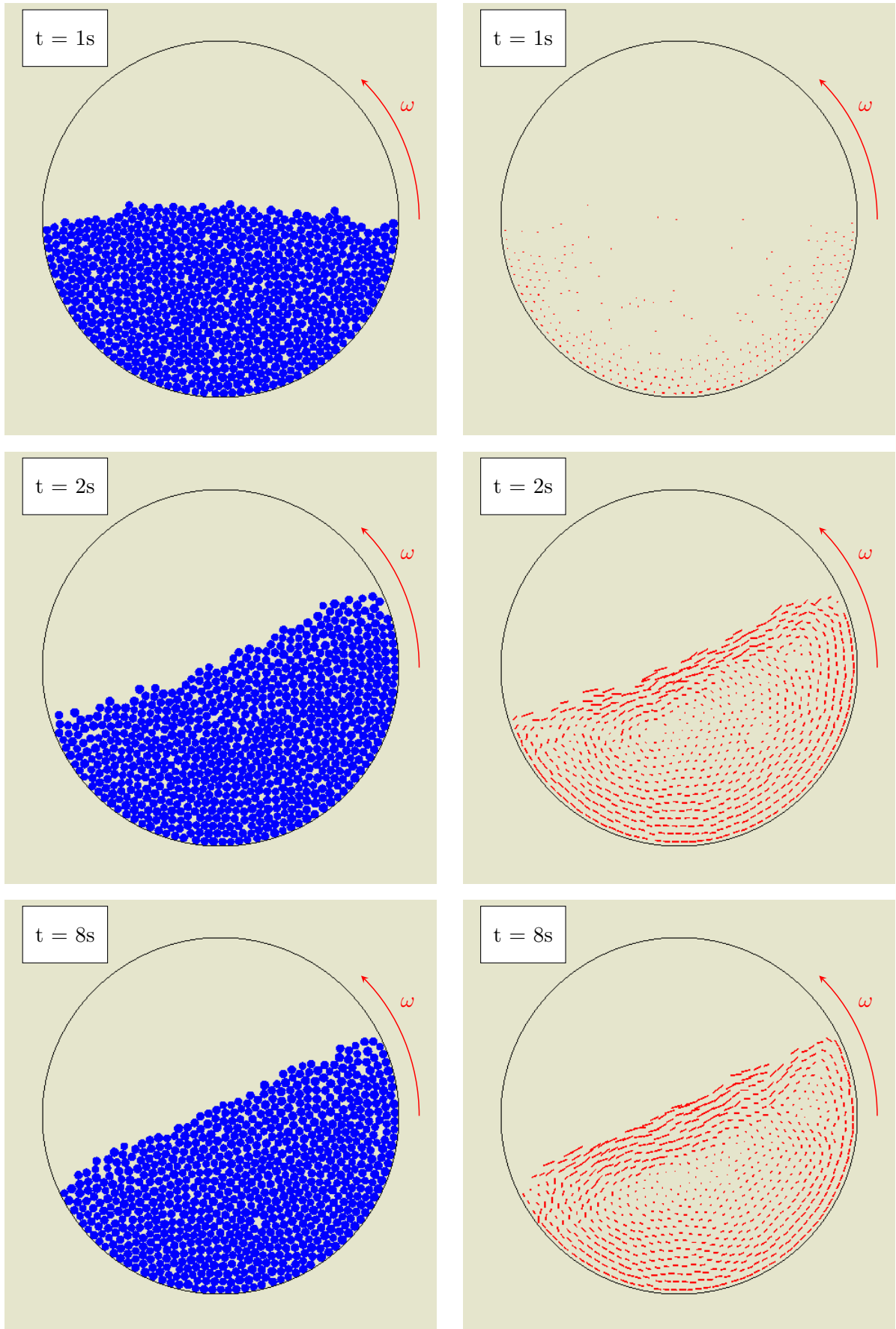


Figure 5.12: Snapshots of the simulation for different times. Left : grains. Right : linear velocity field, scaled by the ratio between the mean radius of the grains and the radius of the cylinder.

The grains reach a stable rolling regime short after $t = 2s$. The velocity fields for $t = 2s$ and $t = 8s$ are qualitatively in good agreement with the results of Yamane et. al for spherical particles, (Yamane et al., 1998). The grains are coarsely separated in three layers : a free-flowing layer at the top, a quasi-static layer at the centre, and a steady flow layer at the bottom. Those grains at the bottom, in contact with the wall, follow its circular motion and have a corresponding velocity. The grains at the top are avalanching towards the left side of the drum, and have a slightly larger velocity than the bottom ones. Since their motion is not dictated by the wall, their velocities are not regularly aligned. As for the grains in the centre, their velocity is small, so that they do not participate much to the flow. Measurements were performed with *ImageJ* every second from $t = 3s$ to $t = 8s$, and averaged, yielding $\theta_d = 24.7233 \pm 0.4531^\circ$, which is significantly higher than the value of θ_r . This increase has already been observed, and a simple empirical relationship has been established between the static angle of repose, the angle of maximum stability θ_m , and the dynamic angle of repose : $\theta_d = (\theta_r + \theta_m)/2$ (Liu et al., 2005).

Again, the experiment was repeated for different coefficients of friction. The results are presented in Fig. 5.13.

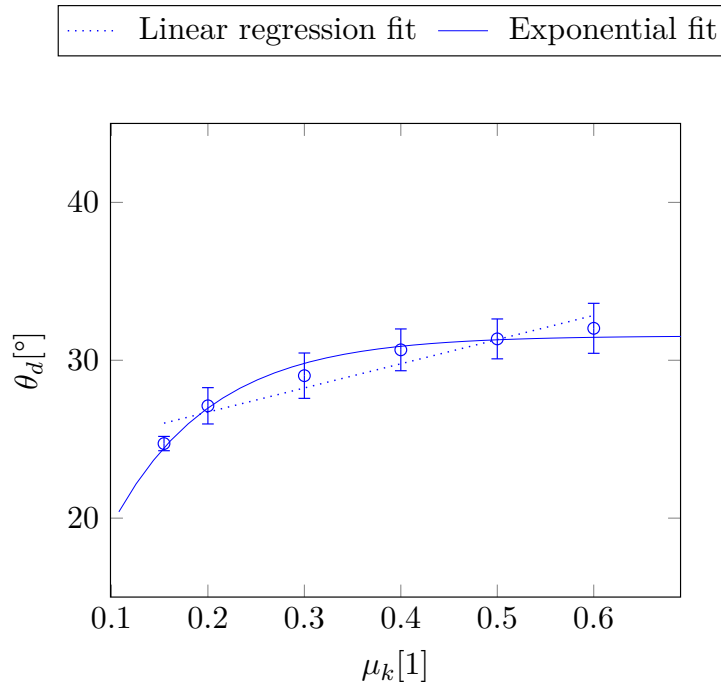


Figure 5.13: Dynamic angle of repose in function of the sliding coefficient.

As θ_r , θ_d increases with increasing friction. However, this increase seems to be less important than for the static case. In fact, Yamane *et al.* reported that the dynamic angle of repose first increased very fast from zero with friction, but that is saturated to a certain value for values of μ_k higher than 0.5, (Yamane et al., 1998). Therefore, the following exponential model was used to fit the data :

$$\theta_d = A - B \cdot \exp(-C \cdot \mu_k)$$

As can be seen in Fig. 5.13, the data follows this model better. This saturation behaviour is in contrast with the one of θ_r . This could be due to the fact that even if the grains undergo high frictional forces due to their mutual interactions, the momentum that allows them to form a flowing slope is bounded first by the particle-wall coefficient of friction and secondly by the rotation speed. Indeed, supposing infinite friction between the grains, i.e. cohesion, the grains would undergo solid rotation with the wall until their weight balances the frictional force from the wall, thus bounding the dynamic angle of repose².

²Although, of course, the dynamic angle of repose would not make any physical sense in that case since the

The reflection above leads to the influence of the rotation speed, which is reported in the literature. Keeping the diameter of the rotating mill constant, the speed is changed via the Froude number with values from $Fr = 0.002$ to $Fr = 0.05$. The sliding friction coefficient was chosen to be 0.1545. The results are shown in Fig. 5.14

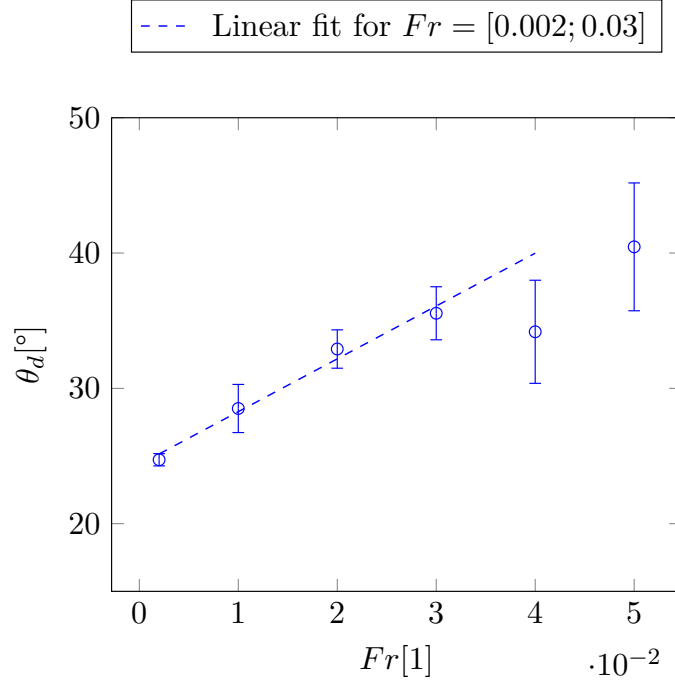


Figure 5.14: dynamic Angle of repose in function of the Froude number for $\mu_k = 0.1545$.

The dynamic angle of repose increases with Fr . This increase is nearly linear for values comprised between $Fr = 0.002$ and $Fr = 0.03$. A similar linear increase was already observed with the rotation speed, for a range of values corresponding to the range of the studied Froude numbers, (Yang et al., 2003), (Yamane et al., 1998). For higher values, the linear prediction falls off. This corresponds to the transition to a cascading regime, as seen in Fig. 5.15.

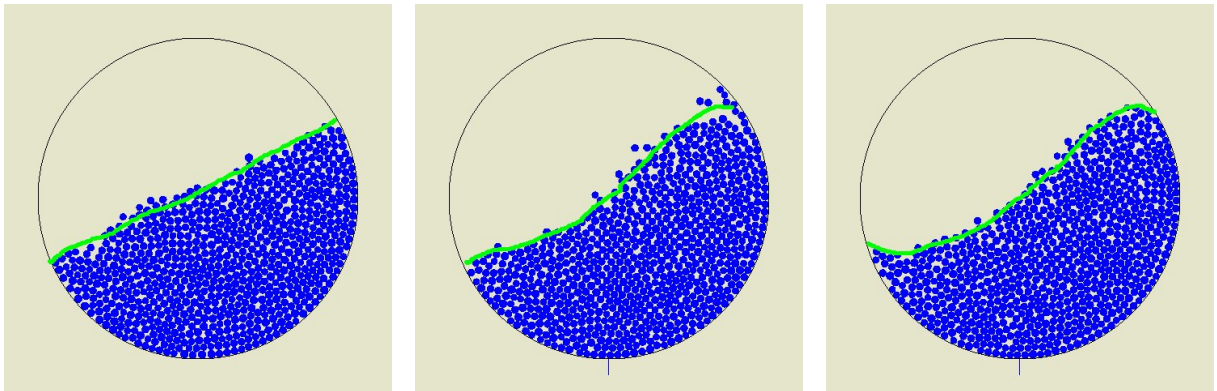


Figure 5.15: Profiles for $Fr = 0.002$, $Fr = 0.03$, and $Fr = 0.05$ (left to right), at $t = 4s$, for $\mu_k = 0.1545$. Notice the characteristic S shaped of the free surface in the cascading regime, in the right figure.

Mellmann determined an empirical relationship for the critical Froude number for the grains could not flow.

transition between rolling and cascading motion, (Mellmann, 2001) :

$$Fr_c \approx 2 \frac{D}{d},$$

with $d = 2rad$ the diameter of the particles. This formula yields $Fr_c = 0.048$, which is in good agreement with the numerical experiment.

The static and dynamic angle of repose for glass beads has been studied with the help of the model. The latter was able to predict a correct static angle of repose for disks in 2D, and reproduced the behaviour of θ_r with increasing friction, as well as the effect of particle size. The effect of polydispersity was investigated, and it was found that highly poly-dispersed systems tend to a constant value of θ_r , while quasi-monodisperse systems, because of the crystal-like ordering, frequent in 2D configurations, show little to no influence of friction on θ_r . The dynamic angle of repose was predicted to be higher than the static one, in agreement with the literature. Its behaviour with increasing friction and rotation speed was also qualitatively reproduced. Since the model seems to be valid for large-scale applications, it is used in the next chapter to study the mixing of particles in a rotating drum.

Chapter 6

An application : mixing of particles

The mixing of granular materials is involved in various industrial fields, such as the agribusiness, the pharmaceutical sector, or the ceramic industry, but also in lotteries, where the balls to be taken need to be homogeneously mixed so that the probabilities are not biased. Several methods can be employed, such as mechanical stirring with blade mixers, static mixers through which the granular media is injected, Turbula-type blenders which use 3D translation and rotation, or even simple rotating mills, as will be studied in this section. In this case, the grains are placed inside a rotating cylinder, just as in section 5.2, and the mixing results of the continuous flow of the grains.

In order to evaluate the homogeneity of the mixture, it is necessary to define a mixing index. This mixing index should be 0 when the particles are perfectly unmixed, and 1 when the mixture is perfectly homogeneous. Several mixing indexes exist in the literature, as described by Godlieb *et al.* The simplest one is the average height method, which initially separates the grains in two groups according to their height, and measures the average height of the upper group. However, this method shows a damped oscillatory behaviour, with values of the mixing index going well above 1. Plus, it can only measure vertical mixing. Another method is the Lacey method, which divides space into a regular grid of cells, and also split the grains in two groups. In each of these cells, the fraction of particles of a chosen group is measured, and the variance of this fraction is compared to the one with perfect mixing and the one with no mixing. Although able to measure mixing in every direction, this method is complex to use, since it requires a grid. A third, simple and suitable method is the neighbour distance method. Before the beginning of the process, each particle's nearest neighbour is determined, the distance between them being of the order of the minimum particle diameter. The principle is to look at the evolution of the sum of the distances between the nearest neighbours through time, which tends to a stationary value dictated by statistics. In order to obtain a mixing index defined over the range $[0;1]$, this sum is normalised by the sum of the distances between the particle and a randomly selected other, (Godlieb *et al.*, 2009). This mixing index M is then given by :

$$M = \frac{\sum_N d_{ij} - d_{min}}{\sum_N d_{ik} - d_{min}},$$

where d_{ij} is the distance between particle i and its initial nearest neighbour, d_{ik} is the distance between a particle and a randomly selected particle, and d_{min} is the minimum diameter of the grains. This method allows measuring the mixing in every direction, but does not depend on a grid.

6.1 Experimental set-up

The parameters used in the mixing experiment are the same as the ones in Table 5.3, except for the Froude number. Its value was chosen to be $Fr = 0.12$, which corresponds to the case

analysed by Xu *et al.* They studied the mixing of the same glass spheres that are simulated in the previous sections in a 2D rotating drum, numerically and experimentally, (Xu et al., 2010). The initial conditions are the same as the ones in section 5.2. The particles are divided in two groups according to their x position. Results are shown in Fig. 6.1 and Fig. 6.2, while the evolution of the mixing index with the mixing time $t_{mix} = t - 1$ is presented in Fig. 6.3.

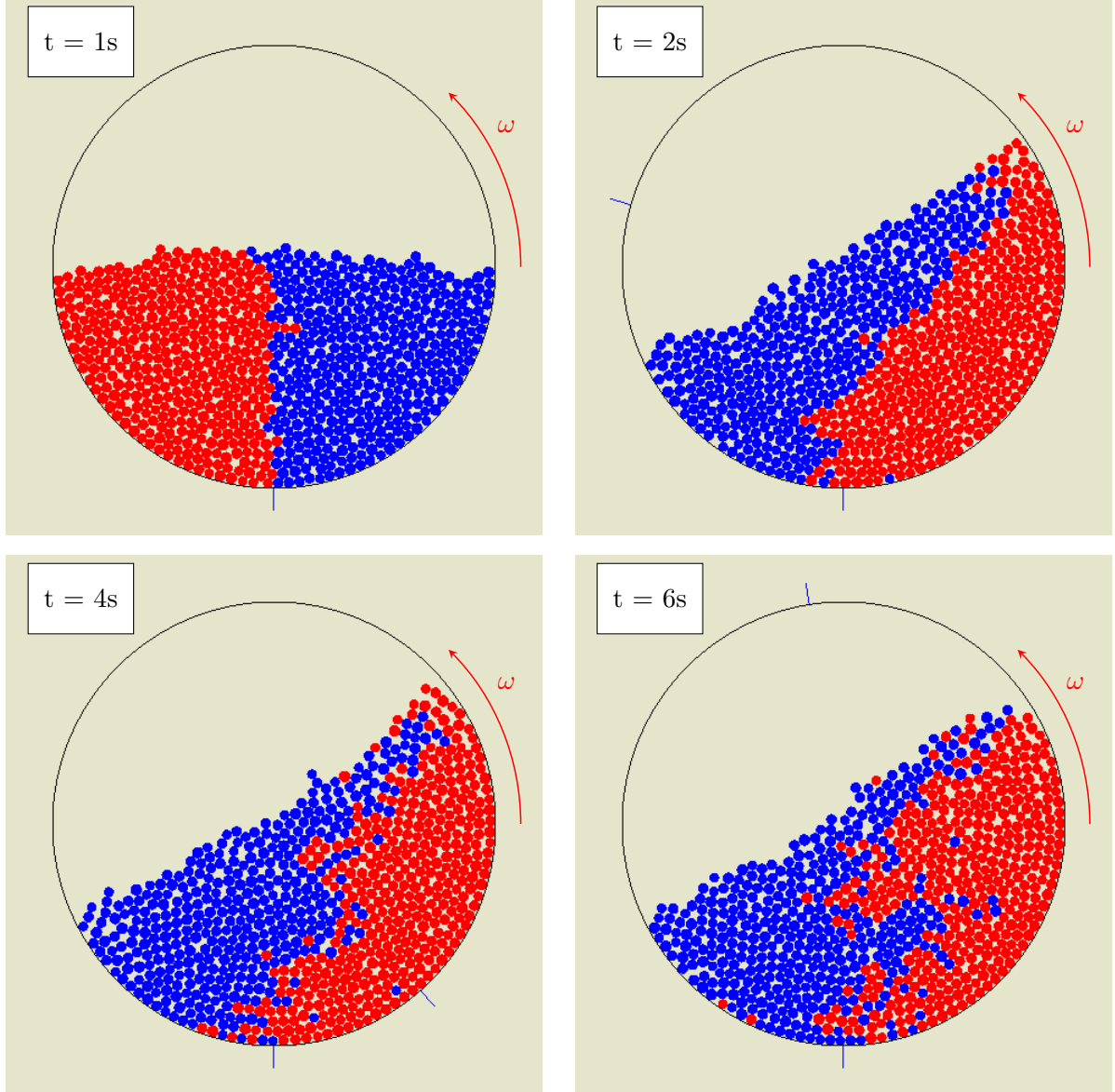


Figure 6.1: Snapshots of the simulation of mixing balls in a rotating drum for times from $t = 1s$ to $t = 6s$. The small interpenetration between the red group and the blue group at time $t = 1s$ is due to the fact that the grains rained down after being split in two groups. The profiles are in good agreement with the experimental and numerical ones obtained by Xu *et al.*

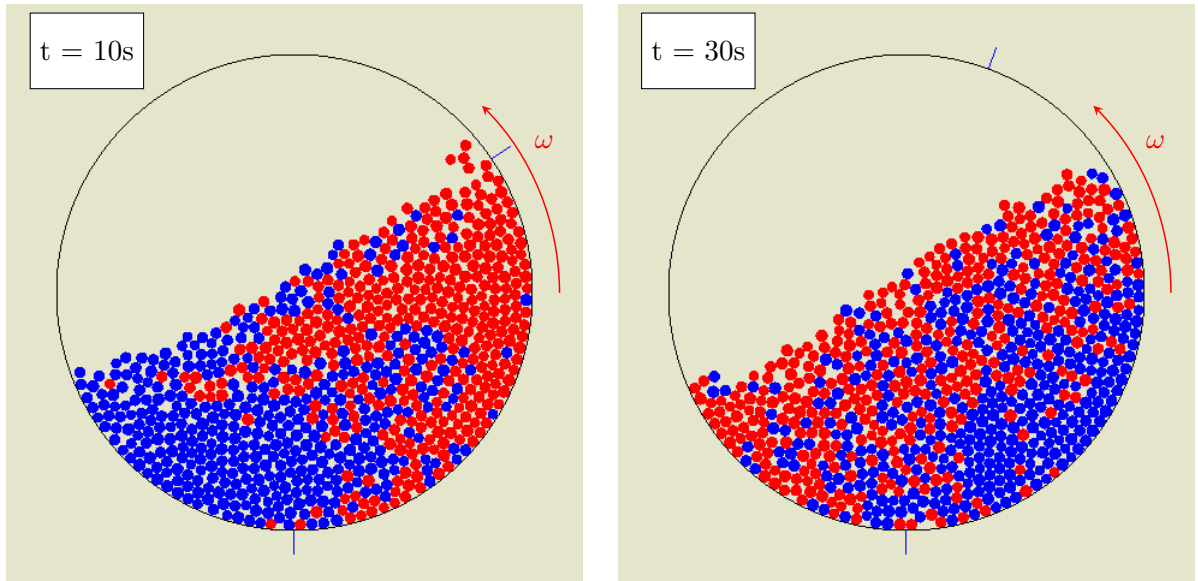


Figure 6.2: Snapshots of the simulation of mixing balls in a rotating drum for times $t = 10s$ and $t = 30s$.

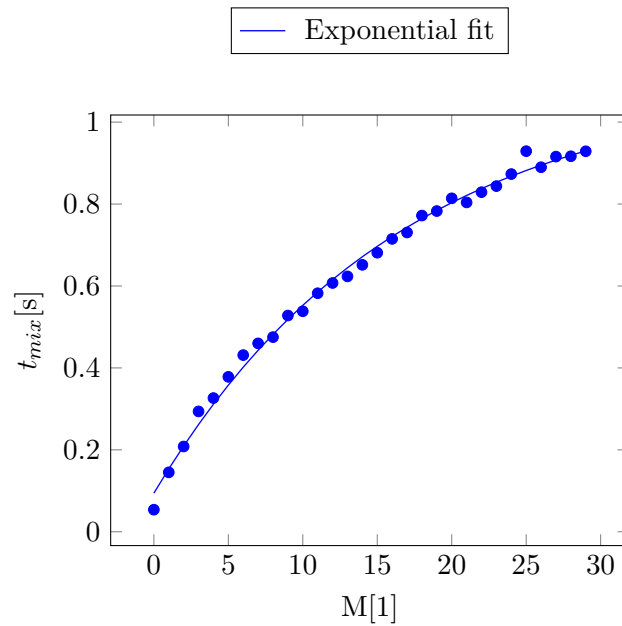


Figure 6.3: Evolution of the mixing index with the mixing time.

As seen in the above graph, the mixing index can be fitted using an exponential model, (Godlieb et al., 2009) :

$$M(t) = 1 - A \cdot \exp(-\lambda \cdot t_{mix}).$$

This model allows extracting¹ a reference value, called the 95% mixing time, or $t_{0.95}$. It is given by :

$$t_{0.95} = \frac{-1}{\lambda} \log\left(\frac{1 - 0.95}{A}\right)$$

¹In some cases, the curve did not fit the data very well, because the increase in the mixing index for short times was too high, while the increase for long times was low, predicting a wrong long-term behaviour. In these cases, the fit was corrected by discarding short times values.

Its value for the experiment was $t_{0.95} = 36.1s$. In Fig. 6.4, the values for $t_{0.95}$ are compared for different Froude numbers.

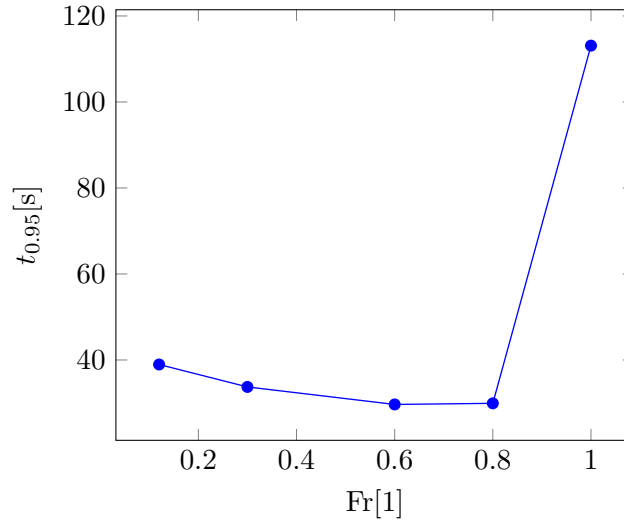


Figure 6.4: $t_{0.95}$ for different Froude numbers.

It was found that the time until 95% mixing decreases with increasing Froude number. The huge increase in $t_{0.95}$ is due to the fact that at $Fr = 1$, the grains are in a centrifuging regime. In this regime, the mixing index reaches a value near 0.75 in about 3s, but then increases very slowly. Except for applications with low mixing requirements, the centrifuging regime is thus to avoid, while the cataracting regime ($0.6 \leq Fr \leq 0.8$) is the fastest. Once this regime is reached, though, $t_{0.95}$ stays constant, indicating that it is useless to feed more power to the rotating mill so that it goes faster, since the efficiency is not improved. Again, $t_{0.95}$ has been compared for different kinetic friction coefficients, which is pictured in Fig. 6.5. The 95% mixing

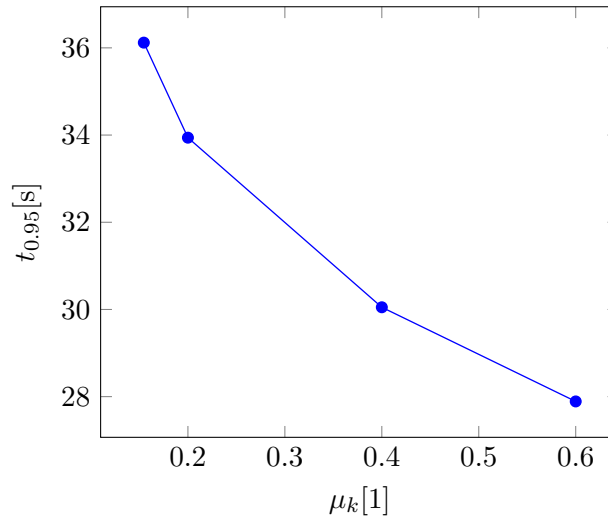


Figure 6.5: $t_{0.95}$ for different μ_k .

times seems to decrease with time, suggesting the use of frictional additives, such as talc, in mixing applications for better efficiency. Finally, a frequent problem in mixing tumblers is the segregation between two species of grains, because of their different size or density. In order to further investigate this issue, a first control simulation was led with half of the particles having a density three times higher than the other half. Snapshots of the simulation are shown in Fig. 6.6.

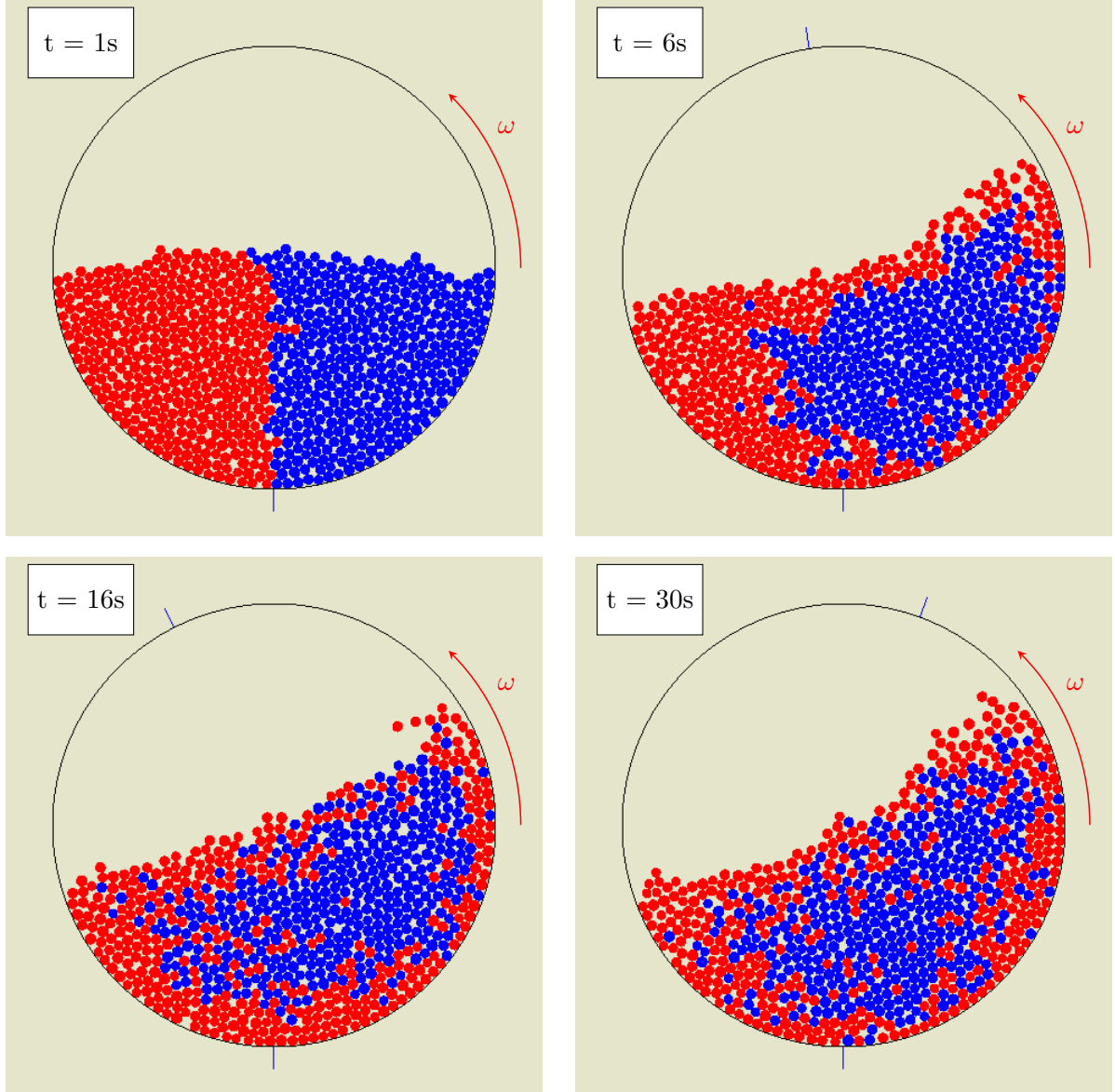


Figure 6.6: Snapshots of the simulation of mixing balls in a rotating drum for times from $t = 1s$ to $t = 30s$. The blue group has a three times higher density than the red group. Again, the profiles are in good agreement with the experimental and numerical ones obtained by Xu *et al.*

Indeed, segregation appears, as heavier blue particles tend to stay grouped in the centre, while the red particles migrate towards the free surface and the circular walls, which agrees with the results of Xu *et al.*, (Xu et al., 2010). The exponential model yields $t_{0.95} = 42.6s$. However, the model does not take the colour, or group, into account², and the time is then underestimated. Based on the observations on the influence of friction and the Froude number, another simulation was led for the same particles, but with higher inter-particle friction ($\mu_k = 0.6$) and Froude number. Regarding the latter, the value $Fr = 0.6$, which was shown to be the one with the best efficiency, resulted in a centrifuging regime. This was because of the increased mass of the grains, who were then able to receive a larger amount of momentum from the walls, since the friction force is bounded indeed by μ_k but also by the normal reaction force. Therefore, the value $Fr = 0.4$ was taken. The results are presented in Fig. 6.7.

²Indeed, when the initial nearest neighbours were defined, the groups were not taken into account, leading to an insensitivity to this variable. This has the advantage over the other mixing indexes to be usable when evaluating the mixing of non-binary mixtures, though.

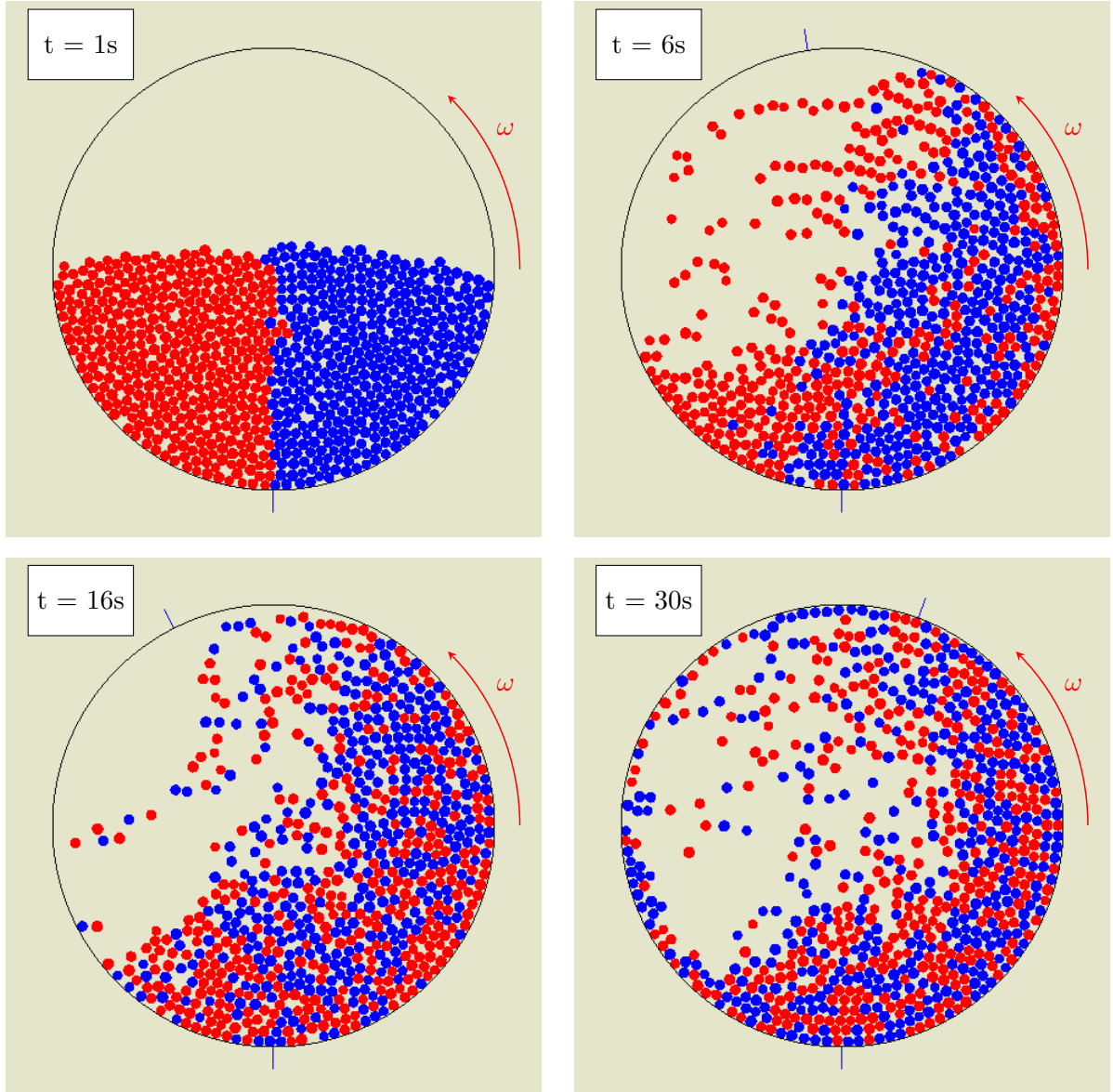


Figure 6.7: Snapshots of the simulation of mixing balls in a rotating drum for times from $t = 1s$ to $t = 30s$. The blue group has a three times higher density than the red group. Friction and Froude number have been enhanced in order to decrease the segregation.

The segregation was strongly decreased by the combined increase of friction and rotation speed, through the Froude number, although the grains are at the onset of centrifuging at $t = 30s$. The exponential model gave $t_{0.95} = 16.31s$, which is much faster than all the previous cases. However, as explained above, this value is only an approximation, and it should be interpreted more as a qualitative criterion rather than an absolute value.

Chapter 7

Conclusion

In this work, the numerical challenge of modelling frictional granular flows is addressed, with the goal to develop an extension to the treatment of the grains in an already existing model for immersed granular flows by Constant *et al.* In the first two chapters, the state of the art in the field of granular media were presented, establishing the theoretical and experimental norms to be compared with, as well as the strengths and weaknesses of different approaches. From several available methods, such as DEM or ED, the Non-Smooth Contacts Dynamics method was chosen, due to its ability to model frictional rigid collisions in a dense granular material.

In the third chapter, the theoretical background of the method is laid out. The behaviour of the grains is derived from the Newton equations of motion. These equations are expressed in a weak integral form, as a balance of momentum, which allows simulating systems with a high density of grains, and where many shocks occur. From the resulting differential measure problem, the discretised equations are obtained through a backward Euler integration scheme. This way, the system is unconditionally stable, allow the use of large time-steps that speed up the calculations. However, the smooth external forces are computed according to an explicit scheme, for the sake of simplicity. Plus, in the presence of sole gravity, which is constant through time and does not depend on the other variables such as position or velocity, the result is equivalent. The implicit contact laws are stated in the local scale, i.e. the scale relative to two particles involved in one contact, because of the binary nature of the contacts. A simple mapping between the global and local scale is laid out, allowing a simple contact resolution. Additionally, the contact algorithm between a grain and a circular wall is refined so that there is no intersection, in order to be able to treat the case of a rotating drum in Chapter 5. The stability expected from the implicit scheme is confirmed by the accurate results for a 1D experiment with large time-steps, as well as by the behaviour of the error in a 2D experiment between a grain and an inclined wall, with the error oscillating in a bounded interval around the analytic solution, and converging linearly with the time-step. This second experiment led to the choice of a 0.005s time-step for the validating experiments of chapter 5.

The implementation of the method requires several improvements from the naive one in order to be computationally efficient. In chapter 4, the details of such an efficient implementation are presented. Notably, improvements on the detection, management and resolution of contacts are detailed. The use of a quadtree build incrementally to recursively divide space in cells containing a maximal number of particles, coupled with the bounding box technique, allows a scaling in $O(\log(N))$ instead of $O(N^2)$ for the time complexity. The management of the contacts uses a queue, and the resolution of the contacts implies the value at the previous time-step, allowing huge time gains in static situations.

In the fifth part of this work, the model is checked against experimental and numerical

results from the literature, based on the angles of repose. The numerical experiments are led for slightly mono-dispersed glass beads. A simple relationship was chosen between the kinematic and static coefficients of friction, because of the unavailability of the latter. This relationship stays rather coarse, and either other values should be found, or a precise theoretical or empirical relationship should be established. Regarding the static angle of repose, a significant deviation from the 3D values of the reference experiment was observed, but for 2D disks the results are in quantitative agreement with literature. The increasing behaviour of the angle of repose with friction was well reproduced by the model. The angle of repose was observed to increase with decreasing particle size, in agreement with literature results. The effect of polydispersity was more surprising. For quasi-monodispersity, crystal like ordering occurred, because of the 2D configuration of the problem, leading to high and widely distributed values. Medium polydispersity showed a classical behaviour, while high polydispersity resulted in a constant angle of repose. The reason of this effect stays unclear, and should be investigated further in the future. As for the dynamic angle of repose, the obtained velocity fields agreed with the ones from literature, and the correct qualitative behaviours have been predicted, notably the saturation of the dynamic angle of repose with increasing friction, as well as a nearly linear increase of the dynamic angle of repose with the rotation speed via the Froude number. However, these results are still only qualitative. Therefore, the simulation parameters should be changed to match some reference ones found in the literature to estimate the quantitative agreement on these aspects.

Finally, the validated model was used to study the mixing of two groups of particles in a 2D rotating drum. The degree of mixing was measured as a ratio between the initial nearest neighbour distance and the distance between random particles, and an exponential model was used to extract $t_{0.95}$, the mixing time to reach a 95% mixed sample. This fitted value is to be taken as a qualitative criterion rather than an absolute quantitative parameter. The profiles from the control simulation were in excellent agreement with the ones found in the literature. The effect of friction and rotation speed were investigated. Regarding friction, a decrease in $t_{0.95}$ was observed with increasing friction, suggesting the use of frictional additives such as talc in mixing tumblers. As for the effect of the rotation speed, it was found that $t_{0.95}$ first decreased with increasing Froude number from $Fr = 0.12$, at fixed cylinder diameter, but reached a stationary value at $Fr = 0.6$, while for $Fr = 1$ a centrifuging regime was reached, yielding bad mixing properties. The problem of density segregation was investigated with a group having a density three times as high as the other one. In the control simulation, segregation was observed as expected, with profiles corresponding well to the ones in literature, and the mixing time was high. A proposed solution was to add a frictional additive modelled by an increased frictional coefficient, coupled with an increase in the rotational speed, and segregation was indeed drastically reduced.

The model seems efficient and yields good results, so it could be implemented into the existing model for immersed granular flows, which should be done in the near future. This implementation could be used to simulate the mixing of granular material in the presence of a fluid, as the actual model only simulates such a mixing process by emulating friction with high fluid viscosity. The experiment on the polydispersity indicated that the diversity of shapes rather than sizes should play a role in the determination of the angle of repose. Therefore, the model could be extended to simulate polygonal particles, which are more representative of a real granular material. The experiments of chapter 5 also showed a significant difference between 2D and 3D results, so the model should be extended accordingly, which implies two new rotation coordinates and velocities, as well as one new position and velocity coordinate, complicating the resolution of the problem in the local frame. Finally, an interesting application of the complete model for frictional immersed flows would be the study of the rheology of macro-molecules, which would be modelled as chains of grains linked by entropic forces. Precisely, Size Exclusion Chromatography could be simulated, and if the model yields good results, this would suppress the need for calibration of these devices.

Bibliography

- Alam, M. and Luding, S. (2002). Rheology of bidisperse granular mixture via event driven simulations.
- Albert, R., Albert, I., Hornbaker, D., Schiffer, P., and Barabasi, A. (1997). Maximum angle of stability in wet and dry spherical granular media. *Physical review E*, 56.
- Armanini, A. (2013). Granular flows driven by gravity. *Journal of Hydraulic Research*, pages 111–120.
- Azanza, E., Chevoir, F., and Moucheron, P. (1999). Experimental study of collisional granular flows down an inclined plane. *Journal of fluid mechanics*, 400:199–227.
- Beakawi Al Hashemi, H. and Baghabra Al-Amoudi, O. (2018). A review on the angle of repose of granular materials. *Powder Technology*, 330:397–417.
- Bizon, C., Shattuck, M., Swift, J., and Swinney, H. (1999). Transport coefficients for granular media from molecular dynamics simulations. *Physical Review E*, 60:4340–51.
- Burkalow, A. (1945). Angle of repose and angle of sliding friction : an experimental study. *Bulletin of the Geological Society of America*, 56:669–707.
- Campbell, C. (1990). Rapid granular flows. *Annual review of fluid mechanics*, 22:57–92.
- Carrigy, M. A. (1970). Experiments on the angle of repose of granular materials. *Sedimentology*, 14:147–158.
- Carstensen, J. and Chan, P. (1976). Relation between particle size and repose angle of powders. *Powder Technology*, 15:129–131.
- Cheng, N. and Zhao, K. (2017). Difference between static and dynamic angle of repose of uniform sediment grains. *International Journal of Sediment Research*, 32:149–154.
- Constant, M., Lambrechts, J., Dubois, F., and Legat, V. (2017). Modèle hybride multi-échelles pour les écoulements granulaires immergés. In *13ème Colloque National en Calcul des Structures*, Presqu’île de Giens (Var).
- Coulomb, C. (1773). Essai sur une application des règles de maximis et minimis à quelques problèmes de statique, relatifs à l’architecture.
- Courrech du Pont, S., Gondret, P., Perrin, B., and Rabaud, M. (2003). Granular avalanches in fluid. *Physical review letters*, 90(4).
- Cundall, P. A. and Strack (1979). A discrete numerical model for granular assemblies. *Géotechnique*, 29(1):47–65.
- Dubois, F. and Radjai, F. (2010). *Modélisation numérique discrète des matériaux granulaires*. Hermès-Lavoisier.

- Dubois, F. and Renouf, M. (2015). Discrete elements methods for the simulation of divided media.
- Dury, C. and Ristow, G. (1998). Boundary effects on the angle of repose in rotating cylinders. *Physical Review E*, 57:4491–4497.
- Fowler, R. and Glastonury, J. R. (1959). The flow of granular solids through orifices. *Chemical Engineering Science*, 10:150–156.
- Godlieb, W., Gorter, S., Deen, N., and Kuipers, J. (2009). Dem and tfm simulations of solids mixing in a gas-solid fluidized bed. In *Seventh International Conference on CFD in the Minerals and Process Industries*, pages 4046 – 4051, Melbourne, Australia.
- Goujon, C., Thomas, N., and Balloz-Dubrujeaud, B. (2003). Monodisperse dry granular flows on inclined planes : role of roughness. *European Physical Journal E*, 11:147–157.
- Henein, H., Brimacombe, J., and Watkinson, A. (1983). Experimental study of transverse bed motion in rotary kilns. *Metallurgical transactions B*, 14B:191–205.
- Irgens, F. (2008). *Continuum mechanics*. Springer.
- Jean, M. (1999). The non-smooth contact dynamics method. *Computer methods in applied mechanics and engineering*, 177:235–257.
- Jop, P., Forterre, Y., and Pouliquen, O. (2006). A constitutive law for dense granular flows. *Nature*, 441:727–730.
- Kochara, S., Halic, T., Iqbal, K., Bayrak, C., and Rowe, R. (2007). Collision detection: A survey. In *Conference Proceedings - IEEE International Conference on Systems, Man and Cybernetics*, pages 4046 – 4051.
- Li, Y., Xu, Y., and Thornton, C. (2005). A comparison of discrete element simulations and experiments for 'sandpiles' composed of spherical particles. *Powder Technology*, 160:219–228.
- Liu, X., Specht, E., and Mellmann, J. (2005). Experimental study of the lower and upper angles of repose of granular materials in rotating drums. *Powder technology*, 154:125–131.
- Liu, Z. (2008). Measuring the angle of repose of granular systems using hollow cylinders. Master's thesis, Southwest Jiaotong University.
- Lube, G., Ruppert, H., Sparks, R., and Freudt, A. (2005). Collapses of two-dimensional granular columns. *Physical Review E*, 72:041301.
- Lun, C., Savage, S., Jeffrey, D., and Chepurniy, N. (1984). Kinetic theoris for granular flows : inelastic particles in couette flow and slightly inelastic particles in a general flowfield. *Journal of fluid mechanics*, 140:223–256.
- Mehta, A. and Barker, G. (1994). The dynamics of sand. *Reports of progress in physics*, 57:383–416.
- Mellmann, J. (2001). The transverse motion of solids in rotating cylinders—forms of motion and transition behavior. *Powder Technology*, 118:251–270.
- Moreau, J. (1994). Some numerical methods in multibody dynamics: application to granular materials. *European journal of mechanics-A/Solids*, 13:93–114.
- Pailha, M. and Pouliquen, O. (2009). A two phase flow description of the initiation of underwater granular avalanches. *Journal of Fluid Mechanics*, 633:115–135.

- Pudasaini, S. (2012). A general two-phase debris flow model. *Journal of geophysical research*, 117.
- Pöschel, T. (1993). Granular material flowing down an inclined chute : a molecular dynamics simulation. *Journal de Physique II*, 3:27–40.
- Radjai, F. and Richefeu, V. (2009). Contact dynamics as a nonsmooth discrete elements method. *Mechanics of Materials*, 41:715–728.
- Rignanese, G.-M., Lherbier, A., Gonze, X., and Charlier, J.-C. (2017). Mapr2451 : Atomistic and nanoscopic simulations. Lecture given at Université Catholique de Louvain, during the 2016-2017 academic year.
- Riley, G., Mann, S., and Jesse, R. (1978). Angles of repose of cohesive powders. *J. Powder Bulk Solids Technol. Journal of Powder & Bulk Solids Technology*, 2:15–18.
- Rognon, P., Roux, J.-N., Naaïm, M., and Chevoir, F. (2007). Dense flows of bidisperse assemblies of disks. *Physics of fluids*, 19:058101.
- Savage, S. and Hutter, K. (1989). The motion of a finite mass of granular material down a rough incline. *Journal of fluid mechanics*, 199:177–215.
- Savage, S. and Hutter, K. (1991). The dynamics of avalanches of granular materials from initiation to runout. part i : Analysis. *Acta Mechanica*, 86:201–223.
- Staron, L. and Hinch, E. J. (2018). Study of the collapse of granular columns using dem numerical simulation.
- Wikipedia contributors (2018). Quadtree. [Online; accessed 16-May-2018].
- Xu, Y., Xu, C., Zhou, Z., Du, J., and Hu, D. (2010). 2d dem simulation of particle mixing in rotating drum : a parametric study. *Particuology*, 8:141–149.
- Yamane, K., Nakagawa, M., Altobelli, S., Tanaka, T., and Tsuji, Y. (1998). Steady particulate flows in a horizontal rotating cylinder. *Physics of fluids*, 10(6):1419–1427.
- Yang, R., Zou, R., and Yu, A. (2003). Microdynamic analysis of particle flow in a horizontal rotating drum. *Powder Technology*, 130:138–146.
- Zhou, Y. C., Xu, B. H., Yu, A. B., and Zulli, P. (2002). An experimental and numerical study of the angle of repose of coarse spheres. *Powder technology*, 125:45–54.

