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PROGRAMA DE PÓS-GRADUAÇÃO EM MODELAGEM MATEMÁTICA E COMPUTACIONAL

NUMERICAL SIMULATION OF GRANULAR MATERIALS: BRAZIL NUT EFFECT AND SEDIMENT TRANSPORT

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MATERIALS: BRAZIL NUT EFFECT AND SEDIMENT
TRANSPORT**

Thesis presented to the Graduate Program in Mathematical and Computational Modeling at Centro Federal de Educação Tecnológica de Minas Gerais, as partial requirement to obtain the degree of Doctor of Philosophy in Mathematical and Computer Modeling.

Research field: Mathematical and Computational Modeling

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Abstract

The simulation of granular materials is studied widely in many research centers around the world, and applied in industries and engineering companies. For the understanding and quantification of granular materials properties, Discrete Element Method (DEM) is used to simulate the behavior of granular materials. Many of the challenges to understanding the behavior of granular materials begin in the dry grain segregation phenomenon. Classically, we have the Brazil-Nut Effect (BNE) - which consists of a confined granular material containing grains of different sizes which, when agitated, displays segregation, with the larger grains rising up to surface. For many years, it was believed that this segregation occurred due to the presence of walls that confine the material. In this thesis we show that in systems with periodic boundary conditions (pbc), BNE can also occur. We also proposed that BNE exhibits resonance effect, and we differentiate systems with walls and pbc by using Large-Deviation function (LDF). We also studied sediment transport that occurs in the interaction between granules and fluids. To simulate the behavior of granular materials immersed in a fluid, we use a Computational Fluid Dynamics (CFD) technique. The solid sediments move in the velocity field transported by the fluid. Three dimensionless parameters are required to describe the transport behavior: the Reynolds number, which relates the inertial forces to the viscous forces, and consequently the fluid turbulence effects; the number of Shields, which is related to the drag forces and the inertial forces of the fluid; and finally, the density ratio between the solid and the fluid phases. It is possible to reproduce the different modes of transport only by changing such dimensionless parameters. In this thesis, we calculate and characterize the saturation time for bedload transport mode in the viscous regime, and we also predict the saturation length for this transport mode. This sediment transport was possible to studied thanks to the sandwich PhD. done in PMMH-ESPCI with CAPES grant No.88881.187077/2018-01.

Keywords: Granular materials. Computer simulations. Discrete Element Method (DEM). Computational Fluid Dynamics (CFD). Brazil-Nut Effect. Sediment transport.

Resumo

A simulação de materiais granulares é estudada nas academias de todo o mundo, também aplicada em indústrias e empresas de engenharia. Para o entendimento e quantificação das propriedades dos materiais granulares, o Método de Elementos Discretos, ou *Discrete Element Method* (DEM), é usado para simular o comportamento de materiais granulares. Muitos dos desafios de se compreender o comportamento de materiais granulares têm início no fenômeno de segregação de grãos secos. Classicamente, temos o efeito castanha do Pará - *Brazil Nut Effect* (BNE) - que consiste em um material granular confinado contendo grãos de diferentes volumes e que, quando agitados, exibem segregação, sendo que os grãos maiores ascendem até a superfície. Por muitos anos, acreditou-se que esta segregação ocorria devido a presença de paredes que confinam o material. Nesta tese mostramos que em sistemas com condição periódica de contorno também pode ocorrer o BNE. Propomos que o BNE se comporta com efeito ressonante, e diferenciamos os sistemas com paredes do com condição periódica de contorno usando a função de grandes desvios - *Large-Deviation function* (LDF). Estudamos também o transporte de sedimentos que ocorre na interação entre granulares e fluidos. Para simular o comportamento de materiais granulares imersos em um fluido, utilizamos uma técnica de Fluidodinâmica Computacional, ou *Computational Fluid Dynamics* (CFD). Os sedimentos sólidos se movem em um campo de velocidades transportados pelo fluido. Três parâmetros adimensionais são necessários para descrever o comportamento do transporte: o número de Reynolds, que relaciona as forças iniciais com as forças viscosas, e consequentemente os efeitos de turbulência do fluido; o número de Shields, que está relacionado com as forças de arraste e as forças iniciais do fluido; e finalmente, a razão de densidade entre o sólido e a fase fluida. É possível reproduzir os diferentes modos de transporte apenas mudando tais parâmetros adimensionais. Nesta tese, calculamos o tempo de saturação para o modo *bedload* no regime viscoso, e também predizemos o tempo de saturação para este modo de transporte. Este estudo de transporte de sedimentos foi possível graças ao doutorado sanduíche realizado no PMMH-ESPCI com a bolsa CAPES No.88881.187077/2018-01.

Palavras Chaves: Materiais granulares. Simulação computacional. Método de Elemento Discreto (DEM). Fluidodinâmica Computacional (CFD). Efeito castanha do Pará (BNE). Transporte de sedimentos.

Résumé

Des simulations de matériaux granulaires ont été étudiées dans les centres de recherche du monde entier, également appliquées dans l'industrie et la société d'ingénierie. Pour comprendre et qualifier les propriétés des matériaux granulaires, la Méthode des Éléments Discrètes, ou *Discrete Element Method* (DEM), est utilisée pour simuler le comportement des matériaux granulaires. De nombreux défis pour comprendre le comportement des matériaux granulaires commencent par le phénomène de ségrégation des grains secs. Classiquement, il y a l'effet noix du Brésil - *Brazil Nut Effect* (BNE) - qui consiste en des matériaux granulaires confinés contenant des grains de différents volumes et qui, lorsqu'ils sont agités, présentent une ségrégation, les plus gros grains remontant jusqu'à la surface. Pendant de nombreuses années, on a cru que cette ségrégation était due à la présence de murs qui confinent le matériau. Dans cette thèse, nous montrons que dans les systèmes avec des conditions aux limites périodiques, le BNE peut également se produire. Nous avons également proposé que le BNE présente un effet de résonance, et nous différencions les systèmes avec des murs et des conditions aux limites périodiques en utilisant la fonction de grande déviation. Nous avons également étudié le transport des sédiments qui se produit dans l'interaction entre les granules et les fluides. Pour simuler le comportement des matériaux granulaires immergés dans un fluide, nous utilisons une technique de Dynamique des Fluides Computationnelle, ou *Computational Fluid Dynamics* (CFD). Les sédiments solides se déplacent dans un champ de vitesses portées par le fluide. Trois paramètres adimensionnels sont nécessaires pour décrire le comportement de transport : le nombre de Reynolds, qui est lié aux forces d'inertie aux forces visqueuses, et par conséquent aux effets de la turbulence des fluides ; le nombre de Shields, qui est lié aux forces de traînée et aux forces d'inertie du fluide ; et enfin, le rapport de densité entre le solide et la phase fluide. Il est possible de reproduire les différents modes de transport simplement en modifiant ces paramètres adimensionnels. Dans cette thèse, nous calculons et caractérisons le temps de saturation pour les modes de transport chargé en régime visqueux, et nous prédisons également la longueur de saturation pour ce mode de transport. Ce transport sédimentaire a pu être étudié grâce au stage de thèse fait au PMMH-ESPCI avec la bourse CAPES 88881.187077/2018-01.

Mots clés: Matériaux granulaires. Simulation par ordinateur. Méthode des éléments discrets (DEM). Dynamique des fluides computationnelle (CFD). Effet de Noix du Brésil (BNE). Transport de sédiments.

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List of Abbreviations and Acronyms

BNE	Brazil-Nut Effect
CFD	Computational Fluid Dynamics
DEM	Discrete Element Method
MD	Molecular Dynamics
LDF	Large Deviation Function
pbc	Periodic boundary condition

List of Symbols

G	Galileos number
R	Reynolds number
Θ	Shields number
ρ	Density
Γ	Dimensionless number that compares shaken acceleration and gravity
ω	Oscillation frequency of shaken systems
ϕ	Packing fraction

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1 Introduction

Granular materials are present in various contexts of nature and in many human activities [2, 3, 4, 5, 6]. Economic activities, like agricultural production, mining and building technology, are essentially linked to the usage of granular materials [3]. For many years, research in granular materials were linked mainly to engineering [7, 8, 9], in order to optimize production process, storing, transportation, and structural applications to these materials. Nowadays, some areas of physics, such as statistical mechanics [10], study intensively the characterization and behavior of these materials, and as well applications, due to the richness of observed phenomena. Its ubiquity reflects the importance of studies about it to better understand their manipulation in the most diverse situations.

Granular materials can be characterized as a cluster of bodies larger than a few hundred micrometers up to the size of asteroids [3, 4]. In addition to the size, another feature of bodies is that they are individually in solid state. Their interactions result in energy dissipation, either by friction or by inelastic collisions interaction. They are not subject to movement caused by thermal fluctuations, and therefore, do not exhibit Brownian motion. More characterizations of granular materials can be found in the Chapter 2 of this thesis.

The aim of this work is to computationally simulate granular materials, using Discrete Element Method (DEM), specifically based on the Molecular Dynamics (MD) [11]. The simulations are in 2D, with grains that have circular geometry, hard-core potential repulsion when in contact, and are under the action of gravity. To simulate the contacts, we also take into account the Coulomb friction between the grains. Once the properties of the materials are defined, such as hardness, friction, mass, position and radius, we apply Newton's laws of motion to perform the simulation. We detail these equations and peculiarities of the simulation of dry granular materials in the Chapter 3.

Among the phenomena presented by the dry granular materials, we were interested this thesis in the Brazil Nut Effect (BNE), related to the segregation of confined grains when submitted to the vibration, and in the presence of a gravitational field. Larger grains segregate to surface, while smaller grains sink to bottom. The Chapter 4 provides more details about the phenomenology of BNE, as well the numerical approach employed. The results and the discussion about BNE phenomena we studied are presented in Chapter 5.

Associated with DEM, we are interested in simulate granular materials carried by fluids and characterize the transport mode of bedload, using Computer Fluid Dynamics (CFD). The fluid flows homogeneously in one direction and varies in another, making the simulation of the fluid been in 1D. In this thesis we describe the technique to simulate 1D flow in viscous regime and a turbulent approach, in Chapter 6, and how to link it with the

granular phase.

We also researched the phenomenon of sediment transport in fluids interested in. The Navier-Stokes [12, 13] equation is used in this work to model the fluid that flows and carries part of the granular materials with. There are some transport modes that are characterized by the way the grains are transported by the fluid, which are briefly described in the Chapter 7. In this thesis, we focused in the bedload transportation mode, and the results of our work are presented in Chapter 8.

1.1 Justification

Because we realize that there is still a lack of understanding in the phenomena involving granular materials, we propose to study in this thesis the techniques that can predict the behavior of the conglomerate, or to characterize some emerging properties of the system that has not yet been reported or documented, as well as to use results already known from the materials, and try to apply them in other areas where measurement is difficult.

Specifically, we will deal with a subject that has not yet been reproduced in the literature: BNE in two dimensions with periodic boundary conditions. To analyze this problem we use computer simulations and the Large Deviation Function (LDF) [14] technique.

We also computed by simulations the saturation time scale¹ and the saturation length scale² of the material for the viscous bedload regime when transported by a fluid. Such measurement is quite difficult to achieve in experiments due to the scales we are treating.

1.2 Motivation

In the context of engineering, it is necessary to understand how the processes are elaborated, in order to adjust them to optimize the production costs, transportation and storage of materials essential to human activities, such as food and ores. In this sense, the understanding of the behavior of these materials, when subjected to certain conditions, allows them to be manipulated in the way of greatest interest, whether due to the need to conserve the material, either due to faster transport or the efficiency of another parameter in which it is intended spend less resources or have the greatest financial, energy or social return.

¹ Saturation time in sediment transport indicates the characteristic time it takes for the material to enter a steady state, leaving a configuration and arriving at the final configuration.

² Saturation length in the sediment transport indicates the characteristic length it takes for the material to enter its normal flux regime, when there is a difference of concentration of the material according to the space.

In grain segregation, problems related to clogging may occur depending on the geometry of the materials [15]. When these materials are subjected to vibration, or when they flow, the larger ones are naturally separated from the smaller ones, thus facilitating the filtration, but making it difficult to mix. These sets of agglomerates can have negative consequences for industrial process, such as wear of silos related to the resistance of materials, corrosion of the silo or granular, rotting or aging of stored food, etc. [16].

Thus, understanding how the granular materials interact and how they are transported, whether transported on a conveyor belt, or carried by the currents of a river, gives the possibility to control its possible effects, or to predict its consequences, such as the amount of residues remaining in the rivers due to the collapse of the Fundão dams in Mariana-MG in November 2015 [17, 18, 19], and the Brumadinho dam in January 2019 [20, 21, 22].

1.3 Workflow

This work is divided into a bibliographic review on granular materials, in Chapter 2, with phenomenology on the study of granular materials. The descriptions of the Chapter 3 relates to the equation of motion and modelling of the granular phase, concerning the interaction forces between grains and how the governing equations are implemented in this system. The Chapter 4 refers in particular to the phenomenon known as BNE and the proposition of this work in studying the dry granular. In Chapter 5 we present the first part of the results of this thesis. The Chapter 6 relates to the equation of motion and modelling the fluid phase, relating to the interaction between grains and fluid in different regimes. The Chapter 7 represents the characterizations of each transport mode, and the descriptions of the transport of materials by fluids in laminar regime. The Chapter 8 contains discussions on the results obtained, referring to the transport of sediments. The Chapter 9 presents the conclusions of this thesis and perspectives for the continuation of this work.

2 Granular Materials

Granular Materials are sets of solid bodies, composed by a given material or different materials. They can have a varied geometries, different densities, friction coefficients, hardness *etc.*, but an individual grain must be larger than $100\mu\text{m}$ [3] to ensure the athermous nature. The solid bodies that composes granular materials should be large enough to do not present kinetic fluctuation induced by thermodynamic temperature. Therefore, Brownian motion do not play a role in those systems. Granular materials interact each other when they are in contact, loosing energy by inelastic collision, as well as by friction.

Inelastic collision occurs when two or more grains collide losing part of their initial kinetic energy, in which they have transformed these loss to heat and they may deform in the process [23]. We are modeling the inelastic collision between two grains in section 6.1.1.1.

2.1 Theory

Examples of granular materials includes sand, stones, soils, drugs, ores, grain foods (rice, corn, soybeans *etc.*), even the asteroid belt and Saturn's rings. The sand alone constitutes 10% of the materials on surface of planet Earth. Besides that, it is estimated that the second most used material in industries are granular materials, using approximately 10% of all the energy on the planet, whether in extraction, transport, or processing, with the most used material being water [3].

Due to the absence of Brownian movements, as well as the dissipation of energy in the contacts, granular systems does not undergo spontaneous relaxation of its stable configurations in the absence of external disturbances, and therefore do not present ergodicity. An ergodic system has the characteristic of visit their micro-states of energy spontaneously, implying that their states are all equiprobable when a very long time is taken in account [10, 24].

To demonstrate this non-ergodicity, we can think about a pile of dry sand that rests at a base. If this base does not oscillate, the structure of the pile does not change, the structure of internal forces will remain unchanged, even if it is heated or cooled. This means that sand grains cannot transit between all equipotential states spontaneously, and then this sand pile will rest with internal configurations (chain-forces, stress tensors, grain contact, *etc.*) unchanged. In the section 2.2, one can find more details.

Granular materials also have particularities regarding their phases-like, analogously to the state of matter. They are presented individually in solid bodies, and when the grains are close to rest, they constitute the equivalent solid phase. However, if the granular system

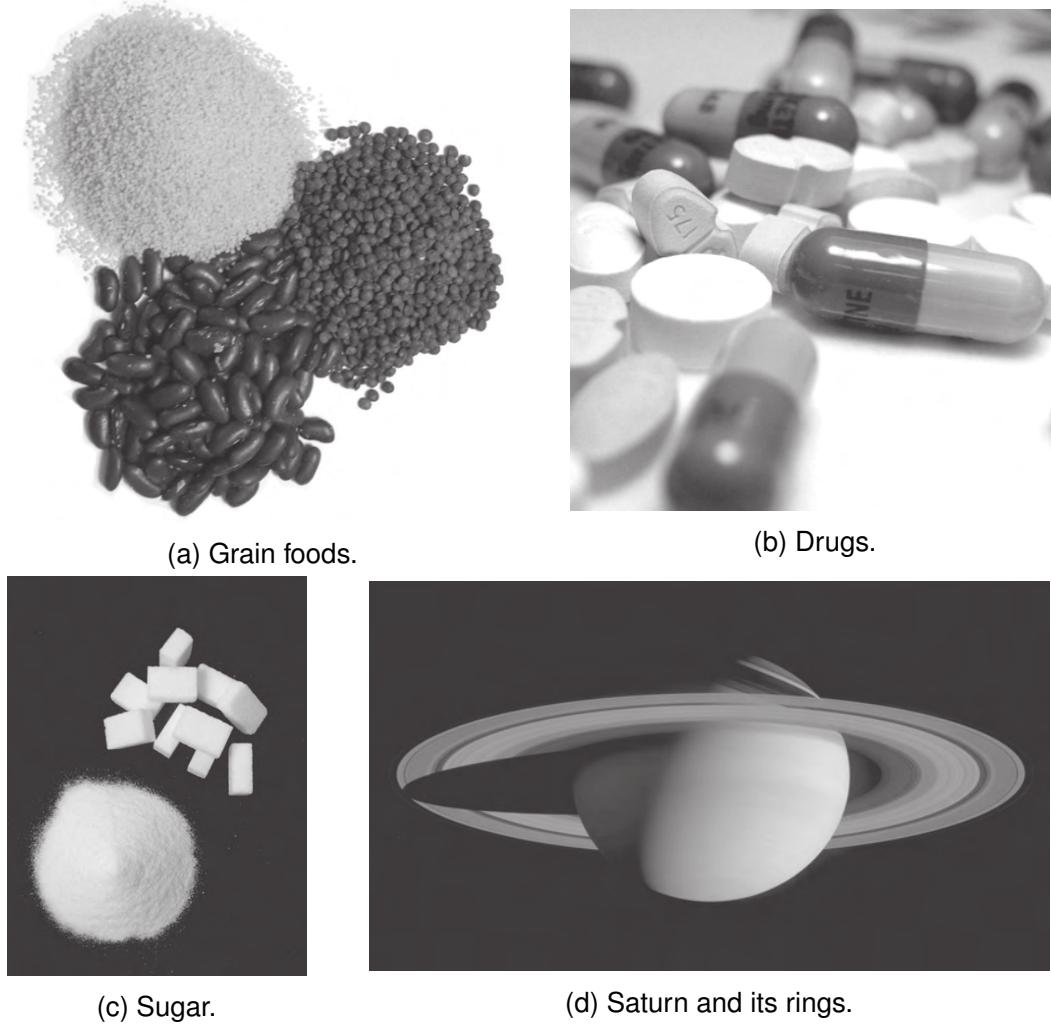


Figure 1 – Examples of granular material. Figures taken from [2].

is slightly agitated, or configured beyond a critical threshold of angle of rest, its behavior can be similar of the liquid. Solid-like and liquid-like granular can coexist and a boundary layer may appear, that indicates the liquid-like flows over the solid-like. When a granular system is vigorously agitated, the behavior is alike gases, they tend to occupy large part of the container which contains them, meaning that its packing fraction (ϕ) is low and the number of contacts between grains are much rarer, compared to the granular liquid-like and solid-like. An example of the granular states is shown in Figure 2, where the solid-like phase is in the bottom, the liquid-like phase is flowing through layers in the middle, and the gaseous-like phase is flowing in a higher disordered portion at top. Such classification is still open in the literature, although there are proposals for what would be the granular temperature of the system, in analogy of thermal temperature [25].

Packing fraction is the measure of the occupied space by the solid portion in relation of the total space occupied by the system.

A differentiation between granular systems can be a direct result of the interaction forces between grains. Systems that have only repulsive interactions are called dry granulars,

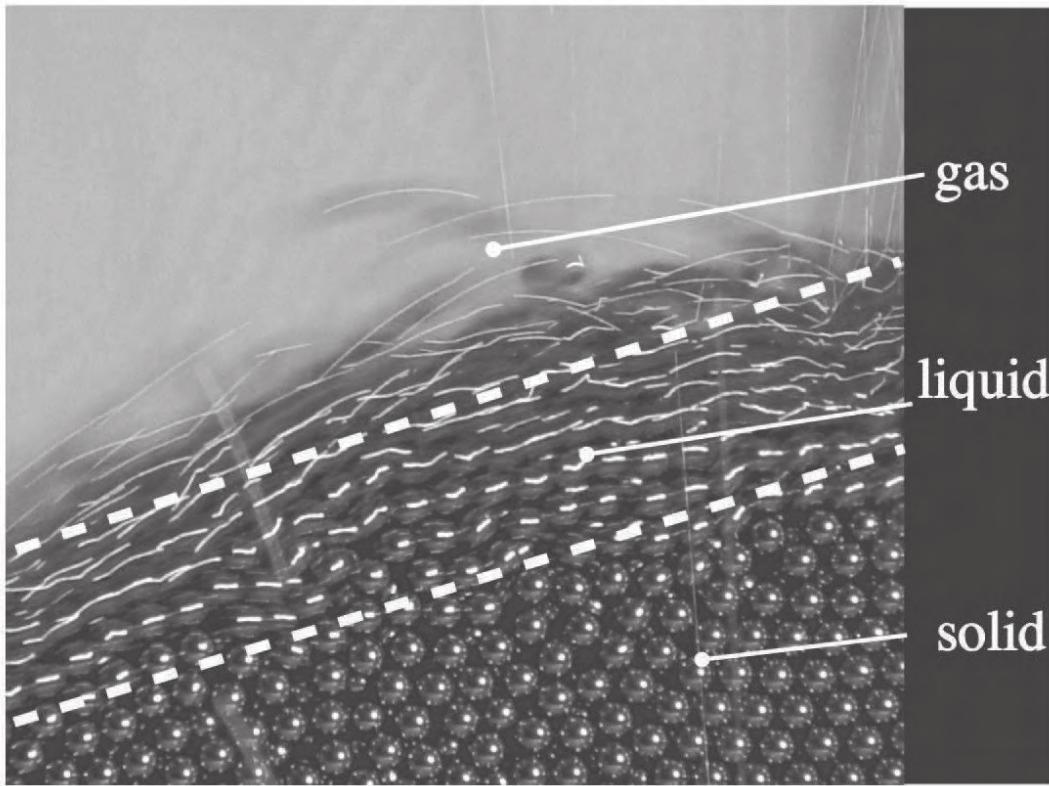


Figure 2 – Example of three granular phases according their kinetic energy. Dashed line is a proposition of the phase-like separations. The gas-like, referred as gas in the Figure, phase is much more agitated and the contact between grains in this region is rare, compared to the other phases-like. The liquid-like phase, referred as liquid in the Figure, is able to move, but still the slide each other. The solid-like phase, referred as solid in the Figure, is an immobile region that grains are in contact each other and this contact does not change over time. Figure taken from [2].

while wet granulars have van der Waals forces in grain-to-grain interactions. In this thesis, we will only consider repulsive contact interactions, although in some cases, there is a fluid surrounding the material. We consider that all the material that is involved by the fluid does not suffer forces of attraction, and therefore, van der Waals force is not included in the interaction between the grains.

2.2 Fenomenology

Perhaps the first image related to granular materials remit to the sand pile. In this case, a static pile of sand is heaped on a surface. In a pile like the one shown in Figure 3, the deposition of the grains forms an angle θ_m as large as possible, called the angle of movement, and when more material is placed on the pile, the upper layers of the pile run down to the base, restoring the angle to the lowest value θ_r , called the angle of repose [3, 5]. The rearrangement of the sand pile after the avalanche can be understood as an example of

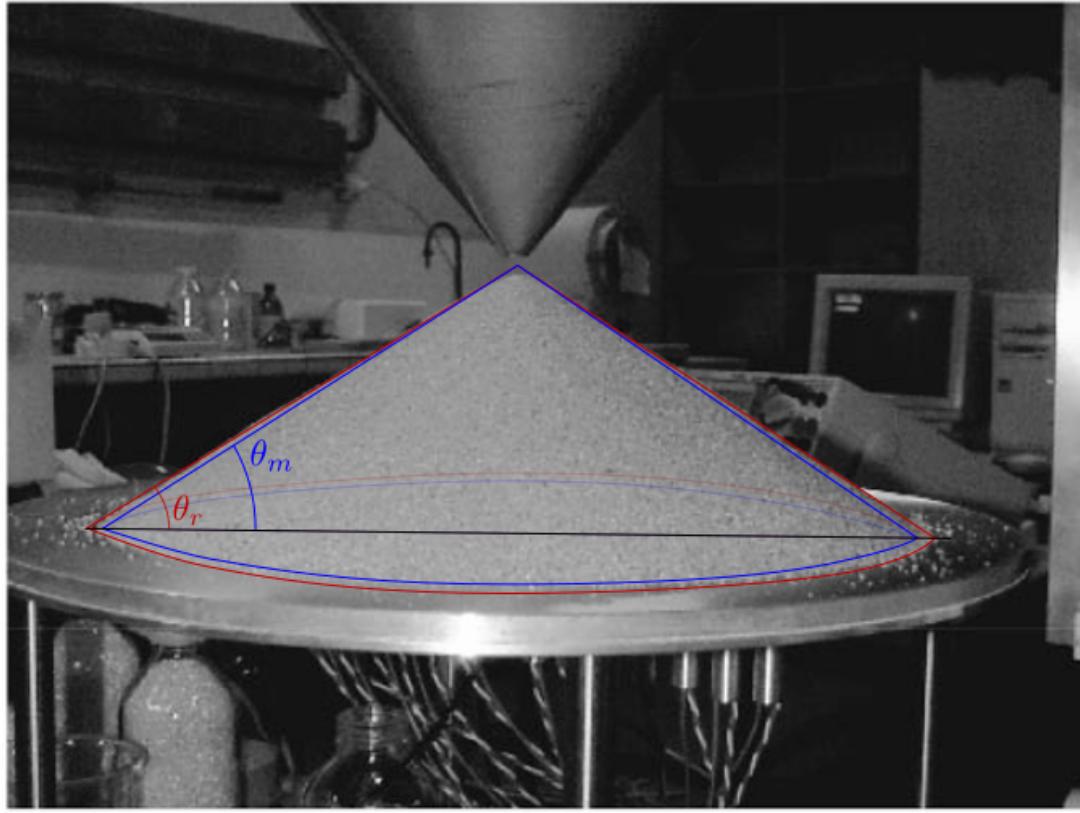


Figure 3 – Example of angle of repose θ_r and angle of movement θ_m in sand. The common values for these angles are $\theta_r = 33^\circ$ and $\theta_m = 35^\circ$. Figure taken from [34].

self-organized criticality in granular materials. A good approximation to the angle of repose is given by:

$$\tan(\theta) = \mu_s, \quad (1)$$

where θ is the angle of repose, and μ_s is the coefficient of static friction of the material's surface.

A system which has no central controller, governed by various agents that interact with rules known in the interaction of agents, and exhibit unforeseen property feature a Complex System. A characteristic property of Complex Systems and granular materials is self-organization. Some authors [26, 27, 28, 29, 30, 31, 32, 33] classify granular materials within the area of study Complex Systems.

Avalanche is the process phenomena that dropping some few grains in a pile part of the surface slides.

Also in sand piles, the preparation method of the system is reflected in the angle of repose [35]. This preparation history allows the system to be configured differently, and therefore, the angle of repose can assume different values using the same material. The angle of repose depends on the relaxation mode in which the pile was made: an inertial mode that relaxation is faster, and a collective mode that relaxation is slower. These dynamics in the angle of repose are called bistability of the angle of repose.

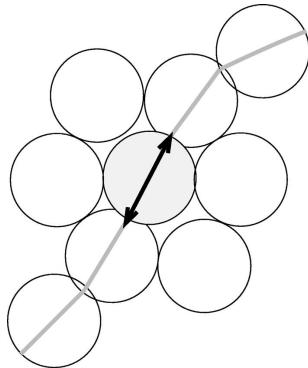


Figure 4 – Portion of an idealized force chain. The transmission of the force coincides with the direction of the contacts between grains, forming a path. Figure taken from [36].

Another common property of dense granular materials is the force chain, which is the force arrangement through the compressed media. Force chains carry most part of the forces of the media and usually the compression stress coincide with the direction of the force chain [36, 37]. The number of grains carrying larger force than the average force decays exponentially with increasing contact force. The force chain is a pathway that the force is transmitted, as shown in Figure 4. The interconnection between two or more branches of force chains forms a force network. The force network is then a subset of the contacts network. The experimental importance of visualizing the chain forces lies in understanding the distribution of the internal forces that sustains the material. As an example, Figure 5 reveals the chain of forces due point force applied on the top of the granular material.

Chains of forces are important to understand the phenomenon that is present in the arching effect. Arches are collective structures that have mutual support, and, consequently, a chain of forces linking the entire structure, being able to support their own weight and that of all the grains above, preventing them from flowing. In the formation of arches, segregation effects can occur, as verified by Magalhães, C. [15] and the flow regimes in a funnel reported by Magalhães, F. [39]. Figure 6 is an example of arch and its chain forces.

To better comprehend the rheology of dense granular materials, there is also the stress tensor, which is a macroscopic quantity of the outer product of contact force between grains and the displacement vector around the analyzed volume [5, 41, 42, 43, 44]. The stress tensor in granular materials shows us the preferable direction of a force propagation in the general form, and with it, one can infer how this granular assembly was built [34], like in Figure 7.

An evidence that the preparation history changes the configuration of the material is described in the references [34, 38]. The circular base shown in Figure 7 was made with two different depositions and the pressure profile is measured along the center. In the experiment, the pressure measured at the base varies according to the deposition, with the deposition made from the funnel having a maximum peak pressure around 0.25 and 0.5 of

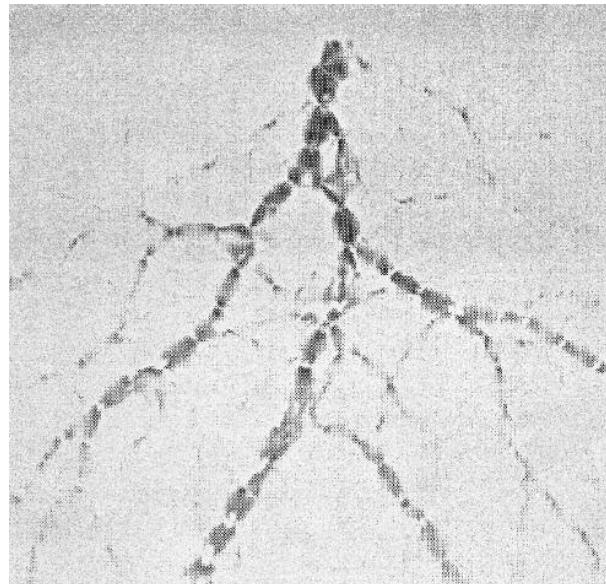


Figure 5 – The application of a point force on top of the material results in the chain of forces, which can be seen in the system's response function, after the gravitational component was subtracted from it. In this case, the system contains photoelastic grains in a two-dimensional space. Photoelastic grains diffract light differently when a force is applied on it. The force applied on a photoelastic grain produces different tensions, which can be seen by lighting it with a polarized light, and then a polarizing plate blocks the non polarized light. The darker, the greater the stress in the material. Figure taken from [38].

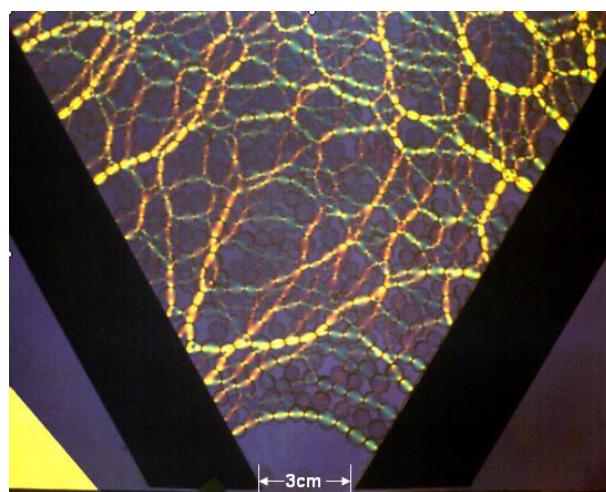


Figure 6 – Arch formation in a funnel. Photoelastic grains were used to display the chain forces, and clearly there is a blocking arch with a chain force sustaining all grains above. Figure taken from [40].

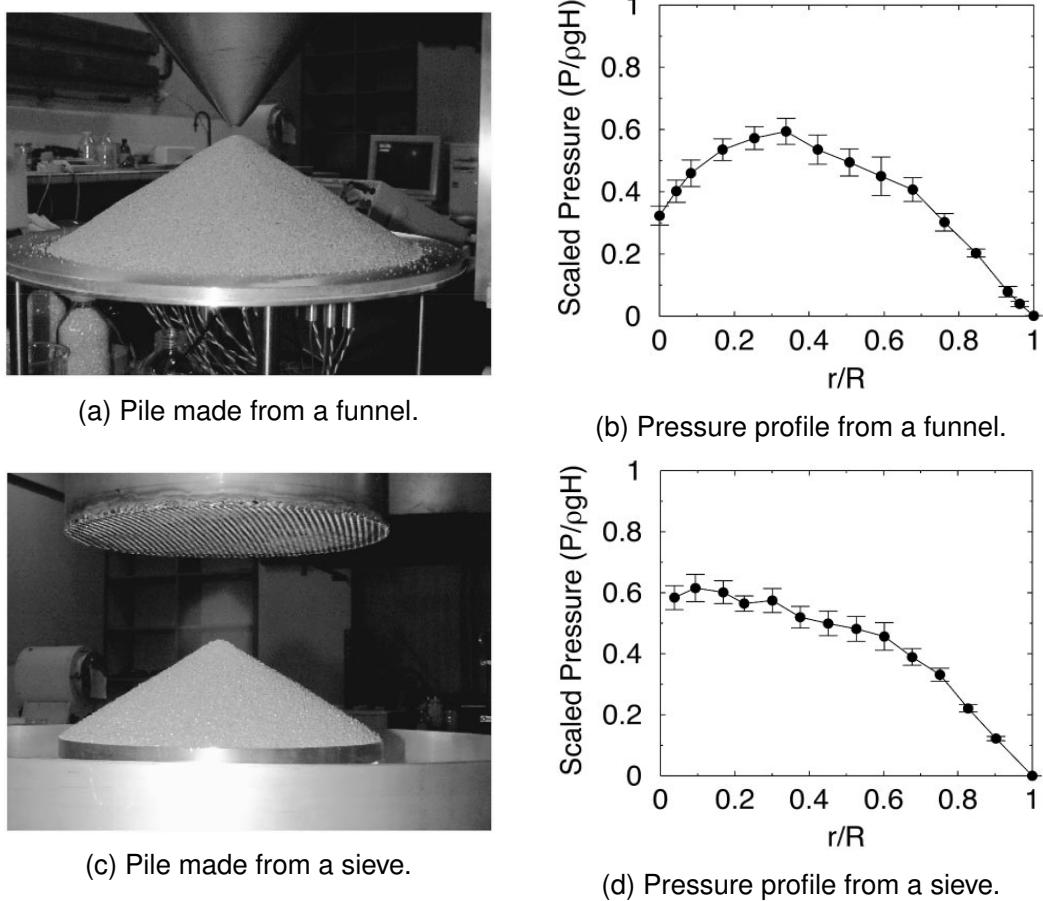


Figure 7 – The preparation of the sand piles reflects on the pressures measured at the bottom of the pile. In the Panels 7a and 7b the deposition from the funnel creates a pressure profile that peaks outside the center of the pile, while in the Panels 7c and 7d the deposition from the sieve creates a pressure profile that has a plateau and decays on the edges. Figures taken from [34].

the table radius r/R , while in the table deposition made from the sieve presents pressure as a kind of plateau between the center of the table and 0.25 of the radius r/R , with the maximum close to the center.

A study by Atman *et al.* [38] shows that different preparation histories of granular materials result in different response functions. As an example, Figure 8 shows two different responses, comparing different geometries of grains: circular and pentagonal. This means that when a localized force is applied over a granular assembly composed by organized assemblies, like the circular grains configuration shown in Panel 8a, the distribution caused by this force, spreads concentrated in two diagonals; while the localized force is applied over a disordered granular assembly, like this pentagonal grains configuration shown in Panel 8b, the distribution caused by this force, spreads more uniformly and deeper than the case applied to organized assembly. The response function of this example is the measurement of the stress after applying the load subtracted from the same preparation before applying the load.

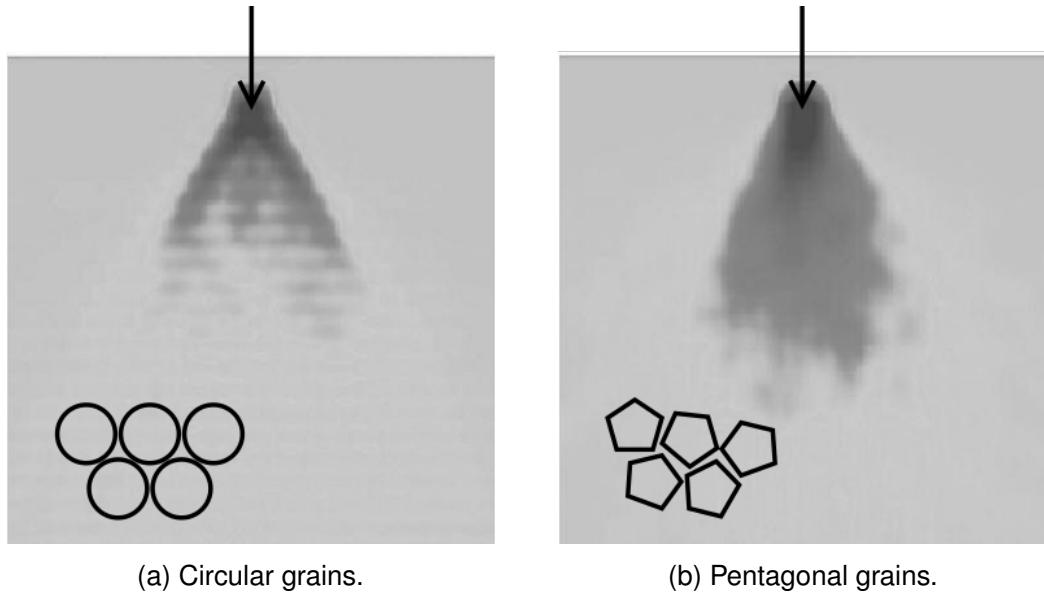


Figure 8 – Different granular systems exhibit different response functions. The main difference between these systems is that Panel 8a has higher organization and circular grains, while Panel 8b has higher disorder and pentagonal grains. Figures taken from [38].

Response function is the response of a system based on different times of the same system, when an input is applied on this different times, then the difference of the states results in the response of this input [4].

One rich property that many researches studied [15, 39, 45, 46, 47] is the jamming effect. Jamming or clogging, is the effect that dense granular materials suffer when a load is applied and these grains do not move. The consequence is that arch may form to hold the material, as in figure 6, but also a cavity may appear if an object is dragged from the inside, like figure 9.

Looking at the scales of granular materials, five separated scales are modeled, according to Radjai *et al.* [49], as shown in Figure 10. From now on, when referred to micro-scale, we are talking about dynamics or measures that accounts the effects on contacts or in particles, like rheological models of grains and inter-particle forces. Meso-scale are the structure of packing, like chain forces, local packing fraction and coordination number. Coordination number is the number of grains in contact with one single grain. Macroscale is related to the effects on the material and the process, like the stress tensor of the agglomerate and the continuum description of granular materials [49].

When a wet confined granular material is under pressure, one can see that the liquid shrinks into the material. This phenomena may be contra-intuitive, since when a liquid is squeezed, it is expelled from the container. If the liquid is mixed with granular material, like sand and sea water on a beach, when someone steps on the sand, the surface near the feet becomes dry. This effect was reported by Reynolds [50].

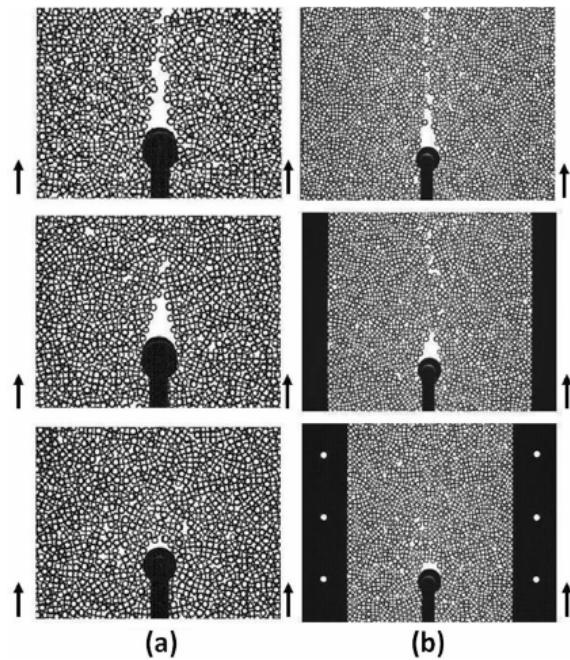


Figure 9 – The cavity behind the intruder varies according to the packing fraction. The packing fraction is increased in the left panels, from top to bottom as follows: $\phi = 0.8050$, $\phi = 0.8208$ and $\phi = 0.8262$, and they have width equals 13.475 times the intruder diameter. The right panels have packing fraction $\phi = 0.8035$ and widths, from top to bottom, equals 10.9, 8.5 and 6.9 times the intruder diameter. Figure taken from [48].

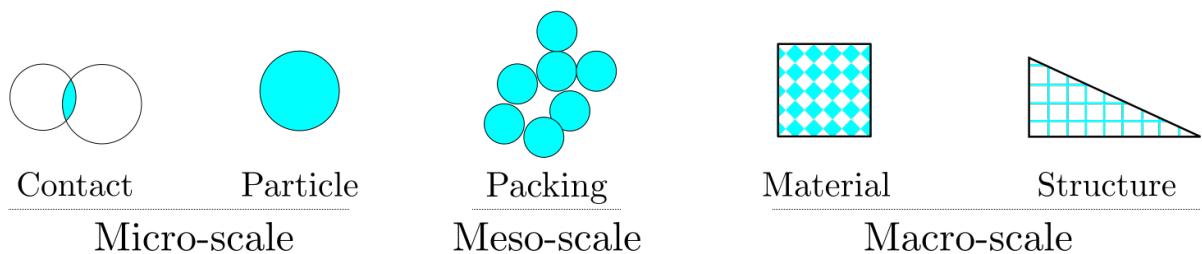


Figure 10 – Scales present in granular measures and effects. The smaller ones are in the contact scale, like contact forces while the higher ones are in landscape scale, like mountains and tectonic formation. Figure adapted from [49].

In the next chapter, we will describe the equations and procedures to carry out simulations of granular materials, taking account the contact model to simulate dry granular systems.

3 Discrete Element Method - DEM

Numerical simulations are widely used to study granular systems, which play an important role in complementing experimental information, which further enhances the understanding of granular physics phenomena. A justification to the use of numerical simulations is the precise control of the input parameters of the simulations and the level of complexity about the object of study. Another advantage is the ease extraction of data, from the grain scale, such as force chains, up to the system scale, such as material shear, showing possible emerging properties and their causes.

The technique to simulate of granular materials that we use in this work is a DEM known in the literature as Molecular Dynamics (MD). The method consists of numerically solving the Newton's laws of motion. An advantage of this method is that any force that can describe the interaction with the elements is accepted in this method.

The technique described in the reference [11] uses the formalisms of analytical mechanics through the interaction potentials between agents, whether Lagrangian or Hamiltonian potentials, to establish the forces acting on each agent. The disadvantage of this type of description is that dissipative forces may not appear, since the description of forces is directly related to potentials. Formally, the system must obey the set of Equations described by the Lagrangian function of the system:

$$\mathcal{L} = \mathcal{T} - \mathcal{V}, \quad (2a)$$

$$\sum_k \left[\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right) - \left(\frac{\partial \mathcal{L}}{\partial q_k} \right) \right] = 0, \quad (2b)$$

$$\vec{F}_i = \nabla \mathcal{L} = -\nabla \mathcal{V}, \quad (2c)$$

where \mathcal{L} represents the Lagrangian function that governs the dynamics of the system, \mathcal{T} the kinetic energy, \mathcal{V} the potential energy, k the number of generalized coordinates of the system, q_k the generalized coordinates, \dot{q}_k the generalized velocities, \vec{F}_i the force exerted on the particle i originated by the gradient of the potential \mathcal{V} .

Other references [1, 7, 15, 24, 39, 41, 42, 43, 51, 52, 53, 54, 55] use the model directly from the acting forces about each element.

3.1 Equations of motion

To carry out the simulation, the set of Equations 14 must be satisfied, which takes into account Newton's laws of motion. Thus, there is information on the agents' states as a

function of time.

$$Translational \begin{cases} \vec{r}_i(t) = \vec{r}_i(0) + \int_0^t \vec{v}_i(t) dt, \\ \vec{v}_i(t) = \vec{v}_i(0) + \int_0^t \vec{a}_i(t) dt, \\ \vec{a}_i(t) = \sum_j \frac{\vec{F}_{i,j}(t)}{m_i}, \end{cases} \quad (3a)$$

$$Rotational \begin{cases} \theta_i^k(t) = \theta_i^k(0) + \int_0^t \vec{\omega}_i^k(t) dt, \\ \vec{\omega}_i^k(t) = \vec{\omega}_i^k(0) + \int_0^t \vec{a}_i^k(t) dt, \\ \vec{a}_i^k(t) = I_i^{k-1} \sum_j \vec{\tau}_{i,j}^k(t), \end{cases} \quad (3d)$$

$$(3e) \quad (3f)$$

where i is the i -th particle of the system, $\vec{r}_i(t)$ is the position vector of the center of mass of the body i at the instant of time t , $\vec{v}_i(t)$ or $\vec{r}_i(t)$ is the velocity vector of the center of mass of the body, $\vec{a}_i(t)$ or $\vec{v}_i(t)$ or $\vec{r}_i(t)$ is the vector of accelerations of the center of mass of the body, $\vec{F}_{i,j}(t)$ is the component of the force that the center of mass of the body suffers from interacting with another body or field j , m_i is the body mass, $\theta_i^k(t)$ is the basis of the body rotation coordinates expressed in the system's k basis, $\vec{\omega}_i^k(t)$ is the pseudovector of angular velocities of the body expressed on the basis k of the system, $\vec{a}_i^k(t)$ is the pseudovector of angular accelerations of the body, I_i^{k-1} is the inverse of the inertia tensor of the body and $\vec{\tau}_{i,j}^k(t)$ is the torque vector that the body suffers from interacting with another body or field. Remembering that the relationship between torque and the force that causes it can be described by the Equation 15:

$$\vec{\tau}_{i,j}(t) = \vec{\chi}_{i,j}(t) \times \vec{F}_{i,j}(t), \quad (4)$$

where the vector $\vec{\tau}_{i,j}(t)$ is the cross product of the vector $\vec{\chi}_{i,j}(t)$, which connects the center of mass of the particle i to the point of application of the force, and the vector $\vec{F}_{i,j}(t)$, the vector of the force caused by interacting with another body or field j . The Equations 14c and 14f express Newton's second law.

The formulation described by the set of Equations 14 covers spaces in 1D, 2D and 3D, but this thesis focuses only on the formulation of 2D systems.

3.1.1 Force model

The forces present in the systems modeled in this Chapter include the contact forces between agents, which belong to the rheological model of grains and the gravitational force. The interaction forces between grain and fluid is described in Chapter 6.

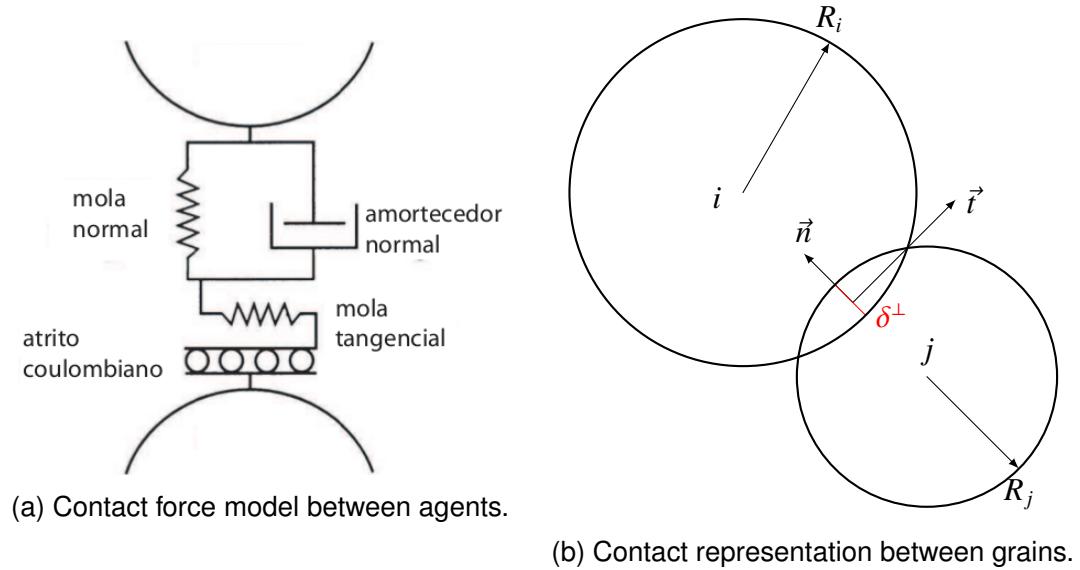


Figure 11 – Force model and representation between two circular grains. Figures taken from [1].

3.1.1.1 Rheological model of grains

The rheological model of the contact between grains we used to simulate granular materials was the rheological model proposed by Kelvin-Voigt [56, 57]. Kelvin-Voigt rheology models the contact force between two grains by a spring and a damper in parallel in the normal direction of contact, as exemplified in Figure 29. The spring portion represents the elastic contribution of the material, related to the Young's modulus, while the damper has the function of dissipate the energy in the inelastic collision between the grains. Additionally, a spring-like element is inserted in the tangential direction. A model proposed in [15] adds a damper-like element in parallel to the tangential spring, modeling the rolling resistance. We chose to use circular geometry for the grains. Because of the circular geometry, all angular momentum variation is caused by torque due to tangential force.

A peculiarity of DEM is that it allows interpenetration between the grains. Therefore, in this model there is no deformation in the contact between two bodies. The maximum interpenetration we allow in our model is controlled by the material's hardness parameter and we impose a maximum penetration of 0.5% of the radius.

To determine the value of the interpenetration, δ , in circular geometry, the Equation 16:

$$\delta_{i,j}^{\perp} = (R_i + R_j - |\vec{r}_j - \vec{r}_i|) \mathcal{H}(R_i + R_j - |\vec{r}_j - \vec{r}_i|), \quad (5)$$

where $\delta_{i,j}^{\perp}$ is the value of the interpenetration between the grains i and j , R_i is the radius of the body i , R_j is the radius of the body j , \vec{r}_i is the position vector of the center of the body i , \vec{r}_j is the position vector of the center of the body j and \mathcal{H} is the Heaviside step function. So, when the distance between the bodies is greater than the sum of the radii, the bodies will not be in contact and the Heaviside step function indicates that the interpenetration

between the grains is null. If the distance between the bodies is lesser than the sum of the radii, the bodies will be in contact and the Heaviside step function indicates that there is interpenetration between grains, by its value being equals to one.

With grains being in contact, the direct consequence of the interpenetration is the appearance of an elastic repulsive force, and the force depends on the interpenetration function δ^\perp . The force expression can be calculated by the Equation 17:

$$\vec{F}_{i,j}^{el} = -k_n (\delta_{i,j}^\perp)^{\frac{D}{2}} \hat{n}_{i,j}, \quad (6)$$

where $\vec{F}_{i,j}^{el}$ is the elastic force that the body j causes to the body i when they come in contact, k_n is the constant related to the elasticity of the material in the direction of contact, $\delta_{i,j}^\perp$ is the interpenetration between the bodies i and j , D is the dimension of the system (in this case, $D = 2$) and $\hat{n}_{i,j}$ is the normal direction of the contact [1, 15, 58]. One can write a potential for this elastic force as: $\mathcal{V} = \frac{1}{2} k_n (\delta_{i,j}^\perp)^2$.

Associated with the elastic force, the damping force is also present. As it is a dissipative force, a potential cannot be associated with the damping force. Most of the energy loss of granular materials is in collision. The Equation 18 describes its behavior:

$$\vec{F}_{i,j}^{am} = -\gamma (\vec{v}_{i,j} \cdot \hat{n}_{i,j}) \hat{n}_{i,j}, \quad (7)$$

where $\vec{F}_{i,j}^{am}$ is the damping force that the body j causes to the body i when they come in contact, γ is the damping constant related to the inelastic collision, $\vec{v}_{i,j}$ is the relative velocity between the centers of mass of bodies i and j and $\hat{n}_{i,j}$ is the normal contact direction [1, 15, 55].

The damping constant is directly linked to the restitution coefficient and can be used equivalently through the transformation shown in the set of Equations 8. Some authors use the restitution coefficient in simulations, such as [24, 51, 55]. In this thesis we will use the damping constant.

$$\epsilon = \exp\left(\frac{-\pi}{\sqrt{\frac{4k_n m}{\gamma^2} - 1}}\right), \quad (8a)$$

$$\gamma = \sqrt{\frac{4k_n m}{\left(\frac{\pi}{\ln(\epsilon)}\right)^2 + 1}}, \quad (8b)$$

where ϵ is the restitution coefficient, γ is the damping constant, k_n is the constant related to the elasticity of the material in the direction of contact and m is the reduced mass $m = \frac{m_i m_j}{m_i + m_j}$.

The friction force is also present in the simulation model. As the surfaces are in contact, there will be a frictional force between them if they tend to move each other. In particular, due to the circular geometry, friction forces will only act in the tangential direction.

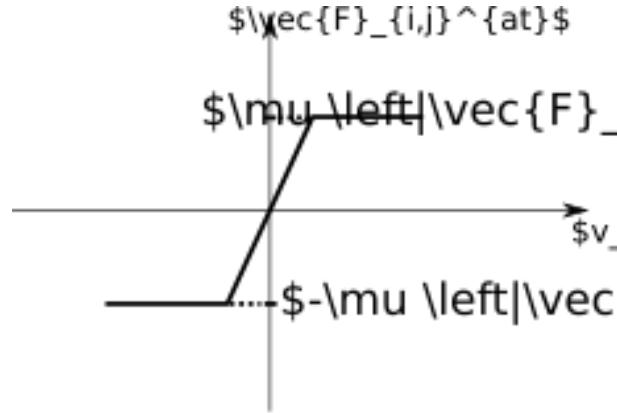


Figure 12 – Friction versus relative velocity between contact. Figure taken from [15].

The relative velocity between the contact point of the bodies is given by the Equation 19 below:

$$\delta_{i,j}^{\parallel} = \vec{v}_{ij} \cdot \hat{t}_{ij} - R_i \omega_i - R_j \omega_j, \quad (9)$$

where $\delta_{i,j}^{\parallel}$ is the relative velocity of the contact point of the bodies i and j , \vec{v}_{ij} is the relative velocity of the centers of mass of the bodies i and j , \hat{t}_{ij} is the tangential vector to the contact surfaces of the bodies i and j , R_i is the radius of the body i , R_j is the radius of the body j , ω_i is the angular velocity of the body i and ω_j is the angular velocity of the body j .

For the tangential force, it is necessary to know the relative displacement of the contact point, as given by the equation 19, applied in the system of Equations 20, which models the friction force with saturation, and is given by:

$$\vec{F}_{i,j}^{at} = \begin{cases} - \int_{t_0}^{t_f} k_t \delta_{i,j}^{\parallel} \hat{t}_{ij} dt, & \text{if } k_t |\delta_{i,j}^{\parallel}| \leq \mu |\vec{F}_{i,j}^n| \quad (\text{Static friction}) \\ - \frac{\delta_{i,j}^{\parallel}}{|\delta_{i,j}^{\parallel}|} \mu |\vec{F}_{i,j}^n| \hat{t}_{ij} & \text{if } k_t |\delta_{i,j}^{\parallel}| > \mu |\vec{F}_{i,j}^n| \quad (\text{Kinetic friction}) \end{cases}, \quad (10)$$

where $\vec{F}_{i,j}^{at}$ is the friction force between the bodies i and j , k_t is the elastic constant of the material in the tangential direction, $\delta_{i,j}^{\parallel}$ is the relative velocity between the contact point of the bodies i and j , \hat{t}_{ij} is the tangential vector to contact surfaces of bodies i and j , μ is the friction coefficient between the surfaces of bodies i and j and $\vec{F}_{i,j}^n = \vec{F}_{i,j}^{el} + \vec{F}_{i,j}^{am}$ is the force normal to the surfaces of bodies i and j .

We chose to model static and dynamic friction to be a single value for simplicity, presented the friction coefficient μ . Figure 12 describe the Coulomb friction we are using in the simulations.

3.1.1.2 The external force: Gravity

For this model, the gravitational influence is approximated by a constant, since the simulation does not take into account that the influence of the bodies' mass is very small, if

compared to the mass of the planet where the simulation is located, as well as the variation of height of the simulated system is very small and is close to the surface of the planet when compared to the radius of the planet. For convenience, we normalize gravity as a unit value.

3.1.2 Temporal discretization

For the computational simulation of solid bodies, the kinematics equations must be rewritten as Taylor series expansions, and we chose the interpolating the velocity equation system by the algorithm known as Velocity Verlet [59, 11]. The equations of motion discretized in time, as a function of the time step Δt , become as in the set of equations 38:

$$\vec{r}_i^{n+1} = \vec{r}_i^n + \vec{v}_i^n \Delta t + \frac{\vec{a}_i^n}{2} (\Delta t)^2, \quad (11a)$$

$$Translacional \left\{ \begin{array}{l} \vec{v}_i^{n+1} = \vec{v}_i^n + \frac{\vec{a}_i^n + \vec{a}_i^{n+1}}{2} \Delta t, \\ \vec{a}_i^{n+1} = \frac{\sum_j \vec{F}_{i,j}^{n+1} + \sum \vec{F}_{i,ext}^{n+1}}{m_i}, \end{array} \right. \quad (11b)$$

$$(11c)$$

$$\theta_i^{n+1} = \theta_i^n + \vec{\omega}_i^n \Delta t + \frac{\vec{\alpha}_i^n}{2} (\Delta t)^2, \quad (11d)$$

$$Rotacional \left\{ \begin{array}{l} \vec{\omega}_i^{n+1} = \vec{\omega}_i^n + \frac{\vec{\alpha}_i^n + \vec{\alpha}_i^{n+1}}{2} \Delta t, \\ \vec{\alpha}_i^{n+1} = I_i^{-1} \sum_j \vec{\tau}_{i,j}^n, \end{array} \right. \quad (11e) \quad (11f)$$

where i is the index of the moving body, j is the index of the body in contact with the body i , n is the time step, \vec{r} is the position of the body, \vec{v} is the velocity of the body, \vec{a} is the acceleration of the body, Δt is the size of the time step, $\vec{F}_{i,j}$ is the contact force between the bodies i and j , \vec{F}_{ext} are the external forces, such as gravity, m is the mass of the body, θ is the angular position of the body, $\vec{\omega}$ is the angular velocity of the body, $\vec{\alpha}$ is the angular acceleration of the body, $\vec{\tau}$ is the torque on the body, I is the moment of inertia of the body.

The set of Equations 38 is written for the 2D system, since there is only one degree of freedom for the rotation, and consequently all equations are written as a function of a single parameter. The velocity approximation as the weighting between the accelerations in the current and future instants of time is the key to the minimization of the imprecision generated by the discretization [11].

3.2 Algorithm

In addition to the equations that govern the system, a series of procedures must be carried out so that the simulation can take place. Each of these steps are essential for the simulation to take place, and are dependent on each other. The Algorithm 7 determines the

routines for executing the simulation. We use the 3rd order Gear Predictor-Corrector with the Velocity Verlet to perform the simulations [11].

Algorithm 1: Given the input of the problem, such as initial positions of bodies, velocities and accelerations, the algorithm assembles a list of bodies that are neighbors delimited by a certain region, then predicts the position and velocity of the bodies at the next instant of time, looks for the contacts that were formed with the prediction, calculates the forces between each body in contact and includes the external forces, and corrects the velocity and acceleration predictions for each body. Thus a DEM step is constructed. Algorithm taken from [1].

```

Input :initial simulation data setup
Output :response and simulation measurements over time
while not reached the stop condition of the simulation do
    if it is time to List the Neighbors then
        | List the Neighbors;
    end
    Predictor;
    Detect Contacts;
    Force Calculation;
    Corrector;
end
```

The algorithm stopping conditions depend on the purpose of the simulation. Some examples, such as static pile stability, energy fluctuations, breaking of force chains, average system velocity, number of time steps, among several other measurable parameters within the simulation can become the stopping criteria of the simulation. In this thesis, we use the number of simulation time steps as the main stopping criterion.

We will briefly discuss each of the routines Algorithm 7. For more details, the references [1, 11, 55] have further explanations about the routines, with examples and detailed algorithms.

3.2.1 Neighbors

Although not the simplest form of the Neighbor-Finding algorithm, it is the most efficient, and is described in [1]. It consists of creating a list of all bodies that belong to a certain region of possible interaction. Creating the list minimizes the number of comparisons during execution, which provides the highest computational performance. The article "Methods of parallel computation applied on granular simulations"[60] reveals the differences between some methods of creating lists of interacting bodies. This article was written during the preparation of this thesis project and is in the Appendix A. The Algorithm 8 refers to the creation of a list of bodies that have the possibility of interacting with each other.

Algorithm 2: Algorithm for creating the list of neighbors. Algorithm taken from [1].

Input: body position
Output: neighbor list
 Divide the space in regions;
foreach body **do**
 | Insert the body in the list of the region it belongs to;
 | Insert the body into adjacent lists of the region it belongs to;
end

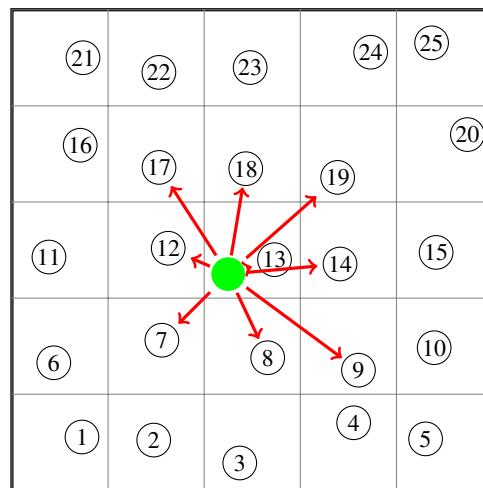


Figure 13 – A busca realizada no algoritmo 8 ocorre entre os corpos com sua região de vizinhança imediatamente adjacente. Figura retirada de [1].

The figure 30 shows the regions that the marked body should be listed. For more details, see the references [1, 11].

3.2.2 Predictor

The prediction routine updates the positions and velocities of the bodies, allowing all forces to be calculated based on the new values. In the set of Equations 38, equations involving terms with index n are updated in this routine. The 9 algorithm shows the structure of the prediction routine.

Algorithm 3: Prediction routine for state variables of bodies. Algorithm taken from [1].

Input :positions, velocities, accelerations and the time step Δt
Output :positions, part of the velocities
forall bodies **do**
 | Calculate new postions;
 | Predict new velocities;
end

3.2.3 Detect contacts

The contact detection routine uses the list of neighbors generated by the Algorithm 8 to check whether the listed body/neighbor pair has interpenetration, described in equation 16, and then generates a new list of bodies that interpenetrate each other to be used in the Algorithm 11. The Algorithm 10 describes this operation.

Algorithm 4: Detect contacts routine. Algorithm taken from [1].

```

Input : Neighbor list
Output : Contact list
forall neighbor bodies do
    Calculate the Interpenetration  $\delta_{i,j}$  between bodies  $i$  and  $j$ ;
    if  $\delta_{i,j} > 0$  then
        | Insert the pair  $i$  and  $j$  in the contact list;
    end
end
```

3.2.4 Force calculation

The routine to calculate the forces uses the contact list generated by the Algorithm 10 to calculate the contact forces between the bodies, such as elastic forces (Equation 17), damping forces (Equation 18) and friction forces (Equation 20). In addition to contact forces, bodies are subjected to gravitational force. The Algorithm 11 contains the execution of the calculation of the forces.

3.2.5 Corrector

The correction routine updates the speeds and accelerations of the bodies. The forces calculated in the force calculation are used here to perform the Velocity Verlet and determine the velocities and accelerations for the next time step. In the set of Equations 38, the equations involving terms with index $n + 1$ are updated in this routine. The Algorithm 12 shows the structure of the correction routine.

3.3 Important parameters

Due to the presented force model, some parameters are important for the simulations. As they are governed by difference equations as a function of the temporal parameter, some criteria must be obeyed for the simulation to be stable. One of the parameters is the time constant Δt , which in our simulations has a direct relationship with the oscillation period of the spring mass model (Kelvin-Voigt rheology), given by $\Delta t = \zeta \sqrt{m_{min}/k_n}$, where ζ is an adjustment value, m_{min} is the smallest mass of the system, and k_n is the spring constant. The

Algorithm 5: In this routine, the resultant forces are calculated for each body. The force \vec{N} is the normal force, contribution of the elastic force \vec{F}^{el} and the damping force \vec{F}^{am} (Equations 17 and 18), F^d is the rolling force of one body on the other, which must be compared with the maximum static friction force μN . Algorithm taken from [1].

```

Input :positions, velocities and contact list
Output :acting forces and torques in the bodies
foreach body do
    Apply gravity force;
    foreach body in the contact list do
        Calculate the normal forces  $\vec{N}$ ;
        Calculate the rolling forces  $F^d$ ;
        if  $|F^d| < \mu|\vec{N}|$  then
             $\vec{F}^{at+} = \vec{F}^d\hat{t}$ ;
        else
             $\vec{F}^{at+} = \mu\text{sign}(\vec{F}^d)N\hat{t}$ ;
        end
        Calculate torque;
    end
end

```

Algorithm 6: Rotina de correção das variáveis dos corpos. Retirado de [1].

```

Entrada :resultante das forças e o passo de tempo  $\Delta t$ 
Saída :estado dos corpos prontos para o próximo passo de tempo
foreach corpo do
    Calcular as acelerações;
    Corrigir as velocidades;
end

```

factors that stabilize the simulations, they must have $\zeta < 1/10$ [1, 15, 11]. In this thesis we will use the factor of 1/10 for non-vibrated systems and 1/100 for vibrated systems.

Another important parameter is the damping factor γ , or the restitution coefficient ϵ . Due to the dissipative nature of granular materials, $\epsilon \approx 0$, which approximates $\gamma \approx 2\sqrt{k_n m_{min}}$, because we will have critical regimes in the spring mass equation when we use the smallest mass of the two bodies, and for all others, the damping will be subcritical [53, 51].

We model the walls for the BNE problem as smooth walls. The technique we use is to create a virtual body that has only the fixed component that it does a boundary, while it is free to move in the other direction, coinciding to be in the closest position of the free bodies.

In the next chapter we will describe the Brazil nut Effect (BNE) and how we set up the simulation that leads to this effect.

4 Brazil Nut Effect (BNE)

Historically, the phenomenon known as BNE was identified in Brazil nut exports, which were taken in containers on ships leaving Brazil, and whenever they arrived at their destination, it was observed that the largest nuts were at the top. Initially it was thought that Brazilian traders arranged the nuts so that the largest were on top and the smaller and broken ones at the bottom. After investigation, it was verified that the larger nuts rise due to the vibration that the containers suffered during transport [15].

The BNE occurs when grains of different sizes segregate, causing larger grains segregate from smaller ones. The segregation effect can be seen when a system is shaken, or a shear cycle is imposed [5]. This phenomenon is associated with the granular phase of the system. In a solid-like granular system, the larger grain is static. With agitation, the system changes to a liquid state, allowing the movement of grains in the system [61]. The movement of the material occurs in convection currents that form close to the walls, or with the ratchet effect [62, 63, 64], both cases allow small grains fill the space previously occupied by the larger grain, rising the larger grain. Figure 18 shows the evolution of the convection currents in a confined media. Once smaller grains collectively move to fill the void left by larger grains, smaller grains impede their downward motion; these correlations are at the basis of the observed size segregation. The ratchet effect is the granular solid-like behavior in below larger grains and the granular liquid-like behavior, where larger grains can move. The ratchet effect is also related to the Reynolds dilatancy, since the stress increases and the granular configuration changes.

One of the firsts attempts to explain the BNE was made by Rosato *et al.* [61] using Monte Carlo simulations and inspired many works to classify the roles of the parameters. As an example of the larger grain rising with respect to time, Figure 15.

The most important number used in the BNE studies is the dimensionless accele-



Figure 14 – Evolution of the vibrated bed. Top Panels are without intruder, while bottom Panels are with an intruder. Black and yellow layers are made of mustard grains. Figure taken from [62].

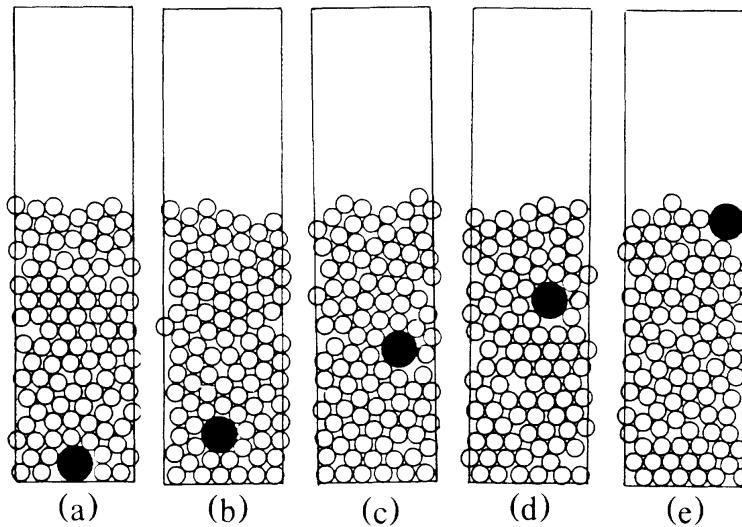


Figure 15 – Temporal evolution of shaken system of particles with periodic boundary conditions using Monte Carlo simulation. Initial configuration in Panel (a) and equally time spaced from Panels (a) to (e). Figure taken from [61].

ration, shown in the equation 12. The dimensionless number is a comparison between the maximum amplitude of the vibrational acceleration and gravity.

$$\Gamma = \frac{A\omega^2}{g}, \quad (12)$$

where Γ a dimensionless number that compares shaken acceleration with gravity, A is the system amplitude of the vibration, ω is the frequency of vibration, and g is the value of gravity. When $\Gamma > 1$, then the intruder can rise, since the ascending part of the oscillation rises the magnitude of the chain forces in the media, but when the system is descending the lighter grains occupies the void space left by the bead, causing the ratchet effect. If $\Gamma < 1$, then the intruder is not able to move, since chain forces stays there. This is the basic explanation, but not all cases work like it, as we see in some of our simulations, in Chapter 5.

An experimental problem is proposed in [63], like we study in Chapter 5. In their experiment a metallic bead is placed at bottom and then agitated. They use a cylinder silo and spherical grains with size ratio between intruder and media of 3, and Γ varies from 2.6 to 3.4, which leads the bead to rise over the media. There is a collapse of the curves involving the intruder position, the amplitude of the vibration A and the oscillation period ω like in figure 16. What we could find in our simulations is that frictionless walls also cause the bead to rise through convection currents, and the ascent ratio is similar with and without friction on the walls, see Figure 25.

The BNE is also influenced by the fluid that surrounds the media. In some cases, the air is relevant in the convection currents, and then leading to segregation, while vacuum leads to mixing [65, 63]. A more viscous fluid than air, like water, changes the regime of ascension of the bead, and the main mechanism that explains it is not the drag it self but the

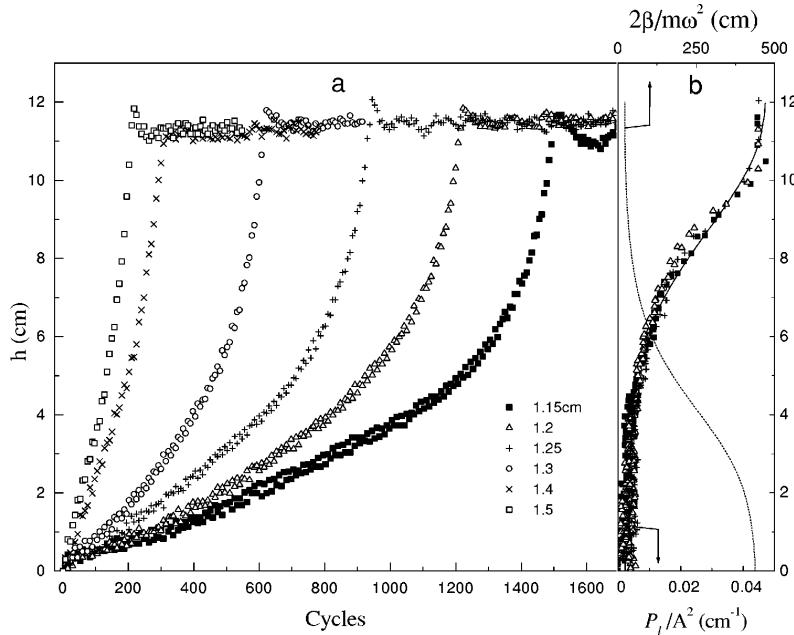


Figure 16 – Evolution of the bead in an agitated media within a cylinder silo. Panel (a) shows the height of the intruder versus time, while Panel (b) shows the collapse of the curves. Figure taken from [63].

enhance of the ratcheting effect [64].

Several phase diagrams were observed for some of the BNE parameters. The two main variables usually analysed are the ratio of the diameters of grains and the ratio of densities of grains, as shown in Figure 17. Another BNE phase diagram proposed by [62] takes into account the dimensionless acceleration Γ and the vibration threshold velocity $v_c = A\omega$.

Another correlated phenomena to BNE is the Reverse BNE (RBNE), in which the bead instead of rises it sinks. Many works enhanced the characterization of BNE and RBNE, in theoretical field, experimental results and numerical simulations [66, 67??, 68, 69, 70, 71, 72, 73, 74]. Some of these diagrams are presented here in Figures 19, 21 and ??.

Recently the Reference [75] experimentally shows that in a mixture of irregular ellipsoidal shape firstly reorient vertically, but without changing significantly their height; secondly, the grains rise upwards, and while doing so, they still tend to stay vertically aligned; and finally, when the grains reach the top, they tend to realign horizontally on the surface.

If the intruder of the media has a non uniform distribution geometry, like a polar particle, inserted in a layer of circular grains, and when the media is agitated, the intruder starts to "self-propel" at the direction it is oriented [76]. This is another property that non uniform shaken granular exhibit, reorienting the position or "propelling-itself".

Next Chapter, we describe the results of our BNE simulations using the techniques presented in Chapter 3.

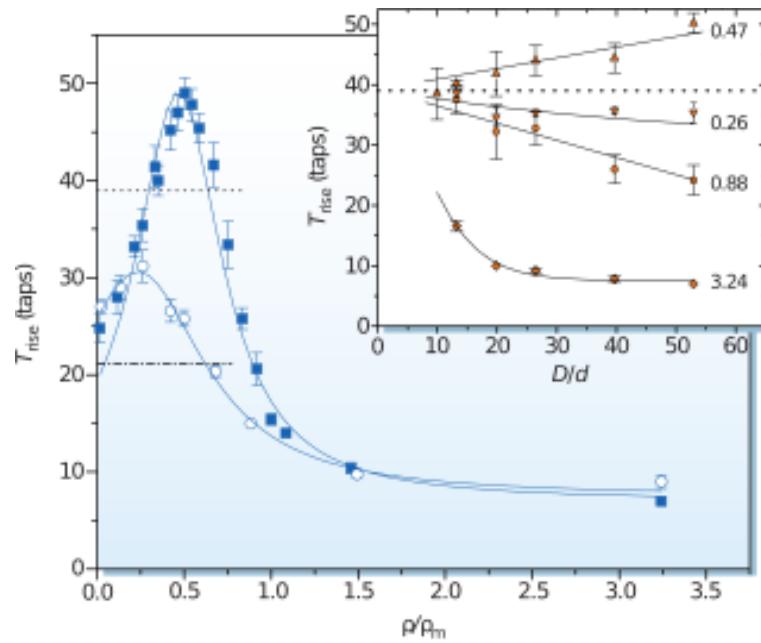


Figure 17 – BNE dependence on density and size ratio. The ascent time T_{rise} in the main Panel versus density rate, with size ratio of 5.08 between intruder and grains with different atmospheric pressures: 1 atm. in squares (■) and 90 torr in circles (○). The ascent time T_{rise} versus the size ratio for different density ratios: 0.44, 0.48, 0.88 and 3.1. Figure taken from [65].

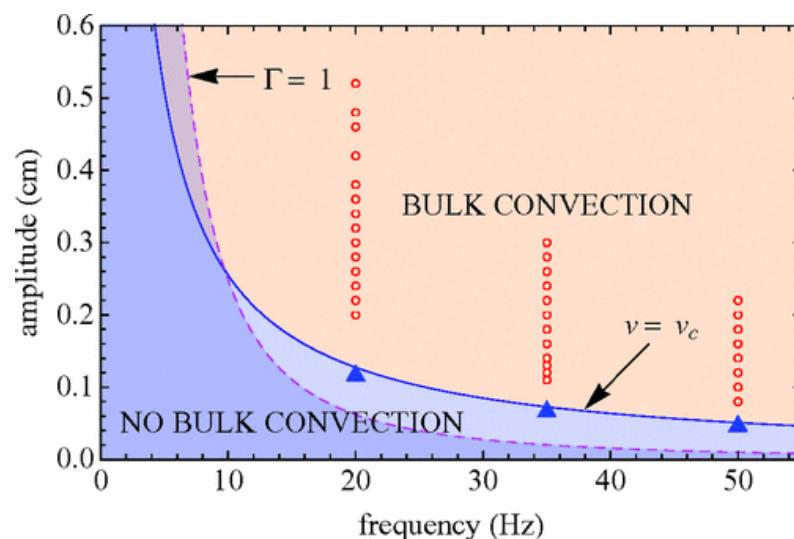


Figure 18 – BNE dependence on the dimensionless acceleration Γ and a critical velocity v_c . Values of $\Gamma < 1$ makes the intruder not rise, but also a $v < A\omega$. Figure taken from [62].

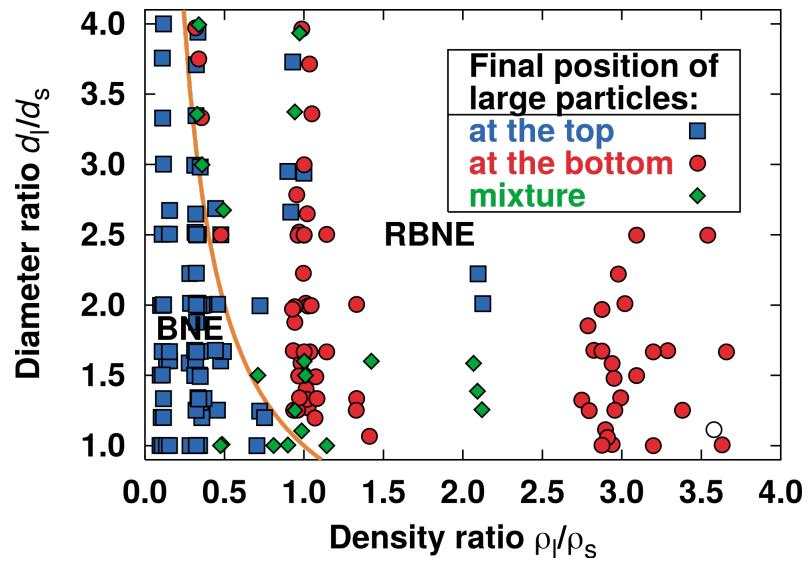


Figure 19 – BNE and RBNE dependence on the density ratio and the size ratio in vibrated base. The diagram shows the regime where beads rises in blue (■) causing the BNE, sinks in red (■) and is mixed in green (■). Figure taken from [71].

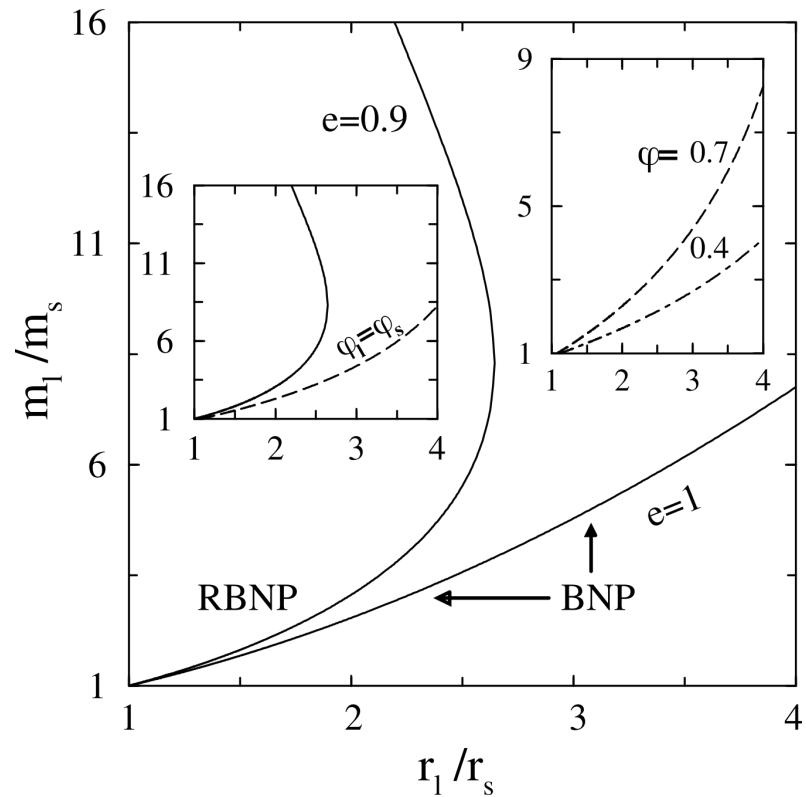


Figure 20 – BNE and RBNE dependence on the density ratio and the size ratio in vibrated base. The diagram shows the BNE-RBNE regime extracted from analytical equations of the forces in the system. e is the restitution coefficient, ϕ is the packing fraction, ϕ_l is the portion of the packing fraction related to the intruders, ϕ_s is the packing fraction of the other grains. Left inset: phase diagram with $e = 0.9$, $\phi_l/\phi_s = 10^{-8}$ (solid curve) and $\phi_l/\phi_s = 1$ (dashed curve). Right inset: phase diagram with $e = 0.9$, $\phi_l/\phi_s = 1$, $\phi = 0.7$ (dashed curve) and $\phi = 0.4$ (dot-dashed curve). Figure taken from [72].

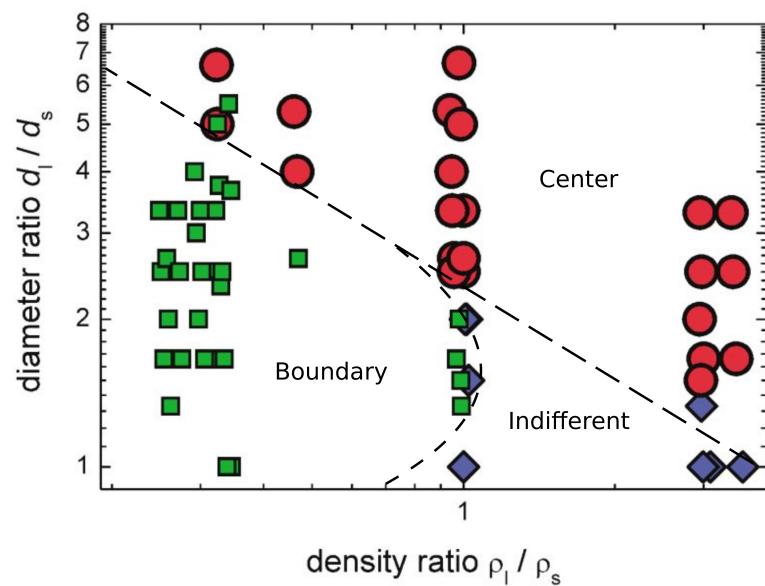


Figure 21 – BNE and RBNE dependence on the density ratio and the size ratio in swirling base. The diagram shows the regime where beads segregates in red (●), aggregates in green (■) and is indifferent in blue (◆). Figure taken from [66].

5 Análise e Discussão dos Resultados

- BNE

Nesta parte da tese, utilizaremos 2500 grãos. O diâmetro médio do grão é $d = 1 \pm 2.5\%$, distribuídos uniformemente. O diâmetro do intruso é de $D = 5$ vezes o diâmetro médio dos grãos. A densidade de todos os grãos é a mesma, e vale $\rho = 1/\pi$, e portanto a massa média dos grãos é de $m = 0,25$, exceto quando estiver ressaltado nas figuras. A constante de mola na direção normal é de $k_n = 1000$ e a tangencial é de $k_t = 750$. A atuação do amortecedor é no regime crítico ($\gamma = 2\sqrt{mk}$), e vale aproximadamente $\gamma = \sqrt{10}$. O atrito dos grãos valem $\mu = 0,5$, tanto entre grãos, quanto entre paredes, quando houver. O passo de tempo ($dt = pT$) vale aproximadamente $dt = \frac{1}{2000\sqrt{10}}$, utilizando a fração de $p = 0,01$ do período de oscilação do modelo de contato massa mola $T = \sqrt{\frac{m}{k}}$. A largura da caixa é de $L = 37.5$ diâmetros de grão.

Inicialmente, estudamos o sistema com paredes no fundo e nas laterais, formando uma caixa. Observamos nestas simulações correntes de convecção próximos às paredes.

Percebemos que intrusos mais densos sobem mais lentamente que intrusos menos densos. Os tempos de subida, quando comparados, podem ser ordenados das figuras $23 < 22 < 24$. Assim como as correntes de convecção são mais intensas, o intruso sobe mais rapidamente e cai mais rapidamente, visto na amplitude de $\Gamma = 1,5$ para as figuras 23, 22 e 24, respectivamente.

Quando retirado o atrito entre os grãos e as paredes, temos que o efeito da con-

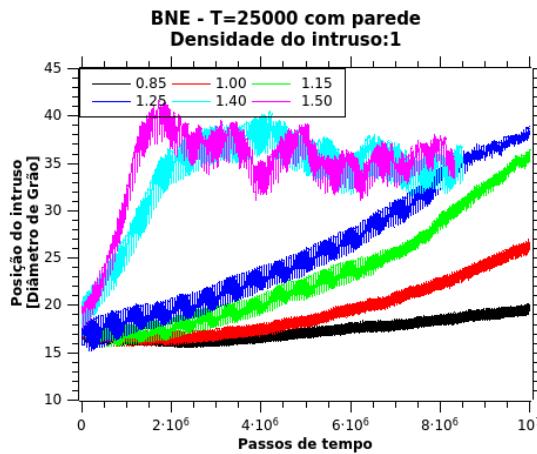


Figure 22 – Média de 10 amostras da subida do intruso em função do adimensional de aceleração. O período de agitação é de 25000 passos de tempo em uma forma senoidal. Este sistema possui atrito nas paredes e densidade do intruso igual a dos grãos.

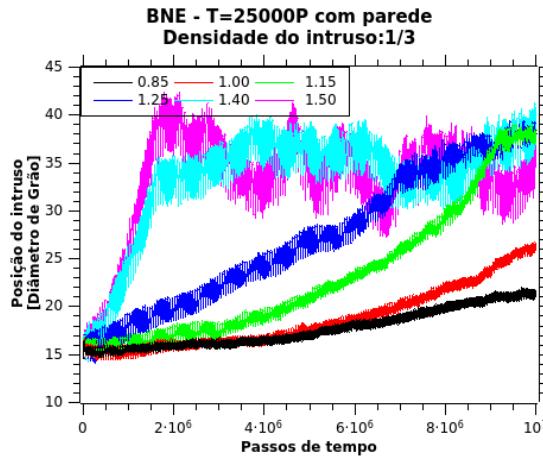


Figure 23 – Média de 5 amostras da subida do intruso em função do adimensional de aceleração. O período de agitação é de 25000 passos de tempo em uma forma senoidal. Este sistema possui atrito nas paredes e densidade do intruso é $\frac{1}{3}$ da densidade dos grãos.

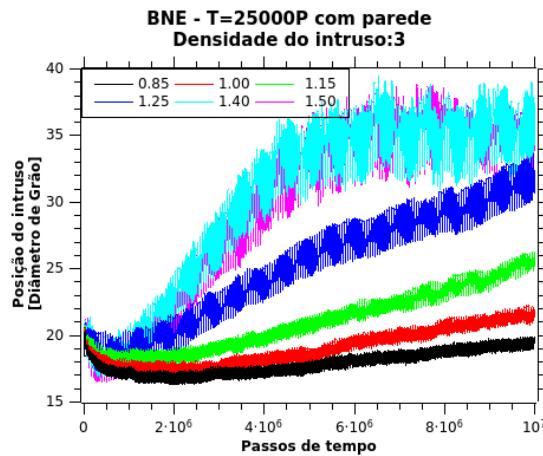


Figure 24 – Média de 5 amostras da subida do intruso em função do adimensional de aceleração. O período de agitação é de 25000 passos de tempo em uma forma senoidal. Este sistema possui atrito nas paredes e densidade do intruso é 3 vezes a densidade dos grãos.

vecção no sistema diminui, ocasionando em uma subida mais lenta que quando o atrito está presente. A figura 25 mostra a subida do intruso no sistema em que as paredes não possuem atrito.

Ao comparar os tempos de subida do sistema que possui atrito nas paredes (figura 22) com o sistema que não possui atrito nas paredes (figura 25), percebemos que o tempo de subida é maior, além de que o sistema que possui agitação menor que a gravidade não sobe, mostrando que um dos fatores que importam para o BNE são as correntes de convecção formadas próximas das paredes.

Quando retiramos o atrito do sistema, o intruso chega ao fundo do sistema, independente da amplitude de vibração. A figura 26 exibe o comportamento do intruso para o

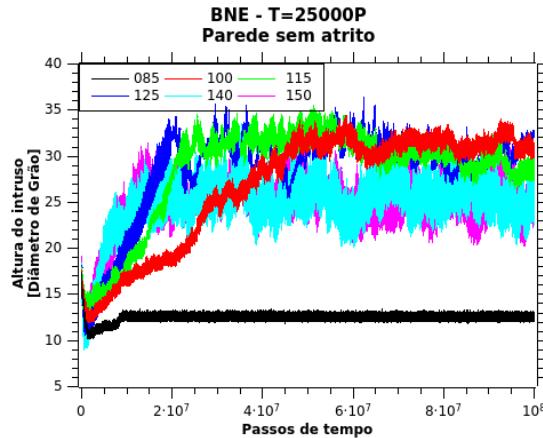


Figure 25 – Média de 3 amostras da subida do intruso em função do adimensional de aceleração. O período de agitação é de 25000 passos de tempo em uma forma senoidal. Este sistema não possui atrito nas paredes.

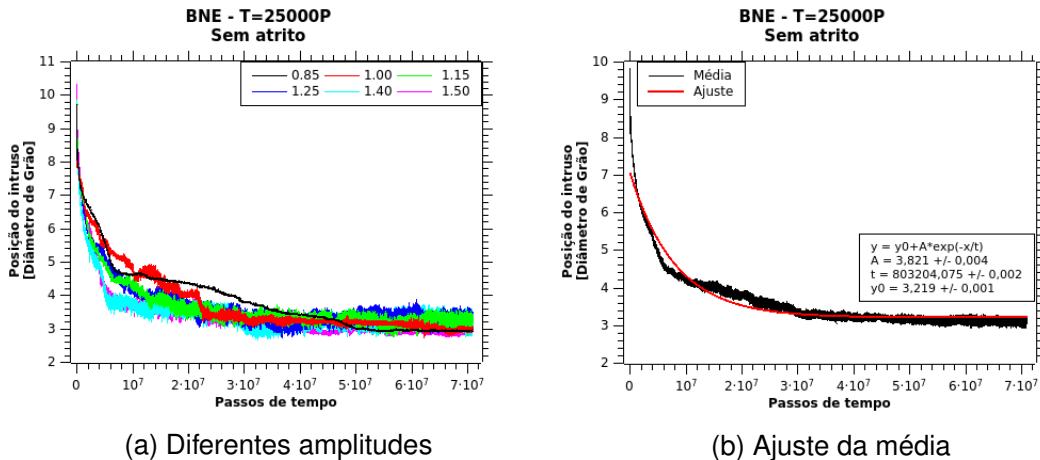


Figure 26 – Amostra da queda do intruso em função do adimensional de aceleração. O período de agitação é de 25000 passos de tempo em uma forma senoidal. Este sistema não possui atrito. A figura 26b possui a média das curvas apresentadas na figura 26a e uma o ajuste de um decaimento exponencial em função do tempo, da posição do intruso até o fundo do sistema.

sistema sem atrito.

Se ao invés de retirarmos o atrito, retirarmos as paredes laterais formando uma condição periódica de contorno de largura 28 diâmetros de grão, verificaremos que o *BNE* não acontece para o período de vibração de 25000 passos de tempo, como mostrado na figura 27.

Já no caso de períodos maiores, o *BNE* ocorre. A figura 28 exemplifica o *BNE* ocorrendo com condição periódica de contorno e período de vibração de 30000 passos de tempo.

Na figura 28b, percebemos que acelerações menores que a gravidade não fazem o intruso ascender, enquanto acelerações próximas da gravidade tem um movimento de

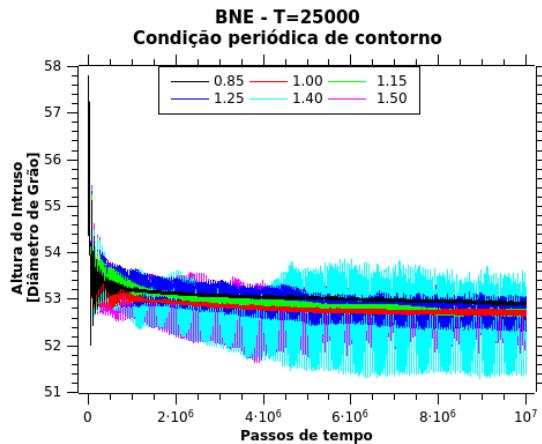


Figure 27 – Média de 5 amostras da posição do intruso em função do adimensional de aceleração. O período de agitação é de 25000 passos de tempo em uma forma senoidal. Este sistema não possui paredes, mas condição periódica de contorno.

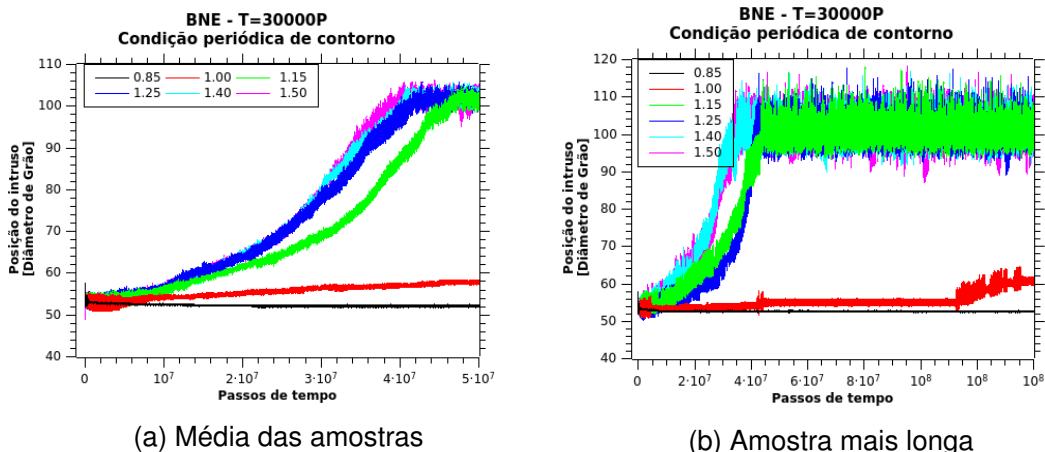


Figure 28 – Média de 10 amostras da subida do intruso em função do adimensional de aceleração. O período de agitação é de 30000 passos de tempo em uma forma senoidal. Este sistema não possui paredes, mas condição periódica de contorno. A figura 28b mostra a amostra com maior passos de tempo de simulação.

ascensão lento e em saltos. Por não haver paredes, as correntes de convecção não se formam no sistema, o que faz com que o intruso atinja o topo e não desça mais.

No próximo capítulo, descreveremos os modos de transporte de grãos quando arrastados por um fluido.

6 Methodology - CFD

Uma forma muito utilizada para estudar sistemas granulares é a realização de simulações numéricas, que têm um papel importante na complementação das informações experimentais, o que aumenta ainda mais a compreensão dos fenômenos da física granular. Uma justificativa é o controle preciso dos parâmetros de entrada das simulações e do nível de complexidade acerca do objeto de estudo. Outra vantagem é a facilidade da medição próxima da escala dos grãos, como as cadeias de forças, até a escala do sistema, como o cisalhamento do material, evidenciando eventuais propriedades emergentes e suas causas.

A técnica de simulação de materiais granulares que utilizamos neste trabalho é um *DEM* conhecido na literatura como Dinâmica Molecular, ou *Molecular Dynamics (MD)*. O método consiste em solucionar numericamente as equações de movimento quando aplicadas forças dinâmicas sobre os elementos a serem simulados. Uma vantagem deste método é que qualquer força que utilize parâmetros dentro da simulação e que possa ser descrita na interação com os elementos é aceita neste método.

A técnica descrita no livro *Computer Simulation of Liquids* [11] utiliza-se dos formalismos da mecânica analítica através dos potenciais de interação entre os agentes, sejam potenciais lagrangianos, sejam potenciais hamiltonianos, para estabelecer a força que atua sobre cada agente. A desvantagem deste tipo de descrição é que forças dissipativas podem não aparecer, uma vez que a descrição das forças está relacionada diretamente com potenciais. Formalmente, o sistema deve obedecer ao conjunto de equações 13 descritas pela função lagrangiana do sistema:

$$\mathcal{L} = \mathcal{T} - \mathcal{V}, \quad (13a)$$

$$\sum_k \left[\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right) - \left(\frac{\partial \mathcal{L}}{\partial q_k} \right) \right] = 0, \quad (13b)$$

$$\vec{F}_i = \nabla \mathcal{L} = -\nabla \mathcal{V}, \quad (13c)$$

sendo que a notação descrita pelo conjunto de equações 13, \mathcal{L} representa a função lagrangiana que rege a dinâmica do sistema, \mathcal{T} a energia cinética, \mathcal{V} a energia potencial, k o número de coordenadas generalizadas do sistema, q_k as coordenadas generalizadas, \dot{q}_k as velocidades generalizadas, \vec{F}_i a força exercida na partícula i originada pelo gradiente do potencial \mathcal{V} .

Já outras referências [1, 7, 52, 15, 53, 54, 39, 24, 51, 55] utilizam o modelo diretamente das forças que agem sobre cada elemento.

6.1 Equações de movimento

Para a realização da simulação, o conjunto de equações 14 deve ser satisfeito, o que leva em consideração as leis de Newton. Assim, tem-se a informação dos estados dos agentes em função do tempo.

$$\vec{r}_i(t) = \vec{r}_i(0) + \int_0^t \vec{v}_i(t) dt, \quad (14a)$$

$$Translacional \left\{ \begin{array}{l} \vec{v}_i(t) = \vec{v}_i(0) + \int_0^t \vec{a}_i(t) dt, \\ \vec{a}_i(t) = \sum_j \frac{\vec{F}_{i,j}(t)}{m_i}, \end{array} \right. \quad (14b)$$

$$(14c)$$

$$\theta_i^k(t) = \theta_i^k(0) + \int_0^t \vec{\omega}_i^k(t) dt, \quad (14d)$$

$$Rotacional \left\{ \begin{array}{l} \vec{\omega}_i^k(t) = \vec{\omega}_i^k(0) + \int_0^t \vec{a}_i^k(t) dt, \\ \vec{a}_i^k(t) = I_i^{k-1} \sum_j \vec{\tau}_{i,j}^k(t), \end{array} \right. \quad (14e)$$

$$(14f)$$

em que i é a i -ésima partícula do sistema, $\vec{r}_i(t)$ é o vetor de posição do centro de massa do corpo i no instante de tempo t , $\vec{v}_i(t)$ ou $\vec{r}_i(t)$ é o vetor de velocidade do centro de massa do corpo, $\vec{a}_i(t)$ ou $\vec{v}_i(t)$ ou $\vec{r}_i(t)$ é o vetor de acelerações do centro de massa do corpo, $\vec{F}_{i,j}(t)$ é a componente da força que o centro de massa do corpo sofre por interagir com outro corpo ou campo j , m_i é a massa do corpo, $\theta_i^k(t)$ é a base das coordenadas de rotação do corpo expressas na base k do sistema, $\vec{\omega}_i^k(t)$ é o pseudovetor de velocidades angulares do corpo expressas na base k do sistema, $\vec{a}_i^k(t)$ é o pseudovetor de acelerações angulares do corpo, I_i^{k-1} é o inverso do tensor de inércia do corpo e $\vec{\tau}_{i,j}^k(t)$ é o vetor de torques que o corpo sofre por interagir com outro corpo ou campo. Lembrando que a relação entre o torque e a força que o causa pode ser descrita pela equação 15:

$$\vec{\tau}_{i,j}(t) = \vec{\chi}_{i,j}(t) \times \vec{F}_{i,j}(t), \quad (15)$$

sendo que o vetor $\vec{\tau}_{i,j}(t)$ é o produto vetorial entre o vetor $\vec{\chi}_{i,j}(t)$, que liga o centro de massa da partícula i ao ponto de aplicação da força, e o vetor $\vec{F}_{i,j}(t)$, o vetor da força causada por interagir com outro corpo ou campo j . As equações 14c e 14f expressam a segunda lei de Newton.

A formulação descrita pelo conjunto de equações 14 abrange espaços em 1D, 2D e 3D, porém esta tese foca apenas na formulação de sistemas em 2D.

6.1.1 Modelo de forças

As forças presentes nos sistemas modelados nesta tese incluem as forças de contato entre os agentes, que pertencem ao modelo reológico dos grãos, as forças de interação entre grão e fluido e a força gravitacional.

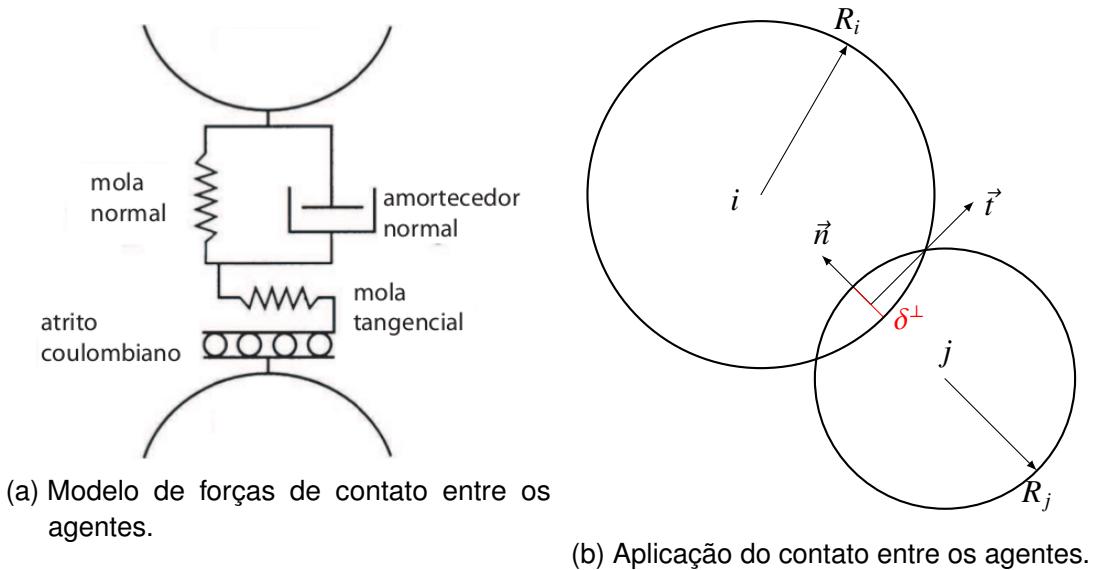


Figure 29 – Modelo de forças e a aplicação do contato entre os agentes. Figuras retiradas de [1].

6.1.1.1 Modelo reológico

O modelo reológico dos agentes utilizado na simulação de *MD* para materiais granulares foi proposto por Kelvin-Voigt [1], com geometria circular pelos agentes. A reologia de Kelvin-Voigt modela a força de contato por uma mola e um amortecedor em paralelo na direção normal do contato, como exemplificado na figura 29. A parcela da mola representa a contribuição elástica do material, relacionado com o módulo de Young, enquanto o amortecedor tem a função de atenuar a energia na colisão inelástica entre os grãos. Adicionalmente, um elemento parecido com uma mola é inserido na direção tangencial. Um modelo proposto em [15] adiciona um elemento parecido com um amortecedor em paralelo à mola tangencial, modelando a resistência ao rolamento. Por causa da geometria circular, toda a variação de momento angular é causada pela força tangencial.

Uma peculiaridade da *MD* é a permissão de inter penetração entre os grãos, e portanto, neste modelo não há deformação no contato entre dois corpos. A inter penetração máxima é controlada pelo parâmetro de dureza do material e impõe penetração de 0.5% dos raios.

Para encontrar o valor da inter penetração δ , na geometria circular, a equação 16:

$$\delta_{i,j}^{\perp} = \left(R_i + R_j - |\vec{r}_j - \vec{r}_i| \right) \mathcal{H}(R_i + R_j - |\vec{r}_j - \vec{r}_i|), \quad (16)$$

em que $\delta_{i,j}^{\perp}$ é o valor da inter penetração entre os grãos i e j , R_i é o raio do corpo i , R_j do corpo j , \vec{r}_i é o vetor de posição do corpo i , \vec{r}_j é o vetor de posição do corpo j e \mathcal{H} é a função de degrau de Heaviside. Então, quando a distância entre os corpos for maior que a soma dos raios, os corpos não estarão em contato e a função degrau de Heaviside indica que a inter penetração entre os grãos é nula.

Com o contato entre os grãos, a consequência direta da interpenetração é o surgimento de uma força elástica repulsiva ao contato, e dependente da função de interpenetração δ^\perp . A expressão da força pode ser calculada pela equação 17:

$$\vec{F}_{i,j}^{el} = -k_n (\delta_{i,j}^\perp)^{\frac{D}{2}} \hat{n}_{i,j}, \quad (17)$$

em que $\vec{F}_{i,j}^{el}$ é a força elástica que o corpo i sente ao entrar em contato com o corpo j , k_n é a constante relacionada a elasticidade do material na direção do contato, $\delta_{i,j}^\perp$ é a interpenetração entre os corpos i e j , D é a dimensão do sistema (no caso, $D = 2$) e $\hat{n}_{i,j}$ é a direção normal do contato [1, 15, 58]. Pode-se escrever um potencial para esta força elástica como: $\mathcal{V} = \frac{1}{2} k_n \delta_{i,j}^{\perp 2}$.

Associado à força elástica, também está presente a força de amortecimento. Por se tratar de uma força dissipativa, não se pode associar um potencial à força de amortecimento. A maior parcela da perda de energia dos materiais granulares está na colisão, e esta é a responsável. A equação 18 descreve seu comportamento:

$$\vec{F}_{i,j}^{am} = -\gamma (\vec{v}_{i,j} \cdot \hat{n}_{i,j}) \hat{n}_{i,j}, \quad (18)$$

em que $\vec{F}_{i,j}^{am}$ é a força de amortecimento que o corpo i sente ao entrar em contato com o corpo j , γ é a constante de amortecimento relacionada a inelasticidade da colisão, $\vec{v}_{i,j}$ é a velocidade relativa entre os centros de massa dos corpos i e j e $\hat{n}_{i,j}$ é a direção normal do contato [1, 15, 55].

A constante de amortecimento está diretamente ligada ao coeficiente de restituição e pode ser utilizada equivalentemente através da transformação mostrada em [1]. Alguns autores utilizam o coeficiente de restituição nas simulações, como [55, 51, 24]. Aqui, utilizaremos a constante de amortecimento.

A força de atrito também está presente no modelo de simulação. Como as superfícies estão em contato, existirá uma força de atrito entre elas, se houver tendência de movimento uma em relação à outra. Em especial, devido à geometria circular, as forças de atrito agirão apenas na direção tangencial. A velocidade de deslocamento entre os pontos de contato dos corpos é dada pela equação 19 a seguir:

$$\delta_{i,j}^{\parallel} = \vec{v}_{ij} \cdot \hat{t}_{ij} - R_i \omega_i - R_j \omega_j, \quad (19)$$

em que $\delta_{i,j}^{\parallel}$ é a velocidade relativa entre os pontos de contato dos corpos i e j , \vec{v}_{ij} é a velocidade relativa entre os centros de massa dos corpos i e j , \hat{t}_{ij} é o vetor tangencial às superfícies de contato dos corpos i e j , R_i é o raio do corpo i , R_j é o raio do corpo j , ω_i é a velocidade de rotação do corpo i e ω_j é a velocidade de rotação do corpo j .

Para a força tangencial, é necessário saber o deslocamento relativo dos pontos de contato, como dada pela equação 19, aplicados no sistema de equações 20, que modela a

força de atrito com saturação, e é dada por:

$$\vec{F}_{i,j}^{at} = \begin{cases} - \int_{t_0}^{t_f} k_t \delta_{i,j}^{\parallel} \hat{t}_{ij} dt, & \text{se } k_t |\delta_{i,j}^{\parallel}| \leq \mu |F_{i,j}^n| \quad (\text{Atrito Estático}) \\ - \int_{t_0}^{t_f} \frac{\delta_{i,j}^{\parallel}}{|\delta_{i,j}^{\parallel}|} \mu |F_{i,j}^n| \hat{t}_{ij} dt, & \text{se } k_t |\delta_{i,j}^{\parallel}| > \mu |F_{i,j}^n| \quad (\text{Atrito Cinético}) \end{cases}, \quad (20)$$

em que $\vec{F}_{i,j}^{at}$ é a força de atrito entre os corpos i e j , k_t é a constante elástica do material na direção tangencial, $\delta_{i,j}^{\parallel}$ é a velocidade relativa entre os pontos de contato dos corpos i e j , \hat{t}_{ij} é o vetor tangencial às superfícies de contato dos corpos i e j , μ é o coeficiente de atrito entre as superfícies dos corpos i e j e $\vec{F}_{i,j}^n = \vec{F}_{i,j}^{el} + \vec{F}_{i,j}^{am}$ é a força normal às superfícies dos corpos i e j .

6.1.1.2 A força externa: Gravidade

Para este modelo, a influência gravitacional é aproximada por uma constante, já que a simulação não leva em conta que a influência da massa dos corpos é muito pequena, se comparada com a massa do planeta em que está situada a simulação, bem como a variação de altura do sistema simulado é muito pequeno e está próximo à superfície do planeta, quando comparada com o raio do planeta. Por conveniência, normalizamos a gravidade como valor unitário.

6.1.1.3 As forças do fluido

A força que o fluido exerce sobre os corpos pode ser entendida como contribuição de diferentes modelos e casos. Uma formulação mais detalhada sobre cada parcela de forças que o fluido exerce sobre cada corpo é descrita pela equação 21:

$$\vec{F}_i^{Fluid} = \vec{F}_i^{Arch} + \vec{F}_i^{Drag} + \vec{F}_i^{Magnus} + \vec{F}_i^{Lift} + \vec{F}_i^{AddedMass} + \vec{F}_i^{Basset}, \quad (21)$$

em que \vec{F}_i^{Fluid} é a contribuição total das forças que o fluido exerce sobre o corpo i , \vec{F}_i^{Arch} é a força de Arquimedes sobre o corpo i , \vec{F}_i^{Drag} é a força de arrasto sobre o corpo i , \vec{F}_i^{Magnus} é a força de Magnus sobre o corpo i , \vec{F}_i^{Lift} é a força de sustentação sobre o corpo i , $\vec{F}_i^{AddedMass}$ é a força de adição de massa sobre o corpo i e \vec{F}_i^{Basset} é a força histórica de Basset sobre o corpo i . Como simplificação do modelo, utilizaremos apenas as forças de Arquimedes e as forças de arraste do fluido [13, 77, 78].

A força de Arquimedes pode ser escrita como na equação 22, enquanto a força de arraste pode ser escrita como na equação 23:

$$\vec{F}_i^{Arch} = \frac{\pi}{6} d_i^3 \vec{\nabla} \cdot \overline{\sigma}, \quad (22)$$

em que \vec{F}_i^{Arch} é a força de Arquimedes no corpo i , d_i é o diâmetro do corpo i e $\vec{\nabla} \cdot \overline{\sigma}$ é o divergente do tensor de tensão do fluido $\overline{\sigma}$, e:

$$\vec{F}_i^{Drag} = \frac{\pi}{8} \rho_f d_i^2 C_d(\mathcal{R}_u) |\vec{u}_f - \vec{v}_i| (\vec{u}_f - \vec{v}_i), \quad (23)$$

em que \vec{F}_i^{Drag} é a força de arraste no corpo i , ρ_f é a densidade do fluido, d_i é o diâmetro do corpo i , $C_d(\mathcal{R}_u)$ é o coeficiente de arrasto em função do número de Reynolds do corpo, descrito pela equação 24, \vec{u}_f é a velocidade do fluido, \vec{v}_i é a velocidade do corpo [77].

$$C_u(\mathcal{R}_u) = \left(\sqrt{C_d^\infty} + \sqrt{\frac{\mathcal{R}_u^c}{\mathcal{R}_u}} \right)^2 \quad (24)$$

em que $C_u(\mathcal{R}_u)$ é o coeficiente de arrasto em função do número de Reynolds do corpo, $C_d^\infty \approx 0.5$ é o coeficiente de arrasto do grão no limite turbulento ($\mathcal{R}_u \rightarrow \infty$), $\mathcal{R}_u^c \approx 24$ é o número de Reynolds de transição do corpo na qual o coeficiente de arrasto torna-se quase constante e a equação 25 que relaciona o número de Reynolds do corpo com os parâmetros do sistema:

$$\mathcal{R}_u = \frac{d_i}{\nu} |\vec{u}_f - \vec{v}_i| \quad (25)$$

em que d_i é o diâmetro do corpo i , ν é a viscosidade dinâmica do sistema, \vec{u}_f é a velocidade do fluido e \vec{v}_i é a velocidade do corpo i [77].

6.1.2 O modelo do fluido

Para o fluido, a equação geral que rege o sistema é a equação de Navier-Stokes, que é a aplicação da segunda lei de Newton para a massa específica em meios contínuos e a aplicação das leis de conservação de massa e de momento [12, 13]. Para a equação da conservação de massa, temos a equação 26:

$$\frac{\partial \rho^f}{\partial t} + \vec{\nabla} \cdot (\rho^f \vec{u}^f) = 0, \quad (26)$$

em que ρ^f é a densidade do fluido, e \vec{u}^f é a velocidade do fluido.

A equação 27 descreve a conservação do momento como:

$$\frac{\partial}{\partial t} (\rho^f \vec{u}^f) + \vec{\nabla} \cdot (\rho^f \vec{u}^f \otimes \vec{u}^f) = \bar{\bar{\sigma}} + p_{ext}, \quad (27)$$

em que ρ^f é a densidade do fluido, \vec{u}^f é a velocidade do fluido, $\bar{\bar{\sigma}}$ é o tensor tensão do fluido e p_{ext} é a pressão causada por agentes externos, como a gravidade e as forças dos corpos que interagem com o fluido.

Na formulação da conservação do momento, existe internamente a conservação da massa, e se escrevermos os termos da equação efetuando-se os produtos internos e as derivadas, teremos a equação 28, que é a equação de Navier-Stokes:

$$\rho^f \frac{\partial \vec{u}^f}{\partial t} + \rho^f (\vec{u}^f \cdot \vec{\nabla}) \vec{u}^f = \vec{\nabla} \cdot \bar{\bar{\sigma}} + p_{ext}, \quad (28)$$

em que ρ^f é a densidade do fluido, \vec{u}^f é a velocidade do fluido, $\bar{\bar{\sigma}}$ é o tensor tensão do fluido e p_{ext} é a pressão causada por agentes externos e que o tensor tensão do fluido pode ser

escrito em função das pressões internas e do cisalhamento do fluido, como na equação 29:

$$\overline{\overline{\sigma}} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} \\ \tau_{yx} & \sigma_{yy} \end{pmatrix}, \quad (29)$$

em que $\overline{\overline{\sigma}}$ é o tensor de tensão do fluido, σ são as componentes de tensão e a pressão do fluido é $p = -\frac{1}{2}(\sigma_{xx} + \sigma_{yy})$, e τ são as componentes do cisalhamento do fluido, sendo que $\tau_{xy} = \tau_{yx}$, indicando que são simétricas.

Uma importante medida é a taxa de deformação do fluido, dada pela equação 30:

$$\dot{\gamma}_{xy} = \frac{1}{2} \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right), \quad (30)$$

em que $\dot{\gamma}_{xy}$ e $\dot{\gamma}_{yx}$ são as componentes do tensor da taxa de deformação, u_x é a velocidade do fluido na direção de escoamento e u_y é a velocidade do fluido na direção da gravidade. As componentes $\dot{\gamma}_{xy}$ e $\dot{\gamma}_{yx}$ são simétricas, sendo também equivalentes às componentes cruzadas do divergente do campo de velocidades.

O cisalhamento do fluido controla algumas características do fluido, como por exemplo o regime de escoamento. A equação que rege o cisalhamento é a equação 36:

$$\tau = \rho^f (\nu + \nu_t) \dot{\gamma}, \quad (31)$$

em que τ é cisalhamento do fluido, ρ^f é a densidade do fluido, ν é a viscosidade intrínseca do fluido, ν_t é a viscosidade que insere turbulência no fluido e $\dot{\gamma}$ é o tensor da taxa de deformação do fluido e é descrito pela equação 30. Para que o escoamento seja laminar em um fluido newtoniano, o termo de viscosidade turbulenta deve ser nulo.

As considerações feitas sobre o fluido são que o fluido é incompressível, que o fluido não circula na direção da gravidade (direção x de escoamento), que possui condição periódica de contorno na direção de escoamento, ou seja, o que acontece de um lado do sistema é o mesmo que acontece no outro e o volume ocupado pelo fluido é o todo o volume não ocupado pelos corpos. As implicações destas condições simplificam as equações 26, 27 e 28. No caso da conservação da massa a implicação da incompressibilidade do fluido é a conservação do volume ao longo de todo o tempo e todo o espaço. Já a condição periódica de contorno na direção do escoamento, em relação à Navier-Stokes, equação 28, implica que a tensão na direção de escoamento seja nula, ou seja, $\sigma_{xx} = 0$ quando não houverem corpos. Para o fluido não circular na direção da gravidade, toda a camada de escoamento é tomada por uma média na direção do escoamento (direção x). Portanto, a simplificação do tensor de tensões do fluido resume-se na equação 32:

$$\vec{\nabla} \cdot \overline{\overline{\sigma}} = \frac{\partial \tau}{\partial y} \hat{x} - \frac{\partial p}{\partial y} \hat{y} \quad (32)$$

em que $\overline{\overline{\sigma}}$ é o tensor de tensão do fluido, τ é a componente do cisalhamento do fluido, p é componente da pressão do fluido, \hat{x} é a direção de escoamento do fluido e \hat{y} é a direção da gravidade.

Aplicando as considerações feitas sobre o fluido na equação de Navier-Stokes, equação 28, tem-se o sistema de equações em relações às direções de escoamento do fluido (x) e da gravidade (y) iguais a:

$$\left\{ \begin{array}{l} (1 - \phi)\rho^f \frac{\partial u_x^f}{\partial t} = (1 - \phi) \frac{\partial \tau}{\partial y} - p_x^{body} \\ 0 = -(1 - \phi) \frac{\partial \sigma_{yy}}{\partial x} - p_y^{body} + (1 - \phi)\rho^f g \end{array} \right. \begin{array}{l} : \hat{x}, \\ : \hat{y}, \end{array} \quad (33a)$$

em que ρ^f é a densidade do fluido, u_x^f é a componente da velocidade na direção do escoamento, ϕ é o coeficiente de compactação dos corpos, τ é a componente do cisalhamento do fluido, σ_{yy} é a componente da tensão no fluido, p_x^{body} é a pressão que os corpos fazem sobre a direção de escoamento x , p_y^{body} é a pressão que os corpos fazem sobre a direção gravitacional y e g é o valor da gravidade.

Para a taxa de deformação do fluido, a aplicação das considerações do fluido resulta na equação 34:

$$\dot{\gamma}_{xy} = \frac{\partial u_x}{\partial y}, \quad (34)$$

em que $\dot{\gamma}_{xy}$ é a componente do tensor da taxa de deformação, u_x é a velocidade do fluido na direção de escoamento e y é a direção da gravidade.

Existem vários modelos de turbulência para serem abordados em um fluido. Neste trabalho escolhemos o modelo de turbulência de Prandtl e o termo viscosidade turbulenta apresenta-se como na equação 35:

$$\nu_t = l^2 |\dot{\gamma}|, \text{ ou seja,} \\ \nu_t = l^2 \left| \frac{\partial u_x}{\partial y} \right|, \quad (35)$$

em que ν_t é o modelo da turbulência, l é um comprimento característico da turbulência e da vorticidade, $\dot{\gamma}$ é a taxa de deformação do fluido, u_x é a velocidade do fluido na direção de escoamento e y é a direção da gravidade.

O cisalhamento do fluido controla algumas características do fluido, como por exemplo o regime de escoamento. A equação que rege o cisalhamento é a equação 36:

$$\tau = \rho^f \left(\nu + l^2 \left| \frac{\partial u_x}{\partial y} \right| \right) \frac{\partial u_x}{\partial y}, \quad (36)$$

em que τ é cisalhamento do fluido, ρ^f é a densidade do fluido, ν é a viscosidade intrínseca do fluido, $l^2 \left| \frac{\partial u_x}{\partial y} \right|$ é a viscosidade que insere o efeito médio da turbulência no fluido e $\frac{\partial u_x}{\partial y}$ é o tensor da taxa de deformação do fluido e é equivalente à equação 30. Para que o escoamento seja laminar em um fluido newtoniano, o termo de viscosidade turbulenta deve ser nulo.

Para a mistura do fluido e do granular, tomamos o comprimento característico da turbulência sempre acima das camadas estáticas do material granular, e portanto

assumimos o comportamento descrito pela equação 37 do comprimento característico da turbulência proposto por van Driest [77]:

$$l(y_b) = \begin{cases} 0 & \text{se } y \leq y_b, \\ \kappa(y - y_b) \left[1 - e^{-(y-y_b)\frac{u_*}{\nu R_{vD}}} \right] & \text{se } y > y_b, \end{cases} \quad (37a)$$

$$(37b)$$

em que $l(y_b)$ é o comprimento característico da turbulência, $\kappa \approx 0,4$ é a constante de von Karman, y é a altura do fluido, y_b é a posição do topo da camada dos sólidos não transportados, u_* é a velocidade característica de cisalhamento imposta no topo do fluido, ν é a viscosidade do fluido e $R_{vD} \approx 26$ é o número Reynolds de van Driest [77]. Porém outros comprimentos característicos da turbulência foram levados em consideração e estão descritos nas referências [77, 78].

6.1.3 Discretização temporal

Para a simulação computacional dos corpos sólidos, as equações da cinemática devem ser reescritas como expansões da série de Taylor, interpolando o sistema de equações de velocidade pelo algoritmo conhecido como *Velocity Verlet* [59, 11]. As equações de movimento discretizadas no tempo, em função do passo de tempo Δt , tornam-se como no conjunto de equações 38:

$$\vec{r}_i^{n+1} = \vec{r}_i^n + \vec{v}_i^n \Delta t + \frac{\vec{a}_i^n}{2} (\Delta t)^2, \quad (38a)$$

$$Translacional \quad \vec{v}_i^{n+1} = \vec{v}_i^n + \frac{\vec{a}_i^n + \vec{a}_i^{n+1}}{2} \Delta t, \quad (38b)$$

$$\vec{a}_i^{n+1} = \frac{\sum_j \vec{F}_{i,j}^{n+1} + \sum \vec{F}_{i,ext}^{n+1}}{m_i}, \quad (38c)$$

$$\theta_i^{n+1} = \theta_i^n + \vec{\omega}_i^n \Delta t + \frac{\vec{\alpha}_i^n}{2} (\Delta t)^2, \quad (38d)$$

$$Rotacional \quad \vec{\omega}_i^{n+1} = \vec{\omega}_i^n + \frac{\vec{\alpha}_i^n + \vec{\alpha}_i^{n+1}}{2} \Delta t, \quad (38e)$$

$$\vec{\alpha}_i^{n+1} = I_i^{-1} \sum_j \vec{\tau}_{i,j}^n, \quad (38f)$$

em que i é o índice do corpo que movimenta, j é o índice do corpo em contato com o corpo i , n é o passo de tempo, \vec{r} é a posição do corpo, \vec{v} é a velocidade do corpo, \vec{a} é a aceleração do corpo, Δt é o tamanho do passo de tempo, $\vec{F}_{i,j}$ é a força de contato entre os corpos i e j , \vec{F}_{ext} são as forças externas, como gravidade e força que o fluido exerce sobre o corpo, m é a massa do corpo, θ é a posição angular do corpo, $\vec{\omega}$ é a velocidade angular do corpo, $\vec{\alpha}$ é a aceleração angular do corpo, $\vec{\tau}$ é o torque sobre o corpo, I é o momento de inércia do corpo.

O conjunto de equações 38 está escrito para o sistema 2D, uma vez que só há um grau de liberdade para a rotação, e consequentemente todas as equações passam

a ser escritas em função de um único parâmetro. A aproximação da velocidade como a ponderação entre as acelerações no instante de tempo atual e futuro é a chave para a minimização da imprecisão gerada pela discretização [11].

Para o fluido, discretizamos a equação 33a de forma explícita¹. Por causa da não linearidade das equações no termo de turbulência, ainda não conseguimos escrever uma expressão implícita² para este sistema. Alguns livros tratam exclusivamente o assunto da discretização da equação de difusão linear e estão referenciados em [79, 80, 81, 82]. A equação para o fluido, em sua forma discretizada torna-se então o sistema de equações 39:

$$\left\{ \begin{array}{l} u_x^{n+1} = u_x^n + \frac{\Delta t}{\rho^f \Delta y} [\tau_k^n - \tau_{k-1}^n] - \frac{\Delta t}{\rho^f} P_k^n, \end{array} \right. \quad (39a)$$

$$\left\{ \begin{array}{l} \tau_k^n = \rho^f \left[\nu + l_k^2 \left| \frac{u_{x_{k+1}}^n - u_x^n}{\Delta y} \right| \right] \left(\frac{u_{x_{k-1}}^n - u_x^n}{\Delta y} \right), \end{array} \right. \quad (39b)$$

em que k é o índice discretização espacial do fluido, n é o passo de tempo, u_x é a velocidade de escoamento do fluido, Δy é o espaçamento da malha do fluido, Δt é o intervalo entre os passos de tempo, ρ^f é a densidade do fluido, τ é o cisalhamento do fluido, P é a pressão que os corpos sólidos fazem no fluido, ν é a viscosidade do fluido e l é o comprimento característico da turbulência.

6.2 Algoritmo

Além das equações que regem o sistema, uma série de procedimentos devem ser realizados para que a simulação possa ocorrer. Cada um destes passos são essenciais para que a simulação ocorra, e são dependentes uns dos outros. O algoritmo 7 determina as rotinas para a execução da simulação. Utilizamos o *Gear Predictor-Corrector* de 3^a ordem com o *Velocity Verlet* para realizar as simulações [11].

As condições de parada do algoritmo dependem do objetivo da simulação. Alguns exemplos, como estabilidade de pilhas estáticas, flutuações de energia, quebra das cadeias de forças, velocidade média do sistema, número de passos de tempo, entre vários outros parâmetros medíveis dentro da simulação podem se tornar o critério de parada da simulação. Nesta tese, utilizamos como principal critério de parada o número de passos de tempo de simulação.

¹ A forma explícita de resolução de um método de equações de diferenças resolve o sistema para o próximo passo de tempo com as operações originais da equação diferencial. Toda a discretização é feita sobre as funções do passo de tempo atual resultando no passo de tempo posterior. A desvantagem desta técnica é o fator de instabilidade da solução que pode vir a ocorrer. A vantagem é que o sistema sempre pode ser escrito por estas equações.

² A forma implícita de resolução de um método de equações de diferenças resolve o sistema do próximo passo de tempo com base nas raízes da equação diferencial do problema. Toda a discretização é feita considerando as raízes que solucionam a equação. A desvantagem desta técnica é o fato de nem sempre existir algoritmo que encontre as raízes. A vantagem é que o fator de estabilidade é mais permissivo.

Algorithm 7: Given the input of the problem, such as initial positions of bodies, velocities and accelerations, the algorithm assembles a list of bodies that are neighbors delimited by a certain region, then predicts the position and velocity of the bodies at the next instant of time, looks for the contacts that were formed with the prediction, calculates the forces between each body in contact and includes the external forces, and corrects the velocity and acceleration predictions for each body. Thus a DEM step is constructed. Algorithm taken from [1].

```

Input :initial simulation data setup
Output :response and simulation measurements over time
while not reached the stop condition of the simulation do
    if it is time to List the Neighbors then
        | List the Neighbors;
    end
    Predictor;
    Detect Contacts;
    Force Calculation;
    Corrector;
end
```

Faremos uma breve discussão a respeito de cada uma das rotinas do algoritmo 7. Para maiores detalhes, as referências [1, 11, 55] possuem maiores explanações sobre as rotinas, com exemplos e algoritmos.

6.2.1 Vizinhos

Apesar de não ser a forma mais simples do algoritmo de localização de vizinhos, esta é mais eficiente, e está descrita em [1]. Consiste criar a lista de todos os corpos que pertencem à uma certa região de possível interação. A criação da lista minimiza o número de comparações feitas durante a execução, o que proporciona o maior desempenho computacional. O artigo "*Methods of parallel computation applied on granular simulations*"[60] revela as diferenças entre alguns métodos da criação das listas de corpos que interagem entre si. Este artigo foi escrito durante a elaboração deste projeto de tese e está no apêndice A. O algoritmo 8 refere-se a criação da lista dos corpos que tem a possibilidade de interação entre si.

A figura 30 mostra as regiões que o corpo marcado deve estar listado. Para maiores detalhes, as referências [1, 11].

6.2.2 Predictor

A rotina de predição atualiza as posições e as velocidades dos corpos, permitindo que todas as forças sejam calculadas em função dos novos valores. No conjunto de

Algorithm 8: Algorithm for creating the list of neighbors. Algorithm taken from [1].

Input: body position
Output: neighbor list
 Divide the space in regions;
foreach body **do**
 | Insert the body in the list of the region it belongs to;
 | Insert the body into adjacent lists of the region it belongs to;
end

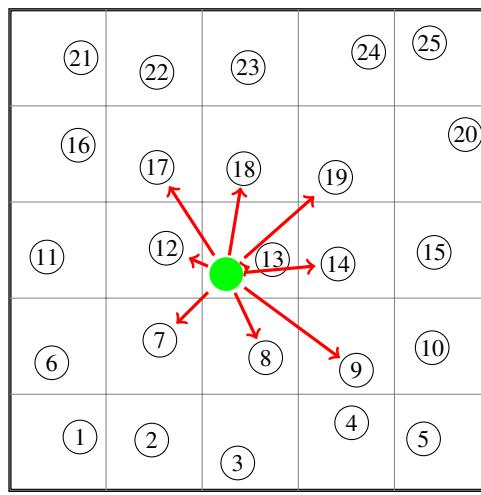


Figure 30 – A busca realizada no algoritmo 8 ocorre entre os corpos com sua região de vizinhança imediatamente adjacente. Figura retirada de [1].

equações 38, equações que envolvem os termos com índice n são atualizados nesta rotina. O algoritmo 9 mostra a estrutura da rotina de predição.

Algorithm 9: Prediction routine for state variables of bodies. Algorithm taken from [1].

Input :positions, velocities, accelerations and the time step Δt
Output :positions, part of the velocities
forall bodies **do**
 | Calculate new postions;
 | Predict new velocities;
end

6.2.3 Detectar contatos

A rotina de detecção de contatos utiliza da lista de vizinhos gerada pelo algoritmo 8 para checar se o par listado corpo/vizinho possuem interpenetração, descrita na equação 16, e então gera uma nova lista de corpos que se interpenetram para ser utilizadas no algoritmo 11. O algoritmo 10 descreve esta operação.

Algorithm 10: Detect contacts routine. Algorithm taken from [1].

```

Input :Neighbor list
Output :Contact list
forall neighbor bodies do
    Calculate the Interpenetration  $\delta_{i,j}$  between bodies  $i$  and  $j$ ;
    if  $\delta_{i,j} > 0$  then
        | Insert the pair  $i$  and  $j$  in the contact list;
    end
end
```

6.2.4 Cálculo de forças

A rotina de calcular as forças utiliza da lista de contatos gerada pelo algoritmo 10 para calcular as forças de contato entre os corpos, como forças elásticas (equação 17), forças de amortecimento (equação 18) e forças de atrito (equação 20). Além das forças de contato, os corpos sofrem a força gravitacional e a interação com o fluido (equações 22 e 23). O algoritmo 11 contém a execução do calculo das forças.

Algorithm 11: In this routine, the resultant forces are calculated for each body. The force \vec{N} is the normal force, contribution of the elastic force \vec{F}^{el} and the damping force \vec{F}^{dam} (Equations 17 and 18), F^d is the rolling force of one body on the other, which must be compared with the maximum static friction force μN . Algorithm taken from [1].

```

Input :positions, velocities and contact list
Output :acting forces and torques in the bodies
foreach body do
    Apply gravity force;
    foreach body in the contact list do
        Calculate the normal forces  $\vec{N}$ ;
        Calculate the rolling forces  $F^d$ ;
        if  $|F^d| < \mu|\vec{N}|$  then
            |  $\vec{F}^{at+} = \vec{F}^d\hat{t}$ ;
        else
            |  $\vec{F}^{at+} = \mu\text{sign}(\vec{F}^d)\vec{N}\hat{t}$ ;
        end
        Calculate torque;
    end
end
```

6.2.5 Corretor

A rotina de correção atualiza as velocidades e as acelerações dos corpos. As forças calculadas no cálculo de forças é utilizada aqui para realizar o *Velocity Verlet* e determinar as acelerações do próximo passo de tempo. No conjunto de equações 38, as equações que

envolvem os termos com índice $n + 1$ são atualizadas nesta rotina. O algoritmo 12 mostra a estrutura da rotina de correção.

Algorithm 12: Rotina de correção das variáveis dos corpos. Retirado de [1].

Entrada : resultante das forças e o passo de tempo Δt
Saída : estado dos corpos prontos para o próximo passo de tempo
foreach corpo **do**
 | Calcular as acelerações;
 | Corrigir as velocidades;
end

6.2.6 Fluido

A rotina de cálculo do fluido consiste na atualização da malha do fluido³ em função do sistema de equações 39. A malha deste fluido é unidimensional, uma vez que consideramos a variação de velocidades apenas na direção y . Assim, consideramos uma malha linear de espaçamento Δy , sendo que Δy é uma fração do grão médio do sistema. Para uma boa amostragem, utilizamos $\Delta y \approx 0.1d$, em que d é o diâmetro médio do grão. Para o cálculo da pressão que o fluido exerce sobre o grão, utilizamos a fração do corpo que pertence à camada em que o mesmo está inserido. A soma de todas as frações de corpos na camada resulta no coeficiente de compactação.

Algorithm 13: Rotina que atualiza os estados do fluido para o próximo passo de tempo.

Entrada : perfil de velocidades e cisalhamento do fluido, forças de arrasto e arquimedes nos grãos, passos de tempo Δt e de espaço Δy
Saída : estado do fluido para o próximo passo de tempo
foreach corpo **do**
 | Calcula as pressões dos corpos no fluido;
end
forall fluido **do**
 | Calcula o cisalhamento do fluido;
 | Atualiza a velocidade do fluido;
end

6.3 Parâmetros importantes

Em decorrência do modelo de forças apresentado, alguns parâmetros são importantes para as simulações. Por serem regidos por equações de diferenças em função do

³ A malha do fluido consiste na divisão geométrica do espaço para realizar simulação, e é baseada em pontos discretos do espaço associados a uma função contínua. Este processo é o método de elementos finitos, ou *Finite Element Method (FEM)* [83].

parâmetro temporal, alguns critérios devem ser obedecidos para que a simulação seja estável. Um dos parâmetros é a constante de tempo Δt , que em nossas simulações possui relação direta com o período de oscilação do modelo massa mola, dado por $\Delta t = \zeta \sqrt{m_{min}/k}$, em que ζ é um valor de ajuste, m_{min} é a menor massa do sistema e k é a constante de elasticidade. Os fatores que estabilizam as simulações que possuem o modelo massa mola devem ter $\zeta < 1/10$ [1, 15, 11]. Nesta tese utilizaremos o fator de 1/10 para sistemas que não são vibrado e 1/100 para sistemas vibrados.

Outro importante parâmetro é o fator de amortecimento γ , ou o coeficiente de restituição ϵ . Pela natureza dissipativa dos materiais granulares, utilizam-se $\epsilon \approx 0^4$, o que aproxima de $\gamma \approx 2\sqrt{km_{min}}$ pois teremos regimes críticos na equação massa mola quando utilizarmos a menor massa dos dois corpos, e para todos os outros, o amortecimento será subcrítico [53, 51].

Para o fluido, três parâmetros adimensionais de controle são importantes: a razão de densidade, descrita pela equação 40, o número de Reynolds, que relaciona as forças iniciais com as forças viscosas, descrito pela equação 41 e o número de Shields, que relaciona as forças de arrasto com as forças iniciais, descrito pela equação 42 [77].

A seguir, a equação que descreve a razão de densidades entre grão e fluido:

$$\mathcal{D}_R = \frac{\rho^{body}}{\rho^f}, \quad (40)$$

em que \mathcal{D}_R é a razão de densidade, ρ^{body} é a densidade do corpo e ρ^f é a densidade do fluido.

O segundo parâmetro adimensional de controle do fluido é o número de Reynolds, dado pela equação:

$$\mathcal{R} = \frac{d}{\nu} \sqrt{(\mathcal{D}_R - 1) gd}, \quad (41)$$

em que \mathcal{R} é o número de Reynolds na escala do corpo, d é o diâmetro médio do corpo, ν é a viscosidade do fluido, \mathcal{D}_R é a razão de densidade e g é o valor de gravidade do sistema.

O terceiro parâmetro adimensional de controle do fluido é o número de Shields, dado pela equação:

$$\Theta = \frac{u_*^2}{(\mathcal{D}_R - 1) gd}, \quad (42)$$

em que Θ é o número de Shields, u_* é a velocidade de cisalhamento imposta para o fluido, \mathcal{D}_R é a razão de densidade, g é o valor de gravidade do sistema e d é o diâmetro médio do corpo.

No próximo capítulo descreveremos o efeito castanha do Pará (*BNE*) e como montamos a simulação que leva a este efeito.

⁴ A relação entre o coeficiente de restituição e o coeficiente de amortecimento podem ser encontrados em [1].

7 Transporte de Sedimentos

O transporte de sedimentos é o movimento de partículas sólidas, carregadas por um fluido em uma certa distância, que escoam na mesma direção. O transporte é uma combinação entre a ação da gravidade no sistema e as forças de arraste do fluido. Um vasto número de fenômenos estão relacionados com o transporte de fluidos, como em processos industriais (ao transportar minérios por um mineroduto), ou a transformação das paisagens (na formação ou desaparecimento de dunas) [2]. O resultado de ação dos diferentes tipos de fluidos, com características diversas, resultam em fenômenos diferentes, como processos causados por água: erosão pluvial, erosão fluvial e assoreamento; e processos causados pelo vento: dunas, desertificação.

Pode-se classificar os tipos de transporte como mostrado na figura 31, em que os sedimentos são retirados de um local e depositados em outro, em diferentes escalas temporais e espaciais. Uma formação pode aparecer na escala de minutos com alguns centímetros de altura nos fundos de rios e oceanos, até formações geológicas de milhares de anos com centenas de quilômetros de extensão.

Materiais sólidos podem ser transportados pelos seguintes modos: *bed load*, que é o transporte de material rolando sobre uma fina camada da base granular e ocorre quando a força gravitacional é a força mais preponderante no sistema [84] ocorrer no fundo dos riachos e lagos e na superfície de um terreno; *saltation*, que é o transporte de material que colide com a base granular em saltos, ocorrendo quando as forças gravitacionais e de arraste são as mais relevantes no sistema, podendo ser visto em rios e nos processos erosivos dos ventos; e finalmente *suspension*, que é o modo de transporte de material em que as forças de arraste causadas pelas flutuações turbulentas passam a ser da ordem de grandeza do peso dos grãos e dominam a dinâmica do sistema [85], podendo ser observado em tempestades de areia ou ao varrer-se a poeira de casa.

Modelos monofásicos não são capazes de reproduzir a física envolvida neste pro-

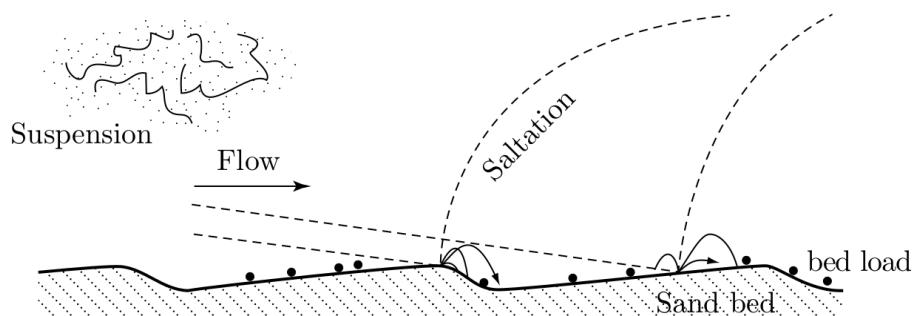


Figure 31 – Diagrama esquemático dos diferentes modos de transporte. Retirado de [2].

blema. Modelos de materiais granulares sem a presença de fluido não exibem as propriedades dos modos de transporte como *bed load*, *saltation* e *suspension*. Assim como os modelos de fluidos sem os sedimentos não são capazes de descrever as propriedades de deposição, de erosão ou mesmo de saturação. Sendo assim, é necessário que o modelo possua as duas fases estejam descritas, sedimento e fluido.

Duas propriedades intrínsecas do arraste são a escala de comprimento de saturação L_{sat} e a escala de tempo de saturação T_{sat} . A escala de comprimento de saturação quantifica a distância característica para que os grãos tenham a densidade máxima transportada pelo fluido q_{sat} . Já a escala de tempo de saturação indica o tempo característico para que a densidade de material transportado decaia quando a velocidade do fluido decair bruscamente, ou para que a densidade de material transportado aumente quando a velocidade do fluido aumentar bruscamente [2].

Visando um modelo que seja capaz de reproduzir tais características, o uso de *Discrete Element Method (DEM)* combinado com o uso de *Finite Element Method (FEM)* simulam o comportamento dos materiais e do fluido, interagindo as diferentes abordagens contínua do fluido e discreta do material granular.

Para descrever o comportamento interativo entre o fluido e o material granular, utilizaremos simulações computacionais baseadas nos trabalhos do professor Dr. Philippe Claudin [77, 86, 87]. Impondo as condições iniciais do fluido, mede-se o tempo necessário para que o novo regime atinja as condições estacionárias. O número de grãos que escoa pelo sistema, no regime estacionário, fornece o fluxo volumétrico saturado q_{sat} , que serve de parâmetro para comparação e medição do tempo de saturação e do comprimento de saturação. Repete-se o processo para cada parâmetro de entrada, quantificando assim, as diferentes transições entre os modos de transporte.

Inicialmente, validamos o fluido, e então, interagimos fluido e grãos. Na validação do fluido observamos se a discretização contempla o modelo contínuo. Montamos uma malha unidimensional espaçada por um tamanho fixo ao longo de uma reta, que denominamos de direção y . A ideia é que haja escoamento na direção perpendicular, denominada de x , e que as camadas não troquem massa ou pressão, mas quantidade de movimento, que se reflete na velocidade do fluido. Tensão de cisalhamento e velocidade do fluido estão intimamente associados pelo conjunto de equações 33a e 36.

Considerando que o cisalhamento do fluido pode ser predominantemente laminar, ou seja, quando o número de Reynolds (equação 41) for muito pequeno (tipicamente $\mathcal{R} < 0.01$), o fluido escoará em regime laminar. Podemos aproximar o cisalhamento por contribuição apenas da parcela de viscosidade do fluido, e teremos então uma equação do tipo difusão linear, e que possui solução analítica no regime estacionário dada pela equação 43:

$$u(y) = \frac{u_*^2}{\nu} y, \quad (43)$$

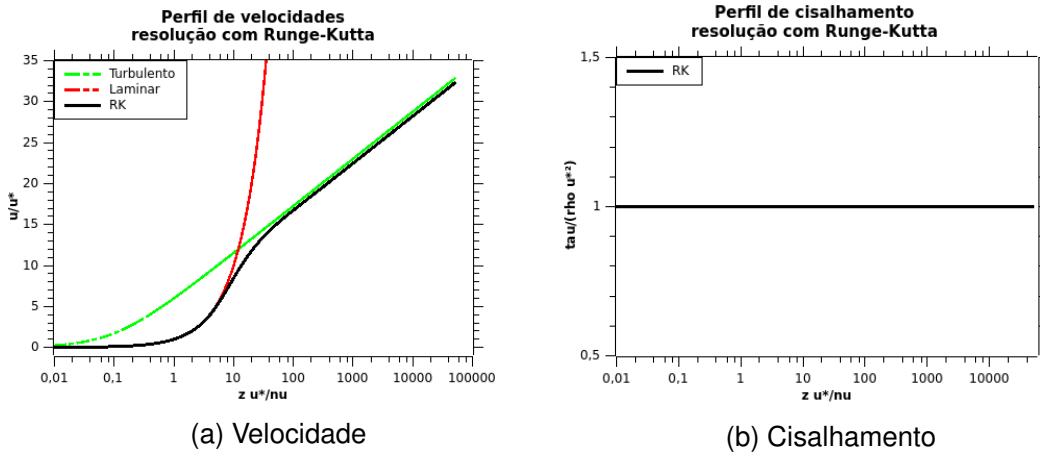


Figure 32 – Resultado do fluido estacionário. Na figura 32a está a solução da equação 45 para a velocidade, utilizando o método de Runge-Kutta de 4^a ordem. Na figura 32b está a solução do cisalhamento.

em que u é a velocidade de escoamento do fluido, u_* é a velocidade característica de cisalhamento imposta ao fluido, ν é a viscosidade do fluido e y é a altura da coluna de fluido.

Considerando que o cisalhamento do fluido pode ser predominantemente turbulento, ou seja, quando o número de Reynolds (equação 41) for muito grande (tipicamente $\mathcal{R} > 1000$), o fluido escoará em regime turbulento. Podemos aproximar o cisalhamento por contribuição apenas da parcela de viscosidade turbulenta, e teremos então o regime estacionário dado pela equação 44.

$$u(y) = \frac{u_*}{\kappa} \ln \left| 1 + \frac{u_*}{0,1\nu} y \right|, \quad (44)$$

em que u é a velocidade de escoamento do fluido, u_* é a velocidade característica de cisalhamento imposta ao fluido, ν é a viscosidade do fluido, $\kappa \approx 0,4$ é a constante de von Karman e y é a altura da coluna de fluido [77].

Para descobrir o regime estacionário do fluido, utilizamos o método de Runge-Kutta de 4^a ordem sobre a equação 45, que é a equação de van Driest [77], e encontramos a curva da figura 32.

$$\left(\nu + l^2 \left| \frac{\partial u}{\partial y} \right| \right) \frac{\partial u}{\partial y} = u_*^2, \quad (45)$$

em que ν é a viscosidade do sistema, u é a velocidade de escoamento do fluido, u_* é a velocidade característica do cisalhamento imposto ao fluido e l é o comprimento de mistura da turbulência, dado pela equação 37b.

As simulações do fluido colapsam em uma única curva com diferentes valores do número de Reynolds. A figura 33 contém os perfis de velocidade normalizados para diferentes números de Reynolds. A validação das simulações é obtida por meio da comparação entre o

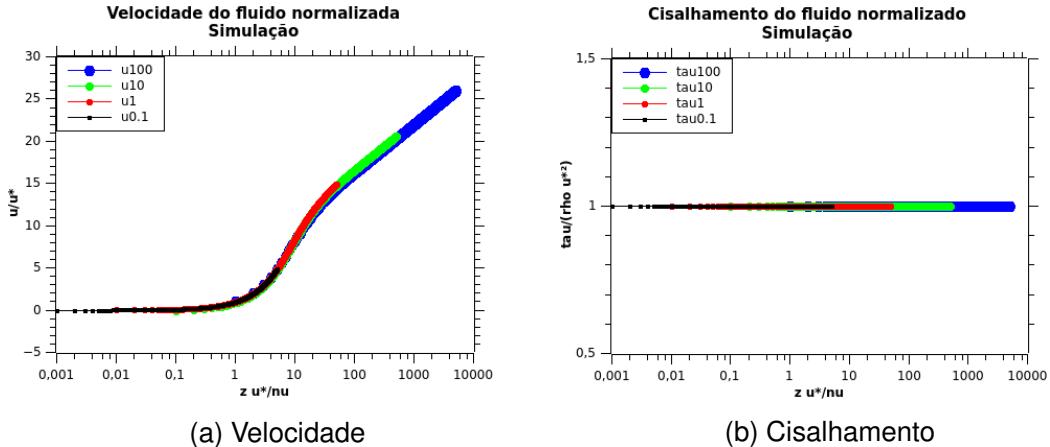


Figure 33 – Resultado do fluido estacionário. Na figura 33a está a evolução do conjunto de equações 33a e 36 com a observação da velocidade. Na figura 33b está o cisalhamento. Em ambos os casos, há variação do número de Reynolds para cada uma das curvas.

cisalhamento do fluido no regime estacionário e o esperado nas equações do cisalhamento, em regime estacionário. Apesar da velocidade apresentar um perfil não linear por inserção da turbulência, observamos que o cisalhamento é constante ao longo do perfil de alturas. Com a constância do cisalhamento, tem-se a indicação de que o sistema é invariante no tempo, e portanto está no regime estacionário.

Comparando os perfis do método de Runge-Kutta de 4^a ordem para resolver as equações 43, 44 e 45, vimos na figura 32a que o perfil laminar encaixa-se para números de Reynolds baixos e que o perfil turbulento encaixa-se em números de Reynolds altos. Por se tratar do regime estacionário, o perfil de cisalhamento é uma constante, como na figura 32b.

Após checado que as simulações do fluido convergem para a solução apresentada pelo Runge-Kutta de 4^a ordem, apresentado na figura 33a, e que o perfil de cisalhamento do fluido é constante ao longo de toda altura, apresentado na figura 33b, inserimos os grãos no sistema e verificamos se as propriedades ainda continuam válidas.

A figura 34 mostra o cisalhamento de um sistema com 8000 grãos, com dispersão dos diâmetros em 20%, constante de mola na direção normal $k_n = 1000$, constante de mola na direção tangencial $k_t = 750$, coeficiente de amortecimento $\gamma = 13,6265$, coeficiente de atrito $\mu = 0,5$, distribuídos em uma base de 200 diâmetros de grão, com condição periódica de contorno, imersos em um fluido de razão de densidade 1/2, número de Reynolds $\mathcal{R} = 0.1$ e número de Shields $\Theta = 0.01$. O resultado é amostrado em 20 simulações, com o cálculo de tensão de cisalhamento nos grãos descrito pela equação 46 [5, 88]:

$$\sigma_{xy} = \sum_i \sum_j \frac{\vec{F}_{i,j} \cdot \hat{x} \vec{r}_{i,j} \cdot \hat{y}}{2d\sqrt{\pi}} \int_0^1 e^{-\frac{y - r_{i,j} - r_{i,j} \cdot \hat{y} s}{w}} ds, \quad (46)$$

em que σ_{xy} é o perfil de cisalhamento que os grãos sofrem, i e j são os índices dos grãos que estão em contato, $\vec{F}_{i,j} \cdot \hat{x}$ é a componente x da força de contato entre os grãos, $\vec{n}_{i,j} \cdot \hat{y}$ é a

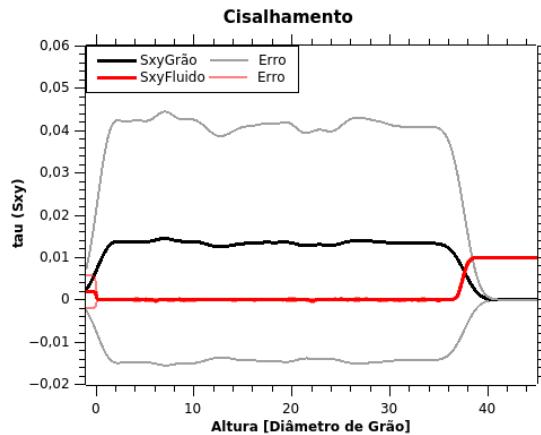


Figure 34 – Perfil de cisalhamento dos grãos e do fluido no regime estacionário.

componente do vetor de contato entre os grãos, d é o diâmetro médio dos grãos, y é a altura do perfil analisado, $r_i \cdot \hat{y}$ é a posição do grão e a integral é uma função de *coarse-graining*, que deve ser positiva e normalizada. Neste caso escolhemos a função gaussiana para melhor suavização do perfil de cisalhamento.

Para o sistema da figura 34 escolhemos os parâmetros do número de Shields e de Reynolds que não arrastassem os grãos, para podermos analisar a influência do fluido no regime estacionário. O perfil de cisalhamento transmitido do fluido para os grãos encaixa-se dentro da faixa esperada, apesar dos cisalhamentos não serem os mesmo, a convergência não é exata por se tratar da interação do meio contínuo com o meio discreto.

Até agora, estivemos preocupados com a consistência física do problema. Os próximos passo são reproduzir os modos de transportes *bead load* e *saltation* descritos por Orencio Durán [77] e medir os tempos de para a acomodação do regime estacionário, determinando assim o tempo de saturação dos modos de transporte dos sedimentos.

8 Análise e Discussão dos Resultados

- CFD

9 Conclusões Parciais

Para os as simulações do BNE conseguimos reproduzir as propriedades de ascensão do intruso com diferentes densidades, diferentes amplitudes de vibração e diferentes frequências de vibração, observando a importância do atrito nas paredes do sistema. Mais do que isso, conseguimos realizar o BNE em um sistema que possui condição periódica de contorno e suas diferenças para o sistema de caixa fechada.

Para o sedimento de transportes, conseguimos validar as propriedades físicas que regem o sistema, condizendo simulação com a conservação de movimento. Validamos o fluido de acordo com a literatura e acoplamos grão e fluido de forma a interagirem sobre as leis da física.

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Apêndices

APÊNDICE A – Artigos publicados

A seguir os artigos publicados desde o início desta pesquisa. O primeiro artigo apresentado refere-se a publicação feita sobre este doutoramento, com resultados mistos das técnicas utilizadas na dissertação de mestrado [1] e este projeto de tese. O segundo e terceiro artigos apresentados referem-se a publicações feitas durante a dissertação, mas que expressam as técnicas utilizadas neste projeto de tese.

A.1 *Large-deviation quantification of boundary conditions on the Brazil nut effect*

This paper was published on the Physical Review E, and it is one of the main themes of this thesis, referring to chapter 4.

A.2 *Methods of parallel computation applied on granular simulations*

Este artigo foi publicado no quatrienal do congresso *Powders & Grains 2017*, que é o maior congresso sobre materiais granulares, e que está em sua 8^a edição.

Methods of parallel computation applied on granular simulations

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Abstract. Every year, parallel computing has become cheaper and more accessible. As consequence, applications were spreading over all research areas. Granular materials is a promising area for parallel computing. To prove this statement we study the impact of parallel computing in simulations of the BNE (Brazil Nut Effect). This property is due the remarkable arising of an intruder confined to a granular media when vertically shaken against gravity. By means of DEM (Discrete Element Methods) simulations, we study the code performance testing different methods to improve clock time. A comparison between serial and parallel algorithms, using OpenMP® is also shown. The best improvement was obtained by optimizing the function that find contacts using Verlet's cells.

1 Introduction

Granular materials have high relevance in Nature as well in humans activities like in mining, in food industry, in construction technology [3–9]. Basically, granular materials are everywhere, from sand to snow, from iron ore pellets to corn grains, from dust to stones. This ubiquity justify the high importance to know their behavior in order to use and manipulate them under different situations.

Several phenomena displayed by granular materials are quite surprising, and in general is a very difficult task to predict the behavior of a substantial quantity of granular material subjected to external loading, a very common situation. Perform experiments under controlled environment is the most desired approach to acquire knowledge about these systems, but most of time only with a detailed modeling of the system is possible to verify theoretical hypothesis. Thus, it is essential to develop a reliable computational model able to predict and reproduce granular behavior under different situations, and increasing system sizes.

Given the importance and presence of granular materials in the world, simulations offer lots of advantages for testing possible characteristic states, to predict behaviors, to save money in execution of projects, and to help plan next moves in engineering for instance. But some disadvantages may be present also, as the increasing of computation time for large systems sizes. With the increasing number of agents in simulation, higher is the computation

time. Most cases, this increasing relation is quadratic in time because the nature of operations.

To improve simulations, and save time, more than one machine can execute the tasks at same time. Parallelization can solve single parts of the problem separately and get them together as part of the final solution, saving total operation time. Also, many researchers are using parallel computation resources in scientific programs to simulate DEM in particles systems [1, 2]. These DEMs are commonly used to simulate different kind of systems, like dense granular materials.

Is possible to perform parallelization in clusters of pc's or multicore computers, since they have more than one CPU (Central Processing Unit) available, that exchange information between them. In the model we use, some operations can be done separately, each one in one processor. More processors used, generally result in lower total execution time from a given job. The increasing number of cores in processors nowadays has turned this possibility very accessible. Also, GPUs (Graphics Processing Units) are becoming a cheaper option to improve a lot computational power.

Given all these possibilities to improve simulations, we propose to measure different techniques to simulate a paradigmatic example of granular system, the Brazil Nut Effect (BNE), and compare the performance of the algorithms. The BNE is a typical segregation phenomena observed in granular materials, which still have several open issues to be explored by simulations. We present results of BNE with frictional and frictionless walls.

In section 2, the methodology to simulate the system is shown, with different proposals to improve the time spent

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on serial and parallel algorithms, and some results. In section 3, the BNE results using these codes. In section 4, the main conclusions we got from our experiments.

2 Methods to save time in simulations

To simulate granular systems computationally, some models can be used [10]. One of this models considers rigid grains which are allowed to display some degree of interpenetrations, which are used in Kelvin-Voight rheology model, Cundal-Strack elastic contact in normal directions, and Coulomb friction in tangent direction, as shown in figure 1. By this, MD (Molecular Dynamics, that is a DEM) can be used [10–12] to integrate the motion equations of the grains directly from Newtons' laws. By choosing an appropriated time step, several different methods can be used to integrate these equations.

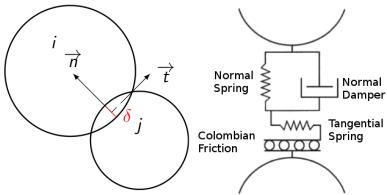


Figure 1. Force model between grain's interactions. i and j are particles that have contact each other. δ is the interpenetration value between the contact ij . n is the direction of the normal contact force. t is the direction of the tangential friction force.

In MD, a predictor-corrector method is used, and its scheme can be seen in Figure 2. The routine *Predict states* solves the kinematic equations over all grains over a single step. The routine *Detect contacts* find grains in contacts each other and store into a list. For the implementation without routine *Set list of neighbors*, *Detect contacts* look for all possible pair of grains for contacts, at every time step, and requires two loops over all grains. Otherwise, *Detect contacts* focus the search to the list of neighbor grains, and require one loop over the neighbor list. Both cases, it is produced a list of contacts, with the predicted states. The routine *Calculate forces* calculate the contact forces and also gravitational, requiring one loop over all particles and one loop over the list of contacts. The routine *Correct predicted states* corrects the predicted states and requires one loop over all particles. If the routine *Set list of neighbors* have Verlet's list implemented, it will search all possible pairs of neighboring grains, and requires two loops over all grains with a given frequency. If the routine *Set list of neighbors* have Verlet's cells implemented, it will search all neighbors grains' dividing the space in regions and look for possobli pair of contact grains only inside a cell and its neighboring cells. It requires one loop over all grains and other over all grains in the cells' neighbors.

To parallelize the simulation, all barriers should be identified to do a proper implementation. The first barrier is a temporal barrier, and happens in simulation each step. This first barrier can't be jumped by the temporal

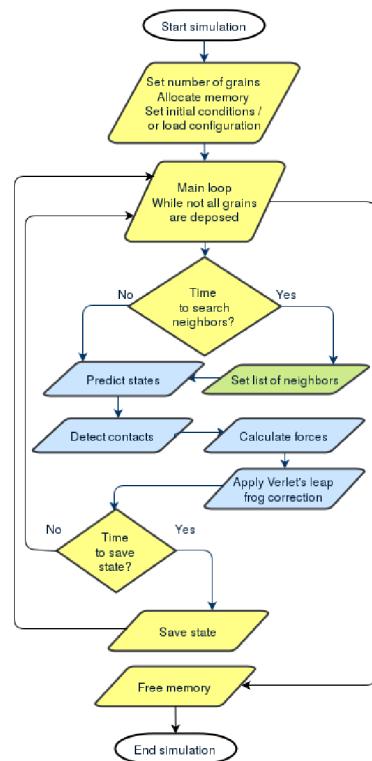


Figure 2. Flowchart of the simulation to simulate granular system using MD. Yellow operations can't be parallelized. Blue operations can be parallelized using CPUs. Green operation is the function that consume most processing, and can be parallelized based onto the type of implementation: *Set list of neighbors* as Verlet's list is the first improvement to reduce time in simulations. *Set list of neighbors* as Verlet's cells is the second improvement to reduce time in simulations.

dependency of the system, as future depends on all past calculation done. Each particle can be treated independently, and at that point, the following routines *Predict states*, *Detect contacts*, *Correct predicted states* and *Set list of neighbors*, using Verlet's list, have no barrier to parallelize, so all loops were done to distribute all calculations to each processor available independently to read and write on memory. In the routine *Set list of neighbors*, using none of Verlet's improvement, the *Set list of neighbors* have no function, once all time steps the contact is calculated inside *Detect contacts*, and no barrier is present in parallelization. If the routine *Set list of neighbors* is using Verlet's cells, one barrier happens to insert grains in the cell it belongs, because to write on one same cell, two processors may try to do at same time. In the routine *Calculate forces* a barrier may happen, depending on implementation. If the 3rd Newton's law is applied on both bodies at same computational sequence when one contact happen, a barrier should be present to prevent memory concurrency by two or more contacts in a particle. This implementation gives an advantage of computation in serial execution that reduces the calculation by half, but a disadvantage in parallel execution by one barrier. The way done here is to calculate the pair of action and reaction separately, in each particle's loop.

The most expansive routine is detect contacts that searches all grains in contact each other, and its computational complexity can be written in function of the number of grains (n), as $O(n^2)$ with Verlet's list, and $O(n \log n)$ with Verlet's cells. Other routines have computational complexity $O(n)$. So, the total complexity of this algorithm can be written as $O(n^2)$ for Verlet's list, and $O(n \log n)$ for Verlet's cells.

2.1 Time spend

The clock time to simulate the system depends on the number of particles, the number of steps the system is simulated, the dynamic of the grains, the number of process running on the machine or cluster, the machine or cluster itself, the method used to implement the solution and many other controllable and uncontrollable variables.

To have an optimized parallel code, one need to know how much time serial functions costs, and their parallelizable portion. The results of time spent by each routine, in seconds, can be found on table 1, table 2 and table 3. The function *Detect contact* is the one which displays best results for application of parallization algorithm. In fact, Verlet's list and Verlet's cells are optimizations for the search algorithm. Both saves computational time and store closer grains into one list. The system do not update the neighbor list all steps of simulation, but only at a given frequency.

Table 1 shown the profile of serial runs of the code with 10^3 grains. For this number of grains, Verlet's cells and Verlet's list have little impact on execution times, but the simple search is the slowest, as expected. Table 2 have the profile of serial running of the code for 10^4 grains, and at this number of grains, Verlet's cells are faster than Verlet's list. Table 3 have the profile of serial running of the code for 10^5 grains, only for Verlet's list and Verlet's cells, because the simplest implementation got no result running after one week with this number of grains, and Verlet's cells are still faster than Verlet's list.

To compare and understand the parallelization, some metrics are defined. One of them is the performance of the system, that is the clock time measured by running that code. Faster codes gives lower results. Our results of performance can be found in figure 3, and for simulations with number of grains higher than 10^3 , Verlet's cells gives best results.

The speedup is the comparison between clock time of execution in serial and the clock time of execution in parallel of same algorithm. It gives the tendency of the parallelization of the code. Best results gives higher curves. Our results of speedup, shown in figure 4, evince that parallelization decreased clock time to perform simulations above than 10^3 particles in the system. We can also conclude that *Detect contacts* without Verlet's implementations and Verlet's list are much more parallelizable than Verlet's list.

The efficiency is the comparison between speedup and the number of processors used. It gives the average utilization of each processor in the algorithm. Best results tends

Table 1. Clock time spent, in seconds, on each routine of serial running of the code for 10^3 grains for 10^3 time steps.

Function	Simplest	List	Cells
Predict states	0.01	0.03	0.03
Detect contact	22.47	0.15	0.18
Calculate forces	0.01	0.01	0.01
Correct states	0.01	0.04	0.02
List of neighbors	--	0.22	0.01

Table 2. Clock time spent, in seconds, on each routine of serial running of the code for 10^4 grains for 10^3 time steps.

Function	Simplest	List	Cells
Predict states	0.27	0.19	0.21
Detect contact	2048	1.98	1.84
Calculate forces	0.09	0.06	0.05
Correct states	0.27	0.34	0.30
List of neighbors	--	23.18	0.05

Table 3. Clock time spent, in seconds, on each routine of serial running of the code for 10^5 grains for 10^3 time steps.

Function	Simplest	List	Cells
Predict states	--	2.93	2.87
Detect contact	--	19.87	19.77
Calculate forces	--	0.93	0.86
Correct states	--	3.87	3.73
List of neighbors	--	2,322.96	0.59

to have value 1, the full use of each processor. Figure 4 shown us that *Detect contacts* without Verlet's implementations and Verlet's list uses more the computational resources at same time than Verlet's cells implementation. For higher number of grains, they occupy more the computational resources, justifying the good use of parallelization with large systems.

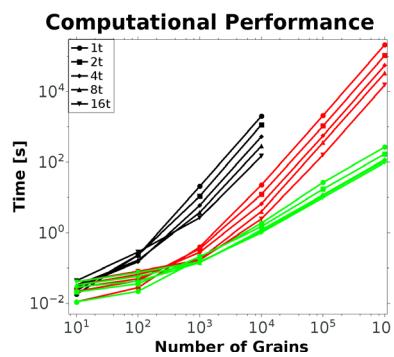


Figure 3. Performance of the system. This compares the results without Verlet's methods (in black), Verlet's list (in red) and Verlet's cells (in green). The number of processors used to simulate varies from 1 to 16, indicated on the legend.

3 Brazil Nut Effect (BNE)

The system has been validated comparing results with the theory of BNE [8, 9, 13, 14]. BNE is a segregation phe-

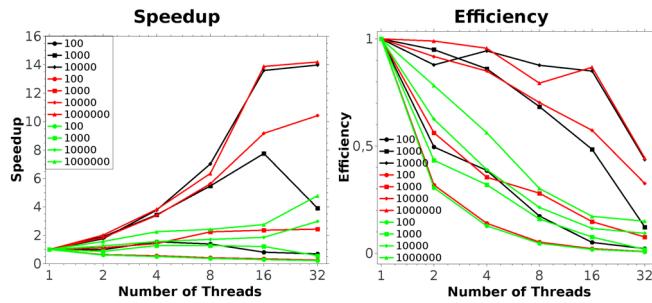


Figure 4. Speedup and Efficiency of the system. This compares the results without Verlet's methods (in black), Verlet's list (in red) and Verlet's cells (in green). The number of grains used to simulate varies from 100 to 1000000, indicated on the legend.

nomena which occurs when a system is shaken and a grain which is larger than the other grains in the media, rises to the surface. Friction is also an important influence to BNE, as can be seen in Figure 5, the larger grain rises in both cases for dimensionless accelerations higher than 1.00, but comparing friction walls with frictionless walls, the intruder with friction walls rises much more than the one without friction.

The parameters of the simulated system were: 2500 grains, uniform polydispersion of the radius of grains around 5%, friction coefficient of 0.5 between grains, and between grains and walls, normal spring stiffness of 1000 adimensional unities [3], tangential spring stiffness of 750 a.u., the radius of the intruder equals 3 times the radius of the larger grains in the media, density of the system equals to π^{-1} in a. u., critical damping coefficient in normal direction, time step of one tenth of the typical colision time for the smallest grains in the system. An imposed sinusoidal force is submitted to the box at 2500 a.u. and the dimensionless acceleration, $\Gamma = A\omega^2/g$, is varying between 0.85 to 1.5.

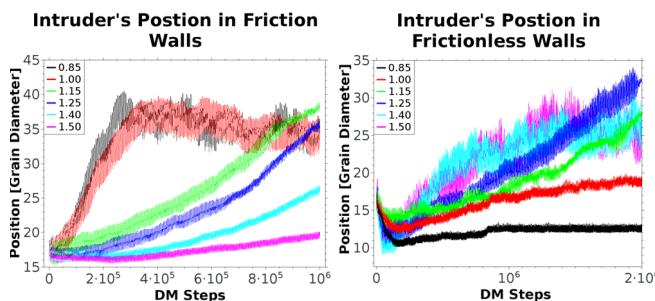


Figure 5. BNE with different amplitudes on the vibration. At left, grains have friction with walls. At right, walls have no friction.

4 Conclusions

We have presented the performance of serial and parallel MD code to simulate granular systems, with 3 different

implementations on the computational function that costs most. The implementation that shown best performance was Verlet's cells, and parallelization present higher gain with increasing number of grains. The BNE simulations evince that intruder's ascension is faster and get higher stationary positions when friction is present at grains and walls.

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A.3 *Mechanical properties of inclined frictional granular layers*

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Mechanical properties of inclined frictional granular layers

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Abstract We investigate the mechanical properties of inclined frictional granular layers prepared with different protocols by means of DEM numerical simulations. We perform an orthotropic elastic analysis of the stress response to a localized overload at the layer surface for several substrate tilt angles. The distance to the unjamming transition is controlled by the tilt angle α with respect to the critical angle α_c . We find that the shear modulus of the system decreases with α , but tends to a finite value as $\alpha \rightarrow \alpha_c$. We also study the behaviour of various microscopic quantities with α , and show in particular the evolution of the contact orientation with respect to the orthotropic axes and that of the distribution of the friction mobilisation at contact.

Keywords Granular systems · Elasticity · Jamming · DEM simulations

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1 Introduction

The nature of the jamming transition in granular systems has been investigated during the last decade, see recent reviews [29, 45]. Many studies have focused on frictionless discs or spheres, typically controlled in volume fraction ϕ or in pressure P [30, 32, 33], showing that the jamming transition is critical (scaling exponents, diverging length scale) [14, 32, 46] and related to isostaticity [1–3, 31, 32, 37, 44]. As the system loses its mechanical rigidity at the transition, its shear modulus G is found to vanish as a power law with respect to the distance to jamming $\phi - \phi_c$, where ϕ_c is the critical volume fraction. The properties of frictional granular packings have also been investigated, see e.g. [40], but, in this context of elastic properties close to jamming, most of the studies have considered homogeneous systems under isotropic pressure [1–3, 11, 22, 23, 39, 42, 47]. In the frictional case, the Liu-Nagel jamming concept [27, 28] must be revised [9]. In particular, jamming and isostatic points do not coincide any more [45], and one thus can expect a finite shear modulus at the transition.

In this paper, we consider static layers of frictional grains under gravity, by means of two-dimensional discrete element simulations (standard Molecular Dynamics [36]), and investigate their mechanical properties through the analysis of their stress response to a localized overload \mathbf{F}_0 at the layer surface, a technique particularly developed by and dear to R.P. Behringer, see e.g. [5, 16]. Expanding the work published in [8], we present here the detailed analysis of layers prepared with three different protocols. The outline is as follows. We first describe the numerical system, its preparation and the computation of the stress response. In the next section, we present an orthotropic elastic analysis of the stress profiles, and detail the fitting procedure. Then, a section is

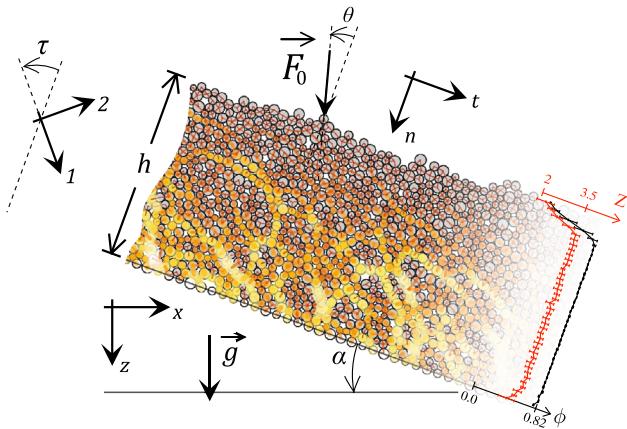


Fig. 1 System set-up and notations. x is the horizontal axis. z is the vertical one, along which acts gravity \mathbf{g} . The granular layer (here GG preparation), of average thickness h , is inclined at an angle α with respect to horizontal. t and n are the axis respectively tangential and normal to the layer. A localized force \mathbf{F}_0 , which makes an angle θ with respect to n , is applied on a grain close to the surface of the layer. The stress responses σ_{nn} and σ_{tn} to this overload are measured at the bottom of the layer (fixed grains in white). Axis $(1, 2)$, making an angle τ with respect to (n, t) , are those of the orthotropic elastic analysis. Black line volume fraction profile $\phi(n)$. Red line coordination number profile $Z(n)$. These are for the GG preparation. *Orangish colors* on grains: force chains (color figure online)

devoted to the measure and the interpretation of the microscopic data. Finally, conclusions and perspectives are drawn.

2 Numerical simulations

2.1 Numerical model and set-up

The numerical model is that described in [5, 18], with $N=3,600$ polydisperse frictional discs coupled, when overlapping, by normal and tangential linear springs, tangential forces being limited by the Coulomb condition with a friction coefficient $\mu = 0.5$. The typical thickness of the layer is $h \simeq 23$ grain diameters, i.e. a system aspect ratio around $1/6$. The layers are prepared at a *fixed* angle α with respect to the horizontal (see Fig. 1 for notations), and unjamming is approached as α is close to α_c , the critical value above which static layers cannot be equilibrated at that angle and always flow. Note that this unjamming point α_c is close in spirit to the situation of a jammed solid sheared up to its yield-stress [24]. It is also close, but different, to progressively tilted granular layers, which eventually loose their mechanical stability, see e.g., [21, 43].

In our simulations, the volume fraction in the layer is fairly uniform all through the layer depth (see Fig. 1) and roughly independent on the inclination angle. The control parameter for the jamming/unjamming transition is then the sole angle α . This situation is therefore qualitatively different to the homogeneous configurations submitted to isotropic pres-

sure cited above, and is effectively closer to an experimental set-up. No external pressure applied to the topmost layer of particles, i.e. the pressure in the system is due solely to the gravitational force acting on the particles themselves.

2.2 Three preparation protocols

Three different system preparations have been carried out: a grain-by-grain (GG), a rain-like (RL) and an avalanched (AV) deposition of the particles on a rough substrate consisting of fixed but size-distributed particles, inclined at the desired angle α . In the GG protocol, grains are added to the layer one after the other, with no initial velocity, at random t -positions and in contact with those already deposited. The time lag between two successive drops is sufficiently large to ensure the relaxation of the system before the next deposit. As for the RL preparation, all N grains are initially put at regular ‘flying’ positions above the bed, with no contact between the particles and no velocity. Then gravity is switched on, and they all fall down like a rain. Finally, for the AV preparation, we start from an initial steady and homogeneous flow running at a large inclination, then abruptly set the angle to the desired value of α and reduce the kinetic energy of the whole system. The layer is prepared when all grains have eventually reached static equilibrium (see [5] for more details).

Above a certain inclination α_c , these preparation procedures do not converge towards a static layer—the grains do not stop moving. The ‘solid-liquid’ transition occurs rather abruptly, over a typical inclination range $\Delta\alpha \simeq 0.5^\circ$ where only part of the simulations converge. This allows for a value of this critical angle defined at this precision. For both GG and AV preparations, we get $\alpha_c \simeq 20.8^\circ$. We have not studied systematically enough the RL preparation for inclinations around 20° to determine its critical angle with a good precision. However, we expect RL and AV data to be very similar close to α_c as in both cases the grains flow down the slope over long distances—typically several times the system size—before stopping, so that the initial configuration is effectively forgotten.

These three preparations mainly differ in their contact orientation (see Fig. 5). Their volume fractions does not vary much from $\alpha = 0^\circ$ to α_c . Typical values are $\phi \simeq 0.82$ for GG and $\phi \simeq 0.81$ for RL and AV. These are slightly larger than—or similar to—the critical value, estimated in our system at $\phi_c \simeq 0.81$ [12, 34, 39].

2.3 Stress response profiles

Once a layer is deposited, stabilized in an equilibrium state, an additional force \mathbf{F}_0 is applied on a grain close to the free surface, and a new equilibrium state is reached. Taking the difference between the states after and before the overload, one can compute the contact forces in response to \mathbf{F}_0 . Intro-

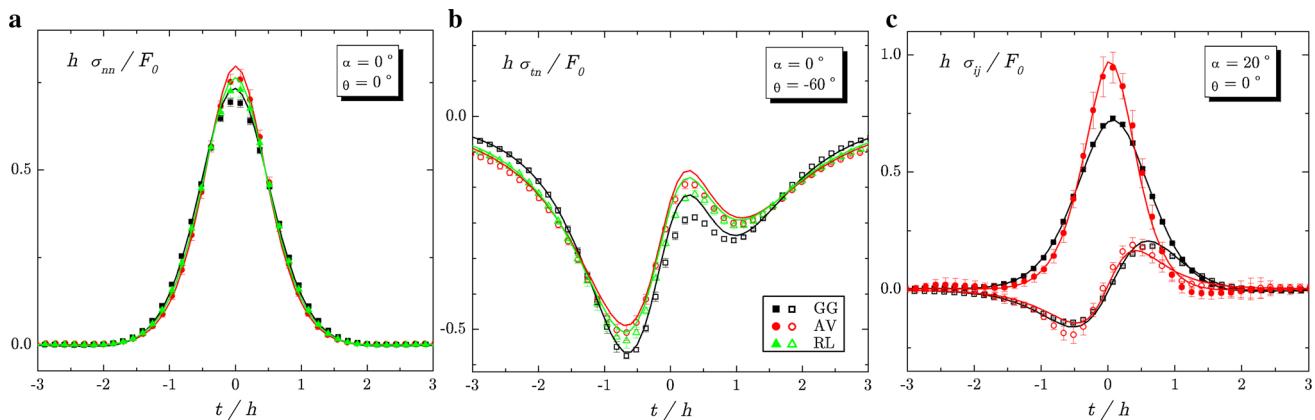


Fig. 2 Stress profiles for the different preparations. The layer inclination α and the overload angle θ are indicated in legend for each panel. Symbols numerical data (filled symbols σ_{nn} , empty symbols σ_{tn} , color

code see legend). Lines elastic fits (see Table 1 for the corresponding values of the fitting parameters) (color figure online)

Table 1 Values of the elastic parameters corresponding to the fits displayed in Fig. 2

$\alpha(^{\circ})$	Prep.	G/E_1	E_2/E_1	ν_{21}	$\tau(^{\circ})$
0	GG	0.403	0.80	0.20	93
	RL	0.303	0.69	0.23	93
	AV	0.275	0.71	0.26	91
20	GG	0.262	0.49	0.17	66
	AV	0.248	0.93	0.27	94

ducing a coarse graining length w , the corresponding stress response can be determined. Taking w of the order of few mean grain diameters (here $w = 6\langle d \rangle$) as well as an ensemble averaging of the data (here, for each tilt angle α , we average over 120–150 independent force loads, distributed on typically 10 layers in total), make the stress profiles quantitatively comparable to a continuum theory [18], such as elasticity, as discussed below. The amplitude of the overload was kept constant for all simulations: $F_0 = 1.0\langle m \rangle g$, where $\langle m \rangle$ is the average mass of the grains. This value is sufficiently small to ensure a linear [6, 7] and reversible response of the system for all values of α , including close to α_c .

Some examples of stress bottom profiles $\sigma_{nn}(t)$ and $\sigma_{tn}(t)$ are displayed in Fig. 2 for different values of the inclination α and of the angle θ that the overload force makes with the normal direction (see Fig. 1). Note that, as we deal with linear elasticity, the stresses can be rescaled by F_0/h . The normal stress data σ_{nn} show classical bell-shaped profiles, which do not differ much for all three preparations when the layer is horizontal ($\alpha = 0$) and the overload vertical ($\theta = 0$), see panel (a). However, one can distinguish between the preparations, especially GG from the two others, looking at the shear stress profiles σ_{tn} in response to a non-normal overload force ($\theta = -60^\circ$), see panel (b). The difference between GG and AV profiles is enhanced for the data at an inclination close to α_c , see panel (c).

3 Orthotropic elastic analysis

Experimental and numerical works have shown that the linear stress response of granular systems to a point force is well described by (possibly anisotropic) elasticity [4, 5, 17, 19, 20, 26, 38]. In this section, we introduce the framework of orthotropic elasticity, with which numerical response profiles such as those displayed in Fig. 2 can be fitted. The details of the computation of elastic response are available in “Appendix”.

3.1 Orthotropic elasticity

Orthotropic elasticity is characterized by a stiff axis (here labelled 1) and a soft one (labelled 2), associated to two Young moduli E_1 and $E_2 < E_1$, and to two Poisson coefficients ν_{12} and ν_{21} (note that, for symmetry reasons, $\nu_{12}/E_1 = \nu_{21}/E_2$). There is also a shear modulus G involved in the corresponding relation between stress and strain tensor components (Eq. 4). A last parameter of this modeling is the angle τ that the axes (1, 2) make with (n, t) (see Fig. 1).

Orthotropic stress responses to a point force \mathbf{F}_0 have been analytically computed in [35] for a semi-infinite medium ($h \rightarrow \infty$). For a given τ , they only depend on two combinations of the elastic parameters, noted R and T , (Eq. 14). For an elastic slab of finite layer thickness h , a semi-analytical integration, following the computation performed in [38] for isotropic elasticity, must be done (see “Appendix”). Rough bottom boundary conditions (zero displacement) are imposed. Besides the coefficients R and T , these bottom conditions involve a Poisson coefficient, say ν_{21} , so that, in total, five dimensionless numbers (τ , R , T , ν_{21} and θ) must be specified to produce the normalized bottom stress responses $\sigma_{ij}h/F_0$ as functions of the reduced tangential coordinate t/h .

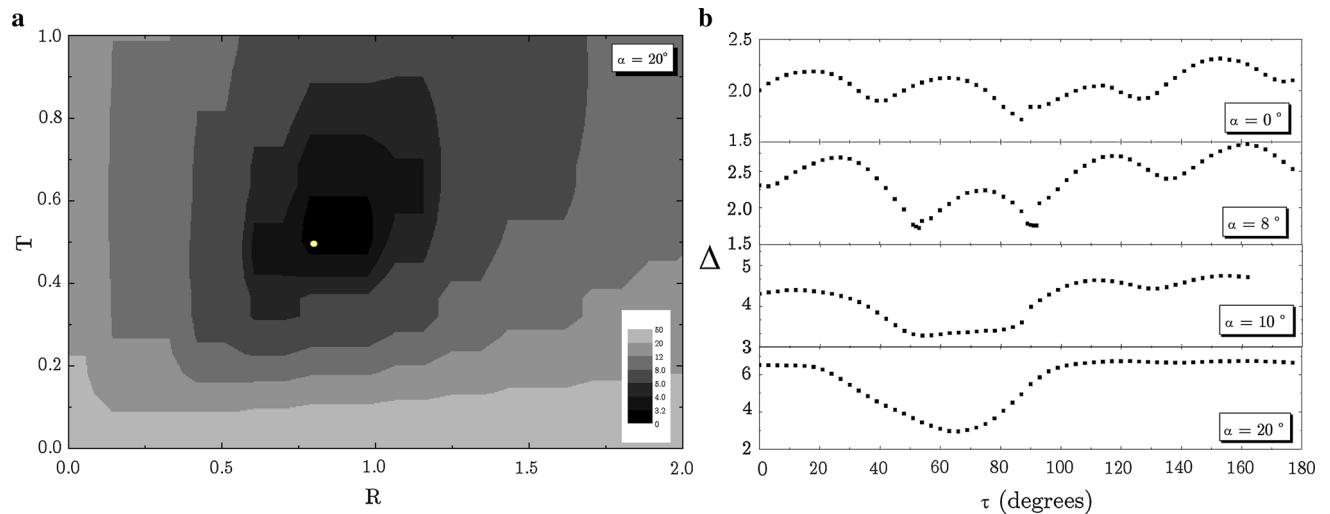


Fig. 3 Fitting technique. **a** Contour plot, in the \$(R, T)\$ parameter plane, of the normalized difference \$\Delta\$ (Eq. 1) between the numerical data and the elastic prediction. The other parameters are \$\nu_{21} = 0.15\$ and \$\tau = 66^\circ\$. The layer inclination is \$\alpha = 20^\circ\$. White bullet location of the best fit. **b**

Difference \$\Delta\$ as a function of the orthotropic angle \$\tau\$ for four values of \$\alpha\$ (see legends). These are GG data. For each of these points, all other parameters are also set to their best fitting values

3.2 Fitting numerical data

The idea is to fit the elastic response profiles to the numerical data, in order to extract the effective elastic parameters of the layer. For a given inclination \$\alpha\$, the four numbers \$\tau\$, \$R\$, \$T\$ and \$\nu_{21}\$ must be adjusted to reproduce at the same time the profiles measured for all three stress components \$\sigma_{nn}\$, \$\sigma_{tn}\$ and \$\sigma_{tt}\$, and for all overload angles \$\theta\$. This is achieved by minimizing the RMS difference

$$\Delta = \sqrt{\frac{1}{N_p} \sum_{\{i,j\}, \theta} \sum_{k=1}^{N_p} \left(\frac{\sigma_{ij}^k|_{\text{num}} - \sigma_{ij}^k|_{\text{elas}}}{\delta\sigma_{ij}^k} \right)^2}, \quad (1)$$

where \$N_p\$ is the number of data points in the profiles, and \$\delta\sigma_{ij}^k\$ is the standard deviation around the mean stress computed from the ensemble averaging.

An example of a contour plot of \$\Delta\$ in the \$(R, T)\$ plane, for given \$\tau\$ and \$\nu_{21}\$, is shown in Fig. 3a. There is a clear deepest point, which corresponds to the best fit. In Fig. 3b, we display \$\Delta\$ as a function of the orthotropic angle \$\tau\$, each point of these curves corresponding to the best fitting \$R, T\$ and \$\nu_{21}\$. These curves have been computed for the GG data at different inclination angles. It shows how the minimum, corresponding to the best fitting \$\tau\$, changes rather abruptly from \$\simeq 90^\circ\$ to \$\simeq 60^\circ\$ around \$\alpha \simeq 9^\circ\$ (see also next section and Fig. 5c).

Some of these fits are displayed in Fig. 2, for various angles \$\alpha\$ and \$\theta\$, and for the different preparations. The overall agreement between the elastic predictions and the numerical data is quantitatively good. In Fig. 4, we show the elastic modulus ratios \$G/E_1\$ and \$E_2/E_1\$ extracted from these fits, as func-

tion of the inclination. \$G/E_1\$ decreases with \$\alpha\$ but does not vanish close to the critical angle, in agreement with the observation that frictional granular systems remain hyperstatic at the unjamming transition [1–3, 23, 42]. Such a discontinuous behaviour at the transition has also been seen in simulations by Otsuki and Hayakawa [34] investigating the rheology of sheared frictional grains close to jamming, and in experimentally created shear-jammed states reported in [9]. The sudden drop of \$G/E_1\$ around \$\alpha \simeq 9^\circ\$ is associated with the change of the orthotropic directions mentioned above. The behaviour of \$E_2/E_1\$ also present an overall decrease with \$\alpha\$, except for the AV data close to \$\alpha_c\$. The complete interpretation of this behavior of the AV data is not entirely clear, but it is clearly related to an increase of friction mobilization at the contacts (see Figs. 5, 6 and discussion below).

4 Microscopic variables

In addition to the above global mechanical properties of the system, we have studied the evolution of various microscopic quantities with \$\alpha\$. The first one of interest is the coordination number \$Z\$, i.e. the average number of contacts per grain, here computed in the bulk of the layer, where it is fairly uniform—it obviously drops down close to the surface. \$Z\$ monotonously decreases with \$\alpha\$ for the GG preparation, while it stays approximately constant for RL and AV data (Fig. 5a). In all cases, it stays always far from the isostatic value \$Z_{\text{iso}} = 3\$ (for frictional grains in 2D). Grains of the bulk that only carry their own weight do not contribute much to the global stability of the contact network. As for so-called rattlers in gravity-free packings (see [13], chap. 6), these grains can be

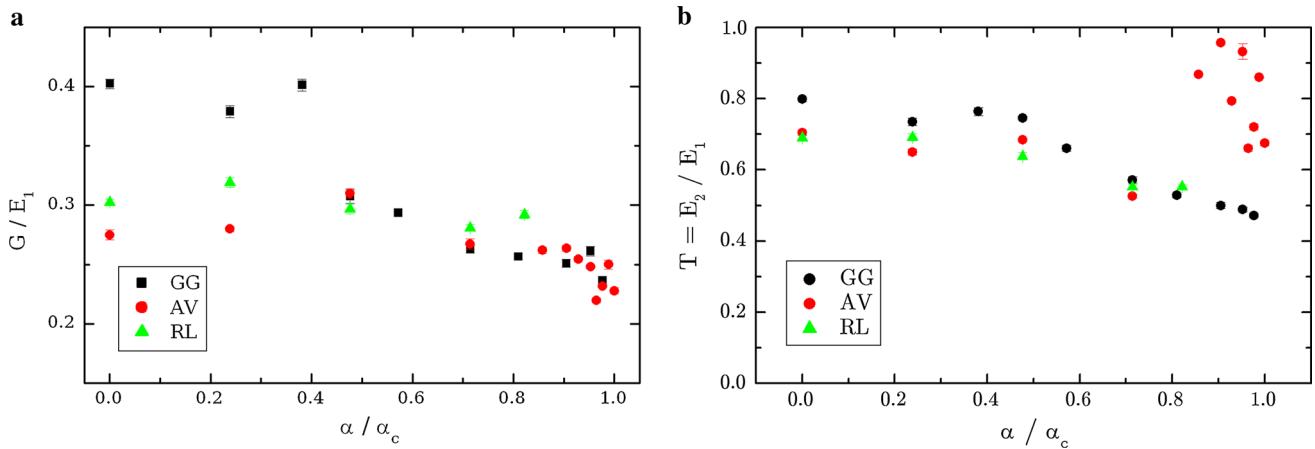


Fig. 4 Shear and Young moduli ratios G/E_1 (**a**) and E_2/E_1 (**b**) as functions of α/α_c . These data include all three preparations GG, RL and AV, see legend (color figure online)

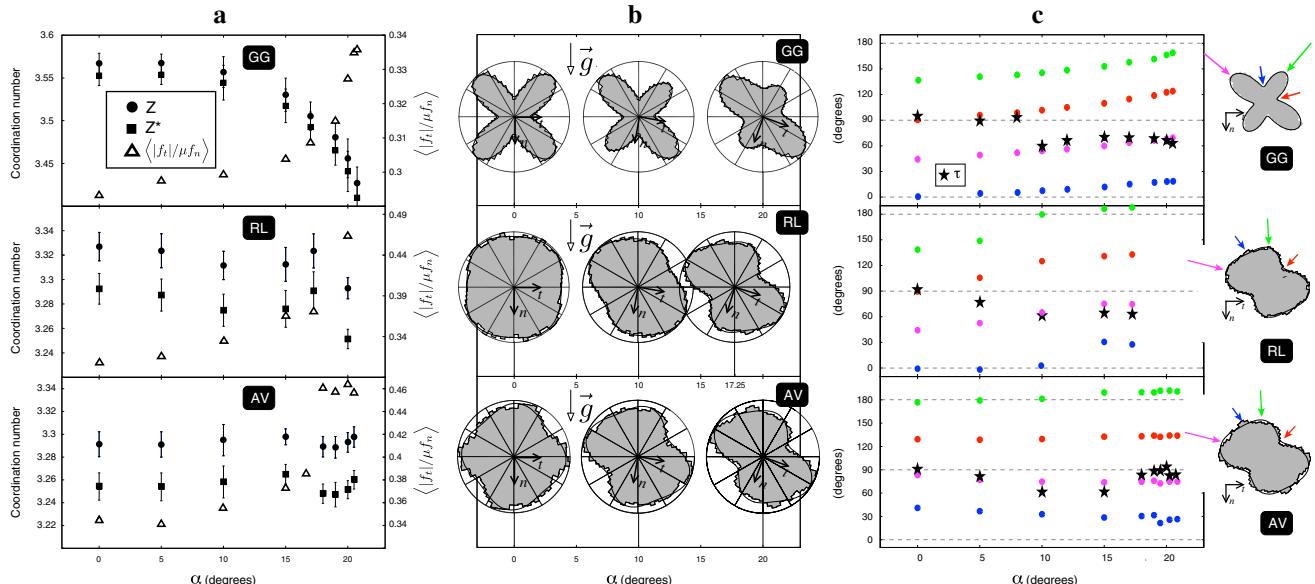


Fig. 5 Microscopic data for the three preparation protocols GG (top), RL (middle) and AV (bottom). **a** Coordination number Z (circle) and modified ('rattlers' removed) coordination number Z^* (square) as functions of the inclination of the layer α . Right y-axis: relative importance of the average friction mobilisation at contact (triangle). **b** Contact angle polar distributions at three inclination angles α . Solid black line fourth-

order Fourier fit. Gravity is vertical (black arrow). **c** Fitted orthotropic elastic angle τ as a function of α (star). The four characteristic angles of the contact angle distribution, computed with respect to the direction n , are also shown—these angles corresponds to the directions of the lobes, and those in between the lobes, see sketch and corresponding coloured arrows in legend (color figure online)

removed from the contact counting, leading to a modified coordination number of the layer Z^* (see Fig. 5a). However, we find that their number is roughly independent of α .

We have also studied the friction mobilisation at the contact level. In the MD simulations, the number of contacts with a ratio of the tangential force f_t to the normal force f_n strictly equal to the microscopic friction μ is zero when static equilibrium is reached. However, some of them are effectively close to the Coulomb criterion. We have first computed the average $\langle |f_t|/\mu f_n \rangle$. This quantity, displayed in Fig. 5a, increases as $\alpha \rightarrow \alpha_c$ for all three preparations, but its overall varia-

tion is weaker for the GG data (see right y-scales), as could be expected. More precisely, we also display in Fig. 6a, b the probability distribution function of the friction mobilisation at contact for the two preparations GG and AV, and for several inclinations. For the GG preparation, the distribution is only slightly skewed towards larger values of $|f_t|/\mu f_n$ when α is increased, but nothing particular happens close to $|f_t|/\mu f_n = 1$. For the AV preparation, however, a peak close to $|f_t|/\mu f_n = 1$ appears for $\alpha \gtrsim 18^\circ$, corresponding to quasi-sliding contacts. Figure 6d shows that they are uniformly distributed all through the layer depth. Following [23, 25, 41], we

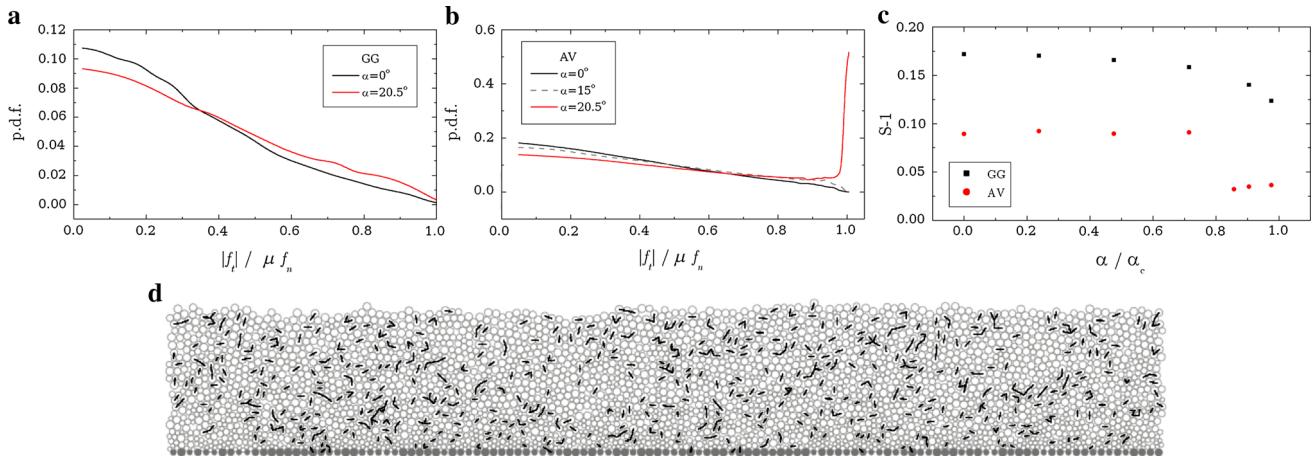


Fig. 6 Probability distribution function of the friction mobilisation at contact $|f_t|/(\mu f_n)$ for the GG (a) and the AV (b) preparations. The distributions for several values of α are displayed. For the AV preparation, the distribution at $\alpha = 18^\circ$ is not shown but is identical to that

at $\alpha = 20.5^\circ$. c Redundancy factor, as defined in [25], as a function of α/α_c . d Spatial distribution of quasi-sliding contacts (bold dashes) in an AV-layer at $\alpha = 20.5^\circ$ (color figure online)

have computed the redundancy factor S , i.e. the ratio of the total number of force degrees of freedom at contacts over the number of equilibrium equations, taking into account these quasi-sliding contacts: $S = (2n_c - n_s)/(3N)$, where n_c is the total number of contacts and n_s is the number of quasi-sliding contacts—recall the system is two-dimensional. We see that S decreases with α (see Fig. 6c), and, for the AV preparation, approaches 1 (the isostatic value), though remaining above this value at α_c .

Finally, we have studied contact angle distributions. Three of these distributions are represented as polar diagrams for $\alpha = 0, 10$ and 20 (or 17.25 for RL) degrees in Fig. 5b. Let us first comment the GG data. The four strongly pronounced lobes are typical of this preparation [13] (chap. 6). The vertical and horizontal directions are always in between these lobes. When the layer is horizontal ($\alpha = 0^\circ$), the orthotropic stiff and soft directions are also found to be (almost) along the horizontal and vertical axis respectively. Note that the fitting procedure effectively gives here $\tau = 93^\circ$ in this case, while $\tau = 90^\circ$ (or 0°) would have been expected for symmetry reasons. This effectively indicates the typical precision we have on the measure of this orthotropic angle. Close to the critical slope, however, the orthotropic orientations are close to those of the lobes, the stiff one being in the direction of the slope. As evidenced in Fig. 5c, the transition between these two microscopic configurations occurs around $\alpha \simeq 9^\circ$, i.e. well below α_c , in correspondence with the drop of G/E_1 between 8° and 10° (see Fig. 4). The polar distributions computed with RL and AV data are more isotropic than in the GG case (Fig. 5b). However, although the lobes are less pronounced, the overall behaviour of the RL data is similar to the GG ones. In the AV case, the orthotropic direction roughly follows that of the lobes over the all range of inclination.

5 Conclusions

To sum up, we have simulated 2D frictional and polydisperse granular layers under gravity inclined at an angle α , and investigated their mechanical and microscopic properties when the unjamming transition is approached. This work tells us what to expect in real experiments, i.e. a layer that becomes elastically softer as $\alpha \rightarrow \alpha_c$, as e.g. inferred from acoustic experiments on a granular packing in the vicinity of the transition [10]. More precisely, the shear modulus G and the stiff Young modulus E_1 both decrease with respect to the soft modulus E_2 , but not to the point at which the system would lose its rigidity before avalanching. In particular, as evidenced by the comparison of the curves in Figs. 4 and 5a, the shear modulus is not found to be a linear function of $Z - Z_{\text{iso}}$ (or $Z^* - Z_{\text{iso}}$), in contrast with the finding of [42] on homogeneous frictional systems, close to isostaticity. In fact, in agreement with the analysis of [21], the idea that the whole granular layer reaches the isostatic limit at the critical angle α_c is too simple because it ignores the anisotropy and inhomogeneity of the packing induced by the preparation and the gravity field. Interestingly, in the simple shear geometry considered in [25], the redundancy factor S does tend to 1 when the critical state is reached, but here remains (slightly) above this value for the avalanched layers, even though some (quasi) sliding contacts appear.

As for perspectives, similarly to what we did for the GG layers in [8], one should compute the vibration modes for the AV layers, taking into account the presence of these quasi-sliding contacts. Also, it could be interesting to use granular simulations with a rolling resistance [15] in order to explore a wider range of ϕ , Z and α .

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Appendix: Orthotropic elastic response

In this Appendix, we detail elastic calculations on a 2D orthotropic slab of finite thickness h . Following the notations of Fig. 1, we note (1, 2) the orthotropic directions, while (n, t) are the directions respectively normal and tangential to the slab. We note τ the angle between axes (1, 2) and (n, t). For the sake of the computation of the stress profiles in response to a force \mathbf{F}_0 applied at the free surface, one can switch off gravity, and the mechanical equilibrium of the system writes

$$\partial_n \sigma_{nn} + \partial_t \sigma_{tn} = 0 \quad \text{and} \quad \partial_n \sigma_{tn} + \partial_t \sigma_{tt} = 0, \quad (2)$$

where σ_{ij} is the stress tensor. We define the strain tensor u_{ij} from the displacement field u_i as $u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$. It verifies the compatibility condition:

$$\partial_n^2 u_{nn} + \partial_t^2 u_{tt} - 2\partial_n \partial_t u_{tn} = 0. \quad (3)$$

Introducing the two Young moduli E_1 and $E_2 < E_1$, the shear modulus G and two Poisson coefficients ν_{12} and ν_{21} , the generalised Hooke’s law relating strain and stress tensors writes, in the orthotropic axes, as follows:

$$\begin{pmatrix} u_{11} \\ u_{22} \\ u_{12} \end{pmatrix} = \begin{pmatrix} \frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & 0 \\ -\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & 0 \\ 0 & 0 & \frac{1}{2G} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{pmatrix}. \quad (4)$$

We call \mathcal{W}_\dagger this 3×3 compliance matrix. It must be symmetric and these coefficients thus verify $\nu_{12}/E_1 = \nu_{21}/E_2$. Elastic energy is well defined if all moduli E_1, E_2, G are positive and $1 - \nu_{12}\nu_{21} > 0$. In (n, t) axes, we have

$$\begin{pmatrix} u_{nn} \\ u_{tt} \\ u_{tn} \end{pmatrix} = \mathcal{W}_\tau \begin{pmatrix} \sigma_{nn} \\ \sigma_{tt} \\ \sigma_{tn} \end{pmatrix} \quad \text{with} \quad \mathcal{W}_\tau = \mathcal{Q}^{-1} \mathcal{W}_\dagger \mathcal{Q} \quad (5)$$

and the rotation matrix

$$\mathcal{Q} = \begin{pmatrix} \cos^2 \tau & \sin^2 \tau & 2 \cos \tau \sin \tau \\ \sin^2 \tau & \cos^2 \tau & -2 \cos \tau \sin \tau \\ -\cos \tau \sin \tau & \cos \tau \sin \tau & \cos^2 \tau - \sin^2 \tau \end{pmatrix}. \quad (6)$$

The matrix \mathcal{W}_τ can be made explicit as follows:

$$\mathcal{W}_\tau = \frac{1}{E_2} \begin{pmatrix} A & -C & 2D \\ -C & B & 2F \\ D & F & H \end{pmatrix}, \quad (7)$$

with

$$A = T \cos^4 \tau + \sin^4 \tau + 2R \cos^2 \tau \sin^2 \tau, \quad (8)$$

$$B = \cos^4 \tau + T \sin^4 \tau + 2R \cos^2 \tau \sin^2 \tau, \quad (9)$$

$$C = \nu_{21} + \cos^2 \tau \sin^2 \tau (2R - 1 - T), \quad (10)$$

$$D = \cos \tau \sin \tau [(\sin^2 \tau - \cos^2 \tau)R + \cos^2 \tau (1 + T) - 1], \quad (11)$$

$$F = \cos \tau \sin \tau [(\cos^2 \tau - \sin^2 \tau)R + \sin^2 \tau (1 + T) - 1], \quad (12)$$

$$H = \nu_{21} - 2 \cos^2 \tau \sin^2 \tau (2R - 1 - T) + R, \quad (13)$$

and where we have introduced the two dimensionless numbers

$$T = \frac{E_2}{E_1} = \frac{\nu_{21}}{\nu_{12}}, \quad \text{and} \quad R = \frac{1}{2} E_2 \left(\frac{1}{G} - \frac{\nu_{12}}{E_1} - \frac{\nu_{21}}{E_2} \right). \quad (14)$$

With the four roots X_k ($k = 1, \dots, 4$) of the biquadratic equation $X^4 + 2RX^2 + T = 0$, that is

$$X = \pm \sqrt{-R \pm (R^2 - T)^{1/2}}, \quad (15)$$

the general solution of the problem can be written as sums of Fourier modes:

$$\sigma_{nn}(n, t) = \sum_{k=1}^4 \int_{-\infty}^{+\infty} b_k(q) e^{iqt+iY_k q n} dq, \quad (16)$$

$$\sigma_{tt}(n, t) = \sum_{k=1}^4 \int_{-\infty}^{+\infty} b_k(q) Y_k^2 e^{iqt+iY_k q n} dq, \quad (17)$$

$$\sigma_{tn}(n, t) = - \sum_{k=1}^4 \int_{-\infty}^{+\infty} b_k(q) Y_k e^{iqt+iY_k q n} dq, \quad (18)$$

where $Y_k = (X_k - \tan \tau)/(1 + X_k \tan \tau)$. The four functions b_k are determined by the boundary conditions at the top and the bottom of the slab.

At the free surface ($n = 0$), the overload force imposes two components of the stress:

$$\sigma_{nn} = F_0 \cos \theta \Delta(t) \quad \text{and} \quad \sigma_{tn} = F_0 \sin \theta \Delta(t), \quad (19)$$

where θ is the angle between \mathbf{F}_0 and the direction of the n axis (see Fig. 1), and where $\Delta(t)$ is a normalised function which tells how this force is distributed along the surface—e.g. a Dirac or a Gaussian of width w_F . We need here its Fourier transform $s(q)$. For the Gaussian case, $s(q) = \frac{1}{2\pi} \exp(-\frac{1}{2} w_F^2 q^2)$. We typically take $w_F \rightarrow 0$ (a δ -peak). These top conditions (19) then give

$$\sum_{k=1}^4 b_k = F_0 \cos \theta s(q) \quad \text{and} \quad \sum_{k=1}^4 b_k Y_k = -F_0 \sin \theta s(q). \quad (20)$$

At the bottom of the slab ($n = h$), we impose rigid and rough conditions, i.e. vanishing displacements in both t and

n directions: $u_t = u_n = 0$. In order to get equations on the functions b_k , we must transform these conditions into equations on the stress components. Taking its derivative along t , the condition $u_t = 0$ gives $u_{tt} = 0$, i.e.

$$-C\sigma_{nn} + B\sigma_{tt} + 2F\sigma_{tn} = 0, \quad (21)$$

leading to

$$\sum_{k=1}^4 b_k \left[-C - 2FY_k + BY_k^2 \right] e^{iY_k q h} = 0. \quad (22)$$

Similarly, the condition $u_n = 0$ gives, after a double derivative along t , the relation $2\partial_t u_{tn} = \partial_n u_{tt}$, leading to

$$\sum_{k=1}^4 b_k \left[2D + (C - 2H)Y_k + 4FY_k^2 - BY_k^3 \right] e^{iY_k q h} = 0. \quad (23)$$

The four linear Eqs. (20, 22, 23) can be inverted, leading to large but analytic expressions for the functions b_k . Integrations over q involved in Eqs. 16–18 must, however, be computed numerically. Finally, the stress components, made dimensionless by F_0/h , can be plotted for given values of the five parameters τ , T , R , v_{21} and θ , as functions of t/h at a given depth (e.g. $n = h$). We checked that the results are insensitive to the value of w_F/h , as long as it remains small.

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A.4 *Non-Gaussian behavior in jamming / unjamming transition in dense granular materials*

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Non-Gaussian behavior in jamming / unjamming transition in dense granular materials

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Abstract. Experiments of penetration of a cylindrical intruder inside a bidimensional dense and disordered granular media were reported recently showing the jamming / unjamming transition. In the present work, we perform molecular dynamics simulations with the same geometry in order to assess both kinematic and static features of jamming / unjamming transition. We study the statistics of the particles velocities at the neighborhood of the intruder to evince that both experiments and simulations present the same qualitative behavior. We observe that the probability density functions (PDF) of velocities deviate from Gaussian depending on the packing fraction of the granular assembly. In order to quantify these deviations we consider a q -Gaussian (Tsallis) function to fit the PDF's. The q -value can be an indication of the presence of long range correlations along the system. We compare the fitted PDF's obtained with those obtained using the stretched exponential, and sketch some conclusions concerning the nature of the correlations along a granular confined flow.

Keywords: jamming/unjamming transition, granular systems, q -gaussian distributions, flow in channels

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INTRODUCTION

Due to its importance for technological applications as well for better understanding of natural phenomena, in last years increasing interest has been paid on the so-called jamming/unjamming transition in confined granular systems [1, 2, 3, 4, 5]. Of particular interest is the clogging of granular material around an intruder – or obstacle– which is a quite common situation in the industry (transport and confining materials) or civil engineering (pile driving for deep foundations). From the mechanical point of view, this type of experiment may provide a better understanding of yielding in granular media by observing directly the structural and dynamic features of the mechanisms which govern the plasticity in dense granular media [4, 5, 6]. Thus, the study of the rheology of a confined granular system close to the jamming became one of the key points of current research, and one of the fundamental issues on current research is to characterize the velocity distribution which governs the system at different jamming/unjamming situations. It is well known that, assuming molecular chaos hypothesis, the expected distribution for a set of colliding particles is that from Maxwell-Boltzmann theory, the Gaussian distribution with its typical bell-shape format and, indeed, it is observed in dilute granular systems and granular

gases [7, 8]. However, previous studies in different confining situations (jamming) [9, 10, 11] have shown that the measured distribution usually deviates a lot from the Gaussian, and the function generally used to fit the data in this scenario is the stretched exponential [12, 13].

In this work, we propose to investigate the grain velocities' distribution around the intruder as a function of the packing fraction of the granular system, in order to verify a possible connection between the characteristic exponent of the distribution and the degree of jamming. We have fitted the data by two kinds of probability distribution functions (PDF's). First, we have considered the stretched exponential,

$$f_\alpha(x) = A * \exp(B * (x - x_0)^\alpha), \quad (1)$$

where A , B , and x_0 are free parameters usually employed in the fit function, and α is the degree of the distribution. Second, we have used the q -Gaussian which was proposed by C.Tsallis [14] as a generic distribution to describe pdf in non-extensive systems:

$$f_q(x) = \frac{\sqrt(D)}{C} (1 - Dx^2(1 - q))^{-\frac{1}{1-q}}, \quad (2)$$

where D is an adjustable parameter (analogous to the inverse of temperature in the Boltzmann-Gibbs formula-

METHODOLOGY

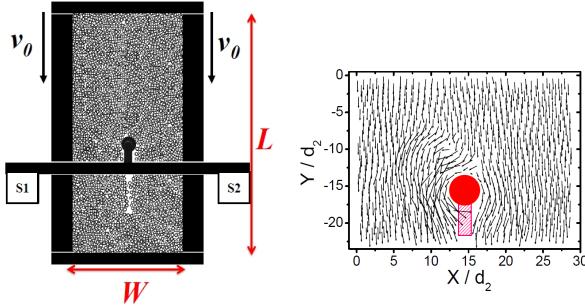


FIGURE 1. Schematic of the experiment. The containing box of dimensions $W = 54 d_2$ and $L \leq 94 d_2$ is placed horizontally over a translating plate and filled with the bidisperse mixture with 7 : 4 proportion of large to small disks. The arrows on both sides indicate the movement of the box at velocity v_0 ; the small circle in the middle marks the intruder, which is fixed in the laboratory frame and connected to two force sensors S1 and S2. The right panel shows a typical displacement map obtained between two successive snapshots with a magnification factor of 50.

tion) and C is a normalization factor. In the fitting procedure, we let D and C vary as free parameters. For tangential velocity distributions for q -gaussian as well as for stretched exponential fits, we also included a 4th parameter, x_0 in order to consider distributions not centered at the origin. The parameter q , which gives the name of this q -Gaussian PDF, is the control parameter which allows to recover the usual Gaussian distribution when $q = 1$, while for $q > 1$ we should expect long range correlations along the system. The major advantage of this particular choice for the PDF is its ability to fit all the data range with a single function, and no need to use a combination of stretched exponential and Gaussian to fit separately the tail and the central part of the distribution [3]. Another interesting feature of the q -Gaussian is the possibility to link directly the value of the q to the length of correlations along the system. For $q = 1$, we expect short range correlations, as assumed in the molecular chaos hypothesis; for $q > 1$, long-range correlations should arise in the system, and the distribution exhibits heavy tails. Thus, we expect that for unjammed, looser systems, the velocity distribution should be rather well described by Gaussian functions or q -Gaussians with $q \rightarrow 1$, while for jammed situations we expect to find a good fit with $q > 1$.

The paper is structured as the following: in the next section we present the experimental set up and the simulation method, and the analysis technique to build the distributions. Next, we compare the fitted exponent values for the experiments and simulations, and their dependence with the packing fraction ϕ and temporal evolution. Finally, we sketch some conclusions.

The experimental setup was already presented in details previously [5] and consists in an horizontal rectangular box filled with a bidisperse mixture of grains – see Figure 1. with $d_2 = 1.25 d_1$, where d_2 (d_1) is the diameter of the large (resp. small) species. In the experiments shown, typically around ~ 6500 grains were used. The packing fraction ϕ was adjusted to $0.8 < \phi < 0.84$, typically below or equal the jamming packing fraction for a frictional granular medium. A CCD camera of 1600×1200 pixels placed above the set-up recorded images every $d_2/30$ displacement of the box, while the box was pulled at a constant velocity v_0 along the tangential t direction. Then an image analysis software is used to localize the positions of grains in each image. By calculating the displacement of each grain between successive images, we construct the cumulative velocity PDF and fit with the q -Gaussian function and stretched exponential, as shown in Figure 2. More precisely, we measured the velocity distributions along the normal v_n and tangential v_t directions of box displacement. We used a minimum square method to obtain the best fit values for the PDF's using equations 1 and 2 as fitting functions.

The simulation is designed to be closer as possible to the experimental situation. We have used a molecular dynamics (MD) code in 2 dimensions, with velocity Verlet implementation and 3rd order Gear predictor-corrector [15]. The rheology for the particles was a modified version of the original Cundall-Strack model [16], with the contact between grains represented as normal and tangential springs, and Coulomb friction between grains. The simulated system has the same geometry, number of grains and aspect ratio as the experimental setup, but the range of packing fraction values simulated was a bit different from the experiments, since we can better explore the parameter space with simulations. Besides, the microscopic parameters were chosen in order to get the best performance for the code, and do not correspond literally to the values expected if a direct conversion of the experimental values was made. Thus, in normalized units the values used for the parameters were: $k_n = 1000$, $k_t = 750$ for the normal and tangential spring stiffnesses, and $\mu = 0.5$ for the friction coefficient. We have used a critical damping in the normal direction of the contacts, but no damping in the tangential one, only Coulomb friction dissipates energy in tangential contact direction. (Please find in [17] the precise definitions of the normalized unities and in [18] more details concerning the simulation method. The normalization of length used here was the width of the system, W).

We ran simulations with the same number of realizations as performed in the experiments. Then we averaged the same number of snapshots to build the velocity pdf's (the “snapshots” in simulations correspond to the config-

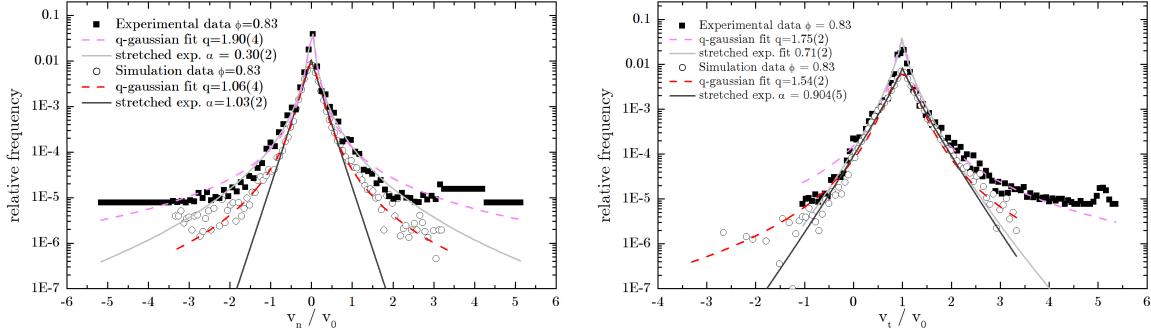


FIGURE 2. Velocities PDF's for experimental data and simulations. The distribution along the normal direction of displacement is shown at left while the distribution along the tangential direction is shown at right.

urations taken at the same frequency as in the experiment – at each $d_2/30$ displacement of the box. Thus, we were able to compare directly simulations with experimental data - Figure 2.

The distributions usually considered about 160 consecutive snapshots, and we averaged the velocities obtained from the displacements calculated between 2 consecutive snapshots (please find interesting features when different values of snapshots are used to calculate the displacement [19]). A typical experiment runs along 1600 snapshots and we can obtain the temporal evolution of the distribution. We show here only the results for distributions taken in front of the intruder in a region corresponding to the right panel of Figure 1. We study the temporal evolutions of the best fit parameters for the two PDF's used to fit the data as well the dependence of the fitted value at the half time of the experiment in function of the initial packing fraction ϕ .

DISCUSSION

In figures 2 we show some results for the velocities PDF's at the same packing fraction, for experiments and simulations. Despite not observing a perfect match, most of the qualitative features observed in the experimental PDF's were successfully reproduced by simulation and, sometimes, even quantitatively. For example, the distributions for $v_{n,t}/v_0 < 1$ show a remarkable match. Moreover, some observations were common to all packing fractions:

- First, it is clear that the confinement provoked by the presence of the intruder induces strong correlations for grains velocities, expressed by heavy tail distributions.
- Due probably to the box aspect ratio, longer than wider, we observe that the confining effect – jamming – is stronger in the normal velocities distribu-

tion than in tangential one. Thus, we have systematically verified that the stretched exponential fits v_n distributions better than q -Gaussian, since the systems are almost completely correlated along this direction.

- The v_t distributions were frequently asymmetrical, with heavy tails with different sizes for $v_t/v_0 > 1$ and $v_t/v_0 < 1$. The long heavy tails for $v_t/v_0 > 1$ systematically were better fitted by q -Gaussian.

The asymmetry observed in the tangential case can be explained considering the rectangular region of snapshot around the intruder: since the intruder is placed in the central bottom part of the region, most of the particles in average were placed in front of the intruder and moving with the same velocity as the box. As they approached the intruder, due to the flux conservation in average, the grains gained velocity, and competed to pass aside the intruder. Other grains which are located just in front of the intruder slowed down, and an excess of small velocities is observed in the distributions. The recirculation of grains just in the vicinity of the intruder (see the right panel in Figure 1) contributes for the negative values of velocities.

Another feature is the excess of velocities for experimental distributions close to $v_t/v_0 = 1$ and $v_n/v_0 = 0$, compared with simulations. This is probably due to the limited experimental frame of observation: When a new grain enters in the window observation, its preceding position is not known. Thus its first velocity is arbitrarily set to 0 in normal direction and to v_0 in the tangential one. Therefore we systematically observe an excess of velocities v_n close to zero or v_t close to v_0 in experiments compared with simulations where all the velocities are known, even outside the window observation.

Figure 3 shows the temporal evolution of the fitted parameter q from the q -Gaussian PDF's at the same value of packing fraction. We observe that the values obtained in the experiments are almost constant (except at the

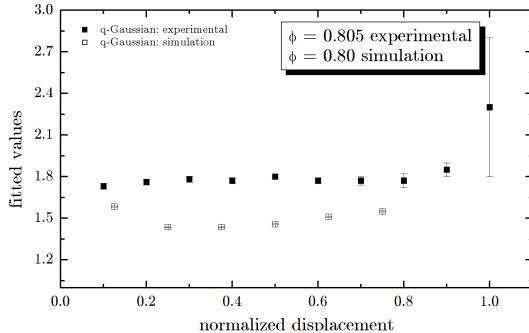


FIGURE 3. Temporal evolution of the exponents of the PDF's used to fit the data, for the packing fraction $\phi = 0.805$ in the experimental case, and $\phi = 0.8$ in simulation. Both plots show the q -Gaussian best fit for v_t in function of the normalized displacement of the containing box.

end of travelling), while in the simulations we observe a rather small but non-monotonic variation with time.

Figure 4 shows results for the fitted exponents q in function of the packing fraction. Clearly, the simulation data show a clear tendency for $q \rightarrow 3/2$ as the packing fraction increases. The experimental results, however, do not show clearly this feature, which could be due to the excess of experimental velocity v_t close to v_0 , as previously discussed. Another possible explanation, is the absence of friction between grains and the table in the case of the simulation. In simulations, since we considered the 2D case, we have no manner to implement this friction. In the experiments, the region in front of the intruder attains progressively a critical packing fraction as the box moves, and we can observe voids and inhomogeneities in the packing of grains. In simulations, the system is considerably more homogeneous, and maybe it can explain why the simulation displays monotonic dependence on the values of the fitted parameters with the packing fraction while the experimental results are inconclusive.

CONCLUSIONS AND PERSPECTIVES

We have presented experimental and simulation results for the velocity PDF's of confined granular systems in the presence of an intruder. We fit the data with q -Gaussian and stretched exponential functions, and sketch the temporal evolution of the fitted values. We verified that the system exhibits strong correlations in both normal and tangential directions, expressed by the $q > 1$ and $\alpha < 1$, but we could not verify quantitative concordance between the simulations and experiments. In simulations, a clear monotonic tendency was verified, pointing to $q \rightarrow 3/2$ and $\alpha \rightarrow 1$ as ϕ increases, but the experimental values do not display any clear tendency.

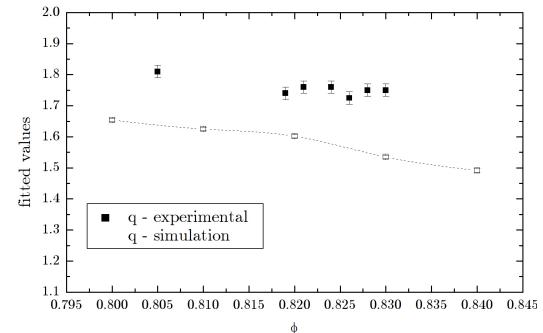


FIGURE 4. Dependence of the fitted values with the packing fraction. The best fitted values of the pdf used - q -Gaussian - were shown in function of the packing fraction at the half-time of the experiment, for v_t distribution.

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APÊNDICE B – Códigos

Coloquei os códigos utilizados para este projeto de tese em um GIT para a maior comodidade e facilidade do acesso. O endereço eletrônico é <<https://github.com/BoscoWarhammer/Doutorado>>.