Proceeding Series of the Brazilian Society of Computational and Applied Mathematics

Pattern Formation in Confined Granular Systems

Nathália Mello Mascarenhas Paixão[1]

Programa de Pós Graduação em Modelagem Matemática e Computacional, CEFET-MG, Belo Horizonte, MG

Allbens Atman Picardi Faria[2]

Instituto Nacional de Ciência e Tecnologia – Sistemas Complexos
Departamento de Física e Matemática, CEFET-MG, Belo Horizonte, MG

Abstract. There are many open questions involving the displacement of granular materials in confined systems, in particular, the flow through a Hele-Shaw cell in the quasistatic regime. It was shown that, in some cases, there is a spontaneous formation of fingers during the injection of grains into a confined system. In this work, the objective is to study the pattern formation in this kind of flow, using Molecular Dynamics simulations. Some parameters were chosen to determine their role in the development of fingers: the friction coefficient between the particles, the friction coefficient between the grains and the cell plates, the grain size distribution (monodisperse, polydisperse or bidisperse systems). The force distribution was analyzed, as well the stress components.

We have observed that the monodisperse systems have a higher tendency for fingers formation, displaying a hexagonal symmetry. We also evince a higher stress field close to the fingers tips, in analogy to the Saffman-Taylor fingering phenomenon.

Keywords. Granular materials, Pattern formation, Quasistatic flow, Molecular Dynamics

1 Introduction

A comprehensive description of the physics of granular materials still is a major challenge due to the peculiar collective behavior associated to different phenomena observed on these systems since they can display solid, liquid, or gas features depending on the experimental conditions [7, 8]. Among the enormous variety of subjects studied in this field, the spontaneous pattern formation plays a major role. It may occur in many kind of systems: vibrating beds, dense granular flows, driven granular gases, flow in rotating drums, quasistatic granular flow etc [2].

The objective of this work is to study the underlying mechanisms associated to the pattern

[1] nathmellomp@gmail.com
[2] atman@dppg.cefetmg.br

formation during the quasistatic displacement of grains in a Hele-Shaw cell. The experimental setup and the initial modeling was already done before [9], an example of experimental realizations can be seen in the Figure 1. The system consists in two parallel plates with a small gap between them (large enough to barely put one grain). The upper plate has a hole the size of which is about 2.5 grain ratio. The grains were inserted one by one in a quasistatic regime. In these experiments, there is a spontaneous finger formation in some systems.

Figure 1: An experiment of grains inserted in a Hele-Shaw cell. Legend: Transition from rounded to fingered pattern as the ratio R between the size of the injected grain and the size of the grain composing the initial layer is increased. (a) carbon steel injected in a polystyrene monolayer: R=1/1.5. (b) polystyrene injected in polystyrene: R=1/1. (c) polystyrene injected in carbon steel: R=1.5/1. The cell spacing is 6.3 ± 0.1 mm and the largest grain has a diameter of 5.9 ± 0.1 mm. All figures are 600 mm wide (Extracted from [9]).

Now, our intention is to investigate the stress propagation along the system and its relationship with the finger phenomena already reported. Our conjecture is that these phenomena have a direct analogy with the well-known Saffman and Taylor problem, where the fingering formation occurs in the fluid-fluid displacement in a Hele-Shaw cell, when the pushed liquid is less viscous than the displaced liquid [10].

To study this system, simulations were done using a common technique to model granular materials, the Molecular Dynamics (3rd order Gear predictor-corrector velocity Verlet algorithm) [4], which consists in a method to integrate differential equations numerically, where the time is discretized [1]. Some parameters were tested in the simulations to determine when the finger formation is enhanced or when it leads to circular patterns. After, stress measurements were made in order to evaluate the stress evolution when the fingers were formed. The measurement of the stress tensor is the usual tool to analyze granular systems. The stress tensor is a macroscopic measurement, but it is computed from microscopic quantities, which are, in the case of granular materials, the contact forces between grains. In quasistatic flows, the dynamic contribution of the stress can be neglected [3].

DOI: 10.5540/03.2016.004.01.0065

2 Metodology

The systems were simulated computationally by means of a 2D Molecular Dynamics (MD) algorithm. In this model, the grains are simulated as discs and there are forces between them only when they are in physical contact, the sum of the radii of the grains is smaller than the distance between their centers, implying to an overlap, δ. The interaction is divided in normal and tangential forces that in the both cases are modeled as springs. The forces are computed using the Hooke's law for elastic materials, thus the grains do not deform plastically. It is necessary to use two stiffness constants, for the normal and tangential directions, K_n and K_t respectively. Damping force was also introduced in the model [4].

In order to simulate the energy loss due to the interaction between the grains and the cell plates, the parameter η (ranging between 0 and 1) was introduced in the algorithm, in analogy with "drag friction". To determine which parameters enhance the pattern formation, we have performed simulations varying: the friction coefficient between the particles, the drag coefficient, η, the grain size distribution (monodisperse, polydisperse or bidisperse systems), and the stiffness constants ratio between injected and displaced grains.

We have considered an initial substrate with 4065 grains in some cases, and in others cases with 3781 grains, both in a hexagonal lattice. It was pushed up to 3500 grains. This base was important to confine the system, and it was made similarly with the real experiments. The inserted grains were 1.5 greater than the biggest grain of the base. The elastic modulus in the tangential direction was 0.75 of the elastic modulus in the normal direction. The damping reproduced an oscillation slightly sub-critical for the smallest grain of the system.

The instantaneous stress profile was calculated for several configurations during the run in accordance to the Equation 1. We have used a normalized Gaussian coarse graining function, $\varphi(R)$, with a characteristic width w (typically $w = 6d$, where d is the mean grain diameter). The best choice for w and the number of samples needed to obtain a robust measurement of the stress tensor were determined after [5].

$$\sigma_{\alpha\beta}(\vec{r}) = \frac{1}{2} \sum_{i,j;i\neq j} f_{ij\alpha}\, \vec{r}_{ij\beta} \int_0^1 ds\, \varphi\left[\vec{r} - \vec{r}_i + s\vec{r}_{ij}\right] \quad (1)$$

The letters i and j are the grains labels, α and β are Cartesian components, $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, where $\vec{r}_i$ is the mass center of the grain i and $\vec{r}_j$ is the mass center of the grain j, and f_{ij} is the contact force magnitude between the both grains.

3 Results

We show in this section some results concerning the different geometries of the displacement of grains – Figure 2, where the black lines represent the forces between grains that are in contact, and the width is proportional to the intensity of the force. It is worth to note that when the injected grains are monodisperse we observe an enhancement of the finger formation, and also the forces are oriented along the fingers directions.

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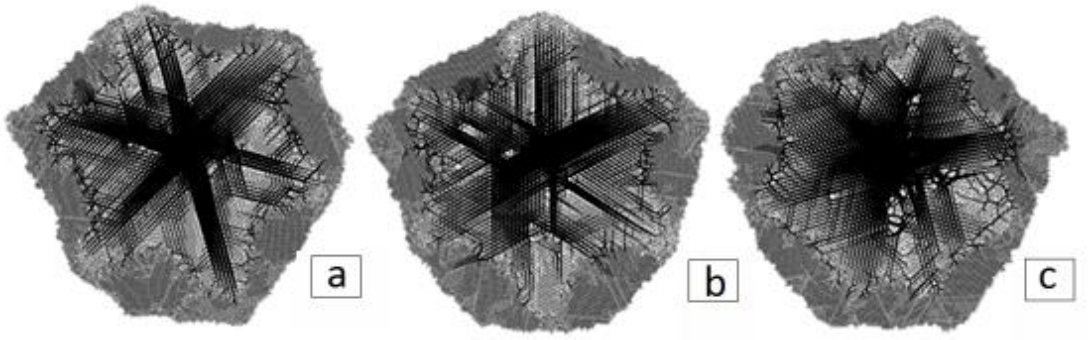

Figure 2: Simulation of monodisperse granular materials using Molecular Dynamics. Legend: Displacement of grains through a Hele-Shaw cell with a monodisperse base and 2500 monodisperse injected grains, for different friction coefficient, μ, between grains. a) μ=0.10. b) μ=0.50. c) μ=0.90.

In most of the cases, the patterns present a hexagonal symmetry, but sometimes, a pentagonal pattern can be observed, particularly, when the drag friction is high. We have noted that the value of the stiffness ratio between injected and displaced grains equal to 10 gives configurations closer to the experiments [9]. The stiffness ratio lower than 1 implies to unrealistic interpenetration between grains.

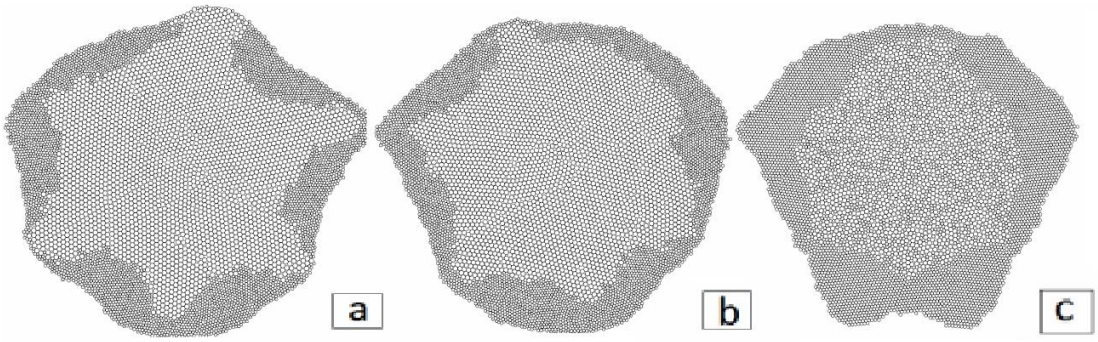

Figure 3: Simulations of differents granular systems using Molecular Dynamics. Legend: Displacement of grains through a Hele-Shaw cell, for different grains granulometries. a) Polydisperse base and monodisperse injected grains. b) Base and injected grains polydisperse. c) Monodisperse base with bidisperse injected grains.

We believe that the finger formation is associated with the crystallization of the lattice formed by the contact force network that could explain why the monodisperse systems display the best fingering patterns. The simulations using bidisperse grains do not crystallize and, consequently, there is no fingering formation, as can be seen in the Figure 3.c. The polydisperse systems also have problems to crystallize, but, when the system is only slightly polydisperse, it can crystallize and it is possible to observe fingering formation, Figure 3.b. From these results, it is possible to make a conjecture that for a given value of polydispersity, the fingering formation could be enhanced or vanish (in the nature, it is impossible to have a

strictly monodisperse system). We intend to find the range of polydispersity values associated to the fingering formation.

The Figure 4 displays only the forces between inserted grains with magnitude greater than the mean force. It is important to emphasize that the mean force of the region depends of the distance of the contact point to the center of the system (place where the grains were inserted). This was necessary because the stress in the regions closer to the center has bigger intensity, and it decreases in the regions more far away. It is possible to infer, qualitatively, that the force chains are oriented along the fingers directions in monodisperse system (Figure 4.a). In the other hand, in polydisperse systems (Figure 4.b), the force chains do not have a preferential direction. The force chains have more the power to push the grains than the other forces (but the later cannot be neglected). Because of this, if in the polydisperse systems the force chains can be oriented in random directions, it is expected to appear a circular pattern. Similarly, as in the monodisperse systems the force chains have preferential directions, the grains are pushed to the fingers directions.

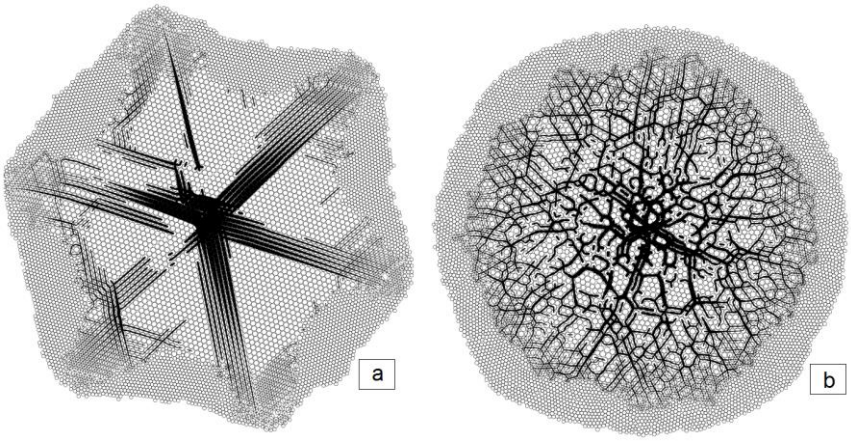

Figure 4: Simulations of two different granular systems using Molecular Dynamics. Legend: Pattern formation in simulations of granular materials flowing through a Hele-Shaw cell, with the force chains represented. a) Base and inserted grains monodisperse, hexagonal pattern. b) Base monodisperse and grains inserted polydisperse, circular pattern.

The crystallization is correlated with the force propagation models to granular materials. The fact that there is a preferential direction along the force chain network is associated with the hyperbolic model for stress propagation, leading to fingering formation, while bidisperse systems without preferential direction leads to smooth circular patterns and elliptical forces propagation model [6, 9].

The stress measurement in granular assemblies is relevant because it reveals the macroscopic behavior of the system, if there are force chains, it does not mean that the system is anisotropic, only the stress tensor can confirm that. In the Figure 5.a, the stress profile was generated 2000 times steps after the beginning of the inserting of the last grain, and the Figure 5.b represents the stress profile after 2500 times steps after the beginning. Near to the center, it is clear that the stress is greater, it occurs because the grains are pushed there. For places with the same distance from the center, the stress has bigger intensity in the fingers directions (the

signal is negative because it is a compression, there is no tensile forces). This is a proof that in monodisperse systems the model is anisotropic, where the forces propagate in the fingers directions. The Figure 5.c represents the subtraction between the stress profiles of the figures 5.b and 5.a. It is possible to see the stress evolution while the grain is inserted, there are some regions that the compression increases and regions that it decreases because of the relaxation.

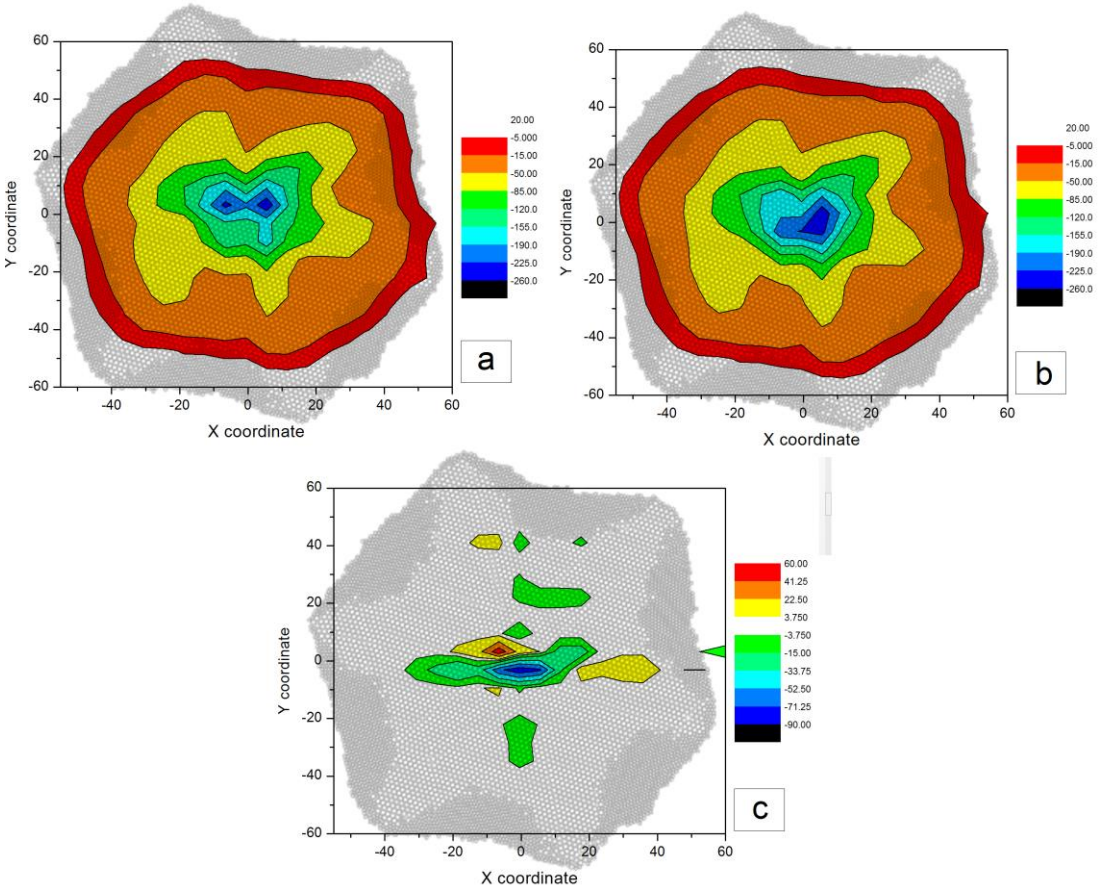

Figure 5: Stress profiles in simulation of monodisperse granular materials. Legend: Simulation of grains flowing through a Hele-Shaw cell where 3500 grains were inserted in the system. a) 2000 times steps of the insertion of the last grain. b) 2500 times steps of the insertion of the last grain. c) Subtraction of the stress profiles of the two configurations presented.

4 Conclusions

The fingering pattern formation during the displacement of granular materials through a Hele-Shaw cell occurs most of the times in systems where the grains are monodisperse distributed. This phenomenon is associated with the crystallization of the grains which is in according to the hyperbolic models of force propagation in triangular lattices.

The stress components are greater at the region which the fingers are formed.

DOI: 10.5540/03.2016.004.01.0065

Acknowledgments

I would like to thank for the financial support of CNPq, for the discussions with the professor Gaël Combe, from Grenoble, France, and for the financial support for an internship of the International Affairs Office of the CEFET-MG.

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