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Self-organizing processes in granular materials

PhD Thesis Book

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Introduction

> *Who could ever calculate the path of a molecule? How do we know that the creations of worlds are not determined by falling grains of sand?*
> *(Victor Hugo, Les Misérables)*

Is it true that the movement of an individual grain of sand is contributing in some way to the overall behavior of the world around us? Is it true that the macroscopic world is extremely sensitive to the precise motion of microscopical substances? The thoughts of Victor Hugo gave inspiration not only to myself but also many scientists to date [Bak96, Jaeger96] when thinking about granular particles.

While the behavior of a single grain - solid body interacting by frictional contacts - can be easily understood, the properties and behavior of a collection of grains are very complex. Granular materials display a surprising range of collective behavior such as convection, size separation, and pattern formation, e.g., when they are poured or shaken.

According to [deGennes99] if measured by tons, the material most manipulated by man is water, and the second most manipulated is granular matter. It is estimated that in the chemical industry roughly half of the products and at least three-quarters of the raw materials are in the form of granular solids on a weight basis [Nedderman05]. If one thinks further about the tons of wheat, sugar, ore, cement, and sand that have to be stored and transported every day, the importance of granular materials becomes evident.

The range of phenomena one can observe while conducting experiments with granular particles is so wide, that we still lack a generally acknowledged theory based on first principles, describing the behavior of granular matter. In contrast to other forms of matter, like solids, gases, and liquids, only fragments of such a theory exist in this field. Due to this, granular materials are the subject of research for a long time, and understanding their behavior on the small scale can cause enormous improvement on large-scale applications. Well-known scientists like Coulomb, Faraday, Hagen, Hertz, Huygens, Reynolds, de Gennes, Edwards, and others laid down the principles in the last centuries.

A well-known example of granular materials is sand, where the grains are mostly silica, of around 100 microns in size, rounded by collisions. It is not surprising, that the pioneering experiments were done in deserts, like the Sahara. Bagnold was one of the pioneers who systematically studied the behavior of sand and collected his findings in his book *Physics of Blown Sand and Sand Dunes* [Bagnold54]. It was first published in 1941 and since then it is used as a basic reference.

As definition, according to [Jaeger92] one can state, that granular materials are many-body systems, *"large conglomerations of discrete macroscopic particles"* with short-range particle interactions of dissipative nature. All motions of granular materials need to be sustained by the external pumping of energy to overcome the loss of energy in particle interactions.

Objectives

First of all the aim of my work was to understand the geometrically frustrated packing and ordering of particles in a container which is at the transition between two and three dimensions. This is called a $2+\varepsilon$-dimensional system. Our aim was to study the effect of shaking by means of discrete element method (DEM) simulations and experiments. A few studies had been done earlier with colloidal and granular particles [Han08, Harth15]. Our aim was to find out whether the system behaves like the two-dimensional case, when the locally optimal configuration is optimal in the global sense as well, thus the densest state can be achieved by simple dynamical processes or is it like the three-dimensional case, where the locally optimal tetrahedral configuration is not space filling. This hinders the realization of the densest configuration by shaking. In order to study this, we conducted experiments, DEM, and Monte Carlo simulations.

This 2+ε-dimensional system turned out to be an excellent opportunity to test Edwards theory [Edwards89, Mehta89, Mehta90, Edwards94, Edwards98, Edwards02, Blumenfeld06, Baule18] in case of granular materials. Although granular materials are athermal systems in non-equilibrium, Edwards proposed a theory describing the ensemble of jammed granular states in the framework of equilibrium statistical physics. Our aim was to test the applicability of this theory to our system and give its description by deriving its partition function. As the number of different configurations is limited in our system, it is possible to calculate the partition function and the corresponding observables analytically. This system makes it possible to study the case of coupled subsystems as well. By creating a coupled system one could study the zeroth law of thermodynamics in the case of granular systems.

In the second part of my work, we studied the behavior of granular particles flowing out of a cylindrical container, a silo. First of all, we were interested in the phenomenon of clogging: When the diameter of the hopper outlet is only a few times larger than the particle size, stable structures can form above the orifice to arrest the flow [Garcimartín10, Tang11, Hidalgo13, Tang16]. The aim of our DEM study supported by experiments was to understand the structure of the clogged states, the geometry of the structure above the orifice. The main question was to decide whether the structure is a three-dimensional dome or it is more like a complex structure of two-dimensional arches spanning above the orifice.

After studying the clogged states in three-dimensional silos, we studied the continuous flow of particles. Several experimental and numerical studies have shown that for frictional hard grains the discharge rate of a silo is constant and independent of the filling height [Nedderman82, Mankoc07, Pacheco-Martinez08, Ahn08, Balevičius11, Oldal12]. However, other studies [Balevičius07] reported time-dependent discharge rates for lower values of the friction coefficient. Another study based on a continuum model [Staron12] reported a transition from granular-like (constant flow rate) to liquid-like (decreasing flow rate) behavior with decreasing effective friction of the granular material. Our aim is to study the effect of particle parameters on their outflow behavior. In our DEM simulations supported by experiments we systematically change the interparticle friction and particle stiffness to understand their effect on the silo flow of granular particles.

New scientific contribution (Thesis statements)

1. **DEM and Monte Carlo simulation of the compaction of uniform spheres in a $2{+}\varepsilon$-dimensional container.**

   I have shown by means of discrete element method (DEM) simulations and experiments that the $2{+}\varepsilon$-dimensional narrow system, filled with monodisperse spherical particles, subjected to shaking approaches its ground state, the triangular lattice with bands or zigzag structures of particles touching alternatively the two sides of the cell. However, this ground state is never reached due to the formation of perfectly ordered incompatible domains. I have shown that the system is driven by the area change of local configurations in a two particle radius space and by the antiferromagnetic vertical alignment, which is supported by Monte Carlo simulations. My DEM simulations revealed that defects in the triangular lattice play an important role in the dynamics because they act as activation sources and help the development of an optimized configuration. By means of Monte Carlo simulations, I explained why it is impossible for the system to reach its ground state: This would necessitate unfavorable events with very small probability. These results are published in [P1].

2. **Application of the Edwards theory to the $2{+}\varepsilon$-dimensional system of uniform spheres by deriving its partition function and comparing the results with DEM simulations and experiments.**

   Under the guidance of János Török I have shown that the $2{+}\varepsilon$-dimensional system can be described by the Edwards ensemble, the partition function can be formulated analytically, and the observables can be calculated analytically. I have shown that the calculation matches reasonably well with simulations. By connecting two well-defined systems I have shown that the case of coupled subsystems can only be described by the Edwards ensemble if the stress equilibrium is taken into account at the microstate level and the partition function of the full system is calculated. The calculations supported by my DEM simulations showed that the Edwards ensemble fails to help in combining subsystems when there is volume exchange not only between the subsystems but also between the subsystems and the environment. These results are published in [P2].

3. **Studying the clogging and outflow behavior of granular particles from a silo by DEM simulations supported by experiments.**

   (a) I have studied the three-dimensional clogging by means of DEM simulations with spherical and elongated particles. The simulations revealed, in accordance with experiments, that on average a structure taller than a hemisphere is visible above the orifice, however, by studying single cases, sparser regions and rathole-like structures can be found. I developed a triangulation method to precisely describe the surface of the clogged structure. The DEM simulations have shown that in the case of elongated particles sometimes a vertical wall is made of horizontally placed particles around the orifice which is closed by the hemisphere-like object found in the case of spherical particles. I have shown that the clogged structure above the orifice is a primary, two-dimensional arch supported by secondary arches. The interparticle force network of the system shows an onion-like layered structure: Cupolas are built upon each other concentrically in semi-ellipsoidal layers. Cupolas farther from the orifice hold larger forces and transmit them to the silo base or wall far from the orifice, reminiscent of the Janssen effect. These results are published in [P3].

(b) I have studied the effect of particle stiffness and coefficient of friction on the gravity-driven silo flow behavior of spherical particles in DEM simulations. My results supported the experimental findings which revealed that the interparticle friction has a much stronger effect for soft grains than for hard grains. In the case of soft grains with high friction coefficient the flow rate is constant (granular-like behavior), while for grains with low surface friction the flow rate decreases systematically with the height of the granular bed. I have shown that the case of hard grains is different: The flow rate is basically constant except for the special limit case of frictionless grains. These results are published in [P4].

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[P2] S. Lévay, D. Fischer, R. Stannarius, E. Somfai, T. Börzsönyi, L. Brendel, and J. Török, “Interacting jammed granular systems”, *Physical Review E*, **103**, 042901 (2021). Supplementary movies of the paper can be found here and here.

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Other publications

[O1] S. Lévay and J. Török, “Multiple shear bands in granular materials”, *EPJ Web of Conferences*, **140**, 03084 (2017).

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