Ph.D. RESEARCH POSITION

Mechanics and rheology of granular chain packings: numerical study of a model system of athermal polymer

At Lab. PMMH (www.pmmh.espci.fr), CNRS/ESPCI/Paris 6/Paris 7, Paris, France

Profile

You are highly motivated and you are deeply committed to research. You are able to work independently and as part of a team. You are equipped with an analytical and critical mind-set and you communicate clearly and concisely.

Qualification

Master's degree in physics or related§background in computational physics§programming skills (e.g.C/C++, Python, Matlab)§experience in particle simulations (SPH, DEM)

Application

One single pdf including your research statement, your CV and, if applicable, a list of your publications. Please send your application to sylvain.patinet@espci.fr. Applications will be considered until the **1st of September**.

Thesis's summary (abstract):

The aim of this thesis is to study numerically the mechanical properties of an athermal analog of polymers: a packing of granular chains. By taking advantage of the analogy, polymer/granular chain, we will study the effect of the chain length and its concentration in this original macroscopic system, allowing straightforward comparison with experiments.

The first part of this thesis will be devoted to the determination of the static mechanical properties of the packing, focusing in particular on the study of the jamming transition. The second objective of this thesis topic will focus on understanding the dynamical properties of granular chains. To this end, two types of protocols will be implemented: the vibration of the packing and its loading with different shear rates to study the variation of the effective viscosity of the system.

The simulations will use a particle dynamics code that we have just developed and validated. They will be compared with model experiments carried out in collaboration with the Interfaces and Complex Fluids Laboratory of the University of Mons in Belgium.

Context

Compared to other materials, our understanding of the link between microscopic phenomena and macroscopic mechanical properties is much less advanced for polymers. This state of affairs stems essentially from the issues encountered in atomic-scale modeling of these systems. The first difficulty lies in the relatively low reliability of the interatomic potentials used in the atomistic simulations with respect to the size of the systems involved and the chemical complexity of polymers. Above all, polymeric systems are composed of extremely long macromolecules, which can reach several hundreds of thousands monomers, and most often have an amorphous structure. Under these conditions, being able only to simulate a representative structure of the experiments, and/or at thermodynamic equilibrium, constitutes a still open challenge.

In addition to these technical difficulties, one observes that polymers have so far did not benefit much of macroscopic analogies when compared to other amorphous systems. These analogies are particularly fruitful when we consider for example the work done in recent decades to compare athermal glasses and granular materials, the similarity of their microscopic relaxation processes, the

glass and jamming transitions... In addition, the use of macroscopic athermal analogues allows a much easier experimental access to particle dynamics.

The thesis aims to answer these two challenges by proposing to study numerically the mechanical and rheological properties of a system composed of granular chains. To this end, we propose to implement simulations of discrete elements where the monomers of the chains are considered as grains interacting via classical contact laws, like Hertz or Hooke. Along the chains, the adjacent grains are also linked together by attracting bonds and angular potentials in order to account for the longitudinal forces and the bending rigidity of the chain. The dynamics is that of a classical granular system, with or without dissipation. This simplified system has several advantages. The first of these lies in the possibility of a direct comparison between simulations and macroscopic experiments. The interaction potentials are indeed well known and their parameters can be easily measured. Moreover, the initial configurations of the stacking of the chains used in simulations can be either reproduced from the measured experimental conformations, or, more simply, be generated following the experimental protocol. Last but not least, this system of granular chains, acting as athermal molecules, allows a strong analogy with polymers.

This approach has already paid off. By experimentally and theoretically studying the mechanical stiffness of these granular chain assemblies, we were able in a first work to understand their resistance to deformation as a function of the length of the chains [1]. The bonds between the grains of a given chain produce topological constraints for other chains that result in interlocking points. Their modeling has been carried out with a powerful analogy in which the granular chains are considered as polymer chains, in the melted state or in solution. It is now a question of extending this first result by taking advantage of the possibilities offered by numerical simulations.

Objectives

We propose in this thesis to extend this approach by using numerical simulations of granular chains, allowing us to have access to the contact statistics in order to establish the links between microstructure and mechanical properties. The approach will consist in systematically studying the effect of the length of the chains as well as their concentration. We will first consider the static mechanical properties and then, in a second step, the dynamical properties through the study of the rheology of packings. The simulations will be confronted to experiments carried out by our partners of the Interfaces and Complex Fluids Laboratory of the University of Mons in Belgium with whom we already collaborated on this subject [1]. A preliminary study on system made it possible to develop the numerical code (massively parallel) and lay the foundations for a quantitative comparison with experiments. An example dealing with the angle of repose of a granular chain packing is shown in figure 1.

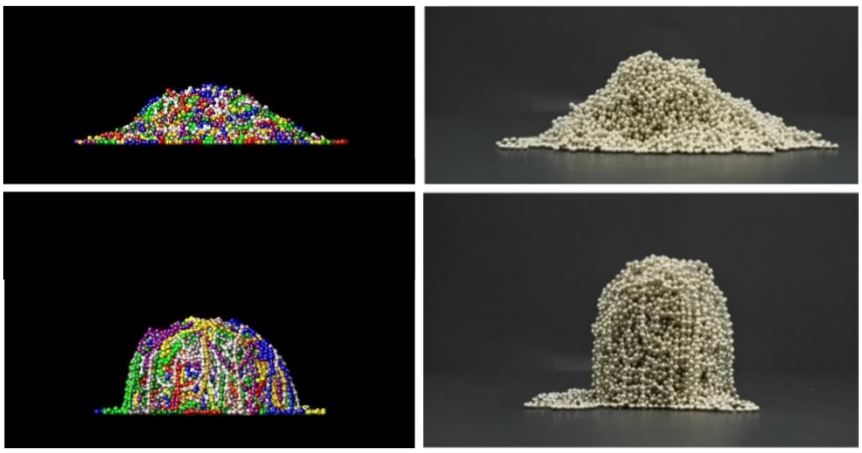

Figure 1: Static equilibrium reached after removal of a cylindrical container obtained numerically (left) and experimentally (right) for granular chains consisting respectively of 5 (left) and 30 (right) grains. One observes a transition from flow to preservation of the original shape as the length of chains in the packing is increased.

The first part of this thesis will be dedicated to the study of the static mechanical properties of packings. By exploiting the analogy between dense granular materials and thermal liquids, we will determine for which parameters the system moves from a "soft" state to a "solid" state (and acquires a finite shear modulus) by varying the density and the length of the chains. We will study the evolution of the number of macroscopic constraints in relation with the number of degrees of freedom in order to determine a phase diagram for this jamming transition. Here too, this study will benefit from the analogy with the polymers for which a variation of the glass transition temperature with the molecule size is observed. The second static configuration studied will concern more directly the problem of the storage of granular materials. We will consider the case of a silo filled with particles, whose height is large compared to its typical width, and which shows an apparent weight at the bottom largely underestimating the total weight of grains it contains. This is the Janssen effect that has been relatively little studied in the case of nonspherical particles.

Once the static properties of the packing are determined, the second objective of this thesis project will focus on understanding the dynamical properties of granular chains. To this end, two types of protocols will be implemented: the vibration of the packing and its loading at different shear rates. The vibrated configurations will make it possible to study, in the case of athermal polymers, the phenomena conventionally associated with glassy systems, such as relaxation or aging. Regarding the rheology, we will study how the effective viscosity of the packing of granular chains varies according to their length. This approach will allow us to revisit Edwards' model of a polymer chain, and its tube, and the reptation model proposed by de Gennes. Depending on the progress of the project, we will try to extend the study to the influence of the chain topology, for example in the case of star polymers showing exponential growth of relaxation times and viscosities depending with the number of entanglements by arm.

Expected results

In the long term, the approaches developed should make it possible to bring a better knowledge of the phenomena involved. By studying a hard spheres limit, this work could thus serve as a basis for a better understanding of the mechanical properties of polymers. Beyond the academic aspect, the study of granular materials is also of strong practical interest. They are in fact widely present in nature and frequently used in industry, since they are well suited for transport, storage and packing. Works on granular media, however, have so far been often confined to ideal spherical particles, sometimes elongated, but very rarely in the form of a chain. The study of these systems could therefore be interesting in other areas such as textiles, biological fibbers, new building materials...

References

[1] D. Dumont, M. Houze, P. Rambach, T. Salez, S. Patinet and P. Damman, Phys. Rev. Lett. 120, 088001 (2018) [*COVER*, *NEWS & VIEWS*, *PHYSICS*, *PRL EDITORS' SUGGESTION*, *CNRS*, *ESPCI PARIS*, *LOMA*] (pdf).