PhD subject

Mechanics and rheology of stacks of granular chains: numerical study of a model athermal polymer system

Laboratory PMMH, ESPCI, Paris, France

Profile

Master of Science — excellent level in science and general culture. A good level of English is required. The essential skills sought for this doctorate are: human qualities, communication, creativity, autonomy and adaptation, pedagogical qualities and a strong motivation for research. A good level of programming, data analysis, physics and mechanics of materials is particularly appreciated.

Application

The doctoral contract is scheduled for three years, starting in the fall. Please send your application to sylvain.patinet@espci.fr and philippe.claudin@espci.fr: a detailed CV, cover letter, detailed exam results, master's notes, names and contact details of professors and supervisors who have followed your work, letters of recommendation, master's thesis, journal and conference articles or any other document establishing your skills for this doctorate.

Thesis supervisors : Sylvain Patinet and Philippe Claudin

Doctoral school : ED 391, Sciences mécaniques, acoustique, électronique et robotique de Paris

Laboratory :

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Keywords : Discrete simulations, granular media, mechanics, statistical physics

Thesis summary

This thesis aims to numerically study the mechanical properties of an athermal analogue of polymers: a stack of granular chains. By taking advantage of the analogy, polymer/granular chain, we study the effect of the length of the chains and their concentration in this original system, allowing a direct comparison with the experiment.

The first part of this thesis will be dedicated to determining the static mechanical properties of stacks, particularly the study of the jamming transition. The second objective of this thesis topic will focus on understanding the dynamic properties of granular chains. For this, two types of protocols will be investigated: the vibration of the stack and its shear for different deformation rates to study the variation of the effective viscosity of the system. The simulations will be carried out using a particle dynamics code we have just developed and validated. They will be compared with model experiments carried out by our collaborators.

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 essentially stems from the obstacles encountered by modelling these systems at the atomic scale. The first difficulty lies in the reliability of the interatomic potentials used in the atomistic simulations concerning the size of the systems involved and the chemical complexity of the polymers. Above all, polymeric systems are composed of highly long macromolecules and most often have an amorphous structure. Under these conditions, being only able to simulate a structure representative of the experiments and/or at thermodynamic equilibrium constitutes a problem that is still open and particularly significant. In addition to these technical difficulties, there is also an observation: polymers have so far benefited little from macroscopic analogies compared to other

amorphous systems. These analogies are, however, particularly fruitful when one thinks, for example, of the work carried out in recent decades to compare glasses and athermal granular materials (similarity of their microscopic processes of relaxation and the glass and jamming transition). In addition, using an athermal macroscopic analogue allows much easier experimental access to particle dynamics.

The proposed thesis subject aims to answer these two obstacles by proposing to numerically study the mechanical and rheological properties of a system composed of granular chains. For this, we propose implementing simulations of discrete elements where the monomers of the chains are modelled as grains interacting via classical friction contact laws. Along the chains, the adjacent grains are also linked by bonds and angular potentials to account for the longitudinal forces and the bending stiffness of the chain. This simplified system has several advantages—the first of these lies in the possibility of a direct comparison between simulations and macroscopic experiments. On the one hand, the interaction potentials are well known, and their parameters can be easily measured. On the other hand, the initial configurations of the stacking of the chains used in the simulation can either be reproduced from the measured experimental conformations or, more simply, be generated by following the experimental protocol. Finally, this system of granular chains, playing the role of athermal molecules, allows a strong analogy with polymers.

This approach has already borne fruit. By studying experimentally and theoretically the mechanical stiffness of these assemblies of granular chains, we could 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, which result in points of lock. Their modelling was carried out with a powerful analogy in which the granular chains are considered polymer chains. It is now a question of taking advantage of this first result by taking advantage of the possibilities offered by numerical simulations.

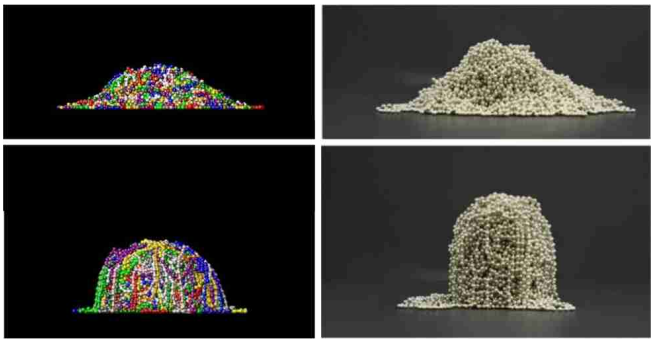

Figure 1: Granular chain stacks at static equilibrium after removal from a container obtained numerically (left) and experimentally (right) for chains consisting of 5 (left) and 30 grains (right). The system exhibits a transition between flow and preservation of the original shape depending on the length of the chains.

Expected results

By studying a limit of the hard sphere type, this work could thus serve as a basis for a better understanding of the mechanical properties of polymers. Beyond academics, studying granular materials also presents substantial practical interests. They are widely distributed in nature and frequently used in industry since they lend themselves well to transport, storage, and packaging. On the other hand, work on granular media has often been confined to ideal spherical particles, sometimes elongated but very rarely in the form of a chain. These systems could therefore be interesting in other areas such as textiles, biological fibres, and 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).