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, pedagogy and a strong motivation for research. A good level of programming, data analysis, in physics and mechanics is particularly appreciated.

Application

The doctoral contract is scheduled for three years. 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 : CNRS UMR 7636 Physique et Mécanique des Milieux Hétérogènes – ESPCI Paris

Websites : https://www.pmmh.espci.fr/ and https://blog.espci.fr/spatinet/

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

Thesis summary

This thesis aims to numerically investigate the mechanical properties of an athermal analogue of polymers: stacks of granular chains. By leveraging the analogy between polymers and granular chains, we will examine the influence of chain length and concentration in this novel system, facilitating a direct comparison with experimental data. The first phase of this research will focus on characterizing the static mechanical properties of granular stacks, with particular attention to the jamming transition. The second objective of this study is to explore the dynamic properties of granular chains under external perturbations. These approaches will allow us to probe the evolution of the system's effective viscosity under different conditions. The numerical simulations will be conducted using a newly developed and validated particle dynamics code. The results will be systematically compared with experimental data obtained by our collaborators, ensuring a robust theoretical-experimental dialogue that enhances our understanding of these complex systems.

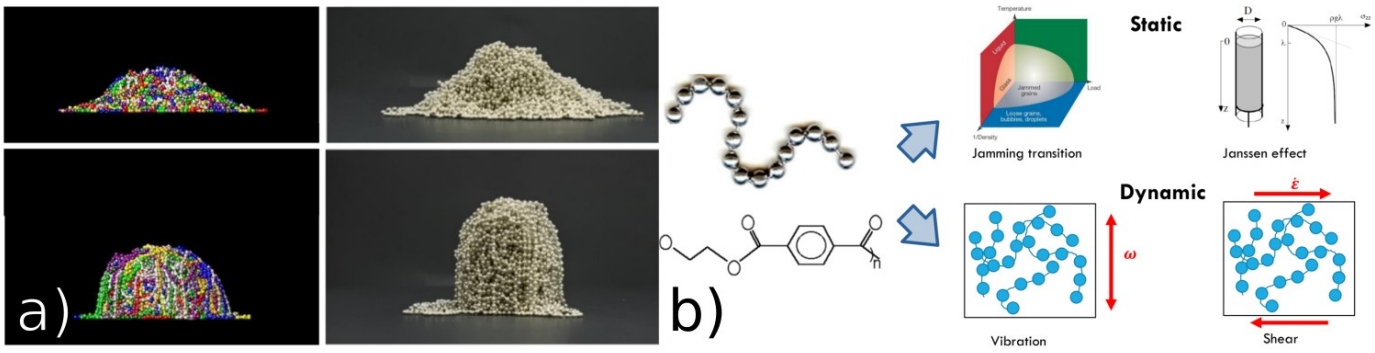

Figure 1: (a) Granular chain stacks after container removal, obtained numerically (left) and experimentally (right), for chains composed of 5 (top) and 30 grains (bottom). Depending on chain length, the system undergoes a transition from flow to the preservation of its original shape.
(b) Granular chain/polymer analogy. This study aims to investigate this novel system in both static (jamming transition and Janssen effect) and dynamic (compaction/melting under vibration and effective viscosity) conditions.

Context

Compared to other materials, our understanding of the relationship between microscopic phenomena and macroscopic mechanical properties in polymers remains significantly less developed. This gap primarily arises from the challenges of modeling these systems at the atomic scale. One of the main difficulties lies in the reliability of interatomic potentials used in atomistic simulations, given the size of the systems involved and the inherent chemical complexity of polymers. Moreover, polymeric materials have extremely long macromolecules that typically exhibit amorphous structures. Under these conditions, simulating a representative structure that aligns with experimental observations and/or thermodynamic equilibrium remains an open and significant challenge.

Beyond these technical obstacles, another critical limitation is the relative scarcity of macroscopic analogies applied to polymers, in contrast to other amorphous systems. Such analogies have proven particularly insightful in the past, as demonstrated by extensive research comparing glasses and athermal granular materials—two systems that share striking similarities in their microscopic relaxation processes and the phenomena of glass and jamming transitions. Furthermore, employing an athermal macroscopic analogue provides much easier experimental access to particle dynamics, offering a promising alternative for studying polymer-like behavior.

This thesis aims to address both challenges by numerically investigating the mechanical and rheological properties of a system composed of granular chains. To achieve this, we propose implementing discrete element simulations, where the monomers of the chains are modeled as grains interacting through classical frictional contact laws. Along each chain, adjacent grains will be connected by bonds and angular potentials to account for longitudinal forces and bending stiffness. This simplified system presents several key advantages. First, it enables direct comparisons between simulations and macroscopic experiments. The interaction potentials are well characterized, and their parameters can be readily measured. Moreover, the initial chain stacking configurations in the simulations can either be reconstructed from experimentally observed conformations or, more simply, generated by replicating the experimental protocol. Finally, this system of granular chains—acting as athermal analogues of polymer molecules—offers a robust framework for drawing meaningful parallels with polymer physics.

This approach has already yielded promising results. By studying both experimentally and theoretically the mechanical stiffness of granular chain assemblies, we have been able to characterize their resistance to deformation as a function of chain length [1]. The bonds between grains within a given chain impose topological constraints on neighboring chains, leading to localized locking points. Modeling these interactions through a polymer-chain analogy has proven to be a powerful conceptual tool. The next step is to leverage these initial findings by exploiting the full potential of numerical simulations to deepen our understanding of these complex systems.

Expected results

By exploring a limiting case akin to hard-sphere systems, this work could provide a foundational framework for a deeper understanding of the mechanical properties of polymers. Beyond its academic relevance, the study of granular materials holds significant practical interest. Granular media are ubiquitous in nature and extensively used in industry due to their favorable transport, storage, and packaging properties. However, research on granular systems has traditionally focused on idealized spherical particles—occasionally elongated but rarely arranged in chain-like structures. Investigating such systems could thus open new avenues in diverse fields, including textiles, biological fibers, and innovative building materials, where the mechanics of interconnected granular assemblies play a crucial role.

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).