Jamming of Hard-Spheres through the Lens of Constrained Optimization

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It has recently been discovered that jamming criticality of spheres-based models defines a broad universality class. Yet, computational techniques to produce jammed packings are still somewhat limited. Moreover, most of available methods are based on energy minimization algorithms, and are therefore designed for soft-spheres configurations. Naturally, generating a critical jammed packing of strictly hard-spheres (HS) is more complicated due to the singular interaction between such type of particles.

Here, we present an algorithm that allows to accurately reach the jamming point of HS configurations through a series of linear optimization problems. Within our approach, the exact, non-convex optimization problem associated to HS jamming is replaced by a sequence of simpler linear problems. Nevertheless, in all cases the non-overlapping constraints imposed by the HS interaction are strictly satisfied.

Importantly, we prove that upon convergence our algorithm produces a stable, well defined jammed state of HS, that corresponds to a (possibly local) optimum of the exact problem. We also show that our method allows to easily construct the full network of contact forces from the Lagrange multipliers associated to the non-overlapping constraints.

This new framework to tackle the jamming problem of HS as a constrained optimization problem also leads to a proxy of the entropy function of HS configurations. Given that entropy is the relevant thermodynamic potential for this type of systems, our approach yields a more precise description of the free-energy landscape. We further exploit this analogy to explore how the vibrational modes of HS can be studied using a cost function derived from the exact jamming optimization problem.

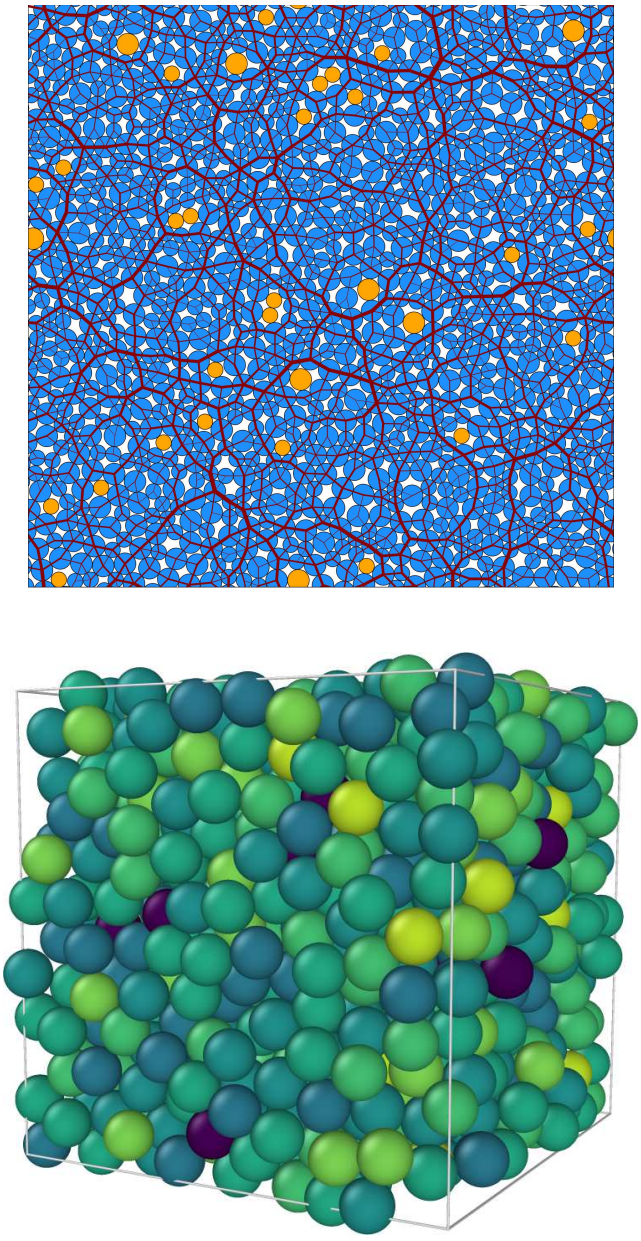

Fig. 1. Top panel: Bidisperse jammed packing of $N = 1024$ disks, showing the full network of contacts and rattlers highlighted in orange. The forces magnitude are indicated by the thickness of the lines. Bottom panel: Monodisperse jammed packing of $N = 1024$ spheres, coloured according to their number of contacts.