Master equation for the probability distribution functions of forces in two-dimensional jammed soft particles

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1. Introduction

Mechanics of dense athermal particles, e.g. granular materials, has wide practical applications, while there are many difficulties to predict their responses to global deformations due to their non-affinity. In contrast, the statistical mechanics, e.g. based on the Edwards ensembles, has been developed to explain their static properties. However, we are still lacking a connection between the non-affine responses and microscopic descriptions of jammed soft particles.

In this study, we use molecular dynamics (MD) simulations of two-dimensional jammed soft particles. We measure the conditional probability distributions (CPDs) of particle overlaps and formulate a master equation for the probability distribution functions (PDFs) of overlaps, which gives microscopic descriptions of the stress, coordination number, and energy density, as basis for a macroscopic, continuum approach to large scale problems [1].

2. Non-affine evolution of the PDFs

At first, we generalize force chain networks by using the Delaunay triangulations, where not only the particles in contact, but also the nearest neighbors are uniquely connected by the Delaunay edges (Fig. 1(a)). We introduce a "generalized overlap" between particles as the difference between the sum of radii and the Delaunay edge length, where the overlap between the nearest neighbors, i.e. the particles in a "virtual contact", is defined as negative. Then, we apply isotropic compression or decompression to the static packings with different distances from the jamming point. Just after the (de)compression, the packing exhibits an affine response, where the PDF of generalized overlaps shifts to the right-hand-side in Fig. 1(b). However, the force balance between the particles is broken by (de)compression and the system is relaxed to a new static state, where the PDF is broadened and generates a discontinuous "jump" around the zero-overlap (Fig. 1(b), note the PDFs after deformations are almost same in virtual contacts).

3. Transitions of generalized overlaps

During the relaxation, (virtual) contacts change in different ways and we categorize them into the four types: contact-to-contact (CC), virtual-to-virtual (VV), virtual-to-contact (VC), and contact-to-virtual (CV), respectively, where the changes, (VC) and (CV), represent closing and opening contacts, respectively. Such transitions can be summarized in scatter plots of generalized overlaps. Figure 1(c) displays a sketch of the scatter plot, where the difference between affine and non-affine responses is characterized by linear fitting functions for scattered data and fluctuations around them. We find that the magnitude of non-affinity is determined by the amount of deformation and distance from jamming, e.g. the difference in slope is linearly scaled by the ratio between them (Fig. 1(d)).

4. CPDs and the master equation

From the results of transitions of generalized overlaps, we find that the CPD in (CC) is given by a Gaussian distribution, indicating individual stochastic evolution of contacts, while the CPD in (VV) is found to be a stable distribution, implying multi-scale correlations between virtual contacts (even though the mean change of virtual contacts is mostly affine). The CPDs in (VC) and (CV) show exponential decays from the zero-overlap, where the difference between characteristic length scales induces the discontinuous "jump" in the PDFs. We formulate a master equation from the CPDs, where a good agreement between its numerical solution and the PDFs obtained through MD simulations is established as long as the incremental deformation steps are kept much smaller than the distance from jamming (Fig. 2).

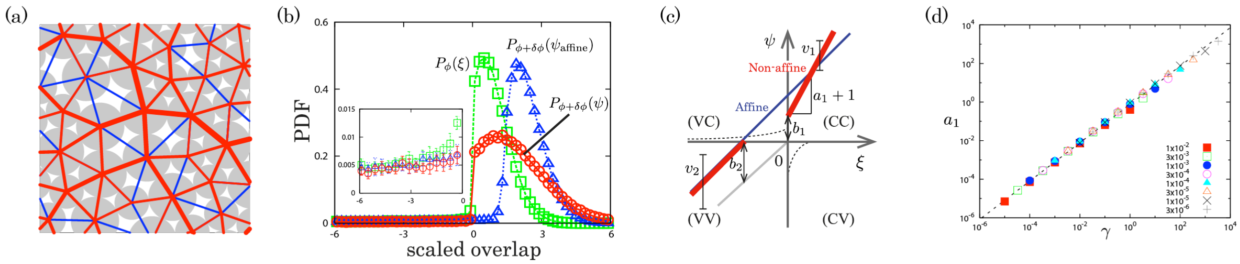

Figure 1 : (a) An extended force chain network, where the red and solid lines connect the particles in contact and virtual contact, respectively. The width of red solid line is proportional to the strength of interparticle force. (b) The PDFs of generalized overlaps before compression, just after compression (affine response), and after relaxaiton (non-affine response). (c) A sketch of scatter plot of overlaps in (CC), (VV), (VC), and (CV). The blue and red solid lines represent linear fitting functions for affine and non-affine changes of overlaps. (d) A double-logarithmic plot of the non-affinity quantified by the difference in slopes of the linear fitting functions against the ratio between the amount of compression and distance from the jamming point.

5. Conclusion

In conclusion, we propose a master equation for the PDFs of generalized overlaps by taking into account the non-affinity of the system. The non-affinity in contacts and fluctuations around mean are more pronounced near jamming, as linearly scaled by the ratio between the amount of deformation and distance from jamming, and the numerical solutions of the master equation indicate that the stochastic evolution of the generalized overlaps is a Markovian.

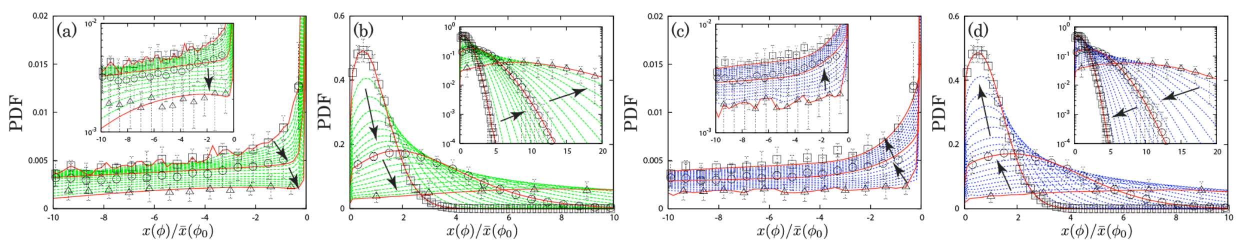

Figure 2 : Non-affine evolution of PDFs of overlaps during isotropic compressions ((a) and (b)) and decompression ((c) and (d)). The open symbols are the results of MD simulations, while the red solid and green or blue dotted lines are the solutions of the master equation. The numerical solutions develop in the directions indicated by the arrows.

Publications in 2014

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[2] C. Sanli, K. Saitoh, S. Luding, and D. van der Meer, "Collective motion of macroscopic spheres floating on capillary ripples: Dynamic heterogeneity and dynamic criticality", *resubmitted to* Phys. Rev. E (Rapid Communication), arXiv:1309.3804 (2014).

[3] A. Singh, V. Magnanimo, K. Saitoh, and S. Luding, "Effect of cohesion on shear banding in quasi-static granular material", *resubmitted to* Phys. Rev. E, arXiv:1312.7133 (2014).

[4] S. Takada, K. Saitoh, and H. Hayakawa, "Simulation of cohesive fine powders under plane shear", *submitted to* Phys. Rev. E, arXiv:1311.7322 (2014).