Characterization of static and dynamic structures in granular materials

Summary of Ph.D. thesis

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Introduction

Granular materials, besides their central technological importance, possess a surprisingly rich phenomenology. Their behavior is only partially understood, which makes these materials a currently active research field of physics and engineering. The natural aim of research is, in particular, to relate the well-known micro-mechanics on grain level to collective properties on large scales.

The grains in a granular material are macroscopic objects, where the interparticle interactions are dissipative. Without agitation grains come to rest under gravity or external pressure and the material freezes into a jammed state. In such a dense packing contact forces develop due to hard core repulsion (as grain deformations are typically very small) and friction. The forces form a highly inhomogeneous network through the disordered system of contacts, involving strong forces with spatial correlations on larger distance than the grain size (force chains) and also screened regions where grains experience no or little force.

Important and unsettled questions are how mechanical properties of the material depend on the force network and the contact network, and what the governing principles are that determine the macroscopic stress under external load. Equally important is the problem of describing the behavior when the material is unable to sustain an incompatible load (e.g. large shear stress) and starts flowing.

Objective and applied methods

The first part of my Ph.D. work is related to stress transmission in static granular systems in the limit case of perfectly rigid particles. Here I performed extensive hard particle simulations based on a discrete element method, the so-called contact dynamics. Whenever it was possible I also applied analytical tools.

On one hand I addressed the question of statical indeterminacy of contact forces: Whether the mechanically admissible force state is unique or there are more solutions for the same contact structure, and how this depends on friction. If there is an ensemble of force solutions, what the extent of indeterminacy is and what the properties of the solution set are. These questions are closely related to properties of the mechanical response given by the material to perturbations of the external load.

On the other hand my goal was to study a model where transmission of mechanical torque is allowed at the contacts and to find out how macroscopic stress is altered by the presence of contact torques. The model was motivated by cohesive nano-powders.

Besides the above static systems I also investigated flow properties and shear band formation in slowly sheared granular materials. Here my aim was to find a model for the nontrivial shape of shear bands that was observed in modified Couette cell experiments. In order to solve the proposed model I applied both numerical and analytical techniques.

New results

1. I studied the contact dynamics method of hard particle simulations. I showed that the relaxation of forces in the iterative calculation is a diffusion process, which is crucial regarding the computational time: it scales with the number of particles n as $n^{1+2/D}$ in D dimensions [2].
   When lowering the accuracy, linear scaling can be achieved, but that leads to effective softening of the particles due to systematic errors. I showed that this pseudo-elastic situation exhibits sound propagation with finite speed and can be described by a damped wave equation [1]. This behavior corresponds to a linear spring-dashpot model of contacts. I determined the dependence of the spring constant and the damping coefficient on the simulation pa-

rameters: on the number of iterations and on the size of the time step.

2.a. The problem of contact forces in a hard disk packing can be statically indeterminate. I proposed a technique based on the contact dynamics algorithm that allows to explore the ensemble of mechanically admissible force states [3]. I proved that these solutions form a convex (hence connected) set in the space of contact forces [6]. I showed that the "physical" force state determined by the construction history is special among the solutions, it does not correspond to a uniform measure in the force space, contrary to the usual assumption.

2.b. With the help of simulations [2] I found that friction induce indeterminacy of the contact forces. I demonstrated that the force fluctuations over the above force-ensemble (see 2.a) vanish proportionally to friction, and in the frictionless case, in agreement with the isostatic structure, forces are statically determined [3].
I found that fluctuations do not grow monotonically with increasing friction. The explanation of this counterintuitive phenomenon is that during packing construction large friction stabilizes the structure and leads to lower connectivity of the contact network, which overcompensates the freedom caused by the opening of the Coulomb angle. This effect confines the undetermined contacts into small separated regions in space (surrounded by fully determined contact forces) and thus suppresses considerably the average fluctuations of forces [6].

3. Based on three dimensional contact dynamics simulations [2] I studied the effect of contact torques on the porosity of cohesive powders [5]. I showed that rolling and torsion torques have significant effect on stabilizing pores and that the presence or absence of contact torques leads to qualitatively different stress transmission through the porous material: Under external load without torques, strong tensile forces develop and they cancel a large part of the pressure exerted by the compressive contacts. If contact torques are switched on, tensile forces are reduced significantly and only a small part of compressive forces is “wasted” against the effect of the tensile ones.

4. I presented a theoretical analysis of shear band formation in granular materials in the narrow band limit [4]. For a modified Couette cell I gave a geometric argument that links the shape of the shear band with its surface position as the function of the filling height, and obtained results in good agreement with experiments. I proposed a simple model based on the principle of least dissipation and solved numerically the variational problem. I showed that the model reproduces well the behavior of the open shapes (that is, shapes of bands reaching the top surface of the material) of shear bands found in experiments. I also predicted the existence of closed shapes for large filling heights or large pressure. The model exhibits first order phase transition between open and closed shapes, accompanied by hysteresis. I solved the model analytically in the large pressure limit.

List of publications

Publications related to my Ph.D. work

[**1**] Tamás Unger, Lothar Brendel, Dietrich E. Wolf, János Kertész, *Elastic behavior in contact dynamics of rigid particles*, Phys. Rev. E, **65**, 061305 (2002).

[**2**] Tamás Unger, János Kertész; *The Contact Dynamics Method for Granular Media*, in Modeling of Complex Systems, p. 116, ed. P.

L. Garrido and J. Marro, (American Institute of Physics, Melville, New York, 2003).

[**3**] Tamás Unger, János Kertész; *Frictional indeterminacy of forces in hard-disk packings*, Int. J. of Mod. Phys. B, **17**, 5623 (2003).

[**4**] Tamás Unger, János Török, János Kertész, Dietrich E. Wolf; *Shear band formation in granular media as a variational problem*, cond-mat/0401143 (2004), accepted for publication in Phys. Rev. Letters.

[**5**] Guido Bartels, Tamás Unger, Dirk Kadau, Dietrich E. Wolf, János Kertész; *The effect of contact torques on porosity of cohesive powders*, cond-mat/0403110 (2004), submitted to Granular Matter.

[**6**] Tamás Unger, Dietrich E. Wolf, János Kertész; *Force indeterminacy in the jammed state of hard disks*, cond-mat/0403089, (2004), submitted to Phys. Rev. Letters.

Additional publications

[**7**] Tamás Unger, Zoltán Rácz; *Concentration profiles and reaction fronts in $A + B \rightarrow C$ type processes: Effect of background ions*, Phys. Rev. E, **61**, 3583 (2000).

[**8**] Zénó Farkas, Guido Bartels, Tamás Unger, Dietrich E. Wolf; *Frictional coupling between sliding and spinning motion*, Phys. Rev. Lett., **90**, 248302 (2003).