Vici Progress Report, January 2014.

Thomas Weinhart

Project description

This report briefly describes the ongoing activities related to the aforementioned project and provides a road map of the same for the users' committee. The project is mainly concerned with the micro-macro transition required to obtain the *bulk properties* of a system of granular particles directly from the particle properties. This requires a description of a discrete granular system (the positions and velocities of, and forces on, each particle) in terms of density, velocity, and stress. In particular, we focus on the definition of the macroscopic stress near external boundaries as they appear in most granular systems but still lack a proper definition. Shallow steady granular flow down an incline over a rough bottom is chosen as an industry-relevant reference system.

Summary of Ongoing Efforts and Accomplishments:

A) An expression for the stress near an external boundary and in mixtures:

To obtain bulk density, velocity, and stress, we choose the coarse-graining method described by Isaac Goldhirsch (Goldhirsch 2010) as it has several advantages over other methods, including: *i)* the fields automatically satisfy the conservation equations of continuum mechanics; *ii)* it is not assumed that the particles are rigid or spherical, and *iii)* the results are valid for single particles (no averaging over ensembles of particles is required).

In order to obtain a micro-macro transition of systems that include external boundaries such as walls (and most systems do), we extended the stress definition to stress fields near external boundaries, allowing for more accurate statistics near system boundaries (Weinhart, Thornton et al. 2012). We further extended the coarse-graining method in (Weinhart, Luding et al. 2013) to account for partial stresses and drag between constituents in mixtures.

The smoothing length w is the key parameter of the coarse-graining method; For granular flows, two distinct coarse-graining length scale ranges are identified in (Weinhart, Hartkamp et al. 2013), where the fields are almost independent of the smoothing length w. The smaller, sub- particle length scale, $w \ll d$, resolves oscillations in the macroscopic fields which are caused by layers in the flow. The larger, particle length scale, $w \approx d$, leads to smooth stress and density fields. The kinetic stress becomes scale-dependent for $w \approx d$; however, this scale-dependence can be quantified and removed.

B) Closure rules for shallow granular flow down an incline over a rough bottom.

Shallow free-surface granular flow down an incline over a rough bottom is chosen as a reference system. We previously showed that the closure relations can be obtained as functions of the micro-parameters such as the geometric roughness of the base. As the flow behaviour depends strongly on the roughness of the bottom, the roughness was varied by changing the diameter of the basal particles, λd, where d is the diameter of the flowing particles. For steady flows, a linear relationship could be found between the Froude number and the flow height scaled by the stopping height $h_{stop}(\theta;\lambda=1)$, which is the height below which the flow arrests at a given inclination for a base with $\lambda=1$. This relationship yields a closure relation for the friction parameter of the continuum shallow water equations and thus a micro-macro transition has been established (Weinhart, Thornton et al. 2012).

Recently, we established a closure for the friction parameter as a function of microscopic contact friction of flowing particles with the base (Thornton, Weinhart et al. 2012), and for the segregation rate of polydispersed steady flows as a function of polydispersity (Thornton, Weinhart et al. 2012). In (Weinhart, Luding et al. 2013), we applied the mixture coarse-graining formulation to confirm two assumptions on the segregation dynamics in particle simulations of bidispersed chute flows: Firstly, the large constituent supports a fraction of the stress that is higher than their volume fraction. Secondly, the interaction force between the constituents follows a drag law that causes the large particles to segregate to the surface. This work is currently extended to take into account both density and size segregation in dense, sheared granular flows.

C) A local and objective description of the stress tensor under shear

A local and objective description of the complete stress tensor under shear was developed both for molecular (Hartkamp, Ghosh et al. 2012) and granular flows (Weinhart, Hartkamp et al. 2013). For plane strain flow, each tensor can be expressed in an inherently anisotropic form with only four objective, coordinate frame invariant variables. For example, the stress is decomposed as: i) the isotropic pressure, ii) the "anisotropy" of the deviatoric stress, i.e., the ratio of deviatoric stress (norm) and pressure, iii) the anisotropic stress distribution between the principal directions, and iv) the orientation of its eigensystem. The strain rate tensor sets the reference system, and each objective stress (and fabric) variable can be then related, via discrete particle simulations, to the inertial number, I. This represents the plane strain special case of a general, local, and objective constitutive model. The resulting model is compared to existing theories and clearly displays small, but significant deviations from more simplified theories in all variables.

D) Validation of closure relations with medium-scale experiments and simulations

Three projects are currently in progress to validate the measured closure rules for granular flows by comparing continuum simulations of medium scale experiments/ simulations such as the flow through a contraction, the flow impacting an inclined plane, and the flow front of a granular avalanche.

E) Development of an open-source code for particle simulations, MercuryDPM

The micro-macro transition methods described in the previous chapters are implemented in MercuryDPM (Thornton, Krijgsman et al. 2013, Thornton, Weinhart et al. 2013). MercuryDPM is an open-source code for particle simulations developed within the Multi

Scale Mechanics group and is actively developed by Thomas Weinhart, Anthony Thornton and Dinant Krijgsman. MercuryDPM is a very versatile, easily understandable code. Thus, it enables the transition of scientific knowledge to users in industry and academia.

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VICI Yearly report 2014

D. Krijgsman

January 23, 2014

Title of the project Bridging the gap between particulate systems and continuum theory

Project aim

The gap between discrete (micro) and continuum (macro) concepts for the modelling and understanding of particulate systems is bridged by micro-macro transition methods. Modern discrete particle-based models describe the particles in detail, but are of limited value for studying industrial processes and natural phenomena since too many particles are involved. Continuum methods, on the other hand, are readily applied in engineering applications. However, continuum methods rely on empirical constitutive laws with phenomenological parameters that disregard both the discrete nature of particles and the micro-structure. Micro-macro transition methods are being developed to combine the advantages of discrete and continuum models.

Furthermore simulations of realistic granular systems are extremely difficult due to huge computational costs. A significant proportion of these cost is associated with the detection of (possible) contacts. Different state of the art methods for contact detection are only suitable for mono dispersed systems. However realistic granular examples usually consist of particles with hugely varying radius.

Progress

Constitutive modelling

A novel local constitutive model based on observations from discrete element simulations has been developed for small-scale deformations of a quasi steady bi-axial geometry. The model consists of non-linear evolution equations for both shear stress and anisotropy, where the anisotropy is used to model the history dependence of the material. The main advantage of the model is that it only consists of 5 material parameters, where comparable constitutive usually require many more. Several discrete particle simulations were performed to test the models accuracy for various deformation modes. In (Krijgsman and Luding 2013) paper this has been done for small cyclic pure shear, where it has been shown that the model is able qualitatively model the transient as well as the limit cycles. For larger scale cycle shear the work is still in progress (Krijgsman and Luding 2013). In this paper also a comparison with different other constitutive models (e.g. granular solid hydrodynamics) will be given. Future work will include extending the model to generic three-dimensional cases and implementing it in a finite element method. The objective is to predict stresses and strains in macro scale applications, taking into account the evolution of the microscopic material structure.

Contact detection

A contact detection method based on a hierarchical grid is developed. The improvement of the algorithm stems from the fact that in granular media most interactions between particles is short ranged. Therefore it is not necessary to test the interactions for particles pairs which are quite distant. This idea for monodisperse flows is incorporated in the Linked Cell method, where the domain is partitioned in different cells (which sizes equal to the particle diameters). In each cell the number of particles is low ($O(1)$) for all possible parameters. For polydisperse flows however the cells have to be as big as the biggest particle in the system. Therefore the number of particles in each cell increases with increasing polydispersity, rendering the algorithm useless for polydisperse flows.

The idea of the new method is to use different grids to partition the particle (i.e. use a grid with small spacing for the small particles and a grid with large spacing for larger particles). Due to this multiple grid the average number of particles per cell is kept low and the method performs excellent for all kinds of particle simulations. For the algorithm to perform optimally the correct number of levels and their sizes have to be determined. In (Krijgsman, Ogarko et al. 2014) we describe the method and suggested four different methods of choosing the number of levels and their sizes.

Mercury DPM

The quick contact detection methods described in the previous chapters is implemented in MercuryDPM (Thornton, Krijgsman et al. 2013, Thornton, Weinhart et al. 2013). MercuryDPM is an open-source code for particle simulations developed within the MultiScale Mechanics group and is actively developed by Thomas Weinhart, Anthony Thornton and Dinant Krijgsman. MercuryDPM is a very versatile, easily understandable code. Thus, it enables the transition of scientific knowledge to users in industry and academia.

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MULTISCALE MECHANICS GROUP (MSM)/TS/CTW
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JANUARY 21, 2014

VICI Report (Project No. 10828)

To: VICI and Industrial Partners of project VICI No. 10828

From: Nicolás Rivas, PhD Student

Subject: Bridging the gap between particulate systems and continuum theory

1 Background

1.1 Granular materials

Granular materials research is relevant for two main reasons. On the one hand, collections of grains are a very common material in every day life; we find them in cosmetic powders, cereals, vitamin pills, sand and rocky terrains, and many others. They also constitute over 75% of all raw material feedstock to industry, making their study relevant for many different processes, where the prediction of their behavior under different circumstances could provide big advantages.

On the other hand, granular materials are remarkably interesting and complex physical systems. Due to the dissipative nature of the interaction between grains it becomes necessary to constantly inject energy in order to keep grains moving, making it a prototype scenario for non-equilibrium dynamics. Agitated or free flowing collections of grains present many of the fundamental features of complex dynamics, as emergence of patterns, self-organization, phase transitions, and others. The ability to experimentally and numerically observe the micro dynamics of the grains in each of these phenomena makes granular assemblies highly relevant in the study of non-equilibrium systems.

1.2 Aim and approach

Particle simulations can now correctly predict grains behavior in a wide range of circumstances, but are mainly limited to spherical geometries, or/and to a low number of particles. Moreover, several continuum equations that describe granular flows have been proposed, but fail to accurately predict the behavior for a wide range of densities and geometries. This project focuses on establishing a connection between both approaches by carefully studying a particular system and its phase transitions, with the goal comparing micro and macro dynamics.

One common procedure in continuum theories for granular materials is taking the Navier-Stoke equations for regular fluids, interpret the fluid density ρ as the granular number density n, and then modify the *transport coefficients*, expanding their validity for a wider range of densities and inelasticities[1, 2]. In this project this approach is used for a driven granular system, consisting in a vertically shaken shallow box filled with grains (see Fig. 1). This system presents many different inhomogeneous stable states that depend on the parameters of energy injection, geometry, and grain properties and number[3, 4, 5]. Studying the transition and stability of these states, from both a microscopic and macroscopic approach, may lead to a better understanding of the out-of-equilibrium statistical physics behind complex granular systems. Two main aspects motivate this research: the development and comparison of a set of simulation tools, both microscopic (molecular dynamics), and macroscopic (granular-hydrodynamics equations solver), in order to see the limits and advantages of each approach in different scenarios; and the study of the vertically vibrated shallow granular system from a physical point of view, in order to further understand the complex behaviors present in driven granular systems.

2 Progress Report

In the context of the VICI project 10828, *Bridging the gap between particulate systems and continuum theory*, the following is a progress report on the granular and hydrodynamic model-

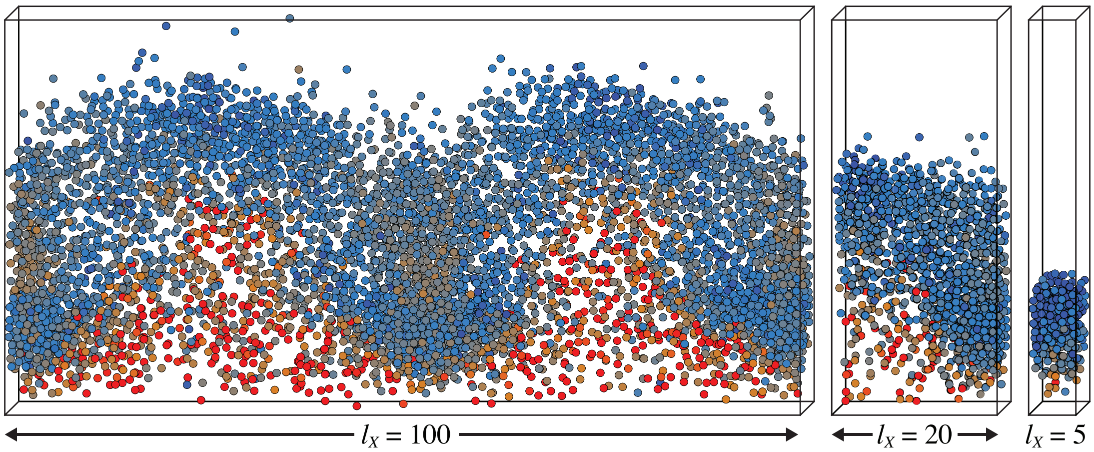

Figure 1: Snapshots of three vertical narrow box systems with the same number of filling layers $F = N\tilde{d}^2/\tilde{l}_x\tilde{l}_y = 12$, with N the total number of particles, $\tilde{d}$ the (dimensional) diameter of the spherical particles, and $\tilde{l}_x$ and $\tilde{l}_y = 5\tilde{d}$ the (dimensional) width and depth of the container, respectively; and energy injection parameters, but different widths $\tilde{l}_x$. From left to right, $\tilde{l}_x = 100\tilde{d}$, $\tilde{l}_x = 20\tilde{d}$, and $\tilde{l}_x = 5\tilde{d}$. The rightmost corresponds to the *column* geometry. Particles are coloured according to their kinetic energy.

ing of a vibrated quasi-two-dimensional granular system.

2.1 Characterization of low-frequency oscillations

In the vertically vibrated granular bed geometry, a density inverted state was previously observed for sufficient energy input, where a highly packed phase is sustained by a low-density, high-temperature one. This state was named Leidenfrost, due to the analogy over the water-over-vapour phenomena present in regular fluids. We took this study further by progressively reducing the length of the container, until the limit of a square base just a few particles in size. Our goal was to further simplify the system in order to more easily identify its fundamental aspects. At this point, having suppressed convection, coherent and collective oscillations of the dense phase, order of magnitudes slower than the energy injection frequency, were identified and studied [6]. We characterized these oscillations (see Fig. 2) and showed that their frequency can be accurately modeled by continuum hydrodynamic equations, yielding further insight into the applicability of continuum equations to granular media, even for a very low number of particles.

Outlook

Our model makes several assumptions in order to obtain the simplest possible estimate for the frequency of oscillations. Some of these assumptions could be relaxed and see how do they affect the accuracy of the prediction. Furthermore, the relation of the oscillations to the Leidenfrost to convective state transition could be further studied. Finally, size particle scalings have already yielded interesting insight into what drives the oscillations; see further §2.4

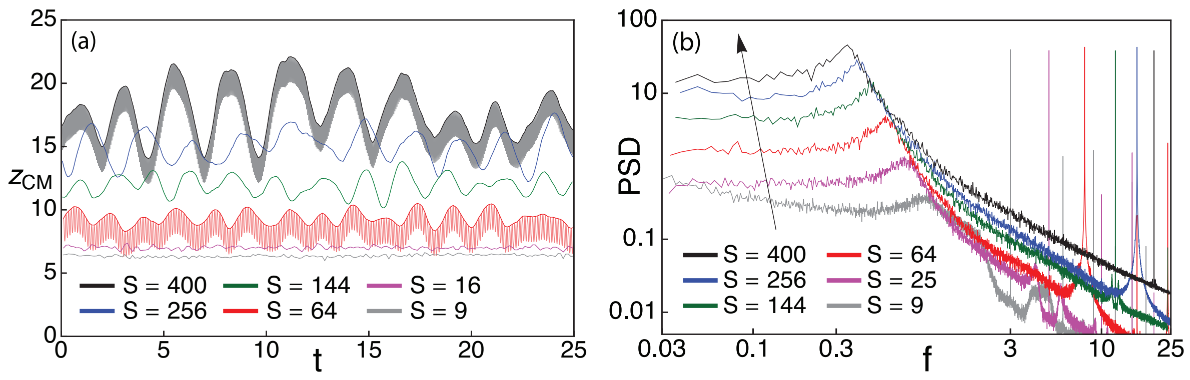

Figure 2: (a) Centre of mass evolution, $z_{cm}(t)$, for shaking amplitude $A_f = 1.0$ and different dimensionless shaking strengths $S = \omega_f^2$, as a function of time in gravity timescale units $t_g = \tilde{t}(\tilde{g}/\tilde{d})^{1/2}$. The light colour data are taken with sub-period resolution, while dark colour data are taken every oscillation cycle at the point of maximum wall amplitude. (b) Fast Fourier transform of the centre of mass of the particles, $z_{cm}(t)$, for $A_f = 1.0$ and several different S. The arrow indicates the direction of increasing S. Different amplitudes, not shown, present the same qualitative behaviour.

2.2 Experimental observation of low-frequency oscillations

Low frequency oscillations (LFOs) of a granular bed in a density-inverted state were experimentally observed for the first time [7]. LFOs, thought to play an important role in the transition between the Leidenfrost and convective states of a vibrofluidised granular bed, were observed over a range of driving frequencies and amplitudes, with particles of varying materials and size, and using containers of different materials. The experimentally acquired results showed a close qualitative and quantitative agreement with both theory and simulations across the range of parameters tested. The influence of sidewall dissipation on LFOs and vertical density profiles was also explored, with simulational and experimental results once again agreeing. Experimental data was acquired using Positron Emission Particle Tracking (PEPT), a non-invasive technique whereby a single particle, physically identical to the others in the system, is 'labelled' with a β^+-emitting isotope.

Outlook

Experimental data could be acquired for higher effective shaking strengths by using a smaller setup and particles, thus allowing for a better comparison between theory and experiments. Moreover, experiments have already been realized and experimental data is being analyzed in a setup where particle tracking is done using a high speed camera, which could provide further insight into the nature of low-frequency oscillations.

2.3 Segregation and phase coexistence on mass binary systems

Unlike in molecular fluids, segregation or demixing occurs spontaneously in driven granular mixtures of different size and/or density particles, which can be a nuisance/blessing in pro-

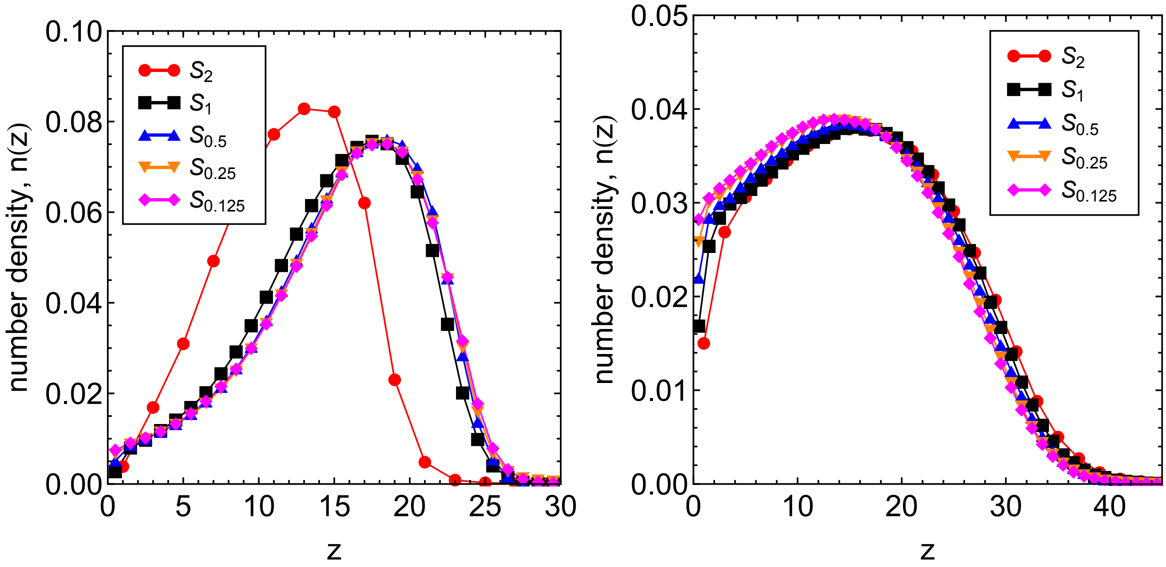

Figure 3: Time-averaged vertical number density profiles, $n(z)$, for systems shown in the inset, where the subscript corresponds to the particles size. For restitution coefficient $r_1 = 0.9$, and $\omega_1 = 100$ (left), and $r_1 = 0.99$, $\omega_1 = 20$ (right).

cessing industries dealing with granular materials. Understanding segregation-driven patterns and finding ways to control them remains a key challenge in granular physics research. We found patterns displaying the coexistence of sub-harmonic/harmonic and asynchronous states, resembling Chimera states, along with partial convection, in experiments and simulations on vertically vibrated binary mixtures of equal-size but different mass particles [8]. The segregation of heavier and lighter particles along the horizontal direction was shown to be the progenitor of such phase-coexisting patterns. We also demonstrated that the buoyancy-driven granular convection can be controlled by adding a very small amount of heavier particles at the same energy cost, the origin of which is tied to the breakdown of equipartition of granular energy.

Outlook

In some regions of the phase space there is considerable disagreement between simulations and experiments: this should be studied further. Wider systems could lead to a better understanding of the natural scales of each state in the coexisting scenarios, and provide a way of studying the interface between them. Transitions between states presenting coexistence could present new dynamics not previously observed in dynamical systems; careful experimental work would be needed for their precise characterization.

2.4 Particle size scaling and hydrodynamic limit convergence

We studied the influence of the number of particles in the vertically vibrated bed of grains, specifically in the transition from a Leidenfrost to a convective state [9]. First, proper scalings of the system parameters were found in order to make the granular hydrodynamic equations invariable to the particles size. The validity of these scalings is being studied in different geometries, which provide useful insights into the influence of finite size in granular dynamics. Fig. 3 shows the vertical density profiles for many different particle sizes, and how these converge to a given profile as $d \to 0$. The system was also simulated through the Leidenfrost/convection transition for almost two order of magnitudes in particle sizes, and observations are being made into the influence of fluctuations and number of particles on the probability of transition. In the column geometry limit the scalings have shown that low-frequency oscillations decrease in amplitude as the number of particles is increased, showing that fluctuations in the momentum transfer from the gaseous to the solid phase in the Leidenfrost state could be the driving mechanisms of the oscillations.

Outlook

The particle size scalings found can be useful in many other granular systems in order to study the role of fluctuations in the system (as fluctuations are inherently related to the number of particles present). In our studied geometry, we are actively working on determining the convergence conditions and speeds for both the column and the wide geometries, as a function of grains interaction parameters. Furthermore, an order parameter was proposed to characterize the transition from Leidenfrost to convection that shows a remarkable dependence on particle size, showing that the transition region gets narrower as the number of particle increases; this is being actively researched. Finally, we believe this to be a promising new approach for the solution of hydrodynamic equations with discrete particle simulations; we expect to show the proper limits and the expected convergence rates of this method, and compare the results with actual solutions of the granular hydrodynamic equations.

2.5 Granular hydrodynamics solution

Outlook

Active work is still being done in order to solve the granular hydrodynamic equations with the apropiate boundary conditions. Initially, the simplest approach was tried, using a constant temperature boundary condition corresponding to the oscillating bottom wall, and a zero density upper boundary condition as the top free surface. The parameters of the simulations where set with the goal of observing the Leidenfrost state: a density inversion state, where a low density region near the vibrating bottom sustains a high density region. We where not able to obtain the known Leidenfrost density profile. Other classical boundary conditions where tried but none was adequate. This motivated the use of more complex boundary conditions, which demanded the use of state-of-the-art numerical methods, particularly space-time discrete Galerkin methods.

Substantial progress has been made on the numerical tools necessary to obtain a solution of the granular hydrodynamic equations. A new version of *hpGEM* software was developed, which is now stable and under active development to add the necessary features for our system. Furthermore, we have began to implement our equations in the *FEniCS* partial differential equations solver, with the final goal of comparing our new code with an existing and actively used alternative. All necessary equations have been already appropriately discretized for the chosen algorithms.

3 General outlook

The main challenge remaining is the solution of the relevant granular hydrodynamic equations for our system. With this, we could conclude our research comparing finite-size, discrete particle simulations with both experiments and continuum solutions. Also, the path from micro to macro state could be continously traveled using the size scalings previously mentioned, which would definitely help us better understand the micro-macro transition present in this particular case.

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MULTISCALE MECHANICS GROUP (MSM)/TS/CTW
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JANUARY 24, 2014

VICI Report (Project No. 10828)

To: VICI and Industrial Partners of project VICI No. 10828

From: Kuniyasu Saitoh, PostDoc

Subject: Stochastic approach to non-affine response in jammed granular packing

Introduction

Overview of statistical mechanics of granular assemblies

Dense packing of granular materials is a common subject in science and technology, as well as flow [1-6], contact modeling [7], glassy dynamics of granular materials [8] and nano-materials [9,10]. Although the understanding of its mechanics has a great importance in many industrial applications, we have not fully understood the physics of granular assemblies because they are inherently *out of equilibrium* due to the dissipation of energy and absence of temperature. Despite their non-equilibrium nature, their static properties have been widely investigated by analogy with critical phenomena, where some quantities (pressure, coordination number, the first peak of radial distribution function, elastic moduli, shear viscosity, etc.) show remarkable critical behaviors around a rigidity transition density, the so-called *jamming point* [11]. Therefore, it is challenging to explain these observations by *statistical mechanics*, e.g. based on the Edwards ensemble or force ensemble theories, where all configurations of particles are assumed to be equally probable under a constant volume or force and torque balances of particles, respectively. Further studies of these ideas lead us to the exploration into statistical weights, i.e. *probability distribution functions (PDFs) of forces*, and many theoretical investigations have been devoted to determine the functional forms of them, though there is still much debate about the tails of the PDFs and how the closing/opening of contacts affects the PDFs at small forces.

Aim and approach

Our aim of this work is to predict and describe how the PDFs of forces change under global deformations. Because it is almost impossible to expect the changes of individual forces, we take a different approach from the previous studies, where we regard forces or overlaps as *stochastic variables* and measure *conditional probability distributions (CPDs) of forces or overlaps* by molecular dynamics (MD) simulations. Under isotropic (de)compressions, the CPDs show striking features of not only forces, but also closing and opening contacts as well as inter-particle gaps. Then, we introduce a *master equation* for the PDFs, where a good agreement between the numerical solutions and the MD simulations is established. Interestingly, the solutions are independent of history, i.e. show *the Markov property*, and reversible as long as an increment of area fraction $\delta\phi$ is much smaller than the distance from the jamming point $\phi - \phi_J$. We also find that the ratio $\delta\phi/\phi - \phi_J$ governs the mechanical response of granular packing, i.e. the degree of *non-affinity* [12].

In the following, we explain our Method and Results. We summarize our results and show outlook in the end of this report.

Method

Molecular dynamics simulations

The method is molecular dynamics (MD) simulations of two-dimensional frictionless particles, where a normal force between particles in contact is modeled by a linear elastic spring and linear viscosity proportional to the relative speed in the normal direction. A global damping force proportional to the particle's velocity is also introduced to enhance the relaxation, where the damping coefficient is the same with the viscosity coefficient between particles in contact.

Preparation of static packing

At first, we randomly distribute a 50:50 binary mixture of particles in a square periodic box, where the ratio of different radii is 1.4 (to avoid crystallization) and each pair of particles initially does not contact. To make static packing of the particles, we gently adjust every radii until the mean overlap over all particles reaches a desired value and every acceleration of particles drops below a threshold.

Isotropic compressions and decompressions

We compress/decompress the static packing by increasing/decreasing every radius and relaxing the system until every acceleration of particles drops below the threshold again. Then, the area fraction of particles increases/decreases by a certain magnitude and we compare the static packing before and after the compression/decompression.

Results

Non-affine responses to (de)compressions

The mechanical response of granular packing is significantly different from that of elastic bodies, where elastic bodies show *affine response* to applied global deformations. The affine response could be correct, if the force balance of each granular particle does not change by deformations. However, the particles are randomly arranged (Fig. 1(a)) and the force balance must be broken by deformations. Figures 1(b) and (c) display displacement vectors of granular particles after isotropic compressions, where the displacements randomly distribute in space, i.e. the system shows *non-affine response*.

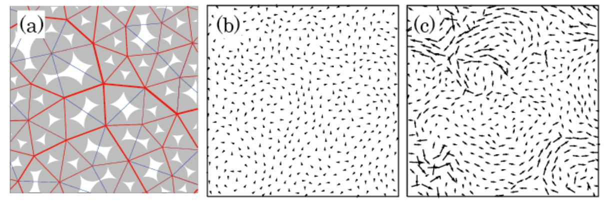

Fig. 1. (a) A force chain network in granular packing. (b) and (c): Displacement vectors of particles after isotropic compressions.

Microscopic insights into the non-affine responses

To understand the origin of non-affine deformations, we study responses of inter-particle overlaps. In Figs. 2(a) and (b), we show overlaps before compression and after relaxation, respectively, where we introduce inter-particle gaps as negative overlaps. Here, we can see four kinds of responses of overlaps: (CC) positive to positive, (VV) negative to negative, (CV) positive to negative, and (VC) negative to positive, respectively. Note that the cases (iii) and (iv) represent *closing and opening contacts*, respectively. The statistics of these responses can be studied by the PDFs of overlaps. Figure 2(c) displays the PDFs before compression, "just" after compression, and after relaxation. Here, the PDF "just" after compression corresponds to affine response. The PDF after relaxation is clearly different from affine response, where it is broadened through rearrangements of particles and closing/opening contacts come into play.

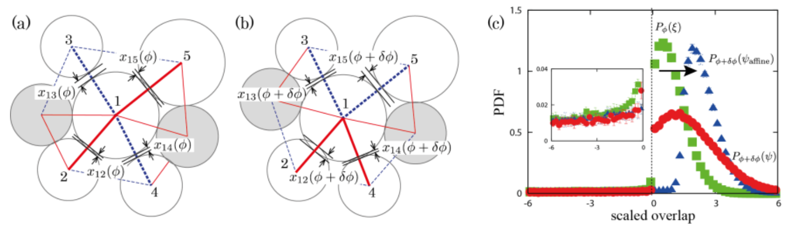

Fig. 2. (a) and (b): Overlaps (a) before compression and (b) after relaxation. (c) The PDFs of scaled overlaps before and "just" after compression, and after relaxation.

Power law scaling of the non-affinity

In our system, each granular particle contacts with surrounding particles, where the number of contacts are always above 4. Therefore, it is almost impossible to predict how an overlap changes during the relaxation. On the other hand, we can easily imagine that an overlap changes *randomly* as shown in Fig. 3(a), where an overlap ξ changes to ψ after the relaxation. The overlaps after the relaxation must distribute around its mean value $\bar{\psi}$ with a certain width υ (Fig. 3(a)). To figure out such random changes, we plot ξ and ψ on a scatter plot. Figure 3(b) is the scatter plot of overlaps, where the blue and red dots are the results of affine and non-affine deformations, respectively. If we look at the positive region (CC), both the blue and red dots distribute around linear functions of ξ, where the slope for affine deformation is exactly one, while that for non-affine response is larger than one, i.e. the slope is given by $a_1 + 1$. This "additional" slope a_1 represents the deviation from affine response and we find that it can be linearly scaled by the ratio between an increment of area fraction and the distance from the jamming point (Fig. 4), i.e. $a_1 \sim \gamma \equiv \delta\phi/\phi - \phi_J$. Therefore, if the system is very close to ϕ_J, the response is highly non-affine even though the applied strain is very small.

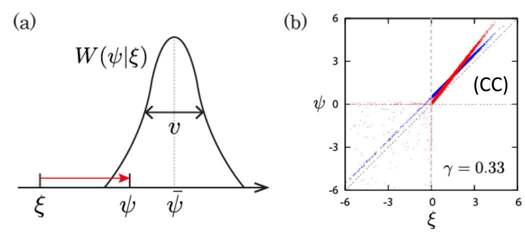

Fig. 3. (a) A sketch of conditional probability of overlaps. (b) A scatter plot of scaled overlaps.

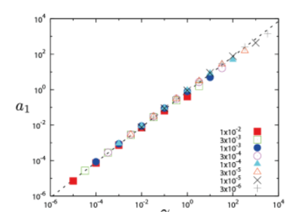

Fig. 4. Power law scaling of the additional slope a1.

Conditional probability distributions of overlaps

We introduce the conditional probability distribution (CPD) of overlaps $W(\psi|\xi)$ as

$$P_{\phi+\delta\phi}(\psi) = \int_{-\infty}^{\infty} W(\psi|\xi) P_{\phi}(\xi)\, d\xi$$

where $P_{\phi+\delta\phi}(\psi)$ and $P_{\phi}(\xi)$ are the PDFs after relaxation and before compression, respectively. Depending on the signs of overlaps, the CPDs can be defined in the four regions, (CC), (VV), (CV), and (VC), as shown in Fig. 5. From our simulations, we find that the CPDs are well described by the *stable distribution family*, e.g. the CPD in (CC) is *Gaussian distribution* and that in (VV) is approximated by the *Holtsmark distribution*.

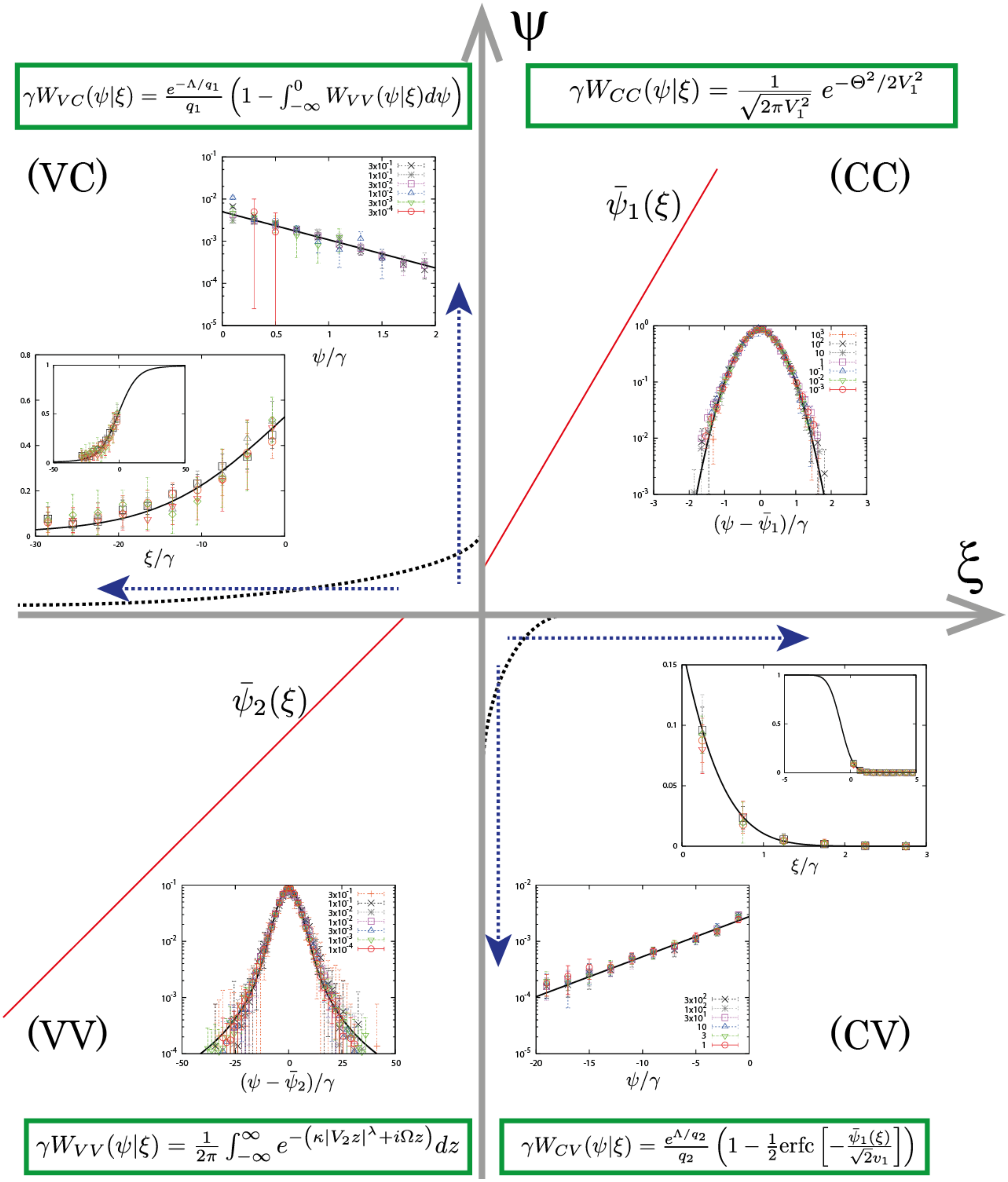

Fig. 5. Conditional probability distributions in (CC), (VV), (VC), and (CV).

The insights one gets from this result is interesting: The Gaussian CPD in (CC) means that the fluctuations of overlaps around the mean value are uncorrelated, though the change of mean overlap shows non-affine responses. On the other hand, the fluctuations of negative overlaps can be infinitely large as described by the Holtsmark distribution function.

Master equation for the PDFs of overlaps

By using the CPDs, we now introduce the *master equation* for the PDFs of overlaps as

$$\frac{\partial}{\partial \phi} P_\phi(\psi) = \int_{-\infty}^{\infty} \{W(\psi|\xi) P_\phi(\xi) - W(\xi|\psi) P_\phi(\psi)\} \, d\xi$$

which describes the changes of the PDFs under compression as well as decompression. Figure 6 displays the numerical solutions of the master equation (solid lines), where we can see a very good agreement between the solutions and the PDFs obtained through the MD simulations (open symbols). From this result, we can confirm the *Markov property of overlaps* and *reversibility*, i.e. the PDFs are independent of history. Note that we can see the agreement only if the ratio $\gamma = \delta\phi/(\phi - \phi_J)$ is infinitesimally small, otherwise both the Markov property and reversibility are broken down.

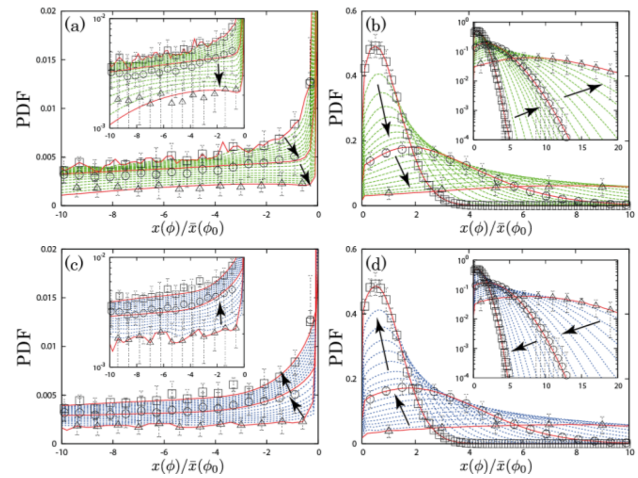

Fig. 6. Numerical solutions of the master equation under compressions ((a) and (b)) and decompressions ((c) and (d)).

Stochastic model of an overlap and Fokker-Planck equation for the PDFs

From our results of mean overlap $\bar{\psi}(\xi)$, we can propose a stochastic model of a single overlap, where the response of an overlap to compression or decompression is described by a *Langevin equation*

$$\frac{dx}{d\phi} = \frac{A}{\phi - \phi_J} x + (1 - A) A_m + \zeta$$

Here, the last term in the right-hand-side is a noise, where its distribution follows the Gaussian CPD in (CC). From the Langevin equation, we can derive the *Fokker-Planck equation* for the PDFs of overlaps

$$\frac{\partial}{\partial \phi} P_\phi(x) = \frac{(A_m V_1)^2}{2} \frac{\partial^2}{\partial x^2} P_\phi(x) - \frac{\partial}{\partial x} \{\alpha(x) P_\phi(x)\}$$

and solve it with the boundary values of the PDFs at zero-overlap (Fig. 7(a)). Figure 7(b) shows the numerical solutions of the Fokker-Planck equation (solid lines), where we can see a good agreement with the MD simulations (open symbols).

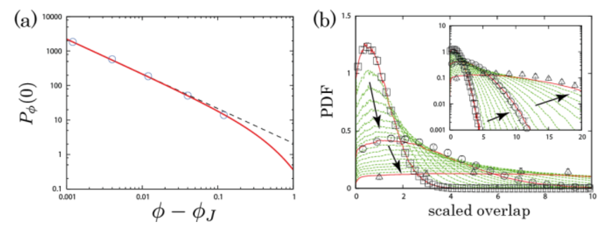

Fig. 7. (a) Boundary values of the PDFs plotted against distance from the jamming point. (b) Numerical solutions of the Fokker-Planck equation under compressions.

Summary

We studied the response of two-dimensional granular packing to isotropic (de)compression. From the scatter plots of overlaps, we quantify the non-affine deformations by the ratio $\gamma = \delta\phi/(\phi - \phi_J)$ and conclude that the non-affinity diverges at the jamming point. Measuring the CPDs of overlaps, we introduce the master equation of the PDFs of overlaps. The CPDs are well approximated by the stable distributions, where the Gaussian CPD indicates uncorrelated fluctuations of overlaps after the relaxation, while the Holtsmark CPD shows large correlations of inter-particle gaps. The numerical solutions of the master equation well describe the results of MD simulations if the increment of area fraction is much smaller than the distance from the jamming point. We also propose a stochastic model of an overlap and derive the Fokker-Planck equation for the PDFs of overlaps, where the solutions also well predict the changes of the PDFs.

Outlook

The response of granular packing to *pure or simple shear* is our current subject, where the PDFs and CPDs are extended to include angles between particles in contacts [13]. The extension to the three-dimensions is also important to practical applications as well as that to frictional grains. More theoretical analysis of our stochastic approach is also necessary.

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