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From particles in steady state shear bands via micro-macro to macroscopic rheology laws

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Abstract. Particulate systems and granular matter are discrete systems made of many particles; they display interesting dynamic or static, fluid- or solid-like states, respectively – or both together. The challenge of bridging the gap between the particulate, microscopic picture towards their continuum description (via the so-called micro-macro transition) is one of today's challenges of modern research. This short paper gives a brief overview of recent progress and some new insights about local granular flow rules for soft particles.

Keywords: Micro-macro transition, flow rules, rheology, macroscopic friction

1 Introduction

Particulate systems pose many challenges for academia and industry. From molecular dynamics simulations of many atoms or particles, one can extract scalar fields like density or temperature, as well as vectorial fields like velocity, or tensors like stress, strain-rate, and structure (fabric). Given sufficiently good statistics the data can have a quality that allows to derive constitutive relations that describe the local rheology and flow behavior [1-6] of fluids (e.g. atoms confined in a nano-scale channel [4]) or granular systems, which are non-Newtonian, with particular relaxation behavior, anisotropy etc. [1-3,5,6]. With attractive forces involved, like van-der Waals forces or liquid-bridges, this leads to cohesion added on top of the already non-trivial dynamics of granular matter [2,6-8]. Dependent on the energy input (e.g. through an applied shear-rate), the particles can flow like a fluid, jam or un-jam, or be solid with interesting anisotropic structure (contact- and force-networks) [9,10].

The goal of the present paper is to use the micro-macro transition proposed by Isaac Goldhirsch [11,12] to determine three-dimensional local rheology laws that go beyond the $\mu(I)$-rheology [13], which predicts well the flow behaviour of rigid particles, where only the inertial number is relevant. However, for real particles also the confining stress (softness) has to be taken into account as control parameter, as presented below. Additionally relevant parameters are not discussed in this study, namely cohesiveness and granular temperature or fluidity.

2 Phenomenology

In granular systems, the interplay between strain, stress and anisotropy can lead to dilatancy that is only one of the interesting micro-mechanical mechanisms related to the ‘memory’ of the packing. Starting from a dense packing, shear motion is only possible if the grains “unlock” from their dense arrangement. Shearing for long time, the initial state is forgotten and a steady state (sometimes referred to as critical state) is reached. The evolution of the steady state anisotropy (micro-structure) is independent from the direction-dependency (“anisotropy”) of stress, both in rates as well as in principal directions, i.e., tensorial eigen-system orientations [3-5]. In steady state, a certain proportionality and relative orientation establishes, which is subject of ongoing research. Thus, particulate systems behave in various ways like a non-Newtonian fluid [3,4], as observed by modern particle simulations, from which all the macroscopic scalar, vectorial, and tensorial fields can be obtained [3-7]. The micro-macro transition translates the information about particle positions, velocities and forces into the continuum fields density, displacement (gradient) structure, and stress, using smoothing and time-averaging (in stready state). In a particular geometry, i.e., the split bottom ring shear cell, see Fig. 1, the fields are functions of the height and the radial distance from the symmetry axis, so that a wide range of local densities, strain-rates and pressures are covered. Having available this information from the micro-macro transition, the next step is to formulate general, local constitutive relations that allow to predict the systems flow behaviour in inhomogeneous systems [5,7-9]. Similar methods and approaches can also be applied to solid-like systems [10] – all are based on the original ideas of coarse-graining from micro-to-macro [11,12], following the ideas of Isaac Goldhirsch [3,11,12]. Macroscopic data can be obtained as functions of particle- and contact-properties like particle sizes, stiffness, friction as well as system parameters like the external shear-rate.

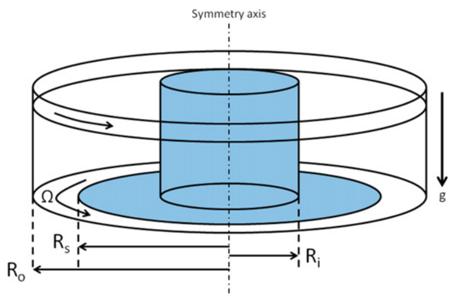

Fig. 1 Schematic plot of the ring-shear cell with the relevant geometry parameters.

Examples of the most basic element tests, i.e., small and representative systems with relevance for the micro-macro approach, involve homogeneous systems like the tri-axial box with pure-shear deformations [9,10], and planar flows with a mix of simple- and pure-shear [4]. Examples for inhomogeneous systems are simple-shear in avalanches on inclined planes [3], or the split-bottom ring-shear cell [5-8]. One simulation of a homogeneous system allows for just one data-set, obtained with a good statistics due to global averaging. In inhomogeneous systems, on the other hand, by means of a suitable local and time averaging, a single simulation allows for the collection of plenty of data-sets (including the particle density, displacement, velocity or velocity gradient, stress and fabric for the micro-structure).

3 Results

Here, a short summary of recent results on formulating the local granular rheology is presented and concluded with an outlook for future research.
When formulating a granular rheology, the starting point is the successful, simple, and elegant so-called $\mu(I)$-rheology [5,13], which relates the so-called macroscopic (bulk) friction, i.e., the shear-stress to pressure ratio $\mu = \tau / p$, in a sheared particulate system to the inertial number, i.e., the dimensionless strain-rate:

$$I = \dot{\gamma} d_0 \Big/ \sqrt{p'/\rho}$$

with shear rate $\dot{\gamma}$, diameter d_0 = 0.0022 m, mass-density ρ = 2000 kg/m^3, and pressure p'. The relation that describes well a wide variety of flows [13] of hard, cohesionless particles, at various strain rates is:

$$\mu(I) = \mu_0 + (\mu_\infty - \mu_0)\,\frac{1}{1 + I_0/I} \qquad (1)$$

where $\mu_0 = 0.15$ and $\mu_\infty = 0.42$ represent the zero and infinite strain rate limits, respectively, and the characteristic dimensionless strain-rate is I_0 = 0.06, where inertia effects considerably kick in. Since the simulations presented below concern particle simulations with a very small coefficient of particle contact friction, μ_p = 0.01, the dependence of the coefficients in Eq. (1) on friction is not considered.

The first correction to the $\mu(I)$-rheology is relevant for soft particles, as based on the results by Singh et al. [5]; it was originally given as linear additive term to the above rheology for small strain-rates [5], however, it can also be rephrased as multiplicative correction factor:

$$\mu(I,p) = \mu(I)\left(1 - \left(\frac{p}{p_0}\right)^{1/2}\right) \tag{2}$$

with the dimensionless pressure $p = p' d_0 / k$, the characteristic pressure at which this correction becomes considerable, $p_0 = 0.9$, and the stiffness $k = 100$ N/m. This correction accounts for a range of particle stiffness (or softness), but also for different magnitudes of gravity, as in a centrifuge or on the moon. This approach allows describing granular flows using a local approach, in opposition to non-local models, saving the beautiful simplicity of locality and extending the basic model by including neglected features. Additional corrections for cohesive particles involve the so-called Bond-number (*Bo*), as studied elsewhere [6,7] and ignored in the following.

Both dimensionless numbers can be expressed as a ratio of time-scales, namely $I = t_{\dot\gamma}/t_p$ and $p = \left(t_p/t_c\right)^2$, where the subscripts denote strain-rate, pressure and contact duration, respectively.

In order to complete the rheology for soft, compressible particles, a relation for the density as function of pressure and shear rate is missing:

$$\phi(I,p) = \phi_c\left(1 + \frac{p}{p_\phi^c}\right)\left(1 - \frac{I}{I_\phi^c}\right) \tag{3}$$

with the critical or steady state density under shear, in the limit of vanishing pressure and inertial number, $\Phi_c = 0.648$, the strain rate for which dilation would turn to fluidization, $I_\phi^c = 0.85$, and the typical pressure level for which softness leads to huge densities, $p_\phi^c = 0.33$ (double, due to the linear contact model). Note that both correction terms are valid only for sufficiently small arguments: Too large inertial numbers would fully fluidize the system so that the rheology should be that of a granular fluid, for which kinetic theory applies, while too large pressure would lead to enormous overlaps, for which the contact model and the particle simulation become questionable. In the following, the considered inertial numbers are $I < 0.1$, while the pressures are $p < 0.01$.

A small correction to the functional form of Eq. (3) removes the invalidity for large arguments, while remaining identical to first order Taylor expansion for small arguments:

$$\phi(I,p) = \phi_c \exp\left(\frac{p}{p_\phi^c}\right)\exp\left(-\frac{I}{I_\phi^c}\right) \tag{4}$$

From a rapid and moderate external rotation frequency, *f*, of the split-bottom ring shear cell, with split at $R_s = 0.085$ m, representative data from Ref. [5]

are plotted in Fig. 2 against the radial position. Higher confining stress corresponds to a higher density, deeper below the free surface, while the density is reduced in the shear band, proportional to the local shear-rate, due to dilatancy. Overall the simulation data agree very well with the corrected density from the analytical Eq. (3), where only local information enters, besides some scatter and more systematic deviations in the tails of the shear band, away from the split, where the local strain rates are very small.

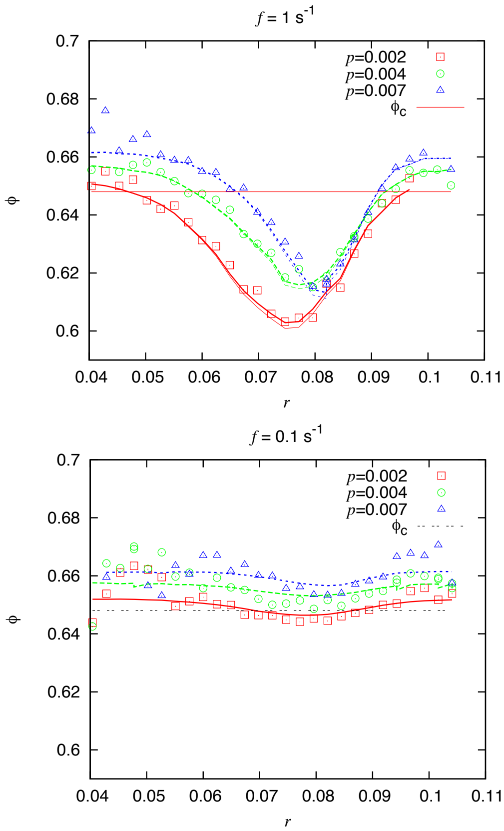

Fig. 2 Density for rapid (top) and moderate (bottom) rotation frequency, plotted against the radial distance r, with data from particle simulations in Ref. [5], using the external rotation rates, $f = \Omega/2\pi$, given above the panels, filtered at three different (approx.) pressure levels, p, as given in the inset (i.e. red, green and blue correspond to: close to the surface, in the middle, and closer to the bottom). The lines correspond to Eq. (3), with all parameter values given in the main text; the horizontal lines give the low stress and strain-rate limit, ϕc. The thin lines in the top-panel represent Eq. (3) while the thicker lines represent the improved form in Eq. (4).

The macroscopic friction, i.e., the shear stress ratio, is plotted in Fig. 3, against the radial position for the same data-sets, in comparison with the classical rheology of Eq. (1) and the pressure-dependent rheology, Eq. (2). The pressure dependence is improved when using the latter, especially in the tails, for the slower rotation rate, where the classical rheology has no pressure dependence. Nevertheless, in the tails the stress ratio does not agree well with theory, indicating a missing additional correction term that accounts for a combination of very low strain-rate and finite granular temperature effects playing a dominating role in those regimes, see Ref. [5] for more details.

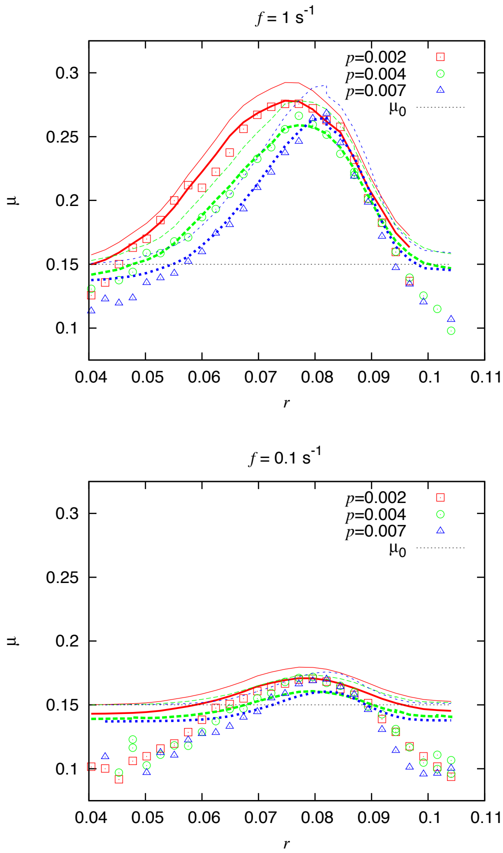

Fig. 3 Shear stress ratio, μ, for the same simulations as in Fig. 2. The lines correspond to Eq. (1), the classical rheology (thin lines), or Eq. (2), the corrected soft rheology (thick lines), with parameters as given in the main text. The horizontal dotted lines give the constant low strain-rate limit, μ_0.

Conclusions and Outlook

In conclusion, particle simulations and the micro-macro transition can guide the development of new rheological particle-flow models that include and combine various mechanisms, which are quantified by dimensionless numbers. The original rheology for hard, cohesionless particles was generalized to include the effect of large confining stress and softness (or compressibility) of the particles. Both density and shear stress ratio are well predicted by the improved, pressure dependent rheology model, especially in the centre of the shear band. However, in the tails deviations still occur, which can be due to several reasons: (i) the statistics is much worse in areas where the strain rate is small, (ii) the system has not yet reached the true steady state – as reported in Ref. [14], (iii) there can be non-local effects as encompassed, e.g., by a "fluidity" variable, as used in Ref. [15-18], or there are additional local corrections needed, as proposed in Ref. [19] and reported as relevant for the present system in Ref. [5].

Ongoing research is aiming at finding such further corrections for very small strain rates, but also for cohesive particles. As next step the implementation of such multi-purpose, generalized flow/rheology models into continuum solvers is in progress. Final step is the development of fully tensorial flow models, as suggested in Refs. [3,4], that are needed to account for all the non-Newtonian aspects of particulate and granular matter.

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