About particles, micro-macro, and continuum theory
Shear-bands, memory of jamming and dilatancy

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Abstract

Particulate systems and granular matter are discrete systems that are made of many particles in interesting dynamic or static, fluid- or solid-like states. The challenge of bridging the gap between the particulate, microscopic picture (via micro-macro transition methods) towards their continuum description is one of todays topics of actual research. This short paper gives a brief overview of recent research and an update on some new results.

Introduction

Particulate systems are posing many challenges for theory and applications. From molecular dynamics simulations of many atoms or particles, one can extract scalar fields like density or temperature, as well as velocity, i.e. vectorial fields, or tensors like stress, strain, and structure (fabric). Given sufficiently good statistics the data can have a quality that allows to derive constitutive relations about the rheology and flow behavior of complex fluids (like atoms confined in nano-geometry, or granular particle systems) that behave strongly non-Newtonian, with particular relaxation behavior, anisotropy etc. [1]. 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]. Dependent on the energy input (shear-rate), the particles can flow like a fluid, jam and un-jam, or be solid with a very interesting anisotropic structure (contact-and force-networks).

Phenomenology

The interplay between strain, stress and anisotropy leads to dilatancy and an interesting 'memory' of the packing: the evolution of anisotropy (micro-structure) is independent from the direction-dependency ("anisotropy") of stress, both in evolution rates as well as in principal directions, i.e., tensorial eigen-system orientations. The particulate systems behave in various ways like a non-Newtonian fluid [3,4], as observed by modern particle simulations, from which macroscopic scalar, vectorial, and tensorial fields are measured [3,4,5,6,7]. Having available all tensorial information from the particle simulations, obtained via the micro-macro transition, the next step is to formulate constitutive relations that allow to predict the systems flow behaviour [5,7,8,9]. Similar methods and approaches can also be applied to solid-like systems [10] – all are based on the original ideas of coarse-graining [11,12]; the basic approach to coarse graining follows the ideas of Isaac Goldhirsch [3,11,12] for the micro-to-macro, starting from micro/atomistic/particle simulations, which can be carried out for many different flow situations.

Examples of basic element tests, i.e., small and representative systems with relevance for the micro-macro approach, involve planar flows [4] like avalanche on inclined planes [3], the split-bottom ring-shear cell [5,6,7,8], or the tri-axial box [9,10]. All have in common that plenty of data on the particle systems density, displacement, velocity and velocity gradient, stress and fabric (micro-structure) can be obtained as functions of particle and contact properties like particle sizes, stiffness, cohesion, or friction as well as system parameters like the external shear-rate.

Results

Here, a short summary of recent research on formulating the granular rheology is presented and concluded with an outlook for future reseach.

When formulating a granular rheology, the starting point is the so-called $\mu(I)$-rheology [5,13], which relates the shear-stress to pressure ratio $\mu = \tau / p$ in a sheared particulate system to the dimensionless strain-rate

$$I = \dot{\gamma} d_0 \sqrt{\varrho/p} \,, \tag{1}$$

with shear rate $\dot{\gamma}$, diameter d_0, mass-density ρ, and pressure p. The relation that describes well a wide variety of flows of hard particles at various strain rates is:

$$\mu(I) = \mu_0 + (\mu_\infty - \mu_0)\frac{1}{1 + I_0/I} \qquad \mu_0 = 0.15,\ \mu_\infty = 0.42, \text{ and } I_0 = 0.06,$$

with the limits of μ, for zero and infinite strain rate, designated by the respective symbols, and the characteristic dimensionless strain-rate I_0 where inertia effects considerably kick in. Since the simulations presented below concern the very small coefficient of particle contact friction $\mu_p = 0.01$, 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 given as a 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 particle stiffness k. This correction accounts for a wide range of different particle stiffness, but also for different gravity, as in a centrifuge or on the moon. Additional corrections for cohesive particles involved the so-called Bond-number (*Bo*) as studied elsewhere [6,7].

In order to complete the rheology for soft, compressible particles, a relation between the density and the 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 state density for vanishing pressure and inertial number, $\phi_c = 0.648$, the characteristic strain rate for which dilation kicks in, $I_\phi^c = 0.85$, and the typical pressure level where softness leads to huge densities, $p_\phi^c = 0.33$ (due to the linear contact model). Representative data from Ref. [5], see Fig. 1, agree very well with the corrected rheology.

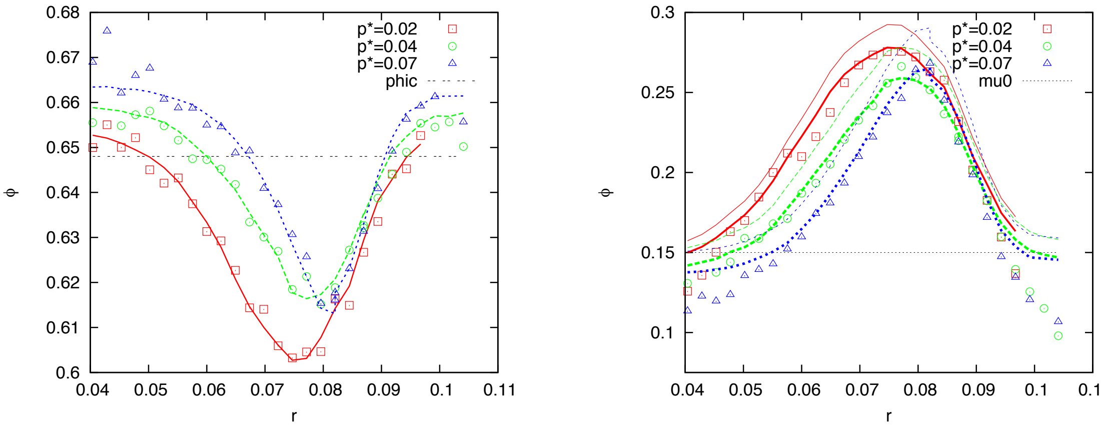

Fig. 1: Density (left) and shear stress ratio (right), plotted against the radial distance r, with data from the particle simulations in Ref. [5], using the external rotation rate $f = 1\ s^{-1}$, selected at three different pressure levels, as given in the inset (i.e. red, green and blue correspond to: close to the surface, in the middle, and closer to the bottom). The lines in the right panel correspond to Eqs. (1), thin lines, (2), thick lines; the lines in the left panel correspond to Eq. (3), with all parameters given in main text; the horizontal lines give the low stress and strain-rate limits: ϕ_c (left) and μ_0 (right).

The shear stress ratio in the tails does not agree well with theory, indicating a missing 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.

Conclusion 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 softness (or compressibility) of the particles, and ongoing research is applying aiming at finding further correction terms for cohesive particles as well as for the poorly understood limit of very small strain-rates (tails). As next step, also the implementation of such multi-purpose, more general flow models into continuum solvers is ongoing as well as the development towards the fully tensorial flow models that are needed to catch all the non-Newtonian aspects of particulate and granular matter.

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