Constitutive Relations from Particle Simulations

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Abstract. Particulate systems like powders, soil or granular matter are discrete, disordered systems displaying dynamic and static, fluid - and solid-like states. The transients between fluid - and solid-like behavior can be intermittent and sometimes both states coexist in steady-state. Bridging the gap between the particulate, microscopic picture (velocities, forces) on the particle scale and their continuum description (strain and stress) via a so-called micro-macro transition is the goal of this paper. The generalized local constitutive relation for the stress in critical state granular flows involves not only density and strain rate but also the jamming-density and the granular temperature.

Keywords: Particle models · Micro-macro transition · Continuum rheology

1 Introduction

Particulate systems are interesting and challenging for academia and of practical relevance for industry, civil engineering and geo-sciences. Molecular dynamics-like discrete particle simulations provide in-depth microscopic insight and allow to extract scalar fields like density or granular temperature, vector fields like the flow velocity, or tensors like stress, strain-rate, and structure (fabric) [1–13]. Either one carries out many simulations of a homogeneous representative volume element (REV) for each state-point [7] or one performs local micro-macro coarse graining on an inhomogeneous system, in which case a few simulations might be sufficient. Given satisfactory statistics, such data-sets can have a quality that allows deriving constitutive relations that describe the local rheology and flow behavior 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]. Attractive forces, like van-der Waals adhesion or liquid-bridges, lead to macro-cohesion added on top of the already non-trivial dynamics of granular matter [2, 6, 8, 9]. 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) [10, 11, 13].

The goal of the present paper is by using particle simulation data and the local coarse graining (micro-macro transition) procedure proposed by Isaac Goldhirsch [12, 13] to determine three-dimensional local rheology laws (in steady state shear in a split-bottom ring shear cell [1, 2, 5, 6, 8, 9]) that go beyond the classical $\mu(I)$-rheology [14].

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This constitutive relation can predict surprisingly well (neglecting all but one non-Newtonian mechanism [3] and not accounting for very small strain-rates [5, 15]) the steady-state flow behavior of rigid, cohesionless particles, where the inertial number is the only relevant dimensionless number relating shear-rate to the confining pressure time-scale. However, for real particles also the effect of large confining stress or, inversely, softness has to be taken into account as additional control parameter [5–9]. As new ingredients to the generalized rheology that complements the static contributions to stress, also the dynamic time-scale set by the so-called granular temperature [7] or fluidity [16–18] has to be considered. For a discussion of many of the relevant time-scales of the involved micro-mechanisms and the dimensionless numbers formed by ratios of those see Refs. [9, 19], and for experiments see Ref. [20] and references therein.

In granular systems, the interplay between strain, stress and microstructure (including anisotropy) is one micro-mechanism that can lead to dilatancy [21–23], related to the 'memory' of the packing. The transitions of granular systems from (jammed) solid to fluid and, oppositely, from un-jammed to (shear) jammed was studied in detail in Refs. [7, 23]. 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 of the tensors establishes, which is subject of ongoing research [5, 6].

Besides the anisotropy of the micro-structure [11, 23] an additional (isotropic) state-variable was identified as a necessary ingredient to describe the slow, quasi-static transitions between fluid - and solid-like states. As mind-changing concept, the transition point itself was proposed as the new state-variable [22, 23]; however, it could be related to various other possible variables like contact/coordination number, isotropic fabric, or the fraction of rattlers [23] and is thus not a unique choice but rather a question of convenience and matter of taste which variable one choses to use.

Starting from a static, dense packing, shear motion is only possible if the grains "unlock" from their dense, jammed arrangement. Shearing for long time, the initial state is forgotten and a steady state (critical state) is reached. The dynamics of the tails of shear bands involves a very slow approach to steady state due to the small strain rate [5, 9, 15]. The local steady state rheology was shown to be valid also in transient states [24] but requires corrections for very small strain rates [5, 9, 25].

In a particular geometry, i.e., the split bottom ring shear cell, see Refs. [1, 2, 5, 6, 8, 9] and references therein, the fields are functions of position (height and radial distance from the symmetry axis), so that a wide range of local densities, strain-rates and pressures are covered by data from a single (inhomogeneous) simulation [5, 6, 8, 9]. Having available this information, the next step is to formulate general, local constitutive relations [9] that allow to predict the systems flow behavior in more general inhomogeneous systems and applications. Similar methods and approaches can also be applied to solid-like systems [11] – all are based on the original ideas of coarse-graining from micro-to-macro [3, 12, 13], following the ideas of Isaac Goldhirsch [12]. Macroscopic data can then be related to microscopic particle - and contact-properties like particle size distributions, stiffness, friction as well as system state parameters like strain-rate (the scale of which is set by the externally applied shear-rate).

2 Theory

In the following, a short summary of recent results and some new insights on formulating a generalized local granular rheology are presented, starting with the shear rheology, but then focusing more on the hydrostatic stress, density, jamming density, strain-rate and granular temperature. Note that the rheology (constitutive relations) are expressed in dimensionless form to make them generally applicable. When parameters are given in dimensional form, those are input parameters for the simulations and to give an indication of what physical experiments the simulations are supposed to model.

When formulating a granular rheology, the starting point is the surprisingly simple and elegant so-called $\mu(I)$-rheology [5, 14] that relates – in a sheared particulate system – the so-called macroscopic (bulk) friction, i.e., the shear-stress to pressure ratio $\mu = \tau/p$, to the inertial number, i.e., the dimensionless strain-rate $I = \dot{\gamma}\, d_0/\sqrt{p'/\rho}$ with local shear rate $\dot{\gamma}$, diameter $d_0 = 0.0022$ m, particle mass-density $\rho = 2000\,\mathrm{kg/m^3}$, and dimensional pressure p'. The relation that describes nicely a surprisingly wide variety of flows [14] of rigid and cohesion-less particles at various strain rates is:

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

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, where inertial effects considerably kick in, is $I_0 = 0.06$. Note that the simulations presented below only concern particle simulations with a very small coefficient of particle contact friction, $\mu_p = 0.01$; the dependence of the coefficients in Eq. (1) on friction are considered elsewhere [21].

Corrections to the $\mu(I)$-rheology become necessary for soft particles and/or high confining stress, as shown by Singh et al. [5]; originally, linear terms were added to the above rheology for small strain-rates [5], however, these can better be re-phrased as multiplicative correction factors [9] allowing for more elegant mathematical treatment so that the original rheology is modified by multiplicative forms that tend to $f \sim 1$ if the respective mechanism is not active. The pressure/softness correction f_p appears as:

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

with the dimensionless pressure $p = p'\, d_0/k$ (corresponding to the typical overlap/deformation of particles relative to their diameter), the characteristic pressure at which this correction becomes considerable, $p_0 = 0.9$, and the particle contact stiffness $k = 100$ N/m. In Ref. [5], where the linear correction was calibrated by local ring-shear

cell data, it was shown that this correction accounts for a wide range of particle stiffness (or softness), but also for different magnitudes of gravity, as in a centrifuge or on the moon.[1]

Note that the pressure dependent correction function, in its linear form, has an unreasonable zero-crossing; this is avoided by the exponential form in Eq. (2); both forms are identical in first order and thus practically identical for all values of confining pressures considered in the particle simulations [5, 9]; a decision about the functional form is not really possible with the available data and remains an open issue for future research. Several additional corrections functions f were presented in Ref. [9] but are dropped here for the sake of brevity; also cohesion involves a dimensionless number, the so-called Bond-number (Bo), as studied elsewhere [6, 7, 9, 19] and ignored in the following. The two dimensionless numbers in Eq. (2) can be expressed as ratios of time-scales, namely $I = t_p/t_{\dot{\gamma}}$ and $p = \left(t_c/t_p\right)^2$, where the subscripts refer to strain-rate, $\dot{\gamma}$, pressure, p, and contact duration, c, respectively [19]. There are many ways of constructing the dimensionless numbers that control the flow behavior and to implement the correction terms they are responsible for, however, here we choose multiplicative functions that are in first order proportional additive corrections, as shown in Ref. [5].

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, $\phi_c = 0.648$, valid for a given material with a certain polydispersity [9, 19], 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, $p_\phi^c = 0.33$. Note that both correction terms in Eq. (5) were first determined as additive corrections [5], identical to the multiplicative form for sufficiently small arguments. Too large inertial numbers are not allowed since they would lead to negative densities; large I would fully fluidize the system so that the rheology should be that of a granular fluid, for which standard kinetic theory applies [7]. Too large pressures would lead to enormous deformations/overlaps (or even breakage), for which the contact model and the particle simulation become questionable.

Two small adaptations of the correction functions in Eq. (3) remove the invalidity for large I, and uses an analogous but not necessarily plausible correction form for pressure, p, while remaining identical to first order Taylor expansion for small arguments:

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

[1] Using either one of the correction terms alone, without the other, leads to slightly different coefficients in Eqs. (1) and (2), e.g., when the I-dependence is neglected for the case of very small gravity and thus very small confining stress, one observes a slightly different $\mu_0 = 0.17$ due to the considerable inertial number at small p, see Eq. (14) and Fig. 5 in Ref. [5]. Thus, correction functions should always be applied together!

This new form, Eq. (4), allows for an elegant rephrasing (inversion) and express pressure as a function of density, critical state density, and inertial number, yielding:

$$p = p(\phi, I) = p_\phi^c \left(\log\left(\frac{\phi}{\phi_c}\right) - \left(-\frac{I}{I_\phi^c}\right)\right) = p_\phi^c \varepsilon_V + \frac{I}{I_p} \tag{5}$$

with the implicit definition of the (virtual, elastic) volumetric strain, $\varepsilon_V = \log(\phi/\phi_c)$, and the dynamic strain-rate non-Newtonian pressure dilatancy coefficient $I_p = I_\phi^c / p_\phi^c$. The volumetric (elastic) strain ε_V in the first term is defined relative to the stress-free reference state, where ϕ_c, is also termed the critical state density (in the zero-pressure limit of a very slowly sheared system in steady state). The factor $p_\phi^c \sim \phi C$ hides its dependence on the coordination number and can be seen as the dimensionless bulk modulus in the static limit. For the dimensional pressure $p' = pk/d_0$, all contributions should in fact be additive, which allows for further contributions (anisotropy is not considered here, but discussed in detail elsewhere [6, 11, 23]) as, e.g., the pressure from standard kinetic theory, $p'_{SKT}(\phi, T_g)$, proportional to the granular temperature, T_g [7]:

$$p'(\phi, \phi_c, I, T_g) = p'(\phi, \phi_c, I) + p'_{SKT}(\phi, \phi_c, T_g) \tag{6}$$

When the system is left at rest, $I = 0$, for vanishing T_g, the *SKT* correction vanishes, and the first term in Eq. (5) survives, for $\phi > \phi_c$ representing a linearly elastic stress-strain relation, as introduced in Ref. [21] for non-sheared systems, and confirmed later in [10, 11, 23] under shear. For $I > 0$, the second term in Eq. (5) represents the (non-Newtonian) pressure-dilatancy, i.e., an over-pressure due to the applied shear, as defined for dense fluids in Ref. [4]; for more details see references therein. Note that the rheological property dilatancy (decrease of density or increase of volume) in pressure-controlled systems, is equivalent to this pressure-dilatancy in a volume-controlled system. The dependence of the last term in Eq. (6) on the softness was studied in Ref. [7], but is not visible here, as it is subject to ongoing research.

3 Conclusions

Particle scale simulations and the micro-macro transition can guide the development of new rheological constitutive models that include and combine various mechanisms as quantified by dimensionless numbers. The original rheology for hard, cohesionless particles [14] was generalized to include the effect of large confining stress or softness (or compressibility) [5] as well as various other effects [9]. Both density and shear stress ratio are well predicted by the improved, inertial - and pressure-dependent rheology model, at least in the center of the shear band [5, 6, 9]. In the tails, however, 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 Refs. [5, 9, 15], *(iii)* there can be non-local effects as encompassed, e.g., by a "fluidity" variable, as used in Refs. [16–18, 25], or there are additional local corrections needed, as proposed in Refs. [9, 21–24] and reported as

relevant for the present system in Refs. [5, 9]. The present paper was adding a kinetic contribution to the hydrostatic stress that allows to link the elastic regime to the standard kinetic theory of collisional granular gases in the respective dense/static/solid and dilute/collisional/fluid cases.

Ongoing research is aiming at finding and calibrating all the necessary additional corrections for very small strain rates [5, 9, 21], for very small pressure close to the free surface [9, 19], and also for cohesive particles [9, 19]. The next step is the implementation of such multi-purpose, generalized scalar flow/rheology models into continuum solvers. The final challenge is the development of fully tensorial flow models, as shown in Refs. [3, 4], that are needed to account for a variety of non-Newtonian aspects of atomistic, particulate and granular matter and include not only the microstructure (fabric) tensor [5, 11] but also the granular temperature [7] as introduced above, as well as other ratios of time-scale or other combinations of dimensionless numbers in the correction functions.

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