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Hydrodynamic fluctuations and averaging problems in dense granular flows

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ABSTRACT: We analize the properties of dense granular systems by assuming a hydrodynamical description, based on conservation laws for the particle number density and linear momentum. We combine analytical methods and experimental and numerical results obtained by ensemble-averaging of data on creep during compaction and molecular dynamics simulations of convective flow.

1 INTRODUCTION

In spite of the early and in many aspects successful hydrodynamical approach applied by Haff (P. K. Haff 1983 1986) to granular systems, there still remain many unsolved questions, since the behavior of a granular mass is fundamentally different from that of typical fluids. For instance, in addition to the ordinary source of hydrodynamic fluctuations –which in this case can't be removed by taking the thermodynamic limit, the fact that solid grains in a dense arrangement can't be regarded as points in any length scale leads to a second source of fluctuations; it operates at distances much larger than the typical diameter of the particles and is related to the appearance of extensive arrangements inside the system. Given a mean density not far away from the close-packing limit, different actual realizations in the configuration space of the particles may lead to departing dynamic properties and, ultimately, in generating completely different time-sequences. This contribution is what we call non-local noise. Both, local and non-local noise, are always present but their relative importance strongly depends on the forcing applied to the system, measured by the parameter $\mathcal{F}g = f/\rho g$, f being the volume density of the forcing and g the acceleration of gravity.

We propose the existence of two regimes; in the weak-forcing limit, $\mathcal{F}g \lesssim 1$, the non-local component of the noise dominates, and consequently one expects very long relaxation rates and non-self-averaging quantities. In this limit, only ensemble averaging is meaningful, as in every possible realization the system explores a small region of the configurational space. The glass-like behavior is most apparent. In the opposite limit, $\mathcal{F}g \gg 1$, the system is not easily trapped in an immobile arrangement, and one can safely assume that in a sufficiently long time it explores the representative part of the configuration space. Time averaging can substitute ensemble averaging only in this limit. Consistently with this picture, the critical density, ρ_c, is not unique in general, but is a distributed quantity depending on the configurational state, Γ. Actually, we shall see that experimental data on compaction at weak forcing display quenched behavior, and the final density may vary over more than 10%. Instead, our numerical study of granular convection under strong forcing indicates a much narrower histogram of maximal achieved densities, ρ_c, despite the fact the number of particles and the used number of samples for averaging were much smaller.

We show that it is possible to understand both limits within the frame of hydrodynamic equations, which are in general stochastic equations including both local and non-local noise. It is be-

yond of the scope of this paper a detailed analysis of the properties of such equations, which is extensively done elsewhere. Our aim is to present some results of our study of the evolution of the mean hydrodinamic fields, comparing them with their observed behavior in a sample of cases.

2 HYDRODYNAMIC EQUATIONS

By hydrodynamic equations we mean balance equations for mean mesoscopic hydrodynamic fields. The lack of an intermediate length scale –contrary to what happens in simple fluids for instance, containing a sufficiently large number of particles such that local fluctuations fade away, adds on the above exposed problem of non-local fluctuations due to the intrinsic granular nature of the system, operating at length scales where hydrodynamic fields can already be defined. The former can be modelled as the usual additive stochastic contribution to the dissipative flows and comes related to the existence of some kind of "temperature", the latter enters via distributed kinetic coefficients (depending on the configurational state Γ). In the continuum approach, conservation of mass and linear momentum read

$$\partial_t \rho + \nabla(\rho \mathbf{v}) = 0, \tag{1a}$$

$$\rho \partial_t v_i = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i, \tag{1b}$$

in the Stokes approximation, and where f_i are the components of the volume density of forcing. As for the terms constituting the stress tensor σ_{ij} a few comments are in order. Provided that the granular particles may be modelled as sufficiently hard spheres, we neglect any elastic contribution other than that introduced by pressure effects, and assume that the non-equilibrium part of σ_{ij} is a local functional of the derivatives of the local velocity,

$$\sigma_{ij} = -p\delta_{ij} + \eta(\rho,\Gamma)\Big(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{v}\Big) + \zeta(\rho,\Gamma)\delta_{ij}\nabla\cdot\mathbf{v} + \xi_{ij}. \tag{2a}$$

where p is the pressure and η and ζ the shear and volume viscosities, respectively.

2.1 *The role of temperature and the pressure term*

Our molecular dynamic simulations indicate that the evolution of the velocity field in dense granular flow is nearly independent from the granular, temperature, defined as the mean fluctuational part of the velocity. Effectively, well inside the bulk, the quantity $\delta v/v$, measuring such fluctuational deviations from the mean velocity v, is typically about six orders of magnitude smaller than close to the boundary. This and other evidences allow us to suppose that granular flows in dense systems can't be sustained by a temperature-based mechanism alone –unlike Rayleigh-Benard convection in simple fluids, for instance. Note that the equation for the energy balance has been omitted; consistently with the observation that the granular temperature plays no significant role, its evolution appears decoupled from the previous system of equations. Similarly, one cannot account for elastic contributions in the high density limit only by using a thermal pressure. Therefore, one has to model such terms by means of an artificial equation of state which must help to resolve the delicate limit $\rho \to \rho_c$. We assumed the most simple dependence, $p = p_0/(1-\rho/\rho_c)$, where p_0 represents a certain constant, in our numerical integration of the hydrodynamic equations in the strong forcing regime.

2.2 The viscosity

Accordingly, the model that we adopt for the viscosity is not thermal, but glass-like. In dense clusters, in order to move, a complex rearrangement of particles has to occur making use of voids. Similar properties are exhibited by glasses. Available experimental data and our numerical results indicate the presence of a factor $\exp[c/(1-\rho/\rho_c))]$ in the mean flow rates, where c is a dimensionless number. This formula is related to the Vögel-Fultcher law for glasses (see N. F. Mott & E. A. Davis 1979); it measures the number of attempts needed for one step in the direction of average flow in a dense granular system. Sufficiently close to ρ_c, we then expect a shear viscosity of the form

$$\eta(\rho,\Gamma) = \eta_0(\rho,\Gamma)\exp\Big(\frac{c}{1-\rho/\rho_c(\Gamma)}\Big). \tag{3}$$

and a similar dependence for the bulk viscosity, $\zeta(\rho,\Gamma)$.

3 RESULTS

We focus on two different examples which are representative of each regime. For the weak forcing limit, we use data on compaction of sand during tapping experiments (J. B. Knight et al. 1995). For the strong forcing limit we perform exten-

sive ensemble averaging of samples generated by molecular dynamic simulations of vertical shaking, –other geometries can be studied, see for example (S. E. Esipov et al., 1996) for an study under horizontal shaking, comparing them with results from the integrated hydrodynamic equations for the mean fields.

3.1 *Weak forcing limit. Application to compaction experiments*

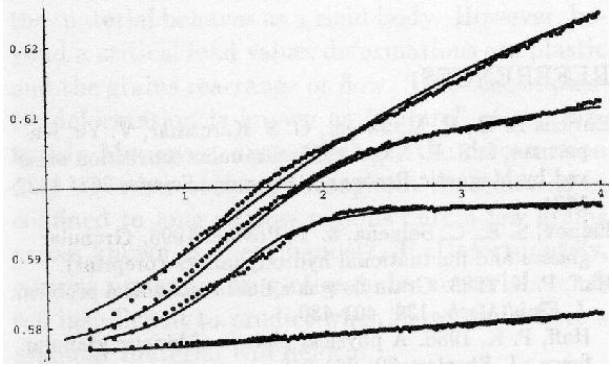
These results provide additional support for the existence of non-local noise, and evidence that the mean flows are of hydrodynamic nature even in very dense limits. Beginning with a loosely packed sand at volume fraction $\rho_0 = 0.57$ the authors report a logarithmic density growth,

$$\rho_c - \rho(t) = \frac{A}{1 + B\ln(1 + t/\tau)}, \qquad (4)$$

where A, B, τ, ρ_c are four fitting parameters. It can be shown that it is possible to retrieve such a dependence by integration of hydrodynamic equations. Omitting further details about calculations and average over non-local noise, one finds after integration of the 1-dimensional version of (1) at late times

$$\bar{\rho_c} - \rho(t) = \frac{c}{\ln[(\int_0^t dtF)/c\bar{\eta}_0]}, \qquad (5)$$

$\bar{\rho}_c$ and $\bar{c}$, already averaged over non-local noise, are constants which depend on, say, the amplitude of forcing, but do not change over time. The quantity F is related to the integral of the density of forcing and is left unspecified. Equation (5) can be compared with experimental fit, (see Figure 1) assuming $\int_0^t dtF = t\langle F\rangle$, where the average is taken over a period of repeated tapping. We find $A/B = \bar{c}$, $\tau = c\bar{\eta}_0/\langle F\rangle$.



This is a three parameter fit. It demonstrates that hydrodynamics may be used for analyzing experimental data. Different fitting values of $\bar{\rho}_c$, $\bar{c}$ support the assumption that granular configurations with different ρ_c, c (different states Γ) do not communicate at weak forcing.

3.1 *Strong forcing limit*

This case is object of a more complete study. It is well known that sand under periodic vertical shaking and gravity in a container develops typical convective rolls, with sand going upwards inside, and downwards along the vertical walls. The motion is evidenced, for example, by the bulging colored stripes resulting from NMR experiments (E. E. Ehrichs et al. 1995), which represent cycle-averaged displacements. Again, it is possible to show that the system of equations (1) can be integrated to give a good fit of the experimental data (S. E. Esipov et al., 1996). A major understanding of the motion requires, however, a time-resolved analysis, and we show how this can be done via molecular dynamics simulations.

The details of the simulations will be omitted here, it suffices to say that we used a polydisperse sample of 2000 soft spheres in a tall rectangular container, and the chosen values for the friction parameters reproduce correctly the experimental NMR images mentioned above. $\mathcal{F}g$ was about 2. The following steps summarize the procedure we used:

1. Time discretization. Each period of shaking is divided in an equal number of frames, where positions of particles are recorded.

2. Spatial discretization and averaging. Using a high resolution grid, the container is divided in cells of the size of the order of one particle. Time averaging –which can replace ensemble averaging in this case, is performed with data of the corresponding frames of more of 100 periods of shaking.

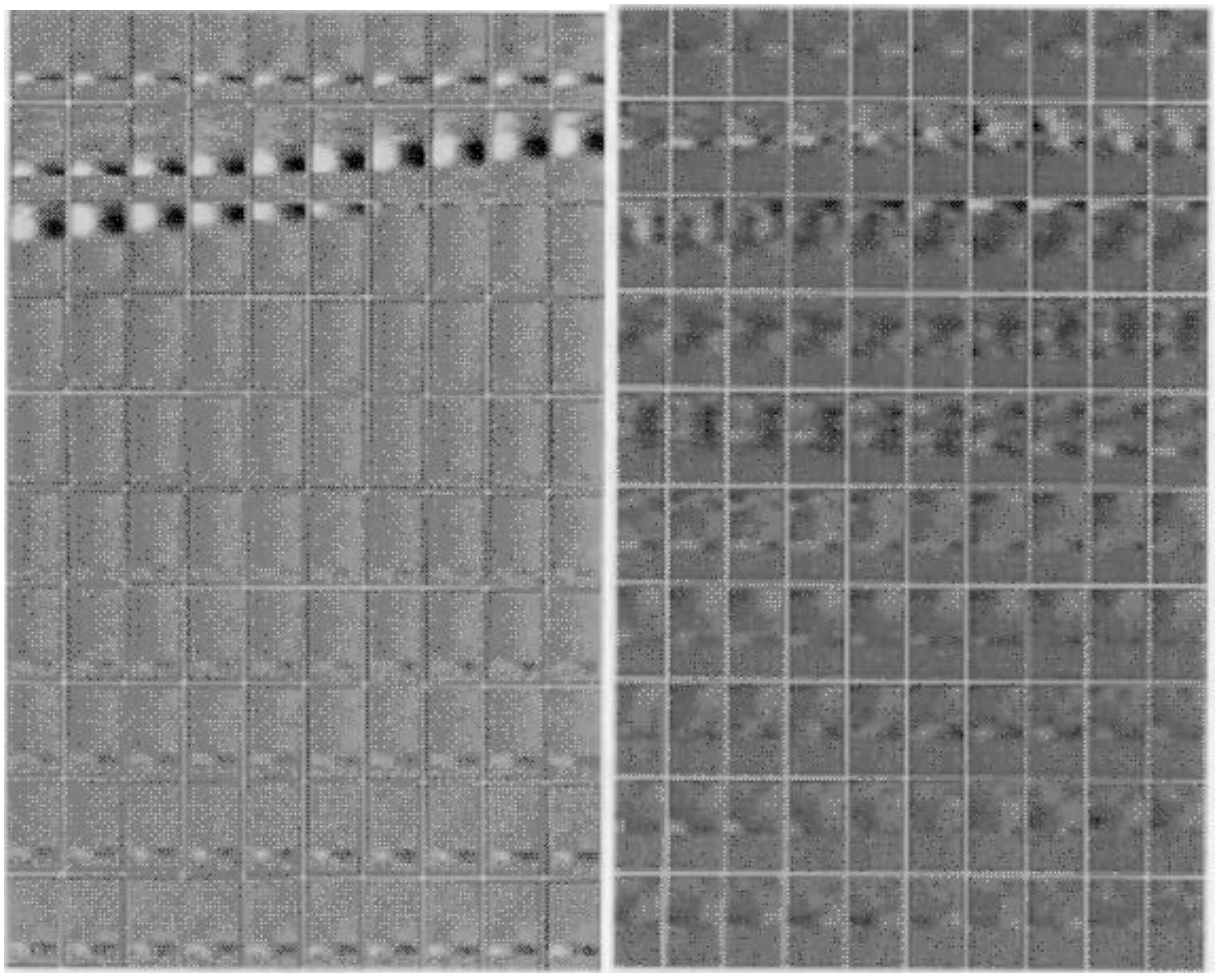
3. Mean density, velocity and temperature (mean fluctuational velocity) are obtained and displayed. As an example, we reproduce in Figure 2a the horizontal component of the velocity, v_x. Observe that the motion is complex and unexpected, in the sense that one cannot infer from the sequence of pictures of v_x (neither from v_y, not shown) the direction of the global motion.

4. Test of the hydrodynamic equations. By using the mean hydrodynamic fields obtained in 3., the system of equations (1) is checked. Selected frames provide fitting values for c=0.15 and $\rho_c = 1.01$ $\max(\rho)$. η_0 was found to be about 300 cpoise by comparing histograms of the tangential force and the velocity gradient close to the walls, whereas the observation that the flow is mostly divergence-free

allows us to neglect the effects of ζ.

5. Study of boundary conditions. We obtained effective boundary conditions for the flow that reproduce to some extent the assumptions of microscopic friction during collisions, but we also found that the motion of sand along the vertical walls comes accompanied by dramatic periodic changes in the density and the stress.

6. The previous results are used to integrate numerically the system of hydrodynamic equations. In Figure 2b we show comparatively the sequence obtained for v_x.



4. CONCLUSIONS

1. Hydrodynamic equations provide an adequate theoretical frame for the study of dense granular systems.

2. Temperature-based mechanisms can be practically dismissed in the description of dense granular flows.

3. Averaging of data from molecular dynamic simulations is an useful tool to reveal the details of the evolution of hydrodynamic fields.

4. Results of numerical integration of the system of hydrodynamic equations show a qualitative agreement with the evolution of hydrodynamic fields.

REFERENCES

Ehrichs E. E., H. M. Jaeger, G. S. Karczmar, V. Yu. Kuperman, & S. R. Nagel 1995. Granular convection observed by Magnetic Resonance Imaging. *Science* 267: 1632-1634.

Esipov, S. E., C. Salueña, & T. Pöschel 1996. Granular glasses and fluctuational hydrodynamics (preprint).

Haff, P. K. 1983. Grain flow as a fluid mechanical problem. *J. Fluid Mech.* 134: 401-430.

Haff, P. K. 1986. A physical picture of kinetic granular flows. *J. Rheology* 30: 931-948.

Knight, J. B., C. G. Fandrich, C. N. Lau, H. M. Jaeger, & S. R. Nagel, 1995. Density relaxation in a vibrated granular material. *Phys. Rev. E* 51: 3957-3963.

Mott N. F. & E. A. Davis 1979. *Electronic Properties of Non-Crystalline Materials.* NY: Oxford U. Press.