Rapid Granular Flows as Mesoscopic Systems

M-L. Tan

Cambridge Hydrodynamics, Inc., 666 Plainsboro Road, Suite 1000, Plainsboro, New Jersey 08536

I. Goldhirsch

*Department of Fluid Mechanics and Heat Transfer, Faculty of Engineering, Tel-Aviv University,
Ramat Aviv, Tel-Aviv 69978, Israel*
(Received 22 May 1998)

The dissipative nature of the particle interactions is responsible for an *inherent* lack of scale separation in granular systems which is not related to the typical grain/container size ratios. It is demonstrated that rapid granular flows are typically supersonic, shear rates in these systems are nearly always "large," the mean free times are comparable with the macroscopic time scale(s), and the *mean free paths can be of macroscopic dimensions*, the latter indicating *nonlocality*. Additional physical and computational implications are discussed. [S0031-9007(98)07276-7]

PACS numbers: 46.10.+z, 47.50.+d, 47.55.Kf, 83.10.Hh

One of the major questions in the field of granular flows is whether their dynamics can be described by macroscopic equations of motion which are local in space and memory free. In this respect, rapid granular flows [1] which are, by definition, flows in which the particles (grains) interact by practically instantaneous collisions, seem to be good candidates for the construction of such equations of motion. Indeed, kinetic theory has been applied [2] to the study of such systems and to the derivation of appropriate constitutive relations. It turns out that some of the peculiar properties of granular systems, such as their instability to clustering [3], layering [4–5], plug formation [4–5], and, in general, to the creation of microstructures, can be captured by the continuum equations. The collapse phenomenon [6], while not directly a consequence of the continuum equations of motion, may also be partly captured by the continuum equations, at least in one dimension [7].

Hydrodynamiclike equations are usually intimately related to the notion of scale separation, the Navier-Stokes equation(s) for fluids being a classical example. It is for this reason that it is important to understand the degree of scale separation that can be expected in granular systems. It is shown below that such scale separation is nonexistent except when the system is very nearly elastic. Moreover, a few peculiar properties of rapid granular flows, such as the existence of macroscopic mean free paths, are demonstrated.

Consider a simply sheared stationary monodisperse granular system composed of disks (spheres) in two (three) dimensions whose collisions are characterized by a fixed coefficient of normal restitution e. The average velocity $\vec{v}$ is taken to point in the streamwise x direction and depends linearly on the spanwise y coordinate: $\vec{v} = \gamma y \hat{x}$, where γ is the shear rate and $\hat{x}$ is a unit vector in the x direction. Such a flow can be shown to exist on the basis of equations of motion derived from

kinetic theory [2]; it can also be produced in molecular dynamic (MD) simulations [3(a),8]. It can be shown by dimensional analysis and general phenomenological (mean-field) arguments [9] (in agreement with results of kinetic theoretical calculations [2(f),2(g),3(b),3(c),9,10]), that the granular temperature T (notice: here and below T is defined as the mean square of the velocity fluctuations, as is common in the field of granular flows), in this system satisfies

$$T = C \frac{\gamma^2 \ell_0^2}{\epsilon},\tag{1}$$

where $\epsilon \equiv 1 - e^2$ is the degree of inelasticity and ℓ_0 is the equilibrium mean free path (see below), which is given by $1/n\sigma_T$, where n is the (particle) number density and σ_T is the total collisional cross section of two particles. The prefactor C is a function of the degree of inelasticity and the volume fraction, but for our purposes it suffices to know that C is $\mathcal{O}(1)$, its value for dilute and nearly elastic systems being about 0.6 in 2D [2(f)] and 3 in 3D [2(g)].

Consider first the change of the macroscopic velocity over a distance of a mean free path ℓ_0 in the y direction: $\gamma \ell_0$. A shear rate can be considered small if $\gamma \ell_0$ is small with respect to the thermal speed $\sqrt{T}$. Using Eq. (1), one obtains: $\gamma \ell_0/\sqrt{T} = \sqrt{\epsilon}/\sqrt{C}$, i.e., the shear rate is not "small" unless the system is nearly elastic (notice that for, e.g., $e = 0.9 : \sqrt{\epsilon} = 0.44$).

Consider next the mean free time τ, i.e., the ratio of the mean free path and the thermal speed: $\tau \equiv \ell_0/\sqrt{T}$. Clearly, τ is the microscopic time scale characterizing the system at hand and γ^{-1} is the macroscopic time scale characterizing this system. The ratio $\tau/\gamma^{-1} = \tau\gamma$ is a measure of the temporal scale separation in the system. Employing Eq. (1) and the definition of τ, one obtains $\tau\gamma = \sqrt{\epsilon}/\sqrt{C}$, and $\mathcal{O}(1)$ quantity. It follows that there is no temporal scale separation in this system, *irrespective*

    0031-9007/98/81(14)/3022(4)$15.00

of its size or the size of the grains, except when ϵ is very small.

The ratio of the speed $\gamma|y|$ to the thermal speed $\sqrt{T}$ can be rewritten, using Eq. (1), as follows: $\gamma|y|/\sqrt{T} = (\sqrt{\epsilon}/\sqrt{C})(|y|/\ell_0)$. Since, as mentioned, $\sqrt{\epsilon}/\sqrt{C}$ is typically $\mathcal{O}(1)$, except for very nearly elastic systems, the speed is supersonic when the coordinate y is larger (in absolute value) than about a mean free path. The subsonic domain is very small indeed, being limited to a strip (in 2D, and a corresponding volume in 3D) whose width is of the order of a mean free path around the stagnant line (in 2D) or plane (in 3D).

The mean free time is usually defined as the time between consecutive collisions of a particle. It is clear that mean free times depend on the *relative velocities* of the particles, hence they are Galilean invariant. A simple, textbooklike (and mean field) derivation of the above expression for the mean free time τ proceeds as follows: the flux of particles impinging on a given particle is (proportional to) $n\sqrt{T}$, hence the typical number of collisions per unit time experienced by this particle is $n\sigma_T\sqrt{T}$, and thus the mean free time is proportional to $1/n\sigma_T\sqrt{T}$. Following the definition of ℓ_0: $\tau = \ell_0/\sqrt{T}$ (this derivation is somewhat different from standard textbook derivations; the latter start with the derivation of an expression for the mean free path, which, as explained below, is valid for systems in equilibrium in frames of reference in which they are stationary). During a mean free time a "typical" particle traverses a distance that is determined by its *absolute speed*. This distance *is* the mean free path. Thus, the mean free path ℓ is given by $u^*\tau$, where u^* is the average speed of a particle, a quantity that depends on the frame of reference. Indeed, consider a gas in equilibrium viewed from a frame of reference in which the center of mass of the gas moves at a speed u, which is far larger than the thermal speed $\sqrt{T}$. In this case $u^* \approx u$ and the mean free path observed in this frame is $\ell \approx u\tau = u(\ell_0/\sqrt{T})$, i.e., it is much larger than ℓ_0. This observation would have been of philosophical value only, had it been applicable to systems in equilibrium alone. As shown below, it has measurable physical consequences in sheared systems.

Next, we return to the sheared granular system. The velocity $\vec{u}$ of a particle equals $\vec{u} = \gamma y \hat{x} + \vec{v}_{th}$, where $\vec{v}_{th}$ is the thermal component of the velocity (the average of $\vec{v}_{th}^2$ being T). Assuming statistical independence of the thermal and average velocities, the steady-state average of u^2 is given by $\gamma^2 y^2 + T$; hence, the typical speed u^* of a particle can be taken to be $u^* = \sqrt{\gamma^2 y^2 + T}$, which implies that the mean free path, as a function of the spanwise coordinate y is given by

$$\ell(y) = \tau\sqrt{\gamma^2 y^2 + T} = \sqrt{\gamma^2 y^2 + T}\,\frac{\ell_0}{\sqrt{T}}. \qquad (2)$$

At values of y at which the speed is subsonic (following the above consideration this happens when $|y|$ is less than

ℓ_0) one can neglect $\gamma^2 y^2$ with respect to T in Eq. (2), in which case $\ell \approx \ell_0$. However, when $|y| > |\ell_0|$, in particular when $|y| \gg \ell_0$, the thermal speed is far smaller than the average speed, and in this case

$$\ell(y) \approx \ell_0 \frac{\gamma|y|}{\sqrt{T}} = \frac{\sqrt{\epsilon}}{\sqrt{C}}|y| = \frac{\sqrt{\epsilon}}{\sqrt{C}}\frac{|y|}{\ell_0}\ell_0, \qquad (3)$$

i.e., the true mean free path is (much) larger than the equilibrium mean free path for $|y| \gg \ell_0$. Moreover, it is of macroscopic dimensions, being an $\mathcal{O}(1)$ quantity times $|y|$; in particular, if the systems are wide enough (in the spanwise direction) the mean free path can exceed the length of the system (in the streamwise direction). In addition, the angular distribution of the free paths becomes highly weighted towards the streamwise direction for $|y| \gg \ell_0$, since there the thermal velocity is small with respect to the average velocity (thus the direction of motion of a particle is close to $\hat{x}$).

The above results have been tested in MD simulations of a sheared system of 20 000 disks in a square enclosure (of unit side) using Lees-Edwards boundary conditions [3(a),8,11] in the y direction and periodic boundary conditions in the x direction. In these simulations $e = 0.6$, the shear rate is 100 inverse time units and the volume fraction ν is 0.05 (dilute system) or 0.4 (relatively dense system). Figure 1(A) depicts a scatter plot of the free paths (for the $\nu = 0.05$ system) arranged according to the y value of the beginning of each free flight. Figure 1(B) shows $\ell(y)$ (computed for each y by averaging over the free paths in a narrow strip around y) as a function of y
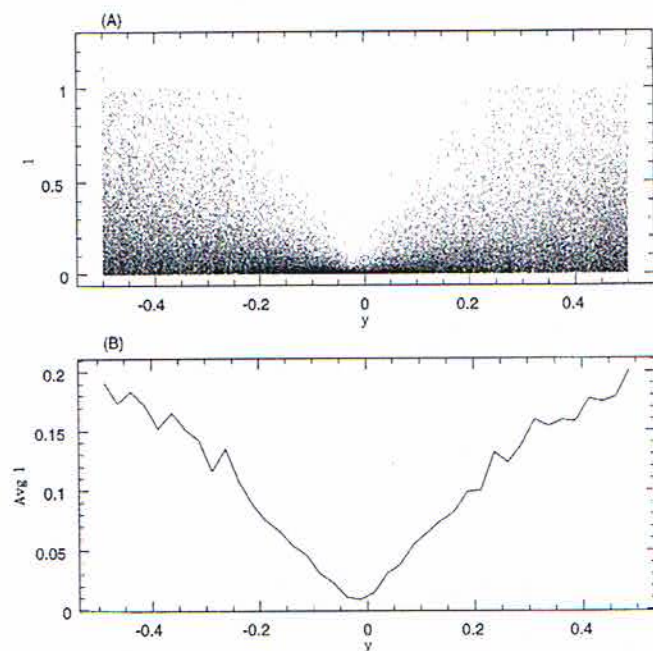

FIG. 1. (A) Scatter plot of the distribution of free paths ℓ versus y for a system in which the macroscopic velocity vanishes at the centerline ($y = 0$). Here, $\nu = 0.05$. (B) The mean free path (Avg ℓ) as a function of y.

(with $-0.5 < y < 0.5$). The linear dependence of $\ell(y)$ on $|y|$ is prominent. Notice that while the maximal value of $\ell(y)$ is 0.2, some free paths [cf. Fig. 1(A)] exceed the length of the system. Thus strong *nonlocality* is observed.

Another interesting, y dependent, property is exhibited by the rms of the *collisional pressure* fluctuations; Fig. 2 [the parameters are the same as in Fig. 1], depicts this quantity as a function of y (here the range of y is $0 < y < 1$). The solid line corresponds to $\vec{v} = \gamma(y - 0.5)\hat{x}$, the dashed line corresponds to $\vec{v} = \gamma(y - 0.25)\hat{x}$, and the dotted line corresponds to $\vec{v} = \gamma y \hat{x}$. In all three cases presented, the fluctuations are maximal at or near the stagnant line. The average collisional pressure is 4 orders of magnitude smaller than the peak value of the rms fluctuations. A possible explanation of this phenomenon is that in the deep supersonic domain there is an ordering of the particles (which violates "molecular chaos"), an expected phenomenon in "strongly sheared" systems (cf., e.g., [2(a),12]); this order must also be long ranged, as the free paths are long. In the subsonic domain such positional order is essentially absent (and the assumption of "molecular chaos" holds). The width of the peaks in Fig. 2 is about an order of magnitude larger than a naive estimate of the width of the subsonic strip; we suspect that this broadening is related to the diffusion of fluctuations. Incidentally, since the simulation employs a Lees-Edwards boundary condition, the above result signals a breakdown of the (normally assumed) homogeneity of such a system. One could say that homogeneity is broken when the mean free path is comparable with the size of the system (i.e., the system can differentiate between different values of y). This may also imply that the use of dissipative devices to absorb energy in simulations of elastic sheared systems may produce undesired results due to the above phenomenon. Figure 3 depicts a similar result to that shown in Fig. 2 for $\nu = 0.4$ (the stagnant line being at $y = 0.5$). While the free paths may not be as large for a denser system as in the dilute limit, they are still far larger than the corresponding equilibrium mean free paths, hence this property is of rather general nature. Figure 4 shows a similar effect in an elastic system prepared at a low enough temperature (with respect to the square of the maximal mean velocity). All other parameters are the same as in Fig. 2. Panel 4A corresponds to an early time (30 collisions per particle after initiation) and panel 4B corresponds to a later time (100 collisions per particle after initiation). Since the system is elastic, it heats up with time until it becomes entirely subsonic, in which case the effect disappears. In contrast, an inelastic sheared system possesses an internal energy sink and it reaches a steady state, in which the effect stays put.

Another phenomenon, which is common to granular and elastic fluids, but is enhanced in the realm of the former, is the "normal stress difference" [2(f),2(g),10]. It can be shown that this effect follows from the Burnett correction in the framework Chapman-Enskog expansion [2(f),2(g),10]. The anisotropy of the normal stress is usually negligibly small in molecular systems (in air at STP conditions the degree of anisotropy of the normal stress is 10^{-20}) and rather prominent [$\mathcal{O}(1)$] in granular systems (a result that can be obtained by substituting the above expression for T in the Burnett formula for the stress tensor). Only in highly sheared dilute molecular systems it is possible to observe normal stress differences; as explained above, granular systems are always "highly sheared" and thus they can serve as testing grounds for effects such as the Burnett effect which is difficult to measure otherwise.
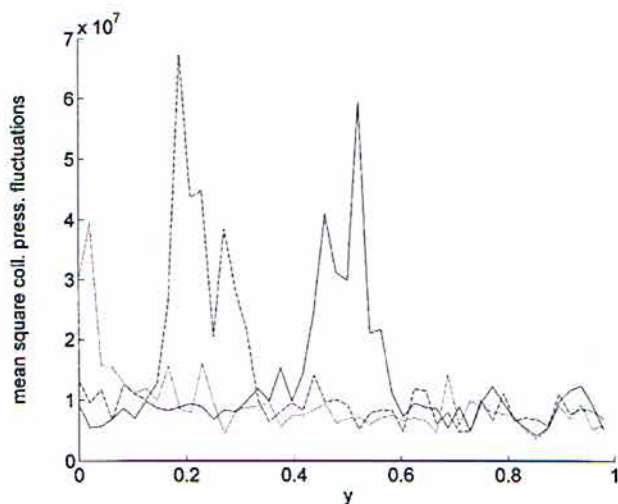
FIG. 2. The mean square fluctuaton, or variance, of the collisional pressure as a function of y (averaging is performed over narrow horizontal strips). The three curves correspond to different choices of the stagnant line (see text).
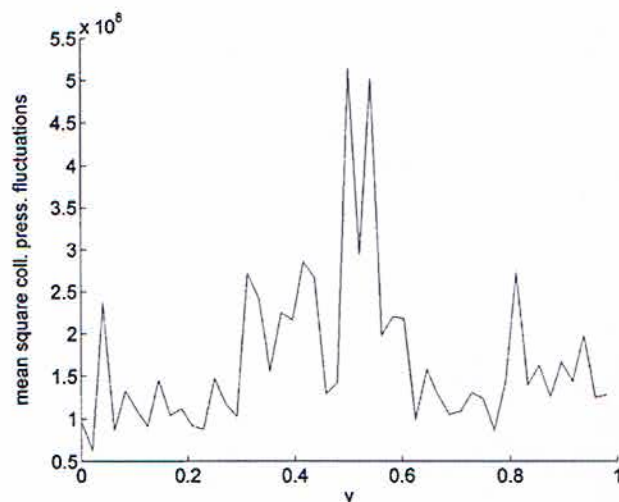
FIG. 3. The variance of the collisional pressure as a function of y for $\nu = 0.4$ (the other parameters being as in the previous plots). The macroscopic velocity vanishes at $y = 0.5$.
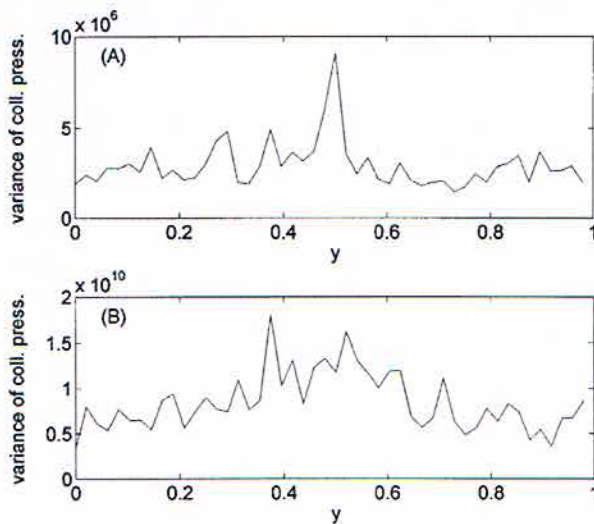
FIG. 4. (A) The variance of the collisional pressure as a function of the y coordinate for an *elastic* system whose macroscopic velocity vanishes at $y = 0.5$. Here $\nu = 0.05$ and $N = 20\,000$. The initial temperature of the system is adjusted so that the thermal speed is much smaller than the magnitude of the macroscopic velocity near the boundaries of the system (the average temperature in the system is 0.1, while the shear rate is 100). (B) The same system as in (A) at a later time when the temperature is higher due to heating by the shear.

Another manifestation of the mesoscopic nature of granular systems is the dependence of their constitutive relations on the coarse graining scales [13(c)] and the strong fluctuations of stress [13] observed in these systems. Still another mesoscopic property of granular systems has been discovered [14] in free (or unforced) systems: It turns out that the latter systems exhibit enhanced long-range velocity correlations. We wish to add that static and quasistatic granular systems exhibit (micro)structures (such as arches and stress chains) which can span the entire "width" of the system, and they should be considered to be mesoscopic as well.

As has been the experience in mesoscopic solid state physics, mesoscopic systems exhibit many different physical properties than macroscopic ones. In particular, average or averaged properties may obscure typical effects in such systems, and thus the process of (ensemble) averaging should be approached with care. Large mean free paths, as discussed above, indicate that the effective interactions (say, in a coarse-grained description) may be long ranged and that the effect of boundaries may be of greater importance in granular systems than in corresponding elastically colliding systems.

We believe that derivations of equations of motion for granular systems should proceed with these findings in

mind; among other things, one needs to account for the violation of molecular chaos (e.g., develop a theory or model for the two particle distribution function, f_2, cf., e.g., [2(a),12], when a kinetic approach is employed). When nonlocality is prominent (and especially when transient and/or strongly inhomogeneous systems are considered) nonlocal equations may be required; alternatively, it may be possible to use an extended set of hydrodynamic variables to restore locality (electrostatics is long ranged but Maxwell's equations, which account for a finite speed of light, are local).

[1] C. S. Campbell, Annu. Rev. Fluid Mech. **22**, 57 (1990).
[2] Cf., e.g., (a) J. T. Jenkins and S. B. Savage, J. Fluid Mech. **130**, 187 (1983); (b) J. T. Jenkins and M. W. Richman, Phys. Fluids **28**, 3485 (1985); (c) C. K. K. Lun and S. B. Savage, J. Appl. Mech. **154**, 47 (1987); (d) C. K. K. Lun, J. Fluid Mech. **223**, 539 (1991); (e) A. Goldshtein, and M. Shapiro, J. Fluid Mech. **282**, 75 (1995); (f) I. Goldhirsch, N. Sela, and S. H. Noskowicz, Phys. Fluids **8**, 2337 (1996); (g) N. Sela and I. Goldhirsch, J. Fluid Mech. **361**, 41 (1998), and references therein.
[3] (a) M. A. Hopkins and M. Y. Louge, Phys. Fluids A **3**, 47 (1991); (b) I. Goldhirsch and G. Zanetti, Phys. Rev. Lett. **70**, 1619 (1993); (c) I. Goldhirsch, M-L. Tan, and G. Zanetti, J. Sci. Comp. **8**, 1 (1993).
[4] M-L. Tan, Ph.D. thesis Princeton University, 1995.
[5] (a) R. Jackson, C-H. Wang, and S. Sundaresan, J. Fluid Mech. **308**, 31 (1996); (b) M. Alam and P. R. Nott (to be published).
[6] S. McNamara and W. R. Young, Phys. Fluids A **4**, 496 (1992).
[7] N. Sela and I. Goldhirsch, Phys. Fluids **7**, 507 (1995).
[8] (a) M-L. Tan and I. Goldhirsch, Phys. Fluids **9**, 856 (1996); (b) I. Goldhirsch and M-L. Tan, Phys. Fluids **8**, 1752 (1996).
[9] P. K. Haff, J. Fluid Mech. **134**, 401 (1983).
[10] I. Goldhirsch and N. Sela, Phys. Rev. E **54**, 4458 (1996).
[11] A. W. Lees and S. F. Edwards, J. Phys. C **5**, 1921 (1972).
[12] J. F. Lutsko, Phys. Rev. Lett. **77**, 2225 (1996).
[13] (a) C. O'Hern, B. Miller, and R. P. Behringer, Phys. Rev. Lett. **77**, 3110 (1996); (b) S. B. Savage, in *Disorder and Granular Media*, edited by D. Bideau and A. Hansen, (North-Holland, Amsterdam, 1993) Vol. 2; (c) B. J. Glasser and I. Goldhirsch (to be published).
[14] T. P. C. van Noije, M. H. Ernst, R. Brito, and J. A. G. Orza, Phys. Rev. Lett. **79**, 411 (1997).