Close-Packed Floating Clusters: Granular Hydrodynamics Beyond the Freezing Point?

Baruch Meerson,[1] Thorsten Pöschel,[2] and Yaron Bromberg[3]
[1]*Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem 91904, Israel*
[2]*Institut für Biochemie, Charité, Monbijoustrasse 2, 10117 Berlin, Germany*
[3]*School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel*
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Monodisperse granular flows often develop regions with hexagonal close packing of particles. We investigate this effect in a system of inelastic hard spheres driven from below by a "thermal" plate. Molecular dynamics simulations show, in a wide range of parameters, a close-packed cluster supported by a low-density region. Surprisingly, the steady-state density profile, including the close-packed cluster part, is well described by a variant of Navier-Stokes granular hydrodynamics (NSGH). We suggest a simple explanation for the success of NSGH beyond the freezing point.

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Continuum modeling of flow of macroscopic grains remains a challenge [1–5]. The best known version of continuum theory here is the Navier-Stokes granular hydrodynamics (NSGH) for a system of inelastic hard spheres [6,7]. The applicability of NSGH is limited to *rapid* granular flows [8]. By definition, these flows are dominated by binary particle collisions, while multiparticle interactions are negligible. Despite this drastic simplification, the validity of the NSGH demands several additional assumptions, some of which can be rather stringent. Under the *molecular chaos* assumption, the NSGH is derivable systematically from more fundamental kinetic equations for inelastic hard spheres [7,9,10]. Going over from kinetic equations to hydrodynamics, one should assume scale separation: The mean-free path of the particles should be much smaller than the characteristic length scale, and the mean time between two consecutive collisions much shorter than any characteristic time scale, described hydrodynamically. The inelasticity of particle collisions brings immediate complications. Already at moderate inelasticity $q = (1 - r)/2$ (where r is the coefficient of normal restitution of the particle collisions), the scale separation may break down, even in the low-density limit [11,12]. The normal stress difference [12] and deviations of the particle velocity distribution [11,13] from the Maxwell distribution also become important for moderately inelastic collisions. Therefore, the NSGH is expected to be accurate only for small inelasticity, $q \ll 1$.

Additional complications appear at large densities. Here the *molecular chaos* assumption breaks down, already for *elastic* hard spheres, when the packing fraction approaches the freezing point value $\phi_f \simeq 0.49$ (in three dimensions) or 0.69 (in two dimensions). As the kinetic equations become invalid, the constitutive relations (CRs), necessary for the closure of hydrodynamics, are not derivable from first-principles anymore. This is the regime considered in this work. We consider an ensemble of monodisperse, nearly elastic hard spheres in such conditions that the standard NSGH [6,7] breaks down because of large densities, *not* large inelasticity. Our main objective is to check whether a variant of NSGH can still be used in an extreme case when the packing fraction is close to the maximum possible value, corresponding to hexagonal packing of spheres.

We will focus on granular materials fluidized by a rapidly vibrating bottom plate in a gravity field. Vibrofluidized granular materials exhibit fascinating pattern-formation phenomena that have attracted much recent interest [14]. In the high-frequency and small-amplitude limit of vibrofluidization, there is no direct coupling between the vibration and the collective granular motion. In a simplified description of this limit, one specifies a constant granular temperature at an immobile bottom plate. In a wide range of parameters, molecular dynamics (MD) simulations of this system show an (almost) close-packed cluster of particles, floating on a low-density fluid (see below). The close-packed floating cluster is an extreme form of the *density inversion*, a phenomenon well known in vibrofluidized granular materials. Lan and Rosato [15] were apparently the first to observe density inversion in three-dimensional MD simulations. Kudrolli *et al.* [16] observed a floating cluster in a reduced-gravity experiment: a slightly tilted two-dimensional system of steel spheres rolling on a smooth surface and driven by a vibrating side wall. Recently, a pronounced density inversion has been observed, in two- and three-dimensional vibrofluidized granular beds, by Wildman *et al.* [17].

An accurate hydrodynamic description of almost close-packed floating clusters seems a very difficult task, as the packing fraction here is far beyond the freezing point. Still, we will attempt to use a variant of NSGH for this purpose. This attempt will prove successful, and we will suggest an explanation. Here is the model problem we are working with. Let $N \gg 1$ nearly elastic hard spheres of diameter d and mass m move in a two-dimensional box with periodic boundary conditions in the x direction (period L_x) and infinite height. The driving base is located at $y = 0$. Gravity acceleration g acts in the negative

y direction. Upon collision with the base, the particle velocity is drawn from a Maxwell distribution with temperature T_0 (which is measured in the units of energy). The kinetic energy of the particles is being lost by inelastic hard-core collisions parametrized by a constant inelasticity parameter $q \ll 1$. Figure 1 shows a typical snapshot of an almost close-packed floating cluster, observed in an event-driven MD simulation of this system. Hexagonal packing is apparent in Fig. 1 [18].

Going over to a hydrodynamic description of zero-mean-flow steady states, we introduce coarse-grained fields: the particle number density $n(y)$, the granular temperature $T(y)$, and the pressure $p(y)$. The maximum possible value of n is the hexagonal close-packing value $n_c = 2/(\sqrt{3}d^2)$. A laterally uniform steady state is described by the momentum and energy balance equations:

$$\frac{dp}{dy} + mng = 0, \qquad \frac{d}{dy}\left(\kappa \frac{d}{dy} T\right) - I = 0, \tag{1}$$

where κ is the thermal conductivity and I is the energy loss rate by collisions. To proceed, we need CRs: an equation of state (EOS) $p = p(n, T)$ and relations for κ and I in terms of n and T. First-principles CRs are available only in the low-density limit (well below the freezing point). Grossman *et al.* [11] derived a set of approximate *global* CRs for a version of NSGH that assumes nearly elastic collisions, but is not limited to low densities. Grossman *et al.* employed free volume arguments in the close vicinity of the hexagonal packing and suggested simple interpolations between the hexagonal-packing limit and low-density limit. These interpolations include two fitting constants α and γ (see below). The optimum values of these constants were found by a comparison with MD simulations of a system of inelastic hard spheres driven by a thermal wall at zero gravity [11].

Notice that, prescribing global CRs of *any* type, one grossly simplifies the delicate issue of phase coexistence that is expected to occur here in close analogy to the system of *elastic* hard spheres [19,20]. Still, we will use the simple CRs [11] to attempt a NSGH description of the close-packed floating clusters. In our notation, the CRs [11] read

$$p = nT\frac{n_c + n}{n_c - n}, \qquad \kappa = \frac{\mu n(\alpha l + d)^2 T^{1/2}}{m^{1/2} l}, \tag{2}$$

and $I = 4(\mu/\gamma l) q n m^{-1/2} T^{3/2}$. Here l is the mean-free path of the grains,

$$l = \frac{1}{\sqrt{8} n d}\frac{n_c - n}{n_c - an}, \tag{3}$$

and $a = 1 - (3/8)^{1/2}$. According to Grossman *et al.*, $\alpha = 1.15$ and $\gamma = 2.26$. We adopted this value of γ, but found better agreement between the hydrodynamics and MD (see below) for $\alpha = 0.6$. The value of $\mu = \mathcal{O}(1)$ drops out from the steady-state problem.

Recently, a more accurate global EOS $p = p(n, T)$ has been suggested [20]. Still, in the absence of comparably accurate relations for κ and I, employing a more accurate EOS in Eqs. (1) would be an excess of accuracy.

Equations (1) should be complemented by three boundary conditions. One of them is $T(0) = T_0 = \text{const}$. Integrating the first of Eqs. (1) over the height from 0 to ∞ and using the conservation of the total number of particles, $\int_0^\infty n(y)\, dy = N/L_x = \text{const}$, we obtain the second boundary condition: $p(0) = mgN/L_x$. The third one is a zero heat flux (that is, a constant granular temperature) at $y \to \infty$ [21,22]. In practice, one should use the shooting method, varying the heat flux $-\kappa\, dT/dy$ at $y = 0$ until the third condition is satisfied with desired accuracy.

Let us measure y in units of the gravity length scale $\lambda = T_0/(mg)$ (note that λ/d should be large enough to fluidize the granulate at the bottom). We rewrite Eqs. (1), in scaled form, as three first-order equations:

$$\frac{dP}{dy} + \frac{1}{Z} = 0, \qquad \frac{d\Phi}{dy} = \Lambda Q(Z) P^{3/2}, \tag{4}$$

$$\frac{d}{dy}[F_2(Z) P^{3/2}] = \frac{\Phi}{F_1(Z)}. \tag{5}$$

Here $Z(y) = n_c/n(y)$ is the inverse scaled density, $P(y) = p(y)/(n_c T_0)$ is the scaled pressure, and $-\Phi(y)$ is the scaled heat flux. The functions F_1, F_2, and Q are

$$F_1(Z) = \frac{[\alpha Z(Z-1) + \sqrt{32/3}(Z-a)]^2}{(Z-a)(Z-1)Z^2},$$

$$F_2(Z) = \frac{(Z-1)^{3/2} Z^{3/2}}{(Z+1)^{3/2}},$$

$$Q(Z) = \frac{(Z-a)(Z-1)^{1/2}}{(Z+1)^{3/2} Z^{1/2}}.$$

Finally, $\Lambda = (64/\gamma)\, q\, (\lambda/d)^2$ and $f = (\sqrt{3}\, d^2 N)/(2\lambda L_x)$ are two scaled governing parameters. Parameter Λ

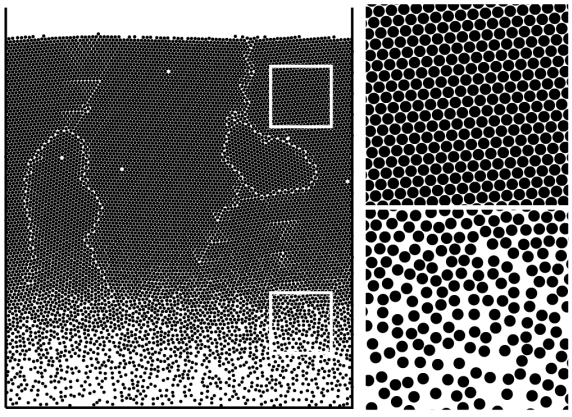

FIG. 1. A snapshot showing the close-packed floating cluster. The parameters are $N = 10^4$, $L_x = 100$, $T_0 = 2\sqrt{3} \times 10^2$, $r = 0.988\,15$, and $g = d = m = 1$. The figures on the right are magnifications of the indicated areas.

controls the relative role of the inelastic heat losses and heat conduction, while f is the *effective* area fraction of the grains (it can be smaller or greater than unity). The boundary conditions at the base become

$$P(0) = f \quad \text{and} \quad Z(0) = \frac{1 + f + (1 + 6f + f^2)^{1/2}}{2f}. \quad (6)$$

Using the hydrodynamic formulation, we first determine the condition for a density inversion. At too small inelasticity q (the rest of the parameters fixed), there is no density inversion, such as in the elastic case $q = 0$, where $T(y) = \text{const}$ and $n(y)$ goes down monotonically. At large enough q, the temperature $T(y)$ drops rapidly with y. To maintain the hydrostatic balance, $n(y)$ should *increase* with the height, on an interval of heights between $y = 0$ and the location of the density maximum $y = y_c$. In our hydrodynamic formulation, the density inversion occurs, at fixed f, when $\Lambda > \Lambda_c$, where $\Lambda_c = \Lambda_c(f)$ is a critical value. The density inversion is born at $y = 0$: $\Lambda = \Lambda_c(f)$ corresponds to dn/dy vanishing at $y = 0$. Using this condition together with Eqs. (4)–(6), we obtain

$$\Phi(0) = -\frac{3}{2} f^{1/2} \frac{F_1[Z(0)]F_2[Z(0)]}{Z(0)}. \quad (7)$$

For a given f, Eq. (7) prescribes the heat flux at the base $y = 0$ that corresponds to the birth of the density inversion. Using shooting, we determine, for every f, the critical value $\Lambda_c(f)$, demanding that the temperature approaches a constant value at large heights. This procedure yields the critical curve $\Lambda = \Lambda_c(f)$ shown in Fig. 2. The density inversion occurs above the critical curve $\Lambda = \Lambda_c(f)$, and it is more and more pronounced, at fixed f, as Λ grows. Figure 3(a) shows the density profiles at $f = 0.25$ and three different values of $\Lambda > \Lambda_c$. One can see that, at large enough Λ, a hexagonally packed cluster appears. The scaled parameters $\Lambda = 20\,015$ and $f = 0.25$ correspond to the snapshot shown in Fig. 1. Noticeable is a steep (exponential) density fall at the upper boundary of the cluster; the exponent corresponds to the very low temperature there. Figure 3(b) shows the scaled temperature for these three cases.

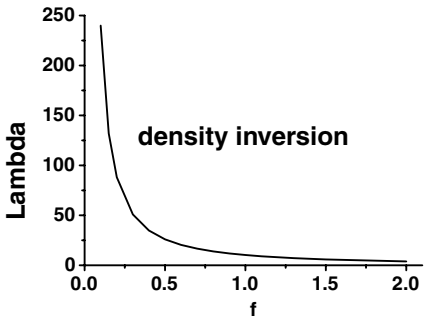

FIG. 2. The critical value Λ_c of the hydrodynamic inelasticity parameter Λ for a density inversion versus the effective area fraction f. At small f one obtains $\Lambda_c \sim f^{-2}$.

Figure 4 compares the density profiles, predicted by this hydrodynamics (solid curves), with the profiles found in MD simulations with $N = 10^4$ particles of diameter $d = 1$, mass $m = 1$, and $r = 0.988\,15$. The (periodic) box width is $L_x = 100$, the gravity acceleration $g = 1$. The MD simulations were done for three different values of the temperature at the base: $T_0 = 100\sqrt{3}$, $200\sqrt{3}$, and $300\sqrt{3}$. The hydrodynamic parameters in these three cases are $f = 0.5$ and $\Lambda = 5004$, $f = 0.25$ and $\Lambda = 20\,015$, and $f = 0.167$ and $\Lambda = 45\,036$, respectively. One can see that the agreement between hydrodynamics and MD simulations is surprisingly good.

An additional argument in favor of hydrodynamics follows from the dimensional analysis of the problem. The full set of parameters includes d, m, r, g, T_0, N, and L_x. One can always choose $d = m = g = 1$, so there are actually *four* independent parameters. This number reduces to *three* for an x-independent steady state, as N and L_x enter the problem only through N/L_x. It is crucial that hydrodynamics further reduces the number of parameters: now only *two* scaled parameters Λ and f appear. This prediction is very robust, as it is independent of the particular form of the functions F_1, F_2, and Q (and of the values of α and γ). We verified this prediction in MD simulations by varying N, T_0, and r, but keeping $\Lambda = 20\,015$ and $f = 0.25$ constant. After rescaling the coordinate y by $\lambda = T_0/(mg)$, the resulting density profiles almost coincide with each other (see Fig. 5). A small shift between the two profiles, observed in Fig. 5, is apparently caused by small vertical oscillations of the granulate. In this example, the oscillation amplitude is about three particle diameters [26].

As already mentioned, the global CRs completely ignore the issue of coexistence, beyond the freezing point, of different phases of the granulate: the liquidlike phase, the random close-packed phase, etc. So why are they so successful? We believe the reason is the following. The vibrofluidized steady state, considered in this work, has a zero mean flow. Therefore, the viscosity terms in the hydrodynamic equations vanish. This fact is not merely a technical simplification. The shear viscosity of granular flow is finite in the liquidlike phase, and *infinite* in the (multiple) domains of the random close-packed phase.

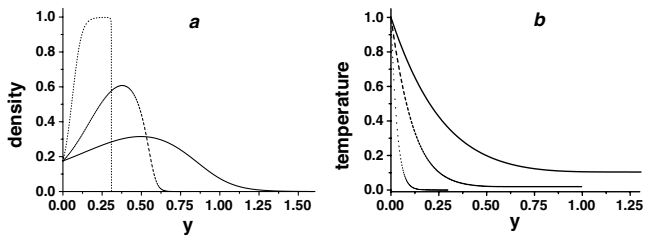

FIG. 3. Scaled density (a) and temperature (b) versus the scaled height y for $f = 0.25$ and $\Lambda = 500$ (solid lines), 2000 (dashed lines), and 20 015 (dotted lines). The dotted lines correspond to the snapshot shown in Fig. 1.

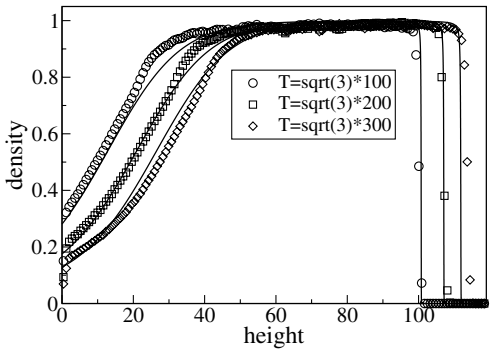

FIG. 4. Scaled density versus the height y as predicted by hydrodynamics (solid curves) and observed in MD simulations, for three different values of the temperature at the base. The parameters are described in the text. The height is measured here in units of d.

The effective *total* viscosity of the system is expected to *diverge* when the coarse-grained density slightly exceeds the freezing density. This invalidates *any* NSGH for sufficiently dense flows, and necessitates the introduction of an order parameter and a different type of the stress-strain relation into the theory (cf. Ref. [3]). Luckily, these complications do not appear for a zero-mean-flow state. Indeed, the EOS, heat conductivity, and inelastic heat loss rate do not exhibit any singularity around the freezing point, and all the way to the hexagonal close packing. Therefore, the NSGH remains reasonably accurate far beyond the freezing point. A future work should address the important question about the range of applicability of the NSGH (actually, of any binary collision model) for solid yet vibrated phase, versus the granular statics approach.

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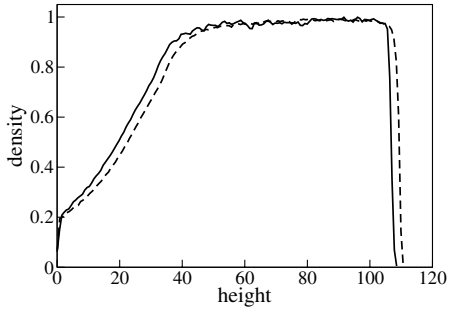

FIG. 5. Checking the hydrodynamic scaling. The solid line corresponds to the MD simulation shown in Fig. 1. The dashed line corresponds to another simulation: with $N = 2 \times 10^4$, $L_x = 100$, $T_0 = 4\sqrt{3} \times 10^2$, $r = 0.997\,051$, and $g = d = m = 1$. For the dashed line, the height y is shrunk by a factor of 2.

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