Compaction in Granular Solid Hydrodynamics

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Compaction is considered and embedded into broader granular behavior. Reversible compaction is related to the pressure exerted by agitated grains, a quantity relevant to dense flow. Irreversible compaction is derived from the loss of elastic deformation, the physics behind elasto-plastic flows.

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Granular compaction – density increase by gentle perturbation of the grains – is a ubiquitous phenomenon, relevant in many contexts such as efficient packaging, or when establishing the structural stability of off-shore windmills that are subject to continual surfs. Compaction has been studied widely but is not yet fully understood, see the review \cite{1}, which carefully considers the phenomenon and cites many useful references. There are two compaction branches: In the irreversible one, the density increases monotonically; in the reversible one, one observes compaction and loosening, depending on whether the perturbation is weakened or strengthened.

Granular solid hydrodynamics (GSH) is a set of partial differential equations \cite{2} constructed to model granular medium in all its facets, though qualitatively at present. It was first employed to calculate static stress distribution for various geometries, including sand piles, silos, and point load, achieving results in agreement with observation \cite{3}. It was then employed to consider slowly strained granular solid \cite{4}, and found to yield response envelopes similar to those from the hypoplastic theory \cite{5}. Recently, the critical state – generally considered a hallmark of granular behavior \cite{6} was identified as a steady-state, elastic solution of GSH \cite{7}. Uniform dense flow, fluidization and jamming were also considered \cite{8}, finding broad agreement to experiments, and more narrowly focused existing theories \cite{3,10}. Finally, the velocity of elastic waves were calculated as a function of the stress \cite{11}.

Here, we use GSH to consider compaction. At present, “geometric frustration models” \cite{1} are employed to account for the irreversible branch, and the Edward entropy $S_{Ed}$ \cite{12} for the reversible one. Both are again narrowly focused. Moreover, the notion of $S_{Ed}$ entails hidden assumptions that merit closer scrutiny.

Derived in compliance with general principles, GSH consists of:

- five conservation laws for the density respectively of the energy $\rho w$, mass $\rho$, and momentum $\rho v_{i}$,
- an evolution equation for the elastic strain $\varepsilon_{ij}$,
- balance equations for two entropy densities, the true and the granular one, $s$ and $s_{g}$.

Two entropies are necessary because of granular media’s \textit{two-stage irreversibility}:

Macrosopic energy, kinetic and elastic, dissipates into mesoscopic, inter-granular degrees of freedom, mainly granular jiggling and the collision-induced, fluctuating elastic deformation. After a characteristic time, the energy degrades further into microscopic, inner-granular degrees of freedom, especially phonons. The two entropies account respectively for the energy of the meso- and microscopic degrees of freedom.

Now a brief presentation of the GSH-equations, tailored for the purpose of granular compaction. (See \cite{2} for the complete theory.) An important quantity of GSH is the energy density $w$, that in its local rest frame is a function of the above listed four variables, $w_{0}(\rho, \varepsilon_{ij}, s_{g}, s)$. The conjugate variables:

- true temperature $T \equiv \partial w_{0}/\partial s$,
- elastic stress $\sigma_{ij} \equiv -\partial w_{0}/\partial \varepsilon_{ij}$,
- chemical potential $\mu \equiv \partial w_{0}/\partial \rho$,
- granular temperature $T_{g} \equiv \partial w_{0}/\partial s_{g}$, and gaseous pressure $P_{T} \equiv \mu p + s_{g} T_{g} + s T - w_{0}$, are given once $w_{0}$ is.

The Cauchy stress is given as $(1-\alpha)\pi_{ij} + P T_{ij}, [\alpha$ is explained below Eq (2),] of which only the trace is needed here,

$$P = (1-\alpha)\pi_{\ell\ell}/3 + P_{T}, \quad (1)$$

In GSH, the elastic strain $\varepsilon_{ij}$ is taken as the portion of the strain that deforms the grains and leads to reversible storage of elastic energy. The energetically indifferent rest, such as rolling and sliding, is the plastic portion. Again, only $\Delta \equiv -\varepsilon_{\ell\ell}$ is relevant. Its evolution, taken as

$$\partial_{t} \Delta + (1-\alpha)\varepsilon_{\ell\ell} = -\Delta/\tau, \quad 1/\tau = \lambda T_{g}, \quad (2)$$

accounts for two facts: First, only the portion $1-\alpha$ of the strain rate $\dot{\varepsilon}_{ij} \equiv \frac{1}{2}(\nabla_{i} v_{j} + \nabla_{j} v_{i})$ deforms the grains, changing $\Delta$ and the energy $w_{0}(\Delta)$ – the rest is plastic. That the same $\alpha$ appears in Eq (1) is a result of the Ousager relation. But it may also be understood via an analogy to a bicycle gear shift: A bigger $\alpha$ implies more pedaling at reduced torque, both with the same factor. Second, when grains jiggle and $T_{g}$ is finite, the grains briefly lose contact with one another. The result is a slow relaxation of granular deformation – as expressed by $\Delta/\tau$. The full tensorial version of Eq (2) is closely related to hypoplasticity, and yields a realistic account of the elasto-plastic dynamics of granular media, see \cite{4}.

Because Eqs (12) are fairly general, it is the energy density $w$ that encodes the material-specific information. The expression we consistently employed to study static
stress distribution and hypoplastic deformation is: \( w_0 = w_1(u_{ij}, \rho) + w_2(s_g, \rho) + w_3(s, \rho) \), where \( w_1 \) is the macroscopic, \( w_2 \) the mesoscopic, and \( w_3 \) the microscopic contributions. We take them (if without shear strain and away from the virgin consolidation line) as
\[
w_1(u_{ij}, \rho) = B \Delta^{2.5}/2.5, \quad w_2(s_g, \rho) = s_g^2/(2\rho b), \quad (3)
\]
and \( w_3 = cp/m \). Explanations: • The elastic energy \( w_1 \) contains the lowest order term in \( \Delta \). Being 2.5 rather than two, the exponent accounts for the Hertz-like contacts between the grains and the Coulomb yield \([13]\). As granular systems are slightly stiffer at higher densities, the elastic coefficient \( B \) grows slowly and monotonically with \( \rho \). In the present context, however, we may approximate \( B \) as a constant – of around 8 GPa for river sand and 7 GPa for glass beads \([3]\) – because the density dependence of \( w_1 \) is the dominant one. • \( w_2 \) contains the lowest order term in an expansion in \( s_g \). The exponent is two because \( w_3 \) has a minimum at \( s_g = 0 \). The density dependence of \( b(\rho) = b_0(1-\rho/\rho_{cp})^a \), with \( a = 0.1 \), is chosen to reproduce the observed, volume-dilating pressure contribution from agitated grains, \( P_F \sim w_2/(\rho_{cp} - \rho) \), that diverges at the random close packing density \( \rho_{cp} \), see \([10]\). The value for the constant \( b_0 \) depends on the scale we choose for \( T_g \). Requiring (somewhat arbitrarily but adhering to convention) that \( \frac{1}{2} k_b T_g \) is, in the rarified limit of granular gas, the kinetic energy of a single grain, we find \( b_0 \approx 10^{-25} \text{J}/(\text{Kg} \cdot \text{Kelvin}^2) \). Finally, \( c, m \) are respectively the average internal energy and mass per grain. Being linear in \( \rho \), \( w_3 \) does not contribute to \( P_F \) and is not relevant for compaction. Given Eq (3), the associated pressure may be calculated from Eq (11) as
\[
P = (1 - \alpha)B \Delta^{1.5} + \alpha p^2 b T_g^2/[2(\rho_{cp} - \rho)]. \quad (4)
\]
Eqs (24) are all one needs to account for both branches of compaction. This ends the presentation of GSH.

Assuming constant \( T_g, P \) while evaluating Eqs (24) simplifies the calculation and focuses the attention on the universal aspects of granular compaction. The underlying physics is: At given \( T_g \), the elastic deformation \( \Delta \) relaxes according to Eq (2). To maintain the constant pressure \( P \), the density must increase as prescribed by Eq (1). This is the irreversible branch of compaction. Relaxation stops at \( \Delta = 0 \), when the pressure is purely temperature generated, \( P = P_F = \alpha p^2 b T_g^2/[2(\rho_{cp} - \rho)] \), and the density assumes the final value \( \rho_f \),
\[
2\rho_{cp}/\rho_f = 1 + \sqrt{1 + 2ab_0 \rho_{cp} T_g^2/P}, \quad (5)
\]
obtained by taking \( b = \text{const} \). Modifying the magnitude of perturbation now, \( \rho_f \) will adjust – becoming larger the smaller \( T_g \) is. This further density modification is of thermodynamic origin and reversible.

Changing \( T_g \) midway, with \( \Delta \) still finite, leads to a change in \( \Delta \) as well, if \( P \) of Eq (4) is given. This disrupts the relaxation of \( \Delta \), in essence resetting its initial condition – as observed in \([14]\) and taken as a memory effect. (Generally speaking, “memory” is usually a result of hidden variables: When all variables have the same values, but the system still behaves differently, we speak of memory, or history-dependence. But an overlooked variable that has different values for the two cases will naturally explain the difference. The manifest and hidden variables here, clearly, are \( \rho \) and \( \Delta \), respectively.)

\( T_g \) is of course not always constant, but neither does it have to be. It is constant for constant shear, or sound waves that oscillates faster than \( T_g \) relaxes; it is not for tapping or sinusoidal shear, which give rise to periodic flare-ups of \( T_g \). Yet because compaction is the result of tiny plastic deformation accumulated over many periods, it is the temperature (\( T_g \)), averaged over many periods, that is relevant. On this longer time scale, constant \( T_g \) is an appropriate approximation. Also, the pressure \( P \) is frequently nonuniform, such as when grains are filled in an open vessel, though it is still given. Being local expressions, all above equations remain valid, and we can read off say \( \rho_f(r) \) from Eq (6) if \( P(r) \) is known.

In a complete theory, one needs to go beyond the universal aspects of compaction, and account for how \( T_g \) is excited by the given perturbation and related to its amplitude. We shall not do this here, only note that one can in principle achieve this by solving GSH for given boundary conditions. These include oscillatory shear, intense sound waves, periodic liquid injections, and horizontal tapping in various geometries, but unfortunately not vertical tapping, because particles flying ballistically part of the time is not a phenomenon amenable to any hydrodynamic description.

The simplest perturbation to account for is oscillatory shear. As long as the yield surface is not breached, and the frequency of oscillation small compared to the relaxation rate of \( T_g \), one obtains (from the balance equation for \( s_g \) a quasi linear relationship between \( T_g \) and the strain rate, \( T_g \sim \sqrt{\nu_{ij}\nu_{ij}} \), see \([2, 4]\). Liquid injection is similar but involves spatial variation. A stationary sound field, if uniform, is again simple, as it maintains a constant \( T_g \) via the strain rate that accompanies any sound. When the sound is turned off, \( T_g \) is quickly gone. This increases \( \Delta \) to maintain the pressure, and quenches the density at the value characteristic of \( T_g \). This is why we may stop the perturbation to measure the density. (During the quench, there is an elastic density change that is negligibly small, but may be accounted for anyway.)

If a sand-filled vessel is tapped horizontally, the blow generates a pulse of sound waves. As the pulse propagates through the medium and reflects multiply off the wall, it becomes a more or less uniform sound field – of brief duration but still with an accompanying \( T_g \) that is monotonically related to the strength of the blow. And the quenched density measured after the tap is the one characteristic of this \( T_g \). All these may in principle be evaluated employing GSH. Tapping the vessel vertically,
circumstances are somewhat different, as a fraction of the particles will fly ballistically some of the time. During the flight, the grains will keep their kinetic energy, but gradually lose $\Delta$: When the squeeze from the neighboring grains is suddenly gone after the tap, each grain oscillates around its free shape with a diminishing amplitude. This is puzzling, since compaction seems a succession of brief $\Delta$-relaxation, each picking up the work where the last one left it, and it is unclear why this process is not disrupted by $\Delta$ vanishing repeatedly. A conceivable answer is that these taps are not that strong.

Newer evidence [12] shows that the control parameter of the reversible branch is not the acceleration $\Gamma$, but the initial velocity $t\Gamma$, with $t$ the tap duration. This is consistent with GSH, because with $w_2 \sim s^2 \sim T_g^2 \sim (t\Gamma)^2$, Eq (4) indeed gives $\rho_f$ as a function of $t\Gamma$.

Eqs (23) are now evaluated with $T_g, P$ taken as constants. Starting from Eq (2) and the continuity equation, $\partial_t \rho/\rho = -v\xi$, we obtain $(1-\alpha)\partial_t P/\rho = \partial_t \Delta / \tau$. From this, we eliminate either $\partial_t \Delta$ or $\partial_t \rho$ by employing $\partial_t P(\Delta, \rho) = 0$, arriving respectively at

$$\partial_t \Delta = -\Delta / \tau_{\Delta}, \quad \partial_t \rho = \rho / \tau_{\rho}, \quad (6)$$

with $\tau_{\Delta} \equiv \tau[1 + (1-\alpha)\rho A], \tau_{\rho} \equiv (\tau/\Delta)[1 - \alpha + \rho A]$, and $A \equiv (\partial P/\partial \rho)/\partial P/\partial \Delta = - \partial \Delta / \partial \rho$.. (Employing Eq (4), both $\tau_{\rho}$ and $\tau_{\Delta}$ may be written as a function of either $\Delta$ or $\rho$ alone.) Note $\tau_{\rho}, \tau_{\Delta}$ are not proper relaxation times, as they depend on $\Delta, \rho$. Nevertheless, we see that $\Delta$ diminishes, while $\rho$ grows – or relaxes backward in time. Since $\partial P/\partial \Delta \sim \sqrt{\Delta}$, or $\tau_{\Delta} \to \tau$ for $\Delta \to 0$, $\Delta$ will eventually relax exponentially toward zero, characterized by the constant relaxation rate $1/\tau_{\Delta} = \lambda T_g$ for $T_g = \text{constant}$. At the same time, $\rho$ grows, ever more slowly, with the diminishing rate $1/\tau_{\rho} \sim \Delta^{1.5}/\tau$. It stops completely at $\rho = \rho_f$ for $\Delta = 0$. Integrating Eqs (6) yields $\rho(t)$, accounting for irreversible compaction. The reversible branch corresponds to the change of $\rho_f$ with $T_g$ as given by Eq (5). As this relation is thermodynamic in nature, it holds independent of path.

We conclude that GSH is capable of a transparent, demystified account for the universal aspects of compaction. It describes slow density growth in the presence of granular jiggling, with a characteristic time that diverges towards the end. This happens concurrent with the loss of elastic deformation. The final density, a thermodynamic function of $T_g$, is larger the smaller $T_g$ is. Two things still need to be done: First, since a crucial starting point of GSH is the second law of thermodynamics using a conventional entropy, we need to understand its relation to the Edwards entropy. Second, we shall make contact with experiments, to find agreement that are, in spite of GSH’s qualitative status, satisfactory.

We revisit granular statistical mechanics and the Edwards entropy $S_{Ed}$. Substituting the volume $V$ for the energy $E$, and compactivity $X$ for the temperature $T$, this theory takes $dV = X dS_{Ed}$ as the basic thermodynamic relation for a “mechanically stable agglomerate of infinitely rigid grains at rest” [12]. The entropy $S_{Ed}$ is obtained by counting the number of possibilities to package grains for a given volume, equating it to $e^{S_{Ed}}$. Because a stable agglomerate is stuck in one single configuration, some perturbation is necessary to enable the system to explore the phase space of $S_{Ed}$. This ansatz, we believe, is best appreciated by taking the entropy more generally as $S(E, V, \rho)$, or $dS = (1/T)dE + (P/T)dV$, with $1/T = \partial S/\partial E, P/T = \partial S/\partial V$. For infinitely rigid grains at rest, we have $E \equiv 0$, because the energy remains zero however these non-interacting grains are arranged. Therefore, $dS = (P/T)dV$, or $dV = (T/P)dS \equiv XdS$.

In GSH, grains are neither assumed infinitely rigid, nor always at rest. The energy, containing both elastic and kinetic contributions, does not vanish – though of course does for infinitely rigid grains at rest, for $u_{ij}, v_i, T_g \equiv 0$. Therefore, $S_{Ed}$ is a minimalistic approach, a special limit of GSH. Note, however, the following objections: • Because of the Hertz-like contact between grains, very little material is being deformed at first contact, and the compressibility diverges at vanishing compression. This is a geometric fact independent of how rigid the bulk material is. Infinite rigidity is never a realistic limit for sand. • The number of possibilities to arrange grains for a given volume concerns inter-granular degrees of freedom. These are vastly overwhelmed by the much more numerous configurations of the inner-granular degrees of freedom. Maximal entropy $S$ implies minimal macroscopic and mesoscopic energy. It is quite unrelated to maximal number of possibilities to package grains. • Being an equilibrium consideration, $S_{Ed}$ is meant to account for the reversible branch of compaction. Yet Eq (5) is a consequence of the pressure exerted by agitated grains, not grains at rest. • Granular media have two different equilibria, a solid-like one for $T_g = 0$, when the system is jammed, and a liquid-like one for finite $T_g$, see III of [2]. A relaxing $\Delta$ represents an advance toward the liquid equilibrium, not reflected in $S_{Ed}$. For all these reasons, we are skeptical that $S_{Ed}$, though clearly a simplification, represents a useful limit.

When comparing experimental data to our results, there are some obvious difficulties: • $T_g$ is typically nonuniform, especially when the energy is injected from one side. Nonuniform shear flows, such as convection, will aggravate the problem. • There is boundary dominance when the system’s dimension becomes a few tens of the particle diameter. • Crystallization may happen for mono-disperse particles. • The relation between $T_g$ and the amplitude $\Gamma$ of the perturbation needs to be evaluated for each case individually, and is usually unknown. Moreover, compaction experiments are executed at constant $\Gamma$, yet we consider compaction at constant $T_g$. As $T_g(\Gamma)$ depends in general on $\rho, \Delta, \cdot \cdot \cdot$, the results are not equivalent. • Experimentally, density change is given as a
function of the number \( n \) of discontinuous perturbations such as tapping. The theory specifies the progress of compaction in terms of the time \( t \). The relation \( t(n) \) that will depend on \( \Gamma \) needs to be specified. Given these circumstances, we shall use some of the experimental data to extract \( T_\rho(\Gamma) \) and \( t(n) \), and look for agreement with the rest. This is admittedly much less than a complete calculation, but stays true to the spirit of accounting for the universal aspects of compaction.

Denoting the initial density as \( \rho_0 \), and the final, \( \Gamma \)-dependent one as \( \rho_f \), the measured data of the Rennes group [16] were given as a stretched exponential (or the KWW law): 

\[
\rho_f - \rho = (\rho_f - \rho_0) \exp\left(-\left(\frac{n}{\tau_{\text{KWW}}}\right)^\beta\right),
\]

with \( \beta = 0.6 - 0.8 \), \( \tau_{\text{KWW}} = \tau_0 \times \exp(\Gamma_0/\Gamma) \), \( \tau_0 = 0.9 \), and \( \Gamma_0 = 8 \) (relative acceleration). The Napoli group [17] reported \( \beta = 1 \) for their simulation and experiments, and considered both results in agreement.

On the theoretical side, the GSH parameters are the same we have consistently employed: \( a, B, b_0 \) are as indicated above. In addition, we have \( \lambda = \lambda_0 (1 - \rho/\rho_c) \) with \( \lambda_0 \) constant, and \( B/P = 3 \times 10^6 \) (by taking the average \( P \) as the hydrostatic pressure of 0.1 m and \( \alpha = 0 \)). Assuming an Arrhanius type law for both \( T_\rho(\Gamma) \) and \( t(n) \), we also take \( T_\rho(\Gamma) = e^{-\Gamma_1/\Gamma} \) times \( \sqrt{\lambda/P(2ab_0\rho_f)} \) (with \( \Lambda = 0.28 \) and \( \Gamma_1 = 0.56 \)), and \( t/n = \tau_n e^{-\Gamma_n/\Gamma} \) (with \( \Gamma_n = 7.8 \) and \( \tau_n = 2.2 \times 10^6 \sqrt{b_0\rho_f/\lambda_0^{-1}} \)). Employing \( T_\rho(\Gamma) \), Eq (5) becomes \( 2\rho_c/\rho_f = 1 + \sqrt{1 + \Lambda e^{-2\Gamma_1/\Gamma}} \).

which fits the experimental data, see (a) of Fig 1. Next, we rewrite \( \tau_\rho(\rho, T_\rho) \) as \( \tau_\rho(\rho, \Gamma) \) using \( T_\rho(\Gamma) \) and \( \rho_f(\Gamma) \), and numerically solve the equation \( \partial \rho = \rho/\tau_\rho \). The resultant \( \rho(t) \to \rho(n) \) for various \( \Gamma \) is shown in (b) of Fig 1. (The assumed Arrhanius type laws correspond to the information contained in two of the five curves in Fig 1.)

Summary: Compaction is a generic phenomenon, indifferent to the method of perturbation. GSH echoes this by providing suitable mechanisms for its two branches, yielding a transparent, de-mystified account. This further unifies our understanding of granular behavior as encapsulated by GSH, which has now been shown capable of accounting, in addition, for static stress distribution, elastic waves, elasto-plastic motion, the critical state, dense flow, fluidization, and jamming.

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