Origin of a Repose Angle: Kinetics of Rearrangement for Granular Materials

Anaël Lemaître
Department of Physics, University of California, Santa Barbara, California 93106
SPEC̄ CEA, Centre d'Etudes de Saclay, 91191 Gif-sur-Yvette, France
(Received 17 July 2001; revised manuscript received 12 February 2002; published 22 July 2002; publisher error corrected 13 August 2002)

A microstructural theory of dense granular materials is presented, based on two main ideas: first, that macroscopic shear results from activated local rearrangements at a mesoscopic scale; second, that the update frequency of microscopic processes is determined by granular temperature. In a shear cell, the resulting constitutive equations account for Bagnold's scaling and for the existence of a Coulomb criterion. In a granular flow down an inclined plane, they account for the rheology observed in experiments [Phys. Fluids **11**, 542 (1999)] and for temperature and velocity profiles measured numerically [Europhys. Lett. **56**, 214 (2001)] [Phys. Rev. E **64**, 051302 (2001)].

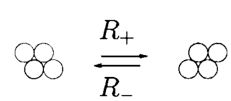
DOI: 10.1103/PhysRevLett.89.064303 PACS numbers: 45.70.Mg, 46.05.+b, 81.05.Rm, 83.10.–y

An upsurge of interest for granular materials has recently stirred the physical literature [1]. The problem is indeed challenging. The situation is paradoxical. Those materials lie at our doorstep, are ubiquitous in everyday life, their understanding is of an extreme interest for numerous practical reasons, ranging from earthquakes or landslides to industrial processes. Yet, there is no satisfactory explanation for the obvious fact that heaps have a slope. Recent advances have been made in experimental and numerical studies. In particular, the flow of a granular layer down an inclined plane is a laboratory model for many realistic situations [2–5]. In this setup, evidence has been given for the existence of a critical curve $H_{\rm stop}(\theta)$, relating the slope θ to the thickness of the granular layer below which the system jams. This relation refines the well-known Coulomb criterion of yield. In the bulk of a dense flow, it is accompanied by Bagnold's scaling, $\sigma \propto \dot{\epsilon}^2$, which relates the shear stress σ to the strain rate $\dot{\epsilon}$ [3,6]. Those experimental findings remain unexplained and add even more constraints to the challenge faced by the theorist. Kinetic theory [7] accounts for the rheology of dilute systems [8], but fails to explain jamming and the rheology of dense systems. Recent theoretical approaches postulate the existence of a repose angle, without explaining how it originates from microscopic motion [9].

This work focuses on structural rearrangements. It draws on the so-called shear transformation zone (STZ) theory [10], recently introduced to account for the behavior of viscoplastic solids. The profound difference between plastic and granular materials at the microscopic level is of particular interest: it has been shown recently that striking similarities accompany jamming transitions in various systems, be they granular materials, glasses, or foams [11]; this observation, however, has not led to the identification of a universal mechanism underlying such similarities, and to a statistical approach for structural systems. More than an isolated model of granular flows, the current work attempts to bridge the gap between two of such systems, thus showing that structural rearrangement is a key to our understanding of dense materials, on very general grounds.

In order to fix ideas, I start with a very brief introduction to rearrangement kinetics in the spirit of [10]. Then, I show how Bagnold's scaling emerges from the microscopic dynamics of the N-body problem for hard spheres. This is necessary to proceed and write macroscopic equations for dense granular materials.

A shear transformation zone (STZ) is defined as a locus within the material where a rearrangement is made possible by the local configuration of the contact network [10]. An important remark that lies at the root of STZ theory is that, once some microscopic shear has occurred somewhere in the material, the system cannot shear further at this point and in this direction (although it may shear backward). This leads to the identification of pairs of types of arrangements which are transformed into one another by a local shear. A local "symmetry" is thus induced by shearing; the local state of the system is determined by the populations of arrangements susceptible to shear in a given direction. To simplify the picture, a single pair of orientations is considered, aligned along the principal axes of the stress tensor, an elementary transformation is sketched as



although an actual STZ might involve more than four grains (say of order 10). Populations of STZ's are denoted n+ and n_-; the rates at which a $\pm \rightarrow \mp$ transformation occurs are denoted $R_\pm$. Macroscopic shear motion results from the balance between local activated rearrangements,

$$\dot{\epsilon} = \mathcal{A}_0(R_+ n_+ - R_- n_-), \tag{1}$$

where $\dot{\epsilon}$ is the off-diagonal component of the rate-of-deformation tensor, and where $\mathcal{A}_0$ is some constant. The rates $R_\pm$ and equations of motion for the populations $n_\pm$ must be specified to close the system.

In order to go further, I need to explain how Bagnold's scaling emerges from the microscopic dynamics of granular materials. It has been observed recently that Bagnold's scaling results from the N-body problem, so long as no time scale is imposed to the system by coupling it, e.g., to a pressure bath [8]. The argument given was based on dimensional considerations, and was expected to hold under the assumption that microscopic dynamics involve only binary collisions. In fact, Bagnold's scaling results from an *exact* invariance of the N-body problem, for hard-sphere systems, in the absence of a thermal or pressure bath. This invariance sets strong constraints on how a theory of dense granular materials can be written.

Consider a system of N grains in contact, submitted to a set of forces F^{c} at each contact point, and to forces $F^{c'}$ at contact points with the boundary. A solution of the system is given by the locations $\vec{r}_i(t)$ of the centers of mass of all grains, their rotations, the sets $c(t)$ and $c'(t)$ of contact points, and the forces as function of time. The interaction between the grains is supposed to be a pure hard-core repulsion, with dissipative collisions; friction may exist provided that the yield criterion at each contact point involves a ratio of forces. Equations of motion introduce no time scale, no scale for the forces network: the system is unchanged if all forces are rescaled as $F^{c,c'} \to F^{c,c'}/F_0$ and time as $t \to t\sqrt{F_0}$: the grains follow the same trajectories, the successive sets c, c' are identical. This invariance holds in a very strong sense: a rescaling of the forces leaves the trajectory of the system *unchanged* in the phase space; only the time coordinate along the trajectory is modified. In a shear cell, it leads immediately to the observation made by Bagnold.

It is noteworthy that kinetic theory correctly incorporates this scaling invariance (although it does not account for dense rheology where Bagnold's scaling is observed). This is performed via the introduction of granular temperature T, which, as opposed to thermodynamic temperature, is a dynamical quantity. In this work, granular temperature is associated with tiny motion of the grains in the surrounding cage made of their neighbors: it determines the smallest time scale in the material; *by definition*, $\sqrt{T}$ is the velocity at which the system evolves along a phase-space trajectory. I can now resume the presentation of STZ theory for granular materials. In the first part of what follows, I study a shear cell and mean-field equations. Then, I consider a granular flow down a plane and show how spatial interactions lead to the emergence of $H_{\mathrm{stop}}(\theta)$.

The invariance presented above has dramatic consequences on how transformation rates can be written for dense granular materials: it is possible to separate the velocity $\sqrt{T}$ at which the system evolves along phase-space trajectories, and the events which occur along these trajectories (collisions or sudden collective rearrangements). The probability that a rearrangement occurs per time unit (in physical space) is the product of the distance (in phase space) spanned by the system per time unit—$\sqrt{T}$—, times the probability that a rearrangement occurs, per unit length, along this trajectory. This latter, intrinsic, probability of rearrangement can depend only on the ratio of stresses σ/P, where σ is the shear stress and P is the pressure. The transition rates are thus written $R_\pm \propto \sqrt{T} f(\pm\sigma/P)$; $\sqrt{T}$ appears as the update frequency of activated processes. Rearrangement is expected to be enhanced by a strong distortion of the force network: the function $f(\sigma/P)$ is a positive, increasing functional of σ/P. An elementary shear is expected to be triggered by a large excess force applied to the transformation zone; recalling that large forces are distributed exponentially in granular packings [12,13], an exponential dependency is expected, and the rates are written [14]

$$R_\pm = R_0\sqrt{T}e^{\pm\mu\sigma/P}.$$

R_0 is some constant, and μ is as an effective friction coefficient that controls the occurrence of elementary rearrangements, and that may depend on the coefficient of static friction between the grains.

Granular temperature is a dynamical quantity which, by definition, is also a scale of specific kinetic energy. Its dynamics results from the balance between the energy produced by the flow and the energy dissipated

$$\dot{T} = \sigma\dot{\epsilon} - \alpha T\sqrt{T}. \tag{2}$$

The second term in the right-hand side (rhs) accounts for collision-mediated energy dissipation (here collisions might be complicated events involving clusters of grains): events occur at the frequency $\sqrt{T}$ and the energy dissipated per event is proportional to T itself; parameter α is related to the restitution coefficient of the grains, and should be sensitive to the volume of the material [15]. Another term in this equation should account for energy dissipated in kinetic friction ($\propto -\dot{\epsilon}P\tan\varphi$); this loss, however, is expected to be lowered by velocity fluctuations [5] and is neglected in the current work.

Equations of motion for the populations $n_\pm$ are required to close the system. They are written [10]

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + \omega(\mathcal{A}_c - \mathcal{A}_a n_\pm). \tag{3}$$

The first two terms on the rhs account for the "internal" dynamics of STZ's, while the last term introduces a coupling of the local arrangements with the mean flow. From a macroscopic standpoint, the flow constantly stirs the grains, thus creating and destroying local configurations. In STZ theory, the rate ω at which the flow induces new configurations is evaluated as the overall work $\sigma\dot{\epsilon}$, normalized by some typical force. In phase space, an elementary shear, $\delta\epsilon$, corresponds to some segment along a trajectory. This segment can be followed at different velocities $\dot{\epsilon}$ depending on the scale of forces. The renewal of geometric configurations along this segment is proportional to $\delta\epsilon$, and can depend only on σ/P, but neither on the scale of forces, nor on the velocity $\dot{\epsilon}$. The assumption $\omega \propto \sigma\dot{\epsilon}$ thus yields $\omega = \sigma\dot{\epsilon}/P$.

Let me now write Eqs. (1) and (3) in a more suitable way. Variables

$$\Delta = \frac{n_- - n_+}{n_\infty}, \quad \Lambda = \frac{n_+ + n_-}{n_\infty}, \quad \text{and } \zeta = \frac{\sigma}{P}$$

are introduced, and the rescaled parameters $n_\infty = 2\mathcal{A}_c/\mathcal{A}_a$, $\epsilon_0 = \mathcal{A}_0\mathcal{A}_c/\mathcal{A}_a$, $\gamma = \mathcal{A}_0\mathcal{A}_c$, and $E_0 = 2\epsilon_0 R_0$. From (1) and (3), it comes

$$\dot{\epsilon} = E_0\sqrt{T}\,\left[\Lambda\sinh(\mu\zeta) - \Delta\cosh(\mu\zeta)\right], \tag{4}$$

$$\dot{\Delta} = \frac{1}{\epsilon_0}(\dot{\epsilon} - \gamma\omega\Delta), \tag{5}$$

$$\dot{\Lambda} = \gamma\frac{\omega\dot{\epsilon}}{\epsilon_0}(1 - \Lambda), \tag{6}$$

T is governed by (2), and $\omega = \dot{\epsilon}\zeta$ (for future use, I do not simplify). Variables Λ and Δ represent the total normalized density of STZ's and the bias between populations $n_\pm$, respectively. These state variables account for a history-dependent texture (or fabric [13]) of the material, and are one of the most interesting aspects of the current model. Since steady state motions are considered in this work, Λ is taken to its asymptotic value, $\Lambda = 1$.

The system (2), (4), and (5) admits multiple jammed solutions, $\dot{\epsilon} = T = 0$; they are stable if $\tanh(\mu\zeta) < \Delta$, where Δ depends on the preparation of the system. In the flowing regime, $\Delta = 1/(\gamma\zeta)$; the flow is stable so long as $\tanh(\mu\zeta) > \Delta$: this is equivalent to $\zeta > \tan\Phi$, with

$$\tanh(\mu\tan\Phi) = \frac{1}{\gamma\tan\Phi}.$$

It is a Coulomb criterion of yield with limit angle Φ. In the flowing regime, the stationary value of T is

$$T = \frac{E_0}{\alpha}K(\zeta)\sigma, \tag{7}$$

with $K(\zeta) = \sinh(\mu\zeta) - \cosh(\mu\zeta)/(\gamma\zeta)$. Bagnold's scaling is recovered from (4)

$$\dot{\epsilon}^2 = [E_0K(\zeta)]^3\frac{\sigma}{\alpha}. \tag{8}$$

The factor $K(\zeta)$ depends on the ratio of forces. This is consistent with the observation by Bagnold that this scaling holds in a region of experimental parameters where the ratio $\zeta = \sigma/P$ is constant [6].

Let me now consider a granular flow of thickness H down an inclined plane. Axis x is taken along the descent, and axis y perpendicular to the plane. Uniform solutions in direction x are looked for; variables $\dot{\epsilon}$, Δ, and T depend on y only. The velocity field is oriented along axis x and the velocity profile $u(y)$ is related to the strain rate by $u'(y) = 2\dot{\epsilon}(y)$. The plane makes an angle θ above the horizontal; the stress tensor obeys Cauchy equations, leading to $P(y) = \rho g(H - y)\cos\theta$ and $\sigma(y) = \rho g(H - y)\sin\theta$, where ρ is the mass density of the material, and g the gravity.

I first neglect spatial effects, e.g., diffusive terms that arise in the equation for T: this corresponds to the limit $H \gg 1$. The local equations are identical to those presented earlier, but σ and P vary in depth. In the flowing regime, $\Delta = 1/(\gamma\tan\theta)$ is uniform; the stability criterion is the same for all layers within the flow: the systems jams if $\theta < \Phi$, and flows otherwise. When it flows, T and $\dot{\epsilon}$ are given by Eqs. (7) and (8), respectively, with σ a linear function of y. Temperature T grows linearly with the depth, and Eq. (8) leads to

$$u(y) = \frac{4}{3}[E_0K(\tan\theta)]^{3/2}\frac{\sqrt{\rho g\sin\theta}}{\sqrt{\alpha}}[H^{3/2} - (H - y)^{3/2}].$$

The linear increase of T with depth, this velocity profile, and the rheology $u(H) \propto H^{3/2}$ agree remarkably well with experimental and numerical findings [2,3].

I finally complete this approach with the introduction of spatial interactions, in order to study flows with a finite thickness. Equation of motion for T should present a diffusive term. This term, however, neither changes the stationary values of Δ in a flow, $\Delta = 1/(\gamma\tan\theta)$, nor the yield criterion $\tanh(\mu\zeta) > \Delta$: it softens temperature and velocity profiles, but does not account for the emergence of the curve $H_{\mathrm{stop}}(\theta)$. For pedagogical purposes, I neglect thermal diffusion, and show that spatial interaction via the renewal of STZ's is sufficient to account for $H_{\mathrm{stop}}(\theta)$.

STZ's are mesoscopic structures that result from arrangement of several grains. Unlike temperature, they do not diffuse, because the motion of individual grains cannot *transport* configurations: the motion of individual grains *renews* configurations. STZ evolve either by internal rearrangements or by aggregation/elimination of grains carried by the neighboring flow. A spatial coupling comes up quite naturally from this picture, since the flow at a given point contributes to the evolution of nearby configurations. The rate ω is now written

$$\omega(\vec{r}) = \frac{1}{2\ell}\int \omega^0(\vec{r} + \vec{R})k(\vec{R})\mathrm{d}\vec{R}, \tag{9}$$

with $\omega^0 = \dot{\epsilon}\sigma/P$. The integral kernel $k(R)$ is the probability that a change at $\vec{r} + \vec{R}$ affects arrangements at $\vec{r}$. Consider, for example, a grain carried at point $\vec{r} + \vec{R}$. In order to interact with the local configuration at $\vec{r}$, this first grain must come into contact with a second grain, at distance $R - D$ from $\vec{r}$ (with D the diameter of a grain). This second grain must also come into contact with a third grain at distance $R - 2D$, etc., thus forming a chain between $\vec{r}$ and $\vec{r} + \vec{R}$. If p denotes the probability that the first grain interacts with the second, $k(R)$ verifies,

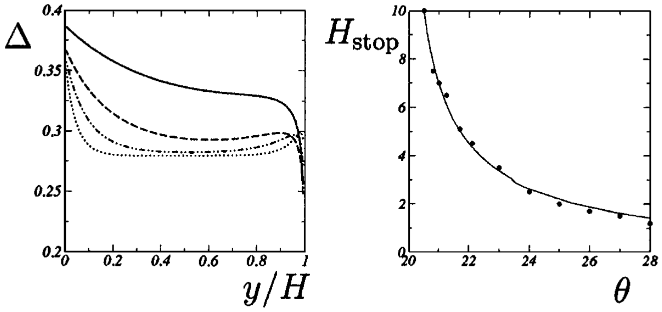


FIG. 1. (left) The state variable Δ as a function of y/H, for values of the parameters $\gamma = 10.23$, $\mu = 0.98$, $\ell = 0.99$, angle $\theta = 24°$, and several values of H: $H = 5$ straight line, $H = 10$ dashed, $H = 20$ dot-dashed, $H = 40$ dotted. (right) H_{stop} from experimental data by Pouliquen [2] (circles) compared to the phase diagram obtained from the current theory (straight line), with $\gamma = 10.23$, $\mu = 0.98$, $\ell = 0.99$. These curves do not depend on parameters E_0 and α.

$k(R) = pk(R - D)$, whence an exponential form, $k(R) = \exp(-R/\ell)$.

Let me now study a flow governed by constitutive Eqs. (2), (4), and (5), and where ω is given by (9). The value of Δ in a steady state is now $\Delta = \dot{\epsilon}/\gamma\omega$, and varies in space. Typical profiles are displayed in Fig. 1 (left). The major consequences of spatial interaction appear at the boundaries. At the top of the flow, Δ vanishes because $\dot{\epsilon} \to 0$, while ω remains nonzero. At the bottom of the flow, only the upper half plane $y > 0$ contributes to the integral expression of ω: this results in an increase of Δ. The system is more isotropic, liquidlike, at the top; it is more textured, solidlike, at the bottom.

The nonuniformity of Δ has dramatic consequences on the stability of the flow. The jamming criterion $\tanh(\mu\zeta) > \Delta$ is controlled by the maximum value reached by Δ at $y = 0$. Moreover, as seen in Fig. 1 (left), Δ globally increases with decreasing H. If the lowest layers jam, the jamming criterion is again verified for the upper layers: jamming propagates upward, leading to the complete arrest of the flow. This process determines a critical height $H_{\text{stop}}(\theta)$, displayed in Fig. 1 (right) and compared with experimental data. The fit is remarkable.

Of course, the introduction of thermal diffusion and dilatancy should slightly blur this picture; it is also expected to account for the deviation from Bagnold's scaling observed in [2], close to the boundaries. The jamming mechanism, however, seems essentially captured at this level of approximation. The detailed analysis of complete equations including those various effects will be addressed in future works.

The results presented in this Letter are twofold. First, the role of activated rearrangements in granular matter has been evidenced, hence providing a microstructural interpretation for the Coulomb criterion. Second, the importance of granular temperature, as opposed to thermodynamic temperature, has been shown; the fact that microscopic collisions determine the update frequency of activated rearrangements lies at the root of Bagnold's scaling. Those features contribute to the existence of a jamming criterion $H_{\text{stop}}(\theta)$ and to temperature and velocity profiles consistent with recent observations.

This work was supported by the W. M. Keck Foundation, and the NSF Grant No. DMR-9813752, and EPRI/DoD through the Program on Interactive Complex Networks.

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[14] Unlike thermodynamic temperature, granular temperature does not measure a volume in the phase space, or a Boltzmann weight for activated processes. The thermodynamic interpretation of temperature as a volume in phase space does not result immediately from its definition as kinetic energy, but from the coupling of the system to a thermal bath, which blends nearby trajectories: the system follows a bundle of trajectories and it is legitimate to use ensembles.
[15] Volume dependence is not considered in the current approach. This is permitted in first approximation because density profiles are flat in a flow down an inclined plane [3]. Moreover, the scaling argument presented here indicates that, in a shear cell, the volume depends on σ/P only; this again is consistent with [6].