Granular materials, such as sand or powders, for many respect are similar to fluids or solids, even though in absence of external drive they rapidly come rest, due to strong dissipation and negligible thermal energy scales (they are non-thermal systems), in disordered states very similar to glasses. As standard thermodynamics is not applicable to describe them, it is natural to ask whether we can even refer to granular packs as “states”. The problem of finding the correct theoretical framework where to describe granular media is in fact of deep relevance to civil engineering, geophysics and physics.

Edwards proposed a thermodynamic description for static granular media, which was partially investigated by recent experiments. These experiments have established that a granular system subject to a tapping dynamics, such as subsequent mechanical oscillations of the container, may lose memory of its initial state and reach a stationary state of volume fraction only dependent on the tapping intensity, a precondition for a statistical mechanics description of static granular material to be possible. The study of out-of-equilibrium (aging) slowly sheared granular assemblies is also useful for the validation of the statistical mechanics of granular media, but it is inherently restricted to a small range of very high volume fractions, where the system is jammed.

Here we give strong evidences supporting the existence of a thermodynamical and statistical mechanical description of granular media. First we demonstrate, via Molecular Dynamics (MD) simulations, that granular packs at rest are genuine thermodynamic states, as they are characterized by a small set of parameters regardless of the procedure with which they are generated. Then we show, via Monte Carlo (MC) simulations, that these states can be described in terms of equilibrium distributions proposed by Edwards. The coincidence between time averages (MD) and ensemble averages (MC) is a strong evidence in favour of the statistical mechanics approach to granular media. For details of materials and methods, see the supplementary materials available online.

MD simulations: time averages – We run Molecular Dynamics simulations of $N = 1600$ monodisperse spherical grains of diameter $d = 1\text{cm}$ and mass $m = 1\text{g}$. Grains, under gravity, are confined in a box with a square basis of length $L = 10\text{cm}$ (see Fig. 1), with periodic boundary conditions in the horizontal directions. The bottom of the box is made of other immobile, randomly displaced, grains (to prevent crystallization). Two grains in contact interact via a normal and a tangential force. The former is given by the spring-dashpot model, while the latter is a single pulse the flow velocity, directed against gravity, $V > 0$ for a time $\tau_0$; then the fluid comes to rest. The flow pulse dynamics is repeated up to reach stationary conditions (see Fig. 2).

As in a recent experiment, the system is immersed in a fluid and, starting from a random configuration, it is subject to a dynamics made of a sequence of flow pulses where the fluid flows through the grains (see Fig. 3). In a single pulse the flow velocity, directed against gravity, is $V > 0$ for a time $\tau_0$; then the fluid comes to rest. We model the fluid-grain interaction via a viscous force proportional to the fluid grain relative velocity: $F_{fg} = -A(v - V)$ where $v$ is the grain and $V$ is the fluid velocity. The prefactor $A = \gamma(1 - \Phi)_1^{-3.65}$ is dependent on the local packing fraction, $\Phi$, in a cube of side length $3d$ around the grain, and the constant is $\gamma = 1\text{ Ns/cm}$. During each pulse, grains are fluidized and then come to rest under the effect of gravity. The tapping dynamics, therefore, allows for the exploration of the phase space of the mechanically stable granular packs. When the system
is subject to such a tap dynamics, it compactifies until it reaches a stationary state where its properties do not depend on the dynamics history. Fig. 2 shows that the volume fraction of our system increases by following a stretched exponential law, Eq. 1.

\[ \Phi(t) = \Phi_\infty - (\Phi_\infty - \Phi_0) \exp\left(-\frac{t}{\tau_c}\right), \quad (1) \]

in agreement with the experiment by P. Philippe et al. [20]. The relaxation time diverges as the tapping intensity decreases, indicating the presence of a glassy like behavior which will be discussed elsewhere [21]. As the thermodynamics approach to granular media aims to describe stationary states, all of measures shown below (averaged over 32 runs) are recorded after the application of a long sequence of flow pulses, when the system is at stationarity.

We plot in Fig. 3 the stationary values of the volume fraction, \( \phi(V, \tau_0) \) (measured in the bulk of the system), and its fluctuations, \( \Delta \phi(V, \tau_0) \), recorded after a sequence of such flow pulses of duration \( \tau_0 \) and velocity \( V \). \( \Delta \phi \) is by definition the standard deviation of \( \phi \) around its average value at stationarity. Actually, the volume fraction probability distributions is Gaussian [13, 15]. \( \phi \) decreases with \( V \) and with \( \tau_0 \); the stronger the pulse, i.e., the larger \( V \) or \( \tau_0 \), the fluffier the pack settled after it. Similarly, \( \Delta \phi \) increases with \( V \) and \( \tau_0 \).

Even though, \( \phi \) depends on both the parameters of the dynamics, \( V \) and \( \tau_0 \), we show now that such stationary states are indeed genuine “thermodynamic states”, i.e., they can be described, in this system, by one macroscopic parameter. Actually, the upper panel of Fig. 4 shows that when \( \Delta \phi \) is parametrically plotted as function of \( \phi \), the scattered data of Fig. 3 collapse, within numerical approximation, onto a single master function. This is a clear indication that \( \Delta \phi \) and \( \phi \) are in a one-to-one correspondence, no matter how the state with packing fraction \( \phi \) is attained. Our claim is that such a property should be found for any macroscopic observable of the system: we checked some of them, including the energy and its fluctuations and the coordination number of grains. Actually, in Fig. 4 lower panel we show that the whole radial distribution function \( g(r) \) of a pack is characterized only by its corresponding value of \( \phi \), i.e., states attained with different dynamical protocols \((V, \tau_0)\) but having the same \( \phi \), have the same \( g(r) \). From these results we derive our first conclusion: at stationarity, we can describe the pack with only one parameter, e.g., \( \phi \), independently of the dynamical protocol. Such a parameter characterizes, thus, the “thermodynamics state” of the system.

**MC simulations: ensemble averages** – Our second important step is to identify the correct Statistical Mechanics distribution for these states. Under a very strong assumption (discussed for instance in [10, 13, 22, 24, 25, 26, 27, 28, 29, 31]), Edwards proposed to use for the grains of a powder the standard machinery of Statistical Mechanics. He suggested, however, to consider a reduced configurational space: the system at rest (i.e., not in its “fluidized” regime) is described by a flat ensemble average restricted to its blocked configurations (i.e., its mechanically stable microstates). Under these hypotheses [13, 24, 27], the canonical ensemble probability, \( P_r \), to find the blocked microstate \( r \), of energy \( E_r \), is:

\[ P_r \propto e^{-\beta_{\text{conf}} E_r}, \quad (2) \]
where the inverse of $\beta_{\text{conf}}$ is the conjugate parameter of the energy, called \textit{configurational temperature}, $T_{\text{conf}}$.

In order to check whether such a Statistical Mechanics scenario applies, we compared ensemble averages over the distribution of Eq. 2 with those over the flow tap dynamics. For instance, the average value of $\phi$ over the distribution of Eq. 2 is

$$\langle \phi \rangle (T_{\text{conf}}) = \frac{\sum_r \phi_r \exp(-E_r/T_{\text{conf}})}{\sum_r \exp(-E_r/T_{\text{conf}})},$$

where the sum runs over all blocked microstates, and $\phi_r$ is the volume fraction of microstate $r$. We evaluated these ensemble averages by use of a Monte Carlo method which is an extension of that introduced in Ref. [6] to the frictional case [15] (frictional forces are essential to assure the stability of granular packs with small volume fraction). Fig. 4 shows, as empty circles, the functions $\langle \Delta \phi \rangle (\langle \phi \rangle)$ (resp. $\langle g(r) \rangle (\langle \phi \rangle)$) for the same ensembles independently calculated from Eq. 2 within numerical errors, they scale on the same curves, pointing out that the inverse of $\beta_{\text{conf}}$ is the conjugate parameter, e.g., $\phi$, irrespectively of the dynamical protocol used to arrive at $\phi$. The dotted line is a linear best fit. A similarly good collapse is also found (lower panel) when we plot the radial distribution function $g(r)$ for the same ensembles obtained from the data of Fig. 3 via the use of the static fluctuation dissipation relation [15].

The empty circles in both panels are the corresponding ensemble averages over the pulse dynamics scenario applied to arrive at $\phi$. We evaluated these ensemble averages by use of the Monte Carlo procedure, while time averages are obtained via the Monte Carlo procedure, while time averages are obtained from the data of Fig. 3 via the use of the static fluctuation dissipation relation.

Conclusions – Summarizing, in the present MD simulations of a non-thermal monodisperse granular system under flow pulse, we find that the stationary configurations of the system can be fully described by only one parameter, e.g., $\phi$, and can be, thus, considered genuine “thermodynamic states”. Within our numerical accuracy, we also showed that a Statistical Mechanics based on the distribution of Eq. 2 is grounded to describe these “states”. We could derive as well the equation of state, $\phi(T_{\text{conf}})$, of the system.
These evidences strongly support the existence of a fundamental theory of dense granular media and address, thus, a variety of important issues in the next future, such as response functions in a granular system, mixing/segregation phenomena, the nature of their jamming transition and phase diagram [3, 22, 23, 32].

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Contents:

1. The Statistical Mechanics approach to granular media.
2. Configurational temperature and dynamical temperature.
3. Monte Carlo method.
Volume fraction fluctuations in the stationary state

Figure A Probability distributions of the volume fraction $\Phi$ in the steady state reached by the system subject to the flow pulses dynamics. The data, obtained by averaging over the stationary dynamics in 32 different runs starting from random initial conditions, are Gaussian distributed (plain lines). The standard deviations of these distributions are the volume fraction fluctuations, $\Delta \Phi$, plotted in Fig. 3.
Statistical Mechanics approach to granular media
In the Statistical Mechanics of powders introduced by S. Edwards (S.F. Edwards and R.S.B. Oakeshott, Physica A 157, 1080, 1989) it is postulated that the system at rest can be described by suitable ensemble averages over its “mechanically stable” states. Edwards proposed a method to individuate the probability, \( P_r \), to find the system in its mechanically stable state \( r \), under the assumption that these mechanically stable states have the same a priori probability to occur. This is the simplest assumption one can imagine: it is the assumption of standard Statistical Mechanics (equiprobability of microstates) with the additional constraint of mechanical stability. A possible approach to find \( P_r \) is as follow (A. Fierro et al., Europhys. Lett. 59, 642, 2002; Phys. Rev. E 66, 061301, 2002; Europhys. Lett. 60 684, 2002). \( P_r \) is obtained as the maximum of the entropy,

\[
S = - \sum_r P_r \log P_r
\]

with the macroscopic constraint, in the case of the canonical ensemble, of fixed system energy \( E = \sum P_r E_r \) (here \( E_r \) is the energy of the mechanically stable microstate \( r \)). For a granular medium at rest in the gravity field, \( E_r \) is the sum of the gravitational energy, and of the interaction energy between grains:

\[
E_r = \sum_i m g z_i + \sum_{i \neq j} V_{ij},
\]

where \( z_i \) is the height of grain \( i \) (with mass \( m \)) and \( V_{ij} \) is the interaction (elastic energy) between grain \( i \) and \( j \) in the microstate \( r \): \( V_{ij} = 0 \) if grains \( i \) and \( j \) are not in contact, otherwise

\[
V_{ij} = \frac{1}{2} k_n |\delta_{ij}|^2 + \frac{1}{2} k_t |\vec{u}_{ij}|^2,
\]

where \( \delta_{ij} \) is the overlap between grain \( i \) and \( j \), and \( \vec{u}_{ij} \) is their shear displacement. The interaction energy \( V_{ij} \) is derived by the normal and the tangential forces acting on the contacting grains (we use the model L3 described in L.E. Silbert et al., Phys Rev E 64, 051302, 2001): \( \vec{f}_n = k_n \delta_{ij}, \vec{f}_t = k_t \vec{u}_{ij} \).

From Edwards’ hypothesis, in analogy to the Gibbs result, you derive that:

\[
P_r = Z^{-1} \exp (-\beta_{conf} E_r)
\]

where \( \beta_{conf} \) is a Lagrange multiplier, called inverse configurational temperature, enforcing the above constraint on the energy:

\[
\beta_{conf} = \frac{\partial S_{conf}}{\partial E}, \quad S_{conf} = \ln \Omega_{stable}(E).
\]

The configurational temperature is \( T_{conf} = \beta_{conf}^{-1} \). Here \( \Omega_{stable}(E) \) is the number of mechanically stable states with energy \( E \). \( Z \) is fixed by the normalization condition \( \sum_r P_r = 1 \), where the sum is restricted to \( \Omega_{stable} \), i.e., to the mechanically stable states.

We note here that for stiff grains the elastic energy \( \sum_{i \neq j} V_{ij} \) is much smaller than the gravitational energy \( \sum_i m g z_i \) (the elastic energy is strictly zero in hard sphere systems). Accordingly \( E_r \) is to a good approximation proportional to the gravitational energy, i.e. to the volume of the system, as originally suggested by Edwards.
Configurational temperature and dynamical temperature
We describe here the two different definitions of temperature for granular systems mentioned in our paper.

Configurational temperature
As discussed above, the configurational temperature is the inverse of the derivative of the configurational entropy with respect to the energy. It is therefore an ‘equilibrium’ temperature, defined for a granular system at stationarity under a given dynamics allowing the exploration of mechanically stable states.

In our main text we have validated Statistical Mechanics approaches to powders by showing that, within numerical errors, the granular packs we consider are characterized, at stationarity, by a single parameter regardless of the dynamical procedure with which they were prepared (they are in a thermodynamic ‘state’), and that time averages coincide with ensemble averages over the distribution detailed above. This result justifies the use of Edwards ‘equilibrium’ partition function to make analytical calculations, and particularly to derive the following equilibrium fluctuation-dissipation relation (Coniglio and Nicodemi Physica A 296, 451 (2001)),

$$\beta_{conf}(E) = \beta_{conf}(E_0) - \int_{E_0}^{E} \frac{dE}{\Delta E^2}$$

which relates the energy and its fluctuations. This relation can be exploited to experimentally measure the configurational temperature (Nowak et al., Powder. Tech. 94, 79, 1997; Knight et al., Phys. Rev. E 57, 1971, 1998; Schröter and Swinney, Phys. Rev. E 71, 030301(R), 2005).

Dynamical temperature
In thermal glassy systems far from stationarity, dynamical off-equilibrium fluctuation-dissipation relations hold. Particularly, in the aging dynamics of mean-field glassy models in contact with a very small bath temperature, $T_{bath}$, generalized out-of equilibrium fluctuation-dissipation relations were discovered where the role of the external temperature is played by a ‘dynamical temperature’ $T_{dyn} \neq T_{bath}$, equal for all slow modes (L.F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. 71, 173, 1993). This scenario was later extended to aging granular materials (for a review see P. Richard et al., Nat. Mat. 4, 121, 2005, and references therein), were the dynamical temperature is defined and measured via a dynamical, off-equilibrium fluctuation dissipation relation,

$$\langle (r(t) - r(t_w))^2 \rangle = T_{dyn} \frac{\delta(r(t) - r(t_w))}{\delta f}$$

where $r$ is the position of a grain, $f$ a constant perturbing field, and $t_w$ the ‘waiting’ time. As the dynamical temperature is defined far from stationarity and, conversely, the configurational temperature at stationarity, Makse and Kurchan have shown that in granular packs, at very high density, the two are equal within numerical errors (Nature 415, 614, 2002). At low volume fraction, on the contrary, the dynamical temperature appears to be no longer defined, as the granular system is no longer jammed and flows as soon as an external perturbation is applied, as shown by Potiguar and Makse (European Physical Journal E 19, 171, 2006).
Monte Carlo method to test the Statistical Mechanics approach to granular materials at rest

In order to test the Statistical Mechanics approach to granular media one has to compare time averaged data, obtained as explained in the text, with ensemble averaged data obtained by sampling Edwards distribution, eq.(2) in the text,

\[ P_r = Z^{-1} \exp(-\beta_{\text{conf}} E_r). \]  

(6)

where \( E_r \) is the energy of the state \( r \),

\[ E_r = \sum_i m g z_i + \sum_{i \neq j} V_{ij}. \]  

(7)

As the Statistical Mechanics approach to granular media deals with mechanically stable states, the phase space of interest (over which eq. (6) must be sampled) is not the usual phase space, \( \Omega_{\text{tot}} \{ \vec{r}, \vec{v}, \vec{\omega} \} \) (here \( \vec{r} \) is the 3N vector of grains c.o.m. positions, \( \vec{v} \) their velocities, and \( \vec{\omega} \) their angular velocities). Instead it is the subset \( \Omega_{\text{stable}} \subset \Omega_{\text{tot}} \{ \vec{r}, 0, 0 \} \) of all states \( r \) where the forces and the torques acting on each single grain sum to zero, and grains neither translate nor rotate.

Since the states to be considered are so highly constrained it is difficult to sample the distribution of eq. (6) via a standard Monte Carlo procedure. For instance, if a state \( r \) is stable, then there is little chance to transform it in a new mechanically stable state \( r' \) via the displacement of a single particle. Introducing many particles Monte Carlo moves is also useless as the probability of selecting a collective move that transform a mechanically stable state into a new mechanically stable state is practically zero.

A Monte Carlo (MC) method to explore \( \Omega_{\text{stable}} \) was proposed by H.A. Makse and J. Kurchan, Nature 415 614 (2002), which uses the following computational trick. The MC algorithm explores the usual phase space, \( \Omega_{\text{tot}} \), but in this phase space one introduces an auxiliary energy \( E_{\text{aux}} \) which measures the degree of ‘mechanical instability’ of a pack in a microstate \( r \). In the present case, we have defined:

\[ E_{\text{aux}} = \sum_{i=1}^{N} |m \vec{g} \vec{d} + \sum_{j \neq i} (\vec{f}_{ij} + \vec{f}_{ji})| + \sum_{i=1}^{N} |\vec{T}_i|, \]  

(8)

where \( \vec{T}_i \) is the total torque acting on grain \( i \). The first term of the above equation enforce the balance of forces on each single grain, and the second the balance of torques. Different expressions could be used for \( E_{\text{aux}} \), the important point being that \( E_{\text{aux}}(r) \geq 0 \ \forall r \), and that \( E_{\text{aux}}(r) = 0 \) if and only if the state \( r \) is mechanically stable.

Then one samples via a standard Monte Carlo procedure the distribution

\[ P_r = Z^{-1} \exp(-\beta_{\text{conf}} E_r - \beta_{\text{aux}} E_{\text{aux}}(r)). \]  

(9)

where \( T_{\text{aux}} = \beta_{\text{aux}}^{-1} \) is the so-called ‘auxiliary temperature’ which controls the equilibrium value of the auxiliary energy. By definition of \( E_{\text{aux}} \), in the limit \( T_{\text{aux}} \rightarrow 0 \) we have:

\[ \lim_{T_{\text{aux}} \rightarrow 0} P_r = \lim_{T_{\text{aux}} \rightarrow 0} \frac{\mathcal{P}_r}{Z} = \lim_{T_{\text{aux}} \rightarrow 0} E_{\text{aux}} = 0. \]  

(10)

Therefore in the limit \( T_{\text{aux}} \rightarrow 0 \) we sample the distribution of mechanically stable states \( (E_{\text{aux}} = 0) \) with probability \( P_r \), as desired. This is precisely the limit which is considered in by Makse and Kurchan method.

In our simulations we start by sampling eq. (9) in the phase space of all granular packs at the desired value of \( T_{\text{conf}} \) and at \( T_{\text{aux}} > 0 \) via a Monte Carlo procedure (see below). Then
we slowly decrease the auxiliary temperature (carefully checking for thermalization) until \( T_{aux} = 0 \). By repeating this procedure several times we generate several packs (a total of 172) at the desired configurational temperature. These packs are then used to compute ensemble averages relative to the chosen value of \( T_{conf} \).

**Implementation of the Monte Carlo method**

In our definition of mechanical stability (eq. (8)) we also include tangential forces (neglected in H.A. Makse and J. Kurchan, Nature 415 614, 2002). Tangential forces model friction, which is essential for our purposes since, under gravity, frictionless stable packs are only found for high volume fractions.

In MD simulations friction has important effects on the dynamics of the system: the frictional force between two grains depends on their shear displacement. In the Monte Carlo algorithm, however, it is convenient to consider the frictional force between two grains (that is their shear displacement) as an independent variable. This leads to the definition of two kind of MC moves: standard single particle displacement, and variation of the tangential shear displacement. The idea of separating geometrical properties of the pack (particle displacement) from the tangential forces (tangential shear variation) has been exploited previously in the literature, even though in a different contest and with simpler models (as for example in T.Unger, J.Kertész, and D. E. Wolf, Phys. Rev. Lett. 94, 178001 (2005); S. McNamara, R. Garcma-Rojo, and H. Herrmann, Phys. Rev. E 72, 021304 (2005)). Below we discuss briefly the two moves.

**Single-particle displacement**

One selects a particle \( n \) in position \( \vec{r}_n \) and a random displacement vector \( \vec{\Delta} \), with \(|\vec{\Delta}| < \lambda \) and \( \lambda \) dynamically varied in order to obtain an acceptance probability \( p_{acc} = 0.5 \). The displacement of particle \( n \) from position \( \vec{r}_n \) to position \( \vec{r}_n + \vec{\Delta} \) induces a variation \( \Delta E_r \) of the energy (eq. (4)), and of the auxiliary energy, \( \Delta E_{aux} \) (eq. (8)), of the system. \( \Delta E_{aux} \) is due to:

1. changes of the overlaps \( \vec{\delta}_{ni} \) between the displaced particle \( n \) and a particle \( i \), and therefore of the normal force \( \vec{f}_{ni} \). In particular contacts may disappear (after the displacement \( |\vec{\delta}_{ni}| < 0 \)), or appear (before the displacement \( |\vec{\delta}_{ni}| < 0 \), after the displacement \( |\vec{\delta}_{ni}| > 0 \)).

2. variations of the shear displacements \( \vec{u}_{ni} \), and therefore of the tangential force \( \vec{f}_{t_{ni}} \). If particles \( i \) and \( n \) are in contact both before and after the displacement of particles \( n \), we consider particle \( n \) as sliding over particle \( i \), inducing a variation of the shear displacement \( \vec{u}_{ni} \). If the displacement of particle \( n \) creates (destroys) a contact, then the shear displacement \( \vec{u}_{ni} \) is created (destroyed) accordingly.

The shear displacement is rescaled by a factor \( \mu |\vec{f}_{t_{ij}}|/k_t |\vec{u}_{ni}| \) if the Coulomb condition is violated. A move of this kind is accepted with probability \( \exp(-\beta_{conf} \Delta E_r - \beta_{aux} \Delta E_{aux}) \).

**Shear-displacements variation**

In this MC move one varies the tangential force between two contacting grains, respecting the Coulomb criteron. Two particles \( n \) and \( m \) are selected. If they are in contact one varies their shear displacement \( \vec{u}_{nm} \) of a random amount \( \Delta \), with \(|\Delta| < \sigma \) and \( \sigma \) dynamically varied in order to obtain an acceptance probability \( p_{acc} = 0.5 \). \( \Delta \) is actually chosen in such a way that \( \vec{u}_{nm} + \Delta \) (and therefore the tangential force) lies in the plane tangent to both grains in their point of contact. Before varying \( \vec{u}_{nm} \) by \( \Delta \) this latter is rescaled in order to satisfy the Coulomb criterion, if necessary.

The tangential move leads to a variation of both the energy of the system, \( E_r \) (as the elastic energy in tangential interaction between the two particles varies), and of its auxiliary en-
energy, $E_{aux}$. As before, the move is accepted with probability $\exp(-\beta_{conf}\Delta E_r - \beta_{aux}\Delta E_{aux})$.

Generation of mechanically stable states with the MC algorithm

Here we show how the volume fraction of the system evolves during the MC procedure. First we thermalize the system at the desired value of $T_{conf}$ and at $T_{aux} = 0.04$ mgd (upper panel). Different values of $T_{aux}$ may be convenient in different runs. Then we slowly decrease the auxiliary temperature until the system reaches a mechanically stable state (lower panel). We check that the same results are obtained with slower cooling rates.