Rhéologie (plasticité) et blocage (jamming) d'un granulaire sec modélisé comme un graphe

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Résumé. Un matériau granulaire dense et sec, avec friction tangentielle infinie, est modélisé comme un graphe connexe de grains reliés par des contacts purement répulsifs. Chaque grain peut donc soit rouler sans glisser sur un autre, soit s'en déconnecter. La stabilité sous cisaillement du granulaire est assurée par la présence de circuits impairs de grains en contact qui les empêchent de rouler l'un sur l'autre. Le matériau granulaire se trouve alors dans l'un de deux états thermodynamiques : solide fragile, bloqué ("jammed") par les circuits impairs, ou fluide sec, en leur absence. La dynamique du granulaire au voisinage de la transition de blocage, dans un tambour tournant à vitesse angulaire constante autour d'un axe horizontal, saute de manière intermittente entre les états solide et fluide. Dans l'état solide fragile, le granulaire suit un cycle limite alternant avalanches et entraînement par le tambour. C'est un comportement de "stick-slip" dans un solide soumis a une friction solide (entrainement par le tambour) et à une force de rappel (gravité). Dans l'état fluide, la force de friction est visqueuse, et le matériau granulaire tend vers un point fixe de pente constante. Si la friction tangentielle est supposée nulle, la modélisation comme un graphe et la frustration causée par les circuits impairs restent valables puisque la force entre grains demeure scalaire et répulsive.

Abstract. Dry granular matter, with infinite tangential friction, is modeled as a connected graph of grains linked by purely repulsive contacts. The degrees of freedom of a grain are non-slip rotation on, and disconnection from another. The material stability under shear (jamming) is ensured by odd circuits of grains in contact that prevent the grains from rolling on each other. A dense hard granular material has two possible states : fragile solid, blocked by odd circuits, and dry fluid or bearing, in the absence of odd circuits, that flows under shear by creation and glide of a pair of dislocations as in plasticity of continuous media. We did introduce the notions of blob, a region of the material containing only even circuits, and of critical contact that closes an odd circuit. The granular material is then represented, at low energies and critical applied shear, as a chain of blobs connected by critical contacts. A granular material inside a cylindrical drum rotating at constant velocity around its horizontal axis alternates intermittently between solid and fluid states. As a fragile solid, it follows a limit cycle of avalanches (slip) and stuck rotations with the drum. This is the stick-slip behavior of a solid subjected to solid friction (to the driving drum) and gravity. In the fluid state, the friction is viscous and the granular material flows to a fixed point with constant slope. For a vanishing tangential friction, the graph description with the frustrating odd circuits is still valid, because the force between grains remains a scalar and repulsive.

1 Introduction

We consider in this paper dry granular materials with a tangential friction that is either a) infinite [1,2] or b) vanishing [3,4]. In both cases, the granular material can be modeled as a *graph*, with in a), the dynamical variables carried by the vertices (non-slip rotation of a grain on another), whereas in b) they are carried by the edges (deformation of struts). Infinite tangential friction and non-slip rotation of the grains (a) provide a direct *mechanism* for the physical behavior of the granular material (unjamming a fragile solid into a dry fluid), and this is why we shall discuss first this model [1,2], and show that conditions b) lead, albeit indirectly, to the same geometrical organization of granular matter and the same dynamics.

Experimentally, dry granular materials have two possible states of flow under shear : a dry fluid [5,6] in which the particles roll without slip on top of each other (bearings), and a fragile solid [3,4], blocked by frustrating arches of particles in contact. The sudden transition between these two states relies on small, extended fluctuations in the medium, typical of second order transitions, unlike the melting of ordinary solids which is first-order. The fragile solid is geometrically frustrated. Indeed, flow is blocked by arches or circuits made of *odd* number of particles in contact with each other, which stabilize the solid state. In that case the particles (spheres, say) cannot roll freely on each other, thereby blocking any movement [7,8]. An odd circuit is fragile because it is inoperative once a single link is broken. This induces a long-range effect (arches can be large in a material without any global symmetry or regular ordering [9,10]) that leads to a second-order transition with scaling laws. Here the rheology takes place at various scales, from the smallest (dislocation glide determining the plasticity) to the largest (arches of size L of the system, responsible for jamming). Unjamming under external shear occurs as intermittency [11,12] rather than with hysteresis as in ordinary second-order phase transitions, because the line defect responsible for jamming (the R-loop) has negligible line tension.

A granular material is represented by a configuration of hard core spheres defining a graph where the center of each sphere is a vertex. Vertices are connected by links or edges depending on whether two adjacent spheres are in contact or not. Grains are made of spheres of radius R_i with i being the label of the individual sphere with arbitrary choice of the numbering since there is no intrinsic long-range ordering. We then define an adjacency matrix $\mathbf{A}$ of size $n \times n$, where n is the number of vertices. The elements $A_{i,j}$ are 1 if grain i and j are in contact, 0 else. We define also a valence matrix $\Delta_{i,j} = z_i \delta_{i,j}$, where $z_i = \sum_j A_{i,j}$ is the degree or valency of the vertex i.

2 Odd circuits, arches and critical contacts

The rotation (without slip) of spheres in contact is a connection from one grain to the other along paths. In the absence of odd circuits, this connection is independent of the path chosen (pure gauge) [9,10,7,8]. An odd circuit blocks or frustrates the free rotation. The dynamics of the graph is built from the scalar degree of freedom θ_i of each sphere. The system can be described by analogy with a system of springs of coupling constant k_s connecting the vertices considered as particles with moment of inertia I, kinetic energy T and potential V, but here the springs are struts with a repulsive interaction (stress-free contact is $\theta_i = -\theta_j$)

$$T = \sum_i \frac{1}{2} I \dot{\theta}_i^2, \quad V = k_s \sum_{i,j} A_{i,j} \left[1 - \cos\left(\theta_i + \theta_j\right)\right]. \tag{1}$$

The linearized Euler-Lagrange equations are given by the characteristic set of relations $(-\lambda \mathbf{1} + \mathbf{M})\,\theta = 0$ where $\mathbf{M} = \mathbf{\Delta} + \mathbf{A}$ is the dynamical matrix and $\lambda = I\omega^2/k_s$ the eigenvalue. Consider now a unitary matrix $\mathbf{O}$ such that $\mathbf{O^{-1}} = \mathbf{O}$ and $O_{i,j} = (-1)^i \delta_{i,j}$. In the case where only even circuits are present in the system, $\mathbf{M}$ is transformed according to $\mathbf{OMO^{-1}}$=$\mathbf{O\Delta O^{-1}}$+$\mathbf{OAO^{-1}}$=$\mathbf{\Delta} - \mathbf{A}$. $\mathbf{Q} = \mathbf{\Delta} - \mathbf{A}$ is a standard dynamical matrix for a system made of springs. $-\mathbf{Q} + z_0 \mathbf{I}$ ($z_0 > z_{max}$) is a positive matrix and the theorem of Perron-Frobenius applies. Since $\sum_j Q_{i,j} = 0$, it has $\lambda = 0$ as lowest non-degenerate eigenvalue, and *Woodstock* eigenvector $\theta'_i = \sum_j O_{i,j}\theta_j = 1$, or $\theta_i = (-1)^i$.

This transformation is equivalent to coloring as $(-1)^i$ the grains enumerated by labels i. $\mathbf{O}$ is a gauge transformation : it transforms both the coupling constants $\mathbf{M'} = \mathbf{OMO^{-1}}$ and $\theta' = \mathbf{O}\theta$. The critical links are identified as the only links where a pair of grains in contact have the same color. Without them, circuits are made of an even number of vertices, therefore the mapping defines a set of zero modes, one for each subgraph of even circuits (which we call *blob*). Odd circuits, through critical links, prevent the material behaving as a fluid. In their presence, the lowest eigenvalue is strictly positive (see [9,10] for details). This eigenvalue serves as an order parameter for the blocked phase, which is proportional to c, the number of critical links. Odd circuits block the system and prevent the material from behaving as a fluid. The lowest eigenvalue λ_{min} is bounded by $4c/n$ [9,10] from variational and algebraic arguments.

The set of critical links defines a minimal surface encircled by a loop. This R-loop [13] is the vorticity of the irreducible odd circuits with one critical link each (see Fig. 1). The forces in the fragile solid are concentrated on the frustrated arches blocking the material, and the lowest eigenvalue λ_{min} is a measure of the frustration. The existence of R-loops explains why it is impossible to describe continuously a granular material without defects. The "dry fluid" is in fact a perfect three-dimensional bearing [7,8] which does not resist shear, but is compressible. Under shear the grains rearrange and separate themselves to eliminate the odd circuits, and the material, albeit "dry", can contain more interstitial fluid such as water.

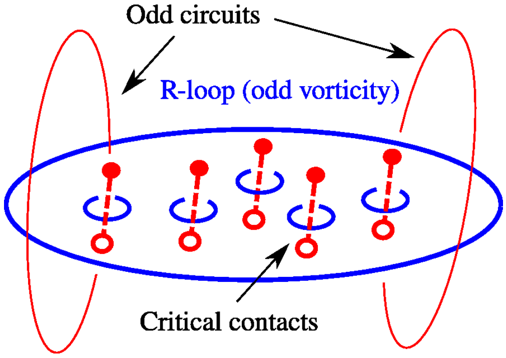


Figure 1. Minimal surface enclosing the critical links in a three-dimensional system. Each odd circuit has one critical link which crosses a surface bounded by a closed loop, R-loop. Several circuits can share the same critical link. The shortest is irreducible by definition.

The ratio c/n, with $c \sim L^{d-1}$ and $n \sim L^d$, is inversely proportional to the linear size L of the d-dimensional system, which is also the size of the largest R-loop near the transition fragile solid-dry fluid [9,10]. By contrast, in ordered crystallization, the R-loops are small, localized, and c/n is finite.

3 Chain of *blobs* (dry fluid domain represented by a generalized vertex) connected by critical contacts

For each R-loop, one can construct a chain of *blobs*, connected by one critical contact. The blobs are alternatively above and below the surface bounded by the R-loop. Blobs are regions of connected vertices without odd circuits, with zero eigenvalue or energy. The soft mode has, in each blob $\mathcal{B}_\alpha$, $\theta'_i = \theta_\alpha$ uniform and arbitrary. Blobs also interact with each other through non-critical links.

The granular material is thus represented as chains of blobs. Fig. 2 represents a typical chain of such blobs $\mathcal{B}_\alpha$, interacting with each other by effective coupling constants $J_{\alpha,\beta}$ for adjacent blobs of same parity α and β and by critical couplings $J^*_{\alpha,\beta}$ between consecutive blobs. Under shear, each blob can flow by plasticity (dislocation creation et glide). But the collapse of the material as a whole occurs by breaking all critical contacts. Near critical shear, only the largest R-loop survives (see Fig. 1 and 2). We can define an effective Hamiltonian for the low-lying energy states, since blobs are connected by a few links [1,2] : We can also add a time-dependent external periodic driving force (shear) of strength h_0 and phase $\theta_0(t) = \Omega t$. The elementary excitations of one particle is non-slip rotation on, and disconnection from another. A state of the material is given by the $\{\theta_\alpha\}$. The relative importance of the non-critical couplings between blobs depends on the surface-to-volume ratio of the blobs, which is small close to the unjamming transition where one largest R-loop remains and the blobs are large (see Fig. 2). The elementary excitations of the granular material are those of a chain of blobs, each with uniform θ_α, connected by critical couplings $J^*_{\alpha,\alpha+1}$. Accordingly, the density of states of low energy is a constant, independent of the energy in all space dimensions d [3,4,9,10,14].

We can identify two lowest energy states : A large enough external force h_0 imposes a homogeneous solution $\theta_\alpha = \theta_0(t)$. The penalty of such choice is located in the critical links. The other possibility is to minimize the energy in these critical links, leading to only two alternating solutions $\theta_\alpha = \pm(-1)^\alpha \theta_0(t)$, which penalizes the blobs, rotating in the direction opposite to the driving shear : If h_0 is large, the homogeneous configuration has lower energy ; physically the driving force tends to override the internal frustration forces located in the critical links. Otherwise, if h_0 is a finite threshold $\sim J^*$, the dynamics is imposed by the critical links.

The granular material may be forced to break the odd circuits, leading to the homogeneous state. Conversely, if odd circuits are reconnected, the system reverts to the alternative state. We can describe this transition by the averaged quantity $\theta = \sum_\alpha \theta_\alpha / N_{blob}$ and the dynamics by $\dot{\theta}$. For the homogeneous state, $\theta = \theta_0$, $\dot{\theta} = \Omega$. Otherwise, the average $\theta \simeq 0$ in the alternating state. This transition is related to the intermittency phenomena seen recently in [11,12] where a cylinder, half filled with glass beads, is set to rotate around its fixed, horizontal axis of revolution at a rate Ω. The angle $\theta(t)$ between the surface of the granular material and the horizontal plane switches intermittently between a fixed point of fluctuating, continuous flow (the homogeneous state, $\theta(t) \simeq$ constant, $\dot{\theta}(t) \simeq 0$), and a limit cycle of driven rotation $\dot{\theta}(t) = \Omega$ and large avalanches $\dot{\theta}(t) < \Omega$, that are indeed the two alternating states (stick-slip of the fragile solid) [1,2]. In the fragile solid state, the driving shear is due to the drum or to gravity. In the first alternative the chain of blobs is stuck to the drum, driven from the bottom, and $\theta_\alpha = (-1)^\alpha \Omega t$. When the chain of blobs is driven from the top, by gravity, $\theta_\alpha = -(-1)^\alpha \theta(t)$, where $\theta(t)$ is the angle defined just above, this situation describing avalanches.

4 Dynamics on graphs [15,16]

For a vanishing tangential friction [3,4], as for an infinite tangential friction, the force between two grains in contact is a scalar and the granular material can be modeled as a graph, with vertices representing the grains, and edges, the contacts between grains. A graph $\Gamma = \{V, E, F\}$ consists of several vector spaces $C_s(\Gamma) = \{C_0(\Gamma), C_1(\Gamma), C_2(\Gamma)\}$, involving vertices $i = 1...n (s = 0)$, edges $\gamma = 1...m (s = 1)$ and, possibly, circuits $J = 1...R_1 (s = 2)$ as vectors. A general vector in $i-$vector space is called an $i-chain$. Different (graded) vector spaces are related by the boundary operators ∂ or incidence matrices $E^{(0)}_{i\gamma} = \pm 1$ if edge γ is incident on (bounded by) vertex i, $= 0$ otherwise, $E^{(1)}_{\gamma J} = \pm 1$ if edge γ is part of circuit J. This requires an orientation of the edges and of the circuits. Poincaré's identity states that the boundary of a boundary is zero, thus $\partial . \partial = \mathbf{0}$ or $\mathbf{E^{(0)}}.\mathbf{E^{(1)}} = \mathbf{0}$: Circuits belong to the kernel of $\mathbf{E^{(0)}}$. One recovers the $n \times n$ adjacency matrix A_{ij} by the identity

$$\mathbf{E^{(0)}}.\mathbf{E^{(0)t}} = \mathbf{\Delta} - \mathbf{A} \tag{2}$$

independent of the orientation of the edges, where Δ is the diagonal, valence matrix defined above and $\mathbf{E^{(0)t}}$ denotes matrix $\mathbf{E^{(0)}}$ transposed. Consequently, like $\mathbf{E^{(0)}}$, $\mathbf{\Delta} - \mathbf{A}$ is of rank $n - 1$. Moreover, the $R_1 = m - (n - 1)$ edges not on a spanning tree (tree on Γ reaching all its vertices) form a basis for independent circuits (the famous 1847 result of Kirchhoff) [15,16]. The cyclomatic or first Betti number of the graph R_1 is the dimensionality of circuit space. The choices of any particular spanning tree, and of the orientation of the edges, are severely reduced in hard granular materials by the concept of *blobs* and *critical links* that constitute basic edges not on a spanning tree.

For an infinite tangential friction, the dynamical variables are the angles of rotation of the grains θ_i, located on the vertices of the graph. The physical state of the granular material is a vector $\mathbf{v} = \{v_i\} \in C_0(\Gamma)$. The Hamiltonian of the system is obtained from the dynamical matrix $\mathbf{M}$. It describes a chain of blobs α (each in a ground state of zero energy $\theta_\alpha \mathbf{a}$, $\mathbf{a} = \{a_i\} = (1, -1, 1, -1, ...)$ alternatively on the vertices of the blob), interacting through critical links that carry a finite energy.

For a vanishing tangential friction, the dynamical variables are strained struts, located on the edges of the graph. The physical state is a vector $\mathbf{e} = \{e_\gamma\} \in C_1(\Gamma)$. Consider two edges incident on the same vertex. They should have opposite orientations to represent struts (see Fig. 3a and 3b). This is possible for even circuits only (circuits with an even number of struts). For each odd circuit, there is one *critical edge* carrying a finite energy J^*. It specifies the odd circuit, gives it its orientation and is not on the spanning tree. Thus, $\mathbf{e} = \{e_\gamma\} = (1, -1, 1, -1, ... -1)$ for even circuits, $\mathbf{e} = (1, -1, 1, -1, ... -1; 1)$ for odd circuits (the critical edge component is 1, separated by a ;), and

$$E^{(1)t}_{J\gamma} e_\gamma = 0, \text{ even circuit}; E^{(1)t}_{J\gamma} e_\gamma = 1, \text{ odd circuit}. \tag{3}$$

The orientation is consistent at each vertex of degree z_i (i.e. all incident edges have the same orientation), except at the vertex bounding a critical edge with the wrong orientation (Figs 3b and 3c), hence

$$E^{(0)}_{i\gamma} e_\gamma = \pm(z_i - 2) \text{ if a critical edge is incident on vertex } i \text{ with the wrong orientation,}$$
$$E^{(0)}_{i\gamma} e_\gamma = \pm z_i \text{ everywhere else.} \tag{4}$$

We recover the chain of blobs interacting through critical links, obtained for infinite tangential friction. But here as for electric networks, the physical state vectors are in the edge-space of Γ, where they obey the circuit and vertex equations above (known as *Kirchhoff's laws* in electrical networks, where the right-hand side = 0) [15]. Here, the critical edges are **not** on the spanning tree : they form the basis for (independent) odd circuits. Out of the R_1 independent circuits, c are specified by the critical edges. Within the blobs, the spanning tree remains arbitrary (Fig. 2).

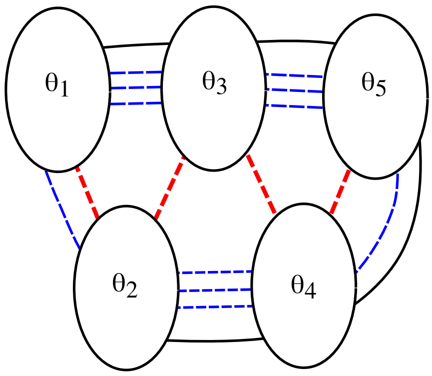
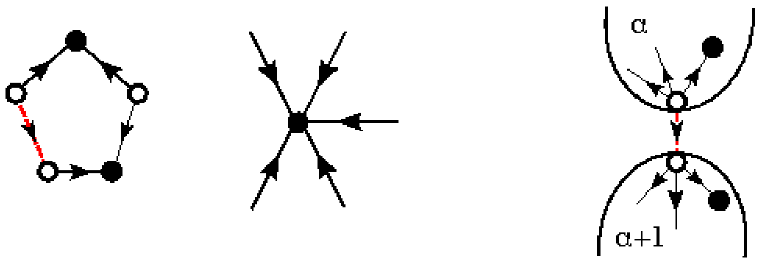


Figure 2. Chain of blobs representing the granular material near unjamming as grains in contact through struts (zero tangential friction). The blobs θ_α are dry fluid domains (each spanned by an arbitrary tree) connected by critical (red, thick-dashed) or non-critical links (blue thin-dashed and black lines). The black lines and the blobs constitute a spanning tree for the material. Cf. the nearly identical figure in [1,2] illustrating infinite tangential friction.

Each blob α has an arbitrary spanning tree, with a non-frustrated dynamics. It can be described by the variable θ_α (see Fig. 2) as a renormalized vertex in a general graph (the non-critical links between two blobs are multiple, whereas there is only one critical link between two (vertices of different) blobs). Only one non-critical link between two blobs is needed to constitute a spanning tree (in Fig. 2, one would need a non-critical link between blobs 5 and 4, or between blobs 1 and 2), so that the c critical links and almost all non-critical links constitute a basis for independent circuits.

The last section of this paper was motivated by a stimulating discussion at Yale (O'Hern group and NR, Nov.'11).



(a) (odd) circuit (b) vertex ($z_i = 5$) (c) critical edge between blobs α and $\alpha + 1$

Figure 3. Physical state for vertices (grains) connected by struts. In (c) the critical edge is incident on blob α with the proper orientation. The critical edge (red, thick-dashed line), $\notin$ the spanning tree, imposes the orientation of the circuit.

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