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Some numerical methods in multibody dynamics: application to granular materials

J. J. MOREAU

ABSTRACT. – The unilaterality of non-penetration constraints, the velocity jumps which occur in case of collisions, the irregularity of the law of dry friction are 'nonsmooth' features of the dynamical systems in view. Numerical methods are presented, which face nonsmoothness without resorting to mollifying approximation procedures. A careful formulation of contact laws generates algorithms which, at every step of the time-discretization, are ready to face possible collisions on the same footing as permanent contacts. These algorithms prove efficient enough to treat on microcomputers or small workstations the dynamical motion of systems involving a few thousands of bodies.

Granular materials are modelled as collections of spherical beads. The concerned numerical technique has recently permitted to discover a mechanism underlying the phenomenon of size-segregation in a granular material contained in a vertically shaken vessel. This mechanism, which connects segregation with the convection currents induced by boundary friction, has been exhibited independently by some experimentalists. The numerical assessment of boundary forces, presented here, throws some light on the generation of boundary currents.

1. Introduction

Several computational techniques are currently used in the dynamics of collections of bodies, during the motion of which contacts, generally subject to friction, are susceptible to occur or to break.

The most popular ones, commonly called Distinct Element or Discrete Element Methods, derive from the pioneering work of P. A. Cundall [Cundall, 1971][Cundall & Strack, 1979] or are adapted from the procedures applied in numerical Molecular Dynamics. They consist in approximating the mechanical constraint of *non inter-penetrability* of each body pair by some close-range steep repulsion law. In addition, on every time interval where two bodies are close enough to be viewed as contacting (numerically, they may appear to overlap a little), they are assumed to exert on each other some dissipative forces, depending on velocities in a smooth way which mimicks friction. Thereby, the evolution problem is approximately reduced to the integration of a system of second order differential equations, to which classical methods are applied. The steeper the approximate laws of interaction, the more realistic are the results, at the price of reducing the time-step length for the sake of numerical stability.

Alternatively, while approximating non inter-penetrability in the same way as above, one may model the inelasticity of possible collisions by assigning different repulsion coefficients to loading

and to unloading [Walton & Braun, 1986]. Friction, on the other hand, may be handled by applying directly the law of Coulomb [Walton, 1993a,b].

Many significant simulations of motions have been obtained by some of these computation techniques, for systems of bodies which may either be fully deformable or treated as macroscopically rigid.

A different approach is presented in this lecture, characterized by the absence of smoothing approximation.

Precisely, the problems in view are *nonsmooth* in three respects :

- The geometric effect of non inter-penetrability is expressed by a set of inequalities, instead of the equalities associated with traditional (bilateral) mechanical constraints. In other words, non inter-penetrability is a unilateral constraint, which makes that, in the space of the configuration variables, the feasible set is a region limited by a collection of surfaces. The boundary of such a region is liable to present a great number of multi-dimensional singularities, a situation similar to what is commonly met in problems arising from Operation Research. This is *nonsmoothness in space*. Furthermore, the physical realization of non inter-penetrability, like that of any mechanical constraint, rests on the action of 'forces of constraint' or 'reactions'. These forces vanish as soon as the concerned bodies separate out, while during contact no function is available to express them completely : all what is known is that reactions belong to some configuration-dependent sets. In regard to such irregular relationships between forces and configurations, one may say that *non-smoothness in force-law* goes with non-smoothness in space.
- In the event of a collision, the function of time which represents the system velocity is expected to be discontinuous. This is *nonsmoothness in time*.
- If the friction considered at contact points is of the *dry* sort, for instance Coulomb's friction, it is governed by a relationship between the reaction force and the local relative velocity which makes another instance of nonsmoothness in force-law.

Motivated, in particular, by the needs of Operation Research and Economics, formal and computational developments have taken place in recent decades, giving birth to a mathematical domain called 'Nonsmooth Analysis' (see e.g. [Clarke, 1989][Hiriart-Urruty & Lemarechal, 1993]). This includes 'Multivalued Analysis', i.e. the treatment of set-valued functions (see e.g. [Aubin & Frankowska, 1990]). The application of such tools to mechanical topics has been systematized under the title of 'Nonsmooth Mechanics' [Moreau et al., 1988][Moreau & Panagiotopoulos, 1988]. The approach presented in this lecture has been developed in this spirit.

We propose to call this approach the *Contact Dynamics method*.

Another numerical strategy, also avoiding the use of mollifying approximations in multibody dynamics, has recently been proposed [Hogue & Newland, 1993]).

At the mathematical level, the study of nonsmooth dynamical problems (existence of solutions, possible cases of uniqueness, approximation procedures, etc.) is the subject of current research [Monteiro Marques, 1993][Paoli & Schatzman, 1993].

2. Outline and discussion

Let be chosen a division of the time-interval I , with origin t_0 , into (usually equal) subintervals. At every of these time-steps, the proposed algorithms will be ready to face collisions on the same

footing as lasting contacts. This is equivalent to treating the latter as successions of mini-collisions. Significantly in [Baraff, 1991], a paper with mechanical insight but aimed at the production of artistic Computer Graphics animations, the same attitude is preconized on the basis of computational complexity assessments.

This uniform treatment is made possible by imposing on the information available about the physical circumstances of contact to be stated under a standardized formalism that we call a 'complete contact law' : see Sec. 5 below. This formalism takes care automatically of the non inter-penetrability constraint and of the possibility of some contacts to break in the course of the motion, but leaves widely open the choice of phenomenological descriptions for friction and for collisions.

In the sort of applications we are to present at the end of this lecture, namely the dynamics of dry granular materials, the law of Coulomb is generally accepted as a fairly good representation of friction.

More problematic is the modelling of collisional processes. By referring to rigid body collisions, one means that the involved bodies show sufficiently small deformation for being geometrically considered as rigid at the global observation scale [Stronge, 1990][Brach, 1991][Wang & Mason, 1992]. In most of the literature devoted to this subject, authors tend to analyse such a collision as a microscopic phenomenon localized in the vicinity of the impact locus : at this scale, material deformability is taken into account (using models of elastic, visco-elastic or elasto-plastic behaviour), as well as the evolution of the small contact zone in which stick and slip regions may be distinguished [Maw et al., 1981]. Situations to which such an analysis is relevant certainly exist but, in general, the consequences of collisions are not localized. For instance, material dissipation in the vicinity of the impact is not the only cause of the energy loss observable at the macroscopic level. Even if the bodies are assumed perfectly elastic, energy conservation cannot be expected. In fact, disturbances are likely to propagate from the collision locus to the whole system and also, if the latter is linked with some external support, to the outside world. After contact recedes, a state of vibration should persist. At the macroscopic observation level, this does not contradict the rigidity assertion, but the energy involved in microscopic agitation may not be negligible. Also as a consequence of vibrations, a collision may, at the microscopic time-scale, split into several separate contact episodes : an example of such a double bounce is calculated in closed form in [Timoshenko, 1948, Chap. 12]. Finite element computation of the collision of two elastic bodies performed in our laboratory has shown the same. This makes the outcome of a collision strongly depend on the shape of the concerned bodies.

Fortunately, the case of spherical objects, widely invoked in the simulation of granular materials, proves more tractable. A collision law involving three parameters, identified as the *friction coefficient*, the *normal restitution coefficient* and the *tangential restitution coefficient* has been discussed [W, 1993a][Lun & Bent, 1993] and experimentally found acceptable [Foerster et al., 1994].

In view of this complexity, we choose to be content with a pragmatic description of collisions, whose validity has to be investigated, in each class of applications, by comparing the results of calculations with some calibrated experiments. It consists in asserting that a complete contact law, of the same form as that which applies to standing contact, holds between the contact percussion and a certain formal local velocity. The latter is constructed by an averaging procedure involving the (known) local velocity before collision and the (unknown) local velocity after (see Sec. 6 below). In the case of spherical bodies, the resulting formulas are found strictly equivalent to those produced by

the above mentioned model, based on normal and tangential restitution coefficients, thus have the same domain of acceptability.

The efficiency of CD methods in the dynamics of granular materials mainly stems from that, once a time-discretization has been chosen, all the collisions which are detected as occurring on a given time-step are treated together. This of course entails some trade-offs which have to be assessed. It seems immaterial that the ordering of the collisions, which mechanically should be successive, is only internal to the algorithm (it depends on the objects numbering; randomizing it in the course of computation has not been judged useful). In fact, the problems in view are physically undeterministic, since a slight change in the initial conditions is enough to produce, after a short time, a completely different sequence of positions and collisions. A more critical observation is that each collision is treated as occurring only once between the involved bodies in the considered time-step. An accumulation of bounces, such as those of a ping-pong ball coming to rest, is thus viewed as a single collision as soon as the successive bounces are all comprised in the time-step. This could result in underestimating the global energy loss arising from inelastic collisions. This source of error may be checked by repeating computation with the time step reduced to half : if no change is found in the energy vs time curve, one may conclude that no harm was done.

Another delicate matter is that, in compact assemblies, the bodies involved in a collision may be part of clusters of objects previously in contact. The propagation of impulses through such clusters raises questions of the same nature as sound in granulate materials.

Anyway, the ultimate criterium of the usefulness of a computation method consists in comparison with calibrated physical experiments. In [Clément et al., 1992][Duran et al., 1993][Rajchenbach et al. 1993] a two-dimensional experimental set-up is described. A container is made of two parallel vertical glass plates and of lateral boundaries of various shapes (circular when spinning drum experiments are devised, rectangular for shaken boxes). Metallic spherical beads with uniform diameter, to which the space available between the glass plates has been adjusted, are introduced. Also, when size-segregation is investigated, larger circular objects with bead-inserts securing correct guiding by the glass plates are added. The high friction coefficients (say 0.8) needed in some experiments is provided by using oxidized aluminium beads or chemically corroded steel beads. Restitution is naturally higher with steel than with aluminium. The fairly large size of the beads (usually 1.5 mm in diameter) makes the effect of air negligible, as it has been tested by counter experiments performed in a void.

Visually, the concordance between these physical experiments and the animations displayed on the computer screen seems almost perfect. Due to the majority of objects having the same diameter, cristal-like arrangements are generally formed whose dynamical behaviour involves some delicate features : dislocations, propagation of defects, etc.. very well reproduced by CD computations. One of these specific effects is the sporadic occurrence, in the upper corners of a vertically vibrated rectangular pack of beads, of *dislocation vortices*. Figure 1 shows how this is rendered on the computer.

Heaps at the surface of vibrated packs of beads are also reproduced by computation [M, 1993].

Such experiments involving the dynamics of very dense assemblies make severe tests for numerical models. Quantitative comparison is currently in progress.

Inertia of the concerned bodies plays an essential part in CD algorithms. This does not preclude the use of the method in computing the *quasi-static* evolutions of granular materials familiar in many situations of civil engineering [Yemmas, 1993]. In that case, one is tempted to view the inertia terms

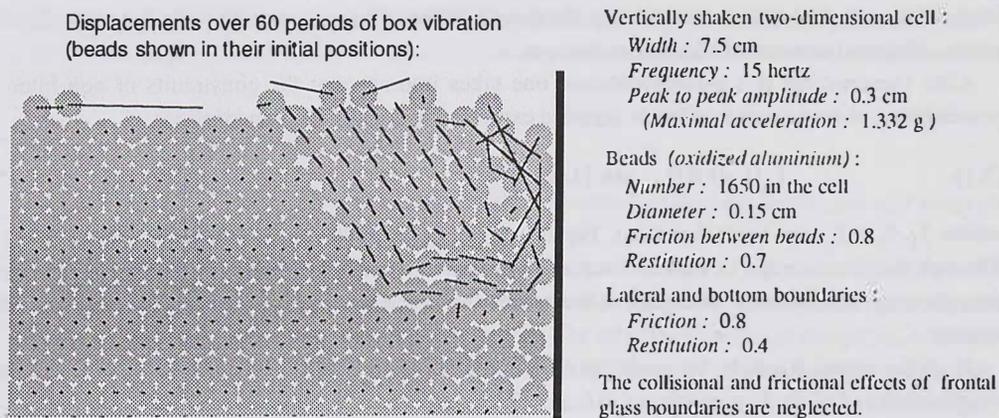


Fig. 1. – Corner circulation in a vertically shaken box.

(Numerical simulation for comparison with experiments of E. Clément, J. Duran & J. Rajchenbach [Clément 1992])

as mere numerical mollifiers whose values might be adjusted for the sake of computation efficiency. Actually, it proves safer to keep these terms with their true physical values. In fact, the experiments commonly made with assemblies of cylinders (Schneebeli materials) show that, however slow the evolution of the control parameters may be, the deformation of the pack takes place through local crises which essentially are dynamical processes [Meftah & al., 1993]. An example of evolution of this sort is shortly presented in [Jean, 1994], where the results of a CD method are compared with those obtained by Cundall's TRUBAL software.

The applications of CD methods have not been limited to round granules. Simulations of buildings made of rectangular blocks assembled without mortar (the case of ancient Greek monuments) supported by quaking ground have been performed. A series of drawings may be found in [Jean & Moreau, 1992] showing the progressive damage and the partial collapse of a wall due to ground oscillation. In this case too, the validity of the assumed contact laws has to be checked. Comparisons with the experiments described in [Ageno & Sjinopoli, 1991] and [Raous, 1993] induce to make the normal and tangential restitution coefficients equal to zero for problems of this sort. More elaborate contact laws remain to be designed, in order to describe masonry with mortar bonds. There is no algorithmic difficulty in making such laws depend on the motion history.

The use of CD methods in the numerical treatment, through finite elements, of dynamic or quasi-static problems involving *deformable bodies* is out the scope of this lecture [Jean, 1993].

The dominant features of all CD algorithms is that they are time-discretization schemes *of the implicit type with regard to velocities*.

3. Analytical setting

Let the configurations of the system members be parametrized, at least locally, through generalized coordinates, say $q = (q^1, q^2, \dots, q^n)$. As usual such a reduction to finite freedom is assumed to result

from (bilateral) ideal constraints, namely the strict rigidity of the system members and the possible action of internal or external frictionless linkages.

After constructing this parametrization, one takes into account the constraints of non interpenetrability ; their geometric effect is assumed expressed by a finite set of inequalities

$$(3.1) \quad f_{\alpha}(t, q) \leq 0, \quad \alpha \in \{1, 2, \dots, \kappa\},$$

where $f_1, f_2, \dots, f_{\kappa}$ are given functions. Equality $f_{\alpha} = 0$ corresponds to the occurrence of a *contact*. Through the presence of t in such an inequality, provision is made for the case where the inequality describes the confinement of a part of the system by some external boundaries with prescribed motion.

In all the sequel, it will be assumed that each of the functions f_{α} is C^1 , with $\partial f_{\alpha} / \partial q \neq 0$ at least in a neighbourhood of the hypersurface $f_{\alpha} = 0$ of \mathbf{R}^{n+1} .

For every imagined motion $t \rightarrow q(t)$ and for t such that the derivative $\dot{q}(t) \in \mathbf{R}^n$ exists, the kinetic energy has an expression of degree 2 in \dot{q} , say

$$(3.2) \quad \mathcal{E}_k(t, q, \dot{q}) = \frac{1}{2} A_{ij}(t, q) \dot{q}^i \dot{q}^j + B_1(t, q) \dot{q}^i + C(t, q),$$

where A is a symmetric positive definite $n \times n$ -matrix, $B \in \mathbf{R}^n$ and $C \in \mathbf{R}$. In the usual case of *scleronomic* (i.e. time-independent) parametrization, A is constant in t , while B and C vanish.

As far as *smooth*, i.e. twice differentiable, motions are concerned, the system Dynamics is governed by Lagrange's equations, here written as an equality in \mathbf{R}^n

$$(3.3) \quad A(t, q) \ddot{q} = F(t, q, \dot{q}) + \sum_{\alpha} r^{\alpha}.$$

The expression F comprises standard terms of Lagrange's equations and the covariant components, relative to the parametrization (q), of some applied forces supposed given as functions of time, position and velocity. The element r^{α} of \mathbf{R}^n is made of the covariant components of the *contact forces* experienced by the system in case the contact $f_{\alpha} = 0$ holds. Their construction rests on the standard definition of the covariant components in \mathbf{R}^n of forces located in physical space, so this construction is connected as follows with the system kinematics.

First suppose that inequality $f_{\alpha} \leq 0$ expresses the mutual non inter-penetrability of some pair of members of the system, say \mathcal{B} and \mathcal{B}' , so that equality $f_{\alpha} = 0$ corresponds to these two bodies touching each other at some point of space denoted by M_{α} . This we shall assume to be an isolated contact point, but other contacts, corresponding to different values of α , may also be in effect between the same bodies at the same instant. For every imagined motion $t \rightarrow q(t)$ bringing the system through the considered contact position for some value of t , the velocities \mathcal{V}_{α} and \mathcal{V}'_{α} of the respective particles of \mathcal{B} and \mathcal{B}' passing at point M_{α} let themselves be expressed as affine functions of the value u of the derivative \dot{q} . The same is thus true for the *relative velocity* $\mathcal{U}_{\alpha} = \mathcal{V}'_{\alpha} - \mathcal{V}_{\alpha}$ of \mathcal{B} with respect to \mathcal{B}' at this point, say

$$(3.4) \quad \mathcal{U}_{\alpha} = G_{\alpha} u + \mathcal{W}_{\alpha},$$

where $G_{\alpha}: \mathbf{R}^n \rightarrow \mathbf{R}^3$ denotes a linear mapping, depending on t and q . No attention is paid at this stage to the imagined motion preserving contact or not. The term $\mathcal{W}_{\alpha} \in \mathbf{R}^3$, a known function of t and q , vanishes in the usual case of a scleronomic parametrization.

Let \mathcal{R}^α denote the contact force that body \mathcal{B} experiences at point M_α from body \mathcal{B}' ; then \mathcal{B} experiences from \mathcal{B}' the force $-\mathcal{R}^\alpha$. Classically, the covariant components of this pair of forces are expressed by

$$(3.5) \quad r^\alpha = G_\alpha^* \mathcal{R}^\alpha,$$

with $G_\alpha^*: \mathbf{R}^3 \rightarrow \mathbf{R}^n$ denoting the transpose of G_α (the convention of implicit summation will never be applied to Greek indices).

Similar formulas hold if inequality $f_\alpha \leq 0$ represents the confinement of a part \mathcal{B} of the system by some external boundary with prescribed motion. Assume that equality $f_\alpha = 0$ corresponds to contact taking place at some point, here again denoted by M_α . The relative velocity, at this point, of \mathcal{B} with respect to the boundary has an expression of the form (3.4), where \mathcal{W}_α now takes into account the known velocity of the boundary, while r^α in (3.5) equals the covariant components of the force \mathcal{R}^α alone, acting on \mathcal{B} . Its counterpart $-\mathcal{R}^\alpha$, exerted by \mathcal{B} upon the boundary, is no more in this case a force experienced by the system.

In both cases; the following relationship is found [M, 1988b] to hold between $\partial f_\alpha / \partial q$ and the normal unit vector \mathbf{n}^α at point M_α to the two contacting bodies, *directed toward* \mathcal{B}

$$(3.6) \quad \exists \lambda \geq 0 \quad \text{such that} \quad G_\alpha^* \mathbf{n}^\alpha = -\lambda \partial f_\alpha / \partial q.$$

In all the sequel, we shall assume that the mapping G_α is *surjective* of \mathbf{R}^n to \mathbf{R}^3 ; equivalently, its transpose G_α^* is *injective* of \mathbf{R}^3 to \mathbf{R}^n . Only some special positions of certain linkages may give rise to 'wedging' effects which break this assumption.

4. Nonsmooth formulation

Due to the bodies being treated as perfectly rigid, possible collisions appear as instantaneous processes. The velocity function $t \rightarrow u(t) = \dot{q}(t)$ of the time interval I into \mathbf{R}^n is expected to be discontinuous at the corresponding instants. Of course, this is only a formal way of condensing the available information regarding a very brief episode, during which u is differentiable and governed by the differential equations of regular Dynamics, but with 'very large' contact forces.

The natural mathematical setting allowing for the function u to exhibit jumps consists in assuming that this function has *locally bounded variation* from I into \mathbf{R}^n (notation: $u \in \text{lbv}(I, \mathbf{R}^n)$), i.e. it has bounded variation on every compact subinterval of I . Classically, with every such u , an \mathbf{R}^n -valued measure on I is associated, called the *differential measure* or *Stieltjes measure* of u and denoted in this paper by du . The reader may refer to [M, 1988a] as an expository text on this subject (see also [Moreau & Valadier, 1987][M, 1989] for some specific aspects).

On every subinterval where u possesses a continuous derivative, say u'_t , one has $du = u'_t dt$ i.e. the measure du admits u'_t as *density function* relative to the Lebesgue measure dt of this time interval (this is more generally true if u is a *locally absolutely continuous function* so that u'_t is an element of $L^1_{\text{loc}}(I, dt; \mathbf{R}^n)$).

Any $u \in \text{lbv}(I, \mathbf{R}^n)$ possesses at every point t of I a *right-limit* and a *left-limit*, respectively denoted by $u^+(t)$ and $u^-(t)$ (by convention the left-limit at the initial instant t_0 is interpreted as $u(t_0)$).

and the symmetric convention applies to the possible final point of I). Typically, for every compact subinterval $[a, b]$ of I , one has

$$(4.1) \quad \int_{[a,b]} du = u^+(b) - u^-(a).$$

This holds in particular for $a=b$, i.e. the integral of the measure du over the singleton $\{a\}$ equals the jump of u at point a . Thus the point a carries an *atom* of the measure du if and only if the jump is nonzero.

The traditional *theory of percussions* rests on the integration of both members of the differential equation (3.3) over the 'very short' interval of a collision process. Since the term F remains bounded on the interval, its integral is negligible, as well as the change of the configuration function q . All what is left is this equality, valid at the instant t of the collision

$$(4.2) \quad A(t, q) (u^+(t) - u^-(t)) = \sum_{\alpha} P^{\alpha}.$$

The terms P^{α} here equal the respective integrals, over the very short time interval, of the covariant components of the 'very large' contact forces. By definition, these integrals constitute the covariant components of the *contact percussions*.

The velocity function u constitutes the central unknown of the evolution problem, to which the configuration function $t \rightarrow q(t)$ is related through

$$(4.3) \quad q(t) = q(t_0) + \int_{t_0}^t u(s) ds$$

The differential equation (3.3), valid on any interval of smooth motion, may then be written as

$$(4.5) \quad A(t, q) u'_t = F(t, q, u) + \sum_{\alpha} r^{\alpha}.$$

Let us regard both members as the density functions, relative to the Lebesgue measure dt on the considered time interval, of some \mathbf{R}^n -valued measures. The equality of these measures

$$(4.6) \quad A(t, q) du = F(t, q, u) dt + \sum_{\alpha} dR^{\alpha}$$

is equivalent to the differential equation (4.5) holding all over I . This may be called a *measure differential equation*. The terms $dR^{\alpha} = r^{\alpha} dt$ in this writing constitute the *contact impulsion* measures. In such a smooth case they happen to admit density functions with regard to dt which properly express reaction *forces*. In contrast, for the collisional situation described in the foregoing, percussions contribute in the contact impulsion through vector measures which do not possess densities relative to dt . Contact percussions actually are *atoms* of the contact impulsion measures and the elements P^{α} of \mathbf{R}^n equal the densities of these atoms relative to δ_t , the Dirac measure at the point t of I .

This is a general fact that, for a finite collection of \mathbf{R} -valued or \mathbf{R}^n -valued measures on the interval I , such here are dt, du, dR^{α} , there exists (non uniquely) a positive real measure, say $d\lambda$, relative to which they possess respective density functions $\iota_{\lambda} \in L^1_{loc}(I, d\lambda; \mathbf{R})$, $u'_{\lambda} \in L^1_{loc}(I, d\lambda; \mathbf{R}^n)$, and $R^{\alpha}_{\lambda} \in L^1_{loc}(I, d\lambda; \mathbf{R}^n)$. An alternative writing of the measure differential equation (4.6) therefore is

$$(4.7) \quad A(t, q) u'_{\lambda}(t) = F(t, q, u) \iota'_{\lambda}(t) + \sum_{\alpha} R^{\alpha}_{\lambda}(t),$$

holding for every t in I (with the possible exception of a $d\lambda$ -negligible subset : equivalently one may assign null values to the respective density functions on such a subset, so as to make (4.7) actually hold everywhere in I).

The element $R_\lambda^{\prime\alpha}(t)$ of \mathbf{R}^n consists of the covariant components of a 3-dimensional vector of physical space, localized at the contact point M_α , say $\mathcal{R}_\lambda^{\prime\alpha}(t)$, and the same correspondence as in (3.5) holds, namely

$$(4.8) \quad R_\lambda^{\prime\alpha}(t) = G_\alpha^*(t, q) \mathcal{R}_\lambda^{\prime\alpha}(t)$$

REMARK 1. In (4.1) the function u appears only through its left- and right-limits : the value that it may take at some discontinuity point is immaterial there. The same is true for (4.3), since classically the set of the discontinuity points of an lbv function is countable, hence negligible in the integration with respect to dt . So the values that one may assign to the velocity function at the exact instants of collisions bear at the present stage no dynamical significance. This latitude will be exploited in the forthcoming Sections.

REMARK 2. One may ask why the treatment of such nonsmooth effects as collisions should rest only on measure differential equations, instead of more general evolution laws involving time-distributions of higher order. Some justification of this peculiarity may be found in [M, 1989a] : the unilaterality of the non inter-penetrability constraint imposes on contact impulses a *sign* condition. Now it is known that a signed distribution is automatically of order zero, i.e. it equals a measure. Let us stress that the present formulation owes nothing to a so-called *principle of constraint*, according to which "constraints shall be maintained by forces, so long as this is possible; otherwise, and only otherwise, by impulses".

5. The general form of a contact law

As already said, in CD methods, one starts with the choice of a subdivision of the investigated time interval. Over each subinterval, persistent contacts are to be treated on the same footing as possible collisions. Also some previously effective contacts may get loose at some instant and, even in the case of smooth motions, this is known to be a nontrivial matter. The traditional approach to contact break consists in tentatively calculating the motion under the assumption that all contacts present at a considered instant remain effective. If the calculation of contact forces in the course of such a motion yields, at a further instant, an unfeasible direction, one concludes that some contacts should break at this instant, so the continued motion has to be calculated differently. But contacts which break are not necessarily those for which unfeasible contact forces were just found (for the frictionless case, see [Delassus, 1917][M, 1963]).

In order that the algorithms handle all such circumstances correctly, one has to design carefully the *contact laws*, i.e. the admitted relationships between the local velocities and the corresponding contact forces - more generally the densities of contact percussions with regard to a base measure $d\lambda$. For each contact assumed to correspond to a certain constraint function f , such a law has the form

$$(5.1) \quad \text{law}(t, q, \mathcal{U}, \mathcal{R}) = \text{true.}$$

For legibility, the index α specifying the concerned contact has been dropped and one simply writes \mathcal{K} instead of $\mathcal{K}_\lambda^\alpha$. Strictly speaking, the normal unit \mathbf{n} and the mapping $G: \mathbf{R}^n \rightarrow \mathbf{R}^3$ make sense only if contact holds, i.e. if $f(t, q) = 0$. For constructing numerical methods (as well as in the study of existence of solutions [Monteiro Marques, 1993]), the definition of these two elements is assumed extended, in a smooth arbitrary way, to values of t and q laying in a neighborhood of the hypersurface $f=0$.

One is looking for motions which, in addition to the dynamical equation (3.3), actually taken under its nonsmooth form (4.6), satisfy the geometrical conditions of non inter-penetrability (3.1). *Contact laws will be formalized in such a way that they take care of that also.*

Here is the key concept.

DEFINITION. A relation of the form (5.1) is said to be a complete contact law if it involves the three following implications

$$(5.2) \quad f(t, q) < 0 \Rightarrow \mathcal{K} = 0,$$

$$(5.3) \quad f(t, q) \geq 0 \Rightarrow \mathbf{n} \cdot \mathbf{u} \geq 0,$$

$$(5.4) \quad \mathbf{n} \cdot \mathbf{u} > 0 \Rightarrow \mathcal{K} = 0.$$

Let us comment on the importance of (5.3). Put

$$(5.5) \quad \mathcal{K}(t, q) = \begin{cases} \{ \mathbf{u} \in \mathbf{R}^3 : \mathbf{n} \cdot \mathbf{u} \geq 0 \} & \text{if } f(t, q) \geq 0 \\ \mathbf{R}^3 & \text{if } f(t, q) < 0, \end{cases}$$

called the set of the *right-admissible* values for the relative velocity of the two concerned bodies at the contact point M . The following is easily established [M, 1986b] :

Let I be a time-interval with origin t_0 and let a motion $q: I \rightarrow \mathbf{R}^n$ be defined through a locally integrable velocity function $u: I \rightarrow \mathbf{R}^n$ by relation (4.3). If $\mathcal{U}(t) = G(t, q)u(t) + \mathcal{W}(t, q)$ belongs to $\mathcal{K}(t, q(t))$ for almost every t and if inequality $f(t, q(t)) \leq 0$ holds at the initial instant t_0 , then this inequality holds for every $t \in I$.

In other words, provided the initial position is correct, the non inter-penetrability condition $f \leq 0$ is automatically taken care of by (5.3). Observe that this statement is sensitive to the ordering of time. In the symmetric assertion involving, instead of the initial instant t_0 , the possible final point of I , one should replace \mathcal{K} by $-\mathcal{K}$, which may be viewed as the set of the *left-admissible* values of \mathbf{u} .

The importance of (5.4) will only become apparent in the next Sections, devoted to the treatment of collisions and to numerical algorithms.

In order to demonstrate that the concept of a complete contact law has more theoretical consistency than a mere programming trick, two usual examples are presented below.

Let us first recall a standard definition of Convex Analysis.

Let C denote a convex subset of \mathbf{R}^3 and let $a \in C$. The subset

$$(5.6) \quad N_C(a) = \{ \mathbf{x} \in \mathbf{R}^3 : \forall y \in C \quad \mathbf{x} \cdot (y-a) \leq 0 \}$$

is called *the (outward) normal cone to C at point a*. In the context of Convex Analysis, it proves consistent to define $N_C(a) = \emptyset$ if $a \notin C$. For every $a \in C$, $N_C(a)$ contains at least the zero of \mathbf{R}^3 and reduces to this single element whenever a is an interior point of C .

The normal cone more generally makes sense when a pair of arbitrary linear spaces is considered, with a bilinear pairing playing the role of the dot product of \mathbf{R}^3 . That is a common situation in Mechanics, the two linear spaces then consisting of 'forces' and 'velocities', paired through the bilinear form 'power'.

EXAMPLE 1 : *Frictionless contact.*

Let us denote by $\mathcal{N}(U)$ the normal cone at point $U \in \mathbf{R}^3$ to the convex set $\mathcal{X}(t, q)$ defined in (5.5). For $f(t, q) \geq 0$, the latter is a closed half-space, so $\mathcal{N}(U) = \{0\}$ if $\mathbf{n} \cdot U > 0$ and $\mathcal{N}(U) = \emptyset$ if $\mathbf{n} \cdot U < 0$. If U lies in the boundary of the half-space, $\mathcal{N}(U)$ consists of the half-line generated by $-\mathbf{n}$. For $f(t, q) < 0$ the set $\mathcal{X}(t, q)$ equals the whole of \mathbf{R}^3 , so $\mathcal{N}(U) = \{0\}$ for every U in this case. Consequently, in the writing

$$(5.7) \quad -\mathcal{R} \in \mathcal{N}(U)$$

a complete contact law is formulated.

This relation implies in particular that, in case of proper contact, \mathcal{R} belongs to the half-line generated by \mathbf{n} : this is the traditional *no friction* assumption.

EXAMPLE 2 : *De Saxcé's formulation of Coulomb's law.*

With a contact exhibiting dry friction, one associates the *cone of Coulomb* C , a convex cone of \mathbf{R}^3 (with vertex at the origin) containing the vector \mathbf{n} in its interior. In the traditional case, C is axisymmetric about \mathbf{n} , but considering more general convex cones provides for the formulation of anisotropic friction.

Let T denote the orthogonal plane to \mathbf{n} in \mathbf{R}^3 . Every elements U and \mathcal{R} of \mathbf{R}^3 may uniquely be decomposed in the form

$$\begin{aligned} U &= U_T + U_N \mathbf{n}, & U_T &\in T, & U_N &\in \mathbf{R}, \\ \mathcal{R} &= \mathcal{R}_T + \mathcal{R}_N \mathbf{n}, & \mathcal{R}_T &\in T, & \mathcal{R}_N &\in \mathbf{R}. \end{aligned}$$

Let $D_1 = \{ \mathcal{R}_T \in T : \mathcal{R}_T + \mathbf{n} \in C \}$ (the 'unit section' of C) and define in T the real function

$$\mathcal{T} \in T \rightarrow \varphi_1(\mathcal{T}) = \sup \{ \mathcal{T} \cdot S \in \mathbf{R} : S \in -D_1 \}.$$

In the traditional case of isotropic friction with coefficient μ , one simply has $\varphi_1(\mathcal{T}) = \mu \|\mathcal{T}\|$. Put the convention $C = \{0\}$ if $f < 0$. Using arguments of Convex Analysis, one establishes [De Saxcé, 1992] that the relation between U and \mathcal{R} consisting of the system of conditions

$$(5.8) \quad U \in \mathcal{K} \quad \mathcal{R} \in C, \quad -U \cdot \mathcal{R} = \varphi_1(U_T) \mathcal{R}_N$$

with \mathcal{K} defined as in (5.5), is a complete contact law which reduces to the law of Coulomb in the standard case. Furthermore, one may prove that for every pair (\mathcal{V}, S)

$$\forall \mathcal{V} \in \mathcal{K}, \quad \forall S \in C \quad \mathcal{V} \cdot S + \varphi_1(\mathcal{V}_T) S_N \geq 0,$$

so that (5.8) expresses that the real function $(\mathcal{V}, \mathcal{S}) \rightarrow \mathcal{V} \cdot \mathcal{S} + \varphi_1(\mathcal{V}_T) \mathcal{S}_N$, separately convex with regard to \mathcal{V} and \mathcal{S} , attains at the point $(\mathcal{U}, \mathcal{R})$ its minimal value relative to the product set $\mathcal{X} \times \mathcal{C}$ and that this minimal value is zero. This is a special case of what De Saxcé calls the method of 'bipotentials', useful in the numerical treatment of various dissipative laws.

6. Collisions

Let us come back to the setting of Sec. 4. At the instant t_c of a collision, the velocity function $t \rightarrow u(t) \in \mathbf{R}^n$ is expected to present a jump between well defined limits $u^-(t_c)$ and $u^+(t_c)$. Concerning a contact of index α , active at this instant (this in particular may be the contact suddenly introduced by the collision) a jump is expected for the local velocity, as expressed by (3.4). It has been observed in Sec. 4 that the value that one might ascribe to u at the very instant t_c has no relevance to the equations of Dynamics. If a contact law of the form (5.1) has then to be invoked, what value of u_α shall be used? The choice of this value is part of the model adopted to describe the mechanical effect of the collision. The complexity of this effect has been stressed in Sec. 2 and we choose here a pragmatic approach, primarily aimed at making the algorithms work whatever are the circumstances met. Fortunately as already said, in the case of spherical bodies the resulting collision model coincides with that which has been discussed by other authors and experimentally tested. The case of bodies of other shapes is still an object of research.

For every α a contact law of the form (5.1) is declared to hold between the contact impulsion S^α and the local *average velocity* u_α^a defined through its normal and tangential components as follows

$$(6.1) \quad u_{\alpha N}^a = \frac{\rho_\alpha}{1+\rho_\alpha} u_{\alpha N}^- + \frac{1}{1+\rho_\alpha} u_{\alpha N}^+ \in \mathbf{R}$$

$$(6.2) \quad u_{\alpha T}^a = \frac{\tau_\alpha}{1+\tau_\alpha} u_{\alpha T}^- + \frac{1}{1+\tau_\alpha} u_{\alpha T}^+ \in T.$$

Here ρ_α and τ_α are chosen constants with values in the interval $[0,1]$. The meaning of ρ_α is made clear by this observation:

Suppose that the contact law accepted for the considered contact is *complete* in the sense of Sec. 5. It readily results from condition (5.2) to (5.3) that, as far as S^α does not vanish, one has $n \cdot u_\alpha^a = 0$, i.e. in view of (6.1)

$$(6.3) \quad u_{\alpha N}^+ = -\rho_\alpha u_{\alpha N}^-,$$

which mean that ρ_α is identical to *Newton's restitution coefficient* in this case.

But for cases where several contacts are present in the system at time t_c , it is essential to observe that (6.3) is not secured anymore if the mathematical treatment yields $S^\alpha = 0$. This is precisely what makes the above formulation able to handle in a logical way the problem, familiar in the earthquake engineering literature, of the *rocking* of a slender rectangular block supported by a fixed horizontal plane. For simplicity, assume the lower edge slightly concave, so that contact can only occur through the two lower corners. Let the left corner remain in contact for an episode where the block rotates to the right, until the right corner collides. If at this time Newton's assumption was applied to both contact points, no rocking could be found.

Similarly, if the admitted contact law involves a sufficient amount of dry friction (or implying $u_{\alpha T}^a = 0$ in a certain situation, one finds

$$(6.4) \quad u_{\alpha T}^+ = -\tau_{\alpha} u_{\alpha T}^-.$$

In view of (6.3) and (6.4), ρ_{α} and τ_{α} may respectively be called the *normal* and *tangential restitution coefficients*.

If the admitted contact law is the (complete) law of Coulomb, the friction coefficient μ_{α} has also to be included in the data relative to the considered contact. There is no algorithmic difficulty in making all these coefficients depend on circumstances. In particular, they may be functions of u_{α}^a so that the restitution coefficients may depend on the strength of the collision and that the collisional friction coefficient may be different from the static or dynamic friction coefficients used for lasting contacts.

One may convince oneself of the importance of the coefficient τ_{α} by applying the above formalism to the bounce of a ball against a plane and discussing the consequences of possible backspin.

An important issue is the *energy balance* of a collision. Authors [Stronge, 1990][Brach, 1991][Wang & Mason, 1992] stress that, in collisions involving bodies deprived from the customary symmetry properties, a treatment based on Newton's restitution assumption may yield an increase in the system energy, even though the system is scleronomic. In general, the prevention of such an unphysical consequence when the above model is used, would require that the three coefficients satisfy certain inequalities. Let us only observe that, when the trick of using an average local velocity first appeared [M, 1988b], this was with ρ_{α} and τ_{α} assuming the single value $\rho \in [0,1]$ for all contacts. The energy balance of a collision for a multicontact system may in this case be drawn from (4.2) in the form

$$(6.5) \quad \mathcal{E}_k^- - \mathcal{E}_k^+ = \frac{1}{2} A_{ij} (u_i^+ - u_i^-)(u_j^+ - u_j^-) \delta - \sum_{\alpha} u_{\alpha}^a \cdot S^{\alpha},$$

with $\delta = 1 - \rho / (1 + \rho) \in [0,1]$ called the *dissipation index*. The first term on the right-hand side is sure to be nonnegative since the matrix A is positive definite. If the contact laws admitted to hold at the various contacts points are all dissipative (such is the law of Coulomb), this equality entails a decrease of kinetic energy. Incidentally, equality (6.5) is only a special case of the expression of the *differential measure* of the function $t \rightarrow \mathcal{E}_k$ in Nonsmooth Dynamics, obtained through the *Differential Calculus of functions with locally bounded variation* [M, 1988a](see also [Moreau & Valadier, 1987]).

REMARK 1. As early as [Lecornu, 1905] it has been recognized that, in the dynamics of systems involving dry friction, velocity jumps may occur even in the absence of collision. Such an event is due to paroxysms in the contact forces, similar to the *locking* effect commonly observed in the statics of the same systems. One may call them *frictional catastrophes*. They logically appear in the framework of Nonsmooth Dynamic, as demonstrated in [M, 1988b] (on this subject, see also [Wang & Mason, 1992] or for an account of early literature on unilateral constraints and frictional contact [Pérès, 1953]).

REMARK 2. If the contact law invoked in conjunction with the above averaging trick is the *complete law of frictionless contact* (5.7), the coefficient τ_α becomes immaterial. If in addition ρ_α is made equal to zero, one obtains the 'standard inelastic shocks' introduced by [M, 1985], a paper which may be read as an introduction to the present treatment of collisions in multicontact systems.

7. A model algorithm

Algorithms based on the foregoing may affect diverse forms (see e.g. [Jean, 1993, 1994]). Here is a typical set-up, which has in fact been used in computing the examples of Sec. 8.

Let $[t_I, t_F]$, $t_F = t_I + h$, denote an interval of the time discretization. Starting with q_I, u_I , the approximate values of q and u at time t_I , the objective is to calculate q_F, u_F , the approximate values at the end of this interval.

IDENTIFICATION OF CONTACTS

Introducing the middle time $t_M = t_I + \frac{1}{2}h$ and a test position $q_M = q_I + \frac{1}{2}h u_I$, the set of the contacts to be treated as active is estimated as

$$J = \{\alpha : f_\alpha(t_M, q_M) \leq 0\}.$$

DISCRETIZATION OF THE MEASURE DIFFERENTIAL EQUATION (4.6)

$$A(q_M)(u_F - u_I) = h F(t_M, q_M, u_I) + \sum_{\beta \in J} G_\beta^*(t_M, q_M) S^\beta,$$

where $S^\beta \in \mathbf{R}^3$ denotes the impulsion at contact β . In short

$$(7.1) \quad u_F = u_I + h A^{-1} F + A^{-1} \sum_{\beta \in J} G_\beta^* S^\beta.$$

CONTACT LAWS

$$(7.2) \quad \forall \alpha \in J : \quad \text{law}_\alpha(u_{\alpha N}^a, u_{\alpha T}^a, S^\alpha) = \text{true},$$

where the average local velocity u_α^a is defined according to Sec. 6 :

$$(7.3) \quad u_{\alpha N}^a = \frac{\rho_\alpha}{1 + \rho_\alpha} u_{\alpha N}^- + \frac{1}{1 + \rho_\alpha} u_{\alpha N}^+$$

$$(7.4) \quad u_{\alpha T}^a = \frac{\tau_\alpha}{1 + \tau_\alpha} u_{\alpha T}^- + \frac{1}{1 + \tau_\alpha} u_{\alpha T}^+.$$

Possibly ρ_α and τ_α , the normal and tangential restitution coefficients assigned to the contact α , will be made dependent of the impact velocity u_α^- . Here u_α^- and u_α^+ are estimated through (3.5), with u_F and u_I playing the roles of u^+ and u^- respectively, namely

$$(7.5) \quad u_\alpha^- = G_\alpha u_I + \mathcal{W}'_\alpha, \quad u_\alpha^+ = G_\alpha u_F + \mathcal{W}'_\alpha.$$

If the contact α takes place between a body of the system and some external boundary with prescribed motion, the term \mathcal{W}'_α equals the negative of the boundary velocity vector at the estimated contact point at time t_M while, for a contact occurring between two members of the system, this term vanishes.

FINAL POSITION

$$q_F = q_M + \frac{1}{2} h u_F.$$

ITERATIVE PROCEDURE

The heaviest part of the computation consists of solving the system of conditions (7.1) to (7.5). Contact laws considered in the foregoing Sections were *positively homogeneous* with regard to velocities. This allows one to replace conditions (7.2) to (7.5) by

$$\forall \alpha \in J: \text{law}_\alpha(\rho_\alpha G_{\alpha N} u_I + G_{\alpha N} u_F + (1 + \rho_\alpha) \mathcal{W}_{\alpha N}, \tau_\alpha G_{\alpha T} u_I + G_{\alpha T} u_F + (1 + \tau_\alpha) \mathcal{W}_{\alpha T}, s^\alpha) = \text{true},$$

to be joined with (7.1). Here is a relaxation technique, amounting to treat a succession of single-contact problems.

Let an estimated solution $u_F^{\text{esti}}, s_{\text{esti}}^\beta$, β running through J , be obtained, with (7.1) satisfied. One attempts to construct a corrected estimate, say $u_F^{\text{corr}}, s_{\text{corr}}^\beta$, by altering only s^α , i.e. $s_{\text{corr}}^\beta = s_{\text{esti}}^\beta$ for $\beta \neq \alpha$. The new estimate is restrained to satisfy (7.1), i.e. since the old estimate satisfies the same,

$$(7.6) \quad u_F^{\text{corr}} = u_F^{\text{esti}} + A^{-1} G_\alpha^* (s_{\text{corr}}^\alpha - s_{\text{esti}}^\alpha),$$

and to satisfy the law of contact α under the form written above. By applying G_α to both members of (7.6) one gives to this contact law the following form

$$(7.7) \quad \text{law}_\alpha(\mathcal{U}_\alpha^{\text{const}} + G_\alpha u_F^{\text{esti}} + H_\alpha (s_{\text{corr}}^\alpha - s_{\text{esti}}^\alpha), s_{\text{corr}}^\alpha) = \text{true},$$

where the expression $\mathcal{U}_\alpha^{\text{const}}$, an element of \mathbf{R}^3 , is defined through its normal and tangential components

$$\mathcal{U}_{\alpha N}^{\text{const}} = \rho_\alpha G_{\alpha N} u_I + (1 + \rho_\alpha) \mathcal{W}_{\alpha N}$$

$$\mathcal{U}_{\alpha T}^{\text{const}} = \tau_\alpha G_{\alpha T} u_I + (1 + \tau_\alpha) \mathcal{W}_{\alpha T}.$$

and $H_\alpha = G_\alpha A^{-1} G_\alpha^*$ is a symmetric positive definite 3×3 matrix.

Solving (7.7) with regard to the unknown s_{corr}^α is, in usual cases, easy. The above computation will then be iterated, with α ranging cyclically through J . The decision of stopping iterations may be taken on observing the magnitude of $s_{\text{corr}}^\alpha - s_{\text{esti}}^\alpha$ and this turns out to be equivalent to checking the precision at which each pair u_α^a, s^α satisfies the corresponding contact law. Observe that, provided this precision check is made, the operator H_α in (7.7) may be replaced by any other mapping with zero limit at the origin: this may be used in tricks for accelerating convergence.

Clearly, this algorithm tolerates a certain amount of violation of the impenetrability constraints. By adjusting the step-length and the stopping criterium, one may keep these errors arbitrarily small and prevent their accumulation.

The iterated calculation is very simple, but needs to be repeated many times in case of numerous contacts. Since equation (7.1) is only preserved from one iteration to the next through the conservation condition (7.6), one should think of the possible accumulation of arithmetic errors. For safety, one may refresh u_F^{esti} from time to time, by returning to (7.1) while keeping the constructed approximate values of s^β : this proves useful only for motions involving thousands of contacts.

Technically, let us also observe that in many usual applications, the $n \times n$ matrix A is constant and diagonal. G^α is a $3 \times n$ matrix, but only the elements corresponding to the two bodies involved in contact α are nonzero. So the treatment of large collections of bodies does not require the handling of large matrices.

The convergence of this algorithm has not been proved and not even the existence of a solution to the problem it addresses. Uniqueness certainly does not hold in general, since the mechanical problem of determining the reactions in a closely packed collection of rigid bodies (for instance a wall made of rectangular blocks) is usually hyperstatic.

REMARK. At every time-step, the above algorithm is ready to face *velocity jumps*, would they result from collisions or arise as *frictional catastrophes* (Sec. 6). It also manages correctly the possible breaking of contacts, automatically overcoming the difficulties recalled at the beginning of Sec. 5.

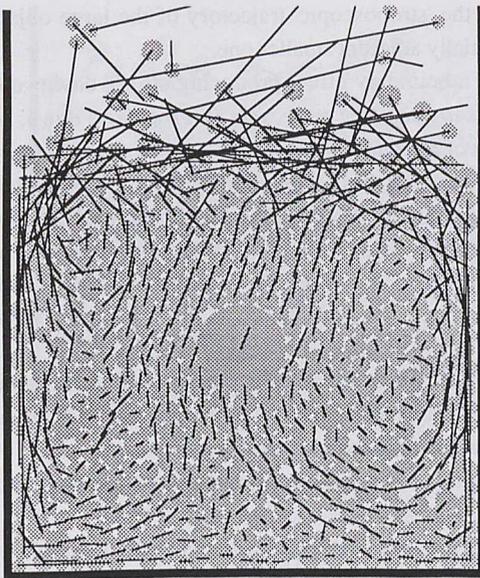
8. Size segregation in vertically shaken granular materials

When a vessel containing grains of different sizes is vertically shaken, one commonly observes a progressive accumulation of larger grains at the top of the pack, even if they are denser than the rest. Similar segregation may also occur in other situations of granular dynamics : flow on a slope, rotating drum (deceptively intended to act as a mixer), etc. and is a nuisance in industrial processes such as the preparation of pharmaceuticals. This is commonly called the 'Brazil nut effect' [Rosato et al., 1987].

The case of vertical shake, to which this lecture is restricted, has been the subject of a fairly large number of studies tending to explain the segregative effect on the basis of statistical mechanics [Mehta & Barker, 1991] or proposing explicit mechanisms at the scale of individual particles [Jullien et al., 1992][Duran et al., 1993]. The same authors have also made use of computer simulations, but not of the properly dynamic sort. These simulations, based on geometry and random drawings (in so-called 'Monte Carlo methods'), are rather meant to test the consequences of tentative conceptions; they may be viewed as an aid to reasoning.

In real situations, several different and possibly antagonistic effects are liable to intervene, so that phenomena may depend qualitatively on the experimental parameters. Anyway, computer simulations performed by the CD method [M, 1993] strongly suggests that past physical experiments, intended to display size-segregation by shaking, produced no proof of any tendency of the larger objects to migrate upwards relatively to the rest of the material. The created animations of two- or three-dimensional granular motions show that, if such a tendency exists, it was anyway masked by an extremely apparent *convection* effect.

Figure 2 is extracted from a series of two-dimensional computations. The upper-left drawing shows the positions of grains at some reference instant. From the center of each, a line is drawn representing the grain displacement after exactly 16 shakes of the containing vessel. An overall circulatory flow is very visible, in which the large object takes part in the same way as its surroundings. Animations show it reach the agitated top region (the long straight lines appearing in this region are the net results of the ballistic flights that small objects perform with only few collisions) then drift to one corner where it remains indefinitely. A less vivid demonstration is



Vertically vibrated vessel :
 Frequency : 20 hertz
 Peak to peak amplitude : 2.5 mm(max. acceleration : 2g)

Two-dimensional circular objects :
 Number : 500
 Larger object : \varnothing 5 mm
 Smaller objects : \varnothing uniformly distributed between 0.75 and 1.5 mm

Contact parameters :
 Friction coefficient : 0.8 everywhere
 Tangential restitution : 0 everywhere
 Normal restitution : 0.9 between circular objects
 0.6 with boundaries

LEFT : stroboscopic displacements over 16 vibration periods (initial positions shown in grey).
 BELOW : stroboscopic trajectories of the large object and of an initially adjacent smaller one over 600 vibration periods.

The downward boundary currents appear too thin to recycle the large object.

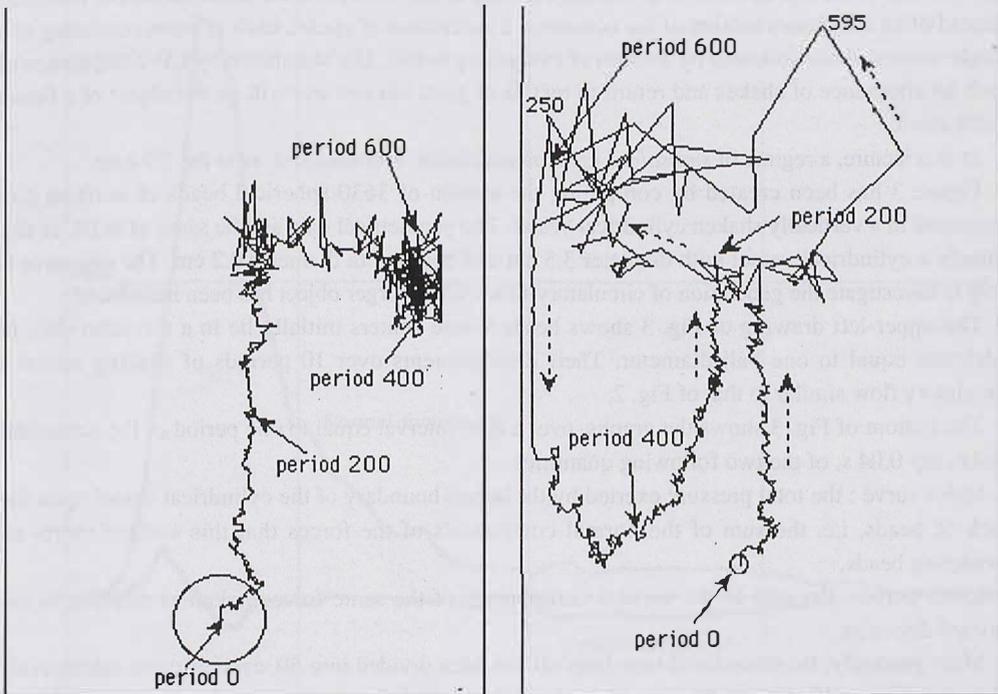


Fig. 2. – Boundary-induced circulation and size-segregation (two-dimensional example).

provided by the bottom drawings of Fig. 2, where the 'stroboscopic' trajectory of the large object over 600 shakes may be compared with that of an initially adjacent smaller one.

The motor of the circulatory flow appears to be a boundary effect producing strong downward currents in thin boundary layers. *Boundary currents are too thin to recycle large objects down*, so size-segregation may be viewed as the result of a sort of *filtration*.

Repeated numerical experiments, with wider vessel and the number of object augmented proportionally, show the same boundary layers but naturally slower general circulation. The two upper corner vortices, already mentioned in Sec. 2, may be identified in this set-up too and are able to take rather large objects into limited incursions downwards. When collections of objects with dispersed sizes are considered, the relative accumulation of the larger ones in the upper part of the vessel manifests itself statistically.

Friction is essential in the generation of boundary currents. Computation performed in the same conditions as above, except that the friction coefficient between beads and boundaries is made equal to zero, yields no circulatory flow and the large object does not move upwards.

Three-dimensional computation, involving spherical beads in a square-based vessel, has produced completely similar results.

Only one month before the distribution of the book [M, 1993], there appeared the paper [Knight et al., 1993] reaching the same conclusion on the basis of three-dimensional experiments : size segregation was found the result of friction induced downward boundary currents, too thin to take large objects back down once these have been brought to the top by the central upward overall motion. The difficulty of observing internal currents in the bead pack led these authors to consider, instead of an oscillatory motion of the container, a succession of cycles, each of them consisting of a single vertical shake followed by a return of everything to rest. The simulation by CD computation of such an alternance of shakes and return to rest is of great interest and will be the object of a future publication.

In this lecture, a regime of *sinusoidal vertical oscillation* is considered, as in the 2D case.

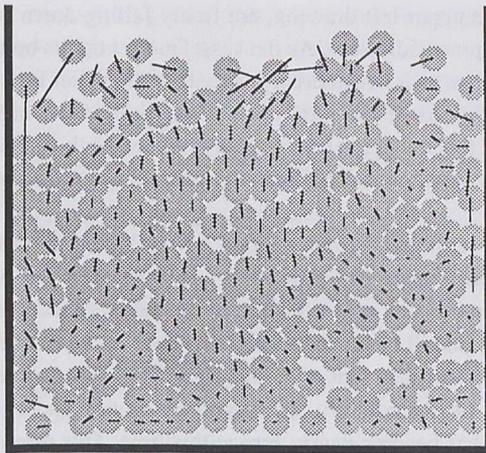
Figure 3 has been created by computing the motion of 3630 spherical beads of uniform size contained in a vertically shaken cylindrical vessel. The geometrical data are the same as in [K. et al.], namely a cylindrical vessel with diameter 3.5 cm and beads with diameter 0.2 cm. The objective is only to investigate the generation of circulatory flows, so no larger object has been introduced.

The upper-left drawing of Fig. 3 shows beads whose centers initially lie in a meridian slice of thickness equal to one ball diameter. Their displacements over 10 periods of shaking reveal a circulatory flow similar to that of Fig. 2.

The bottom of Fig. 3 shows the graphs, over a time interval equal to one period of the sinusoidal shake, say 0.04 s, of the two following quantities

- upper curve : the total pressure exerted by the lateral boundary of the cylindrical vessel upon the pack of beads, i.e. the sum of the normal components of the forces that this surface exerts on contacting beads,
- lower curve : the sum of the vertical components of the same forces, taken as positive in the upward direction.

More precisely, the considered time interval has been divided into 50, each of these subintervals corresponding to 40 steps of the algorithm. At each point of division is plotted the average value of the concerned quantity over the 40 precedings steps. Of course, at every step of the algorithm, 'force' means the quotient of a computed impulse by the step duration. At time 0, the vessel is at its lowest



Cylindrical vessel : \varnothing 3.5 cm

Vertical vibration : frequency 25 hertz,
peak to peak amplitude 0.2 cm
(maximal acceleration 2.51 g)

Beads : \varnothing 0.2 cm, total number 3630

Contact parameters : friction 0.8,
normal restitution 0.95,
tangential restitution 0.4

LEFT : Beads with centers initially located in a
meridian slice of thickness 0.2 cm :
stroboscopic displacements over 10 periods
of vessel vibration

BELOW : Total reaction exerted by the lateral cylindrical boundary upon the pack of beads
(normal and vertical components, time interval : 1 period)

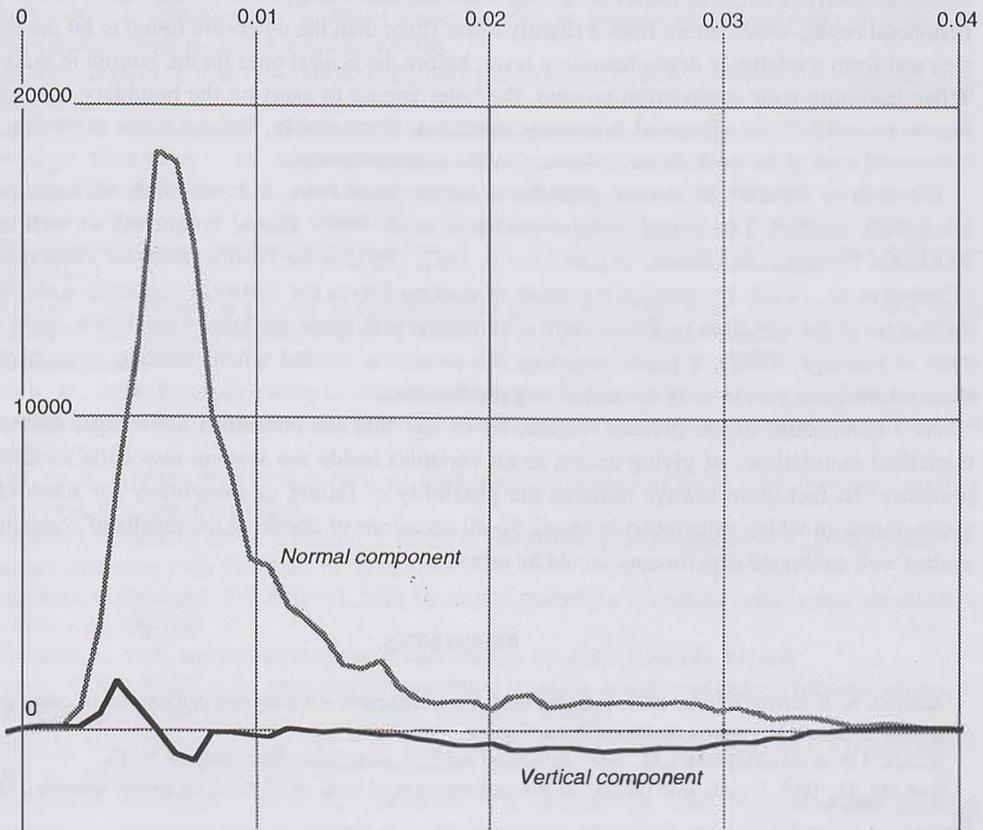


Fig. 3. – Beads in vertically shaken cylindrical vessel.

position and beads, in the positions shown on the upper left drawing, are freely falling down with little internal agitation so the peripheral forces are practically zero. As the vessel moves up, its bottom hits the lowest beads, generating a collision wave which considerably increases the mean internal pressure of the pack. It was found that the variations of the total normal reaction of the lateral boundary, plotted here, nearly reproduce those of this mean internal pressure. As the pack performs its flight loose from the vessel bottom, its internal agitation is progressively damped by collisions so the mean internal pressure decreases.

The time variation of the vertical component of the total force exerted by the lateral boundary shows a *negative average*. The significant effect takes place between $t=0.015$ and $t=0.030$, approximately. During this episode, the granular material is very fluid and its contact with the lateral boundary displays an overall *upward sliding*. Peripheral beads therefore have their upward motion damped: their maximal altitude is found notably lower than that of the others and the latter come to occupy the corresponding vacant space at the top. On the contrary, the downward motion undergoes no boundary damping, because the pack pressure has become nearly zero at this time. This repeated over many periods clearly results in an average downward boundary current.

The contrasty evolution of the vertical component which takes place between $t=0$ and $t=0.01$ should be ascribed to brutal events occurring when the descending beads hit the vessel bottom. The peripheral beads, which return from a slightly lower flight than the others are found to hit the bottom first and form a relatively dense boundary layer, before the central ones hit the bottom in their turn. When initiating their compaction process, the latter appear to exert on the boundary beads some forces provoking the observed boundary reactions. Presumably, these events occurring in a compacted state of the pack do not influence the circulatory currents.

Circulatory currents in shaken granular materials have been, independently of segregation, intensively studied. The experiments of [Laroche et al. 1989] should be quoted, as well as the Molecular Dynamic simulations of [Gallas et al. 1992, 1993] or the Distinct Element simulations of [Tamura et al., 1993]. Frequently, the mode of shaking leaves the vertical boundaries fixed, while the bottom of the container performs vertical vibrations with space-modulated amplitude. Such is the case in [Savage, 1988], a paper stressing the prudence needed when, starting from physical observations, one tries to infer the underlying mechanisms.

As a conclusion to the present lecture, let us say that the enormous advantage, offered by numerical simulations, of giving access to all variables inside the system, also calls for extreme prudence. In fact there always remains the possibility of failure or inaccuracy for some of the assumptions on which calculation is based. So all occasions of checking the results of computation against well calibrated experiments should be seized.

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