New computation methods in granular dynamics

Jean Jacques Moreau

New computation methods in granular dynamics

J.J.Moreau
Laboratoire de Mécanique et Génie Civil, URA CNRS 1214, Université Montpellier II, France

ABSTRACT : The dynamics of collections of bodies, treated as perfectly rigid, involves nonsmooth mathematical relations, arising from the unilaterality of impenetrability constraints, from the formulation of dry friction and from the velocity jumps produced by possible collisions. The presented numerical methods treat nonsmoothness without resorting to regularization procedures. The examples shown concern populations of balls contained is a vertically vibrated rectangular box. First, a comparison is made with some experiments performed by other authors, about the paradoxical shape taken by the free surface when vibration is not strong enough to fluidize it. Other examples reveal an unexpected mechanism of size segregation.

1 INTRODUCTION

Numerical methods have been developed for a few years in our laboratory, devoted to computing the motion of mechanical systems with transient contacts. One is then in the presence of unilateral constraints : since some parts of the system may enter into contact or get loose from each other, but can never interpenetrate, the permitted configurations are characterized by inequalities (possibly an infinite set of them). In the configuration space, this defines a region with corners and edges, instead of the smooth submanifolds which, in the traditional Analytical Dynamics, are associated with constraints. In the case of contact, we take dry friction into account under its simplest phenomenological description, namely the law of Coulomb. The latter consists in a relationship between the sliding velocity and the contact force which assumes different analytical forms, depending on the sliding status ; and this relationship does not permit to express any of the two vector variables as a function of the other. Furthermore, if collisions occur, one should expect velocity jumps, so that the evolution cannot be governed as a whole by differential equations nor differential inclusions in the classical sense. For all these reasons, the investigated problems belong to Nonsmooth Mechanics, a domain for which theoretical and numerical methods have specifically been elaborated in recent years (Moreau, Panagiotopoulos and Strang 1988, Moreau and Panagiotopoulos 1988).

Traditionally, the numerical approach to nonsmoothness rests on smoothing procedures, i.e. the investigated problems are approximated by regular ones to which usual computation methods are applied. For instance, impenetrability is replaced by a steep repulsion potential acting when the concerned bodies come close to each other. This is similar to the "penalty methods" used in Constrained Optimization. The drawback is that the need of precision leads to introduce very stiff repulsion laws, so the numerical stability of the consequent integration procedures requires fine time-discretization and much computing power. Since the pioneering work of P. A. Cundall (1971), significant results have however been obtained in that way (most recently : Gallas, Herrmann and Sokolowski 1992a,b, Y-h Taguchi 1992) .

In contrast, we have decided to face nonsmoothness without resorting to regularization procedures. This results in algorithms efficient enough to treat on a microcomputer the dyna-

mics of rigid body collections involving, say, 1000 contacts. Examples presented in the forthcoming have however been computed on larger workstations. A frontal program on Macintosh have been developed to prepare the data and to analyse the results ; in particular, this program can exploit the numerical files in creating successions of bitmap images on a hard disk, to be displayed as movie-like animations. Current applications are not limited to granulate materials ; for instance, the dynamical behaviour of pieces of stonework supported by quaking ground is also actively investigated.

All the above methods compute motions by solving the equations of Dynamics. Their aim is to investigate phenomena on the same footing as experiments, preferably in interaction with them. This places them at a different epistemological level than Monte Carlo or Cellular Automata simulations, the purpose of which is to develop and test the consequences of a priori conceptions.

2 COLLISIONS

We restrict ourselves in this communication to the treatment of bodies as perfectly rigid. A common weakness of all numerical simulations developed in that framework lies in the difficulty of getting precise phenomenological information about collisions. Possible bounces are ascribed to some non analyzed microscopic elasticity. The traditional restitution coefficient of Newton can be experimentally identified only in the special case of the normal impact of spherical bodies. Recall that, if this coefficient is less that 1, bounce exhibits energy loss. A widespread conception is that such a dissipation should be the result of viscosity or plasticity effects localized in the vicinity of the impact locus. Actually, even if the colliding bodies are made of a perfectly elastic material, some loss of kinetic energy must be expected at the macroscopic level. In fact, dynamical disturbances emanate from the impact and are likely to propagate throughout the concerned bodies. The amplitude of such vibrations may be small enough for the bodies to be described as rigid at the chosen level of observation, while, in view of the velocities involved in the vibration, the latter may carry nonnegligible energy. After the end of the collision process, vibration should last for a certain time before internal dissipation progressively converts its energy into heat. Similarly, if a part of the investigated system collides with some fixed external boundary, an amount of energy is liable to propagate into the surrounding world. If the external boundary moves, the energetic balance becomes still more complicated and the system may receive energy from the surrounding world. This is the case of a collection of rigid grains contained in a shaked vessel.

Common observation, as well as the computations made in our laboratory with body deformations taken into account through the finite element method, show that restitution greatly depends on the shape of the colliding bodies and on the impact location.

Newton's restitution hypothesis involves the impinging and bouncing velocities only through their normal components. In the case of the oblique collision of, say, spherical bodies, friction is expected to transfer angular momentum. However short the collision process is, friction in the contact zone may evolve in a complex way, exhibiting microepisodes of slip and stick. As early as 1880, Darboux (see also Pérès 1953) applied to rigid body collisions a multiple scaling method : the very short duration of the contact interaction is parametrized through a microtime, say τ. In applying the equations of rigid dynamics to the collision process, one treats the velocities of the involved bodies as unknown functions of τ, while positions are considered as constant. Coulomb law is invoked, so as to relate, for every τ, the contact force with the sliding velocity at the contact point. Here again, it is implicitely assumed that microdeformations are concentrated in the vicinity of the impact locus. In our opinion, the probable global microdeformation of the bodies limits the applicability of the approach.

Anyway, Newton's hypothesis proves inadequate as soon as several contacts are present at the time of a collision. This is demonstrated by the familiar example 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. The left corner remains in contact for an episode during which the block rotates to the right, then the right corner collides. If at this time Newton's assumption was applied to the left contact, no rocking could be found.

A numerical method must be able to treat

collisions in multicontact situations. A decisive test is provided by the transmission of impulse across a row of contacting balls, a classical experiment displayed in many scientific museums.

Incidentally, it has long been recognized that, in mechanical systems involving dry friction, velocity jumps may also occur in the absence of collision as the result of a sort of locking. Concerning such "frictional catastrophes" (impossible in the free dynamics of bodies as regular as homogeneous balls) one may refer to the author's contribution in Moreau & Panagiotopoulos 1988: 1-82.

Our computing policy rests on a synthetic formulation of contact which applies to collision instants as well as to episodes of persistent contact. After time-discretization, this formulation generates algorithms which, at every time-step, are ready to face possible collisions or frictional catastrophes.

3 FORMALIZATION OF CONTACT LAWS

Let the generic position of the considered system be labelled by generalized coordinates, say $q \in R^n$. The geometric effect of impenetrability constraints are expressed by inequalities of the form $f_\alpha(t,q) \leq 0$, the subscript α ranging in practice through a finite set (the presence of t in such inequalities pertains to the confinement of some parts of the system by boundaries with prescribed motion). Inequality holds as equality when contact occurs at some point, say M_α, of physical space. The central object, in mathematical formulations as well as in computation, is the velocity function $t \to u(t) \in R^n$ from which the motion $t \to q(t)$ can be retrieved through time-integration.

Since we are to face collisions, the function u should not be expected continuous. The most natural setting consists in assuming that it has bounded variation from the investigated time-interval I to R^n (for theoretical arguments supporting this assumption, see Moreau 1989). Then, at every $t \in I$, the function is sure to possess a left-limit $u^-(t)$ and a right-limit $u^+(t)$ (by convention $u^-(t_0)=u(t_0)$ if t_0 equals the beginning of I). With such a function, a R^n-valued measure on the interval I is classically associated, called the differential measure or Stieltjes measure of u, possibly denoted by du. If u is discontinuous at some point t of I, the measure du possesses an atom at this point, namely the R^n-valued Dirac measure whose value equals the jump $u^+(t)-u^-(t)$. In contrast, on any subinterval throughout which u admits a (Lebesgue-integrable) derivative u', one has du=u'dt, whith dt denoting the Lebesgue measure (for a systematic exposition of such mathematical technicalities, the reader may refer to the author's contribution in Moreau, Panagiotopoulos & Strang 1988: 1-74). The equations of dynamics may then be written as an equality of R^n-valued measures on the interval I. This readily generates integration schemes : on every interval, say (t_i,t_{i+1}), of the time-discretization, the measure equality is replaced by the equality of the corresponding integrals. Then $u(t_{i+1})$ plays the role of u^+ and $u(t_i)$ the role of u^-. In this formulation, forces and percussions are treated on the same footing : classical forces are the densities relative to dt of diffuse impulsions, while percussions arising from collisions appear through their actual values (or equivalently through their densities relative to some atomic base measures).

At the heart of the problem lies the formulation of laws governing contact effects at any instant where some of the inequalities $f_\alpha \leq 0$ hold as equalities. The geometrical inspection of the parametrization (q) allows one to express the relative velocity $\mathcal{U}_\alpha \in R^3$ of the contacting bodies at point M_α as a q-dependent linear function of $u \in R^n$; in the case of a velocity jump, the same expression applies to the left- and right-limits. Since one is in want of phenomenological relations representing the whole collision process approximately, it proves expedient to construct some formal velocity $\mathcal{U}_\alpha^a$ as a weighted mean of the left- and right-limits. We choose to apply different weight coefficients when treating normal and tangential components, namely

$$\mathcal{U}_{\alpha N}^a = \frac{\rho_\alpha}{1+\rho_\alpha}\,\mathcal{U}_{\alpha N}^- + \frac{1}{1+\rho_\alpha}\,\mathcal{U}_{\alpha N}^+$$

$$\mathcal{U}_{\alpha T}^a = \frac{\tau_\alpha}{1+\tau_\alpha}\,\mathcal{U}_{\alpha T}^- + \frac{1}{1+\tau_\alpha}\,\mathcal{U}_{\alpha T}^+$$

Clearly $\mathcal{U}_\alpha^a$ equals $\mathcal{U}_\alpha$ whenever the latter is continuous. By a contact law we mean a relation between $\mathcal{U}_\alpha^a$ and the corresponding contact force or percussion denoted by $\mathcal{R}_\alpha$. Let n_α denote the normal unit vector to the contacting bodies at point M_α, with such a direction that $n_\alpha . \mathcal{U}_\alpha > 0$ corresponds to separation. Strictly

speaking, n_α makes sense only for $f_\alpha=0$; by convention, its definition is extended to neighbouring configurations.

Let us say that a contact law is complete if it involves the three following implications

$$f_\alpha(t,q) < 0 \Rightarrow \mathcal{R}_\alpha = 0.$$
$$f_\alpha(t,q) \geq 0 \Rightarrow n_\alpha . \mathcal{U}_\alpha^a \geq 0$$
$$n_\alpha . \mathcal{U}_\alpha^a > 0 \Rightarrow \mathcal{R}_\alpha = 0.$$

If all possible contacts are governed by laws agreeing with this definition, one easily establishes (see the author's contribution in Moreau & Panagiotopoulos 1988: 1-82) that the calculated motion satisfies $f_\alpha(t,q(t)) \leq 0$ for every α, and every $t \in I$, provided this is true at the initial instant t_0 .

Assuming a complete contact law readily secures the implication

$$\mathcal{R}_\alpha \neq 0 \Rightarrow n_\alpha . \mathcal{U}_\alpha^a = 0.$$

which, in view of the definition of $\mathcal{U}_\alpha^a$, becomes

$$\mathcal{R}_\alpha \neq 0 \Rightarrow n_\alpha . \mathcal{U}_\alpha^+ = -\rho_\alpha n_\alpha . \mathcal{U}_\alpha^-$$

In the event $\mathcal{R}_\alpha \neq 0$, this allows one to identifie ρ_α with Newton's restitution coefficient, but not for $\mathcal{R}_\alpha = 0$; such is the key to a consistent treatment of collisions in the case of multiple contacts.

In view of this, we respectively call ρ_α and τ_α the normal and the tangential restitution coefficient of contact α.

Coulomb's law of dry friction may easily be programmed in the form of a complete contact law. It will then be applied at every time-step of the algorithm, for every contact detected as active in this time step. The problem of determining the corresponding values of the contact impulsions $\mathcal{R}_\alpha$ and, consequently, an estimate value of the velocity function at the end of the interval, is solved by an iteration procedure. Uniqueness of solution is not guaranteed. The reader may refer to Jean & Moreau 1992 for more detail.

4 COMPARISON WITH EXPERIMENTS

The first occasion of comparing directly our computations with observations was provided by the experiments made by M. Raous (1993) on the rocking of rectangular blocks supported by a horizontal table which performs sinusoidal horizontal oscillation. Satisfactory agreement with the simulation is obtained in this case by taking the normal restitution coefficient equal to zero. This conclusion also agrees with the findings of A. Ageno and A. Sinopoli (1993) in experiments motivated by the dynamics of dry stone buildings (ancient Greek monuments) under earthquakes.

In the proper domain of granular dynamics, the currently continued experiments of E. Clement, J. Duran and J. Rajchenbach (1992) permit well controlled comparison.

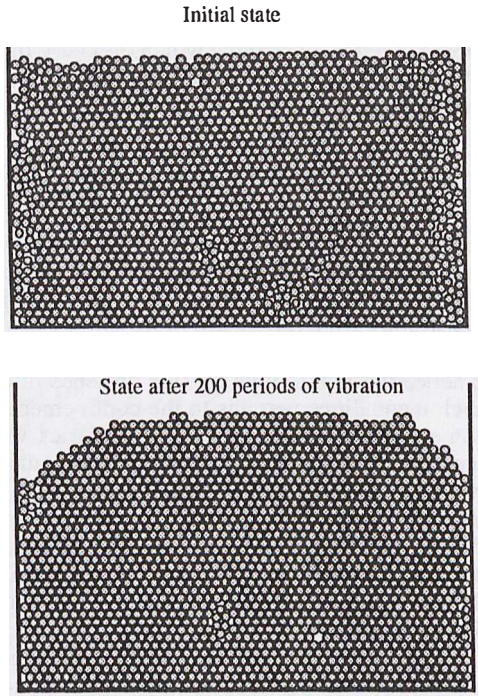

Figure 1

A collection of spherical beads with the same diameter (usually 1.5 mm) is placed in a rectangular cell with two parallel vertical glass walls of slightly greater spacing, allowing one to observe two-dimensional granular motion. The cell is given a vertical sinusoidal vibration with frequency in the range 10-30 hertz. Amplitude is adjusted in such a way that the maximal acceleration $a\omega^2$ little exceeds gravity (for instance 1.1g to 1.5g). In view of their

uniform diameter, beads arrange themselves into a cristal-like hexagonal packing. For aluminium beads, whose normal restitution coefficient is estimated at 0.7, no fluidization occurs in the top layers. Because of surface oxidization, the friction coefficient between beads is as high a 0.8. The following phenomenon is observed. The top of the pack, initially a horizontal straight line due to preparatory shaking, progressively builds a heap. The process emanates from the two lateral boundaries whose average effect appears to drag the contacting beads downward. If $a\omega^2$ has values of order 1.1g to 1.3g, this effect is localized in the two upper corners. Randomly in time, vortices appear in these corners, heaving some fragments of the bead pack into small heaps. As they grow, these two lateral heaps eventually merge into a single one, with maximal height at center.

When $a\omega^2$ is made greater, the downward drag exerted by lateral walls extends lower. This is precisely what happens in our simulation presented on fig.1, which corresponds to a collection of 1650 beads with $a\omega^2=1.63g$. The downward currents affecting the two lateral boundary layers attain the cell bottom. Some beads are consequently forced into the bulk, generating rectilinear dislocations and the upsurge of central fragments of the hexagonal packing.

5 SIZE SEGREGATION IN VIBRATED PARTICULATE MATERIAL

We have applied the same program to various examples of two-dimensional collections of circular objects with non uniform sizes, contained in a vertically shaked box. In all the examples shown below, the box motion is the same : frequency 20 hertz, $a\omega^2=2g$. Contact between objects has friction 0.8, normal restitution 0.9, tangential restitution 0. Contact of objects with walls has friction 0.8, normal restitution 0.6, tangential restitution 0. Computation is aimed at exhibiting the upward segregation of larger objects immersed in a population with diameters uniformly distributed between 1.5 mm and 0.75 mm. Such a dispersion of sizes prevents the formation of a cristal-like packing but here again, due to the large value of $a\omega^2$, the downward flow localized in boundary layers is very apparent.

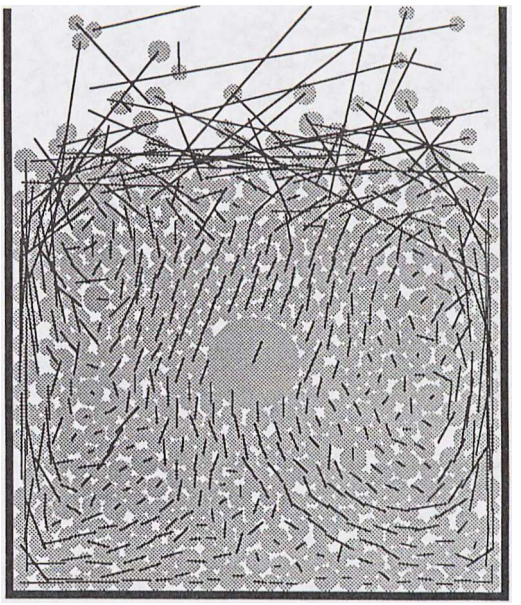

Figure 2

Figure 2 shows a single large immersed object with diameter 5 mm. For each of the 500 objects in presence, the total displacement of its center over some time interval, covering 16 vibration periods, is drawn as a straight line starting from the center of the initial position. This clearly displays a circulatory flow of the whole population. The large object takes part in this flow, without any visible tendency to go up faster than its surroundings. Animations created by the program show it reach the fluidized top region and then drift to one of the upper corners where it remains indefinitely. Apparently, the boundary layer is too thin to recycle it down, while the rest of the population continues to take part in circulatory currents. The motion is also affected by random fluctuations of various scales.

For comparison, figure 3 shows the computation results when boundary friction is made equal to zero, all other data keeping the same values as above. No current now appears along the vertical walls, no general convective flow affects the bulk and the large object stays at bottom.

The case of several large objects yields similar results.

On the other hand, one may make the box

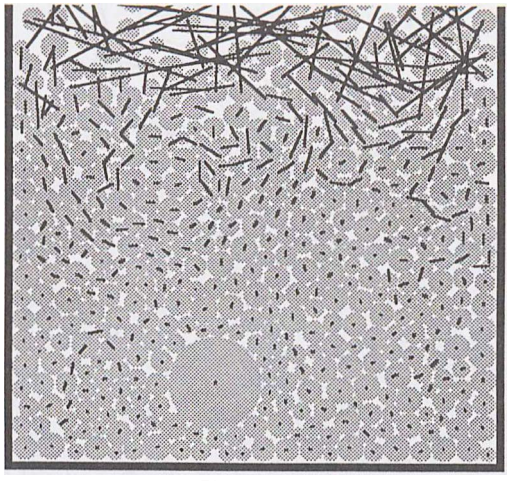

Figure 3

wider while increasing the total number of objects proportionnally so as to obtain the same height of granulate material. If boundary friction is nonzero the same downward boundary currents as in the preceding are visible, but the upward convective flow induced in the rest of the box is naturally slower.

In view of such simulations, one may suspect that some experiments made in the past, with a view to produce size segregation, actually consisted in non segregating upward convection while the downward boundary currents acted as filters. Experimental evidences however seem to exist of segregation occurring in the bulk of a granulate material. We expect to attain situations of this sort by suitably adjusting the computation data.

6 CONCLUSION

The numerical methods presented above work in three-dimensional situations as well. They today appear sufficiently validated to be used in the exploration of granular dynamics, including some slow shearing motions of compact granulate materials, not presented here. In our view, their major utility lies in joint use with experiments. The three parameters of the assumed contact laws, namely the friction coefficient and the two restitution coefficients, have to be adjusted so that the computed results match as well as possible some feasible measurements of the experimental set-up. Then computation allows one to estimate the values of experimentally inaccessible quantities, which may be of great help for understanding phenomena.

REFERENCES

Ageno, A. & A. Sinopoli 1991. Indagine teorica e sperimentale sul problema dell'urto fra blocchi rigidi. *Conv. Ing. Sismica,* Palermo.

Clément, E., J. Duran & J. Rajchenbach 1992. Experimental study of heaping in a two-dimensional "sandpile". *Phys. Rev. Lett.* 69: 1189-1192.

Cundall, P. A. 1971. A computer model for simulating progressive large scale movements of blocky rock systems, *Proc. Symp. of the Int. Soc. of Rock Mech.*, Nancy, France, 1: 132-150.

Darboux, G. 1880. *Bull. Sci. Math.*1, 146-.

Gallas, J. A. C., H. J. Herrmann & S. Sokolowski 1992 a. Molecular dynamics simulation of powder fluidisation in two dimensions. *J. Phys.* 2: 1389-.

Gallas, J. A. C., H. J. Herrmann & S. Sokolowski 1992 b. Convection cells in vibrating granular media. *Phys. Rev. Lett.* 69: 1371-1374.

Jean, M. & J. J. Moreau 1992. Unilaterality and dry friction in the dynamics of rigid body collections. In A. Curnier (ed.), *Proc. Contact Mech. Int. Symp.:* 31-48. Lausanne: Presses Polytechniques et Universitaires Romandes.

Moreau, J. J., P. D. Panagiotopoulos & G. Strang 1988. *Topics in nonsmooth mechanics.* Basel, Boston, Berlin: Birkhäuser.

Moreau, J. J. & P. D. Panagiotopoulos 1988. *Nonsmooth mechanics and applications,* CISM Courses and Lectures, n° 302. Wien, New York: Springer-Verlag.

Moreau, J. J. 1989. An expression of classical dynamics. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 6 (suppl.): 1-48.

Pérès, J. 1953. *Mécanique Générale*. Paris: Masson.

Raous, M. 1993. Experimental analysis of the rocking of a rigid block. *3rd Panamerican Congress of Appl. Mech.* Sao Paulo, Brasil.

Taguchi, Y-h. 1992. New origin of a convective motion : elastically induced convection in granular materials. *Phys. Rev. Lett.* 69: 1367-1370.