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Indetermination in the numerical simulation of granular systems

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ABSTRACT: In the dynamics of systems exhibiting dry frictional contacts, the problem of finding the motion consequent to initial positions and velocities may admit multiple solutions. This indeterminacy is inherent in the information that the model handles. The values of contact forces are a natural complement of data. When coming to time-stepping computation, one is thus induced to treat these values as part of each state description. This is automatic in Molecular Dynamics methods since contact forces are connected with the formal elastic deviations passed from step to step. In Contact Dynamics it is left as an option, leaving the alternative of exploring at each time-step the whole set of possible contact forces and accelerations; indetermination clouds are then displayed for the force at a chosen contact or for the acceleration of a chosen object. In an equilibrium configuration, the set of the possible values of contact forces is similarly investigated.

1 INTRODUCTORY EXAMPLE

Figure 1 shows a two-dimensional model: a circular rigid body B lies in contact with two fixed circular obstacles. At time t_0 , it is released under the action of gravity with zero velocity. Friction at contact points is governed by Coulomb law. Given the geometry of the system, a possible evolution consists in B losing contact and falling freely. But, if the friction angle γ is large enough, B may also remain *wedged*. In the latter case, contact forces remain undetermined in some range.

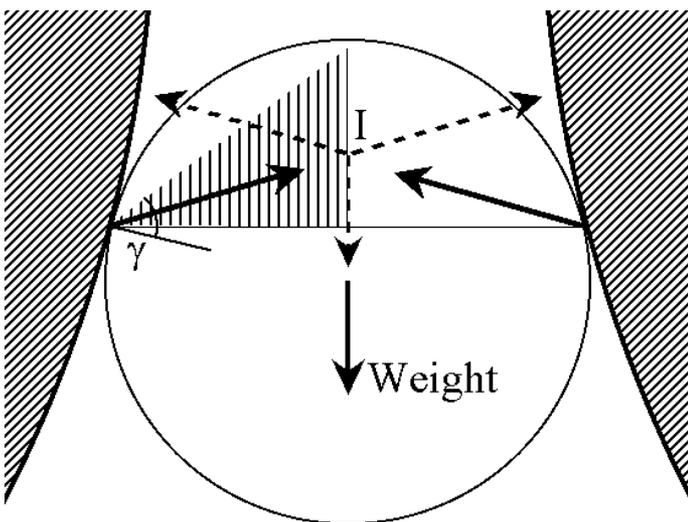


Figure 1. Any position of I on some vertical segment corresponds to contact forces values balancing gravity and compatible with Coulomb friction.

Which of these two motions should be predicted depends on some additional data concerning the “intensity of wedging”. The form of such data depends on the analyst’s state of information.

Imagine first that a recording of the evolution of the active forces (gravity and action of an operator) exerted on B prior to t_0 is available. By using a more elaborate model, accounting for infinitesimal elastic deformations and infinitesimal motions at contact points, one might reconstruct the history of contact forces and finally decide whether the values of these forces at time t_0 agree with B detaching or not.

However, the possibility of the above hysteretic analysis does not exclude the existence of state variables whose values at time t_0 would convey a summary of history sufficient for predicting further evolution. A natural measure of the intensity of wedging precisely consists of the values of contact forces at time t_0 (agreeing with Coulomb law).

It is developed in this contribution that situations of frictional contact may be satisfactorily handled in the framework of perfectly hard bodies, provided the values of contact forces are included in the description of each state of the system.

2 TIME-STEPPING COMPUTATION

A widespread method for the numerical simulation of granular systems is derived from the techniques used in *Molecular Dynamics*, hence referred to as MD. It consists of approximating the impenetrability constraints, when two bodies come close to each

other, by repulsion forces steeply dependent on the mutual positions. Friction forces are similarly approximated, yielding an evolution problem governed by differential equations smooth enough for being handled through standard integration methods. In this way, the interaction forces are connected with fictitious deviations passed from step to step, so that the numerical scheme complies with the proposition made in the foregoing of including these forces in the description of each state.

Another approach entitled *Contact Dynamics* will be preferred here in view of its ability to explore also the plurality of solutions. It faces the essential nonsmoothness of the impenetrability constraints and of dry friction without resorting to any regularizing alteration of the model (for a recent exposition, see Moreau 2004a). The dynamics of a system with n degrees of freedom is formulated in terms of two functions of a time-interval $[0, T]$ to \mathbf{R}^n , the *position function* $t \rightarrow q$, and the *velocity function* $t \rightarrow u$. In the simplest case, q equals the time-integral of u ; the relationship only becomes slightly more complicated when u consists for instance of the components of the spin vectors of rigid bodies.

The geometric effect of impenetrability is expressed by a finite set of inequalities $f_\alpha(t, q) \leq 0$, with equality corresponding to contact. In addition, some mechanical information about each contact should be available in terms of a *contact law*, i.e. a relationship connecting local kinematic data to the contact forces whose respective generalized components are noted $r_\alpha \in \mathbf{R}^n$. Coulomb law in particular may be written in such a form.

Classical (smooth) Mechanics formulates the system dynamics as an \mathbf{R}^n -valued differential equation governing the function u and involving q as a t -dependent parameter, say $du/dt = E(t, q, u, \Sigma r_\alpha)$. But in the present context, the nonsmoothness arising from contact unilaterality and dry friction is liable to entail discontinuities for the function u . The suitable mathematical framework is that of u being an \mathbf{R}^n -valued function of t with *bounded variation*, so that the differential equation of the classical case is replaced by a “measure-differential equation” MDE.

This means that the derivative du/dt should now be understood as an \mathbf{R}^n -valued *measure* on $[0, T]$, with punctual *atoms* at the instants of possible collisions. Mechanical actions, either contact forces or contact percussions or also given as functions of t, q, u , are described through \mathbf{R}^n -valued measures on $[0, T]$.

Time-stepping approximation is constructed by integrating both members of MDE on each interval of the time grid, say $[t_i, t_f]$, $t_f = t_i + h$. Starting from the approximant u_i of $u(t_i)$ delivered by the antecedent step, the objective is to calculate an approximant u_f of $u(t_f)$. Concomitant unknown is the contact impulsion $s = \Sigma s_\alpha$, i.e. the integral of Σr_α over $[t_i, t_f]$. The discretized MDE has to be complemented by some

impulsional form of the contact laws, connecting each s_α with an estimate U_α of the local relative velocity of the contacting bodies. If one chooses as U_α the value associated with the unknown u_f , the discretization scheme so constructed turns out to be of the *implicit* type. Whatever is the procedure additionally used to update q at the end of the step, such an implicit character secures numerical stability, allowing one to use considerably larger step-lengths than in MD methods. The price to pay is that the core of the calculation at each time-step consists of a highly nonlinear and nonsmooth problem.

Various techniques are available to solve the core problem (Renouf & Alart 2004a), possibly parallelized (Renouf et al. 2004b). The most commonly used is a nonlinear Gauss-Seidel procedure which suits well the present needs. It consists in reviewing contacts cyclically again and again, solving for each of them a single-contact problem in which the other contact forces are treated as known and updating interactions until some convergence criterium is met.

By connecting the contact impulsions s_α with u_f , the foregoing numerical scheme turns out to treat possible collisions as perfectly *inelastic*. An improvement, leading to a core problem of exactly the same form, consists in connecting each s_α with some weighted mean of u_f and u_i (possibly using different weights for normal and tangential components). In the special case of a binary collision this is found equivalent to the introduction of some Newton *restitution coefficients*, but in general offers the advantage of handling also multicontact situations.

The Gauss-Seidel iterative procedure has to be launched from some *initial guess* of the impulsions s_α . This guess may consist of zero values but, in case of dense collections of rigid bodies, one considerably accelerates convergence by starting from the values found for these impulsions at the antecedent step for the contacts which were already active.

In the latter case, computation does comply with the proposition made in the foregoing of treating contact forces as state variables passed from step to step and very little indeterminacy is observed.

Otherwise, given a time-step, the Gauss-Seidel procedure allows one to explore the plurality of the solutions. One possibility is to execute a large number of runs of the convergent iteration process, each time with initial guess drawn at random from some plausible range. Any solution then has a chance to be approached. Alternatively, one may launch all runs from zero initial guess while choosing at random, for each run, an ordering of the cyclic review of contacts. The limit of a run depends on this ordering. With κ contacts, the number of solutions attained in the latter way equals at most $(\kappa - 1)!$ which has been found sufficient to generate a significant outline of the solution set (Moreau 2003, 2004b).

To determine whether a given position is an *equilibrium*, a single computation step is enough: start-

ing with $u_i=0$, one checks whether $u_f=0$. The values found for the contact impulses s_α yield the respective contact forces as $r_\alpha=s_\alpha/h$.

3 GRANULAR FLOW ON A SLOPE

Figure 2 shows a detail of the flow of $N=355$ circular bodies on a ground parallel to the lower edge of the picture, under periodic lateral conditions, with gravity corresponding to ground sloping down to the right by 24° . Friction: 0.5; restitution of possible collisions: 0. Flow is not in stationary regime but in a phase of overall acceleration.

A certain computation step is investigated by repeated runs of the Gauss-Seidel procedure at zero initial guess, each run using a reviewing order selected at random. The acceleration vector of a grain center is affected by a dispersion shown on the figure. On the contrary, if the same exploration is performed with the contact forces of antecedent step taken as initial guess, almost no dispersion is visible.

In other numerical experiments of the same sort, no indetermination was visible. Further study is thus needed to discover the governing parameters and to explain why the dispersion produces a line, not an extended cloud. The disposition of contact points at which the sliding velocity equals zero may be determinant. In fact, at these points, Coulomb law only restrains the contact force in a conical region, while at sliding contacts this law involves the very direction of the force.

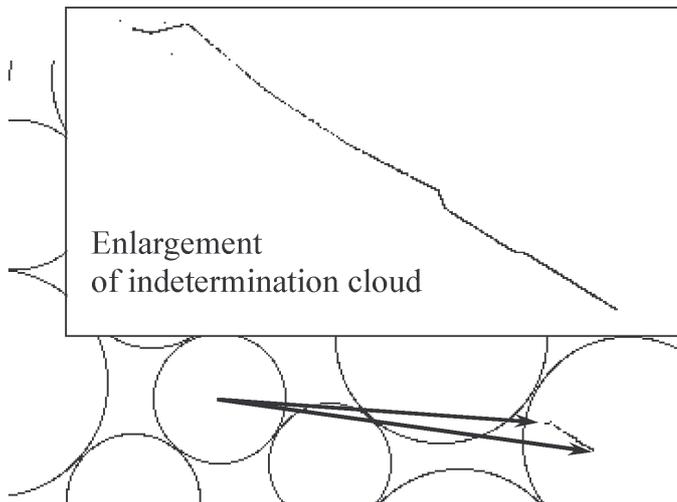


Figure 2. Indetermination of the acceleration vector of a grain.

4 AN EQUILIBRIUM STATE

Figure 3 presents a detail of a collection of $N=28$ frictional circular bodies in equilibrium under gravity. The number of contact points being denoted by κ , the problem is to calculate the element ρ of $\mathbf{R}^{2\kappa}$ consisting of the components of the contact forces.

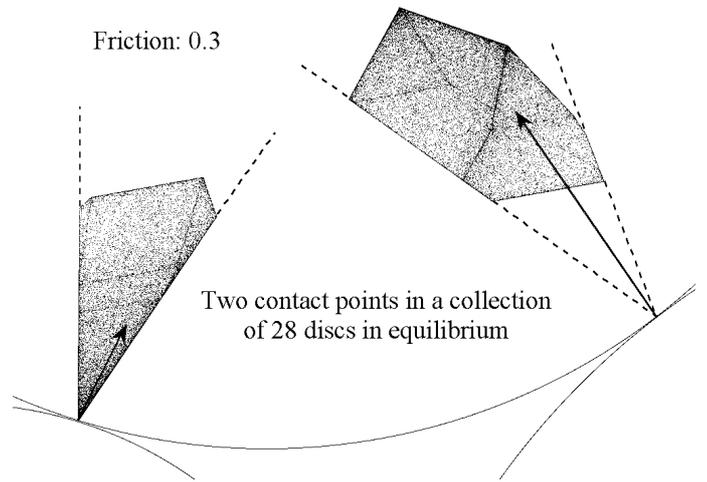


Figure 3. Indetermination clouds for two contact forces.

The $3N$ independent equations of equilibrium restrain ρ in an affine submanifold A of $\mathbf{R}^{2\kappa}$ with dimension $2\kappa-3N$. Coulomb law requires of each contact force, say ρ_α , to belong to an angular region C_α of the corresponding copy of \mathbf{R}^2 . This is equivalent to ρ belonging to a polyhedral cone C in $\mathbf{R}^{2\kappa}$, the Cartesian product of regions C_α . The set of equilibrium solutions in $\mathbf{R}^{2\kappa}$ thus equals the intersection $A \cap C$, a convex hyperpolyhedron. Coming back to an individual contact, the set of the possible values of the contact force equals the Cartesian projection of $A \cap C$ onto the corresponding copy of \mathbf{R}^2 .

Repeated independent runs of the Gauss-Seidel algorithm, with changes in the ordering of contact reviews, are used to explore the set of solutions.

On Figure 3, for two contact points in the assembly, the programme has drawn a dot at the extremity of each computed value of the contact force. The resulting clouds provide outlines of the projections of $A \cap C$. Of course, they are included in the respective angular regions C_α .

A surprise is the appearance inside these clouds of some ghost images of edges and vertices of the high-dimensional polyhedron. This shows that in $\mathbf{R}^{2\kappa}$ the points are a little denser in the vicinity of the boundary of $A \cap C$.

For a similar collection of discs in equilibrium, an investigation in statistical spirit of force indeterminacy has been conducted by Unger et al. 2004.

5 THE MESSAGES FROM HISTORY

Figure 4 presents a 2D model of a phenomenon which gave rise to vivid discussions in recent years: a pile of conical overall shape is constructed by pouring grains from a localized source onto horizontal ground. Measurements reveal that the pressure distribution on ground does not relate to the height of material above. A local minimum of pressure may even be found at the vertical of the apex.

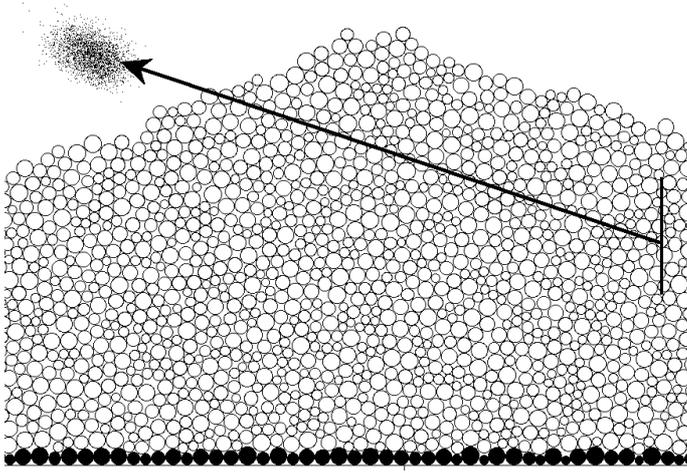


Figure 4. Resultant force transmitted across a vertical cut.

This necessarily means that some central portion of the pile has part of its weight supported by *arching* actions from the surrounding bank. In the present 2D simulation, a vertical cut is drawn through the granular matter. The programme calculates the total force transmitted across this line segment, i.e. the resultant vector of the contact forces exerted by grains with centers on one side upon antagonists on the other side. The vector obtained, approximately parallel to the free surface, confirms the arching trend of force transmission throughout the lateral bank.

Repeated runs of the Gauss-Seidel algorithm with zero initial guess but changes in review ordering have been applied to the equilibrium problem concerning the considered arrangement of grains. For each solution obtained, the programme draws a dot at the endpoint of the transmitted force, thus a cloud wick reflects the plurality of solutions.

The arrangement of grains is the result of simulating the whole construction process of the pile. If at each time-step of this simulation, the initial guess of iterations is made of the antecedent contact forces, practically no indeterminacy is found. What the above cloud reveals is the indeterminacy ensuing in the final step from the decision of ignoring antecedent forces.

Summing up, at each instant of the time-stepping procedure, the message from history consists of two parts: the geometric arrangement of grains and the contact forces. The small size of the above cloud shows that the geometric information is by itself enough for the computation to display the arching effect whatever is the indeterminacy.

In experiments of this sort, one should keep in mind that varying slightly the cut position may produce changes in transmitted force of definitely larger amplitude than the above indetermination. In fact in the example shown only 10 contacts are involved in the force transmission across the segment.

The reader interested in force transmission through granular matter may refer to Moreau 1999, 2004a, where 3D simulations of pile construction are presented. Cuts are drawn in the bulk, either vertical

(pieces of cylindric surfaces coaxial to the pile) or parallel to the free surface (pieces of conic surfaces). In the latter case, the transmitted force is found vertical, an easily explained feature amounting to the assertion, commonly made in Civil Engineering, that the peripheral bank lies in a state of *incipient failure*. For cylindric cuts, the transmitted force is found parallel to a generating line of the conical surface of the pile, revealing the same arching effect as in the foregoing 2D example. The author's interpretation is that these two observations are mathematically equivalent thanks to a *reciprocity formula* ensuing from the symmetry of the Cauchy stress, a tensor classically defined as an average over a granular sample covering the considered cuts.

6 CONCLUSION

The preceding section provides the reassuring example of a simulation where indeterminacy is not large enough to mask the investigated feature.

One should observe that the present paper, essentially algorithmic, calls for a return to the theoretical formulations of the considered mechanical problems, independently of any time-stepping computation technique. Then it doesn't make sense anymore to distinguish between input and output values of contact forces. What the foregoing actually reflects is an *incremental* version of Coulomb law.

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