A COMPUTATIONAL MODEL FOR MULTIPLE COLLISIONS OF RIGID BODIES: AN EXTENSION OF A-CD² METHOD

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Abstract. The A-CD² method gives a mechanical description for instantaneous collisions between rigid bodies. This method considers a solid that moves with constant velocity in the intervals $[t_1, t_c[$ and $]t_c, t_2]$. The contact points at t_c are computed with the current position and the new velocities, due to the collision at t_c , are calculated by means of a constrained optimization problem. Several applications have used this method. When the solid is governed by a torque free motion, the velocities are not necessarily constants, because depend on the moments of inertia. This behavior is not included in the A-CD² method, since constant velocities are considered. An extension includes the use of the Euler equations for modeling the angular velocities, when the body is torque free. Therefore, non constant angular velocities are obtained when the moments of inertia are different.

An important result is the reduction in the computational complexity of the original algorithm, from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$, mainly due to the contact detection stage. This reduction allows to handle problem 20 times larger than the original. Numerical simulations for granular layers motion are presented.

1 INTRODUCTION

Collision between rigid bodies is an important class of processes arising in several natural events, for instances, avalanches, molecules and asteroids collisions, and also in many important engineering and industrial problems e.g., mining, construction, transport, among others.

Thus, it is important to develop computational models for collision simulations in order to complement expensive experiments, which usually requires resources and equipments that are expensive. A computational simulation allows to considerably reduce the use of special equipments and other resources, and still allowing to obtain a very close description of the dynamics of the phenomenon, with the goal of analyzing and studying the evolution of collisions in time.

The approach presented in [1], named A-CD² obtains the new velocities of a set of solids, after a collision, by solving a constrained minimization problem. Currently this method allows us to simulate a system with no more than 1500 solids. The problem is mainly computational: the contact detection algorithm has computatinal complexity $\mathcal{O}(n^2)$, where *n* is the number of solids in the system. Therefore, an efficient computational method is presented, where an algorithm with linear computational complexity is achieved, and an interior point method for the constrained optimization problem is used. Now, simulations with more than 5000 solids is achieved, and the computational time has been decreased considerably. Numerical simulations for the constitution of compact grain layers is obtained, where the solids is concentrated in a point with the objective to have a layer of rigid bodies in equilibrium.

2 METHODS

2.1 A-CD² METHOD

A theory for multiple collisions in granular flow, based on the representation of the medium as a collection of rigid bodies [4] is presented in [1, 2, 10]. When rigid bodies get into collision, it is no longer possible to solve the classical equation of motion because velocities are not differentiable: the application of the principle of virtual work in association with appropriate constitutive laws relating internal stress and velocities allows to obtain a set of equations of motion, valid both for smooth and for non-smooth evolutions. In particular, this approach allows us to overcome the limits of the classical penalty method, it does not require the definition of gap functions, and satisfy the actual physical condition of non-interpenetration of the particles. Moreover, compared to [5] or [6] the existence and the uniqueness of the solution of the Clausius-Duhem inequality has been proved [10]. This approach is called Atomized efforts Contact Dynamics respecting the Clausius-Duhem inequality (A-CD²). It describes multiple bodies contact dynamics (according to the Clausius-Duhem inequality) by means of an "atomization" of the efforts exerted during contact.

According to obtain the velocities after the collision, this approach, for the sake of simplicity, it exposed for a single point, with mass m, colliding once to a rigid fixed surface in a time interval $[t_1, t_2]$ and having instantaneous velocity discontinuity, before generalizing the formulation to a simulataneous collision of N rigid solids [4, 10].



Figure 1: Point - plane system: a particle with mass m and a fixed plane.

As the collision is assumed to be instantaneous, the velocity \boldsymbol{u} of the point is discontinous at the instant t_c of the impact, having a left and right limit noted \boldsymbol{u}^- and \boldsymbol{u}^+ . The contact force is concentrated in time, becoming a percussion \boldsymbol{P}^{int} [4]. In Figure 1 we show the interaction between the point and the rigid fixed plane with one collision in the time interval, the description of the point trajectory $\boldsymbol{x}(t)$ in $[t_1, t_2]$ and the collision at time t_c .

Interior forces considered in the particle motion at interval time $[t_1, t_2]$ are defined by their work. Let us consider a contact force \mathbf{f}^{int} , which is concentrated in time, such as the internal percussion \mathbf{P}^{int} . An exterior percussion \mathbf{P}^{ext} could be taken into account, not depending on \mathbf{u} , and also applied to the point at the instant of collision. External forces \mathbf{f}^{ext} also are considered and are not depending on the velocities. The equations of motion assume the following form on $[t_1, t_2]$ [8]

$$m \frac{d\boldsymbol{u}}{dt} = -\boldsymbol{f}^{int} + \boldsymbol{f}^{ext}$$
 almost everywhere (1)

and

$$m\left(\boldsymbol{u}^{+}(t_{c})-\boldsymbol{u}^{-}(t_{c})\right)=-\boldsymbol{P}^{int}+\boldsymbol{P}^{ext}\qquad\text{everywhere}\qquad(2)$$



Figure 2: Motion of a rigid body.

If we consider now a solid, not a point (see Figure 2), we have [8]

$$m \left(\boldsymbol{u}^{+} - \boldsymbol{u}^{-} \right) = -\boldsymbol{P}^{int} + \boldsymbol{P}^{ext}$$

$$I \left(\boldsymbol{\omega}^{+} - \boldsymbol{\omega}^{-} \right) = -\boldsymbol{g} \boldsymbol{A} \times \boldsymbol{P}^{int} + \boldsymbol{g} \boldsymbol{B} \times \boldsymbol{P}^{ext}$$
(3)

where $\boldsymbol{\omega}$ is the rotational velocity of the solid, \boldsymbol{g} is the center of mass, \boldsymbol{A} is the point where the internal percussion is applied and \boldsymbol{B} is the point where the external percussion is applied.

The following minimization problem:

$$\inf_{\boldsymbol{x}} F(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{x} \rangle + \Phi(\boldsymbol{x}) - \langle 2 \, \boldsymbol{u}^{-} + \boldsymbol{b}, \boldsymbol{x} \rangle \tag{4}$$

where the function $\Phi(\boldsymbol{x}) = \Phi^d(\boldsymbol{x}) + \mathbb{1}_K(\boldsymbol{x})$ and $K = \left[\frac{\boldsymbol{u}-\boldsymbol{N}}{2}, \infty\right] \Phi = \Phi^d + \mathbb{1}_K$ is a pseudopotential of dissipation, which is convex, positive and null in the origin [7, 8, 10, 12] and

$$\boldsymbol{P}^{int} \in \partial \Phi\left(\frac{\boldsymbol{u}^{-} + \boldsymbol{u}^{+}}{2}\right) \quad \text{where } \Phi = \Phi^{d} + \mathbb{1}_{K}$$
(5)

i.e. the internal percussion is derived from a pseudopotential of dissipation, divided in a dissipative Φ^d and reactive $\mathbb{1}_K$ percussion. Particularly, the reactive percussion can be replaced by the constraints $\varphi_k(\boldsymbol{x}) \leq 0$ defining the set Ω .

The collision problem is now a constrained minimization problem, where the solution gives us the new velocities of solids at some discrete time Δt . The function $F(\boldsymbol{x})$ is quadratic due to the choice of the dissipative percussion Φ^d (quadratic) and the set of constraints $\varphi_k(\boldsymbol{x}) \leq 0$, $k = 1, n_c$ (non - interpenetration condition) where n_c is the total number of contact points.

Thus, the constrained minimization problem is given by:

$$\inf_{\boldsymbol{x}\in\Omega} F(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{x} \rangle + \Phi^{d}(\boldsymbol{x}) - \langle 2 \, \boldsymbol{u}^{-} + \boldsymbol{b}, \boldsymbol{x} \rangle$$

where $\Omega = \left\{ \boldsymbol{x} \in \mathbb{R}^{6N} : \varphi_{k}(\boldsymbol{x}) \leq 0, \quad k = 1, ..., n_{c} \right\}$ (6)

The constraint $\varphi_k(\mathbf{x})$ associated to the contact point A_{ijk} is given by

$$\varphi_k(\boldsymbol{x}) = \left(\boldsymbol{d}_{ij}^{\boldsymbol{u}/\boldsymbol{2}^-}\left(\boldsymbol{A}_{ijk}\right) - \boldsymbol{d}_{ij}^{\boldsymbol{x}}\left(\boldsymbol{A}_{ijk}\right)\right) \cdot \boldsymbol{N}_k$$
(7)

where N_k is the normal vector at contact point A_{ijk} , and

$$\boldsymbol{d}_{ij}^{\boldsymbol{u}}\left(\boldsymbol{A}_{ijk}\right) = \left(\boldsymbol{u}_{i} + \boldsymbol{\omega}_{i} \times \boldsymbol{g}_{i} \boldsymbol{A}_{ijk}\right) - \left(\boldsymbol{u}_{j} + \boldsymbol{\omega}_{j} \times \boldsymbol{g}_{j} \boldsymbol{A}_{ijk}\right)$$
(8)

is the actual relative velocity of solids i and j at the contact point A_{ijk} You can see more details in [1, 10, 11].

The function $F(\mathbf{x})$ is possible to write it in the following quadratic matrix form

$$F(\boldsymbol{x}) = \frac{1}{2} \boldsymbol{x}^{T} (2M + \Xi) \boldsymbol{x} - \boldsymbol{x}^{T} (2M \boldsymbol{u}^{-} - \boldsymbol{b}^{\text{ext}})$$
(9)

where $M \in \mathbb{R}^{6N \times 6N}$ is the inertia and mass matrix, $\Xi \in \mathbb{R}^{6N \times 6N}$ is the pseudopotential of dissipation matrix and $\boldsymbol{b}^{\text{ext}}$ is the external percussion vector. It is possible to show that the matrices M and Ξ are sparse [11].

2.2 CONTACT DETECTION

An important step of our work, is the contact detection step, which determines the points where the solids are in contact. This step is divided in two process: (a) determination of closer solids and (b) computation of contact points. The first part is addressed by a neighborhhod technique. This technique consists in computing, each certain amount of timesteps, the neighborhood for each solid, that means, all solids which are closer. The second part is addressed by a technique called "early out", which consists in to proceed with less expensive tests first before to entry in the more specific overlap tests.

2.2.1 Neighborhood

The neighborhood for each solid is computed using a cell mapping technique [13], applied to a three dimensional space. This technique consists in dividing the space in boxes or cubes, and calculating the cube where each solid belongs, for instance, if a solid i is in the position (x_i, y_i, z_i) , then belongs to the cube with coordinate:

$$\left(\frac{x_i - \min_x}{\operatorname{size}_x}, \frac{y_i - \min_y}{\operatorname{size}_y}, \frac{z_i - \min_z}{\operatorname{size}_z}\right),\,$$

where \min_x, \min_y and \min_z are the minimum coordinates x, y and z respectively, and size_x, size_y and size_z are the each size of the cube. Each cube has three coordinates, which is the position in the space, consequently has a corresponding cube. The neighborhood of the solid will be then, all the solids which are in the closer cubes, i.e. for the cube CUBE(a, b, c) with coordinate (a, b, c), the neighborhood will be formed by the 26 cubes around. In the original simulations, the neighborhood computation of one solid considers the distances with all the remaining solids. Therefore, the computation is order $\mathcal{O}(N^2)$. The call mapping technique is order $\mathcal{O}(N)$, because we are going to compute the distances just with the solids which belong to the 26 cubes around.

2.2.2 Contact Points

In [9] is mentioned a *Bounding Volume* (BV) which is a volume encapsulating one or more objects of more complex nature. The idea is, for the simple shapes, such as boxes or spheres, to have cheaper overlap tests than the complex objects they bound. Using bounding volumes fast overlap rejection test is allowed, because it is only necessary a test against the complex bounded geometry when the initial overlap query for the bounding volumes gives a positive result. In [9] also mentioned that not all geometric objects serve as effective bounding volumes; desirable properties for bounding volumes include inexpensive intersection tests, tight fitting, inexpensive to compute, easy to rotate and transform and use little memory.

The main idea is to apply a technique called "early out", which consists in to procede with less expensive tests first before to entry in the more specific overlap tests. Therefore, the idea of the bounding volumes is that they must have a simple geometry shape, allowing a first fast overlapping test. The contact detection between solids has been separated in two steps: a faster overlap detection and a contact point detection. The first step is made using spheres as BV, therefore the overlap detection is focused in detect if a polyhedron is close enough to another one. The second part is performed when both bounding spheres are overlapped, then, is applied a technique to search the points where the polyhedrons are in contact. Three contact point detections are made: surface, face and edge detection.

3 NUMERICAL RESULTS

A granular material is a collection of solid particles or grains, such that most of the particles are in contact with at least some of their neighboring particles. The term granular layer could be used to describe a type of granular material, in fact, a granular layer is simply a collection of solid particles which is in repose in some surface. In this case it will be considered a granular layer in a plane. The problem arises in building this layer, because the idea is to obtain a very compact granular heap.

An interesting result is that the computational time for N solids, have a linear behavior. It is important to remark that the optimization part was a black case, which it is not possible to change, but all the rest of the computations: contact detection, optimization problem building, velocity updating and geometry setting were computed. In the simulation for N solids, they begin at rest in a random position but directed towards the origin, therefore after some simulation time, solids start to collide forming a heap.



Figure 3: Evolution of 1000 solids forming a heap.



Figure 4: Evolution of 3000 solids forming a heap.

4 CONCLUSIONS

The main goal of this work was to develop a mathematical and computational model for multiple collision of rigid bodies, by means of an extension of the A-CD² method. The new elements addressed in this work was the computational issues detected in the original version and the theoretical development for the rotational velocities of the solids. Theses issues comprise (a) inefficient use of computational memory, (b) convergence problem in the constrained minimization problem method and (c) inadequate mechanical behavior according to the rotational velocity of the solids. For the first issue a dynamical algorithm was presented, where the efficient use of computational memory has been achieved. Mainly in the contact detection module, a dynamical neighborhood algorithm was developed. Regarding the convergence problem, the original version uses Uzawa method to find the solution for the constrained minimization problem. In this work an interior-point method (barrier) has been used, by means of the CPLEX library. The convergence problem has been solved, because the high convexity of the function to minimize the barrier method best suits. Finally, the original approach consider, in a timestep simulation, all velocities constant. In our case, a new set of equations has been presented particularly for the rotational velocity non constant behavior.



Figure 5: Computational time comparison between the original version (red dashed) and the new one (blue continuous) for different amounts of solids.

All these improvements allow us to compute until 3000 solids in a reasonable computational time. In the Figure 5, the cpu time is shown for one iteration, without the CPLEX computational cost. Clearly we observe an improvement between the original version and the new one, where the computational order has been reduced. An important remark is that with the original approach, no more than 1000 solids simulation can be achieved in a reasonable computational time. As final conclusion, this extension offers the possibility to simulate large scale problem, even so, we can continue to obtain more improvements.

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