Impact of interaction laws and particle modelling in discrete element simulations

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Abstract. Among mechanical systems, a large number presents naturally a divided feature: granular media, masonries, metal at the grain level, etc. Some of them, due to external loading, may evolve from a continuous state to a, globally or locally, divided one: fracture, wear, cracks, etc. When numerical studies of such media are performed, Discrete Elements Methods (DEMs) appear as most appropriate tool to face to different problems.

Classically, DEMs are based on some hypotheses concerning contact area, deformations and contact interactions which are in some circumstance questionable, especially when they have a strong influence on the macroscopic behaviour of the media.

Using the Contact Dynamics framework, the paper presents how classical hypothesis could be extended to avoid numerical effects. A reflection is proposed taking into account both physical and numerical aspects. Static and dynamic configuration have been used to illustrate the paper purposes.

Keywords: Discrete Element, contact law, Finite Element
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INTRODUCTION

Among mechanical systems, a large number presents naturally a divided feature: granular media, masonries, ceramics, metal, etc. Some of them, due to external loading, may evolve from a continuous state to a, globally or locally, divided one: fracture, wear, cracks, etc. When numerical studies of such media are performed, Discrete Elements Methods (DEM) appear as an appropriate tool to face the various difficulties of the modelling.

Classically, DEMs are based on some hypotheses concerning contact area, bulk models and interaction laws which are in some circumstance restrictive and questionable, especially when they have a strong influence on the macroscopic behaviour of the media.

Based on the Contact Dynamics (CD) framework, the paper presents how classical hypothesis can be extended to avoid some DEM restrictions. A reflection is proposed to improve both physical and numerical aspects. The section presents the headlines of the mechanical framework used in this paper. Various static and dynamic configuration have been studied to illustrate our purpose.

MECHANICAL MODEL

The method used in this paper relies on the (Non Smooth) Contact Dynamics frameworks developed by Moreau and Jean [1, 2].

Considering a multi-contact problem, the approach leads to a reformulation of the classical equation of dynamics in term of contact unknowns written in the contact frame : the local impulse $\mathbf{p}$ and the relative velocity $\mathbf{u}$. Over a given time interval $[t_i, t_{i+1}[$, starting from a the balance of momentum, the problem is written as a set of transfer equations and interaction laws :

$$\left\{ \begin{array}{l} \mathbb{W}\mathbf{p}_{i+1} - \mathbf{u}_{i+1} = -\mathbf{u}_{free} \\ ContactLaw[\mathbf{p}_{i+1}, \mathbf{u}_{i+1}] \end{array} \right. \quad (1)$$

where $\mathbb{W}$ is the Delassus operator that models the dynamics of the solids at the contact points. The right-hand-side of the first equation of the system (1) represents the free relative velocity, velocity of bodies free of contact forces. The second equation closes the system (1), it assumes that each contact law must be satisfied by each couple $(\mathbf{u}_{i+1}, \mathbf{p}_{i+1})$.

The Delassus operator is equal to $\mathbb{H}^* \tilde{\mathbb{M}}^{-1} \mathbb{H}$ where $\mathbb{H}$ is a linear mapping between the local unknown and the global one while $\tilde{\mathbb{M}}^{-1}$ is the inverse of the mass matrix.

Considering rigid bodies, one obtains:

$$\left\{ \begin{array}{ll} \tilde{\mathbb{M}} & = \mathbb{M} \\ \mathbf{u}_{free} & = \tilde{\mathbb{M}}^{-1}(h(1-\theta)\mathbf{F}_i^{ext} + h\theta\mathbf{F}_{i+1}^{ext}) \end{array} \right. \quad (2)$$

where θ is the time integrator parameter, h the time step and $\mathbf{F}^{ext}$ the external forces.

Considering deformable bodies, in the case of linear case, one obtains:

$$\left\{\begin{array}{ll}\tilde{\mathbb{M}} & =\mathbb{M}+h\theta\mathbb{C}+h^2\theta^2\mathbb{K}\\ \mathbf{u}_{free} & =\tilde{\mathbb{M}}^{-1}(h(1-\theta)\mathbf{F}_i^{ext}+h\theta\mathbf{F}_{i+1}^{ext}+\\ & h\mathbf{F}^{vol}(\mathbf{q}_i+\theta\mathbf{v}_i,\mathbf{v}_{i+1}))\end{array}\right. \quad (3)$$

where $\mathbb{C}$ and $\mathbb{K}$ represents respectively the viscosity and the stiffness matrices and $\mathbf{F}^{vol}$ represents the internal forces of the deformable bodies.

To close the system an interaction law, which must be satisfied by each couple $(\mathbf{u}_{i+1},\mathbf{p}_{i+1})$, must be defined. In the present study we consider only unilateral contact with dry Coulomb's friction. The unilateral contact means that when contact occurs (gap is equal to zero) the normal impulse is positive and when the contact vanishes (gap is positive) it is equal to zero. As proposed by Jean [2], this Signorini condition may be written as follow (subscript $i+1$ is intentionally omitted) :

$$g_{ini}/h+u_n\geq 0 \quad p_n\geq 0 \quad (g_{ini}/h+u_n).p_n=0, \quad (4)$$

where the index n denotes the normal component of the various quantities, g_{ini} is the distance between objects at the beginning of the time step and h the time step. One advantage of this writing is that you are able to implicitly settle that the gap is equal to zero at the end of time step if contact occurs. One drawback is that this writing means a fully plastic shock law.
An alternative writing was proposed by Moreau [3], it is summarized by the so-called *velocity Signorini condition*

$$if \quad g_{ini}\leq 0. \quad \tilde{u}_n\geq 0 \quad p_n\geq 0 \quad \tilde{u}_n.p_n=0, \quad (5)$$

$$otherwise \quad p_n=0 \quad (6)$$

The main advantage of this writing is that it implicitly embed a **collision** law based on the Newton restitution law through $\tilde{u}_n=u_{n,i+1}+e_nu_{n,i}$. The main drawback comes from the fact that you may recover a negative gap. It is important to note that the inelastic shock is not rigorously equal to the restitution law with e_n equal to 0.

The dry Coulomb's friction law enforce that the friction force lies in the Coulomb's cone ($||\mathbf{p}_t||\leq\mu p_n$, μ friction coefficient), and a sliding occurs only when you reach the cone ($||\mathbf{p}_t||=\mu p_n$) and its direction is opposed to the friction force. We can summarize previous explanations by the following relation:

$$||\mathbf{p}_t||\leq\mu p_n \quad ||\mathbf{u}_t||\neq 0\rightarrow\mathbf{p}_t=-\mu p_n\frac{\mathbf{u}_t}{||\mathbf{u}_t||} \quad (7)$$

NUMERICAL RESULTS

In this paper, all the results are obtained using LMGC90 software developed by Dubois and Jean ([4]). Our simulations concern the biaxial compression and shear of a 2D sample made of circular particles either rigid or deformable. We consider the two different contacts law presented before: plastic Signorini Coulomb (IQS), restitution Signorini Coulomb (RST).

Rigid bodies

We consider a sample of 2000 rigid bodies with randomly generated radius between 8 mm − 16 mm ($R_{max}/R_{min}=2$) in an area bounded contained by four rigid frictionless walls (see figure 1). In these simulations we consider rigid particles made of steel with a specific mass equal to 7800 kg/m^3.

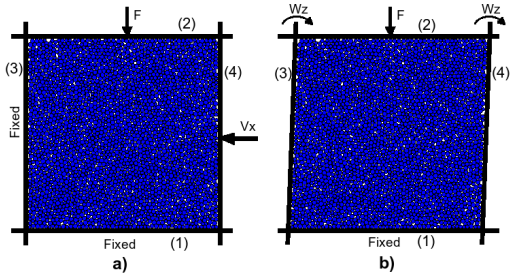

FIGURE 1. *Geometry of the sample and boundary condition. Case a: applied force in Y direction and applied velocity in X direction. Case b: applied force in Y direction and applied rotation velocity around Z direction*

The loads are applied in two phases: isotropic compression followed by a biaxial or a shear load. During the first phase $F_y=F_x$, and during the second phase $F_y=F$, where F is the confining force reached at the end of the first phase. The initial configuration of the second phase is the same for both loads (see figure 1) :

- case (a): walls 1,3 are fixed, a force F equal to 1000 kN is applied on the wall 2 and velocity V of 0.01 m/s is applied on the wall 4 (F,V are linear functions of time so that the force F and the velocity V reach their maximum values at $t=1\ s$).
- case (b): wall 1 is fixed, a force F equal to 1000 kN is applied on the wall 2 and rotation velocity W_z of 0.04 rad/s is applied on walls 3 and 4.

We have conducted our tests with different contact laws: plastic Signorini Coulomb law (IQS) and restitution Signorini Coulomb's law (RST). With the RST contact law, we have tested two different value of normal restitution e_n: 0 and 0.9.

The walls do not interact. The contact between disks and walls is without friction. Gravity forces are neglected. The time step is equal to $1.10^{-3}\ s$ and the simulation time is equal to 4 s.

Since contact between walls and particles is frictionless, the principal directions of stresses and strains coincide with the coordinate axes x and y (see figure 1). Therefore principal strains were calculated directly from wall displacements, whereas principal stresses were obtained as the sum of the normal forces applied by disks on surrounding walls divided by the wall length (and disks thickness !?).

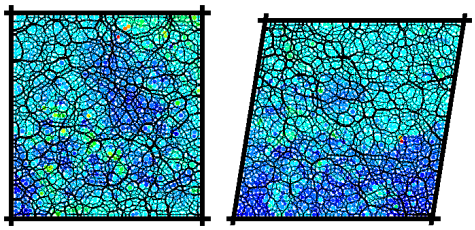

FIGURE 2. *Velocity of particles and contact force network at the end of the load for case a and b*

Figures (2) show the velocity field and the contact force network between particles. When we apply a load (force or velocity) on the walls it is supported by the particles through the contact network.

The orientation and the amplitude distribution of the contact force depends on the external load, the physical parameters and the history. One can see in the figure (3) the compacity evolution with respect to the increasing external load.

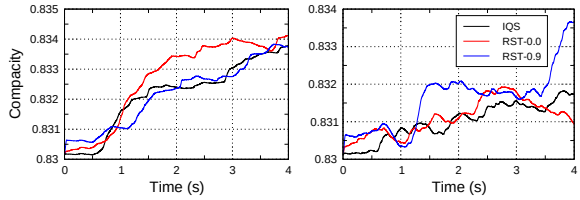

FIGURE 3. *Compacity evolution for case a and b*

One can observe in the figure (3) that :

- case a. The evolutions are more or less the same for the 3 contact laws. The small variations around the mean value are triggered by arch breaking, dilatation induced by shear, etc.
- case b. The evolutions are less similar and more noisy. This may be explained by the different behavior the contact law act. One can observe that the IQS law evolves the more regularly due to its dissipative and fully implicit properties.

When using the CD approach one needs to manage the precision of the computation which depends on the time step, the converging tolerance of the contact solver (Non Linear Gauss-Seidel in the present work), etc. Relevant informations to compare the results are the necessary computational effort represented by the number of iterations and the precision of the results represented by the violation. We can see in the figure (4) the influence of the numerical model on the average number of interation. One can notice that with the contact law RST-0.9 the results are more smooth.

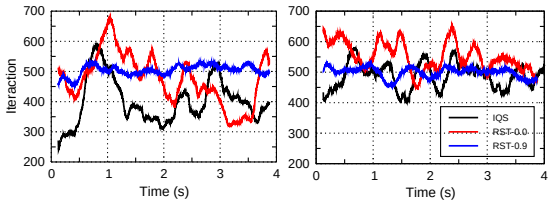

FIGURE 4. *Average number of interations with the different contact laws IQS, RST-0.0 and RST-0.9 for case a (right) and case b (left)*

One can observe in the figures (5 and 6) the mean violation evolution for the different contacts laws. The median radius of the particles is around $10^{-2}m$ which means that for RST law the violation is less than 0.05% of the radius and for IQS law it is less than 10^{-3}% of the radius.

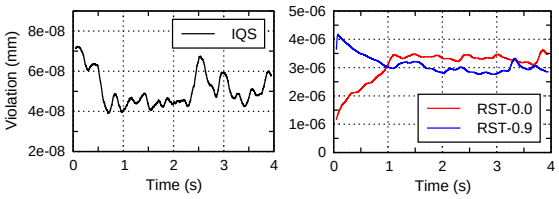

FIGURE 5. *Evolution of the mean violation for case a*

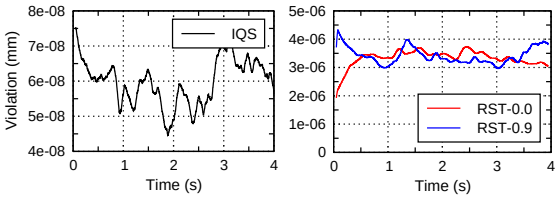

FIGURE 6. *Evolution of the mean violation for case b*

Figures (7 and 8) are showing :

- Left :the angular distribution of the normal contact forces at the end of the simulation. We have obtain a good condordance between diffirent measured quantities. The orientations distributions of contact normale obtained by the two model are identical. we obtain a constant probability, almost independent of the orientation feature when compress a multi disks without gravity.
- Right : the number of contacts as a function of the normal contact force normalized by its mean value at the end of the simulation.

In both cases we obtain very similar results.

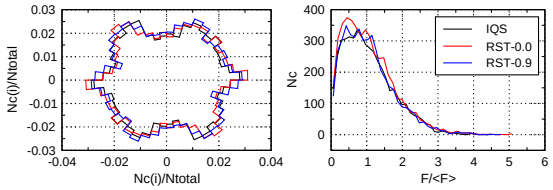

FIGURE 7. *Case a. Left : angular distribution of contact forces. Right : number of contacts as a function of a normalized normal contact forces*

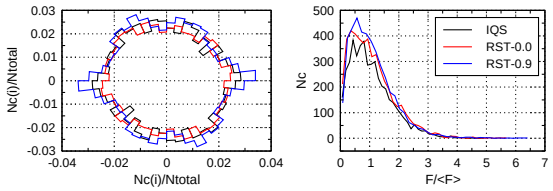

FIGURE 8. *Case b. Left : angular distribution of contact forces. Right : number of contacts as a function of a normalized normal contact forces*

Deformable bodies

In this part, we have considered the same problems as before (see), replacing the rigid particles by deformable ones (see figure 9). The material is considered to stay elastic with a Young modulus $E = 320GPa$ and a Poisson coefficient $\nu = 0.33$. Each particle is meshed with quadrilateral elements. The time step h is equal to $10^{-4}s$.

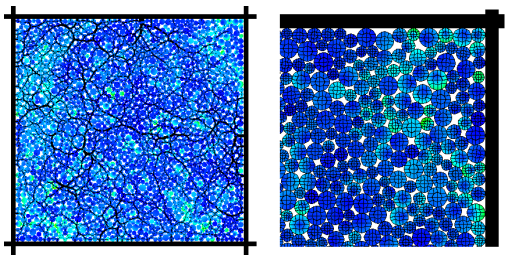

FIGURE 9. *Velocity field and contact force network of the meshed deformable particles*

CONCLUSION

The Contact Dynamics framework allows to use various interaction laws and bulk models. The compared interaction laws allow to obtain similar results, from a macroscopic physical point of view, in various situations. Depending on the required numerical precision or physical precision one is able to choose or switch from one model to the other.

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