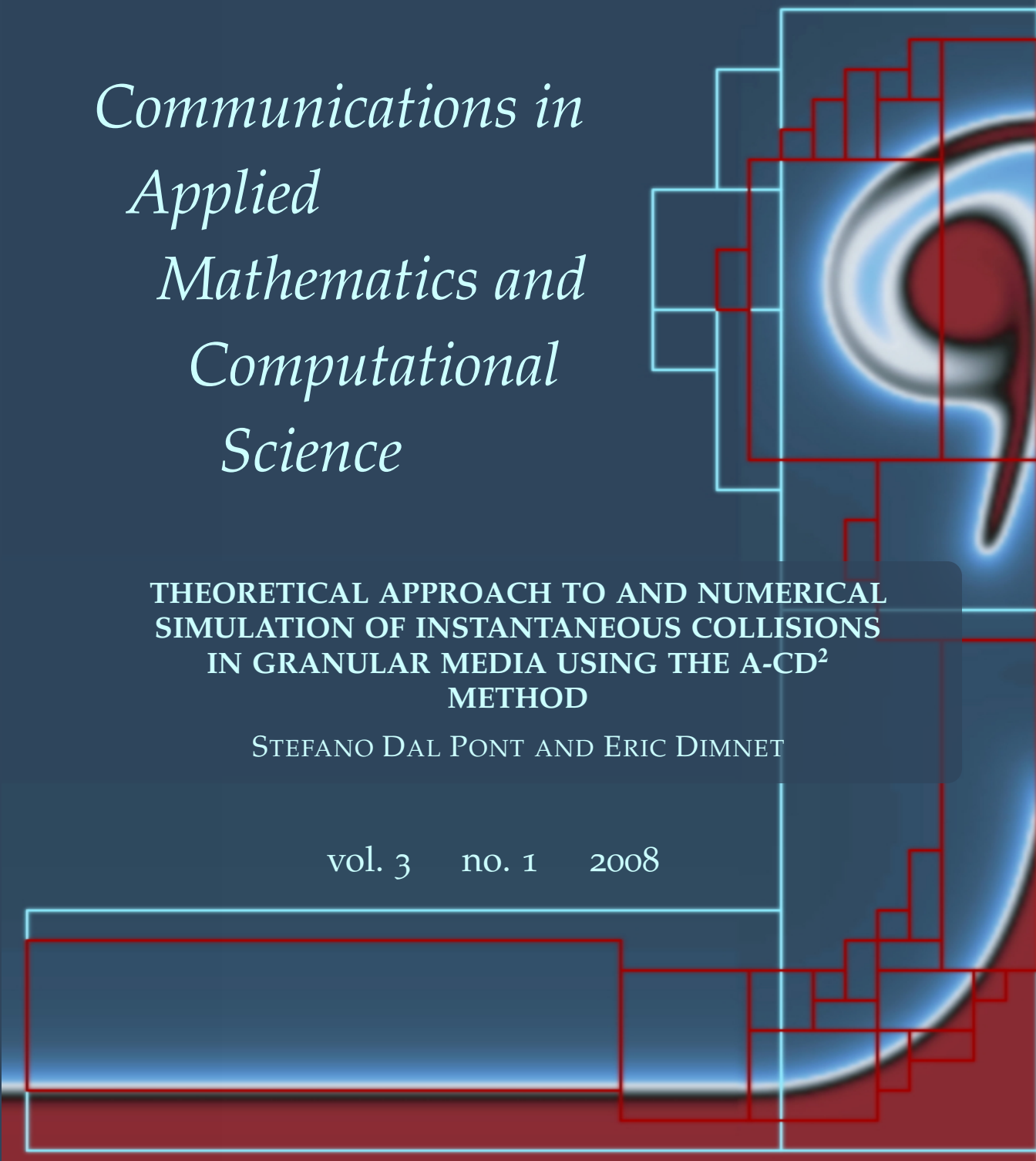
Communications in Applied Mathematics and Computational Science



THEORETICAL APPROACH TO AND NUMERICAL SIMULATION OF INSTANTANEOUS COLLISIONS IN GRANULAR MEDIA USING THE A-CD^2 METHOD

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vol. 3 no. 1 2008

mathematical sciences publishers

COMM. APP. MATH. AND COMP. SCI.
Vol. 3, No. 1, 2008

THEORETICAL APPROACH TO AND NUMERICAL SIMULATION OF INSTANTANEOUS COLLISIONS IN GRANULAR MEDIA USING THE A-CD^2 METHOD

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This paper presents a model for the description of instantaneous collisions and a computational method for the simulation of multiparticle systems' evolution. The description of the behavior of a collection of discrete bodies is based on the consideration that the global system is deformable even if particles are rigid. Making use of the principle of virtual work, the equations describing the regular (that is, smooth) as well as the discontinuous (that is, the collisions) evolutions of the motion system are obtained. For an instantaneous collision involving several rigid particles, the existence and the uniqueness of the solution as well as its satisfaction of a Clausius–Duhem inequality (proving that the evolution is dissipative) are proved. In this approach, forces are replaced by a succession of percussions (that is, forces concentrated in time). The approach is therefore named Atomized stress Contact Dynamics respecting the Clausius–Duhem inequality (A-CD^2). This paper focuses also on nonassociated behaviors, and in particular on Coulomb's friction law. The use of this constitutive law represents a further theoretical and numerical enhancement of the model. The theory is finally illustrated by some numerical examples, using the associated constitutive laws and Coulomb's (nonassociated) friction law.

1. Introduction

Many engineering problems require a description of the contact mechanisms occurring among colliding solids. The classical continuum approach presents several well-known drawbacks, especially when large strains and crack propagation take place. Discrete approaches representing the medium as a granular material have been proposed by many authors [3; 11; 10; 15]. The description of a multiparticle system evolution requires the description of the interactions among these particles both during the regular, smooth evolution as well as in the instant of nonsmooth evolution, that is, during a collision. The velocity discontinuity at the instant of a collision does not allow us to solve the classical smooth equations of motion because velocities are

MSC2000: 78M50.

Keywords: discrete model, instantaneous collisions, principle of virtual work, Coulomb's friction law, A-CD^2 method, granular media.

not differentiable. In this paper, the nonsmooth equations of motions describing a collision derive from the principle of virtual work together with an appropriate set of constitutive laws. Constitutive laws can be both associated as well as nonassociated, that is, Coulomb's friction law can be taken into account. Moreover, the existence and the uniqueness of the solution as well as the satisfaction of the Clausius–Duhem inequality are demonstrated. The Clausius–Duhem inequality assures us that the solution of the equations describing the collisions always corresponds to a dissipative evolution. During the evolution of multibody system each particle undergoes regular stress (forces) and nonregular stress (percussions). In consequence, their movement is a succession of smooth evolutions (with differentiable velocities) mixed with nonsmooth evolutions (collisions with discontinuity of velocity). For this reason, a method which leads to a set of equations describing smooth as well as nonsmooth evolutions is proposed. It results from the general principle of atomization of the stress (see Section 4), known as the Percussion Method (or PM) [11; 5].

The presented method is therefore named *atomized stress contact dynamics respecting a Clausius–Duhem inequality* (A-CD^2). The approach is illustrated by the numerical simulation of two multiparticle systems' evolutions: the dynamic evolution of a granular flow and the quasistatic evolution of a biaxial test.

2. The instantaneous collision model

For simplicity, the mechanical model describing collisions will be first presented by treating the case of a single moving point colliding with a rigid fixed body. This simplified formulation reduces the degrees of freedom (DOFs) of the system and allows one to focus on the shock mechanism.

In the following, the equation of motion will be given in the time interval $[t_1, t_2]$.

We assume that collisions are instantaneous, and thus forces must be modeled by forces concentrated in time. These stresses are contact percussions $\boldsymbol{P}^{\text{int}}$ [5; 4]. The velocity $\boldsymbol{U}$ of the point is therefore discontinuous at the instant of the collision t_c and its left and right limits will be noted $-$ and $+$.

2.1. ***The principle of virtual work.*** Regarding time dependency, we consider that our mechanical system may undergo two kind of actions, forces and percussions. Forces have a density with respect to Lebesgue's measure in time, (that is, they are regular and smooth functions of time). Percussions have a density with respect to Dirac's measure in time (that is, the action is concentrated in an instant). These two actions are named regular stresses (forces) and nonregular stresses (percussions).

Interior stress (both forces $\boldsymbol{r}^{\text{int}}$ and percussions $\boldsymbol{P}^{\text{int}}$) are defined by their work.

The principle of virtual work leads us to choose the following expression for the virtual work of the internal stress [9; 6; 4]:

$$W^{\text{int}}(t_1, t_2, t_c, \boldsymbol{V}) = -\int_{t_1}^{t_2} d\tau\ \boldsymbol{V} \cdot \boldsymbol{r}^{\text{int}}(\tau) - \boldsymbol{P}^{\text{int}}(t_c) \cdot \frac{\boldsymbol{V}^-(t_c) + \boldsymbol{V}^+(t_c)}{2}, \qquad (1)$$

where $\boldsymbol{V}$ is a virtual velocity of the point and t_c is a virtual time of collision. In particular, Equation (1) allows one to establish a duality between the internal percussion $\boldsymbol{P}^{\text{int}}$ and the quantity $\boldsymbol{V}^{\Sigma} = (\boldsymbol{V}^- + \boldsymbol{V}^+)/2$, which can be interpreted as the rate of deformation of the system formed by the point and the fixed body at the collision instant. Similarly, we define $\boldsymbol{V}^{\Delta} = \boldsymbol{V}^+ - \boldsymbol{V}^-$ and likewise for other quantities superscripted by $+$ and $-$.

The virtual work of the acceleration is [5; 9; 6]:

$$W^{\text{acc}}(t_1, t_2, t_c, \boldsymbol{V}) = \int_{t_1}^{t_2} d\tau\, m \frac{d\boldsymbol{U}(\tau)}{d\tau} \cdot \boldsymbol{V}(\tau) + m\boldsymbol{U}^{\Delta} \cdot \boldsymbol{V}^{\Sigma},$$

where m is the mass of the point and $\boldsymbol{U}$ is the actual velocity.

The virtual work of an exterior percussion is [5; 9; 6]:

$$W^{\text{ext}}(t_1, t_2, t_c, \boldsymbol{V}) = \int_{t_1}^{t_2} d\tau\ \boldsymbol{V}(\tau) \cdot \boldsymbol{r}^{\text{ext}}(\tau) + \boldsymbol{P}^{\text{ext}}(t_c) \cdot \boldsymbol{V}^{\Sigma}.$$

The principle of virtual work implies that for any velocity $\boldsymbol{V}$ and any virtual time of collision t_c, the following expression holds:

$$W^{\text{acc}}(t_1, t_2, t_c, \boldsymbol{V}) = W^{\text{int}}(t_1, t_2, t_c, \boldsymbol{V}) + W^{\text{ext}}(t_1, t_2, t_c, \boldsymbol{V}).$$

According to this principle, the equations of motion are written in the following form on $[t_1, t_2]$:

$$m\frac{d\boldsymbol{U}}{d\tau} = -\boldsymbol{r}^{\text{int}} + \boldsymbol{r}^{\text{ext}} \quad \text{almost everywhere}, \qquad (2)$$

and

$$m\boldsymbol{U}^{\Delta} = -\boldsymbol{P}^{\text{int}} + \boldsymbol{P}^{\text{ext}} \quad \text{everywhere}. \qquad (3)$$

Thus, the internal percussion $\boldsymbol{P}^{\text{int}}$ in Equation (3) is the internal stress of the point-fixed body system at the instant of the collision. Due to the duality (established by the principle of virtual work) between $\boldsymbol{P}^{\text{int}}$ and $\boldsymbol{V}^{\Sigma}$ and following the classical mechanical approach, constitutive laws are given by expressing $\boldsymbol{P}^{\text{int}}$ as a function of $\boldsymbol{V}^{\Sigma}$.

An appropriate set of constitutive laws describing the behavior and the interactions between the colliding bodies must now introduced.

2.2. ***The constitutive laws.*** Constitutive laws take into account the interactions among particles during the collision and assure the noninterpenetration of the bodies. These two aspects are made explicit by splitting the internal percussion into a dissipative percussion $\boldsymbol{P}^{\mathrm{d}}$ that takes into account the behavior during the collision and a reactive percussion $\boldsymbol{P}^{\mathrm{reac}}$ that assures the noninterpenetration:

$$\boldsymbol{P}^{\mathrm{int}} = \boldsymbol{P}^{\mathrm{d}} + \boldsymbol{P}^{\mathrm{reac}}. \tag{4}$$

The dissipative percussion. This describes the (dissipative) interactions among the colliding bodies. A general, associated dissipative interaction can be described introducing a pseudopotential of dissipation Φ^{d}, which is a convex and positive function which is null in the origin [14; 11; 7; 8; 17; 5]: $\boldsymbol{P}^{\mathrm{d}} \in \partial \Phi^{\mathrm{d}} \left(\boldsymbol{U}^{\Sigma} \right)$.

The reactive percussion. The term $\boldsymbol{P}^{\mathrm{reac}}$ describes the reaction to the noninterpenetration condition, which implies $U_N^+ \geq 0$ (where $U_N^+ = \boldsymbol{U}^+ \cdot \boldsymbol{N}$, see Figure 1). This percussion is equal to 0 if $U_N^+ > 0$, is nonnull if $U_N^+ = 0$, and implies that the condition $U_N^+ < 0$ cannot hold. All these properties can be naturally written by means of the indicator function [14; 11] in the following way:

$$\boldsymbol{P}^{\mathrm{reac}} \in \partial I_K \left(\boldsymbol{U}^{\Sigma} \cdot \boldsymbol{N} \right), K = \left[\frac{U_N^-}{2}, +\infty \right[.$$

This percussion $\boldsymbol{P}^{\mathrm{reac}}$ is the (mechanical) reaction to the noninterpenetration condition $U_N^+ \geq 0$. From the mathematical point of view, $P^{\mathrm{reac}} = ||\boldsymbol{P}^{\mathrm{reac}}||$ is the Lagrange multiplier associated to the constraint $U_N^+ \geq 0$ (see also Figure 2). Therefore, there is no need to add any penalties to the model.

In particular, because K is convex and contains the origin, the indicator function I_K is a pseudopotential of dissipation [7; 8; 17]. The internal percussion can be

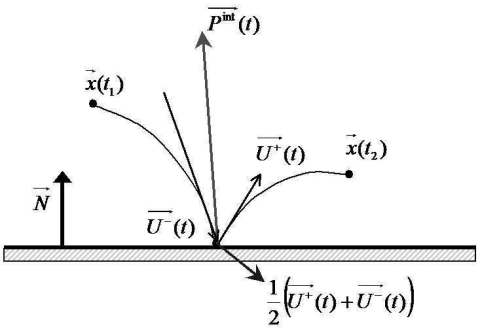

Figure 1. Instantaneous collision between a point and a rigid and fixed plane.

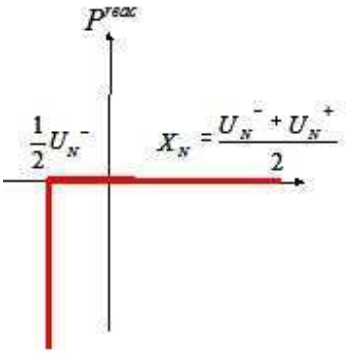

Figure 2. Indicator function.

therefore written in the following form:

$$\boldsymbol{P}^{\text{int}} \in \partial\Phi\left(\boldsymbol{U}^{\Sigma}\right), \quad \text{where} \quad \Phi = \Phi^{\text{d}} + I_K,$$

that is, the internal percussion derives from a pseudopotential of dissipation.

Using the pseudopotential of dissipation and the indicator function is a natural and effective way to introduce into the model both the dissipative character of the evolution and the necessity of the noninterpenetration among particles. Moreover, these mathematical tools are characterized by some properties (for example, convexity) which will be particularly useful in the following (see Section 4).

3. Simultaneous collision of N solids

In the previous section, the main characteristics of the model were presented. In particular, the general equations describing the evolution of the system (Equations (2) and (3)) as well as the general form of the constitutive relationships (4) are presented. This approach can be naturally extended to the case of N colliding solids.

We consider N solids colliding at time t, defined by their mass m_i, a center of gravity G_i and an inertial tensor I_i. Contacts between solids are assumed to be punctual. The k-th contact between the solid i and the solid j takes place at points $A_{i,j,k}$. The set of contact points between the solids i and j is named $S_{i,j}$. If these two solids are not in contact, this set is not necessarily empty. The interactions between distant (not in contact) particles can be taken into account (for details, see [5]). In this paper these interactions will not be considered. Percussion $\boldsymbol{P}^{\text{int}}_{i,j,k}$ is applied at contact point $A_{i,j,k}$. $\boldsymbol{V}_i$ is the virtual velocity of the center of gravity G_i and $\boldsymbol{\omega}_i$ is the virtual rotational velocity. External percussions $\boldsymbol{P}^{\text{ext}}_{i,l}$ are applied at

points $B_{i,l}$ of solid i. S_i' contains the points $B_{i,l}$ on which external percussions are applied on the solid i.

If we define the vector $\hat{V} = (\boldsymbol{V}_i, \boldsymbol{\omega}_i)$ which takes into account both translational and rotational degrees of freedom, we can write the relative velocities of the solids in contact at point $A_{i,j,k}$ in the following form:

$$\boldsymbol{D}_{i,j}(\hat{V}, A_{i,j,k}) = \boldsymbol{V}_i + \boldsymbol{\omega}_i \wedge \overrightarrow{G_i A_{i,j,k}} - (\boldsymbol{V}_j + \boldsymbol{\omega}_j \wedge \overrightarrow{G_j A_{i,j,k}}),$$

where we denote by $\overrightarrow{AB}$ the vector from point A to point B. The relative velocities at the contact points $B_{i,l}$ of solid i are

$$\boldsymbol{E}_i(\hat{V}, B_{i,l}) = \boldsymbol{V}_i + \boldsymbol{\omega}_i \wedge \overrightarrow{G_i B_{i,l}}.$$

In the following, we will focus our attention on the instant of the collision, t. If we denote by $\boldsymbol{U}_i$, $\boldsymbol{\Omega}_i$ the actual velocities of the solid i and by $\boldsymbol{V}_i$, $\boldsymbol{\omega}_i$ its virtual velocities, we can write the principle of virtual work in the following generalized form, which holds for all $\hat{V}$:

$$\begin{aligned} 0 = \sum_{i=1}^{N} \left\{ m_i \boldsymbol{U}^{\Delta} \cdot \left(\boldsymbol{V}_i^{\Sigma} - \boldsymbol{U}_i^{\Sigma} \right) + I_i \boldsymbol{\Omega}_i^{\Delta} \cdot \left(\boldsymbol{\omega}_i^{\Sigma} - \boldsymbol{\Omega}_i^{\Sigma} \right) \right\} \\ + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{A_{i,j,k} \in S_{i,j}} \boldsymbol{P}_{i,j,k}^{\text{int}} \cdot \left\{ \boldsymbol{D}_{i,j}^{\Sigma}(\hat{V}, A_{i,j,k}) - \boldsymbol{D}_{i,j}^{\Sigma}(\hat{U}, A_{i,j,k}) \right\} \\ - \sum_{i=1}^{N} \sum_{B_{i,l} \in S_i'} \boldsymbol{P}_{i,l}^{\text{ext}} \cdot \left\{ \boldsymbol{E}_{i,j}^{\Sigma}(\hat{V}, B_{i,l}) - \boldsymbol{E}_{i,j}^{\Sigma}(\hat{U}, B_{i,l}) \right\}, \end{aligned} \quad (5)$$

where

$$\boldsymbol{D}_{i,j}^{\Sigma}(\hat{V}, A_{i,j,k}) = (\boldsymbol{D}_{i,j}(\hat{V}^+, A_{i,j,k}) + \boldsymbol{D}_{i,j}(\hat{V}^-, A_{i,j,k}))/2,$$

and so on.

As in the previous case, it is necessary to introduce a set of constitutive laws describing the behavior and the interactions among the colliding bodies.

3.1. *Constitutive laws.*

3.1.1. *Associated constitutive law.* Associated constitutive laws can be defined by means of a pseudopotential of dissipation in the following way:

$$\boldsymbol{P}^{\text{int}}_{i,j,k} \in \partial \Phi_{i,j,k}\big(\boldsymbol{D}^{\Sigma}_{i,j}(\hat{U}, A_{i,j,k}).\big) \tag{6}$$

$\Phi_{i,j,k}$ is a pseudopotential of dissipation formed from the sum of the pseudopotential describing the dissipation during the percussion and of the function $\widetilde{I_K} : \boldsymbol{D} \to I_K(\boldsymbol{D} \cdot \boldsymbol{N})$ which assures the noninterpenetration condition. The second term requires the existence of a normal at the contact point (see for example Figure 1), that is, the boundary of at least one colliding solid must be regular at this point. If this condition is not satisfied (for example, a corner-corner collision), an appropriate normal at the contact point must be defined (see [5]).

If we introduce Equation (6) into Equation (5) and apply the inequality of the subdifferential (see for example [11]), we can write for all $\hat{V}$:

$$\begin{aligned} 0 \le \sum_{i=1}^{N} \left\{ m_i \boldsymbol{U}_i^{\Delta} \cdot \left(\boldsymbol{V}_i^{\Sigma} - \boldsymbol{U}_i^{\Sigma} \right) + I_i \boldsymbol{\Omega}_i^{\Delta} \cdot (\boldsymbol{\omega}_i^{\Sigma} - \boldsymbol{\Omega}_i^{\Sigma}) \right\} \\ + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{A_{i,j,k} \in S_{i,j}} \Phi_{i,j,k} \left\{ \boldsymbol{D}^{\Sigma}_{i,j}(\hat{V}, A_{i,j,k}) - \boldsymbol{D}^{\Sigma}_{i,j}(\hat{U}, A_{i,j,k}) \right\} \\ - \sum_{i=1}^{N} \sum_{B_{i,l} \in S_i'} \boldsymbol{P}^{\text{ext}}_{i,l} \cdot \left\{ \boldsymbol{E}_i^{\Sigma}(\hat{V}, B_{i,l}) - \boldsymbol{E}_i^{\Sigma}(\hat{U}, B_{i,l}) \right\} \ge 0. \end{aligned} \tag{7}$$

As every function

$$\begin{aligned} \hat{V} &\to \Phi_{i,j,k}(\boldsymbol{D}_{i,j}(\hat{V}, A_{i,j,k})) \\ &= \Phi_{i,j,k} \left(\boldsymbol{V}_i + \boldsymbol{\omega}_i \wedge \overrightarrow{G_i A_{i,j,k}} - (\boldsymbol{V}_j + \boldsymbol{\omega}_j \wedge \overrightarrow{G_j A_{i,j,k}}) \right) \end{aligned}$$

is a pseudopotential of dissipation, the function

$$\hat{V} \to \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{A_{i,j,k} \in S_{i,j}} \Phi_{i,j,k}(\boldsymbol{D}_{i,j}(\hat{V}, A_{i,j,k})) = \Phi(\hat{V})$$

is also a pseudopotential of dissipation.

The definition of the scalar product

$$\left\langle \hat{U}, \hat{V} \right\rangle = \sum_{i=1}^{N} (m_i \boldsymbol{U}_i \cdot \boldsymbol{V}_i + I_i \boldsymbol{\Omega}_i \cdot \boldsymbol{\omega}_i)$$

allows us to rewrite Equation (7) in the following way:

$$\left\langle \hat{U}^{\Delta} - T^{\text{ext}}, \hat{V} - \hat{U}^{\Sigma} \right\rangle + \Phi(\hat{V}) - \Phi\left(\hat{U}^{\Sigma}\right) \geq 0, \tag{8}$$

for every $\hat{V} \in \mathbb{R}^{6N}$. $T^{\text{ext}} \in \mathbb{R}^{6N}$ is defined by

$$\left\langle T^{\text{ext}}, \hat{V} \right\rangle = \sum_{k=1}^{N} \left(\boldsymbol{R}_k \cdot \boldsymbol{V}_k + \boldsymbol{M}_k \cdot \boldsymbol{\omega}_k \right),$$

where $\boldsymbol{R}_k$ is the resultant of all the exterior percussions applied on the solid k and $\boldsymbol{M}_k$ is the resultant of their angular moment applied with respect to the center of gravity of the solid k.

Given that $\mathbb{R}^{6N}$ has a scalar product defined by $\langle \cdot\,, \cdot \rangle$ and given the definition of subgradient, the formulation (8) is equivalent to the following inclusion:

$$-(\hat{U}^{\Delta} - T^{\text{ext}}) \in \partial\Phi(\hat{U}^{\Sigma}),$$

or, given the definition of $\hat{U}^{\Sigma}$, to the following form:

$$2\hat{U}^{-} + T^{\text{ext}} \in 2\hat{U}^{\Sigma} + \partial\Phi(\hat{U}^{\Sigma}). \tag{9}$$

This inclusion is finally equivalent to the minimization problem

$$\inf \left\{ \langle Y, Y \rangle + \Phi(Y) - \left\langle 2\hat{U}^{-} + T^{\text{ext}}, Y \right\rangle \middle| Y \in \mathbb{R}^{6N} \right\},$$

and the argument X that minimizes this satisfies the Karush–Kuhn–Tucker condition: $0(6N) \in 2X + \partial\Phi(X) - 2\hat{U}^{-} - T^{\text{ext}}$, that is, the inclusion (9).

3.1.2. *Existence and uniqueness of the solution.* The existence and the uniqueness of the solution in the case of an associated constitutive law can be stated by the following theorem:

Theorem 1. If all the constitutive laws derive from a pseudopotential of dissipation, then the problem of the multiple collision of N rigid solids has a unique solution $\hat{U}^{+}$.

The demonstration of this theorem is a direct consequence of the strong convexity of the function

$$Y \to \mathcal{F}(Y) = \langle Y, Y \rangle + \Phi(Y) - \left\langle 2\hat{U}^{-} + T^{\text{ext}}, Y \right\rangle,$$

proved from

$$\left\langle \frac{X+Y}{2}, \frac{X+Y}{2} \right\rangle \leq \frac{1}{4}(\langle X, X\rangle + \langle Y, Y\rangle + 2\langle X, Y\rangle)$$
$$\leq \frac{1}{4}(2\langle X, X\rangle + 2\langle Y, Y\rangle - \langle X-Y, X-Y\rangle)$$
$$\leq \frac{\langle X, X\rangle + \langle Y, Y\rangle}{2} - \frac{2}{8}\langle X-Y, X-Y\rangle,$$

and

$$-\left\langle 2\hat{U}^- + T^{\text{ext}}, \frac{X+Y}{2} \right\rangle = -\frac{\left\langle 2\hat{U}^-, X\right\rangle + \left\langle 2\hat{U}^-, Y\right\rangle}{2}.$$

As Φ is a pseudopotential of dissipation,

$$\Phi\left(\frac{X+Y}{2}\right) \leq \frac{\Phi(X)+\Phi(Y)}{2},$$

and we can state that $\mathbb{R}^{6N}$ is characterized by the scalar product $\langle\,\cdot\,,\,\cdot\,\rangle$ and by the associated norm

$$\mathscr{F}\left(\frac{X+Y}{2}\right) \leq \frac{\mathscr{F}(X)+\mathscr{F}(Y)}{2} - \frac{2}{8}\|X-Y\|^2.$$

Therefore, $\mathscr{F}$ is strongly convex, as it is an α-convex function ($\alpha = 2$). Such functions admit only one minimum on the Hilbert space $\left(\mathbb{R}^{6N}; \langle\,\cdot\,,\,\cdot\,\rangle\right)$, that is, the existence and the uniqueness of the solution is given.

3.1.3. *Dissipative character of the collision.* The constitutive law (6) describing the internal stress derives from a pseudopotential of dissipation:

$$\boldsymbol{P}^{\text{int}}_{i,j,k} \cdot \boldsymbol{D}^{\Sigma}_{i,j}(\hat{U}, A_{i,j,k}) \geq 0 \tag{10}$$

in every point $A_{i,j,k}$ and

$$\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{A_{i,j,k} \in S_{i,j}} \boldsymbol{P}^{\text{int}}_{i,j,k} \cdot \boldsymbol{D}^{\Sigma}_{i,j}(\hat{U}, A_{i,j,k}) \geq 0. \tag{11}$$

This inequality, under the hypothesis that the temperature does not vary during the collision, represents the inequality of Clausius–Duhem of the shock [12].

This inequality shows that the collision is dissipative if no exterior percussion is applied. In this case, the kinetic energy balance (sum of the translational energy

$\frac{1}{2}m\boldsymbol{U}^2$ and the rotational energy $\frac{1}{2}I\boldsymbol{\Omega}^2$) is negative because

$$\begin{aligned}\sum_{i=1}^{N}\left(\frac{1}{2}m_i\cdot\left((\boldsymbol{U}_i^+)^2-(\boldsymbol{U}_i^-)^2\right)+\frac{1}{2}I_i\left((\boldsymbol{\Omega}_i^+)^2-(\boldsymbol{\Omega}_i^-)^2\right)\right)&\\ =\sum_{i=1}^{N}\left(m_i\boldsymbol{U}_i^{\Delta}\cdot\boldsymbol{U}_i^{\Sigma}+I_i\boldsymbol{\Omega}_i^{\Delta}\cdot\boldsymbol{\Omega}_i^{\Sigma}\right)&\\ =-\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\sum_{A_{i,j,k}\in S_{i,j}}\boldsymbol{P}_{i,j,k}^{\text{int}}\cdot\boldsymbol{D}_{i,j}^{\Sigma}(\hat{U},A_{i,j,k})\le 0.&\end{aligned}\tag{12}$$

3.1.4. *Nonassociated constitutive law.* Associated constitutive laws derive from a pseudopotential of dissipation. However, many real behaviors are well modeled by means of nonassociated constitutive laws. In particular, the behavior of brittle materials such as rocks, concrete or ceramics is well represented by Coulomb's friction law. In this case, the tangential components (those in the plane perpendicular to the contact normal) of the percussion are described as follows:

$$||\boldsymbol{P}_T||\le\mu||\boldsymbol{P}_N||,\ \text{where } \mu>0.$$

$$\text{If } ||\boldsymbol{P}_T||<\mu||\boldsymbol{P}_N||,\ \text{then } \boldsymbol{X}_T=\boldsymbol{0}.$$

$$\text{If } ||\boldsymbol{P}_T||=\mu||\boldsymbol{P}_N||,\ \text{then } \exists\lambda \text{ such that } \boldsymbol{X}_T=\lambda\boldsymbol{P}_T.$$

This behavior does not derive from a pseudopotential of dissipation; nevertheless, it can be shown that this problem is also dissipative and can lead to a unique solution. Due to the nonassociated form of Coulomb's friction law, the existence and the uniqueness of the solution can not be directly deduced as in the previous case. However, if the solution exists, Coulomb's law describing the percussions $\boldsymbol{P}_{i,j,k}^{\text{int}}$ corresponding to the solution verifies the inequality (10). This implies also conditions (11) and (12) and assures the dissipative character of the collision.

The problem of the existence and uniqueness of a solution can be approached by a series of solutions obtained by the Tresca associated constitutive law (see Figure 3). It will be shown that this series converges to the unique solution of the problem if the friction coefficient verifies certain conditions.

If at every contact, the value of the normal percussion P_N is known or fixed, the tangential part of the constitutive law derives from a pseudopotential of dissipation:

$$\boldsymbol{P}_T\in\partial\Phi_T\left(\boldsymbol{V}_T^{\Sigma}\right),$$

that is, $\Phi_T(\boldsymbol{V}_T^{\Sigma})=\mu P_N|\boldsymbol{V}_T^{\Sigma}|$, where $\boldsymbol{V}_T$ is the tangential relative velocity between two colliding solids. X is the solution of the problem in which the normal

percussions are known or fixed:

$$X = \arg\inf \left\{ \langle Y, Y\rangle + \Phi(\hat{P}_N(X), Y) - \left\langle 2\hat{U}^- + T^{\text{ext}}, Y\right\rangle \mid Y \in \mathbb{R}^{6N} \right\},$$

where the vector $\hat{P}_N(X)$ contains the (*a priori* unknown) values of P_N and where the pseudopotential $\Phi(\hat{P}_N(X), Y)$ is the sum, for each contact, of the expression

$$\mu P_N \left\| \boldsymbol{V}_T^{\Sigma} \right\|. \tag{13}$$

The Coulomb friction problem is treated by an iterative procedure solving at each iteration a problem in which a Tresca constitutive law (in which the slipping threshold is fixed) is used. As this law is associated (see Figure 3), the solution of the equations is unique. The values of the normal percussions P_N are multiplied by the frictional coefficient and then used in the following iteration as the new slipping thresholds μP_N:

$$X_{n+1} = \arg\inf \left\{ \langle Y, Y\rangle + \Phi(\hat{P}_N(X_n), Y) - \left\langle 2\hat{U}^- + T^{\text{ext}}, Y\right\rangle \mid \mid Y \in \mathbb{R}^{6N} \right\},$$

the existence and uniqueness of the solution is assured by the convergence of the series. It can be shown [5] that two real positive numbers (depending on the grain size) M and M' exist such that, if the friction coefficient μ is the same for every NC contact, the condition implies the uniqueness and the existence of the velocities

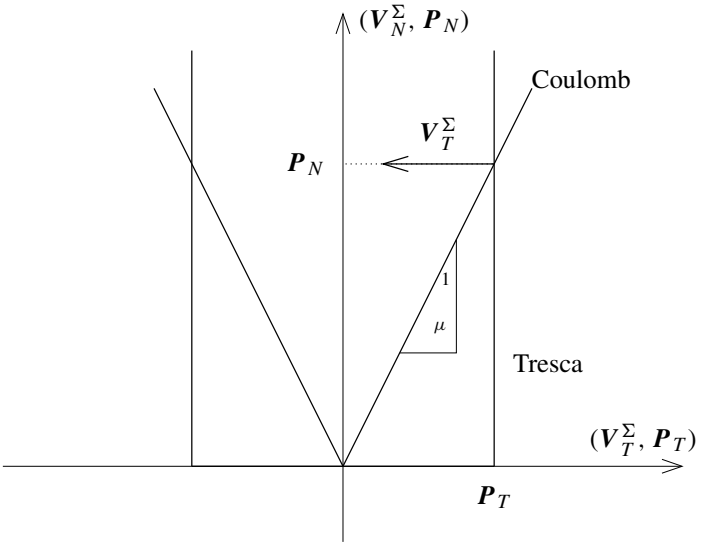

Figure 3. Friction laws: Tresca versus Coulomb.

after the collision:

$$\mu < \frac{1}{16 \cdot NC^{3/2} \cdot M(1+M')^2}.$$

If more than one friction coefficient is given (at different contacts), the inequality should be verified by the largest coefficient.

4. Numerical method

In the previous section, a theory describing rigid bodies collisions was proposed. The full set of equations describing the smooth and nonsmooth evolution of the system are given. To compute an approximation of the evolution described by this set of equations over a time interval $[0, T]$, one must deal with forces having a density with respect to Lebesgue's measure in time and percussions having a density with respect to Dirac's measure in time. The A-CD^2 method consists of approximating all the forces by a succession of percussions, in order to have all the stresses described as percussions.

In the following section, the time-discretization technique of the forces (atomization) is presented. The consequence of the atomization of forces is to make the evolution a succession of instantaneous velocity discontinuities. To solve the equations of velocity discontinuities, a constrained minimization algorithm is proposed.

f^{int} is a vector in $\mathbb{R}^{6N}$ containing the sum of the internal forces (for example, contact forces) exerted on the system during the regular evolution of the system. The coordinates $6(i-1)+1, 2, 3$ represent the three linear momenta in the principal directions exerted on the particle i; the coordinates $6(i-1)+4, 5, 6$ represent the three angular momenta with respect to the center of gravity of i. Similarly, f^{ext} contains the sum of the external forces exerted on the system during the regular evolution of the system (for example, weight; see also Section 4.1). P^{int} and P^{ext} stand for the sums of the internal and external percussions during contacts.

The equations of motion have the following form:

$$\begin{aligned} \frac{dU}{dt} &= -f^{\text{int}} + f^{\text{ext}}, \qquad \text{almost everywhere,} \\ U^{\Delta} &= -P^{\text{int}} + P^{\text{ext}}, \qquad \text{everywhere.} \end{aligned}$$

From time 0 to t, the accumulated stresses R^{int} and R^{ext} are defined by:

$$\begin{aligned} R^{\text{int}}(t) &= \int_0^t d\tau \; f^{\text{int}}(\tau) + \int_0^t d\tau \; \sum_{t_i} P^{\text{int}}(t_i)\delta_{t_i}(\tau), \\ &= \int_0^t d\tau \; f^{\text{int}}(\tau) + \sum_{t_i} P^{\text{int}}(t_i) H(t-t_i), \end{aligned}$$

and

$$R^{\text{ext}}(t) = \int_0^t d\tau\ f^{\text{ext}}(\tau) + \int_0^t d\tau\ \sum_{t_j} P^{\text{ext}}(t_j)\delta_{tj}(\tau),$$
$$= \int_0^t d\tau\ f^{\text{ext}}(\tau) + \sum_{t_j} P^{\text{ext}}(t_j)H(t-t_i),$$

where t_i and t_j are the instants when internal and external percussions are exerted. We can write

$$dV(t) = -dR^{\text{int}}(t) + dR^{\text{ext}}(t).$$

The percussion method (PM) approximates the regular elements of R^{int} and R^{ext} by the percussions. This procedure is named stress atomization. The approximated evolution is obtained by calculating a series of velocities discontinuities separated by constant velocity evolutions. If this procedure is applied to a system formed by solids, this procedure is known as A-CD^2 method. Practically, the application of the A-CD^2 method can be summarized as follows:

- The time length $[0, T]$ is discretized in n regular steps $\left[t_k, t_{k+1}\right]$ of length $\Delta_n = T/n$. In each time step, active forces are "atomized", that is, replaced by percussions exerted at the instant $\theta_k = t_k + \Delta_n/2$.
- All the percussions exerted during the time gap $\left[t_k, t_{k+1}\right]$ are also exerted at the instant θ_k. It follows that velocities are discontinuous at the instants θ_k when the percussions are exerted and are constant elsewhere.

4.1. ***Atomization of a regular force.*** The atomization of a regular force f on the time interval $\left[t_k, t_{k+1}\right]$ consists of replacing it with the percussion P exerted at the instant θ_k. If f depends on a time-dependent quantity y, we can write on $\left[t_k, t_{k+1}\right]$ that

$$\int_{t_k}^{t_{k+1}} d\tau\ f(y(\tau)) \simeq (t_{k+1} - t_k) f\left(\frac{y^+(\theta_k) + y^-(\theta_k)}{2}\right),$$

and thus f can be replaced by the percussion

$$P(t) = \Delta_n f\left(\frac{y^+(\theta_k) + y^-(\theta_k)}{2}\right)\delta_{\theta_k}(t),$$

which is the derivative of

$$E_P(t) = \Delta_n f\left(\frac{y^+(\theta_k) + y^-(\theta_k)}{2}\right)H(t-\theta_k),$$

where δ is the Dirac function and H is the Heaviside function. Practically, three cases must be treated: a constant force, a time dependent force, and position dependent forces.

4.1.1. *Constant force.* The atomization of a constant force f_0 consists of approximating it with a percussion of intensity $f_0\Delta_n$, on any time interval Δ_n. For example, the action of the weight $-\int_{t_k}^{t_{k+1}} d\tau\ g$ at time θ_k is approximated by

$$(0, 0, -g\Delta_n, 0, 0, 0, \dots, 0, 0, -g\Delta_n, 0, 0, 0, \dots, 0, 0, -g\Delta_n, 0, 0, 0).$$

4.1.2. *Time dependent force.* The force $f(t)$ exerted on the system at the time gap $\left[t_k, t_{k+1}\right]$ is replaced by a percussion of intensity $\Delta_n f(\theta_k)$ exerted at the instant θ_k.

4.1.3. *Position dependent force.* The force $f(Y(t))$ exerted on the system at the time $\left[t_k, t_{k+1}\right]$ is replaced by a percussion of intensity $\Delta_n f(Y(\theta_k))$ exerted at the instant θ_k. If we consider, for example, that two points are elastically bounded and note the elongation $x(t)$ at the instant t, the modulus of the elastic force exerted on every point is $k\,|x(t)|$. This force is therefore replaced by a percussion of intensity $\Delta_n k\,|x(\theta_k)|$.

4.2. ***Solution algorithms.*** The atomization of the regular stress, in which forces are replaced by a succession of percussions, makes the velocities become step functions with respect to time. At any instant θ_k velocities are discontinuous while their value is constant elsewhere. Between θ_k and θ_{k+1} every particle moves with a constant velocity. The way in which discontinuities are calculated at the instant θ_k requires further development.

4.2.1. *Constitutive law deriving from a pseudopotential of dissipation.* The percussion responsible for the velocity discontinuity at the instant θ_k are caused either by a collision occurring in the time $[t_k, t_{k+1}]$ or by the atomization of a regular stress in this interval. Under the hypothesis that the percussions derive from a pseudopotential of dissipation, the problem can be written in any of the three following forms:

$$\text{for all } V,\ \left\langle U^{\Delta} - T^{\text{ext}}, V - U^{\Sigma}\right\rangle + \Phi(V) - \Phi\left(U^{\Sigma}\right) \geq 0,$$

$$2U^{-} + T^{\text{ext}} \in 2X + \partial\Phi(U^{\Sigma}),$$

$$\inf_{Y\in\mathbb{R}^{6n}} \left\{\langle Y, Y\rangle + \Phi(Y) - \left\langle 2U^{-} + T^{\text{ext}}, Y\right\rangle\right\}.$$

In particular, if the internal percussions are derived from a pseudopotential of dissipation,

$$X \to \Phi_{i,j,k}(D_{i,j}(X, A_{i,j,k})),$$

the function

$$X \to \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{A_{i,j,k} \in S_{i,j}} \Phi_{i,j,k}(D_{i,j}(X, A_{i,j,k})) = \Phi(X)$$

is a pseudopotential of dissipation that can be divided in two parts:

$$\Phi(X) = \Phi^d(X) + \Phi^r(X).$$

$\Phi^r(X)$ is the sum of all the indicator functions modeling the noninterpenetration conditions and renamed B_l, $l = 1, \ldots, p$ (p is the total number of indicator functions):

$$\Phi^r(X) = \sum_{i=1}^{p} I_{\left[d_l\left(\frac{V^-}{2}\right), +\infty\right[}(\varphi_l(X)),$$

$$d_l(X) = \boldsymbol{D}_{i,j}(X, B_l) \cdot \boldsymbol{N}_l, \quad l = 1, \ldots, p.$$

$\Phi^d(X)$ is differentiable.

The equation is therefore equivalent to:

$$\mathcal{F}(Y) = \langle Y, Y \rangle + \Phi(Y) - \left\langle 2V^- + P^e, Y \right\rangle, \text{ where } Y \in \mathbb{R}^{6N},$$

which implies the following minimization problem:

$$\mathcal{F}(Y) = \langle Y, Y \rangle + \Phi^d(Y) - \left\langle 2V^- + P^e, Y \right\rangle,$$

where

$$Y \in \Omega = \left\{ Y \in \mathbb{R}^{6N} \middle/ \varphi_l(Y) = -d_l(Y) + d_l\left(\frac{V^-}{2}\right) \leq 0,\ l = 1, \ldots, p \right\}. \quad (14)$$

The solution of this minimization problem is a saddle point of the application (Lagrangian) [5]:

$$L(Y, \mu) \in \Omega \times R_+^p \to \mathcal{F}(Y) + \sum_{l=1}^{p} \mu_l \varphi_l(Y).$$

The domain Ω as well as the functions $\mathcal{F}$ and $\Phi^d(Y)$ is convex. This means that if X is a solution of the problem, there exists at least one $\lambda \in R_+^p$ such that (X, λ) is a saddle point of L. If (X, λ) is a saddle point of L, then $X \in \Omega$ and X is a solution of the problem.

This problem is characterized by the following property [1]:

$$L(X, \lambda) = \inf_{Y \in \mathbb{R}^{6N}} \sup_{\mu \in R_+^p} L(Y, \mu) = \sup_{\mu \in R_+^p} \inf_{Y \in \mathbb{R}^{6N}} L(Y, \mu),$$

which leads us to the dual problem (Q), which is the maximization of:

$$G(\mu) = \inf_{Y \in \mathbb{R}^{6N}} L(Y, \mu), \quad \text{with } \mu \in R_+^p.$$

The dual problem can be solved by the Uzawa method, which can be defined as a fixed point gradient method with a projection applied to the dual problem (Q).

Given a point $\mu \in R_+^p$, we denote X_μ as the element that minimizes $L(Y, \mu)$ such that:

$$G(\mu) = L(X_\mu, \mu) = \mathcal{F}(X_\mu) + \sum_{l=1}^{p} \mu_l \varphi_l(X_\mu),$$

which allows one to write $\nabla (G(\mu))_l = \varphi_l(X_\mu)$ of the gradient of $G(\mu)$. The path is denoted ρ and the projection on the domain R_+^p is stated as $\max\{0, \rho\varphi_l(X_\mu)\}$, $l = 1, \ldots, p$.

The algorithm can be therefore summarized as follows:

(i) $\mu^0 \in R_+^p$ is fixed at step 0;

(ii) at every step n,

$$X_n = \arg\min\{\mathcal{F}(Y) + \sum_{i=l}^{p} \mu_l^n \varphi_l(Y), Y \in \mathbb{R}^{6N}\}$$

is calculated;

(iii) μ^{n+1} is updated as $\mu_l^{n+1} = \max\{0, \rho\varphi_l(X_{\mu^n})\}$.

This algorithm allows one to replace the initial constrained minimization problem

$$\arg\min \left\{ \langle Y, Y \rangle + \Phi^d(Y) - \left\langle 2V^- + P^e, Y \right\rangle, \ Y \in \Omega \right\},$$

with a suite of unconstrained minimization problems

$$\arg\min \left\{ \mathcal{F}(Y) + \sum_{l=1}^{p} \mu_l^n \varphi_l(Y), \quad Y \in \mathbb{R}^{6N} \right\}.$$

Further details, as well as the necessary conditions for convergence, can be found, for example, in [2].

4.2.2. *Case of Coulomb's friction law.* Friction problems using Coulomb's constitutive law can be approached by a strategy similar to the one used for demonstrating the existence and the uniqueness of the solution. If $f_{i,j,k}$ stands for the frictional coefficient at contact A_{ijk}, and starting from a first approximation of the normal percussions G_0, the problem can be solved in an iterative way by the associated Tresca's law

$$X_{G_0} = \operatorname{arginf} \left\{ \langle Y, Y \rangle + \Phi(G_0, Y) - \left\langle 2U^- + P^{\text{ext}}, Y \right\rangle \ \middle| Y \in \mathbb{R}^{6N} \right\},$$

where $\Phi(G_0, Y)$ is the pseudopotential of dissipation defined in (13). The unique solution (due to Theorem 1) X_{G_0} allows one to define the new normal stress

$$P^{G_0}_{Ni,j,k} = \boldsymbol{P}^{\text{int}}_{A_{i,j,k}} \cdot \boldsymbol{N}_{A_{i,j,k}} = \boldsymbol{D}_{i,j}(2U^- + P^{\text{ext}} - 2X_{G_0}, A_{i,j,k}) \cdot \boldsymbol{N}_{A_{i,j,k}},$$

constituting the new slipping thresholds of successive iteration of the cycle.

This approach requires the convergence of two imbricated suites (the first one computes the slipping threshold, the second contains the Uzawa algorithm) which consume excessive computation time. It is therefore proposed an original approach that consists of solving one unique suite in which the slipping thresholds and the reactions are updated simultaneously. For simplicity, only a two dimensional case is given (in such a case, the tangent at the contact point has only one dimension).

The original problem 4.2.1 can be therefore modified by defining a further nonslipping condition

$$\psi(X) = 0, \quad s_l(X) = \boldsymbol{D}_{i,j}(X, B_l) \cdot \boldsymbol{T}_l, \quad l = 1, \ldots, p,$$

where $\boldsymbol{T}$ is the tangential direction and by introducing the following problem:

$$\mathcal{F}(Y) = \langle Y, Y \rangle + \Phi^d(Y) - \left\langle 2V^- + P^e, Y \right\rangle, \quad \text{where } Y \in \Omega,$$

$$\Omega = \left\{ Y \in \mathbb{R}^{6N} \Big/ \left[\begin{array}{l} \varphi_l(Y) = -d_l(Y) + d_l\left(\dfrac{V^-}{2}\right) \le 0,\ l = 1, \ldots, p, \\ \\ \psi_l(Y) = -s_l(Y) + s_l\left(\dfrac{V^-}{2}\right) = 0,\ l = 1, \ldots, p \end{array} \right] \right\}, \quad (15)$$

that is, the tangential nonslipping condition enforces the solution lies on path I in Figure 4. Thanks to Theorem 1, this problem has a unique solution. The solution of such a problem can be approached, as in the previous case, by defining

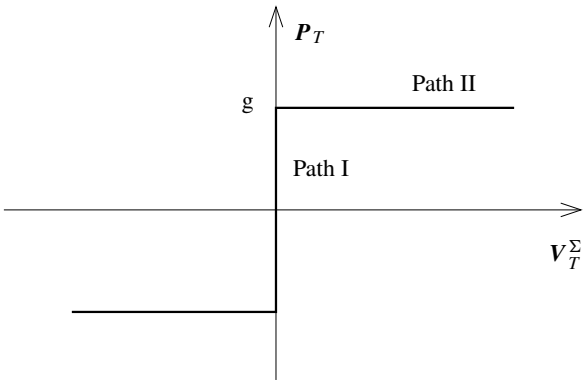

Figure 4. Scheme of Coulomb's law behavior.

a modified Lagrangian taking into account the additional nonslipping condition and, numerically, by means of a modified Uzawa algorithm (see the previous section) [2]:

$$L(Y, \mu, \zeta) \in \Omega \times R_+^p \to \mathcal{F}(Y) + \sum_{l=1}^{p} \mu_l \varphi_l(Y) + \sum_{l=1}^{p} \zeta_l \psi_l(Y).$$

The algorithm is then modified as follows (paths are noted as ρ and ϱ):

(i) $\mu^0 \in R_+^p$ and $\zeta^0 \in \mathbb{R}^p$ are fixed at step 0;

(ii) at every step n,

$$X_n = \arg\min\{\mathcal{F}(Y) + \sum_{i=1}^{p} \mu_l^n \varphi_l(Y) + \sum_{l=1}^{p} \zeta_l \psi_l(Y), Y \in \mathbb{R}^{6N}\}$$

is calculated;

(iii) μ^{n+1} is updated as $\mu_l^{n+1} = \max\{0, \rho\varphi_l(X_{\mu^n})\}$;

(iv) ζ^{n+1} is updated as $\zeta_l^{n+1} = \varrho\psi_l(X_{\zeta^n})$.

If X is a solution of the problem, there exists at least one $\lambda \in R_+^p$ and $\xi \in \mathbb{R}^p$ such that (X, λ, ξ) is a saddle point of L.

The unconstrained minimization has not been yet discussed. However, given the strong convexity of the functions we deal with, the solution can be easily approached by classical newtonian methods (for example, BFGS [1]).

As Lagrange multipliers correspond to the normal (λ associated to the condition φ) and to the tangential (ξ associated to the condition ψ) stress, their values can be directly compared as follows:

$$\begin{aligned} &\text{If } |\lambda| \le \mu|\xi|, \text{ then } \boldsymbol{V}_T^{\Sigma} = \mathbf{0} \text{ and Section 4.2.2 holds.} \\ &\text{If } |\lambda| \le \mu|\xi|, \text{ then } \boldsymbol{V}_T^{\Sigma} = \mathbf{0} \text{ and Section 4.2.2 holds.} \\ &\text{If } |\lambda| > \mu|\xi|, \text{ then Section 4.2.2 is violated.} \end{aligned} \tag{16}$$

In particular, if $|\lambda| > \mu|\xi|$, it means that the tangential nonslipping condition does not hold and contact behavior must follow path II in Figure 4. The problem must be reformulated on contacts where the condition no longer holds, taking into account that tangential slipping occurs. This means that if the k-th contact violates condition (16), the tangential stress is greater than the slipping threshold g, and the problem must be reformulated to take into account that the condition ψ no longer holds on this contact. A further pseudopotential defining the frictional behavior on slipping contacts must be defined, that is, the pseudopotential $\Phi_G^d(Y)$ applies on slipping contacts $m = 1, k$ while the nonslipping condition ψ holds on $n = k+1, p$ slipping

contacts:

$$\Phi^{df} = \sum_i \mu_i |\lambda_i| \| \boldsymbol{V}_{T_i}^{\Sigma} \|.$$

An alternative method consists in extending this sum at all the terms. Adding $|\lambda_l| \| \boldsymbol{V}_{T_l}^{\Sigma} \|$ to a term corresponding to a contact l where the constraint ψ_l is kept does not affect the solution. This further term accelerates the convergence as it acts as a penalty function associated to the constraints ψ_l.

The second step of the computation can be explicitly taken into account by defining the problem modified as follows:

$$\mathcal{J}(Y) = \langle Y, Y \rangle + \Phi_G^d(Y) + \Phi^d(Y) - \left\langle 2V^- + P^e, Y \right\rangle, \quad \text{where } Y \in \Upsilon,$$

$$\Upsilon = \left\{ Y \in \mathbb{R}^{6N} \middle/ \left[\begin{array}{l} \varphi_l(Y) = -d_l(Y) + d_l\left(\dfrac{V^-}{2}\right) \leq 0,\ l = 1, \ldots, p, \\ \psi_j(Y) = -s_j(Y) + s_j\left(\dfrac{V^-}{2}\right) = 0,\ j = k+1, \ldots, p \end{array} \right] \right\}. \tag{17}$$

Equation (17) constitutes, as in the previous case, a constrained minimization problem where the constraints are given by inequalities (that is, the noninterpenetration condition on all the p contacts) and equalities (that is, the nonslipping conditions on n contacts where Equation (16) holds). Slipping behavior on contacts where Equation (16) is violated is taken into account by the pseudopotential Φ^{df}. The algorithm is then modified as follows:

(i) $\mu^0 \in R_+^p$ and $\zeta^0 \in \mathbb{R}^{p-k}$ are fixed at step 0;

(ii) at every step n,

$$X_n = \arg\min\{\mathcal{J}(Y) + \sum_{l=1}^{p} \mu_l^n \varphi_l(Y) + \sum_{i=k+1}^{p} \zeta_j^n \psi_j(Y),\ Y \in \mathbb{R}^{6N}\}$$

is calculated;

(iii) μ^{n+1} is updated as $\mu_l^{n+1} = \max\{0, \rho\varphi_l(X_{\mu^n})\}$;

(iv) ζ^{n+1} is updated as $\zeta_j^{n+1} = \varrho\psi_j(X_{\zeta^n})$.

It should be finally verified that contacts following path I behavior in Figure 4 still respect the nonslipping condition (that is, the tangential percussion is below the slipping threshold). Otherwise the computation should be iterated starting from the new initial condition.

5. Numerical simulations

To illustrate the theory, some numerical simulations based on the described numerical method will be presented.

Molecular dynamics (MD) methods, for example, [16; 18; 15], are often used when approaching similar problems. MD methods consider, in general, the continuum discretized by a collection of rigid disks suitably linked with contact elements. The definition of the contact model reproducing the behavior of the media results from the overlapping of the disks. The mechanical answer is then governed by the contact law which transforms the error of the penalty contact formulation into a displacement field [15]. This approach turns out to be particularly effective in solving quasistatic problems, but less effective in dynamics problems such as fragmentations or granular flows, where gap functions can hardly be defined [13]. The A-CD^2 method turns out to be particularly effective in solving both dynamics problems such as fragmentations or granular flows (as gap functions used in molecular dynamics methods [13] are not required) and quasistatic problems such as compaction.

5.1. ***Associated constitutive law.*** The case of an associated constitutive law has been applied to an example of a landslide formed from 300 rigid regular bodies. Similar results with more than 1200 particles can be found in [4]. In this example, regular stresses (that is, contact forces) exerted on particles are associated to multiple percussions due to collisions. In such a situation, the A-CD^2 method turns out to be well adapted to reproduce such a dynamic case. Let us recall that dissipation is always assured when an associated constitutive law (or a Coulomb's friction law) is used. In these cases, the Clausius–Duhem inequality (Equation (12)) holds. It proves that the evolution is dissipative, regardless of whether the solids are sliding or rolling.

The geometry of the slide is given in Figure 5.

To simulate the dispersion of material properties of an irregular assembly, a random generation of the initial configuration has been set. This means that the bodies have a random number of sides and a random initial rotation. The mass and the inertia modulus of every polygon is therefore calculated according to its random number of sides. In the first part of the analysis, particles are generated as shown in Figure 5. The rigid bodies are then submitted to the action of gravity and the package arranges to a stable position behind a floodgate. After the gate removal, the final, stable configuration of packaging is computed while observing the value of kinetics energy, that is, if kinetics energy is below an established threshold, final stabilized position is considered to be achieved (see Figure 6).

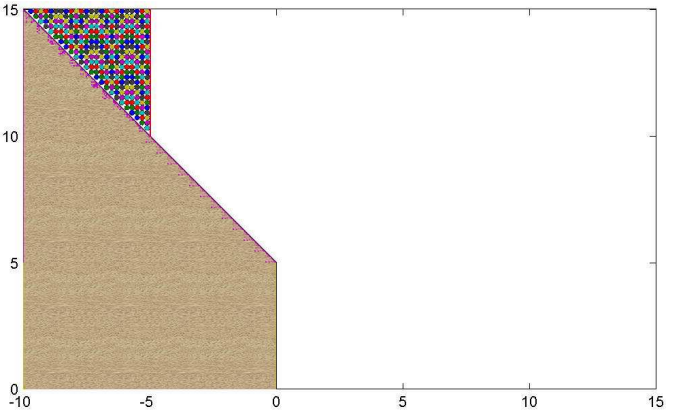

Figure 5. Initial packaging of the polygons.

The constitutive law describing the behavior of the solids during the shock has been chosen in a quadratic form:

$$\Phi = \frac{1}{2} K_T \left(\left(\hat{U}^+ + \hat{U}^- \right) \cdot \boldsymbol{T} \right)^2 + \frac{1}{2} K_N \left(\left(\hat{U}^+ + \hat{U}^- \right) \cdot \boldsymbol{N} \right)^2,$$

$$K_T \geq 0, \quad K_N \geq 0,$$

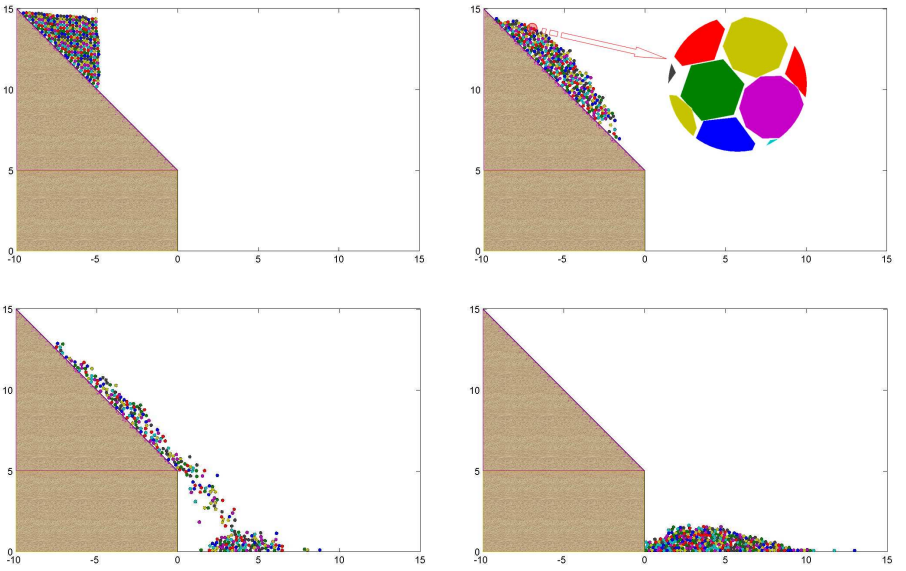

Figure 6. Evolution of the system at $t = 1\,\text{s},\ 2.5\,\text{s},\ 5\,\text{s},\ 10\,\text{s}$.

Radius	Density	K_N	K_T	Δn
0.25 m	$2500\,\mathrm{kg\,m^{-3}}$	$78\,\mathrm{kg\,m^{-1}}$	$78\,\mathrm{kg\,m^{-1}}$	10^{-4} s

Table 1. Parameters used in the numerical simulation of the slide.

where K_T and K_N represent the tangential and the normal elastic constants (see for example [11]) and U is written in a compact form standing for $\hat{U} = (\boldsymbol{U}_i, \boldsymbol{\omega}_i)$). This choice leads to the following form of the functional:

$$\text{Find } U^+ \in C \text{ that minimizes } J(V) = \frac{1}{2}a(V, V) - l(V),$$

which can be solved by the Uzawa method [2].

The parameters describing the packaging as well as the contact laws are summarized in Table 1. The choice of the time step Δn is particularly important as small interpenetrations may occur between θ_k and θ_{k+1}. This numerical problem can be avoided (at a higher computational cost) by decreasing Δn.

5.2. ***Coulomb's friction law.*** The nonassociated constitutive law has been applied for the simulation of a biaxial test. The geometry of the assembled specimen is given in Figure 7. The assembly phase has been performed as in the previous case: the specimen is formed by an irregular packing of 200 particles, obtained by imposing a random geometrical perturbation on the initial (regular) arrangement.

Two horizontal rigid walls are defined as the loading plates. The left and the right external columns of particles constitute flexible boundaries where an external elastic force is continuously exerted. This flexible boundary is stress-controlled and simulates the membrane usually used in biaxial tests. After generation, the particles are compacted, and the biiaxial test is performed by applying the confining force and moving the upper platen. The parameters used in this simulation are presented in Table 2.

The results of the simulation are presented in Figure 7. These results correspond to Mohr–Coulomb's theory. The last image shows the specimen configuration after fracture. The shear band corresponds to a slipping band between particles forming

Parameter	Value
Radius	0.1
Friction coefficient μ	0.1

Table 2. Parameters used in the numerical simulation of the biiaxial test.

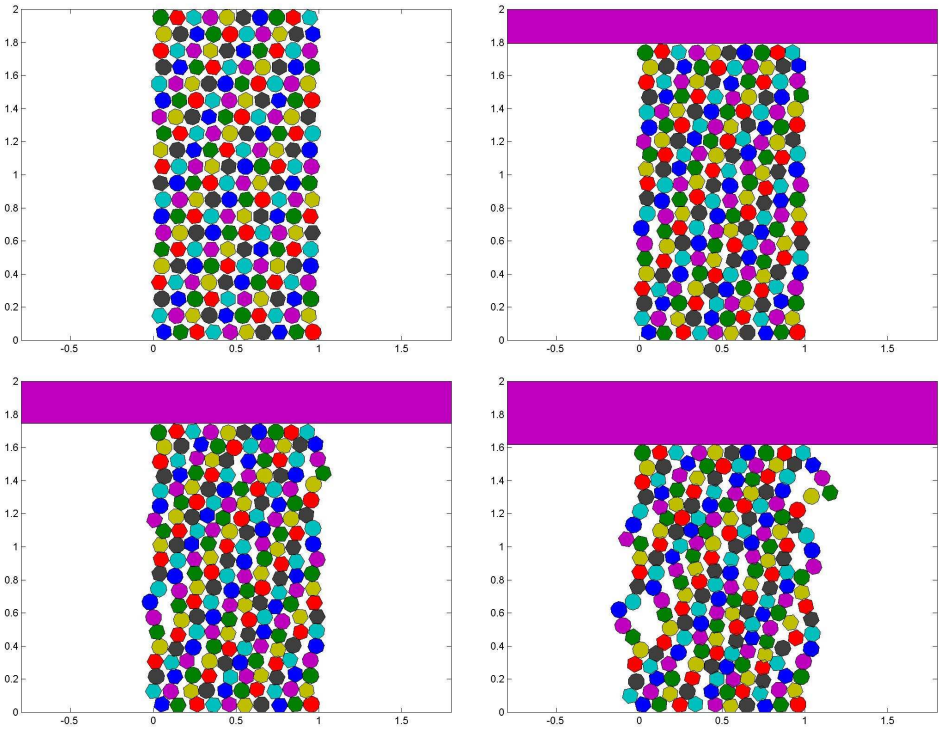

Figure 7. Evolution of the system during the biiaxial test.

an angle of about 50°. The shear bands predicted by Mohr–Coulomb's theory ($\pi/4 \pm \phi/2$ where $\mu = tg\phi$) are therefore respected.

6. Conclusion

This paper has proposed a description of instantaneous collisions among rigid particles respecting the principle of virtual work and a method, named A-CD^2, for describing the evolution of a multiparticle system. This method constitutes a general framework capable of integrating all the stress which are generally present in a mechanical system. The numerical examples that have been presented include features such as gravitational forces, viscous friction, unilateral contact, Coulomb's friction, and elastic forces exerted by a membrane. The proposed method is particularly effective in simulating evolution in which collisions among particles or contact fracture with velocity discontinuity are observed together with regular evolutions. The proposed A-CD^2 method is therefore well adapted for describing the mechanical behavior of granular media.

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Received February 13, 2007. Revised September 24, 2007.

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