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# A primal-dual active set method for solving multi-rigid-body dynamic contact problems

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In this work, an active set type method is considered in order to solve a mathematical problem that describes the frictionless dynamic contact of a multi-body rigid system, the so-called nonsmooth contact dynamics (NSCD) problem. Our aim, here, is to present the local treatment of contact conditions by an active set type method dedicated to NSCD and to carry out a comparison with the various well-known methods based on the bipotential theory and the augmented Lagrangian theory. After presenting the mechanical formulation of the NSCD and the resolution of the global problem concerning the equations of motion, we focus on the local level devoted to the resolution of the contact law. Then we detail the numerical treatment of the contact conditions within the framework of the primal-dual active set strategy. Finally, numerical experiments are presented to establish the efficiency of the proposed method by considering the comparison with the other numerical methods.

## **Keywords**

Granular media, unilateral constraint, rigid body, discrete element method, nonsmooth contact dynamics, semismooth Newton method, primal-dual active set, bipotential, augmented Lagrangian, multi-body contact, numerical simulations

## **1. Introduction**

The simulation of dynamic multi-body contact problems is involved in many engineering applications, such as granular media, masonry, tensegrities, geomaterials, robotic manipulation and mechanical deformable systems. In the case of both deformable bodies and rigid bodies, the numerical solution of multi-contact problems remains a difficult and nontrivial task because contact law is strongly nonlinear, nonsmooth and multivalued. Moreover, the numerical methods used to solve multi-body contact problems depend, in particular, on the mechanical behaviour (deformable or rigid) of the bodies involved.

In most cases, the bodies considered are assumed to be rigid. In a rigid-body model, the contact dynamics method, also called the nonsmooth contact dynamics (NSCD) method, is based on a discrete element method initially developed for the simulation of granular materials. For a survey on the subject, we can refer to Radjai and Richefeu [1]. This very well-known method emerged from a mathematical formulation of nonsmooth dynamics and subsequent algorithmic developments realized by Moreau and Jean [2–7]. In this context, it is important to note that the contact dynamics method deals with the following two major issues: the contact

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law based on complementarity relations between the contact (or impulse) forces and velocities, and nonsmooth motion involving velocity jumps with impulse forces. To give a consistent description of the dynamics, the discrete element method is based on two main computational level tasks: an implicit time-stepping scheme is used to solve the equations of motion at the global level, while an explicit local treatment deals with the evolution of the contact network between rigid bodies. The most commonly used discrete element method is based on the nonlinear Gauss–Seidel (NLGS) method developed by Jean and Moreau [3–6] and it consists of an iterative process pertaining to the Gauss–Seidel method by considering, successively, each contact until convergence is achieved. More sophisticated methods, such as conjugate gradient-type methods, have also been developed (see, e.g., Renouf and Alart [8]) to solve nonsmooth contact dynamics problems. For the local treatment of the contact conditions, several approaches can be considered, such as, for instance, methods based on the bipotential theory and the augmented Lagrangian theory [4, 7, 9–13]. Furthermore, note that when dynamic contact systems are considered without friction, the resulting problem can be formulated as a convex quadratic problem and several other efficient methods based on quadratic programming can be used to solve these nonsmooth dynamical systems [14–16].

When deformable bodies are considered, a time-stepping method and a finite-element method are generally used for the full discretization of the contact problem. A numerical treatment of the contact conditions can then be realized by several numerical approaches. A wide bibliography exists on this subject [17–19]. For instance, Alart and Curnier [20] have introduced an augmented Lagrangian formulation combined with a generalized Newtonian method to solve nondifferentiable but continuous equations arising from frictional contact problems. Several other methods have emerged during the last few years. Amongst them, active set strategies are very successful and are widely used because of their efficiency and simplicity of implementation. In the standard active set approach, which can be found in well-known books of optimization [14, 16, 21], the methods are divided into primal active set methods and dual active set methods. When finding a feasible starting point, primal active set methods generate a sequence of primal feasible iterations until dual feasibility is achieved; hence, an optimal solution is obtained. Dual active set methods for convex quadratic problems generate a sequence of dual feasible iterations until primal feasibility is achieved; hence, an optimal solution is obtained. More recently, primal-dual active set methods have been considered to solve variational problems with unilateral constraints [22–28]. These approaches are characterized by the fact that the active set is defined by a relation described by both the primal and the dual feasibilities, which are enforced together during each iteration. Furthermore, within the framework of semismooth Newtonian techniques [22, 23, 25], it can be proven that the primal-dual active set type methods lead to direct enforcement of the exact contact conditions on nodes related to the active and inactive contact sets.

The contribution of this paper is to propose a primal-dual active set method for the numerical treatment of the contact conditions within the resolution of dynamic multi-rigid-body contact problems. To our knowledge, this is the first time that a primal-dual active set method has been considered for solving such types of contact dynamics problem. Very few works have been devoted to this topic. We can cite, for instance, the work of Sharaf [29], in which a very particular class of rigid-body dynamics problems is considered, and the work of Koziara and Bicanic [30], for which a semismooth Newtonian method is proposed to solve problems dealing with pseudo-rigid bodies. Our goal in this work is to show the performance and efficiency of the primal-dual active set method for NSCD problems, compared with other effective methods based on the bipotential and augmented Lagrangian theories that have been recently developed [13]. For this purpose, several numerical examples of rigid-body contact problems are considered. Furthermore, a comparison of performances of the whole methods can be realized by the use of only one stopping criterion [13].

The remainder of the article is organized as follows. In Section 2, we recall the usual contact conditions commonly used in contact dynamics, and the main traits of the primal-dual active set type method within the framework of a deformable body system. In Section 3, the discrete element method context for solving a dynamic multi-rigid-body contact problem is presented by considering first the equations of motion and then the general algorithm for NSCD problems. After presenting methods based on the bipotential and the augmented Lagrangian theories, Section 4 is devoted to a numerical treatment of the dynamic contact conditions by a primal-dual active set method within the framework of dynamic multi-rigid-body contact problems. After that, in Section 5, we present several numerical simulations to illustrate the performances of the active set method compared with other effective methods. Finally, in Section 6, we conclude by discussing some prospects and future works in continuation of the present study.

## 2. Contact conditions and active set type methods

The aim of this section is to recall the usual contact conditions commonly used in contact dynamics. First, a brief presentation of the contact laws in the case of a deformable body is given; then the dynamic contact conditions for rigid-body systems are provided. Finally, the main traits of the primal-dual active set type method are also briefly recalled to solve dynamic contact problems in the framework of deformable bodies.

### 2.1. Contact conditions

First of all, to simplify the writing, let us consider the contact without friction of a deformable body with a rigid obstacle, the so-called foundation. Note that, in what follows, the contact between two or several bodies can be generalized quite easily by considering an effort on the formalism. For mathematical convenience, we assume that the body occupies a bounded domain  $\Omega \subset \mathbb{R}^d$  ( $d = 1, 2, 3$ ), with a Lipschitz continuous boundary  $\Gamma$ . We denote by  $\mathbf{n}$  the unit inner normal vector on  $\Gamma$  and  $\mathbf{t}$  the associated tangent vector. We use the notation  $\mathbf{u}$  and  $\boldsymbol{\sigma}$  for the local displacement and the local stress tensor at one point of the domain  $\Omega$ , respectively. Also, we denote by  $u_n$  and  $\mathbf{u}_t$  the normal and tangential components of  $\mathbf{u}$  on  $\Gamma$  given by  $u_n = \mathbf{u} \cdot \mathbf{n}$ ,  $\mathbf{u}_t = \mathbf{u} - u_n \mathbf{n}$ . Finally,  $\sigma_n$  and  $\boldsymbol{\sigma}_t$  will represent the normal and the tangential stress on  $\Gamma$ , defined by  $\sigma_n = (\boldsymbol{\sigma} \mathbf{n}) \cdot \mathbf{n}$  and  $\boldsymbol{\sigma}_t = \boldsymbol{\sigma} \mathbf{n} - \sigma_n \mathbf{n}$ . Furthermore, a dot superscript represents the time derivative with respect to the time variable  $t$ , e.g.,  $\dot{u} = \partial u / \partial t$ .

Now, let us consider a potential contact between one point of  $\Gamma$  and the foundation. A potential contact point has the following dynamic content. As long as the normal distance  $u_n$  between the body and the obstacle remains positive (corresponding to a gap), no force is activated and the normal force  $\sigma_n$  is identically zero. But when  $u_n = 0$ , a nonnegative (repulsive) normal force  $\sigma_n$  is mobilized at the contact point and can take indefinitely large values, depending on the forces acting on the body. These conditions define a complementary relation, called Signorini's conditions [31], between  $u_n$  and  $\sigma_n$ . These frictionless contact conditions can be written following the Karush–Kuhn–Tucker conditions, as follows:

$$\begin{cases} u_n \geq 0, \\ \sigma_n \geq 0, \\ u_n \sigma_n = 0, \end{cases} \quad (1)$$

$$\boldsymbol{\sigma}_t = 0. \quad (2)$$

In addition, when contact dynamics are considered, the persistency condition has to be added for energy conservation purposes [18]. Indeed, to eliminate the work of the normal contact reaction at time  $t$  ( $\mathcal{W}_{\text{cont}} = \int_{\Gamma} \sigma_n \dot{u}_n$ ), the following persistency condition has to be considered [32, 33]:

$$\dot{u}_n \sigma_n = 0. \quad (3)$$

This condition means that the normal contact reaction can only appear during persistent contact. One can easily prove [4, 5, 18] that the addition of the persistency condition (equation (3)) to the unilateral contact law (equation (1)) gives the following contact dynamic conditions:

$$\text{if } u_n > 0, \quad \sigma_n = 0 \quad (4)$$

$$\text{if } u_n = 0, \quad \begin{cases} \dot{u}_n \geq 0, \\ \sigma_n \geq 0, \\ \dot{u}_n \sigma_n = 0, \end{cases} \quad (5)$$

In the following, a couple  $(u_n, \sigma_n)$  verifying this set of conditions is denoted by

$$\text{contact\_law}(\dot{u}_n, \sigma_n) = \text{.true.}$$

The previous alternatives in equations (4) and (5) lead to the condition of a complete contact law formulated by Moreau [4, 5]. In the context of nonsmooth motion, the time derivative  $\dot{u}$  is not unique and then the left-limit velocity and the right-limit velocity must be distinguished. Since the actual velocity at time  $t$  is immaterial, the question of velocity jump is crucial and is problematic when the step of time discretization is addressed. As a consequence, in a time-stepping formulation, the discrete forms of the complementarity condition formulated

in displacement ( $u_n \sigma_n = 0$ ) and in velocity ( $\dot{u}_n \sigma_n = 0$ ) are incompatible and cannot be enforced at the same discrete instant.

At this stage, we can distinguish two cases related to the nature of the dynamic contact system considered. In the case where deformable bodies are concerned, the contact conditions formulated in displacement (equation (1)) are usually preferred, with the use of an additional numerical treatment to take into account the persistency condition and thus the energy conservation properties [18, 32–38]. In the case of multi-rigid-body systems, the question of nondissipation of energy is essential to ensure reliable dynamics of the system. Then the contact conditions formulated in velocity (equation (5)) are always used and relate the impulse forces to the velocities. Here, the issue is to predict the velocities of the bodies and the impulse forces acting on the simultaneous multi-contacts. To resume, the choice of the contact model and, more precisely, the choice of the complementarity relation depend on the nature of the physics of the problem (a system of deformable bodies or a multi-rigid-body system) involved in the context of nonsmooth contact dynamics. In the following, we recall the main traits of the primal-dual active set type method in the case of the unilateral contact conditions formulated in displacement to solve a system of deformable bodies. The description of the primal-dual active set method for the solution of multi-rigid-body system will be dealt with in Section 4.3.

## 2.2. Primal-dual active set type method

As mentioned by Hintermuller and colleagues [22, 23], the primal-dual active set type method can be seen as a semismooth Newtonian method, for which the contact conditions can be reformulated in terms of a fixed point problem [39]. Let us recall this usual result in the case of the local unilateral contact conditions formulated in displacement.

**Proposition 1.** *Let  $\gamma > 0$ , the contact conditions in displacement (equation (1)) are equivalent to:*

$$\sigma_n = [\sigma_n - \gamma u_n]_+ \text{ on } \Gamma^c. \quad (6)$$

The proof of Proposition 1 can be found in Abide et al. [28] or Chouly et al. [39]. Here,  $\Gamma^c$  denotes the boundary part of  $\Omega$  in contact.

The main trait of the active set type method is to consider separately the solution of the equation of motion (or the equation of equilibrium)  $\mathcal{R}(\mathbf{u}, \boldsymbol{\sigma}) = \mathbf{0}$  and the solution of the fixed point  $\sigma_n = [\sigma_n - \gamma u_n]_+$ . Here,  $\mathcal{R}(\mathbf{u}, \boldsymbol{\sigma})$  is the generalized nonlinear operator, which includes all the operators related to the acceleration, the constitutive behaviour of the material and the external solicitations. Let us denote by  $\mathcal{S}$  the set of contact nodes of  $\Gamma^c$  and by  $c$  a node of  $\mathcal{S}$ . The solution of equation (6) leads us directly to enforce  $u_n^c = 0$  if the nodes  $c \in \mathcal{S}$  are in a status of contact by checking an active set condition, that is  $\sigma_n^c - \gamma u_n^c \geq 0$  for all  $c \in \mathcal{S}$ . Furthermore, the calculus of the fixed point of equation (6) leads also to the condition  $\sigma_n^c = 0$  in the case of noncontact [22, 23]. Thereby, let us consider the active subset  $\mathcal{A}$  of contact nodes defined by  $\mathcal{A} = \{c \in \mathcal{S} : \sigma_n^c - \gamma u_n^c \geq 0\}$ , and the associated inactive subset:  $\mathcal{I} = \mathcal{S} \setminus \mathcal{A}$ . The general form of the iterative active set algorithm of index  $i$  can be as follows:

- (i) Choose  $(\mathbf{u}^0, \boldsymbol{\sigma}^0)$ , set  $i = 0$ .
- (ii) Set:

$$\mathcal{A}^{i+1} = \{c \in \mathcal{S} : \sigma_n^{c,i} - \gamma u_n^{c,i} \geq 0\}, \quad (7)$$

$$\mathcal{I}^{i+1} = \mathcal{S} \setminus \mathcal{A}^{i+1}. \quad (8)$$

- (iii) Find  $(\mathbf{u}^{i+1}, \boldsymbol{\sigma}^{i+1})$ , such that

$$\mathcal{R}(\mathbf{u}^{i+1}, \boldsymbol{\sigma}^{i+1}) = \mathbf{0}$$

$$u_n^{c,i+1} = 0 \quad \text{for all } c \in \mathcal{A}^{i+1}, \quad (9)$$

$$\sigma_n^{c,i+1} = 0 \quad \text{for all } c \in \mathcal{I}^{i+1}. \quad (10)$$

- (iv) If  $\mathcal{A}^{i+1} = \mathcal{A}^i$  stop, else go to (ii).

The goal of the active set type strategy is to find the correct subset  $\mathcal{A}$  of all nodes that are currently in contact by considering the status of contact that is derived directly through computation of the fixed point of equation

(6). The main trait of this method is to consider exactly the contact conditions at the contact nodes without the need for using additional nodes to determine the normal contact stress, as is the case for the augmented Lagrangian approach. In the case of a nonlinear constitutive behaviour of the material, a standard Newtonian method can be coupled to the active set method to solve the equation  $\mathcal{R}(\mathbf{u}^{i+1}, \boldsymbol{\sigma}^{i+1}) = \mathbf{0}$ . Therefore, at each Newton iteration, stopping criteria related to the pair  $(\mathbf{u}, \boldsymbol{\sigma})$  and the residue  $\mathcal{R}(\mathbf{u}, \boldsymbol{\sigma})$  must be added.

To solve a dynamic multi-rigid-body system with contact, the unilateral contact conditions must be expressed in terms of velocity. Then Proposition 1 can be naturally generalized in the case of a local unilateral contact law expressed in velocity.

**Proposition 2.** *Let  $\gamma > 0$ ; the contact conditions in velocity (equation (5)) are equivalent to:*

$$r_n = [r_n - \gamma \dot{u}_n]_+ \quad (11)$$

where  $r_n$  is the reaction impulse force between two particles in contact.

**Proof.** We use here similar arguments already employed for the proof of Proposition 1 [28].

First, let us assume that the following conditions hold:  $\dot{u}_n \geq 0, r_n \geq 0$  and  $\dot{u}_n r_n = 0$ . We consider successively the cases  $\dot{u}_n > 0$  and  $\dot{u}_n = 0$ . If  $\dot{u}_n > 0$ , the condition  $\dot{u}_n r_n = 0$  implies that  $r_n = 0$ . Thus,  $[r_n - \gamma \dot{u}_n]_+ = [-\gamma \dot{u}_n]_+ = 0 = r_n$ , since  $\gamma > 0$ . If  $\dot{u}_n = 0$  and  $r_n \geq 0$  then  $[r_n - \gamma \dot{u}_n]_+ = r_n$ .

Conversely, we assume now that equation (11) holds. This implies that  $r_n \geq 0$ . Next if  $r_n = 0$ , we have  $[-\gamma \dot{u}_n]_+ = 0$  and this leads to  $\dot{u}_n \geq 0$ , since  $\gamma > 0$ . Finally, if  $r_n > 0$  then  $r_n = r_n - \gamma \dot{u}_n > 0$ ; so  $\gamma \dot{u}_n = 0$ , which implies  $\dot{u}_n = 0$ , since  $\gamma > 0$ .  $\square$

The goal of the next section is to propose a general algorithm for NSCD, for which the dynamic contact condition (equation (11)) is treated by an active set type method.

### 3. Nonsmooth contact dynamics (NSCD)

After presenting the equations of motion of a dynamic multi-rigid-body contact problem, the general algorithm for solving the full problem is described. This general algorithm is based on two main computational level tasks: the global level, with the solution of the equations of motion, and the local level, devoted to the contact resolution. At this stage, we briefly recall several methods dedicated to the numerical contact resolution. These methods are based on the bipotential theory and the augmented Lagrangian theory.

#### 3.1. Equations of motion

Classically [3, 4, 6, 7], the motion of a multi-contact system is described using a global generalized coordinate  $\mathbf{q}$  describing the centre position and the rotation of each particle (for  $N_p$  particles,  $\mathbf{q} \in \mathbb{R}^{\tilde{d} \times N_p}$ , where  $\tilde{d} = 6$  for a three-dimensional problem and  $\tilde{d} = 3$  for a two-dimensional problem). Owing to the possible shocks between particles, it is necessary to introduce the generalized velocity denoted by  $\dot{\mathbf{q}}$  as a function of bounded variations and its associated differential measure  $d\dot{\mathbf{q}}$ . Then the equations of motion must be formulated in terms of a differential measure equation:

$$\mathbb{M}d\dot{\mathbf{q}} + \mathbf{F}^{\text{int}}(t, \mathbf{q}, \dot{\mathbf{q}})dt = \mathbf{F}^{\text{ext}}(t, \mathbf{q}, \dot{\mathbf{q}})dt + d\mathbf{R}, \quad (12)$$

where

- $\mathbb{M}$  represents the generalized mass matrix;
- $\mathbf{F}^{\text{int}}$  and  $\mathbf{F}^{\text{ext}}$  represent the internal and external forces, respectively;
- $d\mathbf{R}$  is a nonnegative real measure, representing the reaction forces and impulses between particles in contact.

For the sake of simplicity and without lost of generality, only the external forces are considered in the following. The internal forces are neglected because the general case can be easily derived through a linearizing procedure.

Then, for the numerics in a time-stepping approach, we consider that the time interval of interest  $[0, T]$  is discretized by introducing uniform time instants  $t_k$  defined by  $t_{k+1} = t_k + \Delta t$  for  $k = 0, \dots, N_T - 1$ , where

$\Delta t = T/N_T$  is the time step and  $N_T$  is the number of time steps. Then equation (12) is integrated over each time interval  $[t_k, t_{k+1}]$ , and approximated using a  $\theta$ -method with  $\theta \in [\frac{1}{2}, 1]$  for stability reasons [5, 8].

Therefore, the classical approximation of equation (12) yields

$$\begin{cases} \mathbb{M}(\dot{\mathbf{q}}_{k+1} - \dot{\mathbf{q}}_k) = \Delta t(\theta \mathbf{F}_{k+1} + (1 - \theta)\mathbf{F}_k) + \mathbf{P}_{k+1} \\ \mathbf{q}_{k+1} = \mathbf{q}_k + \Delta t\theta\dot{\mathbf{q}}_{k+1} + \Delta t(1 - \theta)\dot{\mathbf{q}}_k \end{cases} \quad (13)$$

where  $\mathbf{P}_{k+1}$  represents the value of the total impulsion over the time step, which contains the contribution of smooth contact and the local percussion densities exerted during shocks, and  $\mathbf{F}_k$  (or  $\mathbf{F}_{k+1}$ ) is the external force computed at time  $t_k$  (or  $t_{k+1}$ ).

We will denote  $\dot{\mathbf{q}}_k^{\text{free}} = \dot{\mathbf{q}}_k + \mathbb{M}^{-1}\Delta t(\theta \mathbf{F}_{k+1} + (1 - \theta)\mathbf{F}_k)$  as the free velocity (the velocity when the contact impulses vanish). Then, the first equation in equation (13) becomes

$$\dot{\mathbf{q}}_{k+1} = \dot{\mathbf{q}}_k^{\text{free}} + \mathbb{M}^{-1}\mathbf{P}_{k+1}. \quad (14)$$

To write the contact law, for a contact node  $x^c$  (note that  $c, 1 \leq c \leq N_c$ , is used as a label for contact nodes, where  $N_c$  is the total number of contact nodes), it is necessary to define the local-global mapping

$$\begin{cases} \mathbf{v}^c = H^*(\mathbf{q}, c)\dot{\mathbf{q}} \\ \mathbf{P} = H(\mathbf{q}, c)\mathbf{p}^c \end{cases} \quad (15)$$

where  $\mathbf{v}^c$  is the local relative velocity between the two bodies in contact and  $\mathbf{p}^c$  is the contact impulse ( $\mathbf{v}^c, \mathbf{p}^c \in \mathbb{R}^d$  where  $d$  is the dimension of the problem) and  $H(\mathbf{q}, c)$  is the matrix of the local-global mapping that permit to compute the variables  $\mathbf{v}^c$  and  $\mathbf{p}^c$  in the local frame at a contact node  $x^c$  from the global variable  $\dot{\mathbf{q}}$  and  $\mathbf{P}$ . For duality reasons,  $H^*$  is the transpose of matrix  $H$ . We recall that  $\mathbf{p}^c$  can be decomposed into the sum of a normal component  $p_n^c$  and a tangential component  $\mathbf{p}_t^c$ , as  $\mathbf{p}^c = p_n^c \mathbf{n} + \mathbf{p}_t^c$ . We also denote by  $\mathbb{H}(\mathbf{q})$  the total-global mapping, for  $\mathbf{v}$  and  $\mathbf{p}$  in  $\mathbb{R}^{d \times N_c}$  (vectors composed of all relative velocities and contact impulses, respectively):

$$\begin{cases} \mathbf{v} = \mathbb{H}^*(\mathbf{q})\dot{\mathbf{q}} \\ \mathbf{P} = \mathbb{H}(\mathbf{q})\mathbf{p} \end{cases} \quad (16)$$

Let us notice that even if  $H(\mathbf{q}, c)$  and  $H^*(\mathbf{q}, c)$  have good theoretical properties, this is not necessarily the case for  $\mathbb{H}$  and  $\mathbb{H}^*$ . In the discretization, a prediction of  $\mathbf{q}$  is computed to estimate the mapping  $\mathbb{H}(\mathbf{q})$  (see equations (18) and (19)).

Using equations (13) and (16), the discretization of the motion of a multi-contact system, with contact between particles can be written:

$$\begin{cases} \tilde{\mathbf{v}}_{k+1} = \tilde{\mathbf{v}}_k^{\text{free}} + \mathbb{W}\mathbf{p}_{k+1} \\ \text{contact\_law}(\tilde{\mathbf{v}}_{k+1}^c, \mathbf{p}_{k+1}^c) = \text{.true} \quad \forall c \in \{1, 2, \dots, N_c\} \end{cases} \quad (17)$$

where  $\mathbb{W} = \mathbb{H}^*\mathbb{M}^{-1}\mathbb{H}$  is the Delassus operator, and  $\tilde{\mathbf{v}}_k^{\text{free}} = \mathbb{P}^*\dot{\mathbf{q}}_k^{\text{free}}$  is the relative free velocity. Notice that a Newtonian impact law is also considered in the first part of equation (17) (see equation (21))[3], which modifies  $\mathbf{v}_k$  and  $\mathbf{v}_k^{\text{free}}$  as  $\tilde{\mathbf{v}}_k$  and  $\tilde{\mathbf{v}}_k^{\text{free}}$ , respectively. The second part of equation (17) is the implicit frictionless contact law that is in our case the classical Signorini condition with  $\mathbf{p}_t^c = \mathbf{0}$ .

### 3.2. Resolution of the global problem: the nonlinear Gauss–Seidel method (NLGS)

In this section, we describe the algorithm used at the global level to solve the problem of equation (17). Following the ideas of Jean and Moreau [3, 7, 9], we use the NLGS algorithm, which is the most commonly used. It involves considering each contact successively until convergence is achieved. The numerical criterion used to state the convergence will be studied later in this paper.

This method is intrinsically sequential but it is possible to use a simple multi-threading technique, which consists of splitting the contact loop onto several threads. This method has been studied by Reouf et al. [40] for the case of a local algorithm based on the augmented Lagrangian method.

Notice that it is also possible at this stage to consider more sophisticated methods, such as conjugate gradient-type methods [8]. However, these techniques do not significantly speed up the convergence. This is why they are not considered in the rest of this paper. The time-stepping method combined with the NLGS algorithm takes the following form:

- Loop on the step time  $k$ :

- Prediction of a position (for computation of the local-global mapping):

$$\mathbf{q}_{k+\frac{1}{2}} = \mathbf{q}_k + \frac{\Delta t}{2} \dot{\mathbf{q}}_k; \quad (18)$$

- Initialization of the motion:  $\dot{\mathbf{q}}_{k+1}^0 = \dot{\mathbf{q}}_k^{\text{free}}$  (initialization of the contact forces with  $\mathbf{P} = 0$ );
- Loop on  $j \geq 0$  (NLGS), until convergence:

- \* Loop on the contacts  $c$ :

- Computation of the local-global mapping

$$\mathbf{v}^i = H^*(\mathbf{q}_{k+\frac{1}{2}}, c) \dot{\mathbf{q}}_k; \quad \text{velocity at the beginning of the time step} \quad (19)$$

$$\mathbf{v}^{c,jf} = H^*(\mathbf{q}_{k+\frac{1}{2}}, c) \dot{\mathbf{q}}_{k+1}^j; \quad \text{predicted velocity at the end of the time step} \quad (20)$$

- Newton shock law (using formal Moreau velocity)

$$\tilde{\mathbf{v}}_n^{c,j+1} = \frac{\mathbf{v}_n^{c,jf} + e_n \mathbf{v}_n^i}{1 + e_n}; \quad (21)$$

- Computation of the contact law

$$\text{contact\_law}(\tilde{\mathbf{v}}_n^{c,j+1}, \mathbf{p}^{c,j+1}) = \text{.true}; \quad (22)$$

- Actualization of the generalized displacement

$$\dot{\mathbf{q}}_{k+1}^{j+1} = \dot{\mathbf{q}}_{k+1}^j + \mathbb{M}^{-1} H(\mathbf{q}_{k+\frac{1}{2}}, c) \mathbf{p}^{c,j+1}.$$

- \* End of the loop on contacts  $c$ .

- End of the loop on  $j$  of NLGS. When the convergence is reached, actualization of the velocity:

$$\dot{\mathbf{q}}_{k+1} = \dot{\mathbf{q}}_{k+1}^{j+1}$$

- Actualization of the generalized displacements:  $\mathbf{q}_{k+1} = \mathbf{q}_{k+\frac{1}{2}} + \frac{\Delta t}{2} \dot{\mathbf{q}}_{k+1}$

- End of the loop on the step time  $k$ .

## 4. Numerical computation of the local contact impulses

We present in this section three methods to compute the local contact forces in the previous algorithm (equation (22)). The first two are based on the work of Alart and Curnier [20], de Saxcé and Feng [41] and Fortin et al. [12] and are classical, and will be useful to evaluate the third method, which is based on the primal-dual active set method. Moreover, the first two methods have been developed in the more general problems of frictional contact problems, which are no longer convex.

Let us notice that for all of the proposed methods, an assumption on the existence and the uniqueness of the one-contact problem is needed. This property is verified here by the positive sign of the reduced element of the Delassus matrix.

### 4.1. A Newtonian or augmented Lagrangian technique to solve the contact problem

The first method, developed by Alart and Curnier [20], is based on the optimization of an augmented Lagrangian problem. In the case of a contact problem with friction, the method can be written as follows. For a given contact point  $c$  ( $1 \leq c \leq N_c$ ), one can define the Cartesian product of an infinite half cylinder with section equal to a

ball  $\mathcal{B}(0, \mu \mathbf{p}^c)$  of radius  $\mu \mathbf{p}^c$  by  $\mathcal{C}(\mu \mathbf{p}^c) = \mathbb{R}^+ \times \mathcal{B}(0, \mu \mathbf{p}^c)$ , where  $\mu$  is the friction coefficient. Then the granular type contact problem is given by

$$\mathbf{p}^c \in \operatorname{argmin}_{\mathbf{s} \in \mathcal{C}(\mu \mathbf{p}^c)} J_c(\mathbf{s}), \quad (23)$$

where

$$J(\mathbf{s}) = \frac{1}{2} \mathbf{s} \cdot \mathbb{W}_{cc} \mathbf{s} + \left( \mathbf{v}^{c, \text{free}} - \tilde{\mathbf{v}}^c + \sum_{\alpha=1, \alpha \neq c}^{N_c} \mathbb{W}_{c\alpha} \mathbf{p}^\alpha \right) \cdot \mathbf{s}$$

where  $\mathbb{W}_{c\alpha}$  is the reduced element of the Delassus matrix, related to the contacts  $c$  and  $\alpha$ . Then the projected gradient method can be applied to solve the minimization problem (equation (23)). Therefore, for each iteration  $j$  of the NLGS algorithm, this approach leads to the following form of the contact reaction as a saddle point of an augmented Lagrangian problem:

$$\mathbf{p}^{c, j+1} = \operatorname{proj} \left( \mathbf{p}^{c, j} - \rho \left( \mathbf{v}^{c, \text{free}} - \tilde{\mathbf{v}}^c + \sum_{\alpha=1, \alpha \neq c}^{N_c} \mathbb{W}_{c\alpha} \mathbf{p}^\alpha + \mathbb{W}_{cc} \mathbf{p}^{c, j} \right), \mathcal{C}(\mu \mathbf{p}^c) \right), \quad (24)$$

where the function  $\operatorname{proj}(\mathbf{v}, \mathcal{C})$  is the orthogonal projection of  $\mathbf{v}$  on the convex set  $\mathcal{C}$ . Equation (24) can be formulated equivalently as follows:

$$\begin{aligned} \boldsymbol{\tau}^{j+1} &= \operatorname{proj}(\boldsymbol{\tau}^{j+1}, \mathcal{C}(\mu \mathbf{p}^c)) \\ \text{where } \boldsymbol{\tau}^{j+1} &= \mathbf{p}^j - \rho \mathbf{v}^j \quad \text{and} \quad \mathbf{v}^j = \mathbf{v}^{c, \text{free}} - \tilde{\mathbf{v}}^c + \sum_{\alpha=1, \alpha \neq c}^{N_c} \mathbb{W}_{c\alpha} \mathbf{p}^\alpha + \mathbb{W}_{cc} \mathbf{p}^{c, j}. \end{aligned} \quad (25)$$

Here,  $\boldsymbol{\tau}^{j+1}$  is the augmented contact reaction and  $\rho$  is the arbitrary positive parameter. This method, which is based on an augmented Lagrangian technique with a projected gradient solver, will be referred to as the standard augmented Lagrangian (SAL) method.

It is also possible to use an iterative Newtonian method to find the minimum of  $J$  by seeking the solution as a zero of the function  $\tilde{f}_c(\chi)$  where, for a contact  $c$ ,  $\chi = (\mathbf{p}^c, \tilde{\mathbf{v}}^c)$  and

$$\tilde{f}_c(\chi) = \begin{pmatrix} \tilde{\mathbf{v}}^c - \tilde{\mathbf{v}}^{c, \text{free}} - \sum_{\alpha=1}^{N_c} \mathbb{W}_{c\alpha} \mathbf{p}^\alpha \\ \tilde{\mathbf{Z}}^c \end{pmatrix},$$

in which the vector  $\tilde{\mathbf{Z}}^c$  is the error on the prediction of the reaction

$$\tilde{\mathbf{Z}}^c(\mathbf{p}^c, \tilde{\mathbf{v}}^c) = \mathbf{p}^c - \operatorname{proj}(\boldsymbol{\tau}^c, \mathcal{C}(\mu \mathbf{p}^c)), \quad (26)$$

This method, which is based on an augmented Lagrangian technique and a quasi-Newtonian solver, will be referred to as the enhanced augmented Lagrangian (EAL) method. The idea of the enhancement is to consider, for the approximation of the gradient of  $\tilde{f}_c$ , not only the part of  $\tilde{f}_c$  that is always differentiable, as in the standard case, but all the part of  $\tilde{f}_c$  that is differentiable, especially when  $\boldsymbol{\tau}^c$  is in the interior of  $\mathcal{C}(\mu \mathbf{p}^c)$ . This idea is also used in the next section with the bipotential, where it is explained in more detail [13].

#### 4.2. A bipotential technique to solve the contact problem

It is also possible to use the notion of a bipotential, introduced by Fortin, de Saxé and colleagues [10–12, 41]. Using this framework, a couple  $(\mathbf{v}, \mathbf{p})$  satisfies the Signorini's contact conditions if and only if

$$b_c(\mathbf{w}, \mathbf{s}) + \mathbf{w} \cdot \mathbf{s} \geq b_c(\mathbf{v}, \mathbf{p}) + \mathbf{v} \cdot \mathbf{p} = 0 \quad \forall \mathbf{w}, \mathbf{s} \quad (27)$$

where  $b_c$  is the bipotential

$$b_c(-\mathbf{v}, \mathbf{p}) = \Psi_{\mathbb{R}^+}(v_n) + \Psi_{K_\mu}(\mathbf{p}) + \mu p_n \|\mathbf{v}_t\| \quad (28)$$

$\Psi_C$  stands for the indicator function of the set  $C$ :  $\Psi_C(x) = 0$  if  $x \in C$ ,  $\Psi_C(x) = +\infty$  if  $x \notin C$ , and  $K_\mu$  is the set defined by

$$K_\mu = \{\mathbf{p} = p_n \mathbf{n} + \mathbf{p}_t : \|\mathbf{p}_t\| - \mu p_n \leq 0\}. \quad (29)$$

The minimization of equation (27) is classically realized using a Uzawa method without considering the singular term  $\Psi_{\mathbb{R}^+}(\tilde{\mathbf{v}}_n^{c,j})$ . This minimization can also be viewed as the proximal point of the augmented force  $\mathbf{p} - \rho \tilde{\mathbf{v}}$ , with respect to the function  $\mathbf{p} \mapsto \rho b_c(-\tilde{\mathbf{v}}, \mathbf{p})$  [10, 12, 41]:

$$\mathbf{p} = \text{prox}(\mathbf{p} - \rho \tilde{\mathbf{v}}, \rho b_c(-\tilde{\mathbf{v}}, \mathbf{p}))$$

The bipotential method with an Uzawa solver will be referred to as the standard bipotential (SBP) method.

Then, following the ideas developed by Joli and Feng [42] for the case of continuum mechanics and adapted by Dumont [13] for the case of granular materials, to solve the local problem with a Newton-like method, it is necessary to reformulate the problem. Therefore, for each contact  $c$ , the local problem to be solved can be written as

$$\begin{cases} \tilde{\mathbf{v}}_{k+1}^c = \tilde{\mathbf{v}}_k^{c,\text{free}} + \sum_{\alpha=1}^{N_c} W_{c\alpha} \mathbf{p}^\alpha & \forall c = 1, \dots, N_c \\ \mathbf{p}^c = \text{proj}(\boldsymbol{\tau}^c, K_\mu) \end{cases} \quad (30)$$

where  $\boldsymbol{\tau}^c = \mathbf{p}^c - \rho \tilde{\mathbf{v}}$  is the augmented reaction used in equation (24). This problem can be written equivalently as

$$\begin{cases} \tilde{\mathbf{v}}_{k+1}^c - \tilde{\mathbf{v}}_k^{c,\text{free}} - \sum_{\alpha=1}^{N_c} W_{c\alpha} \mathbf{p}^\alpha = 0 & \forall c = 1, \dots, N_c \\ \mathbf{p}^c - \text{proj}(\boldsymbol{\tau}^c, K_\mu) = 0 \end{cases} \quad (31)$$

Remembering now that we want to use a Newton algorithm to solve these equations inside the NLGS loop on the variable  $j$ , we define now, for each contact  $c = 1, \dots, N_c$ , the function

$$f_c^j(\boldsymbol{\chi}) = \begin{pmatrix} \tilde{\mathbf{v}}^{c,j} - \tilde{\mathbf{v}}_k^{c,\text{free}} - \sum_{\alpha=1}^{N_c} W_{c\alpha} \mathbf{p}^{\alpha,j} \\ \mathbf{Z}^{c,j} \end{pmatrix}$$

where:

- the vector  $\mathbf{Z}^c$  is the error in the prediction of the reaction

$$\mathbf{Z}^{c,j}(\mathbf{p}^{c,j}, \tilde{\mathbf{v}}^{c,j}) = \mathbf{p}^{c,j} - \text{proj}(\boldsymbol{\tau}^{c,j}, K_\mu). \quad (32)$$

- $\boldsymbol{\chi}_c = (\mathbf{p}^{c,j}, \tilde{\mathbf{v}}^{c,j})^t$ .
- $\boldsymbol{\chi} = (\chi_1, \chi_2, \dots, \chi_{N_c})^t$ .

The first equality in the relation  $f(\boldsymbol{\chi}) = 0$  is the equation of motion for the bodies in contact, and the second relation is related to the friction condition between the bodies in contact, written within the bipotential framework [13, 43]. Then a Newtonian algorithm of index  $l$  is used to solve the problem  $f(\boldsymbol{\chi}) = 0$ . This algorithm can be written, for a contact  $c$ , as follows:

- Initialization:

$$\boldsymbol{\chi}_c^0 = (\mathbf{p}^0 = \mathbf{p}^{c,j}, \tilde{\mathbf{v}}^0 = \tilde{\mathbf{v}}^{c,j})^t, \quad \ell = 0$$

- Loop on  $\ell$ , until convergence:

- $\boldsymbol{\tau}_\ell^c = \mathbf{p}^\ell - \rho \tilde{\mathbf{v}}^\ell$
- Resolution:

$$\left[ \frac{\partial f_c}{\partial \boldsymbol{\chi}^c}(\boldsymbol{\chi}^\ell) \right] \Delta \boldsymbol{\chi}_c = -f_c(\boldsymbol{\chi}^\ell) \quad (33)$$

- Actualization:  $\chi_c^{\ell+1} = \chi_c^\ell + \Delta\chi_c$
- End of the loop on  $\ell$  until convergence,  $\tilde{\mathbf{v}}^{c,j+1} = \tilde{\mathbf{v}}^\ell$  and  $\mathbf{p}^{c,j+1} = \mathbf{p}^\ell$ .

For a two-dimensional problem, the matrix

$$\left[ \frac{\partial f_c}{\partial \chi^c}(\chi^\ell) \right]$$

is equal to

$$\left[ \frac{\partial f_c}{\partial \chi^c}(\chi) \right] = \begin{bmatrix} -W & Id_{2 \times 2} \\ A_c & B_c \end{bmatrix} \quad (34)$$

where

$$A_c = \begin{bmatrix} \frac{\partial Z_c}{\partial p_n} & \frac{\partial Z_c}{\partial r_t} \end{bmatrix} \quad (35)$$

$$B_c = \begin{bmatrix} \frac{\partial Z_c}{\partial v_n} & \frac{\partial Z_c}{\partial v_t} \end{bmatrix} \quad (36)$$

In the case with no friction ( $\mu = 0$ ), the matrices  $A_c$  and  $B_c$  take different forms according to the contact status:

- First case: contact

$$A_c = [\mathbf{0}; \mathbf{t}]$$

$$B_c = [\rho \mathbf{n}; \mathbf{0}]$$

- Second case: no contact. In this case

$$A_c = Id_{2 \times 2} \quad B_c = 0_{2 \times 2}$$

The previous bipotential technique with the use of a Newtonian solver will be referred to as the enhanced bipotential (EBP) method.

### 4.3. A primal-dual active set method for NSCD

This section is devoted to the numerical treatment of the contact conditions by a primal-dual active set method within the framework of multi-rigid-body dynamic contact problems.

For this purpose, it is necessary to define the active set defined in equations (7) and (8), and to compute the contact conditions on each set only in terms of contact impulses, using the local general equations of motion (equation (17)) in the form of equation (11). We recall that  $\mathcal{S}$  denotes the set of potential contact particles and  $c \in \mathcal{S}$  represents a potential contact between two particles. Moreover, let us consider the active subset  $\mathcal{A}$  of contact defined by  $\mathcal{A} = \{c \in \mathcal{S} : p_n^c - \gamma \tilde{v}_n^c \geq 0\}$ , and the associated inactive subset:  $\mathcal{I} = \mathcal{S} \setminus \mathcal{A}$ . With these notations, the numerical computation of the local contact step inside the NLGS iteration loop of index  $j$  leads to the following primal-dual active set algorithm:

- Compute:  $\tau_n^{c,j+1} = p_n^{c,j} - \gamma \tilde{v}_n^{c,j}$  for each  $c \in \mathcal{S}$ .
- Set:

$$\mathcal{A}^{j+1} = \{c \in \mathcal{S} : \tau_n^{c,j+1} \geq 0\}, \quad (37)$$

$$\mathcal{I}^{j+1} = \mathcal{S} \setminus \mathcal{A}^{j+1}. \quad (38)$$

- Find  $(\mathbf{v}^{j+1}, \mathbf{p}^{j+1})$  such that

$$\text{if } c \in \mathcal{A}^{j+1} \text{ then } \tilde{v}_n^{c,j+1} = 0 \text{ and } \mathbf{p}_t^{c,j+1} = \mathbf{0}, \text{ (contact)} \quad (39)$$

$$\text{Computation of the local contact force: } p_n^{c,j+1} = p_n^{c,j} - \tilde{v}_n^{c,j} / W_{nn}. \quad (40)$$

$$\text{if } c \in \mathcal{I}^{j+1} \text{ then } p_n^{c,j+1} = 0, \text{ and } \mathbf{p}_t^{c,j+1} = \mathbf{0} \text{ (no contact).} \quad (41)$$

- Convergence obtained for the active sets when :  $\mathcal{A}^{j+1} = \mathcal{A}^j$  and  $\mathcal{I}^{j+1} = \mathcal{I}^j$ .

We can remark that the term  $\tau_n^{c,j+1}$  computed in the first step is similar to the augmented expression (equation (25)) used for the methods presented in the two previous sections. The main trait of the active set type method is to enforce directly and exactly the contact conditions that are found when the problems considered in equations (24) and (31) are solved with a Newtonian type solver. Unlike the augmented Lagrangian approach, another trait of the active set type method is the nonuse of additional nodes for determination of the normal contact stress. Indeed, the computation of  $p_n^{c,j+1}$  for all  $c \in \mathcal{A}^{j+1}$  is obtained a posteriori, see equation (40). The method described in this section, which is based on a primal-dual active set approach, will be referred to as the primal-dual active set (PDAS) method.

Let us notice that only one iteration of the active set method is realized for one contact at each global iteration of the NLGS method, as in the case of the SBP method, and unlike the other methods. A numerical study showed that considering several iterations of the active set method at each NLGS step did not improve the method.

#### 4.4. Stopping criterion

Since each numerical solution of the presented method ends the NLGS iteration with different properties (some of the methods are exact for the dynamic, some of the methods are exact for the contact law, and the others are not exact for either), it is necessary to use an identical stopping criterion for all the methods, which is able to take into account all types of error. Even if such very robust stopping criteria exist in the literature [21], we propose here a criterion that permits each type of error to be exhibited separately. This criterion, developed from that proposed by Fortin et al. [11] has been extended in the case of the Newtonian and bipotential (EBP) method, where some terms are naturally vanishing in the original Uzawa and bipotential (SBP) method. This stopping criterion  $\varepsilon_{\text{glob}}$  has been proposed in such a way that both the error in the equation of motion  $\varepsilon_{\text{motion}}^c$ , the error in the Signorini contact law  $\varepsilon_{b_c}$  and the error of penetration  $\varepsilon_{\text{pen}}^c$  must be sufficiently small. Therefore, the numerical solution provides good properties related to both the equation of motion and the Signorini contact law.

This criterion can be stated as

$$\varepsilon_{\text{glob}} = \frac{1}{N_c} \sum_{c=1}^{N_c} [\varepsilon_{\text{motion}}^c + \varepsilon_{b_c} + \varepsilon_{\text{pen}}^c] \quad (42)$$

where:

- $\varepsilon_{\text{motion}}^c = \|\tilde{\mathbf{v}}^c - \tilde{\mathbf{v}}_m^c\|$ , where  $\tilde{\mathbf{v}}_m^c = \tilde{\mathbf{v}}^{c,i} + \sum_{\alpha=1}^{N_c} W_{c\alpha} \mathbf{p}^\alpha$ , so  $\varepsilon_{\text{motion}}$  measures the error on the equation of motion (see equation (30); this term vanishes for the SBP and SAL methods);
- $\varepsilon_{b_c} = |\tilde{\mathbf{v}}^c \cdot \mathbf{p}^c|$  is the absolute value of the bipotential, which must vanish if and only if the couple  $(\tilde{\mathbf{v}}^c, \mathbf{p}^c)$  verifies the Signorini contact law;
- $\varepsilon_{\text{pen}}^c = -\min(0, \tilde{v}_n^c)$  is the value of the penetration.

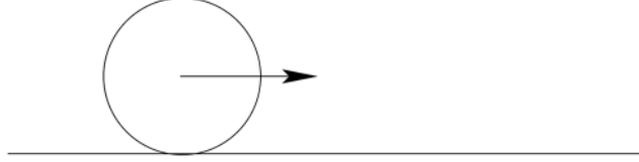
One can notice that it is absolutely necessary to verify in the criterion that there is no penetration, because nothing in the presented algorithm ensures that this condition is satisfied at the end of the loop. Moreover, if this condition is not satisfied, the other part of the bipotential can be negative or vanish, even if the couple  $(\tilde{\mathbf{v}}, \mathbf{p})$  is not a solution.

## 5. Numerical simulations

In this section, several numerical examples are solved to illustrate the performances of the PDAS method, compared with various other methods (SBP, SAL, EBP and EAL). Three numerical examples of increasing complexity are considered: the sliding of one ball on a plane obstacle, the sedimentation of a collection of balls and a poly-disperse collection of balls falling over an inclined plane.

### 5.1. Sliding of one ball on plane obstacle

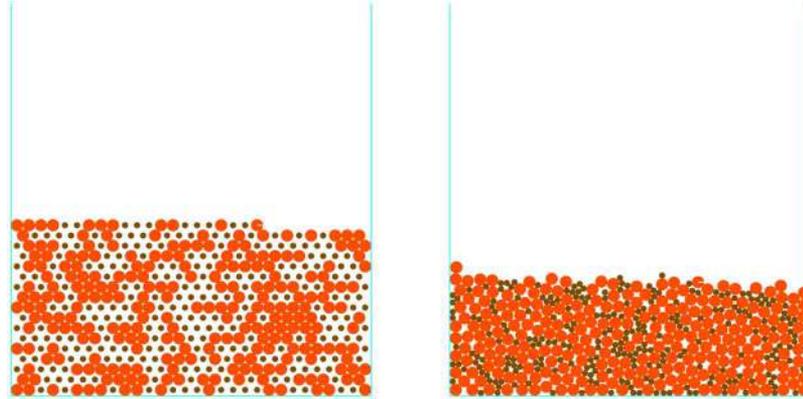
In this first example, a ball posed on a horizontal plane is considered (see Figure 1) with a nonvanishing initial horizontal velocity ( $v_0 = 1.5 \text{ m} \cdot \text{s}^{-1}$ ). There is only one point contact between the ball and the plane. Since there is no friction, the ball slides on the horizontal plane, without rolling. The final time is equal to  $T = 0.2 \text{ s}$  and the number of time steps is fixed to 2000 with  $\Delta t = 10^{-4} \text{ s}$ .



**Figure 1.** Sliding of one ball on plane obstacle.

**Table 1.** Results for example 1. For each method are provided the number of nonlinear Gauss–Seidel iterations for each time step (second column), the total CPU time (third column) and the CPU time devoted to the computation of the contact forces (fourth column).

	Iterations	CPU time (s)	Contact forces CPU time (s)
Standard bipotential	18	4.10	$1.29 \times 10^{-1}$
Standard augmented Lagrangian	17	4.07	$1.11 \times 10^{-1}$
Enhanced bipotential	2	4.00	$8.40 \times 10^{-2}$
Enhanced augmented Lagrangian	2	4.02	$9.5 \times 10^{-2}$
Primal-dual active set	1	3.91	$7.7 \times 10^{-2}$



**Figure 2.** Sedimentation of a collection of balls (left: initial state; right: final state).

The results for this example with sliding are presented in Table 1. In this example, one can notice (see Table 1) that all the methods need a similar total CPU time to compute the solution. However, the time necessary to compute the contact forces is smaller for the three last methods. Moreover, the PDAS method needs only one iteration of NLGS, meaning that good status for the contact is found directly. For the EBP and EAL methods, two iterations of NLGS are necessary, whereas for the standard methods, since there is no convergence for the contact law within each NLGS iteration, 18 iterations are necessary to obtain convergence.

Let us notice that this value also strongly depends on the penalization parameter, unlike the other methods, which are relatively independent of the parameters [13].

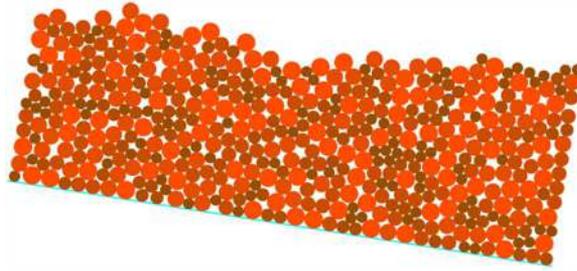
## 5.2. Sedimentation of a collection of balls

In this second example, the sedimentation of a collection of 500 rigid balls, with radii ranging from 0.25 mm to 0.5 mm, in a box is considered (see Figure 2). The stopping criterion is equal to  $\varepsilon_{\text{glob}} = 10^{-7}$ . The time step is equal to  $\Delta t = 5.10^{-5}$  s and the number of time steps is equal to 1000.

This example is representative of multi-rigid-body contact problems, owing to the large number of rigid bodies considered and the large proportion of computing time necessary for the local treatment of the contact compared with the total CPU time. According to Table 2, one can observe in this example that the active set method provides the best results in terms of computing time, both for the total time and the time devoted to the treatment of the contact. The EBP and the EAL methods need similar computing time and the SBP and

**Table 2.** Results for example 2. For each method is provided the total CPU time (second column) and the total CPU time necessary to compute the contact forces (third column).

	CPU time (s)	Contact forces CPU time (s)
Standard bipotential	265.43	235.4
Standard augmented Lagrangian	259.89	232.79
Enhanced bipotential	143.68	126.99
Enhanced augmented Lagrangian	148.49	131.81
Primal-dual active set	135.19	120.42



**Figure 3.** Balls falling over an inclined plane (initial state).

**Table 3.** Results for example 3. For each method is provided the total CPU time (second column) and the total CPU time necessary to compute the contact forces (third column).

	CPU time (s)	Contact forces CPU time (s)
Standard bipotential	6790	6724
Standard augmented Lagrangian	6704	6660
Enhanced bipotential	3967	3956
Enhanced augmented Lagrangian	3699	3676
Primal-dual active set	3058	2977

SAL methods also provided comparable results but with a larger computing time, essentially resulting from the computation of the contact forces.

### 5.3. Example of a poly-disperse collection of balls falling over an inclined plane

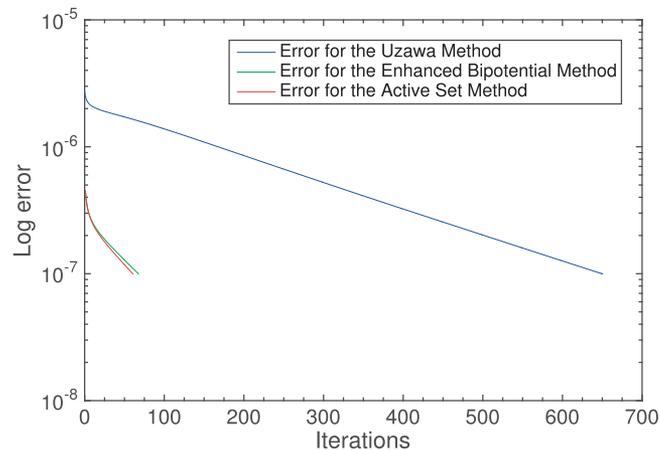
The third example concerns the falling of a poly-dispersed collection of 500 balls over an inclined plane, with a slope equal to  $10^\circ$ . The radii of the balls range from 0.6 mm to 1 mm (see Figure 3). The balls in contact with the plane are sticking. The stopping criterion is equal to  $\varepsilon_{\text{glob}} = 10^{-7}$ . The time step is equal to  $\Delta t = 10^{-5}$  s and the number of time steps is equal to 10000.

The interest of this example lies in the fact that the balls can have very different velocities, which makes simulation using the SBP and SAL methods difficult, since the convergence and the optimal parameters depend strongly on the cinematics. Indeed, the slope of the plane has been chosen in such a way that the balls close to the bottom have small velocity, by contrast with the balls on the top.

As expected, one can observe in Table 3 that the two first methods are not efficient, since they are 75% more computationally expensive than the others. The EBP and EAL methods provide very similar results in terms of time consumption. Once again, the PDAS method is slightly faster than the other methods, with a gain of 17.3% compared with the EAL method.

To study the convergence of the NLGS method at one time step, Figure 4 shows the convergence of the NLGS method for three different treatments of the contact, namely the SBP, the EAL and the PDAS methods.

One can observe in Figure 4 that convergence of the NLGS algorithm associated with the SBP method is very slow, unlike that associated with the two other methods, which provide very close results. Note that the convergence is faster with the PDAS method.



**Figure 4.** Convergence of the NLGS method for various treatments of the contact law at the 1000th time step.

## 6. Conclusion

In this article, we have proposed an adaptation of the active set method to solve the contact dynamics problem with several rigid particles. Numerical tests show that this method is efficient and fast compared with standard methods. These first encouraging results leads us to envisage taking into account friction, using Coulomb's law within the framework of the active set method. We refer to Hintermuller et al. [26, 27] and Kunisch and Stadler [25] for the treatment of frictional and cohesive contact.

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## References

- [1] Radjai, F, and Richefeu, V. Contact dynamics method. *CGP-Gateway.org* [http://www.cgp-gateway.org/Methods/Contact\\_Dynamics/](http://www.cgp-gateway.org/Methods/Contact_Dynamics/) (2013, accessed 8 March 2017)
- [2] Moreau, JJ. Application of convex analysis to some problems of dry friction. *Trends in Applications of Pure Mathematics to Mechanics* 1979; 2: 263–280.
- [3] Moreau, JJ. Unilateral contact and dry friction in finite freedom dynamics. In: Moreau, JJ and Panagiotopoulos, P-D (eds.) *Non smooth mechanics and applications (CISM Courses and Lectures, vol. 302)*. Vienna: Springer-Verlag, 1988, 1–82.
- [4] Moreau, JJ. Some numerical methods in multibody dynamics: application to granular materials. *Eur J Mech A Solids* 1994; 13(4-suppl.): 93–114.
- [5] Moreau, JJ. Numerical aspect of sweeping process. *Comput Methods Appl Mech Eng* 1999; 177: 329–349.
- [6] Jean, M, and Moreau, JJ. Unilaterality and dry friction in the dynamics of rigid body collections. In: Curnier, A (ed.) *Contact mechanics international symposium*. Lausanne: Presses Polytechniques et Universitaires Romanes, 1992, 31–48
- [7] Jean, M. The non smooth contact dynamics method. *Comput Methods Appl Mech Eng* 1999; 177: 235–257.
- [8] Renouf, M, and Alart, P. Conjugate gradient type algorithms for frictional multicontact problems: applications to granular materials. *Comput Methods Appl Mech Eng* 2004; 194(18–20): 2019–2041.
- [9] Jourdan, F, Alart, P, and Jean, M. A Gauss-Seidel like algorithm to solve frictional contact problems. *Comput Methods Appl Mech Eng* 1998; 155: 31–47.
- [10] Fortin, J. *Simulation numérique de la dynamique des systèmes multicorps appliquée aux milieux granulaires*. PhD Thesis, University of Lille, France, 2000.
- [11] Fortin, J, Hjjaj, M, and de Saxcé, G. An improved discrete element method based on a variational formulation of the contact law. *Comput Geotech* 2002; 29: 609–640.
- [12] Fortin, J, Millet, O, and de Saxcé, G. Numerical simulation of granular materials by an improved discrete element method. *Int J Numer Methods Eng* 2005; 62: 639–663.
- [13] Dumont, S. On enhanced descend algorithms for solving frictional multi-contact problems: applications to the discrete element method. *Int J Numer Methods Eng* 2013; 93: 1170–1190.
- [14] Nocedal, J, and Wright, SJ. *Numerical optimization (Springer Series in Operations Research)*. New York: Springer Verlag, 1999.
- [15] Acary, V, and Brogliato, B. *Numerical methods for nonsmooth dynamical systems: applications in mechanics and electronics*. Berlin: Springer, 2008.

- [16] Cottle, RW, Pang, J, and Stone, RE. *The linear complementarity problem. (Classics in Applied Mathematics, no. 60)*. Philadelphia: SIAM, 2009.
- [17] Wriggers, P. *Computational contact mechanics*. Chichester: Wiley, 2002.
- [18] Laursen, T. *Computational contact and impact mechanics*. Berlin: Springer, 2002.
- [19] Kikuchi, N, and Oden, JT. *Contact problems in elasticity: a study of variational inequalities and finite element methods*. Philadelphia: SIAM, 1988.
- [20] Alart, P and Curnier, A. A mixed formulation for frictional contact problems prone to Newton like solution methods. *Comput Methods Appl Mech Eng* 1991; 92: 353–375.
- [21] Facchinei, F, and Pang, JS. *Finite-dimensional variational inequalities and complementarity problems (Springer Series in Operations Research, vols. I–II)*. New York: Springer Verlag, 2003.
- [22] Hintermuller, M, Kovtunenkov, V, and Kunish, K. Semismooth Newton methods for a class of unilaterally constrained variational problems. *Adv Math Sci Appl* 2004; 147: 513–535.
- [23] Hintermuller, M, Ito, K, and Kunish, K. The primal-dual active set strategy as a semismooth Newton method. *SIAM J Optim* 2002; 13: 865–888.
- [24] Hueber, S and Wohlmuth, BI. A primal-dual active set strategy for non-linear multibody contact problems. *Comput Methods Appl Mech Eng* 2005; 194(27–29): 3147–3166.
- [25] Kunisch, K, and Stadler, G. Generalized Newton methods for the 2D-Signorini contact problem with friction in function space. *ESAIM Math Model Numer Anal* 2005; 39(4): 827–854.
- [26] Hintermuller, M, Kovtunenkov, VA, and Kunisch, K. Constrained optimization for interface cracks in composite materials subject to non-penetration conditions. *J Eng Math* 2007; 59(3): 301–321.
- [27] Hintermuller, M, Kovtunenkov, VA and Kunisch, K. Obstacle problems with cohesion: a hemi-variational inequality approach and its efficient numerical solution. *SIAM J Optim* 2011; 21(2): 491–516.
- [28] Abide, S, Barboteu, M, and Danan, D. Analysis of two active set type methods to solve unilateral contact problems. *Appl Math Comput* 2016; 284: 286–307.
- [29] Sharaf, IM. An active set algorithm for a class of linear complementarity problems arising from rigid body dynamics. *Pakistan J Stat Oper Res* 2016; 12(2): 339–352.
- [30] Koziara, T, and Bicanic, N. Semismooth Newton method for frictional contact between pseudo-rigid bodies. *Comput Methods Appl Mech Eng* 2008; 197: 2763–2777.
- [31] Signorini, A. Sopra alcune questioni di elastostatica. *Atti della Società Italiana per il Progresso delle Scienze* 1933; 21(II): 143–148.
- [32] Laursen, T, and Chawla, V. Design of energy conserving algorithms for frictionless dynamic contact problems. *Int J Numer Methods Eng* 1997; 40: 863–886.
- [33] Armero, F, and Petocz, E. Formulation and analysis of conserving algorithms for frictionless dynamic contact/impact problems. *Comput Methods Appl Mech Eng* 1998; 158: 269–300.
- [34] Simo, J, and Tarnow, N. The discrete energy-momentum method. Part I: Conserving algorithms for nonlinear elastodynamics. *Z Angew Math Phys* 1992; 43: 757–793.
- [35] Gonzalez, O. Exact energy and momentum conserving algorithms for general models in non linear elasticity. *Comput Methods Appl Mech Eng* 2000; 190: 1763–1783.
- [36] Hauret, P, and Le Tallec, P. Energy-controlling time integration methods for nonlinear elastodynamics and low-velocity impact. *Comput Methods Appl Mech Eng* 2006; 195: 4890–4916.
- [37] Ayyad, Y, and Barboteu, M. Formulation and analysis of two energy-consistent methods for nonlinear elastodynamic frictional contact problems. *J Comput Appl Math* 2009; 228: 254–269.
- [38] Acary, V. Energy conservation and dissipation properties of time-integration methods for nonsmooth elastodynamics with contact. *Z Angew Math Mech* 2015; 96(5): 585–603.
- [39] Chouly, F, Hild, P, and Renard, Y. A Nitsche finite element method for dynamic contact: 1. Space semi-discretization and time-marching schemes. *ESAIM Math Model Numer Anal* 2015; 49(2): 481–502.
- [40] Renouf, M, Dubois, F, and Alart, P. A parallel version of the non smooth contact dynamics algorithm applied to the simulation of granular media. *J Comput Appl Math* 2004; 168: 375–38.
- [41] de Saxcé, G, and Feng, Z-Q. New inequality and functional for contact with friction: the implicit standard material approach. *Mech Struct Mach* 1991; 19: 301–325.
- [42] Joli, P, and Feng, Z-Q. Uzawa and Newton algorithms to solve frictional contact problems within the bi-potential framework. *Int J Numer Methods Eng* 2008; 73(3): 317–330.
- [43] Feng, Z-Q, Joli, P, Cros, J-M et al. The bi-potential method applied to the modeling of dynamics problems with friction. *Math Comput* 2005; 36: 375–383.