

NUMERICAL SIMULATION FOR A GRANULAR FLOW

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Keywords: Discret model, multi-particle system, Uzawa method, Conjugate Gradient method.

Abstract. The numerical simulation for a multi-particle system of rigid polyhedrons is presented. The computational method that is applied, *Atomized efforts Contact Dynamics respecting the Clasius-Dunheim inequality*, assumes that the particles have constant velocities on small time intervals and the forces due to contacts or gravity are applied only in the limits of such intervals under the form of percussions. Therefore the velocities of the particles have instantaneous time-discontinuities at discrete time. A constrained minimization problem must be solved to get the new velocities of each particle after the time interval. The convergence of the Uzawa method applied to this problem is studied and the conjugate gradient method is applied for solving the unconstrained minimization step.

1 INTRODUCTION

A solid particle in a granular flow has smooth evolutions and instantaneous velocity jumps due to the collisions as well. The velocity-discontinuity at the instant of the collision does not allow the use of classical smooth equations of motion. In this work, the non-smooth equations of motion which describe a collision are obtained by an appropriate set of constitutive laws and applying the principle of virtual work. Clausius-Dahem inequality assures that the solution of the equations describing the collisions always corresponds to a dissipative evolution. The numerical method used to compute the evolution results from the general principle of atomization of efforts of $A - CD^2$ approach (Dal Pont and Dimnet, 2006; Dimnet, 2002a,b).

2 INSTANTANEOUS COLLISION MODEL

The mechanical model describing collision will be first presented by treating the case of a single moving point colliding with a rigid fixed body. In the following, the equation of motion will be given in the time interval $[t_1, t_2]$. We assume instantaneous collisions, thus forces must be modeled by forces concentrated in time. These sorts of efforts are identified as contact percussions \overrightarrow{P}^{int} . Velocity is therefore discontinuous at the instant of the collision t_c and its left and right limits will be noted by \overrightarrow{U}^- and \overrightarrow{U}^+ .

2.1 Principle of virtual work

Interior forces, \overrightarrow{r}^{int} and \overrightarrow{P}^{int} which are forces concentrated in time, are defined by their work. Principle of virtual work leads us to choose the following expression for the virtual work of the internal forces (Dimnet, 2006):

$$W^{int} \left(t_1, t_2, t_c, \overrightarrow{V} \right) = - \int_{t_1}^{t_2} \overrightarrow{r}^{int}(\tau) \overrightarrow{V}(\tau) d\tau - \overrightarrow{P}^{int}(t_c) \frac{\overrightarrow{V}^-(t_c) + \overrightarrow{V}^+(t_c)}{2} \quad (1)$$

where \overrightarrow{V} is a virtual velocity of the point and t_c is a virtual time of collision. The virtual work of the acceleration efforts is (Dimnet, 2002b):

$$W^{acc} \left(t_1, t_2, t_c, \overrightarrow{V} \right) = \int_{t_1}^{t_2} m \frac{d\overrightarrow{U}(\tau)}{d\tau} \overrightarrow{V}(\tau) d\tau + m \left(\overrightarrow{U}^+(t_c) - \overrightarrow{U}^-(t_c) \right) \frac{\overrightarrow{V}^-(t_c) + \overrightarrow{V}^+(t_c)}{2} \quad (2)$$

where m is the mass of the point and \overrightarrow{U} is the current velocity.

Principle of virtual work applies to any velocity \overrightarrow{V} and any time t_c , therefore the following expression holds:

$$W^{acc} \left(t_1, t_2, t_c, \overrightarrow{V} \right) = W^{int} \left(t_1, t_2, t_c, \overrightarrow{V} \right) \quad (3)$$

According to this principle, motion equations assume the following form on $[t_1, t_2]$:

$$m \frac{d\overrightarrow{U}}{d\tau} = -\overrightarrow{r}^{int} \quad \text{almost everywhere} \quad (4)$$

and

$$m \left(\overrightarrow{U}^+ - \overrightarrow{U}^- \right) = -\overrightarrow{P}^{int} \quad \text{everywhere} \quad (5)$$

Due to the duality in the sense of the internal work between \overrightarrow{P}^{int} and $\frac{\overrightarrow{V}^-(t_c) + \overrightarrow{V}^+(t_c)}{2}$ and following the classical mechanical approach, constitutive laws are given by expressing \overrightarrow{P}^{int} as a function

of $\frac{\vec{V}^-(t_c) + \vec{V}^+(t_c)}{2}$. An appropriate constitutive law describing the behavior and the interactions between the colliding bodies has to be now introduced.

2.2 Constitutive laws

Constitutive laws take into account the interactions among particles during the collision and assure de non-interpenetration of the bodies. These two aspects are made explicit by splitting the internal percussion into a *dissipative percussion* \vec{P}^d , take into account the behavior during the collision and a *reactive percussion* \vec{P}^{react} assuring the non-interpenetration, which can as well be considered as a reaction to the non-interpenetration condition:

$$\vec{P}^{int} = \vec{P}^d + \vec{P}^{react} \quad (6)$$

1. An associative dissipative interaction can be described introducing a pseudo-potential of dissipation Φ^d , which is convex, positive function and null at the origin (Dimnet, 2002b; Moreau, 1966; Frémond, 1995):

$$\vec{P}^d \in \partial\Phi^d \left(\frac{\vec{U}^- + \vec{U}^+}{2} \right) \quad (7)$$

2. All the properties of the reactive percussion can be written by means of indicator functions (Moreau, 1966; Frémond, 1995):

$$\vec{P}^{react} \in \partial I_K \left(\frac{\vec{U}^- + \vec{U}^+}{2} \right) \cdot \vec{N}, \quad \text{with } K = \left[\frac{\vec{U}^- \cdot \vec{N}}{2}, \infty \right[\quad (8)$$

In particular, as K is convex and contains the value 0, the indicator function I_K is a pseudo-potential of dissipation. The internal percussion can be therefore written in the following form:

$$\vec{P}^{int} \in \partial\Phi \left(\frac{\vec{U}^- + \vec{U}^+}{2} \right) \quad \text{where } \Phi = \Phi^d + I_K \quad (9)$$

i.e. the internal percussion derives from a pseudo-potential of dissipation.

2.3 Simultaneous collision of N solids

Instantaneous collision model of a point colliding with a fixed point presented before can be generalized for N colliding bodies. Contact among solids is assumed to be punctual. It considers N solids colliding at time t , each one with mass m_i , center of gravity \vec{G}_i and an internal tensor I_i . The k^{th} contact between the solid i and the solid j takes place at point \vec{A}_{ijk} . \vec{P}_{ijk}^{int} is applied at contact point \vec{A}_{ijk} . \vec{V}_i is the virtual velocity of the center of gravity \vec{G}_i and $\vec{\omega}_i$ is the virtual rotational velocity.

Let be the vector $\vec{\nu} = (\vec{V}_i, \vec{\omega}_i)$, and $\vec{\nu} = (\vec{U}_i, \vec{\Omega}_i)$ therefore the relative velocities of the solids in contact at point \vec{A}_{ijk} can be written in the following form:

$$\vec{D}_{ij} \left(\vec{\nu}, \vec{A}_{ijk} \right) = \left(\vec{V}_i + \vec{\omega}_i \times \vec{G}_i \vec{A}_{ijk} \right) - \left(\vec{V}_j + \vec{\omega}_j \times \vec{G}_j \vec{A}_{ijk} \right) \quad (10)$$

Let be $\vec{U}_i, \vec{\Omega}_i$ the current velocities and $\vec{V}_i, \vec{\omega}_i$ the virtual velocities of the solid i , then the principle of virtual work for all $\vec{\nu}$ can be written in the following form:

$$W^{acc}(\vec{\nu}) = \sum_{i=1}^N m_i (\vec{U}^{\dagger} - \vec{U}^{\neg}) \left(\frac{\vec{V}^{\neg} + \vec{V}^{\dagger}}{2} - \frac{\vec{U}^{\neg} + \vec{U}^{\dagger}}{2} \right) + I_i (\vec{\Omega}^{\dagger} - \vec{\Omega}^{\neg}) \left(\frac{\vec{\omega}^{\neg} + \vec{\omega}^{\dagger}}{2} - \frac{\vec{\Omega}^{\neg} + \vec{\Omega}^{\dagger}}{2} \right) \quad (11)$$

$$W^{int}(\vec{\nu}) = - \sum_{i=1}^{N-1} \sum_{j=i+1}^N \sum_{A_{ijk}} \vec{P}_{ijk}^{int} \left(\frac{\vec{D}_{ij}(\vec{\nu}^{\dagger}, \vec{A}_{ijk}) + \vec{D}_{ij}(\vec{\nu}^{\neg}, \vec{A}_{ijk})}{2} \right) - \vec{P}_{ijk}^{int} \left(\frac{\vec{D}_{ij}(\vec{v}^{\dagger}, \vec{A}_{ijk}) + \vec{D}_{ij}(\vec{v}^{\neg}, \vec{A}_{ijk})}{2} \right) \quad (12)$$

$$W^{acc} - W^{int} = 0 \quad (13)$$

Introducing the internal percussion (9) into (12) and introducing (11),(12) into (13) and applying the inequality of the sub-differential (Frémond, 1995) the following expression holds:

$$\forall \vec{\nu} \rightarrow \sum_{i=1}^N m_i (\vec{U}^{\dagger} - \vec{U}^{\neg}) \left(\frac{\vec{V}^{\neg} + \vec{V}^{\dagger}}{2} - \frac{\vec{U}^{\neg} + \vec{U}^{\dagger}}{2} \right) + I_i (\vec{\Omega}^{\dagger} - \vec{\Omega}^{\neg}) \left(\frac{\vec{\omega}^{\neg} + \vec{\omega}^{\dagger}}{2} - \frac{\vec{\Omega}^{\neg} + \vec{\Omega}^{\dagger}}{2} \right) + \sum_{i=1}^{N-1} \sum_{j=i+1}^N \sum_{A_{ijk}} \Phi_{ijk} \left(\frac{\vec{D}_{ij}(\vec{\nu}^{\dagger}, \vec{A}_{ijk}) + \vec{D}_{ij}(\vec{\nu}^{\neg}, \vec{A}_{ijk})}{2} \right) - \Phi_{ijk} \left(\frac{\vec{D}_{ij}(\vec{v}^{\dagger}, \vec{A}_{ijk}) + \vec{D}_{ij}(\vec{v}^{\neg}, \vec{A}_{ijk})}{2} \right) \geq 0 \quad (14)$$

Introducing an external percussion applied by the gravity and considering the scalar product:

$$\langle \vec{\nu}, \vec{\nu} \rangle = \sum_{i=1}^N m_i \vec{U}_i \cdot \vec{V}_i + I_i \vec{\Omega}_i \cdot \vec{\omega}_i \quad (15)$$

It is possible to rewrite (14) in the following way:

$$\left\langle \vec{v}^{\dagger} - \vec{v}^{\neg} - T^{ext}, \frac{\vec{\nu}^{\dagger} + \vec{\nu}^{\neg}}{2} - \frac{\vec{v}^{\dagger} + \vec{v}^{\neg}}{2} \right\rangle + \Phi \left(\frac{\vec{\nu}^{\dagger} + \vec{\nu}^{\neg}}{2} \right) - \Phi \left(\frac{\vec{v}^{\dagger} + \vec{v}^{\neg}}{2} \right) \quad (16)$$

Given that \mathbb{R}^{6N} has a scalar product defined by $\langle \cdot, \cdot \rangle$ and given the definition of sub-gradient, the formulation (16) is equivalent to the following inclusion:

$$- \left(\vec{v}^{\dagger} - \vec{v}^{\neg} - T^{ext} \right) \in \partial \Phi \left(\frac{\vec{v}^{\dagger} + \vec{v}^{\neg}}{2} \right) \quad (17)$$

or given $\vec{X} = \left(\frac{\vec{v}^+ + \vec{v}^-}{2}\right)$, the following more concise form:

$$2\vec{v}^- + T^{ext} \in 2\vec{X} + \partial\Phi(\vec{X}) \tag{18}$$

This inclusion is finally equivalent to the minimization problem:

$$\begin{aligned} & \inf_{\vec{X} \in \Omega} \langle \vec{X}, \vec{X} \rangle + \Phi(\vec{X}) - \langle 2\vec{v}^- + T^{ext}, \vec{X} \rangle \\ & \text{where } \Omega = \left\{ \vec{X} \in \mathbb{R}^{6N} \mid \phi(\vec{X}) : d_l\left(\frac{\vec{v}^-}{2}\right) - d_l(\vec{X}) \leq 0, \quad l = 1, p \right\} \\ & \text{and } d_l(Z) = D_{ij}(Z, A_{ijl}) \cdot \vec{N}_l \end{aligned} \tag{19}$$

2.4 Numerical solution of the minimization problem

The solution of the minimization problem (19) is a saddle point of the Lagrange function (Dimnet, 2002b):

$$L(\vec{X}, \mu) \rightarrow F(\vec{X}) + \sum_{l=1}^p \mu_l \phi_l(\vec{X}) \tag{20}$$

The domain Ω as well as the applications $F(\vec{X})$ and $\phi_l(\vec{X}), l = 1, p$ are convex; this means that if \vec{X}^* is a solution of the problem, it exists at least one $\mu^* \in \mathbb{R}_+^p$ such that (\vec{X}^*, μ^*) is a saddle point of $L(\vec{X}, \mu)$.

The function defined in (19) with few steps of linear algebra is possible to get a quadratic form:

$$F(X) = \vec{X}^T(M + \Xi)\vec{X} - 2\vec{X}^T M \vec{U}^- - \vec{X}^T T^{ext} \tag{21}$$

where $M \in \mathbb{R}^{6N \times 6N}$ is the mass and inertia matrix with the following form:

$$M = \begin{bmatrix} M_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & I_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & 0 & M_2 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & 0 & I_2 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & 0 & \ddots & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & 0 & M_k & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 & I_k & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 & M_N & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I_N \end{bmatrix} \quad \text{where } M_i, I_i \in \mathbb{R}^{3 \times 3} \tag{22}$$

furthermore the matrix $\Xi \in \mathbb{R}^{6N \times 6N}$, is the internal percussion which depends of each contact between two solids; therefore we must consider the internal percussion due to the normal and tangential velocity of each solid involve in the contact, then:

$$\Xi = \frac{1}{2} (\kappa_N \Xi_N + \kappa_T \Xi_T) \tag{23}$$

where κ_N and κ_T are the normal and tangential coefficient respectively.

Let consider for each contact the vector $\vec{C}_k \in \mathbb{R}^6 N$ and the matrices $R_k, S_k \in \mathbb{R}^{3 \times 6N}$ which are used for the computation of the matrix Ξ . Let assume that in the contact k are involved the solid i and j , then the vector \vec{C}_k and matrices R_k, S_k have the following form:

$$\vec{C}_k = \left[\dots \ 0 \ \vec{C}_k^i \ 0 \ \dots \ 0 \ \vec{C}_k^j \ 0 \ \dots \right]^T \quad \text{where } \vec{C}_k^i, \vec{C}_k^j \in \mathbb{R}^6 \quad (24)$$

$$R_k = \left[\dots \ 0 \ R_k^i \ 0 \ \dots \ 0 \ R_k^j \ 0 \ \dots \right]^T \quad \text{where } R_k^i, R_k^j \in \mathbb{R}^{3 \times 6} \quad (25)$$

$$S_k = \left[\dots \ 0 \ S_k^i \ 0 \ \dots \ 0 \ S_k^j \ 0 \ \dots \right]^T \quad \text{where } S_k^i, S_k^j \in \mathbb{R}^{3 \times 6} \quad (26)$$

Therefore,

$$\Xi_N = \sum_{k=1}^{nc} \vec{C}_k \vec{C}_k^T \quad (27)$$

$$\Xi_T = \sum_{k=1}^{nc} (R_k - S_k) (R_k - S_k)^T \quad (28)$$

where nc is the number of contacts. Finally:

$$\Xi = \frac{1}{2} \left(\kappa_N \sum_{k=1}^{nc} \vec{C}_k \vec{C}_k^T + \kappa_T \sum_{k=1}^{nc} (R_k - S_k) (R_k - S_k)^T \right) \quad (29)$$

Obviously, both the matrix M and the matrix Ξ are sparse; this characteristic allow us to make the numerical computations easier.

The constraints of the minimization problem are linear assuring the non-interpenetration between the solids. In the matricial form the constraints are given by:

$$\Phi_i(\vec{X}) : b_i - \vec{a}_i^T \vec{X} \leq 0, \quad \text{where } b_i = \vec{a}_i^T \frac{\vec{U}^-}{2}, \quad \vec{a}_i = \vec{C}_i, \quad \forall i = 1, nc \quad (30)$$

2.5 The Uzawa method

The Uzawa method had been used to solve the minimization problem and implies a succession of unconstrained minimization problem (Ciarlet, 1989). The method is given by:

Algorithm 1 Uzawa method

Require: $\vec{\mu}_0 \in \mathbb{R}_p^+$ is the initial vector for the Lagrange multipliers and \vec{X}_0 a starting point.

1: Let be $\gamma_0 = 1$ and $n = 0$

2: **while** $|\gamma_n| \leq \varepsilon$ **do**

3: Compute $\vec{X}_{n+1} = \operatorname{argmin} \left\{ F(\vec{X}) + \sum_{l=1}^p \mu_l^n \phi_l(\vec{X}), \quad X \in \mathbb{R}^{6N} \right\}$

4: Compute $\mu_{n+1}^l = \max \left\{ 0, \mu_n^l + \varrho \phi^l(\vec{X}_{n+1}) \right\}, \quad \forall l = 1, p$

5: Compute $\gamma_{n+1} = \sum_{l=1}^p \mu_{n+1}^l \phi^l(\vec{X}_{n+1})$

6: $n \rightarrow n + 1$

7: **end while**

The step 3 was solved by the *conjugate gradient method* (Nocedal and Wright, 1999) applied to the equation:

$$\nabla F(\vec{X}^*) + \sum_{l=1}^p \mu_l \nabla \Phi_l(\vec{X}^*) = 0 \tag{31}$$

which is the condition for a *stationary point* of the function (Nocedal and Wright, 1999); in our case, this stationary point is the minimum of the function. From (21) we have that (31) is given by:

$$2(M + \Xi)\vec{X}^* - 2M\vec{U}^* - \vec{T}^{ext} + \sum_{l=1}^p \mu_l (-\vec{C}_l) = 0 \tag{32}$$

$$2(M + \Xi)\vec{X}^* = 2M\vec{U}^* + \vec{T}^{ext} + \sum_{l=1}^p \mu_l \vec{C}_l \tag{33}$$

Therefore the conjugate gradient method is in the following form:

Algorithm 2 Conjugate gradient method

Require: \vec{x}_0 in \mathbb{R}^{6N} is the initial vector.

- 1: Compute $\vec{r}_0 = 2M\vec{U}^* + \vec{T}^{ext} + \sum_{l=1}^p \mu_l \vec{C}_l - 2(M + \Xi)\vec{x}_0$
 - 2: Set $\vec{p}_0 = \vec{r}_0, k \rightarrow 0$
 - 3: **while** $\|\vec{r}_0\| \geq \varepsilon$ **do**
 - 4: $\alpha_k = \frac{\vec{r}_k^T \vec{p}_k}{\vec{p}_k^T (2M + 2\Xi) \vec{p}_k}$
 - 5: $\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$
 - 6: $\vec{r}_{k+1} = \vec{r}_k - \alpha (2M + 2\Xi) \vec{p}_k$
 - 7: $\beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$
 - 8: $\vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$
 - 9: $k \rightarrow k + 1$
 - 10: **end while**
-

The convergence of the Uzawa method has been a very hard work to find the optimal parameter ϱ . In (Ciarlet, 1989) is mentioned that this parameter is bounded by:

$$0 \leq \varrho \leq \frac{2\alpha}{\|C\|^2}$$

where $\langle \nabla F(\vec{X}) - \nabla F(\vec{Y}), \vec{X} - \vec{Y} \rangle \geq \alpha \|\vec{X} - \vec{Y}\|^2$ (34)

In this case, due to the high convexity of F (Dimnet, 2006), the value of α could be estimate in function of the maximal inertia of the solids and the matrix C which is the coefficient matrix of the constraints; in this case it was used the *frobenius norm* to get an estimation of $\|C\|^2$. It was used the *complementary slackness condition* for the convergence of the Uzawa method, this condition is given by (Nocedal and Wright, 1999):

$$\sum_{l=1}^p \mu_l \phi_l(\vec{X}^*) = 0 \tag{35}$$

3 NUMERICAL RESULTS

Numerical simulations were running with different amount of solids $N = 27, 54, 200, 480, 648$. The surface was considered as a slope with angle $\pi/4$ and the initial position of the solids was set in $h = 1[m]$ from the ground. For the time step it was assigned $\Delta t = 10^{-4}[s]$. The experiments were run in an IBM iDataplex machine, Intel Xeon X5550, 3GB.

In the table 1 is shown the different results that it was obtained: the total computation time and the number of contacts. In the figure 1 is shown some pictures of the simulation.

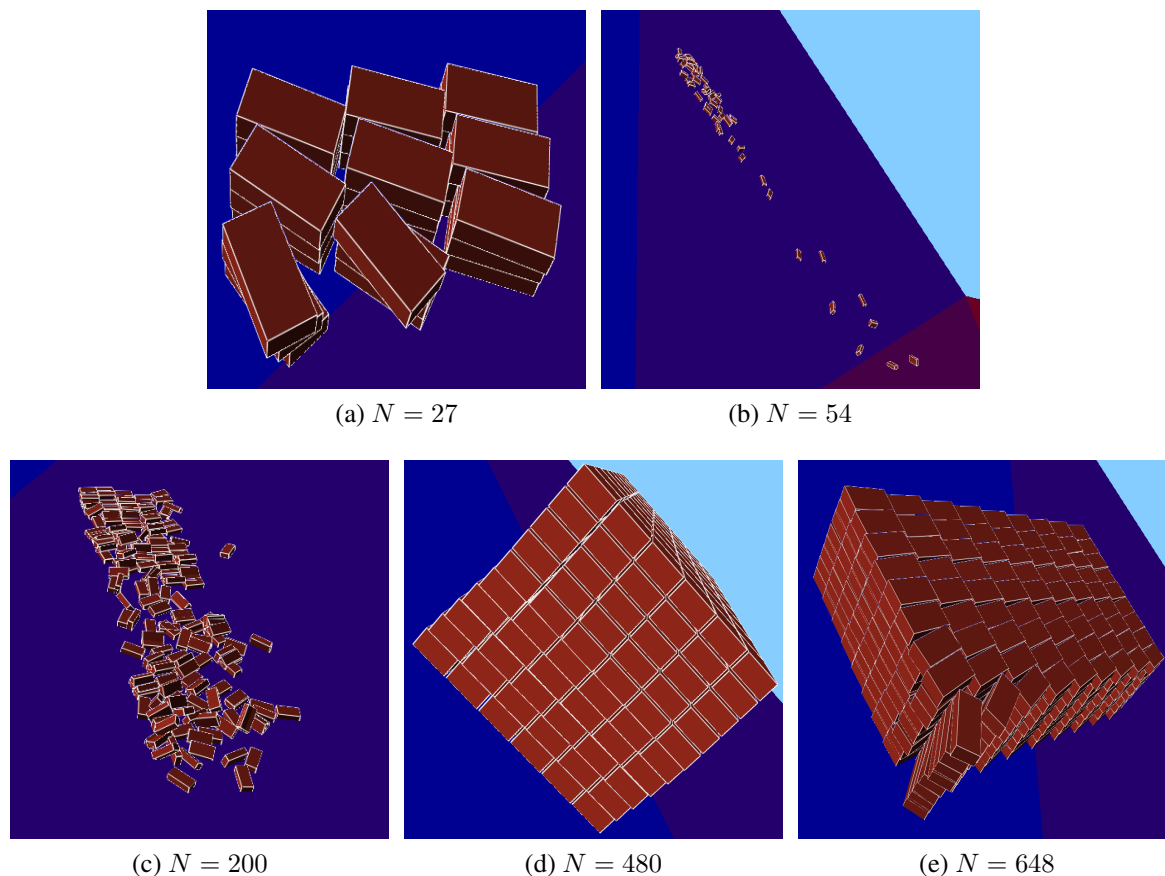


Figure 1: Numerical results with different amount of solids.

Number of solids	Total number of contacts	Number of iterations	Total time in sec.
27	85050	5000	2180.84
54	305504	2000	3284.75
200	944094	2000	27412.96
480	1421032	2000	109651.84
648	8172457	5000	151210.10

Table 1: Computation time for different amount of solids.

Acknowledgments. This research was supported by the Chilean grants: FONDECYT 1100805 and CCTVal FB/24GH/10. Partial support was also received from CONICYT (Chile) PhD. Grant and DGIP Grant (Universidad Técnica Federico Santa María).

4 CONCLUSIONS

In these kind of numerical simulations, it shows that it is necessary include a parallel computational technique to solve the minimization problem (for each solid it adds 6 variables to the system). Some real flow experiments (Manzella and Labiouse, 2009) use a huge amount of solids, in the order of 5000 to 10000 bricks; then, it is a great challenge to perform this numerical simulation with that amount of solids.

In reference to the method that was used, Uzawa method, it was found an important characteristic about the parameter ρ . At the end of the numerical simulation it was necessary to get the solution with the maximal number setting in the method (500 iterations), but at the beginning it was not necessary to get the solution with the maximal numbers of iterations; then, a future aspect to review is to obtain some adaptive parameter with the goal to get the convergence with less amount of iterations.

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