IV International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2015
E. Oñate, M. Bischoff, D.R.J. Owen, P. Wriggers & T. Zohdi (Eds)

ACTIVE-SET BASED QUADRATIC PROGRAMMING ALGORITHM FOR SOLVING INNER OPTIMIZATION PROBLEMS WITH INEQUALITIES IN GRANULAR DYNAMICS SIMULATIONS

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Key words: Granular Materials, Contact Problems, DVI, MPRGP

Abstract. Active-set algorithm for solving inner optimization problem in multi-body dynamics is presented. The efficiency of our algorithm is demonstrated on the solution of simple simulation with thousands of moving spherical particles and static box obstacles. We discuss the solvability and the uniqueness of solution of the problem and the influence of solution to resulting velocity during time-stepping schema.

1 Introduction

In this paper, we are interested in granular dynamics problems; in particular, namely simple multibody dynamics problems. These problems that may deal with from hundreds to billions of discrete rigid bodies interacting through contact, impact, or mutual constraints, such as simulation of the movement of granular matter, are one of the most challenging issue in computer-aided kinematics and dynamics of mechanical systems. Many real-world systems contain or interact with granular material, as granular material belongs among the most manipulated materials. For instance, such a material is utilized in a variety of fields, from sand, gravel, or nanoscale powders to large boulders in the civil industry. Devices consisted of rigid bodies interacting through frictional contacts and mechanical joints pose numerical solution challenges because of the discontinuous nature of their motion, see Pfeiffer and Glocker [1].

Usually, these simulations are performed using discrete element method (DEM, see for instance Cundall [2], Avci and Wriggers [3]; a penalty method where the computation of interaction force is based on the kinematics of the interaction, some representative parameters, and an empirical force law.

From our point of view, an other method is more interesting. It is more similar to the solution of linear elasticity contact problems, because the problem is consisting of a differential variational inequality (DVI, see Pang and Stewart [4], Renouf and Alart [5], Heyn [6]). The method is sometimes referred to the Lagrange multiplier approach. It enforces non-penetration of rigid bodies via a constraint-based approach. In the DVI method, a linear inequality constrained quadratic optimization problem with symmetric positive semidefinite Hessian matrix must be solved at each time step of the simulation. The unknowns in the problem are the normal contact forces between interacting bodies. The efficient solution of inner optimization problem in DVI brings us to the development of Quadratic programming (QP) algorithms. Our research in the solution of particle dynamics simulations is motivated by the results achieved by Heyn et al. [7].

Authors used our Modified Proportioning with Reduced Gradient projection algorithm (MPRGP) to solve DVI efficiently in spite of the fact that all theoretical results supporting the convergence of MPRGP were valid only for the strictly convex cost functions. Only recently, we successfully extended the theory and explained the convergence of the MPRGP for the problems with more general convex quadratic cost function, see Dostál and Pospíšil [8].

In the paper, we are interested in simple simulations with sphere and box particles, but our algorithms can be easily generalized to particle problems with general geometry.

The first subsection consists of short review of the numerical solution concept and time-stepping scheme. The aim of the paper is not to develop new simulations techniques or to modify the mathematical modelling process. However, we are interested in numerical aspect of the inner QP optimization problem and our proofs of the solvability are based on the object structures. Therefore, we decided to present short review. We present the formulation of the problem and derivation of optimization problem. The presented theory and ideas in these subsections can be considered as a short review of Heyn [6].

In the second section we present own new results in the mathematical aspect of the optimization problem solvability.

In the next section, we present our active-set based algorithm Modified Proportioning with Reduced Gradient Projection (MPRGP). This algorithm was successfully used to solve a linear elasticity contact problems with up to more than 40 million of nodal variables, see Dostál et. al [9]. This method combines the conjugate gradient steps with the reduced gradient projection steps and adaptive precision control of the solution of the auxiliary problems. Special attention is paid in the discussion of the solvability of optimization problem. The performance of the algorithm is demonstrated by the solution of a 3D particle dynamics problem.

The last subsection includes the numerical experiments and results. We have implemented algorithms in C programming language with CUDA library, and we performed simulations on GPU card. The problem of granular dynamics is suitable for solving on such a massively parallel architectures. However, the aim of the paper is not to develop

optimal implementation, but the development of algorithms. Much more efficient implementation was presented by the team from Simulation-Based Engineering Lab (SBEL) University of Wisconsin-Madison in Chrono::Engine software [10].

2 Time-stepping schema and formulation of optimization problem

In this short section, we review the basic of multi-body simulations. For more informations see, for instance, Haug [11] and Heyn [6].
Let us consider the system of $n_b \in \mathbb{N}$ rigid bodies (*particles*) in vector space $\{(x, y, z) \in \mathbb{R}^3\}$. Each particle has 6 degrees of freedom - location of centre of gravity $[r_x, r_y, r_z]^T$ and unit quaternion of rotation $[e_0, e_1, e_2, e_3]^T$. For every body $T_{(i)}, i = 1, \ldots, n_b$ in the system in given time t, let us denote $q^t_{(i)} \in \mathbb{R}^7$ as a *vector of generalized position* and $v^t_{(i)} \in \mathbb{R}^6$ as a *vector of generalized velocities*. In our simulations, the rotation of the body is represented by the unit quaternion of rotation and the angular velocity is represented by Euler angles. The position of bodies in the next time-step can be evaluated using time-stepping schema

$$q^{(t+h)} = q^{(t)} + h.Qv^{(t)} \ ,$$

where h is *sufficiently small* time step. Here, Q denotes the matrix of linear mapping between derivative of position vector and vector of velocities, see Haug [11]. This equation can be considered as a discretized numerical solution of the first Newton law using Euler method.
The same method is also used for the computation of velocities. The increment in the next time-step depends on the mass of each body, affecting external forces $F_{ext}(t, q, v)$, and contacts and other limiting conditions. This situation is described by second Newton law, i.e.

$$v^{(t+h)} = v^{(t)} + hM^{-1}(F_{ext} + F_C) \ , \tag{1}$$

where M is generalized mass matrix, F_C is a vector of forces induced by contact constraints, and F_{ext} is a vector of external forces. In our simple simulation, the vector of external forces represents the gravity force affecting each body.
The contact between two bodies T_A and T_B constitutes forces and torques

$$\begin{aligned} F_A &= -\tilde{\gamma} n_A(C) \ , & F_B &= \tilde{\gamma} n_A(C) \ , \\ M_A &= C^A \times F_A \ , & M_B &= C^B \times F_B \ , \end{aligned}$$

where $n_A(C)$ is outward unit normal to the body T_A at the contact point $C = [C_x, C_y, C_z]^T \in \mathbb{R}^3$ in global coordinate system, and $\tilde{\gamma} \geq 0$ is unknown size of the force. Force F_B causes the change of the position of the body T_B (the components of the generalized velocity vector corresponding to the position of gravity center). The change of rotation of the body T_B (the components of the generalized velocity vector corresponding to the rotation) is effected by associated torque M_B. Analogically, forces F_A and M_A change the position

and rotation of body T_A. All forces can be expressed by one vector

$$F_C = \begin{bmatrix} F_A \\ M_A \\ F_B \\ M_B \end{bmatrix} = \begin{bmatrix} -\tilde{\gamma} n_A(C) \\ C^A \times F_A \\ \tilde{\gamma} n_A(C) \\ C^B \times F_B \end{bmatrix} = \begin{bmatrix} -\tilde{\gamma} n_A(C) \\ -\tilde{\gamma} \tilde{C}^A n_A(C) \\ \tilde{\gamma} n_A(C) \\ \tilde{\gamma} \tilde{C}^B n_A(C) \end{bmatrix} = \underbrace{\begin{bmatrix} -n_A(C) \\ -\tilde{C}^A n_A(C) \\ n_A(C) \\ \tilde{C}^B n_A(C) \end{bmatrix}}_{=:D \in \mathbb{R}^{12,1}} \tilde{\gamma} \ , \tag{2}$$

where we used the matrix representation of the vector product

$$\tilde{C}^B = \begin{bmatrix} 0 & -C_z^A & C_y^A \\ C_z^A & 0 & -C_x^A \\ -C_y^A & C_x^A & 0 \end{bmatrix}, \quad \tilde{C}^B = \begin{bmatrix} 0 & -C_z^B & C_y^B \\ C_z^B & 0 & -C_x^B \\ -C_y^B & C_x^B & 0 \end{bmatrix}.$$

The unknown size of the force $\tilde{\gamma}$ is constrained by the non-penetration conditions of the bodies, which can be described by *gap function* $\Phi : \mathbb{R}^{7+7} \to \mathbb{R}$. It holds

- $\Phi([q_A, q_B]) = 0, \tilde{\gamma} \geq 0$ if the bodies are in contact,
- $\Phi([q_A, q_B]) > 0, \tilde{\gamma} = 0$ if the bodies are not in contact,
- $\Phi([q_A, q_B]) < 0$ if the bodies penetrate each other.

Merging these observations, we obtain the *complementarity condition*

$$\begin{aligned} \Phi(q) &\geq 0, \\ \tilde{\gamma} &\geq 0, \\ \Phi(q) &\perp \tilde{\gamma}. \end{aligned}$$

Instead of these conditions, we can consider more numerically stable conditions (see Anitescu [12])

$$\begin{aligned} \tilde{\gamma} &\geq 0, \\ \tfrac{1}{h}\Phi(q) + D^T v^{(t+h)} &\geq 0 \ , \\ \tfrac{1}{h}\Phi(q) + D^T v^{(t+h)} &\perp \tilde{\gamma}. \end{aligned} \tag{3}$$

This problem can be reformulated to the quadratic programming problem with bound constraints, see next theorem. For simplicity we denote $\gamma = t.\tilde{\gamma}$.

Lemma 1. *The solution of the optimization problem*

$$\min_{\gamma \geq 0} \frac{1}{2} \gamma^T N \gamma + r^T \gamma \ , \tag{4}$$

where

$$N = D^T M^{-1} D, \tag{5a}$$

$$r = \frac{1}{h}\Phi + D^T M^{-1} k, \tag{5b}$$

$$k = M v^{(t)} + h.F_{ext}, \tag{5c}$$

is equivalent to the solution of original problem

$$M(v^{(t+h)} - v^{(t)}) = hF_{ext} + D^T\gamma, \tag{6a}$$

$$\frac{1}{h}\Phi(q) + D^T v^{(t+h)} \geq 0, \tag{6b}$$

$$\frac{1}{h}\Phi(q) + D^T v^{(t+h)} \perp \gamma, \tag{6c}$$

$$\gamma \geq 0. \tag{6d}$$

Proof. The proof is based on the Karush-Kuhn-Tucker optimality conditions. See Heyn [6]. □

The algorithm in every time-step has the form of Algorithm 1.

Algorithm 1: **Time-stepping schema.**

Given $t, h, q^{(t)}, v^{(t)}$.
  find contacts
  if *there is a contact*
    set up N, r *from contacts*
    solve the problem

$$\gamma = \arg\min_{\gamma \geq 0} \frac{1}{2}\gamma^T N\gamma + r^T\gamma$$

    $v^{(t+h)} = v^{(t)} + M^{-1}(hF_{ext} + D\gamma)$
  else
    $v^{(t+h)} = v^{(t)} + hM^{-1}F_{ext}$
  endif
  $q^{(t+h)} = q^{(t)} + h.Qv^{(t)}$

Return $q^{(t+h)}, v^{(t+h)}$.

3 The solvability and uniquess of the solution

In this section, we prove that the inner optimization problem has always solution. However, since kernel of Hessian matrix is non-trivial, it can have infinite number of solutions. We show that the resulting velocity is independent of the choice of the solution of inner optimization problem.

Lemma 2. *Let* $A \in \mathbb{R}^{n,n}$ *be a symmetric positive definite matrix and let* $B \in \mathbb{R}^{n,m}$ *be a rectangular matrix.*

Then

$$\operatorname{Ker} B^T AB = \operatorname{Ker} B, \tag{7a}$$

$$\operatorname{Im} B^T AB = \operatorname{Im} B^T. \tag{7b}$$

Proof. See Laub [13] or Dostál [14]. □

Lemma 3. *The optimization problem* (4) *is a quadratic programming problem with symmetric positive semidefinite Hessian matrix and right-hand side vector from the image of Hessian matrix, i.e.*

$$\forall x \in \mathbb{R}^{n_c} : \langle Nx, x\rangle \geq 0 \tag{8a}$$

$$r \in \operatorname{Im} N \tag{8b}$$

Proof. At first, we prove (8a). It is necessary to show that $\forall x \in \mathbb{R}^{n_c} : \langle Nx, x\rangle \geq 0$. We use that $M \in \mathbb{R}^{6n_b,6n_b}$ is symmetric positive definite. Therefore, the inverse is also symmetric positive definite and it induces the norm in $\mathbb{R}^{6n_b}$. Furthermore, we can write

$$\langle Nx, x\rangle = \langle D^T M^{-1} Dx, x\rangle = \langle M^{-1} Dx, Dx\rangle = \|Dx\|^2_{M^{-1}} \geq 0 \ .$$

If we take a look into the formula for the right-hand side vector

$$r = \frac{1}{h}\Phi + D^T M^{-1} k \ ,$$

we can use Lemma 2 and simplify the proof of (8b) into the proof of

$$\Phi \in \operatorname{Im} D^T \ . \tag{9}$$

At first, let us define the vector spaces $\mathcal{V}, \mathcal{W} \subset \mathbb{R}^{nc}$

$$\mathcal{V} = \operatorname{span}\left\{\begin{bmatrix}1\\-1\\0\\0\\\vdots\\0\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\\-1\\\vdots\\0\\0\end{bmatrix}, \dots \begin{bmatrix}0\\0\\0\\0\\\vdots\\1\\-1\end{bmatrix}\right\}, \quad \mathcal{W} = \operatorname{span}\left\{\begin{bmatrix}1\\1\\0\\0\\\vdots\\0\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\\1\\\vdots\\0\\0\end{bmatrix}, \dots \begin{bmatrix}0\\0\\0\\0\\\vdots\\1\\1\end{bmatrix}\right\} .$$

We take a better look into the structure of matrix $D \in \mathbb{R}^{6n_b,n_c}$ whose blocks are given by (2). This matrix always consists of the pairs of contacts - the contact between the body T_A and the body T_B (denoted by contact AB) as well as the contact between body B and A (denoted by contact BA). For the sake of simplicity we consider the construction

of matrix $D \in \mathbb{R}^{6n_b,n_c}$ with consecutive collocation of the contact pairs. Then each pair of columns corresponds to the pair of contacts and the nonzero rows corresponding to the indexes of the bodies in this contact is given by (2). The submatrix for one pair of contacts AB and BA has the structure

$$D_{\mathcal{R},\mathcal{C}} = \begin{bmatrix} -n_A(C_{AB}) & n_B(C_{BA}) \\ -\widetilde{C}^A_{AB} n_A(C_{AB}) & \widetilde{C}^A_{AB} n_B(C_{BA}) \\ n_A(C_{AB}) & -n_B(C_{BA}) \\ \widetilde{C}^B_{AB} n_A(C_{AB}) & \widetilde{C}^B_{BA} n_B(C_{BA}) \end{bmatrix}, \tag{10}$$
$$\mathcal{R} = \{\text{indexes of } v_A, \text{indexes of } v_B\},$$
$$\mathcal{C} = \{\text{index of contact } AB, \text{index of contact } BA\} .$$

The key ingredient of the proof is a small observation − the contact forces in the contact points $C_{AB} = C_{BA}$ have opposite directions and the outward unit normals of the bodies in the contact are also opposite. Thus $n_A = -n_B$ and the submatrix (10) can be written in simplier form

$$D_{\mathcal{R},\mathcal{C}} = \begin{bmatrix} -n_A & -n_A \\ -\widetilde{C}^A n_A & -\widetilde{C}^A n_A \\ n_A & n_A \\ \widetilde{C}^B n_A & \widetilde{C}^B n_A \end{bmatrix},$$

where we used notations $n_A = n_A(C_{AB}) = -n_B(C_{BA})$, $C^A = C^A_{AB} = C^A_{BA}$, and $C^B = C^B_{AB} = C^B_{BA}$.
Using this structure, it is easy to check that

$$\begin{aligned} \forall v \in \mathcal{V}: &\quad Dv = 0, \\ \forall w \in \mathcal{W} \setminus \{0\}: &\quad Dw \neq 0. \end{aligned}$$

Furthermore, we proved that $\mathcal{V} \subset \operatorname{Ker} D$ and $\mathcal{W} \cap \operatorname{Ker} D = \{0\}$. Using this and $\operatorname{Im} D^T \perp \operatorname{Ker} D$, we can write

$$\left.\begin{array}{l} \operatorname{Ker} D \supset \mathcal{V} \perp \mathcal{W} \\ \mathcal{W} \cap \operatorname{Ker} D = \{0\} \end{array}\right\} \quad \Rightarrow \quad \mathcal{W} \perp \operatorname{Ker} D \quad \Rightarrow \quad \mathcal{W} \subset \operatorname{Im} D^T .$$

To prove (9), notice that $\Phi \in \mathcal{W}$ because the gap function has the same value for both contacts AB and BA (the distance between bodies T_A and T_B is the same as distance between bodies T_B and T_A). □

The previous lemma proves that the cost function is bounded from below. Using the clasical results given by Frank and Wolfe [15], we can conclude that the optimization problem (4) has always solution.

Lemma 4. *The velocity in the next time-step $v^{(t+h)}$ given by Algorithm 1 is independent of the choice of the solution of the optimization problem* (4).

Proof. Let $\bar{\gamma}_1, \bar{\gamma}_2$ denote different solutions of optimization problem (4). Then the velocity in the next time-step given by Algorithm 1 is given by

$$\begin{aligned} v^{(t+h)}(\bar{\gamma}_1) &= v^{(t)} + M^{-1}(hF_{ext} + D\bar{\gamma}_1), \\ v^{(t+h)}(\bar{\gamma}_2) &= v^{(t)} + M^{-1}(hF_{ext} + D\bar{\gamma}_2). \end{aligned}$$

Thus the difference of these velocities reads

$$v^{(t+h)}(\bar{\gamma}_1) - v^{(t+h)}(\bar{\gamma}_2) = M^{-1}D(\bar{\gamma}_1 - \bar{\gamma}_2) \ .$$

Since the solutions of quadratic programming problem differ by the vector from the kernel of Hessian matrix, see Dostál [14] and $\operatorname{Ker} N = \operatorname{Ker} D$ (see Lemma 2), we can write

$$v^{(t+h)}(\bar{\gamma}_1) - v^{(t+h)}(\bar{\gamma}_2) = M^{-1}0 = 0.$$

□

4 Modified Proportioning with Reduced Gradient Projection

For solving problem (5), we are using an active-set based algorithm. This algorithm is based on the decomposition of the set of indices of all constraints $\mathcal{M} = 1, \ldots, n_c$ into two disjoint subsets subject to the value of the constraint function

$$\mathcal{F}(\gamma) := \{j \in \mathcal{M} : \gamma_j > 0\}, \quad \mathcal{A}(\gamma) := \{j \in \mathcal{M} : \gamma_j = 0\}.$$

Using this decomposition, we decompose the gradient of the cost function $g(\gamma) = \nabla f(\gamma) = N\gamma + r$ in every iteration γ^k into *free* and *chopped* gradient

$$\begin{aligned} &\varphi_j(\gamma^k) = g_j \ \text{ for } j \in \mathcal{F}(\gamma^k), \quad &&\varphi_j(\gamma^k) = 0 \ \text{ for } j \in \mathcal{A}(\gamma^k), \\ &\beta_j(\gamma^k) = 0 \ \text{ for } j \in \mathcal{F}(\gamma^k), \quad &&\beta_j(\gamma^k) = \min\{g_j, 0\} \ \text{ for } j \in \mathcal{A}(\gamma^k). \end{aligned}$$

Modified Proportioning with Reduced Gradient Projection (MPRGP, see Algorithm 2) is an efficient algorithm for the solution of convex quadratic programming problems with simple bounds. The basic version was proposed independently by Dostál [16] and Friedlander and Martínez [17]. It can be considered as a modification of the Polyak algorithm. Dostál and Schöberl in [18] combine the proportioning algorithm with the gradient projections [19]. They use the constant $\Gamma > 0$, the test to decide about leaving the face, and three types of steps to generate the sequence of iterates γ^k that approximate the solution.

The precision of the solution of auxiliary problems is controlled by norm of violation of Karush-Kuhn-Tucker condition in each inner iterate γ^k by

$$\Gamma\|\varphi(\gamma^k)\| \geq \left\|\beta(\gamma^k)\right\|,$$

while $\Gamma > 0$ and γ^k satisfying this inequality is called as *proportional*. If $\gamma \in \Omega$, i.e. $\gamma \geq 0$, we call γ *feasible*.

Algorithm 2: **Modified Proportioning with Reduced Gradient projection (MPRGP).**

Step 0 {*Initialization of parameters*}
$\gamma^0 \in \Omega$, $\overline{\alpha} \in \left(0, \|N\|^{-1}\right]$, $\Gamma > 0$

Step 1 {*Proportioning step - removes indices from* $\mathcal{A}(\gamma^k)$}
If γ^k *is not proportional then define*
$\gamma^{k+1} = \gamma^k - \alpha_{CG}\beta(\gamma^k)$ *by proportioning,*
$\alpha_{CG} = \frac{\beta^T(\gamma^k)g(\gamma^k)}{\beta^T(\gamma^k)A\beta(\gamma^k)}$ *minimizes* $\phi(\gamma^k - \alpha\beta(\gamma^k))$ *with respect to* α

Step 2 {*CG step*}
If γ^k *is proportional then generate*
$\gamma^{k+1} = \gamma^k - \alpha_{CG}p^k$ *by trial cg step,*
$p^{k+1} = \varphi(\gamma^k) - \beta_{CG}p^k$, $\beta_{CG} = (\varphi^T(\gamma^k)Ap^k)/((p^k)^TAp^k)$

Step 3 {*Expansion step - expands* $\mathcal{A}(\gamma^k)$}
If $\gamma^k \in \Omega$ *then accept it else generate*
$\gamma^{k+1} = P_+(\gamma^k - \overline{\alpha}\varphi(\gamma^k)) = \gamma^k - \overline{\alpha}\widetilde{\varphi}(\gamma^k)$ *by projection to feasible set*

Every solution $\overline{\gamma}$ of auxiliary problem satisfies the Karush-Kuhn-Tucker conditions expressed by the relation

$$\varphi(\gamma) = 0 \quad \wedge \quad \beta(\gamma) = 0,$$

hence as a stopping criteria, we are using the Euclidean norm of the *projected gradient*

$$g^P(\gamma) = \varphi(\gamma) + \beta(\gamma) = \frac{1}{\alpha}(\gamma - P_+(x - \alpha g(\gamma))),$$

where P_+ is the projection to set of feasible vectors defined as

$$P_+(\gamma)_i = \max\{\gamma_i, 0\}.$$

More details about implementation of the algorithm may be found in [18]. A short review of optimal QP algorithms can be found in Dostál and Pospíšil [20].

5 Numerical experiment

In this section, we present the numerical results showing the efficiency of our algorithm on the simulation of 32810 spherical particles. During the first stage of the simulation, small particles are poured into box represented by five walls. The initial position of the particles and final position can be found in Fig. 3. Afterwards, in $t = 0.3$ s, we add large

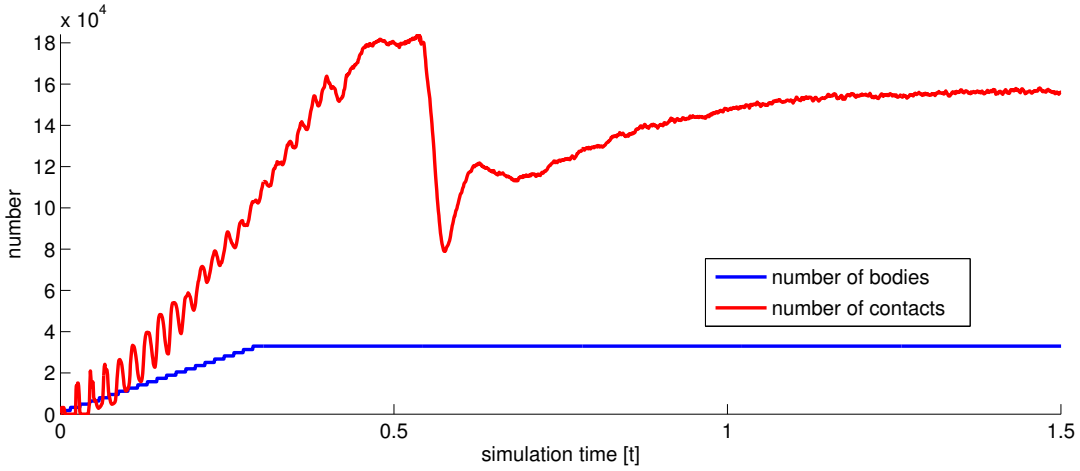

Figure 1: The number of bodies and contacts in the system during the simulation.

spherical particle to study the behaviour of the impact. The material of the bodies is represented by density $\rho = 2800$ kg $\cdot$ m^{-3}. Small particles have radius $r = 0.011$ m and the large one $r_2 = 0.15$ m. The stepsize of the time-stepping scheme is $h = 8 \cdot 10^{-4}$ s.

Algorithm was implemented in C programming language in CUDA environment [21]. For contact detection, we are using our own implementation of the Moving Bounding-Box algorithm [22]. We demand the relative stopping tolerance

$$\|g^P(\gamma)\| \leq 10^{-4} \cdot \|r\|.$$

The number of bodies in the system and the number of contacts can be found in Fig. 1. The number of iterations and the Hessian matrix multiplications (the most time-consuming operation) depends on the dimension of the inner problem, see Fig. 2.

6 Conclusion

In our paper, we proved the solvability of inner optimization problem in multi-body dynamics and presented the results of our active-set algorithm for the solution of optimization problem in particle dynamics. Our numerical experiment shows the efficiency of the algorithm.

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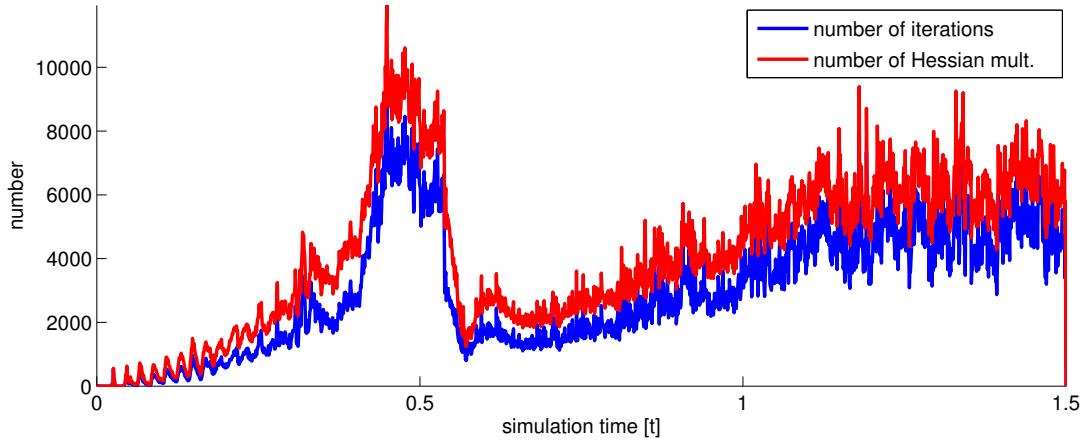

Figure 2: The number of iterations and Hessian multiplications during the simulation.

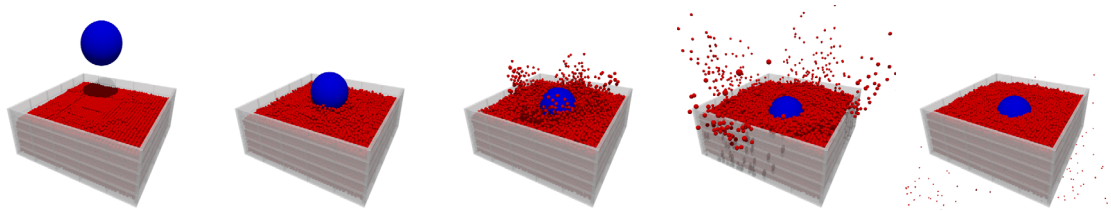

Figure 3: The state of the benchmark simulation in $t = 0.4$ s, 0.56 s, 0.64 s, 0.8 s, 1.44 s.

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