Using the fractional interaction law to model the impact dynamics in arbitrary form of multiparticle collisions

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I. INTRODUCTION

Nature of particulate flows offers the physics and engineering communities an opportunity to analyse the interesting behaviour of granular materials. From a phenomenological point of view such a flow, being halfway between a solid and a liquid state, is not well understood because the basic physics is extremely complex. In a local state, the simplest form of the granular dynamics is as follows - during an arbitrary extortion particles move individually and during collisions particles may exchange their momenta and energies. Therefore the collision process plays a dominant role in the development of theoretical studies and also in the performance of simulations. For an understanding of the collision process we need to consider a simple situation, focusing on what happens when two particles collide. In other words, we need to be able to distinguish the following basic phenomena: static contact, cohesion, attrition, erosion and fragmentation. These phenomena may occur simultaneously or respectively when an individual particle impacts with another. After impact separation or clusterisation of the two particles occurs. In addition, the particles may gain or loss mass. Here we will focus on the dynamics of the collision process which may be decomposed into impact and contact processes. However, as the contact process is formed, we can also notice rebound or static contact, or permanent contact, called cohesion. These processes exist simultaneously when we analyse the dynamics of colliding particles. With regard to the granular dynamics involving many particles in motion, we can observe multiparticle collisions, especially when particle concentration is very dense, because collisional times between several binary particle contacts are higher in comparison to their separation times. Multiparticle collisions occur when an individual particle collides with neighbouring particles, so that those contacts have direct a influence on each other. Only, an infinitesimally short collisional time is required for binary collisions. In all the considered cases the collision process between the two particles is characterised through the collisional time, which is dependent on the impact energy and the physical properties of the contacting surfaces. Moreover, after impact dissipation of energy occurs between the colliding particles. Therefore the simulations of such dynamics are limited by assumptions concerning the collision process. One of the major aspects which needs to be taken into account in the simulations is how to control (correlate) the collisional time and the energy dissipation associated with an individual particle during the dynamics of multiparticle collisions.

Generally two different ways exist to model the dynamics of a granular material. The continuum approach is based on binary collisions of smooth spherical particles. Unfortunately, the introduction of real quantities such as distribution of particle dimensions, particle shapes, their surface wetness and roughness, etc., greatly limit the application of continuum models. Balzer et al. inform us that the kinetic theory is useful for the modelling of gas-solid flow applications in industry: where the geometry involved is complex (many different inlets or/and outlets). However, the kinetic theory cannot reflect the real dynamics involved in multiparticle collisions because the collisional time is defined only for binary collisions.

The discrete deterministic approach more realistically reflects the collision process. Note that multiparticle collisions in the discrete approach are decomposed into several binary collisions. In this approach one may distinguish two general methods. The molecular dynamics method takes into account an expression for the repulsive force acting between a pair of contacting par-
particles. In this method particles virtually overlap when a contact occurs. The overlap reflects the quantitative deformations of particle surfaces because the modelling of realistic deformations would be much too complicated. The interaction laws in the molecular dynamics method define basic models of the repulsive force for two colliding particles. They are valid for particle collisions which are independent from one another. The next method, called the event driven method, assumes instantaneous changes in the direction and value of particle velocities according to conservation equations each time a binary contact occurs. As shown in the basic difference between the event driven and molecular dynamics methods is the collisional time between a pair of particles. In the event driven method this time is ideally zero. Note that this situation is quite different for the molecular dynamics method, where the contact time is greater than zero and is dependent on parameters describing the structure of two contacting surfaces, and is of course dependent on the impact energy. However, the repulsive force models in the molecular dynamics method underestimate the energy dissipation in multiparticle collisions. (This is the so-called “detachment effect”) but in the event driven method an inelastic collapse occurs.

In this paper we will focus on the molecular dynamics method because this gives us a chance to correlate the collisional time and the energy dissipation during multiparticle collisions. We shall introduce a novel mathematical description of this method taking into account the division of the collision process into an impact phase, a contact phase and another phase occurring after the contact phase. We assume that the impact phase and the phase formed after the contact phase are infinitesimally short in time. Consequently, we will analyse the well-known interaction laws of the repulsive force in the contact phase in order to examine several difficulties within the collisions.

On the base of preliminary results we shall introduce a novel form of the repulsive force defined under fractional calculus. We will also demonstrate the basic properties of this force and focus on what happens with the collisional time and the energy dissipation for multiparticle collisions. This analysis is necessary in computational simulations of the cluster dynamics. Within the cluster one may notice non-permanent contact and/or cohesion phenomena between several pairs of colliding particles.

II. THE DISCRETE MODEL OF MOTION OF FOR INDIVIDUAL PARTICLE

Let us turn our attention to a set of spherical particles moving under arbitrary exertion. The spherical shape of the particle makes only the mathematical description easier and does not make the model in any way poorer. The reader may find in more information concerning the molecular dynamics technique adapted to arbitrary form particle shapes. The particles are numbered by the discrete index $i = 1, \ldots, np$, where $np$ is the total number of considered particles. We describe an individual particle through its radius $r_i$ (or diameter $d_i$), mass $m_i$, inertia moment $J_i$, position $x_i$ of the mass centre, linear speed $\dot{x}_i$ and angular velocity $\omega_i$. With regard to the collision of two individual particles we also introduce the natural function $j(i)$ ($j(i) \neq i$ by assumption) of a particle $i$ in order to find the particle index of a particle in a set of particles $np$. Several papers present different algorithms that detect particle collisions, being dependent on their shapes, and consequently that to find the natural function $j(i)$. For a binary collision we neglect phenomena which cause a change in the mass of an individual particle. Thus in our discrete model we do not take into account fragmentation, attrition and erosion which eventually take place during the collision process. These phenomena will be the subject of future investigations.

However, after the contact, which is the second phase of the collision process, rebound, non-permanent contact (static contact) or cohesion can arise simultaneously. In this paper, we will try to model above the phenomena by introducing a novel mathematical description and a novel form of the repulsive force into the molecular dynamics method.

A. Mapping local coordinates onto global ones and defining the overlap

Starting from the description shown in Fig. let us introduce several definitions before formulating the motion equations. First, we assign local coordinates as $(\xi, \eta, \zeta)$ and global ones as $(x, y, z)$. When we consider a contact which eventually takes place between two particles then the normal unit vector $e_{\xi j(i)}$ that connects the particle’s centres of mass reads

$$e_{\xi j(i)} = \frac{x_{j(i)} - x_i}{\|x_{j(i)} - x_i\|} = \left[ e_x^{\xi j(i)}, e_y^{\xi j(i)}, e_z^{\xi j(i)} \right],$$  \hspace{1cm} (1)

where $\| \cdot \|$ represents a norm calculated from the relative coordinate $x_{j(i)} - x_i$. Tangential unit vectors which operate on a tangent plane (rotated by $\pi$ to the normal) become

$$e_{\eta j(i)} = \left[ e_y^{\xi j(i)}, -e_x^{\xi j(i)}, 0 \right] \frac{\|x_{j(i)} - x_i\|}{\|x_{j(i)} - x_i\|_{x,y}},$$  \hspace{1cm} (2)

$$e_{\xi j(i)} = e_{\eta j(i)} \times e_{\xi j(i)},$$  \hspace{1cm} (3)

where $\| \cdot \|_{x,y}$ represents the norm which is calculated only in the tangent plane. When a particle hits a wall we redefine unit vectors putting $xb_{n(i)}$ instead of $x_{j(i)}$, where $xb_{n(i)}$ is a point whose coordinates issue from the line that crosses the particle’s centre of
reduce the penetration width of the particles defined as mass and is perpendicular to the wall. The general form of the base vectors is presented as follows

$$\mathbf{e}_{j(i)} = \begin{bmatrix} \mathbf{e}_{\xi j(i)} \\ \mathbf{e}_{\eta j(i)} \\ \mathbf{e}_{\zeta j(i)} \end{bmatrix}.$$  (4)

FIG. 1: Scheme illustrates particle collisions with useful notations.

Fig. 1 presents the “virtual overlap” $\| \mathbf{\zeta}_{j(i)} \|$ of two particles experiencing a contact. With regard to Fig. 1, we define the overlap as

$$\| \mathbf{\zeta}_{j(i)} \| = r_{j(i)} + r_i - \| \mathbf{x}_{j(i)} - \mathbf{x}_i \|,$$  (5)

which is associated with the particles having spherical forms. Note that only positive values of formula (5) indicate a contact while negative ones confirm that the considered particles are in separation. This means that they move individually. As presented in previous section and in Fig. 1, the overlap reflects the penetration depth of the particles in a direction which connects the particle’s centres of mass, pointing from $i$ to $j(i)$. We also introduce the penetration width of the particles defined as the direction perpendicular to the previous one. Thus we have

$$\| \mathbf{\eta}_{j(i)} \| = \| \mathbf{\xi}_{j(i)} \|$$

$$= 2 \sqrt{r_i^2 - \left( r_i + \frac{1}{2} \| \mathbf{\zeta}_{j(i)} \| \right)^2 \frac{2r_{j(i)} - \| \mathbf{\zeta}_{j(i)} \|}{\| \mathbf{\zeta}_{j(i)} \| - (r_i + r_{j(i)})}^2}$$  (6)

valid for $\| \mathbf{\zeta}_{j(i)} \| \geq 0$. Let $\mathbf{c}_{j(i)}$ be a vector which defines a point $C_{j(i)}$ of the application of the repulsive force, and which is taken as the mass centre of the overlapping region $\mathbb{5}$ as shown in Fig. 1. Taking into consideration the fact that particles have only spherical forms and collide when their overlap $\mathbb{5}$ is positive we obtain

$$\mathbf{c}_{j(i)} = \mathbf{x}_i + \left( r_i - \frac{\| \mathbf{\zeta}_{j(i)} \| (r_{j(i)} - \| \mathbf{\zeta}_{j(i)} \|)}{r_i + r_{j(i)} - \| \mathbf{\zeta}_{j(i)} \|} \right) \mathbf{e}_{\zeta j(i)}.$$  (7)

Thus, at the beginning of a collision we have

$$\mathbf{c}_{j(i)} = \frac{r_i \mathbf{x}_i + r_{j(i)} \mathbf{x}_{j(i)}}{r_i + r_{j(i)},}$$  (8)

and one can find an explicit time $t_{j(i)}^b$ where the overlap $\mathbb{5}$ is zero. Above notation allows us to analyse multiparticle collisions where an individual particle $i$ collides with neighbouring particles $j(i)$. Therefore many overlaps $\mathbb{5}$ indexed $j(i)$ on the particle $i$ may occur. This allows us to formulate the motion equations in the right form.

Next we introduce the relative velocity of a particle $i$ and a particle $j(i)$ at point $C_{j(i)}$ as

$$\mathbf{\tilde{u}}_{j(i)} = \mathbf{\tilde{u}}_{j(i)}^l + \mathbf{\tilde{u}}_{j(i)}^r = \mathbf{\dot{x}}_i - \mathbf{\dot{x}}_{j(i)}$$

$$- (\mathbf{\omega}_i \times \mathbf{s}_{i,j(i)} + \mathbf{\omega}_{j(i)} \times \mathbf{s}_{j(i),i}),$$  (9)

where $\mathbf{\tilde{u}}_{j(i)}^l$ and $\mathbf{\tilde{u}}_{j(i)}^r$ are linear and rotational relative velocities and $\mathbf{s}_{i,j(i)}$ and $\mathbf{s}_{j(i),i}$ are branch vectors connecting the mass centres of particles $i$ and $j(i)$ with the point $C_{j(i)}$ of application of the repulsive force. Note that above values are defined for the global system of coordinates $(x, y, z)$. To change this to the local system of coordinates we need to use the scalar product of the base vectors $\mathbb{11}$ per the vector of the relative velocity. Calculating the branch vectors we obtain the following dependencies in the local system $(\xi, \eta, \zeta)$ as

$$\mathbf{s}_{i,j(i)}' = \begin{bmatrix} 0, 0, -\| \mathbf{\xi}_{j(i)} \| \end{bmatrix}, \mathbf{s}_{j(i),i}' = \begin{bmatrix} 0, 0, -\| \mathbf{\zeta}_{j(i)} \| \end{bmatrix},$$  (10)

where

$$\| \mathbf{\xi}_{j(i)} \| = \| \mathbf{c}_{j(i)} - \mathbf{x}_i \|$$

$$= r_i - \frac{\| \mathbf{\zeta}_{j(i)} \|}{\| \mathbf{\zeta}_{j(i)} \| - (r_i + r_{j(i)})},$$  (11)
\[ \left\| \vec{\zeta}_j(i) \right\| = \left\| \vec{c}_j(i) - \vec{x}_j(i) \right\| \]
\[ = r_j(i) - \left\| \zeta_j(i) \right\| \leq \frac{1}{2} \left\| \zeta_j(i) \right\| - r_i. \]  
(12)

In the global system of coordinates the branch vectors become
\[ \mathbf{s}_{i,j}(i) = \mathbf{e} \cdot \nabla \mathbf{r}_{i,j}(i), \quad \mathbf{s}_{j,i}(i) = \mathbf{e} \cdot \nabla \mathbf{r}_{j,i}(i), \]  
(13)

Using Eqs. (4) and (9) we translate the linear and rotational relative velocities in the global system of coordinates to the local one as
\[ \mathbf{u}_{\xi j}(i) = \mathbf{e} \cdot \mathbf{u}_{\xi j}(i), \quad \mathbf{u}_{\zeta j}(i) = \mathbf{e} \cdot \mathbf{u}_{\zeta j}(i), \]  
(14)

where \( \mathbf{u}_{\xi j}(i), \mathbf{u}_{\zeta j}(i) \) are the relative velocities operating in the normal direction to the contacting surfaces as shown on Fig. 1, and \( \mathbf{u}_{\xi j}(i) = \left[ \mathbf{u}_{\xi j}(i), \mathbf{u}_{\zeta j}(i) \right], \mathbf{u}_{\zeta j}(i) = \left[ \mathbf{u}_{\zeta j}(i), \mathbf{u}_{\zeta j}(i) \right] \) denote vectors of the relative velocities acting in the tangential direction (rotated by \( \frac{\pi}{2} \) to the normal). Additionally we use the same translation as presented by expression (14) for calculations \( \omega'_i = \mathbf{e} \cdot \omega_i, \quad \omega'_j(i) = \mathbf{e} \cdot \omega_j(i) \) in order to obtain the angular velocities for particles \( i \) and \( j(i) \) in the local system of coordinates \( (\xi, \eta, \zeta) \).

If a collision between a particle and a wall takes place, the overlap is defined as
\[ \left\| \eta^b_{j(i)} \right\| = r_i - \left\| \mathbf{x}_{\eta j(i)} - \mathbf{x}_i \right\|, \]  
(15)

and also we have
\[ \left\| \eta^b_{j(i)} \right\| = 2 \sqrt{\frac{1}{2} \left( 2r_i - \left\| \zeta^b_{j(i)} \right\| \right)} \]  
(16)

which is valid for \( \left\| \zeta^b_{j(i)} \right\| \geq 0 \). In this case the point of application \( \mathbf{c}^b_{j(i)} \) is defined by the following formula
\[ \mathbf{c}^b_{j(i)} = \mathbf{x}_i \left( r_i - \frac{5}{8} \left\| \zeta^b_{j(i)} \right\| \right) + \mathbf{e}^b_{j(i)}, \]  
(17)

where
\[ \mathbf{e}^b_{j(i)} = \frac{\mathbf{x}_{\eta j(i)} - \mathbf{x}_i}{\mathbf{x}_{\eta j(i)} - \mathbf{x}_i} \]  
(18)

becomes a normal unit vector which is perpendicular to the wall. When a particle-wall collision begins we obtain \( \mathbf{c}^b_{j(i)} = \mathbf{x}_i + r_i \mathbf{e}^b_{j(i)} \). Moreover, one can find the explicit time \( t^b_{j(i)} \) when the overlap is zero. Expressions (9)–(14), defined for a particle-particle collision, may be redefined in simple way for a particle-wall collision when \( \dot{x}_j(i) \) and \( \omega_j(i) \) are zeros and unit vectors are also redefined as explained in previous considerations.

For example a component of the branch vector (11) is redefined for a particle-wall collision and takes the following form
\[ \left\| \mathbf{u}^b_{j(i)} \right\| = r_i - \frac{5}{8} \left\| \mathbf{z}_{j(i)} \right\|. \]  
(19)

We neglect here any additional expressions necessary to describe the particle-wall collision. The reader can do this very easily in the same way as explained previously.

Summarising our considerations, we introduced the above mathematical description which is necessary for the formulation of the motion equations and is also necessary for some forms of the repulsive force, acting for both particle-particle and particle-wall collisions.

**B. Motion equations**

The molecular dynamics method requires a discrete deterministic approach in order to the model motion of an individual particle. Note that the particle may collide or lose contact with other particles. Therefore in motion equations we need to add or reject some forms of the repulsive force and/or the attractive force in order to simulate the particle dynamics more realistically. In this paper we neglect the attractive force and we will concentrate only on the repulsive force. Against this background, let us describe the motion of an individual particle by the following two sets of equations
\[ \begin{align*}
\mathbf{m}_i \ddot{x}_i &= \sum_l \mathbf{F}_l \\
\mathbf{J}_i \omega_i &= \sum_l \mathbf{M}_l
\end{align*} \]  
(20)

suitable for particle motion without any collision, and
\[ \begin{align*}
\mathbf{m}_i \ddot{x}_i &= \sum_{j(i),j(i) \neq i} \mathbf{P}^\text{coll}_{j(i)} + \mathbf{P}^\text{coll}_{j(i) \neq i} + \sum_l \mathbf{F}_l \\
\mathbf{J}_i \omega_i &= \sum_{j(i),j(i) \neq i} \mathbf{M}^\text{coll}_{j(i)} + \sum_l \mathbf{M}_l
\end{align*} \]  
(21)

which takes into account multiparticle collisions. The above sets of equations exist simultaneously over time and are dependent on the detection of a contact and the administration of the repulsive force-overlap path during the contact. In both Eqs. (20) and (21) \( \mathbf{F}_l \) denotes an arbitrary force which extorts the motion of a particle, \( \mathbf{M}_l \) is an arbitrary torque, \( \mathbf{P}^\text{coll}_{j(i)} \) is a collisional force composed of the repulsive and friction forces and acts between a pair of colliding particles, \( \mathbf{F}^\text{coll}_{j(i)} \) is also the collision force operating on a particle-wall collision, \( \mathbf{M}^\text{coll}_{j(i)} \) and \( \mathbf{M}^\text{coll}_{j(i) \neq i} \) are collisional torques definitively operating on particle-particle and particle-wall collision.

We need to define some of the criteria necessary for handling the above two sets of equations over the time of
the calculations. It was evidently shown in the previous subsection that for the beginning of a collision the overlap given by expression (13) or (14) is zero. Thus we have the impact phase. However, some of the criteria for determining when the collision ends are unclear. Correctly predicting the separation time of two colliding particles is crucial in the calculation. Most papers assume the particles separate at the time when the overlap returns to zero. As proved in [35], the repulsive force changes direction at the time when the overlap returns to zero. This is contrary to experimental evidence, also shown and compared with some models in [35], when the force does not change direction. An attractive force operating in opposite direction to the repulsive force has different origins and is not taken into account here.

At this crucial point of our considerations, we need to introduce some definitions in order to predict correctly the beginning time of a particle collision and the time when the collision ends. Let us consider the time of calculations $t \in (0, T)$ where $T$ represents the total time in which the calculations are performed. We also define the time step $\Delta t$ in which we trace the system dynamics. Follow on from previous explanations we start with some conditions.

**Definition 1** If, within a time interval $(t, t + \Delta t)$ detects the beginning of a collision between a pair of particles is detected then the overlap (14) should fulfill the following conditions

$$\left\| \mathbf{\zeta}(t) \right\| \leq 0 \quad \text{and} \quad \left\| \mathbf{\zeta}(t + \Delta t) \right\| \geq 0$$

and therefore

$$\left\| \mathbf{\zeta} \left( t_{b}^{b(i)} \right) \right\| = 0,$$  \hspace{1cm} (22)

and then time $t_{b}^{b(i)} \in (t, t + \Delta t)$ is the time when the collision starts.

**Definition 2** If, within a time interval $(t, t + \Delta t)$ the end of a collision is formed then the overlap (14) and the normal component of the repulsive force $R_{\zeta j(i)}$ should fulfill the following conditions

$$\left\| \mathbf{\zeta}(t) \right\| \geq 0 \quad \text{and} \quad \left\| \mathbf{\zeta}(t + \Delta t) \right\| \leq 0$$

and $R_{\zeta j(i)}(t) > 0$ and $R_{\zeta j(i)}(t + \Delta t) > 0$ \hspace{1cm} (23)  

and therefore

$$\left\| \mathbf{\zeta} \left( t_{e}^{e(i)} \right) \right\| = 0,$$

and then time $t_{e}^{e(i)} \in (t, t + \Delta t)$ is the time when the collision ends.

In formulae (22) and (23) $R_{\zeta j(i)}$ represents a normal component of the repulsive force. In the next subsection we will introduce a definition of this force.

**Definition 3** If, within a time interval $(t, t + \Delta t)$ the overlap and the normal component of the repulsive force $R_{\zeta j(i)}$ behave as follows

$$\left\| \mathbf{\zeta}(t) \right\| > 0 \quad \text{and} \quad \left\| \mathbf{\zeta}(t + \Delta t) \right\| > 0$$

and $R_{\zeta j(i)}(t + \Delta t) \to 0^{+},$

then time $t_{e}^{e(i)} = \Delta t + t$ is the time when the collision ends.

**Definition 4** When the condition (24) is fulfilled then linear and rotational components (14) of the relative velocity predict the following states after the collision:

- rebound of particles without particle deformations for $\mathbf{u}_{\zeta j(i)}^{lin} \left( t_{e}^{e(i)} \right) \neq 0$ and $\mathbf{u}_{\zeta j(i)}^{lin} \left( t_{e}^{e(i)} \right)$ has an opposite direction (sign) to $\tilde{\mathbf{u}}_{\zeta j(i)}^{lin} \left( t_{b}^{b(i)} \right)$,

- torsion for $\mathbf{\omega}_{\zeta j(i)} \left( t_{e}^{e(i)} \right) - \mathbf{\omega}_{\zeta j(i)} \left( t_{e}^{e(i)} \right) \neq 0$ or sliding for $\tilde{\mathbf{u}}_{\zeta j(i)}^{lin} \left( t_{e}^{e(i)} \right) \neq 0$ or rolling for $\tilde{\mathbf{u}}_{\zeta j(i)}^{rot} \left( t_{e}^{e(i)} \right) \neq 0$

- non-permanent or permanent stick of particles without particle deformations for $\tilde{\mathbf{u}}_{\zeta j(i)}^{lin} \left( t_{e}^{e(i)} \right) = 0$, and for $\tilde{\mathbf{u}}_{\zeta j(i)}^{rot} \left( t_{e}^{e(i)} \right) = 0.$

**Definition 5** When the condition (24) is fulfilled then components (14) of the relative velocity predict the same states as described by definition 4 but particle deformations are noted.

**Definition 6** When the condition (24) is fulfilled then the normal component $\tilde{\mathbf{u}}_{\zeta j(i)}^{lin} \left( t_{e}^{e(i)} \right)$ of the relative velocity (14) predicts adhesion-induced plastic deformations of particles or breakage of particles depending on the hardness of the contacting surfaces.

On the base of previous assumptions and definitions 1 and 2 we introduce the collisional time between a pair of contacting particles as $t_{\text{coll}} = t_{e}^{e(i)} - t_{b}^{b(i)}$. This time is determined by conditions (22) and (23) simultaneously. In other words, when the overlap changes sign faster than the repulsive force changes direction or vice versa then the collision is finished. If particles are still in contact then the total contact time is significantly greater than the collisional time. If particles are separated then the total contact time equals the collisional time. As presented in the first section, the collisional process composes the impact phase, the contact phase and the last phase formed after the contact phase. Moreover, when the formulation of the first and the last phases is infinitesimally short in time then the collisional time is predicted.
by the contact phase. The contact phase is predicted by the repulsive force-overlap path. The adhesion or cohesion states extend the contact phase over time to infinity. In our approach adhesion and cohesion are eventually formed after the impact and they represent completely different phenomena which definitely result from the collision process. Generally, when we model impact dynamics we need to consider the balance between the repulsive force which is a direct reaction to the impact, and the attractive forces which are a result i.e. cohesion of particles. Therefore, our collisional time \( \tau_{j(i)} \) also becomes the time of relaxation in which the collision process is stopped and novel states are formed. Most papers neglect this fact and identify the total contact time, which may increase to infinity, as the collisional one.

Extending our considerations we notice that definition 4 is suitable for the elastic collisions of particles because there are no deformations in contacting particles - the overlap tends to zero faster than the repulsive force changes direction. In definition 5 we observe the opposite situation - the repulsive force changes direction faster than the overlap tends to zero. In our approach the collision process is fully controlled by the repulsive force except for the situation presented by formula (25) in definition 3. On the basis of definition 6, which results from definition 3, we are able to explain that the local stresses associated with deformations of contacting particles become sufficiently large so as to exceed the elastic limit of the materials to a result plastic flow occurs and the behaviour of particle adhesion differs from that predicted by the elastic deformation theory. Adhesion-induced plastic deformations of contacting materials are evidently shown in some experiments. Therefore we have two possible states resulting from the impact: particle clusterisations when the colliding materials are soft, and fragmentation of particles when the colliding materials are hard.

Summarising this subsection we formulated two general forms of the motion equations and discussed precisely how to handle them.

C. Collisional forces, collisional torques and the fractional interaction law

With regard to motion equations we introduce a mathematical description of the collisional forces and torques occurring in such a system. In the normal direction to the contacting surfaces we apply only a repulsive force, completely neglecting any attractive forces. In one can find some forms of attractive forces and their physical meanings. In a tangential plane we introduce a system of friction forces and torques. According to the friction mechanism, the tangential friction force is one of four types: torsion with sliding friction, sliding friction, rolling friction or static friction. Torsion friction occurs when colliding particles differ by their angular velocities in the normal direction \( \omega_{\xi j(i)} \) and \( \omega_{\zeta j(i)} \). Torsion with sliding friction is for colliding particles which have different angular velocities in the normal direction and different linear velocities in the tangential plane. Sliding friction happens when slipping occurs in colliding particles. When the relative linear velocity of the particles in the tangent direction reduces to zero, sliding friction is replaced by rolling friction. If the external forces are sufficiently small, the rolling friction reduces the velocity until particle motion stops and static friction occurs. Considering the impact dynamics, we implemented the following mechanism in general form: torsion with sliding friction can change to rolling friction and the rolling friction tends to static friction. More details concerning the modelling of torsion, sliding and rolling friction can be found in. Here we show a description of the collisional force in global coordinates \((x, y, z)\) as

\[
P_{j(i)}^{\text{coll}} = \begin{cases} P_{j(i)}^{\text{sta}} & \text{for } \|\mathbf{u}_{\text{lin}}^{\text{fin}}\|_j - \|\mathbf{u}_{\text{rot}}^{\text{rot}}\|_j = 0 \\ P_{j(i)}^{\text{rol}} & \text{for } \|\mathbf{u}_{\text{lin}}^{\text{fin}}\|_j - \|\mathbf{u}_{\text{rot}}^{\text{rot}}\|_j = 0 \\ P_{j(i)}^{\text{sli}} & \text{for } \|\mathbf{u}_{\text{lin}}^{\text{fin}}\|_j - \|\mathbf{u}_{\text{rot}}^{\text{rot}}\|_j > 0 \end{cases} \quad (26)
\]

where \( P_{j(i)}^{\text{sta}} \) is the force acting in a static friction state, \( P_{j(i)}^{\text{rol}} \) is the force occurring in a rolling state and \( P_{j(i)}^{\text{sli}} \) is the force coupling the torsion-sliding state. The emphasis in this paper is on the impact dynamics the static friction is only implemented in a simple form. A more detailed model of the static friction state requires analysis of the tangential displacement and possibly the inclusion of time dependent effects. According to Fig. 4 we need to define the collisional force in the local system of coordinates \((\xi, \eta, \zeta)\). Using a matrix of the base vectors we introduce transition from the local system to the global ones as

\[
P_{j(i)}^{\text{sli}} = \mathbf{e}_j^{\text{t}}(i) \cdot P_{j(i)}^{\text{sli}}(i), \quad P_{j(i)}^{\text{rol}} = \mathbf{e}_j^{\text{t}}(i) \cdot P_{j(i)}^{\text{rol}}(i), \quad (27)
\]

where \( P_{j(i)}^{\text{sli}}(i) \) and \( P_{j(i)}^{\text{rol}}(i) \) are forces defined in the local system of coordinates as

\[
P_{j(i)}^{\text{sli}} = \begin{bmatrix} T_{\xi j(i)}^{\text{sli}} \\ T_{\eta j(i)}^{\text{sli}} \\ -R_{\zeta j(i)}^{\text{sli}} \end{bmatrix}, \quad P_{j(i)}^{\text{rol}} = \begin{bmatrix} T_{\xi j(i)}^{\text{rol}} \\ T_{\eta j(i)}^{\text{rol}} \\ -R_{\zeta j(i)}^{\text{rol}} \end{bmatrix}. \quad (28)
\]

In expression \( T_{\xi j(i)}^{\text{sli}}, T_{\eta j(i)}^{\text{sli}}, T_{\xi j(i)}^{\text{rol}}, T_{\eta j(i)}^{\text{rol}} \) represent components of the friction force in a plane \((\xi, \eta)\) for torsion-sliding and rolling states, \( R_{\zeta j(i)}^{\text{sli}} \) is a sum of the normal components of attractive and repulsive forces operating during a collision. As assumed in this paper, we neglect attractive forces and concentrate only on forms of the repulsive force. Some forms of the attractive forces can be found in but the most well-known forms of the repulsive force are in. On the basis of preliminary results we now introduce a model of the repulsive force in general form called the fractional interaction law. Thus we have...
\[
R_{\xi_j(i)} = \begin{cases} 
\max \left[ 0, c_{j(i)} k_{j(i)} \xi_j(i) \right] & \text{for } \xi_j(i) \geq 0 \\
0 & \text{for } \xi_j(i) < 0 
\end{cases}
\]

where \(c_{j(i)}\), \(k_{j(i)}\) are damping and spring coefficients with the same meaning as in the linear interaction law \[4\], \(\|\xi_j(i)\|\) represents the overlap defined by formula \[9\], \(t^b_{j(i)}\), \(t^e_{j(i)}\) are start and stop times of a collision (not a total contact) predicted by several definitions in the previous subsection, as explained in \[12\] \(\alpha_{j(i)}\) is the conversion degree of impact energy into viscoelasticity of the material and \(\nu_{j(i)} D^{\alpha_{j(i)}}_{\cdot j(i)} \left(\|\xi_j(i)\|\right)\) represents general form of the differential and integral operator of fractional order. According to fractional calculus \[23\] \[31\] we introduce the definition of this operator in the following form

\[
\nu_{j(i)} D^{\alpha_{j(i)}}_{\cdot j(i)} \left(\|\xi_j(i)\|\right) = \begin{cases} 
\sum_{t=b}^{n-1} \frac{(t-t^b_{j(i)})^{\alpha(j(i))}}{\Gamma(t-\alpha_{j(i)}+1)} \|\xi_j(t)\| + \nu_{j(i)} D^{\alpha_{j(i)}}_{\cdot j(i)} \left(\|\xi_j(t)\|\right) & \text{for } \alpha_{j(i)} \geq 0 \\
\nu_{j(i)} D^{\alpha_{j(i)}}_{\cdot j(i)} \left(\|\xi_j(t)\|\right) & \text{for } \alpha_{j(i)} < 0 
\end{cases}
\]

where \(t\) denotes actual time of calculations \(t \in (t^b_{j(i)}, t^e_{j(i)})\), the sum represents the initial conditions,

\[
\nu_{j(i)} D^{\alpha_{j(i)}}_{\cdot j(i)} \left(\|\xi_j(t)\|\right) = \begin{cases} 
\frac{1}{\Gamma(n_{j(i)}-\alpha_{j(i)})} \int_{t^b_{j(i)}}^{t} \frac{d^{\alpha_{j(i)}}_{\cdot j(i)}}{(t-\tau)^{n_{j(i)}-\alpha_{j(i)}}+1} \|\xi_j(t)\| d\tau & \text{for } n_{j(i)}-1 < \alpha_{j(i)} < n_{j(i)} \\
\frac{1}{\Gamma(\beta_{j(i)})} \int_{t^b_{j(i)}}^{\nu_{j(i)}} \frac{d^{\beta_{j(i)}}_{\cdot j(i)}}{(t-\tau)^{\beta_{j(i)}-1}} \|\xi_j(t)\| d\tau & \text{for } \beta_{j(i)} \in \mathbb{R}^+ \\
\frac{1}{\Gamma(\beta_{j(i)}-1)} \int_{t^b_{j(i)}}^{\nu_{j(i)}} \frac{d^{\beta_{j(i)}-1}_{\cdot j(i)}}{(t-\tau)^{\beta_{j(i)}-1}} \|\xi_j(t)\| d\tau & \text{for } \beta_{j(i)} \in \mathbb{N} 
\end{cases}
\]

where \(n_{j(i)} = [\alpha_{j(i)}] + 1\) and \([\cdot]\) denotes an integer part of a real number, and \(\nu_{j(i)} D^{\alpha_{j(i)}}_{\cdot j(i)} \left(\|\xi_j(t)\|\right)\) is the Riemann-Liouville fractional integral.

and \(\beta_{j(i)} = -\alpha_{j(i)}\). Eqn. \[32\] represents the form of the repulsive force acting in the normal direction to the contacting surfaces.

Now we introduce additional definitions of forces operating in the tangent plane. Here we define the normal force as \(N_{\cdot j(i)} = [0, 0, R\xi_j(i)]\). According to \[2\] we define the friction force which is coupled between torsion-sliding friction as

\[
T'_{\cdot j(i)} = -\mu \left(\|n'_{\cdot j(i)}\|\right) F(\lambda_{j(i)})
\]
where the friction coefficient is
\[
\mu \left( \| \mathbf{u}'_{j(i)} \| \right) = \mu_d + (\mu_s - \mu_d) e^{-a \| \mathbf{u}'_{j(i)} \|},
\]
where \( a \) is a numerical constant, \( \mu_s \) and \( \mu_d \) are static and dynamic coefficients of friction. Moreover in formula (33) the function \( \mathcal{F}(\lambda_{j(i)}) \) is defined according to (35) as
\[
\mathcal{F}(\lambda_{j(i)}) = \begin{cases} 
\frac{\lambda_{j(i)}^2 + 1}{\lambda_{j(i)}} & \text{for } \lambda \leq 1 \\
\frac{\lambda_{j(i)}^2 + 1}{\lambda_{j(i)}} - 1 & \text{for } \lambda > 1
\end{cases}
\]
where \( K(\lambda_{j(i)}) \) and \( E(\lambda_{j(i)}) \) are the complete elliptic integral functions of the first and the second kind, \( \lambda_{j(i)} \) is the dimensionless quantity defined as
\[
\lambda_{j(i)} = \frac{\| \mathbf{u}'_{j(i)} - \mathbf{a}'_{j(i)} \|}{\| \eta_{j(i)} \| \| \omega_{\xi} - \omega_{\xi j(i)} \|}.
\]

The limiting values of the function \( \mathcal{F}(\lambda_{j(i)}) \) are \( \mathcal{F}(0) = 0 \) for torsion without sliding and \( \lim_{\lambda_{j(i)} \to \infty} \mathcal{F}(\lambda_{j(i)}) = 1 \) for sliding without torsion.

According to (36) we define the rolling friction force as
\[
T'_{j(i)} = \frac{1}{m_i + \frac{1}{m_{j(i)}} \| \mathbf{j}_{j(i)} \|^2 + \| \eta_{j(i)} \|^2 \| \mathbf{r}_{j(i)} \|^2} \left( \frac{1}{J_i} \mathbf{ss}_{j(i)} \times \mathbf{N}_{j(i)} \times \mathbf{s}_{j(i)} - \frac{1}{J_{j(i)}} \mathbf{ss}_{j(i)} \times \mathbf{N}_{j(i)} \times \mathbf{s}_{j(i)} + \mathbf{A}_{j(i)} \right),
\]
where
\[
\mathbf{ss}_{j(i)} = \begin{bmatrix} \| \eta_{j(i)} \| \| \mathbf{u}'_{j(i)} \| \| \mathbf{u}'_{j(i)} \| \| \mathbf{a}'_{j(i)} \| \| \mathbf{a}'_{j(i)} \| \end{bmatrix}.
\]

The above expressions are necessary for the definitions of some collisional torques. Therefore we have the collisional torque operating from particle \( i \) to particle \( j(i) \) as
\[
M^\text{coll}_{i,j(i)} = \begin{cases} 
0 & \text{for } \| \mathbf{u}'_{j(i)} \| = \| \mathbf{u}'_{j(i)} \| = 0 \\
M^\text{rot}_{i,j(i)} & \text{for } \| \mathbf{u}'_{j(i)} \| - \| \mathbf{u}'_{j(i)} \| = 0 \\
M^\text{slip}_{i,j(i)} & \text{for } \| \mathbf{u}'_{j(i)} \| - \| \mathbf{u}'_{j(i)} \| > 0
\end{cases}
\]
where \( M_{i,j}^{sl}(k) \) is the coupled torsion-sliding torque, \( M_{i,j}^{rol}(k) \) represents the coupled torsion-rolling torque. Note that transition from the local system of coordinates to the global ones reads

\[
M_{i,j}^{sl}(k) = e^{T}_{j}(k) \cdot \left( \dot{M}_{i,j}^{sl}(k) + \dot{M}_{i,j}^{tor}(k) \right),
\]

\[
M_{i,j}^{rol}(k) = e^{T}_{j}(k) \cdot \left( \dot{M}_{i,j}^{rol}(k) + \dot{M}_{i,j}^{tor}(k) \right).
\]

We define the torsion torque as \( \dot{M}_{i,j}^{tor}(k) = \left[ 0, 0, M_{i,j}^{tor}(k) \right]^T \)

and according to [3] we obtain

\[
M_{i,j}^{tor}(k) = -\frac{1}{2} \mathcal{T} \left( \lambda_{i,j}(k) \right) \| \eta_{j}(k) \| \mu \left( \| \tilde{\omega}_{i,j}(k) \| \right),
\]

where the function \( \mathcal{T} \left( \lambda_{j}(k) \right) \) reads

\[
\mathcal{T} \left( \lambda_{j}(k) \right) = \begin{cases}
\frac{1}{9} (4-2\lambda_{j}(k)) E \left( \lambda_{j}(k) \right) + (\lambda_{j}(k)-1) K \left( \lambda_{j}(k) \right) & \text{for } \lambda_{j}(k) \leq 1 \\
\frac{1}{9} (4-2\lambda_{j}(k)) E \left( \frac{1}{\lambda_{j}(k)} \right) + \left( 2\lambda_{j}(k)-5 + \frac{3}{\lambda_{j}(k)} \right) K \left( \frac{1}{\lambda_{j}(k)} \right) & \text{for } \lambda_{j}(k) > 1
\end{cases}
\]
where \( \alpha \in \mathbb{R}^+ \), \( n = [\alpha] + 1 \) and \([\cdot]\) denotes an integer part of a real number, \( A_i = f^{(n)}(t_i) \) where \( f^{(n)} \) is the derivative of integer order \( n \). Note that in formula (46) \( f(t) \) denotes the overlap \( C \). Taking the above assumptions into account we obtain the discrete form of the Riemann-Liouville fractional integral \( \mathcal{D}_t^\alpha f(t) \) as

\[
t_{n} T_{t_{n}}^{\alpha} f(t) = \frac{1}{\Gamma(\alpha + 1)} \left[ A_1 (t_n - t_0)^{\alpha} + \sum_{i=2}^{nt} (A_i - A_{i-1}) (t_n - t_{i-1})^{\alpha} \right], \tag{47}
\]

where \( \beta \in \mathbb{R}^+ \) and \( B_i = f(t_i) \). The Discrete forms of the fractional operators makes it possible to integrate the system (21) by using any predictor-corrector procedure [20] with correction of the time step \( h \). The correction of the time step provides measures that allow us to determine the begin time when particles enter into a collision and the end time of particle collisions. It should be noted that the begin and end times are determined by several definitions presented in the previous section.

Taking formulae (20), (40) into account in calculations of particle contacts we need to find an accurate time needed to detect the switching between torsion-sliding, sliding and rolling processes. As described in the paper [20], a simple way to calculate the switching time is to use a linear approximation method.

Next we consider a problem occurring in the calculations of friction forces [26], [30] and the torsional torque [12]. When the relative velocity at the contact point changes from negative to positive or from positive to negative, it indicates that the signum function \( \text{sign}(x) \) changes sign very fast in above expressions. This is not desirable as it influences the stability and convergence of the numerical calculations in a significant way. Therefore we modified the signum function introducing

\[
\text{sign}(x) = \begin{cases} 
-1 & \text{for } x \leq -\epsilon_2 \\
\frac{x - \epsilon_1}{\epsilon_2 - \epsilon_1} & \text{for } -\epsilon_2 \leq x \leq -\epsilon_1 \\
0 & \text{for } -\epsilon_1 \leq x \leq \epsilon_1 \\
\frac{x - \epsilon_1}{\epsilon_2 - \epsilon_1} & \text{for } \epsilon_1 \leq x \leq \epsilon_2 \\
1 & \text{for } x \geq \epsilon_2
\end{cases}, \tag{48}
\]

where \( x \) is the actual value registered during a contact (the relative velocity), \( \epsilon_1, \epsilon_2 \) are numerical coefficients. This function is robust for \( x \to 0 \) and gives a satisfactory result.

IV. RESULTS AND THEIR ANALYSIS

To illustrate the benefits of the fractional interaction law [29] in the dynamics of arbitrary multiparticle collisions, first we will demonstrate how this law operates in simple cases connected with one dimensional problem. First we will simulate a central collision between two particles. Fig. 2 shows the dynamics of a two-particle collision, which is represented by some variations in the overlap \( ||C|| \) (1), the linear relative velocity \( \zeta = \dot{u}^{lin}_{\zeta} \) (14) and the repulsive force \( R_{\zeta} \) (20) over time for different levels of the conversion degree \( \alpha \). Here we neglect the index \( j(i) \) because only two particles collide. Moreover, all vectors are converted to scalar values when a one dimensional problem is considered. For the figure we have \( m_{eff} = \frac{m_1 m_2}{m_1 + m_2} = 7.06858 \cdot 10^{-6} \text{kg}, r_1 = r_2 = 3 \cdot 10^{-3} \text{m}, k = 5000 \frac{N}{m}, c = 0.1 \text{kg/s} \). The initial relative velocity is set at \( \zeta = 0.5 \frac{m}{s} \) and three groups of variations in the conversion degree are taken into account. The first group is for \( \alpha < 0 \) (left column), the second is for \( 0 \leq \alpha \leq 1 \) (middle column) and the third represents \( \alpha > 1 \) (right column). Within the range \( 0 \leq \alpha \leq 1 \) we observe that collisional time \( t_c \) increases when \( \alpha \) is increased. It should be noted that the collisional time is registered when the repulsive force \( R_{\zeta} \) reaches zero, as presented in several definitions in the previous sections. Therefore, the overlap \( ||C|| \) has some values at the time when a collision ends and deformations of the particle surfaces are noted. Analysing the behaviour of the relative velocity \( \zeta \) over time we notice that this velocity changes direction for small values of \( \alpha \), which means that particle rebounds dominate. When \( \alpha \) increases we can see that the relative velocity tends to zero, which means that particles stick together. In other words, if \( \alpha = 0 \), no viscous term in Eqn. (20) may occur and all the impact energy must be due to elasticity. In this case the overlap reaches zero at the same time as the repulsive force reaches zero. If \( \alpha = 1 \), on the other hand, the impact energy is transferred.
FIG. 2: Behaviour of the overlap (top), relative velocity (middle) and force (bottom) over time for the fractional interaction law.

Extending our considerations for $\alpha > 1$ we observe (right column on Fig. 2) that the repulsive force is not generated and tends to zero for $t_c \to \infty$, and therefore the overlap increases to high and unrealistic values. Moreover, the relative velocity does not change direction and particles undergo the next time steps of the calculations. According to definition 6, presented in the previous section, the fragmentation of particles or permanent cohesion of particles is a direct result of the plastic flow of their contacting surfaces. The contacting surfaces are destroyed because deformations of contacting particles become sufficiently large so as to exceed the elastic limit of the materials, and we noticed particle clusterisations. This process is observed experimentally in [12, 28], and may be modelled by the fractional interaction law [20].

Next we considered the behaviour of the overlap, relative velocity and repulsive force for $\alpha < 0$ (left column on
Larger negative values of the conversion degree $\alpha$ decreases the collisional time. The relative velocity changes direction but at the end time reaches larger absolute values in comparison to the initial relative velocity. As this is unrealistic all the solutions for $\alpha < 0$ are not taken into account. The aim of this example is to show the power of fractional calculus where more solutions are obtained in comparison to classical differential and integral operators having integer order. However, we need to choose which solutions obtained by fractional calculus are suitable physically.

In Fig. 3 we constructed several mappings for the relative velocity-overlap (left), force-overlap (middle) and force-relative velocity (right) where $\alpha$ changes from negative to positive values. Analysing these mappings we found a set of criteria necessary to predict different states of particle collisions included in definitions in the previous section. It should be noted that small positive values of $\alpha$ predict particle rebounds when particle deformations are practically neglected. When $\alpha$ tends to unity we also observe particle rebounds but particle deformations are visible and more energy is dissipated. As indicated in the left chart in Fig. 3 when $\alpha$ is above unity the repulsive force is not generated and this indicates instability in particle collisions. This instability takes the form of particle fragmentation or permanent clusterisation of particles after the collision. Therefore the conversion degree $\alpha$ is a ratio of the impact energy over the specific energy needed for the destruction of particle surfaces. This assumption should be validated experimentally, and this is the aim of our future investigations. Note that when the physical properties of colliding granular materials and the impact energy are fixed we still observe different values of energy dissipation after the collision. This can be easily seen when we compare the particle collisions for smooth surfaces of particles and for rough ones. The fractional interaction law can simulate this because the conversion degree $\alpha$ can change.

In order to compare the fractional interaction law with other interaction laws, changes over time of the overlap, the relative velocity and the repulsive force for two-particle collision were presented. We assumed parameters of colliding particles to be $r_1 = r_2 = 3 \times 10^{-3} m$, $m_{eff} = 7.06858 \cdot 10^{-6} kg$, $\zeta = 0.5 \frac{m}{s}$. Moreover, we assumed the collision time between two colliding bodies the $t_c = 10^{-4} s$ and the restitution coefficient $e_r = 0.5$. These assumptions are necessary to calculate the set of coefficients required by different interaction laws, depending on the type of interaction law chosen. In Table I we list all the coefficients. Some of the expressions applied to calculate the coefficients for linear [13] and hysteretic [33] laws can be found in [25]. The formulae of the coefficients used in the linear interaction law assumed that at the end time of a collision the overlap is zero. In Table I the “linear1” represents the above case. We assumed that the repulsive force reaches zero at the end time of a collision. Thus we have a set of coefficients called “linear2” also used for the linear interaction law. For the non-linear [15] and fractional laws we performed a numerical test to find the values of coefficients which allow us to keep the assumed collision time and the restitution coefficient in a two-particle contact. It should be noted that we obtained many sets of coefficients for the fractional interaction law. Therefore for this law we establish the spring coefficient which has the same value as for the linear interaction law. Fig. 4 shows the behaviour of the overlap (top chart), the relative velocity (middle chart) and the repulsive force (bottom chart) over time where different interaction laws are taken into account. Analysing this figure we can confirmed that the interaction law fulfilled our assumptions concerning the collisional time and the restitution coefficient. It should be noted that the repulsive force changes direction in the linear interaction law (linear1) for the set of coefficients calculated under the formulae found in [25]. This shows a deficiency in numerical calculations and should be rejected. Some changes in the values of the above coefficients give satisfactory results in the linear interaction law (linear2). However, the repulsive force in the linear interaction law has a value at the beginning time which is independent on the set of coefficients used. This is also unrealistic behaviour in the linear law.

Using different interaction laws we observed different overlaps at the end time of a collision. The highest value of overlap is for the hysteretic law and decreases for the fractional through the non-linear to the linear one. Note that for the fractional law we can find another set of coefficients in order to fulfil our assumptions and to obtain another value of the overlap at the end time of collision. When we determine all parameters necessary to describe the dynamics of particle impacts then we obtain some values of the collisional time and the restitution coefficient for this case. However when we still keep the above parameters and increase or decrease the surface roughness of colliding particles then we obtain values of the collisional time and the restitution coefficient differing in comparison to the previous values. As we did not change physical properties of this granular material therefore we have to save the steady value of the spring coefficient in all interaction laws. Changing only the damping coefficient in the linear and non-linear laws and the unloading slope $k_2$ in the hysteretic law we do not have any guarantee that we will obtain accurate values of the col-
FIG. 3: Mapping the relative velocity-overlap (left), force-overlap (middle) and force-relative velocity (right) for the fractional interaction law.

FIG. 4: Comparison of the overlap (top), relative velocity (middle) and force (bottom) over time for different interaction laws.

Collisional time and the restitution coefficient reflecting the above cases. This is a disadvantage of the well-known interaction laws. In the fractional interaction law we have an additional parameter called the conversion degree $\alpha$ which causes some changes in the collisional time and the restitution coefficient. However, this requires some experimental data involving the impact dynamics of smooth and rough particles. These data will provide measures that allow some links to be made between the experiment and the coefficients of the fractional law.

In order to verify the validity of the interaction laws for multiparticle collisions, the energies dissipated at each contact were compared. Here we introduce a measure of energy dissipation during multiparticle collisions which is the ratio of the kinetic energy evaluated in time over the initial kinetic energy. We define the total ratio of energy lost through multiparticle collisions as

$$\varepsilon = 1 - \frac{\sum_{i=1}^{nc} m_i \dot{x}_i^2}{\sum_{i=1}^{nc} m_i^0 (\dot{x}_i^0)^2}, \tag{49}$$

where the superscript 0 refers to the initial kinetic energy examined at time $t = 0$ s and $nc$ is the total number of colliding particles.

We used a set of particles $np$ vertically stacked over a bottom plate as shown in [18, 25]. We assumed the following conditions $r_i = 0.0015 m$, $m_i = 1.41 \cdot 10^{-5} kg$, $\dot{x}_i = -0.5 \frac{m}{s}$, for $i = 1, \ldots, np$. Gravity is set at zero. Taking into account the results presented by [18] we calculated the energy dissipation as a function of the number of considered particles $np$, which becomes the number of colliding particles $nc$ when at the begin time of the collision the distances between spheres equal zero $r_j^0 = 0 m$, for $j = 1, \ldots, nc$. Note that $j = 1$ represents a collision between the first particle and the bottom plate and $j = nc$ is a collision between the topmost particles. We also assume the collisional time between two colliding bodies $t_c = 10^{-4} s$ and the restitution coefficient $e_r = 0.945$. These assumptions are necessary to calculate some coefficients depending on the type of
interaction law chosen. The coefficients represent a collision between two particles or between a particle and the bottom plate, where the plate mass is infinite.

Fig. 5 shows the energy dissipation as being dependent on the number of collisions \( nc \) for different interaction laws used in the molecular dynamics method and also in the event driven method \[1, 22\]. For linear, non-linear and hysteretic laws we noted the same dependencies as in \[15, 22\]. This means that the “detachment” effect occurs. First, we considered the fractional interaction law for a steady value of the conversion degree \( \alpha_{ji} = 0.0258 \), for all binary collisions. In this case we obtained similar results for the hysteretic and fractional interaction laws. Thus the “detachment” effect also occurs in the fractional interaction law for the steady value of \( \alpha_{ji} \). As written in \[15\] the kinetic energy obtained from the event driven technique is dissipated totally for \( nc : (1 - \epsilon_s) \) large. It should be noted that the basic interaction laws are valid for a two-particle collisions which are completely independent of other collisions. However, in multiparticle collisions we need to include mutual dependencies between several binary collisions. Taking this fact into account, we can obtain satisfactory results when the conversion degree \( \alpha_{ji} \) changes in relation to the number of colliding particles. This was explained more precisely in \[15\].

Therefore we propose \( \alpha'(nc) \sim 1 + \exp(-nc) \) in order to keep a qualitative agreement with the event driven method. It should be noted that we cannot estimate correctly \( \alpha'(nc) \) by direct comparison with the event driven technique. We require experimental data involving multiparticle collisions. This data will provide measures that allow some links to be made between several coefficients in the fractional interaction law and the experiment.

The last example simulates the dynamics of five particles in three dimensional space for two values of the parameter \( \alpha \). The first value \( \alpha = 0.01 \) indicates the strong repulsive state, i.e. particles rebound almost without dissipation of their energy. The second one for \( \alpha = 0.97 \) represents the weak repulsive state where most of the impact energy is converted into material viscoelasticity. In the real behaviour of granular materials we can easily observe such states, when we consider the collisions for contacting particles with smooth surfaces and for rough ones. For this simulation we assumed the following conditions \( r_1 = 0.02 \ m, \ r_2 = 0.01 \ m, \ r_3 = 0.007 \ m, \ r_4 = 0.005 \ m, \ r_5 = 0.009 \ m, \ g_1 = g_2 = 2000 \ \frac{kg}{s^2}, \ g_2 = g_3 = g_5 = 1000 \ \frac{kg}{s^2}, \ x_1 = [0.0, 0.1, 0.23] \ m, \ x_2 = [0.001, 0.125, 0.205] \ m, \ x_3 = [-0.002, 0.090, 0.198] \ m, \ x_4 = [-0.004, 0.120, 0.186] \ m, \ x_5 = [-0.001, 0.1, 0.18] \ m \). Moreover, we consider a situation where a particle with an initial linear velocity \( \mathbf{u}_1 = [0, 0, \frac{m}{s}] \) collides at different moments in time with particles which initially do not move \( \mathbf{u}_j = [0, 0, 0 \ \frac{m}{s}] \) for \( j = 2, \ldots, 4 \). Particles do not rotate initially \( (\omega_1 = 0, \frac{1}{s}) \), gravity is set to zero and \( k = 1000 \ \frac{kg}{s}, \ c = 1 \ \frac{kg}{s} \) for each pair of colliding particles. We also simplified values of the friction coefficients putting into Eq. \[34\] \( a = 0 \) and \( \mu_s = 0.5 \) for each pair of colliding particles. Fig. 6 shows the trajectories of the mass centres of five particles in three dimensional space for strong and weak repulsions as a reaction to the impact dynamics. The particles are
numbered from "1" to "5". This simulation does not reflect the real motion of particles because we neglect external forces, i.e. the gravitational force. We can only show how the fractional interaction law operates in the above conditions as being dependent on the conversion degree $\alpha$. In the strong repulsive state ($\alpha = 0.01$) we observe linear particle trajectories. As $\alpha$ is increased and reaches the weak repulsive state ($\alpha = 0.97$) we noticed different particle trajectories in comparison to the previous state. According to the results presented in Fig. 2 we can say that duration over time of the repulsive force, which is longer over time for higher values of $\alpha$, has a significant influence on the particle trajectories.

In order to explain more precisely what happens to particle trajectories in strong and weak repulsive states, the velocities of one individual particle were analysed. Fig. 7 shows in global coordinates $(x, y, z)$ the linear and angular velocities of particle "1" over time. In this figure the dashed lines represent particle velocities in the strong repulsive state, whereas continuous lines indicate the weak repulsive state. We can observe clear jumps in particle velocities over time for the strong repulsive state. This is a result of the duration of a collision determined by the collisional time between a pair of contacting particles. In this state we can notice binary collisions because several collisional times between the different pairs of contacting particles have shortest values in comparison to their separation times, where particles move individually. However, in the weak repulsive state we observe continuous changes in particle velocities without the distinction of any jumps. This means that several collisional times between the pairs of contacting particles overlap each other. The binary collisions are not distinguished here.

Moreover, we analysed, in the local system of coordinates $(\xi, \eta, \zeta)$, the angular velocities over time of particle "1", which collides with the particle "5". In the strong repulsive state we observe smaller values of $\omega_\xi$ and $\omega_\eta$ (these velocities are angular velocities predicted in the tangent plane as shown in Fig. 1) in comparison to the weak repulsive state. This means that torsion-sliding friction dominates in the strong repulsive state, where binary collisions are noted. In the weak repulsive state we observe that the angular velocities $\omega_\xi$ and $\omega_\eta$ have higher values than in the strong repulsive state. Thus we expect
the torsion-rolling state between particles "1" and "5". However multiparticle collisions are noted in the weak repulsive state.

In order to prove where binary or multiparticle collisions occur, some distributions of collisional times over the duration time of calculations are presented. Fig. 8 presents the sequence of segments of collisional times over the time of observation for strong and weak repulsive states. Continuous segments represent collisional times for FIG. 8: Sequence of collisional times depending on strong (\(\alpha = 0.01\)) and weak (\(\alpha = 0.97\)) repulsions.

weak repulsion whereas strong repulsion is denoted by the dashed segments. Each segment represents one binary collision between a pair of contacting particles, i.e. "1"-"3" means the collision between particle "1" and particle "3". Analysing this figure we observe longer collisional times for the weak repulsive state in comparison to the collisional times for the strong repulsive state. Moreover the collisional times overlap in the weak repulsive state, therefore multiparticle collisions occur.

V. CONCLUDING REMARKS

We used the molecular dynamics method to model the motion of individual spherical particles in three-dimensional space. We introduced a novel mathematical description of this method which takes into account the division of the collision process into an impact phase, contact phase and another phase formed after the contact phase. We assumed that the impact phase and the phase formed after the contact phase are infinitesimally short in time. We redefined the collisional time so that it is predicted by the repulsive force-overlap path. The force can control the energy dissipation and the collisional time for an individual particle colliding with many other particles. In multiparticle collisions we included the friction mechanism needed for the transition from coupled torsion-sliding friction through rolling friction to static friction. Therefore our model includes multiparticle collisions in arbitrary forms. Using the fractional interaction law one can determine different states of particle repulsions, i.e. strong and weak repulsive states. In the strong repulsive state binary collisions dominate, and torsion-sliding friction is the main friction mechanism. However, within the multiparticle collisions rolling friction is observed to be much stronger. The presented numerical results can be used to realistically model the impact dynamics of an individual particle in a group of colliding particles. In order to tune the model coefficients we require experimental data involving multiparticle collisions. This data provides measures that allow some links to be made between several coefficients in the fractional interaction law and the experiment.

Acknowledgments

This work was supported by the State Committee for Scientific Research (KBN) under the grant 4 T10B 049 25.

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