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A community detection method for network structure analysis of force chains in granular medium in a rotating drum

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Abstract. We analyze the motion of granular matter in a partially filled drum rotating around the horizontal axis. The motion of granular medium is simulated using the discrete element model (DEM). As the drum rotates, the free surface sloping angle changes periodically as it attains the limit repose angle leading to an avalanche, after which its value is reduced to below the repose angle. Systems of this type are of interest from both theoretical and application viewpoints: similar setups are used in industry, such as rotary kilns and mixers; besides, dynamics of granular matter leads to macroscopic effects, such as segregation and emergence of patterns. Observable macroscopic effects depend largely on the underlying structure of force chains arising from pairwise mechanical contacts between the particles. Discrete element simulations produce the data for each individual particle: position, translational and rotational velocity, force vector between the interacting particle pairs. These data about the microscopic state must be processed to obtain the observable macroscopic states. Particle configurations at each time moment available from DEM simulations can be represented as graphs: each particle is represented as a graph vertex, the vertex pairs are connected by edges if the respective particle pairs are in contact, and the edge weights are proportional to the interaction force. After the graph for a particle state is created, the algorithms of the graph analysis can be applied to analyze the corresponding state of granular matter. Among such algorithms, we use the community detection algorithms to analyse the emergence of force groups among the particles, i.e., the groups of particles that have stronger mechanical forces among the particles in the group than the forces with particles that do not belong to the given group. Such groups are structures of larger scale than the usual force chains. Distribution of group sizes (number of particles belonging to the group) and their positions depend on the rotation velocities of the drum; in turn, they influence the variation of the repose angle and the process of the avalanches. We report the relations between the characteristics of the detected force groups and the observable effects in the granular matter obtained by DEM simulations.

Keywords: discrete element method, granular matter, network theory, graph, community detection.

Introduction

Granular media is a form of matter consisting of multiple solid particles interacting through mechanical forces. This type of media is widely encountered in nature, technology and industry. Besides, the phenomena exhibited by this matter are interested from theoretical point of view and the models developed for its simulation can be applied to problems in various fields.

Mechanical behaviour of granular media is determined by multiple interactions of the constituent particles giving rise to the bulk properties such as compressive stress, flow properties, uneven distribution of particles by their size, density, etc. in moving matter. In theoretical analysis, the most detailed information is provided by simulations based on the discrete element model (DEM) (Džiugys & Peters, 2001). These simulations provide the data of each individual particle i at certain time moments: the position (coordinate) $\mathbf{x}_i$, linear velocity $\mathbf{v}_i$, angular velocity $\mathbf{w}_i$, force of mechanical interaction $\mathbf{F}_{ij}$ between the particles i and j. Other parameters can be included in simulations depending on the particular task, e.g., the particle temperature, structural composition (Peters, Džiugys, & Navakas, 2011), etc. The set of these parameters at the time moment t_i provides a "microscopic" state of the simulated matter. However, bulk properties of granular matter, such as density distribution, porosity, pressure forces upon the container walls, repose angle, as well as macroscopic phenomena, such as avalanches, bulk motion, are more accessible in experimental research and observable in practical applications. The relevant set of bulk properties can be thought of as a "macroscopic" granular state.

In order to derive the "macroscopic" properties of granular media from DEM simulations, as well as to gain insight into the mechanisms underlying it, processing of the simulation data is required to identify the larger scale structures. Force chains are among the structures usually encountered when analysing mechanical properties in granular media. The usual approach to identify force chains is to use thresholding that provides the "backbone" of the particulate system consisting of the particles with the strongest interactions. However, this approach neglects the influence of particles exposed to weaker forces that provide the stability for the major force chains against, e.g., buckling (Campbell, 2003). A larger scale structures of interacting particles thus have to be analysed to get a more comprehensive picture of force distributions in a granular pack. The system of the force chains can be understood as a network (Papadopoulos, Porter, Daniels, & Bassett, 2018) for which the appropriate techniques of mathematical graph analysis can be applied. A "community detection" technique of the graph analysis (Fortunato, 2010; Fortunato & Hric, 2016) is a promising approach that has been applied for a number of cases in granular media analysis (Navakas, Džiugys, & Peters, 2010; Basset, Owens, Daniels, & Porter, 2012; Basset, Owens, Porter, Manning, & Daniels, 2015).

Here, we analyse the application of this approach to the problem of varying free surface landscape in a rotating drum partially filled with granular packed bed consisting of a number of spherical particles. Motion of granular media in a rotating drum is an illustrative example as it entails a number of interesting physical phenomena (Dury & Ristow, 1999a, 1999b; Hill, Gioja, Amaravadi, & Winter, 2005; Prigozhin & Kalman, 1998). Among others, evolution of the slope angle (inclination) of the free surface is interesting from the point of view of applications (calculating the repose angle in bulk storage and handling, landslides and avalanches in geomechanics), as well as theoretical and numerical analysis of the underlying structure of forces in the bulk materials leading to avalanches and the observable structure of the free surface. This evolution of the free surface slope is analysed using the DEM data.

Simulation method

The system under consideration is a horizontal drum partially filled with $N_p = 1900$ spherical particles (Figure 1). The particle radii are distributed at random in the range from $r_{\min} = 5\times10^{-4}$ m to $r_{\max} = 10^{-3}$ m. The drum radius is $R = 0.05$ m. For easier visualisation and estimation of results, as well as shorter simulation times, a quasi-2D problem is simulated: the centers of all the particles are located in the same vertical plane xy ($z = 0$), perpendicular to the drum axis, but all the particle parameters, such as volumes, moments of inertia, etc., are calculated for 3D spheres. The analysis, presented below, can be readily applied to the 3D cases. The particle motion was simulated for the time period from $t_0 = 0$ s to $t_f = 100$ s with the time step $\Delta t = 5\times10^{-6}$ s at different angular drum rotation velocities: $V_r = 0.1$; 0.5; 1.0; 5.0; 10.0 rad/s. The particle data were recorded every 2000 iterations, i.e., every 0.01 s. The initial particle positions are such that the free surface of the packed bed is nearly horizontal. As the drum rotates, this angle gradually increases until it reaches a certain value (repose angle) after which either an avalanche starts, or the packed bed slides over the inner surface of the drum, until the free surface angle attains a certain smaller value.

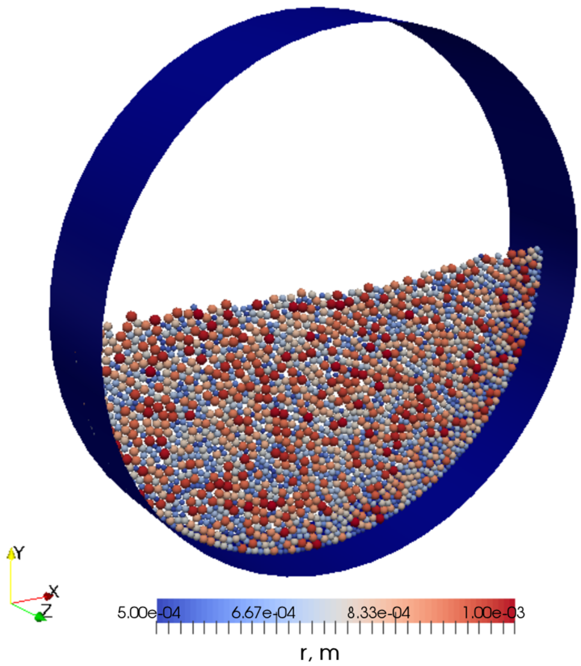


Figure 1. Granular media (spherical particles) in a rotating drum.
The particles are colored according to their radii r

When determining the free surface inclination angle, it was assumed that this surface is sufficiently flat, i.e., it is close to a straight line in the 2D plane where the particle centers are located. The top particles of the bed were identified and their center positions (x_i, y_i) were approximated by a straight line $y_i = kx_i + b$. The angle of the free surface is $\varphi = tan^{-1}(k)$. The particles were considered to be a part of the surface if they were located at the boundary of the packed bed and their distance to the inner surface of the drum was larger than the diameter of the largest particle, $2r_{\max}$ (some particles could be erroneously assigned to the surface in cases when cavities appear in the depth of the bed near the drum surface; the number of such particles was insignificant, therefore, they had negligible influence to determination of the surface angle). Some of the surfaces determined at different time moments and at different drum rotation velocities are shown in Figure 2. At sufficiently large drum rotation velocity, the top particles detach from the main bulk (Figure 2d), therefore, the definition of the free surface in this case becomes vague; the linear fit underestimates the slope angle in these cases. On the other hand, detachment of a large number of particles indicates the onset of the avalanche.

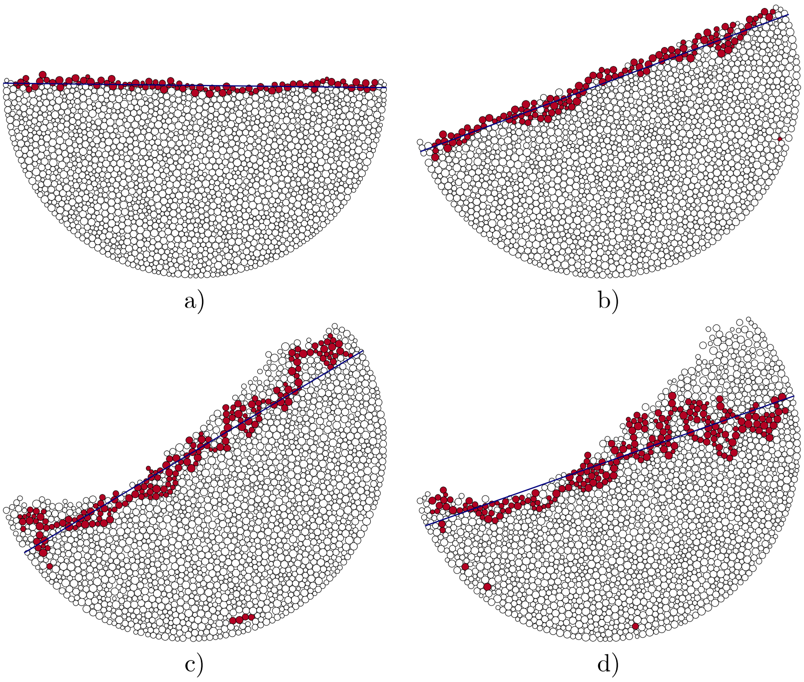


Figure 2. Detection of the surface of granular bed in a rotating drum at different time moments t and different drum rotation velocities V_r: $t = 0$ s, $V_r = 5$ rad/s (a); $t = 10$ s, $V_r = 5$ rad/s (b); $t = 15$ s, $V_r = 20$ rad/s (c); $t = 20$ s, $V_r = 20$ rad/s (d). The surface particles are colored in red, and the linear approximation of the surface is shown by the blue line

The evolution of the surface slope at different drum rotation velocities is shown in Figure 3; for clearer presentation, only the period $0 \le t \le 10$ s is shown. The values of this angle have large scatter throughout the time, therefore, the general trends are better illustrated by the histogram of the values (Figure 4).

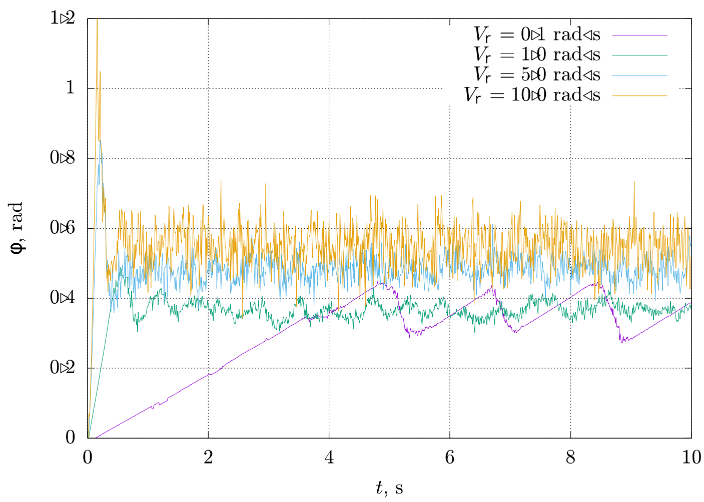


Figure 3. Evolution of the free surface inclination angle at different drum radial velocities V_r for the period $0 \le t \le 10$ s

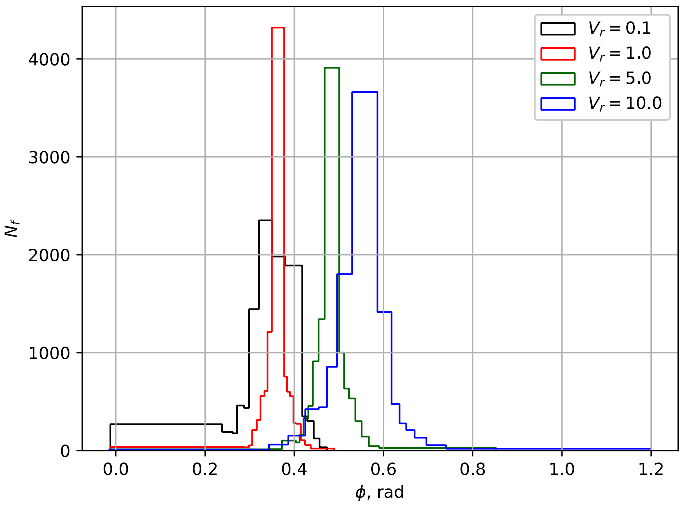


Figure 4. Histograms of the free surface inclination angle distribution at different drum radial velocities V_r

Positions of the particles at the initial time moment $t = t_0 = 0$ s and a later time $t = 15$ s, as well as the forces of interaction, are shown in Figure 5; the particles in this figure are colored according to the sum of moduli of the forces acting upon the respective particle i: $\mathbf{F}_i = \sum_j \left|\mathbf{F}_{ij}\right|$, and the forces between the particle pairs $\mathbf{F}_{ij}$ are shown by lines with thicknesses proportional to the force moduli $|\mathbf{F}_{ij}|$.

DEM simulations provide the data, among other, about the particles that are in mechanical contacts and the interaction forces among them. Given this information for a certain time moment, an interaction graph can be built. The particles are represented by the vertices of this graph, and the vertices i,j are connected by the graph edges if the respective particles i,j are in contact. The edge weight $w_{i,j}$ between the vertices i,j is proportional to the force of mechanical interaction $\mathbf{F}_{i,j}$ between the particles i,j:

$$w_{ij} = \frac{\left|\mathbf{F}_{ij}\right|}{\max\limits_{i,j}\left|\mathbf{F}_{ij}\right|}. \quad (1)$$

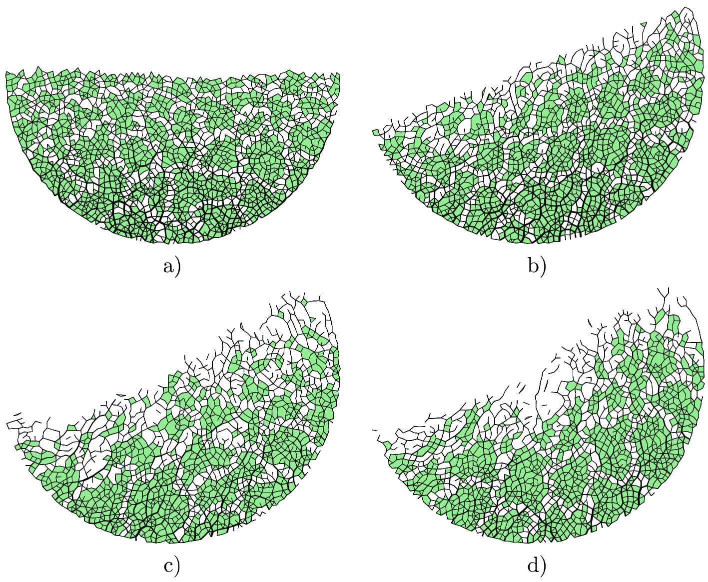
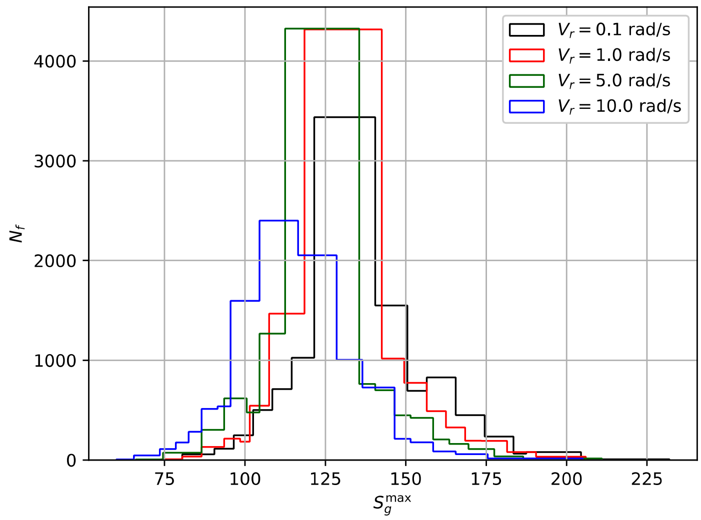


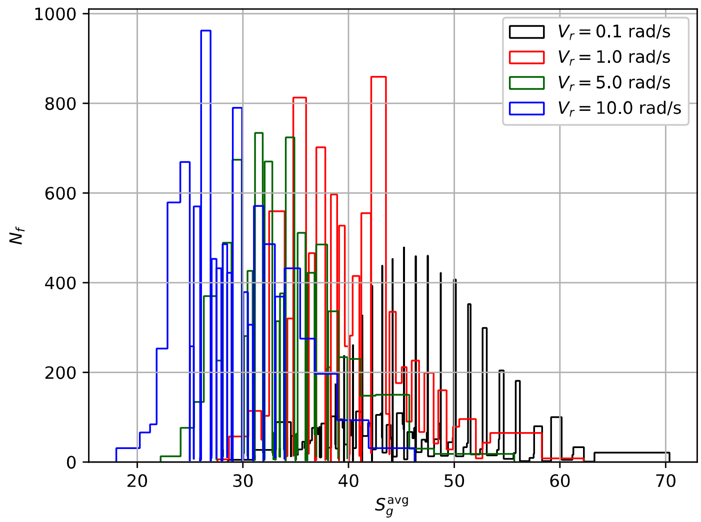
Figure 5. Particle "force clusters" identified using the "walktrap" community detection algorithm at different time moments t and the drum angular velocity V_r: $t = 0$ s (a; initial positions, equal for all the values of V_r); $t = 10$ s, $V_r = 1$ rad/s (b); $t = 10$ s, $V_r = 5$ rad/s (c); $t = 15$ s, $V_r = 5$ rad/s (d). The clusters are highlighted by green polygons produced by connecting the centers of the outermost particles of the respective cluster; the forces between the particle pairs are shown by black lines with thicknesses proportional to respective force moduli. Not to obstruct the clusters in the picture, the particles are not shown

The interaction graphs were constructed for the time moments at every 2000 iterations of DEM simulation (every 10^{-2} s), from the particle data available for these moments. The edge weights were assigned as defined by Eq. (1). Having built the interaction graph for a certain particle configuration (at the selected time moment), the force clusters were identified from the respective graphs using the "walktrap" community detection algorithm (Pons & Latapy, 2006), implemented in the *igraph* library (Csárdi & Nepusz, 2006).

Locations of the force groups identified using this method are shown in Figure 5. As can be expected, the largest clusters appear near the bottom where the compression forces are strongest. The upper area near the surface becomes unstable periodically as the drum rotates and the surface avalanches appear as the particles in this area having weak contacts become loose. Since the results of DEM simulations were recorded every 2000 iterations (10^{-2} s), the graphs were constructed for these time moments. During the period between two consecutive recorded time moments, the graph structures change significantly. Evolution of the cluster structure over time is rather chaotic, analogous to the case of the surface slope angle (Figure 4), therefore, it is more illustrative to analyse the distribution histograms of the cluster parameters. The histograms of sizes of the clusters (i.e., the numbers of the particles contained in the respective clusters) at the respective time moments t_i, $t_0 \leq t \leq t_f$, are shown in Figure 6. Distributions of the maximum cluster size are similar for the rotation velocities $V_r < 10$ rad/s, but this maximum size becomes noticeably smaller at $V_r = 10$ rad/s. The largest groups appear near the bottom of the packed bed where most of the particles move at similar velocity to that of the drum wall, whereas near the surface, small groups of loosely connected particles, or individual particles, detach from the surface and initiate the avalanches. The number of detached particles is larger for higher rotation velocities, and large number of small particle groups influence the average cluster size in these cases.



a)



b)

Figure 6. Histograms of maximum (a) and average (b) sizes of particle clusters (i.e., number of particles therein) identified from the interaction force moduli $|\mathbf{F}_{ij}|$ at different drum rotation angular velocities V_r

Conclusions

An approach for identification of larger scale structure of force chains was applied for the problem of evolution of the slope angle of the free surface of particle bed in a rotating drum. Depending on the angular rotation velocity of the drum, different regimes of evolution of the surface slope angle can be noticed. These regimes are reflected in the sizes of the detected particle force clusters. A more detailed analysis of the community structure of force chains can reveal the underlying mechanisms influencing the slope angle evolution and initiation of the avalanches on the free surface.

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