A novel approach to investigate the network of granular material using modified 3D DEM simulation

Fang Hu*, Peng Hu

1 Department of Information Engineering, Sichuan Staff University of Science and Technology, Chengdu, Sichuan, 610101, China
2 Calibration and testing centre, Sichuan water resources bureau, Chengdu, Sichuan, 510106, China
*Corresponding author’s e-mail: hf_sc@126.com

Abstract. Recently it is increasingly popular to draw upon concepts and tools from the network science to help with the analysis of granular material as this method is perfectly suitable for the granular system and provides new prospective into investigating the micro-macro relationship. However, 2D simulation brings insufficient and unrealistic results while 3D simulation requires huge workloads. It is of great significance to put forward a quick and accurate method to calculate the network-related indexes of a granular material. In this study, a modified open-source discrete element code, YADE is employed to simulate a series of tri-axial compression tests on specimens composed of polydisperse-sized spheres with varying particle diameter. The contact network evolution is studied real time with satisfactory calculation speed under the help of GPU and SQL Server parallel computing. The general evolution pattern of contact network during loading is illustrated from the view of network metrics. The initial void ratio, coordination number together with the clustering coefficient and the average shortest path of the system are shown. Particles with similar size tend to form a looser packing, resulting in smaller shear force and less connectivity of the whole system. The proposed approach is strong at improving the efficiency of the calculation when investigating the contact network of the granular material.

1. Introduction
Granular materials are made up of a large number of grains in contact. Their macroscopic behavior is complicated, highly related to the arrangement and interactions of constituent particles [1–4], as well as attributes of individual particles (e.g. shape, size, and crush resistance). In granular materials subject to loading, the relentless rearrangement of particles (or contacts) conforming to a somehow self-organized pattern leads to a specific evolution of the internal network of interactions [5]. This network is also referred to as contact network. To improve modeling the behavior of these granular media, it is therefore essential to comprehensively understand the evolution of contact network and link the characteristics of contact network to macro-scale bulk properties. The vital first step is to develop measures that quantitatively identify the features of contact network responsible for these bulk properties. However, capturing and characterizing the nature of the highly complex and dynamic contact network can be challenging.

The network theory, which is the study of graphs where discrete objects are viewed as nodes and their weighted or unweighted relations are treated as edges [6], has received wide applications in numerous fields including mathematics, physics, climate, sociology, transportation [7]. Recently, ideas
from network science are also applied in the analysis of contact network in granular systems. The contact network can be subdivided into elementary loops, and the closed loops are composed of a set of contacting nodes. Regarding these three levels, namely the node level, the loop level and the whole network level, we can use various quantitative indexes provided by the network theory to characterize the contact network. The node-level parameters such as degree and clustering coefficient, loop properties such as its geometry (e.g. size, shape, and orientation) and valence, and the network-level parameters such as the shortest path are explicitly investigated in many researches [8-11]. By systematically investigating the evolving area and valence of the loops under different initial porosities, [12] interprets the mechanism of shear dilatation in granular materials. The average shortest path is proven linearly correlating with the parameters of the Cam-Clay model [13]. Contact network provides a new and effective insight for understanding phenomenon and predicting the macroscopic behavior of granular materials. However, huge workloads are required to compute the network information in a 3D simulation where over tens of thousands of particles are involved. Using traditional calculation method, it will take hours to calculate the network metrics for a given time step. It is therefore desired to put forward an efficient method to compute. This study introduces such a method based on GPU-aided parallel computation and combined with SQL Server, this method is proven capable of computing data at any time step with a satisfactory speed. The DEM simulation tool, workflow of our proposed approach and the simulation setup will be introduced in the next section, followed by the interpretation of the simulation results where we carefully pick two time-consuming network metrics to present. Last, the conclusion is given.

2. Methodology

2.1. DEM contact model

Yade is an open-source DEM(Discrete Element Method) simulation tool[14] where a granular material is simulated as an assembly of individual particles and their interactions are calculated and updated at every time step by the second Newton’s Law. A simple linear force-displacement contact model together with Coulomb’s friction law is utilized in this study. The normal contact force $f_n$ is calculated as follows:

$$f_n = \begin{cases} -k_u u_n n_n, & \text{if } u_n > 0 \\ 0, & \text{otherwise} \end{cases}$$

(1)

where $u_n$ is the penetration depth of two particles in contact, $n_n$ represents the normal direction vector, and $k_u$ is the normal stiffness defined as:

$$k_n = \frac{2E r_a r_b}{(r_a + r_b)}$$

(2)

where $E$ is the Young’s modulus of the two contacting particles with radius $r_a$ and $r_b$. The tangential stiffness $k_t$ equals the normal stiffness multiplied by the Poison’s ratio. The tangential contact force $f_t$ is calculated in an incremental manner as follows:

$$f_t = \begin{cases} (f_t)_0 -k_t \Delta u, & \text{if } |f_t| \leq \mu |f_n| \\ -\mu |f_n| n_t, & \text{otherwise} \end{cases}$$

(3)

where $(f_t)_0$ is the shear(tangential) contact force acquired from the previous time step, $\Delta u$ is the increment of the relative tangential displacement, $n_t$ denotes the direction vector of $u$, $\mu$ is the inter-particle friction coefficient, $|\cdot|$ returns the magnitude of a vector.
In addition, a simple non-viscous damper is introduced to dissipate kinematic energy and take into account the quasi-static condition. The damping force is defined as:

\[ f_{\text{damping}} = \alpha f^* \]  

(4)

where \( \alpha \) represents the damping coefficient, and \( f^* \) is the resultant force of an individual particle. It should be noted that the direction of the damping force is opposite to the relative velocity of the particle.

2.2. Contact network extraction

The most time-consuming step when calculating the network metrics lie in the extraction of the contact network from the DEM tool. It is therefore crucial to improve the efficiency of this step. For acceleration, a novel approach is proposed, as shown in Fig.1. At any specific time step \( t \), the majority (90\%) of the contact pairs in the particulate system are outputted into a SQL Server database. The selection criterion is based on the average coordination number. The contact information of particles with more than one contacting pairs is transferred to the SQL Server database. The head database will distribute workloads to several calculator databases and is in charge of organizing data. In the SQL Server, a modified Delaunay triangulation method \cite{2} is adopted to establish the contact network of the granular system, where parallel computation as well as the GPU acceleration method is employed. The modification enables the parallel computation of up to 12 threads simultaneously, making the establishment of a contact network composed of 10,000 particles complete within 0.01s. On the other hand, the minority of the contact pairs which are with zero or only one contact are left to the Yade to complement the updating of the network metrics. The data transferring is accomplished via a Python script. The Pore Finite Volume aka Yade’s “FlowEngine” in Yade is used to cope with the GPU acceleration, which is strong at the asymptotic nature of triangulation costs, volume calculation costs, and force calculation costs\cite{15}. In SQL Server, the Parallel Page Supply is used to handle the parallel computation. This workflow is perfectly run in a standard personal desktop using Intel Core i7 CPU (3.1 GHz) and Nvidia GeForce GTX 1060 6GB GPU.

2.3. Simulation setup

In our simulation, 10,000 polydispersed-size spheres are used to generate the dense sample where the friction angle of inter-particle and particle-wall is both set to zero followed by a minor vibration of the wall to further compact the sample. By changing the particle diameter ratio \( D_{\text{min}}/D_{\text{max}} \) from 0.2 to 1 with an interval of 0.2, five different samples are prepared. For polydispersed-sized samples, the size distribution is uniform with only the different maximum and minimum value. Then, the drained biaxial compression simulation is conducted, which includes two steps, namely an isotropic
compression stage and a shear loading stage. At first, every sample is isotropically compressed using a servo-control mechanism under a confining pressure of 100 kPa until the kinetic energy of the whole system is smaller than $10^{15}$ J, which manifests a desired stable state. Afterwards, the sample is vertically compressed by moving the top rigid wall downward at a constant velocity of 0.01 m/s. This loading rate is cautiously chosen to be small enough to satisfy a quasi-static condition. As shearing starts, the confining pressure on the lateral walls remains constant by the servo-control. All samples are sheared to an axial strain of 30%, when a critical state is reached and the re-organization of the internal texture becomes nearly steady. The major simulation parameters are listed below. To guarantee the accuracy, all the samples are sheared for 3 times independently and the results shown below are averaged as well. During compression and shearing, the recording and calculation of network metrics are in effect and data are consecutively recorded.

| Parameter                                | Value       |
|------------------------------------------|-------------|
| Young's modulus $E$ (GPa)                | 15          |
| Poison’s ratio                           | 0.35        |
| Density                                  | 2650 kg/m$^3$ |
| Particle number                          | 10000       |
| Particle diameter ratio($D_{min}/D_{max}$) | 0.2,0.4,0.6,0.8,1 |
| Inter-particle friction angle            | 38°         |
| Damping coefficient $\alpha$             | 0.3         |
| Confining pressure                      | 100 kPa     |

3. Results

3.1. Strength property and initial packing

Figure 2. (a) The packing sample, (b) the initial void ratio and coordination number against different particle diameter ratio.

The initial packing is shown in Fig.2(a). And the packing as well as the strength is plotted against the particle diameter ratio in Fig.2(b). After the isotropic compression, the initial void ratio increases with the particle diameter ratio. The critical internal friction angle is computed as well, suggesting a different tendency from void ratio. The shear strength represented by the friction angle decreases with the particle diameter ratio.

3.2. Network metrics

The clustering coefficient of a node $i$ is defined as the ratio of the number of triangles connected this node to the number of triples centered on this node, where a triple centered on node $i$ is a set of two edges connected to the node. This metric is highly computational-costly as we have to calculate every node’s clustering coefficient. And this metric is significant because it is a straight reflection of the network connectivity. As shown in Fig.3 (a), the average clustering coefficient of the system drops quickly at the beginning of the shearing, followed by fluctuations over a relatively steady value. When
looking at the effect of different particle diameter ratio, it is reached that the clustering coefficient goes up with the decrease of the particle diameter ratio, indicating that the uninform-sized sample is poor in connectivity. This observation conform to previous research [16].

The shortest path of a network is the average shortest path length between any two nodes in a network. This metric requires even larger workloads than the clustering coefficient as the time complexity approaches O(n!). We present the average shortest path length of the system at two stages, namely the beginning of the shearing and the steady state, to investigate the effect of the particle diameter ratio. As shown in figure 3 (b), it is evident that with higher particle diameter ratio, the average shortest path goes up. It is again reinforced that when conducting numerical simulation on granular material, the size polydispersity should be considered so as to reach a more uniform sample.

Figure 3. (a) The clustering coefficient and (b) the average shortest path length against different particle diameter ratio.

4. Conclusions
This study puts forward a novel approach for computing the network system of a granular material with high efficiency aided by the GPU acceleration and parallel computation. By using SQL Server to share the computation loads, the approach shortens the cumbersome calculation time of network metrics. Its capability is demonstrated by a series of 3D DEM tri-axial test simulations where polydisperse-sized spheres are sheared. The results show that particles with uniform size result in a looser packing, a smaller clustering coefficient and larger average shortest path. Such computational-costly metrics are monitored real-time, demonstrating the calculation capability of our proposed calculation approach. This approach is a promising tool to help with the analysis of the network science as well as other engineering scenarios.

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References
[1] Bassett, D.S., Owens, E.T., Daniels, K.E., Porter, M.A.: Influence of network topology on sound propagation in granular materials. Phys Rev E Stat Nonlin Soft Matter Phys. 86, 4515–4516 (2012)
[2] Radjai, F., Wolf, D.E., Jean, M., Moreau, J.J.: Bimodal Character of Stress Transmission in Granular Packings. Phys.rev.lett. 80, 61–64 (1998)
[3] Radjai, F., Roux, S., Moreau, J.J.: Contact forces in a granular packing. Chaos. 9, 544–550 (1999)
[4] Bi, D., Jie, Z., Chakraborty, B., Behringer, R.P.: Jamming by shear. Nature. 480, 355 (2011)
[5] Tordesillas, A., Behringer, B., Lin, Q., Shi, J., Zhang, J.: Structural Stability and Jamming of Self-Organized Cluster Conformations in Granular Materials. In: APS March Meeting (2011)
[6] Börner, K., Sanyal, S., Vespignani, A.: Network Science. Annu. Rev. Inf. Sci. Technol. 41, 537–607 (2010)
Bollobás, B.: Modern Graph Theory. Grad. Texts Math. 184, (1998)

Giusti, C., Papadopoulos, L., Owens, E.T., Daniels, K.E., Bassett, D.S.: Topological and geometric measurements of force-chain structure. Phys. Rev. E. 94, 032909 (2016).

Nguyễn, N.S., Magoariec, H., Cambou, B.: Analysis of local behaviour in granular materials. Comptes Rendus - Mec. 342, 156–173 (2014).

Ren, J.: Nonlinear Dynamics and Network Properties in Granular Materials under Shear. (2013)

Jensen, R.P., Bosscher, P.J., Plesha, M.E., Edil, T.B.: DEM simulation of granular media-structure interface: Effects of surface roughness and particle shape. Int. J. Numer. Anal. Methods Geomech. 23, 531–547 (1999).

Oda, M., Konishi, J., Nemat-Nasser, S.: Experimental micromechanical evaluation of strength of granular materials: Effects of particle rolling. Mech. Mater. 1, 269–283 (1982)

Ouadfel, H., Rothenburg, L.: 'Stress-force-fabric’ relationship for assemblies of ellipsoids. Mech. Mater. 33, 201–221 (2001). https://doi.org/10.1016/S0167-6636(00)00057-0

Liu, Q.B., Xiang, W., Budhu, M., Cui, D.S.: Study of particle shape quantification and effect on mechanical property of sand. Yantu Lixue/Rock Soil Mech. 32, 190–197 (2011). https://doi.org/10.16285/j.rsm.2011.s1.121

Sallam, a. M., Ashmawy, a. K.: Effect of particle shape and angularity on dilation of granular soils: a discrete element approach. Proc. 17th Int. Conf. Soil Mech. Geotech. Eng. (ICSMGE 2009). 4 (2009). https://doi.org/10.3233/978-1-60750-031-5-417

Saint-Cyr, B., Szarf, K., Voivret, C., Azéma, E., Richefeu, V., Delenne, J.-Y., Combe, G., Nouguier-Lehon, C., Villard, P., Sornay, P., Chaze, M., Radjai, F.: Particle shape dependence in 2D granular media. EPL (Europhysics Lett. 98, 44008 (2012). https://doi.org/10.1209/0295-5075/98/44008