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Temporal variation of contact networks in granular materials

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Abstract

For analogue granular materials simulated using DEM, contact networks are often drawn by joining the centroids of contacting particles. Although a limited amount of research has been done to characterise the temporal aspects of such contact networks at a micro-scale, many simple questions regarding the duration of contacts in evolving granular systems remain unanswered. This paper addresses this gap in the existing knowledge by using the open-source code LAMMPS to run and analyse nine (3D) triaxial simulations of 20,164 polydisperse spherical particles. Contacts which exist for a long duration are preferentially oriented in the direction of the major principal stress while the fabric anisotropy for contacts with a given duration increases with duration. Regardless of simulation conditions, there is a linear relationship between the percentage of contacts present for a given duration and contact duration, despite the non-linear overall behaviour of the material. The forces transmitted by contacts increase, on average, with increasing duration. The total number of unique contacts which appear during triaxial compression increases linearly after 10% axial strain, although the number of contacts, both total and subdivided into strong and weak force subnetworks, remains quite stable. The majority of contacts in these evolving granular systems, even those participating in strong force chains, are formed and lost repeatedly.

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Keywords

Discrete element modelling; dynamic networks; triaxial simulations; contact duration; granular materials

1) Introduction

In any granular material, a contact network can be created, in principle, by joining the centroids of contacting particles to create edges. Because the particles comprising a granular material can change position over time, and hence contacts are continually created and lost, the contact network is dynamic [1]. Creating the contact network for real granular materials can be difficult as it is necessary to accurately find the positions of particles inside a three-dimensional sample without disrupting those at the periphery. This remains true despite the development of advanced techniques such as micro-computed tomography [2], magnetic resonance imaging and techniques based on the measurement of acoustic emissions [3].

Discrete element modelling (DEM) simulations can easily generate data on the contact network for analogue granular materials. For 2D simulations, contact networks can be plotted where each contact in the network is represented by a line connecting the centroids of the contacting particles, the thickness of which is proportional to the magnitude of the force transmitted at the contact, e.g., [4,5]. Researchers have developed criteria to identify strong force chains within these contact networks [6,7] and have statistically characterised the distribution of contact forces in their systems [8]. Other researchers have studied granular media using complex networks and graph theory, often using data obtained from 2D simulations of disks, e.g., [9-12]. Although a limited amount of research has been done to characterise the temporal aspects of contact networks at a micro-scale, little prior research has considered how long a contact exists for when an assembly is subjected to controlled loading or deformation, especially using 3D triaxial loading with a realistic grading. In one of the few prior papers exploring this subject, analysis of a 2D dataset revealed that the proportion of contacts which are present at any initial time in a simulation of cohesive grains decreases
exponentially with time [13].

The objective of this paper is to address this gap in the existing knowledge by studying the evolution of the contact network with specific reference to two per-contact quantities: duration and transitivity. Duration is the proportion of the simulation for which a contact exists while transitivity studies the transitions of a contact between different defined states (e.g., present/absent) as the simulation progresses. It is now well established that the buckling of force chains is an important mechanism underlying soil failure [14-16]. The duration and transitivity of the contacts participating in the stronger force chains that transmit the majority of the applied stress must have a significant influence on the behaviour of the system as a whole. One can infer that longer-duration contacts are an indicator of more stable force chains and so the frequency of rupture and creation of contacts within the strong force network is a measure of the stability of the strong force chains. The data used for this study was obtained by running nine triaxial compression simulations using assemblies of polydisperse spheres.

2) DEM simulations

The numerical samples used in this paper all contain 20,164 spherical particles bounded by a periodic cell to eliminate boundary effects; periodic cell boundary conditions have been used previously for DEM simulations in geomechanics [e.g., 17,18]. The deformation field in a periodic cell is homogenous [19] which is not true for a sample bounded by rigid walls [20]. The particle size distribution (PSD) used for all the samples is shown on Figure 1 and is representative of Toyoura sand. A digitized PSD of a real Toyoura sand measured by sieve analysis [21] is also provided on Figure 1 for comparison. Particles smaller than 0.116 mm were omitted from the numerical sample for computational tractability.

These simulations were run using the open-source, MPI-parallelised code LAMMPS [22] which is maintained and distributed by researchers at the Sandia National Laboratories. Although primarily used for molecular dynamics, some functionality has been added to the code to facilitate its use for DEM simulations of granular materials. The authors have made
some modifications to the base code including the addition of a stress-control algorithm for periodically-bounded samples which includes the ability to maintain either the volume or the mean effective stress of the sample at a constant value by adjusting the positions of lateral boundaries to compensate for axial shearing. Following the approach of Barreto [23], this modified version of the code was successfully validated using the expressions developed by Thornton [24] for the stress ratios in a face-centred cubic assembly of monosized rigid spheres.

Initially the particle radii were generated and stored in order of decreasing size. The largest particle was placed inside the periodic cell at a position chosen using a random number generator. A trial position was then randomly selected for the second-largest particle, and a check was done to ensure that if the particle were placed at this position, it would not overlap any pre-existing particles. Particles were, however, permitted to intersect the periodic boundaries. If there was no inter-particle overlap, it was placed inside the cell; otherwise another random position was chosen. As each particle was placed inside the cell without overlap, the algorithm moved to the next-largest particle until all particles had been placed inside the cell. At that stage, opposing pairs of periodic boundaries were moved closer together using a servo-control algorithm until a pre-defined isotropic stress state had been attained and the sample was in a stable equilibrium. The homogeneity of the resultant samples was checked by local analysis of the void ratio, mean particle size and contact density [25].

Nine samples were prepared in total with void ratios, \( e \), defined here as the volume of voids divided by the volume of particles, varying from 0.533 to 0.646. This range of void ratios was achieved by varying both the confining pressure and the particle surface friction coefficient, \( \mu \). The friction coefficients used during sample preparation are given in Table 2 for information. Once sample preparation was complete, the friction coefficient was set at 0.25 for all samples. Local damping, implemented as described by [26], with a coefficient of 0.1 was used throughout the simulations; gravity was inactive. A simplified Hertz-Mindlin contact model was allocated with a shear modulus, \( G \), of 29 GPa and Poisson’s ratio, \( \nu \), of 0.12. The normal component of the contact force between contacting spheres denoted as \( a \) and
is computed according to conventional Hertzian theory, i.e., \( F_n = \frac{4GR_g}{3(1-v)} d \), where \( d \)

is the inter-particle overlap and \( R_g = \sqrt{\frac{R_a R_b}{R_a + R_b}} \). The tangential component, \( F_t \), is calculated incrementally, i.e., \( F_t^i = F_t^{i-1} - \frac{4GR_g \sqrt{d}}{2-\nu} \Delta d_S \), where \( i \) and \( i-1 \) are consecutive timesteps and \( \Delta d_S \) is the increment of relative shear displacement during timestep \( i \). A slip criterion was imposed so that the shear force is limited to \( \mu F_n \). It is noted that this Hertzian implementation differs substantially from the inbuilt LAMMPS ‘pair/gran/hertz/history’ model.

Taking a soil-mechanics approach, each of the nine prepared samples was then subjected to one of the following triaxial loading regimes:

1. **Constant \( \sigma_3' \):** the sample was sheared vertically in compression at a constant strain rate while the minor and intermediate principal effective stresses, aligned with the axes of the periodic cell, were held constant at the initial confining pressure.

2. **Constant \( p' \):** the sample was sheared vertically at a constant strain rate while the positions of the lateral boundaries were adjusted continuously to maintain both a constant mean effective stress (i.e., the arithmetic mean of the three effective principal stresses), \( p' \), and equal horizontal stresses.

3. **Constant volume:** these are similar to the constant-\( p' \) simulations except the volume is held constant rather than \( p' \). These constant-volume simulations are commonly used to simulate undrained loading of a fully saturated soil and inherently assume that the pore fluid is incompressible.

A critical-state line (CSL) which spans several orders of magnitude of \( p' \) was obtained using a range of constant-\( \sigma_3' \), constant-volume and constant-\( p' \) simulations. Using three different triaxial loading regimes allowed the uniqueness of the CSL to be confirmed, i.e., the void ratio and \( p' \) were found at critical state for several constant-\( \sigma_3' \) simulations, and both
constant-volume and constant-p’ simulations beginning at similar void ratio or p’, respectively, were run to confirm that the critical state points are in agreement regardless of test conditions. Furthermore, applying the analysis described in this paper to simulation data obtained using three common loading conditions shows whether or not the contact network and its temporal properties depend on the loading conditions adopted. The main simulation parameters are summarised in Table 1. A strain rate of 1/s was chosen for all simulations as a sensitivity analysis showed that a consistent mechanical response was obtained using strain rates lower than this value. The adoption of periodic cell boundary conditions prevented the formation of shear bands in these simulations. Detailed particle and contact information was written to files at regular intervals during the simulations to facilitate the analysis described in this paper. Each sample was sheared until a critical state had been attained, i.e., until continued loading did not change either the volume or stress state [27]. Therefore, the simulations were terminated at different axial strain levels. The frequency at which the output files were written also differs among the simulations. The exception is the constant-p’ tests, all of which have the same maximum axial strain and number of output files. Table 2 summarises the experimental conditions and critical state parameters for the nine simulations that were run, noting that axial strain is defined using the strain-controlled vertical dimension and critical state parameters were recorded at the end of each simulation when the system response could reasonably be considered to be critical. The mean radial strain decreased quadratically with increasing axial strain.

All the simulations were run on a high-performance computing cluster at Imperial College (cx1) using a timestep of 5.38 ns. Figures 2a-c show the evolution of deviator stress, q, i.e., the difference between the major and minor principal effective stresses, against axial strain for all nine simulations. The stress increases for the constant-σ’ simulations are the smallest: they are approximately one order of magnitude lower than for the constant-p’ tests, which in turn are around an order of magnitude lower than for the constant-volume tests. The volumetric strains for the drained simulations are shown on Figures 2d and 2e, while Figure 2f shows the change in p’ during shearing for the constant-volume simulations. The 0.533-100 sample (the
densest tested) behaves dilatively throughout shearing. $M$, defined as $\frac{q}{p'}$, was calculated at the phase transformation point and is given in Table 2 for all simulations. The maximum $p'$ attained is approximately 35 MPa for the 0.578-1000 sample. Although particles of silica sands are quite robust, such high stresses would cause considerable grain breakage in a real sample [28] which was not modelled in these simulations. Inter-particle overlaps were monitored during the simulations to ensure that they were small relative to particle size (95% of overlaps were required to be smaller than 5%) so that point contact was approximated [29]. All nine simulations discussed in this paper satisfy this overlap criterion. A fundamental proposal of the critical-state soil mechanics framework is that the critical state line is a unique characteristic of a material which does not depend on experimental conditions [30]. Hence the critical states for all nine simulations can be presented on Figure 3 which shows the critical state line in both $e$-$\log(p')$ and $q$-$p'$ space. These critical state parameters are also given in the rightmost columns of Table 2.

3) Probability density functions of contact duration

Contacts are created in a soft-sphere DEM simulation when particles overlap each other, and are lost when the particles subsequently separate. The duration of a contact, $d$, is quantified as the proportion of the simulation for which the contact exists. A contact which is present continuously throughout the simulation has the maximum duration, $d$, of 1. As discussed in Section 2, the simulation data were written to text files at discrete intervals of axial strain. It is assumed that contacts which were present in each output data set are present for the entire strain interval. This assumption was justified by halving the number of output files analysed for one representative simulation, 0.603-1000, and confirming that the trends in contact duration and other results presented in this paper remain the same. The duration of each contact was calculated using MATLAB [31] to sequentially import text files containing the contact force information, including the identities of the contacting particles. When the first text file was imported to MATLAB, all pairs of contacting particles in that file were stored in
a matrix along with the number of files in which the contact was present: one at this stage. Each contact in the second and subsequent files was compared to those already present in this matrix. If present, the number of appearances was incremented; otherwise a new row was appended to the matrix. Once all files were imported, the duration of each contact was quantified as the number of output files in which the contact was present divided by the total number of output files. The total number of possible contacts is \( \binom{20164}{2} = 2.033 \times 10^8 \).

Since particles are geometrically confined by neighbouring particles, the number of unique contacts which are created during simulations of triaxial loading is much smaller than this upper limit. Since most potential contacts are never formed, they are excluded from the analysis for clarity so that durations are strictly positive.

Figure 4 plots the percentage of contacts present \((P_d)\) against their durations, \(d\). Regardless of the simulation conditions, the percentage of contacts present for a given duration \((P_d\) for a given \(d)\) decreases almost linearly as \(d\) increases. The sole exception is contacts which have a duration of one; more of these tend to be present than contacts with durations between 0.9 and 1. Linear regressions were fitted using a least-squares method, omitting the data for durations of zero and one as these outliers skew the regression if included. The \(R^2\) statistics were above 95% for all regressions except for the two constant-volume simulations with the lowest void ratios. The linear nature of the \(P_d\) vs \(d\) relationship is somewhat surprising given the clear non-linearity of the material overall behaviour as illustrated in Figure 2. It would be interesting to correlate the \(P_d\) vs \(d\) relationship with the simulation parameters; however, since the slopes and intercepts of these regressions depend on the number of data points available, the regressions for the constant-\(\sigma'_f\) or constant-volume simulations cannot be meaningfully compared.

Comparing the three constant-\(p'\) simulations (where the numbers of data points were the same), the slopes of the linear regressions increase as the initial confining pressure is increased or the initial void ratio is decreased. Furthermore, there is a clear relationship between the initial confining pressure or void ratio and the proportion of contacts that remain intact throughout the simulation: the samples with initial confining pressures of 5 MPa, 10
MPa and 20 MPa (and void ratios of 0.625, 0.612 and 0.594) have 0.11%, 0.21% or 0.44% of contacts, respectively, with durations of one. The reason for this is particles have less mobility in granular systems with low void ratios, induced by high confining pressures. Hence contacts have a greater likelihood of existing for a long duration in denser than in looser systems in which the particles have greater freedom of movement.

In addition to analysing the durations of all contacts within the contact network, each contact was categorised as strong or weak at each time interval depending on whether the contact force transmitted is above or below the mean contact force, respectively. This approach has been used previously [8,32]. An important caveat to note is that force chains are not being identified explicitly in this study, and membership of the strong subnetwork does not necessarily mean that a contact is part of a strong force chain. The duration data for only the strong contacts is presented in Figure 5. For the data presented in Figure 5, contacts are considered only while they are both present and within the strong subnetwork, but not while the contact force transmitted is below the mean. The duration pattern for the strong forces differs markedly from the overall data presented in Figure 4; however, despite the non-linearity of the material behaviour, a clear pattern emerges again. In this case, rather than having a linear correlation, the number of contacts that are considered to be strong for a given duration decreases exponentially with duration. Few strong contacts are present for more than half of the simulation. Two-parameter exponential regressions of the form \( y = ae^{bx} \) were fitted to the data (\( R^2 > 0.96 \)) as shown on Figure 5. For the constant-\( p' \) simulations, increasing the initial confining pressure or reducing the initial void ratio causes the regression parameter \( a \) to decrease (3.01, 2.80 and 2.56 for the 0.625-5000, 0.612-10000 and 0.594-20000 simulations, respectively) and the parameter \( b \) to increase (-0.059, -0.055, -0.050). The transition of contacts between the strong and weak force subnetworks is discussed further in Section 7.
4) Relationship between duration and orientation of contacts

The second-order fabric tensor is frequently calculated in geomechanics to provide information on average/representative orientations and to quantify the magnitude of the sample anisotropy. The fabric tensor is often calculated using all the contacts in a sample, following the definition of Satake [33]. To better understand the relationship between the orientation and duration of contacts, a modified fabric tensor was calculated:

$$\phi_{ij}^d = \frac{1}{N_d} \sum_{k=1}^{N_d} n_i^k n_j^k$$

(1)

where $N_d$ is the number of contacts with duration $\geq d$ and $n_i^k$ is a unit vector along contact $k$ (the branch vector or unit contact normal for spherical particles). This tensor is symmetric with a trace equal to one. The eigenvalues and eigenvectors of the fabric tensor may be calculated; the eigenvalues give an indication of the extent of clustering of contacts along particular orientations, while the eigenvectors corresponding to these eigenvalues give the orientation of the fabric. The anisotropy of the fabric can be quantified using the deviatoric fabric, $\Phi_d$, which is defined as the difference between the maximum and minimum eigenvalues of the fabric tensor, i.e., the difference between the major and minor fabric components. In an evolving system of transient contacts, the fabric tensor could reasonably be calculated using several different sets of particle centroids. In this study, the branch vector for each contact was calculated in two different ways: the branch vector when the contact was formed for the first time and a mean branch vector calculated while the contact was present. The results using both approaches are similar; hence only the results using the branch vectors at initial contact formation are discussed below.

Figure 6 shows deviatoric fabric, $\Phi_d$, for contacts with duration $\geq d$ against contact duration. $\Phi_d$ increases with increasing duration for all simulations, indicating increased anisotropy. The major fabric (i.e., largest eigenvalue) is oriented approximately vertically (in the direction of shearing and the major principal stress) for all simulations and durations, while the intermediate and minor fabric are approximately horizontal. The increase in deviator fabric
with duration therefore indicates that the contacts that last longer are more likely to have a vertical orientation. This suggests that it is the contacts in the force chains that are known to form in the direction of the major principal stress that are more stable and last longer, in comparison with those contacts that make up the orthogonal, weaker contact force network. This hypothesis is confirmed by reference to the rose diagrams shown on Figure 7 for three representative simulations: 0.627-1000, 0.612-10000 and 0.599-527. These diagrams are plotted by projecting the branch vectors corresponding to contacts onto the x-z plane, quantifying the angles between the branch vectors and this plane, and then assigning each angle to one of 18 bins between 0° and 180°, separated by 10° increments. The length of each segment is proportional to the number of contacts, while the colour indicates the mean duration of contacts in the segment. All contacts in the system are considered in the rose diagrams on the top row of Figure 7, while the diagrams on the bottom row are restricted to contacts with durations ≥ 0.9. Clearly, contacts with long durations are preferentially oriented vertically, i.e., in the direction of shearing, regardless of the simulation conditions.

5) Relationship between duration and contact force

Each contact has a contact force vector associated with it; the normal component of this force acts along the line joining the centres of these idealised spherical particles while the tangential component is coplanar to the circular contact plane. The fabric data and rose diagrams suggest that because the contacts with longer duration are more likely to be orientated in the principal stress direction, they are likely to participate in the strong force network and bear larger contact forces, on average, than those with shorter durations (refer to, e.g., [34]). Thinking about the way in which discrete element models work, this difference in force magnitude will also arise because simulated particles which are in contact must move apart by an amount equal to the inter-particle overlap in order for the associated contact to be lost; the minimum time required for this to occur increases if the overlap (and hence, the contact force) is larger. In the current study, the mean and maximum values of contact force magnitude were recorded for each contact and subsequently binned according to contact duration. The average force
magnitudes were calculated for each duration and simulation, and are plotted on Figure 8. Both the mean and maximum forces increase, on average, with increasing duration. The forces for the constant-\(\sigma'_3\) simulations are approximately one order of magnitude lower than those for the constant-volume or constant-\(p'\) simulations; this difference may be explained by the differences in stress level (Figure 2). The central regions of all the plots, between durations of 0.2 and 0.8, show a linear trend: fitted linear regressions have \(R^2\) values exceeding 0.9 in all cases.

The parameters of these linear regressions are reasonably insensitive to the axial strain, and hence relationships could be sought between the regression parameters and the properties of the samples at critical state. To demonstrate this insensitivity to strain, consider the simulation denoted by 0.627-1000 which was run to an axial strain of 40.3%. If the maximum axial strain is reduced to 29.3%, the slope, \(m\), and intercept, \(c\), of the maximum force regression change by 6.4% and 17.7%, respectively, while for the mean force regression, the corresponding changes are 2.3% and 8.9%. If the axial strain is further reduced to 18.6%, less than half of the full range, the respective differences compared to the full strain range become 18.2% and 37.1% for the maximum forces, and 0.3% and 20.8% for the mean forces. Although some of these differences appear substantial, they are considerably smaller than the differences between simulations: the smallest difference between any of the parameters obtained for different constant-\(\sigma'_3\) simulations is a factor of two. The situation is similar for the constant-volume and constant-\(p'\) tests. Once this insensitivity to strain had been established, it was found that the slopes, \(m\), and intercepts, \(c\), of the fitted linear regressions are related in a similar way to the mean effective stress at critical state as shown on Figure 9. The system is highly complex and it is difficult to relate these correlations to the mechanical behaviour meaningfully.

If only the strong force subnetwork is considered, the trends in the data observed in Figures 8 and 9 remain. Figure 10 plots the mean force magnitudes against the duration of these strong contacts. As expected, the mean force magnitudes are larger for the strong contact case than when all contacts are considered. There is more scatter in Figure 10 than in Figure 8 due to
the limited availability of data at large durations when the strong subnetwork membership restriction is imposed. As before, linear regressions were fitted to the central parts of these force-duration plots ($R^2 > 0.92$). The slopes of these regressions, considering only the strong force subnetwork, are larger than the slopes of the corresponding regressions which consider all contacts on Figure 8 by a factor of 1.6, on average. The intercepts too are larger (by a factor of 2.25) when analysis is restricted to the strong force subnetwork. A relationship was found between the slopes, $m$, and intercepts, $c$, of the regressions shown on Figure 10 and $p'$ at critical state as shown on Figure 11. Again, it is worth noting that although these trends emerge from the simulations, a link to the mechanics of the system response is not evident.

6) Evolution of the number of contacts with strain

Even though the magnitudes of the principal stresses within the granular assemblies increase greatly prior to the critical state, particularly for the constant-volume simulations, the total number of contacts changes little as shown on Figure 12. This indicates that an increase in stress compared to the initial confining pressure is due to an increase in the average force at each contact rather than a major increase in the number of contacts: a fact which has been widely established in the literature (e.g., evolution of coordination number in [17]). Figure 12 also indicates that the number of contacts categorised as strong or weak remains relatively stable as the simulations progress. As contacts are continuously being created and lost during a simulation, and because contacts may transfer between the strong and weak subnetworks, the number of contacts and relative proportions in the strong and weak subnetworks appear to achieve what can be termed a dynamic equilibrium.

The samples are initially percolating and subject to a finite mean stress and so contacts are present in the system at the onset of shearing. As triaxial loading proceeds, some of these contacts are lost; however, these contacts may potentially reform subsequently. If contacts are reformed, these may be distinguished from contacts which are being formed for the first time. The total number of unique (distinct) contacts which have appeared in the system is plotted against axial strain on Figure 13. At low strain, the total number of unique contacts rises
sharply; after axial strains of around 10%, the increase becomes more gradual and has a linear trend. For the constant-volume and constant-$p'$ simulations, it is interesting to note the strong similarity among simulations regardless of the initial void ratio or confining pressure. For sample 0.533-100, the large increase in the number of unique contacts at small strains indicates substantial particle rearrangement. The void ratio and confining pressure for this sample are both the lowest of all simulations, and although a low void ratio would tend to inhibit particle rearrangement, the use of a low confining pressure of only 100 kPa has the dominant effect on contact formation. The difference between the 0.533-100 sample and the others on Figure 13 may be due to the extremely strongly dilative volumetric response of this sample throughout shearing, as shown on Figure 2d, which differs from the initial contraction followed by a limited dilation of the looser samples.

7) Transitivity of contacts

The duration of a contact quantifies the total fraction of the entire simulation length for which it exists. The calculated duration may be either a single continuous interval or several non-contiguous time intervals. Although two contacts may have the same duration, the manner in which this duration is distributed can have significant implications for the contacting particles, and at a larger scale, for the simulation as a whole. The number of times that each contact was formed during a simulation, i.e., the transitivity of the contact between present and absent states, was analysed to supplement the duration data.

Figure 14 shows the percentage of contacts in each simulation which form once, twice, etc. The majority of contacts are formed more than once in all cases. For the constant-$\sigma'_3$ simulations, more than 70% of contacts are created multiple times which is larger than the corresponding proportions for the constant-$p'$ or constant-volume tests. For the latter, between 30% and 45% of contacts are formed only once in the system, which may be attributable to the imposed geometrical constraint of maintaining a constant volume. It is always the case that the percentage of contacts decreases monotonically as the number of times that contacts
are created increases. It should be noted that there is a small skew in the data, common to all simulations, caused by the reduced timeframe for contacts created at the end of the simulation to be lost subsequently. For example, contacts which are created for the first time at the very end of a simulation cannot be lost as no further data are output from the simulation.

Since the number of times that a contact is created depends on both the maximum axial strain reached and the frequency with which data files are written, the transitivity results are not mutually comparable except those of the constant-p’ simulations. There is a clear relationship between the initial confining pressure or void ratio and the contact transitivity: on average, contacts are created least often when the initial confining pressure is highest and the void ratio is lowest, while transitivity is highest for an initial confining pressure of 5 MPa and void ratio of 0.625. This is explained by the greater mobility of particles in loose systems compared to denser systems in which particles are ‘locked in’ to their initial positions.

The categorisation of any particular contact as strong or weak may change during the simulation if the rates of change of force transmitted at the contact and the mean force for all contacts differ. Therefore the transitivity of contacts between the strong and weak subnetworks may also be studied. For each contact, the number of times that contact moved from the weak to the strong subnetwork, or entered the strong subnetwork concurrently with contact formation, was quantified. These data are shown on Figure 15. The trends are broadly similar to those seen on Figure 14 with one key difference: the methodology adopted in this paper disregards contacts which never form during a simulation so the smallest permissible number of times a contact forms is one, whereas it is possible for contacts to remain within the weak subnetwork throughout their duration. Hence the smallest permissible number of times a contact enters the strong subnetwork is zero. This is the case for between 15% and 25% of contacts, i.e., a large majority of contacts form part of the strong subnetwork at some stage during the simulation. For all simulations except 0.533-100, more contacts enter the strong subnetwork exactly once than any other possibility. For the constant-p’ simulations, the transitivity of contacts between the strong and weak subnetworks is increased by choosing a low initial confining pressure or high void ratio, as was the case for contact transitivity
between present and absent states.

Although there is a marked visual similarity between Figures 14 and 15, there is no clear relationship between the number of times a contact is formed and the number of times a contact enters the strong subnetwork (though it should be emphasized that the distinction between strong and weak contacts is somewhat arbitrary, being based on whether the contact force is above or below the mean contact force, respectively). The product-moment correlation coefficient, $r$, between these two properties is 0.222 when averaged for all simulations with a standard deviation of 0.104 between simulations: a very weak correlation in all cases. Correlations were also evaluated between these two properties and the mean and maximum forces borne by each contact during the simulations. The results are given in Table 3, and indicate that these four correlations are also weak. These correlations indicate that contacts which are formed large numbers of times are not necessarily ‘rattlers’ within voids, but can participate in strong force chains. This is further confirmed by noting that 20.3% of contacts are formed more than five times for the 0.627-1000 sample and 94.1% of these contacts appear in the strong subnetwork at some stage during the simulation. For typical constant-volume (0.599-527) and constant-p’ (0.612-10000) simulations, 81.3% and 92.6% are the respective percentages of contacts which are formed more than five times and are also present in the strong subnetwork during the simulation.

8) Discussion and conclusions

This paper has examined the duration and transitivity of contacts in a percolating granular material subject to nine different triaxial compression tests. These temporal properties have an important influence on soil behaviour as they dictate the ability of a force chain to consistently transmit force through a sample. Each of the numerical samples was sheared until a critical state was attained. Analysis of the contact force network revealed the following:

1. Considering three types of triaxial compression test (strain-controlled constant-$\sigma'_3$, constant-p’ and constant-volume), there is a clear correlation between contact
duration and contact orientation. The fabric anisotropy for contacts with a given duration increases with duration. As the orientation of the principal fabric is always vertical, this increase in anisotropy indicates that the longer-lasting contacts have a directional bias in the vertical direction. Rose diagrams confirmed this conclusion that was originally developed using a second-order fabric tensor.

2. Considering again all three types of triaxial compression test, there is a systematic trend in contact durations. The percentage of contacts present for a given duration was plotted against duration; in all cases, the correlation was linear with a negative slope even though the material overall behaviour is non-linear. This finding was explored by categorising, at each output stage, contacts as either strong or weak depending on whether the contact force is above or below the mean contact force, respectively. It was found that the percentage of contacts present in the strong subnetwork decreases exponentially with increasing duration.

3. The mean and maximum forces transmitted by a contact increase with contact duration. When the means in each bin were plotted against duration, the central parts of the plots, between durations of 0.2 and 0.8, were linear for both the total network of contacts and the strong subnetwork. The slopes and intercepts of linear regressions fitted to these central regions were related to \( p' \) at critical state.

4. Some correlations with the simulation parameters and the duration trends could be explored using the three constant-\( p' \) simulations, all of which 201 data files and so could be meaningfully compared. The percentage of contacts which exist for the entire simulation increases with increasing confining pressure and decreases with increasing initial void ratio. For the strong subnetwork, the parameters describing the exponential regressions fitted to the constant-\( p' \) data were related to the initial confining pressure and void ratio.

4. Prior analyses of response to compression induced shear (e.g., [17]) have revealed that the mechanical coordination number achieves a stable value after only a small amount of shearing. This study has found that the total number of unique contacts
which appear during triaxial compression increases linearly after 10% axial strain; its rate of change is similar for most of these simulations. As shearing progresses, there is potential for particles which were initially far apart to come into contact so that new contacts are continuously being formed. However, the number of contacts remains quite stable during these simulations. This is also true for the number of contacts in the strong and weak subnetworks.

5. The majority of contacts which are formed in the system (55-80%) are formed more than once. Correlations between contact transitivity and the force transmitted by the contact are weak. Typically over 90% of those contacts which are formed more than five times appear in the strong subnetwork during the simulation, thus indicating that contacts which are formed large numbers of times are not simply ‘rattlers’ within voids but can participate in strong force chains.

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10) References


[25] Huang, X., Hanley, K.J., O'Sullivan, C., Kwok, F.: Effect of sample size on the response of DEM samples with a realistic grading. Accepted for publication in
Particuology (2013)


Figure 1: Particle size distribution within the simulated samples compared with the equivalent distribution for a real Toyoura sand.
Figure 2: Evolution of deviator stress, $q$, in kPa against axial strain (%) for the nine simulations (a-c), volumetric strain against axial strain for both sets of drained simulations (d and e) and mean effective stress, $p'$ (kPa) against axial strain for the constant-volume simulations (f)

Figure 3: Critical state line in e-log($p'$) and $q$-$p'$ space
Figure 4: Percentage of contacts present against duration, $d$. Trendlines are also shown for the plots for linear regressions fitted to the data.

Figure 5: Percentage of contacts present for duration $d$ in the strong subnetwork against duration, where strong contacts are identified as those bearing a contact force greater than the mean. The trendlines are for fitted exponential regressions.

Figure 6: Deviatoric fabric, calculated using the subset of contacts with durations $\geq d$, against contact duration, $d$. 

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Figure 7: Rose diagrams showing the orientations of the branch vectors to the vertical for three representative simulations: 0.627-1000, 0.612-10000 and 0.599-527, respectively. The top row shows all contacts in the system while the bottom row shows only contacts with durations ≥ 0.9. Branch vectors used in the calculation are those when the contact is initially formed. The colours indicate the mean duration of contacts in each segment.

Figure 8: Average contact forces for contacts binned by duration, for which the contact forces were defined in two different ways: the maximum contact force while the contact was present and the mean contact force during this duration. Linear regressions were fitted to the central parts of the plots between durations of 0.2 and 0.8.
Figure 9: Illustration of the linear relationship between the natural logarithm of $p'$ at critical state and both the slopes, $m$, and intercepts, $c$, of the linear regressions shown on Figure 8

Figure 10: Average contact forces for contacts in the strong network binned by duration. As for Figure 8, the contact forces were defined in two different ways: the maximum contact force while in the strong subnetwork and the mean contact force during this duration. Linear regressions were fitted to the central parts of the plots between durations of 0.2 and 0.8

Figure 11: Illustration of the linear relationship between the natural logarithm of $p'$ at critical state and both the slopes, $m$, and intercepts, $c$, of the linear regressions shown on Figure 10
Figure 12: Evolution of the number of contacts, total as well as subdivisions into strong and weak contacts, with axial strain (%)

Figure 13: Increase of the number of unique contacts which appear in the simulations against axial strain (%)

Figure 14: Percentage of contacts which are formed $n$ times during the simulations against $n$
Figure 15: Percentage of contacts which enter the strong network $n$ times during the simulations against $n$