Shear bands as bottlenecks in force transmission

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Abstract – The formation of shear bands is a key attribute of degradation and failure in soil, rocks, and many other forms of amorphous and crystalline materials. Previous studies of dense sand under triaxial compression and two dimensional analogues from simulations have shown that the ultimate shear band pattern may be detected in the nascent stages of loading, well before the band’s known nucleation point (i.e., around peak stress ratio), as reported in the published literature. Here we construct a network flow model of force transmission to identify the bottlenecks in the contact networks of dense granular media: triaxial compression of Caicos Ooid and Ottawa sand and a discrete element simulation of simple shear. The bottlenecks localise in the nascent stages of loading – in the location where the persistent shear band ultimately forms. This corroborates recent findings on vortices that suggest localised failure is a progressive process of degradation, initiating early in the loading history at sites spanning the full extent, yet confined to a subregion, of the sample. Bottlenecks are governed by the local and global properties of the sample fabric and the grain kinematics. Grains with large rotations and/or contacts having minimal load-bearing capacities per se do not identify the bottlenecks early in the loading history.

Introduction. – The lack of a full understanding of shear band mechanics on par with fracture mechanics has been a glaring limitation of predictive models of degradation and failure of dense granular media [1]. Despite a long history of scientific inquiry, many aspects of the origin and evolution of shear bands remain a mystery [1–8]. Knowledge of the origin of shear bands is important for a wide range of practical applications. Shear bands have a deleterious impact on the performance of materials critical to the built environment (e.g., soil and rocks) [1–4]. On the other hand, their properties may prove favourable in other settings, for example, the recovery of petroleum and natural gas found in shale and tight rock formations rely on their rich pores as conduits for flow [6]. From a fundamental perspective, intense research interest has been paid to shear bands as a unifying signature of failure for a broad class of everyday materials known as “soft matter” [5, 9]. Although specific causal mechanisms may differ from one material type to another (e.g., force chain buckling in dense granular media [4, 10] versus STZ transitions in amorphous media [9]), evidence suggest a common root: heterogeneities in the initial fabric which predispose the sample deformation to localise to a particular subregion, once a critical (yield) stress is reached [1, 7–9]. A recent study of shear band formation in dense Hostun sand under triaxial compression, using data obtained from high resolution x-ray \(\mu\)-CT, showed that this subregion becomes incised in the sample much earlier than previously thought [5]. Specifically, the ultimate shear band pattern proved to be encoded in the grain kinematics from the beginning of loading [5]. Corroborative evidence from discrete element simulations further confirmed that this pattern plainly manifests in grain motions earlier than the known precursor of force chain buckling [5, 7]. Under-
standing the implication of these findings in the context of the traditional continuum theory for shear bands [2] has obvious import, especially since the practical analysis of geotechnical structures and geomaterial phenomena is entirely performed in the realm of continuum mechanics [2–4,8]. To that end, the nonaffine displacement field (i.e., the deviation of grain displacements from the affine or uniform strain) presents an essential starting point for analysis, keeping in mind that the continuum deformation of a material under uniform boundary conditions would be uniquely described by this affine strain in the absence of inhomogeneities and instabilities [1,7,8]. A subsequent study, designed to unravel the structural significance of vortices in the early pre-failure regime, showed that such system-wide patterns are also evident in the motions of 3-cycles, i.e., structures comprising three grains in mutual contact, as early as the first strain interval of the test [1]. Moreover, a multi-scale spatio-temporal analysis revealed that the vertical motions induced a preferential and progressive degradation of the most stable subgroup, so-called persistent 3-cycles, along a subregion where the shear band ultimately forms, to the extent that their complete eradication in this subregion marks the full development of the shear band in space and time [1]. Three-cycles give rigidity to granular systems, providing lateral support and rotational frustration to major load-bearing force chains (e.g., [10–12] and refs. therein). As such, their progressive loss in the region where the shear band ultimately forms may explain why force chain buckling initiates there, precipitating collective force chain buckling and in turn the shear band. Given the symmetric boundary conditions and the initially (globally) isotropic state of these samples, the initial bias and attendant instabilities could arguably be attributed to heterogeneities in the microstructural fabric (e.g., contact network) [1,8]. Here we probe this possibility by examining the development of bottlenecks in force transmission through the contact network – from the perspective of network flow theory [13,14].

Many problems dealing with the transmission of information or matter in various systems (e.g. multiprocessor scheduling, circuit partitioning, traffic engineering, pipeline networks, underground mine design, etc.) can be solved by an abstraction to a graph or network [15]. These problems invariably involve quantifying the functionality of the system as a transmission medium and identifying internal structural details that can inhibit transmission. In this context, the maximum flow and the minimum cut are two of the most broadly applied and rich algorithmic problems in network flow theory [15]. The maximum flow determines how much can be transmitted through the network between two artificial nodes in the network (so-called source and sink), whereas the minimum cut represents a set of edges in the network that form the bottlenecks of transmission. Consider, for example, the traffic flow within a network of interconnected two-way roads. In that case, the maximum flow signifies the maximum flow rate of vehicles between two points, (e.g., from a downtown intersection to a freeway on-ramp) over all feasible routes between those points, without exceeding the capacity of any road in the network. Since the minimum cut represents the bottlenecks, these are the roads that need to be widened in order to increase the maximum flow; widening any other road not belonging to the minimum cut will not increase traffic flow.

Preliminary studies of 2D simulation data explored the efficacy of the network flow approach using simple models (see [14] and refs. therein). Here we exploit the most recent advances in high resolution x-ray μ-CT which deliver both individual grain contacts and kinematics for many stages of the loading history of 3D sand samples, including the failure regime where the shear band is fully developed. Our aim is to elucidate a possible root cause of shear bands with respect to force transmission by solving the maximum flow-minimum cut problem using a more realistic model of a contact’s load-bearing capacity. In this model, we take full advantage of the empirical data for each grain, structural and kinematical, for many stages of the loading history.

Data. – Three systems are studied. System A is from a discrete element (DEM) simulation of a simple shear test. Systems B and C are from triaxial compression tests (constant confining pressure) of two types of sand, Caicos Ooid and Ottawa, respectively. The data for each system comprise individual grain contacts, displacements and rotations for each equilibrium state of the test. The salient aspects are summarised briefly below: complete details are reported elsewhere [6,16–18].

System A: DEM simulation of simple shear. As described in [6], this simulation involves an assembly of 129,000 polydisperse spheres subjected to simple shear, with height, width and depth of 118 mm × 50.6 mm × 12.7 mm. Particles are enclosed within periodic boundaries on the four vertical sides, and contained on the top and bottom with an additional single layer of spheres. These thin capping layers break periodicity in the vertical direction and serve as rough rigid platens with which shearing displacements are induced. From an isotropic state, the assembly is horizontally sheared across its height in the direction of its width while maintaining constant vertical normal stress and constant width and depth. Thin shear zones (i.e., micro-bands) appear throughout the assembly shortly after the start of loading, but are non-persistent. A horizontal persistent shear band, of thickness 13–16 times the mean grain diameter, becomes fully developed at 9% strain, extending across the entire width of the assembly.
System B: Triaxial compression of Caicos Ooid sand. A dense, cylindrical dry sand specimen of around 70,000 grains in a latex membrane, 24 mm in height and 11 mm in diameter, is submitted to triaxial compression subject to 100 kPa cell pressure, as described in [16, 17]. Axial strain is controlled at 21 μm min⁻¹. Caicos Ooid grains are very rounded with diameters in the range 200–600 μm. The initial porosity is 35% and no inhomogeneity or anisotropy is evident in the 3D distribution of porosity. The uncontrolled flow rate during deposition can, however, cause horizontal bands of material with larger grains: this leads to fewer intergranular contacts in such bands, albeit at equal porosity within the resolution of measurement. Grain rotations and local strain begin to show inhomogeneities from [0.91, 1.82]% [17], which develop into a fully mature shear band by the increment [5.48, 6.38]%, i.e., approximately halfway between peak stress and the beginning of the residual stress plateau.

System C: Triaxial compression of Ottawa sand. A cylindrical sample of dry F35 Ottawa sand, comprising around 27,000 grains, height of 20.6 mm and diameter of 10.25 mm, was submitted to triaxial compression under a constant confining pressure of 400 kPa, as described in [18]. Grain diameters are in the range 300-425 μm. The initial porosity is 35%. Peak stress is reached at approximately 3.5% axial strain and stretches out to approximately 7% strain, where the principal stress ratio decreases and approaches residual stress plateau at about 12% strain. Grain rotations localise into a single shear band that initiates at around [3.5, 5]% strain, becoming fully developed by 12% strain.

The network flow model. – Forces in a granular material are transmitted through the particle contacts. Thus, we construct a flow network \( \mathcal{N} = (V, E, C, s, t) \) [13–15] based on the contact network of the material. \( V \) is the set of intermediate nodes that represent the particles. \( E \) is the set of edges that connect nodes in \( V \) whose corresponding particles are in physical contact. \( C = \{c_{(i,j)} : (i, j) \in E \} \) is the set of edge capacities: this represents the force-bearing capacity of, or the maximum force units that can be transmitted through, the contact corresponding to edge \( (i, j) \). Two artificial nodes direct the flow: the source node \( s \) and the sink node \( t \). Since the applied compression is in the vertical direction, we may assign the top and bottom loading platens to act as a global source \( s \) and global sink \( t \), respectively, such that edges connected to \( s \) and \( t \) are given infinite capacity [13, 15]. Force flow is symmetric, \( c_{(i,j)} = c_{(j,i)} \); hence, reversing the source and sink assignment would not alter the flow. We solve the maximum flow-minimum cut problem for \( \mathcal{N} \) subject to two constraints. Capacity constraint I: the flow along an edge cannot exceed its capacity, \( f_{(i,j)} \leq c_{(i,j)}, \forall (i,j) \in E \). Capacity constraint II: the flow is conserved at every node except at the source or sink, \( \sum_{u \in V} f_{(u,v)} = \sum_{u \in V} f_{(v,u)}, v \neq \{s,t\} \). Given a feasible flow \( f \), the net flow leaving the source node \( s \) is the same as the net flow entering the sink node \( t \). This is quantified by the flow value \( |f| \): \( |f| = \sum_{u \in V} f_{(s,u)} = \sum_{u \in V} f_{(u,t)} \). The maximum flow problem is an optimisation problem: find a flow \( f \) such that \( |f| \) is maximum [15]. It is a dual of the minimum cut problem: find a partition of the flow network into two disjoint sets \( S \) and \( T \) with \( s \in S, t \in T, S \cup T = V \), such that the capacity of the cut, i.e., sum of the capacities of the edges in the cut, \( c(S,T) = \sum_{u \in S,v \in T} c_{(u,v)} \), is minimum. By the maximum flow-minimum cut theorem, the maximum flow \( f \) is the capacity of the minimum cut [15].

For each of systems A, B, and C, we construct a model of force transmission as a flow through a series of consecutive contact networks, \( \mathcal{N}(\epsilon) \), each representing an equilibrium state of a small assembly of grains. For a given model input, i.e., \( \mathcal{N}(\epsilon) \) and the force-bearing edge capacities \( c_{(i,j)} \), we find the maximum flow and the minimum cut. Since contact forces cannot be directly measured for natural granular materials, we construct a proxy measure for \( c_{(i,j)} \) that exploits the microstructural and kinematical data for the sand samples B and C. Two local quantities are considered: (i) the resistance to relative motion at the contacts, as measured by the relative grain displacement; and (ii) the local topology of the contact, in particular, the number of 3-cycles that the edge is part of (i.e., 3-cycle membership). We base the latter on recent studies that have demonstrated 3-cycles are the mechanical structures that give rigidity to granular systems (e.g., [10–13]). The strong stabilising influence exerted by 3-cycles, established in simulations and experiments, can be tied to the dual support they provide to load-bearing force chain columns, specifically preventing force chain failure by buckling via two mechanisms: they (i) prop-up and restore alignment of grains in force chains, and (ii) frustrate relative rotations at contacts. Incorporating both grain kinematics and local contact topology, we propose the following unitless edge capacity,\

\[
c_{(i,j)} = \frac{1 + \alpha}{|\Delta u_{(i,j)}|^n},
\]

where \( \alpha \) is the 3-cycle membership of edge \( (i, j) \), \( |\Delta u_{(i,j)}| \) is the magnitude of the relative displacement vector of the particles corresponding to nodes \( i \) and \( j \) normalised by the mean particle diameter, and parameter \( n \) is a positive integer. For all samples, the minimum cut achieves its maximum predictive power for \( n = 2 \); no further improvements in the minimum cut prediction are observed for \( n \geq 2 \). Overall, the higher the number of stabilising 3-cycles that a contact is part of and/or the smaller the relative displacement between the two contacting grains, the higher is the load-bearing capacity of that contact. Thus, system properties that influence the edge capacities are those that contribute to: (i) the structural connectivity of the sample (i.e., how densely connected is the contact network) such as initial density (or porosity), number of grains, grain size distribution and the confining pressure;
cannot provide a direct measure of force. Since the edge capacities in Eq. (1) are not expressed in terms of force quantities, the maximum flow (friction). Since the edge capacities in Eq. (1) are not expressed in terms of force quantities, the maximum flow is only a relative measure of force, the maximum flow can only provide a direct measure of force.

Results. – The stress response of all three samples is typical of dense granular materials (Fig. 2(a,b,c)). The stress ratio initially rises to a peak, then decreases, before levelling off to a plateau or residual stress in the failure regime. All samples exhibit dilatancy in the pre-failure regime; global dilatancy ceases as each sample deforms in the presence of a single persistent shear band in the failure regime [6, 16–18]. For each equilibrium state, the model output comprises the contact network and the edge capacity function, while the model output comprises the maximum flow and the minimum cut. It is useful to keep in mind what specific aspects of the edge capacities in Eq. (1) influence the model output. First, the maximum flow depends solely on the absolute edge capacities in the cut, while the minimum cut depends solely on the relative edge capacities. Thus, if we scale all the edge capacities by, say, 10, the maximum flow scales by 10, but the minimum cut stays the same. Second, since $c_{i,j}$ in Eq. (1) is only a proxy measure for force, the maximum flow can only provide a proxy for the load-bearing capacity of the sample: a relative measure of the maximum force that could be transmitted through the contact network in the direction of applied compression. From the evolution of the maximum flow, we see that the functionality of each system as a medium for force transmission progressively degrades prior to failure (Fig. 2(a,b,c)). This degradation is due to dilatancy. The concomitant loss of connectivity as the sample dilates destroys available conduits for force transmission. In the subsequent failure regime, the maximum flow levels off to a near-constant residual value, though small fluctuations can be seen in system A. This suggests that force transmission is governed by the dynamics inside the shear band, a process shown to be driven by the continual creation and destruction of force chains [1,8,10]. That these fluctuations do not manifest to the same degree in B is due to the much lower temporal resolution in the experiment compared to that achieved in the simulation (only one measurement was taken in the failure regime for C, hence we cannot probe further). We note comparable values of the residual maximum flow values, for systems A and B, $3.95 \times 10^{-3}$ and $5.85 \times 10^{-4}$, respectively; that for system C is an order of magnitude less, $2.91 \times 10^{-5}$. These residual values, measured relative to the initial maximum flow, reflect the significant degradation in the ability of each system to transmit forces in the failure regime (note the normalised maximum flow in Fig. 2(a,b,c) is on a logarithmic scale). Overall, the evolution of maximum flow in these samples is in accord with earlier results from DEM simulations of 2D samples under biaxial compression [14].

To assess the predictive power of the minimum cut, we first examine shear band evolution in the early stages of loading using the raw data on grain kinematics and the location and plane of the persistent shear band. No evidence of the shear band manifests until around peak stress ratio; see §1 of [19]. This is corroborated by the spatial distributions of grain rotations, which have long been regarded as a reliable indicator of the spatial extent of shear bands in both simulations and experiments [16, 17]: see Fig. 3(a-c, left) and §2 of [19]. Now compare the grain rotations in Fig. 3(a-c, left) against the location of the bottlenecks from the minimum cut in Fig. 3(a-h, right). In the early stages of loading, the minimum cut literally “draws a line in the sand” indicating the region where the shear band will ultimately form. The extent to which the bottlenecks are related to grain rotations is informative, since the edge capacity does not directly depend on grain rotations. We focus first on system A, where many more measurements were taken at much higher temporal resolution than those attained in either experiment. Initially, grain rotations are negligible in A (Fig. 3(a, left; top row)). Although rotations progressively increase with strain in the stages leading up to peak stress, they remain spatially dispersed throughout the sample, thus providing no indication of where the persistent shear band ultimately forms: see Fig. 3(b, left; top row) and §2 of [19]. By contrast, the bottlenecks localise very early in the loading history — persisting in the same location of the sample from as early as 0.8% shear strain to the end of the

Fig. 1: Depiction of the proposed network flow model for an assembly of 10 grains, compressed in the vertical direction, and their displacement vectors (top left). The contact network through which force is transmitted with 3-cycles highlighted (top right). A flow network is constructed (bottom left): each edge has a force-bearing capacity given by Eq. (1). The top (bottom) wall is represented by a global source (sink) node. The maximum flow–minimum cut problem is solved (bottom right). Edges in the minimum cut (dashed) form a distributed set of bottlenecks, separating the sample into two grain assemblies: red versus blue grains. No more than the maximum flow of 20 force units can be transmitted through the contact network between the top and bottom walls.
Shear bands as bottlenecks in force transmission

Fig. 2: Evolution with strain of the maximum flow (blue cross), normalised by the largest maximum flow value across all states of the test, and principal stress ratio (black curve) as a function of strain for systems A (a), B (b), C (c).

Fig. 3: Particle rotations and minimum cut from the start (column (a)) to the end (column (c)) of loading history, for systems A (row A), B (row B) and C (row C). Each pair of images shows the sample at the beginning of the strain interval; grain colours represent information across the strain interval. Increasing values of rotations (left) are coloured from cool dark blue (lowest) to hot red (highest). In the minimum cuts (right), green particles identify source/sink nodes; grains are coloured by their location on the source (red) or sink (blue) side of the minimum cut. Strain intervals: for A [0,0.0,0.001]% (a), [0.8,0.801]% (b), [12.0,12.01]% (c); for B [0,0.176]% (a), [0.914,1.82]% (b), [10.94,11.85]% (c); for C [0.1]% (a), [1.2]% (b), [12,17.5]% (c). See [19] for additional results.

As patterns can be plainly visualised in 2D, we further tested our findings on the minimum cut for two physical experiments in 2D, reported elsewhere [10,12]. The system in [10] deforms in the presence of a single persistent shear band. The system in [12] maintained uniform deformation throughout loading: shear bands do not form. Minimum cuts, accumulated over many stages of the test, show a persistent localisation in the shear band for the system in [10]; by contrast, the cuts do not localise in the pure shear test where the sample deforms in the absence of shear bands [12] (see also §3 of [19]). Overall, our results on the minimum cut suggest that the early and persistent localisation of bottlenecks in force transmission is what ultimately leads to the formation of the shear band, which plainly manifests in the localisation of grain rotations. These findings are consistent with the preferential and progressive destruction of the most stable 3-cycles observed in the early stages of the loading history — at sites spanning the full extent, yet confined to a subregion, of the sample [1]. We found in [1] that such initial spatial bias predisposed co-located force chains to undergo collective buckling, which in turn led to the shear band forming in that subregion of the sample.

Turning to the sand samples, Caicos Ooid (B) and Ottawa (C), we see essentially the same trend as observed for A, though keep in mind that the temporal resolutions of the measurements of individual grain contacts and kinematics are significantly lower for these: see Fig. 3(a-c, right; middle-bottom rows) and §2 of [19]. With continued
advancements in high resolution imaging and grain tracking, we expect a concomitant improvement in the early prediction of the ultimate location of the shear band for real granular materials by the method of minimum cut — without need for information on contact forces.

Conclusion. – We examined force transmission in three dense granular systems: a discrete element simulation of simple shear (A) and triaxial compression of Caicos Ooid (B) and Ottawa sand (C). At each equilibrium state in the deformation history, we mapped the contact network into a flow network and solved the maximum flow—minimum cut problem. Prior to failure, a progressive decline in the functionality of each sample as a medium for force transmission is evident in the monotonic decrease in the functionality of each sample as a medium for force transmission is evident in the monotonic decrease in the functionality of each sample as a medium for force transmission is evident in the monotonic decrease in force transmission begins from one equilibrium state to another, the bottlenecks become spatially localised early in the loading history — in the region where the persistent shear band ultimately forms. These findings are all consistent with recent results from a multi-scale analysis of vortices from simulations and experiments in 2D [1,8].

Local as well as global properties of the fabric contribute to the formation and location of bottlenecks. Weakly supported grains undergoing large rotations with minimal load-bearing contact capacities do not reliably identify the bottlenecks in the pre-failure regime: here, such grains remain spatially dispersed in the sample even when the bottlenecks could already identify the ultimate location of the persistent shear band.

The early prediction of failure through bottlenecks in force transmission opens new opportunities for detection as well as manipulation of impending failure in granular systems. This study casts light on the pressing need for new knowledge on shear bands, derived from state-of-the-art developments from experiment, simulation and data analysis, to be incorporated in the continuum theory for shear bands [8]. The combination of new opportunities for early detection of failure direct from data, along with improved predictive continuum models of granular failure, can potentially catalyse step change advances in design, development and risk management of a wide range of granular media phenomena.

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