Direct observation of turbulent like vortex-cluster formation in three-dimensional granular flow

Norihiro Oyama,1 Hideyuki Mizuno,2 and Kuniyasu Saitoh3,4
1 Mathematics for Advanced Materials-OIL, AIST-Tohoku University, Sendai 980-8577, Japan
2 Graduate School of Arts and Sciences, The University of Tokyo, Tokyo 153-8902, Japan
3 Research Alliance Center for Mathematical Sciences, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan
4 WPI-Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

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We study the statistical property of dynamics in three dimensional dense granular systems driven by a simple shearing deformation by molecular dynamics simulation. As is the case in two dimension, the velocity fluctuations show typical characteristics of turbulent flow such as the non-Gaussian broader probability distribution, the strong spatial correlation and the energy cascade. We also successfully extracted collective clusters like vortex filaments which are unique structure for three dimensional systems. The size distribution analysis of extracted clusters allows us to define a characteristic length diverging at the close packing fraction.

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Turbulence is frequently observed in nature and represents a non-equilibrium system characterized by cascades of kinetic energy [1]. Because the cascade process, i.e. kinetic energy injected at macroscopic scale is transferred to smaller scales without dissipation and finally dissipates at microscopic level, is ubiquitous, the research of turbulent flows has been aimed for a wide range of different materials, e.g. incompressible fluids [1,2], plasma [1,3], quantum vortex [4,5], bacterial suspensions [6,7], and liquid crystals [8,9]. Nearly all these examples address continuum media and, as typical in statistical physics, the observed turbulence strongly depends on spatial dimensionality [10].

In contrast to the turbulent flows in continuum media, physicists have studied “turbulent-like” complex motions of discrete particles, which are characteristic of disordered systems like glass, emulsions, colloidal suspensions, and granular materials [10]. Then, it has been widely observed that non-affine velocities of discrete particles exhibit vortex structures [10,11], their probability distribution functions (PDFs) show the tails much wider than normal distributions [12,13], and their spatial correlations unveil the collective behavior of disordered materials [14]. Recently, their similarity with usual turbulence has been pointed out by numerical simulations [15-17] and experiments [18] of granular materials, where the cascade process is associated with turbulence except that kinetic energy injected by external forces dissipates through inelastic interactions between granular particles [19]. In addition, the cascade process has been evidenced by the power-law decay of the spectrum of non-affine velocities [20], which is reminiscent of energy cascades in granular materials. However, all these aspects of granular turbulence have been studied intensively in two dimensional (2D) systems and much less attention has been paid to three-dimensional (3D) granular materials.

In this letter, we demonstrate granular turbulence in 3D systems by means of molecular dynamics (MD) simulations for the first time. By extracting vortex-clusters, which is defined based on both the relative distance between particles and the similarity of vorticity, we illustrate that the collective behavior seen in 3D granular turbulence is quite similar to vortex filaments, or the ones in usual fluid turbulence. The cluster analysis also allows us to extract a length scale diverging at the close packing fraction of regular crystal, \(\varphi^* \approx 0.74\), which is much higher than the jamming transition density, \(\varphi_c \approx 0.64\).

**Numerical methods.**— We use MD simulations of 3D granular particles. To avoid crystallization, we randomly distribute a 50:50 binary mixture of \(n = 65536\) particles in a \(L \times L \times L\) periodic box, where different kinds of particles have the same mass, \(m\), and different radii, \(R_i\) and \(R_S\) (with their ratio, \(R_i/R_S = 1.4\)). The force between the particles, \(i\) and \(j\), in contact is modeled by a linear spring-dashpot [21], i.e. \(f_{ij} = -(k_s\zeta_{ij} - \eta \ddot{r}_{ij})\dot{r}_{ij}\) if \(\zeta_{ij} > 0\) and \(f_{ij} = 0\) otherwise. Here, \(\dot{r}_{ij}\) is the unit vector pointing from the center of particle \(j\) to particle \(i\) and \(\zeta_{ij} \equiv R_i + R_j - r_{ij}\) with the particle radii, \(R_i\) and \(R_j\), and the inter-particle distance, \(r_{ij}\), represents the overlap between the particles. In the contact force, we introduce a spring constant, \(k_s\), and viscosity coefficient, \(\eta\), such that the restitution coefficient is given by \(e = \exp(-\pi/\sqrt{2mk_s}/\eta^2 - 1) \approx 0.7\) [22]. Then, we apply simple shear deformations to the system by the Lees-Edwards boundary conditions [23]. In each time step, every particle position, \(\mathbf{r}_i = (x_i, y_i, z_i)\) \((i = 1, \ldots, n)\), is replaced with \((x_i + \Delta \gamma y_i, y_i, z_i)\) and equations of motion are numerically integrated with a small time increment, \(\Delta t\). Here, \(\Delta \gamma\) represents a strain step so that the shear rate is defined as \(\dot{\gamma} \equiv \Delta \gamma/\Delta t\).
Our system is specified by two control parameters, i.e.,
the volume fraction of granular particles, \( \varphi \), and the shear rate, \( \dot{\gamma} \). We estimate the jamming point as \( \varphi_c \approx 0.64 \) and fix the shear rate to \( \dot{\gamma} t_0 = 2.5 \times 10^{-5} \) with the time unit, \( t_0 \equiv \eta/\kappa_s \), where the shear stress hardly depends on the shear rate if \( \dot{\gamma} t_0 \lesssim 2.5 \times 10^{-5} \) (see Supplemental Material (SM) for flow-curves). In the following analyses, we exploit only the data in steady states, where the total strain is greater than unity.

Statistics of non-affine velocities.— To investigate turbulent-like complex motions of granular particles, we analyze their non-affine velocities, \( \delta \mathbf{u}_i \equiv \mathbf{u}_i - \dot{\gamma} \mathbf{y}_i \mathbf{e}_x \) (defined as fluctuations of particle velocities \(^{[25]}\)), where \( \mathbf{u}_i \) and \( \mathbf{e}_x \) are the velocity of \( i \)-th particle and the unit vector parallel to the \( x \)-axis, respectively. Figure 1(a) displays the PDFs of each component of non-affine velocities, \( \delta \mathbf{u}_\alpha = (\delta u_x, \delta u_y, \delta u_z) \), where every PDF is symmetric around \( \delta u_\alpha = 0 \) (\( \alpha = x, y, z \)) and comparable if the volume fraction, \( \varphi \), is the same so that there is no preferred direction for velocity fluctuations. Although such an isotropic behavior is common in 2D flows \(^{[13–15]}\), where all particles move in-plane, we confirm that out-of-plane motions are also equiprobable. As shown by the arrows in Fig. 1(a), the PDFs become broader with the increase of \( \varphi \) and significantly deviate from the normal distribution (the dashed line). Therefore, strong correlations between the non-affine velocities in dense 3D systems are indicated by the wide (almost exponential) tails of the PDFs. Note that the PDFs are getting wider even if the volume fraction exceeds the jamming point, \( \varphi > \varphi_c \).

To quantify the correlations between non-affine velocities, we introduce spatial correlation functions as \( C(r) = \langle \delta \mathbf{u}(r) \cdot \delta \mathbf{u}(0) \rangle / \langle \delta \mathbf{u}(0) \cdot \delta \mathbf{u}(0) \rangle \) \(^{[13,19]}\), where the non-affine velocity field is defined as \( \delta \mathbf{u}(r) \equiv \sum_i \delta \mathbf{u}_i \delta(r-r_i) \) with the delta function, \( \delta(r) \). Here, the ensemble averages, \( \langle \cdots \rangle \), are taken over time and different positions for the origin, \( \mathbf{0} \). Because the non-affine velocities are isotropic in space (Fig. 1(a)), we further take spherical averages such that the correlation functions are given by functions of the distance, i.e., \( C(r) \) with \( r \equiv |r| \). Figure 1(b) displays semi-logarithmic plots of normalized correlation functions, where the distance is scaled by the mean particle diameter, \( d_m \equiv R_L + R_S \). In this figure, the correlation functions monotonously decrease with the increase of the distance and we describe their tails by exponential cutoff, \( C(r) \sim e^{-r/\xi_c} \) (the dotted lines), to introduce a correlation length as \( \xi_c \). We show the dependence of \( \xi_c \) on the volume fraction, \( \varphi \), in the inset of Fig. 1(a): If the system is below jamming, \( \varphi < \varphi_c \), the correlation length increases with the volume fraction, while it plateaus above jamming, \( \varphi > \varphi_c \). Therefore, the length scale extracted from the spatial correlation functions does not diverge at any volume fractions and cannot characterize collective motions above jamming, which we will unveil by analyses of vortex-clusters.

Energy cascades in 3D granular flows.— In addition to the collective motions of granular particles, cascades of kinetic energy can be quantified by the Fourier transform of \( C(r) \), i.e., the spectrum of non-affine velocities, \( E(k) = \rho_0 / 2 \langle |\delta \mathbf{u}(k)|^2 \rangle \). Here, \( \rho_0 \equiv mn/L^2 \) is the mass density and the Fourier transform of non-affine velocities is given by \( \delta \mathbf{u}(k) = \sum \delta \mathbf{u}_i e^{-i k \cdot r} \), with the wave number vector, \( \mathbf{k} \), and imaginary unit, \( i \). The spectrum, \( E(k) \), is an analog of energy spectrum \(^{[25]}\), where its integral over the whole \( \mathbf{k} \)-space gives granular temperature \(^{[32]}\). Because spatial distributions of the non-affine velocities are isotropic, we also take a spherical average...
of the spectrum such that $E(k)$ with $k = |k|$. Figure 2 shows our results of the spectra, where we increase the volume fraction as listed in the legend. As can be seen, the spectrum exhibits the well-established power-law decay, $E(k) \sim k^{-5/3}$ (as indicated by the dashed line), if the system is above jamming, $\varphi > \varphi_c$ (while it decays only weakly below jamming, $\varphi < \varphi_c$). We find that the range of power-law is more than one decade from the system size, $k \sim 2\pi/L$, to about three particle diameters, $2\pi/3d_m$. Moreover, the exponent, $-5/3$, can be derived from a simple dimensional analysis in the similar way Kolmogorov performed \cite{13}. Therefore, the cascade processes of kinetic energy in dense granular flows are associated with usual turbulence and rather complicated structures of non-affine velocities, e.g. “vortices of all possible scales” \cite{11}, can be expected in 3D systems.

Analyses of vortex-clusters.— As we mentioned, the spatial correlation functions cannot characterize complex structures of the non-affine velocities above jamming. Therefore, we turn our attention to the vorticity field, i.e. $\omega(r) = \nabla \times \delta u(r)$. In 2D flows, the vorticity points to the out-of-plane $z$-axis \cite{27}. However, they can rotate in 3D systems and their 3D structures, e.g. vortex filaments, are important aspects of fully developed turbulence \cite{11}. Here, we calculate the vorticity field by the coarse-graining (CG) method as \cite{33,34}

$$\omega(r) = \rho(r)^{-2} \sum_{i=1}^{N} \sum_{j=1}^{N} \psi_j(r) \left[ \nabla \psi_i(r) \times \delta u_{ij} \right] , \quad (1)$$

where $\rho(r)$ and $\delta u_{ij} = \delta u_i - \delta u_j$ are the number density field (which is also calculated by the CG method) and the relative non-affine velocity between the particles, $i$ and $j$, respectively. On the right-hand-side of Eq. (1), the CG kernel for the $i$-th particle is given by a Gaussian function, $\psi_j(r) \equiv e^{-|r-r_j|^2/d_m^2}$ (see SM \cite{31} for full details). Figure 3(a) displays a snapshot of the vorticity, Eq. (1), at each particle position, i.e. $\omega_i \equiv \omega(r_i)$, where the volume fraction is given by $\varphi = 0.66 > \varphi_c$. This figure, we observe that the vorticity distributes heterogeneously in space and there is no preferred direction as in the case of non-affine velocities (Fig. 1(a)). In SM \cite{31}, we show that the PDFs of vorticity are symmetric around zero and exhibit exponential tails (as in usual turbulence \cite{36}) above jamming. To detect 3D structures of vorticity (like vortex filaments), we identify clusters of $\omega_i$ by a similar method used for Janus particles \cite{37,38}: If two particles, $i$ and $j$, are in contact, we compute the angle between $\omega_i$ and $\omega_j$ as $\theta_{ij} \equiv \cos^{-1}(\vec{\omega}_i \cdot \vec{\omega}_j)$, where $\vec{\omega}_i \equiv \omega_i/|\omega_i|$ represents the direction of vorticity. Then, if the angle is smaller than a threshold, i.e. $\theta_{ij} < \theta_c$, we include the particles in a same cluster. We call these clusters vortex-clusters. Figure 3(b) shows a snapshot of vortex-clusters, where we adjust the threshold to $\theta_c = \pi/6$ to obtain their smooth morphologies \cite{37,38}. As can be seen, the 3D structures of vorticity are nicely visualized and it should be noted that their bending, twisting, and branching, of vortex-clusters (Fig. 3(b)), fail to detect the non-trivial 3D structures, e.g. bending, twisting, and branching, of vortex-clusters (Fig. 3(b)).

We quantify the size of vortex-clusters to explain collective motions of granular particles above jamming. Figure 4(a) displays the PDFs of cluster size, $P(N)$, where $N$ is the number of particles in a vortex-cluster. In this figure, all the tails are well described by the power-law with an exponential cutoff, i.e. $P(N) \sim N^{-\alpha} \exp(-N/N_C)$. Therefore, adjusting the exponent, $\alpha$, and characteristic size, $N_C$, we estimate a characteristic length scale from $\xi_C \equiv N^{1/3}_C$. We find that the exponent slightly decreases with the increase of volume fraction below jamming, $\varphi < \varphi_c$, while it converges to $\alpha \approx 1$ above jamming, $\varphi > \varphi_c$. On the other hand, the characteristic size, $n_C$, further increases above jamming such that the length scale, $\xi_C$, does not plateau in $\varphi > \varphi_c$ (the inset of Fig. 4(a)). That is a remarkable difference from the correlation length of non-affine velocities, $\xi$, because the spatial correlation functions, $C(r)$, fail to detect the non-trivial 3D structures, e.g. bending, twisting, and branching, of vortex-clusters (Fig. 3(b)). The dependence of $\xi_C$ on the volume fraction is well described by the Vogel-Fulcher-Tammann-type equation \cite{39}.

$$\xi_C(\varphi) = \xi_C^0 \exp[A(\varphi^*/\varphi) - \varphi)] \quad \text{(the solid line in the inset of Fig. 4(a))},$$

where $\varphi^* \approx 0.74$ adjusted to the data is very close to the close packing fraction of the FCC crystal. The divergence at the close packing fraction can be understood intuitively, i.e. the shearing external force on the perfect crystal would lead to a rigid body rotation of the whole system in which the correlation length is infinite. Interestingly, the length scales, $\xi$ and $\xi_C$, agree

![FIG. 2. Double logarithmic plots of the spectra, $E(k) / E(0)$, where the wave number $k$ is scaled by the mean particle diameter as $kd_m/2\pi$. The volume fraction, $\varphi$, increases as listed in the legend and the dashed line depicts the power-law decay $E(k) \sim k^{-5/3}$ which the scaling analysis predicts for mesoscopic scale \cite{33}.](image-url)

![FIG. 3. Analysis of vortex-clusters.](image-url)

![FIG. 4. Quantitative analysis of vortex-clusters.](image-url)
FIG. 3. (a) The vorticity, Eq. (1), at each particle position, i.e., $\omega_i$ (the arrows), where the color represents its magnitude, $|\omega_i|$. (b) Two large vortex clusters are extracted from (a) where color different clusters are depicted by different colors and the darkness represents the magnitude. In both (a) and (b), only subsystems are visualized and the volume fraction and shear rate are given by $\varphi = 0.66$ and $\gamma t_0 = 2.5 \times 10^{-5}$, respectively.

with each other if the system is below jamming, indicating that the non-trivial 3D structures of vortex-clusters are characteristic above jamming.

The simple morphology of clusters can be quantified by the polar order parameter $\psi(N)$ of the vorticity vectors of component particles as a function of the cluster size $N$. The polar order $\psi(N)$ is defined as $\psi(N) = \left(\frac{1}{N} \sum_i |\tilde{\omega}_i|\right)$. The calculated results are shown in Fig. 4(b). When all vorticity vectors are completely parallel, $\psi(N) = 1$, and when the directions are completely random, $\psi(N) \sim 1/\sqrt{N}$. Also, especially in the current situation, if all vectors are distributed within $\theta_C$ from a unique axis of order, $\psi$ is larger than a critical value $\psi_C = \cos \theta_C \approx 0.866$. We call such a cluster a “uniaxial cluster”. On the other hand, the order parameter $\psi$ is less than $\psi_C$ for the case of “multi-axial clusters” where multiple uniaxial clusters are merging into a single one with bridging particles in between individual uniaxial clusters. We stress that such multi-axial clusters can not be realized in 2D systems where all vorticity vectors must be parallel. Interestingly, the characteristic cluster sizes $N_C$ for unjammed systems all meet $\psi(N_C) > \psi_C$. In other words, most clusters in the unjammed regime are uniaxial. On the other hand, in jammed regime, $\psi(N_C)$ becomes less than $\psi_C$ which means multi-axial clusters are observed rather frequently. Different branches of multi-axial clusters are treated as uncorrelated by the simple spatial correlation function $C(r)$, while within a branch or a uniaxial-cluster, $C(r)$ can detect the correlation. This might be the reason why we see clear discrepancy between $\xi_S$ and $\xi_C$ only in the jammed regime.

Summary. — To conclude, we confirmed that the granular turbulence does take place in 3D systems. Such a turbulent-like property is quantified by the PDF or the spatial correlation function of the non-affine velocities, and by the energy spectrum whose power-law behavior can be explained also theoretically. We also successfully extracted the collective structure equivalent to conventional vortex filaments, by looking at coarse-grained vorticities on particle. The extracted cluster allows us to define a characteristic length scale which diverges at around the close packing density $\varphi^* \sim 0.74$.

We confirmed that statistical properties of non-affine velocities were consistent with those in 2D flows [26] and found that the spectra of non-affine velocities showed the power-law decay with the same exponent for 3D turbulence. The spatial correlation functions cannot characterize complex structures of the non-affine velocities above jamming.

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* oyama.norihiro@aist.go.jp
FIG. 4. The volume fraction dependence of the results of the cluster analysis. (a) The PDFs of the cluster size $N$. The dashed line depicts the power-law decay $P(N) \sim N^{-\chi}$ and the dotted lines represent the fitting curve. The inset shows two distinct characteristic length $\xi_C$ (circles) and $\eta$ (triangles) as functions of the volume fraction. The solid line in the inset depicts the VFT law fitting of $\xi(\varphi)$. (b) The polar order parameter $\psi(N)$ of clusters as a function of $N$. The dashed line indicates the critical value $\psi_C$. The inset sketches are schematic images of uniaxial and multiaxial clusters. In both (a) and (b), colors are as in Fig. and in (a), $\varphi$ increases as indicated by the arrow.

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tally share the origin of the power law behavior.

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