Statistical Law of Turbulence in Granular Gas

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Abstract. A novel description of granular gases from the viewpoint of “fluid turbulence” is presented. In the large-scale simulation by event-driven molecular dynamics simulations, we obtained clear evidence for the energy and enstrophy (square of vorticity) cascade, in which we found $-5/3$ (3D) and $-3$ (2D) exponents predicted by the Kolmogorov and Kraichnan-Leith-Bachelor energy spectrum, respectively. The growth of the Reynolds number based on the Taylor microscale confirmed that the cascade regimes were that of fully developed turbulence. During the evolving process of the regime in fully developed turbulent inhomogeneous state, we discovered a new regime arose from the collision between “clusters”, in which the previous theoretical predictions of the energy decay in this regime collapse.

1. Introduction
Granular gases are fascinating systems from the viewpoint of extending classical equilibrium statistical physics. They are defined by the fact that the characteristic time of granular motion driven by external forces (e.g., gravity or a vibrating plate) is small compared to the mean free time between inelastic collisions (See, review papers [1, 2]) Because granular motion is strongly affected by the energy source in general, the inelastic hard sphere (IHS) model without gravity, called the “freely evolving granular gas”, has been much investigated as a simple model, using methods based on several different levels of analysis. These levels include the microscopic (molecular dynamics (MD)) [3 - 8], the mesoscopic (Enskog-Boltzmann equation) [9, 10] and the macroscopic (Navier-Stokes (NS) equations, Ginzburg-Landau theory) [11 - 14].

In the inviscid limit of three-dimensional (3D) and two-dimensional (2D) incompressible NS turbulence (i.e., the Euler equation at high Reynolds number), energy and enstrophy are conserved in time. The enstrophy $Z$ in 2D is defined by $Z = \frac{1}{2} \langle (\nabla \times u)^2 \rangle$, where $(\nabla \times u)$ and $u = (u_x, u_y)$ are the vorticity and the velocity, respectively. We also define the rate of volumetric dilatation as $Q = \frac{1}{2} \langle (\nabla \cdot u)^2 \rangle$. As a result, the most prominent dynamic features of 2D turbulence are two fluxes in the k-space. By dimensional analysis, a $-5/3$ (3D) or $-3$ (2D) power law in energy spectrum is derived under the assumption that the energy spectrum only depends on the energy or enstrophy flux and the wave number, which is called Kolmogorov or Kraichnan-Leith-Bachelor (KLB) theory,

$$E(k) = Ce^{2/3}k^{-5/3}, \quad (3D)$$
$$E(k) = C'\eta^{2/3}k^{-3}, \quad (2D)$$

where $C$ and $C'$ are constant; $\epsilon$ and $\eta$ are the energy and enstrophy transfer rate, respectively [15 - 17]. These cascade mechanisms are phenomenological, highly nontrivial and difficult to understand especially at the microscopic molecular level.
In the granular system, although these analogies have been pointed out by several authors [18, 19, 20], there are very few studies related to turbulence, because the dissipation mechanism of viscosity in the NS equation is viewed as completely different from that of inelastic collisions. First, Taguchi found numerically that the energy spectra from particle displacements at mid-depth in a 2D vibrated granular bed, which was composed of a few hundred particles, have a $-5/3$ exponent, similar to Kolmogorov scaling in 3D turbulence [18]. Then, neglecting the influence of gravity, a 2D granular gas with a Langevin-type thermostat was studied by Peng and Ohta in a system with about $10^3$ particles [19]. Radjai and Roux [20] reported the spatial power-law spectrum of the particle displacements, as in Taguchi’s work, in the quasi-static motions of the dense granular flow with a Parrinello-Rahman type boundary in a 2D MD model. All studies were performed in 2D and showed the power-law scaling of the energy spectrum and some relationship to NS turbulence. However, the special features of 2D NS turbulence were not shown. The main possible reasons for this are the following: (a) the statistical errors are quite large because of the small number of particles, (b) the system size is too small and is comparable to the minimal spatial correlation lengths (such as the Kolmogorov dissipative length), (c) no systematic parameter surveys exists, and (d) the unique features of 2D turbulence are not well-known in the granular physics community.

In our previous study [21], we have investigated the macroscopic statistical properties on the freely evolving quasi-elastic IHS model by performing a large-scale event-driven molecular dynamics with mainly $512^2$ particles system and found that remarkably analogous to an enstrophy cascade process in the decaying 2D fluid turbulence. We found that there are four typical regimes in the freely evolving inelastic hard disk system, which are homogeneous, shearing (vortex), clustering and final state. In the shearing regime, the self-organized macroscopic coherent vortices become dominant. In the clustering regime, the energy spectra are close to the expectation of KLB theory and the squared two-particle separation strictly obeys Richardson law. In this paper, we have performed the simulation with $2048^2$ for 2D and $128^3$ for 3D particles system. The present system in 2D is 16 times larger than that of previous our works. We have confirmed the previous study on a clear quantitative evidence of the enstrophy cascade. To compare with the direct numerical simulation (DNS) of fluid turbulence quantitatively, we discuss the Reynolds number based on the Taylor microscale in our simulation.

2. Model and Numerical method

The freely decaying IHS model is so simple that the system is completely characterized by only three parameters: the restitution coefficient $r$, the total number of disks $N$, and the packing fraction $\nu$. The system size $L$ in units of disk diameter $\sigma$ is $L/\sigma = \sqrt{\pi N/\nu}/2 \ (2D)$ and $\sqrt[3]{4\pi N/(3\nu)}/2 \ (3D)$. All disks are identical, so the system is mono-dispersive. For the dissipation, the normal restitution coefficient $r$ for binary instantaneous collision is introduced (i.e., parallel to the relative position of the two colliding disks in contact).

Even in the quasi-elastic thermodynamic limit, the system becomes unstable and several spatio-temporal scales appear. The standard evolution scenario is that spatial instabilities occur from the initial homogeneous cooling state (HCS: 1st stage) to the velocity field (shearing regime: 2nd stage), and then to the density field (clustering regime: 3rd stage). Finally, global structures in the system (final attractor regime: 4th stage) appear as a non-equilibrium steady state, or local inelastic collapse occurs.

The system consists of up to about 4.2 million hard disks (2D) or 2.1 million hard spheres (3D) placed in a square or cubic box with periodic boundaries without any external force. To perform a large scale simulation, a simple and efficient event-driven algorithm is used [22]. Initially, the system is prepared in the equilibrium state (i.e., the density is uniform and the disk velocities are Maxwell-Boltzmann distributed) by a long preparation run in an elastic system (i.e., $r = 1$; the so-called the Alder solid-fluid transition occurs when the packing fraction is $\nu \sim 0.70$ for 2D and
Figure 1. The energy spectra at the onset of clustering regime (3rd stage) are shown. The exponents develop a maximum close to $-3$ for 2D (the left) and $-5/3$ for 3D (the right). The parameters are set at $(r, N, \nu)=(0.99637, 2048^2, 0.60)$ for 2D and $(0.95, 128^3, 0.40)$ for 3D, respectively.

Because the total energy is monotonically decreasing in a freely evolving process, constant energy in time can be realized by attaching a thermostat. There are several types of thermostats to keep the total kinetic energy constant, roughly categorized as deterministic or stochastic. The advantage of a deterministic thermostat is that the trajectory of particles does not change compared with the non-thermostat case. Here, we introduce the new-scaled time $t_s$, which is described by $t_s = \int_0^t \beta(t)^{-1} dt$, where $\beta(t) = \sqrt{T(0)/T(t)}$, where $T(t)$ is the average kinetic energy per particle as a function of the usual time $t$. Introducing a new-scaled time $t_s$ instead of $t$ is completely equivalent to adding a deterministic thermostat to the hard sphere system [23, 24].

3. Results

3.1. Energy Spectrum

In Fig. 1, the energy spectra $E(k)$ (power spectra of the “kinetic temperature” field, which are discretized by grids of size the disk diameter $\sigma$) at $(N, \nu) = (2048^2, 0.60)$ for 2D (left) and $(128^3, 0.40)$ for 3D (right) with respect to the nondimensional wave number divided by the energy dissipation for inelastic collisions $\sqrt{1-r^2}$ are shown. Although the local equilibrium assumption in a granular system is not valid, we regard the granular temperature as the “kinetic temperature” since the restitution coefficient is set near the elastic case between collisions and the system is still regarded as homogeneous state in density before the clustering regime.

Our large-scale simulations show that $E(k)$ develops towards exponents $-3$ (2D) and $-5/3$ (3D) for small wavenumbers (large scale), until the onset of the clustering regime (3rd stage) [21], as is expected by the KLB and Kolmogorov theory for freely decaying 2D and 3D NS fluid turbulence, respectively.

In 2D case, we calculated the time evolution of the dissipation rate for the scaled enstrophy $-d\tilde{Z}/dt_s$ and found that the enstrophy peak is a criterion to estimate the boundary time between the shearing regime (2nd stage) and the clustering regime (3rd stage). The enstrophy dissipation is almost finished around $t_s \sim 500$, at which time the exponent of the energy spectrum reaches...
Figure 2. Developed turbulent patterns in the vorticity (left) and temperature (right) fields around \( t_s \sim 500 \) in 2D. The parameters are the same as in the left of Fig. 1.

In Fig. 1, we can also estimate the characteristic spatial scales \( K_d = k \sigma / \sqrt{1 - r^2} \sim 2 \) (2D) and \( \sim 4 \) (3D) as the minimal dissipative domain, which are composed of about \( \sim 10^3 \) disks and \( \sim 10^2 \) spheres, respectively. Although the particle number in the dissipative domain depends on the packing fraction and the restitution function, we also confirmed that the values of the minimal wavenumber \( K_d \) scaled with a function of the restitution coefficient \( \sqrt{1 - r^2} \), as predicted by kinetic theory. Figure 3 shows various values of \( E(k) \) in 2D, scaled by a function of the restitution coefficient over a wide parameter space when the packing fraction is fixed at \((N, \nu) = (2048^2, 0.60)\). During the evolution of \( E(k) \) for small wavenumbers, the minimal dissipation scale \( K_d \) appears not to change. Even when the systems have already evolved to the beginning of the clustering instability, the scaling behavior for the minimal dissipation is valid. When the restitution coefficient is close to unity, we found that the inertial range grows gradually. This suggests that the Reynolds number becomes higher in the quasi-elastic limit.

3.2. Microscale Reynolds Number

In the study of fluid turbulence, the dimensionless Reynolds number \( Re \) is estimated to characterize the quantitative measurement of the turbulent state, which is given by the ratio of inertial forces to viscous forces. To analyze the small-scale statics in the DNS of NS turbulence, the Taylor’s microscale Reynolds number is often used. In this subsection, we also estimated the Taylor microscale Reynolds number in the granular gas.

The Taylor microscale \( \lambda \) in homogeneous isotropic incompressible \( D = 2 \) or \( 3 \) dimensional NS turbulence with zero mean velocity can be derived as,

\[
\lambda = \sqrt{\frac{D(D + 2) \nu_{\text{vis}} \langle u_x^2 \rangle}{\langle \epsilon \rangle}},
\]

where \( \nu_{\text{vis}} \) and \( \langle \epsilon \rangle \) are the kinematic viscosity and the energy dissipation rate, respectively. For a hard core fluid, the kinematic viscosity \( \nu_{\text{vis}} = \eta_E / \rho \) can be derived by the density \( \rho (= mn) \) and Enskog shear viscosity \( \eta_E \), which can numerically be estimated by the expression of the Enskog theory for hard disk systems by Gass(1971) [25] with the third Sonine polynomial approximation in 2D and by Wainwright(1964) [26] with the equation of state by Ree & Hoover (1967) [27] in 3D.
Figure 3. Scaling behavior of the energy spectra at the onset of the 3rd stage for different restitution coefficients $r$ at a fixed $(N, \nu) = (2048^2, 0.60)$.

For example, the expression of Enskog shear viscosity $\eta_E$ for 2D is,

$$\eta_E = \eta_0 \gamma \rho \left\{ \frac{1}{\gamma \rho \chi} + 1 + \gamma \rho \chi \left( \frac{1}{4} + \frac{2}{\pi \gamma_0(3)} \right) \right\},$$

(4)

where $\eta_0 = (\gamma_0(3)/2\sigma)\sqrt{mkT/\pi}$, $\gamma \rho = \pi \sigma^2 n/2 = 2y$, $\chi = (1 - 7y/16)/(1 - y)^2$ (Enskog scaling factor), $y = \pi \sigma^2 n/4$, and $n$ is number density. Here we use in the third Sonine polynomial approximation $\gamma_0(3) = 1.022$.

The Reynolds number based on Taylor microscale $\lambda(t_s)$ can be estimated as,

$$R_\lambda(t_s) = \frac{\langle u_s^2 \rangle^{1/2} \lambda(t_s)}{\nu_{vis}}.$$

(5)

Because we can obtain both the energy dissipation rate $\langle \epsilon \rangle$ via Haff’s law and the kinematic viscosity via Enskog theory, we can roughly estimate $R_\lambda \sim 10$ at $t_s = 0$. However, $R_\lambda$ increases to 327 (2D) and 1470 (3D) at the onset of the deviation from Haff’s law in the kinetic energy decaying functions. Although the granular gas system is well described as the compressible macroscopic fluid equations, we can regard that the system is still almost homogeneous in the early stage of relaxation. Therefore, before the clustering regime begins, the derivation of Taylor’s microscale expression may be considered valid. This assumption is also confirmed to be fairly good approximation by the calculation of the fluctuation of density as shown in the Fig. 1 of Ref. [21].

3.3. Asymptotic Energy Decay after Haff’s Law and Cluster Collision Regime

During the 1st stage, uniform granular gas remains homogeneous, however, the kinetic energy (or velocity) decreases via inelastic collisions in time. In this regime, the granular temperature $T(t)$ decays according to Haff’s law,
The relationship between time $t$ and scaled time $t_s$ (left) and the total kinetic energy per particle divided by its initial energy $T(t)/T(0)$ in terms of $t_s$ in the evolving process of granular gas (right) are shown.

\[
\frac{T(t)}{T(0)} = \frac{1}{(1 + t/\tau_0)^2} \equiv \exp\left(-2\tau_0 \tau\right)
\]

where $\tau$ is collision number and $\tau_0$ is a fitting parameter, which can also be estimated explicitly by the kinetic theory in dilute case.

In the clustering regime, due to inhomogeneous in density, $T(t)$ deviate from Haff’s law. In our large simulation (e.g., parameters are set at $(N, \nu, r) = (2048^2, 0.60, 0.9964)$), the relationship between $t$ and $t_s$ are consistent with the Haff’s law at 1st to 2nd stages and becomes $t \sim t_s^2$ after 3rd stages (the left of Fig. 4). We confirmed that the energy decay is also consistent with the Haff’s law before clustering regime (the right of Fig. 4).

The long time (asymptotic) behavior of $T(t)/T(0)$ in a system of freely IHS model are predicted by several theories [28, 29], which are using mode coupling theory and extension of inelastic (sticky) hard rods gas. In 2D case, both theories predict $T(t)/T(0) \sim \tau^{-1}$ and $\sim t^{-1}$, respectively. In the 3rd stages, although we confirmed that the theoretical predictions are consistent with our simulations in relatively dilute system, the deviation is gradually observed in relatively dense system. In the right of Fig. 4, we can estimate that $T(t)/T(0) \sim t^{-3/4} \sim \tau^{-2}$, where $\tau \sim t_s^{3/2} \sim t_s^{3/4}$. Therefore, we found that the exponent of power decay in the 3rd stage at the dense system seems to be slower than that of dilute case, which cannot be explained by the previous theories.

Moreover, we found that the power law of the kinetic energy decay at 3rd stage is also collapsed after $t_s \sim 800$ in the right of Fig. 4. To investigate the reason of this deviation, we focus on the collision rate during the evolving process in terms of $t_s$, which increases rapidly at this regime. Based on the detail analysis of dynamics, we conclude that this deviation comes from collisions between “clusters”. In the 3rd stage, several large clusters are created and distributed separately in space. Eventually those clusters composed of large number of inelastic particles collide each other at this regime (after $t_s \sim 800$). This regime (new 4th regime: cluster collisions) can clearly be seen more than a few million particles system, which cannot be resolved in the
relatively small particles system. In the actual simulation, the spatial distribution of the rate of volumetric dilatation $Q(x)$ defined in Sec. 1 clearly show that the propagation of semicircular shape density shock wave in the clusters appears in this regime. The theoretical prediction of asymptotic behavior of energy decay after the clustering regime is not valid at high density and large scale system. This new finding might be considered to be important in the late stage of aggregation process in the system composed of many granular particles (such as the formation of the planetesimal (an ultimately small fraction of a planet)). We are now analyzing this regime in detail, which will appear elsewhere in the near future.

4. Concluding remarks
In this study, we showed several analogous features of both 2D and 3D NS turbulence in granular gases using the well-defined simple IHS model. By extensive event-driven molecular dynamics and systematic estimations of the spatial correlation in a wide parameter space, typical features of 2D and 3D NS turbulence (i.e., the enstrophy and energy cascade) were found in the relatively dilute early stages of the granular gas. We also found that the maximum of the enstrophy dissipation rate is a clear criterion to determine the time between the shearing and clustering regimes in 2D. The energy spectra were the same as expected from KLB(2D) and Kolmogorov(3D) theory at the onset of the clustering stage. The minimal dissipation scale depended on the restitution coefficient and could be scaled by a function of the restitution coefficient. In the quasi-elastic limit, because the features of turbulence clearly appear, the system has a high Reynolds number with Taylor microscale $R_\lambda \sim 327$ (2D) and $R_\lambda \sim 1470$ (3D) in our simple estimation. In general, because the laboratory and industrial turbulent flows are characterized by $R_\lambda \sim O(10^2 \sim 10^3)$, it is quite reasonable that the granular gas system shows the specific laws of turbulent behavior. These results suggest that the granular gas in the quasi-elastic and thermodynamic limit is strongly related to both 2D and 3D NS turbulence. It is indeed interesting that modern large scale molecular dynamics simulation can allow us to check the validity of the macroscopic NS equation and its numerical solution by DNS directly. These molecular dynamics simulations are hence an important bridge between the microscopic and macroscopic levels, and offer another route to approach the problem of fluid turbulence.

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