Extraction of Turbulent-like Vortex-Cluster in 3D Granular Flow

(arXiv:1805.05449)

MathAM-OIL, AIST-Tohoku U

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Agenda

- Introduction

  Turbulence & Granular Turbulence
- Numerical Methods

  Molecular Dynamics Simulation under Simple Shear
- Results (arXiv:1805.05449)

  3D Granular Turbulence & Its Complicated Structure
- Summary & Overview

Granular Turbulence

- Today's topic -

- Why is it regarded as a turbulence?
- How nontrivial is it?

Ubiquity of Turbulence

Tuebulent Behaviors in the Nature

- Newtonian fluid
- Quantum vortex
- Plasma
- Topological defects in liquid crystals
- Bacterial suspension

▶ Most examples are suitable for the continuum description

Granular Turbulence

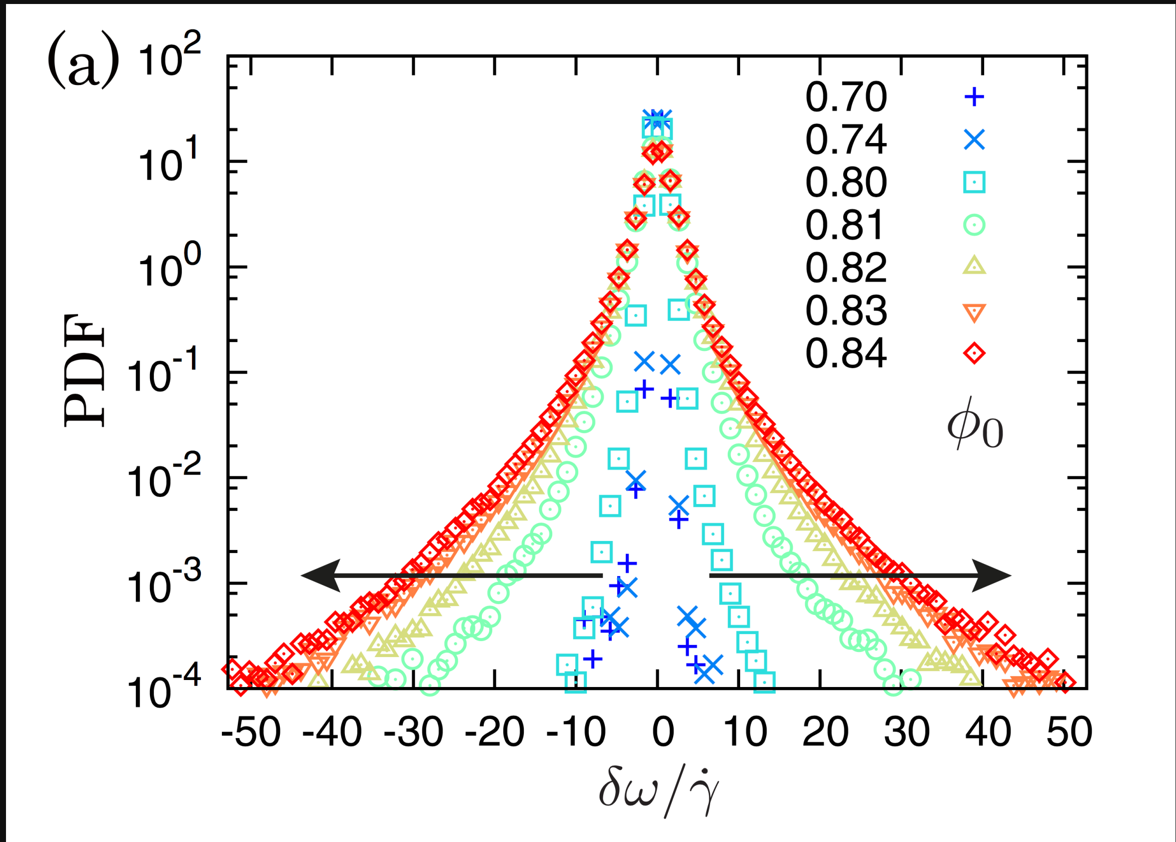
Turbulence in a discrete system!!

- Only reported on 2D systems

F. Radjai and S. Roux, *Phys. Rev. Lett.*, 2002, **89**, 064302

2D granular turbulence 1

Non-Gaussian (broader) probability distribution function of the vorticity

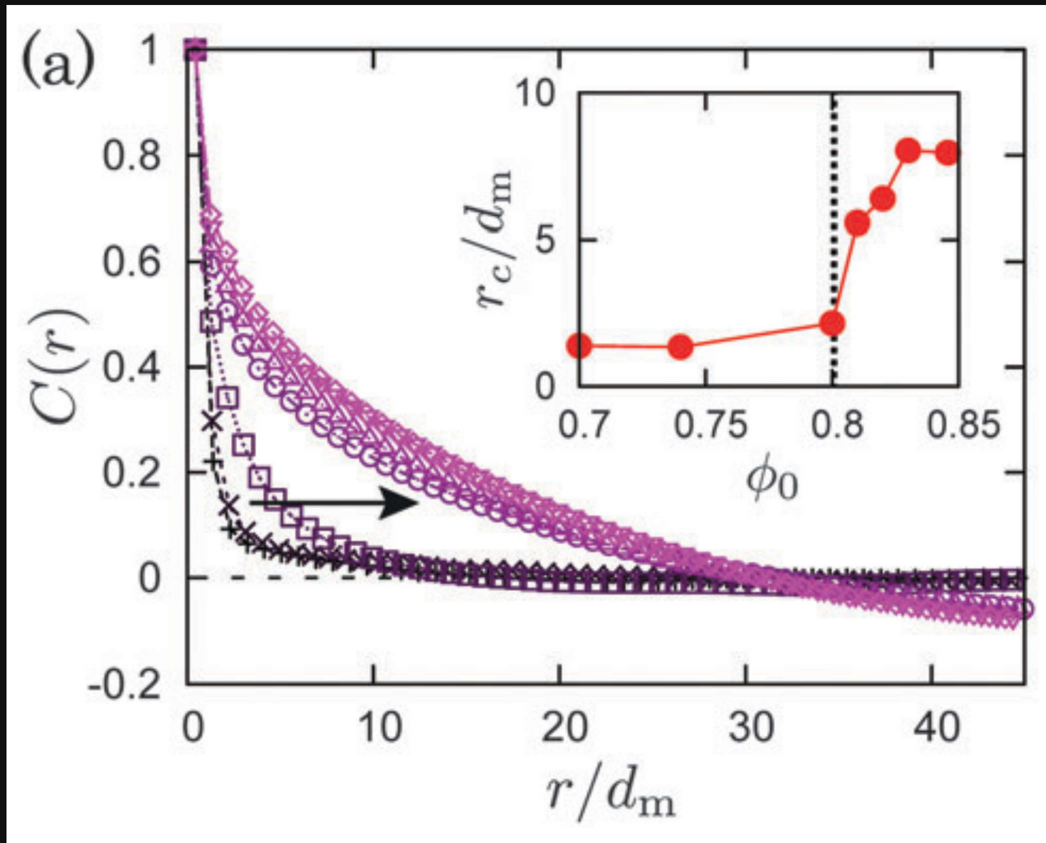


K. Saitoh and H. Mizuno, *Phys. Rev. E,* 2016, **94**, 022908

- The distribution is isotropic also

2D granular turbulence 2

Long-ranged spatial correlation of the non-affine velocity

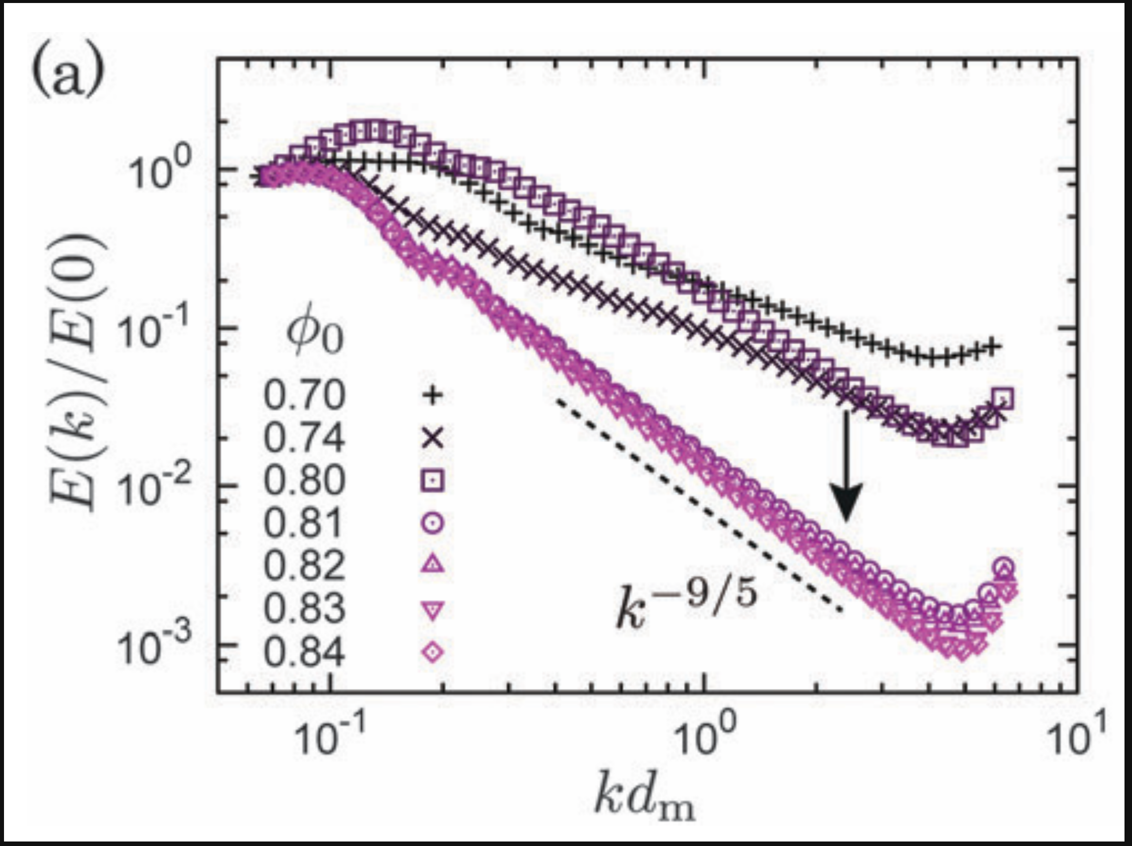


K. Saitoh and H. Mizuno, *Soft Matter*, 2016, **12**, 1360

- Correlation becomes long-ranged discontinuously at φ_j

2D granular turbulence 3

The power-law decay of the energy spectrum

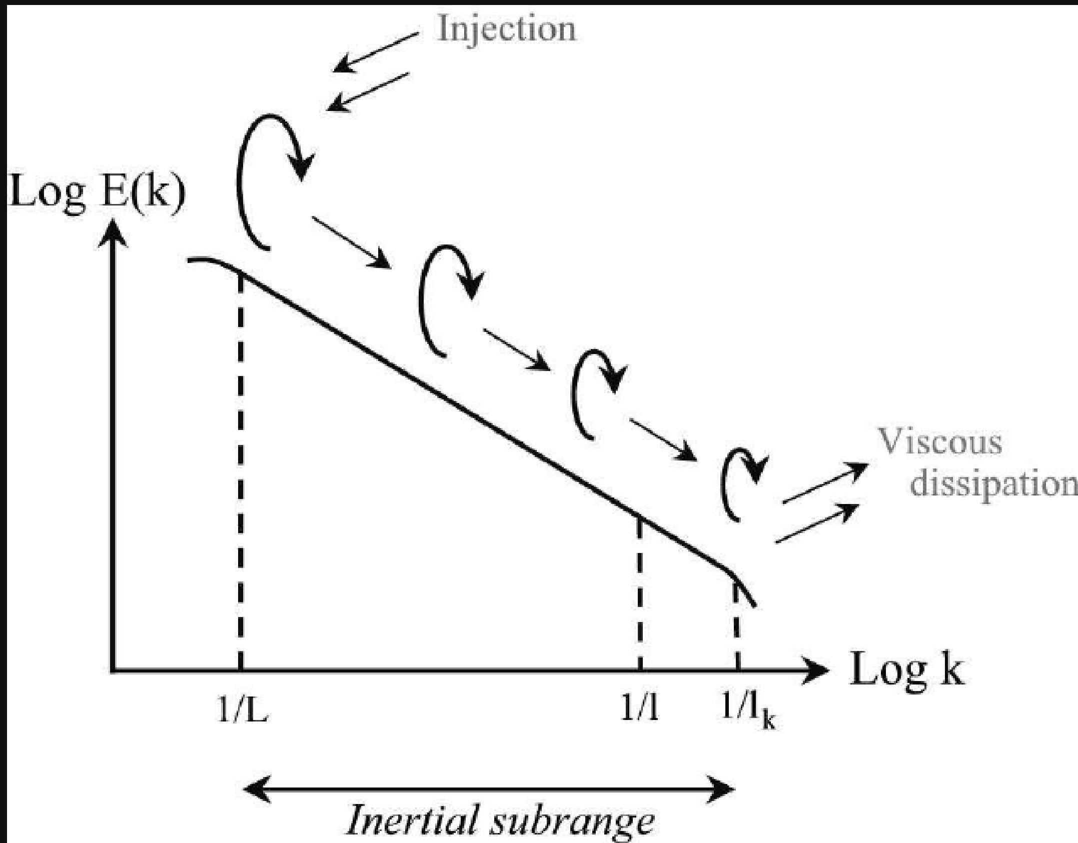


K. Saitoh and H. Mizuno, *Soft Matter*, 2016, **12**, 1360

- Energy cascade = characteristic feature of turbulence

Intuitive Picture of Energy Cascade

Inertial subrange



(from Wikipedia)

Questions to be Answered

- What if in 3D = "more realistic" systems?
- Dimensionality affects the statistical properties?
- What is unique for 3D?
  (3D complicated structure?)

Numerical Methods

- MD simulation with external shear -

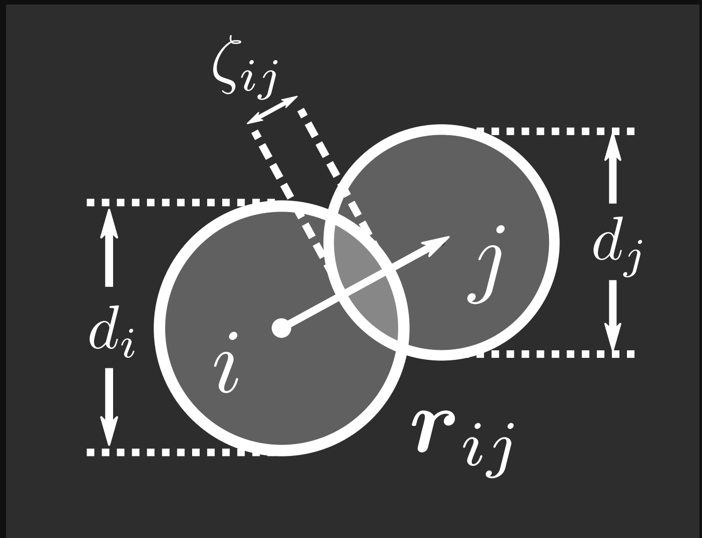
Particle Interaction

- Linear spring-dashpod model -

$$\boldsymbol{f}_{ij} = \begin{cases} -\left(k_\mathrm{s}\zeta_{ij} - \eta\dot{\zeta}_{ij}\right)\tilde{\boldsymbol{r}}_{ij} & (\zeta_{ij} > 0) \\ 0 & (\mathrm{otherwise}) \end{cases}$$

$$\zeta_{ij} = \frac{1}{2}\left(d_i + d_j\right) - r_{ij}$$

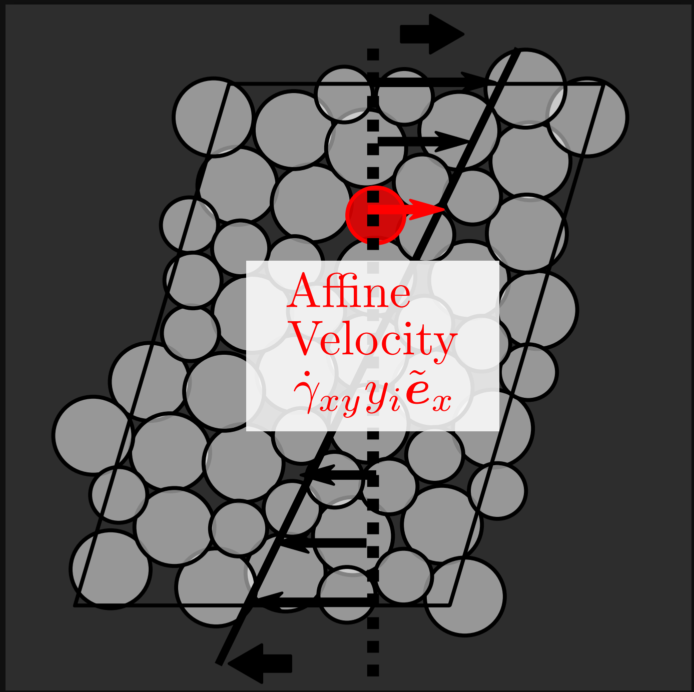
(k_s :spring constant, η : damping coefficient)



Steady simple shear
- with Lees-Edwards boundary condition -

$$\dot{\boldsymbol{r}}_i = \boldsymbol{u}_i = \delta\boldsymbol{u}_i + \dot{\gamma}_{xy} y_i \tilde{\boldsymbol{e}}_x$$

$$\delta\dot{\boldsymbol{u}}_i = \frac{1}{m}\sum_{j\neq i} \boldsymbol{f}_{ij}$$



Steady simple shear
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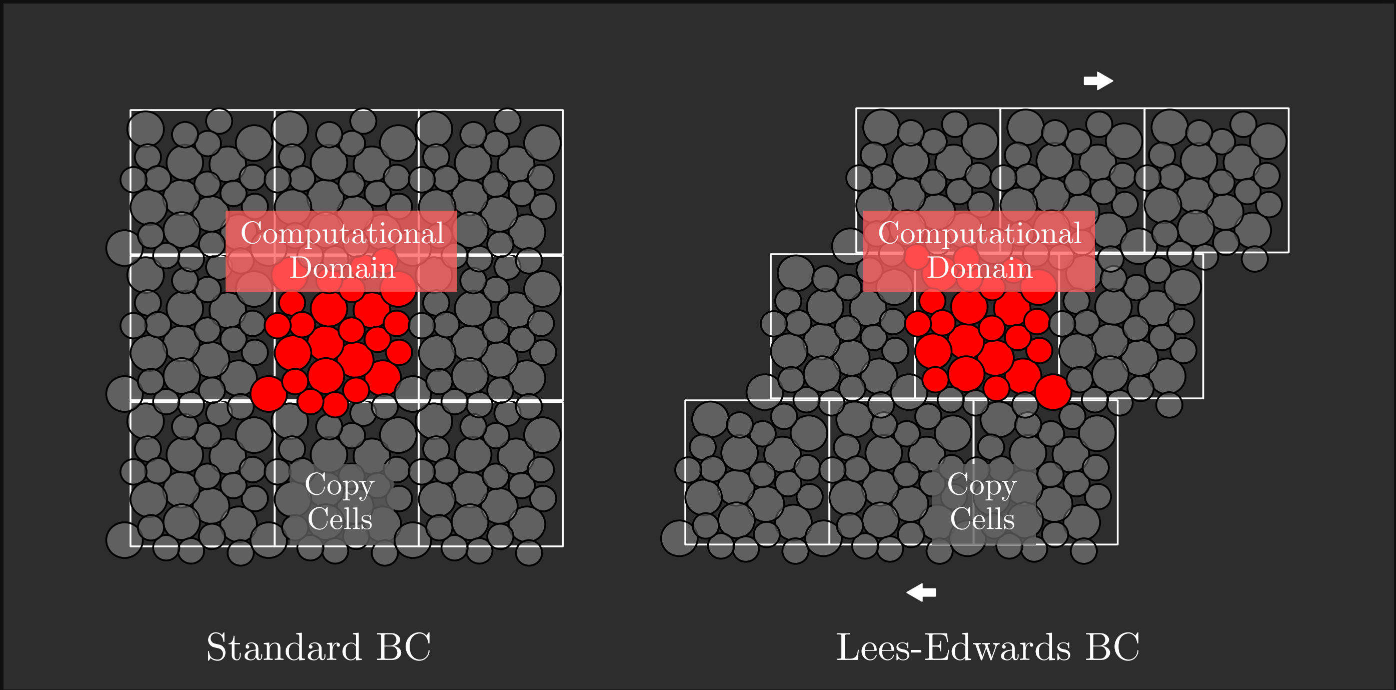
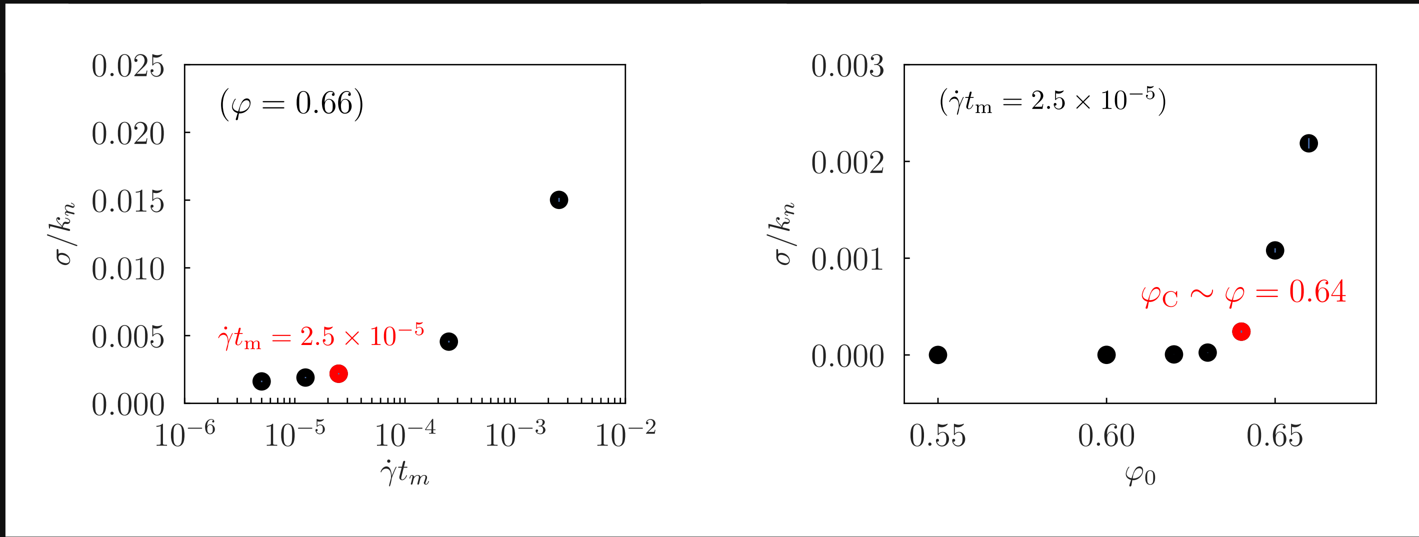


Parameters

50% : 50% binary mixture	$d_\mathrm{A} = 1$ and $d_\mathrm{B} = 1.4$
Number of particles	N = 65536
Shear rate	$\dot{\gamma} t_\mathrm{m} = 2.5 \times 10^{-5}$
Mean volume fraction	$\varphi = 0.6 - 0.66$ $(\varphi_\mathrm{c} \sim 0.64)$
Spring constant	$k_\mathrm{s} = 40$
Viscosity	$\eta = 1$

Flow Curves of the Current System



- Jamming transition point: around 64 %
- $\dot{\gamma}t_{\mathrm{m}} = 2.5 \times 10^{-5}$ is used

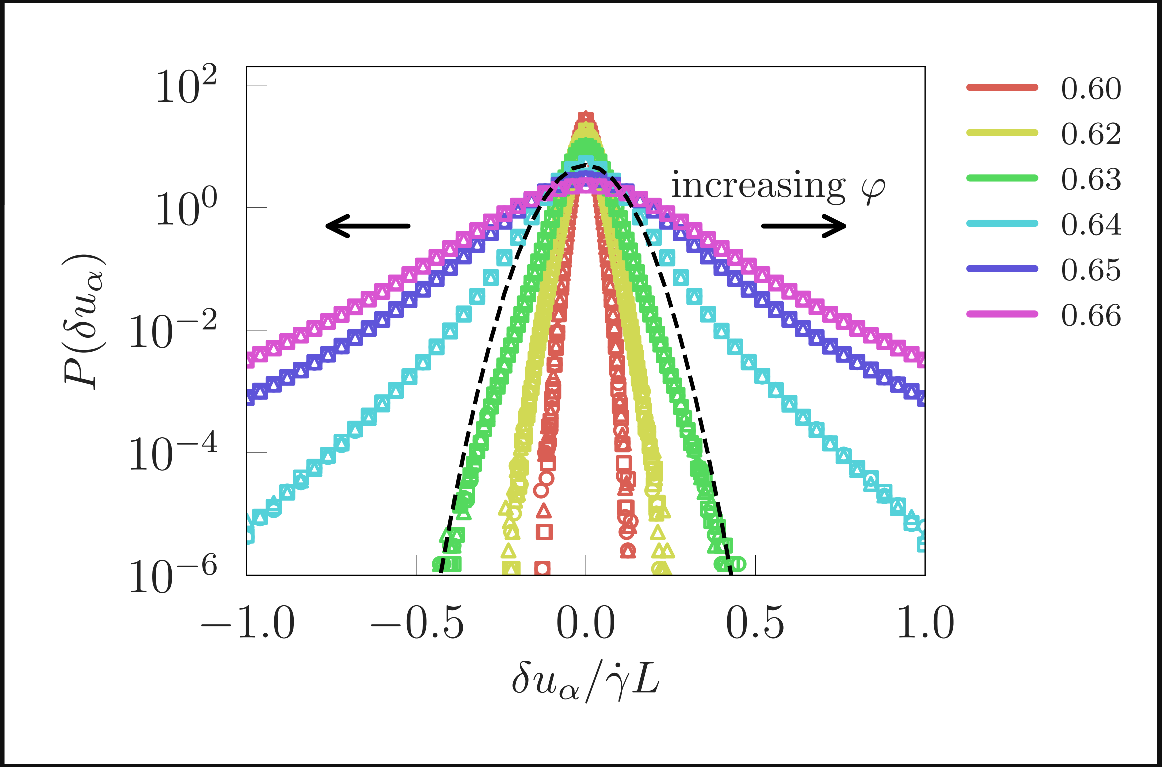
Results

- in 3D systems -

(arXiv:1805.05449)

PDF of Non-affine Velocities

Isotropic and non-Gaussian (broader)

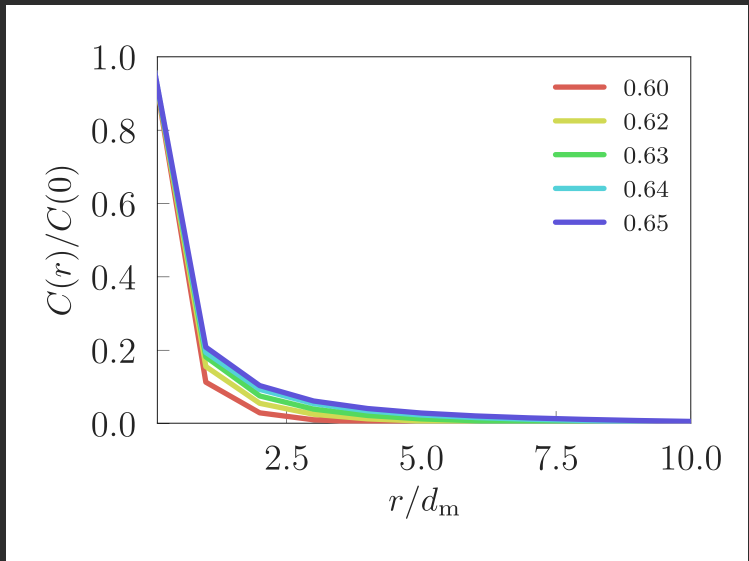


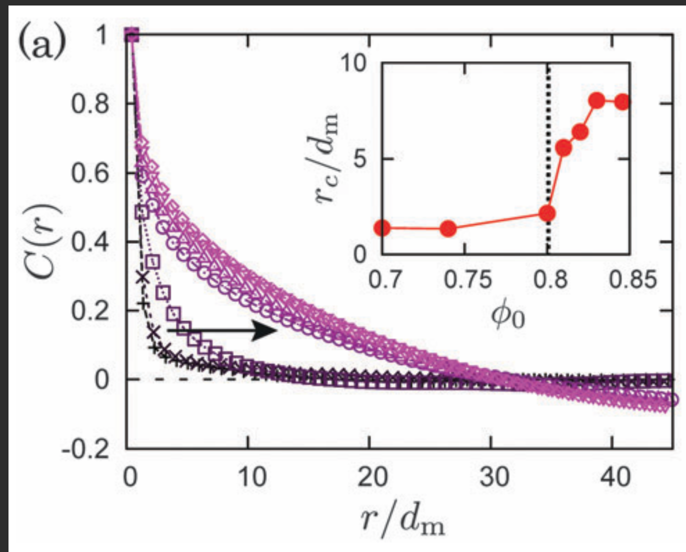
- Suggest the spatial correlation

Simple Spatial Correlation

Spherically averaged

$$C(r) = \langle \delta \boldsymbol{u}(r) \cdot \delta \boldsymbol{u}(0) \rangle$$





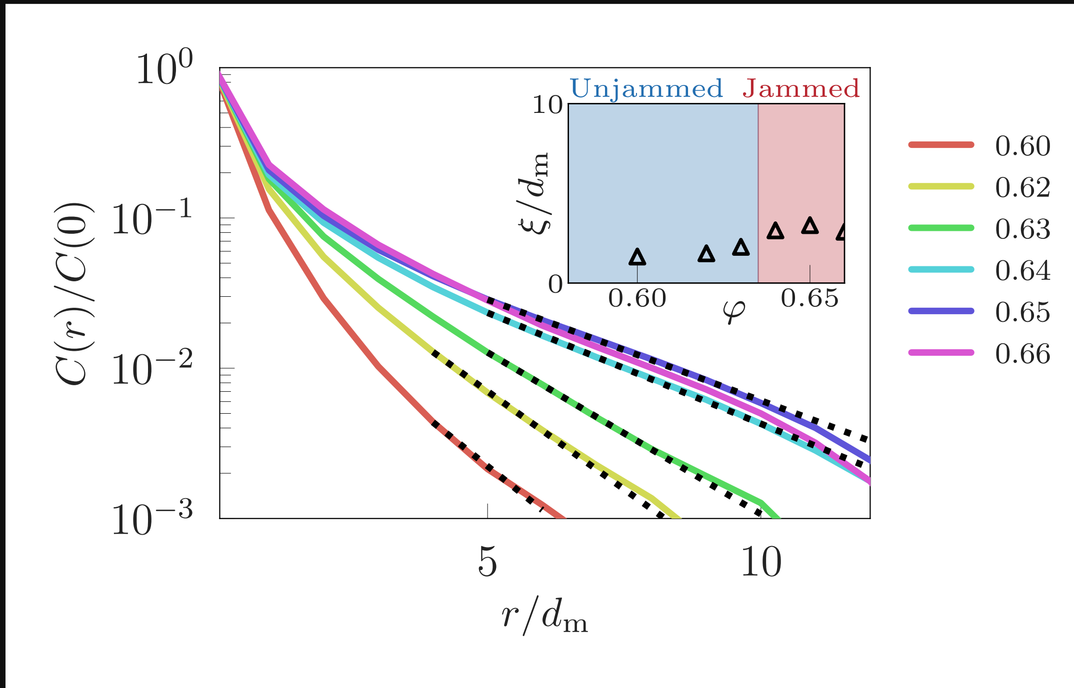
K. Saitoh and H. Mizuno, *Soft Matter*, 2016, **12**, 1360

- Spatially correlated..?

Exponential Cutoff

Introduction of the correlation length ξ_S

$$C(r) \sim \exp\left(-r/\xi_S\right)$$

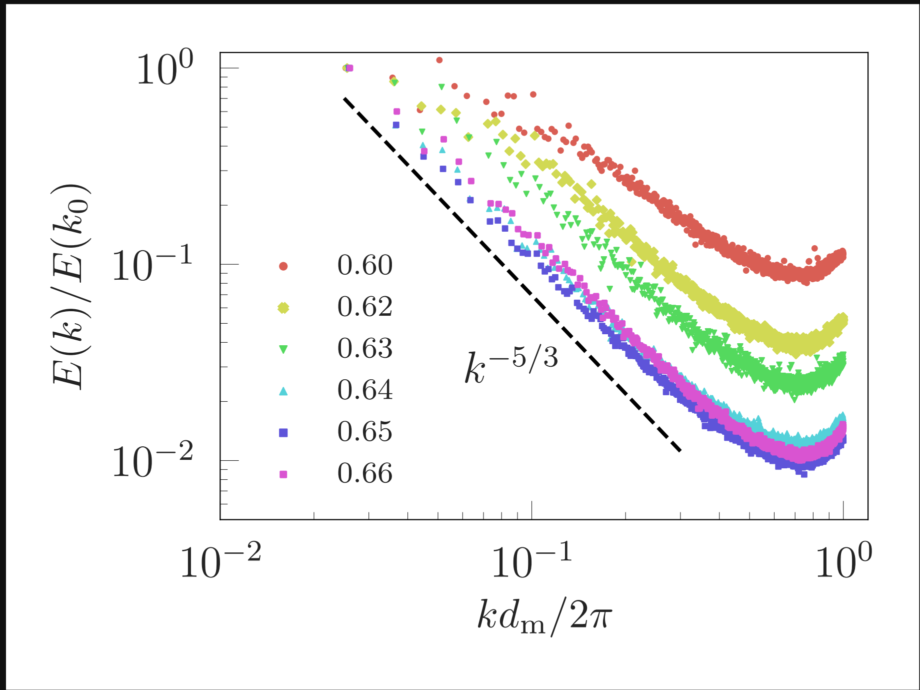


- Correlation length ξ_S saturates at the onset of jamming (Consistent with the 2D results)

Energy Spectrum

Fourier space counterpart of the spatial correlation

$$E(k) = \frac{\rho_0}{2}\langle|\delta\hat{\boldsymbol{u}}(k)|^2\rangle$$



$$\delta\hat{\boldsymbol{u}}(\boldsymbol{k}) = \sum_{i=1}^{N_\mathrm{p}} \delta\boldsymbol{u}_i \mathrm{e}^{-I\boldsymbol{k}\cdot\boldsymbol{r}_i}, \qquad \mathcal{E} \equiv \frac{1}{2}\langle|\delta\boldsymbol{u}|^2\rangle = \int_0^\infty E(k)4\pi k^2 \mathrm{d}k$$

Universality Assumptions

- Kolmogorov 41 theory -

A. Kolmogorov, *Doklady Akademiia Nauk SSSR*, 1941, **30**, 301-305

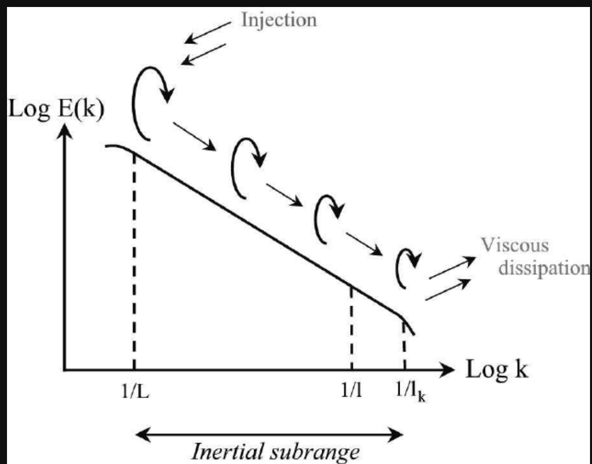
Local similarity assumption

$\phi(k) \sim \epsilon^{\alpha}\nu^{\beta}$ at intermediate length scale and $Re \gg 1$

(ϵ:energy injection, ν: dissipation)

Inertial subregion assumption

$\phi(k) \sim \epsilon^{\alpha}$ at intermediate length scale and $Re \to \infty$



(from Wikipedia)

Dimensional Analysis
- Kolmogorov 41 theory -

Energy spectrum

$$\mathcal{E} \equiv \frac{1}{2}\langle|\delta \boldsymbol{u}|^2\rangle = \int_0^\infty \phi(k)\mathrm{d}k$$

$$\phi(k) = [L^3 \cdot T^{-2}]$$

Average Dissipation Rate and Kinematic Viscosity

$$\epsilon \equiv \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} = [L^2 \cdot T^{-3}]$$

$$\nu = [L^2 \cdot T^{-1}]$$

Scaling Relation

$$\phi(k) = \epsilon^{\frac{1}{4}}\nu^{\frac{5}{4}}\left(k \cdot \epsilon^{-\frac{1}{4}}\nu^{\frac{3}{4}}\right)^{\delta}$$

$$\delta = -\frac{5}{3}$$

- Macro energy injection vs. continuum dissipation

Dimensional Analysis
- 41-like approach to granular turbulence-

Energy spectrum

$$\mathcal{E} = \int_0^\infty E(k) 4\pi k^2 \mathrm{d}k$$

$$E(k) = [L^5 \cdot T^{-2}]$$

Energy Injection per Particle and Inelasticity of Collisions

$$\chi \equiv \sigma \cdot \dot{\gamma} / \rho_n = [L^5 \cdot T^{-3}]$$

$$\eta = [T^{-1}]$$

Scaling Relation

$$E(k) = \chi \eta^{-1} \left(k \cdot \chi^{\frac{1}{5}} \eta^{-\frac{3}{5}} \right)^\delta$$

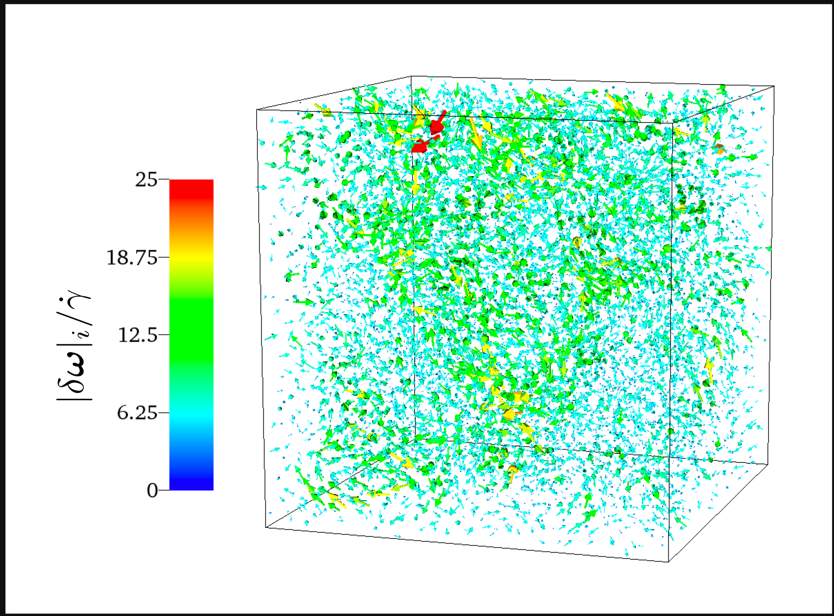
$$\delta = -\frac{5}{3}$$

- Per-particle energy injection vs. dissipation due to collisions

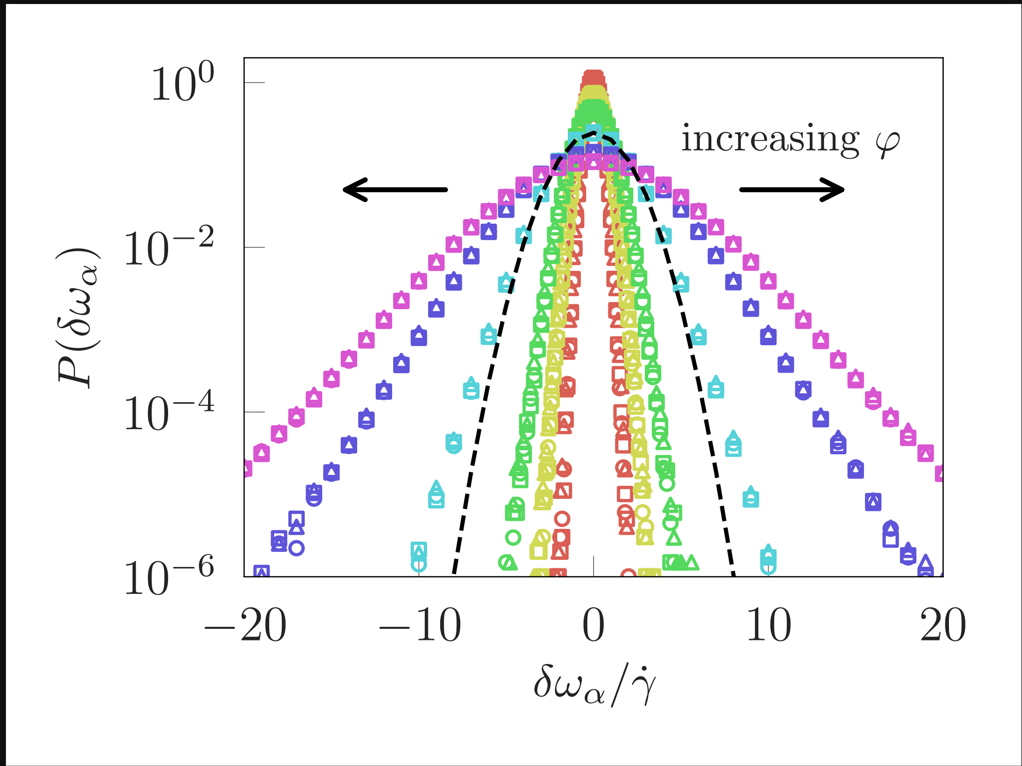
Coarse-Grained Vorticity Field

$$\delta\boldsymbol{\omega}(\boldsymbol{x}) = \rho^{-2}(\boldsymbol{x}) \sum_{i=1}^{N} \sum_{j=1}^{N} \Psi_j(\boldsymbol{x}) \left[\nabla\Psi_i(\boldsymbol{x}) \times \delta\boldsymbol{u}_{ij}\right]$$

$$\left(\begin{array}{ll} \Psi(\boldsymbol{r}) = \exp(-(\boldsymbol{r}/d_{\mathrm{m}})^2) & \text{Gaussian kernel} \\ \rho(\boldsymbol{r}) = \sum_{i=1}^{N} \Psi(\boldsymbol{r} - \boldsymbol{r}_i) & \text{particle density field} \\ \delta\boldsymbol{u}(\boldsymbol{r}) = \rho^{-1}(\boldsymbol{r}) \sum_{i=1}^{N} \delta\boldsymbol{u}_i \Psi(\boldsymbol{r} - \boldsymbol{r}_i) & \text{non-affine velocity field} \end{array}\right)$$



Probability Distribution of Vorticity



- Non-Gaussian (broader) distribution
- Completely isotropic in 3D, while they are (implicitly) aligned in 2D

The turbulent-like collectivity does exist

then...

how about its spatial structure?

Questions to be Answered

- ☑ What if in 3D = "real" systems?

  : Granular turbulence can be observed

- ☑ Dimensionality affects the statistical properties?

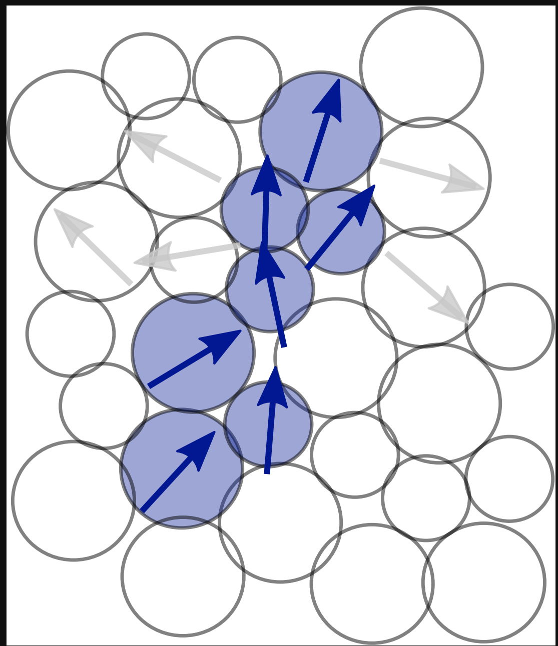
  : The exponent of the energy spectrum differs

- ☐ What is unique for 3D?

  : Vortex filaments with complicated shape?

Vortex-Clusters

- defined w.r.t both the relative position and the vortex affinity -



- condition 1:

  $\zeta_{ij} > 0$

  (particles are touching)

- condition 2:

  $\theta_{ij} \equiv \cos^{-1}(\hat{\delta\boldsymbol{\omega}}_i \cdot \hat{\delta\boldsymbol{\omega}}_j) < \theta_{\mathrm{C}}$

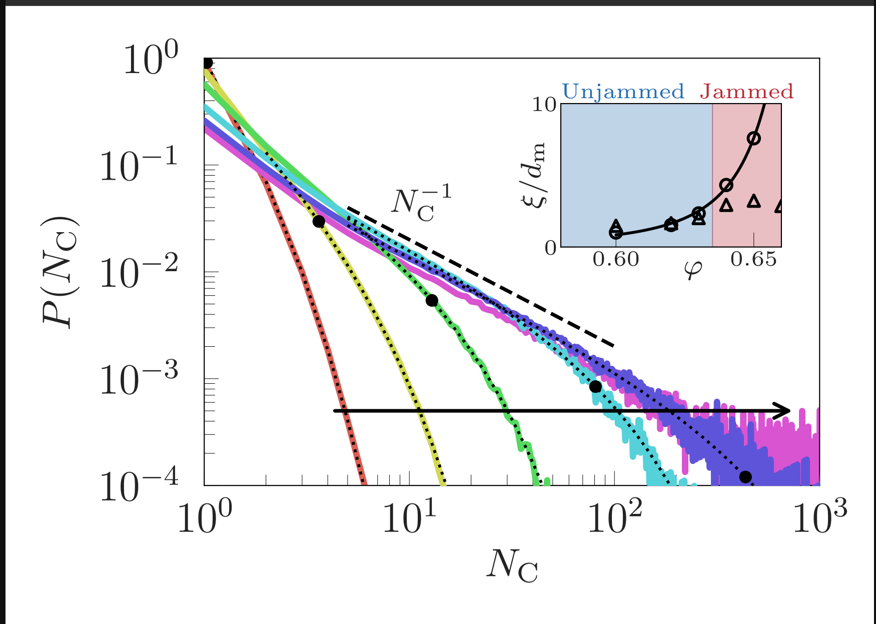
  $(\theta_{\mathrm{C}} = \frac{\pi}{6})$

- $\hat{\delta\boldsymbol{\omega}}_i$: the unit vorticity vector of particle i

▶ Equivalent object to the vorticity filament

Size Distribution

Power-law nature of the turbulent structure



- Power law with exponential cutoff:

  $P(N_C) \sim N_C^{\alpha} \exp(-N_C/\nu_C)$

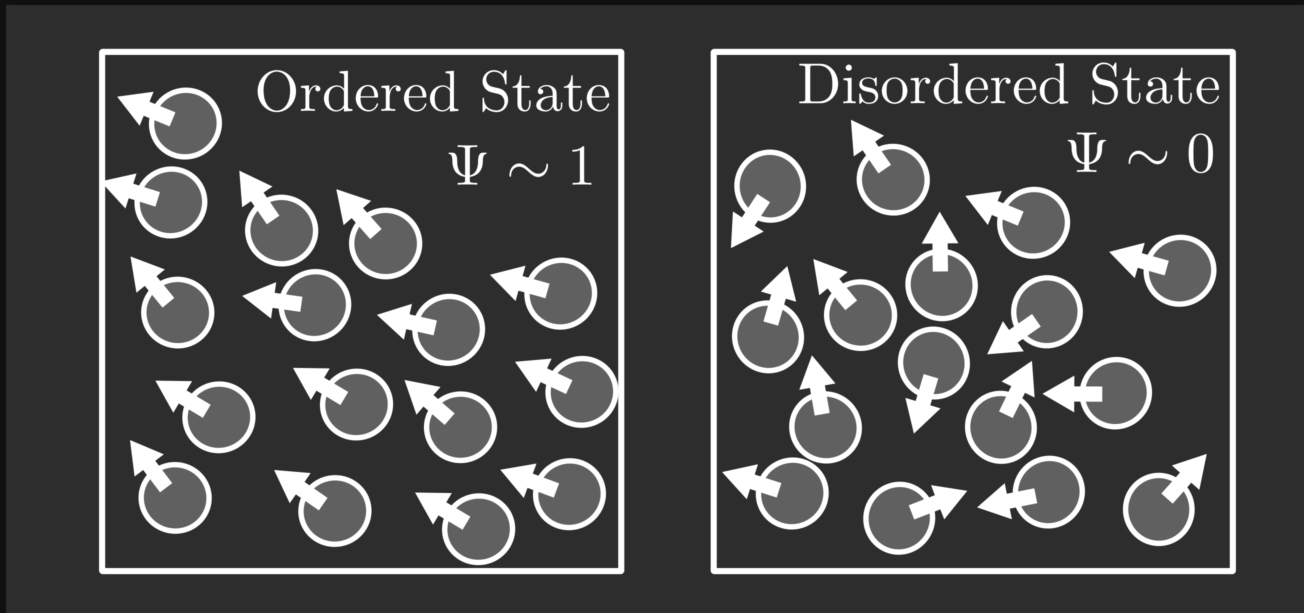
  (ν_C: characteristic cluster size)

- Characterisitic length $\xi_C = \nu_C^{1/3}$ reaches the system size at $\varphi = 0.66$

Polar Order Parameter 1

- Intuitive morphology detection -

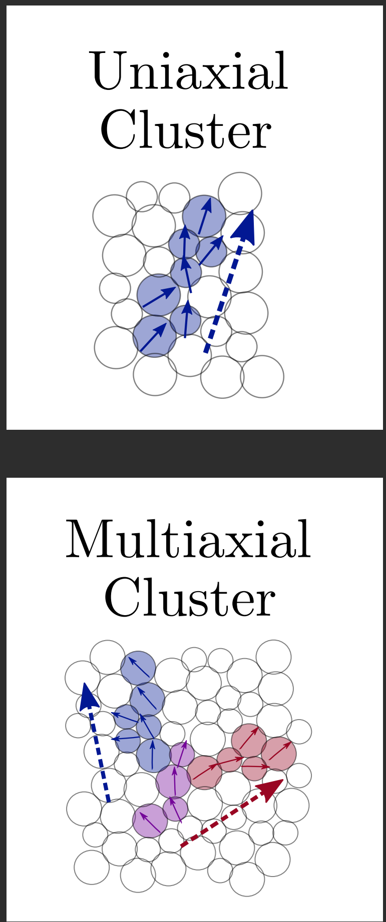
$$\psi(N) = \frac{1}{N} |\sum_{i}^{N} \delta\hat{\omega}_i|$$



$\psi(N) \sim 1$: Ordered state, $\psi(N) \sim 0$: Disordered state

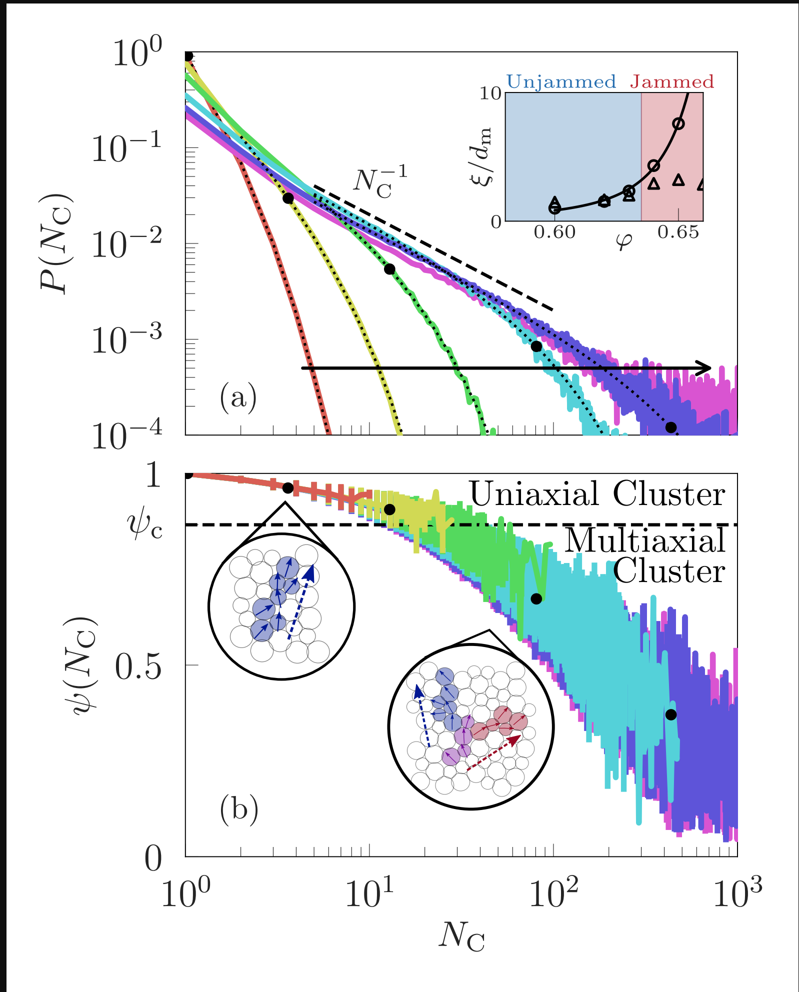
Polar Order Parameter 2

- Threshold for the multi-axiality -



- $\psi(N) = \frac{1}{N} | \sum_{i}^{N} \delta\hat{\omega}_i |$
- $\psi(N) \geq \psi_C$: uniaxial cluster
- $\psi(N) < \psi_C$: multiaxial cluster
- $\psi_C = \cos\theta_C \approx 0.866$
- Multiaxial clusters:
  merge and division of clusters

Size Distribution and the Polar Order Parameter



- Clusters with size of N_C are multiaxial above jamming

Summary

- answered questions in this work -

☑ What if in 3D = "more realistic" systems?

: Granular turbulence can be observed

☑ Dimensionality affects the statistical properties?

: The exponent of the energy spectrum differs

☑ What is unique for 3D?

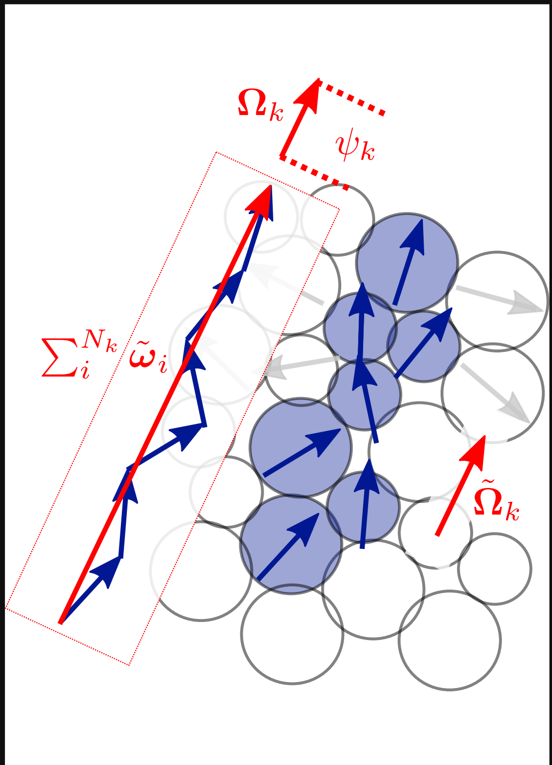
: Multiaxial vortex-clusters are formed

THE END

Thank You for Your Kind Attention!!

Appendix

Critical Polar Order

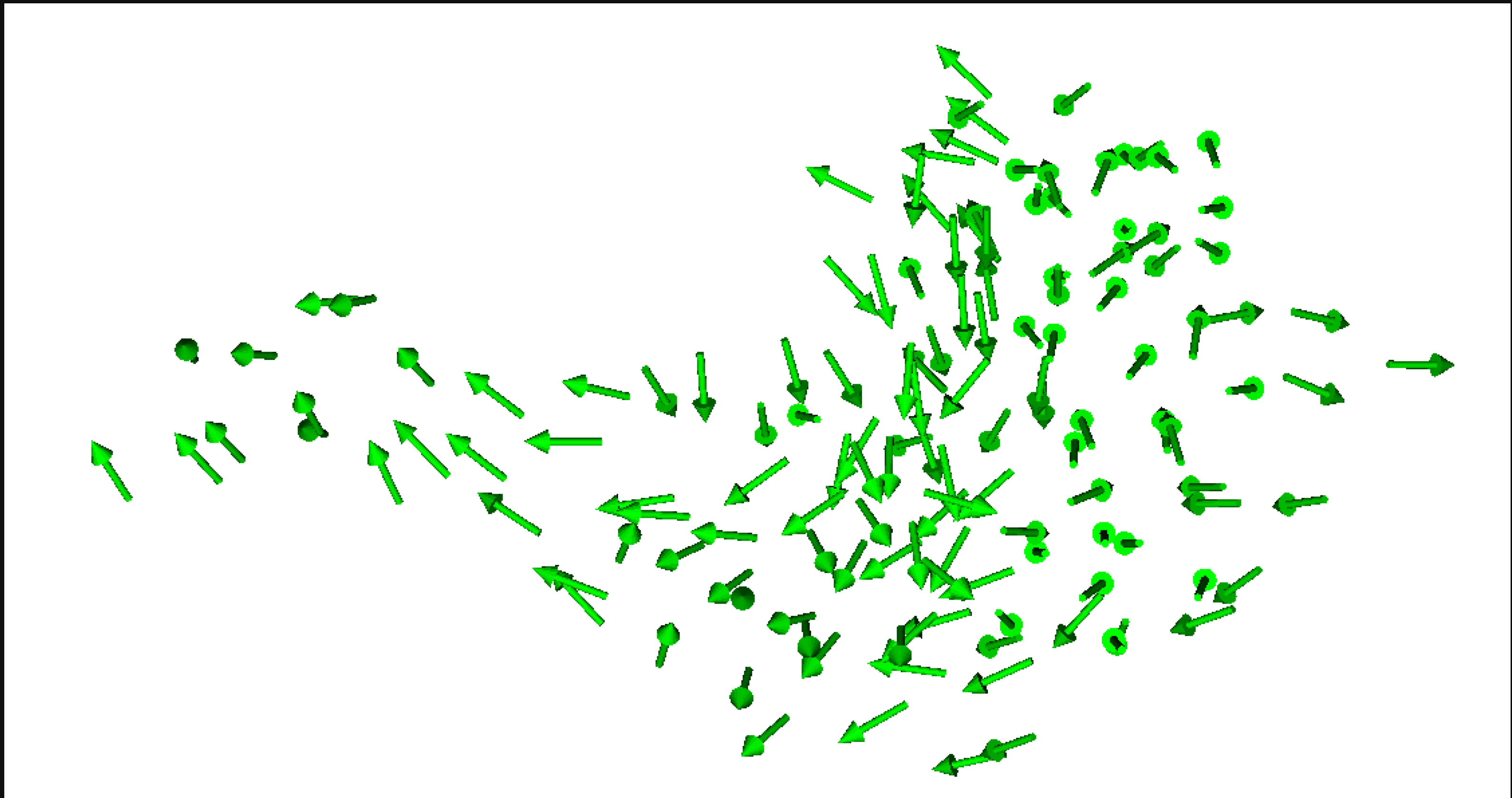


- $\psi_k \equiv |\frac{1}{N_k} \sum_i^{N_k} \tilde{\omega}_i| = |\Omega_k|$
- $$\psi_k^2 = \frac{1}{N_k^2} |\sum_k^{N_k} \omega_i|^2 = \frac{1}{N_k^2} \sum_i^{N_k} \sum_j^{N_k} (\omega_i \cdot \omega_j)$$
- $\sum_i^{N_k} \tilde{\Omega}_k \cdot \tilde{\omega}_i = \frac{1}{\psi_k N_k} \sum_i \sum_j^{N_k} (\tilde{\omega}_i \cdot \tilde{\omega}_j)$
- $$\psi_k^2 = \frac{1}{N_k} \psi_k \sum_i^{N_k} \tilde{\Omega}_k \cdot \tilde{\omega}_i = \frac{1}{N_k} \psi_k \sum_i \cos\theta_i$$
- $\psi_k = \frac{1}{N_k} \sum_i^{N_k} \cos\theta_i \; (\tilde{\Omega}_k \cdot \tilde{\omega}_i = \cos\theta_i)$

▶ If $\theta_i < \theta_c$ for all i, $\psi_k < \psi_c \equiv cos\theta_c \sim 0.866$

Snapshot

Multiaxial cluster with a size of $N_c = 141$



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