

Deformation mechanisms in granular flows

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Statement of originality

This is to certify that, to the best of my knowledge, the content of this thesis is my own work. This thesis has not been submitted for any degree or other purpose.

The intellectual content of this thesis is the product of my own work, and all the assistance received in preparing this thesis and the sources are acknowledged.

Date: 28 August 2024

Parisa Shekari Namin

Authorship attribution statement

Chapter 3 of this thesis is published as ‘Size of heterogeneous deformations in sheared granular flows’ in the Physical Review Fluids Journal. I was the primary researcher, the lead author, and analysed the data under the guidance and supervision of Associate Professor Pierre Rognon and Dr. Benjy Marks.

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Abstract

Understanding the evolution of deformation fields in sheared granular flows is essential to elucidate their complex flow behaviours. This thesis investigates the mechanisms driving local deformation in dense granular flows, utilising discrete element simulations in plane shear configurations. The research focusses on the spatiotemporal evolution of kinematic fields and their relation to the constitutive laws that govern granular flows at the continuum scale. It reveals that the particle rearrangements within these flows are neither spatially uniform nor temporally steady, particularly at lower inertial numbers.

The findings demonstrate a diffusive propagation mechanism for shear deformation, where local particle rearrangements trigger further rearrangements nearby, creating zones of increased deformation. This mechanism suggests a connection between distant regions of the flow, propagating across a mesoscopic distance that varies with the inertial number. These insights provide a potential microscopic basis for non-local behaviour observed in continuum-scale models. Key findings include the characterisation of length scales and Representative Volume Elements (REVs) associated with kinematic heterogeneities, such as velocity fluctuations, deformation, and nonaffine deformation, and the identification of the role of kinematic clusters in these processes.

The results of this thesis contribute to bridging the gap between continuum and discrete descriptions of granular flows by elucidating the microstructural processes underlying their rheological behaviours. The findings emphasise the importance of incorporating large-scale structures and micromechanics of deformation into the development of more accurate continuum models.

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CHAPTER 1

Introduction

Granular media are prevalent in both industrial (pharmaceutical manufacturing, mining operations, and processing of food grains) and geophysical contexts (such as landslides, sediment transport in rivers, and soil behaviour during earthquakes), making them one of the most challenging materials to model on a large scale. Despite their widespread use, understanding their kinematic properties has remained a persistent scientific challenge. The 125th anniversary issue of *Science* identified the development of a comprehensive theory for the motion of granular media as one of the 125 crucial gaps in scientific knowledge (AAAS 2005).

Granular media consist of numerous individual particles, each with its own material properties, such as shape, size, roughness, elasticity, and restitution. Accurately modelling these diverse properties and their distributions is inherently complex. In addition, granular media often exhibit segregation during flow, causing property distributions to vary over space and time. Even when a granular mixture remains homogeneous, its mechanical behaviour can change on the basis of its flow history, and the absence of significant thermal fluctuations makes many equilibrium principles inapplicable. Furthermore, the grain size in the granular material is not negligible to the size of the experimental setup, which means that the impact of the microscopic scale cannot be ignored even when considering the continuum limit (Kamrin et al. 2024).

Several fundamental questions remain unresolved with respect to the motion of granular materials: *How do granular grains deform internally at the microscale? How is the bulk behaviour of the flow (far from the boundaries) captured by the concept of Representative Elementary Volume (REV)?* These questions are at the core of this thesis, which aims to

investigate flow kinematics, deformation fields, and nonaffine deformation in granular flow under plane shear.

Chapter 2 provides a critical overview of the developments in continuum theories and the discrete particle approach, which serve as alternatives to continuum descriptions for understanding granular flow. This thesis aims to develop a robust micromechanical understanding of the grain-scale kinematics that underlie continuum-scale behaviours. This thesis mainly employs theoretical investigations supported by numerical simulations. The numerical methods are detailed mainly in the literature review chapter, with additional details provided in each subsequent chapter.

Granular flows exhibit complex behaviours, characterised by heterogeneous and transient kinematic fields reminiscent of turbulence. A critical parameter that significantly impacts the flow behaviour is characterising the length scale of kinematic heterogeneities, such as velocity fluctuations, shear rate, vorticity, and dilation rate, by identifying Representative Elementary Volume (REV) size. Although continuous models have been developed to explain the non-local behaviour of granular flows on the grain scale, there is not much information available on velocity fluctuation, deformation heterogeneities, and the associated length scales, and REV sizes. *The main question here revolves around understanding the mechanisms that govern the emergence and evolution of kinematic fields that influence the REV size in the shear granular system, particularly at low inertial numbers, where they appear to diverge.* Chapter 3 sheds some light on these questions by providing the variation in REV size as a function of the inertial number, demonstrating a characteristic power law that ranges from a few grain diameters at high inertial numbers to several dozen grain diameters at low inertial numbers. The results underscore a striking contrast between macroscopic and microscopic deformations in granular flows, emphasising the spatial correlations that develop at low inertial numbers and partitioning the flow into ‘cold’ and ‘hot’ zones with varying strain rates.

Another critical aspect of granular flow deformation is understanding the mechanisms behind the propagation of internal deformations. Although the deformation of granular materials has been explored in the literature, the key mechanisms driving micro-deformations remain elusive. This thesis also explores this fundamental question: *How do internal deformations*

propagate within these materials under various conditions and what are the main driving factors? Chapter 4 addresses this by investigating the spatial and temporal correlations of velocity fluctuations, deformation, and nonaffine deformation in granular flows across a range of inertial numbers. Key factors identified in this research include structural rearrangements, stress fluctuations, strain-dependent non-affine motion, and self-activated processes.

This thesis mainly employs numerical investigations and simulations. The general approach involves a statistical analysis of the granular flows, where a large number of grains are numerically simulated within a homogeneous representative volume element under simple shear conditions, interacting via integrated contact forces using Newton's laws. This simple shear configuration minimises the effects of walls and intruders that other geometries might introduce. The system parameters are sampled through separate steady-state simulations to map the desired measurements, such as grain kinematics. This method constructs a comprehensive picture of the granular system by measuring grain kinematics, including velocity fluctuations, shear strain, and squared non-affine displacement, allowing for simultaneous probing to complement the analytical findings.

Chapter 3 of this thesis has been published in the Physical Review Fluids Journal. As a result, some overlap between the literature review and the introductory section of Chapter 3 is inevitable. However, this overlap has been minimised whenever possible, with the literature review chapter aiming to provide a broader context for the research presented.

CHAPTER 2

Literature review

Granular material flow has been a topic of scientific inquiry for several decades, with initial research efforts dating back to the mid-20th century. Early studies focused primarily on understanding the fundamental behaviours of granular materials under various conditions. The advent of Discrete Element Method (DEM) simulations and advanced experimental techniques significantly propelled this field forward. DEM, in particular, has become a cornerstone in the study of granular materials, allowing researchers to simulate and analyse the complex interactions between individual particles. Experimental methods have also evolved, providing detailed insight into the behaviour of granular flows through high-speed imaging and advanced measurement techniques. Recent research has concentrated on granular deformation and explored how these materials respond to different stress and strain conditions. Despite these advances, significant gaps in our understanding remain, particularly concerning the microscopic mechanisms that drive deformation, its clustering, and kinematic behaviours in granular materials. This active field of research continues to evolve, with ongoing studies aiming to bridge these knowledge gaps and develop a more comprehensive understanding of granular material flow.

This review of the literature provides a comprehensive overview of the field, guiding the reader through the development of key concepts with a focus on deformation and kinematics at the microscale. Section 2.1 begins by explaining the rheology of shear flows and rheology models and introduces the relevant dimensional numbers associated with this flow configuration. Section 2.2 discusses the current understanding of grain velocities in granular flows. Section 2.3 reviews the recent literature on velocity gradients and deformation rates, highlighting primary measurement methods and the latest findings. Sections 2.4 and 2.5 are dedicated

to understanding microscopic deformation and nonaffine displacement in granular packing, respectively. Finally, the statistical methods for measuring microscopic heterogeneity are summarised in Section 2.6.

2.1 Granular materials under shear

2.1.1 Simple shear flows

Simple shear flow of cohesionless grains with slight polydispersity and without interstitial fluid is a common approach to understanding the rheology in dense granular flows. This approach takes into account the transfer of momentum and the dissipation of energy between grains in direct contact with the walls (Da Cruz et al. 2005). The granular material in such systems is sheared, with the velocity gradient- also known as the shear rate $\dot{\gamma} = \frac{2u}{H}$ - being homogeneous and the normal stress P kept constant during flow, where u is the shearing velocity at the boundaries. To avoid flow heterogeneity induced by solid walls, periodic boundary conditions as presented in Figure 2.1, are used (Lees and Edwards 1972).

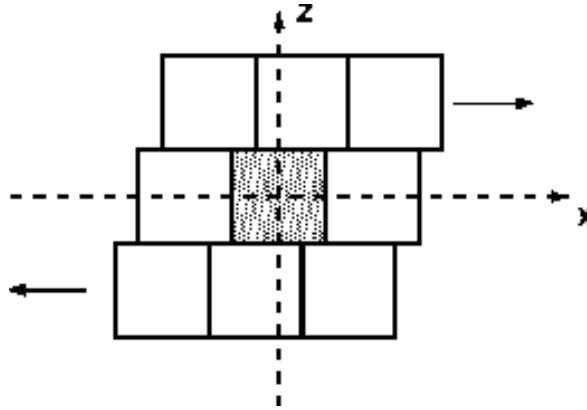


FIGURE 2.1: Lees and Edwards boundary conditions (Lees and Edwards 1972).

The number of grains typically consists of particles $8000 \sim 13,000$, with a mean diameter of d , a mass of m and a density ρ (Ma et al. 2020; Mei et al. 2023; Wang et al. 2021). To prevent shear-induced crystallisation, a uniform polydispersity of $d \pm 20\%$ is introduced in the grain diameters (Luding 2001; Da Cruz et al. 2005). Simple shear flow has been extensively

investigated in the literature, both in 2D and in 3D, considering the effects of boundary conditions as presented in Figure 2.2.

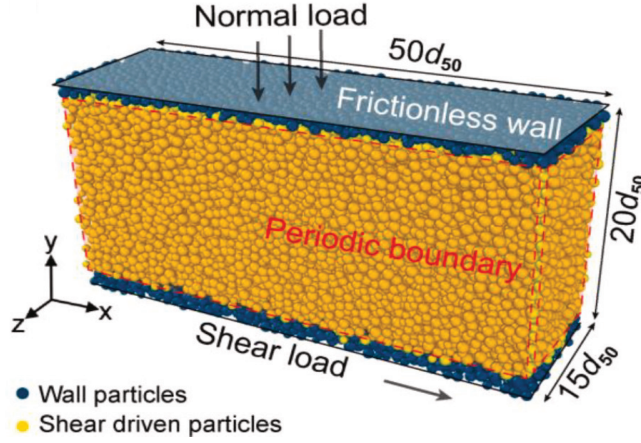


FIGURE 2.2: Simple shear flow geometry with frictionless walls (Mei et al. 2023).

The behaviour of granular materials in simple shear flows is significantly influenced by the characteristics of individual grains and their interactions. Linear elastic repulsion is governed by the stiffness coefficients k_n and k_t , which determine the normal and tangential components of the contact force. Viscous dissipation, characterised by the coefficient of restitution e , accounts for the energy lost during collisions between grains. Tangential friction, represented by the friction coefficient μ , influences the resistance to sliding between grains. These parameters collectively determine the general rheological properties of the granular flow.

2.1.2 Dimensional analysis

In the absence of gravity, the shear flow is homogeneous, with the shear rate $\dot{\gamma}$ and stresses remaining uniform throughout the flow. A key dimensionless number in this context is the inertial number I , which also remains homogeneous:

$$I = \dot{\gamma} d \sqrt{\frac{\rho}{P}} = \dot{\gamma} \sqrt{\frac{m}{Pd}}. \quad (2.1)$$

This number represents the ratio of the time scales associated with shear flows: the shear time $\frac{1}{\dot{\gamma}}$ for one shear deformation, the inertial time $t_i = d\sqrt{\frac{\rho}{P}}$, that is, the characteristic displacement time of a grain with diameter of d under pressure P , or the collision time τ_c

(Da Cruz et al. 2005; Jop 2015). Furthermore, the ratio k_n/P is a dimensionless number that represents the rigidity of the grains (Da Cruz et al. 2005). This ratio is typically chosen to be low enough to allow larger time steps and to reduce computational costs, but large enough to ensure that it does not influence the flow properties of the material. Although stiffer grains are expected to produce similar results, softer grains could affect flow dynamics, although such highly deformable grains are rarely encountered (Singh et al. 2015).

The Bond number, which characterises the ratio of cohesive forces to gravitational forces, is significant in the study of cohesive granular flows. This parameter is often used to predict the flowability of various powders, such as pharmaceutical or ceramic powders with polydispersed particle size distributions (Giraud et al. 2021). The Froude number F_r , representing the ratio of inertial forces to gravitational forces, is commonly used in studies of granular flows in inclined planes and in rotating drums (Zhu et al. 2020). The granular temperature Θ , which measures the kinetic energy of the particles, also influences the rheological properties of the granular materials (Kim and Kamrin 2020).

It is important to note that the friction coefficient μ , defined as the ratio between shear stress and normal stress, and the solid fraction ϕ , representing the volume fraction of solids in the material, are dimensionless critical numbers influencing the packing density and flow properties of granular materials (Barker et al. 2021; Radjai 2021). These parameters are captured by the aforementioned dimensionless numbers and will be discussed further in the rheology models section.

2.1.3 Rheology in granular material

2.1.3.1 Inertial rheology

Inertial rheology, also known as the frictional rheology $\mu(I)$ model (MiDi 2004; Da Cruz et al. 2005), describes the flow behaviour of granular materials comprising small, hard, quasi-monodisperse particles that flow steadily under finite pressure. This model establishes a direct relationship between the shear stress to pressure ratio, $\mu \equiv \tau/P$ (Kamrin et al. 2024), and the inertial number I , as introduced in Section 2.1.2. In dense granular flows, this relationship is

often observed to be approximately linear (Da Cruz et al. 2005):

$$\mu(I) = \mu_s + bI. \quad (2.2)$$

where μ_s represents the internal friction corresponding to the Mohr-Coulomb friction law (Nedderman 1992). The local rheology described by a friction coefficient $\mu(I)$ can be understood as a specific instance within the broader framework of the theory of mixing length. As illustrated in (MiDi 2004), when the stress ratio τ/P is defined by $\mu(I)$ and the pressure P is expressed as $P = \frac{\rho d^2 \dot{\gamma}^2}{I^2}$, it leads to $\tau = \rho \frac{\mu(I) d^2}{I^2} \dot{\gamma}^2$. This relationship suggests that the coherence length is a function of the local properties of the flow and is given by:

$$l(I) = \frac{\sqrt{\mu(I) d}}{I}. \quad (2.3)$$

The $\mu(I)$ model is regarded as a local rheology model that relates the stress tensor σ and the velocity gradient ∇v in steady-state flow. However, this model does not account for scenarios in which the grains are either not small, not quasi-monodisperse, or flow inhomogeneously (Koval et al. 2009). To address these limitations, the following sections will briefly review nonlocal continuum models and particle segregation models.

2.1.3.2 Nonlocal rheology models

Nonlocal effects on granular material arise from various sources, highlighting the limitations of local rheology models. The finite size of grains relative to the system's geometry can lead to behaviours that local models cannot capture (Tüzün and Nedderman 1979). Local rheology models often fail in scenarios with significant strain rate gradients, such as in inhomogeneous flows, where the $\mu(I)$ model does not accurately predict the creeping decay of shear rates deep into the bulk, emphasising the importance of a grain size effect (Koval et al. 2009).

Nonlocality also affects the flow arrest criterion in systems with thin features, such as the stoppage of thin granular layers on inclined planes. These phenomena demonstrate that the granular material behaves more strongly as the geometric scale becomes comparable to the grain size (Pouliquen 1999; Silbert et al. 2001; Silbert et al. 2003; Zuriguel et al. 2014). Another intriguing nonlocal effect is known as secondary rheology. In this phenomenon,

probes inserted into a body of granular media can be moved with an arbitrarily small force, provided that the material is flowing somewhere within the system, even if the primary flow is distant from the probe. In contrast, when the granular body is static, a specific yield force must be exceeded to initiate the movement of the probe (Kamrin et al. 2024). These factors illustrate that the intrinsic length scale of the grains competes with flow gradients and significantly impacts the overall flow behaviour, necessitating a nonlocal approach in granular flow modelling.

A continuum theory for partially fluidized granular flows was developed by (Aranson and Tsimring 2002), incorporating mass and momentum conservation laws alongside an order parameter that delineates the transition between static and flowing states. This order parameter, a key variable in the theory, represents the fraction of static contacts among particles within a specified volume. While challenging to measure experimentally, it can be derived through molecular dynamics simulations, enabling the estimation of phenomenological parameters. Although this model has been proposed for broader applications; including other granular flows, binary mixtures, and granular materials that are wet, cohesive, or subject to additional vibrations, no “microscopic” theory of granular flow yet exists, analogous to the Ginzburg-Landau theory of superconductivity (Ginzburg and Landau 1950).

Several models have been proposed to extend the $\mu(I)$ model to account for nonlocal phenomena in granular materials. The nonlocal granular fluidity model (NGF), proposed by (Kamrin and Koval 2012), introduces a state field called granular fluidity, which satisfies a set of equations that incorporate diffusion and pressure-weighted viscosity. It captures nonlocal phenomena such as nonlocal creep, thin-body strengthening, and secondary rheology. Although the underlying physics of NGF is not fully understood, a connection between granular fluidity and temperature has been established (Kim and Kamrin 2020). The I-gradient model proposed by (Bouzid et al. 2015) attempts to extend $\mu(I)$ directly by supposing:

$$\mu = \mu(I)(1 - v\nabla^2 I/I). \quad (2.4)$$

This model predicts nonlocal creep in $2D$ and rate independence but cannot capture thin-body strengthening. In addition, other models rely on system-wide integral equations, such as a

body-wide self-activation model, where flow perturbations influence the shear rate at every point (Pouliquen and Forterre 2009), a model that convolves local rheology over a kernel (Nott 2017), and an integrated formulation of eddy viscosity (Miller et al. 2013).

The local constitutive laws have also struggled to account for the effect of wall perturbations flows under simple shear. To measure the characteristic length scale of such flows by using the kinetic viscosity $\nu(m^2/s^{-1})$, it is been suggested to present the friction law as:

$$\tau = \mu_s \sigma + \rho \nu \dot{\gamma}. \quad (2.5)$$

where $\nu = \frac{1}{\rho} \frac{\partial \dot{\gamma}}{\partial \tau}$. The kinetic viscosity has been suggested to be expressed as a function of a typical time scale $\dot{\gamma}^{-1}$ and a length scale l_v (Rognon et al. 2015):

$$\nu \propto l_v^2 \dot{\gamma}. \quad (2.6)$$

and,

$$l_v \propto \frac{d}{\sqrt{I}}. \quad (2.7)$$

It is important to note that at low inertial numbers, the momentum diffuses over a characteristic length scale that is significantly larger than the grain size d . Additionally, the scaling of l_v with I is proposed to be analogous to the scaling of the ‘cooperativity length’ with I , as measured by (Kamrin and Koval 2012).

2.1.3.3 Granular kinetic theory

Granular kinetic theory, developed by (Haff 1983; Brilliantov and Pöschel 2010), is an approach that links the granular viscosity to a collisional temperature T , which satisfies a diffusive energy balance equation. Essentially, this theory incorporates the granular temperature as a measure of the fluctuating kinetic energy of the particles, enabling predictions of the granular viscosity and other rheological properties. Further extensions of this theory to the dense regime have been proposed by (Jenkins and Berzi 2010; Berzi 2014), where the ratio of shear stress to pressure is defined as $\tau/P = \left(\frac{f_2 f_3}{f_1^2 L} \right)^{1/2}$. In case of the simple shear flow in dense granular materials, the relation between the inertial number and concentration

is described by the following equation:

$$I = \left(\frac{\nu f_3}{f_1 f_2 L} \right)^{1/2}. \quad (2.8)$$

where L represents the correlation length, and the parameters f_1 , f_2 , and f_3 are derived from the work of (Berzi 2014).

2.1.3.4 Particle segregation models

Particle segregation models are essential for understanding how particles of different sizes, shapes, and densities separate under shear in granular flows. Recent advances in this area include models that couple rheological descriptions with segregation dynamics to predict the evolution of particle concentration and distribution. (Barker et al. 2021) presents a framework that unifies rheology and segregation theories, providing a comprehensive approach to model granular flows. This model accounts for the advection of particle concentrations, the feedback of particle size properties on bulk flow, and the influence of shear rate, pressure, and gravity on segregation rates. Furthermore, density-driven segregation was explored in shear cells, demonstrating how segregation can be successfully modelled using a continuum approach that incorporates effective viscosity and friction coefficients (Tirapelle et al. 2021). These studies highlight the complexity of segregation phenomena and the need for advanced modelling techniques to accurately predict and control segregation in granular materials.

2.1.3.5 Continuum models with yield criteria

Continuum models with yield criteria are pivotal in describing the behaviour of granular materials under various loading conditions. These models typically integrate constitutive elasto-viscoplastic relations and yield criteria to capture the transition between different phases, such as solid-like and fluid-like states. For example, (Tiwari and Klar 2024) proposed a mesh-free particle method to simulate granular flows using an elasto-viscoplastic model with a yield criterion based on $\mu(I)$ rheology (Tiwari and Klar 2024). This approach allows for an accurate simulation of the collapse of the granular column and the motion of the rigid body in granular materials. Another significant contribution is by (Massoudi 2023),

who reviewed fundamental concepts for the derivation of constitutive relations for the stress tensor of granular materials, emphasising the importance of yield criteria and dilatancy in continuum mechanics (Massoudi 2023). These models are crucial for applications where granular materials transition between static and dynamic states, such as in storage and handling processes in industrial settings.

These models are predicated on the assumption of the existence of a finite-size representative elementary volume (REV), which is defined as the minimum volume of material needed to obtain a behaviour similar to any larger volume. The existence of a REV has been demonstrated in granular packing. Refer to 2.6.4 for the review of previous studies on the measurement of REV size in granular flow.

2.2 Grains velocity fluctuations

Grain velocity fluctuations in dense granular flows are influenced by shear rate and confining pressure. Specifically, relative velocity fluctuations are dependent on the inertial number, I (MiDi 2004), rather than the softness of the grains κ (Macauley and Rognon 2021). Previous studies have proposed a consistent scaling law for relative velocity fluctuations, suggesting an exponent of $\beta = 0.5$ for the following power law (Da Cruz et al. 2005; Macauley and Rognon 2021; Kharel and Rognon 2017):

$$\frac{\delta v}{\dot{\gamma} d} \approx \alpha I^\beta. \quad (2.9)$$

Figure 2.3 illustrates the distribution of force and velocity in simple shear flows. It can be observed that, while the scaling law for force fluctuations depends on both the inertial number and the softness values, the scaling law for vertical velocity fluctuations depends solely on the inertial number. To elucidate the physical mechanisms underlying the velocity and force fluctuations, it has been suggested that grain motions in dense granular flows follow a random walk (Macauley and Rognon 2021).

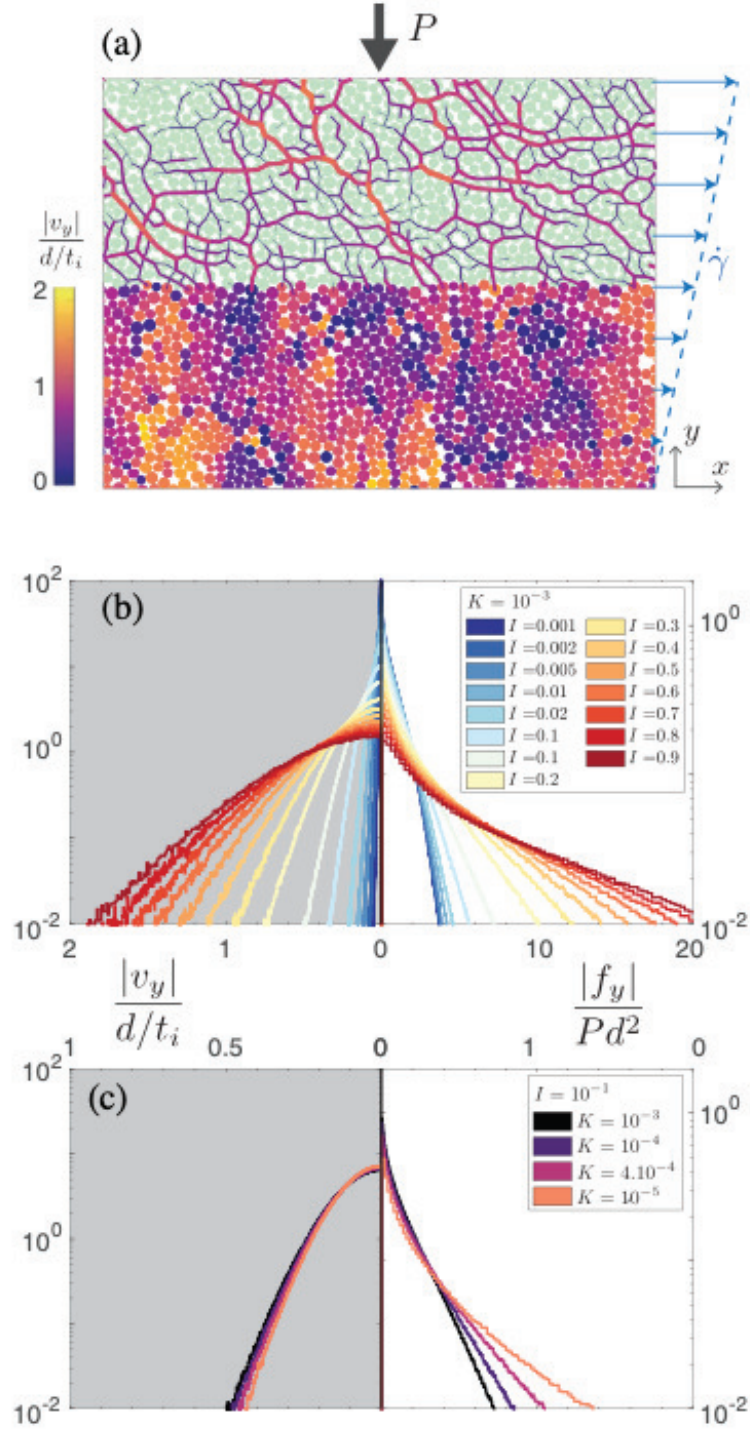


FIGURE 2.3: Force and velocity distributions. (a) Plane shear under prescribed pressure and shear rate. (b) and (c) show the probability density functions (PDFs) of grain velocity (left) and contact forces (right) for different inertial numbers and different softness (Macauley and Rognon 2021).

2.3 Velocity gradient and deformation rate

The pair velocity, or the relative velocity between neighboring grains i and j at the contact point, excluding the rotation rate ω_{ij} (Rognon et al. 2015), is given by:

$$v_{ij} = v_j - v_i. \quad (2.10)$$

To incorporate the effect of ω_{ij} into the calculation of the relative velocity of the grains, Da Cruz et al. (2005) suggests the following formulation:

$$v_{ij} = v_j - v_i + \frac{1}{2}(d_i\omega_i + d_j\omega_j)\vec{t}_{ij}. \quad (2.11)$$

where the normal component of the above expression represents the time derivative of the normal deflection at the contact, and the tangential component corresponds to the time derivative of the tangential relative displacement.

The heterogeneity in grain and pair velocities, as evidenced above, indicates that the deformation rate within the flow is not homogeneous and probably deviates from the macroscopic shear rate $\dot{\gamma}$. The velocity gradient tensor, derived from the velocity field by taking its spatial gradient, is fundamental to determine the strain rate in various configurations. In other words, the velocity gradient tensor captures the local deformation and rotation of grains in the granular flow, allowing for a detailed analysis of the flow dynamics and the development of nonlocal behaviours near walls. To investigate the heterogeneity in the deformation rate, the local velocity gradient tensor for each grain has been presented by (Marmottant et al. 2008; Rognon et al. 2015) using the following formula:

$$F_{\alpha\beta} = \langle l_{ij} \times l_{ij} \rangle^{-1} \cdot \langle l_{ij} \times v_{ij} \rangle. \quad (2.12)$$

In this equation, $\cdot$ signifies the dot product, $\times$ represents the outer product, and $^{-1}$ denotes the inverse of the tensor. Angle brackets $\langle \rangle$ indicate averaging over all pairs of neighbouring grains i and j . Here, l_{ij} is the vector between the centres of two grains and v_{ij} is their relative velocity, as presented in Figure 2.4. Grains are considered neighbours if their centre-to-centre distance is less than $1.5d$ to $2d$. The tensor F provides a spatial average of the velocity gradient in this region.

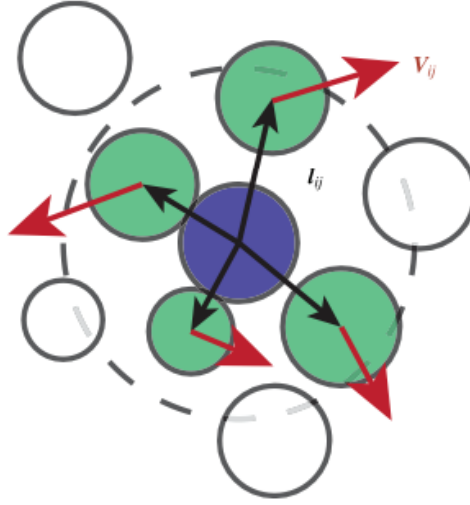


FIGURE 2.4: Local velocity gradient measurement. The local velocity gradient tensor can be estimated for each grain considering the neighbouring grains, their relative position, and relative velocity. Here, the velocity gradient associated with the dark central grain (purple online) involves the lighter grains (green online), but excludes the white grains, which are farther away than the cutoff distance represented by the dashed circle (Rognon et al. 2015).

The cutoff distance is chosen to be as small as possible to obtain local information while ensuring that enough neighbours are included to evaluate the velocity gradient. Different cutoff values were tested with no significant change in the results.

2.3.1 Deformation rate

The velocity gradient can be expressed as the sum of the shear strain rate tensor $\dot{\epsilon}_s$ and the vorticity tensors w (Bechtel and Lowe 2015).

$$F_{\alpha\beta} = \dot{\epsilon}_s + w. \quad (2.13)$$

where the symmetric tensor $\dot{\epsilon}_s$ and skew tensor w are defined as follow:

$$\dot{\epsilon}_s = \frac{F_{xy} + F_{yx}}{2}, w = \frac{F_{xy} - F_{yx}}{2}. \quad (2.14)$$

It is important to note that the F_{yx} component of the tensor $F_{\alpha\beta}$ is equal to the shear rate $\dot{\gamma}$ (Rognon et al. 2015). The third kinematic quantities, the volumetric strain rate $\dot{\epsilon}_v$ (trace of F)

defined as:

$$\dot{\epsilon}_v = F_{xx} + F_{yy}. \quad (2.15)$$

2.3.2 Quantitative analysis and experimental observations

Recent studies have further investigated the fluctuations in grain velocity, velocity gradient and deformation rate in granular flows and their implications for industrial applications and the study of natural phenomena. The velocity profiles and shear rates averaged in depth of granular flows in inclined flume experiments are shown to vary significantly with grain size, indicating that particle size plays a crucial role in the influence of granular flow dynamics (Li et al. 2022).

The scaled velocity profiles in dense granular flows follow a universal exponential function independent of the average volume fraction and channel width in the vertical rectangular channel with periodic boundary conditions in the other two directions (Debnath et al. 2022). This study identifies four distinct zones in the dense granular flow within a vertical channel: the plug zone, the dense shear zone, the loose shear zone, and the wall shear zone. The velocity profiles show no significant changes between the plug and shearing zones, but the shear rate shows a clear distinction between these zones. In the plug zone, the shear rate is effectively zero, while in the dense shear zone, it decreases monotonically. The average flow velocity has been observed to be proportional to $\sqrt{W}$, where W is the width of the channel, and the universal scaling of the velocity and thickness of the boundary layer does not apply to the smallest channel width, probably due to finite-size effects. In such cases, both the particle diameter and the channel width become relevant length scales, affecting the flow properties.

The effect of walls on the behaviour of dense granular materials in simple shear flow has been studied by analysing profiles of stresses, solid fraction, and shear rate. Modelling of wall perturbations involves expressing the kinetic viscosity as a function of a typical time scale and a length scale (Rognon et al. 2015). The study finds that the shear rate profiles in dense granular flows are effectively captured by the eddy viscosity model, with the shear rate being maximum near the walls and $\dot{\gamma}(y) \propto \Delta y^{-1/2}$ when the distance from the wall is greater than

2d. The measured time-averaged velocity and the shear rate profiles taken into account with the inertial number and the effect of the walls are presented in Figure 2.5.

In addition, the spatial distribution of the vorticity and its associated length scales was investigated as shown in Figure 2.6 and Figure Figure 2.7 , respectively.

The associated length scale is found to scale as when approaching the walls, rather than the linear scaling usually assumed in traditional eddy viscosity model:

$$l_w(y) \propto (\Delta y/d)^{1/2}. \quad (2.16)$$

There is a direct link between the local shear rate and vorticity, and it highlights how vorticity is influenced by the shear rate, particularly near the walls where the vorticity is higher:

$$w(y) \approx \frac{\dot{\gamma}(y)}{2}. \quad (2.17)$$

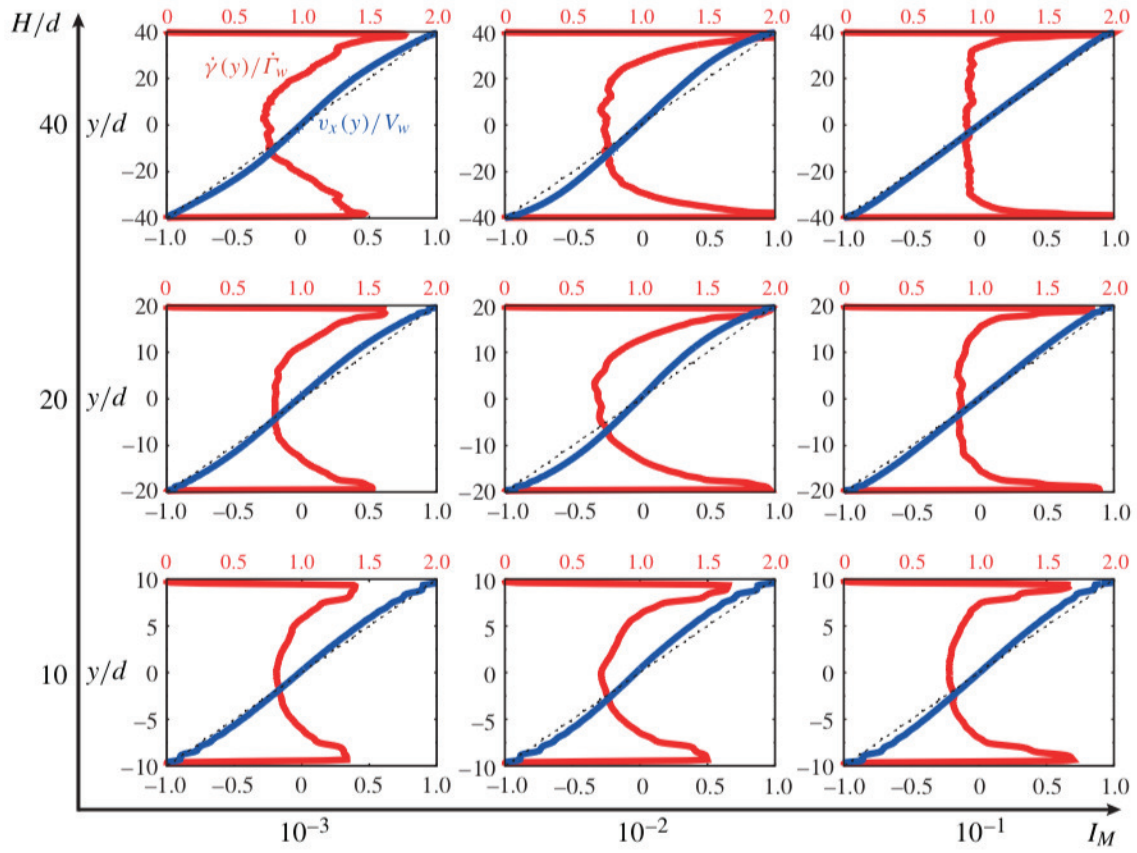


FIGURE 2.5: Time-averaged velocity and shear rate profiles for flows with various inertial numbers I and widths H as indicated by arrows. The velocity profile $v_x(y)$ normalised by the wall velocity V_w . For the colour code refer to (Rognon et al. 2015).

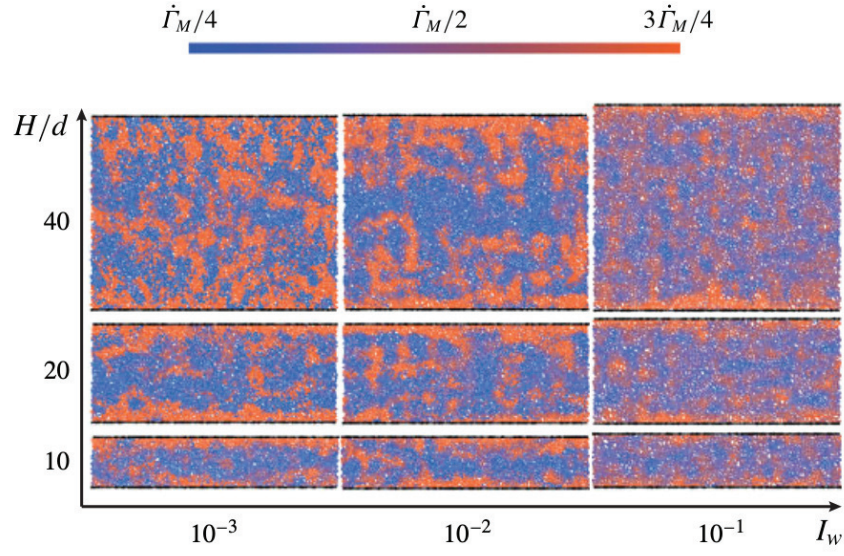


FIGURE 2.6: Vorticity field. Snapshots for different system widths, H , and different inertial numbers, I as indicated by the arrows. (Rognon et al. 2015).

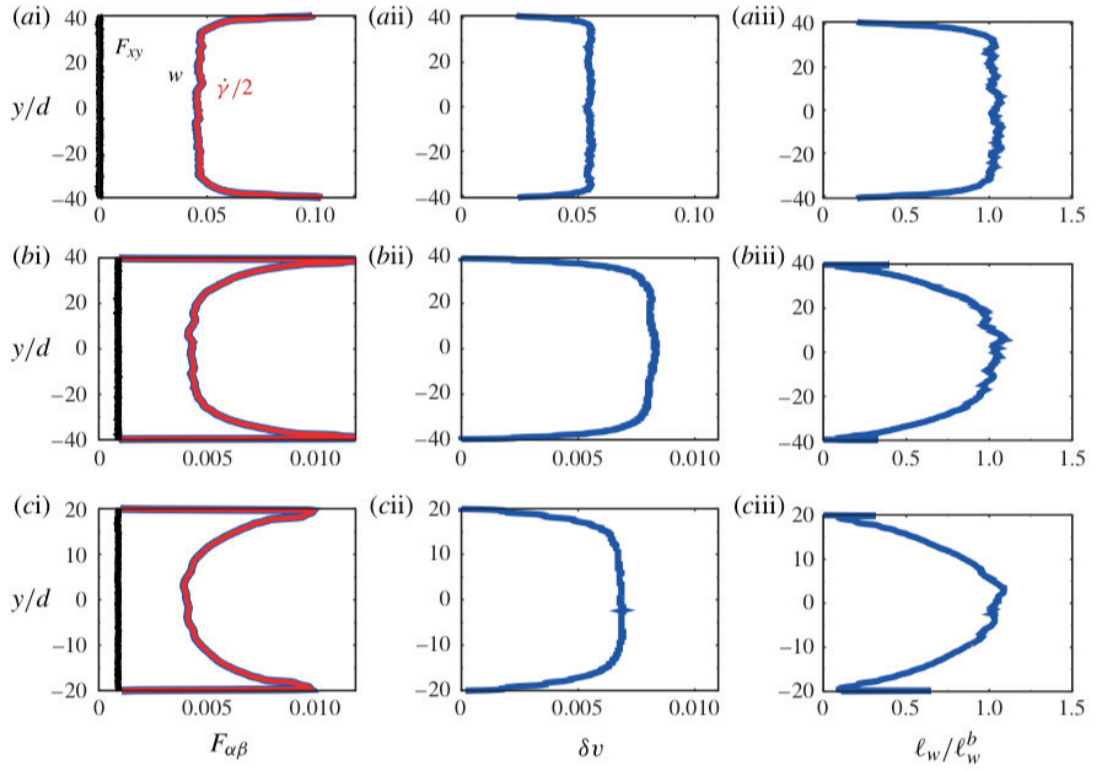


FIGURE 2.7: Vorticity and vorticity length scale. (a) $H/d = 40$, $I = 0.1$; (b) $H/d = 40$, $I = 0.01$; (c) $H/d = 20$, $I = 0.01$. (i) the shear rate $\dot{\gamma}$, vorticity w and F_{xy} profiles. (ii) the velocity fluctuations profiles δv , (iii) the deduced vorticity length scale w (Rognon et al. 2015).

2.4 Microscopic deformation

Recent studies have focused on understanding the micromechanical origins of macroscopic flow behaviour in granular materials. For example, the role of force chains on the grain scale has been investigated. These chains influence the flow dynamics and stability of granular materials under shear (Tian and Liu 2019). Furthermore, the effect of particle shape and size distribution on flow properties has been explored, revealing that polydispersity can improve the stability and flowability of granular materials (Pan et al. 2022; Cantor et al. 2018).

Granular materials under shear exhibit localised deformation, plastic deformations, and slip avalanches. Slip avalanches in granular materials refer to large-scale sudden slippages or shifts within the material that occur when internal stresses exceed a certain threshold. These events involve a rapid reorganisation of the grains, leading to a sudden release of accumulated stress, similar to phenomena observed in earthquakes and landslides. Stress avalanches in the granular material are suggested to be related to the spatial and temporal evolution of microscopic plastic events (Ma et al. 2021) and are induced by the interaction of these microscopic plastic events (Nicolas et al. 2018).

Microscopic observations in amorphous solids indicate that a comprehensive description of the macroscopic state of the deforming body requires not only stress and strain, but also certain average characteristics of the ‘shear transformation zones (Falk and Langer 1998). These zones are small regions, potentially composed of as few as five to ten molecules, arranged in configurations particularly susceptible to inelastic rearrangements under shear stresses. To identify these arrangements, a commonly used method is to measure the magnitude of nonaffine displacement during a specific time interval. The following section highlights some of the previous findings in this regard.

2.4.1 Shear strain and volumetric strain

Experimental studies and numerical simulations have revealed spatial and temporal correlations of plastic heterogeneity of granular materials (Ma et al. 2019a; Karimi and Barrat

2018). The link between microscopic dynamics and plastic flow in granular materials has been developed through the conduct of experiments and particle-based numerical simulations.

Quasi-static shear experiments have been conducted in a 3D disordered granular system to study plastic deformation and investigate the link between microscopic dynamics and plastic flow in granular materials (Cao et al. 2018). This study revealed that highly distorted coplanar tetrahedra are the structural defects responsible for microscopic plasticity in disordered granular packing. However, these defects may not fully capture the complexity of all possible mechanisms that contribute to deformation in granular materials. Moreover, the plastic events were discrete in space and exhibited specific orientations aligned with the principal stress direction. X-ray microtomography has also been used to image individual sand grains in 3D, followed by binarization and segmentation to separate grains (Andò et al. 2012). This imaging technique enables the observation of deformation mechanisms in real time during loading tests. A novel approach in that study was the introduction of an approach called ID-Track for quantifying individual grain kinematics in sand samples undergoing loading. Although this method tracks grains based on unique geometrical features for identification and matching between images, allowing for the measurement of displacements and rotations, there may be trade-offs in precision, particularly in capturing subtle rotational movements of grains during deformation tests.

The dense packing of the granular material has also been simulated under biaxial compression using the combined finite- and discrete-element method. This method has allowed the collection of a large amount of particle-level kinematical data including particle angular velocity, granular temperature, and local strain. The spatiotemporal data analysis provided new insights into strain localisation in dense granular materials, revealing clustered patterns during shearing. This was evidenced by high Moran values I , positive scores Z and statistically significant p , indicating the inherent short-range order in granular systems. A correlation was established between localised modes with different particle kinematics and the spatial distributions of local Moran statistics and the quadrant location map, suggesting a connection between particle behaviour and the spatial patterns of strain localisation (Ma et al. 2019b).

2.5 Nonaffine displacement

A key question in understanding grain-level deformation is identifying where irreversible plastic rearrangements occur. This involves pinpointing locations where molecular or particle displacements are nonaffine, meaning that they significantly deviate from what can be described by a linear strain field. Previous research suggests that at very small strain scales, nonaffine motions originate in particles that experience large stress fluctuations due to the fragility of the contact force network and the short lifespan of force chains. In contrast, plastic deformation at larger strain scales is characterised by structural rearrangements and shear transformations. Between these two scales, cooperative dynamics and long-range dynamical heterogeneity play a crucial role in the annihilation and merging of plastic zones, particularly at strain scales close to the structural relaxation time (Ma et al. 2021).

2.5.1 Nonaffine displacement and plastic activities

In the context of molecular dynamics simulations, nonaffine displacement can be calculated by analysing the positions of particles at different time steps and evaluating the deviations from expected displacements based on applied stress, which could provide information on heterogeneity and localised plastic events that contribute to the general deformation behaviour of the material. Nonaffine displacement D_{min}^2 is determined by minimising the mean square difference between the actual displacements of neighbouring particles relative to a central one and the hypothetical displacements they would undergo in a region of uniform deformation described by a locally affine tensor ϵ_{ij} (Falk and Langer 1998). Thus, given a system-scale strain increment, the corresponding D_{min}^2 can be computed as:

$$D^2(t, \Delta t) = \sum_n \sum_i (r_n^i(t) - r_0^i(t) - \sum_j (\delta_{ij} + \epsilon_{ij}) \times [r_n^j(t - \Delta t) - r_0^j(t - \Delta t)])^2. \quad (2.18)$$

where the indices i and j represent spatial coordinates and the index n encompasses the particles within the interaction range of the reference particle. Here, $r_n^i(t)$ denotes the i^{th} component of the position of the particle n^{th} at time t . A neighbourhood is defined when $R_{ij} \leq 2d$ (Liu et al. 2021; Wang et al. 2020; Boattini et al. 2020; Mei et al. 2023) to

$R_{ij} \leq 2.5d$ (Ma et al. 2021; Falk and Langer 1998), and it is assumed that this range is large enough to encompass the local neighbours of the particles within the time interval Δt . In the computation of D^2 , the summation is performed on neighbouring particles j situated within the cutoff distance from particle i . This computation is then subject to minimisation with respect to the local strain tensor ϵ_{ij} . The determination of this tensor is accomplished using the methodology that was initially outlined by (Falk and Langer 1998), as presented below:

$$X_{ij} = \sum_n [r_n^i(t) - r_0^i(t)] \times [r_n^j(t - \Delta t) - r_0^j(t - \Delta t)]. \quad (2.19)$$

$$Y_{ij} = \sum_n [r_n^i(t - \Delta t) - r_0^i(t - \Delta t)] \times [r_n^j(t - \Delta t) - r_0^j(t - \Delta t)]. \quad (2.20)$$

$$\epsilon_{ij} = \sum_k X_{ik} Y_{jk}^{-1} - \delta_{ij}. \quad (2.21)$$

D_{min}^2 has been widely used as an indicator to investigate microscopic plasticity in various materials, including granular materials (Cao et al. 2018; Cubuk et al. 2017; Zhai et al. 2022; Mei et al. 2023), metallic glasses (Wang and Jain 2019), and colloidal systems Ghosh et al. 2017; Liu et al. 2021. Particles exhibiting nonaffine displacements exceeding a specified threshold are typically involved in microscopic plastic events. Figure 2.8 shows the intensity plots D_{min}^2 for a particular system that undergoes plastic deformation.

In recent years, the combination of nonaffine displacement measurements with machine learning approaches has significantly advanced research in understanding the relationship between microscopic structure and plasticity. This integration has greatly enhanced our understanding of the nature of microscopic plasticity in amorphous solids. A study by (Ma et al. 2021) used a combined finite- and discrete element method (FDEM) to explore the microscopic dynamics of plastic flow in granular materials. This method involved simulating the simple shearing of irregularly shaped particles and tracking particle-scale dynamics once a steady state was reached. The research highlighted the initiation, annihilation and merging of zones of intense plastic activity on different time scales or strain scales. The findings demonstrated that nonaffine motions originated from particles that experienced significant stress fluctuations at small strain scales. By examining the spatiotemporal variability of plastic activity and the transient nature of highly mobile clusters, it was confirmed that the

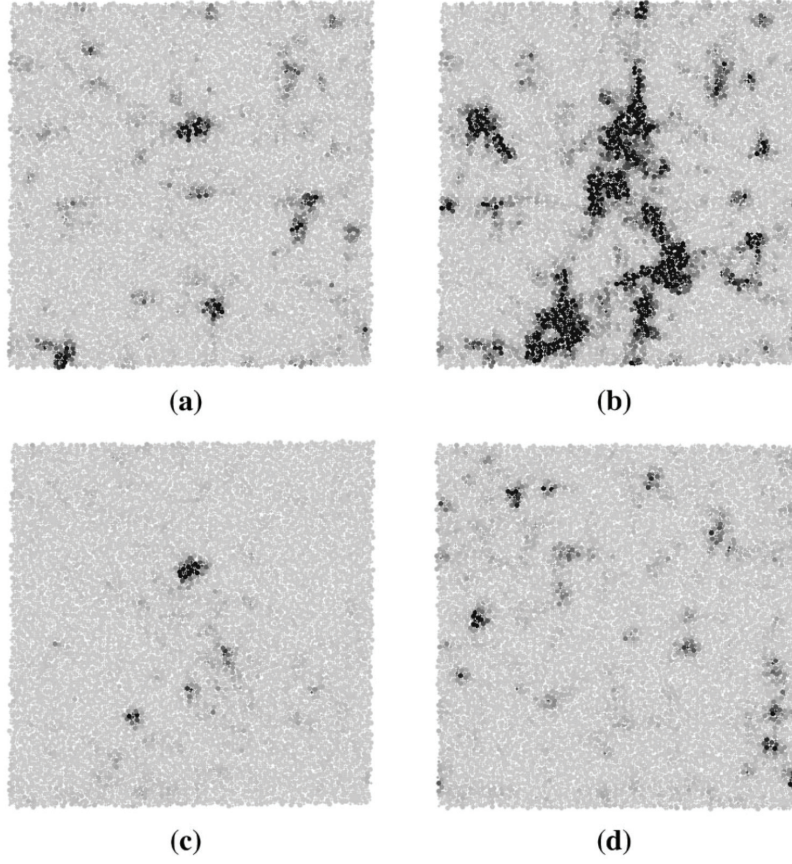


FIGURE 2.8: Intensity plots of D_{min}^2 , the deviation from affine deformation, for various intervals. (a – c) show deformation during one simulation in which the stress has been rapidly ramped up to a value lower than the yield stress and then remained constant. (d), the initial system and the time interval are the same as in (a), but the stress has been applied in the opposite direction. The grey scale in these figures has been selected so that the darkest spots identify molecules for which $|D_{min}| \approx 0.5a_{sl}$ (Falk and Langer 1998).

dynamic nature of plastic deformation in granular materials. This variability underscores the complexity of plastic behaviour and the necessity of considering both spatial correlation and temporal evolution when studying plastic heterogeneity in sheared granular materials. The effect of different time and strain intervals on the spatial distribution of D_{min}^2 and the process of initiation, annihilation, and merging of the intense plastic cluster is shown in Figure 2.9.

Another significant study by (Mei et al. 2023) employed a novel data-driven framework based on a 3D convolutional neural network (CNN) to establish a quantitative link between particle-scale dynamics and macroscopic responses of granular materials in 3D. The research

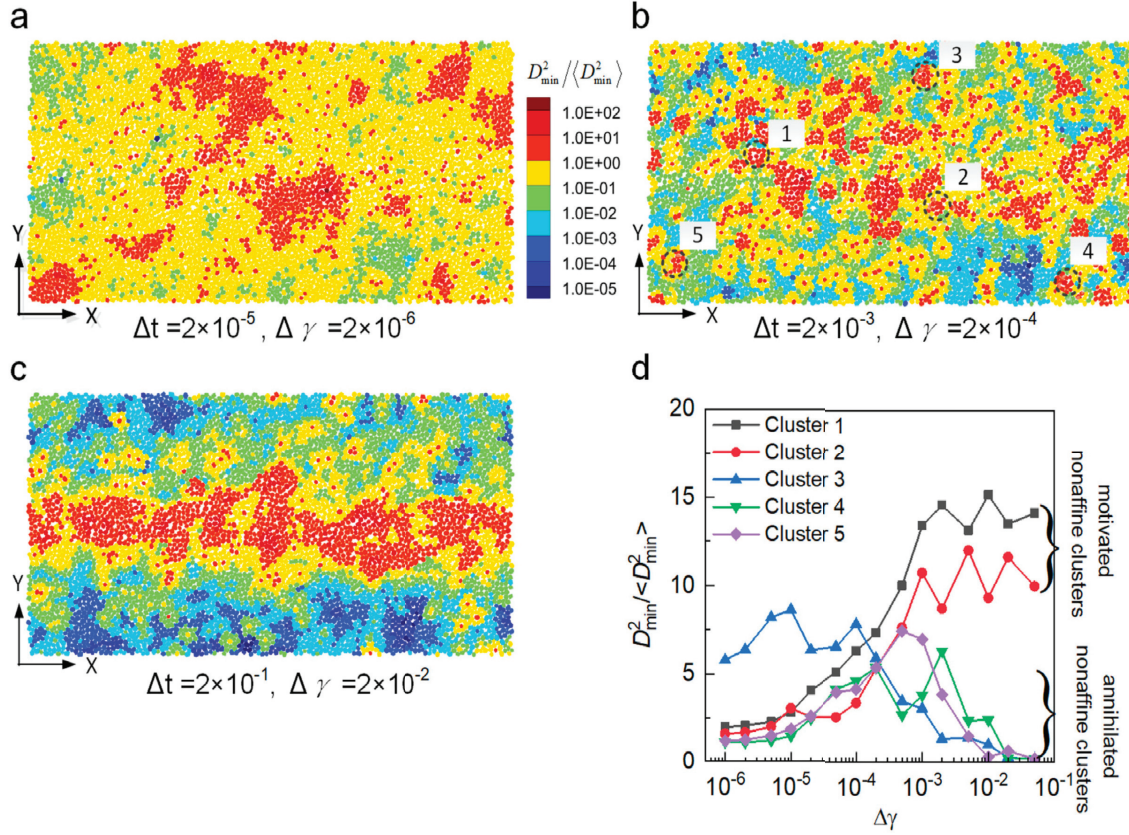


FIGURE 2.9: Spatial distributions of D_{min}^2 . (a – c) show the spatial distributions of D_{min}^2 for different strain intervals $\Delta\gamma$. The particles are colour-coded using the same logarithmic colour scales. Five clusters are circled that have undergone obvious shear transformations and local rearrangements. (d) Evolutions of cluster nonaffinity as a function of the strain interval $\Delta\gamma$ (Ma et al. 2021).

revealed that mesoscopic structures, particularly active clusters that exhibit high microscopic dynamics, play a crucial role in determining macroscopic responses. The spatial patterns of microscopic dynamics were identified as key factors controlling stress fluctuations in granular materials. The study distinguished two distinct mechanisms responsible for these spatial patterns during the stick and slip regimes: free volume-induced structural rearrangements during the stick regime and contact network dynamics during the slip regime. The research emphasised the importance of spatial clustering of microscopic dynamics in the governance of slip avalanches and highlighted the spatial pattern of microscopic dynamics as a critical factor influencing macroscopic stress fluctuations in granular materials.

2.6 Measurement of Microscopic heterogeneity

2.6.1 Spatial correlation

The measurement of spatial correlation in granular materials is essential to understand the microstructural organisation and collective behaviour of granular assemblies. Spatial correlation functions, such as the normalised correlation function, quantify how the positions, velocities, or rearrangements of grains are correlated over different spatial separations. The normalised correlation function for nonaffine displacement $C_{D_{min}^2}(r)$ is defined as:

$$C_{D_{min}^2}(r) = \frac{\langle D_{min}^2(0)D_{min}^2(r) \rangle - \langle D_{min}^2 \rangle^2}{\langle [D_{min}^2]^2 \rangle - \langle D_{min}^2 \rangle^2}. \quad (2.22)$$

where, $D_{min}^2(0)$ and $D_{min}^2(r)$ represent the nonaffine displacements of neighbouring grains within the distance of r , with brackets indicating the average of all pairs of particles (Ma et al. 2021; Cubuk et al. 2017).

Additionally, the spatial auto-correlation of plasticity or any given dataset can be quantified using Moran's I , which objectively measures how similar one element is to others surrounding it. This single quantitative metric defined as:

$$I = \frac{N}{\sum_i \sum_j w_{ij}} \frac{\sum_{i=1}^N \sum_{j=1}^N w_{ij} (D_{min,i}^2 - \langle D_{min}^2 \rangle) (D_{min,j}^2 - \langle D_{min}^2 \rangle)}{\sum_{i=1}^N (D_{min,i}^2 - \langle D_{min}^2 \rangle)^2}. \quad (2.23)$$

where N is the number of particles and w_{ij} is the spatial weight matrix. $w_{ij} = 1$ for neighbouring particles with a cut-off distance of 1.5, and $w_{ij} = 0$ otherwise (Liu et al. 2018). Moran's I evaluates whether the observed pattern is clustered ($0 < I \leq 1$), dispersed ($-1 < I \leq 0$), or random (≈ 0).

Moran's I is often transformed to Z score for statistical application, and computed as :

$$Z_I = \frac{I - E(I)}{\sqrt{Var(I)}}. \quad (2.24)$$

where $E(I) = \frac{-1}{N-1}$ is the expected value of Moran's I under the null hypothesis of no spatial autocorrelation and $Var(I)$ is the variance of Moran's I . The value p is the probability of

incorrect rejection of the null hypothesis. The Z score and the corresponding p value help to decide whether to reject the null hypothesis (Ma et al. 2019b).

To quantitatively characterise nonaffine clusters, clusters are typically constructed by connecting the highest 10% particles D_{min}^2 that are closest neighbours. The radius of gyration R_g is calculated as:

$$R_g^2 = \frac{\sum_{i=1}^s A_i (r_i - \bar{R})^2}{\sum_{i=1}^s A_i}. \quad (2.25)$$

where the summation is over s particles belonging to the cluster, A_i is the area of particle i , $\bar{R}$ is the center of mass of the cluster defined by:

$$\bar{R} = \frac{\sum_{i=1}^s A_i r_i}{\sum_{i=1}^s A_i}. \quad (2.26)$$

It has been suggested that the radius of gyration R_g has a growth in the power law with the size of the cluster s , but its relationship with the value of the inertial number has not yet been explored (Ma et al. 2021).

2.6.2 Temporal correlation

The temporal auto-correlation function C for kinematic measurements K including nonaffine displacement D_i^2 , for a specific reference time t and time interval Δt , is defined as:

$$C(\Delta t) = \frac{\frac{1}{n} \sum_{i=1}^n (K_i^t - \bar{K}^t)(K_i^{t+\Delta t} - \bar{K}^{t+\Delta t})}{\sigma(K^t)\sigma(K^{t+\Delta t})}. \quad (2.27)$$

here, $\sigma(K^t)$ denotes the standard deviation of the variable K_i across all n particles in the shear cell at time t . A characteristic correlation time τ is then defined by the integral:

$$\tau = \int_{\Delta t=0}^{\infty} C(\Delta t) \partial \Delta t. \quad (2.28)$$

2.6.3 Variogram

The variogram method is a geostatistical approach used to assess the representative volume element (REV) size for various structural, kinetic and kinematic properties of granular

materials. The variogram represents the variance in a homogenised property as a function of the sampling volume or distance. By tessellating the domain of interest into subdomains and calculating the homogenised property within each subdomain, variograms help to understand the variance evolution across different sampling volumes.

The variance of homogenised properties across all subdomains is calculated, and the process is repeated for increasing subdomain sizes to analyse the variance across different volumes. The variance decay with increasing sampling volume was analysed to identify the transition from statistical heterogeneity to statistical homogeneity, with different decay rates indicating different levels of homogeneity (Shahin et al. 2022).

2.6.4 Representative Elementary Volume (REV)

In granular mechanics, identifying the REV size has been a topic of extensive research. The existence of a REV has been demonstrated in granular packings subjected to quasi-static loading, focussing on structural and mechanical properties such as porosity (De Cola et al. 2016), stress, and energy dissipation (Wiącek and Molenda 2016; Shahin et al. 2022). The size of the REV was found to be influenced by various factors, including the type of material, elastic properties, geometry (Wiącek and Molenda 2016; Costanza-Robinson et al. 2011; Al-Raoush and Papadopoulos 2010), boundary conditions (Wiącek and Molenda 2016), and loading patterns (Shahin et al. 2022).

Measurement of the Representative Volume Element (REV) is crucial in materials science and engineering to understand the behaviour of materials on a macroscopic scale by examining their microscopic properties. The explanation of how researchers typically measure REV is summarised in the following section.

2.6.4.1 Geostatistics methods and autocorrelation functions

Researchers apply geostatistical methods to analyse the spatial variability of material properties. This involves statistical techniques that help in understanding how a property changes

over space and at what scale this property becomes homogeneous across the sample. Similarly to variograms, autocorrelation functions assess the spatial correlation of properties at different distances to find the REV. This approach is particularly useful for determining the homogeneity of microstructural features in a material, ensuring that the chosen volume accurately represents the larger material

2.6.4.2 Experimental methods

. Experiments such as X-ray tomography and 3D X-ray diffraction are carried out to collect data on the structural, kinetic, and kinematic variables of the material. These nondestructive testing methods provide a detailed view of the material's internal structure and behaviour under different conditions. By analysing these high-resolution images, researchers can quantify the microstructural features and estimate the REV by identifying the volume over which these features remain consistent.

2.6.4.3 Numerical methods

The discrete element method (DEM) and finite element analysis (FEA) complement experimental data by allowing researchers to model and simulate the behaviour of granular materials under various conditions and analyse the distribution of stress and deformation within the material. These simulations help in validating the experimental measurements and in exploring the effects of different boundary conditions and system size on REV sizes.

2.6.4.4 Image analysis

Image analysis techniques are employed to process and analyse the microscopic images obtained from experimental methods. These techniques involve quantifying the geometric and topological properties of the microstructure, such as grain size, shape, and distribution. Image analysis can be combined with statistical methods to assess the homogeneity of these properties across different volumes, helping to determine the REV. Advanced image processing algorithms have been developed to automate this process, making it more efficient and accurate.

2.6.4.5 Cluster analysis

Cluster analysis is used to group similar data points within microstructural images, based on their properties. This method helps to identify distinct regions within the material that may require separate REV's. By clustering the data, researchers can ensure that the REV chosen is truly representative of the dominant microstructural characteristics and that it accounts for any significant heterogeneity within the material. This approach is particularly useful in complex materials with multiple phases or varying grain sizes.

2.7 Concluding remarks

Based on the literature review, despite numerous studies on granular material shear flow, several critical aspects remain underexplored, revealing significant gaps in our current understanding.

One key area that requires further investigation is the evolution of deformation at the micro-scale over extended timescales that far exceed the structural relaxation time. Understanding how localised failure develops and progresses over these longer durations is crucial to building more accurate predictive models of granular material failure under shear. The behaviour of individual grains often diverges from the average global response of the granular system, especially in how velocity and deformation interact. Although grain velocity is known to not always align with shear direction, our understanding of the shear process itself is incomplete, particularly regarding the microstructures of kinematics at the grain scale. Advancing this knowledge necessitates a detailed examination of deformation rates and spatial correlations, acknowledging that the presence of heterogeneities requires a sufficiently large Representative Volume Element (REV) to capture these effects accurately.

Furthermore, the impact of varying parameters, such as particle size, shape, boundary conditions, and different loading conditions, on strain localisation is not yet fully understood. These factors influence material behaviour and require extensive investigation to elucidate their effects. Moreover, the role of external factors, such as temperature and moisture content,

which can significantly impact strain localisation, has not been adequately explored. Insights into how these environmental conditions influence granular systems could lead to better predictions and control of material behaviour in real-world applications.

Another area that needs further study is the determination of the existence and size of Representative Volume Elements (REVs) in granular flows. Unlike continuous materials, where REVs are more commonly defined, the discrete nature of granular materials introduces unique challenges. The methods used to measure REVs in continuous materials are not necessarily applicable to granular systems, and this discrepancy has not yet been thoroughly addressed in the literature. Innovative and parametric methods are required to accurately define REVs in granular flows. Typically, the identification of an REV is constrained by both lower and upper bounds, with recent studies focussing primarily on the lower bound, which pertains to the representation of homogenised behaviour. However, further research is needed on re-examining the lower bound and identifying the upper bound of the REV, particularly in terms of incorporating local heterogeneity into numerical analysis of spatial processes. This would provide a more comprehensive framework for understanding and modelling the behaviour of granular materials.

Much of the current research has focused on plastic deformation in quasi-static flow under a single inertial number, leaving the behaviour under diverse flow conditions largely unexplored. Understanding how these different conditions affect plastic deformation is crucial for a complete understanding of material behaviour. To fully grasp the mechanisms of plastic deformation, it is essential to investigate the relationship between the microstructural properties and kinematics of granular materials and the spatiotemporal variability of plastic activity.

In addition, the mechanisms underlying microscopic plastic deformation in granular materials are not fully understood. Specifically, the processes by which microscopic plastic events originate and merge to produce macroscopic plastic deformation require further investigation for the development of continuum models. Bridging this knowledge gap is essential to connect microscale dynamics with macroscale behaviour of granular materials, which remains a challenging undertaking in material science, geology, and industrial applications. Additionally, it is important to develop nonlocal continuum models that account for the specific timescale

of deformation propagation, where particle interactions are not instantaneous but occur over measurable durations. Recognising the importance of large-scale structures and clusters will aid in the development of more accurate continuum models that better capture the complex behaviour observed at the grain scale.

CHAPTER 3

Size of heterogeneous deformation in sheared granular flows

This article will investigate the identification of a REV size based on kinematics in granular flows to develop homogenisation theories and understand the effective behaviour of granular flows as a continuum scale. The study begins by establishing the continuum description of granular flows, which is based on continuity equations for the conservation of mass and momentum. It highlights the importance of REV, which is influenced by various factors such as material type and loading patterns, and suggests that the REV size in granular flows may be larger than the grain diameter due to the development of correlated grain motion, termed ‘granulence’. The discrete element method is used to analyse local kinematic quantities across a range of inertial numbers, revealing that the REV size increases at lower inertial numbers and is characterised by a power-law relationship.

The findings indicate that the REV size, which is crucial for developing homogenisation theories for granular flows, diverges at low inertial numbers, suggesting that kinematic structures within the flow may not fully develop in smaller systems. This has implications for understanding deviations in constitutive laws for granular viscosity and diffusivity, particularly in flows near boundaries. The results also propose that similar large REV sizes may be observed in other soft materials exhibiting correlated particle motion, thereby broadening the relevance of the study beyond granular flows.

This article is taken directly from work published in *Physical Review Fluids* (Shekari et al. 2023). I was the primary researcher and lead author under the guidance and supervision of Associate Professor Pierre Rognon and Dr. Benjy Marks.

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Size of heterogeneous deformations in sheared granular flows

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Sheared granular materials spontaneously develop heterogeneous and transient kinematic fields which resemble turbulence. We focus here on characterizing the length scale of these heterogeneities. We simulate plane-shear flows and measure the local grain velocity, velocity fluctuation, shear rate, vorticity, and dilation rate. The results show that these quantities are widely distributed, even more so at low inertial numbers. We relate this effect to spatial correlations that develop at low inertial numbers, where the flow becomes partitioned into “cold” patches with lower than average strain rate and “hot” zones where the strain rate is concentrated. We finally extract a characteristic length scale for the size of these heterogeneities, corresponding to the size of a representative elementary volume. This size is found to vary from a few grain diameters at high inertial number to a few dozen grain diameters at low inertial number, following a characteristic power law. These insights into representative elementary volume (REV) size may be of importance to further develop continuum models for granular flows, capturing local and nonlocal effects.

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I. INTRODUCTION

A continuum description for granular flows is key to predict the behavior of many natural events and industrial processes. This description hinges on continuity equations capturing mass and momentum conservation. Each law relates a diffusion coefficient—diffusivity or viscosity—to spatially averaged deformations and stresses. Examples of such laws include the $\mu(I)$ frictional rheology [1,2], nonlocal models [3–5], and scaling laws for shear-induced diffusion [6–8]. These laws are predicated on the assumption of the existence of a finite size representative elementary volume (REV), which is defined as the minimum volume of material needed to obtain a behavior similar to any larger volume.

The existence of a REV has been demonstrated in granular packings subjected to quasistatic loading, focusing on structural and mechanical properties such as porosity [9], and stress and energy dissipation [10,11]. The size of the REV was found to be influenced by various factors, including the type of material, elastic properties, geometry [10,12,13], boundary conditions [10], and loading patterns [11]. In contrast, the existence and size of REV in granular flows remains to be established.

While a single grain diameter is an intuitive lower bound for a REV, analysis of granular flow internal kinematics suggest that it could, in fact, be much larger. These studies have revealed the spontaneous development of the correlated motion of grains, a process coined “granulence” by analogy with velocity correlations observed in turbulent flows [14,15]. The structure of these granular clusters yields some mesoscopic length scale which is likely to affect the REV size [16–20]. For example, a configuration that is too small to let granular clusters develop to their full size could behave differently to a larger configuration able to accommodate larger clusters. The drop

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in effective viscosity observed near flow boundaries is an empirical confirmation of this relation [21–23].

This work attempts to measure the REV size in granular flow by focusing on their internal kinematics. In discrete element method simulations of plane-shear flows covering a range of inertial numbers (Sec. II), we first measure local quantities including grain velocity, relative velocity (Sec. III), and local velocity gradient tensors (Sec. IV), and analyze their statistical distribution. We then extract a REV size based on the local rate of shear and vorticity (Sec. V), with a particular interest in its variation with the inertial number.

II. PLANE SHEAR FLOWS

We use the discrete element method (DEM) to simulate plane-shear flows of dry, cohesionless grains. The simulated system is presented in Fig. 1(a). It consists of a two-dimensional assembly of 10^4 grains with a mean diameter d , mass m , and density ρ . To prevent shear-induced crystallization, a uniform polydispersity of $d \pm 20\%$ is introduced in the grain diameters. The system is two dimensional (x and y directions only) and Lees-Edwards periodic boundary conditions [24] are used to avoid flow heterogeneity induced by solid walls [22]. The shear rate $\dot{\gamma} = \frac{2u}{H}$ and normal stress P are prescribed and kept constant during flow, where u is the shearing velocity at the boundaries and H is the system size in the y direction, which varies to maintain a constant value of P . The system size in the x direction is kept constant at $100d$.

Grains interact through direct contact via a contact force comprised of a linear elastic repulsion, a viscous dissipation, and tangential friction. The associated mechanical parameters are the normal stiffness $k_n = 10^3 P$, the coefficient of restitution set to 0.5, and the coefficient of friction set to 0.5. The choice of these parameters was found to only mildly influence the rheological behavior of the packing [2,25]. The ratio k_n/P is selected to be as low as possible to enable larger time steps and therefore reduce computational time, while large enough not to affect the flowing properties of the material. It is expected that stiffer grains would yield similar results. In contrast, softer grains could affect the flow dynamics [25], although such highly deformable grains are seldom.

In the absence of gravity, this configuration yields homogeneous, steady shear flows. Here, homogeneous means that when averaged over time, the shear rate $\dot{\gamma}$ and the stresses are the same anywhere in the flow. This implies that the inertial number [1,2] is also homogeneous,

$$I = \dot{\gamma} t_i,$$

where $t_i = d\sqrt{\frac{\rho}{P}}$ is the inertial time. At any point in time, however, local fluctuations may arise, which will be the focus of the analysis below.

A series of steady flows was simulated covering a range of inertial numbers $10^{-3} \leq I \leq 1$. The lower values correspond to a quasistatic regime, while the higher values correspond to a collisional regime. Each flow is prepared by preshearing an initially loose and random packing over five shear deformations. This is sufficient to reach a steady regime during which macroscopic stresses and solid fractions are no longer evolving. The grain's velocity and position are then recorded every 1/20th of a shear deformation, for a duration of 15 shear deformations. This forms the database analyzed below.

III. GRAIN AND PAIR VELOCITIES

We first consider individual grain velocities, given by $\vec{v}^i$ for the velocity of grain i in the x and y directions, with components v_x^i and v_y^i . We define the nonaffine components $\delta\vec{v}^i$ as

$$\delta v_x^i = v_x^i - y^i \dot{\gamma}, \quad \delta v_y^i = v_y^i. \quad (1)$$

Here, $\delta\vec{v}^i$ measures the deviation from the time-averaged flow field, which is $y\dot{\gamma}$ in the x direction and 0 in the y direction. We refer to $\delta\vec{v}^i$ as the velocity fluctuation. Figures 1(b) and 1(c) illustrate

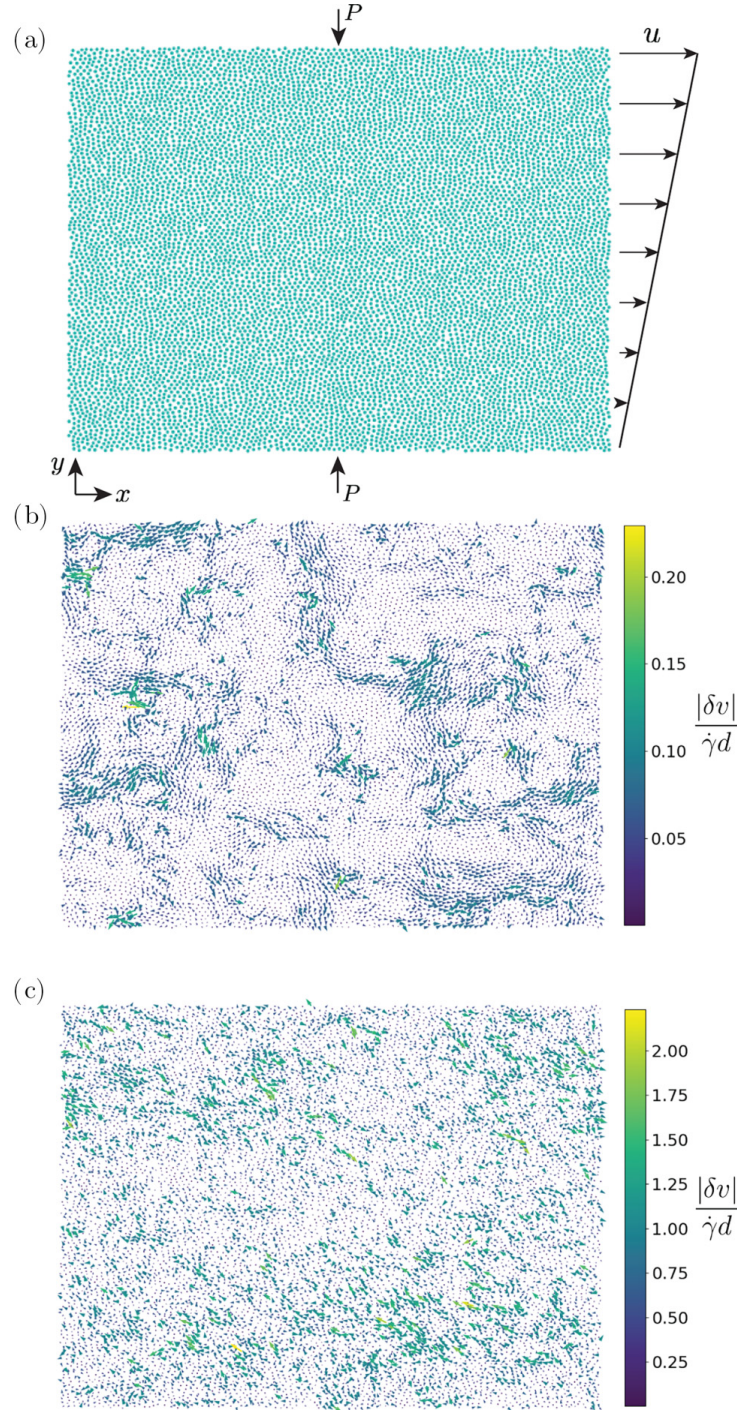


FIG. 1. Velocity fluctuations in plane-shear flows. (a) Schematic of the plane-shear flow configuration, featuring a snapshot of the grain packing under applied pressure P and shear velocity u . The system dimension is $100d \times 80d$. (b),(c) Snapshots of grain velocity fluctuations for inertial numbers $I = 0.01$ and $I = 0.5$, respectively. The arrows represent the velocity fluctuations δv in both the x and y directions for each grain, with the arrow base located at the center of the grain.

fields of velocity fluctuation in two snapshots taken in flows with $I = 0.01$ and $I = 0.5$, respectively. In agreement with previous findings [6,14,26], these snapshots show that grains are not simply following the average flow field. They feature large fluctuations, with some spatial correlations at low inertial number.

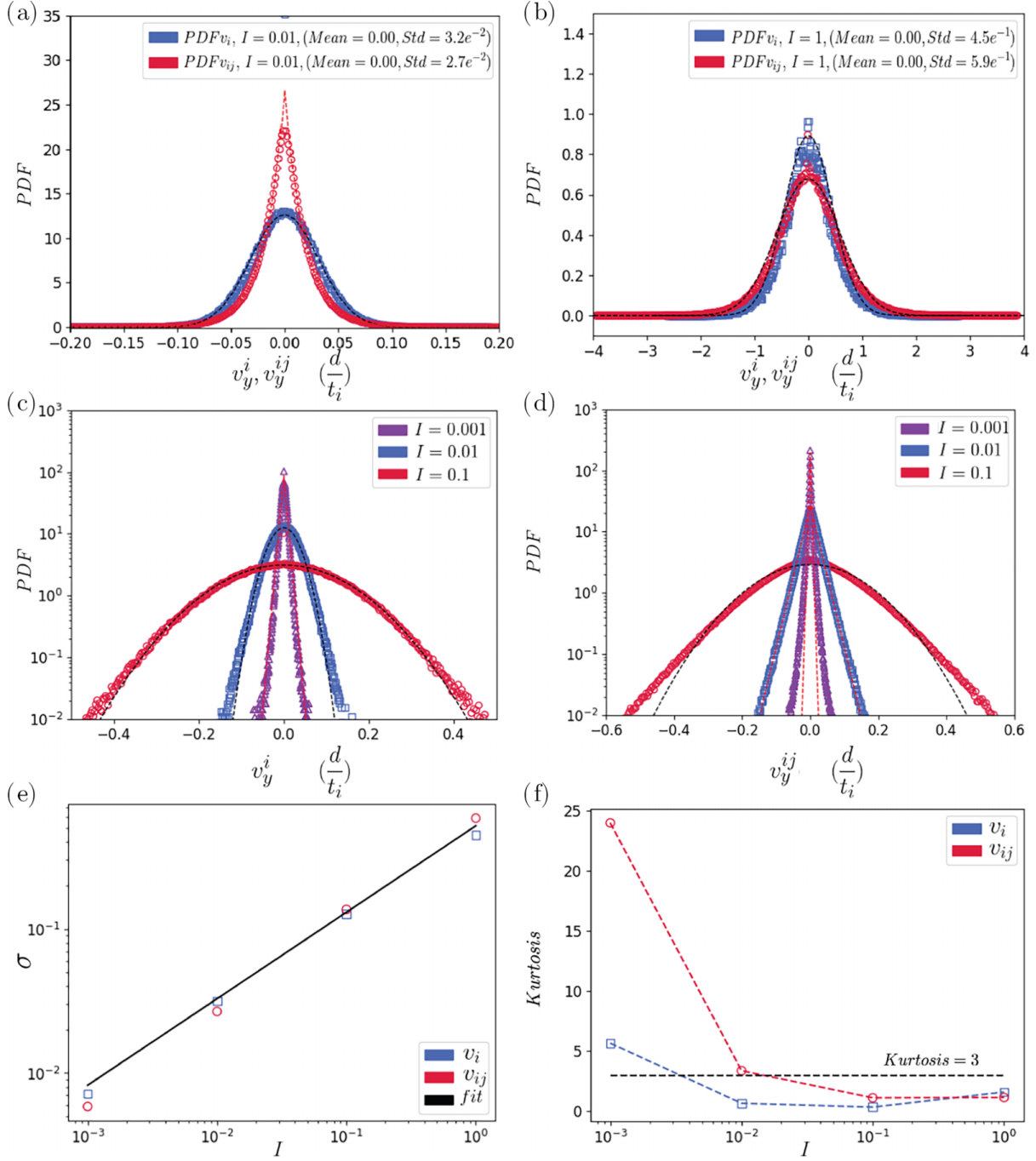


FIG. 2. Velocity and relative velocity distributions in plane-shear flows. (a),(b) Distributions of grain velocity (v_y^i) and grain relative velocity (v_y^{ij}) in the y direction for two different inertial numbers $I = 0.01$ and $I = 1$, respectively. Black lines are normal distribution fits; red line is an exponential distribution fit. Means and standard deviation of the distributions are given in the legends. (c),(d) Distributions of v_y^i and v_y^{ij} for a range of inertial numbers. (a)–(d) Velocities are in units of d/t_i . (e) Standard deviation of velocity fluctuations $\sigma(\delta v_y^i)$ (blue) and $\sigma(\delta v_y^{ij})$ (green) for different inertial numbers I , and power law in Eq. (3) (black line). (f) Kurtosis of v_y^i (blue) and v_y^{ij} (green) for different inertial numbers.

To highlight the existence of cooperative motion suggested in Fig. 1(b), we next consider the relative velocity of pairs of grains in the y direction, defined as

$$\delta v_y^{ij} = v_y^j - v_y^i, \quad (2)$$

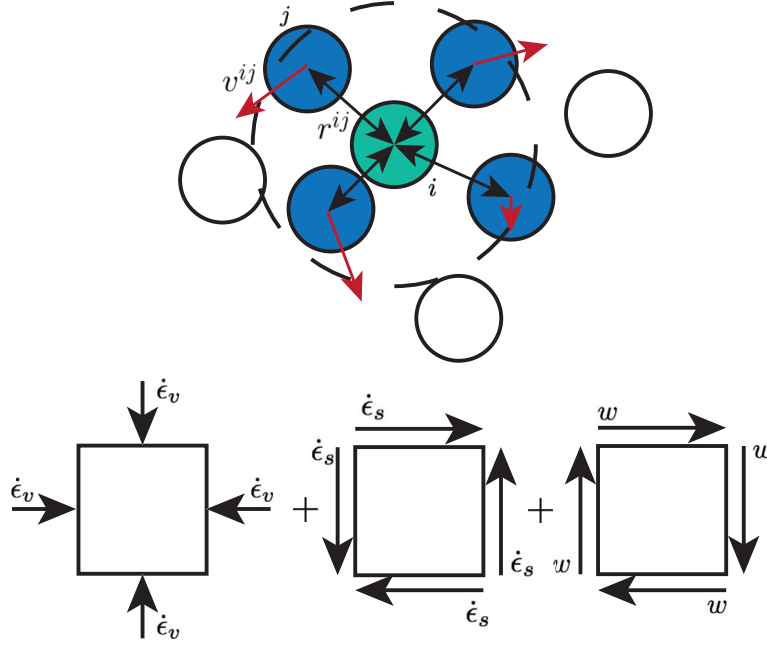


FIG. 3. Velocity gradient and decomposition into deformation rates. Top: Illustration of how the velocity gradient tensor F is calculated for a single grain (green) including close neighbors (blue) using Eq. (4); the calculation involves relative position (r^{ij}) and relative velocity (v_y^{ij}). The cutoff distance used to define neighboring grains in this study is $|r^{ij}| \leq 2d$, which is highlighted as the dashed circle. This cutoff distance is chosen to evaluate the velocity gradient on the smallest possible zone while ensuring that enough neighbors are present to determine F . Bottom: Decomposition of the velocity gradient tensor into volumetric strain rate, shear strain rate, and vorticity, corresponding to the trace, symmetric, and antisymmetric parts of F .

for all neighboring pairs of grains i and j . Two grains are deemed neighbors if their center-to-center distance is less than $2d$. Pairs that are farther away are excluded. The rationale for considering pair relative velocities is that their distribution can indicate the presence of spatial correlation within a distance $2d$. In the absence of spatial correlation, grain and pair velocities should be equally distributed. In contrast, some differences in their distribution should arise in the presence of spatial correlation.

Figures 2(a) and 2(b) compare the probability density functions (PDFs) of these two quantities including all grains, all pairs, and all time steps at two inertial numbers $I = 0.01$ and $I = 1$. At high inertial number, grain and pair velocities both follow a normal distribution. At low inertial number, grain velocities follow a normal distribution, while pair velocities follow an exponential distribution. Consistent with the representation in Fig. 1, this suggests the development of spatially correlated motion at low inertial number. This transition, or lack of transition, from a normal to an exponential distribution is further illustrated in Figs. 2(c) and 2(d).

How much the grain and pair velocities deviate from the mean flow—which is null in this direction—is measured by the standard deviation of these distributions, $\sigma(v_y^i)$ and $\sigma(v_y^{ij})$. Figure 2(e) shows that in spite of the difference in the shape of these distributions, standard deviations of grain and pair velocities follow a similar power law of the inertial number,

$$\frac{\sigma(\delta v_y^i)}{d/t_i} \approx \frac{\sigma(\delta v_y^{ij})}{d/t_i} \approx \alpha I^{n_I}. \quad (3)$$

The results are consistent with exponents $n_I \approx 0.60$ and coefficient $\alpha \approx 0.50$. Such a power law for v_i is consistent with previous results [2,8,27]. A power exponent $n_I = 1$ would yield $\delta v_y^{ij} \propto \dot{\gamma}d$, which means that velocity fluctuations are entirely driven by the characteristic shear velocity $\dot{\gamma}d$, with no effect of the inertial time t_i . A power exponent less than 1 means that the two standard

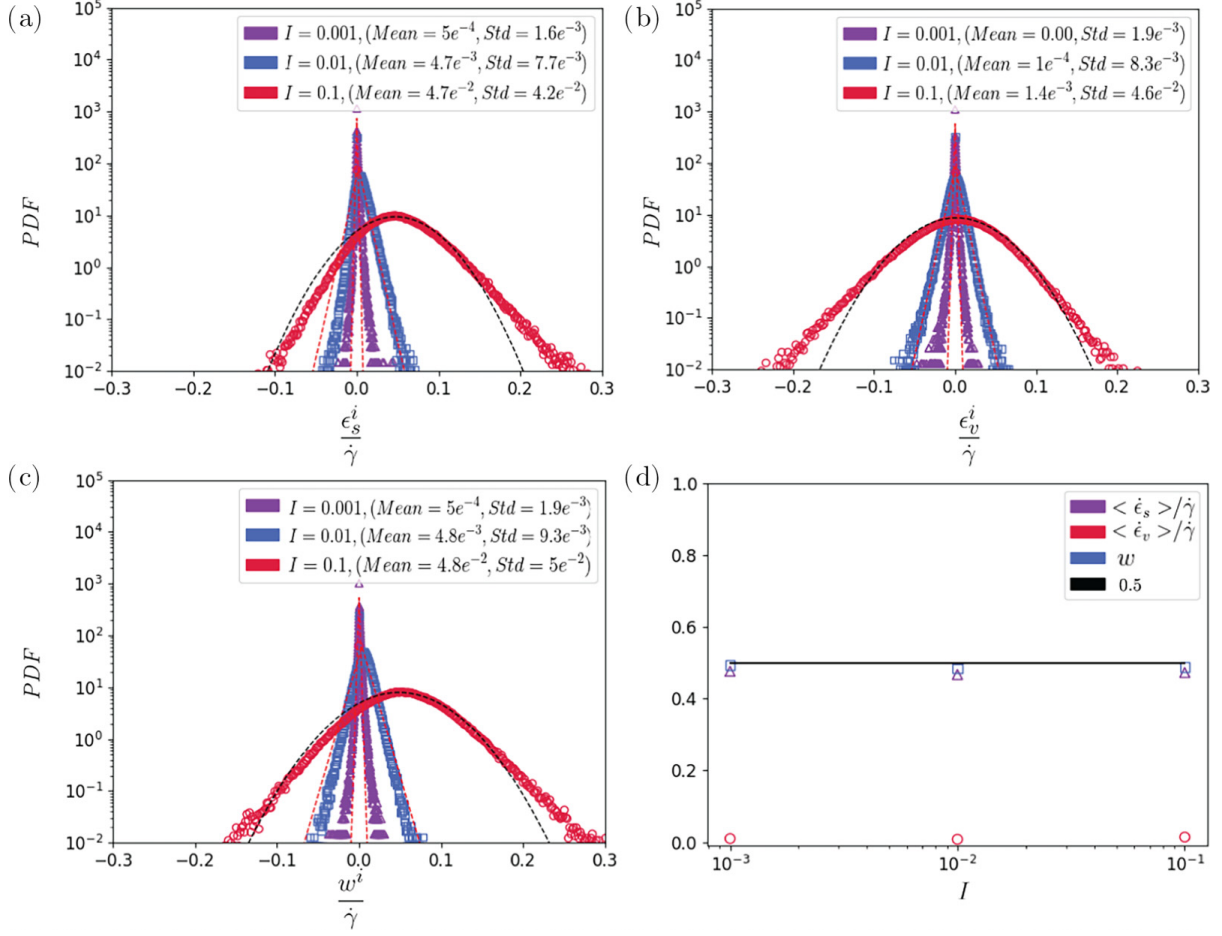


FIG. 4. Distribution of local deformation rates. (a) Shear strain rate ($\dot{\epsilon}_s$), (b) volumetric strain rate ($\dot{\epsilon}_v$), and (c) vorticity (w) for different inertial number I . (a)–(c) Means and standard deviations of the distributions are indicated in the legends. (d) Means $\langle \dot{\epsilon}_s \rangle$ (green line), $\langle \dot{\epsilon}_v \rangle$ (red line), and $\langle w \rangle$ (blue line) of these distributions normalized by the macroscopic shear rate $\dot{\gamma}$, including a black line at 0.5 for visual reference.

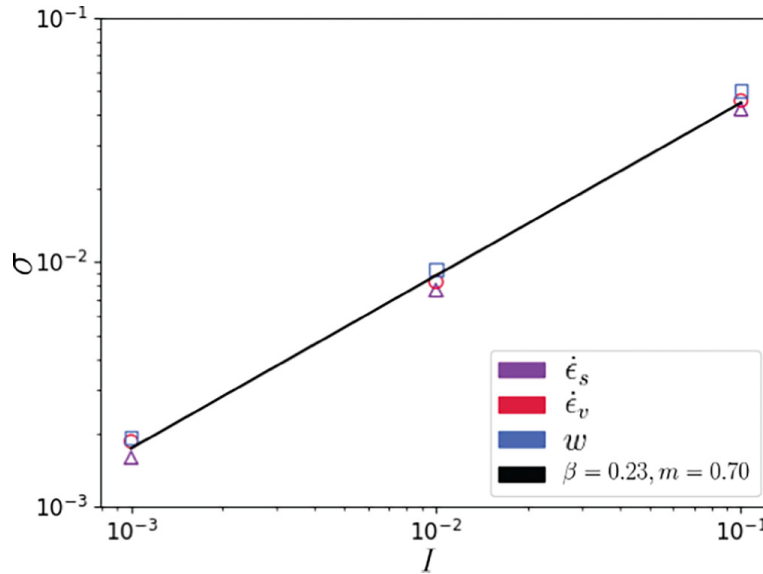


FIG. 5. Fluctuations of deformation rates, represented by the standard deviation of the local shear strain rate $\sigma(\dot{\epsilon}_s)$, volumetric strain rate $\sigma(\dot{\epsilon}_v)$, and vorticity $\sigma(w)$ in unit t_i^{-1} at different inertial number. The black line is the power law in Eq. (6) with $\beta = 0.23$, $m = 0.70$.

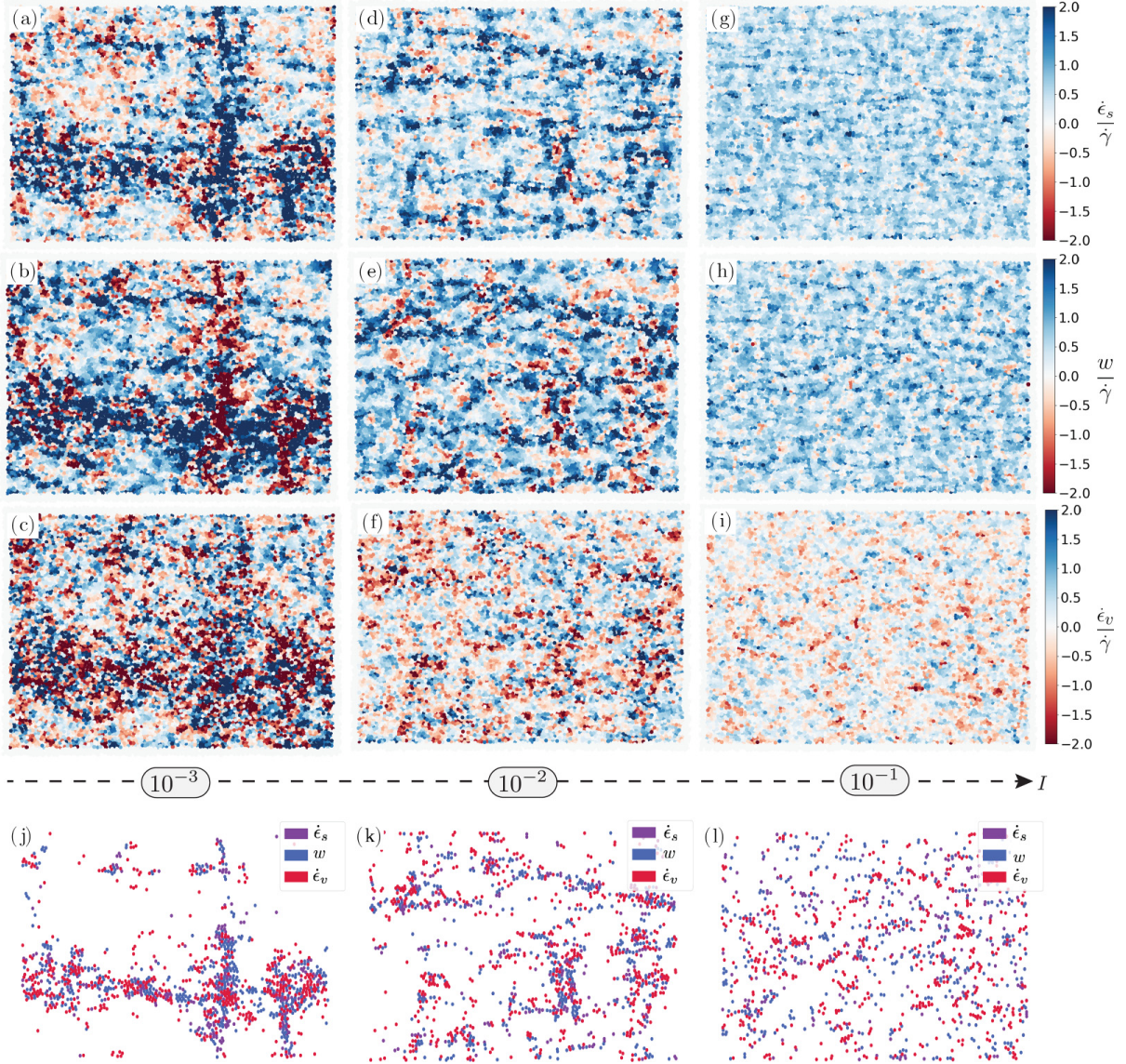


FIG. 6. Spatial distribution of kinematic fields. (a)–(i) Normalized shear strain rate, volumetric strain rate, and vorticity fields at three different inertial numbers $I = 0.001$, $I = 0.01$, and $I = 0.1$, respectively. (j)–(l) Spatial distribution of extreme values in each kinematic field at the same inertial numbers.

deviations become sensitive to the inertial time t_i and are much larger than the characteristic shear velocity $\dot{\gamma}d$ at low inertial numbers. A qualitative interpretation is that velocity fluctuations become driven by inertial rearrangements, which characteristic time t_i is independent of the shear time $\dot{\gamma}^{-1}$.

Compared to a normal distribution, an exponential distribution features higher probability near the mean value—zero in our case—and a higher probability very far from the mean. The transition from a normal to an exponential distribution for the pair velocities can then be understood as resulting from a partitioning of the flow into (i) “cold” zones with low pair velocities comprised of most pairs, and (ii) “hot” zones with high pair velocities comprised of few outlier pairs. The measure of the kurtosis of these distributions, shown in Fig. 2(f), further highlights the increasing presence of outliers at low inertial number. For individual grain velocity, the value of the kurtosis remains near 3, which is the value expected for a normal distribution. In contrast, pair velocity distributions exhibit significant excess kurtosis, with values reaching 25 at the lower inertial number. These high values are driven by, and thus reflect the increasing presence of, outliers in these distributions.

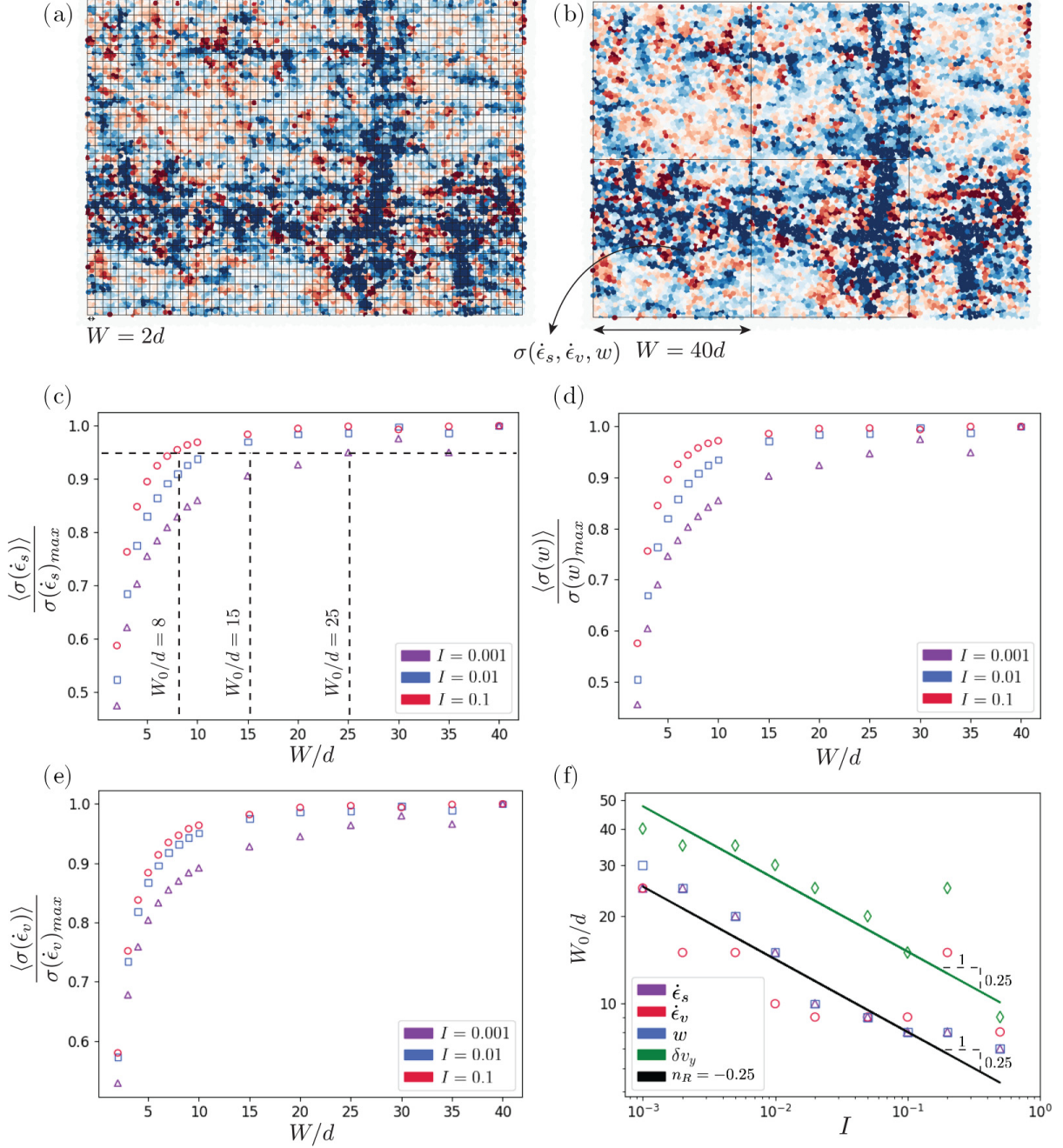


FIG. 7. REV size. (a),(b) Illustrations of the window size ($W = 2d$ and $40d$) used to measure standard deviations σ of kinematic quantities, and the mean of these standard deviations $\langle \sigma \rangle$ including all windows and all times. (c)–(e) Evolution of the mean standard deviation as a function of the window size W , normalized by its maximum value defined as $\sigma_{\max} = \langle \sigma \rangle(W = 40d)$. Dashed lines on (c) show the method used to extract a minimum REV size W_0 for different inertial numbers. (d) Minimum REV size W_0 obtained from shear strain rate, volumetric strain rate, and vorticity velocity fluctuation in the y direction, as a function of the inertial number. The green and black lines correspond to the power law in Eq. (7).

IV. VELOCITY GRADIENT AND DEFORMATION RATE

The heterogeneity in grain and pair velocities evidenced above suggests that the rate of deformation within the flow is also not homogeneous and is likely to deviate from the macroscopic shear rate $\dot{\gamma}$. To evidence heterogeneities in the deformation rate, we measured the local velocity gradient

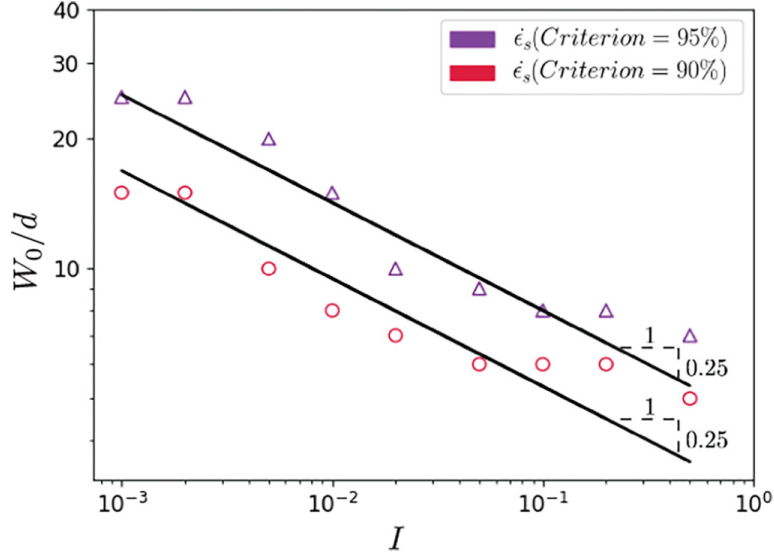


FIG. 8. Effect of criterion on REV. REV size of shear strain rate for two criteria of 95% and 90%. Lines are best fit using Eq. (7).

tensor defined for each grain as [22,28]

$$F^i = \langle r^{ij} \otimes r^{ij} \rangle^{-1} \cdot \langle r^{ij} \otimes v^{ij} \rangle. \quad (4)$$

The symbols $\cdot$ and $\otimes$ denote the tensor product and the outer product, respectively, and $^{-1}$ represents the inverse of the tensor. $\langle \cdot \rangle$ represents an average over all pairs of neighboring grains j ; and r^{ij} is the center-to-center vector between two grains and v^{ij} their relative velocity vector. Pairs are considered neighbors if their center-to-center distance is less than $2d$. F^i is a second-rank tensor that measures a spatial average of the velocity gradient in this zone, as illustrated in Fig. 3. The distance $2d$ is chosen to be as small as possible to obtain local information while ensuring that enough neighbors are included to evaluate the velocity gradient.

In the following, we will focus on three kinematic quantities extracted from this tensor: the shear strain rate $\dot{\epsilon}_s^i$ (symmetric part of F), the vorticity w^i (antisymmetric part of F), and the volumetric

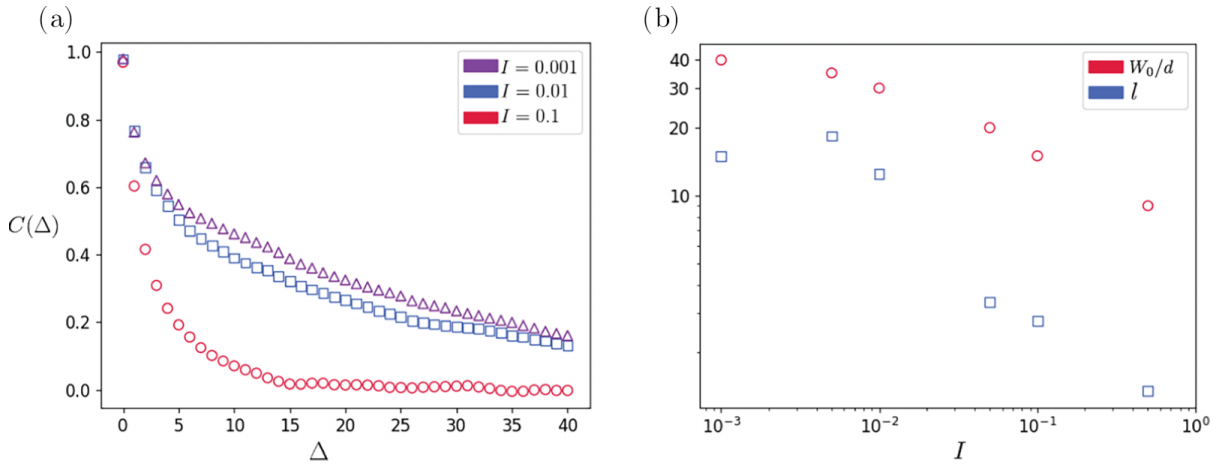


FIG. 9. Spatial correlation of v_y . (a) The dependence of the v_y spatial correlation to the controlling parameter $\Delta(d)$, where d is the average diameter of the grains. (b) The comparison between the extracted minimum REV size W_0/d and correlation length (l) obtained from v_y for different inertial numbers.

strain rate $\dot{\epsilon}_v^i$ (trace of F), defined as

$$\dot{\epsilon}_s^i = \frac{F_{xy}^i + F_{yx}^i}{2}; \quad w^i = \frac{F_{xy}^i - F_{yx}^i}{2}; \quad \dot{\epsilon}_v^i = F_{xx}^i + F_{yy}^i. \quad (5)$$

For reference, the macroscopic deformation rates of the plane-shear configuration are $\dot{\gamma}/2$ for the shear strain rate and the vorticity and 0 for the volumetric strain rate.

Figure 4 shows that the microscopic deformations rate are, on average, equal to their macroscopic counterpart. However, they are widely distributed. Shear strain rate, and vorticity and volumetric strain rate all follow a normal distribution at high inertial number and transition to an exponential distribution at low inertial numbers, which is similar to the distribution of pair velocities. Figure 5 shows that their standard deviations $\sigma(\dot{\epsilon}_s^i)$, $\sigma(\dot{\epsilon}_v^i)$, and $\sigma(w^i)$ follow a similar power law of the inertial number,

$$\frac{\sigma(\dot{\epsilon}_s^i)}{1/t_i} \approx \frac{\sigma(\dot{\epsilon}_v^i)}{1/t_i} \approx \frac{\sigma(w^i)}{1/t_i} \propto \beta I^m, \quad (6)$$

with best-fit values of $\beta = 1.48$ and $m = 0.70$. Here, too, a power $m = 1$ would mean that all standard deviations would simply scale with the macroscopic shear rate $\dot{\gamma}$. A power less than one indicates that the inertial number affects these standard deviations, which become increasingly greater than $\dot{\gamma}$ at low inertial number. These distributions mean that there exist zones in the flow with a shear strain rate larger or smaller than the macroscopic one. Similarly, there exist zones rotating faster or slower than the macroscopic vorticity, and zones which are dilating or contracting while the flow is macroscopically neither dilating or contracting.

Figures 6(a)–6(i) evidence the spatial distributions of these three quantities. They highlight a spatially random distribution at high inertial number and large spatial correlations at low inertial number. Figures 6(j)–6(l) help one to visualize where the zones of extreme values of shear strain rate, volumetric strain rate, and vorticity coincide. They represent only grains with outlier values: $|x - \langle x \rangle| > 2\sigma(x)$, with x being either $\dot{\epsilon}_s^i$, $\dot{\epsilon}_v^i$, or w^i , $\langle \cdot \rangle$ the mean value of the distribution, and σ its standard deviation. These results show that at high inertial number zones of extreme vorticity, the volumetric and shear strain rates do not coincide and are rather seemingly randomly distributed within the flow. In contrast, they do coincide at low inertial number, where the flow features “hot” zones with extreme values of all three quantities and “cold” zones with close to average values of all of these quantities.

V. REPRESENTATIVE ELEMENTARY VOLUME

The distribution and spatial correlation of kinematic fields evidenced above suggest that microscopic strain rates spontaneously feature a mesoscopic organization at low inertial number. One could expect that their associated length scale constitutes a lower bound for the size of a representative elementary volume in these flows.

To determine the size of a REV, we propose the statistical method illustrated in Figs. 7(a) and 7(b). The flow is first split into square cells of size W . The standard deviation σ of a kinematic quantity ($\dot{\epsilon}_s$, $\dot{\epsilon}_v$, or w) is measured in each cell, and averaged over all cells and all time steps. We refer to the resulting averages $\langle \sigma(\dot{\epsilon}_s) \rangle$, $\langle \sigma(\dot{\epsilon}_v) \rangle$, and $\langle \sigma(w) \rangle$. A REV would exist if there is a finite cell size W_0 for which these quantities are similar to those measured in larger cells.

Figures 7(c)–7(e) show the evolution of these quantities with the cell size W . For the shear strain rate, the volumetric strain rate, and the vorticity, they are minimal for small cells ($W = 2d$). They gradually increase for larger cells before reaching a plateau. The explanation for this increase is that smaller cells are more likely to be fully contained within a hot zone or a cold zone. They would then include grains undergoing a similar kinematic, which yields small standard deviations within the cell. On the contrary, large cells are more likely to contain grains belonging to both hot and cold zones, featuring different kinematics.

As illustrated in Fig. 7(c), we propose to define a REV size W_0 as the cell size required to reach a mean standard deviation 95% of the maximum value: $\langle \sigma(W_0) \rangle = 0.95 \langle \sigma(W = 40d) \rangle$. Taking the example of the shear strain rate, Fig. 7(c) shows that the REV size W_0 depends on the inertial number I : it becomes larger at lower inertial numbers.

Figure 7(f) presents the REV size W_0 obtained from the shear strain rate, volumetric strain rate, vorticity, and velocity fluctuations in the y direction. REV sizes related to the shear strain rate and vorticity are similar. They are generally larger than the REV size related to the volumetric strain rate. Accordingly, we propose to define the REV size of the flows based on shear strain rate and vorticity. Results are then consistent with a power law of the inertial number,

$$\frac{W_0}{d} \approx \zeta I^{n_R}, \quad (7)$$

with an exponent $n_R = -0.25$ and $\zeta = 4.5$. The REV size related to velocity fluctuations exhibits a power law with a similar exponent, but with a larger prefactor $\zeta = 9$. In the range of inertial numbers explored here, the REV size W_0 varies from a few grain diameters at high inertial numbers to a few dozen grain diameters at $I = 10^{-3}$. These values are dependent on the choice for the threshold (95%). Nonetheless, the REV results obtained with a different threshold (see Appendix A) show that this choice only affects the prefactor ζ , but not the power exponent n_R . Furthermore, Appendix B compares the value of the REV obtained with v_y with its spatial correlation length. While the REV size appears to be consistently larger than the correlation length, both quantities appear to increase as I decreases and diverge in the limit of $I \rightarrow 0$.

Extrapolating the law (7) to lower inertial number would lead to large REV sizes, for instance, $W_0 \approx 450d$ for $I = 10^{-8}$, a value commonly encountered in sheared fault gouge during earthquakes [29]. Experimental studies have revealed that REV dimensions for the volume fraction and energy dissipation in quasistatic flow conditions under simple shear are equal to $5d$ and $25d$, respectively [11]. Furthermore, for triaxial compression, a representative cubic element with a side length of $5.33d$ is introduced to capture the contact fabric, which is characterized by the coordination number and the contact fabric anisotropy [30]. The results presented here suggest that REV size based on internal kinematics may be much larger than these values in quasistatic flows. Further still, extrapolating our results to $\dot{\gamma} \rightarrow 0$ predicts a diverging REV size. This would correspond to an absence of a finite REV.

VI. CONCLUSION

This paper highlights a striking contrast between the macroscopic and microscopic deformation in granular flows. In macroscopically homogeneous shear flows, local strain rates are found to be widely distributed and spatially correlated, even more so at low inertial number. This observation resulted in the identification of a kinematics-based representative elementary volume, the size of which significantly increases and seemingly diverges at low inertial number. This REV size represents the characteristic size of instantaneous kinematic structures spontaneously developing within the flow.

This REV size is a fundamental piece of information to further develop homogenization theories explaining the effective behavior of granular flows as a continuum. It may be particularly useful to better understand the origin of finite-size effects. For instance, let us assume that constitutive laws for granular viscosity $\mu(I)$ and diffusivity $D(I)$ are measured in a large enough system—larger than the REV. The existence of a large REV size W_0 suggests that deviations from these laws could arise in flows at a distance from a boundary $h < W_0$, as kinematic structures would not have enough space to fully develop. The granular viscosity and diffusivity could then become a function of h : $\mu(I, h)$ and $D(I, h)$. Such deviations were indeed observed in experimental and simulated sheared flows in Refs. [6,21,22].

These results further suggest that large REV size may also develop in other soft materials which feature correlated particle motion; these include suspensions of grains [31–33], cohesive granular flows [34,35], foams [36,37], and suspensions of deformable particles (blood, emulsions) [38,39].

APPENDIX A: THE EFFECT OF THRESHOLD ON REV SIZE

Figure 8 shows the REV related to $\dot{\epsilon}_S$ obtained using two different thresholds: 95% and 90%. The results indicate that this choice is affecting the prefactor of the power law, but not its exponent.

APPENDIX B: COMPARING REV AND CORRELATION LENGTH

To measure the spatial correlation C of velocity in the y direction, we used the following expression:

$$C(\Delta) = \frac{\langle v_y^i v_y(y_i + \Delta) \rangle}{\langle (v_y^i)^2 \rangle}, \quad (\text{B1})$$

where $\langle . \rangle$ is an average over all grains i , v_y^i is the y velocity of that grain, and $v_y(y_i + \Delta)$ is the velocity at a distance Δ_y from the position of that grain. This velocity must be defined by some spatial average of the grain velocity near the position $(x_i; y_i + \Delta)$. We used the following coarse-graining function to estimate this average:

$$v_y(\Delta) = \frac{\sum_{j=1}^n v_y^j w(x_j - x_i, y_i + \Delta - y_j)}{\sum_{j=1}^n w(x_j - x_i, y_i + \Delta - y_j)}, \quad (\text{B2})$$

with the weight function defined as

$$w(X, Y) = e^{-\frac{X^2 + Y^2}{l^2}}. \quad (\text{B3})$$

The length scale of the coarse graining l is set to be one grain diameter. Grains located much farther than l from the coordinate $(x_i; y_i + \Delta_y)$ will have virtually no influence on the coarse-grain velocity. Finally, the correlation length ℓ is defined as

$$\ell = \int_0^\infty C(\Delta) \partial \Delta, \quad (\text{B4})$$

which is approximated by $\ell = \int_0^{20d} C(\Delta) \partial \Delta$. Figure 9 shows the autocorrelation function and compares the associated length scale ℓ to the REV (W_0). It appears that the REV size is consistently larger than the correlation length ℓ , but that both quantities diverge in the limit of $I \rightarrow 0$. This divergence is consistent with the results in Ref. [40].

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CHAPTER 4

Propagation of microscopic deformation in dense granular material

The research paper will investigate the kinematics of granular flows, with a focus on the propagation and evolution of local deformation and nonaffine deformation fields under simple shear. It begins by highlighting the importance of velocity fluctuations, their correlation length, and the influence of the inertial number. The study employs discrete element simulations to analyse plane shear flows, detailing the setup, boundary conditions, and the effects of polydispersity on the flow behaviour.

The key findings demonstrate that microdeformations are intricately linked to grain velocity fluctuations and exhibit unsteady evolution with pronounced spatial and temporal correlations, particularly at lower inertial numbers. This paper also introduces scaling laws for kinematic heterogeneities, revealing a diffusive propagation mechanism for shear deformation and particle rearrangements at the microscale. This mechanism aligns with continuum models that describe granular flows, especially those that incorporate nonlocal behaviours. It shows that the deformation in two distant regions of the flow is interconnected, propagating across a mesoscopic distance that increases as the inertial number decreases.

Variogram analysis effectively captures the spatial correlations, offering a robust approach to quantifying the minimum REV size to capture microdeformation heterogeneities in granular flows under plane shear. The findings provide a potential microscopic rationale for the nonlocal behaviour observed in granular flows at the continuum scale, enhancing our understanding of the dynamics of granular materials under shear deformation. These insights have practical implications for engineering applications.

Propagation of internal deformations in dense granular flows

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This paper analyses how local deformation develops in dense granular flows. In simulated plane shear flows, we measure the spatio-temporal correlations of local kinematic fields including particle velocity, local deformation, and nonaffine deformation. All of these fields exhibit an unsteady evolution and significant spatial correlations, which become larger at low inertial numbers. The characteristic correlation length and time scales are expressed as power laws of microscopic inertial time and macroscopic shear time. These scaling laws highlight a mechanism of diffusive propagation of the shear deformation and particle rearrangements: particle rearrangements trigger further rearrangements in their vicinity, forming zones in the flow with higher deformation than others. This mechanism provides a possible microscopic rationale for nonlocal behaviour observed at the continuum scale.

I. INTRODUCTION

A continuum description of granular flows is often required to model and predict the dynamics of natural events and industrial processes. Examples include landslides [1], earthquakes [2], snow avalanches [3], bulk material handling, mineral processing, pharmaceutical manufacturing [4]. Like any other fluids, granular flows are described using continuity equations. This bypasses the need of capturing the motion of every single particle, which is generally impractical owing to their large number. Rather, the granular nature of the material is embedded in effective transport coefficients: the assumption is that, at any point in the flow, a viscosity η relates the shear stress to the shear rate and a diffusivity $\mathcal{D}$ relates the flux of particle mass to the concentration gradient.

The $\mu(I)$ rheology rationalised the dependence of the granular viscosity with two flow parameters, the shear rate $\dot{\gamma}$ and the normal stress P , and two particle parameters, their size d and their density ρ [5–7]. The inertial number $I = \dot{\gamma}t_i$ was found to govern the ratio of the friction coefficient μ of the shear to the normal stress. This number compares two time scales. The first is the global shear time $\dot{\gamma}^{-1}$, which measures the time it takes for two layers of particles to experience a shear displacement of d . The second time scale is the inertial time $t_i = d\sqrt{\rho/P}$. It measures the time of an idealised rearrangement, where a particle is pushed into a free space on a distance d under the action of a force Pd^2 . Similarly, the inertial number was found to govern the coefficient of diffusion $\mathcal{D}(I)$ [8–11].

This description is qualified as *local*, which means that the two transport coefficients are entirely governed by the local value of the inertial number I at the location of interest and are unaffected by the nature of the flow or the presence of boundaries in the vicinity. Several observations pointed out that granular flows are in fact nonlocal. For example, measuring $\mu(I)$ in a flow that is homogeneous, where I and stresses are constant in space, gives a different result than measuring the same relation in flows featuring a gradient of stress and/or a gradient of I . Similarly, the granular viscosity is not the same far or close to solid

boundaries. This suggests the existence of a mesoscopic length scale that is larger than one particle, over which the material behaviour is somehow coupled. The existence of such a length scale and the possibility of nonlocal behaviours were foreshadowed with the introduction of $\mu(I)$ rheology [6]. A dimensional analysis of the granular viscosity scaling with I pointed out that it embeds a length scale that increases and diverges when $I \rightarrow 0$ [12]; a parallel with the Prandtl mixing length in turbulent flows allowed the explanation of drops in viscosity near solid boundaries reminiscent of turbulent boundary layers [12, 13]. Several nonlocal continuum models were introduced to complement the local $\mu(I)$ rheology and capture the behaviour of flows in complex geometries [14–17]. In spite of their differences, all these models involve a characteristic ‘nonlocal’ length reflecting how far one part of the flow can influence another part, a length that diverges when $I \rightarrow 0$.

Nonlocal behaviours observed and modelled at the continuum scale suggest the existence of a microscopic process that connects distant parts of the flow. However, the exact nature of this process remains to be established. Recent advances suggest that this process would involve individual grain motion via the field of velocity fluctuations. Specifically, fluidity, the quantity that is nonlocal, has been shown to be the product of velocity fluctuations and a function of the solid fraction [18]. Consistently, fields of velocity fluctuations exhibit long-range spatial correlations, which are short-lived [8, 19, 20]. These show that granular flow involves large patches of grains, or clusters, which virtually move as a rigid body within the flow for short periods of time. Consistent with nonlocal continuum models, the size of these clusters increases and diverges when $I \rightarrow 0$.

We have recently shown that these velocity fields were associated with fields of deformation rate, also featuring wide distributions and large spatial correlations [21], and the recent analysis in [22] showed a mechanism of propagation of local deformation, by which local rearrangements are likely to trigger more rearrangements in their vicinity. This observation is consistent with the assumption of a self-activated relation of stresses at the core of the nonlocal continuum model proposed in [14]. This suggests that the way local deformations propagate in granular flow could be a physical process conducive to non-locality. However,

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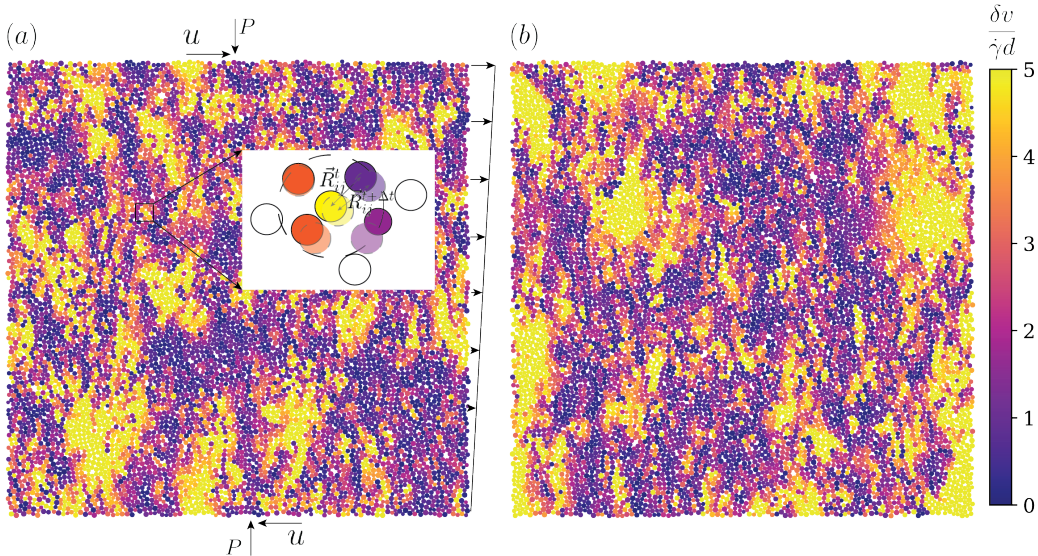


FIG. 1. **Plane shear configuration and fields of velocity fluctuations.** (a) and (b) show two consecutive velocity fields taken during the same flow ($I = 0.01$). Particles are coloured according to the norm of their velocity fluctuations. The time period between the snapshot corresponds to a global shear deformation $\Gamma = 0.125$. (a) illustrates the plane shear flow setup, including the prescribed shear velocity u , the resulting shear rate $\dot{\gamma}$ and the normal stress P .

the typical size and time scale governing this propagation, their relation to the velocity fluctuations, and their dependence with the inertial number remain to be established.

To advance this topic, in this paper, we focus on observing how local deformations occur within sheared granular flows. Our approach is to simulate homogeneous and steady flow at different inertial numbers, to measure kinematic quantities including velocity fluctuation, local deformation, and nonaffine deformation, and to measure their spatial and temporal correlation. The paper is organised as follows: our numerical method and the metric used are introduced in section II, the results in terms of spatio-temporal correlation of these kinematic quantities are presented in section III, and the main features of the process of propagation of deformation are discussed in section IV.

II. METHOD

This section presents the simulated granular flows, the way kinematic quantities such as velocity fluctuations, local deformation, and nonaffine deformation are measured, and the statistical tools used to quantify their spatial and temporal correlations.

A. Simulated plane shear flows

We analyse a set of in-silico granular flows previously presented in [21]. Flows are simulated using a discrete element method (DEM). The flow geometry is plane shear with a prescribed shear rate $\dot{\gamma}$ and a prescribed normal stress P , as illustrated in Figure 1.

The particles are cohesionless disks which interact only by elasto-dissipative and frictional contact; there is no long range interaction or gravity. The disks are

quasi-monodisperse with an average diameter of d , a mass of m and a density ρ . Their diameters are uniformly distributed in the range $d \pm 20\%$. This slight polydispersity prevents shear-induced crystallisation. Particles interact *via* pairwise contacts involving a linear elastic force normal to the contact with a spring stiffness $k_n = 10^3 P d$ and a viscous normal force tuned to produce a coefficient of restitution of $e = 0.5$. Tangential contact forces involve a linear elastic force with stiffness $k_t = k_n/2$, capped by a sliding Coulomb criterion with a coefficient of friction of $\mu_p = 0.5$.

To enable a faster simulation time and larger shear cells, we focused on two-dimensional systems. An assembly of 10^4 disks is sheared in a cell of length $L = 100d$ in the shear direction x . In the transverse direction y , the cell width H is about $80d$. H is not fixed; it can vary to let the packaging dilate or contract as a way to control the internal stress P . Lees-Edwards periodic boundary conditions are used in the two directions [23] to avoid the introduction of solid boundaries and the heterogeneity they would induce [12]. We will discuss below whether this cell size is large enough not to limit the development of mesoscopic kinematic structures.

With the Lee-Edwards boundary condition, an external velocity gradient $\frac{2u}{H}$ is prescribed by translating the top and bottom copy of the shear cell at a constant velocity $\pm u$ in the shear direction. The cell width H adapts to the external normal stress P so that the internal normal stress P_{int} converges to P in steady states; this is ensured by prescribing an inertial dynamics $\ddot{H} = (P - P_{int})/Lm$. In the steady flows analysed below, P_{int} equates P with some minor fluctuations, and H is nearly constant during flows. Furthermore, the solid fraction and the velocity gradient are homogeneous: When averaged over time, the velocity profile $v_x(y)$ is linear. As a result, the velocity gradient $\dot{\gamma} = \frac{\partial v_x}{\partial y} = \frac{2u}{H}$ is spatially constant. The

global shear deformation of the cell steadily increases in time as $\Gamma = \frac{\dot{\gamma}}{2}t$.

Flows are prepared by placing the particles randomly without contact in a loose configuration. Then both normal stress and the shear rate are applied. Flows experience a transient during which the solid fraction increases as H decreases, leading to a steady state. The advantage of the plane shear configuration in a biperiodic domain is that these steady flows are homogeneous: they are controlled by a single value of the inertial number $I = \dot{\gamma}t_i$; with $t_i = \sqrt{m/P}$ the inertial time [5, 6]. Here, ‘steady and homogeneous’ means that quantities such as solid fraction, stresses, and deformation rates are statistically similar at any point in the flow and at any point in time. However, they exhibit spatiotemporal fluctuations, which will be the object of the analysis below.

B. Measuring deformation and nonaffine deformations

Our analysis focusses on kinematic quantities including grain velocity, nonaffine velocities, local deformation, and nonaffine deformation. This section presents these quantities, how they are related and how they are measured from DEM simulations.

1. Grain velocity and nonaffine velocity

With DEM, the velocity of any particle i , $\vec{v}^i$, is known at any time. It typically varies over time and is different from particle to particle. It is useful to split this velocity into two components, its affine component governed by the shear flow and its nonaffine component $\delta\vec{v}^i$ defined as:

$$\delta v_x^i = v_x^i - \dot{\gamma}y^i, \quad \delta v_y^i = v_y^i. \quad (1)$$

Here v_x^i and v_y^i are the velocity of particle i in the shear and transverse direction, and y^i is the position of particle i . The nonaffine velocity measures how the velocity of a particle differs from the average flow velocity field, which is $\dot{\gamma}y$ in the shear direction and 0 in the transverse direction. We will refer to $|\delta\vec{v}^i|$ as velocity fluctuations.

Figure 1 shows two snapshots of the velocity fluctuations taken in a flow with $I = 0.01$. The time period between the two snapshots is short, corresponding to a global shear deformation $\Gamma = 0.125$. This figure highlights some key features of the velocity fluctuations, which have been previously established. Firstly, many particles are not simply following the main flow - this would yield $|\delta\vec{v}^i| = 0$. Some experience velocity fluctuations that are more than five times larger than the shear velocity $\dot{\gamma}d$. Secondly, the spatial distribution of velocity fluctuations is not random. The shear cell is comprised of ‘hot’ zones where the particles have large velocity fluctuations and ‘cold’ zones where the velocity fluctuations are small or null. Lastly, these zones are short-lived: after a global deformation Γ much smaller than one, new ‘hot’ and ‘cold’ zones appear at seemingly unrelated locations.

2. Local deformation and nonaffine deformation

Particle velocity and local deformation are related as follows: the local deformation is the integral over time of the velocity gradient tensor F_i . The local velocity gradient tensor around a particle i can be calculated at any point in time considering some neighbouring particles j , using this formula [12, 21, 24]:

$$F_i = \langle \vec{R}_{ij}^t \otimes \vec{R}_{ij}^t \rangle^{-1} \cdot \langle \vec{R}_{ij}^t \otimes \vec{v}_{ij}^t \rangle. \quad (2)$$

$\vec{R}_{ij}$ is the center-to-center vector between a pair of particles i and j and $\vec{v}_{ij} = \vec{v}_{ij}$ is the relative velocity of these two particles. In (2), the symbols $\cdot$ and $\otimes$ denote the tensor product and the outer product, respectively; the power -1 is the inverse of the tensor. The angled brackets denote an average including all particles j within a distance d_{avg} from i ($|\vec{R}_{ij}| \leq d_{avg}$). This in effect produces a spatial average on a distance d_{avg} . The choice of d_{avg} is arbitrary. To obtain a measurement as local as possible, we choose d_{avg} to be as small as possible. However, when d_{avg} is too small, there may be no or not enough neighbour particle j within this distance to enable the determination of F_i . We found that choosing $d_{avg} = 2d$ was the best compromise and used this value in the following. We also checked that varying this value slightly within $1.5d$ and $3d$ did not significantly affect the results.

In [21], we analysed the spatial variation of the shear strain rate $\dot{\epsilon}_{i,s}$ (the symmetric part of F_i), the rotation rate (the antisymmetric part of F_i), and the dilation rate (trace of F_i), as well as their temporal correlations. These quantities exhibit spatial correlations similar to that of the velocity fluctuations: the characteristic correlation length was found to be much larger than one particle size and to increase at low inertial numbers.

We now consider the local deformation ϵ_i around individual particles. It is given by the integration over a period of time Δt of the deformation rates: $\epsilon_i(\Delta t) = \int_{\tau=t}^{t+\Delta t} F_i^\tau d\tau$; here t is a reference time taken during steady flow. Alternatively and consistent with (2), the local deformation can be calculated in terms of the relative position of the pair of grains at time t and time $t + \Delta t$ as:

$$\epsilon_i(\Delta t) = \langle \vec{R}_{ij}^t \otimes \vec{R}_{ij}^t \rangle^{-1} \cdot \langle \vec{R}_{ij}^t \otimes \vec{R}_{ij}^{t+\Delta t} \rangle. \quad (3)$$

In the following we will focus on local shear deformation ϵ_i^s , which is the symmetric part of ϵ_i .

ϵ_i measures the average deformation around a particle i considering a number of neighbouring particles j . If both i and j followed perfectly the mean shear flow, their relative position would evolve over time as $\vec{R}_{ij}^{t+\Delta t} = \epsilon_i(\Delta t) \cdot \vec{R}_{ij}^t$. However, the prevalence of velocity fluctuations implies that this scenario is unlikely and that the relative position of any pair of particles is likely to deviate from this average deformation. The square nonaffine displacement D_i^2 is a metric that was introduced to quantify the magnitude of these deviations around a particle i . It is defined as [25, 26]:

$$D_i^2(\Delta t) = \langle \left(\vec{R}_{ij}^{t+\Delta t} - \epsilon_i(\Delta t) \cdot \vec{R}_{ij}^t \right)^2 \rangle. \quad (4)$$

The angle brackets denotes the average over neighbouring particles j with are within a distance $2d$ of i at time t . $\bar{R}_{ij}^{t+\Delta t}$ is the actual relative position of i and j at time $t + \Delta t$, whereas $\epsilon_i(\Delta t)\bar{R}_{ij}^t$ would be their relative position had this pair of particles perfectly followed the local deformation ϵ_i .

The physical dimension of D_i is a length and that of D_i^2 a length square. $D_i = 0$ means that all neighbouring particles exactly follow the local deformation. $D_i > 0$ means that at least some neighbouring particles deviate from this. Large values of D_i have been associated with topological rearrangements that occur around i within the period of time t to $t + \Delta t$, which are conducive to microscopic plastic deformation. This metric has been extensively used to monitor the appearance of particle rearrangements in granular materials [22, 27–29] and colloidal systems and colloidal systems [30, 31] and plastic deformation in metallic glass [25, 26].

We are interested in measuring the extent to which kinematic quantities such as velocity fluctuations, deformation, and nonaffine deformation are correlated spatially and temporally. The following two sections describe the metric used to do so. For simplicity and generality, we consider a scalar K_i that can be any of the quantities listed above for a particle i , and $\bar{K}^t = \frac{1}{n} \sum_{i=1}^n K_i^t$ is the average of K considering all n particles in the shear cell at time t .

C. Temporal auto-correlation

The temporal auto-correlation function C is defined for a given reference time t and a given time interval Δt as:

$$C(\Delta t) = \frac{\frac{1}{n} \sum_{i=1}^n (K_i^t - \bar{K}^t)(K_i^{t+\Delta t} - \bar{K}^{t+\Delta t})}{\sigma(K^t)\sigma(K^{t+\Delta t})}. \quad (5)$$

The operator $\sigma(K^t)$ is the standard deviation of K_i considering all n particles in the shear cell at time t . A characteristic correlation time τ is defined as:

$$\tau = \int_{\Delta t=0}^{\infty} C(\Delta t) \partial \Delta t. \quad (6)$$

In practice, flows do not last an infinite amount of time, so calculating this integral up to $\Delta t \rightarrow \infty$ is not possible. However, when the correlation function drops from 1 to about 0 in a finite period of time, the correlation time τ can be approximated by $\tau \approx \int_0^{t_{max}} C(\Delta t) \partial \Delta t$. The criteria for the choice of t_{max} is $t_{max} \gg \tau$. As we shall see in the following, correlation times typically are shorter than the shear time $\dot{\gamma}^{-1}$. As our studied flows are steady, the temporal correlation time can be measured using any reference time t to obtain a time-average value of τ .

D. Spatial correlations

We consider three methods to quantify spatial correlations, based on the spatial auto-correlation function, the variogram and a clustering algorithm. This

section presents these methods and their complementary.

1. Auto-correlation function

The first way to measure spatial correlations is by using the spatial auto-correlation function ξ , defined for a spatial distance Δ as:

$$\xi(\Delta) = \frac{\frac{1}{n} \sum_{i=1}^n (K_i^t - \bar{K}^t)(K_i^t(\Delta) - \bar{K}^t)}{\sigma(K^t)^2}. \quad (7)$$

The sum runs on all n particles in the shear cell. Measuring this auto-correlation function requires knowledge of the value of the quantity $K_i(\Delta)$, which is the value of K at a distance Δ from the position of the particle i . This distance can be taken along any direction; we will focus on the correlation in the transverse direction y . This value K is estimated using a coarse graining function, which is used to interpolate K considering the grains located near this position. Amongst several possible choices, we use the following function, written here for a correlation along the y direction:

$$K_i(\Delta) = \frac{\sum_{j=1}^n K_j w(x_j - x_i, y_i + \Delta - y_j)}{\sum_{j=1}^n w(x_j - x_i, y_i + \Delta - y_j)}. \quad (8)$$

where w is chosen to be a Gaussian weigh; w gives more importance for particles located closer to the location on interest:

$$w(x, y) = e^{-\frac{x^2 + y^2}{l^2}}. \quad (9)$$

The parameter l defines a characteristic range of influence: particles located further than l contribute much less to the coarse grained value $K_i(\Delta)$ than particles within a distance l . Coarse graining is a form of spatial averaging and l represents the characteristic length of this averaging. The spatial correlation length is defined as the integral of the correlation function ξ :

$$\ell = \int_{\Delta=0}^{\infty} \xi(\Delta) \partial \Delta. \quad (10)$$

As no flow is infinitely large, the integral can not be calculated up to $\Delta \rightarrow \infty$. When the correlation function drops from 1 to nearly 0 within a finite distance Δ , the correlation length can be approximated by $\ell = \int_{\Delta=0}^{\Delta_{max}} C(\Delta) \partial \Delta$, using $\Delta_{max} \gg \ell$. The distance ℓ represents some average length of the kinematic structures in a flow. However, it contains no information on the possible distribution in size of these structures.

2. Variogram and representative element volume

The variogram method is designed to directly evidence the existence and size of a representative element volume (REV), as discussed in [21]. A variogram is constructed by measuring the variance of a kinematic quantity K considering particles within a

zone (disk in 2D or sphere in 3D) of radius h , and to observe how this variance evolves when h is increased. A finite-size REV exists if there exists a value h_0 above which the variance no longer depends on h . This means that a volume of size h_0 is large enough to statistically represent any larger volume, as far as the variance of the quantity is concerned.

In our bidimensional systems, the variance σ^2 of a quantity K is measured on a sample of p particles located within a disk of radius h by:

$$\sigma_K^2(h) = \frac{1}{p-1} \sum_{i=1}^p (K_i - \bar{K})^2. \quad (11)$$

with $\bar{K} = \frac{1}{p} \sum_{j=1}^p K_j$. We then average this variance by considering a series of disk with the same radius h , but centred at different, random position in the shear cell. This yields the value $\langle \sigma^2(h) \rangle$. A variogram corresponds to the function $\langle \sigma^2(h) \rangle$, which is calculated by considering disks of different radii h .

Variograms typically exhibit low variance at low h , which increases as h increases. A finite-size REV exists if $\langle \sigma^2(h \rightarrow \infty) \rangle$ tends to a finite value. Then, a REV size h_0 can be defined as the value h_0 for which the variance is close enough to $\langle \sigma^2(h \rightarrow \infty) \rangle$. However, this requires a definition of what is considered ‘close enough’, which is arbitrary. The maximum radius h that can be tested in our flow geometry is limited to half the width of the shear cell $H/2 = 40d$. We therefore chose to define the REV size h_0 as the radius that leads to a variance equal to 95% of the variance at $h = 40d$:

$$\langle \gamma(h_0) \rangle = 0.95 \langle \gamma(h = 40d) \rangle. \quad (12)$$

The length h_0 is a measure of the degree of spatial correlation of the quantity K . We will analyse below how it compares to the auto-correlation length ℓ .

3. Clustering algorithm

Spatial correlation and variograms measure the average size of the kinematic structures in the shear cell. However, the nature of these metrics is that they do not identify individual structures. Clustering methods are designed to do so.

A cluster is defined as a group of adjacent particles that share similar kinematic properties. This definition relies on two arbitrary criteria to select whether a pair of particles is adjacent and whether their kinematic properties are similar. We will seek to cluster outlier particles, that is, particles that have an extreme value of a kinetic quantity K . The first criterion is based on a threshold value K_c : particles with $K_i > K_c$ may belong to a cluster. Too large values of K_c would exclude most particles and create no or few clusters; too small values of K_c would include most particles and produce a single very large cluster. Rather than a fixed value of K_c , a second criterion is to set a fixed number of particles with the most extreme value of K , for example $X_c = 10\%$ of the total number of particles. We will discuss the choice of K_c and X_c in the following.

The ‘adjacent’ criteria is defined as follows: two eligible particles are considered to belong to the same cluster if their centre-to-centre distance is smaller than a specified distance, chosen to be $2d$. The clustering algorithm then groups adjacent eligible particles into clusters. The results is a list of individual clusters at a given time. Each cluster is comprised of a number of particles, with a minimum of 3.

The size of each cluster c is defined by their radius of gyration r_c :

$$r_c^2 = \sum_{i=1}^{n_c} (\vec{R}_i - \vec{R}_0)^2. \quad (13)$$

n_c is the total number of particles in this cluster, $\vec{R}_i$ is the position of particle i and $\vec{R}_0 = \sum_{i=1}^{n_c} \vec{R}_i / n_c$ is the centre of mass of the cluster. The average size R_g of the clusters in the shear cell is defined by the average of the cluster size weighted by the number of particles they are comprised of:

$$R_g^2 = \frac{\sum_{c=1}^{N_c} n_c r_c^2}{\sum_{c=1}^{N_c} n_c}. \quad (14)$$

where N_c is the total number of clusters in the shear cell.

III. RESULTS

We now use the method presented in the previous section to measure the spatial and temporal correlations of the following kinematic quantities: velocity fluctuations δv_y , shear deformation ϵ_i and nonaffine deformation D_i .

A. Velocity fluctuations

1. Temporal correlation

Figure 2 shows the temporal auto-correlation of the velocity fluctuations for different values of the inertial numbers. The time interval Δt is expressed in unit global shear deformation as $\Gamma = \Delta t \dot{\gamma} / 2$, where Γ . Consistent with the snapshots in Figure 1, the auto-correlation function drops to about zero well before the cell undergoes a unit shear deformation. The auto-correlation time $\tau^{\delta v_y}$ measured using (6) is consistent with the power law of the inertial number:

$$\tau^{\delta v_y} \dot{\gamma} \approx a I^b. \quad (15)$$

The best fit of the measured values of τ yield $a = 0.47$ and $b = 0.50$. Previous works reported power exponents of 0.5, which are consistent with this value [8, 11]. This power law points out that (i) the velocity fluctuations remain correlated during a small fraction of the shear deformation Γ as $I < 1$, and (ii) this fraction becomes smaller as I decreases and tends to 0.

In the inertial number range reported here, the autocorrelation time of the velocity fluctuation ranges

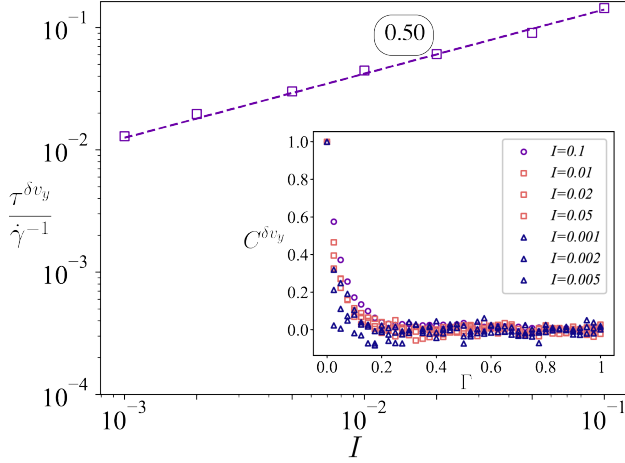


FIG. 2. **Temporal correlation of the velocity fluctuations** δv_y . The autocorrelation function C using (5) is measured at a specific reference time t as a function of global deformation Γ for various inertial numbers. The auto-correlation time $\tau^{\delta v_y}$, expressed in units of $\dot{\gamma}^{-1}$, is determined using (6) and plotted against the inertial number. Each point represents an average including 5 reference times spanning over a global shear deformation of 1Γ . The line is the best fit for the power law of (15).

from 10^{-2} to 10^{-1} times the shear time $\dot{\gamma}$. The power law (15) implies that the velocity fluctuation correlation time is not simply driven by the shear time, but also involves the inertia time t_i : rearranging (15) shows that the correlation time is a geometric average of the shear time and the inertial time:

$$\tau \propto \left(\frac{1}{\dot{\gamma}}\right)^{1-b} t_i^b. \quad (16)$$

2. Spatial correlations

Figure 3 compares the three methods used to measure the spatial correlation of the velocity fluctuations, which are based on spatial auto-correlations, variogram and clustering. Figure 3 also reports the dimensionless quantity $\sigma(\delta v)/\dot{\gamma}d$; where $\sigma(\delta v_y)$ is the standard deviation of velocity fluctuations. Several studies equate $\sigma(\delta v_y)/\dot{\gamma}d$ with a characteristic mesoscopic length of the velocity fluctuation referred to as ‘lever’ length, ℓ^{lever} [8, 20]. Consistent with previous results, our data indicate a negative power law with the inertial number:

$$\frac{\ell^{lever}}{d} = \frac{\sigma(\delta v_y)}{\dot{\gamma}d} \approx aI^b. \quad (17)$$

with a best fit obtained with $a = 0.35$ and $b = -0.5$; this power exponent was found to be dependent on the particle friction coefficient [8, 20]. This scaling law indicates that the width of the particle velocity distribution is not solely governed by the velocity shear scale $\dot{\gamma}d$; it can vastly exceed this scale and is a function of the inertial velocity d/t_i :

$$\sigma(\delta v_y) \propto (\dot{\gamma}d)^{1+b} \left(\frac{d}{t_i}\right)^{-b}. \quad (18)$$

with $b < 0$, the spread of the velocity fluctuation distribution is meant to be a geometric average of the shear and inertial velocities scales.

Although $\frac{\sigma(\delta v_y)}{\dot{\gamma}d}$ is commonly used to define a mesoscopic length, it is not a direct measurement of the spatial correlations of the velocity of particles. The spatial auto-correlation lengths $\ell^{\delta v_y}$, the average cluster size $R_g^{\delta v_y}$ and the REV $h_0^{\delta v_y}$ directly measure these spatial correlations. Qualitatively, these three metrics are similar to the lever length; they increase when the inertial number decreases. However, they do feature some quantitative and qualitative differences. All three metrics are significantly larger than ℓ^{lever} . These lengths increase with the inertial number, but with a power exponent ranging from 0.2 to 0.3, which is significantly lower than 0.5. Furthermore, the REV size reaches a value of $h_0^{\delta v_y} \approx 30d$ at $I = 0.01$ and plateaus at lower inertial numbers.

The snapshots of Figures 3 highlight the effect of the inertial number on the spatial distribution of the velocity fluctuation. At high inertial number ($I = 0.1$), Figure 3g shows that velocity fluctuations do not show a large spatial correlation. This is confirmed by the result of the clustering analysis in Figure 3c where most clusters are rather small, with a gyration radius of the order of a few particle size. At low inertial number ($I = 0.001$), Figure 3d shows that velocity fluctuations feature large ‘hot’ zones (in yellow) and large ‘cool’ zones (in purple). Clustering analysis identifies a few large clusters of particles with high velocity fluctuations. Their gyration radius is a few dozen particles in size, nearly as large as the shear cell width H .

These kinematic structures are detected by the auto-correlation function and by the variogram as presented in Figures 3e and 3f, respectively. The auto-correlation functions of velocity decrease with Δ faster at high inertial number than at low inertial number. Consistently, the variogram increases sharply with distance h at high inertial numbers and more gradually at low I . Interestingly, the REV size is much larger than any other length as shown in Figure 3b. For example, at $I = 0.005$, the REV size is $h_0^{\delta v} \approx 30d$, while the autocorrelation length and the cluster size are about $10d$ and the lever length is only $4d$. A possible reason for this difference is that both the auto-correlation and the cluster algorithm provide an average size of the kinematic structures, while the REV may be more sensitive to the size of the largest structures - indeed, a REV should be large enough to encompass the largest of the structures. It seems that, at low inertial numbers, some kinematic structures could grow larger than the width of the shear cell $H/2 = 40d$ if the cell were wider; their maximum size is capped by $H/2$ in this cell.

B. Shear deformation

The velocity of a particle is an instantaneous quantity; in contrast, local deformations are defined with respect to an interval of time Δt . Figure 4 shows a series of snapshots representing the evolution of local

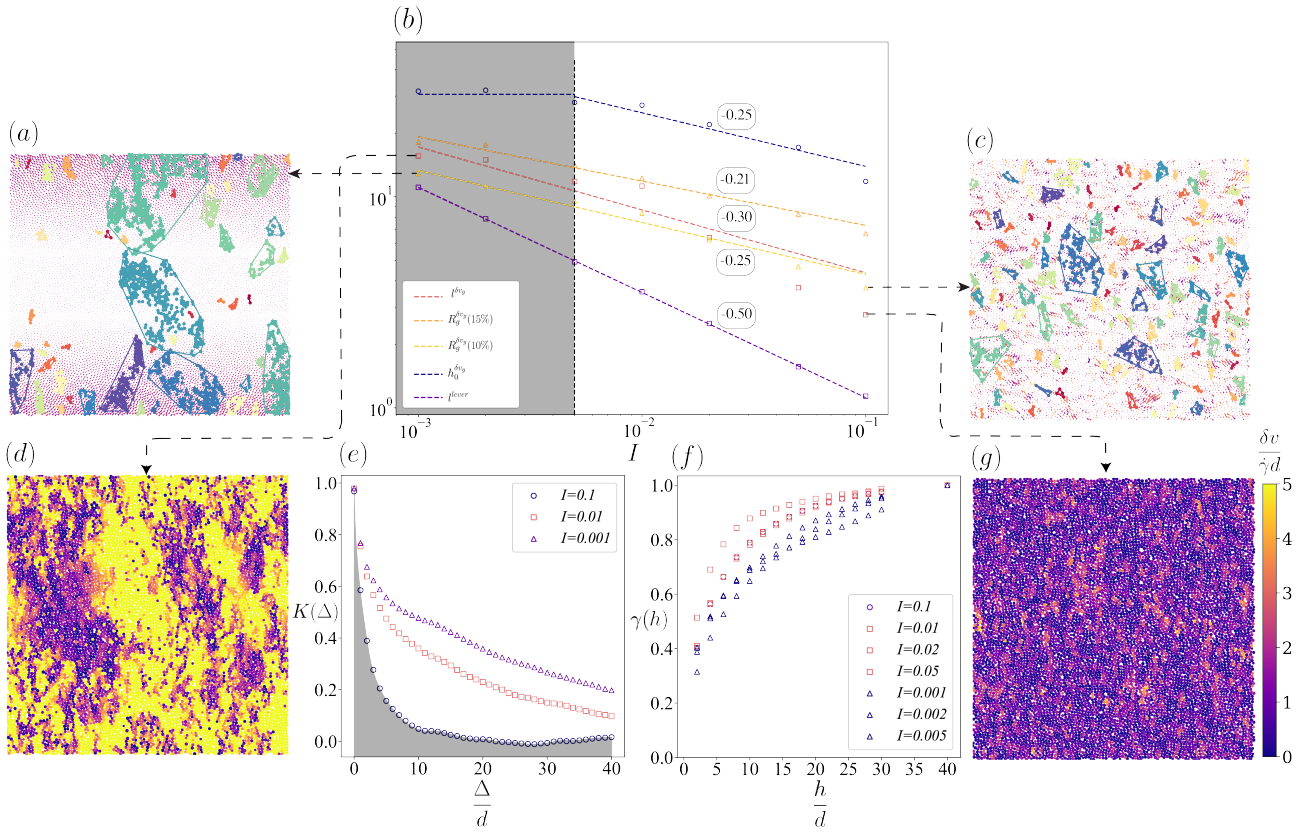


FIG. 3. **Velocity fluctuation δv_y .** (a) and (c) show the velocity of all particles (represented as vectors) and the results of the clustering algorithm for flows with inertial numbers $I = 0.001$ and $I = 0.1$, respectively. Particles within the same cluster are depicted in the same colour, with cluster perimeters outlined for clarity; particles not belonging to any cluster are omitted. Clusters are identified by selecting the top 15% of the particles with the highest velocity fluctuations. (d) and (g) illustrate the spatial fields of velocity fluctuations, where particles are coloured according to the magnitude of $|\delta \vec{v}_i|$ for the inertial numbers $I = 0.001$ and $I = 0.1$, respectively. (e) provides examples of spatial auto-correlation function ξ using (7) in the y direction, and (f) displays the variogram measured in particles at a specific reference time. (b) compares different measures of spatial correlation length as a function of the inertial number, including auto-correlation length ℓ^{lever} , representative element volume $h_0^{\delta v_y}$, and the size of the cluster $R_g^{\delta v_y}$, determined by considering the top 10% or 15% of the particles with the highest velocity fluctuations; the dashed line represents power laws with the power exponent listed on the figure.

shear deformation around each grain i as this time interval increases. Time is converted into a global shear deformation $\Gamma = \Delta t \dot{\gamma}$. The local shear deformation is heterogeneous: Some zones experience much more shear deformation (in yellow) than others (purple). After a relatively small global deformation $\Gamma = 0.5$, some particles have already experienced a shear deformation greater than 1. In contrast, some particles experience virtually no shear deformation even when the global deformation has reached $\Gamma = 1$. The snapshots in Figure 4 further evidence two features. First, local deformations are correlated in space, and the size of zones of lower/higher deformation is larger at low inertial number. Secondly, these zones appear to grow with time and to be advected with the flow: their shape stretches and rotates as the global shear progresses.

The following sections seek to quantify these visual observations using the statistical tools presented in Section II.

1. Temporal correlation

We first developed an ad hoc metric to highlight how some particles experience large shear deformation earlier than others, whereas other particles experience virtually no shear deformation even after a significant global deformation. This metric is the proportion p of particles whose shear deformation ϵ_s^i is lower than a selected threshold. We chose 0.5 here as an example. Figure 5 shows the evolution of this proportion p as the shear cell undergoes a global deformation that increases from 0 to 2. The curves $p(\Gamma)$ exhibit a characteristic S-shaped shape. If all particles experienced the same deformation, the local deformation would be homogeneous and equal to the global deformation anywhere in the shear cell. As a consequence, $p(\Gamma)$ would be a step function with a step occurring at $\Gamma = 0.5$ set by the choice of the threshold; a higher threshold would shift the step to larger values of Γ . In these shear flows, the spread of the S-shaped function $p(\Gamma)$ shows that some particles experience a much larger shear deformation early on, while others experience little shear for a long time. This spread is larger at

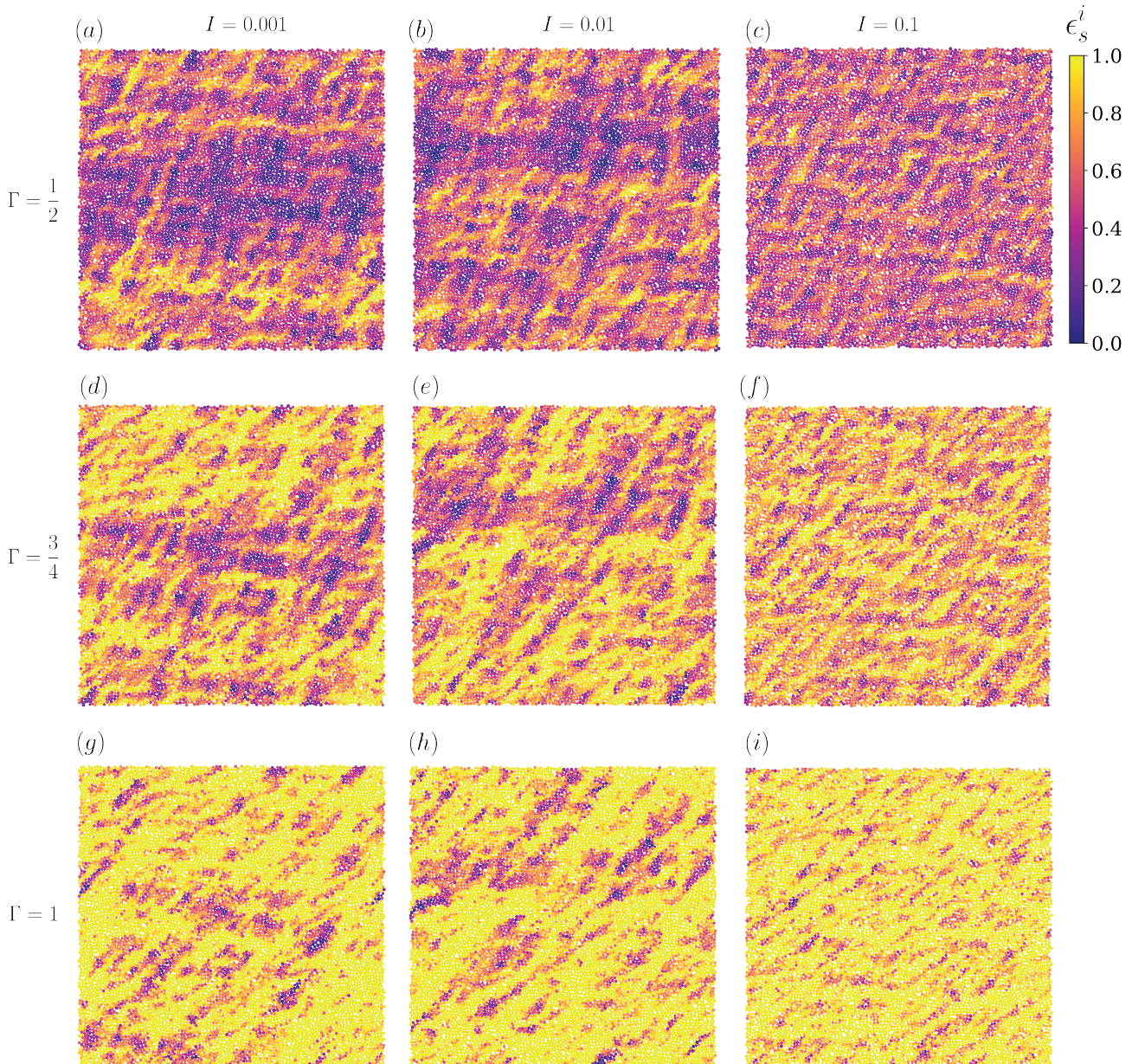


FIG. 4. **Spatio-temporal evolution of the local shear deformation.** Snapshots show particles coloured according to their local deformation ϵ_s^i measured at different time intervals, expressed in global deformation Γ (lines). By definition: $\epsilon_s^i(\Gamma = 0) = 0$. The three columns represent flows with different inertial numbers $I = 0.001$, $I = 0.01$, and $I = 0.1$.

lower inertial number.

Figure 6 shows the temporal evolution of local shear deformation for a few particles. It confirms that the local deformation does not increase continuously and equally for all particles. Rather, it exhibits a step-like evolution that includes phases of sustained and rapid growth followed by phases with little or no growth. The temporal auto-correlation of ϵ_s^i , shown in Figure 6 provides more information on the persistence of extreme values of shear deformation. In particular, the auto-correlation time appears to be nearly independent of the inertial number:

$$\tau^{\epsilon_s^i} \dot{\gamma} \approx 0.3. \quad (19)$$

this implies that local deformations are correlated for a period of time solely governed by the global deformation as it corresponds to a fraction of Γ - about

0.3Γ - with no effect of the inertial time. This qualitatively and quantitatively differs from the velocity correlation time $\tau^{\delta v}$. First, $\tau^{\delta v}$ is a function of the inertial time and $\tau^{\epsilon_s^i}$ is not. Second, the correlation time of the shear deformation is much larger than that of the velocity fluctuation, especially at low inertial numbers. For instance, at $I = 0.001$, $\tau^{\delta v} \approx 8.10^{-3}/\dot{\gamma}$ while $\tau^{\epsilon_s^i} \approx 0.3/\dot{\gamma}$.

2. Spatial correlations

We seek to characterise the spatio-temporal correlations observed in Figure 4 using the clustering method. The aim is to detect clusters of particles that have undergone a local deformation greater than or equal to a selected threshold, $\epsilon_s^i \geq 0.5$, and to de-

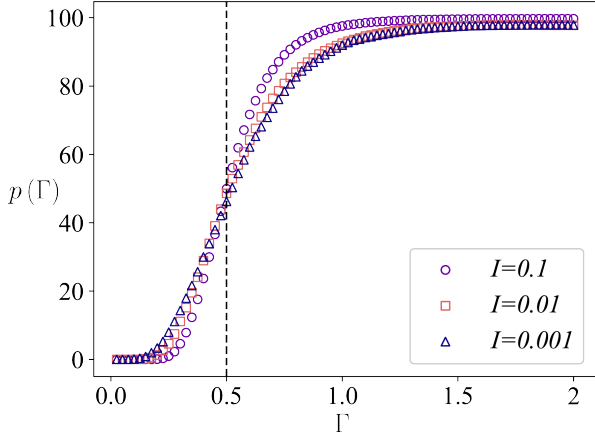


FIG. 5. **Local shear deformations breakthrough.** The plot shows the percentage p of particles whose local shear deformation ϵ_s^i has exceeded a threshold value of 0.5 as the global shear deformation Γ progresses. By definition, $\epsilon_s^i(\Gamma = 0) = 0$.

test how these clusters evolve when the time interval increases. Here, also, the value 0.5 is arbitrary and does not influence the conclusion of this analysis. As global deformation Γ progresses, the survival curves and snapshots in Figure 4 show that more and more particles will pass this threshold and become eligible to belong to a group. Figures 7(a) to (c) and Figures 7(f) to (f) show the evolution in the number of clusters $N_c^{\epsilon_s^i}$ and their average gyration radius $R_g^{\epsilon_s^i}$ as the shear deformation progresses, in flows with different inertial numbers I . These curves point out a two-stage process by which the deformation is distributed in the system. First, at relatively low deformation - approximately less than 0.3, both the number of clusters and their size increase; this corresponds to a growth stage during which new particles exceeding the deformation threshold 0.5 either join a preexisting cluster and increase its size or form a new cluster. Then, at larger deformation, the average size of the cluster continues to increase until it reaches the width of the shear cell $40d$; in the mean time, the number of clusters decreases to eventually reach 1; this is a coalescence stage where new particles that exceed the threshold tend to bridge two preexisting clusters forming a single larger cluster. Eventually, the system consists of a single cluster that includes all the particles, as they have all exceeded the threshold.

During the growth phase, the cluster size increases more rapidly and the number of clusters is lower than at low inertial number. This suggests a qualitative difference in the propagation of deformation between low and high inertial numbers. At high inertial numbers, particles pass the 0.5 threshold at locations that are not related to the location of particles that have previously passed this threshold. In contrast, at low inertial numbers, particles are more likely to pass the 0.5 threshold if they are located near a zone where this threshold has been passed. This is reminiscent of a self-activated process in which local deformation seeds are propagated in some locations and propagate from this point as the global deformation progresses.

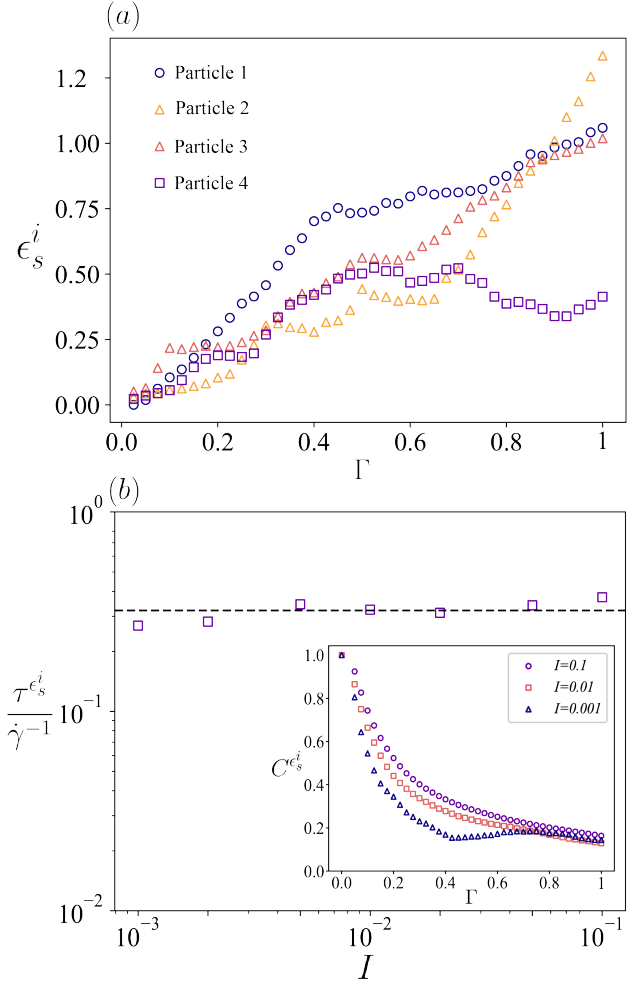


FIG. 6. **Temporal correlation of the local shear deformation ϵ_s^i .** (a) The evolution of local shear deformation for four randomly selected particles in a flow with an inertial number $I = 0.01$. (b) Inset- Auto-correlation function C as defined in (5), measured at a specific reference time t as a function of the global deformation Γ for different inertial numbers. Main Auto-correlation time $\tau^{\epsilon_s^i}$, in unit of $\dot{\gamma}^{-1}$, calculated using (6), as a function of the inertial number; with each point represent an average including 5 reference times spanning over a global shear deformation of 1Γ . The line indicates $\tau^{\epsilon_s^i} = 0.3\dot{\gamma}^{-1}$.

This spatio-temporal correlation of the local deformation is further reflected by the analysis of the spatial distribution of extreme shear deformation. For this analysis, we first applied the clustering algorithm considering a fixed number of particles rather than a total of particles that had passed a threshold. We consider at any point in time Γ 15% of the particles that have experienced the largest shear deformation. We found that the average cluster size $R_g^{\epsilon_s^i}$ is then independent of Γ and follows the power law of the inertial number as shown in Figure 8:

$$R_g^{\epsilon_s^i} \propto aI^b. \quad (20)$$

with a best fit obtained with $a = 1.65$ and $b = -0.30$. We found a similar power law, albeit with a larger prefactor $a = 4.86$ when measuring the REV of the local deformation using the variogram method - here

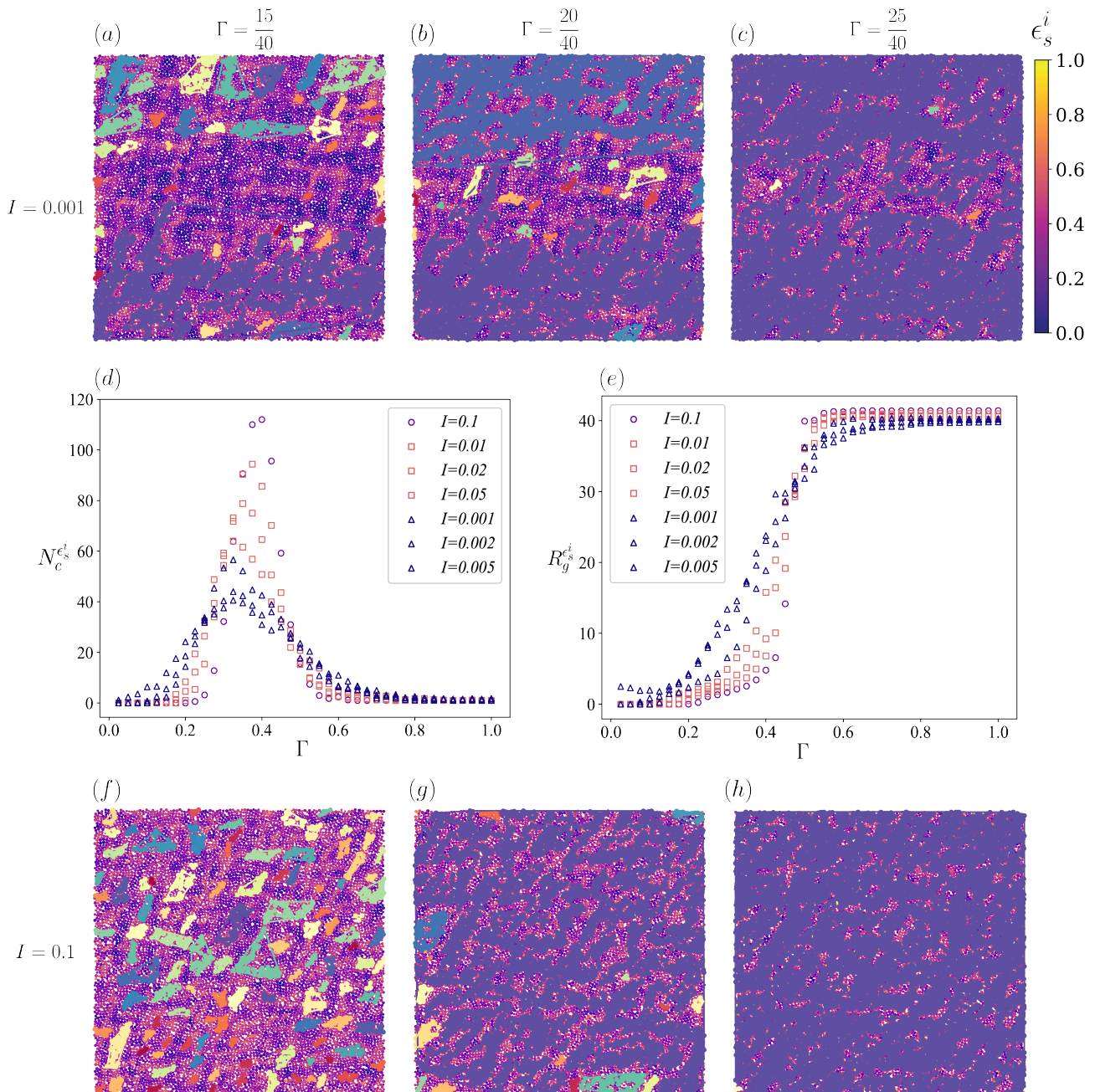


FIG. 7. **Shear strain.** (a) to (c) and (f) to (h) show the evolution in the number of clusters $N_c^{\epsilon_s^i}$ as the shear deformation progresses, in flows with inertial numbers $I = 0.001$ and $I = 0.1$, respectively. (d) shows the evolution of the shear strain radius of gyration, and (e) presents number of clusters in a range of inertial numbers. At relatively low deformation, both the number of clusters and their size increase, where new particles exceed the deformation threshold 0.5 and join a pre-existing cluster with increase its size or form a new cluster. In larger deformations, the average size of the cluster continues to increase until it reaches the width of the shear cell $40d$; and the number of clusters decreases to eventually reach 1; where the system eventually consists of a single cluster that includes all particles, as they have all exceeded the threshold.

to, the choice of Γ did not influence the results. This power law is similar to that of the spatial correlation of the velocity fluctuations.

C. Nonaffine deformation

The analysis of the local deformations highlighted their spatio-temporal correlations, and pointed out a possible mechanisms of propagation. We now consider

whether this mechanism involves the propagation of particle rearrangement. To this end, we measured the evolution of the nonaffine local deformation $D_i^2(\Gamma)$, as defined in Section II. In fact, relatively large values of these quantities have been shown to be a signature of a local topological rearrangement of particles. A threshold value of $D_i^2(\Gamma) \approx 0.5d^2$ ($D_i \approx 0.7d$) was proposed as an indicator of particle rearrangement. Like local deformations, $D_i^2(\Gamma)$ generally increases as global shear Γ progresses. Figure 9 shows the heterogeneous

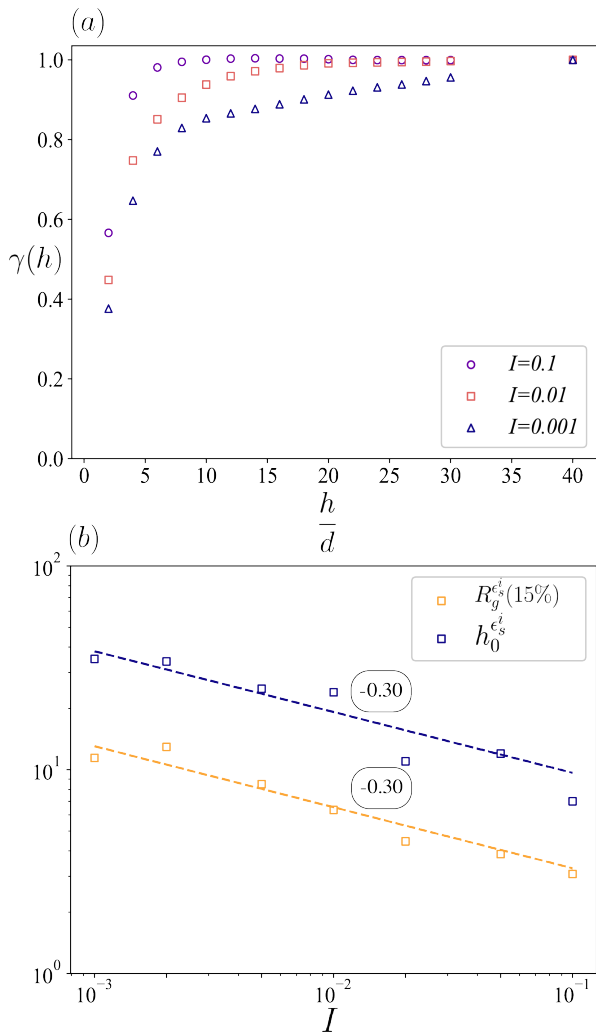


FIG. 8. **Shear strain variogram and length scale.** (a) shows the variogram of shear strain measured in particles at specific reference time. (b) compare different measure of the spatial correlation as a function of the inertial number, including representative element volume h_0^{ϵ} , and the size of the cluster R_g^{ϵ} , determined by considering the top 15% of the particles with the highest shear strain.

field of local deformation. The shear cell comprises some zones with higher values of D_i^2 and others with lower values. The characteristics of these zones match those of shear deformation; they are larger in low inertial numbers, appear to grow, and are advected with the flow as Γ increases.

1. Temporal correlation

Figure 10 shows the auto-correlation function of the nonaffine displacement. Like shear deformation, non-affine displacement is correlated on a period of time that is virtually independent on I , and solely driven by the global deformation Γ :

$$\tau^{D_i^2} \propto 0.2\Gamma. \quad (21)$$

2. Spatial correlation

We analyse the spatio-temporal evolution of the nonaffine deformation using the method presented in Section III B 2 for the local deformation. First, we use the clustering method to identify when and where particles exceed a nonaffine deformation threshold of $D_i^2 > 0.5$. The goal is to identify particles having experienced some rearrangements in their neighbourhood and thus to map the evolution of rearrangements. Figure 11 shows the evolution of the rearrangement clusters as global deformation increases. In terms of shear deformation, there is initially a growth phase during which both the size and the number of rearrangement clusters increases. Once the global deformation is larger than about 0.3, these clusters coalesce: the system features larger and fewer clusters. Eventually, all the particles experienced some rearrangement in their vicinity, and the shear cell was composed of a single cluster that included all the particles. During the growth phase, the rearrangement clusters are larger and fewer at low inertial numbers than at high inertial numbers. This means that, at low inertial numbers, new rearrangements are more likely to occur near the location where rearrangements have already occurred as Γ progresses.

The spatial organisation of particle rearrangements is further reflected in the analysis of the spatial distribution of extreme nonaffine deformation. For this analysis, we applied the clustering algorithm considering a fixed number of particles rather than all particles having passed a threshold: at any point in time Γ 15% of the particles that have experienced the largest non-affine deformation are eligible to belong to a cluster.

We found that the average cluster size $R_g^{D_i^2}$ is then independent of Γ and follows the power law of the inertial number as shown in Figure 12:

$$R_g^{D_i^2} \propto aI^b. \quad (22)$$

with a best fit obtained with $a = 1.2$ and $b = -0.27$. We found a similar power law, albeit with a larger prefactor $a = 4.18$ when measuring the REV of the local deformation using the variogram method - here to, the choice of Γ did not influence the results. This power law is similar to that of the spatial correlation of the velocity fluctuations and that of the shear deformation.

IV. DISCUSSION

We now interpret the results of the spatio-temporal analysis of the kinematic fields presented in the previous section to identify some features of the micro-mechanisms of deformation occurring in these flows.

The most significant feature is that local deformations do not grow steadily and are not distributed uniformly even though the global deformation is steady and uniform. The unsteady and heterogeneous nature of particle velocities has long been recognised in dense granular flows [8, 19, 20], and we have recently shown

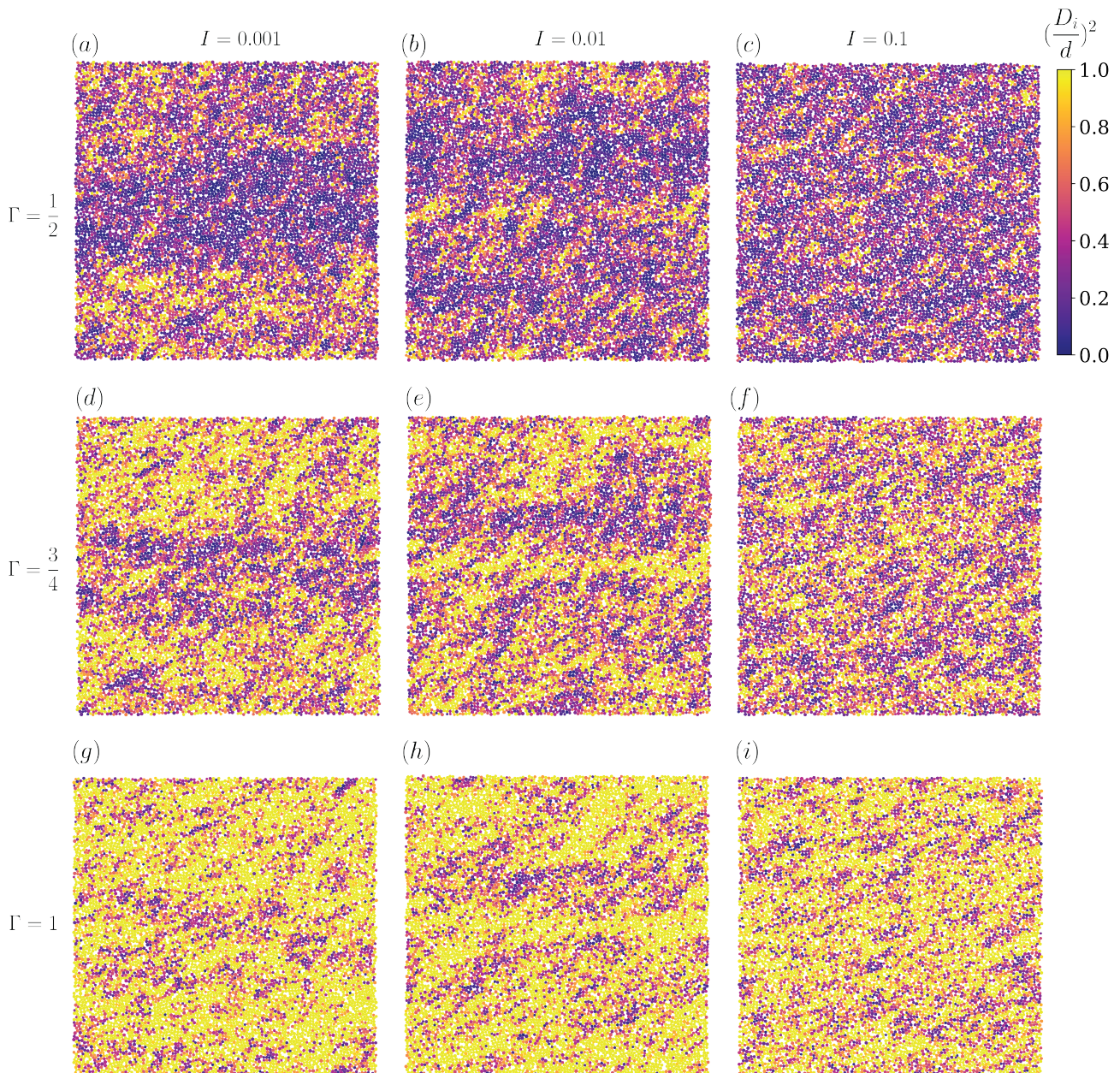


FIG. 9. **Evolution of the nonaffine displacement** $D_i^2(\Gamma)$. The snapshots show the nonaffine displacement $D_i^2(\Gamma)$ of each particle in different time intervals corresponding to the increasing values of global shear deformation Γ , in flows with inertial numbers of $I = 0.001$, $I = 0.01$ and $I = 0.1$.

that these translate into heterogeneous rates of local deformation [21]. The observations made here about local deformations complete these findings.

A. Particle velocity and diffusivity

Shear flows under prescribed normal stress involve two time scales: the macroscopic shear time $\dot{\gamma}$ and the microscopic inertial time t_i . In dense flows, $I = \dot{\gamma}t_i < 1$ means that the inertial time is much shorter than the shear time. Both time scales are involved in the scaling of the velocity fluctuations and that of their auto-correlation time: $\sigma(\delta v) \propto d\dot{\gamma}/\sqrt{I}$ and $\tau^{\delta v} \propto \dot{\gamma}^{-1}\sqrt{I}$, as measured in Section III A.

The interpretation of velocity fluctuations and their correlation times in the context of shear-induced dif-

fusion provided two information [8]. First, particles exhibit random walk trajectories that involve steps that last $\tau^{\delta v_y}$ during which the particles move at a velocity $\sigma(\delta v)$; the length of these steps is then of the order of the size of the particle d : $\sigma(\delta v)\tau^{\delta v_y} \propto d$. Second, particle random walks yield a diffusive behaviour of particles characterised on the continuum scale by an effective diffusivity $\mathcal{D}$. The Green-Kubo relation relates this diffusivity to the velocity fluctuation and their auto-correlation time as: $\mathcal{D} = \sigma^2(\delta v)\tau^{\delta v_y}$, which yields the following scaling law:

$$\mathcal{D} \propto \frac{d^2}{\tau^{\delta v_y}} = \frac{d^2\dot{\gamma}}{\sqrt{I}}. \quad (23)$$

In diluted systems, where there is a lot of free space between particles, the step of a random walk could

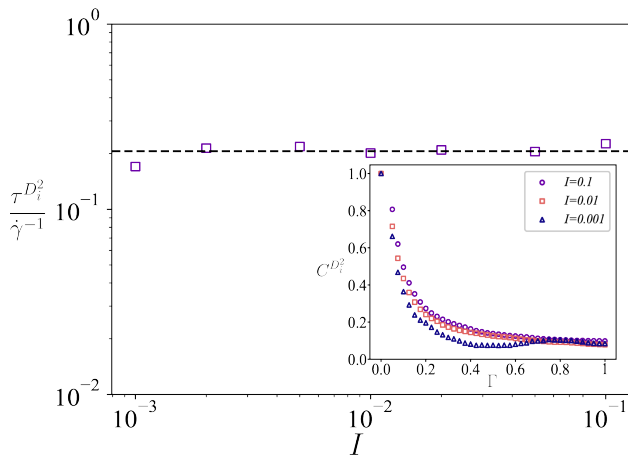


FIG. 10. **Temporal correlation of the nonaffine displacements.** Inset temporal auto-correlation function C of the square nonaffine displacements D_i^2 for flows with inertial numbers of $I = 0.001$, $I = 0.01$ and $I = 0.1$. Main Auto-correlation time scale $\tau^{D_i^2}$ is as a function of the inertial number; and the dashed line represents $\tau^{D_i^2} = 0.2/\dot{\gamma}$.

correspond to a free flight during which a particle is not interacting with any other particle. In dense systems, there is no such free flight as the particles experience multiple sustained contact at any point in time. For a particle to take a step of length d , nearby particles must move away over a distance of the order of d , leading to some local deformation of the order of $d/d \sim 1$. This topological rearrangement has been observed in granular flows and in other particle flows [27, 32].

This suggests that local deformations occur during short events lasting $\tau^{\delta v_v}$; shorter than the shear time $\dot{\gamma}^{-1}$, that yields an increment in deformation of the order of 1, followed by little or no further deformation during the rest of the shear time. This step-like development of local deformation is consistent with the auto-correlation times $\tau^{\epsilon_s} \simeq \tau^{D_i^2}$ measured in sections IIIB and IIIC, which are both of the order of the shear time $\dot{\gamma}^{-1}$.

B. Diffusion of local-deformation

Our results show that local shear deformation and particle rearrangement do not occur steadily or randomly in space. Rather, they seemingly propagate from ‘seed’ events: once a local deformation of the order of 1 has occurred somewhere in the shear cell, further similar events are likely to occur in its vicinity. The result is the existence of clusters consisting of particles with higher deformation than average in the flow; or similar clusters of particles that have undergone more rearrangements than others, as measured by D^2 . We found that the spatial correlation length of these clusters is a power law of the inertial number:

$$\frac{R_g^{\epsilon_s}}{d} \simeq \frac{R_g^{D_i^2}}{d} \propto I^{-\frac{1}{4}}. \quad (24)$$

and that these clusters are sustained during a time interval $\tau^{\epsilon_s} \simeq \tau^{D_i^2} \propto \dot{\gamma}^{-1}$. This scaling is consistent with a mechanism of diffusion of the deformation, involving a diffusivity $\mathcal{D}$ given by (23). Considering an arbitrary period of time Δt , this mechanism predicts that the deformation would diffuse on a distance $\sqrt{\Delta t \mathcal{D}} \propto I^{-\frac{1}{4}}$, which is compatible with the measured size of deformation clusters.

V. CONCLUSION

This analysis of the local kinematic fields in plane shear flows sheds some light on the micromechanisms governing the deformation within dense granular flows. Interestingly, within a material subjected to a steady and uniform external loading, particle velocities, local deformations, and particle rearrangements are found to occur in a way that is neither uniform in space nor steady in time.

Spatio-temporal analysis of these kinematic quantities revealed a mechanism of propagation of the local deformation. In response to a small global deformation, a small fraction of the particles experience a significant local shear deformation of the order of 1. This corresponds to some particle rearrangements, which occurs in a period of time corresponding to the velocity auto-correlation time, which is much shorter than the global shear time. As the global deformation progresses, further rearrangements occur preferentially in the vicinity of pre-existing rearrangements. This leads to an apparent propagation of the local deformation and rearrangements. We observed that this propagation lasts for a period of time on the order of one global shear deformation and covers a larger distance in this period as the inertial number is smaller. The measured scaling law (24) for the size of the cluster is compatible with diffusive propagation of the deformation process using the same diffusivity as for shear-induced diffusion (23), which is itself related to particle velocity fluctuations and their auto-correlation time.

The mechanism of propagation of local deformation is compatible with continuum models describing granular flows, in particular their nonlocal behaviours. This indicates that the deformation occurring at two distant parts of the flow is coupled, as the deformation propagates over some mesoscopic distance. Consistent with continuum nonlocal models, this mesoscopic distance increases at low inertial number. Furthermore, this propagation is found to be diffusive, which defines a time scale for this coupling. To further establish the link between this microprocess and continuum non-local modelling, the next step would be to analyse the propagation of local deformation in flows including a gradient in stress and shear rate, including a solid boundary [33] or subjected to transient loading.

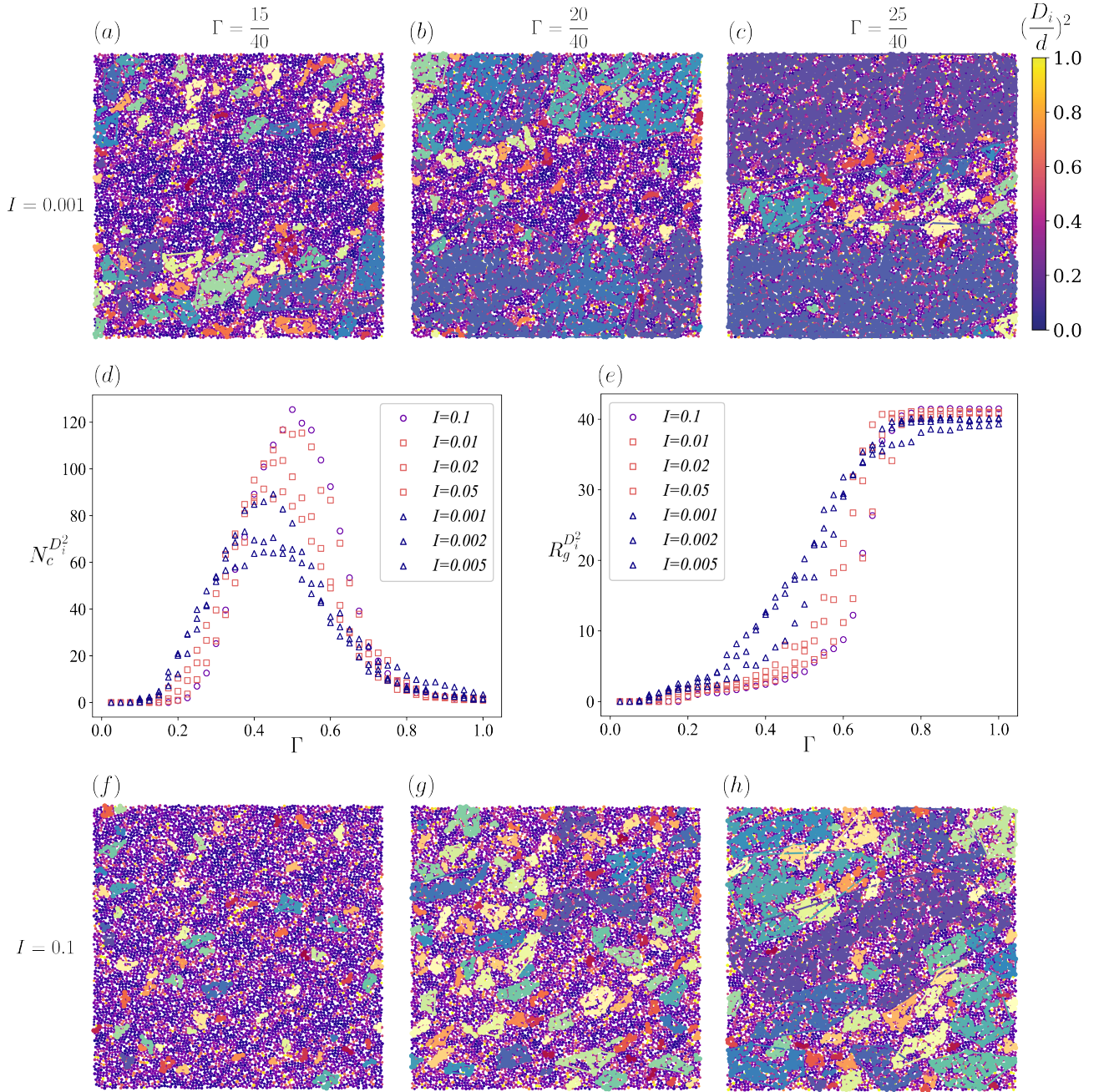


FIG. 11. **Nonaffine displacement.** (a) to (c) and (f) to (h) show the evolution in the number of clusters $N_c^{D_i^2}$ as the shear deformation progresses, in flows with inertial numbers $I = 0.001$ and $I = 0.1$, respectively. (d) shows the evolution of the nonaffine displacement radius of gyration, and (e) presents number of clusters in a range of inertial numbers.

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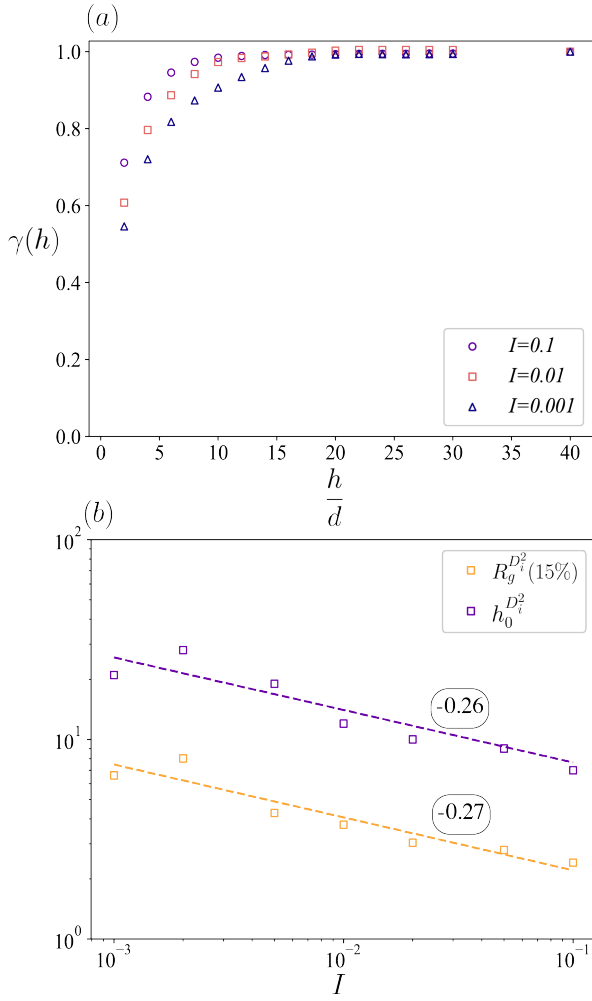


FIG. 12. **Squared nonaffine displacement variogram and length scale.** (a) shows the variogram of nonaffine displacement in particles at specific reference time. (b) compare different measure of the spatial correlation as a function of the inertial number, including representative element volume $h_0^{D_i^2}$, and the size of the cluster $R_g^{D_i^2}$, determined by considering the top 15% of the particles with the highest nonaffine displacement.

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CHAPTER 5

Conclusion and outlook

This thesis provides analysis and development of local kinematic fields, including particle velocity, local deformation, and nonaffine deformation, in granular flows under plane shear. It revealed the length scales associated with flow kinematic heterogeneities such as velocity fluctuations, shear rate, vorticity, and dilation rate. Furthermore, it elucidates the spatio-temporal propagation and diffusion mechanisms of these local kinematic fields, highlighting the role of kinematic clusters in these processes.

Chapter 3 focused on heterogeneous deformation and demonstrated that kinematic measures exhibit significant spatial and temporal correlations, particularly at lower inertial numbers. This chapter established a characteristic length scale for the size of kinematic heterogeneities, corresponding to the size of a Representative Volume Element (REV). The REV size was found to vary with the inertial number, ranging from a few grain diameters at high inertial numbers to several dozen grain diameters at lower inertial numbers. Our results suggested that the REV size diverges at $I \rightarrow 0$, which challenges the existence of a REV in this limit.

It is noteworthy that the REV was measured using the method introduced in Chapter 3, where the system was divided into square cells of size W and the standard deviation of a kinematic quantity within each cell was calculated. If the shape of the windowed cells were to change from square to rectangular—extending only in one direction—the calculated standard deviation of kinematic measures is expected to slightly vary, likely resulting in a different final value of the REV. This suggests that the REV determination may be sensitive to cell shape, an aspect that could be explored further in future studies.

These findings have important implications for homogenisation theories, which can leverage the information embedded in the defined REV size to better explain the effective behaviour of granular materials as a continuum and understand the origins of finite-size effects. Constitutive laws for granular viscosity, $\mu(I)$, and diffusivity, $D(I)$, were measured in systems that exceeded the REV size. A large REV suggests that deviations from these constitutive laws may arise in flows where the distance from a boundary is less than the REV size. In such cases, kinematic structures do not have sufficient space to fully develop, causing the granular viscosity and diffusivity to depend on the proximity to the boundary, thereby introducing system size effects and modifying these laws accordingly.

In practical applications, defining a kinematic-based REV becomes essential in situations where granular materials exhibit significant heterogeneity or non-local behavior at the grain scale, particularly under low-shear or boundary-constrained conditions. Such a REV definition is critical in fields like geotechnical engineering, where localized failures or zones of liquefaction under low confinement may lead to instability, posing safety risks in construction and natural hazard scenarios.

Chapter 4 established a diffusive propagation mechanism for shear deformation and particle rearrangements. This mechanism potentially explains the nonlocal behaviour of the granular flow at the continuum scale. It was discovered that particle rearrangements trigger further rearrangements nearby, creating localised zones of increased deformation. This process suggests an interconnection of deformation between distant regions of the flow, propagating across a mesoscopic distance. Consistent with continuum nonlocal models, this mesoscopic distance increases as the inertial number decreases. Additionally, the diffusive nature of this propagation introduces a timescale for this coupling effect.

This chapter also examined the extent of microscopic propagation during a unit of shear deformation and proposed scaling laws for the size of deformation clusters that align with diffusive propagation models. Similarly to shear-induced diffusion, the associated diffusivity parameters are linked to fluctuations in particle velocity and autocorrelation time.

An additional contribution of Chapter 4 was an extension to Chapter 3 for the determination of the REV size in granular flows. A combination of statistical methods, including autocorrelation functions, standard deviation analysis, variograms, and clustering algorithms, was used to measure the REV size. The REV size determined using the variogram method was found to be larger than that obtained with other methods, introduced the minimum size for the REV in granular flows under simple shear.

The approach of this thesis was to use a simplified "flow" problem to gain an understanding of kinematic fields at the microscale before introducing additional complexities. This was explored using a simple shear flow with periodic boundary conditions in both directions to investigate heterogeneous flow kinematics. This approach provided detailed insights into grain-scale kinematics, serving as a foundation for studying more complex granular flows that involve noncircular particles, solid boundaries, or transient loading conditions.

As an initial extension, this thesis examined the kinematic fields, their spatiotemporal evolution, and their propagation mechanisms at the grain scale. Future research could build on this work by exploring how these mechanisms are influenced by different flow configurations and assessing the impact of particle size diversity, as observed in polydisperse systems. In such systems, cluster size is expected to vary with particle size, where larger particles frequently serve as stable anchors, while smaller particles form mobile, dynamic sub-clusters around them. This structural diversity indicates that clusters persist in a polydisperse environment, although their stability and morphology differ significantly from those in monodisperse systems. Additionally, the diffusive process in polydisperse systems may be sensitive to grain size. Larger particles exhibit reduced mobility, impeding the movement of smaller particles and resulting in non-uniform diffusion rates that depend on local particle size distribution. This size sensitivity potentially introduces spatial and temporal complexity into the diffusion profile.

Future research should explore the effects of confining stress, interparticle friction, and particle stiffness on the evolution of kinematic fields, which in turn may influence the REV size in steady-state simple shear flows of granular materials. It is anticipated that higher confining stress may reduce the REV size by encouraging more uniform particle interactions, while

varying interparticle friction could introduce shear resistance and alter particle rearrangements, potentially increasing REV size. Particle stiffness may also impact REV size, as stiffer particles may experience reduced deformation under stress, leading to smaller kinematic fluctuations and thus a smaller REV size. Additionally, the shape of particles, including factors such as angularity, aspect ratio, and irregularity, should be incorporated into future studies. The shape of the particles can have a significant impact on particle rearrangements, packing densities, and the development of force chains, which in turn influence kinematic fields and REV size. In systems with highly angular or elongated particles, the development of stable clusters may be hindered, leading to a smaller REV, while more spherical particles may facilitate larger, more uniform structures.

Moreover, future studies should aim to connect the propagation of local deformation across micro- and macroscale flows, integrating these insights with continuum models. This thesis identified a specific time scale for the propagation of deformations, where particle interactions are not instantaneous but occur over a measurable duration. This aspect remains underexplored in existing continuum models, and recognising the importance of large-scale structures and clusters will help develop more accurate continuum models that better capture the complex behaviours observed at the grain scale.

The analysis of local kinematic fields in plane shear flows has provided valuable insights into the micromechanisms governing deformation within dense granular flows in 2D. However, this thesis did not explore the evolution of stress fields in granular materials or their correlation with the propagation of deformation, which presents an avenue for future research. While both 2D and 3D systems may exhibit similar types of kinematic structures, such as clusters, shear zones, and velocity fluctuations, the overall dynamics and microstructural evolution is expected to differ between the two cases. In 2D systems, the lack of the third dimension can lead to different packing structures, force chain networks, and particle rearrangements, which in turn may affect the development of kinematic heterogeneities and the associated length scales, such as the REV.

By examining the microstructural processes responsible for rheological behaviours, this thesis contributes to bridging the gap between continuum and discrete descriptions of granular flows.

Understanding these kinematic processes provides clarity on their continuum-scale responses and helps to elucidate the conditions under which specific constitutive models succeed or fail.

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