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Quantification of heavy particles segregation in turbulent flows: a Lagrangian approach

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Preferential concentration of particles in turbulence is studied numerically by quantifying the Lagrangian compressibility of the particulate phase. The compressibility of the particle velocity field predicted by the "Full Lagrangian method" (Osiptsov 1984) is compared with the mesoscopic Eulerian particle velocity field (Février et al. 2005) both in a direct numerical simulation of turbulence and in a synthetic flow field. We demonstrate that the Lagrangian method, in contrast to the Eulerian, accurately predicts the compressibility of the particle velocity field even when the latter is characterized by singularities. Results show that the particle clustering occurs predominantly in regions where the particle velocity field is compressed.

1. Introduction

The way particles suspended in a turbulent flow are transported and segregated by turbulent structures is crucial in many atmospheric and industrial applications such as powder production and formation and growth of PM10 particulate and droplet growth in clouds. In recent years, this phenomenon has been studied from different viewpoints. Eulerian methods, such as 'box-counting', represent a classical approach to the problem recently employed by Février et al. 2005, and Simonin et al. 2006. According to this method, the "mesoscopic Eulerian formalism" (MEF), the velocity of particles dispersed in turbulent flows can be seen as the sum of two contributions: a continuous turbulent velocity field shared by all particles referred to as the Mesoscopic Eulerian Particle Velocity Field (MEPVF) and a random velocity component we refer to as Random Uncorrelated Motion (RUM) (Reeks 2004). The latter component is dominant in the case of particle with large inertia, thus leading to ballistic particle motion, and negligible in the case of infinitesimally small particles. One of the main disadvantages of Eulerian 'box counting' methods is that they require a large number of particles to obtain accurate statistics, and thus have a high computational cost.
In contrast, a high computational efficiency can be obtained using the "Full Lagrangian method" (FLM), a method initially developed by Osiptsov (2000) and later followed by Reeks (2004) and Healy & Young (2005). This method evaluates the size of an infinitesimally small volume of particles and its changes in the course of time along each particle trajectory. The rate of deformation of this volume is related to the

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compressibility of the particle velocity field (e.g. Aris 1989) which is an indicator of particle concentration.
In the present study we exploited the FLM and compare it to the MEF. Particle tracking simulations have been performed in a simple two-dimensional synthetic turbulent flow and the two methods have been benchmarked in a direct numerical simulation of turbulence.

2. Mathematical – Physical model

In this work, we study the dispersion of identical, rigid and spherical particles in a carrier flow of density ρ and kinematic viscosity υ. Particles are assumed to be heavy (i.e. $\rho_p/\rho >> 1$ where ρ_p is the particle concentration) and spherical with radii a_p much smaller than the smallest length scale of the flow. Upon neglecting gravity and Brownian motion, the equations of motion are (Maxey et al. 1983):

$$\frac{d\vec{x}_p}{dt} = \vec{v}, \qquad \frac{d\vec{v}}{dt} = \frac{1}{St}(\vec{u} - \vec{v}), \tag{1}$$

Where $\vec{x}_p$ and $\vec{v}$ are the position and the velocity of the particle respectively, and $\vec{u} = \vec{u}(\vec{x}_p, t)$ denotes the velocity of the carrier flow at the position of the particle. All variables have been made dimensionless by a typical time scale T and a typical velocity scale U. The parameter $St = 2\rho_p a_p^2/(9\rho\upsilon T)$ is the Stokes number which represents the particle response time to changes in the flow.
Let $\vec{v}_E$ denote the MEPVF. In a continuum approach in which the spatial derivatives of $n\vec{v}_E$ are finite, the particle number concentration $n(\vec{x}, t)$ evolves by (Balkovsky et al. 2001): $\partial_t n + \nabla \cdot (n\vec{v}_E) = 0$. Along the trajectory of a particle which moves with velocity $\vec{v}_E$, we have:

$$\frac{dn}{dt} = -n(\nabla \cdot \vec{v}_E). \tag{2}$$

Where $\nabla \cdot \vec{v}_E$ denotes the compressibility of the particle velocity field. It is clear that the number concentration along the trajectory of a particle is directly related to the compressibility. For sufficiently small Stokes numbers, $\vec{v}_E = \vec{u} - St\vec{u} \cdot \nabla\vec{u} + \mathrm{O}(St^2)$ (Balkovsky et al. 2001, Maxey 1987, Elperin et al. 1996, and Chun et al. 2005), and consequently in an incompressible flow:

$$\nabla \cdot \vec{v}_E \cong -St\nabla \cdot (\vec{u} \cdot \nabla\vec{u}) = -StQ \tag{3}$$

Here the quantity Q denotes the Okubo-Weiss parameter (Okubo 1970) and (Weiss 2001). For finite Stokes number an analytical expression for $\nabla \cdot \vec{v}_E$ is not available, and it needs to be determined numerically.
The MEF approach provides a way to calculate $\nabla \cdot \vec{v}_E$ Février et al. 2005. It is based upon a division of the calculation domain into grid cells. Averaging the velocities of all

the particles inside a cell gives $\vec{v}_E$, defined in the center of a cell. By taking the spatial derivatives using a finite difference method, one can obtain $\nabla \cdot \vec{v}_E$ at each cell centre. Simonin et al. 2006 observed that the long term average properties of the MEPVF are independent from the initial conditions of the particles.

As an alternative method to calculate $\nabla \cdot \vec{v}_E$ we employ the FLM. We consider the fractional volume of particles surrounding the particle and follow its evolution as the particle moves through the turbulent carrier flow. Upon defining a unit deformation tensor as $J_{ij} \equiv \partial x_{p,i}(\vec{x}_0, t) / \partial x_{0,j}$, we can differentiate Eq. 1 with respect to $\vec{x}_0$ in order to obtain (Osiptsov 1984, Reeks 2004, and Healy &Young 2005):

$$\frac{dJ_{ij}}{dt} = \dot{J}_{ij}, \qquad \frac{d\dot{J}_{ij}}{dt} = \frac{1}{St}(J_{kj}\frac{\partial u_i}{\partial x_k} - \dot{J}_{ij}). \tag{4}$$

The initial conditions are chosen as $J_{i,j}(0) = \delta_{ij}$ and $\dot{J}_{ij}(0) = \partial u_i(\vec{x}_0, 0) / \partial x_j$. Along a particle trajectory the instantaneous value of J corresponds to the inverse of the particle number concentration, so that using Eq. 2 and averaging over all particle trajectories gives a relation between J and $\nabla \cdot \vec{v}_E$ (Aris 1989):

$$\frac{d}{dt}\langle \ln |J| \rangle = < \nabla \cdot \vec{v}_E > \tag{5}$$

Eq. 5 may result in J becoming equal to zero momentarily, which is equivalent to a singularity in the particle velocity field $(\nabla \cdot \vec{v}_E = -\infty)$. Therefore the FLM is able to detect singularities in the spatial distribution of particles, in contrast to the MEF which is ultimately based on a difference equation.

3. A numerical study

In this section we first compare the two methods in a simple two-dimensional synthetic flow field (Babiano et al. 2000). Secondly, we investigate the compressibility of the particle velocity field in a DNS of statistically stationary homogeneous isotropic turbulence.

3.1 Kinematic simulation

The time-dependent stream function Ψ which describes the flow is:

$$\Psi(x, y, z) = \cos(x + g(t)) \cos y, \tag{6}$$

where A and w are respectively the amplitude and the frequency of the sinusoidal function $g(t) = A\sin(wt)$. The velocity field follows from $\vec{u} = (\partial\Psi / \partial y, -\partial\Psi / \partial x)$. Particles are injected at random positions $\vec{x}_0 = \vec{x}_p(0)$ inside the periodic domain $[0,2\pi] \times [0,2\pi]$ with the same velocity as the fluid at the corresponding position, $\vec{v}(0) = \vec{u}(\vec{x}_0, 0)$. Using Eq. 1, we trace 10^6 particles to determine the value of $< \nabla \cdot \vec{v}_E >$ with the MEF, with 60 grid cells in each direction. Alternatively we follow 10^4

particles using Eqs. 1 and 4, and determine $<\nabla \cdot \vec{v}_E>$ from Eq. 5. We present the results from both methods in Fig. 1, together with the estimate for small St, Eq. 3. For a small Stokes number such as $St = 0.05$ (Fig. 1a), the three lines collapse. This is expected, since Eq. 3 is exact in the limit of infinitely small St. If $St = 0.2$ (see Fig. 1b), there is still an excellent correspondence between the result from the MEF and the FLM. The analytical estimate, however, is quite different because the particles do not precisely follow the oscillations in the flow field due to their inertia. Therefore the lines for $<\nabla \cdot \vec{v}_E>$ are shifted to the right with respect to the curve obtained with the analytical calculation . The graph for $St = 0.5$ (Fig. 1c) is qualitatively different from the previous two, as it contains sharp negative peaks in the value of $<\nabla \cdot \vec{v}_E>$. These intermittent events correspond to a sudden collapse of the volume occupied by the particles so that $J \approx 0$ and $<\nabla \cdot \vec{v}_E> \rightarrow \infty$. This phenomenon is due to RUM, i.e. singularities in the flow field where particle trajectories cross and J vanishes. The agreement between the MEF and the FLM is nonetheless very good, although the peaks tend to be a bit steeper in the Lagrangian method. If particles are perfectly ballistic $(St \rightarrow \infty)$, we expect $<\nabla \cdot \vec{v}_E>$ to be zero for most instants of time, interrupted only by intermittent negative peaks when two particle trajectories cross. This behavior is examplified by Fig. 1d for $St = 2$.

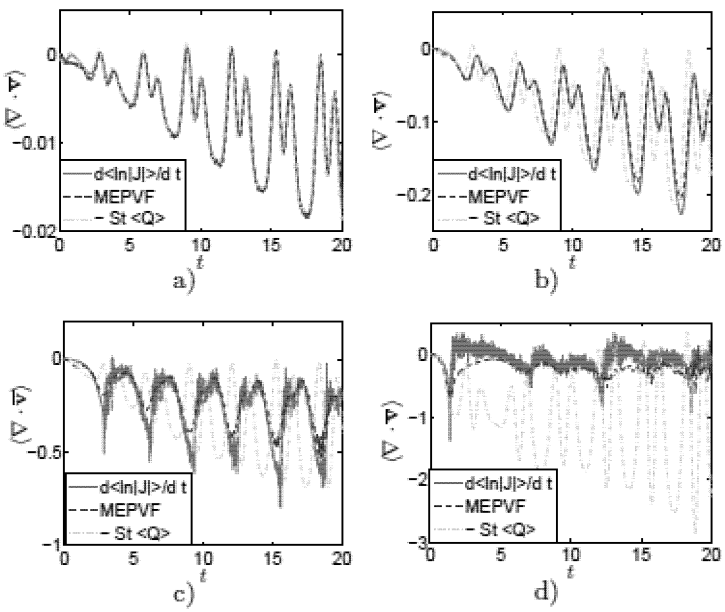

Fig. 1: (Color online) Compressibility of the particle velocity field in the synthetic flow ($A = \pi, \omega = 1$) *as a function of time, measured by the FLM (red solid line) and the MEF (blue dashed line. Maxey's estimate is plotted as well (green dash-dotted line). a)* $St = 0.05$*, b)* $St = 0.2$*, c)* $St = 0.5$*, d)* $St = 2$.

3.2 Direct numerical simulation

The three-dimensional incompressible Navier-Stokes equations are solved using a finite volume method on a staggered grid (128^3 cells) in a triply-periodic cubic domain. The discretization in time is achieved by a second-order Runge-Kutta scheme. The Reynolds number based on the Taylor microscale is $\mathrm{Re}_\lambda = 51$. To determine the MEPVF, we consider one fluid flow realization in which we inject an ensemble of O ($20 \cdot 10^6$) particles with $St = 1$, based on the Kolmogorov time scale. For the FLM, we inject O (10^5) particles with a uniform random distribution into the turbulent flow at $t = 0$. The time of injection is chosen to be the end of the transient of the particle kinetic energy of the MEPVF. Eqs. 1 and 4 are solved for a time span of approximately 10 times the Kolmogorov time scale, and the compressibility of the particle velocity field is computed from Eq. 5. Fig. 2 displays the particle-averaged value of $\nabla \cdot \vec{v}_E$, as a function of time, for the MEF and the FLM. We observe that the correspondence between the two methods is good with the exception of an initial transient. The small difference is probably due to the influence of RUM whose effects are included in the quantification of J but not in the MEF. Apparently, $< \nabla \cdot \vec{v}_E >$ approaches a negative constant, both in the FLM and in the MEF. This indicates that the particle number concentration, measured along the particle trajectories, increases continuously.

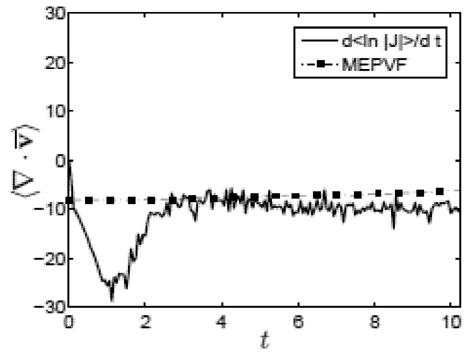

Fig. 2: Compressibility of the particle velocity field as a function of time in a DNS of turbulence for particles with $St = 1$. The solid lines denotes the compressibility measured by the Lagrangian method, whereas the dotted line is obtained using the MEPVF.

4. Conclusion

We have employed the FLM to determine the compressibility of the particle velocity field. The agreement with the MEF approach is generally very good, suggesting that the FLM can indeed be used in the quantification of particle clustering in turbulence. Furthermore, the latter is a more accurate and computationally more efficient way with respect to the MEF which is as intuitive as complicated, its complication being caused by the large number of particles required to determine steep concentration gradients;

specifically, there may be regions devoid of particles close to regions of particle accumulation.

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