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Measuring segregation of inertial particles in turbulence by a full Lagrangian approach

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Preferential concentration of inertial particles in turbulence is studied numerically by evaluating the Lagrangian compressibility of the particle velocity field using the "full Lagrangian method." This is compared with the "mesoscopic Eulerian particle velocity field" 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. In particular we use the method to evaluate the growth rates of spatial moments of the particle number density which reflect the fractal structure of segregation and the occurrence of singularities.

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Suspensions of small heavy particles in turbulent flows are found in a variety of processes such as droplets in clouds [1], soot particles in postcombustion devices, and reacting particles in chemical process facilities [2]. It is well known from experiments [3], numerical simulations [4,5], and theoretical studies [1,6] that particles in turbulent flows tend to concentrate preferentially due to their inertia. While being influential in many of these natural and industrial processes, this "demixing" is of fundamental interest in statistical physics, since it is associated with the behavior of a nonlinear system far from equilibrium, combining the properties of kinetics and hydrodynamics with caustics superimposed on multifractal structures [5,7,8].

Inertial particles are generally ejected from regions of high vorticity and accumulate in regions of high strain rate, thereby inducing nonzero gradients in the particle number density, $n(\mathbf{x},t)$, i.e., the number of particles situated inside an infinitesimally small volume located at position $\mathbf{x}$ at time t. Preferential concentration is associated with a nonzero compressibility of the particle velocity field $\overline{\mathbf{v}}(\mathbf{x},t)$ which is defined as the mean velocity of particles at a certain position $\mathbf{x}$ at time t. Indeed, it is well known [9–11] that the particle velocity field may be compressible even if the turbulent carrier flow is incompressible. Local gradients of $n(\mathbf{x},t)$ and $\overline{\mathbf{v}}(\mathbf{x},t)$ control the rates of interparticle collisions, coalescence, breakup, and possibly sedimentation and resuspension.

One possibility of measuring the local concentration of discrete particles and the particle velocity field is to use "box counting" (see, e.g., [12]). This method is as intuitive as it is complicated, its complication being caused by the large number of particles required to determine steep concentration gradients; in particular, there may be regions devoid of particles close to regions of particle accumulation. In the present study we propose an alternative method to quantify the compressibility of the particle velocity field, namely, the "full Lagrangian method" (FLM) [13–15] and compare it to the "mesoscopic Eulerian formalism" (MEF) [11,16], which is essentially a box counting method. We show that the FLM can be used to predict local concentration gradients at small scales in a more accurate and computationally cheaper way than the MEF. The potential of the FLM is illustrated in a simple two-dimensional synthetic turbulent flow field and we benchmark the two methods in a direct numerical simulation (DNS) of turbulence. Finally, we demonstrate that the FLM can be used to determine any spatially averaged moment of the particle number density.

In this work, we study the dispersion of identical, rigid, and spherical particles in a carrier flow of mass density ρ and kinematic viscosity ν. Particles are assumed to be heavy (i.e., $\rho_p/\rho \gg 1$ where ρ_p is the particle density) with radii a_p much smaller than the smallest length scale of the flow. Upon neglecting gravity and Brownian effects, the equations of motion are [17]

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}}{dt} = \frac{1}{\mathrm{St}}(\mathbf{u}-\mathbf{v}), \tag{1}$$

where $\mathbf{x}_p$ and $\mathbf{v}$ are the position and velocity of the particle, respectively, and $\mathbf{u}=\mathbf{u}(\mathbf{x}_p,t)$ denotes the velocity of the carrier flow at the position of the particle. All variables have been made dimensionless by a typical time scale $\mathcal{T}$ and a typical velocity scale $\mathcal{U}$. The parameter $\mathrm{St}=2\rho_p a_p^2/(9\rho\nu\mathcal{T})$ is the Stokes number, which represents the ratio between the inertia driving the particle and the viscous damping action of the fluid.

Février *et al.* [16] have proven that 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 called the mesoscopic Eulerian particle velocity field (MEPVF) and denoted by $\overline{\mathbf{v}}$, and a random velocity component we refer to as random uncorrelated motion (RUM) [14] (alternatively called "sling effect" [1] or "crossing trajectories effect" [18]). The latter component is

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dominant in the case of large inertia, thus leading to a ballistic particle motion and negligible in the case of infinitesimally small particles. In a continuum approach in which the spatial derivatives of $n\bar{\mathbf{v}}$ are finite, the particle number density $n(\mathbf{x},t)$ evolves by [6] $\partial_t n+\nabla\cdot(n\bar{\mathbf{v}})=0$. In regions devoid of particles $\bar{\mathbf{v}}$ is formally undefined, but the number density is zero there and consequently $n\bar{\mathbf{v}}=0$ as well. Along the trajectory of a particle which moves with velocity $\bar{\mathbf{v}}$, we have

$$\frac{dn}{dt} = -n(\nabla\cdot\bar{\mathbf{v}}), \tag{2}$$

where $\nabla\cdot\bar{\mathbf{v}}$ denotes the *compressibility* of the particle velocity field. If the initial number density is uniform and normalized so that $n(\mathbf{x},0)=1$, Eq. (2) can easily be integrated in order to obtain [6] $n=\exp[\int_0^t(\nabla\cdot\bar{\mathbf{v}})dt']$. It is clear that the number density along the trajectory of a particle is directly related to the compressibility. For sufficiently small Stokes numbers, $\bar{\mathbf{v}}=\mathbf{u}-\mathrm{St}\mathbf{u}\cdot\nabla\mathbf{u}+\mathcal{O}(\mathrm{St}^2)$ [6,9,10,19], and consequently in an incompressible flow,

$$\nabla\cdot\bar{\mathbf{v}} \simeq -\mathrm{St}\,\nabla\cdot(\mathbf{u}\cdot\nabla\mathbf{u}) = -\mathrm{St}Q, \tag{3}$$

where Q denotes the Okubo-Weiss parameter [20,21]. For finite Stokes numbers however an analytical expression for $\nabla\cdot\bar{\mathbf{v}}$ is not available and it needs to be determined numerically.

The MEF approach provides a way to calculate $\nabla\cdot\bar{\mathbf{v}}$ [11,16] based upon a division of the calculation domain into grid cells. Averaging the velocities of all the particles inside a cell gives $\bar{\mathbf{v}}$ defined in the center of a cell. By taking the spatial derivatives using a finite difference method, one can obtain $\nabla\cdot\bar{\mathbf{v}}$ at each cell center.

As an alternative method to calculate $\nabla\cdot\bar{\mathbf{v}}$ 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 $J_{ij}\equiv\partial x_{p,i}(\mathbf{x}_0,t)/\partial x_{0,j}$, we can differentiate Eq. (1) with respect to $\mathbf{x}_0$ in order to obtain [13–15]

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

The initial conditions are chosen as $J_{ij}(0)=\delta_{ij}$ and $\dot{J}_{ij}(0)=\partial u_i(\mathbf{x}_0,0)/\partial x_j$. Along a particle trajectory $|J|\equiv|\det(J_{ij})|=n^{-1}$, so that using Eq. (2) and averaging over all particle trajectories gives a relation between J and $\nabla\cdot\bar{\mathbf{v}}$ [22]:

$$\frac{d}{dt}\langle\ln|J|\rangle = \langle\nabla\cdot\bar{\mathbf{v}}\rangle. \tag{5}$$

Equation (4) may result in J becoming equal to zero, which is equivalent to a singularity in the particle velocity field ($\nabla\cdot\bar{\mathbf{v}}=-\infty$). 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. A method similar to the FLM was proposed by Falkovich and Pumir [23], first for infinitesimally small St and subsequently for any St [24], who used a nonlinear equation for the time evolution of the deformation tensor. Although their method is well suited for detecting singularities in the particle velocity field—and thus for the determination of collision rates—its main disadvantage is that the calculation necessarily finishes once a singularity has been encountered [15]. It is therefore not ideally suited for the long-time calculations of the compressibility, which is the main objective of the present study.

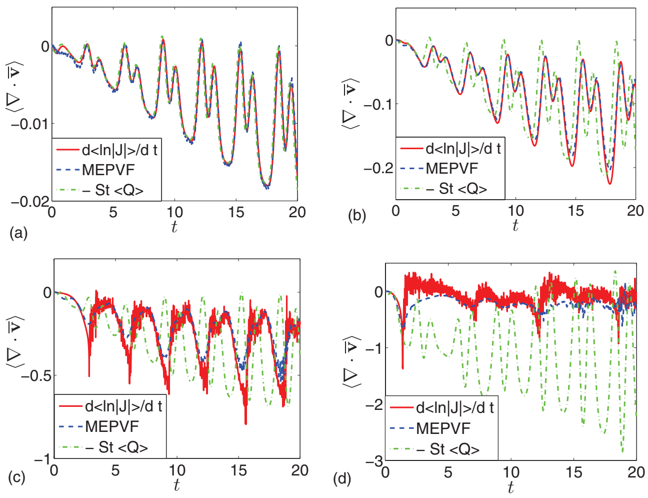

FIG. 1. (Color online) Compressibility of the particle velocity field $\langle\nabla\cdot\bar{\mathbf{v}}\rangle$ in the synthetic flow ($A=\pi$, $\omega=1$) as a function of time, measured by the FLM ($d\langle\ln|J|\rangle/dt$; red solid line), and by the MEF (MEPVF; blue dashed line). Maxey's estimate, Eq. (3), is plotted as well (green dash-dotted line). (a) St=0.05, (b) St=0.2, (c) St=0.5, and (d) St=2.

We compare the FLM and the MEF in a simple two-dimensional synthetic flow field. The time-dependent stream function Ψ is [25]

$$\Psi(x,y,t) = \cos[x + A\sin(\omega t)]\cos y, \tag{6}$$

and the velocity field follows from $\mathbf{u}=(\partial\Psi/\partial y,-\partial\Psi/\partial x)$. Particles are injected at random positions $\mathbf{x}_0=\mathbf{x}_p(0)$ inside the periodic domain $[0,2\pi]\times[0,2\pi]$ with the same velocity as the fluid at the corresponding position, $\mathbf{v}(0)=\mathbf{u}(\mathbf{x}_0,0)$. Using Eq. (1), we trace 10^6 particles to determine the value of $\langle\nabla\cdot\bar{\mathbf{v}}\rangle$ with the MEF with 60 grid cells in each direction. Alternatively we follow 10^4 particles using Eqs. (1) and (4) and determine $\langle\nabla\cdot\bar{\mathbf{v}}\rangle$ 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. 1(a)], 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. 1(b)], there is still an excellent correspondence between the result from the MEF and the FLM. The value of $-\mathrm{St}\langle Q\rangle$, 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 $\langle\nabla\cdot\bar{\mathbf{v}}\rangle$ are shifted to the right with respect to the curve $-\mathrm{St}\langle Q\rangle$. The graph for St=0.5 [Fig. 1(c)] is qualitatively different from the previous two, as it contains sharp negative peaks in the value of $\langle\nabla\cdot\bar{\mathbf{v}}\rangle$. These intermittent events correspond to a sudden collapse of the volume occupied by the particles so that $J\sim 0$ and $\langle\nabla\cdot\bar{\mathbf{v}}\rangle\to-\infty$. 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

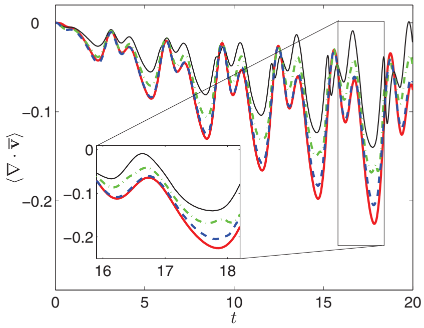

FIG. 2. (Color online) Compressibility of the particle velocity field $\langle \nabla \cdot \bar{\mathbf{v}} \rangle$ in the synthetic flow ($A=\pi$, $\omega=1$) as a function of time for St=0.2, measured by the FLM ($d\langle \ln|J|\rangle/dt$; red solid line), and by the MEF on three different grid resolutions: 10×10 grid cells (thin solid black line), 20×20 grid cells (dash-dotted green line), and 60×60 grid cells (dashed blue line).

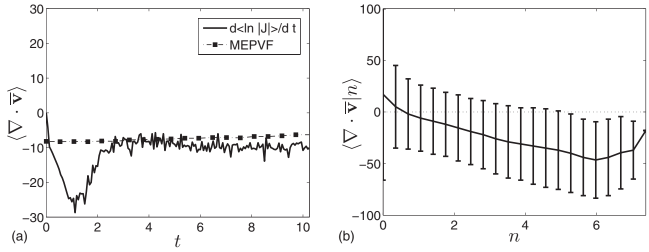

FIG. 3. (a) Compressibility of the particle velocity field $\langle \nabla \cdot \bar{\mathbf{v}} \rangle$ as a function of time in a DNS of turbulence for particles with St =1. The solid line denotes the compressibility measured by the Lagrangian method ($d \ln|J|/dt$), whereas the dotted line represents the Eulerian method using the MEPVF. (b) Instantaneous conditional average $\langle \nabla \cdot \bar{\mathbf{v}} | n \rangle$, determined from the MEPVF, as a function of the particle number density in a DNS of turbulence for particles with St=1. Error bars show the rms of the distribution of $\nabla \cdot \bar{\mathbf{v}}$.

FLM is nonetheless very good, although the peaks tend to be a bit steeper in the Lagrangian method. If particles are perfectly ballistic ($\mathrm{St}\to\infty$), we expect $\langle \nabla \cdot \bar{\mathbf{v}} \rangle$ to be zero for most instants of time, interrupted only by intermittent negative peaks when two particle trajectories cross. This behavior is exemplified by Fig. 1(d) for St=2.

We can relate the onset of RUM to a specific value of St. This value can be evaluated by neglecting the flow time dependence and setting $A=0$ or $\omega=0$, thus considering a flow field made of an array of counter-rotating vortices with hyperbolic regions between them. When the inertial particles move from one vortex to another, they statistically cross the separatrix of the vortices near the hyperbolic stagnation points (x_h, y_h). The stream function containing these points can be approximated by a Taylor expansion up to third order: $\Psi \simeq \pm (x-x_h)(y-y_h)$. Particles can cross the separatrix only if St>0.25 [26], when particle inertia is sufficient to overcome the damping action of the fluid. We also note that the value St=0.25 is the threshold for which J can become equal to zero [14]. Indeed, Figs. 1(a) and 1(b) are very smooth whereas Figs. 1(c) and 1(d) are characterized by intermittent negative peaks. Our result is very much in agreement with previous studies [18,24] which show that RUM has an activation dependence on the Stokes number in real turbulence consisting of different time and length scales.

The difference between the results from the FLM and the MEF can be illustrated by a convergence test of the grid cells in the MEPVF. Figure 2 depicts a similar result as in Fig. 1(b), but with three different resolutions of the MEPVF. As the mesh becomes finer, the small-scale fluctuations in the particle number density are better predicted and the values of $\langle \nabla \cdot \bar{\mathbf{v}} \rangle$ are generally lower. The result from the FLM coincides almost perfectly with the solution of the finest mesh in the MEPVF, thus confirming the consistency of the FLM approach and illustrating its potential.

Now we investigate the compressibility of the particle velocity field in a DNS of statistically stationary homogeneous isotropic turbulence. 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 $\mathcal{O}(20\times 10^6)$ particles with St=1, based on the Kolmogorov time scale. For the FLM, we inject $\mathcal{O}(10^5)$ particles with a uniform random distribution into the turbulent flow at $t=0$. All particles are released with the initial velocity equal to the local fluid velocity. Equations (1) and (4) are solved for a time span of approximately ten times the Kolmogorov time scale, and the compressibility of the particle velocity field is computed from Eq. (5).

Figure 3(a) displays the particle-averaged value of $\nabla \cdot \bar{\mathbf{v}}$, 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, $\langle \nabla \cdot \bar{\mathbf{v}} \rangle$ approaches a negative constant, both in the FLM and in the MEF. This indicates that the particle number density, measured along the particle trajectories, increases continuously.

Figure 3(b) quantifies the joint correlation between the particle number density and $\nabla \cdot \bar{\mathbf{v}}$ calculated from the MEPVF at one instant of time $t=10$. We observe that a locally increased particle number density is positively correlated with a compression of the MEPVF.

Finally, we show how the FLM allows us to determine the moments of the particle number density averaged over space. Because $n=|J|^{-1}$ along the trajectory of each particle, the αth moment of the particle number density averaged over all particles is $\langle n^\alpha \rangle = \langle |J|^{-\alpha} \rangle$. The particle average of any variable Φ, $\langle \Phi \rangle$, is related to the value spatially averaged over a domain Ω, $\bar{\Phi}$, by $\langle \Phi \rangle = \Omega^{-1}\int_\Omega n\Phi d\mathbf{x} = \overline{n\Phi}$. In the present study, the flows are periodic in space and the number of particles in the domain remains constant. Hence:

$$\overline{n^\alpha} = \langle |J|^{1-\alpha} \rangle, \qquad \forall\, \alpha \in \mathbb{R}. \tag{7}$$

Thus, any space-averaged moment of the particle number density can be obtained from Lagrangian statistics of J.

We determine $\overline{n^\alpha}$ in the synthetic flow using Eq. (7) and show the result in Fig. 4 for St=0.2 (a) and St=0.5 (b), for

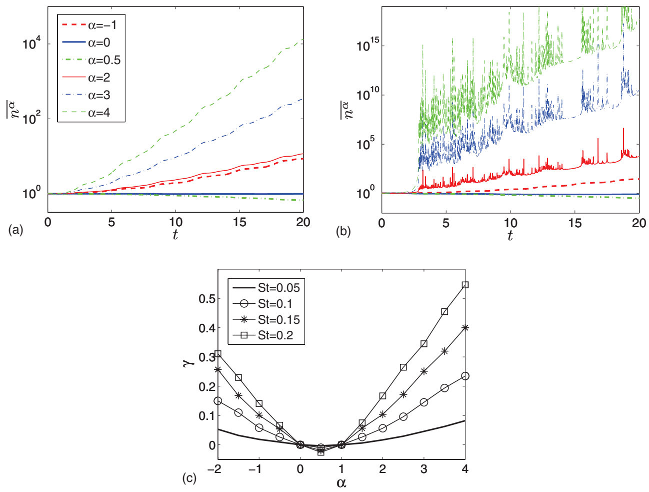

FIG. 4. (Color online) [(a) and (b)] Spatial average of the moments of the particle number density $\overline{n^\alpha}$ as a function of time in the synthetic two- dimensional flow $(A=\pi,\omega=1)$ for St=0.2 (a) and St=0.5 (b), for six different values of α; the legend is valid for both graphs. (c) Coefficient γ as a function of α for four different Stokes numbers.

six different values of α. The value $\alpha=1$ is not plotted, since it is trivially equal to 1; see Eq. (7). If St=0.2, the second, third, and fourth moments of n increase approximately exponentially with time. Because $\bar{n}=1\,\forall\, t$, the particles are clustered in smaller and smaller areas. The same qualitative behavior is visible in Fig. 4(b) for St=0.5, although the resulting values for $\overline{n^\alpha}$ for $\alpha>1$ are even higher by several orders of magnitude. The high intermittent peaks correspond to events when $J=0$ and can be attributed to the presence of RUM in this case where St>0.25.

If St is sufficiently small so that the effect of RUM is negligible, then we find after a sufficiently long time: $\overline{n^\alpha} \propto \exp(\gamma t)$, where γ is a function of St and α alone. We calculate γ as a function of α on the basis of the results for $\langle |J|^{1-\alpha}\rangle$, for four different St and plot the results in Fig. 4(c). All graphs pass through the α axis at $\alpha=0$ and $\alpha=1$ as expected. For all Stokes numbers considered, $\gamma\leq 0$ if $0\leq\alpha\leq 1$, and $\gamma>0$ otherwise. Figure 4(c) shows that γ is approximately proportional to St. These results are in perfect agreement with Balkovsky *et al.* [6] who predicted theoretically that γ is convex function of α at a given Stokes number, i.e., $\partial^2\gamma/\partial\alpha^2\neq 0\,\forall\,\alpha$. Here, Balkovsky's theoretical prediction for the number density has actually been confirmed in a numerical simulation. Our results are also in qualitative agreement with [27], who investigated experimentally the spatially coarse-grained moments of the particle number density and their dependence on the normalized box size. The reason why we have been able to obtain the high-order moments $\overline{n^\alpha}$ is because we calculated the moments of the particle number density by the FLM instead of by a classical Eulerian box-counting method which would have had too limited a spatial resolution to detect clustering on increasingly small scales.

In conclusion, we have explored the possibility of employing the FLM to determine the compressibility of the particle velocity field. The agreement with the Eulerian MEF approach is generally very good suggesting that the FLM can indeed be used in the quantification of particle clustering in turbulence. Finally, we have explained how the FLM can be used to determine any spatially averaged moment of the particle number density. By doing so, we have unambiguously demonstrated the existence of singularities in the particle velocity field.

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