A lattice model for the Eulerian description of heavy particle suspensions

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Abstract

Modeling dispersed solid phases in fluids still represents a computational challenge when considering a small-scale coupling in wide systems, such as the atmosphere or industrial processes at high Reynolds numbers. A numerical method is here introduced for simulating the dynamics of diffusive heavy inertial particles in turbulent flows. The approach is based on the position/velocity phase-space particle distribution. The discretization of velocities is inspired from lattice Boltzmann methods and is chosen to match discrete displacements between two time steps. For each spatial position, the time evolution of particles momentum is approximated for simulating the dynamics of diffusive heavy inertial particles. The approach is based on the Eulerian-Lagrangian direct numerical simulation (see, for instance, Balachandar and Eaton 2010; Toschi and Bodenschatz 2009) for recent reviews). This approach is particularly suited for monitoring the fluctuations occurring at dissipative scales. However, direct numerical simulations are quickly too computationally expensive for studying particle suspensions in realistic settings. On the one hand, a large-scale system, such as a chemical reactor, an atmospheric cloud or a protoplanetary disk, contains a prohibitively large number of particles. On the other hand, the substantial Reynolds numbers of natural and industrial flows require the use of large-scale models, such as large-eddy simulations. Eulerian-Lagrangian methods, where the dispersed phase is modeled by point particles, show some difficulties in correctly predicting modifications of the carrier flow by the dispersed phase, particle-to-particle interactions and near-wall effects.

Some of these shortcomings can be circumvented using Eulerian-Eulerian methods (see Fox 2012 for a review). The main difficulty then relies in finding a fluid description of the dispersed particulate phase. In principle, this is achieved by prescribing a closure for the kinetic hierarchy of moment equations. When considering an ensemble of particle trajectories, one naturally introduces the phase-space density at least for particles with a large-enough response time. For particles with smaller inertia, one relies on the use of stochastic Langevin models (Pozorski and Apte 2009; Shotorbani and Mashayek 2006). In addition the constraints on the number of particles can be relaxed using super-particles approaches, which then necessitates some modeling for collisions (Rein et al. 2010; Shima et al. 2009). However, as stressed for instance by Portela and Oliemans (2006), Lagrangian methods prove some difficulties in correctly predicting modifications of the carrier flow by the dispersed phase, particle-to-particle interactions and near-wall effects.

1. Introduction

Particle-laden turbulent flows are found in numerous natural and industrial situations, ranging from droplet growth in clouds and dust accretion in early stellar systems, to turbulent mixing in engines and industrial sprays. In such situations, the processes that need being modeled and quantified involve the fine-scale dynamical properties of the particles, like preferential concentration, collisions and coalescences, chemical reactions, and modulation of the fluid flow by the particles. To address specific microphysical issues, one usually study simultaneously the turbulent flow and the dispersed phase using Eulerian-Lagrangian direct numerical simulation (see, for instance, Balachandar and Eaton 2010; Toschi and Bodenschatz 2009) for recent reviews). This approach is particularly suited for monitoring the fluctuations occurring at dissipative scales. However, direct numerical simulations are quickly too computationally expensive for studying particle suspensions in realistic settings. On the one hand, a large-scale system, such as a chemical reactor, an atmospheric cloud or a protoplanetary disk, contains a prohibitively large number of particles. On the other hand, the substantial Reynolds numbers of natural and industrial flows require the use of large-scale models, such as large-eddy simulations. Eulerian-Lagrangian methods, where the dispersed phase is modeled by point particles, show some advantages: they allow for an easy implementation of polydispersity and are rather insensitive to subgrid-scale fluctuations, at least for particles with a large-enough response time (Wang and Squires 1996). For particles with smaller inertia, one relies on the use of stochastic Langevin models (Pozorski and Apte 2009; Shotorbani and Mashayek 2006). In addition the constraints on the number of particles can be relaxed using super-particles approaches, which then necessitates some modeling for collisions (Rein et al. 2010; Shima et al. 2009). However, as stressed for instance by Portela and Oliemans (2006), Lagrangian methods prove some difficulties in correctly predicting modifications of the carrier flow by the dispersed phase, particle-to-particle interactions and near-wall effects.

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\[ f(x, v, t) = \langle \delta(x_p(t) - x) \delta(v_p(t) - v) \rangle, \]

where the fluid velocity realization is fixed and the average \( \langle \cdot \rangle \) is both over the particle ensemble (different realizations of the initial conditions and/or average over a large number of particles) and over the molecular diffusion of the particles (with diffusion constant \( \kappa \)). The phase-space density then solves the diffusion-transport equation

\[ \partial_t f + v \cdot \nabla_x f - \nabla_v \cdot \left[ f(\mathcal{F}(x, v, t)/m_p) - \nabla_v \cdot (\kappa \nabla_v f) \right] = 0, \]

where \( \mathcal{F} \) is the force exerted by the fluid on a particle located at \( x \) with a velocity \( v \) and \( m_p \) is the particle mass. This Fokker–Planck equation is exact and fully describes the dynamics of

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small particles in the phase space. The drift terms are completely prescribed by a given realization of the fluid flow. To obtain an Eulerian description of particles dynamics that depends on the spatial variable \( x \) only, the usual approach consists in deriving the equations for the various moments of the velocity \( v \). To close the resulting hierarchy, additional assumptions are needed. They naturally arise when focusing on given asymptotics (see, e.g., Carrillo et al., 2008). For instance, when the particles experience a very strong viscous drag with the flow (small Stokes numbers), an effective particle velocity can be written (Maxey 1987) leading to close this hierarchy at the zeroth order and to write an explicit equation for the transport of particle density. This then serves as a basis for deriving subgrid-scale models for large-eddy simulations (see, e.g., Shotorban and Balachandar 2007). First-order closures lead to writing an evolution equation for a particle velocity field that is coupled to the fluid flow. Again, such methods are limited to asymptotically small values of the Stokes number, as they are inadequate to deal with multi-streamed particle distributions. It is indeed well known that the trajectories of finite-Stokes-number particles can cross, leading to the formation of regions where the particle velocities are multivalued and cannot be described in terms of a spatial field. This phenomenon is usually referred to as particle-trajectory crossing (Chen 2000), sing effect (Falkovich et al., 2002) or caustic formation (Wilkinson and Mehlig, 2005) and has important impacts in estimating collision rates (see, e.g., Bec et al., 2005). Higher-order closures, such as ten-moment equations, can also be proposed depending on the specific forces applied on the particles. They account for the dispersion in particle velocities and can thus catch some aspects of multi-streaming (using either algebraic or quadrature closures Desjardins et al., 2008; Fevrier et al., 2005).

In principle, accessing the full multi-streaming dynamics of particles requires solving the kinetic equation \( \square \) in the entire \((2 \times d)\)-dimensional position-velocity phase space. \((d \) denotes here the dimension of the physical space.) A clear difficulty which is then faced is the prohibitive computational cost of integrating a partial differential equation in a space with such a large dimensionality. Attempts have nevertheless been made by decreasing the number of relevant degrees of freedom. This can be easily done, for instance, by considering one-dimensional flows (see, e.g., Carrillo et al., 2008 and references therein). Other approaches are based on the physical observation that the distribution of particle velocities is usually rather concentrated along a given number of branches in phase space. This led for instance Liu et al. (2011) to capture implicitly the velocity dispersion by applying a level-set method in phase space. The proposed lattice-particle method is directly compared to the results of direct Lagrangian simulations. Section 3 is devoted to the one-dimensional case with a random Gaussian flow. Section 2 shows the results of coupled Navier–Stokes and lattice particles simulations in two dimensions for turbulent flows, either in the direct cascade of enstrophy or in the inverse cascade of kinetic energy.

2. Description of the method

The solutions \( f(x, v, t) \) to the Liouville (or Fokker–Planck) equation \( \square \) are defined in the full position-velocity phase-space \( \Omega \times \mathbb{R}^d \), where \( \Omega \) designates a \( d \)-dimensional bounded spatial domain. To simulate numerically the dynamics, we divide the phase-space in \((2 \times d)\)-dimensional hypercubes. We then approximate \( f(x, v, t) \) as a piecewise-constant scalar field on this lattice. Positions are discretized on a uniform grid with spacing \( \Delta x \) in all directions. In principle, \( f \) has to be defined for arbitrary large velocities. We however assume that relevant values of \( v \) are restricted to a bounded interval \([-V_{\text{max}}, V_{\text{max}}]^d\), where \( V_{\text{max}} \) has to be specified from physical arguments based on the forces \( \mathcal{F} \) applied on the particles. Velocities are assumed to take \( N^d \) values, so that the grid spacing reads \( \Delta v = 2V_{\text{max}}/N_v \). Figure 1 illustrates the phase-space discretization in the one-dimensional case with \( N_v = 5 \). The various cells in position-velocity contain a given mass of particles. All these particles are assumed to have a position and velocity equal to that at the center of the cell.

![Figure 1: Sketch of the lattice dynamics in the \((x, v)\) position-velocity phase space. The solid curve is the fluid velocity profile; the greyscale tiling represents the discretization of particles mass in phase space. The black horizontal arrows show advection, while the blue and red vertical arrows are forcing and diffusion, respectively.](image)

The three phase-space differential operators appearing in Eq. 2, namely the advection, the particle forcing, and the diffusion, are applied one after the other, following an operator...
For the advection step, we use a technique inspired from the Lattice-Boltzmann method (see, e.g., [Succi 2001]). The time stepping is chosen, so that a discrete velocity exactly matches a shift in positions by an integer number of gridpoints. Namely, we prescribe \( \Delta x = \Delta v \Delta t \). All the particle phase-space mass located in \([-\Delta v/2, \Delta v/2]\) does not move; that in \([\Delta v/2, 3\Delta v/2]\) is shifted by one spatial gridpoint to the right and that in \([-3\Delta v/2, -\Delta v/2]\) to the left, etc. All the mass is displaced from one cell to another according to its own discrete velocity value. This evolution is sketched by black horizontal arrows in Fig. 1. This specific choice for the time-stepping implies that the advection (in space) is treated exactly for the discrete system. The next steps consist in applying the force acting on the particles and the diffusion. The corresponding terms in Eq. (2) are conservation laws, which suggests using a finite-volume approximation. The time evolutions due to forcing and diffusion are performed successively. In both cases, we use classical schemes (see below), where zero-flux conditions are imposed on the boundary of \( \Omega \), and 0/3 diffusion is approximated using finite differences. These steps are illustrated by the horizontal blue and red arrows in Fig. 1.

A few comments on the convergence and stability of the proposed method. Clearly, except for specific singular forcings, all the linear differential operators involved in Eq. (2) are expected to be bounded. We can thus invoke the equivalence (or Lax–Richtmyer) theorem for linear differential equations that ensures convergence, provided the scheme is stable and consistent (see [LeVeque 2002]).

For the operator associated to particle acceleration, we use in this study either a first-order upwind finite-volume scheme or a higher-order flux limiter by following the strategy proposed by Hundsdorfer et al. (1995). The upwind scheme is first-order accurate and is well-known for being consistent and stable if it satisfies the Courant–Friedrichs–Lewy (CFL) condition. This requires that the time needed to accelerate particles by the grid size \( \Delta v \) is larger than the time step \( \Delta t \). This leads to the stability condition

\[ \text{CFL} = (\Delta t/\Delta v)_{\text{max}} |F(x,v,t)|/m_p < 1. \]  

The upwind scheme is however known to suffer from numerical diffusion, and obviously, one should only expect to recover the correct dynamics only when the numerical diffusion \( \kappa_{\text{num}} \) is much smaller than the physical one \( \kappa \). The average numerical diffusion can be estimated as \( \langle \kappa_{\text{num}} \rangle \approx \langle F \rangle \Delta t/\Delta v \). To limit the effects of this numerical diffusion, we have also used a flux-limiter scheme. While taking benefit of a higher-order approximation where the field is smooth, it uses the ratio between consecutive flux gradients to reduce the order in the presence of strong gradients only. The limiter is a nonlinear function of the phase-space density field and the stability is ensured provided that it is total-variation diminishing (TVD; see [LeVeque 2002]).

Among the various TVD limiters available on the market, we choose the scheme of [Koren 1993] with parameter 2/3.

For the term associated to diffusion, the flux at the interface between two velocity cells is computed using finite differences. The resulting finite-volume scheme is thus equivalent to compute a discrete Laplacian on the velocity mesh. The stability condition is then given by

\[ \frac{\kappa \Delta t}{\Delta v^2} < \frac{1}{2}. \]  

To summarize, the stability and convergence of the proposed method is ensured when both (3) and (4) are satisfied.

From now on we restrict ourselves to small and heavy particles whose interaction with the carrier fluid is dominated by viscous drag and diffusion. In that case, we have

\[ \frac{d v_p}{dt} = -\frac{1}{\rho_p} \langle v_p - u(x_p, t) \rangle + \sqrt{2\kappa} \eta(t), \]  

where \( \eta(t) \) is the standard \( d \)-dimensional white noise and the fluid velocity field \( u(x,t) \) is prescribed and assumed to be in a (statistically) stationary state. This Stokes drag involves the viscous particle response time \( \tau_p = 2 \rho_p a^2/(9 \rho v) \), with \( a \) the diameter of the particles, \( \rho \) the viscosity of the fluid, \( \rho_p \gg \rho \) the particle and fluid mass densities, respectively. Inertia is quantified by the Stokes number \( St = \tau_p/\tau_t \), where \( \tau_t \) is a characteristic time of the carrier flow. The diffusion results from the random collisions between the considered macroscopic particle and the molecules of the underlying gas. Assuming thermodynamic equilibrium, the diffusion coefficient reads \( \kappa = 2 k_B T/(m_p \tau_p) \), where \( k_B \) is the Boltzmann constant and \( T \) the absolute temperature. The effect of diffusion is measured by the non-dimensional number \( \mathcal{K} = \kappa \tau_t/U_t^2 \) ( \( U_t \) being a characteristic velocity of the fluid flow). Such a specific dynamics leads to appropriate estimates for the bound \( V_{\text{max}} \) in particle velocity. One can indeed easily check that when \( \kappa = 0 \), we always have \( |v_p| \leq \max_{x,p} |u(x,t)| \). In a deterministic fluid flow, as for instance when \( u \) is stationary, this gives the natural choice \( V_{\text{max}} = \max_{x,p} |u(x,t)| \). However, in most situations, the maximal fluid velocity is not known a priori. One then relies on the statistical properties of \( u \), as for instance its root-mean square value \( u_{\text{rms}} = \langle u_i^2 \rangle^{1/2} \). Usually the one-time, one-point statistics of fluctuating velocity fields (being random or turbulent) are well described by a Gaussian distribution. This ensures that by choosing \( V_{\text{max}} = 3 u_{\text{rms}} \), the probability that a particle has a velocity out of the prescribed bounds is less than 1\%.

In practice, it is known that the typical particle velocity decreases as a function of the Stokes number. It was for instance shown by [Abrahamson 1975] that \( \langle |v_p|^2 \rangle \propto u_{\text{rms}}^2/\pi St \) at very large Stokes numbers. An efficient choice for \( V_{\text{max}} \) should account for that.

In the next two sections we investigate two different cases: First a one-dimensional random Gaussian carrier flow with a prescribed correlation time and, second, a two-dimensional turbulent carrier flow that is a solution to the forced incompressible Navier-Stokes equation.
3. Application to a one-dimensional random flow

3.1. Particle dynamics for $d = 1$

In this section, we test our method in a one-dimensional situation. For that, we assume that the fluid velocity is a Gaussian random field, which consists in the superposition of two modes whose amplitudes are Ornstein–Uhlenbeck processes, namely

$$u(x, t) = A_1(t) \cos(2\pi x/L) + A_2(t) \sin(2\pi x/L)$$

$$\frac{dA_i(t)}{dt} = -\frac{1}{\tau_i} A_i(t) + \sqrt{\frac{2}{\tau_i}} \xi_i(t)$$

where the $\xi_i$ are independent white noises with correlations $\langle \xi_i(t) \xi_j(t') \rangle = \delta(t - t')$. This flow is by definition fully compressible (potential) and spatially periodic with period $L$. It is characterized by its amplitude $\langle (u(x, t))^2 \rangle = u_{rms}$ and its correlation time $\tau_i$, which are fixed parameters. We focus on the case when the Kubo number $Ku = \tau_i u_{rms}/L$ is of the order of unity.

We next consider particles suspended in this flow and following the dynamics $\Xi$. The relevant Stokes number is then defined as $St = \tau_p u_{rms}/L$ and the relative impact of diffusion is measured by $\mathcal{K} = \kappa L/u_{rms}$. When diffusion is neglected ($\mathcal{K} \rightarrow 0$), the particles distribute on a dynamical attractor (see Fig. 2 Left) whose properties depend strongly on $St$. These strange attractors are typically fractal objects in the phase space and they are characterized by their fractal dimension spectrum [Hentschel and Procaccia 1983]. The locations of particles are obtained by projecting these sets on the position space and might thus inherit the associated clustering [Bec 2003]. The dimension that is relevant for binary interactions between particles is the correlation dimension $D_2$, which relates to the probability of having two particles within a given distance, namely

$$p_2^s(r) = \mathbb{P}(|x_p^{(1)}(t) - x_p^{(2)}(t)| < r) \sim (r/L)^D_2, \text{ for } r \ll L,$$  

where $x_p^{(1)}$ and $x_p^{(2)}$ denote the positions of two different particle states. Note that as we consider $a$ to be in a statistically stationary state, $p_2^s$ is independent of time. The correlation dimension $D_2$ varies from $D_2 = 0$ for a point concentrations to $D_2 = 1$ for a homogenous mass distribution. In the example of Fig. 2 (Left) $D_2 \approx 0.7$. The variations of $D_2$ as a function of the Stokes number are displayed in the inset of Fig. 3. $D_2$ indeed varies from 0 at small Stokes numbers to values close to one. For $St = 0$, the particles concentrate on a point; their distribution is said to be atomic and $D_2 = 0$. This is a consequence of the compressibility of the one-dimensional (potential) flow. Actually this behavior persists for finite Stokes numbers, up to a critical value $St^*$, as shown by Wilkinson and Mehlhig [2003] in the case where $\tau_f \ll L/u_{rms}$ (that is $Ku \rightarrow 0$). We observe here $St^* \approx 0.6$. For $St > St^*$, the dimension increases and tends to a homogenous distribution ($D_2 = 1$) at large particle inertia.

When one has only access to the Eulerian density of particles, the distribution of distances cannot be directly inferred from (8). One then relies on the coarse-grained density of particles $\rho_c(x, t) = \int_{r^2/2} dx' \int dv f(x + x', v, t)$. (9)

It is known that, under some assumptions on the ergodicity of the particle dynamics, the second-order moment of this quantity scales as $\langle r^2 \rangle \propto r^{D_2-1}$ (see, e.g., [Hentschel and Procaccia 1983]. In one dimension, this second-order moment is exactly the same as the radial distribution function. This quantity will be used in the next sections to address the physical relevance of the lattice-particle method. It is of particular interest when considering collisions between particles. Indeed, as explained for instance by Sundaram and Collins [1997], the ghost-collision approximation leads to write the collision rate between particles as the product of two contributions: one coming from clustering and entailed in the radial distribution function, and another related to the typical velocity differences between particles at a given distance. This second quantity relates to the particle velocity (first-order) structure function

$$S_1(r) = \left\langle \frac{(\mathbb{E}^{(1)} - v^{(2)}_p)(x_p^{(1)} - x_p^{(2)})}{r} \right\rangle = r \int_{-r/2}^{r/2} dx' \int dv f(x + x', v, t).$$

This is the average of the amplitude of the velocity difference between two particles that are at a given distance $r$. As the probability of distances, this quantity behaves as a power law $S_1(r) \sim r^{D_2-1}$ for $r \ll L$ (see, e.g., [Bec et al. 2005]. The exponent $\xi_1$, shown in the inset of Fig. 3 decreases from 1 at $St = 0$, corresponding to a differentiable particle velocity field, to 0 when $St \rightarrow \infty$, which indicates that particle velocity differences become uncorrelated with their distances. Again, when working with the phase-space density one cannot use (10) but relies on

$$S_1(r) = \left\langle \frac{\int dv \int dv' f(x, v) f(x + r, v') |v - v'|}{\int dv \int dv' f(x, v) f(x + r, v')} \right\rangle.$$  

As the second-order moment of the coarse-grained density, this quantity will also be used as a physical observable for benchmarking the method.

In the above discussion, we have neglected the effects of diffusion. It is for instance expected to alter clustering properties by blurring the particle distribution at small scales. This is illustrated in Fig. 3 where one can compare the instantaneous phase-space particle positions in the absence of diffusion (Left) and when it is present (Right) at the same time and for the same realization of the fluid velocity. At large scales, identical patterns are present, but diffusion acts at small scale and smoothes out the fine fractal structure of the distribution. One can easily estimate the scales at which this crossover occurs. Diffusion is
responsible for balancing Stokes drag and diffusion in the particle dynamics, namely \( \nu^2/\tau_p \approx \kappa \), so that \( \nu_2 \sim \tau_p^{3/2} \kappa^{1/2} \). This dispersion in velocity is responsible for a dispersion in positions on scales of the order of \( \ell_d = \tau_p \nu_2 \sim \tau_p^{3/2} \kappa^{1/2} = St^{1/2} K^{1/2} L \). Hence, when diffusion is small enough and \( \ell_d \ll L \), the spatial distribution of particles is unchanged by diffusion at length scales \( r \gg \ell_d \), and the probability that two particles are at a distance less than \( r \) behaves as \( p_2^\tau(r) \sim (r/L)^D \). For \( r \ll \ell_d \), diffusion becomes dominant, the particles distribute in a homogeneous manner and \( p_2^\tau(r) \propto r^d \), with \( d = 1 \) being the space dimension. By continuity at \( r = \ell_d \), we get \( p_2^\tau(r) \sim (\ell_d/L)^D(r/\ell_d) \) at small scales.

![Figure 3: Cumulative probability \( p_2^\tau(r) \) of inter-particle distances for various diffusivities]  

This picture is confirmed numerically as shown in Fig. 3 which represents the scale-behavior of \( p_2^\tau(r) \) for a fixed Stokes number and various values of the diffusivity \( \kappa \). One clearly observes the homogenous distribution \( \propto r^d \) at small scales and the fractal scaling \( \propto r^D \) in an intermediate range. The predicted transition between the two behaviors is indicated by the vertical lines at the diffusive scale \( \ell_d \). A homogeneous distribution is recovered for \( r \sim \ell_d \).

Velocity statistics are also altered by the presence of diffusion. The structure function \( S_r \) is expected to behave as \( r^4 \) for \( \ell_d \ll r \ll L \) and to saturate to a constant value when \( r \ll \ell_d \). By continuity, the value of this plateau should be \( \sim \ell_d^4 \sim K^{1/2} \). Note finally that the slow convergence \( \ell_d/L \propto \sqrt{K} \) as \( K \to 0 \) implies that very small values of the diffusion are needed in order to clearly recover the statistics of diffusive-less particles as an intermediate asymptotics.

3.2. Lattice-particle simulations

We now turn to the application of the lattice-particle method described in Sec. 2 to this one-dimensional situation. We compare the results to Lagrangian simulations where we track the time evolution of \( N_p \) particles randomly seeded in space with zero initial velocity. We choose and normalize the initial phase-space density \( f(x,v,0) \) to match the Lagrangian settings. The distribution is uniform over the cells, concentrated on a vanishing velocity and the total mass is such that \( \sum_{i=1} f(x_i,v_i,0) \Delta x \Delta v = N_p \). In all simulations, the maximum velocity is set to \( v_{max} = u_{rms} = 1 \) and we have chosen \( L = 2\pi \) and \( \tau_L = 1 \). In these units, the time step is kept fixed at \( \Delta t = \Delta x/\Delta v = 2^{1/2} \pi \approx 0.05 \). The number of discrete velocities is of the form \( 2^n + 1 \) and is varied between \( N_v = 3 \) to 129. The number of spatial collocation points is then given by \( 2^{n+6} \) and thus varies between \( N_c = 128 \) to 8192. Note that, because of the CFL condition, this choice restricts the number of discrete velocities that can be used to \( N_v < 1 + 128 St \).

![Figure 4: Position-velocity phase-space positions of Lagrangian particles (black dots) on the top of the field obtained by the lattice-particle method (colored background). The diffusivity is here \( \kappa = 10^{-3} (K = 6.28 \times 10^{-3}) \) and \( St = 2 \).]  

Figure 4 represents simultaneously the phase-space distribution of Lagrangian particles and the numerical approximation obtained by the particle-lattice method for \( N_v = 129 \). Clearly, one observes that the model fairly reproduces the distribution of particles, including the depleted zones, as well as the more concentrated regions. Furthermore, the method is able to catch multivalued particle velocities. We have for instance up to three branches in \( v \) for \( x \approx \pi/2 \). It is important to emphasize that numerical diffusion is of course present, and that it has to be smaller than the physical diffusion \( \kappa \) in order for the model to be consistent with the Lagrangian dynamics.

To get a more quantitative insight on the convergence of the method, we next compare the coarse-grained densities obtained from the Lagrangian simulation and the lattice-particle approximation of the phase-space density. The first, denoted \( \rho^E \), is computed by counting the number of particles contained in the different boxes of a tiling of size \( r \). The second is written as \( \rho^E \) and is obtained by summing over velocities and coarse-graining over a scale \( r \) the phase-space density obtained numerically. To confirm the convergence of the method, we measure for a fixed \( r \) the behavior of the \( L_2 \)-norm of the difference between \( \rho^E \) and \( \rho^E \), namely

\[
\| \rho^E - \rho^E \| = \left( \rho^E(x,t) - \rho^E(x,t) \right)^{1/2},
\]
where the angular brackets $\langle \cdot \rangle$ encompass a spatial and a time average. Figure 5 shows the behavior of the relative $L_2$-error as a function of the number of velocity gridpoints $N_v$, for various values of the Stokes number, as labeled. One observes that the error decreases when the resolution increases, giving strong evidence of the convergence of the method. The error is found proportional to the velocity grid spacing $\Delta v$, indicating that the method is first order. The constant is a decreasing function of the Stokes number. This indicates that the method is more accurate for particles with strong inertia. The reason for this trend will be addressed in the sequel.

To assess the ability of the proposed method to reproduce physically relevant quantities, we now compare statistics obtained using the lattice method with those using a Lagrangian approach. We focus on the clustering and velocity difference properties that were introduced and discussed in Section 3.1.

Figure 6 shows for given values of the Stokes number and of the diffusivity, the second-order moment of the coarse-grained density $\langle \rho^2 \rangle$, as a function of $r$ for $St = 1.9$, $K = 10^{-2}$, and various lattice velocity resolutions $N_v$, as labeled.

Figure 5: Relative $L_2$-error of the lattice-particle method for evaluating the coarse-grained density $\rho_L$, on a scale $r = L/128$, as a function of the number of velocity gridpoints $N_v$ and for various values of the Stokes number, as labeled.

Figure 6: Convergence of the second-order moment of the coarse-grained density $\langle \rho^2 \rangle$, which is shown as a function of $r$ for $St = 1.9$, $K = 10^{-2}$, and various lattice velocity resolutions $N_v$, as labeled.

Figure 7: Three snapshots of the Lagrangian particles (black dots, for $K = 0$) and of the lattice-particle Eulerian solution (colored background) in the $(x, v)$ plane for different times: At $t < \tau_4$ (Left) the solution is well approximated at large scales; At $t = \tau_4$ (Center) an order-unity fraction of the mass is concentrated on a scale less than $\ell_4$. At $t > \tau_4$ (Right), the Eulerian and Lagrangian solutions diverge exponentially fast with differences appearing at the largest scales.

Clustering event followed by the divergence of the solutions, is shown in Fig. 7. Starting from a correctly reproduced distribution, the major part of non-diffusive Lagrangian particles concentrate into a subgrid region while the Eulerian approximation is stacked at scales of the order of $\ell_4$. At a later time, the two distributions diverge and the diffusive particles fill faster larger scales. The probability with which one encounters such a configuration strongly depends on the Stokes number and on the spatial dimension. In the one-dimensional case, such events are rather frequent but become sparser when the Stokes number increases. This is essentially due to the compressibility of the carrier flow. For incompressible fluids in higher dimensions, we expect a negligible contribution from these events.

To close this section on one-dimensional benchmarks of the lattice-particle method, we report some results on velocity difference statistics. For that, we have measured the first-order structure function $S_1(r)$ of the particle velocity, using (10) in the Lagrangian case and (11) for solutions obtained with the lattice-particle method. Figure 8 shows the relative error of $S_1(r)$ for of gridpoints $N_v$ becomes larger (i.e. when $\Delta v \to 0$). At sufficiently high velocity resolutions, the method is able to capture the large-scale velocity properties of the concentration of the particles. The second-order moment of density then saturates to a value lower than that expected from Lagrangian measurements. The situation is very different at very low resolutions where the data obtained from the lattice-particle method deviates much, even at large scales. This corresponds to the case when the numerical diffusion in velocity is larger than the physical diffusion.

These strong deviations stem from a non-trivial effect of diffusion that lead to finite-scale divergences of the solutions associated to different values of $K$. In the absence of diffusion, there is a finite probability that an order-one fraction of mass gets concentrated on an arbitrary small subdomain of the position-velocity phase space. This corresponds to a violent fluctuation where the local dimension approaches zero. At the time when this occurs, the mass distribution associated to a finite value of the diffusion will get stacked at a scale $\ell_d$. Because of the chaotic nature of the particle dynamics, the two mass distributions, with and without diffusion will experience very different evolutions and diverge exponentially fast. Such a strong
fixed values of the separation $r$, the Stokes number, and the diffusivity, as a function of the velocity resolution. Clearly, when the number of gridpoints $N_v$ increases, the error decreases, following a law approximatively proportional to the grid spacing $\Delta v$. The inset shows the same quantity but, this time, for a fixed resolution ($N_v = 33$) and as a function of the Stokes number. One clearly observes a trend for this error to decrease with $St$. There are two explanations for this behavior. First, as seen above, there are strong clustering events leading to differences between the Lagrangian and lattice solutions that can persist for a finite time. When the Stokes number increases, such events become less probable. The second explanation relies on the fact that particles with a larger Stokes number experience weaker velocity fluctuations. This implies that for a fixed value of $V_{\text{max}}$, the particle velocity is more likely to be fully resolved at large values of $St$. As seen in the inset of Fig. 8 the downturn of the error is compatible with a behavior $\propto St^{-1/2}$. It might thus be proportional to the expected value of the root-mean-squared particle velocity when $St \gg 1$ (Abrahamson [1975]), favoring the second explanation. We will turn back in Sec. 4.2 for the two-dimensional case on the effect of the maximal resolved velocity $V_{\text{max}}$ onto the convergence of the lattice-particle method.

4. Application to incompressible two-dimensional flows

We extend in this section the lattice-particle method to two-dimensional flows. For the particle acceleration, we again make use of a flux-limiter scheme.

4.1. Cellular flow

We first consider a fluid flow that is a stationary solution to the incompressible Euler equations (and to the forced Navier–Stokes equations). It consists of a cellular flow field, a model that have often been used to investigate mixing properties, as well as the settling of heavy inertial particles (see, e.g., Bergougnoux et al. [2014] Maxey and Corrsin [1986]). The velocity field is the orthogonal gradient of the $L$-periodic bimodal stream function $\psi(x, y) = U \sin(\pi(x + y)/L) \sin(\pi(x - y)/L)$ (the typical velocity strength is here denoted by $U$). The cellular flow has been here tilted by an angle $\pi/4$ in order to avoid any alignment of the separatrices between cells with the lattice that leads to spurious anisotropic effects.

Figure 9 shows two snapshots for two different values of $St = \tau_p U/L$ of the stationary particle distribution (black dots), together with the density field evolved by the lattice-particle dynamics. For the smallest Stokes number (Left panel), one observes that the particle distribution is concentrated along the separatrices between the different cells. One also observes that it develops entangled structures in the vicinity of the hyperbolic stagnation points of the flow. These loops, which are aligned with the stable direction, corresponds to oscillations in the particle dynamics that occurs when their inertia makes them cross the unstable manifold with a too large velocity. At larger $St$, the particle distribution is somewhat broader but is this time centered on specific trajectories that do not perform the aforementioned oscillation but rather cross ballistically the heteroclinic separatrices. These results show that the lattice-particle method is able to reproduce the complex dynamics of particles in a two-dimensional steady flow. The fine structures of the spatial distribution are fairly reproduced, as long as the numerical diffusion surpasses numerical errors.

4.2. Heavy particles in 2D turbulence

We next turn to the study of the model in non-stationary fluid flows that are solutions to the forced two-dimensional incompressible Navier–Stokes equations

$$\partial_t u + u \cdot \nabla u = -\nabla p + \nu \nabla^2 u - \alpha u + f, \quad \nabla \cdot u = 0. \quad (13)$$

The linear damping term involving the coefficient $\alpha$ originates from Ekman friction (in geophysical flows), Rayleigh friction (in stratified fluids) or the friction induced by the surrounding air in soap-film experiment. The flow is maintained in a statistical steady state by the forcing $f$ that is assumed to be concentrated over a specific scale $\ell_f$. The fluid velocity field $u$ is computed numerically using a pseudo-spectral, fully de-aliased GPU solver for the vorticity-streamfunction formulation of the Navier-Stokes equation [13].
The two-dimensional Navier-Stokes equation is known to develop two cascades (see, e.g., Boffetta and Ecke, 2012). Kinetic energy undergoes an inverse cascade with a rate $\varepsilon$ toward the large scales $\ell \gg \ell_\Omega$ where it is dissipated by the linear damping. The enstrophy $\langle \omega^2 \rangle$ (where $\omega = \partial_x u_y - \partial_y u_x$ designates the vorticity) experiences a direct cascade to the small scales $\ell \ll \ell_\Omega$ with a rate $\eta$ and is then dissipated by molecular viscosity. These different cascades are associated to different behaviors of the velocity power spectrum. For $k \ll k_\ell \ll k_\Omega$, the inverse energy cascade promotes a $k^{-5/3}$ Kolmogorov law, as in the three-dimensional direct cascade. At small scales, i.e. for $k \gg k_\ell$ in the direct enstrophy cascade, the flow is characterized by long-living vortices and the spectrum follows a $k^{-3}$ Batchelor–Kraichnan law with a logarithmic correction.

Dimensional analysis predicts that the direct enstrophy cascade is associated to a unique timescale $\tau_\Omega = \eta^{-1/3}$. Investigating heavy particle dynamics at the small scales of two-dimensional turbulence thus requires comparing their response time to $\tau_\Omega$. The relevant parameter is then the Stokes number defined as $St = \tau_p/\tau_\Omega$. For $St \ll 1$, particles almost follow the flow and tend to distribute homogeneously in space. When $St \gg 1$, they completely detach from the fluid and experience a ballistic motion leading again to a space-filling distribution. Non-trivial clustering effects occur when the Stokes number is order one. This is illustrated in Fig. 10 which shows a snapshot of the particle distribution in the position space on top of the turbulent vorticity field in the direct enstrophy cascade. Due to their inertia, particles are ejected from vortices and concentrate in high-strain regions. There, the combination of stretching, folding and dissipation induced by their dynamics makes them converge to a dynamical attractor with fractal properties. Such a behavior is quantitatively measured by the correlation dimension $D_2$ defined in Eq. (8). The evaluation of $D_2$ as a function of $St$ resulting from Lagrangian simulations is presented in Fig. 11. At $St = 0$, unlike in the one-dimensional case where the dimension of the attractor is 0, particles follow the streamlines of the incompressible two-dimensional flow, fill the position space, and hence $D_2 = 2$. Clustering then increases with inertia to attain a minimum at $St \approx 0.2$. It then decreases again as the velocity of particles separate from that of the fluid and disperse in the velocity space, leading to a space-filling distribution $D_2 = 2$ when $St \to \infty$.

The velocity distribution of particles is itself having a behavior that is very similar to the one-dimensional case. This is clear from Fig. 11 where the scaling exponent $\zeta_1$ of its first-order structure function (see Eq. (10)) is represented as a function of the Stokes number. For $St \ll 1$, the particles are as if advected by a smooth velocity field and $\zeta_1 \approx 1$. When $St \gtrsim 1$, particles with very different velocities can come arbitrarily close to each other and $\zeta_1 \to 0$.

Particle properties in the inverse energy cascade are more difficult to characterize because of the scale-invariance of the velocity field. In particular, neither the moments of the coarse-grained density nor the particle velocity structure functions display any scaling behavior. What has been nevertheless observed numerically by Boffetta et al. (2004) is that the particle spatial distribution is dominated by the presence of voids whose sizes obey a universal scaling law. Chen et al. (2006) argued that such voids are related to the excited regions of the flow and that particles tend to follow the calm regions where the zeros of the fluid acceleration are more probable.

In the sequel we apply the lattice method to both the direct and the inverse two-dimensional cascades. Resolving both cascades in the same simulation would require a tremendous scale separation and thus number of gridpoints (see Boffetta and Musacchio, 2010). For that reason we consider the two cases separately.

4.2.1. Direct enstrophy cascade

The fluid flow is integrated by a pseudo-spectral method on a uniform square spatial grid using a stream-function formu-
lution of the Navier-Stokes equation $E$. To maintain a de-
veloped turbulent state, a stochastic forcing is applied in the
wavenumber shell $1 \leq |k| < 4$ of Fourier space while the kinetic
energy accumulating at large scales is removed by a linear fric-
tion. The particle dynamics is simulated using a spatial lattice
with the same resolution as the fluid and with various numbers $N_v^2$ of discrete velocities. The acceleration step is done via a
flux limiter scheme as described in Sec. 2. Results are com-
pared to particle trajectories obtained from Lagrangian simula-
tions. Figure 12 shows the instantaneous particle distributions
obtained from the two approaches. The qualitative agreement is
excellent, reproducing correctly depleted zone as well as more
concentrated regions.

To get more quantitative informations on the relevance of
the method, we have performed a set of simulations with a
$512^2$ resolution and in which both the number of discrete ve-
locities $N_v^2$ and the maximum velocity $V_{\text{max}}$ are varied. Fig-
ure 13 shows measurements of the second-order moment of the
coarse-grained density $\rho_v$ obtained by integrating the phase-
space density $f(x, v, t)$ with respect to velocities and over space
in boxes of length $r$. This is the two-dimensional version of
Fig. 6 and the statistics of $\langle \rho_v^2 \rangle$ have a very similar behavior as
in the one-dimensional case. Here $St = 0.5$, $V_{\text{max}} = 3.9 \, \text{u}_{\text{rms}}$, and $N_v$ is varied from 9 to 21. One clearly observes that the
statistics obtained from the lattice method converges to that ob-
tained from Lagrangian simulations.

The interplay between the choices of $N_v$ and of $V_{\text{max}}$ requires
some further comments. On the one hand the method converges
when both $\Delta v = 2 \, V_{\text{max}}/N_v \to 0$ and $V_{\text{max}} \to \infty$. On the other
hand, the computational cost is $\propto N_v^2$. One can thus wonder if
for a fixed cost there is an optimal choice of $V_{\text{max}}$ that minimizes
the error obtained with the lattice method. Focusing again on
the second-order statistics of the particle mass distribution, we
have measured the average with respect to $r$ of the error made
on the density moment $\langle \rho_v^2 \rangle$ defined as

$$E(N_v, V_{\text{max}}) = \langle (\rho_v^2) \rangle - \langle (\rho_v^2) \rangle / \langle (\rho_v^2) \rangle,$$  \hspace{1cm} (14)

where

$$\overline{f(r)} = \frac{1}{L^2} \int_0^L \overline{|f(r)|} \, r \, dr.$$  \hspace{1cm} (15)

Figure 14 (top) represents this quantity as a function of $V_{\text{max}}$ for
different values of the cost $N_v^2$. One clearly observes that
there is indeed for a fixed $N_v$ a specific choice of $V_{\text{max}}$ where
the error is minimal. The optimal value of the maximal velocity
increases with $N_v$. On the right of the minimum, the error is in
principle dominated by a $\Delta v$ too large. This is confirmed by
the collapse of the various curves on the right of their minima
that can be seen in the bottom of Fig. 14 where $E$ is represented as a

![Figure 12: Snapshot of the position of Lagrangian particles (black dots), to-
going with the density field obtained from the lattice method (colored back-
ground, from white: low densities to red: high densities) for
1024² and lattice simulations were performed with 1024² spatial gridpoints
associated to $1^2$ discrete velocities.](image)

![Figure 13: Second-order moment of the coarse-grained density $\rho_v$ as a function
of $r$ for $St = 0.5$ and $K' = 1.0$ for $10^{-1}$ in the direct cascade, both from Lagrangian
measurement (black line) and the lattice method with different $N_v$, as labeled.](image)

![Figure 14: Distance-averaged error $E$ of the second-moment of the mass density
as defined in (14) as a function of the maximal velocity $V_{\text{max}}$ (top) and of the
velocity grid spacing $\Delta v = 2 \, V_{\text{max}}/(N_v - 1)$ (bottom) for various values of the
velocity resolution $N_v^2$ and for $St = 0.5$.](image)
function of $\Delta v$. In the left of the minimum, the error should be
dominated by a too small value of $V_{\text{max}}$. One can indeed guess
an asymptotic collapse for $V_{\text{max}} \propto u_{\text{rms}}$ on the upper panel of
Fig. [14] or equivalently, the fact that the curves separate from
each other at small values of $\Delta v$ in the lower panel.

The value of the error at the optimal $V_{\text{max}}$ decreases from $N_r = 9$ to $N_r = 13$ but then seems to saturate (or to decrease
only very slowly) at higher values of $N_r$. One cannot exclude
that this behavior corresponds to a logarithmic convergence of $E$
when $N_r \to \infty$. This slow dependence is also visible in the
bottom panel where the collapse of the various curves seems to
extend weakly on the left-hand side of the minima for $N_r = 13,
17$ and $21$. Accordingly, a small difference in $N_r$ is not
evertheless observed at small scales. We obtained

4.2.2. Inverse energy cascade

To complete this study we have also tested the proposed lat-
tice method in a two-dimensional turbulent flow in the inverse
kinetic energy cascade regime. The stochastic forcing is now
acting at small scales ($400 \lesssim |k| \lesssim 405$) and we made use of
hyper-viscosity (here eighth power of the Laplacian) in order to
truncate the direct enstrophy cascade. The kinetic energy accu-
ulated at large scales is again removed using a linear friction
in the Navier–Stokes equation (13).

The particle Stokes number is now defined as $St = \tau_p/L$
using the large-eddy turnover time $\tau_L = L/u_{\text{rms}}$. Since small-scale statistics are dominated by
forcing and are thus irrelevant. The flow is integrated with a
resolution of $2048^2$ gridpoints while the lattice-particle method
is applied for $St \approx 0.1$ on a coarser grid with $512^2$ points.

Figure 15 shows that the lattice-particle method is able to
reproduce the main qualitative features of the particle spatial
distribution at scales within the inertial range of the inverse en-
ergy cascade. This is confirmed in Fig. [15] which represents the
relative error $E$ defined in Eq. (14) of the second-order moment
$\langle \rho_r^2 \rangle$ of the density $\rho_r$, coarse-grained over a scale $r$. The
Lagrangian integration was performed with $2 \times 10^4$ particles (with
no physical diffusion) and the lattice method on a 512$^2$ spatial
grid with $N_r^2 = 9^2$ discrete values of the particle velocity. One
clearly observes that the error decreases at the largest scales of
the flow.

Figure 15: Snapshot of the position of Lagrangian particles (black dots), to-
gether with the density field obtained from the lattice method (colored back-
ground, from white: low densities to red: high densities) for $St = 0.1$ in the
inverse energy cascade. The fluid flow was integrated using a resolution of $2048^2$
and lattice simulations were performed with $512^2$ spatial gridpoints associated to $9^2$ discrete velocities.

5. Conclusions

We have presented a new Eulerian numerical method to
model the dynamics of inertial particles suspended in unsteady
flow. This lattice-particle method is based on the discretization
in the position-velocity phase space of the evolution equation
for the particle distribution. The spatial grid is chosen such
that particles with a given discrete velocity hop by an integer
number of gridpoints during one time step, an idea close to that
used in lattice-Boltzmann schemes. We have shown that the
model reproduces the correct dynamical and statistical proper-
ties of the particles, even with a reasonably small amount of ve-
locity gridpoints. Some deviations from Lagrangian measure-
ments are nevertheless observed at small scales. We obtained
evidence that they are due to numerical diffusivity acting in the
space of velocities. The proposed method is anyway intended to
describe large scales where such deviations disappear. It might
hence be a suitable candidate for developing large-eddy mod-
els for particle dynamics. Indeed, as equation (2) is linear in $f$, some techniques of subgrid modeling used in scalar turbulent
transport (see, for example, Girimaji and Zhou, 1996) could be
adapted.

Our approach consists in always imposing the same mesh
for particle velocities, independently of the spatial position and
of the local value of the fluid velocity. This is well-adapted
for particles with a large Stokes number. Their velocity ex-
periences small fluctuations and is generally poorly connected
to that of the fluid. In addition, the method is accurate at the largest scales and can hence catch the structures appearing in the spatial and velocity distributions of large-Stokes-number particles. Such considerations indicate that the proposed lattice-particle method is suitable for modeling particles with a sufficiently strong inertia. Conversely, particles with a weak inertia develop fine-scale structures in their distribution. They result from tiny departures of their velocity from that of the fluid. Our method, applied with a fixed velocity resolution, might not be able to catch such deviations. However, a more suitable idea for this case is to use a variation of our approach where, instead of a full resolution of the particle velocity, one considers its difference with that of the fluid. This would of course require changing scheme for integrating advection.

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