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Monte Carlo Studies of Effective Diffusivities for Inertial Particles

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Summary. The transport of inertial particles in incompressible flows and subject to molecular diffusion is studied through direct numerical simulations. It was shown in recent work [9,15] that the long time behavior of inertial particles, with motion governed by Stokes' law in a periodic velocity field and in the presence of molecular diffusion, is diffusive. The effective diffusivity is defined through the solution of a degenerate elliptic partial differential equation. In this paper we study the dependence of the effective diffusivity on the non–dimensional parameters of the problem, as well as on the streamline topology, for a class of two dimensional periodic incompressible flows.

1 Introduction

Inertial particles play an important role in various applications such as atmosphere science [6,16] and engineering [5,8]. The presence of inertia leads to many exciting phenomena and in particular to the fact that the distribution of particles in turbulent flows is homogeneous, i.e. particles tend to cluster [1,2,17,18]. Whilst the problem of passive tracers, where inertia is neglected, has attracted the attention of many scientists over the last decades, cf. [7,11], the number of theoretical investigations concerning inertial particles is still rather small.

The purpose of this paper is to study the long time behavior of particles which move in steady, periodic two–dimensional incompressible velocity fields and are subject to molecular diffusion, using Monte Carlo simulations. The particle motion is governed by Stokes's law

$$\tau \ddot{x} = v(x) - \dot{x} + \sigma \dot{\beta}. \tag{1}$$

Here $\tau > 0$ is the Stokes' number, which can be thought of as the non–dimensional particle relaxation time. The field $v(x)$ is the (given) fluid velocity, $\sigma > 0$ is the molecular diffusivity and $\dot{\beta}$ stands for white noise, i.e. a mean zero Gaussian process with covariance

$$\langle \dot{\beta}_i(t)\dot{\beta}_j(s)\rangle = \delta_{ij}\delta(t-s),$$

where $\langle\cdot\rangle$ stands for ensemble average. It was shown in recent work [9,15] that, for periodic velocity fields $v(x)$, the long time behavior of inertial particles which move according to (1) is governed by an effective Brownian motion. To be more precise, let

$$x^\epsilon(t) := \epsilon x\left(\frac{t}{\epsilon^2}\right). \tag{2}$$

The process $x^\epsilon(t)$ satisfies the rescaled equation

$$\tau\epsilon^2\ddot{x} = \frac{1}{\epsilon}v\left(\frac{x}{\epsilon}\right) - \dot{x} + \sigma\dot{\beta}. \tag{3}$$

The results of [9,15], see Theorem 1 in Sect. 2, imply that $x^\epsilon(t)$ converges, as ϵ tends to 0, to a Brownian motion with covariance $\mathcal{K}$, the *effective diffusivity*.

Now, the effective diffusivity is defined in terms of the solution of a degenerate Poisson equation, see equations (8) and (9) below. It is expected that $\mathcal{K}$ depends on the parameters of the problem τ and σ in a complicated, highly non linear way. Moreover, the diffusivity is also expected to depend non–trivially on the topology of the streamlines of $v(x)$, as happens for passive tracers [11]. Our goal is to gain some insight into such dependencies by means of direct numerical simulations for a class of two dimensional flows.

Similar problems have been investigated within the context of massless tracer particles which move according to equation (1) with $\tau = 0$:

$$\dot{x} = v(x) + \sigma\dot{\beta}. \tag{4}$$

It has been known for a long time [3] that the long time behavior of passive tracers moving in periodic flows is diffusive, with an effective diffusivity $\mathcal{K}_0$ which can be computed in terms of a Poisson equation with periodic boundary conditions, the cell problem. It is a well documented fact that the functional dependence of the effective diffusivity on the molecular diffusivity depends crucially on the streamline topology. For example, in the case of cellular flows–i.e. flows with closed streamlines–both diagonal components of $\mathcal{K}_0$ scale linearly with σ:

$$\mathcal{K}_0 \sim \sigma, \quad \sigma \ll 1\,.$$

On the contrary, for shear flows the component of $\mathcal{K}_0$ along the direction of the shear is inversely proportional to the square of σ [19]:

$$\mathcal{K}_0 \sim \frac{1}{\sigma^2}, \quad \sigma \ll 1\,.$$

In [12] lower and upper bounds on the dependence of $\mathcal{K}_0$ for $\sigma \ll 1$ were derived and the concepts of maximally and minimally enhanced diffusion were introduced. Recall that for pure molecular diffusion (i.e. Brownian motion) the diffusion coefficient is $\mathcal{K}_0 = \frac{\sigma^2}{2}$.

The problem of studying the properties of the effective diffusivity becomes even more involved in the case of the inertial particles for two reasons. First, there are two non–dimensional parameters to consider, the Stokes number τ, together with the molecular diffusivity σ. Second, the Poisson equation that we need to solve in order to compute $\mathcal{K}$, equation (9) below, is degenerate and is posed on $2\pi\mathbb{T}^d \times \mathbb{R}^d$, where $\mathbb{T}^d$ denotes the d–dimensional unit torus; this renders analytical investigations on the dependence of $\mathcal{K}$ on τ and σ very difficult. Furthermore, the direct numerical solution of the cell problems is a non–trivial issue and hence Monte Carlo methods are natural.

In order to gain some insight into this difficult and interesting problem we resort to direct numerical simulations of (1) for a two–dimensional one–parameter velocity field, the Childress–Soward flow [4]

$$v_{CS}(x) = \nabla^{\perp}\psi_{CS}(x), \quad \psi_{CS}(x) = \sin(x_1)\sin(x_2) + \delta\cos(x_1)\cos(x_2). \tag{5}$$

Here $\delta \in [0, 1]$. This family of flows is useful for numerical experiments because as, δ ranges from 0 to 1, the flow ranges from pure cellular to pure shear. In Figs. 1a, 1b and 1c we present the contour plots of the Childress–Soward stream function $\psi_{CS}(x)$ for $\delta = 0.0$, $\delta = 0.5$ and $\delta = 1.0$, respectively.

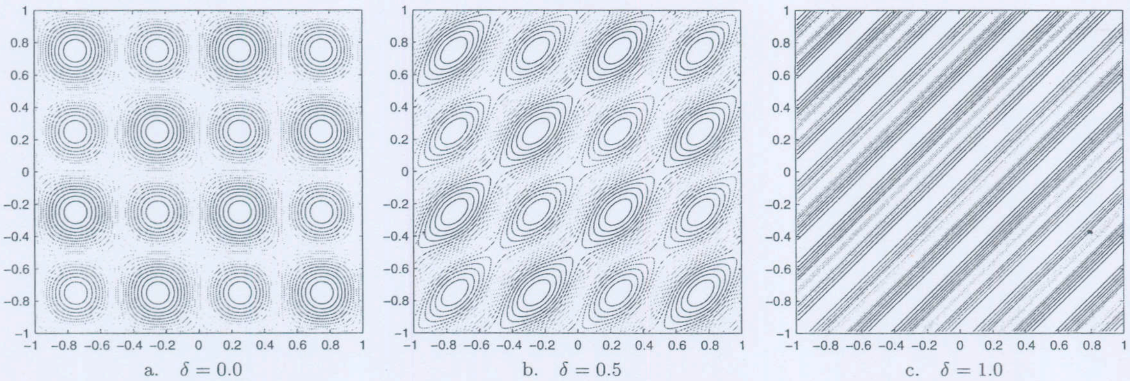


Fig. 1. Contour plot of $\psi_{CS}(x)$ for $\delta = 0.0$, $\delta = 0.5$ and $\delta = 1.0$.

The numerical results reported in this paper indicate that the presence of inertia can lead to a tremendous enhancement in the effective diffusivity, beyond the enhancement in the absence of inertia, for certain values of the parameters of the problem. However, it is shown that the effective diffusivity depends very sensitively on the streamline topology. In particular, for shear flows the presence of inertia seems to have a negligible effect on the effective diffusivity.

The rest of the paper is organized as follows: in Sect. 2 we review the results on periodic homogenization for inertial particles that were obtained in [9, 15].

In Sect. 3 we present the results obtained through Monte Carlo simulations concerning the dependence of $\mathcal{K}$ on τ, σ and δ for the Childress–Soward flow. Section 4 is reserved for conclusions.

2 Periodic Homogenization for Inertial Particles

We consider the motion of inertial particles moving in incompressible velocity fields $v(x)$ subject to molecular diffusion. Under the assumption that the density of the particles ρ_p is much greater than the density of the surrounding fluid ρ_f, $\frac{\rho_f}{\rho_d} \ll 1$, this gives rise to equation (1) [14]. Generalizations of equation (1) which are valid for the case $\frac{\rho_f}{\rho_d} \sim 1$ can also be treated by augmenting $v(x)$ to include added mass effects. We refer to [14] for the model and to [15, sec. 4.7] for details of the homogenization result in this case.

Upon introducing the particle velocity $y = \sqrt{\tau}\dot{x}$, as well as the auxiliary variable $z = x/\epsilon$, we can rewrite the rescaled equation (3) as a first order system:

$$\begin{aligned} \dot{x} &= \frac{1}{\sqrt{\tau}\epsilon} y \,, \\ \dot{y} &= \frac{1}{\sqrt{\tau}\epsilon^2} v(z) - \frac{1}{\tau\epsilon^2} y + \frac{\sigma}{\sqrt{\tau}\epsilon} \dot{\beta} \,, \\ \dot{z} &= \frac{1}{\sqrt{\tau}\epsilon^2} y, \end{aligned} \tag{6}$$

with the understanding that $z \in 2\pi\mathbb{T}^d$ and $x, y \in \mathbb{R}^d$. The "fast" process $\{z, y\} \in 2\pi\mathbb{T}^d \times \mathbb{R}^d$ is Markovian with generator

$$\mathcal{L} = \frac{1}{\sqrt{\tau}} \left(y \cdot \nabla_z + v(z) \cdot \nabla_y \right) + \frac{1}{\tau} \left(-y \cdot \nabla_y + \frac{\sigma^2}{2} \Delta_y \right) .$$

It is proved in [15], using the results of [13], that the process $\{z,\, y\}$ is ergodic and that the unique invariant measure possesses a smooth density $\rho(y, z)$ with respect to Lebesgue measure. This density satisfies the stationary Fokker–Planck equation

$$\mathcal{L}^* \rho = 0 \,,$$

where $\mathcal{L}^*$ is the adjoint of the generator of the process:

$$\mathcal{L}^* = \frac{1}{\sqrt{\tau}} \left(-y \cdot \nabla_z - v(z) \cdot \nabla_y \right) + \frac{1}{\tau} \left(\nabla_y (y\,) + \frac{\sigma^2}{2} \Delta_y \right) .$$

The main result of [9,15] is that, provided that the fluid velocity is smooth and centered with respect to the invariant measure $\rho(y, z)$, the long time behavior of the inertial particles is diffusive, with an effective diffusivity which can be computed through the solution of a degenerate Poissson equation. More precisely we have the following theorem.

Theorem 1. *Let $x^\epsilon(t)$, defined in (2), be the solution of the rescaled equation (3), in which the velocity field $v(z) \in C^\infty(2\pi\mathbb{T}^d)$ satisfies*

$$\int_{2\pi\mathbb{T}^d}\int_{\mathbb{R}^d} v(z)\,\rho(y,z)\,dzdy = 0. \tag{7}$$

Then the process $x^\epsilon(t)$ converges weakly, as $\epsilon \to 0$, to a Brownian motion on $\mathbb{R}^d$ with covariance $\frac{1}{2}\mathcal{K}$. Here

$$\mathcal{K} = \frac{1}{\sqrt{\tau}}\int_{2\pi\mathbb{T}^d}\int_{\mathbb{R}^d} y \otimes \Phi(y,z)\rho(y,x)\,dydz \tag{8}$$

and the function $\Phi(y,z)$ is the solution of the Poisson equation

$$-\mathcal{L}\Phi(y,z) = \frac{1}{\sqrt{\tau}}y. \tag{9}$$

The notation $\otimes$ denotes the tensor product between two vectors in $\mathbb{R}^d$. We will sometimes refer to $\mathcal{K}$ as the *inertial effective diffusivity.* The proof of this theorem, which is based on the martingale central limit theorem, can be found in [9], together with bounds on the rate of convergence. It is straightforward to show that the effective diffusivity $\mathcal{K}$ is a nonnegative matrix. We also remark that the centering condition (7) ensures the absence of a large scale mean drift. Sufficient conditions for (7) to hold are derived in [15]. In the case where (7) does not hold, a Galilean transformation with respect to the mean drift brings us back to the situation described in Theorem 1.

The asymptotic behavior of $\mathcal{K}$ as τ tends to 0 was also investigated in [15]. It was shown that, as τ tends to 0, $\mathcal{K}$ converges to $\mathcal{K}_0$, the effective diffusivity for the passive tracers case:

$$\mathcal{K} = \mathcal{K}_0 + \mathcal{O}(\tau). \tag{10}$$

The effective diffusivity $\mathcal{K}_0$ is also computed through the solution of a Poisson equation:

$$-\mathcal{L}_0\chi = v(x), \quad \mathcal{L}_0 = v(x)\cdot\nabla + \frac{\sigma^2}{2}\Delta, \tag{11a}$$

$$\mathcal{K}_0 = \frac{\sigma^2}{2}I + \int_{2\pi\mathbb{T}^d} v(x)\otimes\chi(x)\,dx. \tag{11b}$$

Here I stands for the identity matrix on $\mathbb{R}^d$. We will refer to $\mathcal{K}_0$ as the *tracer effective diffusivity.* It still an open question whether the higher order corrections in (10) are of definite sign. Notice that for $\mathcal{K}_0$ the cell problem (11a) is a uniformly elliptic PDE with periodic boundary conditions and is amenable to direct numerical simulation, e.g. by means of a spectral method. This is no longer true for the cell problem (9), which is a degenerate elliptic equation posed on $\mathbb{R}^d \times (2\pi\mathbb{T}^d)$, and we use Monte Carlo methods in this case.

3 Numerical Results

In this section we study numerically the effective diffusivity $\mathcal{K}$ for equation (1) for the Childress–Soward velocity field (5). We are particularly interested in analyzing the dependence of $\mathcal{K}$ on the non–dimensional parameters of the problem τ, σ and δ.

The results of [15] enable us to check that the Childress–Soward flow satisfies condition (7) and hence the absence of ballistic motion at long scales is ensured. Moreover, the symmetry properties of (5) imply that the two diagonal components of the effective diffusivity are equal, whereas the off–diagonal components vanish. In the figures presented below we use the notation $K := \mathcal{K}_{11} = \mathcal{K}_{22}$.

We compute the effective diffusivity using Monte Carlo simulations: we solve the equations of motion (1) numerically for different realizations of the noise and we compute the effective diffusivity through the formula

$$\mathcal{K} = \lim_{t\to\infty} \frac{1}{2t} \langle (x(t) - \langle x(t) \rangle) \otimes (x(t) - \langle x(t) \rangle) \rangle,$$

where $\langle \cdot \rangle$ denotes ensemble average. We solve the stochastic equations of motion using Milstein's method, appropriately modified for the second order SDE (1) [10, p. 386]:

$$x_{n+2} = (2-r)x_{n+1} - (1-r)x_n + r\Delta t v(x_{n+1}) + \sigma r \Delta t \mathcal{N}(0,1) \ .$$

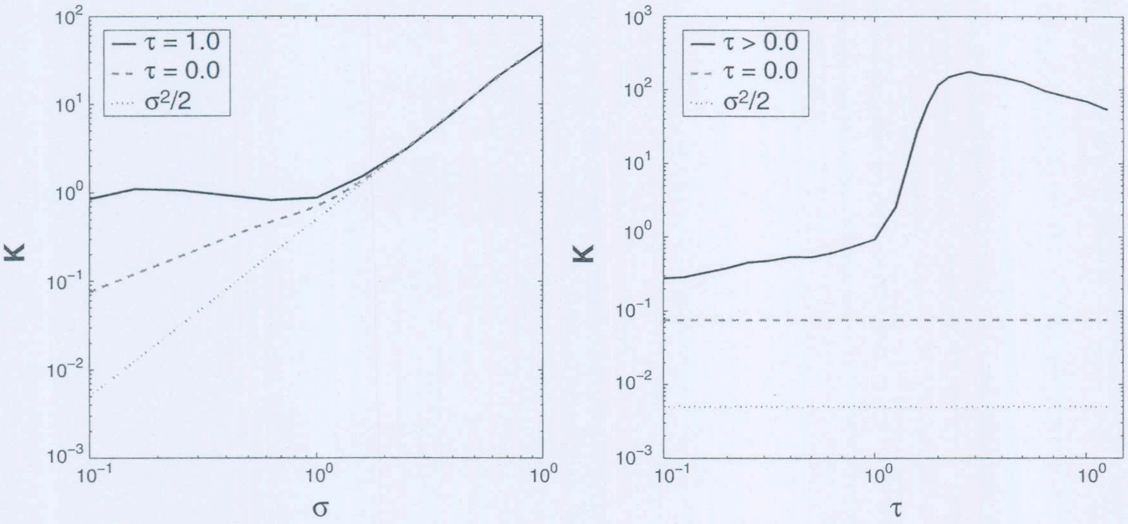
where $r = \frac{\Delta t}{\tau}$. This method has strong order of convergence 1.0. We use $N = 1024$ uniformly distributed particles in $2\pi\mathbb{T}^2$ with zero initial velocities and we integrate over a very long time interval (which is chosen to depend upon the parameters of the problem) with $\Delta t = 5.10^{-4} \min\{1, \tau\}$.

We are interested in comparing the effective diffusivities for inertial particles with those for passive tracers. The latter are computed by solving the cell problem (11a) by means of a spectral method similar to that described in [12].

We perform two sets of experiments: first, we fix $\sigma = 0.1$ and compute the effective diffusivity for τ taking values in $[0.1, 10]$. Then, we fix $\tau = 1.0$ and compute $\mathcal{K}$ for σ taking values in $[0.1, 10]$. We perform these two experiments for various values of the Childress–Soward parameter $\delta \in [0, 1]$. The choice $\delta = 0.0$ corresponds to closed streamlines, whereas the choice $\delta = 1.0$ leads to a flow with completely open streamlines, i.e. a shear flow. The results of our numerical simulations for $\delta = 0.0$, 0.25, 0.5, 0.75, 1.0 are reported in Figs. 2 to 6.

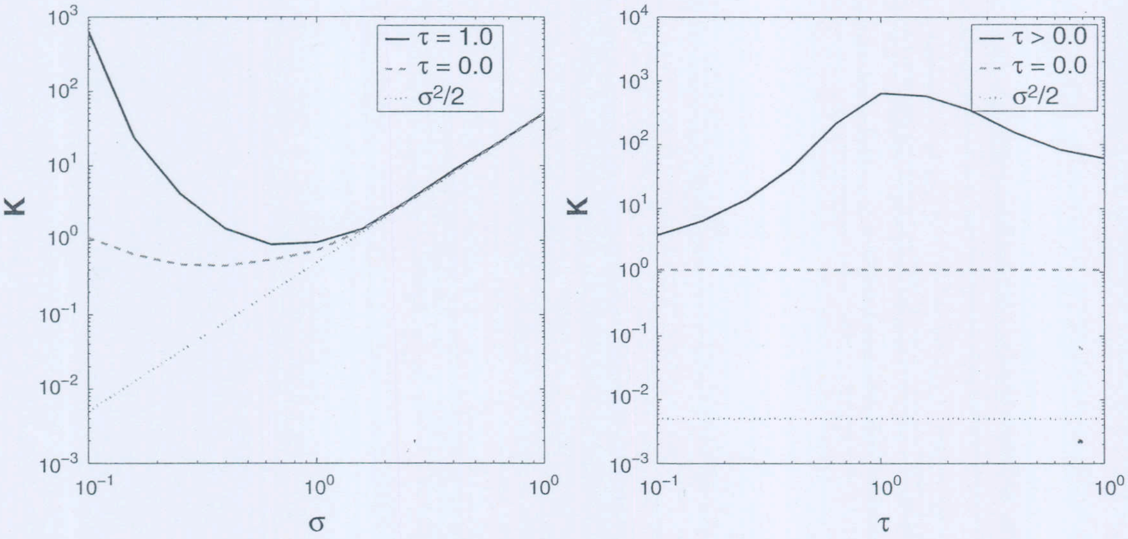
Several interesting results can be drawn from our numerical simulations. First, a resonance occurs when the Stokes' number $\tau = \mathcal{O}(1)$, which leads to a tremendous enhancement in the effective diffusivity. In particular, for $\delta = 0.25$ and $\delta = 0.5$, Figs. 3 and 4, the effective diffusivity for $\tau = \mathcal{O}(1)$ is several orders of magnitude greater than the one for $\tau = 0.0$.

On the other hand, the effect of inertia on $\mathcal{K}$ becomes negligible as the streamlines become completely open, Fig. 6. In this case, $\delta = 1.0$ the effective diffusivity for inertial particles behaves very similarly to the effective diffusivity for passive tracers.



a. $\mathcal{K}$ vs σ b. $\mathcal{K}$ vs τ

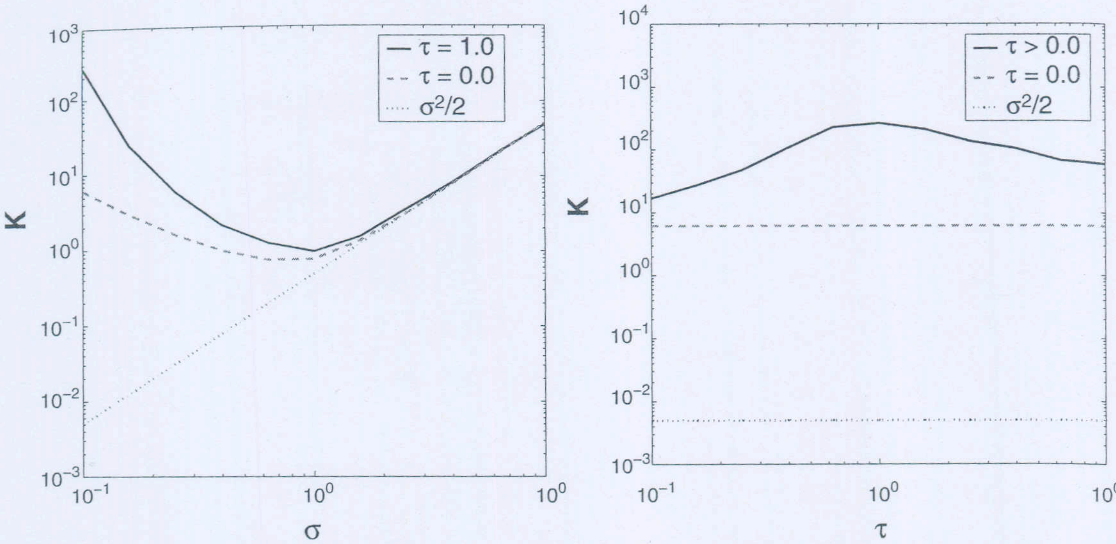
Fig. 2. Effective diffusivity versus σ (with $\tau = 1.0$) and τ (with $\sigma = 0.1$) for $\delta = 0.0$.



a. $\mathcal{K}$ vs σ b. $\mathcal{K}$ vs τ

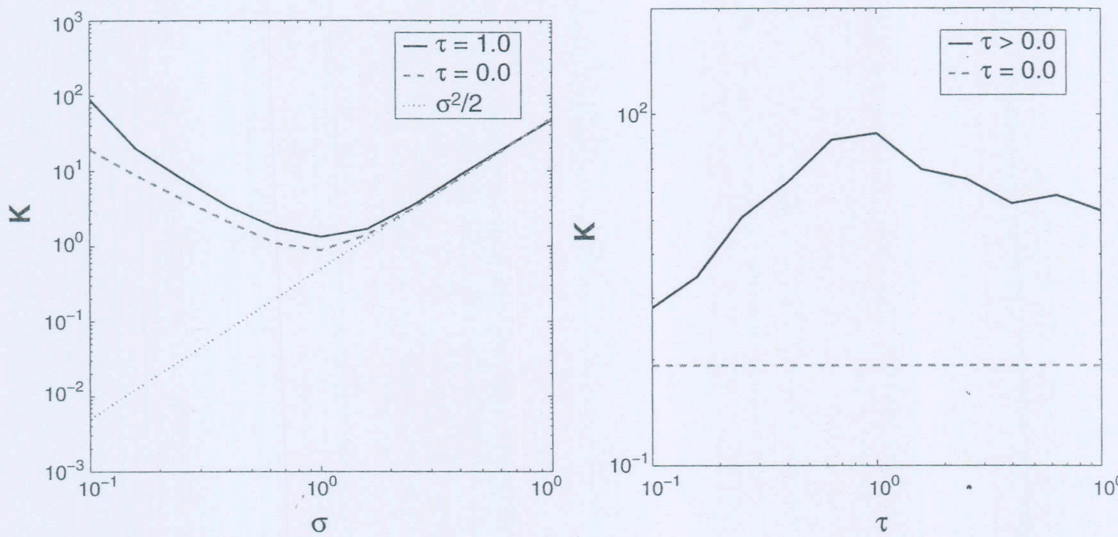
Fig. 3. Effective diffusivity versus σ (with $\tau = 1.0$) and τ (with $\sigma = 0.1$) for $\delta = 0.25$.

The effective diffusivity as a function of δ for inertial particles as well as passive tracers is plotted in Fig. 7, for $\tau = 1.0$ and $\sigma = 0.1$. It becomes clear from this figure that, for τ and σ fixed, the effective diffusivity for inertial particles reaches its maximum for $\delta \approx 0.30$: in contrast to the passive tracers case, the dependence of the inertial effective diffusivity on δ is not monotonic.



a. $\mathcal{K}$ vs σ b. $\mathcal{K}$ vs τ

Fig. 4. Effective diffusivity versus σ (with $\tau = 1.0$) and τ (with $\sigma = 0.1$) for $\delta = 0.5$.



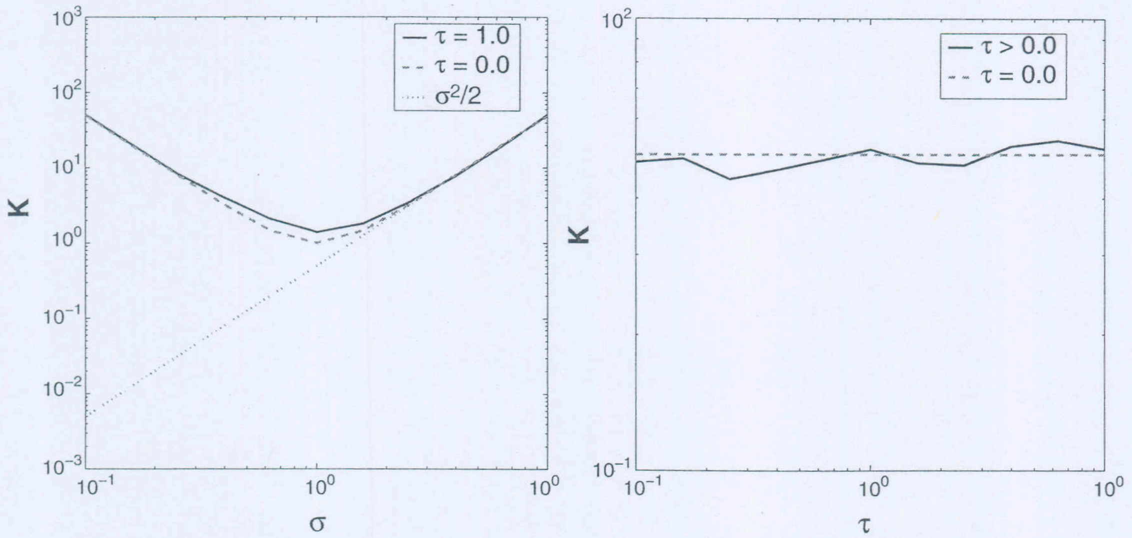
a. $\mathcal{K}$ vs σ b. $\mathcal{K}$ vs τ

Fig. 5. Effective diffusivity versus σ (with $\tau = 1.0$) and τ (with $\sigma = 0.1$) for $\delta = 0.75$.

4 Conclusions

The dependence of the effective diffusivity for inertial particles on the particle relaxation time τ and the molecular diffusivity σ was investigated in this paper by means of Monte Carlo simulations, for a one parameter family of steady two dimensional flows. We illstrated several phenomena of interest:

- the inertial effective diffusivity can be much greater than the tracer effective diffusivity, for certain values of the parameters of the problem;



a. $\mathcal{K}$ vs σ b. $\mathcal{K}$ vs τ

Fig. 6. Effective diffusivity versus σ (with $\tau = 1.0$) and τ (with $\sigma = 0.1$) for $\delta = 1.0$.

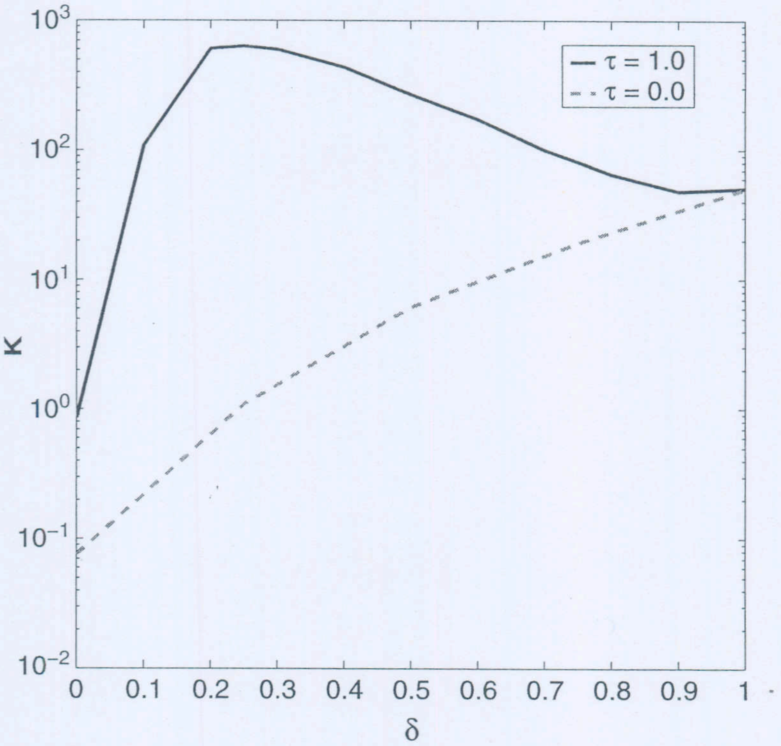


Fig. 7. Effective diffusivity versus δ for $\sigma = 0.1$, $\tau = 1.0$.

- inertia creates interesting effects of enhanced diffusivity, especially for small molecular diffusion, and these effects depend non-trivially on the topology of the streamlines of the velocity field;
- for velocity fields with most, or all, streamlines open the effect of inertia is negligible;
- the effective diffusivity is not montonic in the Stokes number, which measures the strength of the inertial contribution – maxima are observed for Stokes numbers of order 1.

Many questions are open for further study, both analytical and numerical:

- it would be of interest to develop asymptotic studies of the effective diffusivity, in particular to understand the effects of small molecular diffusion and small Stokes number;
- it would be of interest to develop variational characterization of effective diffusivities, as has been very effective for passive tracers [11];
- it is of interest to investigate effective diffusivities for time dependent velocity fields $v(x, t)$, with randomness introduced in space and/or time.

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