Eddy diffusivities in scalar transport

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Standard and anomalous transport in incompressible flow is investigated using multiscale techniques. Eddy-diffusivities emerge from the multiscale analysis through the solution of an auxiliary equation. From the latter it is derived an upper bound to eddy-diffusivities, valid for both static and time-dependent flow. The auxiliary problem is solved by a perturbative expansion in powers of the Péclet number resummed by Padé approximants and by a conjugate gradient method. The results are compared to numerical simulations of tracers dispersion for three flows having different properties of Lagrangian chaos. It is shown on a concrete example how the presence of anomalous diffusion can be revealed from the singular behaviour of the eddy-diffusivity at very small molecular diffusivities.

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I. Introduction

The problem of passive scalars diffusion in incompressible velocity fields has a theoretical and practical importance in many fields of science and engineering, ranging from mass and heat transport in geophysical flows to chemical engineering and combustion \[1\]. The main interest is in the understanding of the mechanisms leading to transport enhancement. Taking into account the molecular diffusion, the motion of a fluid element can be described by the following Langevin equation

\[
\frac{dx}{dt} = v(x, t) + \eta(t),
\]

(I.1)

where \(v(x, t)\) is the Eulerian incompressible velocity field at the position \(x\) and time \(t\), and \(\eta\) is a Gaussian white noise with zero mean and correlation function

\[
\langle \eta_i(t) \eta_j(t') \rangle = 2D_0 \delta_{ij} \delta(t - t').
\]

(I.2)

The coefficient \(D_0\) is the (bare) molecular diffusivity. If \(\theta(x, t)\) denotes the concentration of tracers, the Fokker-Planck equation \[2\] associated to (I.1) is

\[
\partial_t \theta + (v \cdot \partial) \theta = D_0 \partial^2 \theta.
\]

(I.3)

The incompressibility condition \(\partial \cdot v = 0\) is explicitly used in (I.3). Our interest will be mainly concentrated on the long-time behaviour of (I.3). For time scales much longer than the characteristic microscopic time, the evolution of \(\theta(x, t)\) is dominated by long-wave disturbances. The equation for these slow modes can be obtained by the usual “hydrodynamic” analysis \[3\]

\[
\partial_t \langle \theta \rangle = D_{ij}^E \frac{\partial^2}{\partial x_i \partial x_j} \langle \theta \rangle + \ldots \quad i, j = 1, \ldots, d
\]

(I.4)

where \(\langle \theta \rangle\) is the concentration field averaged locally over a volume of linear dimensions much larger than the typical length \(l\) of the velocity field and \(d\) is the space dimension. The corrections in (I.4) involve terms containing at least three derivatives of \(\langle \theta \rangle\), which can be neglected in the weak gradients limit \(|\partial \langle \theta \rangle|/\langle \theta \rangle \ll l^{-1}\). Eq. (I.4) then reduces to a diffusion equation, with an effective diffusion tensor \(D_{ij}^E\) (the eddy-diffusivity tensor). The latter has a direct practical importance since it measures the spreading for very long times of a spot of tracers:

\[
D_{ij}^E = \lim_{t \to \infty} \frac{1}{2t} \langle (x_i(t) - \langle x_i \rangle) (x_j(t) - \langle x_j \rangle) \rangle , \quad i, j = 1, \ldots, d.
\]

(I.5)

where \(x(t)\) is the position of a tracer at time \(t\) and the average is taken over the initial positions or, equivalently, over an ensemble of test particles. Note that the existence of
the limit in (I.3) ensures that the transport is a standard diffusion process, at least for a very large time. This is the typical situation, but there are also cases showing the so-called anomalous diffusion: the spreading of particles does not vary linearly with time but as a power law $t^\gamma$, with $\gamma \neq 1$ (where $\gamma > 1$ and $\gamma < 1$ correspond to superdiffusive and subdiffusive behaviours, respectively). Transport anomalies indicate the presence of strong correlations in the dynamics, even at large time and space scales. An interesting possibility is the one discussed in [4]. The flow is periodic, but the Lagrangian phase space is a complicated self-similar structure of islands and cantori. Particles are thus transported in a coherent way longer and longer as $D_0$ is decreased, finally leading to anomalous diffusion in the absence of any molecular diffusion.

The aim of this paper is using multiscale techniques [5] to study standard and anomalous diffusion. The multiscale formalism is introduced in Section II, where the calculation of eddy-diffusivities is reduced to the solution of an auxiliary equation. From the latter, upper and lower bounds for eddy-diffusivities are derived in the general case of time-dependent flows. The calculation of the exact analytical expression of the eddy-diffusivity for parallel flows and random flows $\delta$-correlated in time is also reviewed. Random flows with a short correlation time are discussed more thoroughly in Appendix 1. Numerical methods are generally needed to solve the auxiliary equation leading to the eddy-diffusivity tensor for a generic flow. Two possibilities are discussed in Section III. The first one is to perform a Padé resummation of the series expressing the eddy-diffusivity in powers of the Péclet number. The second is the use of a conjugate gradient algorithm. Both methods are used in Section IV to analyze three flows having a standard diffusive transport (the $ABC$ [6, 7, 8], the $BC$ and a two dimensional time-dependent flow). The results are compared to numerical simulations of tracers dispersion, i.e. numerical integrations of (I.1). The flows have been chosen since they can be considered as prototypes for three very different situations with respect to Lagrangian chaos [9, 10], i.e. the chaotic properties of the deterministic equation obtained from (I.1) suppressing the noise. If the latter equation is integrable, as for the $BC$ flow, the diffusion process is expected to be strongly sensitive to the detailed geometric structure of the Eulerian field and to the presence of molecular diffusion. For a non-integrable flow we expect a competition between coherent transport in the non-chaotic regions (which turns out to be dominant in the $ABC$ flow) and random advection. The limiting case is the one of a strongly turbulent flow, like the time-dependent flow, where molecular transport can be ignored on a large range of scales and chaotic advection is dominant. The study of anomalous diffusion is presented in Section V, where the flow introduced in [4] is analyzed. A singular behaviour of the eddy-diffusivity at high Péclet numbers is shown to be a signature of anomalous transport. A reliable procedure for predicting the presence of anomalous diffusion is thus provided.
II. The multiscale technique

A general method for studying transport processes is the so-called multiscale technique
(also known as homogenization [4]). The idea is to exploit the scale separation in the
dynamics. Specifically, let $v(x, t)$ be an incompressible velocity field, periodic both in space
and time. (The technique can be extended to handle the case of a random, homogeneous
and stationary velocity field with some non-trivial modifications in the rigorous proofs of
convergence [11].) The scalar field $\theta(x, t)$ evolves according to the Fokker-Planck equation
(1.3). The units are chosen in such a way that the periodicities of $v$ are $O(1)$. In order
to avoid trivial sweeping effects, the average of the velocity field over the periodicities is
supposed to vanish. We shall be interested in the dynamics of the field $\theta$ on large
scales assumed to be $O(1/\epsilon)$, where $\epsilon \ll 1$ is the parameter controlling the scale separation.
Because we expect the scalar field to have a diffusive dynamics, the associated time scale
is $O(1/\epsilon^2)$.

The presence of the small parameter $\epsilon$ naturally suggests to look for a perturbative
approach. The perturbation is however singular [12] since a constant field is a trivial
solution of (1.3). The origin of this phenomenon can be grasped in the following simple
situation. Let the large-scale field have a single wavenumber $\epsilon$. Because of the advection
term in (1.3), a small-scale field $\tilde{\theta}$ is produced and the wavenumbers spaced from those of
$v$ by multiples of $\epsilon$ are generally excited. The interaction between the latter modes and
those of $v$, due again to the advection term, is responsible for the transport coefficients
renormalization. The essential shift of order $\epsilon$ in the wavenumbers of $\tilde{\theta}$ with respect
to those of $v$ is missed by regular perturbation expansions. Asymptotic methods, like
multiscale techniques, are thus needed.

In addition to the fast variables $x$ and $t$, let us then introduce slow variables as $X = \epsilon x$
and $T = \epsilon^2 t$. The prescription of the technique is to treat the two sets of variables as
independent. It follows that

$$
\partial_i \mapsto \partial_i + \epsilon \nabla_i; \quad \partial_t \mapsto \partial_t + \epsilon^2 \partial_T,
$$

(II.1)

where $\partial$ and $\nabla$ denote the derivatives with respect to fast and slow space variables,
respectively. The solution is sought as a perturbative series

$$
\theta(x, t; X, T) = \theta^{(0)} + \epsilon \theta^{(1)} + \epsilon^2 \theta^{(2)} + \ldots,
$$

(II.2)

where the functions $\theta^{(n)}$ depend a priori on both fast and slow variables. By inserting (II.2)
and (II.1) into (1.3) and equating terms having equal powers in $\epsilon$, we obtain a hierarchy
of equations. The solutions of interest to us are those having the same periodicities as
the velocity field. The first equation, corresponding to $O(\epsilon^0)$, is

$$
\partial_t \theta^{(0)} + (v \cdot \nabla) \theta^{(0)} = D_0 \partial^2 \theta^{(0)}.
$$

(II.3)
By using Poincaré inequality, one can show \cite{13} that for periodic solutions
\[
-\partial_t \int (\theta(0))^2 \, dV = D_0 \int (\partial \theta(0))^2 \, dV \geq D_0 \left( \frac{2\pi}{L} \right)^2 \int (\theta(0))^2 \, dV,
\]  
(II.4)
where \(L\) is the spatial periodicity length of \(\mathbf{v}\) (supposed for simplicity to be the same in all directions) and the integral is over the periodicity box. The inequality (II.4) implies that the solution will relax to a constant with respect to fast variables, i.e.
\[
\theta^{(0)}(\mathbf{x}, t; \mathbf{X}, T) = \theta^{(0)}(\mathbf{X}, T).
\]  
(II.5)
It can be also easily checked that the transient has no effect on the large-scale dynamics. The equations at order \(\epsilon\) and \(\epsilon^2\) are
\[
\partial_t \theta^{(1)} + (\mathbf{v} \cdot \nabla) \theta^{(1)} - D_0 \partial^2 \theta^{(1)} = -\mathbf{v} \cdot \nabla \theta^{(0)},
\]  
(II.6)
\[
\partial_t \theta^{(2)} + (\mathbf{v} \cdot \nabla) \theta^{(2)} - D_0 \partial^2 \theta^{(2)} = -\partial_T \theta^{(0)} - (\mathbf{v} \cdot \nabla) \theta^{(1)} + D_0 \nabla^2 \theta^{(0)} + 2D_0 \mathbf{\partial} \cdot \nabla \theta^{(1)}.
\]  
(II.7)
Since the equation (II.6) is linear, its solution can be written as
\[
\theta^{(1)}(\mathbf{x}, t; \mathbf{X}, T) = \theta^{(1)}(\mathbf{X}, T) + \mathbf{w}(\mathbf{x}, t) \cdot \nabla \theta^{(0)}(\mathbf{X}, T),
\]  
(II.8)
where the first term on the r.h.s. is a solution of the homogeneous equation and the vector field \(\mathbf{w}\) has a vanishing average over the periodicities and satisfies
\[
\partial_t \mathbf{w} + (\mathbf{v} \cdot \nabla) \mathbf{w} - D_0 \partial^2 \mathbf{w} = -\mathbf{v}.
\]  
(II.9)
Due to the incompressibility of the velocity field, the average over the periodicities of the l.h.s. in (II.6) and (II.7) is zero. For the equations to have a solution, the average of the r.h.s. should also vanish (Fredholm alternative). The resulting solvability conditions provide the equations governing the large-scale dynamics, i.e. the dynamics in the slow variables. From (II.7) we obtain
\[
\partial_T \langle \theta^{(0)} \rangle = D_0 \nabla^2 \langle \theta^{(0)} \rangle - \langle \mathbf{v} \cdot \nabla \theta^{(1)} \rangle,
\]  
(II.10)
where the symbol \(\langle \cdot \rangle\) denotes the average over the periodicities. The solvability condition for (II.6) is trivially satisfied, reflecting the absence of \(\alpha\)-type effects \cite{14, 15}. By plugging (II.8) into (II.10) we obtain the diffusion equation
\[
\partial_T \theta^{(0)}(\mathbf{X}, T) = D^{E}_{ij} \nabla^2 \theta^{(0)}(\mathbf{X}, T),
\]  
(II.11)
where the eddy diffusivity tensor is
\[
D^{E}_{ij} = D_0 \delta_{ij} - \frac{1}{2} \left[ \langle v_i w_j \rangle + \langle v_j w_i \rangle \right].
\]  
(II.12)
Remark that the structure of the eddy-diffusivity tensor will reflect the rotational symmetries of \(\mathbf{v}\) and is in general non-isotropic.
II..1 Inequalities for the eddy-diffusivity

Two important inequalities can be derived from the auxiliary equation (II.9) and the expression (II.12) of the eddy-diffusivity. Let us consider the \( i \)-th and the \( j \)-th components of (II.9) and multiply by \( w_j \) and \( w_i \), respectively. Taking the sum and averaging, the time derivative and the advective term vanish and we obtain

\[
-\frac{1}{2} \left( \langle v_i w_j \rangle + \langle v_j w_i \rangle \right) = D_0 \langle \partial w_i \cdot \partial w_j \rangle. \tag{II.13}
\]

From (II.13) and (II.12) it follows

\[
D_{ij}^E = D_0 \left[ \delta_{ij} + \langle \partial w_i \cdot \partial w_j \rangle \right]. \tag{II.14}
\]

This expression of the eddy-diffusivity clearly shows that the correction to the molecular contribution is positive definite. Large-scale scalar transport is therefore enhanced in the presence of a small-scale incompressible velocity field. The cause is that for the advection-diffusion equation (I.3) the integral of \( \theta^2 \) over the whole space is a decreasing function of time. When the dynamics does not possess the latter property the large-scale transport can actually be depleted, rather than increased. For momentum transport in Navier-Stokes flow the depletion can be so strong that the eddy-viscosity becomes negative, i.e. the average flux is in the same direction as the large-scale gradient \[16, 17\].

The second inequality also is derived from (II.13) but it is an upper bound to eddy-diffusivities. Because of incompressibility, the velocity field can be expressed using a vector potential as \( \mathbf{v} = \text{rot} \mathbf{A} \). By taking the trace of (II.13) and integrating by parts, we obtain

\[
0 \leq D_0 \langle \partial w_i \cdot \partial w_i \rangle = -\langle v_i w_i \rangle = -\langle \mathbf{A} \cdot \text{rot} \mathbf{w} \rangle. \tag{II.15}
\]

Application of the Schwartz inequality leads to

\[
D_0 \langle \partial w_i \cdot \partial w_i \rangle \leq \langle A^2 \rangle^{1/2} \langle (\text{rot} w)^2 \rangle^{1/2} \leq \langle A^2 \rangle^{1/2} \langle \partial w_i \cdot \partial w_i \rangle^{1/2}, \tag{II.16}
\]

whence

\[
\frac{D_{ii}^E}{D_0} \leq d + \frac{\langle A^2 \rangle}{D_0} \equiv d + \text{Pe}^2. \tag{II.17}
\]

The Péclet number is denoted by \( \text{Pe} \). The result (II.17), valid for time-dependent flows also, generalizes a similar inequality known for time-independent velocity fields \[11, 18\]. The inequality (II.17) also provides an upper bound for each eigenvalue since the eddy-diffusivity tensor is positive definite.
II..2 Two exactly solvable cases

By using multiscale techniques, the calculation of eddy diffusivities has been reduced to the solution of the auxiliary equation (II.9). Numerical methods are generally needed to solve it but there are a few cases where one can obtain the solution of (II.9) analytically. We shall briefly review here the case of parallel flows and random flows $\delta$-correlated in time.

The peculiar property of parallel flows is that the velocity is everywhere in the same direction, e.g. in three dimensions

$$ v(x, y, z; t) = (v_x(y, z; t), 0, 0), \quad \text{(II.18)} $$

and $v_x$ cannot depend on $x$ because of incompressibility. The advective non-linearity $v \cdot \partial v$ is thus vanishing. Thanks to the latter, we can easily obtain the solution of the auxiliary equation (II.9) as

$$ \hat{w}(q, \omega) = \frac{\hat{v}(q, \omega)}{i\omega - D_0q^2}. \quad \text{(II.19)} $$

The Fourier transforms of $v_x$ and $w_x$ are denoted by $\hat{v}$ and $\hat{w}$. If $F(q, \omega) = \langle \vert \hat{v}(q, \omega) \vert^2 \rangle$, it follows that the eddy-diffusivity is

$$ D^E_\parallel = D_0 \left( 1 + \int \frac{F(q, \omega) q^2}{\omega^2 + D_0^2 q^4} dq d\omega \right); \quad D^E_\perp = D_0. \quad \text{(II.20)} $$

Here, $D^E_\parallel$ and $D^E_\perp$ are the components of the eddy-diffusivity tensor parallel and orthogonal to the direction of the velocity. For the Kolmogorov flow $v_x = V \cos y$ and the parallel eddy-diffusivity $D^E_\parallel = D_0 + V^2/2D_0$.

Let us now consider random flows having a short correlation time $\tau$. Neglecting the diffusion term in (II.9) we obtain a hyperbolic equation which can be formally integrated along the characteristics

$$ w(x(a, t); t) = - \int_0^t v(x(a, s); s) \, ds + w(a; 0). \quad \text{(II.21)} $$

Here, $a$ denotes the Lagrangian initial position and the Eulerian position at time $t$ is

$$ x(a, t) = a + \int_0^t v(x(a, s); s) \, ds. \quad \text{(II.22)} $$

From (II.21) Taylor’s expression of the eddy-diffusivity tensor immediately follows

$$ D^E_{ij} = \frac{1}{2} \int_0^\infty \left( \Gamma^L_{ij}(s) + \Gamma^L_{ji}(s) \right) ds, \quad \text{(II.23)} $$
where the Lagrangian correlation function is defined as

$$\Gamma^L_{ij}(t - s) = \langle v_i(x(a, t); t) v_j(x(a, s); s) \rangle. \quad (II.24)$$

The operation $$\langle \cdot \rangle$$ denotes either spatial or ensemble averaging which do coincide since the velocity field is supposed homogeneous, stationary and mixing. Note that the convergence of the integral (II.23) is not at all guaranteed. The role of a small, but non-zero, molecular diffusivity can be crucial in this respect \[1\]. In the limit where $$\tau$$ is small, the Lagrangian correlation $$\Gamma^L_{ij}$$ tends to the Eulerian correlation $$\langle v_i(x, t) v_j(x, s) \rangle$$. For a signal $$\delta$$-correlated in time

$$\langle v_i(x, t) v_j(x, s) \rangle = 2 F_{ij} \delta(t - s), \quad (II.25)$$

and the expression (II.23) reduces to

$$D^E_{ij} = D_0 \delta_{ij} + F_{ij}. \quad (II.26)$$

The corrections to this result due to a small, but finite, correlation time will be studied in Appendix 1.

**III. Numerical methods**

Whenever the auxiliary equation (II.9) cannot be solved exactly, numerical methods are needed. In this Section we shall discuss two different methods that we have used: a perturbative expansion and a conjugate gradient algorithm.

In the perturbative method, the solution $$w$$ of the auxiliary equation (II.9) is sought as a power series in the Péclet number $$\text{Pe} \sim 1/D_0$$:

$$w = \text{Pe} w^{(1)} + \text{Pe}^2 w^{(2)} + \cdots. \quad (III.1)$$

We shall concentrate on the time-independent case for simplicity. By inserting the expansion (III.1) into (II.9) the following recursive relation is obtained

$$w^{(1)} = \partial^{-2} \frac{v}{D_0 \text{Pe}}, \quad w^{(2)} = \partial^{-2} \frac{v \cdot \partial w^{(1)}}{D_0 \text{Pe}}, \quad \ldots \quad w^{(n)} = \partial^{-2} \frac{v \cdot \partial w^{(n-1)}}{D_0 \text{Pe}}, \quad \ldots \quad (III.2)$$

Expressions (III.2) and the calculation of the average value in (II.12) are conveniently handled in Fourier space, leading to

$$\frac{D^E_{ij}}{D_0} = \delta_{ij} + \sum_{n \geq 1} (c_n)_{ij} \text{Pe}^{2n}. \quad (III.3)$$
Here, the \( c_n \)'s are numerical coefficients and the series turns out to be in \( Pe^2 \), rather than in \( Pe \). The contribution of order \( 2n + 1 \) in \( < v_i w_j > \) is indeed antisymmetric, as can be easily checked by integrating \( n \) times by parts. The series (III.3) will in general converge for \( Pe < Pe^* \) only, because of singularities in the complex plane. A reliable analytic continuation beyond the disc of convergence can however be performed. In [14] it was indeed shown that the component of the eddy-diffusivity in the arbitrary direction \( \hat{n} \) can be represented as a Stieltjes integral

\[
\frac{D_E}{D_0} = 1 + Pe^2 \int dz \frac{\rho_{\hat{n}}(z)}{1 + Pe^2 z^2},
\]

where \( \rho_{\hat{n}}(z) \) is a positive definite function, possibly singular. The poles of the eddy-diffusivity, considered as a function of a complex variable, are all on the imaginary axis. Moreover, it follows from (III.4) that Padé approximants of (III.3) have some interesting peculiar properties (see e.g. [2]). Let us indeed denote by \( P_n(\text{Pe}) \) the diagonal Padé approximant of order \( n \) for the series (III.3) and by \( P_{n+1}(\text{Pe}) \) the Padé approximant having the numerator and the denominator of degree \( n \) and \( n + 1 \), respectively. The following results hold for every value of the Péclet number: (i) The diagonal sequence \( P_n \) is monotonically increasing and has an upper bound; (ii) The sequence \( P_{n+1} \) is monotonically decreasing and has a lower bound; (iii) The exact value \( P^* \) of the Stieltjes integral satisfies

\[
\lim_{n \to \infty} P_n \leq P^* \leq \lim_{n \to \infty} P_{n+1}.
\]

The difference \( (P_{n+1} - P_n) \) decreases monotonically in \( n \) and provides an upper bound to the error due to the finite order. The quality of the resummation by a finite order approximant can be thus checked self-consistently. Padé approximants are very sensitive to the precision in the computations when the series is extended well beyond its radius of convergence. For small values of the molecular diffusivity, the coefficients in the series (III.3) must be then known with very high precision. In our numerical calculations we used the FORTRAN multiple-precision package MP, written by R.P. Brent [20]. It should be noted, however, that very high precision computations are quite expensive in computers memory costs (see next Section).

The second method that we have used to solve the auxiliary equation (II.9) is a conjugate gradient algorithm [21]. The components of the vector \( w \) are not coupled in eq. (II.9), which is thus equivalent to a set of scalar equations. All of them can be written in Fourier space as

\[
A_{i,j} x_j = b_i, \quad i, j = 1, \ldots, V.
\]

Here, \( V \) is the resolution, \( x_i \) and \( b_i \) are vectors having the \( V \) components equal to the Fourier transform of the relevant components of \( u \) and \( -v \), respectively. Conjugate gradient algorithms are widely used to minimize multidimensional functions when the number
of dimensions is very large. The interested reader is referred to [22] for a comparison with other methods (Gauss-Siedel or Minimal-Residue [21]) in another stiff numerical problem, the inversion of the propagator in lattice quantum chromodynamics. The solution of the problem (III.6) is sought by minimizing the quantity \((Ax - b)^2\) over a sequence of directions orthogonal to the matrix \(A\). In all the applications of the method that we have considered, the matrix \(A\) in (III.6) is sparse (quasi-diagonal). Each iteration of the minimization algorithm can be then performed in \(O(V)\) operations, rather than \(O(V^2)\). For a positive-definite matrix, the rate of convergence of the method can be shown to be exponential [21]. Our matrix \(A\) has actually one zero eigenvalue, corresponding to a constant field. The problem is nevertheless well-posed since both the velocity field and the solution \(w\) are orthogonal to constants, i.e. have zero average. As in any other numerical scheme, the simulations are expected to become more and more demanding as the molecular diffusivity becomes smaller. An increasing number of excited scales requires indeed a greater resolution and the rate of convergence of the method decreases when \(V\) and the Péclet number are increased. It is also to be checked that no eigenvalue is equal to zero within the numerical accuracy because of round-off errors. In the next Section it will turn out that the previous limitations are not very severe and do not forbid to perform high Péclet numbers simulations.

We conclude this Section by briefly describing the numerical scheme used for the numerical simulations of tracers dispersion. The latter are done by uniformly distributing \(N\) particles in the periodicity box and letting them evolve according to the Langevin equation (I.1). The \(i\)-th diagonal element of the eddy-diffusivity tensor is then given by

\[
\sigma_i^2(t) = \lim_{t \to \infty} \frac{1}{2Nt} \sum_{k=1}^{N} \left[ x_i^{(k)}(t) - \frac{1}{N} \sum_{j=1}^{N} x_i^{(j)}(t) \right]^2. \tag{III.7}
\]

The indices \(k\) and \(j\) label the \(N\) particles whereas the index \(i\) denotes the spatial directions \((x, y\) for the two-dimensional and \(x, y, z\) for the three-dimensional case). The numerical integration of the Langevin equation was performed by a Runge-Kutta algorithm, modified to take into account the white noise term [23]. The integration step was \(\Delta t = 0.01\) and the total number of integration steps was \(10^6\). This ensured a good convergence of the quantities (III.7) also for the lowest molecular diffusion coefficients \(D_0\) used. The number of particles used was 1 000 for the three-dimensional and 2 000 for the two-dimensional case.

**IV. Standard diffusion**

The aim of this Section is to apply the methods previously discussed to three flows showing standard diffusion. The criterion in the choice of the flows is to have different mechanisms
of diffusion enhancement, highlighting the influence of Lagrangian chaos on transport at high Péclet numbers. Specifically, we have considered:

- The three dimensional ABC flow \[6, 7, 8\]:
  \[
  \begin{aligned}
  \dot{x} &= A \sin(z) + C \cos(y), \\
  \dot{y} &= B \sin(x) + A \cos(z), \\
  \dot{z} &= C \sin(y) + B \cos(x).
  \end{aligned}
  \tag{IV.1}
\]

with \(A = B = C\). The ABC flow is a Beltrami time-independent solution of Euler’s equations. Eq. (IV.1) shows Lagrangian chaos but the phase space is also made of regular regions, having roughly the shape of a tube parallel to one of the three axes (principal vortices).

- The two dimensional BC flow
  \[
  \begin{aligned}
  \dot{x} &= C \cos(y), \\
  \dot{y} &= B \cos(x),
  \end{aligned}
  \tag{IV.2}
\]

obtained by projecting the flow (IV.1) onto the \(x - y\) plane and translating the \(x\)-coordinate by \(\pi/2\). Eq. (IV.2) is integrable and the streamlines form a closed structure made of four cells in each periodicity box.

- The two dimensional time dependent flow
  \[
  \begin{aligned}
  \dot{x} &= \cos(y) + \sin(y) \cos(t) \\
  \dot{y} &= \cos(x) + \sin(x) \cos(t)
  \end{aligned}
  \tag{IV.3}
\]

This flow is not a solution of Euler’s equations anymore but it is the superposition of the flow (IV.2) with another flow of the same type oscillating with frequency \(\omega = 1\). The motivation for introducing a time dependency is to destroy all possible “regular islands”, like the vortices in (IV.1).

Note that both the flows (IV.1) and (IV.2) have an isotropic eddy-diffusivity tensor. Let us indeed consider the latter for simplicity and perform the following two operations: translation by \(\pi\) and mirror-inversion with respect to one of the axes (e.g. \(x \mapsto \pi - x\) and \(y \mapsto \pi - y\)). From the auxiliary eq. (II.9) it follows that, under the previous operations, one of the components of \(w\) is odd and the other is even, in such a way that \(<v_x w_y> = <v_y w_x> = 0\). The diagonal components are obviously equal because of the symmetry \(x \leftrightarrow y\). For (IV.1) the proof is similar, exploiting the fact that the group of symmetries of the flow is isomorphic to the cubic group [8]. The flow (IV.3) possesses the symmetry \(x \leftrightarrow y\), but it is not mirror-symmetric. The diagonal components of
the eddy-diffusivity will then be equal but the non-diagonal component does not vanish. In Langevin simulations the previous symmetry properties are exploited to reduce the statistical fluctuations by averaging over the directions.

In Figs. 1, 2 and 3 we present the results for the diagonal component of the eddy-diffusivity tensor of (IV.1), (IV.2) and (IV.3), respectively. The curves in each figure correspond to numerical simulations of the Langevin equation, the Padé method and the conjugate gradient algorithm. To attain the highest Péclet number the order of Padé approximants used is 54, 115, 29 and the number of significant digits in the computations is 83, 203, 40, respectively. Concerning the conjugate gradient algorithm, in Fig. 4 it is shown the power spectrum of the auxiliary field \( w \) for the flow (IV.3) at \( D_0 = 0.01 \). It can be seen that the field is resolved enough to ensure the presence of a conspicuous exponentially decaying tail. The conjugate gradient algorithm turns out to be much more efficient at high Péclet numbers than the Padé method. The latter has the advantage of requiring the calculation of the coefficients of (III.3) only: once they are computed, the eddy-diffusivities for all values of \( D_0 \) such that the method works are available. On the other hand, the memory costs for high precision arithmetics are a major drawback and practically restrict the method to moderate Péclet numbers.

From the high Péclet number behaviour of the eddy-diffusivities in the figures it is clear that the three flows have a very different dynamics. The main contribution to diffusion in the flow (IV.1) comes from the particles in the vortices, where the transport is almost ballistic, leading to the observed \( 1/D_0 \) dependence. Because of the presence of closed cells, a non-zero molecular diffusivity is needed to have an effective diffusion in the flow (IV.2), as indicated by the \( \sqrt{D_0} \) behaviour in Fig. 2. The transport for small molecular diffusivities indeed occurs by jumps from one cell to another due to the white-noise term in the Langevin equation [24, 25, 26]. The probability of jumping is controlled by the width of boundary layers located near the separatrices and gives the square-root law. The flow (IV.3) is finally an example of strong Lagrangian turbulence. The particles can diffuse even in the absence of molecular diffusion, chaotic advection is dominant and the eddy-diffusivity attains a finite value independent of the molecular diffusivity. The figures show that for all the flows considered, Langevin simulations and numerical solutions of the auxiliary equation (II.9) do agree. Moreover, in the latter method no problem of finite statistics and simulation times must be overcome. We conclude that multiscale techniques combined with an efficient numerical scheme for the solution of the auxiliary equation (e.g. a conjugate gradient algorithm or a pseudo-spectral code [27]) provide a powerful tool for the calculation of eddy-diffusivities and transport properties.
V. Anomalous diffusion

We shall discuss here how the multiscale formalism presented in the previous Sections can be used for the problem of anomalous diffusion. At a first sight it would seem that multiscale techniques cannot be used anymore. Consider indeed a two-dimensional static parallel flow (II.18). If the power spectrum $F(q)$ defined in Section II.2 is such that

$$F(q) \sim q^\alpha, \quad \alpha \leq 1, \quad \text{for } q \ll 1,$$

then the integral in (II.20) diverges and the eddy-diffusivity is not defined. The divergence is actually reflecting the fact that the transport in the direction of the flow is superdiffusive [28, 29, 30, 31], i.e.

$$\langle x^2(t) \rangle \sim t^{2\nu}, \quad \nu > 1/2,$$

and it is not a standard diffusion. The particles are indeed coherently swept by large-scale modes having wavelengths comparable (or even larger) to the typical length of the scalar field. Scale-separation breaks down and multiscale methods, heavily relying on this assumption, seem to become useless. Let us however cut out the singular part in the integral (II.20) by defining a regularized velocity field $v_L$, such that

$$F_L(q) = \begin{cases} F(q) & \text{if } q > L^{-1} \\ 0 & \text{if } q < L^{-1} \end{cases}$$

The eddy-diffusivity is now finite and exhibits a dependence

$$D_{\parallel}^E(L) \sim L^{1-\alpha}, \quad L \gg 1,$$

on the cut-off length $L$. A standard diffusion is however observed only for spatial and time lengths larger than $L$ and $t^* \sim L^2/D_0$, respectively. For $t \sim t^*$ the system has indeed a crossover [32] and for times shorter than $t^*$ it shows the same behaviour as in (V.2). By matching at $t^*$ the two different regimes, we obtain

$$\nu = \frac{3 - \alpha}{4} \geq 1/2.$$  

For $\alpha = 0$, i.e. a velocity field which is a white noise in space, (V.5) leads to $\nu = 3/4$, the well known result of Matheron and De Marsily [28].

In the previous example the origin of superdiffusion was related to the spatial structure of the velocity field. Another interesting case is the one of velocity fields with very long Lagrangian correlation times. The integral defining the eddy-diffusivity in Taylor’s expression (II.23) may then diverge, indicating the presence of anomalous transport for $D_0 = 0$. Note however that for any $D_0 > 0$ the transport is in general a standard
diffusion (see (11.20) for an example of the role of a small molecular diffusivity). The molecular diffusivity can be thus used as a regularization parameter, similarly to the cut-off length for parallel flows. As in the latter case, by studying the behaviour of the eddy-diffusivity close to the critical point (small $D_0$) one should be able to have some insights into the anomalous behaviour at the critical point ($D_0 = 0$). Specifically, the examples of Section IV show that in the presence of ballistic channels the eddy-diffusivity varies as the inverse of $D_0$ for small $D_0$, while for a system with strong Lagrangian chaos it tends to a constant. If $D_n^E$ denotes the eddy-diffusivity in the arbitrary direction $\hat{n}$, we are thus led to interpret a small $D_0$ behaviour

$$D_n^E \sim D_0^{-\beta}, \quad 0 < \beta < 1$$

as a mark of anomalous diffusion in the direction $\hat{n}$ for $D_0 = 0$. For a practical application of the previous argument we have considered the velocity field [4]

$$\begin{align*}
\dot{x} &= \partial_y \psi + \varepsilon \sin z \\
\dot{y} &= -\partial_x \psi + \varepsilon \cos z \\
\dot{z} &= \psi
\end{align*}$$

(V.7)

where

$$\psi(x, y) = 2 \left[ \cos x + \cos \left( \frac{x + \sqrt{3} y}{2} \right) + \cos \left( \frac{x - \sqrt{3} y}{2} \right) \right].$$

(V.8)

Numerical simulations of (V.7) have led the authors of [4] to conclude that the flow exhibits anomalous diffusion in the $x - y$ plane for some intervals of $\varepsilon$-values in the range $(0, 5)$. In particular, $\varepsilon = 1$ and $\varepsilon = 2.3$ are such that the diffusion is standard and anomalous, respectively. Let us now introduce a small molecular diffusivity and calculate the eddy-diffusivity of the flow (V.7). The auxiliary equation is solved by the conjugate gradient method and the results for $D_{xx}$ are presented in Figs. 5 and 6. It is evident that for $\varepsilon = 1$ the eddy-diffusivity tends to a constant for small $D_0$, while for $\varepsilon = 2.3$ it is observed the behaviour $D_{xx} \sim D_0^{-\beta}$ with $\beta \simeq 0.7$. This value is in rough agreement with the numerical results of [4] using the dimensional relation $\beta = 2

\nu - 1$ obtained by matching the diffusive behaviour with the anomalous behaviour (V.2) at the typical diffusive time $O(1/D_0)$. The criterion (V.6) is thus confirmed and we conjecture that its validity is not restricted to the flow (V.7) only. For a generic flow, anomalies in the zero-diffusivity dynamics could be then captured by introducing a small molecular diffusivity and looking for a singular behaviour of transport coefficients. As shown in the previous section, the advantage with respect to simulations of the Langevin equation is that no problem of statistical fluctuations must be tackled. The previous procedure should then allow to make robust predictions on the presence of anomalous transport.

Acknowledgments

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Appendix 1

We shall derive here the expression of the eddy-diffusivity for incompressible flows having a short correlation time. Specifically, the ratio $\tau_c/\tau_s$ between the correlation and the sweeping time (defined precisely later) is supposed to be small. We shall be particularly interested in 3D isotropic flows. By the latter we mean velocity fields invariant under rotations, but not in general under parity transformations. When the correlation time tends to zero, we recover the case of flows $\delta$-correlated in time. For a Gaussian flow, the first two corrections are shown to be proportional to $(\tau_c/\tau_s)^2$: one of them is related to the correlation length of the flow and the second is due to helicity. The former reduces, while the latter increases the eddy-diffusivity, in agreement with [33].

Let $v(x, t)$ denote a random, homogeneous and stationary incompressible velocity field. We shall suppose the flow to be isotropic, Gaussian and the correlation function
\[ \langle v_i(x, t) v_j(y, s) \rangle = C(|t - s|) B_{ij}(x - y). \] (A.1)

The mean velocity is equal to zero. The temporal correlation function $C(t)$ decays on a time-scale of order $\tau_c$. The spatial correlation function is defined via its Fourier transform as
\[ \tilde{B}_{ij}(k) = P_{ij}(k) \frac{E(k)}{4\pi k^2} - i \frac{1}{2} \epsilon_{ijl} k_l H(k) \frac{1}{4\pi k^4}, \] (A.2)

where $P_{ij} = \delta_{ij} - k_i k_j / k^2$ is the solenoidal projector and $\epsilon_{ijk}$ is the fundamental antisymmetric tensor. The functions $E(k)$ and $H(k)$ will be called the energy and the helicity spectrum since
\[ \frac{1}{2} \langle v^2 \rangle = C(0) \int E(k) \, dk; \quad \langle v \cdot \omega \rangle = C(0) \int H(k) \, dk. \] (A.3)

The helicity is a pseudo-scalar and it is thus vanishing for flows having a center of symmetry (parity-invariance). The helicity spectrum satisfies the inequality (see [34]):
\[ |H(k)| \leq 2 k E(k). \] (A.4)

We shall be interested in the calculation of eddy-diffusivities for very high Péclet numbers. The eddy-diffusivity is given in this limit by Taylor’s expression (II.23)
\[ D_{ij}^E = \frac{1}{2} \int_0^\infty \left[ \langle v_i(x(a, t), t) v_j(a, 0) \rangle \right. \left. + i \leftrightarrow j \right] dt. \] (A.5)

Let us now suppose the correlation time $\tau_c$ of the velocity field to be much smaller than the sweeping time $\tau_s$. The latter is defined as
\[ \tau_s = \frac{\lambda}{(v^2)^{1/2}} = \left( \frac{1}{C(0) \int k^2 E(k) \, dk} \right)^{1/2}, \] (A.6)
and it is roughly the average time it takes for a particle to travel a distance equal to
the correlation length $\lambda$. The dominant contribution in (A.5) will be given by Eulerian
positions $x(a,t)$ close to $a$:

$$x(a,t) = a + \int_0^t ds \, v(a, s) + \int_0^t ds \, (\nabla_t v)(a, s) \int_0^s ds' \, v_t(a, s') + \ldots,$$

(A.7)

and the velocity $v(x(a,t), t)$ in (A.5) is

$$v(x(a,t), t) = v(a, t) + (\nabla_t v)(a, t) \int_0^t ds \, v_t(a, s) +$$

$$\frac{1}{2} (\nabla^2_t v)(a, t) \int_0^t ds \, v_t(a, s) \int_0^s ds' \, v_m(a, s') + \ldots.$$ (A.8)

Eq. (A.8) can now be plugged into Taylor’s expression (A.5), leading to

$$D_{ij}^{E} = \frac{1}{2} \int_0^\infty dt \left[ \langle v_i(a, t) v_j(a, 0) \rangle + \frac{1}{2} \int_0^t ds \, \int_0^s ds' \langle (\nabla_t v_t)(a, t) v_j(a, 0) \rangle \langle v_t(a, s) v_m(a, s') \rangle + \int_0^t ds \, \int_s^\infty ds' \langle (\nabla_t v_t)(a, t) v_m(a, s') \rangle \langle (\nabla_m v_t)(a, s) v_j(a, 0) \rangle \right] + i \leftrightarrow j;$$ (A.9)

where homogeneity, incompressibility and the properties of Gaussian statistics have been
exploited. Eq. (A.9) is valid for a generic Gaussian random flow and the next terms
in the expansion are $O(\tau_c/\tau_s)^4$. Let us now specialize (A.9) to the isotropic case. The
eddy-diffusivity tensor is then proportional to $\delta_{ij}$ and its trace can be calculated by using
(A.1) and (A.2):

$$\text{Tr} \, D_{ij}^{E} = 2 \int E(k) \, dk \int_0^\infty dt \, C(t) -$$

$$- \frac{2}{3} \left( \int E(k) \, dk \right) \left( \int k^2 E(k) \, dk \right) \int_0^\infty dt \, C(t) \int_0^t ds \, \int_0^s ds' \, C(|s - s'|) +$$

$$+ \frac{1}{6} \left( \int H(k) \, dk \right)^2 \int_0^\infty dt \, \int_0^t ds \, C(s) \int_s^\infty ds' \, C(t - s') .$$ (A.10)

In order to estimate the order of magnitude of the various terms in (A.10) it is convenient
to consider the case

$$C(|t|) = \frac{1}{2\tau_s} \chi_{\tau_s}(|t|); \quad \chi_{\tau_s}(|t|) = \begin{cases} 1, & \text{if } |t| \leq \tau_s; \\ 0, & \text{otherwise.} \end{cases}$$ (A.11)
When $\tau_s \to 0$ a flow $\delta$-correlated in time is obtained. In this limit, the only non-vanishing contribution in (A.10) is the first one, which coincides with (II.26). Both corrections in (A.10) are proportional to $$(\tau_c/\tau_s)^2$$, as can be checked by using (A.4) and the Schwartz inequality. If the correlation function $C(t)$ is not (A.11), the constants are changed but not the orders of magnitude, provided the condition $\int C(t) \, dt = 1$ is kept fixed.

Note that for the correlation function (A.11) the helicity contribution in (A.10) is clearly positive while the one related to the correlation length is negative. These results have a simple physical interpretation. It is convenient to consider the Lagrangian correlation time which is proportional to the eddy-diffusivity. The first correction in (A.10) is due to the fact that the presence of a spatial correlation length obviously reduces the Lagrangian correlation time. The second correction depends on the presence of helicity. The latter has the effect that particles move following a helix, instead of a straight line. The mean velocity is however the same since it depends on the energy spectrum only. It will then take a longer time for a particle to escape a strongly correlated region, the Lagrangian correlation time is longer and the eddy-diffusivity is increased. An equivalent remark is that a path following a helix is discriminated against tightly bending back on itself.

A Gaussian flow has been considered but the results can be easily generalized to the general case. If third-order moments do not vanish the first correction will in general be proportional to $\tau_c/\tau_s$. We finally note that the helical term is actually the only one in (A.9) which needed to be symmetrized with respect to the indices $i$ and $j$. The latter fact is related to Onsager’s reciprocity theorem. When the helicity does not vanish, the correlation function will indeed not satisfy the time-reversibility condition $B_{ij}(x) = B_{ji}(x)$ and the velocity field has a preferred sense of rotation. The lack of parity invariance can be thus interpreted as a lack of symmetry with respect to time-reversal, which is responsible for the antisymmetry of transport coefficients.

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FIGURE CAPTIONS

FIGURE 1. The diagonal component $D_{11}^E$ as a function of the bare molecular diffusivity $D_0$ for the three dimensional ABC flow (IV.1) with $A = B = C = 1$. The continuous line is the result of the Padé method. The black and white squares are the results of the conjugate gradient method and direct simulations, respectively.

FIGURE 2. The diagonal component $D_{11}^E$ as a function of the bare molecular diffusivity $D_0$ for the two dimensional BC flow (IV.2) with $B = C = 1$. The continuous line is the result of the Padé method. The black squares are the results of the direct simulations.

FIGURE 3. The diagonal component $D_{11}^E$ as a function of the bare molecular diffusivity $D_0$ for the two dimensional time dependent flow (IV.3). The continuous line is the result of the Padé method. The black and white squares are the results of the conjugate gradient method and of direct simulations, respectively.

FIGURE 4. Log-log plot of the energy spectrum of the auxiliary field $w$ for the (IV.3) flow at $D_0 = 0.01$.

FIGURE 5. The diagonal component $D_{11}^E$ as a function of the bare molecular diffusivity $D_0$ for the three dimensional flow (V.7), (V.8) with $\epsilon = 1$ (standard diffusion).

FIGURE 6. The diagonal component $D_{11}^E$ as a function of the bare molecular diffusivity $D_0$ for the dimensional flow (V.7), (V.8) with $\epsilon = 2.3$ (anomalous diffusion).
