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Effective transport in random shear flows

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We obtain an effective transport description for the superdiffusive motion of random walkers in stratified flow by projection of the process on the direction of stratification. The effective dimensionally reduced motion is shown to describe a correlated random walk characterized by the Lagrangian velocity correlation. We analyze the projected motion through exact analytical solutions for the distribution density for an arbitrary correlated Gaussian noise and derive an evolution equation for the one-point and conditional two-point displacement densities. The latter gives an explicit effective equation for superdiffusive transport in stratified random flow and demonstrates that the displacement density has a Gaussian scaling form for all times.

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Non-Markovian transport and non-Fickian and anomalous diffusion are frequently observed in disordered dynamic systems (e.g., [1–3]). Many studies have focused on the development of effective non-Markovian transport frameworks based on the assumption of heavy-tailed uncorrelated disorder distributions (e.g., [4,3]). Here we study the complementary scenario of non-Markovian processes originating from (strong) correlations by focusing on effective transport in stratified random flow (e.g., [5–7]). Matheron and de Marsily [5] studied the latter as a model for solute transport in stratified porous media and found superdiffusive growth of the distribution density in the direction of stratification. Such anomalous and in general non-Fickian transport features dominate solute transport in geological formations.

Many applications, ranging from performance assessment of nuclear waste repositories in geological media to groundwater remediation, require identifying and quantifying the effective large scale transport dynamics caused by the interaction of medium heterogeneities and microscale transport dynamics [e.g., [8,9]]. The latter implies spatial or stochastic averaging of the microscale transport equations, i.e., dimensional reduction or in general projection of the process (e.g., [10,11]). Such a contraction of information in general leads to a non-Markovian property of the projected process [11] that can be cast into formal effective equations by using the projector formalism proposed by Zwanzig and Mori [12,13], see, e.g., [14] for an application to transport in random media. Here, we derive an explicit effective transport equation and explicit solutions for the distribution densities of the projected process by exploiting the fact that the projected motion of random walkers in stratified flow describes a correlated random walk characterized by its Lagrangian velocity correlation. It has been shown that the latter plays an important role for characterizing non-Fickian transport in heterogeneous media in general (e.g., [15]). In the following, we pose the projection problem for transport in stratified random flow, which is solved by (i) demonstrating that the projected motion of a random walker describes a correlated random walk; (ii) derivation of a (non-Markovian) transport equation for correlated random walks. These steps render an explicit effective transport framework for stratified random media.

Transport of a passive scalar $c(\mathbf{x},t)$ in a stratified flow field $u(y)$ is described by the Fokker–Planck equation (e.g., [5]),

$$\frac{\partial c(\mathbf{x},t)}{\partial t} = -u(y)\frac{\partial c(\mathbf{x},t)}{\partial x} + D\frac{\partial^2 c(\mathbf{x},t)}{\partial y^2}, \tag{1}$$

where the coordinate vector is given by $\mathbf{x}=(x,y)^T$; D is the diffusion coefficient. For simplicity, we restrict this study to an infinite $d=2$ dimensional domain, no diffusion in flow direction. The spatial density $c(\mathbf{x},t)$ and its gradient normal to the boundaries at infinity are zero. The normalized initial distribution $c(\mathbf{x},t=t_0)=\rho(y)\delta(x)$, where $\rho(y)$ is normalized to one, its variance is denoted by a^2. For $a \gg 1$, $\rho(y)$ is assumed to have the scaling form,

$$\rho(y) = \frac{1}{a} f_\rho\left(\frac{y}{a}\right), \tag{2}$$

where $f_\rho(0)$ is constant. The stratified flow field $u(y)$ is a realization of the stationary spatial Gaussian random process $\{u(y)\}$ characterized by the constant ensemble mean velocity $u_E=\overline{u(y)}$ and the correlation of the velocity fluctuations $u'(y)=u(y)-u_E$, which is given by $C_E(y-y')=\overline{u'(y)u'(y')}$. The overbar denotes the ensemble average over all realizations of $\{u(y)\}$.

In order to obtain a simplified effective transport description, the spatial density is projected on the x direction by,

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$$\bar{c}(x,t) \equiv \int_{-\infty}^{\infty} \mathrm{d}y c(\mathbf{x},t). \tag{3}$$

We determine a non-Markovian evolution equation and explicit analytical expressions for the average density $\bar{c}(x,t)$ by formulating the projected transport problem as a correlated random walk.

The starting point is the Langevin equation equivalent to the Fokker-Planck equation (1), which is given by (e.g., [6]),

$$\frac{\mathrm{d}X(t|b)}{\mathrm{d}t} = u_E + u'[Y(t|b)], \quad \frac{\mathrm{d}Y(t|b)}{\mathrm{d}t} = \xi(t). \tag{4}$$

We used here the decomposition $u(y)=u_E+u'(y)$; $\xi(t)$ is a Gaussian white noise with zero mean and correlation $\langle \xi(t)\xi(t')\rangle = 2D\delta(t-t')$, where the angular brackets denote the white noise average. The initial particle position at time $t=t_0$ is given by $[X(t_0|b), Y(t_0|b)]=(0,b)$. Particles are initially distributed along the y axis according to $\rho(b)$. The distribution density $c(\mathbf{x},t)$ in this picture is given by

$$c(\mathbf{x},t) = \int_{-\infty}^{\infty} \mathrm{d}b\rho(b)\langle \delta[x - X(t|b)]\delta[y - Y(t|b)]\rangle. \tag{5}$$

Application of (3) to (5) gives for the average density,

$$\bar{c}(x,t) = \int_{-\infty}^{\infty} \mathrm{d}b\rho(b)\langle \delta[x - X(t|b)]\rangle \equiv \langle \delta[x - X(t)]\rangle_\zeta. \tag{6}$$

The trajectory $X(t)$ describes the $d=1$ dimensional random walk,

$$\frac{\mathrm{d}X(t)}{\mathrm{d}t} = u_E + \zeta(t), \tag{7}$$

with the initial position $X(t=t_0)=0$ and noise $\zeta(t) = u'[y(t,b)]$. The latter is Gaussian distributed because $u'(y)$ is a Gaussian random field. The noise average, denoted by $\langle\cdot\rangle_\zeta$, is defined in (6) and consists of taking the average over the white noise $\xi(t)$ and integration over the source distribution $\rho(b)$. Thus, noise mean and correlation are given by

$$\langle \zeta(t)\rangle_\zeta = \int_{-\infty}^{\infty} \mathrm{d}y \left[\int_{-\infty}^{\infty} \mathrm{d}b\rho(b)u'(y+b) \right] g(y,t|0), \tag{8}$$

$$\langle \zeta(t)\zeta(t')\rangle_\zeta = \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}y' \left[\int_{-\infty}^{\infty} \mathrm{d}b\rho(b)u'(y+b)u'(y'+b) \right] \times g(y,t-t'|y')g(y,t'|0), \tag{9}$$

where $g(y,t-t'|y') = \langle \delta[y-y(t,b)]\rangle_{Y(t')=y'}$ is the conditional density of the transverse diffusion process in (4). For the infinitely extended medium under consideration here, it is given by

$$g(y,t|y') = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(y-y')^2}{4Dt} \right]. \tag{10}$$

In the limiting case of $a \gg 1$ and using the scaling form (2), the expressions in the square brackets in (8) and (9) can be substituted by the respective ensemble averages,

$$\lim_{a\to\infty} \frac{1}{a} \int_{-\infty}^{\infty} \mathrm{d}b f\left(\frac{b}{a}\right) u'(y+b) \equiv \overline{u'(y)} = 0, \tag{11}$$

$$\begin{aligned} \lim_{a\to\infty} \frac{1}{a} \int_{-\infty}^{\infty} \mathrm{d}b f\left(\frac{b}{a}\right) u'(y+b)u'(y'+b) &= \overline{u'(y)u'(y')} \\ &= C_E(y-y'), \end{aligned} \tag{12}$$

where we used (2) and the ergodicity of $\{u(y)\}$. Thus, in this limit the Lagrangian mean $\langle \zeta(t)\rangle_\zeta \equiv 0$. Using (12) in (9), we obtain for the Lagrangian velocity correlation,

$$\langle \zeta(t)\zeta(t')\rangle_\zeta \equiv C_L(t-t') = \int_{-\infty}^{\infty} \mathrm{d}y C_E(y) g(y,t-t'|0). \tag{13}$$

Thus, for sufficiently large source distributions, the noise $\zeta(t)$ can be approximated by a stationary correlated Gaussian noise. The projected motion of a random walker in stratified random flow is a correlated random walk characterized by the correlated Gaussian noise $\zeta(t)$, with zero mean and correlation (13). As such, we can obtain an effective transport framework and a complete effective description for transport in stratified random flow by deriving solutions for the n-point densities of correlated random walks, which are non-Markovian by nature. In the following, we derive explicit solutions for correlated random walks.

Discretizing (7) in time, we obtain

$$X(t_N + \tau) = X(t_N) + u_E\tau + \zeta(t_N)\tau, \tag{14}$$

with the constant time increment τ and discrete time $t_N = N\tau$. The random walk (14) has the sharp initial position $X(t_0)=x_0$ at time $t_0 = N_0\tau$. The random force $\zeta(t_N)$ kicks in at time t_{N_0}. In order to make the process well defined, for $t_N < t_{N_0}$ we consider the process deterministic or driven by white noise. Thus, for $t_N > t_{N_0}$, the evolution of $X(t_N)$ does not depend on the system states previous to t_{N_0}. The series of random velocities $\zeta(t_n)$ $(n=N_0,\ldots,\infty)$ describes the stochastic process $\{\zeta(t_n)\}$. The latter can be described by its characteristic function, which is defined by the Fourier transform of the multivariate distribution density (e.g., [10]),

$$G(\{\kappa(t_n)\}) = \left\langle \exp\left[\mathrm{i}\sum_n \kappa(t_n)\zeta(t_n) \right] \right\rangle_\zeta. \tag{15}$$

The $\{\kappa(t_n)\}$ denote the Fourier variables conjugate to $\{\zeta(t_n)\}$. For the multi-Gaussian correlated processes $\zeta(t)$, it is given by

$$G(\{\kappa(t_n)\}) = \exp\left[-\frac{1}{2}\sum_{nn'} \kappa(t_n)C_L(t_n - t_{n'})\kappa(t_{n'}) \right]. \tag{16}$$

Note that $\{\zeta(t_n)\}$ is Gaussian white noise for $C_L(t_n - t_{n'}) \propto \delta_{nn'}$. Systems driven by strongly correlated noise have been studied in various contexts (e.g., [16]) ranging from Brownian motion in fractals [e.g. [17,18]] to the description of animal movements (e.g., [19]).

The correlated random walk (14) is non-Markovian. Note that a non-Markovian process is not sufficiently characterized by its one-point density and transition probability. Here, for simplicity we focus only on the latter two distributions.

In order to derive an explicit expression for $\bar{c}(x,t)$, we perform a Fourier transform of (6), which gives for $\tilde{\bar{c}}(k,t)$ in discrete time,

$$\tilde{\bar{c}}(k,t_N) = \langle \exp[\mathrm{i}kX(t_N)]\rangle_\zeta, \tag{17}$$

where k is frequency and the tilde denotes Fourier-transformed quantities. From (14) we obtain for $X(t_N)$,

$$X(t_N) = x_0 + \sum_{l=N_0}^{N-1} u_E\tau + \sum_{l=N_0}^{N-1} \zeta(t_l)\tau. \tag{18}$$

Inserting the latter into (17), and subsequently performing the noise average, gives

$$\tilde{\bar{c}}(k,t_N) = \exp\left[\mathrm{i}k\left(x_0 - \sum_{i=N_0}^{N-1} u_E\tau\right)\right] \times G(\{\kappa(t_i)=k\}_{i=N_0}^{N-1};\{\kappa(t_i)=0\}_{i\geq N}), \tag{19}$$

which can be verified by inserting (15) into (19).

For process times t_N that are large compared to the constant time increment, $t_N \gg \tau$, we take the limit to continuous time, set $t_N = t$, and identify

$$\sum_{i=N_0}^{N-1} \varphi(t_i)\tau \equiv \int_{t_0}^{t} \mathrm{d}t'\,\varphi(t) \tag{20}$$

for an arbitrary function $\varphi(t)$. Thus, we obtain from (19) by using (16) and taking the limit of continuous time,

$$\tilde{\bar{c}}(k,t) = \exp\left[-k^2\int_0^{t-t_0} \mathrm{d}t'\,D(t') + \mathrm{i}ku_E(t-t_0)\right], \tag{21}$$

where we defined the time-dependent diffusion coefficient,

$$D(t) = \int_0^t \mathrm{d}t'\,C_L(t'). \tag{22}$$

A similar method was used in Ref. [18] for the derivation of the evolution equation for the one-point density for a generalized Langevin equation with power-law correlated noise. Note that with the same method as outlined above all n-point densities of the correlated random walk (7) can be calculated [23].

Derivation of (21) with respect to time and transforming the resulting equation back to real space, we obtain the following evolution equation for the average concentration,

$$\frac{\partial}{\partial t}\bar{c}(x,t) + u_E\frac{\partial}{\partial x}\bar{c}(x,t) - D(t-t_0)\frac{\partial^2}{\partial x^2}\bar{c}(x,t) = 0 \tag{23}$$

with the initial condition $\bar{c}(x,t=t_0) = \delta(x-x_0)$. Note that the average concentration is identical to the two-point conditional density,

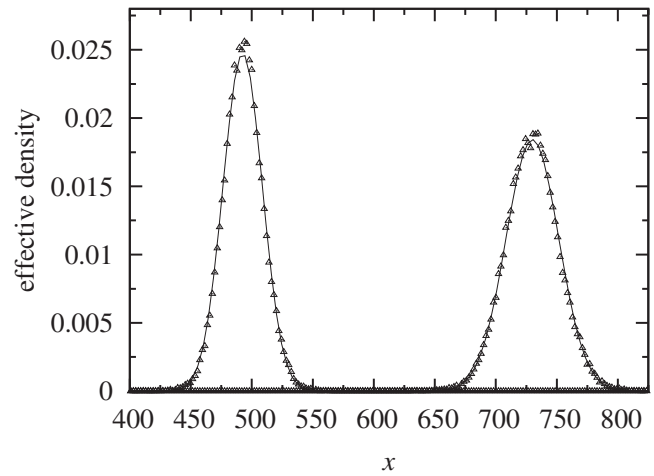

FIG. 1. Effective distributions obtained from (triangles) projection of the random walk (4) to the direction of stratification using numerical random walk simulations and (solid) expression (25), at two different times. The velocity mean and autocorrelation are $u_E = 10$ and $C_E(y) \propto \delta(y)$.

$$P(x,t|x',t') = \langle \delta[x - X(t)]\rangle_\zeta\big|_{X(t')=x'} \tag{24}$$

for $t' = t_0$. As outlined above, for consistency reasons, we assume that the correlated noise is switched on at t_0 while for $t < t_0$ the noise is uncorrelated or zero. Thus, (23) expresses the fact that the system remembers the point in time when the correlated random force is switched on, i.e., the non-Markovianity of the projected process. Seen as the evolution equation for $P(x,t|x',t')$, (23) expresses the system's memory of a measurement at time t'.

The solution of (23) is a Gaussian pulse, i.e.,

$$\bar{c}(x,t) = [2\pi\sigma^2(t)]^{-1/2}\exp[-(x-u_Et)^2/\sigma^2(t)], \tag{25}$$

where we set $t_0 = 0$ and defined the variance $\sigma^2(t)$ by

$$\sigma^2(t) = \int_0^t \mathrm{d}t'\,D(t'), \tag{26}$$

where $D(t)$ is given by the general expression (22). In terms of the Eulerian velocity correlation function, $D(t)$ is given by (e.g., [5,20]),

$$D(t) = \int_0^t \mathrm{d}t' \int_{-\infty}^{\infty} \mathrm{d}y\,C_E(y)g(y,t'|0), \tag{27}$$

which can be obtained by inserting (13) into (22). Note that the average density (25) is always Gaussian, irrespective of the noise correlation $C_L(t)$ and thus of the Eulerian velocity correlation $C_E(y)$. Figure 1 shows the average concentration $\bar{c}(x,t)$ obtained by random walk simulations compared to the analytical solution (25). Analytical and numerical solutions are in perfect agreement.

For times $t \gg \tau_D = l^2/D$ and a $C_E(y)$ that decays sharply on the correlation scale l, it is easy to show that $D(t) \propto \sqrt{t}$; thus we find for the variance (26) $\sigma^2(t) \propto t^{3/2}$. For delta-correlated velocity, i.e., $C_E(y) \propto \delta(y)$, this is exactly so for all times [6].

Thus, for zero bias, i.e., $u_E=0$, and delta-correlated velocity, the projected density $\bar{c}(x,t)$, (25), has the exact scaling form,

$$\bar{c}(x,t) = t^{-3/4} f(x/t^{3/4}), \tag{28}$$

where $f \propto \exp(-u^2)$. The scaling form (28) has been conjectured by [6,21]. However, unlike argued there, the scaling function $f(u)$ has Gaussian shape for all times as the solution $\bar{c}(x,t)$ of (23) for $u_E=0$ is a Gaussian pulse with variance proportional to $t^{3/2}$ according to (25) and (26). This is confirmed by comparison with explicit random walk simulation as illustrated in Fig. 1.

The analysis of effective transport in stratified random flow in terms of correlated random walks is conditioned by (i) the velocity distribution and (ii) the initial distribution of random walkers, which determine the statistical characteristics of the effective correlated noise. For source distributions with an extension of the order of the correlation scale, preasymptotic transport is dominated by the details of the local velocities, which can induce nonlocal terms in the effective transport equation (e.g., [22]). This memory is expected to persist until the distribution is spread out vertically by diffusion over a distance that is much larger than the correlation scale and has sampled a representative part of the flow variability. A line source with a transverse extension that is large compared to the correlation scale wipes this memory out from the very beginning, thus giving the Gaussian scaling form (25) at all times.

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