Intermittency in Passive Scalar Advection

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A Lagrangian method for the numerical simulation of the Kraichnan passive scalar model is introduced. The method is based on Monte Carlo simulations of tracer trajectories, supplemented by a point-splitting procedure for coinciding points. Clean scaling behavior for scalar structure functions is observed. The scheme is exploited to investigate the dependence of scalar anomalies on the scaling exponent ξ of the advecting velocity field. The three-dimensional fourth-order structure function is specifically considered. [S0031-9007(98)06331-5]

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The Kraichnan model of passive scalar advection by a self-similar Gaussian white-in-time velocity field [1] is by now a paradigm for intermittency in turbulent systems. It was shown by Kraichnan [2] that, for advecting velocity fields which are white-in-time (δ correlated), the equal-time correlation functions of the scalar field θ obey closed equations of motion. In his 1994 paper [1] he used this remarkable property and the so-called "linear ansatz" to predict the scaling exponents ζ_n of the nth order scalar structure function S_n for all space dimensions $d \geq 2$ and for all velocity scaling exponents $0 \leq \xi \leq 2$. The predicted ζ_n's are *anomalous*, for example, $2\zeta_2 - \zeta_4 > 0$; in other words, the scaling exponents cannot be predicted by dimensional analysis. Hence, the flatness of scalar increments over a distance r grows $\propto r^{\zeta_4 - 2\zeta_2}$ as $r \to 0$, a phenomenon referred to as "intermittency" [3]. The linear ansatz was revisited via fusion rules in Ref. [4], and its validity in the limit $\xi \to 0$ was questioned in Ref. [5]. A different approach was developed in Refs. [6–8] in which anomalous scaling has its roots in the zero modes (solutions of the unforced problem) of the closed exact equations satisfied by the scalar correlations [9]. Their determination for correlation functions with more than two or three points presents a daunting task which has so far received solutions only via perturbation theory. Three limits have been identified for the Kraichnan model: Large d's [6], small ξ's [7], and ξ's close to the Batchelor limit $\xi = 2$ [8,10]. The first two expansions are regular, while for the third one the relevant small parameter should be $\sqrt{2 - \xi}$. (This is due to the preservation of the collinear geometry in the Batchelor limit, leading to an angular nonuniformity in the perturbation analysis [8,10].)

Numerical simulations have up to now been based on the direct integration of the passive scalar partial differential equation and have been limited to two dimensions [11,12]. Although the predictions of the linear ansatz appear compatible with such simulations, it should be noted that such calculations are highly delicate. To wit, the difficulty of observing for S_2 the known asymptotic scaling [1].

Our aim here is to propose a different numerical strategy based on the Monte Carlo simulation of Lagrangian trajectories [13]. For structure functions of finite order only a finite number of tracer particles is needed. The tracer trajectories are easy to simulate and the calculation at each time step only involves a small number of random vectors, basically, differences of velocities, rather than the whole velocity field. Furthermore, working with the tracers naturally allows one to measure the scaling of the structure functions $S_{2n}^{(L)}(r) = \langle [\theta(\boldsymbol{r}) - \theta(0)]^{2n} \rangle$ vs the integral scale L of the forcing. Physically, this means that the passive scalar variance injection rate (which equals its dissipation rate) and the separation r are kept fixed while the integral scale L is varied. In an anomaly-free theory, e.g., of the Kolmogorov 1941 type, nothing should change in inertial-range statistical quantities. Anomalies will here be measured directly through the scaling dependence on L of the structure functions.

Specifically, let us consider the passive scalar equation

$$\partial_t \theta(\boldsymbol{r}, t) + \boldsymbol{v}(\boldsymbol{r}, t) \cdot \nabla \theta(\boldsymbol{r}, t) = \kappa \nabla^2 \theta(\boldsymbol{r}, t) + f(\boldsymbol{r}, t) . \tag{1}$$

For the Kraichnan model [1], the velocity and the forcing are Gaussian independent processes, both homogeneous, stationary, isotropic, and white-in-time. The velocity is self-similar (no infrared cutoff is needed nor assumed in our procedure); the correlations of its increments are given by

$$\langle v_\alpha(\boldsymbol{r}, t)\, v_\beta(\boldsymbol{r}, 0) \rangle - \langle v_\alpha(\boldsymbol{r}, t)\, v_\beta(0, 0) \rangle = r^\xi \left[(\xi + d - 1)\delta_{\alpha\beta} - \xi \frac{r_\alpha r_\beta}{r^2} \right] \delta(t) . \tag{2}$$

As for the forcing, $\langle f(\boldsymbol{r}, t)\, f(0, 0) \rangle = F(r/L)\, \delta(t)$, where $F(r/L)$ is nearly constant for distances r smaller than the integral scale L and decreases rapidly for $r \gg L$.

When the molecular diffusivity κ is simply ignored, and θ is assumed to vanish in the distant past at $t = -T$, Eq. (1) can be recast as $\theta(\boldsymbol{r}, t) = \int_{-T}^{t} f(\boldsymbol{r}(s), s)\, ds$, with the Lagrangian trajectory defined by the stochastic differential equation $d\boldsymbol{r}(s) = \boldsymbol{v}(\boldsymbol{r}(s), s)\, ds$ and the final condition $\boldsymbol{r}(t) = \boldsymbol{r}$. Using the Wick rule to calculate Gaussian averages over the forcing, the scalar correlations

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can be expressed as averages of time integrals of F over the statistics of Lagrangian trajectories. Furthermore, zero-mode ideas suggest the universality of the scaling exponents with respect to the choice of F. It is then convenient to consider the step function $F = 1$ for $r \leq L$ and $F = 0$ for $r > L$. (The fact that its Fourier transform is not positive definite is not relevant for the sequel as it actually amounts to taking a complex forcing function.) The scalar correlations have then very simple expressions, e.g., for the second- and the fourth-order correlations in the stationary state,

$$\langle \theta(\boldsymbol{r}_1)\,\theta(\boldsymbol{r}_2)\rangle = \langle T_{12}^L\rangle_{\mathcal{L}}\ ; \tag{3}$$

$$\langle \theta(\boldsymbol{r}_1)\,\theta(\boldsymbol{r}_2)\theta(\boldsymbol{r}_3)\theta(\boldsymbol{r}_4)\rangle = \langle T_{12}^L T_{34}^L + T_{13}^L T_{24}^L + T_{14}^L T_{23}^L\rangle_{\mathcal{L}}\ .$$

Here, T_{12}^L is the (random) amount of time that two particles starting at $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and moving backwards in time spend with their mutual distance $|\boldsymbol{r}_1(s) - \boldsymbol{r}_2(s)| < L$, and $\langle\bullet\rangle_{\mathcal{L}}$ denotes the average over the Lagrangian trajectory statistics. Expressions similar to (3) are easily derived for higher order correlations. Note that we can exchange backward and forward motion in time since, according to (2), the statistical properties of $\boldsymbol{v}$ and $-\boldsymbol{v}$ are the same.

In the limit $\kappa \to 0$ this procedure, which ignores molecular diffusion, is actually correct as long as all points $\boldsymbol{r}_i$ are distinct. However, if we, e.g., put $\boldsymbol{r}_1 = \boldsymbol{r}_2$ we find that $\langle\theta^2\rangle$, given by (3) is incorrect: it diverges $\propto T$ as $T \to \infty$. With coinciding points, the correct procedure is the point splitting: the tracer particles must be initially separated by a small distance $O(\epsilon)$, and the value of the correlation function for coinciding points is given by the limit $\epsilon \to 0$. This is finite for any $\xi < 2$ because, even for $\epsilon \to 0$, the particles reach an $O(1)$ separation in a finite time, on account of the Hölder nonsmooth nature of the velocity field (see, e.g., Ref. [14] for this important property of what may be termed a "Richardson walk"). It is then easily checked that $\langle\theta^2\rangle$ coincides with the known value at $\kappa = 0$ of the analytical solution [1] and that for $\xi = 2$ its divergence is logarithmic in ϵ, as it should be in the Batchelor regime.

In our simulations, the point-splitting operation is most conveniently implemented by keeping a nonvanishing amount of "molecular noise." By this we understand that the different particles, in addition to being swept along by the velocity field, are undergoing *independent* Brownian motions with a small diffusivity κ. This Brownian diffusion is relevant only for interparticle distances smaller than the dissipation scale $\eta = O(\kappa^{1/\xi})$. The corresponding stochastic equations of motion for the case of $2n$ tracer particles are

$$d\boldsymbol{r}_i(s) = \boldsymbol{v}(\boldsymbol{r}_i(s), s)\,ds + \sqrt{2\kappa}\ \dot{\boldsymbol{W}}_i(s)\,ds\,, \qquad i = 1,\ldots,2n\,,$$
$$\boldsymbol{r}_i(t) = \boldsymbol{r}_i\,, \tag{4}$$

where $\langle(\dot{W}_i)_\alpha(s)\ (\dot{W}_j)_\beta(s')\rangle = \delta_{ij}\delta_{\alpha\beta}\delta(s - s')$ and $\boldsymbol{r}_i$ is the position at the (final) time t. It can be checked that the $2n$th order scalar correlation functions given by (3), with $\boldsymbol{r}_i$ and t interpreted as Eulerian coordinates, satisfy Kraichnan's closed equations (for details, see Refs. [14,15]).

The Lagrangian method defined by (3) and (4) is numerically implemented as follows. Because of homogeneity only differences in positions and velocities matter, and we can work with $2n - 1$ particles for the moments of order $2n$. The $2n$th order structure function S_{2n} requires $n + 1$ configurations of such particles. For example, $S_2(r) = 2[\langle\theta^2\rangle - \langle\theta(r)\theta(0)\rangle]$. Since the velocity field is white-in-time, equations such as (4) could present the well known Ito–Stratonovich ambiguity [16] which is, however, absent as a consequence of incompressibility. The tracer positions are updated using the classical Euler–Ito scheme of order 1/2 [16]. Thus, during the time interval Δs the Lagrangian positions for each configuration of tracers $(r_i)_\alpha$ ($i = 1,\ldots,2n - 1$ and $\alpha = 1,\ldots,d$) are shifted by $\sqrt{\Delta s}\,[(X_i)_\alpha + (Y_i)_\alpha]$. Here, $(X_i)_\alpha$ and $(Y_i)_\alpha$ are two sets of $(2n - 1)d$ Gaussian random variables chosen independently at each time step and with the appropriate correlations. For example, using $\boldsymbol{r}_2 - \boldsymbol{r}_1,\ldots,\boldsymbol{r}_{2n} - \boldsymbol{r}_1$ as dynamical variables, we have $\langle(X_1)_1(X_2)_3\rangle = \langle[\boldsymbol{v}'(\boldsymbol{r}_2) - \boldsymbol{v}'(\boldsymbol{r}_1)]_1[\boldsymbol{v}'(\boldsymbol{r}_3) - \boldsymbol{v}'(\boldsymbol{r}_1)]_3\rangle$ and $\langle(Y_1)_1(Y_2)_1\rangle = 2\kappa$. (The $\boldsymbol{v}'$ field has no time dependence and the same spatial correlations as the $\boldsymbol{v}$ field.) Individual realizations are stopped when all the interparticle distances become larger than 10 times the largest integral scale of interest $L_{\max}$. The number of realizations needed for the results reported below is from one to several millions. The diffusivity κ is chosen such that the diffusive time at the dissipation scale, $\eta^2/\kappa \propto \kappa^{(2-\xi)/\xi}$, is small compared to the inertial time $\propto (\text{scale})^{2-\xi}$.

A severe test for the Lagrangian method is provided by the second-order structure function S_2, whose expression is known analytically [1]. Its behavior being nonanomalous, a flat scaling in L should be observed. The structure function S_2 measured by the Lagrangian method is shown in Fig. 1 for $\xi = 0.6$ and $d = 3$ (all structure functions are plotted in log-log coordinates). The measured slope is 10^{-3} and the error on the constant is 3%. (These figures are typical also for other values of ξ studied.) Two remarks are in order. First, it follows from the analytic solution that the constant-in-L behavior holds for all $r < L$, including in the dissipative region. Physically, this corresponds to the fact that, as r moves down in the dissipative region, the energy flux becomes smaller and smaller, but still remains independent of L. Second, the asymptotic scaling for $L \ll r$ goes over into the scaling for $\langle\theta^2\rangle$, namely, $L^{2-\xi}$; the transition to the constant-in-L behavior around $r = L$ is very sharp, on account of the step function chosen for F.

We applied our method to the determination of the anomalies for the fourth-order structure function

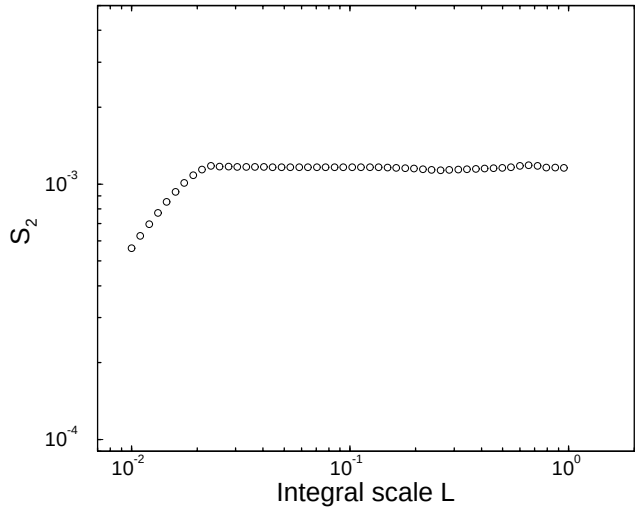

FIG. 1. The 3D second-order structure function S_2 vs L for $\xi = 0.6$. The separation $r = 2.7 \times 10^{-2}$, the diffusivity $\kappa = 1.115 \times 10^{-2}$, and the number of realizations is 4.5×10^6.

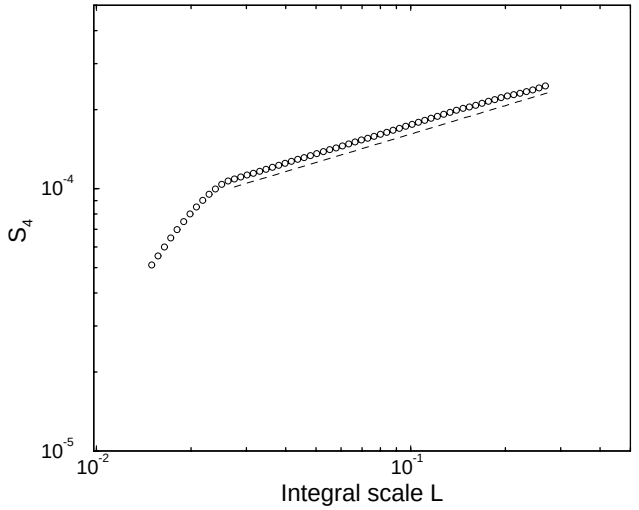

FIG. 3. Same curve as in Fig. 2 for $\xi = 0.9$. The parameters are $r = 2.7 \times 10^{-2}$, $\kappa = 4.4 \times 10^{-4}$, and the number of realizations is 8×10^6.

$S_4(r\,;L) \propto r^{2\zeta_2}(L/r)^{2\zeta_2-\zeta_4}$ in three dimensions. The results are summarized in the curve of the anomalous correction $2\zeta_2 - \zeta_4$ vs ξ presented later in Fig. 5. The three plots of S_4 vs L in Figs. 2, 3, and 4 indicate that the Lagrangian simulations require more and more computational effort when ξ is decreased from 2 to 0. This is due mainly to the fact that the three correlation functions appearing in the expression of S_4 have dominant contributions scaling as $L^{2(2-\xi)}$ and $L^{2-\xi}$, but they are both canceled in the combination giving S_4. Making the subdominant contribution of S_4 to emerge requires stronger and stronger cancellations as ξ decreases. For all the cases reported the scaling is quite clean, as also confirmed by the analysis of local scaling exponents (on octaves ratios), whose fluctuations give the conservative error bars in Fig. 5.

The dot-dashed line in Fig. 5 is the first-order perturbative prediction $(4/5)\xi$, obtained in Ref. [7]. The dashed line is a fit of the form $a\gamma + b\gamma^{3/2}$ with $\gamma = 2 - \xi$ (the parameters are $a = 0.06$ and $b = 1.13$), showing that the data are compatible with an expansion in $\sqrt{\gamma}$. Note that a term $\propto \sqrt{\gamma}$ is ruled out by the Hölder inequality $\zeta_4 \leq 2\zeta_2 = 2\gamma$ [17]. It is interesting to note that the crossing of the curve in Fig. 5 with the monotonically decreasing (in ξ) linear ansatz prediction occurs around $\xi = 1$. This is the point farthest from the two limits $\xi = 0$ and $\xi = 2$ which both have strongly nonlocal dynamics, suggesting a possible relation between

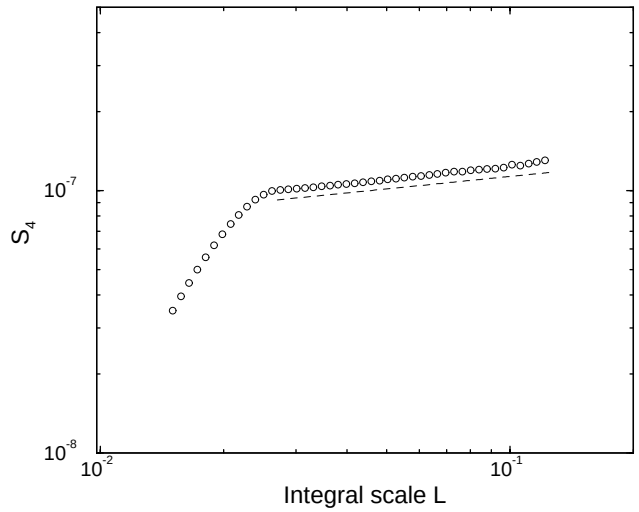

FIG. 2. The 3D fourth-order structure function S_4 vs L for $\xi = 0.2$. The separation $r = 2.7 \times 10^{-2}$, the diffusivity $\kappa = 0.247$, and the number of realizations is 15×10^6.

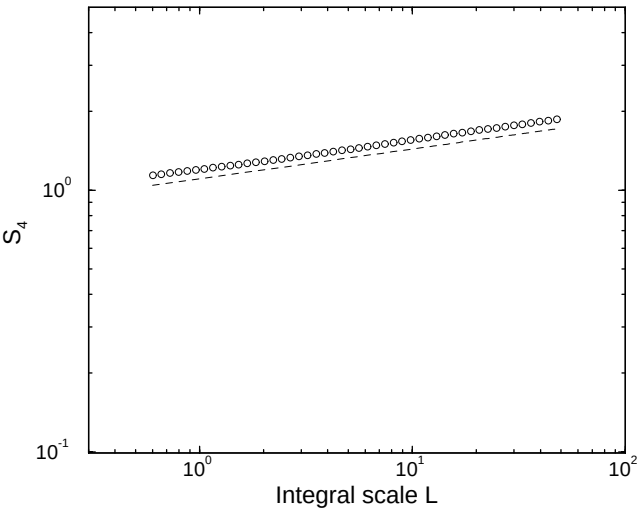

FIG. 4. Same curve as in Fig. 2 for $\xi = 1.75$. The parameters are $r = 2.7 \times 10^{-2}$, $\kappa = 10^{-9}$, and the number of realizations is 1.5×10^6.

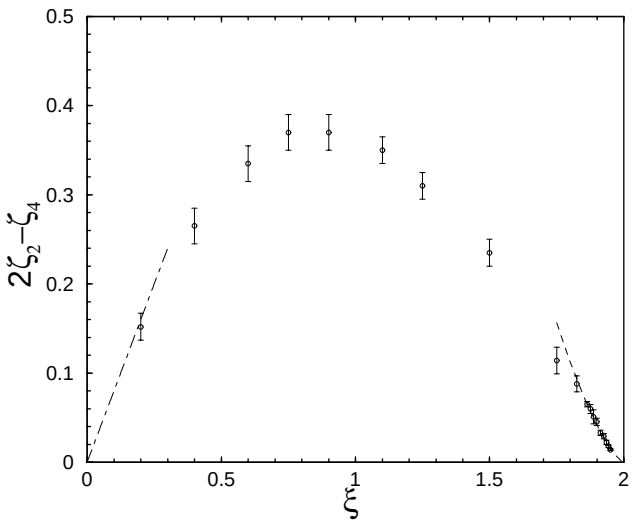

FIG. 5. The anomaly $2\zeta_2 - \zeta_4$ for the fourth-order structure function in the three-dimensional Kraichnan model.

deviations from the linear ansatz and locality of the interactions [20].

We finally note that the two main ingredients of the method reported here have, in fact, a wider range of applicability than the determination of anomalies for the Kraichnan model. First, the Lagrangian tracer method appears more flexible than the integration of the passive scalar partial differential equation. The latter permits in principle measurement of all the observables and somehow corresponds to an infinite number of tracer particles. Changing their number according to which specific correlation function is being investigated seems, however, to be more economic and convenient and should also be of interest for analyzing the advection by more realistic flow. Second, considering the scaling behavior vs the integral scale L, rather than vs the separation r, could be useful in many situations where the injection rate can be controlled; this includes the simulation of Navier–Stokes flow with white-in-time forcing. Such a procedure presents the advantage of giving direct access to the scaling exponent anomalies, which are quantitative measurements of intermittency.

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