Anomalous scaling in passive scalar advection: Monte-Carlo Lagrangian trajectories

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We present a numerical method which is used to calculate anomalous scaling exponents of structure functions in the Kraichnan passive scalar advection model (R. H. Kraichnan, Phys. Fluids 11, 945 (1968)). This Monte-Carlo method, which is applicable in any space dimension, is based on the Lagrangian path interpretation of passive scalar dynamics, and uses the recently discovered equivalence between scaling exponents of structure functions and relaxation rates in the stochastic shape dynamics of groups of Lagrangian particles. We calculate third and fourth order anomalous exponents for several dimensions, comparing with the predictions of perturbative calculations in large dimensions. We find that Kraichnan’s closure appears to give results in close agreement with the numerics. The third order exponents are compatible with our own previous nonperturbative calculations.

The Kraichnan rapid advection model [4] is a simplified model for turbulent advection of a passive scalar \( T(r) \) in which the velocity field scales in space but decorrelates in time infinitely rapidly. The scaling properties of this model are interesting: The structure functions \( S_n(R) \equiv \langle (T(r + R) - T(r))^n \rangle \) depend on \( R \) like power laws, \( S_n(R) \sim R^\zeta_n \), and the exponents \( \zeta_n \) are “multiscaling” in the sense that they are nonlinear functions of the index \( n \) in contraction with classical (Kolmogorov) approaches. The importance of this model lies in the fact that it has been the first example in which the mechanism for multiscaling, which appears also in Navier-Stokes turbulence [2], has been identified [3], and in which a controlled calculation of scaling exponents is possible. As such it is an important laboratory for testing ideas that may pertain also for the understanding of multiscaling in Navier-Stokes turbulence. It is not surprising therefore that it drew enormous attention and theoretical efforts. To date, the scaling exponents in the Kraichnan model have been calculated only in a small part of the parameter space, with an explicit solution in the former case, and by a finite difference scheme in the latter [1].

In a recent article [12], we presented a new interpretation of the phenomenon of anomalous scaling in passive scalar correlation functions: the theory connects between the scaling exponents \( \zeta_n \) and the relaxation rates of the geometric shape formed by \( n \) points advected by the turbulent flow. Starting from a generic distribution in the space of shapes, the stochastic advection can be considered as a relaxation to the invariant measure in this space, while the over-all scale undergoes a Richardson diffusion. In this Letter we apply the theory, using Monte-Carlo methods, to calculate the scaling exponent throughout the entire parameter space [3]. We generate random sample paths for the \( n \) trajectories, and measure the shape relaxation rate by the standard method of analyzing the autocorrelation of the signal. Compared to direct numerical simulation, this method demands relatively modest computing resources: there is no need to keep track of the whole scalar field. The realizations of random velocity are generated only at the instantaneous positions of the advected points, and this amounts to sampling a small set of correlated Gaussian random variables. Hence, it is possible to perform simulations in arbitrary integer dimensions. Another advantage of the Monte-Carlo method is that it is trivially parallelizable, in the sense that the data is collected from numerous independent realizations, whose calculation is completely independent, and may therefore be performed on different machines. Nevertheless, the accurate calculation of the anomalous exponents is still not easy, due to slow convergence rate and the large number of realizations that is therefore required.

The Kraichnan model describes the advection of a passive scalar by a random velocity field \( u \) which is Gaussian, \( \delta \)-correlated in time, incompressible and self similar in space:

\[
\langle (u(r, t) - u(r', t)) \otimes (u(r, t') - u(r', t')) \rangle = h(r - r') \delta(t - t'),
\]

\[
h(r) = \left( \frac{r}{\ell} \right)^\xi \left( 1 - \frac{\xi}{d-1+\xi} \frac{r \otimes r}{r^2} \right).
\] (1)

The passive scalar is driven by a large scale forcing (of scale \( L \)), which is taken Gaussian and \( \delta \)-correlated in time as well. The fundamental objects of the Kraichnan model are the many point correlation functions

\[
\mathcal{F}_{2n}(r_1, r_2, \ldots, r_{2n}) \equiv \langle T(r_1, t)T(r_2, t) \ldots T(r_{2n}, t) \rangle,
\] (2)
where pointed brackets denote an ensemble average with respect to the stationary statistics of the forcing and the statistics of the velocity field.

The correlation functions may be expanded in a series of scale invariant terms, i.e., terms which are homogeneous functions of their variables. The most important term for $R/L \to 0$ is expected to be a zero mode of the Kraichnan partial differential operator $\mathcal{K}$. The functions $\mathcal{F}_{2n}$ contain, in addition to their own zero-modes, also contributions from the zero modes of lower order functions and normal scaling contributions due to the external forcing. These do not contribute however to the $n$th order structure functions, and thus do not affect the scaling exponent $\zeta_n$. The question is how to compute the homogeneity exponents of the zero modes. Kraichnan himself avoided this (difficult) problem and suggested a closure procedure whose main result is a convenient definition of the overall scale and the shape variables is fixed by the sum of edge lengths, and the shape by two angles of the triangle defined by the three points. The configuration of these points can be described by trial and error to minimize the effective action for the evolution operator; its large scale reaches the value $s > s_0$ and the invariant measure, with increasing exponents $\lambda_{n,m}$. Ref. [12] established a correspondence which implies that the exponents $\lambda_{n,m}$ are precisely the set of anomalous scaling exponents of the $n$th order correlation function. The functions $\mu_m$’s are the adjoint family of left eigenfunctions of $\gamma_n$, and are the corresponding scaling structures, namely the zero modes of the Kraichnan operator.

The basic ingredient for the numerical implementation of the shape dynamics for the calculation of scaling exponents is a finite difference approximation of the solution of eqs. (10) describing the random Lagrangian trajectories of the $n$ points. We used the simple Ito-Euler method for this purpose [14], which makes the approximation

$$r_i(t + \delta t) \sim r_i(t) + \sqrt{\delta t} \eta_i(t),$$

where the $\eta_i$ are a set of Gaussian random vectors whose covariance as a function of $s$ is given by the spatial part of the covariance of the $n$ random vectors $u(r_i)$. The results of the difference scheme [14] are then used to calculate the instantaneous scale $s(t)$ using some convenient definition of $s$ (we used the square root of the sum of squares of point separations). We fixed a set of threshold values for $s$ spaced logarithmically, and for each event where the value of $s$ increases for the first time beyond one of the threshold values, we record the instantaneous value of a certain function of the shape $\sigma(Z)$. Once more, the function $\sigma$ is largely arbitrary; however, it has to be a permutation-symmetric function of the coordinates.

To extract the relaxation rates, it is convenient to calculate the autocorrelation of the signal $\sigma(s)$. In fact (for $s < s')$

$$\langle \sigma(s)\sigma(s') \rangle = \int dz'dz'' \beta_0(\mathbf{Z}) \gamma_n(\mathbf{Z}, \mathbf{Z'}, s'/s)\sigma(\mathbf{Z})\sigma(\mathbf{Z'}) = \langle \sigma \rangle_0^2 + \langle \sigma \rangle_0 (\langle \sigma \rangle_1 \left( s'/s \right)^{-\lambda_{n,1}} + \cdots),$$

where $\langle \rangle_m$ denote average with respect to $\beta_m$. Thus, the autocorrelation function of $\sigma$ relaxes to a constant, and the asymptotic relaxation rate is equal to the $n$th order structure function scaling exponent $\zeta_n$. The precise measurement of the scaling exponent is not easy, however, since the signal contains a constant whose fluctuation tend to mask the decaying part which contains the scaling information. Additionally, in the case of $n = 4$ where we consider below, three point contributions contaminate the signal with relatively persistent transients. For this reason a very large number of realizations, $O(10^6)$, is required to measure a scaling exponent, and the function $\sigma$ needs to be tuned carefully to decrease the effect of transients [15]. Indeed, the autocorrelation for any generic definition of $\sigma$ decays asymptotically with an exponent $\zeta_n$, however, for a poorly chosen definition of $\sigma$, the transients may dominate for a very large range. We have tuned our definitions for $\sigma$ by trial and error to expose the asymptotic decay rate as early as possible.
We removed the constant from the autocorrelation signal using two methods, the first was by numerically differentiating the autocorrelation signal, and the second by subtracting the value of the autocorrelation at the farthest separation measured \((s/s_0 = 100)\). Both methods give consistent results though the numerical differentiation is more noisy while subtraction tends to introduce a bias in the large \(s\) results.

In our \(n = 3\) calculations we used

\[ \sigma_3 = \log(l_{12}) + \log(l_{13}) + \log(l_{23}) \]  
and in the four point

\[ \sigma_4 = (l_{12}l_{34})^4 + (l_{13}l_{24})^4 + (l_{14}l_{23})^4. \]

Where \(l_{ij}\) is the distance between points \(i, j\) normalized such that \(\sum_{i<j} l_{ij}^2 = 1\).

The case of third order correlation function exponents deserves attention, being the simplest non-trivial one. The Lagrangian paths are relatively easy to generate in this case, and the number of realizations needed to observe scaling behavior is smaller than in the four point case. Additionally, [11] demonstrated that three point correlation function can be calculated directly by a finite difference scheme, and thus the two calculations can be tested against each other for consistency.

We generated a set of data for three point relaxation rates in 4 dimensions for various values of \(\xi\). The number of required realizations was \(O(10^5)\), except for small values of \(\xi\) where a larger number is required. We also generated data for \(\xi = 1\) for several space dimensionalities, as in the four point case discussed below. In fig. 1 we display a typical data set measuring the relaxation of the three point distribution to its invariant measure.

Similar results were obtained for the three point simulations for other parameter values, with generally a longer scaling range the closer is \(\xi\) to 2. The results are summarized in fig. 2, along with the leading scaling exponents calculated by the method of [11]. We find satisfactory agreement between the predictions of the two methods, providing support for the validity of the present theoretical and numerical framework.

FIG. 2. The leading three point scaling exponent in four dimensions, calculated as a function of \(\xi\) by the present Monte-Carlo method (circles) and by the method of [11]is difficult to estimate the systematic errors in the results of the latter method so no error bars are given. However, we have indications that these errors are smaller the statistical errors, except when \(\xi\) is near 2. In the latter case we use results whose accuracy is higher than those published in[11].

Possibly the main interest in our method is in its ability to provide measurement of \(\zeta_4\) from the simulation of four point relaxation. In measuring \(\zeta_4\) we concentrated on a scan through various dimensions and fixed \(\xi = 1\). The possibility of performing measurements in various dimensions (including the ‘physical’ \(d = 3\) case) exemplifies the superiority of this algorithm with respect to direct numerical simulations, where dimensions larger than 2 are inaccessible due to memory requirements. The \(d\)-scan allows us to test, for the first time, the perturbative large \(d\) expansion results [8,12]. In fig. 3 we show the results of a typical four point calculation.
The results of the three and four point simulations as a function of $d$ are summarized in fig. 4, along with the prediction of large $d$ perturbation theory, and the prediction of Kraichnan’s closure. We find that Kraichnan’s prediction agrees well with the $\zeta_4$ results, whereas the perturbative calculations are still not relevant. We cannot estimate how large $d$ should be to agree with the large $d$ perturbation theory. The prediction for $\zeta_3$ (given in [12]) is in rough agreement with our simulations.

In summary, Lagrangian trajectory approach (developed independently by [13]) is seen to provide a numerical tool allowing us to compute the anomalous exponents of the Kraichnan model, in principle for the entire parameter space. The simulations are based on a new interpretation of anomalous scaling linking it to relaxation rates in the stochastic shape dynamics; the success of the simulations provides further support to this physically appealing picture of anomalous scaling in this model. Finally we note that the basic principles employed here are not specific to the Kraichnan model, and it might be possible to use them in other contexts, perhaps sacrificing some of the simplicity. In particular, the fact that we need to consider only $n$ points simultaneously depends heavily on the $\delta$-correlated nature of the velocity, and would probably not carry over to more realistic situations.

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