A differentiable trajectory approximation to turbulent diffusion

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The problem of turbulent diffusion is posed as determining the time evolution of the probability density of the concentration given those for the fluid velocity components, sources, and the initial concentration. At each time, all variables are elements of the Hilbert space $L_R^2(R^3)$, and a finite-dimensional approximation based on expansions in orthonormal basis functions is developed. An expression for the joint probability density of all the Fourier coefficients is derived, the evaluation of which is shown to be particularly straightforward. Diffusion of material from a single source in an unbounded mildly turbulent fluid is considered as an application.

I. INTRODUCTION

The essential problem associated with turbulent diffusion may be stated as follows: Determine the time evolution of the probability density of the concentration of a passive scalar in a fluid, given knowledge of the probability densities of the fluid velocity components and of the sources and initial distribution of material. More specifically, the instantaneous concentration c of a passive scalar in a fluid having velocity u is governed by the species conservation equation and initial condition

$$\frac{\partial c}{\partial t} + u \cdot \nabla c = \mathfrak{D}\nabla^2 c + S\,, \tag{1}$$

$$c(x,0) = c_0(x)\,, \tag{2}$$

where $\mathfrak{D}$ is the molecular diffusivity of the species in the medium and S is the rate of introduction of material into the fluid. The random nature of the concentration c arises because of the random character of the fluid velocity u.

When attacked from a rigorous point of view, the problem of predicting the probability density of c leads one to the theory of Markov processes in functional spaces, which, although actively being pursued, (starting with Baklan[1]), has not yet yielded results of direct applicability to turbulent diffusion. Hopf[2] introduced ideas for obtaining turbulent solutions to the Navier–Stokes equations. If Hopf's equation for the characteristic functional were solved, that information could be used as input in Eq. (1). A modern justification of some aspects of Hopf's theories has led to increased interest in that approach.[3] The discovery of strange attractors in physical situations[4] motivated the generalization of bifurcation ideas for quasi-periodic solutions, and a complete theory about the nature of turbulence is forming along these lines.[5]

Because of the general feeling that infinite-dimensional theories of turbulence are not yet at the point of practical implementation, most current approaches rely on the concept of the spectrum of turbulence. The wavenumbers of the spectrum can be visualized as the inverse of eddy sizes, and intuitive reasoning can be used to impose structure on the behavior of the eddies through equations involving wavenumbers. We do not choose to invoke spectral arguments in the work that follows.

There have been a number of notable attempts to approach the probabilistic problem defined at the outset in an approximate manner. Cameron and Martin,[6] based on earlier ideas of Wiener, created an L^2 theory for functionals on the trajectories of Gaussian random fields. They showed that any such functional can be expanded in a countable series of functionals X_m, sometimes referred to as the Cameron–Wiener–Hermite polynomials. Least-squares theory allows one to use truncated expansions in the conservation equations satisfied by the original functional to produce a finite set of differential equations that is an approximation for the infinite-dimensional system. This approach has been pursued by Crow and Canavan[7] for the Navier–Stokes equations assuming that the velocity u is a Gaussian functional and by Saffman[8] for turbulent diffusion, with similar considerations for the concentration c. Although criticism of this approach has been expressed because the results fail to reproduce the inertial range behavior of the spectrum of u predicted by Kolmogoroff's theory,[9] the principal drawback of the method lies in the numerical effort required even for low-order approximations. For example, the Cameron–Wiener–Hermite functional can be expressed as

$$X_m = \int K_m \, d\rho_m\,, \quad m = 0, 1, \ldots\,, \tag{3}$$

where K_m is a deterministic, real function of m real variables, and ρ_m is an m-dimensional random measure. Subsituting Eq. (3) into Eq. (1) and collecting terms of like order, one obtains partial differential equations for the K_m, the order and complexity of which increase with m.

In this work we propose an approach to turbulent diffusion by finite-dimensional approximation in the general spirit of Cameron–Wiener–Hermite expansions. By imposing certain restrictions on the class of random functionals being approximated, the level of complexity is reduced substantially from that of the Cameron–Wiener–Hermite approaches. The essential elements of the method are presented in the next section. Then, the problem of predicting the probability density of the concentration of a passive scalar released from a source

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in a fluid of infinite extent is studied. The computational aspects of the method are also briefly discussed.

II. DIFFERENTIABLE TRAJECTORY APPROXIMATION

We are interested in obtaining a solution for the probability density of c in Eq. (1) given probability densities of u, S, and c_0. Because, as we noted earlier, this problem in its most general form requires the theory of Markov processes in infinite-dimensional spaces, with which we are not yet prepared to deal, it is necessary to restrict the scope of the problem being considered. Our purpose is to determine the probability density of c in a situation in which material is released from a source in a fluid commencing at some time, say $t=0$. In such a case it is natural to assume that the initial concentration c_0 decays to zero infinitely far from the source (the origin) as to be square-integrable. (In fact, the most convenient choice of the initial concentration is $c_0=0$.) If so, the concentration at some finite time $t>0$ will also be square-integrable. Because the velocity field contains finite energy, we expect the velocity field to be square-integrable over the entire space. More precisely, the velocity field $u=(u_1,u_2,u_3)$, S, c_0, and c are elements of Hilbert space $X=L^2_R(R^3)$. Subsequently, we denote the inner product of two elements, f,g of X by $\langle f,g\rangle$. The assumption of square-integrable velocity fields is not restrictive, since all velocity fields must contain only finite energy when considered on a large enough spatial scale (see Section 3.6 of Lumley).[10]

One of the important properties of X is that it is separable and, therefore, has a countable complete orthogonal basis $B=(\psi_i, i=0,1,2,\ldots)$. Then, the elements of X are limits of series, the terms of which are the elements of B multiplied by the generalized Fourier coefficients

$$\begin{aligned} u_j(x,t)&=\sum_i \alpha_{ij}(t)\psi_i(x), \quad j=1,2,3\,,\\ c(x,t)&=\sum_i \beta_i(t)\psi_i(x)\,,\\ S(x,t)&=\sum_i \gamma_i(t)\psi_i(x)\,,\\ c_0(x)&=\sum_i \xi_i\psi_i(x)\,. \end{aligned} \tag{4}$$

The Fourier coefficients are given by relations of the form

$$\xi_i=\langle c_0,\psi_i\rangle, \quad i=0,1,2,\ldots\,,$$

The coefficients α_{ij}, β_i, and γ_i are random processes, whereas the ξ_i are random variables. Given specifications of the statistical properties of the α_{ij}, γ_i, and ξ_i, use of Eqs. (4) will reduce the general problem to that of determining the statistical properties of the β_i.

Substituting Eqs. (4) into Eq. (1), and assuming that the derivatives obtained are also in X, we get

$$\chi=\sum_i \dot\beta_i\psi_i+\sum_{k=1}^{3}\sum_i\sum_j \alpha_{ik}\beta_j\psi_i\frac{d\psi_j}{dx_k}-\sum_i\gamma_i\psi_i=0\,. \tag{5}$$

Using the completeness of B, we produce a countable number of equations by means of

$$\langle\chi,\psi_n\rangle=0; \quad n=0,1,2,\ldots\,. \tag{6}$$

The orthonormality of B gives Eqs. (6) the compact form

$$\dot\beta+\Omega\beta-\gamma=0\,, \tag{7}$$

where $\beta=(\beta_0,\beta_1,\ldots)$ and $\gamma=(\gamma_0,\gamma_1,\ldots)$ are in l^2_R and $\Omega=(\omega_{ij})$, where

$$\omega_{ij}=\sum_{k=1}^{3}\sum_l \alpha_{lk}\left\langle\psi_l\frac{d\psi_j}{dx_k},\psi_i\right\rangle. \tag{8}$$

We note that inclusion of the molecular diffusion term $\mathfrak{D}\nabla^2 c$ alters the expression for ω_{ij}, only through the addition of

$$\sum_{k=1}^{3}\left\langle\frac{d^2\psi_j}{dx_k^2},\psi_i\right\rangle\,,$$

with the form of Eq. (7) as a first-order ordinary differential equation in time remaining.

The limitations of this approach are essentially that the coefficients β_i should be differentiable with respect to t, and the α_{ij} and γ_i be sufficiently regular so as to guarantee the existence and uniqueness of solutions. Therefore, we cannot deal with random vector fields in complete generality. (The trajectories of Wiener processes are, for example, nowhere differentiable.) However, we allow each of the coefficients to be random variables at each time, with the condition that their values cannot change abruptly in small time intervals. This class of random fields is wide enough for many applications, particularly those in which measurements of the variables are repeatedly taken to determine their probability distributions.

Then, we can consider Eq. (7), by virtue of the least-squares theory in Hilbert spaces[11] as n-dimensional, with a degree of accuracy directly related to the number n of terms retained in the expansions of the variables.

At this point we are going to assume that the coefficients α and γ do not depend on time so that Eq. (7) is autonomous. If explicit dependence on t is unavoidable, then defining $\beta_{-1}=t$, $\gamma_{-1}=0$, $\beta=(\beta_{-1},\beta_0,\ldots)$ and $\gamma=(\gamma_{-1},\gamma_0,\ldots)$, Eq. (7) becomes

$$\dot\beta+\Omega(\beta_{-1})\beta-\gamma=0\,,$$

which is autonomous but nonlinear. Nevertheless, the theory to be discussed is still valid, although the analytical solutions are not available.

Through the approximations embodied in truncating Eqs. (4), Eq. (1) has been transformed into the finite set of ordinary differential equations, Eq. (7), in which the dependent variables are the coefficients β_i and the parameters are the coefficients α_{ij} and γ_i. The stochastic problem then involves determining the probability density of β_i given those for α_{ij} and γ_i, namely, those characterizing the velocity field and the source, and that for ξ_i, arising from the initial concentration. Let the joint probability density of β, α, and γ be $p(\beta,\alpha,\gamma;t)$. From Eq. (7), p can be shown to satisfy the conserva-

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tion equations

$$\frac{\partial p}{\partial t} + \operatorname{div}(pF) = 0 , \tag{9}$$

where $F(\beta,\alpha,\gamma) = [-\Omega(\alpha)\beta + \gamma, 0, 0]^T$.

The solution of Eq. (9) is[12]

$$p(\beta,\alpha,\gamma,t) = p_0[\Phi(\beta,\alpha,\gamma,-t),\alpha,\gamma]\exp(t\,\mathrm{tr}\,\Omega) , \tag{10}$$

where

$$\Phi(\beta,\alpha,\gamma,t) = \left[\exp(-\Omega t)\left(\int_0^t \exp(\Omega s)\gamma\, ds + \beta\right),\alpha,\gamma\right]^T , \tag{11}$$

and where p_0 is the initial joint probability density of ξ, α, and γ. If ξ, α, and γ are assumed to be mutually stochastically independent,

$$p_0(\xi,\alpha,\gamma) = p_{0_\xi}(\xi)p_{0_\alpha}(\alpha)p_{0_\gamma}(\gamma) . \tag{12}$$

When Ω is invertible, Eq. (9) can be expressed completely in terms of the eigenvalues λ_i and corresponding eigenvectors z_i of Ω and its inverse Ω^{-1}, i.e.,

$$\Phi(\beta,\alpha,\gamma,t) = \left(\sum_j \frac{z_j^T(\beta - \Omega^{-1}\gamma)}{\|z_j\|^2} z_j \exp(\lambda_j t) + \Omega^{-1}\gamma,\alpha,\gamma\right)^T . \tag{13}$$

The standard choice of basis for $L^2(R)$ is

$$\phi_i(x) = d_i \exp(-x^2/2)H_i(x), \quad i = 0,1,2,\ldots , \tag{14}$$

where H_i is the Hermite polynomial of degree i, and

$$d_i = (\pi^{1/2}2^i i!)^{-1/2} . \tag{15}$$

The extension to R^3 can be obtained from

$$\psi_I(x) = \phi_i(x_1)\phi_j(x_2)\phi_k(x_3) , \tag{16}$$

where $I = (ijk)_n$ (the number ijk in base n) and n is the maximum degree of the Hermite polynomials entering the basis elements.

Some properties of the standard basis for X allow us to obtain information about the structure of Ω. Since the Hermite polynomials are generated by

$$H_n(x) = (-1)^n \exp(x^2)\frac{d^n}{dx^n}\exp(-x^2) , \tag{17}$$

they obey certain recursion relations, of which the most useful are

$$\begin{aligned} &\frac{dH_m(x)}{dx} = 2mH_{m-1}(x) , \\ &\frac{d^2H_m(x)}{dx^2} - 2x\frac{dH_m(x)}{dx} + 2mH_m(x) = 0 , \\ &H_{m+1}(x) = 2xH_m(x) - 2mH_{m-1}(x) . \end{aligned} \tag{18}$$

Equations (16) and (18) permit one to express the elements of Ω as linear combinations of integrals containing only ϕ's and their products. These integrals can finally be reduced to either of the forms

$$\begin{aligned} &\int_{-\infty}^{\infty} x^{2m}\exp\left(\frac{-x^2}{2}\right)dx = (2\pi)^{1/2}(2m-1)!! \\ &\int_{-\infty}^{\infty} x^{2m+1}\exp\left(\frac{-x^2}{2}\right)dx = 0 . \end{aligned} \tag{19}$$

As a result, the evaluation of the essential result, Eq. (10) can largely be carried out analytically. Because of the second of Eqs. (19), Ω will be sparse. In addition, Ω can be decomposed into symmetric and skew-symmetric parts, greatly simplifying the evaluation of eigenvalues and eigenvectors.

III. SOURCE IN AN INFINITE FLUID

We will apply the foregoing theory to a simple, idealized case. We consider a fluid in which the three velocity components u_1, u_2, and u_3 are random variables, but temporally and spatially independent. The fact that such functions are not elements of $L^2(R)$ does not prevent us from using the method, because that which is essential for convergence is $c \in X$. When the velocity field is also in X, the basis of X can be used throughout. In the current case, the results cannot be expected to be realistic as $x \to \pm\infty$. Because of the restriction that velocity components are to be temporally and spatially independent, expansion in the Fourier coefficients is not necessary, and we can merely retain u_1, u_2, and u_3 themselves as the random variables characterizing the velocity field. Because the proposed method is new, we have chosen to focus on an example that affords an analytical solution, thereby clearly illustrating the use of the method.

Suppose that there is a single source centered at the origin that commences at $t = 0$ with constant material release rate A. We choose to represent the spatial variability of S in the form

$$S(x,t) = C\psi_0(x) = C\pi^{-3/4}\exp(-\|x\|^2/2) . \tag{20}$$

With the restriction of total mass conservation

$$A = \int_{R^3} C\psi_0\, d\mu \tag{21}$$

(μ denoting Lebesgue measure), C is determined as $A2^{-3/2}\pi^{-3/4}$. Although the spatial dependence of S is specified, the release rate A may be considered as a random variable.

Summarizing, the joint probability density characterizing the concentration distribution is $p(\beta,u_1,u_2,u_3,A,t)$, and the applicable form of Eq. (10) is

$$p(\beta,u_1,u_2,u_3,A,t) = p_0[\Phi(\beta,u_1,u_2,u_3,A,-t),u_1,u_2,u_3,A] \times \exp(t\,\mathrm{tr}\,\Omega) . \tag{22}$$

The elements of Ω in this case are

$$\omega_{ij} = \sum_{k=1}^{3} u_k \left\langle \frac{d\phi_{i_k}(x_k)}{dx_k}, \phi_{j_k}(x_k)\right\rangle \delta_k , \tag{23}$$

where $i = (i_1 i_2 i_3)_n$, $j = (j_1 j_2 j_3)_n$, and δ_k is $\delta_{i_r j_s}\delta_{i_s j_r}$, where δ_{i_m} is the Kronecker delta and $k \neq r \neq s \neq k$.

A first observation tells us that, since the subscript l of Eq. (8) does not appear here, Ω is skew-symmetric. A simple integration by parts using the asymptotic behavior of the ϕ_i's,

$$\left\langle \frac{d\phi_i}{dx}, \phi_j\right\rangle = \int_R \frac{d\phi_i}{dx}\phi_j\, dx = -\left\langle \phi_i, \frac{d\phi_j}{dx}\right\rangle , \tag{24}$$

confirms this statement. Also, calling

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$$\tilde{\omega}_{ij}^{k}=\left\langle \frac{d\phi_{i_k}(x_k)}{dx_k},\phi_{j_k}(x_k)\right\rangle \delta_k\,,\quad k=1,2,3, \tag{25}$$

and using Eqs. (18), we obtain

$$\begin{aligned}\frac{d\phi_i(x)}{dx}&=d_i\exp(-x^2/2)[H_i'(x)-xH_i(x)]\\&=d_i\exp(-x^2/2)\{2iH_{i-1}(x)-\tfrac{1}{2}[H_{i+1}(x)+2iH_{i-1}(x)]\}\\&=d_i\exp(-x^2/2)[iH_{i-1}(x)-\tfrac{1}{2}H_{i+1}(x)]\,,\end{aligned} \tag{26}$$

and

$$\tilde{\omega}_{ij}^{k}=\frac{d_{i_k}}{d_{j_k}}\left(i_k\delta_k^{-}-\frac{1}{2}\delta_k^{+}\right)\delta_k\;;\quad k=1,2,3\,, \tag{27}$$

where $\delta_k^{-}=\delta_{i_k-1,j_k}$ and $\delta_k^{+}=\delta_{i_k+1,j_k}$. We can simplify Eq. (25) to a form suitable for constructing Ω. Since δ^{-} and δ^{+} cannot be simultaneously different from zero, we have:

(i) if $\delta_k^{-}=1$, then $\delta_k^{+}=0$, and $j_k=i_k-1$, which leads to

$$\tilde{\omega}_{ij}^{k}=(i_k/2)^{1/2}\delta_k\,; \tag{28}$$

(ii) if $\delta_k^{+}=0$, by parallel reasoning,

$$\tilde{\omega}_{ij}^{k}=-(j_k/2)^{1/2}\delta_k\,. \tag{29}$$

Equations (28) and (29) indicate that, as expected, Ω can be decomposed into blocks, each of which reflects the number of terms used in the orthogonal expansions. These comments are illustrated in a second-degree ($n=3$) evaluation of Ω, shown in Fig. 1. We have superposed $\tilde{\Omega}_1$, $\tilde{\Omega}_2$, and $\tilde{\Omega}_3$ for economy of space, but it should be noted that $\Omega=u_1\tilde{\Omega}_1+u_2\tilde{\Omega}_2+u_3\tilde{\Omega}_3$. As a consequence, $\Omega=0$, if and only if, $u_1=u_2=u_3=0$.

In this example, $\operatorname{tr}\Omega=0$, so that Eq. (22) becomes

$$\begin{aligned}&p(\beta,u_1,u_2,u_3,A,t)\\&\quad=p_0[\Phi(\beta,u_1,u_2,u_3,A,-t),u_1,u_2,u_3,A]\,,\end{aligned} \tag{30}$$

where

$$\Phi=\left[\exp(-\Omega t)\left(A\int_0^t[\exp(\Omega s)]_1 ds+\beta\right),u_1,u_2,u_3,A\right]^T, \tag{31}$$

where $[\exp(\Omega s)]_1$ denotes the first column of $\exp(\Omega s)$. Physically, $\operatorname{tr}\Omega=0$ indicates that the initial concentration distribution is distorted due to randomness in the velocity field, but that the value of the probability density is not modified by the flow Φ. This observation is in agreement with the classical theory of turbulent diffusion.[13]

This example can be computationally implemented as follows:

(1) Choose the number of terms in the approximate expansion of C, and construct $\tilde{\Omega}_1$, $\tilde{\Omega}_2$, $\tilde{\Omega}_3$.

(2) Measure the values of u_1,u_2,u_3 of interest.

(3) Accumulate records of velocity and calculate approximately the probability density of u_1, u_2, and u_3.

(4) Evaluate Ω and its eigenvalues.

(5) For chosen values of β and t, evaluate $p(\beta,u_1,u_2,u_3,A;t)$

(6) For subsequent actualizations, start at 2.

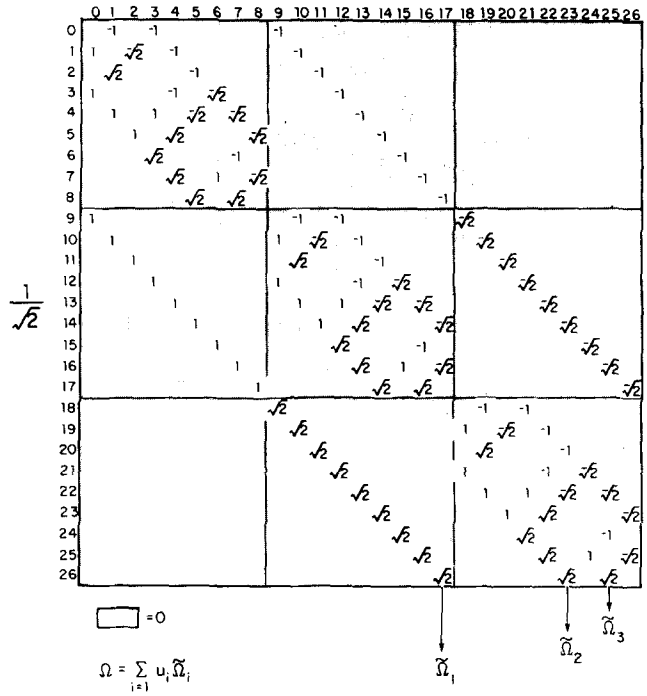

FIG. 1. The square matrix Ω, when the first three terms of the standard basis $\{\phi_i,\ i=0,1,\ldots\}$ of $L_R^2(R)$ are used to generate the $\{\psi_j,\ j=0,1,\ldots\}$, has dimension 27. Numbers ranging from 0 to 26 label the rows and columns, each being the decimal expression of the multi-index $(ijk)_3$ formed by the integers $0\leq i,j,k\leq 2$. For example, $\omega_{15,20}$ is associated with $\psi_{15}(x_1,x_2,x_3)=\psi_{(120)_3}(x_1,x_2,x_3)=\phi_1(x_1)\phi_2(x_2)\phi_0(x_3)$ and $\psi_{20}(x_1,x_2,x_3)=\psi_{(202)_3}(x_1,x_2,x_3)=\phi_2(x_1)\phi_0(x_2)\phi_2(x_3)$. The numbers appearing in the parallel to the diagonal indicated as $\tilde{\Omega}_k\,(k=1,2,3)$ and its reflection, should be multiplied by $u_k/\sqrt{2}$ to obtain Ω. The blank areas represent zeros.

We point out that in this case the sparseness and skew symmetry of Ω enable one to use computational methods of relative simplicity for each of the steps of the algorithm. Another important property that comes from the inspection of the $\tilde{\Omega}_i$ is commutativity, and therefore the following relation can be used

$$e^{\Omega t}=\exp(u_1t\tilde{\Omega}_1)\exp(u_2t\tilde{\Omega}_2)\exp(u_3t\tilde{\Omega}_3)\,. \tag{32}$$

In step (5) we can choose two different forms for evaluating p, depending on the existence of Ω^{-1} [see Eqs. (11) and (13)]. The invertibility of Ω will depend not only on the values of u_1,u_2,u_3, but on the order of the approximation. Consider, for instance, the case $u_1=u_2=0$, $u_2=1$. Then, the blocks

$$\begin{pmatrix}0&-1&0\\1&0&-\sqrt{2}\\0&\sqrt{2}&0\end{pmatrix}$$

are all singular, and, therefore, $\tilde{\Omega}_3=\Omega$ is singular, with eigenvalues $0,\sqrt{3}i,-\sqrt{3}i$. But, if we increase by one the number of basis elements, we get the block

$$\begin{pmatrix}0&-1&0&0\\1&0&-\sqrt{2}&0\\0&\sqrt{2}&0&-\sqrt{3}\\0&0&\sqrt{3}&0\end{pmatrix}$$

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that is invertible (eigenvalues: $\pm(3+\sqrt{6})^{1/2}i, \pm(3-\sqrt{6})^{1/2}i$. Therefore, the eigenvalues will appear in nonzero conjugate pairs (Ω invertible) with another zero eigenvalue when we use an odd number of basis elements (Ω singular).

IV. CONCLUSIONS

We have presented an approach for approximating the solution to a wide class of turbulent diffusion problems, which compares favorably with the Wiener–Hermite expansions in computational effort. The formalism has particular attractiveness in situations in which actual measurements of the velocity field are available from which to construct probability densities of the three components. In obtaining the input Fourier coefficients α, γ, ξ from the data, the same L^2 theory can be used, leading to algebraic rather than differential equations. The extension of the present work to stationary processes with countable spectra can be envisioned (see Sec. 3.12 of Lumley)[10]. However, the functional calculus in spaces other than L^2 is considerably more involved than that for L^2, and this aspect has not been pursued here.

We have used the term "differentiable trajectory" in describing the method to highlight the key assumption that the coefficients β of the concentration c are differentiable. When several sources or sinks are present, the linearity of the conservation equations, transmitted to the equations for the probability density, allows for the superposition of solutions. The convergence of the approximate solutions is an essential advantage of the function space dictated by the physics of the problem.

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