Probability Density Function Method for Langevin Equations with Colored Noise

Peng Wang,[1,*] Alexandre M. Tartakovsky,[1,†] and Daniel M. Tartakovsky[2,‡]
[1]*Pacific Northwest National Laboratory, Richland, Washington 99352, USA*
[2]*University of California, San Diego, 9500 Gilman Drive, La Jolla, California 92093, USA*
(Received 26 October 2012; published 2 April 2013)

Understanding the mesoscopic behavior of dynamical systems described by Langevin equations with colored noise is a fundamental challenge in a variety of fields. We propose a new approach to derive closed-form equations for joint and marginal probability density functions of state variables. This approach is based on a so-called large-eddy-diffusivity closure and can be used to model a wide class of non-Markovian processes described by the noise with an arbitrary correlation function. We demonstrate the accuracy of the proposed probability density function method for several linear and nonlinear Langevin equations.

DOI: 10.1103/PhysRevLett.110.140602 PACS numbers: 05.10.Gg, 02.50.Fz

Langevin equations are ubiquitous in virtually every scientific field, ranging from physics, biology, and chemistry to economics and electronics. They provide a mesoscale description of systems that are subjected to (either internally generated or externally imposed) random excitations (Langevin forces). The classical treatment of Langevin problems approximates these excitations as Gaussian white noise, which is appropriate for Markovian systems. These assumptions are not appropriate for a large class of natural phenomena with temporally correlated and non-Gaussian Langevin forces (see Appendix A1 of Ref. [1] and the references therein). Analysis of such non-Markovian systems, described by Langevin equations with "colored noise," remains an open challenge.

Langevin (stochastic ordinary-differential) equations

$$\frac{dX_i}{dt} = h_i(\mathbf{X}, t) + \sum_{j=1}^{N} g_{ij}(\mathbf{X}, t)\xi_j(t), \qquad i = 1, \ldots, N, \tag{1}$$

describe the temporal evolution of N state variables $\mathbf{X} = \{X_i\}_{i=1}^N$. The dynamics of each system variable $X_i(t)$ consists of a slowly varying (deterministic) part h_i and a quickly varying random part $g_{ij}\xi_j$, in which fluctuations $\xi_j(t)$ have zero mean and a two-point covariance function

$$C_{ij}(t, s) \equiv \langle \xi_i(t)\xi_j(s)\rangle = q_{ij}\delta_{ij}\rho_{ij}(t, s). \tag{2}$$

Here, q_{ij} is the variance, δ_{ij} is the Kronecker delta function, and ρ_{ij} is the correlation function. At any given time t, the system's state is defined by the joint probability $P[X_1 \le x_1, \ldots, X_N \le x_N; t]$ or, equivalently, by its joint probability density function (PDF) $p_{\mathbf{X}}(\mathbf{x}; t)$.

The derivation of equations that govern the dynamics of $p_{\mathbf{X}}(\mathbf{x}; t)$ in systems with uncorrelated in time ("white") noise $\boldsymbol{\xi}(t)$, i.e., with $\rho(t, s) = \tau\delta(t - s)$ (τ is the characteristic time), is relatively straightforward. For $\boldsymbol{\xi}(t)$ with an arbitrary pointwise distribution, these equations are called the Kramers-Moyal expansion (KME); the latter reduces to the Fokker-Planck equation (FPE) if $\boldsymbol{\xi}(t)$ is Gaussian [1]. To render the KME computable, it has to be truncated after a finite number of terms. This truncation can give rise to negative values of PDF (see p. 9 of Ref. [1]).

Treating the Langevin force $\boldsymbol{\xi}(t)$ as white noise is appropriate if fluctuations occur on time scales that are much smaller than that of the mesoscale variables $\mathbf{X}(t)$. Two distinct frameworks have been proposed to deal with non-Markovian systems with colored noise $\boldsymbol{\xi}(t)$.

The first approach introduces an additional Markovian process to describe the evolution of $\boldsymbol{\xi}(t)$. The resulting enlarged system is Markovian and, hence, can be described by a FPE for the joint PDF of $\mathbf{X}$ and $\boldsymbol{\xi}$ (see Sec. 3.5 of Ref. [1]). Then, $p_{\mathbf{X}}$ is obtained by marginalizing a solution of this FPE with respect to $\boldsymbol{\xi}$. Alternatively, the enlarged (Markovian) system of Langevin equations can be solved with the unified colored noise approximation (UCNA) [2]. In UCNA, only limited functional forms of ρ_{ij} allow a Markovian representation. When UCNA is applicable, it is valid only for certain conditions (e.g., large times), and its computational cost soars as the phase dimension increases. It is computationally prohibitive for systems with many degrees of freedom or Langevin forces that cannot be described by simple Markovian processes [1].

The second approach (see Ref. [3] for a review) is to derive an equation for $p_{\mathbf{X}}(\mathbf{x}, t)$ that, unlike KME, has a finite number of terms. This differential equation involves random variables and requires a closure. Most existing closures place restrictions on the noise properties. For example, the decoupling theory (Hänggi ansatz) [2] requires dimensionless $\boldsymbol{\xi}$ to be Gaussian, second-order stationary, and to have small variances $q_{ij} \ll 1$; the small correlation-time expansion [4] is limited to correlation times $\lambda_{ij} \to 0$ and $\lambda_{ij}/q_{ij} \ll 1$; and the functional integral [2] and path integral [5] methods require $\boldsymbol{\xi}$ to be statistically homogeneous.

Our goal is to derive a closed-form computable PDF equation for Langevin equations (1), in which the Langevin force $\boldsymbol{\xi}(t)$ has an arbitrary correlation function and strength. To derive a governing equation for $p_{\mathbf{X}}(\mathbf{x}; t)$, we

adopt the PDF method originally developed in the context of turbulent flows [6]. Let us define a "raw" joint PDF of system states $\mathbf{X}$ at time t

$$\Pi(\mathbf{X}, \mathbf{x}; t) = \prod_{i=1}^{N} \delta[X_i(t) - x_i]. \tag{3}$$

Its ensemble average over random realizations of $\mathbf{X}$ yields $p_{\mathbf{X}}(\mathbf{x}, t)$, the joint PDF of $\mathbf{X}$:

$$\langle \Pi \rangle = \int \prod_{i=1}^{N} \delta_i(X_i' - x_i) p_{\mathbf{X}}(\mathbf{x}', t) dx_1' \cdots dx_N' = p_{\mathbf{X}}. \tag{4}$$

Multiplying the ith Langevin equation (1) with $\partial\Pi/\partial x_i$, using the properties of the Dirac delta function $\delta(\cdot)$, and summing up the resulting N equations yields a stochastic evolution equation for Π

$$\frac{\partial \Pi}{\partial t} = -\nabla_{\mathbf{x}} \cdot (\mathbf{v}\Pi). \tag{5}$$

Here, $\nabla_{\mathbf{x}} = (\partial/\partial x_1, \ldots, \partial/\partial x_N)^{\top}$ and the ith component of the N-dimensional vector $\mathbf{v} = (v_1, \ldots, v_N)^{\top}$ is

$$v_i(\mathbf{x}, t) = h_i(\mathbf{x}, t) + \sum_{j=1}^{N} g_{ij}(\mathbf{x}, t)\xi_j(t). \tag{6}$$

Note that, unlike its turbulent counterpart, the "advective velocity" $\mathbf{v}$ is not divergence free, i.e., $\nabla_{\mathbf{x}} \cdot \mathbf{v} \neq 0$.

Employing the Reynolds decomposition to represent the random fields in (5) as the sums of their ensemble means and respective zero-mean fluctuations and taking the ensemble average of the resulting equation yields an unclosed PDF equation

$$\frac{\partial p_{\mathbf{X}}}{\partial t} = -\nabla_{\mathbf{x}} \cdot (\langle \mathbf{v} \rangle p_{\mathbf{X}}) - \nabla_{\mathbf{x}} \cdot \langle \mathbf{v}' \Pi' \rangle. \tag{7}$$

The same PDF equation was derived using different methods in Refs. [2,7]. It is not computable since it contains the unknown cross covariance $\langle \mathbf{v}'\Pi' \rangle$. A closure approximation is needed to express $\langle \mathbf{v}'\Pi' \rangle$ in terms of $p_{\mathbf{X}}$. In the context of Langevin equations with colored noise, such closures were proposed for particular forms of the correlation function ρ_{ij} (see the introduction).

The formal similarity between (5) and advective transport of a passive scalar in a random velocity field allows us to employ an alternative closure that is variously known as the large-eddy-diffusivity (LED) closure [8] or the weak approximation [9]. This enables us to approximate (7) with a closed-form PDF equation

$$\frac{\partial p_{\mathbf{X}}}{\partial t} = -\nabla_{\mathbf{x}} \cdot (\mathcal{V} p_{\mathbf{X}}) + \nabla_{\mathbf{x}} \cdot (\mathcal{D} \nabla_{\mathbf{x}} p_{\mathbf{X}}). \tag{8}$$

The "eddy-diffusivity" (second-rank) tensor $\mathcal{D}$ and "effective velocity" vector $\mathcal{V}$ are expressed in terms of the two-point "velocity" covariance tensor $\boldsymbol{\rho}_v(\mathbf{x}, t; \mathbf{y}, s) = \langle \mathbf{v}'(\mathbf{x}, t)\mathbf{v}'(\mathbf{y}, s)^{\top} \rangle$ and the mean-field Green's function $G(\mathbf{x}, \mathbf{y}, t - s)$ for (5). The latter is defined as a solution of the deterministic equation $\partial G/\partial s + \langle \mathbf{v} \rangle \cdot \nabla_{\mathbf{y}} G = -\delta(\mathbf{y} - \mathbf{x})\delta(s - t)$, subject to the homogeneous initial (and boundary) conditions corresponding to their (possibly inhomogeneous) counterparts for (5). Specifically, $\mathcal{D}$ and $\mathcal{V}$ are given by [8,9]

$$\mathcal{D}(\mathbf{x}, t) = \int_0^t \int_{\Omega} G \boldsymbol{\rho}_v(\mathbf{x}, t; \mathbf{y}, s) d^N y ds, \tag{9a}$$

$$\mathcal{V}(\mathbf{x}, t) = \langle \mathbf{v} \rangle - \int_0^t \int_{\Omega} G \nabla_{\mathbf{y}} \cdot \boldsymbol{\rho}_v(\mathbf{x}, t; \mathbf{y}, s) d^N y ds. \tag{9b}$$

Recalling the definition of $\mathbf{v}$ in (6) yields

$$\mathcal{D} = \int_0^t \int_{\Omega} G[\mathbf{g}(\mathbf{x}, t) \cdot \mathbf{C}] \cdot \mathbf{g}(\mathbf{y}, s)^{\top} d^N y ds, \tag{10a}$$

$$\mathcal{V} = \langle \mathbf{v} \rangle - \int_0^t \int_{\Omega} G[\mathbf{g}(\mathbf{x}, t) \cdot \mathbf{C}] \cdot [\nabla_{\mathbf{y}} \cdot \mathbf{g}(\mathbf{y}, s)] d^N y ds, \tag{10b}$$

where $\mathbf{C}(t, s)$ is the covariance matrix of the Langevin force $\boldsymbol{\xi}(t)$, whose components C_{ij} are defined in (2).

PDF equations (8)–(10) are the main result of this Letter. They are formally valid for Langevin forces with arbitrary distributions and correlations. The LED approximation accounts only for the first two moments of $\boldsymbol{\xi}$. Yet, it gives accurate and robust approximations of mean system behavior (see Ref. [10] and the references therein). This is all we need since $\langle \Pi \rangle = p_{\mathbf{X}}$.

Unlike the currently used empirical closures, our (two-point) closure rests on the solid mathematical foundation. It can be viewed as a leading-order term in a perturbation expansion in the correlation length of $\mathbf{v}(t)$ [8] and requires both $p_{\mathbf{X}}$ and its gradient to vary slowly in the phase space [9]. Consequently, the accuracy of the approximations of $\mathcal{D}$ and $\mathcal{V}$ can be improved by incorporating higher-order terms, e.g., by employing four-point self-consistent closures [10].

In the remainder of this Letter, we examine the ability of our PDF approach to handle Langevin systems with Gaussian colored noise $\boldsymbol{\xi}$. We consider two distinct transport phenomena: a linear process with additive noise (Brownian motion) and a nonlinear process with multiplicative noise (hydrodynamic dispersion).

Brownian motion.—Classical Brownian motion involves two Langevin equations for particle displacement X and velocity U

$$\frac{dX}{dt} = U, \qquad \frac{dU}{dt} = -KU + \xi(t), \tag{11}$$

where K is the damping factor. The general PDF equation (8) with (10) reduces to

$$\frac{\partial p_{XU}}{\partial t} = -\frac{\partial u p_{XU}}{\partial x} + \frac{\partial K u p_{XU}}{\partial u} + \mathcal{D}_U \frac{\partial^2 p_{XU}}{\partial u^2}, \tag{12a}$$

with

$$\mathcal{D}_U(t) = \int_0^t C(t, s) e^{-K(t-s)} ds. \tag{12b}$$

For uncorrelated (white noise) $\xi(t)$, this equation reduces to the classical Fokker-Planck equation.

Since the Langevin equations (11) are decoupled, we also use the general PDF equation (8) to obtain PDF equations for the marginal PDFs of velocity $p_U(u;t)$ and displacement $p_X(x;t)$

$$\frac{\partial p_U}{\partial t} = \frac{\partial K u p_U}{\partial u} + \mathcal{D}_U \frac{\partial^2 p_U}{\partial u^2}, \tag{13a}$$

$$\frac{\partial p_X}{\partial t} = -\langle U\rangle \frac{\partial p_X}{\partial x} + \mathcal{D}_X \frac{\partial^2 p_X}{\partial x^2}. \tag{13b}$$

Here, $\mathcal{D}_U$ is given by (12b), $\mathcal{D}_X(t) = \int_0^t C_U(t,s)ds$, $\langle U\rangle = U_0 \exp(-Kt)$, and

$$C_U(t,s) = \int_0^t \int_0^s e^{-K(t+s-t_1-t_2)} C(t_1,t_2) dt_1 dt_2. \tag{13c}$$

The mean $\langle U\rangle$ is computed by averaging the second Langevin equation in (11) and integrating the result. The covariance $C_U(t,s)$ is obtained by integrating the second Langevin equation in (11), multiplying the result with $U'(s)$, and taking the ensemble average. The PDF equations (13) are identical to those obtained in Ref. [2] by relying on a closure that is only applicable to linear Langevin equations. In contrast, our PDF method is also valid for nonlinear Langevin equations (1).

As discussed earlier, one of the prevalent approaches to handling colored noise in Langevin systems is to enlarge the phase space. We use the first Langevin equation in (11), which is driven by colored noise $U(t)$ with $C_U(t,s) = q\exp(-|t-s|/\lambda)$, to compare this framework with ours. The extended phase-space approach supplements this Langevin equation with a Langevin equation for $U(t)$—the second equation in (11) in which the Langevin force $\xi(t)$ is treated as white noise—that asymptotically produces the desired correlation structure of U. Then, the PDF of $X(t)$ is found by integrating over u the joint PDF solution p_{XU} of the Fokker-Planck equation (12). Figure 1 compares the PDF of the original non-Markovian process

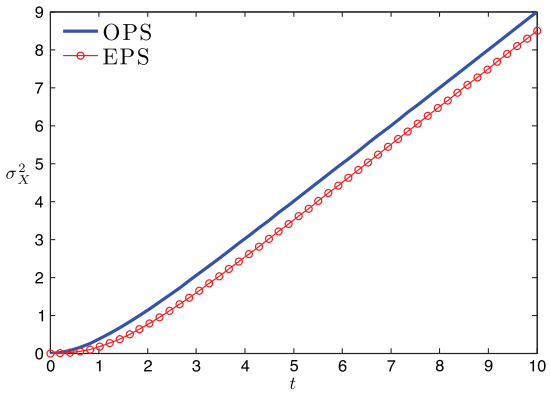

FIG. 1 (color online). Temporal evolution of displacement variance $\sigma_X^2(t)$ in the original (OPS) and extended (EPS) phase spaces: the LED closure for exponentially correlated velocity.

given by (13) and the PDF of the extended Markovian process. Since both PDFs are Gaussian and have the same mean, Fig. 1 shows only the variances of the original and extended processes. While the extended phase-space approach accurately predicts the asymptotic behavior of the growth rate of the variance, it underestimates it at early times ($Kt \ll 1$).

Hydrodynamic dispersion.—In lieu of the second example, we consider a nonlinear Langevin equation that describes dispersion in porous media [11]

$$\frac{dU}{dt} = -KU + g + \sqrt{|U|}\xi(t), \tag{14}$$

where K is the friction coefficient (inversely proportional to the permeability of a porous medium) and g is the gravitational acceleration. The PDF method allows for the noise $\xi(t)$ to be a correlated random process with an arbitrary covariance function C.

According to (8), the PDF of velocity U satisfies the PDF equation

$$\frac{\partial p_U}{\partial t} = -\frac{\partial \mathcal{V} p_U}{\partial u} + \frac{\partial}{\partial u}\left(\mathcal{D}\frac{\partial p_U}{\partial u}\right), \tag{15a}$$

in which the effective velocity $\mathcal{V}(u,t)$ and the macrodispersion coefficient $\mathcal{D}(u,t)$ are given by

$$\mathcal{V} = -Ku + g \pm \frac{\sqrt{|u|}}{2}\int_0^t C(t,s)e^{-K(t-s)}\sqrt{|I|}ds, \tag{15b}$$

$$\mathcal{D} = \sqrt{|u|}\int_0^t C(t,s)e^{-K(t-s)}\sqrt{1/|I|}ds, \tag{15c}$$

where $I = K/\{(Ku-g)\exp[-K(t-s)] + g\}$.

Formally, the PDF equation (15) is valid for an arbitrary covariance function C. As this equation was derived using the LED closure, its accuracy may depend on a specific form of C and a magnitude of the correlation time. In the following, we study the accuracy of the PDF model (15) for two extreme cases of the noise correlation time $\lambda = 0$, i.e., white noise ξ with $C(t,s) = q\tau\delta(t,s)$, and $\lambda = \infty$, i.e., random constant ξ with $C = q$.

For $C(t,s) = q\tau\delta(t,s)$, our PDF equation is exact, as it yields the standard Fokker-Planck equation in the Stratonovich formulation, in which the effective velocity (15b) and the dispersion coefficient (15c) become the leading Kramers-Moyal coefficients [1]

$$\mathcal{V} = -Ku + g \pm q/2, \qquad \mathcal{D} = q|u|. \tag{16}$$

For $C = q$, for finite times, we compare the numerical solution of (15) with the velocity PDF obtained from the Monte Carlo solution of (14). Figure 2 shows a good agreement between these two solutions. For infinite time, Fig. 2 also shows a good agreement between the analytical steady-state solution of (15)

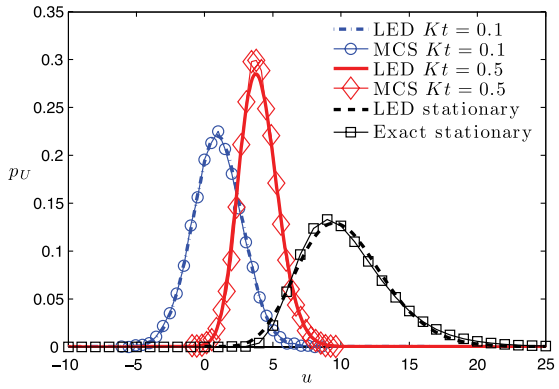

FIG. 2 (color online). Temporal snapshots of the velocity PDF $p_U(u;t)$ for colored noise with infinite correlation length at times $tK = 0.1$, $tK = 0.5$, the stationary solution from the PDF method (17), and the exact stationary solution (18). MCS, Monte Carlo simulation.

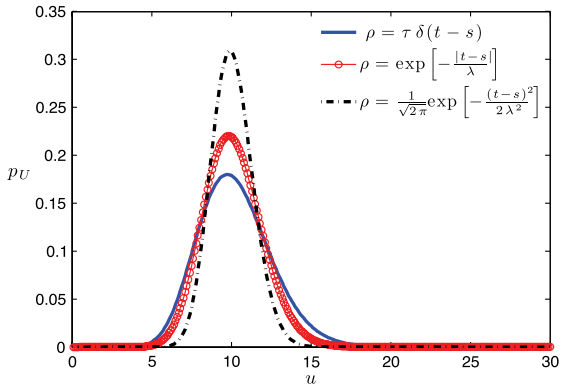

FIG. 3 (color online). Velocity distribution $p_U(u;t)$ at dimensionless time $tK = 10$ for three correlation functions: (1) delta, (2) exponential, and (3) Gaussian.

$$p_U^{\mathrm{ss}}(u) = N \exp\left(\int_u \frac{\mathcal{V}(u)}{\mathcal{D}(u)}\,du\right) \tag{17}$$

(N is the normalizing constant) and the exact steady-state velocity PDF obtained from the steady-state solution of the Langevin equation $U = g/K + \sqrt{|U|}\xi/K$

$$p_U^{\mathrm{ss(exact)}}(u) = \frac{K|U_{\mathrm{st}}| + g}{2|U_{\mathrm{st}}|^{3/2}}\, p_\xi[\xi(U_{\mathrm{st}})]. \tag{18}$$

Given the accuracy of our PDF solutions at both ends of the correlation length spectrum, we expect it to be accurate for intermediate correlation times λ as well.

Finally, we study the effect of the functional form of the noise covariance function C on p_U. While our PDF method does not require $\xi(t)$ to be stationarity, for consistency, we limit our analysis to three stationary correlation functions $C(t,s) = q\rho(|t-s|)$: white noise, exponential function, and Gaussian function. The velocity PDFs plotted in Fig. 3 demonstrate the significant impact of the noise correlation function ρ on the nonlinear dispersion process (14). The white noise yields the longest distribution tail, while the Gaussian correlation leads to the most symmetric velocity PDF. The identical mean velocity at $tK = 10$ is obtained for all three correlation functions.

In summary, we derived a closed-form PDF equation for general nonlinear Langevin equations with arbitrary colored noise. This equation allows a theoretical treatment of a wide class of non-Markovian processes. The PDF equation relies on a LED closure. To demonstrate the accuracy of this closure, we solved linear and nonlinear Langevin equations describing Brownian motion and hydrodynamic dispersion. Our analysis leads to the following conclusions. (1) The LED closure provides a good estimate of the PDFs of system states for both linear and nonlinear Langevin systems with Gaussian colored noise. (2) In contrast with the existing approaches, the LED closure does not impose any restrictions on the noise's correlation function or correlation length. (3) Unlike its counterparts, our approach is applicable for both early and late times. (4) A higher order of accuracy may be achieved by including more terms in the LED approximation (8)–(10), which in turn may relax the requirement of Gaussian noise.

This research was supported by the Advanced Scientific Computing Research Program of the U.S. Department of Energy, Office of Science, and by the Computational Mathematics Program of the Air Force Office of Scientific Research.

*peng.wang@pnnl.gov
†alexandre.tartakovsky@pnnl.gov
‡dmt@ucsd.edu

[1] H. Risken, *The Fokker-Planck Equation: Methods of Solutions and Applications* (Springer, New York, 1989), 2nd ed.
[2] P. Hänggi and P. Jung, *Advances in Chemical Physics* (Wiley, New York, 1995), p. 239.
[3] K. Lindenberg and B. J. West, *The Nonequilibrium Statistical Mechanics of Open and Closed Systems* (VCH, New York, 1990).
[4] R. F. Fox, Phys. Rev. A **33**, 467 (1986).
[5] M. A. Fuentes, H. S. Wio, and R. Toral, Physica (Amsterdam) **303A**, 91 (2002).
[6] H. D. Chen, S. Y. Chen, and R. H. Kraichnan, Phys. Rev. Lett. **63**, 2657 (1989).
[7] R. L. Stratonovich, *Topics in the Theory of Random Noise* (Gordon and Breach, New York, 1967).
[8] R. H. Kraichnan, Complex Syst. **1**, 805 (1987).
[9] S. P. Neuman, Water Resour. Res. **29**, 633 (1993).
[10] M. Dentz and D. M. Tartakovsky, Phys. Rev. E **77**, 066307 (2008).
[11] A. M. Tartakovsky, D. M. Tartakovsky, and P. Meakin, Phys. Rev. Lett. **101**, 044502 (2008).