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New evolution equations for the joint response-excitation probability density function of stochastic solutions to first-order nonlinear PDEs

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ABSTRACT

By using functional integral methods we determine new evolution equations satisfied by the joint response-excitation probability density function (PDF) associated with the stochastic solution to first-order nonlinear partial differential equations (PDEs). The theory is presented for both fully nonlinear and for quasilinear scalar PDEs subject to random boundary conditions, random initial conditions or random forcing terms. Particular applications are discussed for the classical linear and nonlinear advection equations and for the advection-reaction equation. By using a Fourier-Galerkin spectral method we obtain numerical solutions of the proposed response-excitation PDF equations. These numerical solutions are compared against those obtained by using more conventional statistical approaches such as probabilistic collocation and multi-element probabilistic collocation methods. It is found that the response-excitation approach yields accurate predictions of the statistical properties of the system. In addition, it allows to directly ascertain the tails of probabilistic distributions, thus facilitating the assessment of rare events and associated risks. The computational cost of the response-excitation method is order magnitudes smaller than the one of more conventional statistical approaches if the PDE is subject to highdimensional random boundary or initial conditions. The question of high-dimensionality for evolution equations involving multidimensional joint response-excitation PDFs is also addressed.

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1. Introduction

The purpose of this paper is to introduce a new probability density function approach for computing the statistical properties associated with the stochastic solution to first-order nonlinear scalar PDEs subject to uncertain initial conditions, boundary conditions or external random forces. Specifically, we will consider two different classes of model problems: the first one is a fully nonlinear stochastic PDE¹ in the form

$$\frac{\partial u}{\partial t} + \mathcal{N}(u, u_x, x, t; \xi) = 0, \tag{1}$$

where N is a continuously differentiable function, $u_x = \partial u / \partial x$ and ξ is a finite-dimensional vector of random variables with known joint probability density function. The second one is a multidimensional guasilinear PDE

$$\frac{\partial u}{\partial t} + \mathcal{P}(u, t, \boldsymbol{x}; \boldsymbol{\xi}) \cdot \nabla_{\boldsymbol{x}} u = \mathcal{Q}(u, t, \boldsymbol{x}; \boldsymbol{\eta}), \tag{2}$$

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¹ In this paper we will often refer to PDEs with random coefficients as "stochastic PDEs".

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where \mathcal{P} and \mathcal{Q} are continuously differentiable functions, **x** denotes a set of independent variables while ξ and η are two vectors of random variables with known joint probability density function. The boundary and the initial conditions associated with Eqs. (1) and (2) can be random processes of arbitrary dimension.

As is well known. Eqs. (1) and (2) can model many physically interesting phenomena such as ocean waves in an Eulerian framework [1,2], linear and nonlinear advection problems, advection-reaction systems [3,4] and, more generally, scalar conservation laws. The key aspect to determine the statistical properties of these systems relies in representing efficiently the functional relation between their solution and the input uncertainty. This topic, indeed, has received great attention in recent years. Well known approaches are generalized polynomial chaos [5–7], multi-element generalized polynomial chaos [8,9], multi-element and sparse grid adaptive probabilistic collocation [10-12], high-dimensional model representations [13,14], stochastic biorthogonal expansions [15–17] and generalized spectral decompositions [18,19]. However, first-order nonlinear or quasilinear PDEs with stochastic excitation admit an exact reformulation in terms of joint response-excitation probability density functions [20,21]. This formulation has an advantage with respect to more conventional stochastic approaches since it does not suffer from the curse of dimensionality problem, at least when randomness comes only from boundary or initial conditions. In fact, we can prescribe these conditions in terms of probability distributions and this is obviously not dependent on the number of random variables underlying the probability space. Therefore, the PDF approach seems more appropriate to tackle several open problems such as curse of dimensionality, discontinuities in random space [9], and long-term integration [22,23]. In addition, it allows to directly ascertain the tails of probabilistic distributions thus facilitating the assessment of rare events and associated risks. However, if an external random forcing term, e.g., represented in the form of a finite-dimensional Karhunen-Loève expansion, appears within the equations of motion then the dimensionality of the corresponding problem in probability space could increase significantly. This happens because the stochastic dynamics in this case develops over a high-dimensional manifold and therefore the exact probabilistic description of the system necessarily involves a multidimensional probability density function, or even a probability density functional. The evolution equation for the joint response-excitation PDF associated with the solution to Eq. (1) or Eq. (2) can be determined by using different methods. In this paper we will employ a functional integral technique we have recently introduced in the context of nonlinear stochastic dynamical systems [20,24]. This allows for very efficient mathematical derivations compared to those ones based on the more rigorous Hopf characteristic functional approach [25–27] (see also Appendix A).

This paper is organized as follows. In Section 2 we introduce the functional integral representation of the joint responseexcitation PDF associated with the solution to nonlinear stochastic PDEs. This representation is used in Section 3 and Section 4 to derive the exact PDF equations corresponding to Eqs. (1) and (2), respectively. In these sections, we also include specific examples of application to nonlinear advection and advection–reaction systems. By using a Fourier–Galerkin spectral method, in Section 6 we obtain the numerical solution to the response-excitation PDF equations for prototype nonlinear advection and advection–reaction problems. These solutions are compared against those obtained by using multi-element probabilistic collocation. Finally, the main findings and their implications are summarized in Section 7. We also include two appendices where we discuss the Hopf characteristic functional approach to the response-excitation theory and the Fourier–Galerkin systems for the nonlinear advection equation in physical and probability spaces.

2. Functional integral representation of the probability density function

Let us consider a physical system described in terms of partial differential equations subject to random initial conditions, random boundary conditions or external random forcing terms. The solution such initial-boundary value is a random vector field whose regularity properties in space and time are strongly related to the type of nonlinearities appearing in the equations as well as on the statistical properties of the random input processes. In order to fix ideas, let us consider the simple scalar advection–diffusion equation

$$\frac{\partial u}{\partial t} + \zeta(\omega) \frac{\partial u}{\partial x} = v \frac{\partial^2 u}{\partial x^2},\tag{3}$$

with deterministic boundary and initial conditions. The parameter $\xi(\omega)$ is assumed to be a random variable with known probability density function. The solution to Eq. (3) is a random scalar field that depends on the random variable $\xi(\omega)$ in a possibly nonlinear way. We shall denote such functional dependence as $u(x, t; [\xi])$. The joint probability density of $u(x, t; [\xi])$ and ξ , i.e. the solution field at the space–time location (x, t) and the random variable ξ , admits the following integral representation [27]

$$p_{u(\mathbf{x},t)\xi}^{(a,b)} \stackrel{\text{def}}{=} \langle \delta(a - u(\mathbf{x},t;[\xi]))\delta(b - \xi) \rangle, \quad a, b \in \mathbb{R}.$$
(4)

The average operator $\langle \cdot \rangle$, in this particular case, is defined as a simple integral with respect to the probability density of $\xi(\omega)$, i.e.

$$p_{u(x,t)\xi}^{(a,b)} = \int_{-\infty}^{\infty} \delta(a - u(x,t;[z])) \delta(b - z) p_{\xi}^{(z)} dz,$$
(5)

where $p_{\xi}^{(z)}$ denotes the probability density of $\xi(\omega)$, which might be compactly supported (e.g., a uniform distribution in [-1, 1]). Indeed, the support of the probability density function $p_{u(x,t)\xi}^{(a,b)}$ is actually determined by the nonlinear transformation

 $\xi \to u(x,t; [\xi])$ appearing within the delta function $\delta(a - u(x,t; [\xi]))$ (see, e.g., Chapter 3 in [28]). The representation (5) can be easily generalized to infinite dimensional random input processes. To this end, let us examine the case where the scalar field u is advected by a random velocity field U according to the equation

$$\frac{\partial u}{\partial t} + U(x,t;\omega)\frac{\partial u}{\partial x} = v\frac{\partial^2 u}{\partial x^2},\tag{6}$$

for some deterministic initial condition and boundary conditions. Disregarding the particular structure of the random field $U(x, t; \omega)$, let us consider its collocation representation for a given discretization of the space–time domain. This gives us a certain number of random variables { $U(x_i, t_j; \omega)$ } (i = 1, ..., N, j = 1, ..., M), with known joint probability distribution. The random field u solving Eq. (6) at a specific space–time location (x_i, t_j) is, in general, a nonlinear function of *all* the variables { $U(x_n, t_m; \omega)$ }. In order to see this, it is sufficient to write an explicit finite difference numerical scheme of Eq. (6). The joint probability density of the solution field u at (x_i, t_j) and the external advection field U at a different space–time location, say (x_n, t_m), admits the following integral representation

$$p_{u(x_i,t_j)U(x_n,t_m)}^{(a,b)} = \langle \delta(a - u(x_i,t_j;[U(x_1,t_1),\dots,U(x_N,t_M)]))\delta(b - U(x_n,t_m))\rangle,$$
(7)

where the average is with respect to the joint probability of all the random variables $\{U(x_n, t_m; \omega)\}$ (n = 1, ..., N, m = 1, ..., M). The notation $u(x_i, t_j; [U(x_1, t_1), ..., U(x_N, t_M)])$ emphasizes that the solution field $u(x_i, t_j)$ is, in general, a nonlinear function of all the random variables $[U(x_1, t_1), ..., U(x_N, t_M)]$. If we send the number of these variables to infinity, i.e. we refine the space-time mesh to the continuum level, we obtain a functional integral representation of the joint probability density

$$p_{u(x,t)U(x',t')}^{(a,b)} = \langle \delta(a - u(x,t;[U]))\delta(b - U(x',t')) \rangle = \int \mathcal{D}[U]W[U]\delta(a - u(x,t;[U]))\delta(b - U(x',t')),$$
(8)

where W[U] is the probability density functional of random field $U(x, t; \omega)$ and $\mathcal{D}[U]$ is the usual functional integral measure [29–31]. Depending on the specific stochastic PDE, we may need to consider different joint probability density functions, e.g., the joint probability of a field and its derivatives at different space–time locations. The functional representation described above allows us to deal with these different situations in a very practical way. For instance, we have

$$p_{u(x,y,t)u_{x}(x',y',t')u_{y}(x'',y'',t'')}^{(a,b,c)} = \langle \delta(a - u(x,y,t))\delta(b - u_{x}(x',y',t'))\delta(c - u_{y}(x'',y'',t''))\rangle,$$
(9)

where, for notational convenience, we have denoted by $u_x \stackrel{\text{def}}{=} \partial u / \partial x$, $u_y \stackrel{\text{def}}{=} \partial u / \partial y$ and we have omitted the functional dependence on the random input variables (i.e. the variables in the brackets [·] in (8)). Similarly, the joint probability of u(x, y, t) at two different spatial locations is

$$p_{u(x,y,t)u(x',y',t)}^{(a,0)} = \langle \delta(a - u(x,y,t)) \delta(b - u(x',y',t)) \rangle.$$
(10)

In the sequel we will be mostly concerned with joint probability densities of different fields at the *same* space-time location. Therefore, in order to lighten the notation further, sometimes we will drop the subscripts indicating the space-time variables and write, for instance

$$p_{uu_x}^{(a,b)} = \langle \delta(a - u(x, y, t)) \delta(b - u_x(x, y, t)) \rangle, \tag{11}$$

or even more compactly

(1)

$$p_{uu_x}^{(a,b)} = \langle \delta(a-u)\delta(b-u_x) \rangle. \tag{12}$$

2.1. Representation of derivatives

We will often need to differentiate the probability density function with respect to space or time variables. This operation involves generalized derivatives of the Dirac delta function and it can be carried out in a systematic way. To this end, let us consider Eq. (4) and define the following linear functional

$$\int_{-\infty}^{\infty} p_{u(x,t)}^{(a)} \rho(a) \, da = \left\langle \int_{-\infty}^{\infty} \delta(a - u(x,t)) \rho(a) \, da \right\rangle = \langle \rho(u) \rangle, \tag{13}$$

where $\rho(a)$ is a continuously differentiable and compactly supported function. A differentiation of Eq. (13) with respect to t gives

$$\int_{-\infty}^{\infty} \frac{\partial p_{u(x,t)}^{(a)}}{\partial t} \rho(a) \, da = \left\langle u_t \frac{\partial \rho}{\partial u} \right\rangle = \left\langle u_t \int_{-\infty}^{\infty} \frac{\partial \rho}{\partial a} \delta(a - u(x,t)) \, da \right\rangle = \int_{-\infty}^{\infty} -\frac{\partial}{\partial a} \left\langle u_t \delta(a - u(x,t)) \right\rangle \rho(a) \, da. \tag{14}$$

This equation holds for an arbitrary $\rho(a)$ and therefore we have the identity

$$\frac{\partial p_{u(x,t)}^{(a)}}{\partial t} = -\frac{\partial}{\partial a} \langle \delta(a - u(x,t)) u_t(x,t) \rangle.$$
(15)

Similarly,

$$\frac{\partial p_{u(x,t)}^{(a)}}{\partial x} = -\frac{\partial}{\partial a} \langle \delta(a - u(x,t)) u_x(x,t) \rangle.$$
(16)

Straightforward extensions of these results allow us to compute derivatives of joint probability density functions involving more fields, e.g., u(x, t) and its first-order spatial derivative $u_x(x, t)$

$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial t} = -\frac{\partial}{\partial a} \langle \delta(a - u(x,t)) \delta(b - u_x(x,t)) u_t(x,t) \rangle - \frac{\partial}{\partial b} \langle \delta(a - u(x,t)) \delta(b - u_x(x,t)) u_{tx}(x,t) \rangle, \tag{17}$$

where $u_{tx} \stackrel{\text{def}}{=} \partial^2 u / \partial t \partial x$.

2.2. Representation of averages

Let us consider the quantity $\langle \delta(a-u)u \rangle$. By applying well-known properties of Dirac delta functions it can be shown that

$$\langle \delta(a-u)u\rangle = ap_{u(x,t)}^{(a)}.$$
(18)

This result is a multidimensional extension of the following identity that holds for only one random variable $\xi(\omega)$ (with probability density $p_{\xi}^{(2)}$) and a nonlinear function $g(\xi)$ (see, e.g., Chapter 3 of [28] or [32])

$$\int_{-\infty}^{\infty} \delta(a - g(z))g(z)p_{\xi}^{(z)} dz = \sum_{n} \frac{1}{|g'(\hat{z}_{n})|} \int_{-\infty}^{\infty} \delta(z - \hat{z}_{n})g(z)p_{\xi}^{(z)} dz = \sum_{n} \frac{g(\hat{z}_{n})p_{\xi}^{(z_{n})}}{|g'(\hat{z}_{n})|},$$
(19)

where $\hat{z}_n(a) = g^{-1}(a)$ are solutions of g(z) = a. Now, since $g(\hat{z}_n) = g(g^{-1}(a)) = a$, from Eq. (19) it follows that

$$\int_{-\infty}^{\infty} \delta(a - g(z))g(z)p_{\xi}^{(z)} dz = a \sum_{n} \frac{p_{\xi}^{(\hat{z}_{n})}}{|g'(\hat{z}_{n})|} = a \int_{-\infty}^{\infty} \delta(a - g(z))p_{\xi}^{(z)} dz,$$
(20)

which is equivalent to Eq. (18). Similarly, one can show that

$$\langle \delta(a-u)\delta(b-u_x)u\rangle = ap_{uu_x}^{(a,b)},\tag{21a}$$

$$\langle \delta(a-u)\delta(b-u_x)u_x\rangle = bp_{uu_x}^{(a,b)},\tag{21b}$$

and, more generally, that

$$\langle \delta(a-u)\delta(b-u_x)h(x,t,u,u_x)\rangle = h(x,t,a,b)p_{uu_x}^{(a,b)},\tag{22}$$

where, for the purposes of the present paper, $h(u, u_x, x, t)$ is any continuous function of u, u_x , x and t. The result (22) can be generalized even further to averages involving a product of two continuous functions h and q

$$\langle \delta(a-u)\delta(b-u_x)h(x,t,u,u_x)q(x,t,u_{xx},u_{xt},u_{tt},\ldots)\rangle = h(x,t,a,b)\langle \delta(a-u)\delta(b-u_x)q(x,t,u_{xx},u_{xt},u_{tt},\ldots)\rangle.$$
(23)

In short, the general rule is: we are allowed to take out of the average $\langle \cdot \rangle$ all those functions involving fields for which we have available a Dirac delta. As an example, if *u* is a time-dependent field in a two-dimensional spatial domain we have

$$\langle \delta(a-u)\delta(b-u_x)\delta(c-u_y)e^{-(x^2+y^2)}\sin(u)u_xu_y^2u_{xx}\rangle = e^{-(x^2+y^2)}\sin(a)bc^2\langle \delta(a-u)\delta(b-u_x)\delta(c-u_y)u_{xx}\rangle.$$
(24)

2.3. Intrinsic relations depending on the structure of the joint PDF

The fields appearing in the joint PDF are often related by deterministic equations. For instance, in the particular case of (12) we have

$$u_{x}(x,t;\omega) = \lim_{x' \to x} \frac{u(x',t;\omega) - u(x,t;\omega)}{(x'-x)}.$$
(25)

As a consequence, we expect that there exist a certain number of *intrinsic relations* between the joint PDF and itself. In order to determine these relations, let us consider the joint density

$$p_{u(x,t)u_{x}(x',t')}^{(a,b)} = \langle \delta(a - u(x,t))\delta(b - u_{x}(x',t')) \rangle.$$
(26)

By taking the derivative of with respect to x

$$\frac{\partial p_{u(x,t)u_x(x',t')}^{(a,b)}}{\partial x} = -\frac{\partial}{\partial a} \langle \delta(a - u(x,t))u_x(x,t)\delta(b - u_x(x',t')) \rangle.$$
(27)

and then sending $x' \to x$ and $t' \to t$ we obtain the result

$$\lim_{x' \to x} \frac{\partial p_{u(x,t)u_x(x',t)}^{(a,b)}}{\partial x} = -b p_{u(x,t)u_x(x,t)}^{(a,b)}.$$
(28)

This is a *differential constraint* for the joint PDF of u and u_x at (x, t) reflecting the fact these fields are *locally related* by Eq. (25). Additional regularity properties of $u(x, t; \omega)$ yield additional differential constraints for (26). For instance, the existence of the second-order spatial derivative gives

$$\lim_{\alpha'\to \mathbf{x}} \frac{\partial^2 p_{u(\mathbf{x},t)u_{\mathbf{x}}(\mathbf{x}',t)}^{(a,b)}}{\partial \mathbf{x}^2} = b^2 \frac{\partial p_{u(\mathbf{x},t)u_{\mathbf{x}}(\mathbf{x},t)}^{(a,b)}}{\partial a^2} + \frac{\partial}{\partial a} \int_{-\infty}^{b} \lim_{\mathbf{x}\to\mathbf{x}'} \frac{\partial p_{u(\mathbf{x},t)u_{\mathbf{x}}(\mathbf{x}',t)}^{(a,b')}}{\partial \mathbf{x}'} db'.$$
(29)

In principle, if the field *u* is analytic then we can construct an infinite set of differential constraints to be satisfied at every space–time location. In other words, the local regularity properties of *u* can be translated into a set differential constraints involving the joint probability density function (26).

3. Kinetic equations for the PDF of the solution to first-order nonlinear stochastic PDEs

Let us consider the nonlinear scalar evolution equation

$$\frac{\partial u}{\partial t} + \mathcal{N}(u, u_x, x, t) = \mathbf{0},\tag{30}$$

where N is a continuously differentiable function. For the moment, we restrict our attention to only one spatial dimension and assume that the field $u(x, t; \omega)$ is random as a consequence of the fact that the initial condition or the boundary condition associated with Eq. (30) are random. A more general case involving a random forcing term will be discussed later in this section. As is well known, the full statistical information of the solution to Eq. (30) can be always encoded in the Hopf characteristic functional of the system (see Appendix A). In some very special cases, however, the functional differential equation satisfied by the Hopf functional can be reduced to a standard partial differential equation for the one-point one-time characteristic function or, equivalently, for the PDF of the system. First-order nonlinear scalar stochastic PDEs of the form (30) belong to this class and, in general, they admit a reformulation in terms of the joint density of u and its first order spatial derivative u_x at the same space-time location, i.e.,

$$p_{uu_x}^{(a,b)} = \langle \delta(a - u(x,t))\delta(b - u_x(x,t)) \rangle.$$
(31)

The average operator $\langle \cdot \rangle$ here is defined as an integral with respect to the joint probability density functional of the random initial condition and the random boundary condition. A differentiation of Eq. (31) with respect to time yields

$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial t} = -\frac{\partial}{\partial a} \langle \delta(a-u)u_t \delta(b-u_x) \rangle - \frac{\partial}{\partial b} \langle \delta(a-u)\delta(b-u_x)u_{xt} \rangle.$$
(32)

If we substitute Eq. (30) and its derivative with respect to x into Eq. (32) we obtain

$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial t} = \frac{\partial}{\partial a} (\mathcal{N} p_{uu_x}^{(a,b)}) + \frac{\partial}{\partial b} \left\langle \left(\frac{\partial \mathcal{N}}{\partial u} u_x + \frac{\partial \mathcal{N}}{\partial u_x} u_{xx} + \frac{\partial \mathcal{N}}{\partial x} \right) \delta(a-u) \delta(b-u_x) \right\rangle.$$
(33)

Next, let us recall that N and its derivatives are at least continuous functions (by assumption) and therefore by using Eq. (23) they can be taken out of the averages. Thus, the only item that is missing in order to close Eq. (33) is an expression for the average of u_{xx} in terms of the probability density function. Such an expression can be easily obtained by integrating the identity

$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial x} = -b \frac{\partial p_{uu_x}^{(a,b)}}{\partial a} - \frac{\partial}{\partial b} \langle \delta(a-u)\delta(b-u_x)u_{xx} \rangle$$
(34)

with respect to *b* from $-\infty$ to *b* and taking into account the fact that the average of any field vanishes when $b \to \pm \infty$ due to the properties of the underlying probability density functional. Therefore, Eq. (34) can be equivalently written as

$$\langle \delta(a-u)\delta(b-u_x)u_{xx}\rangle = -\int_{-\infty}^{b} \frac{\partial p_{uu_x}^{(a,b')}}{\partial x} db' - \int_{-\infty}^{b} b' \frac{\partial p_{uu_x}^{(a,b')}}{\partial a} db'.$$
(35)

A substitution of this relation into Eq. (33) yields the final result

$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial t} = \frac{\partial}{\partial a} \left(\mathcal{N} p_{uu_x}^{(a,b)} \right) + \frac{\partial}{\partial b} \left[\left(b \frac{\partial \mathcal{N}}{\partial a} + \frac{\partial \mathcal{N}}{\partial x} \right) p_{uu_x}^{(a,b)} - \frac{\partial \mathcal{N}}{\partial b} \left(\int_{-\infty}^{b} \frac{\partial p_{uu_x}^{(a,b')}}{\partial x} db' + \int_{-\infty}^{b} b' \frac{\partial p_{uu_x}^{(a,b')}}{\partial a} db' \right) \right], \tag{36}$$

where N here is a function of a, b, x and t, respectively. Eq. (36) is the correct evolution equation for the joint PDF associated with the solution to an arbitrary nonlinear evolution problem in the form (30). This equation made its first appearance in

[33], although the original published version has many typos and a rather doubtful derivation.² A generalization of Eq. (30) includes an external random force in the form

$$\frac{\partial u}{\partial t} + \mathcal{N}(u, u_x, x, t) = f(x, t; \omega).$$
(37)

Depending on the type of the random field f and on its correlation structure, different stochastic methods can be employed. For instance, if the characteristic variation of f is much shorter than the characteristic variation of the solution u then we can use small correlation space-time expansions. In particular, if the field f is Gaussian then we can use the Furutsu-Novikov-Donsker [34–36] formula (see also [37,38,27]). Alternatively, if we have available a Karhunen-Loève expansion

$$f(\mathbf{x}, t; \omega) = \sum_{k=1}^{m} \lambda_k \xi_k(\omega) \psi_k(\mathbf{x}, t),$$
(38)

then we can obtain a closed and exact equation for the joint probability of u, u_x and all the (uncorrelated) random variables $\{\xi_k(\omega)\}$ appearing in the series (38), i.e.,

$$\mathbf{p}_{u(x,t)u_{x}(x,t)\{\xi_{k}\}}^{(a,b,\{c_{k}\})} = \left\langle \delta(a-u(x,t))\delta(b-u_{x}(x,t))\prod_{k=1}^{m}\delta(c_{k}-\xi_{k})\right\rangle.$$
(39)

For the specific case of Eq. (37) we obtain the PDF equation

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial a} (\mathcal{N}P) + \frac{\partial}{\partial b} \left[\left(b \frac{\partial \mathcal{N}}{\partial a} + \frac{\partial \mathcal{N}}{\partial x} \right) P - \frac{\partial \mathcal{N}}{\partial b} \left(\int_{-\infty}^{b} \frac{\partial P}{\partial x} db' + \int_{-\infty}^{b} b' \frac{\partial P}{\partial a} db' \right) \right] - \left[\sum_{k=1}^{m} \lambda_k c_k \psi_k \right] \frac{\partial P}{\partial a}, \tag{40}$$

where we have used the shorthand notation

<u>م.</u>.

$$P \stackrel{\text{def}}{=} p_{u(x,t)u_x(x,t)\{\xi_k\}}^{(a,b,\{c_k\})}.$$
(41)

Note that Eq. (40) is linear and exact but it involves four variables (t, x, a and b) and *m* parameters $(\{c_1, \ldots, c_m\})$. In any case, once the solution is available³ we can integrate out the variables $(b, \{c_k\})$ and obtain the *response probability of the system*, i.e. the probability density of the solution *u* at every space–time point as

$$p_{u(x,t)}^{(a)} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} p_{u(x,t)u_x(x,t)\{\xi_k\}}^{(a,b,\{c_k\})} db \, dc_1 \cdots dc_m.$$
(42)

The integrals above are formally written from $-\infty$ to ∞ although the probability density we are integrating out may be compactly supported. We conclude this section by observing that the knowledge of the probability density function of the solution to a stochastic PDE at a specific location does *not* provide all the statistical information of the system. For instance, the calculation of the two-point correlation function $\langle u(x,t)u(x',t')\rangle$ requires the knowledge of the joint probability density density of the solution *u* at two different locations, i.e. $p_{u(x,t)u(x',t')}^{(a,b)}$. We will go back to this point in Section 4.

3.1. An example: nonlinear advection problem with an additional quadratic nonlinearity

Let us consider the following quadratic prototype problem (see, e.g., [39], p. 358)

$$\begin{cases} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \left(\frac{\partial u}{\partial x}\right)^2 = 0, \quad v \ge 0, \quad x \in [0, 2\pi], \quad t \ge t_0, \\ u(x, t_0; \omega) = A \sin(x) + \eta(\omega), \quad A > 0, \\ \text{Periodic B.C.}, \end{cases}$$
(43)

where $\eta(\omega)$ is a random variable with known probability density function. If we substitute Eq. (43) and its derivative with respect to *x* into Eq. (32) we obtain

$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial t} = (ab + vb^2) \frac{\partial p_{uu_x}^{(a,b)}}{\partial a} + bp_{uu_x}^{(a,b)} + \frac{\partial}{\partial b} \langle \delta(a-u)\delta(b-u_x)(u_x^2 + uu_{xx} + 2vu_xu_{xx}) \rangle.$$
(44)

At this point we need an explicit expression for the last average at the right hand side of Eq. (44) in terms of the probability density function (31). Such an expression can be easily determined by using the averaging rule (23) and identity (35). We finally get

² The equation numbering in this footnote corresponds to the one in Ref. [33]. First of all, we notice a typo in Eq. (1.5), i.e. two brackets are missing. Secondly, according to Eq. (1.1) f is a multivariable function that includes also x and therefore one term is missing in Eq. (1.6). Also, the final result (1.8) seems to have three typos, i.e., the variable v is missing in the last integral within the brackets (this typo was corrected in the subsequent Eq. (1.9) and there are two signs that are wrong. We remark that these sign errors are still present in Eq. (1.9).

 $^{^{3}}$ Later on we will discuss in more detail numerical algorithms and techniques that can be employed to compute the numerical solution to a multidimensional linear PDE like (40).

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$$\frac{\partial p_{uu_x}^{(a,b)}}{\partial t} = -a \frac{\partial p_{uu_x}^{(a,b)}}{\partial x} + b p_{uu_x}^{(a,b)} + \frac{\partial}{\partial b} (b^2 p_{uu_x}^{(a,b)}) - \nu b^2 \frac{\partial p_{uu_x}^{(a,b)}}{\partial a} - 2\nu \left(b \frac{\partial p_{uu_x}^{(a,b)}}{\partial x} + \int_{-\infty}^b b' \frac{\partial p_{uu_x}^{(a,b')}}{\partial a} db' + \int_{-\infty}^b \frac{\partial p_{uu_x}^{(a,b')}}{\partial x} db' \right). \tag{45}$$

This equation is consistent with the general law (36) with $\mathcal{N}(a, b, x, t) = ab + vb^2$. An alternative derivation of Eq. (45) is also provided in Appendix A.3 by employing the Hopf characteristic functional approach. Note that Eq. (45) is a linear partial differential equation in four variables (a, b, x, t) that can be integrated for $t \ge t_0$ once the joint probability of u and u_x is provided at some initial time t_0 . In the present example, such an initial condition can be obtained by observing that the spatial derivative of the random initial state $u(x, t_0; \omega) = A \sin(x) + \eta(\omega)$ is the *deterministic* function

$$u_x(x,t_0;\omega) = A\cos(x). \tag{46}$$

Therefore, by applying the Dirac delta formalism, we see that the initial condition for the joint probability density of u and u_x is

$$p_{u(x,t_0)u_x(x,t_0)}^{(a,b)} = \langle \delta(a - A\sin(x) - \eta)\delta(b - A\cos(x)) \rangle = \delta(b - A\cos(x))\langle \delta(a - A\sin(x) - \eta) \rangle$$
$$= \delta(b - A\cos(x))\frac{1}{\sqrt{2\pi}}e^{-(a - A\sin(x))^2/2},$$
(47)

provided $\eta(\omega)$ is a Gaussian random variable. At this point it is clear that Eq. (45) has to be interpreted in a weak sense in order for the initial condition (47) to be meaningful. From a numerical viewpoint the presence of the Dirac delta function within the initial condition introduces significant difficulties. In fact, if we adopt a Fourier–Galerkin framework then we need a very high (theoretically infinite) resolution in the *b* direction in order to resolve such initial condition and, consequently, the proper temporal dynamics of the probability function. In addition, the Fourier–Galerkin system associated with Eq. (45) is fully coupled and therefore inaccurate representations of the Dirac delta appearing in the initial condition rapidly propagate within the Galerkin system, leading to numerical errors. However, we can always apply a Fourier transformation with respect to *a* and *b* to Eqs. (45) and (47), before performing the numerical discretization. This is actually equivalent to look for a solution in terms of the joint characteristic function instead of the joint probability density function. The corresponding evolution equation is obtained in Appendix A.3 and it is rewritten hereafter for convenience ($\phi_{uu_x}^{(a,b)}$ denotes the joint characteristic function of *u* and u_x , while *i* is the imaginary unit)

$$\frac{\partial \phi_{uu_x}^{(a,b)}}{\partial t} = ib \frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial b^2} - i \frac{\partial \phi_{uu_x}^{(a,b)}}{\partial b} + i \frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial a \partial x} - iva \frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial b^2} - 2 \frac{iv}{b} \left(\frac{\partial \phi_{uu_x}^{(a,b)}}{\partial x} - a \frac{\partial \phi_{uu_x}^{(a,b)}}{\partial b} - b \frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial b \partial x} \right). \tag{48}$$

The initial condition for this equation is obtained by Fourier transformation of Eq. (47), i.e.

$$\phi_{u(x,t_0)}^{(a,b)} = \frac{1}{\sqrt{2\pi}} e^{ibA\cos(x)} \int_{-\infty}^{\infty} e^{ia\alpha - (\alpha - A\sin(x))^2/2} \, d\alpha.$$
(49)

We do not address here the computation of the numerical solution to the problem defined by Eqs. (45) and (47).

4. Kinetic equations for the PDF of the solution to first-order quasilinear stochastic PDEs

In this section we obtain a kinetic equation for the probability density function associated with the stochastic solutions to multidimensional quasilinear stochastic PDE in the form

$$\frac{\partial u}{\partial t} + \mathcal{P}(u, t, \mathbf{x}; \boldsymbol{\xi}) \cdot \nabla_{\mathbf{x}} u = \mathcal{Q}(u, t, \mathbf{x}; \boldsymbol{\eta}).$$
(50)

In this equation \mathcal{P} and \mathcal{Q} are assumed to be continuously differentiable functions, \mathbf{x} denotes a set of independent variables⁴ while $\boldsymbol{\xi} = [\xi_1, \dots, \xi_m]$ and $\boldsymbol{\eta} = [\eta_1, \dots, \eta_n]$ are two vectors of random variables with known joint probability density function. We remark that Eq. (50) models many physically interesting phenomena such as ocean waves [1], linear and nonlinear advection problems, advection–reaction equations [3,4] and, more generally, scalar conservation laws. We first consider the case where the stochastic solution $u(\mathbf{x}, t; \omega)$ is random as consequence of the fact that the initial condition or the boundary conditions are random. In other words, we temporarily remove the dependence on $\{\xi_k\}$ and $\{\eta_k\}$ in \mathcal{P} and \mathcal{Q} , respectively. In this case we can determine an exact evolution equation for the one point one time PDF

$$p_{u(\boldsymbol{x},t)}^{(a)} = \langle \delta(\boldsymbol{a} - \boldsymbol{u}(\boldsymbol{x},t)) \rangle.$$
(51)

The average here is with respect to the joint probability density functional of the random initial condition and the random boundary conditions. Differentiation of (51) with respect to t yields

⁴ In many applications **x** is a vector of spatial coordinates, e.g., $\mathbf{x} = (x, y, z)$. In a more general framework **x** is a vector of independent variables including, e.g., spatial coordinates and parameters. For example, the two-dimensional action balance equation for ocean waves in the Eulerian framework [1,2] is defined in terms of the following variables $\mathbf{x} = (x, y, \theta, \sigma)$ where θ and σ denote wave direction and wavelength, respectively.

$$\frac{\partial p_{u(\boldsymbol{x},t)}^{(a)}}{\partial t} = -\frac{\partial}{\partial a} \langle \delta(a - u(\boldsymbol{x},t)) [-\mathcal{P}(u,t,\boldsymbol{x}) \cdot \nabla_{\boldsymbol{x}} u + \mathcal{Q}(u,t,\boldsymbol{x})] \rangle.$$
(52)

By using the results of the previous sections it is easy to show that this equation can be equivalently written as

$$\frac{\partial p_{u(\boldsymbol{x},t)}^{(a)}}{\partial t} + \frac{\partial}{\partial a} \left(\mathcal{P}(a,t,\boldsymbol{x}) \cdot \int_{-\infty}^{a} \nabla_{\boldsymbol{x}} p_{u(\boldsymbol{x},t)}^{(a')} da' \right) = -\frac{\partial}{\partial a} (\mathcal{Q}(a,t,\boldsymbol{x}) p_{u(\boldsymbol{x},t)}^{(a)}).$$
(53)

Note that this is a linear partial differential equation in (D + 2) variables, where *D* denotes the number of independent variables appearing in the vector **x**. Such dimensionality is completely independent of the number of random variables describing the boundary conditions or the initial conditions.

As we have previously pointed out, the knowledge of the one-point one-time probability density function of the solution to a stochastic PDE does not provide all the statistical information about the stochastic system. For instance, the computation of the two-point correlation function requires the knowledge of the joint probability of the solution field at two different locations. In order to determine such equation let us consider the joint density

$$p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a,b)} = \langle \delta(a - u(\mathbf{x},t))\delta(b - u(\mathbf{x}',t)) \rangle.$$
(54)

Differentiation of Eq. (51) with respect to time yields

$$\frac{\partial}{\partial t} p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a,b)} = -\frac{\partial}{\partial a} \langle \delta(a - u(\mathbf{x},t)) \delta(b - u(\mathbf{x}',t)) [-\mathcal{P}(u,t,\mathbf{x}) \cdot \nabla) x u + \mathcal{Q}(u,t,\mathbf{x})] \rangle - \frac{\partial}{\partial b} \langle \delta(a - u(\mathbf{x},t)) \delta(b - u(\mathbf{x}',t)) \times [-\mathcal{P}(u,t,\mathbf{x}') \cdot \nabla_{\mathbf{x}'} u + \mathcal{Q}(u,t,\mathbf{x}')] \rangle,$$
(55)

and therefore

(-)

$$\frac{\partial}{\partial t} p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a,b)} + \frac{\partial}{\partial a} \left(\mathcal{P}(a,t,\mathbf{x}) \cdot \int_{-\infty}^{a} \nabla_{\mathbf{x}} p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a',b)} da' \right) + \frac{\partial}{\partial b} \left(\mathcal{P}(b,t,\mathbf{x}) \cdot \int_{-\infty}^{b} \nabla_{\mathbf{x}'} p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a,b)} db \right) \\
= -\frac{\partial}{\partial a} \left(\mathcal{Q}(a,t,\mathbf{x}) p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a,b)} \right) - \frac{\partial}{\partial b} \left(\mathcal{Q}(b,t,\mathbf{x}') p_{u(\mathbf{x},t)u(\mathbf{x}',t)}^{(a,b)} \right).$$
(56)

Next, we consider the full Eq. (50) and we look for a kinetic equation involving the joint probability density of u and all the random variables $\{\xi_i\}$ and $\{\eta_i\}$

$$p_{u(\boldsymbol{x},t)\{\xi_i\}\{\eta_j\}}^{(a,\{b_i\},\{c_j\})} \stackrel{\text{def}}{=} \left\langle \delta(a-u(\boldsymbol{x},t)) \prod_{k=1}^m \delta(b_k-\xi_k) \prod_{j=1}^n \delta(c_k-\eta_k) \right\rangle.$$
(57)

The average here is with respect to the joint probability density functional of the random initial condition, the random boundary conditions and all the random variables $\{\xi_i\}$ and $\{\eta_j\}$. By following exactly the same steps that led us to Eq. (53) we obtain

$$\frac{\partial}{\partial t} p_{u(\boldsymbol{x},t)\{\xi_i\}\{\eta_j\}}^{(a,\{b_i\},\{c_j\})} + \frac{\partial}{\partial a} \left(\mathcal{P}(a,t,\boldsymbol{x},\boldsymbol{b}) \cdot \int_{-\infty}^{a} \nabla p_{u(\boldsymbol{x},t)\{\xi_i\}\{\eta_j\}}^{(a',\{b_i\},\{c_j\})} da' \right) = -\frac{\partial}{\partial a} \left(\mathcal{Q}(a,t,\boldsymbol{x},\boldsymbol{c}) p_{u(\boldsymbol{x},t)\{\xi_i\}\{\eta_j\}}^{(a,\{b_i\},\{c_j\})} \right).$$
(58)

Thus, if **x** is a vector of *D* variables then Eq. (58) involves (D + 2) variables and (n + m) parameters, i.e. $\mathbf{b} = (b_1, \ldots, b_m)$, $\mathbf{c} = (c_1, \ldots, c_n)$. Therefore, the numerical solution to Eq. (58) necessarily involves the use of computational schemes specifically designed for high-dimensional problems such as sparse grid or separated representations [40–42]. However, let us remark that if \mathcal{P} and \mathcal{Q} are easily integrable then we can apply the method of characteristics directly to Eq. (50) and obtain an analytical solution to the problem. Unfortunately, this is not always possible and therefore the use of numerical approaches is often unavoidable.

4.1. Example 1: linear advection

Let us consider the simple linear advection problem

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \sigma\xi(\omega)\psi(x,t), & \sigma \ge 0, \ x \in [0,2\pi], \ t \ge t_0, \\ u(x,t_0;\omega) = u_0(x;\omega), \\ \text{Periodic B.C.}, \end{cases}$$
(59)

where $u_0(x; \omega)$ is a random initial condition of arbitrary dimensionality, $\xi(\omega)$ is a random variable and ψ is a prescribed deterministic function. We look for an equation involving the joint response-excitation probability density function

$$p_{u(x,t)\xi}^{(a,b)} = \langle \delta(a - u(x,t))\delta(b - \xi) \rangle.$$
(60)

The average here is with respect to the joint probability measure of $u_0(x; \omega)$ and $\xi(\omega)$. Differentiation of (60) with respect to *t* and *x* yields, respectively

$$\frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial t} = -\frac{\partial}{\partial a} \langle \delta(a-u)u_t \delta(b-\xi) \rangle, \tag{61a}$$

$$\frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial x} = -\frac{\partial}{\partial a} \langle \delta(a-u)u_x \delta(b-\xi) \rangle. \tag{61b}$$

A summation of Eqs. (61a) and (61b) gives the final result

$$\frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial t} + \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial x} = -\frac{\partial}{\partial a} \langle \delta(a-u)[u_t+u_x]\delta(b-\xi) \rangle = -\frac{\partial}{\partial a} \langle \delta(a-u)\sigma\xi\psi\delta(b-\xi) \rangle = -\sigma b\psi(x,t)\frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial a}.$$
(62)

Thus, the problem corresponding to Eq. (59) can be formulated in probability space as

$$\begin{cases} \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial t} + \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial x} = -\sigma \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial a} b\psi(x,y), \quad \sigma \ge 0, \ x \in [0,2\pi], \ t \ge t_0, \\ p_{u(x,t_0)\xi}^{(a,b)} = p_{u_0(x)}^{(a)} p_{\xi}^{(b)}, \\ \text{Periodic B.C.}, \end{cases}$$
(63)

where we have assumed that the process $u_0(x; \omega)$ is independent of ξ and we have denoted by $p_{u_0(x)}^{(a)}$ and $p_{\xi}^{(b)}$ the probability densities of the initial condition and $\xi(\omega)$, respectively. Eq. (63) is derived also in Appendix (A.1) by employing a Hopf characteristic functional approach. Once the solution to Eq. (63) is available, we can compute the *response probability* of the system as

$$p_{u(x,t)}^{(a)} = \int_{-\infty}^{\infty} p_{u(x,t)\xi}^{(a,b)} \, db \tag{64}$$

and then extract all the statistical moments we are interested in, e.g.,

$$\langle u^m(\mathbf{x},t;\omega)\rangle = \int_{-\infty}^{\infty} a^m p_{u(\mathbf{x},t)}^{(a)} da.$$
(65)

4.2. Example 2: nonlinear advection

A more interesting problem concerns the computation of the statistical properties of the solution to the randomly forced inviscid Burgers equation

$$\begin{cases} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \sigma \xi(\omega) \psi(x, t), & \sigma \ge 0, \ x \in [0, 2\pi], \ t \ge t_0, \\ u(x, t_0; \omega) = A \sin(x) + \eta(\omega) & A \in \mathbb{R}, \end{cases}$$
(66)
Periodic B.C.,

where, as before, ξ and η are assumed as independent Gaussian random variables and ψ is a prescribed deterministic function. Note that the amplitude of the initial condition controls the initial speed of the wave. We look for an equation involving the probability density (60). To this end, we differentiate it with respect to *t* and *x*

$$\frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial t} = -\frac{\partial}{\partial a} \langle \delta(a-u)u_t \delta(b-\xi) \rangle, \tag{67a}$$

$$\frac{\partial p_{u(x,t)\xi}^{(u,t)}}{\partial x} = -\frac{\partial}{\partial a} \langle \delta(a-u)u_x \delta(b-\xi) \rangle, \tag{67b}$$

$$a\frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial x} = -\frac{\partial}{\partial a}\langle \delta(a-u)uu_x\delta(b-\xi)\rangle + \langle \delta(a-u)u_x\delta(b-\xi)\rangle.$$
(67c)

By using Eq. (67b) we obtain

$$\langle \delta(a-u)u_{x}\delta(b-\xi)\rangle = -\int_{-\infty}^{a} \frac{\partial p_{u(x,t)\xi}^{(a',b)}}{\partial x} da'.$$
(68)

Finally, a summation of Eq. (67a) and Eq. (67c) (with the last term given by Eq. (68)) gives

$$\begin{cases} \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial t} + a \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial x} + \int_{-\infty}^{a} \frac{\partial p_{u(x,t)\xi}^{(a',b)}}{\partial x} da' = -\sigma b\psi(x,t) \frac{\partial p_{u(x,t)\xi}^{(a,b)}}{\partial a}, \quad x \in [0,2\pi], \ t \ge t_{0}, \\ p_{u(x,t_{0})\xi}^{(a,b)} = p_{\eta}(a,x)p_{\xi}(b), \\ \text{Periodic B.C.}, \end{cases}$$
(69)

where, as before

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$$p_{\xi}(b) = \frac{1}{\sqrt{2\pi}} e^{-b^2/2}, \quad p_{\eta}(a, x) = \frac{1}{\sqrt{2\pi}} e^{-(a - A\sin(x))^2/2}.$$
(70)

Eq. (69) is derived also in Appendix (A.2) by employing a Hopf characteristic functional approach.

4.3. Example 3: nonlinear advection with high-dimensional random forcing

A generalization of the problem considered in Section 4.2 involves a high-dimensional random forcing term [43]

$$\begin{cases} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \sigma f(t, x; \omega), & x \in [0, 2\pi], \ t \ge 0, \ \sigma \ge 0, \\ u(x, 0; \omega) = A \sin(x) + \eta(\omega), \\ \text{Periodic B.C.}, \end{cases}$$
(71)

where $f(t, x; \omega)$ is a random field with stipulated statistical properties, e.g. a Gaussian random field with prescribed correlation function. For convenience, let us assume that we have available a Karhunen–Loève representation of f, i.e.

$$f(\mathbf{x}, t; \omega) = \sum_{k=1}^{m} \lambda_k \xi_k(\omega) \psi_k(\mathbf{x}, t),$$
(72)

where $\{\xi_k(\omega)\}$ is a set of uncorrelated Gaussian random variables. With these assumptions the space–time autocorrelation of the random field (72) can be rather arbitrary. Indeed, the functions ψ_k can be constructed based on a prescribed correlation structure [16]. Now, let us look for an evolution equation involving the joint probability density function of the solution u and the random variables $\{\xi_1, \ldots, \xi_m\}$

$$p_{u(x,t)\{\xi_j\}}^{(a,\{b_j\})} = \left\langle \delta(a-u) \prod_{k=1}^m \delta(b_k - \xi_k) \right\rangle.$$
(73)

By following the same steps that led us to Eq. (69) it can be shown that

$$\frac{\partial}{\partial t}p_{u(x,t)\{\xi_j\}}^{(a,\{b_j\})} + a\frac{\partial}{\partial x}p_{u(x,t)\{\xi_j\}}^{(a,\{b_j\})} + \int_{-\infty}^{a}\frac{\partial}{\partial x}p_{u(x,t)\{\xi_j\}}^{(a',\{b_j\})}da' = -\sigma\sum_{k=1}^{m}\lambda_k b_k \psi_k(x,t)\frac{\partial}{\partial a}p_{u(x,t)\{\xi_j\}}^{(a,\{b_j\})}.$$
(74)

This is a linear equation that involves three variables (a, t and x) and *m* parameters (b_1, \ldots, b_m) .

4.4. Example 4: advection-reaction equation

Let us consider a multidimensional advection-reaction system governed by the stochastic PDE

$$\frac{\partial u}{\partial t} + \mathbf{U}(\mathbf{x}, t; \omega) \cdot \nabla u = \mathcal{H}(u), \tag{75}$$

where $\mathbf{x} = (x, y, z)$ are spatial coordinates, $\mathbf{U}(\mathbf{x}, t; \omega)$ is a vectorial random field with known statistics and \mathcal{H} is a nonlinear function of *u*. Eq. (75) has been recently investigated by Tartakovsky and Broyda [4] in the context of transport phenomena in heterogeneous porous media with uncertain properties.⁵ In the sequel, we shall assume that we have available a representation of the random field $\mathbf{U}(\mathbf{x}, t; \omega)$, e.g., a Karhunen–Loève series of each component in the form

$$U^{(x)}(\boldsymbol{x},t;\omega) = \sum_{i=1}^{m_x} \lambda_i^{(x)} \xi_i(\omega) \Psi_i^{(x)}(\boldsymbol{x},t),$$
(76a)

$$U^{(y)}(\mathbf{x},t;\omega) = \sum_{j=1}^{m_y} \lambda_j^{(y)} \eta_j(\omega) \Psi_j^{(y)}(\mathbf{x},t),$$
(76b)

$$U^{(z)}(\boldsymbol{x},t;\omega) = \sum_{k=1}^{m_z} \lambda_k^{(z)} \zeta_k(\omega) \Psi_k^{(z)}(\boldsymbol{x},t).$$
(76c)

Note that each set of random variables $\{\xi_i\}$, $\{\eta_j\}$ and $\{\zeta_k\}$ is uncorrelated, but we can have a correlation between different sets. This gives us the possibility to prescribe a correlation structure between different velocity components at the same space-time location. Given this, let us look for an equation satisfied by the joint probability density function

$$p_{u(\boldsymbol{x},t)\{\xi_i\}\{\eta_j\}\{\zeta_k\}}^{(a,\{b_i\},\{c_j\},\{d_k\})} = \left\langle \delta(a - u(\boldsymbol{x},t)) \prod_{i=1}^{m_x} \delta(b_i - \xi_i) \prod_{j=1}^{m_y} \delta(b_j - \eta_j) \prod_{k=1}^{m_z} \delta(d_k - \zeta_k) \right\rangle,$$
(77)

where the average is with respect to the joint probability density functional of the initial conditions, boundary conditions and random variables $\{\{\xi_i\}, \{\eta_i\}, \{\zeta_k\}\}$. By following the same steps that led us to Eq. (53), we obtain

⁵ In [4] it is assumed that \mathcal{H} is random as a consequence of an uncertain reaction rate constant $\kappa(\mathbf{x};\omega)$.

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$$\frac{\partial P}{\partial t} + \left(\sum_{i=1}^{m_x} \lambda_i^{(x)} b_i \Psi_i^{(x)}\right) \frac{\partial P}{\partial x} + \left(\sum_{i=1}^{m_y} \lambda_i^{(y)} c_i \Psi_i^{(y)}\right) \frac{\partial P}{\partial y} + \left(\sum_{i=1}^{m_z} \lambda_i^{(z)} d_i \Psi_i^{(z)}\right) \frac{\partial P}{\partial z} = -\frac{\partial}{\partial a} (\mathcal{H}P), \tag{78}$$

where *P* is a shorthand notation for Eq. (77). Eq. (78) involves five variables (a, x, y, z, t) and $(m_x + m_y + m_z)$ parameters. Thus, the exact stochastic dynamics of this advection–reaction system develops over a high-dimensional manifold. In order to overcome such a dimensionality issue, Tartakovsky and Broyda [4] obtained a *closure approximation* of the response probability associated with the solution to Eq. (75) based on a Large Eddy Diffusivity (LED) scheme. Note that a marginalization of Eq. (78) with respect to the parameters $\{\{b_i\}, \{c_j\}, \{d_k\}\}$ yields an unclosed equation for $p_{u(x)}^{(a)}$.

5. Some remarks on kinetic equations involving high-dimensional joint response-excitation probability density functions

All the equations presented in this paper for the probability density function are linear evolution equations that can be formally written as [44,45]

$$\frac{\partial p}{\partial t} = Hp,\tag{79}$$

where *H* is, in general, a linear operator depending on space, time as well as on many parameters, here denoted by $\{b_i\}$. The parametric dependence of *H* on the set $\{b_i\}$ is usually linear. For instance, the kinetic Eq. (74) can be written in the general form (79) provided we define

$$H \stackrel{\text{def}}{=} L + \sigma B, \tag{80a}$$

$$L \stackrel{\text{def}}{=} -a \frac{\partial}{\partial x} (\cdot) - \int_{-\infty}^{a} \frac{\partial}{\partial x} (\cdot) da', \tag{80b}$$

$$B \stackrel{\text{def}}{=} -\sum_{k=1}^{d} b_k \psi_k(x,t) \frac{\partial}{\partial a}(\cdot).$$
(80c)

A discretization of Eq. (79) with respect to the variables of the system, e.g. *a* and *x* in case of Eq. (74), yields a linear system of ordinary differential equations for the Fourier coefficients⁶ $\hat{p}(t; \{b_i\})$

$$\frac{d\hat{p}(t;\{b_i\})}{dt} = \hat{H}(t;\{b_i\})\hat{p}(t;\{b_i\}).$$
(81)

The matrix $\hat{H}(t; \{b_i\})$ is the finite-dimensional version of the linear operator *H*. The *short-time propagator* associated with the system (81) can be expressed analytically in terms of a Magnus series [46,47]

$$\hat{p}(t; \{b_i\}) = \exp\left[\sum_{k=1}^{\infty} \Omega_k(t, t_0; \{b_i\})\right] \hat{p}(t_0; \{b_i\}),$$
(82)

where the matrices $\Omega_k(t; \{b_i\})$ are

. .

$$\Omega_1(t,t_0;\{b_i\}) = \int_{t_0}^t \widehat{H}(t_1;\{b_i\}) dt_1$$
(83a)

$$\Omega_{2}(t,t_{0};\{b_{i}\}) = \frac{1}{2} \int_{t_{0}}^{t} \int_{t_{0}}^{t_{1}} [\widehat{H}(t_{1};\{b_{i}\}),\widehat{H}(t_{2};\{b_{i}\})] dt_{1} dt_{2},$$

$$(83b)$$

$$\Omega_{3}(t,t_{0};\{b_{i}\}) = \frac{1}{6} \int_{t_{0}}^{t_{1}} \int_{t_{0}}^{t_{2}} \left([\hat{H}(t_{1};\{b_{i}\}),[\hat{H}(t_{2};\{b_{i}\}),\hat{H}(t_{3};\{b_{i}\})]] + [\hat{H}(t_{3};\{b_{i}\}),[\hat{H}(t_{2};\{b_{i}\}),\hat{H}(t_{1};\{b_{i}\})]] \right) dt_{1} dt_{2} dt_{3},\dots$$
(83c)

[,] being the matrix commutator (Lie bracket), i.e. $[A, B] \stackrel{\text{def}}{=} AB - BA$. As is well known, the convergence radius of the representation (82), i.e. the break-down time T_b where we have no guarantee that the solution is in the form (82), depends on the norm of the operator H (see Section 2.7 in [46]). Thus, we cannot expect that the representation (82) in general holds for all $t \ge 0$. However, in some particular cases, e.g. when the matrix $\hat{H}(t; \{b_i\})$ has the structure

$$\widehat{H}(t; \{b_i\}) = \sum_{l=1}^{d} z_k(t) Q_k(\{b_i\}), \quad z_k(t) \text{ are scalar functions, } Q_k \text{ are matrices}$$
(84)

then there exist a global representation of the solution in terms of a product of *d* matrix exponentials [48]. A global representation can also be constructed based on the general the formula (86). To this end, let us partition the integration period [0, T] into *n* small chunks $[t_{i+1}, t_i]$ ($t_{n+1} = T, t_0$) and consider a Magnus expansion within each time interval. This allows us to represent the time evolution of the solution through a product of exponential operators in the form

⁶ In Eq. (81) $\hat{p}(t; \{b_i\})$ denotes a vector of Fourier coefficients.

$$\mathcal{G}(t, t_0; \{b_i\}) = \prod_{j=0}^{n} \exp\left[\sum_{k=1}^{p} \Omega_k(t_{j+1}, t_j; \{b_i\})\right],\tag{85}$$

where, e.g., $\Omega_1(t_{j+1}, t_j; \{b_i\})$ is defined by Eq. (83a) but with integration limits t_j and t_{j+1} . In order to achieve a time integration method order 2*p*, only terms up to Ω_{2p-2} have to be retained in the exponents appearing in (85). We also remark that these exponential operators can be decomposed further by using the Suzuki's formulae [49]. The response probability of the system at a particular time then is obtained by averaging the unitary evolution $\mathcal{G}(t, t_0; \{b\})\hat{p}(t_0; \{b_i\})$ with respect to all the parameters $\{b_j\}$, i.e. over all the possible histories of the system. In other words, once the transformation (85) has been constructed then we can, in principle, integrate out all the variables $\{b_i\}$ and obtain the following expression for the Fourier coefficients of the *response probability*

$$\hat{p}(t) = \langle \mathcal{G}(t, t_0; \{b_i\}) \hat{p}(t_0; \{b_i\}) \rangle_b, \quad t \in [0, T],$$
(86)

where the average $\langle \cdot \rangle_b$ denotes a multidimensional integral with respect to the parameters $\{b_j\}$. It is clear at this point that the computation of the multidimensional integral appearing in Eq. (86) is the key aspect for the calculation of *the response probability* associated with the random wave. Remarkably, this averaging operation is very similar to the computation of the *effective Lagrangian* in the functional integral formalism of classical statistical physics ([29], p. 196). Unfortunately, there is still no explicit analytical formula for the integral of the exponential operator (85) with respect to the parameters b_k (see, e.g., [50–53]) and therefore it seems that an analytical calculation of (86) cannot be performed explicitly. From a numerical viewpoint, however, recent multidimensional extensions [50] of the Van Loan [51] algorithm could lead to effective techniques for the calculation of the average appearing in Eq. (86).

6. Numerical results

The purpose of this section is to provide a numerical verification of the joint response-excitation PDF equations we have obtained in this paper. To this end, we will consider three prototype problems involving randomly forced linear and nonlinear advection equations as well as a nonlinear advection–reaction equation.

6.1. Linear advection

By using the method of characteristics ([54], p. 97; [39], p. 66) it can be proved that the analytical solution to (59) assuming

$$\psi(\mathbf{x},t) = \sin(\mathbf{x})\sin(2t),\tag{87a}$$

$$u_0(x;\omega) = \sum_{k=1}^{10} \eta_k(\omega) \frac{1}{k} \sin(kx+k) + \sum_{k=1}^{10} \zeta_k(\omega) \frac{1}{k} \cos(kx),$$
(87b)

is

$$u(\mathbf{x},t;\omega) = u_0(\mathbf{x}-t;\omega) + \sigma\xi(\omega)Q(\mathbf{x},t),$$
(88)

where

$$Q(x,t) \stackrel{\text{def}}{=} \frac{2}{3}\sin(x-t) - \frac{1}{2}\sin(x-2t) - \frac{1}{6}\sin(x+2t).$$
(89)

Thus, if $\eta_k(\omega)$, $\zeta_k(\omega)$ and $\zeta(\omega)$ are independent Gaussian random variables then we obtain the following statistical moments

$$\langle u(x,t;\omega)^n \rangle = \begin{cases} 0 & n \text{ odd,} \\ (n-1)(n-3)\cdots [Z(x-t)^2 + \sigma^2 Q(x,t)^2]^{n/2} & n \text{ even,} \end{cases}$$
(90)

where

$$Z(x)^{2} \stackrel{\text{def}}{=} \sum_{k=1}^{10} \frac{1}{k^{2}} [\sin(kx+k)^{2} + \cos(kx)^{2}].$$
(91)

Similarly, the analytical solution to the problem (63) for the initial condition

$$p_{u(x,t_0)\xi}^{(a,b)} = \frac{1}{2\pi |Z(x)|} \exp\left[-\frac{a^2}{2Z(x)^2} - \frac{b^2}{2}\right]$$
(92)

is obtained through the method of characteristics as

$$p_{u(x,t)\xi}^{(a,b)} = \frac{1}{2\pi |Z(x-t)|} \exp\left[-\frac{a^2 + b^2 (Z(x-t)^2 + \sigma^2 Q(x,t)^2) - 2ab\sigma Q(x,t)}{2Z(x-t)^2}\right].$$
(93)

An integration of Eq. (93) with respect to *b* form $-\infty$ to ∞ , gives the following expression for the response probability density function (i.e. the probability of $u(x, t; \omega)$)

$$p_{u(x,t)}^{(a)} = \frac{1}{\sqrt{2\pi}|W(x,t)|} \exp\left[-\frac{a^2}{2W(x,t)^2}\right],$$
(94)

where

$$W(x,t)^{2} \stackrel{\text{def}}{=} Z(x-t)^{2} + \sigma^{2}Q(x,t)^{2}.$$
(95)

Note that the statistical moments (90) are in perfect agreement with the moments of the probability density function (94) and therefore the solutions to Eqs. (63) and (59) are fully consistent. The response probability density (64) is shown in Fig. 1 at different time instants. Similarly, in Fig. 2 we plot the variance of the solution field at different times (note that the mean field is identically zero).

6.2. Nonlinear advection

An analytical solution to the problem (66) is not available in an explicit form and therefore we need to resort to numerical approaches. To this end, we employ a Fourier–Galerkin method combined with high-order probabilistic collocation for the simulation of both Eqs. (66) and (69) (see Appendix B). For smooth initial conditions, the spectral convergence rate of the



Fig. 1. Response probability $p_{u(x,t)}^{(\alpha)}$ of the solution to the linear advection problem (59) as computed form Eq. (63). Shown are snapshots of the probability density function at different times for $\sigma = 3$.



Fig. 2. Linear advection equation. (a) Variance of the solution field $u(x,t;\omega)$ in space–time for $\sigma = 3$ and (b) time-slices of the variance in spatial domain.



Fig. 3. Response probability $p_{u(x,t)}^{(a)}$ of the solution to the nonlinear advection problem (66) as computed from Eq. (69). Shown are snapshots of the probability density function at different times.

Fourier–Galerkin method [55] allows us to simulate the time evolution of the probability density very accurately. In addition, the integral appearing in Eq. (69) can be computed analytically. However, the use of a global Fourier series for the representation of the probability density function has also some drawbacks. First of all, the positivity and the normalization condition are not automatically guaranteed. The normalization condition, however can be enforced by using suitable geometric time integrators (see Section 5). Secondly, if the initial condition for the probability density is compactly supported, e.g. a uniform distribution, then the convergence rate of the Fourier series may significantly deteriorate [56] (although the representation theoretically converges to any distribution in L^2).

Given these preliminary remarks, let us now recall that the nonlinear advection equation develops shock singularities in *finite time* (e.g. [39], p. 276; [3,57,58]). Therefore, a careful selection of the simulation parameters and the type of random forcing is necessary in order to avoid these situations.⁷ In particular, we shall consider

$$\psi(x,t) = \sin(x)\sin(20t), \quad \sigma = \frac{1}{2}, \quad A = \frac{1}{2}$$
(96)

in Eqs. (66) and (69). It can be shown that with these choices the solution is smooth for all $t \in [0, 1]$ with probability about 1. The Fourier resolution in the *x* direction is set to N = 100 modes for both u(x,t) and $p_{u(x,t)\xi}^{(a,b)}$ while the resolution for the *a* variable appearing in the probability density is set to Q = 250 modes (see Appendix B for further details). The Gaussian random variables ξ and η in Eq. (66) are sampled first on a 50 × 50 Gauss–Hermite collocation grid (PCM) and then on a multi-element collocation grid of 10 elements of order 10 (ME-PCM) [59] for higher accuracy. Similarly, the dependence on the parameter *b* in Eq. (69) is handled through a multi-element Gauss–Lobatto–Legendre quadrature. Specifically, we have employed 10 equally-spaced finite elements, each element being of order 10. Once the solution to Eq. (69) is available, we can compute the *response* PDF of the system (Fig. 3) and its relevant statistical moments (Fig. 4) at different time instants. These moments are in a very good agreement with the ones obtained from high-order collocation approaches applied to Eq. (66). In order to show this, in Fig. 5 we plot the time-dependent relative errors between the mean and the variance of the field *u* as computed from Eqs. (66) and (69). These relative errors are defined as

$$e_{2}[\langle u \rangle](t) \stackrel{\text{def}}{=} \frac{\|\langle \tilde{u} \rangle - \langle u \rangle\|_{L_{2}([0,2\pi])}}{\|\langle u \rangle\|_{L_{2}([0,2\pi])}}, \quad e_{2}[\sigma_{u}^{2}](t) \stackrel{\text{def}}{=} \frac{\|\tilde{\sigma}_{u}^{2} - \sigma_{u}^{2}\|_{L_{2}([0,2\pi])}}{\|\sigma_{u}^{2}\|_{L_{2}([0,2\pi])}}, \tag{97}$$

where the quantities with a tilde are obtained from probabilistic collocation of Eq. (66) (either Gauss–Hermite or ME-PCM), while $\|\cdot\|_{L_2([0,2\pi])}$ denotes the standard L_2 norm in $[0, 2\pi]$, i.e.

$$\|g(x)\|_{L_{2}([0,2\pi])} \stackrel{\text{def}}{=} \left(\int_{0}^{2\pi} g(x)^{2} dx\right)^{1/2}.$$
(98)

⁷ We remark that the singularities of the nonlinear advection equation subject to random initial conditions, random boundary conditions or random forcing terms are random in space and time. In other words, the location of a shock and the time at which it appears are both random. In this paper we shall limit ourselves to PDEs with smooth solutions.



Fig. 4. Nonlinear advection equation. Time snapshots of the mean (left) and the variance (right) the solution field $u(x, t; \omega)$.



Fig. 5. Nonlinear advection. Relative errors (97) between the mean and the variance of the field *u* as computed from probabilistic collocation of Eq. (66) and integration of the probability density function satisfying Eq. (69). We show two different results: (a) Gauss–Hermite collocation of Eq. (66) on a 50 × 50 grid; (b) ME-PCM of Eq. (66) with 10 finite elements of order 10 for both $\xi(\omega)$ and $\eta(\omega)$ (100 × 100 collocation points).

The error growth in time observed in Fig. 5(a) is not due to a random frequency problem [22,8], but rather to the fact that the response probability of the system tends to split into two distinct parts after time t = 0.5 (see Fig. 3). This yields to accuracy problems when a global Gauss–Hermite collocation scheme is used. A similar issue has been discussed in [9], in the context of stochastic Rayleigh–Bénard convection subject to random initial states (see also [60]). Fig. 5(b) shows that the error growth can be stabilized in time if the ME-PCM method is used. In this case, the maximum pointwise errors between the mean and the variance fields are

$$\max_{\substack{t \in [0,1] \\ x \in [0,2\pi]}} |\langle \tilde{u} \rangle - \langle u \rangle| = 3.0 \times 10^{-7}, \quad \max_{\substack{t \in [0,1] \\ x \in [0,2\pi]}} |\tilde{\sigma}_u^2 - \sigma_u^2| = 1.7 \times 10^{-6}.$$
(99)

In addition to the mean and variance we have examined so far, it also interesting to compare other output functionals such as the *skewness* and the *kurtosis* of the solution field. We recall that these quantities are defined, respectively, as

$$\gamma(\mathbf{x},t) \stackrel{\text{def}}{=} \frac{\kappa_3(\mathbf{x},t)}{\kappa_2(\mathbf{x},t)^{3/2}} \text{ (skewness), } \quad \chi(\mathbf{x},t) \stackrel{\text{def}}{=} \frac{\kappa_4(\mathbf{x},t)}{\kappa_2(\mathbf{x},t)^2} \text{ (kurtosis),}$$
(100)

where $\kappa_i(x, t)$ denotes the *i*-th cumulant of $u(x, t; \omega)$. The skewness and the kurtosis are obviously zero in correspondence of the Gaussian initial state, and they evolve in time as shown in Fig. 6. It is interesting to analyze the L^2 errors between the variance, skewness and kurtosis as computed by ME-PCM and the highly accurate PDF approach. This is done in Fig. 7 where we plot

$$E_{2}[\sigma_{u}^{2}](t) \stackrel{\text{def}}{=} \|\tilde{\sigma}_{u}^{2} - \sigma_{u}^{2}\|_{L_{2}([0,2\pi])}, \quad E_{2}[\gamma](t) \stackrel{\text{def}}{=} \|\tilde{\gamma} - \gamma\|_{L_{2}([0,2\pi])}, \quad E_{2}[\gamma](t) \stackrel{\text{def}}{=} \|\tilde{\chi} - \chi\|_{L_{2}([0,2\pi])}. \tag{101}$$

The tilded quantities here are those obtained from ME-PCM. As expected, ME-PCM loses some accuracy when representing higher-order moments of the solution.



Fig. 6. Nonlinear advection. Skewness (a) and kurtosis (b) of the solution field.



Fig. 7. Nonlinear advection. Absolute L^2 errors (101) between the variance, skewness and kurtosis of the ME-PCM solution relatively to the reference PDF solution. As expected, ME-PCM loses accuracy when representing higher-order statistics.

A fundamental question concerns the *computational cost* required by ME-PCM and PDF approaches. A comparison between the boundary value problems (66) and (69) shows that the PDF method introduces an additional variable in the system (i.e the variable *a*) but, at the same time, it does not suffer from the dimensionality in the boundary and initial conditions. In particular, for the prototype problem we have studied in this section to *validate* our new equations, ME-PCM is moderately faster than the PDF method, at comparable level of accuracy in the variance. This is due to the fact that it is more efficient to sample (66) N^2 times for ξ and η instead of sampling (69) N times for *b*. However, if the initial condition of the system is high-dimensional, then the PDF method overwhelms ME-PCM and other collocation approaches such as sparse grid. This is exemplified in the next section.

6.3. Nonlinear advection-reaction problem with high-dimensional random initial conditions

In order to show the efficiency gain of the PDF methodology with respect to more conventional solution techniques we consider a nonlinear advection–reaction problem [4] subject to a high-dimensional random initial condition. In particular, we examine the dynamics of the system

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = -(u^2 - 1), & x \in [0, 2\pi], \ t \ge 0, \\ u(x, 0; \omega) = u_0(x; \omega), \\ \text{Periodic B.C.} \end{cases}$$
(102)

where

$$u_0(\mathbf{x};\omega) = U + \sigma \sum_{k=1}^{m} [\eta_k(\omega)\sin(k\mathbf{x}) + \xi_k(\omega)\cos_k(k\mathbf{x})], \quad U \ge 0, \quad \sigma > 0,$$
(103)

and $\{\eta_1, \ldots, \eta_m, \xi_1, \ldots, \xi_m\}$ is a 2*m*-dimensional normal random vector with uncorrelated components. In the context of advection–reaction phenomena, $u(x, t; \omega)$ can represent the dimensionless random concentration of a chemical species. Therefore, the initial condition (103) is usually set to be in [0, 1], 1 being the dimensionless equilibrium concentration. Under this hypothesis, the solution to the problem (102) is a smooth random field. In Fig. 8 we plot the set of couples (U, σ) for



Fig. 8. Set of couples (U, σ) for which $u_0(x; \omega)$ in (102) satisfies the condition $0 \le u_0(x; \omega) \le 1$ with probability about one. In figure (a) we plot the results for the case m = 2, m = 10 and m = 40. The triangular-like shaped domain with $U^* = 1/2$ shown in figure (a) holds for arbitrary m with the corresponding value of σ^* given in figure (b). For illustration purposes, we plot several samples of the initial state u_0 for a mean value $U = U^* = 1/2$, perturbation amplitude $\sigma = 2\sigma^*/3$, and different m. As easily seen, high-dimensional random initial conditions are usually quite rough in space.

which the initial condition (103) satisfies $0 \le u_0(x; \omega) \le 1$ with probability nearly one. Note that, by construction, the mean and the variance of $u_0(x; \omega)$ are, respectively

$$|u_0\rangle = U, \quad \sigma_{u_0}^2 = m\sigma^2. \tag{104}$$

The one-point one-time PDF of the solution to (102) satisfies the boundary value problem

$$\begin{cases} \frac{\partial p_{u(x,t)}^{(a)}}{\partial t} + \frac{\partial p_{u(x,t)}^{(a)}}{\partial x} - (a^2 - 1) \frac{\partial p_{u(x,t)}^{(a)}}{\partial a} = 2ap_{u(x,t)}^{(a)}, \quad x \in [0, 2\pi], \ t \ge 0, \\ p_{u(x,0)}^{(a)} = \frac{1}{\sqrt{2\pi m\sigma}} \exp\left[-\frac{a^2}{2m\sigma^2}\right], \\ \text{Periodic B.C.} \end{cases}$$
(105)

Note that this problem is independent of the dimensionality of the random initial condition. In Fig. 9 we plot the time-snapshots of the solution PDF at location $x = \pi$ for a random initial condition (103) defined in terms of 120 random variables (i.e. m = 60), $\sigma = 0.006$ and U = 0.25 (see Fig. 8). It is seen that $p_{u(x,t)}^{(a)}$ tends to $\delta(a - 1)$ as time increases, i.e. $u(x, t; \omega)$ tends to the deterministic equilibrium concentration $u_{eq} = 1$. At this point we remark that the numerical solution of (102) is not viable in practice by using conventional statistical approaches. For example, a tensor product probabilistic grid would require 120^n Gauss–Hermite points in the present case, where *n* denotes the number of collocation points for each random variable appearing in the series expansion (103). Sparse grid collocation [10] can significantly reduce such number of points, although it cannot completely overcome the dimensionality problem. On the contrary, the PDF method yields an exact, low-dimensional, linear evolution equation for the PDF which (102) can be solved efficiently.

7. Summary and discussion

We have obtained and discussed new evolution equations for the joint response-excitation probability density function (PDF) of the stochastic solution to first-order nonlinear scalar PDEs subject to uncertain initial conditions, boundary conditions or random forcing terms. The theoretical predictions are confirmed well by numerical simulations based on an accurate Fourier–Galerkin spectral method. A reformulation of a stochastic problem in terms of the probability density function has an advantage with respect to more conventional stochastic approaches in that it does not suffer from the curse of dimensionality if randomness comes from boundary or initial conditions. In fact, we can prescribe these conditions in terms of probability distributions and this is obviously not dependent on the number of random variables characterizing the underlying probability space. In addition, the PDF method allows to directly ascertain the tails of the probabilistic distribution, thus facilitating the assessment of *rare events* and associated risks. However, if an external random forcing appears within



Fig. 9. Advection–reaction. Time snapshots of the one-point one-time PDF of the solution field at $x = \pi$. The initial condition is defined in terms of 120 random variables, i.e. m = 60 in (103), and $(\sigma, U) = (0.006, 0.25)$. It is seen that $p_{u(x,t)}^{(a)}$ tends to $\delta(a - 1)$ as time increases, i.e. $u(x, t; \omega)$ tends to the (deterministic) equilibrium concentration $u_{eq} = 1$.

the scalar PDE modeling the physical system, then the dimensionality of the corresponding problem in probability space could increase significantly (see the Sections 3–5). This happens because the exact stochastic dynamics in this case develops over a high-dimensional manifold and therefore the exact probabilistic description necessarily involves a multidimensional joint response-excitation probability density function, or even a probability density functional. In order to overcome this issue a *closure approximation* [61,4,62,63] of the evolution equation involving the probability density function can be constructed. This usually yields a system which is amenable to numerical simulation. However, the computation of the numerical solution to an equation involving a probability density function is itself a challenging problem [64,65]. In fact, in addition to the question of dimensionality, which may be handled by using closures or specifically designed algorithms [41,42,40], we have several constraints that have to be satisfied, e.g., the positivity and the normalization condition. Moreover, the probability density function could be compactly supported over *disjoint domains* and this obviously requires the use of suitable numerical techniques such as the discontinuous Galerkin method. Finally, if the boundary conditions or the initial condition associated with the problem in physical space are set to be deterministic then the corresponding conditions in probability space will be defined in terms of Dirac delta functions (see Section 3.1).

A fundamental question is whether the statistical approaches developed in this paper for first-order nonlinear stochastic PDEs can be extended to more general equations involving higher order derivatives in space and time, such as the secondorder wave equation, the diffusion equation or the Klein-Gordon equation. Unfortunately, the self-interacting nature of these higher-order problems is often associated with the existence of nonlocal solutions which, in turn, makes it impossible to obtain a closed evolution equation governing the probability density function a specific space-time location. Even in these nonlocal cases, however, it is possible to formulate an infinite set of differential constraints satisfied locally by the probability density function of the stochastic solution [24,66]. These differential constraints involve, in general, unusual partial differential operators, i.e. limit partial derivatives and, in principle, they allow to determine the probability density function associated with the solution to the underlying stochastic PDE [67]. An alternative and very general approach relies on the use of functional integral techniques [68,30,29,31,69], in particular those ones involving the Hopf characteristic functional (see also Appendix A). These methods aim to cope with the global probabilistic structure of the solution to a stochastic PDE and they have been extensively studied in the past as a possible tool to tackle many fundamental problems in physics such as turbulence [70,25]. Their usage grew very rapidly around the 70 s, when it became clear that the diagrammatic functional techniques can be applied, at least formally, to many different problems in classical statistical physics [68]. However, functional differential equations involving the Hopf characteristic functional are, unfortunately, not amenable to numerical simulation.

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Appendix A. Hopf characteristic functional approach

In this appendix we use the Hopf characteristic functional approach [26,25,71,72] to derive some of the equations for the joint response-excitation probability density function we have considered in the paper. This allow us to show how these equations can be obtained from general principles.

A.1. Linear advection

Let us consider the boundary value problem (59) and introduce the joint characteristic functional of the solution field $u(x, t; \omega)$ and the random variable $\xi(\omega)$

$$F[\alpha(X,\tau),b] \stackrel{\text{def}}{=} \left\langle e^{i \int_{X} \int_{T} u(X,\tau;\omega) \alpha(X,\tau) \, dX \, d\tau + ib\xi(\omega)} \right\rangle,\tag{106}$$

where $\alpha(X, \tau)$ is a test function and the average $\langle \cdot \rangle$ is with respect to the joint probability measure of ξ and η , namely the amplitude of the forcing and the amplitude of the spatially uniform initial condition. The Volterra functional derivative of (106) with respect to u(x, t), i.e. the Gâteaux differential [73] of the functional $F[\alpha, b]$ with respect to α evaluated at $z(X, \tau) = \delta(t - \tau)\delta(x - X)$, is

$$\frac{\delta F[\alpha, b]}{\delta u(x, t)} = i \Big\langle u(x, t; \omega) e^{i \int_{X} \int_{T} u(X, \tau; \omega) \alpha(X, \tau) \, dX \, d\tau + ib\xi(\omega)} \Big\rangle.$$
(107)

A differentiation of Eq. (107) with respect to x and t yields the identity

$$\frac{\partial}{\partial t} \left(\frac{\delta F[\alpha, b]}{\delta u(x, t)} \right) + \frac{\partial}{\partial x} \left(\frac{\delta F[\alpha, b]}{\delta u(x, t)} \right) = i \sigma \psi(x, t) \Big\langle \xi(\omega) e^{i \int_{X} \int_{T} u(X, \tau; \omega) \alpha(X, \tau) \, dX \, d\tau + ib\xi(\omega)} \Big\rangle, \tag{108}$$

where we have used Eq. (59). Eq. (108) is a *functional differential equation* that holds for arbitrary test functions $\alpha(X, \tau)$. In particular, it holds for

$$\alpha(X,\tau)^{+} \stackrel{\text{def}}{=} a\delta(t-\tau)\delta(x-X), \quad a \in \mathbb{R}.$$
(109)

Thus, if we evaluate Eq. (108) for $\alpha = \alpha^+$ we obtain

$$i\langle [u_t(\mathbf{x}, t; \omega) + u_{\mathbf{x}}(\mathbf{x}, t; \omega) - \sigma \psi(\mathbf{x}, t) \xi(\omega)] e^{iau(\mathbf{x}, t; \omega) + ib\xi(\omega)} \rangle = 0.$$
(110)

This condition is equivalent to a partial differential equation involving the *joint characteristic function* of the random variables $u(\mathbf{x}, t; \omega)$ and $\xi(\omega)$

$$\phi_{u(x,t)\xi}^{(a,b)} \stackrel{\text{def}}{=} \langle e^{iau(x,t;\omega)+ib\xi(\omega)} \rangle.$$
(111)

In order to see this, let us notice that

 $a \cdot (a h)$

1.0

$$\frac{\partial \phi_{u(x,t)\xi}^{(u,c)}}{\partial t} = ia \langle u_t(x,t;\omega) e^{iau(x,t;\omega) + ib\xi(\omega)} \rangle, \tag{112a}$$

$$\frac{\partial \phi_{u(x,t)\xi}^{(a,b)}}{\partial u} = ia \langle u_x(x,t;\omega) e^{iau(x,t;\omega) + ib\xi(\omega)} \rangle, \tag{112b}$$

$$\frac{\partial \chi}{\partial t} = i \langle \xi(\omega) e^{iau(x,t;\omega) + ib\xi(\omega)} \rangle.$$
(112c)

A substitution of Eqs. (112a)-(112c) into Eq. (110) immediately gives

$$\frac{\partial \phi_{u(x,t)\xi}^{(a,b)}}{\partial t} + \frac{\partial \phi_{u(x,t)\xi}^{(a,b)}}{\partial x} = \sigma \psi(x,t) a \frac{\partial \phi_{u(x,t)\xi}^{(a,b)}}{\partial b},\tag{113}$$

which is the result we were looking for. An inverse Fourier transformation of Eq. (113) with respect to *a* and *b* gives exactly Eq. (63). In order to see this, let us simply recall the definition of $p_{u(x,t)\xi}^{(a,b)}$ as the inverse Fourier transform of the characteristic function $\phi_{u(x,t)\xi}^{(a,b)}$

$$p_{u(x,t)\xi}^{(a,b)} = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-ial - ibq} \phi_{u(x,t)\xi}^{(l,q)} dl dq,$$

and two simple relations arising from Fourier transformation theory of a one-dimensional function g(x)

$$\int_{-\infty}^{\infty} e^{-iax} \frac{d^n g(x)}{dx^n} dx = (ia)^n \int_{-\infty}^{\infty} e^{-iax} g(x) dx,$$
$$\int_{-\infty}^{\infty} e^{-iax} x^n g(x) dx = i^n \frac{d^n}{da^n} \int_{-\infty}^{\infty} e^{-iax} g(x) dx.$$

A.2. Nonlinear advection

Let us consider the nonlinear advection problem (66) where, for simplicity, we neglect the additive random forcing term at the right hand side. This simplification does not alter in any way the main aspects of the proof presented hereafter.⁸ The Hopf characteristic functional of the solution field is

$$F[\alpha] = \left\langle e^{i \int_{X} \int_{T} u(X,\tau;\omega)\alpha(X,\tau) \, dX \, d\tau} \right\rangle. \tag{114}$$

As before, the Volterra functional derivative of (114) with respect to u(x, t) is

⁸ Indeed, the random forcing function can be included in the Hopf characteristic functional exactly as we have done in Eq. (106).

$$\frac{\delta F[\alpha]}{\delta u(x,t)} = i \Big\langle u(x,t;\omega) e^{i \int_{X} \int_{T} u(X,\tau;\omega) \alpha(X,\tau) \, dX \, d\tau} \Big\rangle.$$
(115)

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A differentiation of Eq. (115) with respect to x and t gives, respectively

$$\frac{\partial}{\partial t} \left(\frac{\delta F[\alpha]}{\delta u(x,t)} \right) = i \left\langle u_t(x,t;\omega) e^{i \int_X \int_T u(X,\tau;\omega) \alpha(X,\tau) \, dX \, d\tau} \right\rangle,\tag{116a}$$

$$\frac{\partial}{\partial x} \left(\frac{\delta F[\alpha]}{\delta u(x,t)} \right) = i \left\langle u_x(x,t;\omega) e^{i \int_X \int_T u(X,\tau;\omega) \alpha(X,\tau) \, dX \, d\tau} \right\rangle.$$
(116b)

Now we perform an additional functional differentiation of Eq. (116b) with respect to u(x',t')

$$\frac{\delta}{\partial u(x',t')} \left(\frac{\partial}{\partial x} \frac{\delta F[\alpha]}{\delta u(x,t)} \right) = - \left\langle u_x(x,t;\omega) u(x',t';\omega) e^{i \int_X \int_T u(X,\tau;\omega) \alpha(X,\tau) \, dX \, d\tau} \right\rangle \tag{117}$$

and then we take the limits for $x' \to x$ and $t' \to t$ to obtain

$$\frac{\delta}{\partial u(x,t)} \left(\frac{\partial}{\partial x} \frac{\delta F[\alpha]}{\delta u(x,t)} \right) = - \left\langle u(x,t;\omega) u_x(x,t;\omega) e^{i \int_X \int_T u(X,\tau;\omega) \alpha(X,\tau) \, dX \, d\tau} \right\rangle.$$
(118)

A summation Eq. (116a) and Eq. (118) gives (taking Eq. (66) into account)

$$\frac{\partial}{\partial t} \frac{\delta F[\alpha]}{\delta u(x,t)} - i \frac{\delta}{\partial u(x,t)} \left(\frac{\partial}{\partial x} \frac{\delta F[\alpha]}{\delta u(x,t)} \right) = 0.$$
(119)

This functional differential equation holds for arbitrary test functions $\alpha(X, \tau)$. In particular it holds for

$$\alpha^+(X,\tau) = a\delta(t-\tau)\delta(x-X).$$

Evaluating Eq. (119) for $\alpha = \alpha^+$ yields

$$\langle (u_t + uu_x)e^{iu(x,t;\omega)a} \rangle = 0.$$
(120)

Let us define the *characteristic function* of the random variable $u(x, t; \omega)$.

$$\phi_{\mu(x\,t)}^{(a)} \stackrel{\text{def}}{=} \langle e^{iu(x,t;\omega)a} \rangle. \tag{121}$$

From the definition (121) it easily follows that

$$\frac{\partial \phi_{u(x,t)}^{(a)}}{\partial t} = ai \langle u_t e^{iu(x,t;\omega)a} \rangle, \tag{122a}$$

$$\frac{\partial \phi_{u(x,t)}^{(a)}}{\partial a} = i \langle u e^{i u(x,t;\omega)a} \rangle,$$

$$\frac{\partial^2 \phi^{(a)}}{\partial a} = i \langle u e^{i u(x,t;\omega)a} \rangle,$$
(122b)

$$\frac{\partial^2 \phi_{u(x,t)a}^{(\omega)}}{\partial a \partial x} = -a \langle u u_x e^{iu(x,t;\omega)a} \rangle + \frac{1}{a} \frac{\partial \phi_{u(x,t)}^{(\omega)}}{\partial x}.$$
(122c)

Substituting Eq. (122c) and Eq. (122a) into Eq. (120) yields the following equation for the characteristic function $\phi_{u(xt)}^{(a)}$

$$a\frac{\partial\phi_{u(x,t)}^{(a)}}{\partial t} - ia\frac{\partial^2\phi_{u(x,t)}^{(a)}}{\partial a\partial x} + i\frac{\partial\phi_{u(x,t)}^{(a)}}{\partial x} = 0.$$
(123)

The inverse Fourier transformation of Eq. (123) with respect to a gives

$$\frac{\partial^2 p_{u(x,t)}^{(a)}}{\partial a \partial t} + a \frac{\partial^2 p_{u(x,t)}^{(a)}}{\partial a \partial x} + \frac{\partial p_{u(x,t)}^{(a)}}{\partial x} = 0.$$
(124)

Taking into account the fact that $p_{u(x,t)}^{(a)}$ vanishes at infinity, together with all its derivatives, we easily see that Eq. (124) is equivalent to

$$\frac{\partial p_{u(x,t)}^{(a)}}{\partial t} + a \frac{\partial p_{u(x,t)}^{(a)}}{\partial x} + \int_{-\infty}^{a} \frac{\partial p_{u(x,t)}^{(a')}}{\partial x} da' = 0.$$
(125)

This coincides with Eq. (69) with $\sigma = 0$.

A.3. Nonlinear advection with an additional quadratic nonlinearity

In this section we discuss the application of the Hopf characteristic functional approach for the derivation of an equation involving the probability density function of the solution to the problem (43). To this end, let us consider the following joint Hopf characteristic functional

$$F[\alpha(X,\tau),\beta(X,\tau)] = \left\langle e^{i\int_{X}\int_{T}u(X,\tau;\omega)\alpha(X,\tau)\,dX\,d\tau + i\int_{X}\int_{T}u_{x}(X,\tau;\omega)\beta(X,\tau)\,dX\,d\tau} \right\rangle,\tag{126}$$

where $\alpha(X, \tau)$ and $\beta(X, \tau)$ are two test fields. Functional differentiation with respect to *u* and *u*_x yields

$$\begin{split} \frac{\delta F[\alpha,\beta]}{\delta u(x,t)} &= \left\langle iu(x,t;\omega)e^{i\int_{X}\int_{T}u(X,\tau;\omega)\alpha(X,\tau)\,dX\,d\tau+i\int_{X}\int_{T}u_{x}(X,\tau;\omega)\beta(X,\tau)\,dX\,d\tau} \right\rangle, \\ \frac{\delta F[\alpha,\beta]}{\delta u_{x}(x,t)} &= \left\langle iu_{x}(x,t;\omega)e^{i\int_{X}\int_{T}u(X,\tau;\omega)\alpha(X,\tau)\,dX\,d\tau+i\int_{X}\int_{T}u_{x}(X,\tau;\omega)\beta(X,\tau)\,dX\,d\tau} \right\rangle, \\ \frac{\delta^{2}F[\alpha,\beta]}{\delta u(x,t)\delta u_{x}(x,t)} &= -\left\langle u(x,t;\omega)u_{x}(x,t;\omega)e^{i\int_{X}\int_{T}u(X,\tau;\omega)\alpha(X,\tau)\,dX\,d\tau+i\int_{X}\int_{T}u_{x}(X,\tau;\omega)\beta(X,\tau)\,dX\,d\tau} \right\rangle. \end{split}$$

By combining different functional derivatives of $F[\alpha, \beta]$ with respect to u and u_x it is straightforward to obtain the following functional differential equation corresponding to Eq. (43)

$$\frac{\partial}{\partial t}\frac{\delta F[\alpha,\beta]}{\delta u(x,t)} - i\frac{\delta^2 F[\alpha,\beta]}{\delta u(x,t)\delta u_x(x,t)} - iv\frac{\delta^2 F[\alpha,\beta]}{\delta u_x(x,t)^2} = 0.$$
(127)

This equation holds for arbitrary test functions α and β . In particular it holds for

$$\begin{aligned} \alpha(X,\tau)^+ &= a\delta(t-\tau)\delta(x-X),\\ \beta(X,\tau)^+ &= b\delta(t-\tau)\delta(x-X). \end{aligned}$$

An evaluation of Eq. (127) for $\alpha = \alpha^+$ and $\beta = \beta^+$ gives us the condition

$$\langle [u_t(x,t;\omega) + u(x,t;\omega)u_x(x,t;\omega) + vu_x(x,t;\omega)^2]e^{iau(x,t;\omega)+ibu_x(x,t;\omega)} \rangle = 0.$$
(128)

Next we show that the integral Eq. (128) is equivalent to a partial differential equation for the joint characteristic function of the random variables $u(x, t; \omega)$ and $u_x(x, t; \omega)$, i.e. the characteristic function of the solution field and its first-order spatial derivative at the same space-time location

$$\phi_{uu_x}^{(a,b)} \stackrel{\text{def}}{=} \langle e^{iau(x,t;\omega) + ibu_x(x,t;\omega)} \rangle.$$
(129)

To this end, let us first notice that

 $\Omega (a,b)$

$$\frac{\partial \phi_{uu_x}^{(a,b)}}{\partial t} = \langle [iau_t + ibu_{xt}]e^{iau(x,t;\omega) + ibu_x(x,t;\omega)} \rangle \stackrel{(43)}{=} \langle [iau_t - ib(u_x^2 + uu_{xx} + 2vu_xu_{xx})]e^{iau(x,t;\omega) + ibu_x(x,t;\omega)} \rangle.$$
(130)

At this point we need an expression for the average appearing in Eq. (130) in terms of the characteristic function. This expression is obtained by observing that

$$\frac{\partial \phi_{uu_x}^{(u')}}{\partial x} = \langle [iau_x + ibu_{xx}]e^{iau(x,t;\omega) + ibu_x(x,t;\omega)} \rangle, \tag{131a}$$

$$\frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial a \partial x} = \langle i u_x e^{i a u(x,t;\omega) + i b u_x(x,t;\omega)} \rangle - \langle [a u u_x + b u u_{xx}] e^{i a u(x,t;\omega) + i b u_x(x,t;\omega)} \rangle = \frac{\partial \phi_{uu_x}^{(a,b)}}{\partial b} + a \frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial a \partial b} - b \langle u u_{xx} e^{i a u(x,t;\omega) + i b u_x(x,t;\omega)} \rangle,$$
(131b)

$$\frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial b \partial x} = \langle i u_{xx} e^{i a u(x,t;\omega) + i b u_x(x,t;\omega)} \rangle - \langle [a u_x^2 + b u_x u_{xx}] e^{i a u(x,t;\omega) + i b u_x(x,t;\omega)} \rangle = \frac{1}{b} \frac{\partial \phi_{uu_x}^{(a,b)}}{\partial x} - \frac{a}{b} \frac{\partial \phi_{uu_x}^{(a,b)}}{\partial b} + a \frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial b^2} - b \langle u_x u_{xx} e^{i a u(x,t;\omega) + i b u_x(x,t;\omega)} \rangle.$$
(131c)

Therefore, by using Eqs. (130), (131b) and (131c) we obtain the following explicit representation for the time derivative appearing in Eq. (128)

$$ia\langle u_{t}e^{iau(x,t;\omega)+ibu_{x}(x,t;\omega)}\rangle = \frac{\partial\phi_{uu_{x}}^{(a,b)}}{\partial t} - ib\frac{\partial^{2}\phi_{uu_{x}}^{(a,b)}}{\partial b^{2}} + i\frac{\partial\phi_{uu_{x}}^{(a,b)}}{\partial b} + ia\frac{\partial^{2}\phi_{uu_{x}}^{(a,b)}}{\partial a\partial b} - i\frac{\partial^{2}\phi_{uu_{x}}^{(a,b)}}{\partial a\partial x} + 2iv\left(\frac{1}{b}\frac{\phi_{uu_{x}}^{(a,b)}}{\partial x} - \frac{a}{b}\frac{\phi_{uu_{x}}^{(a,b)}}{\partial b} + a\frac{\partial^{2}\phi_{uu_{x}}^{(a,b)}}{\partial b^{2}} - \frac{\partial^{2}\phi_{uu_{x}}^{(a,b)}}{\partial b\partial x}\right).$$
(132)

The other terms in Eq. (128) are

$$\langle uu_{x}e^{iau(x,t;\omega)+ibu_{x}(x,t;\omega)}\rangle = -\frac{\partial^{2}\phi_{uu_{x}}^{(a,b)}}{\partial a\partial b},$$
(133a)

$$\langle u_x^2 e^{iau(x,t;\omega)+ibu_x(x,t;\omega)} \rangle = -\frac{\partial^2 \phi_{uu_x}^{(a,b)}}{\partial b^2}.$$
(133b)

Finally, a substitution of Eqs. (132)-(133b) into Eq. (128) gives

$$b\frac{\partial\phi_{uu_x}^{(a,b)}}{\partial t} = ib^2\frac{\partial^2\phi_{uu_x}^{(a,b)}}{\partial b^2} - ib\frac{\partial\phi_{uu_x}^{(a,b)}}{\partial b} + ib\frac{\partial^2\phi_{uu_x}^{(a,b)}}{\partial a\partial x} - ivab\frac{\partial^2\phi_{uu_x}^{(a,b)}}{\partial b^2} - 2iv\left(\frac{\partial\phi_{uu_x}^{(a,b)}}{\partial x} - a\frac{\partial\phi_{uu_x}^{(a,b)}}{\partial b} - b\frac{\partial^2\phi_{uu_x}^{(a,b)}}{\partial b\partial x}\right).$$
(134)

An inverse Fourier transform of Eq. (134) with respect to *a* and *b* yields

$$\frac{\partial^2 p_{uu_x}^{(a,b)}}{\partial b \partial t} = \frac{\partial^2}{\partial b^2} (b^2 p_{uu_x}^{(a,b)}) + \frac{\partial}{\partial b} (b p_{uu_x}^{(a,b)}) - \frac{\partial}{\partial b} \left(b \frac{\partial p_{uu_x}^{(a,b)}}{\partial x} \right) - v \frac{\partial}{\partial b} \left(b^2 \frac{\partial p_{uu_x}^{(a,b)}}{\partial a} \right) - 2v \left[\frac{\partial p_{uu_x}^{(a,b)}}{\partial x} + b \frac{\partial p_{uu_x}^{(a,b)}}{\partial a} + \frac{\partial}{\partial b} \left(b \frac{\partial p_{uu_x}^{(a,b)}}{\partial x} \right) \right], \quad (135)$$

which, upon integration with respect to *b* from $-\infty$ to *b*, gives exactly Eq. (45).

Appendix B. Fourier-Galerkin systems for the nonlinear advection equation in physical and probability spaces

In this appendix we obtain the Fourier–Galerkin system corresponding to the nonlinear advection problem considered in Section 4.2 This allows the interested reader to perform numerical simulations and easily reproduce our numerical results. *Fourier–Galerkin system in physical space.* Let us consider a Fourier series representation of the solution to the problem (66) (periodic in $x \in [0, 2\pi]$)

$$u(\mathbf{x}, t; \omega) = \sum_{n=-N}^{N} \hat{u}_n(t; \omega) e^{in\mathbf{x}}.$$
(136)

A substitution into Eq. (66) and subsequent projection onto the space

$$\mathfrak{B}_{2N+1} = \operatorname{span}\{e^{-ipx}\}_{p=-N,\dots,N} \tag{137}$$

yields

,

$$2\pi \frac{d\hat{u}_p}{dt} + \sum_{n=-N}^{N} \sum_{m=-N}^{N} im\hat{u}_n \hat{u}_m \int_0^{2\pi} e^{i(n+m-p)x} dx = \sigma\xi(\omega) \int_0^{2\pi} \psi(x,t) e^{-ipx} dx.$$
(138)

At this point, let us set $\psi(x, t) = \sin(kx) \sin(jt)$. The integral in Eq. (138) then is easily evaluated as

$$\int_{0}^{2\pi} \psi(x,t) e^{-ipx} dx = -i\sin(jt) \int_{0}^{2\pi} \sin(kx)\sin(px) dx = -i\pi\sin(jt)\delta_{pk} + i\pi\sin(jt)\delta_{(-p)k}.$$
(139)

Therefore, we obtain the following Galerkin system

$$\begin{cases} \frac{d\hat{u}_p}{dt} + i\sum_{m=-N}^{N} m\hat{u}_{p-m}\hat{u}_m = i\frac{\sigma}{2}\xi(\omega)\sin(jt), \quad p = -k, \\ \frac{d\hat{u}_p}{dt} + i\sum_{m=-N}^{N} m\hat{u}_{p-m}\hat{u}_m = -i\frac{\sigma}{2}\xi(\omega)\sin(jt), \quad p = k, \\ \frac{d\hat{u}_p}{dt} + i\sum_{m=-N}^{N} m\hat{u}_{p-m}\hat{u}_m = 0, \quad \text{otherwise.} \end{cases}$$
(140)

The initial condition for $\hat{u}_p(t; \omega)$ is obtained by projection as

$$\hat{u}_p(t_0,\omega) = \delta_{p0}\eta(\omega) + \frac{iA}{2}(\delta_{-1p} - \delta_{1p}).$$
(141)

The solution strategy is as follows:

- 1. we sample $\xi(\omega)$ and $\eta(\omega)$ at suitable quadrature points, e.g., Gauss–Hermite or ME-PCM points [59];
- 2. for each realization of $\xi(\omega)$ and $\eta(\omega)$ solve the system (140) with the initial condition (141).

When the solutions corresponding to all these realizations are available, we compute the mean and the second order moment of the solution as

$$\langle u(\mathbf{x},t;\omega)\rangle = \sum_{n=-N}^{N} \langle \hat{u}_n(t;\omega)\rangle e^{in\mathbf{x}},\tag{142a}$$

$$\langle u(\mathbf{x},t;\omega)^2 \rangle = \sum_{n,p=-N}^N \langle \hat{u}_n(t;\omega) \hat{u}_p(t;\omega) \rangle e^{i(n+p)\mathbf{x}}.$$
(142b)

In a collocation representation the averaging operation can be explicitly written as

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$$\langle \hat{u}_{n}(t;\omega) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{u}_{n}(t;\eta,\xi) e^{-(\eta^{2}+\xi^{2})/2} \, d\eta \, d\xi \simeq \sum_{i=1}^{K_{\eta}} \sum_{j=1}^{K_{\zeta}} w_{i}^{\xi} w_{j}^{\eta} \hat{u}_{n}(t;\eta_{i},\xi_{j}), \tag{143}$$

where $\{\eta_i\}$ and $\{\xi_i\}$ are quadrature points while w_i^{ξ} and w_i^{η} are the corresponding integration weights.

Fourier–Galerkin system in probability space. Let us consider the following Fourier series representation of the solution to the problem (69) (periodic in $[0, 2\pi] \times [-L, L]$)

$$p_{u(x,t)\xi}^{(a,b)} = \sum_{n=-N}^{N} \sum_{m=-Q}^{Q} \hat{p}_{nm}(t,b) e^{inx+ima\pi/L},$$
(144)

where [-L, L] is large enough in order to include the support of the response probability function.⁹ For subsequent mathematical developments it is convenient to set

$$A_{mq}^{(0)} \stackrel{\text{def}}{=} \int_{-L}^{L} e^{i(m-q)a\pi/L} da = \begin{cases} 2L & m = q \\ 0 & m \neq q \end{cases},$$
(145a)

$$A_{mq}^{(1)} \stackrel{\text{def}}{=} \int_{-L}^{L} a e^{i(m-q)a\pi/L} \, da = \begin{cases} 0 & m = q \\ (-1)^{(m-q)} \frac{2L^2}{(m-q)i\pi} & m \neq q \end{cases},$$
(145b)

$$A_{mq}^{(2)} \stackrel{\text{def}}{=} \int_{-L}^{L} a^2 e^{i(m-q)a\pi/L} \, da = \begin{cases} \frac{2}{3}L^3 & m = q\\ (-1)^{(m-q)} \frac{4L^3}{((m-q)\pi)^2} & m \neq q \end{cases}.$$
(145c)

Now, the projection of Eq. (69) onto the Fourier space

$$\mathfrak{B}_{2N+2Q+2} = \operatorname{span}\{e^{-ihx - iqa\pi/L}\}_{\substack{h=-N,\dots,N\\q=-Q,\dots,Q}}$$
(146)

yields the Fourier-Galerkin system

$$\frac{d\hat{p}_{hq}}{dt} = -\frac{i\hbar}{2L} \sum_{m=-Q}^{Q} \hat{p}_{hm} (A_{mq}^{(1)} + B_{mq}) + \sigma \frac{bq\pi}{2L} (\hat{p}_{(h-k)q} - \hat{p}_{(h+k)q}) \sin(jt),$$
(147)

where

$$B_{mq} \stackrel{\text{def}}{=} \int_{-L}^{L} \left(\int_{-L}^{a} e^{ima'\pi/L} da' \right) e^{-iqa\pi/L} da = \begin{cases} A_{0q}^{(1)} + LA_{0q}^{(0)} & m = 0\\ \frac{L}{i\pi m} (A_{0q}^{(0)} - e^{-il\pi} A_{0q}^{(0)}) & m \neq 0 \end{cases}$$
(148)

In order to set the initial condition for \hat{p}_{hq} we need to calculate the projection of $p_n(a, x)$ onto the space (146). This is given by

$$\int_{0}^{2\pi} \int_{-L}^{L} p_{\eta}(a,x) e^{-ihx - iqa\pi/L} da dx = \frac{1}{\sqrt{2\pi}} \int_{0}^{2\pi} e^{-ihx} \int_{-L}^{L} e^{-(a - A\sin(x))^{2}/2} e^{-iqa\pi/L} da dx.$$
(149)

The last integral can be manipulated further

$$\int_{-L}^{L} e^{-(a-A\sin(x))^2/2} e^{-iqa\pi/L} da = e^{-A^2\sin(x)^2/2} \int_{-L}^{L} e^{-a^2/2 + (A\sin(x) - iq\pi/L)a} da \simeq \sqrt{2\pi} e^{-q^2\pi^2/(2L^2) - iq\pi A\sin(x)/L},$$

The error in this approximation is far below the machine precision (10^{-14}) for all $q \in \mathbb{Z}$ if $L \ge 20$, i.e., we can consider it as *numerically exact* for all $a \in [-20, 20]$. Therefore the initial condition for the Fourier Galerkin system (147) is

$$\hat{p}_{hq}(t_0, b) = \frac{p_{\xi}^{(b)}}{4\pi L} e^{-q^2 \pi^2 / (2L^2)} I_{hq}.$$
(150)

where $p_{\xi}^{(b)}$ is Gaussian and we have defined

$$I_{hq} \stackrel{\text{def}}{=} \int_0^{2\pi} e^{-ihx - iq\pi A \sin(x)/L} dx.$$
(151)

These integrals can be evaluated numerically to the desired accuracy. At this point the solution strategy is as follows:

- 1. We sample the variable b at quadrature points in [-20, 20], e.g., at multi-element Gauss-Legendre-Lobatto points.
- 2. For each realization $b = b_k$ we set the initial condition (150) and we integrate the system (147) in time.

⁹ We will set L = 20 in the present numerical study (see the comments before Eq. (150)).

The response probability, i.e. the marginal of Eq. (144) with respect to *b* then can obtained through simple Gauss quadrature. Once the response probability is available, we can compute analytically the mean and the second order moment of *u* as

$$\begin{split} \langle u(x,t) \rangle &= \int_{-L}^{L} a p_{u(x,t)}^{(a)} \, da = \sum_{n=-N}^{N} \sum_{m=-Q}^{Q} \hat{p}_{nm}(t) A_{m0}^{(1)} e^{inx}, \\ \langle u(x,t)^2 \rangle &= \int_{-L}^{L} a^2 p_{u(x,t)}^{(a)} \, da = \sum_{n=-N}^{N} \sum_{m=-Q}^{Q} \hat{p}_{nm}(t) A_{m0}^{(2)} e^{inx}. \end{split}$$

where the matrices $A_{nm}^{(1)}$ and $A_{nm}^{(2)}$ are defined in Eqs. (145b) and (145c) while

$$\hat{p}_{nm}(t) \stackrel{\text{def}}{=} \sum_{i=1}^{K_b} w_i^{(b)} \hat{p}_{nm}(t; b_i)$$
(152)

are Fourier coefficients of the response probability ($w_i^{(b)}$ are quadrature weights).

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