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Dynamically orthogonal field equations for continuous stochastic dynamical systems

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ABSTRACT

In this work we derive an exact, closed set of evolution equations for general continuous stochastic fields described by a Stochastic Partial Differential Equation (SPDE). By hypothesizing a decomposition of the solution field into a mean and stochastic dynamical component, we derive a system of field equations consisting of a Partial Differential Equation (PDE) for the mean field, a family of PDEs for the orthonormal basis that describe the stochastic subspace where the stochasticity 'lives' as well as a system of Stochastic Differential Equations that defines how the stochasticity evolves in the time varying stochastic subspace. These new evolution equations are derived directly from the original SPDE, using nothing more than a dynamically orthogonal condition on the representation of the solution. If additional restrictions are assumed on the form of the representation, we recover both the Proper Orthogonal Decomposition equations and the generalized Polynomial Chaos equations. We apply this novel methodology to two cases of two-dimensional viscous fluid flows described by the Navier–Stokes equations and we compare our results with Monte Carlo simulations.

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1. Introduction

In the past decades an increasing number of problems in continuum theory have been treated using stochastic dynamical theories. Such problems are mainly described by stochastic partial differential equations (SPDEs) and they arise in a number of areas including fluid mechanics, elasticity, and wave theory to describe phenomena such as turbulence [1–5], random vibrations [6–8], flow through porous media [9,10], and wave propagation through random media [11–13]. This is but a partial listing of applications and it is clear that almost any phenomenon described by a field equation has an important subclass of problems that may profitably be treated from a stochastic point of view. This includes problems for which the dynamics is not fully resolved or not sufficiently known to warrant solely a deterministic approach as well as problems for which initial, boundary or parametric uncertainties are significant.

A basic goal of uncertainty quantification is to estimate joint probability distributions for the field variables, given the probabilistic information for the initial state and forcing of the system as well as for the SPDE random coefficients. A complete probabilistic description of the response would either require the knowledge of the response characteristic functional or equivalently the knowledge of the whole Kolmogorov hierarchy of the joint probability distributions of the response stochastic fields at any collection of time instances and spatial locations [9,14]. Given the SPDE that governs the system, it was first shown by Hopf [15] that for the stochastic Navier–Stokes equations, a functional differential equation can be derived that governs the characteristic functional for the response. His approach was later adapted to the problems of stochastic wave propagation by Tatarskii [16] and Lee [17]. This approach, known as the statistical approach to turbulence, has also been developed further by many authors (see, e.g., [18–20]) and provides us with infinite-dimensional transport equations for the characteristic functional that characterizes the stochastic solution. Even though these functional equations contain the full probabilistic information for the dynamical system and their derivation from the SPDE is straightforward [9], their infinite-dimensional character prevents a feasible method of solution.

The Monte Carlo simulation technique is a more practical method that can be readily applied to solve such problems to an arbitrary degree of accuracy, provided a sufficiently large number of samples is used. During the past years significant advances have been made in improving the efficiency of Monte Carlo schemes.

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This includes new sequential Monte Carlo methods (e.g. particle filters, see e.g. [21]) where the probability density function of the response is approximated by a mixture of weighted Dirac functions. A most recent development is the usage of a mixture of weighted Gaussian kernels instead of Dirac functions to provide a more reliable representation of the response pdf [22,23]. In recent years, such particle filters and their variants have been applied to stochastic estimations in various fields including ocean and atmosphere dynamics [24] and structural dynamics [25].

Another approach is based on the generation and evolution of an optimal set of input samples of reduced dimensionality such that the scales and dynamical processes where the dominant, most energetic, uncertainties occur are continuously spanned. This is motivated by the multi-scale, intermittent, non-stationary and non-homogeneous uncertainty fields for ocean dynamics (e.g. [26]). The methodology, referred to as Error Subspace Statistical Estimation (ESSE) [27–30], uses a Karhunen–Loeve (KL) expansion but with time varying and adaptive basis functions. The functions are evolved using stochastic, data-assimilative, ensemble predictions initialized by a multi-scale scheme and evolved through a Monte Carlo approach. Similar ideas have been later applied to the modeling of diffusion processes in random heterogeneous media [31,32]. These methods approximate the response pdf without making any explicit assumption about its form and can thus be used in general nonlinear, non-Gaussian systems. However, a major issue is that the evolution of the dominant uncertainties is through a Monte Carlo scheme and therefore a larger number of samples can still be required for accurate prediction.

Order reduction methods have also been utilized to derive reduced order models which have lower complexity relative to the original SPDE model and which reveal the underlying structure of the system dynamics. A classical approach is the statistical technique of Karhunen–Loeve expansion or Proper Orthogonal Decomposition (POD) (see [33–35]) where the response of the dynamical system is usually assumed to have the form

$$u(\mathbf{x}, t; \omega) = \sum_{i=1}^{s} X_i(t; \omega) u_i(\mathbf{x}), \quad \omega \in \Omega \tag{1}$$

where $X_i(t; \omega)$ are stochastic processes and the family $u_i(\mathbf{x})$ are functions computed from data collected in the course of experiments or from direct numerical simulations. Specifically, $u_i(\mathbf{x})$ s are orthonormal fields that provide an optimal modal decomposition in the sense that a finite collection of these modes can capture the dominant components of the complete infinite-dimensional process. A Galerkin projection of the original governing equations to the low-dimensional subspace identified by the POD basis functions $u_i(\mathbf{x})$ provides the reduced order evolution equations for the unknown stochastic coefficients $X_i(t; \omega)$. The POD concept has been applied to a wide range of areas such as turbulence [34,36,37,35], and control of chemical processes [38–40]. However, the main drawback of the POD method is that the basis functions are chosen a priori and therefore may not be able to efficiently represent the evolving responses generated by nonlinear dynamical processes.

Another main approach is the Polynomial Chaos (PC) expansion pioneered by Ghanem and Spanos [41] in the context of solid mechanics. It is based on the original theory of Wiener on polynomial chaos [42–44]. The stochastic field describing the system response is treated as an element in the Hilbert space of random functions and is approximated by its projection onto a finite subspace spanned by orthogonal polynomials. Specifically, instead of imposing a representation for fixed fields $u_i(\mathbf{x})$ as for the POD method, the stochastic processes $X_i(t; \omega)$ are spectrally represented in terms of fixed multi-dimensional Hermite polynomials,

$$u(\mathbf{x}, t; \omega) = \sum_{i=1}^{s} \Phi_i(\boldsymbol{\zeta}(\omega)) u_i(\mathbf{x}, t), \quad \omega \in \Omega \tag{2}$$

where Φ_i are orthogonal polynomials and $\boldsymbol{\zeta}(\omega)$ are given random variables. A Galerkin projection of the governing equations to the low-dimensional subspace defined by the Φ_is transforms the original SPDE to a set of coupled deterministic PDEs for the unknown family $u_i(\mathbf{x}, t)$. The method has been applied to a series of applications including fluid mechanics [45–49], structural mechanics [41,50,51], and wave propagation in random media [52]. Although for any arbitrary random process with finite second order moments, the PC expansion converges in accord with Cameron–Martin theorem [43], it has been demonstrated that the convergence rate is optimal for Gaussian processes [53], while for other types of processes the convergence rate may be substantially slower. A recent development by Xiu and Karniadakis [54,47] proposes a generalized PC expansion where basis functions from the Askey family of hypergeometric polynomials are used. It is shown that suitable basis functions different from the Hermite polynomials can increase substantially the rate of convergence. Depending on the stochastic coefficients of the original SPDE and the initial stochastic conditions, there is an optimum choice of basis functions through which an optimum rate of convergence can be achieved. However, this choice must be made a priori and this can be a very challenging task especially for non-stationary complex dynamical systems with large number of degrees of freedom (e.g. atmospheric or oceanic dynamics).

The objective of the present work is to utilize a more general expansion,

$$u(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{s} Y_i(t; \omega) u_i(\mathbf{x}, t), \quad \omega \in \Omega \tag{3}$$

where $Y_i(t; \omega)$ are stochastic processes $\bar{u}(\mathbf{x}, t)$ is the statistical mean and $u_i(\mathbf{x}, t)$ are deterministic orthonormal fields, and to derive evolution equations for the $Y_i(t; \omega)$, $\bar{u}(\mathbf{x}, t)$ and $u_i(\mathbf{x}, t)$ without making any assumptions on their form: the original SPDE governing $u(\mathbf{x}, t; \omega)$ is the only information utilized. Using a new dynamical orthogonality condition for the fields $u_i(\mathbf{x}, t)$, we overcome the redundancy of representation (3) and derive an exact set of evolution equations that has the form of an s-dimensional stochastic differential equation for the random coefficients $Y_i(t; \omega)$ coupled with $s + 1$ deterministic PDEs for the fields $\bar{u}(\mathbf{x}, t)$ and $u_i(\mathbf{x}, t)$, where s is the number of modes that we retain in representation (3). In this way, the basis that describes the stochastic subspace is dynamically evolved and is not chosen a priori: it adapts to the stochasticity introduced by the stochastic initial conditions and coefficients, and evolves according to the SPDE governing $u(\mathbf{x}, t; \omega)$. The stochastic coefficients $Y_i(t; \omega)$ are also evolved according to dynamical equations derived directly from the original SPDE allowing us to use any SDE numerical scheme for their solution (e.g. particle methods). For the special case of stochastic excitation that is delta correlated in time, i.e. white noise, an equivalent nonlinear Fokker–Planck–Kolmogorov equation describes the evolution of the joint probability density function for the stochastic processes $Y_i(t; \omega)$.

The derived field equations are consistent with the dynamical orthogonality condition which also implies the preservation of the classical orthonormality condition for the fields $u_i(\mathbf{x}, t)$. If additional suitable assumptions, either on the form of the fields $\bar{u}(\mathbf{x}, t)$ and $u_i(\mathbf{x}, t)$, or on the form of $Y_i(t; \omega)$ are utilized, our novel equations reproduce the reduced order equations obtained by application of the POD or PC method, respectively. We apply our new derived field equations to the two-dimensional stochastic Navier–Stokes equations and compare our results with direct Monte Carlo simulations initiated using the ESSE approach.

2. Definitions and problem statement

Let $(\Omega, \mathcal{B}, \mathcal{P})$ be a probability space with Ω being the sample space containing the set of elementary events $\omega \in \Omega$, $\mathcal{B}$ is the σ-algebra associated with Ω, and $\mathcal{P}$ is a probability measure. Let $\mathbf{x} \in D \subseteq \mathbf{R}^n$ denote the spatial variable and $t \in \mathcal{T}$ the time. Then every measurable map of the form $u(\mathbf{x}, t; \omega), \omega \in \Omega$ will define a random field. In applications, the most important cases are where $n = 2, 3$ therefore in what follows we will assume that $\mathbf{x} \in D \subseteq \mathbf{R}^n,\ n = 2, 3$. For a random field $u(\mathbf{x}, t; \omega), \omega \in \Omega$ we define the mean value operator as

$$\bar{u}(\mathbf{x}, t) = E^{\omega}[u(\mathbf{x}, t; \omega)] = \int_{\Omega} u(\mathbf{x}, t; \omega) \mathrm{d}\mathcal{P}(\omega).$$

The set of all continuous, square integrable random fields, i.e. $\int_D E^{\omega}[u(\mathbf{x}, t; \omega) u(\mathbf{x}, t; \omega)^{\mathrm{T}}] \mathrm{d}\mathbf{x} < \infty$ for all $t \in \mathcal{T}$ (where $\bullet^{\mathrm{T}}$ denotes the complex conjugate operation) and the bilinear form or covariance operator

$$\begin{aligned} &\mathbf{C}_{u(\cdot,t;\omega)v(\cdot,s;\omega)}(\mathbf{x}, \mathbf{y}) \\ &\quad = E^{\omega}\left[(u(\mathbf{x}, t; \omega) - \bar{u}(\mathbf{x}, t))^{\mathrm{T}}(v(\mathbf{y}, s; \omega) - \bar{v}(\mathbf{y}, s))\right], \\ &\qquad \mathbf{x}, \mathbf{y} \in D,\ t, s \in \mathcal{T} \end{aligned} \tag{4}$$

form a Hilbert space [55,11] that will be denoted by $\mathbf{H}$.

For every two elements $u(\mathbf{x}, t; \omega), v(\mathbf{x}, t; \omega) \in \mathbf{H}$ we define the spatial inner product as

$$\langle u(\bullet, t; \omega), v(\bullet, t; \omega) \rangle = \int_D u(\mathbf{x}, t; \omega)^{\mathrm{T}} v(\mathbf{x}, t; \omega) \mathrm{d}\mathbf{x}$$

where the integral on the right hand side is defined in the mean square sense [56]. For the case where the integrands are deterministic the mean square integral is reduced to the classical Riemann integral. In what follows we will use Einstein's convection for summation, i.e. $\sum_i a_i b_i = a_i b_i$ except if the limits of summation need to be shown. A double index that is not summed-up will be denoted as $a_{\bar{i}} b_{\bar{i}}$. We define the projection operator $\boldsymbol{\Pi}$ of a field $u(\mathbf{x}, t), \mathbf{x} \in D$ to an m-dimensional linear subspace spanned by the orthonormal family $\{w_j(\mathbf{x}, t; \omega)\}_{j=1}^m,\ \mathbf{x} \in D$ as follows

$$\begin{aligned} &\boldsymbol{\Pi}_{\{w_j(\mathbf{x},t;\omega)\}_{j=1}^m}[u(\mathbf{x}, t; \omega)] \\ &\quad = \sum_{j=1}^{m} w_j(\mathbf{x}, t; \omega) \left\langle w_j(\bullet, t; \omega), u(\bullet, t; \omega) \right\rangle \\ &\quad = w_j(\mathbf{x}, t; \omega) \left\langle w_j(\bullet, t; \omega), u(\bullet, t; \omega) \right\rangle. \end{aligned}$$

Let us now study in more detail the covariance operator when it acts on an element $u(\mathbf{x}, t; \omega), \omega \in \Omega$ for $s = t$. In this case we will have

$$\begin{aligned} &\mathbf{C}_{u(\cdot,t;\omega)u(\cdot,t;\omega)}(\mathbf{x}, \mathbf{y}) \\ &\quad = E^{\omega}\left[(u(\mathbf{x}, t; \omega) - \bar{u}(\mathbf{x}, t))(u(\mathbf{y}, t; \omega) - \bar{u}(\mathbf{y}, t))^{\mathrm{T}}\right], \\ &\qquad \mathbf{x}, \mathbf{y} \in D,\ t \in \mathcal{T}. \end{aligned}$$

Then the integral operator defined by

$$T_{\mathbf{C}}\phi = \int_D \mathbf{C}_{u(\cdot,t)u(\cdot,t)}(\mathbf{x}, \mathbf{y}) \phi(\mathbf{x}, t) \mathrm{d}\mathbf{x}, \quad \phi \in \mathbf{L}^2 \tag{5}$$

is a compact, self-adjoint, and positive operator in the Hilbert space of deterministic, continuous, square integrable fields, $\mathbf{L}^2$, i.e. all continuous fields $\phi(\mathbf{x}, t)$ such that $\langle \phi(\bullet, t), \phi(\bullet, t) \rangle < \infty$ [35,57]. Therefore the Karhunen–Loeve expansion [56] follows, that is, every random field $u(\mathbf{x}, t; \omega) \in \mathbf{H}$ at a given time t can be written in the form

$$u(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{\infty} Y_i(t; \omega) u_i(\mathbf{x}, t), \quad \omega \in \Omega$$

where $u_i(\mathbf{x}, t)$ are the eigenfunctions, and $Y_i(t; \omega)$ are zero-mean, stochastic processes with variance $E^{\omega}[Y_i^2(t; \omega)]$ equal to the corresponding eigenvalue $\lambda_i^2(t)$ of the eigenvalue problem

$$\int_D \mathbf{C}_{u(\cdot,t)u(\cdot,t)}(\mathbf{x}, \mathbf{y}) u_i(\mathbf{x}, t) \mathrm{d}\mathbf{x} = \lambda_i^2(t) u_{\bar{i}}(\mathbf{y}, t), \quad \mathbf{y} \in D. \tag{6}$$

In most applications of interest we have $\lambda_i(t) \sim \exp(-ci)$ for some $c > 0$ which implies that all the support of the measure $\mathcal{P}$ is approximately contained in a compact set [35]. Therefore, every random field $u(\mathbf{x}, t; \omega) \in \mathbf{H}$ can be approximated arbitrarily well, by a finite series of the form

$$u(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{s} Y_i(t; \omega) u_i(\mathbf{x}, t), \quad \omega \in \Omega \tag{7}$$

where s is a sufficiently large, non-negative integer. Based on the above discussion we define the stochastic subspace $\mathbf{V}_S = \mathrm{span}\{u_i(\mathbf{x}, t)\}_{j=1}^s$ as the linear space spanned by the s eigenfields that correspond to the s largest eigenvalues. Hence, $\mathbf{V}_S$ defines the appropriate subspace where the stochasticity of the random field 'lives' at time t, following ESSE ideas [27,58]. The goal of this work is two-fold:

1. For fixed dimensionality s study how the stochasticity evolves inside $\mathbf{V}_S$. More specifically we seek the equations governing the evolution of the stochastic vector $\{Y_j(t; \omega)\}_{j=1}^s$.
2. Study how $\mathbf{V}_S$ evolves inside $\mathbf{H}$ through the variation of the basis $\{u_j(\mathbf{x}, t)\}_{j=1}^s$.

The SPDE describing the system evolution is assumed to have the form

$$\frac{\partial u(\mathbf{x}, t; \omega)}{\partial t} = \mathcal{L}[u(\mathbf{x}, t; \omega); \omega], \quad \mathbf{x} \in D,\ t \in \mathcal{T},\ \omega \in \Omega \tag{8}$$

where $\mathcal{L}$ is a general (nonlinear), differential operator. Additionally, the initial state of the system at t_0 is described by the random field

$$u(\mathbf{x}, t_0; \omega) = u_0(\mathbf{x}; \omega), \quad \mathbf{x} \in D,\ \omega \in \Omega \tag{9}$$

and the boundary conditions are given by

$$\mathcal{B}[u(\boldsymbol{\xi}, t; \omega)] = h(\boldsymbol{\xi}, t; \omega), \quad \boldsymbol{\xi} \in \partial D,\ \omega \in \Omega \tag{10}$$

where $\mathcal{B}$ is a linear differential operator. For all of the above quantities we assume that the random coefficients have statistical moments of any order.

3. Dynamically orthogonal field equations

In this section we will use representation (7) to derive reduced order field equations describing the mean state of the system, its stochastic characteristics and their interactions. Clearly, representation (7) with all quantities $(\bar{u}(\mathbf{x}, t), \{u_j(\mathbf{x}, t)\}_{j=1}^s, \{Y_j(t; \omega)\}_{j=1}^s)$ varying is redundant and therefore we cannot derive independent equations from the SPDE describing their evolution. Hence, it is essential to impose additional constraints in order to get a well posed problem for the unknown quantities.

To this end we examine more carefully the source of redundancy in representation (7). Specifically, we notice that the variation of the stochastic coefficients $\{Y_j(t; \omega)\}_{j=1}^s$ can express exclusively the evolution of uncertainty within the stochastic space $\mathbf{V}_S$. On the other hand, by varying the basis $\{u_j(\mathbf{x}, t)\}_{j=1}^s$ we can express both the evolution of uncertainty within $\mathbf{V}_S$ and also normal to $\mathbf{V}_S$. Therefore, we see that the source of redundancy comes from the evolution of uncertainty that can be described by both the variation of the stochastic coefficients and the basis. To overcome this difficulty we need to restrict the evolution of the basis $\{u_j(\mathbf{x}, t)\}_{j=1}^s$ to be normal to the space $\mathbf{V}_S$ since the evolution within $\mathbf{V}_S$ can

be described completely by the stochastic coefficients. The above requirement can be elegantly expressed through the following condition

$$\frac{d\mathbf{V}_S}{dt} \perp \mathbf{V}_S \Leftrightarrow \left\langle \frac{\partial u_i(\bullet,t)}{\partial t}, u_j(\bullet,t) \right\rangle = 0, \quad i=1,\dots,s,\ j=1,\dots,s. \tag{11}$$

We will refer to the above condition as the dynamically orthogonal (DO) condition. Note, that the DO condition implies the preservation of orthonormality for the basis $\{u_j(\mathbf{x},t)\}_{j=1}^s$ since

$$\frac{\partial}{\partial t}\left\langle u_i(\bullet,t), u_j(\bullet,t)\right\rangle = \left\langle \frac{\partial u_i(\bullet,t)}{\partial t}, u_j(\bullet,t)\right\rangle + \left\langle \frac{\partial u_j(\bullet,t)}{\partial t}, u_i(\bullet,t)\right\rangle = 0, \quad i=1,\dots,s,\ j=1,\dots,s.$$

To summarize the above discussion, in what follows we will use the DO representation defined by Eq. (7) and the additional properties

1. $\{Y_j(t;\omega)\}_{j=1}^s$ are zero-mean stochastic processes.
2. $\{u_j(\mathbf{x},t)\}_{j=1}^s$ are deterministic fields satisfying the DO condition (11) which are initially orthonormal, i.e. $\langle u_i(\bullet,t_0), u_j(\bullet,t_0)\rangle = \delta_{ij}$.

As it is proven in the following theorem, the DO expansion results in a set of independent, explicit equations for all the unknown quantities. In particular, using the DO expansion we reformulate the original SPDE to an s-dimensional stochastic differential equation for the random coefficients $Y_i(t;\omega)$ coupled with $s+1$ deterministic PDEs for the fields $\bar{u}(\mathbf{x},t)$ and $u_i(\mathbf{x},t)$.

Theorem 1 (*DO Evolution Equations*). *Under the assumptions of the DO representation the original SPDE (8)–(10) is reduced to the following system of equations*

$$\frac{dY_i(t;\omega)}{dt} = \langle \mathcal{L}[u(\bullet,t;\omega);\omega] - E^\omega[\mathcal{L}[u(\bullet,t;\omega);\omega]], u_i(\bullet,t)\rangle, \tag{12}$$

$$\frac{\partial \bar{u}(\mathbf{x},t)}{\partial t} = E^\omega[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]], \tag{13}$$

$$\frac{\partial u_i(\mathbf{x},t)}{\partial t} = \boldsymbol{\Pi}_{\mathbf{V}_S^\perp}\left[E^\omega\left[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]\,Y_j(t;\omega)\right]\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)} \tag{14}$$

where $\boldsymbol{\Pi}_{\mathbf{V}_S^\perp}[F(\mathbf{x})] = F(\mathbf{x}) - \boldsymbol{\Pi}_{\mathbf{V}_S}[F(\mathbf{x})] = F(\mathbf{x}) - \langle F(\bullet), u_k(\bullet,t)\rangle u_k(\mathbf{x},t)$ *and* $\mathbf{C}_{Y_i(t)Y_j(t)} = E^\omega[Y_i(t;\omega)Y_j(t;\omega)]$. *The associated boundary conditions have the form*

$$\mathcal{B}[\bar{u}(\boldsymbol{\xi},t;\omega)]\,|_{\boldsymbol{\xi}\in\partial D} = E^\omega[h(\boldsymbol{\xi},t;\omega)]$$
$$\mathcal{B}[u_i(\boldsymbol{\xi},t)]\,|_{\boldsymbol{\xi}\in\partial D} = E^\omega\left[Y_j(t;\omega)h(\boldsymbol{\xi},t;\omega)\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)}$$

and the initial conditions are given by

$$Y_i(t_0;\omega) = \langle u_0(\bullet;\omega) - \bar{u}_0(\bullet), u_{i0}(\bullet)\rangle$$
$$\bar{u}(\mathbf{x},t_0) = \bar{u}_0(\bullet) \equiv E^\omega[u_0(\mathbf{x};\omega)]$$
$$u_i(\mathbf{x},t_0) = u_{i0}(\mathbf{x})$$

for all $i=1,\dots,s$, *where* $u_{i0}(\mathbf{x})$ *are the eigenfields of the correlation operator* $\mathbf{C}_{u(\cdot,t_0)u(\cdot,t_0)}$ *defined by the eigenvalue problem (6).*

Proof. First we insert the DO representation to the evolution equation (8). We obtain

$$\frac{\partial \bar{u}(\mathbf{x},t)}{\partial t} + \frac{dY_i(t;\omega)}{dt}u_i(\mathbf{x},t) + Y_i(t;\omega)\frac{\partial u_i(\mathbf{x},t)}{\partial t} = \mathcal{L}[u(\mathbf{x},t;\omega);\omega]. \tag{15}$$

By applying the mean value operator we obtain the second equation of the theorem (Eq. (13)), i.e. an evolution equation for the mean part of the representation.

By considering the inner product of the evolution equation (15) with each of the fields $\{u_j(\mathbf{x},t)\}_{j=1}^s$ we have

$$\left\langle \frac{\partial \bar{u}(\bullet,t)}{\partial t}, u_j(\bullet,t)\right\rangle + \frac{dY_i(t;\omega)}{dt}\left\langle u_i(\bullet,t), u_j(\bullet,t)\right\rangle + Y_i(t;\omega)\left\langle \frac{\partial u_i(\bullet,t)}{\partial t}, u_j(\bullet,t)\right\rangle = \left\langle \mathcal{L}[u(\mathbf{x},t;\omega);\omega], u_j(\bullet,t)\right\rangle.$$

Now, the second term on the left hand side vanishes because of orthonormality except one term for which $i=j$. Moreover, the DO condition implies that the third term vanishes completely. Therefore we have the family of s stochastic differential equations

$$\frac{dY_j(t;\omega)}{dt} + \left\langle \frac{\partial \bar{u}(\bullet,t)}{\partial t}, u_j(\bullet,t)\right\rangle = \left\langle \mathcal{L}[u(\bullet,t;\omega);\omega], u_j(\bullet,t)\right\rangle, \quad j=1,\dots,s.$$

Note that by using (13) or by applying the mean value operator to the above equation, we obtain

$$\left\langle \frac{\partial \bar{u}(\bullet,t)}{\partial t}, u_j(\bullet,t)\right\rangle = E^\omega\left[\left\langle \mathcal{L}[u(\bullet,t;\omega);\omega], u_j(\bullet,t)\right\rangle\right], \quad j=1,\dots,s.$$

The quantity $\left\langle \frac{\partial \bar{u}(\bullet,t)}{\partial t}, u_j(\bullet,t)\right\rangle$ expresses the variation of $\bar{u}$ towards directions of the stochastic subspace $\mathbf{V}_S$. Hence, the equation for $\mathbf{Y}(t;\omega)$ will take the final form (12).

As a next step, we multiply equation (15) with $Y_j(t;\omega)$ and apply the mean value operator to get

$$E^\omega\left[\frac{dY_i(t;\omega)}{dt}Y_j(t;\omega)\right]u_i(\mathbf{x},t) + E^\omega\left[Y_i(t;\omega)Y_j(t;\omega)\right]\frac{\partial u_i(\mathbf{x},t)}{\partial t} = E^\omega\left[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]\,Y_j(t;\omega)\right]$$

which can be written as

$$\mathbf{C}_{Y_i(t)Y_j(t)}\frac{\partial u_i(\mathbf{x},t)}{\partial t} + \mathbf{C}_{\frac{dY_i(t)}{dt}Y_j(t)}u_i(\mathbf{x},t) = E^\omega\left[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]\,Y_j(t;\omega)\right] \tag{16}$$

where $\mathbf{C}_{Y_i(t)Y_j(t)} = E^\omega[Y_i(t;\omega)Y_j(t;\omega)]$. By considering the inner product of the last equation with the field $u_k(\mathbf{x},t)$, and using DO condition, we obtain an exact expression for $\mathbf{C}_{\frac{dY_k(t)}{dt}Y_j(t)}$

$$\mathbf{C}_{\frac{dY_k(t)}{dt}Y_j(t)} = E^\omega\left[\langle \mathcal{L}[u(\mathbf{x},t;\omega);\omega], u_k(\bullet,t)\rangle\, Y_j(t;\omega)\right]. \tag{17}$$

Note that this result (17) can also be obtained from the definition of $\mathbf{C}_{\frac{dY_k(t)}{dt}Y_j(t)}$ and from Eq. (12). Now, inserting the last expression to Eq. (16) will result in the equation

$$\mathbf{C}_{Y_i(t)Y_j(t)}\frac{\partial u_i(\mathbf{x},t)}{\partial t} = E^\omega\left[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]\,Y_j(t;\omega)\right] - \boldsymbol{\Pi}_{\mathbf{V}_S}\left[E^\omega\left[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]\,Y_j(t;\omega)\right]\right] = \boldsymbol{\Pi}_{\mathbf{V}_S^\perp}\left[E^\omega\left[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]\,Y_j(t;\omega)\right]\right]$$

where

$$\boldsymbol{\Pi}_{\mathbf{V}_S^\perp}[F(\mathbf{x})] = F(\mathbf{x}) - \langle F(\bullet), u_k(\bullet,t)\rangle\, u_k(\mathbf{x},t).$$

Moreover, since $\mathbf{C}_{Y_i(t)Y_j(t)}$ is positive-definite it can always be inverted and therefore we obtain the final expression (14) for the evolution of the fields $u_i(\mathbf{x},t)$.

Finally, by applying the mean value operator on Eq. (10) for $\mathbf{x} \in \partial D$ we obtain the boundary condition for the evolution of the mean field

$$\mathcal{B}\left[\bar{u}(\boldsymbol{\xi}, t; \omega)\right]|_{\xi\in\partial D} = E^{\omega}\left[h(\boldsymbol{\xi}, t; \omega)\right].$$

Additionally, by multiplying Eq. (10) with $Y_j(t; \omega)$ and applying the mean value operator we obtain for $\mathbf{x} \in \partial D$

$$E^{\omega}\left[Y_j(t; \omega)h(\boldsymbol{\xi}, t; \omega)\right] = \mathbf{C}_{Y_i(t)Y_j(t)}\mathcal{B}\left[u_i(\boldsymbol{\xi}, t)\right]|_{\xi\in\partial D}.$$

Therefore,

$$\mathcal{B}\left[u_i(\boldsymbol{\xi}, t)\right]|_{\xi\in\partial D} = E^{\omega}\left[Y_j(t; \omega)h(\boldsymbol{\xi}, t; \omega)\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)}.$$

The initial conditions for the quantities involved are found by approximating the initial field $u_0(\mathbf{x}; \omega)$ by a truncated Karhunen–Loeve expansion containing s terms. Therefore, the initial conditions $u_{i0}(\mathbf{x})$ for the fields $u_i(\mathbf{x}, t)$ will be the s most energetic eigenfields of the correlation operator $\mathbf{C}_{u(\cdot,t_0)u(\cdot,t_0)}$ defined by the eigenvalue problem (6)

$$\int_D \mathbf{C}_{u(\cdot,t_0)u(\cdot,t_0)}(\mathbf{x}, \mathbf{y})u_{i0}(\mathbf{x})\mathrm{d}\mathbf{x} = \lambda_i^2 u_{i0}(\mathbf{y}), \quad \mathbf{y} \in D.$$

The initial conditions for the stochastic coefficients $Y_i(t; \omega)$ will be given by the projection of the field $u_0(\mathbf{x}; \omega) - \bar{u}_0(\mathbf{x})$ to the orthonormal eigenfields $u_{i0}(\mathbf{x})$ as follows

$$Y_i(t_0; \omega) = \left\langle u_0(\bullet; \omega) - \bar{u}_0(\bullet), u_{i0}(\bullet)\right\rangle,$$

and the initial condition for the mean field will be given by $\bar{u}(\mathbf{x}, t_0) = \bar{u}_0(\mathbf{x}) \equiv E^{\omega}[u_0(\mathbf{x}; \omega)]$. □

As it can be easily verified the evolution equations derived above are consistent with the DO condition that was initially assumed. Also, the initialization procedure for our DO field equations follows the multivariate ESSE approach, e.g. [58,59].

It should be emphasized that the knowledge of the full set of quantities associated with the DO expansion, i.e. $\{Y_j(t; \omega)\}_{j=1}^{s}$, $\bar{u}(\mathbf{x}, t)$, and $u_i(\mathbf{x}, t)$ can lead, through simple random variable transformations [33], to analytic expressions of any statistical quantity of interest (e.g. pdfs of velocity field at particular positions of the domain, spectral representations of the stochasticity etc.) in terms of these DO expansion quantities.

3.1. The case of independent increment excitation (white noise)

A special class of SPDE of great importance is the case where the operator $\mathcal{L}$ can be linearly split into a deterministic part and a stochastic part having the form of derivative of an independent increment process [60], e.g. Brownian motion or Poisson process. More specifically we consider the special case of a system excited by an independent increment (with respect to time) stochastic process and having deterministic boundary conditions, described by the evolution equation

$$\begin{aligned}
&\frac{\partial u(\mathbf{x}, t; \omega)}{\partial t} = \mathcal{D}\left[u(\mathbf{x}, t; \omega)\right] + \sum_{r=1}^{R}\Phi_r(\mathbf{x}, t)\frac{\mathrm{d}W_r(t; \omega)}{\mathrm{d}t}, \\
&\quad \mathbf{x} \in D,\ t \in \mathcal{T},\ \omega \in \Omega \qquad (18)\\
&u(\mathbf{x}, t_0; \omega) = u_0(\mathbf{x}; \omega), \quad \mathbf{x} \in D,\ \omega \in \Omega \\
&\mathcal{B}\left[u(\boldsymbol{\xi}, t; \omega)\right] = h_D(\boldsymbol{\xi}, t), \quad \boldsymbol{\xi} \in \partial D,\ \omega \in \Omega
\end{aligned}$$

where $\mathcal{D}$ is a deterministic, differential operator, $h_D(\boldsymbol{\xi}, t)$ is a deterministic quantity defining the boundary conditions, $\{\Phi_r(\mathbf{x}, t)\}_{r=1}^{R}$ are deterministic, sufficiently smooth fields, and $\{W_r(t; \omega)\}_{r=1}^{R}$ are taken for simplicity to be independent Brownian motions (although the proof follows exactly the same steps for general independent increment processes). In this case an alternative description of the stochasticity inside $\mathbf{V}_S$, can be given in terms of the probability density function $f_{\mathbf{Y}}(y_1, y_2, \ldots, y_s, t)$ for the stochastic vector $\{Y_j(t; \omega)\}_{j=1}^{s}$. For simplicity in what follows we will also use the following notation

$$\begin{aligned}
\mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \mathbf{Y}(t; \omega)\right] &\equiv \mathcal{D}\left[\bar{u}(\mathbf{x}, t) + \sum_{i=1}^{s} Y_i(t; \omega)u_i(\mathbf{x}, t)\right] \\
&= \mathcal{D}\left[u(\mathbf{x}, t; \omega)\right]
\end{aligned}$$

with $\mathcal{U}(\mathbf{x}, t)$ referring to the $s + 1$ fields $\bar{u}(\mathbf{x}, t)$, $\{u_j(\mathbf{x}, t)\}_{j=1}^{s}$. We then obtain the following result.

Corollary 2. *Under the assumption of the DO representation the SPDE (18) is reduced to the following system of equations*

$$\begin{aligned}
\frac{\partial f_{\mathbf{Y}}}{\partial t} &= -\frac{\partial}{\partial y_j}\left[f_{\mathbf{Y}}\left\langle \mathcal{D}\left[\mathcal{U}(\bullet, t), \mathbf{y}\right]\right.\right. \\
&\quad \left.\left. - \int_{\mathbb{R}^s} f_{\mathbf{Y}}(\boldsymbol{\upsilon}, t)\mathcal{D}\left[\mathcal{U}(\bullet, t), \boldsymbol{\upsilon}\right]\mathrm{d}\boldsymbol{\upsilon},\ u_i(\bullet, t)\right\rangle\right] \\
&\quad + \frac{1}{2}\frac{\partial^2}{\partial y_i \partial y_j}\left[f_{\mathbf{Y}}Q_{ij}(t)\right] \qquad (19)
\end{aligned}$$

$$\frac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} = \int_{\mathbb{R}^s} f_{\mathbf{Y}}(\boldsymbol{\upsilon}, t)\mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \boldsymbol{\upsilon}\right]\mathrm{d}\boldsymbol{\upsilon}, \qquad (20)$$

$$\frac{\partial u_i(\mathbf{x}, t)}{\partial t} = \boldsymbol{\Pi}_{\mathbf{V}_S^{\perp}}\left[\int_{\mathbb{R}^s} \upsilon_j f_{\mathbf{Y}}(\boldsymbol{\upsilon}, t)\mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \boldsymbol{\upsilon}\right]\mathrm{d}\boldsymbol{\upsilon}\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)} \qquad (21)$$

where $Q_{ij}(t) = \left\langle \Phi_r(\bullet, t), u_i(\bullet, t)\right\rangle\left\langle \Phi_r(\bullet, t), u_j(\bullet, t)\right\rangle$ *and* $\mathbf{C}_{Y_i(t)Y_j(t)} = \int_{\mathbb{R}^s} \upsilon_i\upsilon_j f_{\mathbf{Y}}(\boldsymbol{\upsilon}, t)\mathrm{d}\boldsymbol{\upsilon}$. *The associated boundary conditions have the form*

$$\begin{aligned}
&\mathcal{B}\left[\bar{u}(\boldsymbol{\xi}, t; \omega)\right]|_{\xi\in\partial D} = h_D(\boldsymbol{\xi}, t) \\
&\mathcal{B}\left[u_i(\boldsymbol{\xi}, t)\right]|_{\xi\in\partial D} = 0
\end{aligned}$$

and the initial conditions are given by

$$\begin{aligned}
&f_{\mathbf{Y}}(\mathbf{y}, t_0) = f_{\mathbf{Y}_0}(\mathbf{y}) \\
&\bar{u}(\mathbf{x}, t_0) = E^{\omega}\left[u_0(\mathbf{x}; \omega)\right] \\
&u_i(\mathbf{x}, t_0) = u_{i0}(\mathbf{x})
\end{aligned}$$

for all $i = 1, \ldots, s$, *where* $u_{i0}(\mathbf{x})$ *are defined in Theorem 1 and* $f_{\mathbf{Y}_0}(\mathbf{y})$ *is the probability density function associated with the random vector* $Y_i(t_0; \omega) = \left\langle u_0(\bullet; \omega) - \bar{u}_0(\bullet), u_{i0}(\bullet)\right\rangle$.

Proof. By using the special form of the SPDE (18) and the zero-mean property of the Brownian motion we obtain from Eq. (12)

$$\begin{aligned}
\frac{\mathrm{d}Y_i(t; \omega)}{\mathrm{d}t} &= \left\langle \mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \mathbf{Y}(t; \omega)\right]\right. \\
&\quad \left. - E^{\omega}\left[\mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \mathbf{Y}(t; \omega)\right]\right], u_i(\bullet, t)\right\rangle \\
&\quad + \left\langle \Phi_r(\bullet, t), u_i(\bullet, t)\right\rangle\frac{\mathrm{d}W_r(t; \omega)}{\mathrm{d}t}.
\end{aligned}$$

This last equation is an Ito stochastic differential equation and can be written equivalently as a transport equation for the probability density function $f_{\mathbf{Y}}(y_1, y_2, \ldots, y_s, t)$

$$\begin{aligned}
&\frac{\partial f_{\mathbf{Y}}}{\partial t} + \frac{\partial}{\partial y_j}\left[f_{\mathbf{Y}}\left\{\left\langle \mathcal{D}\left[\mathcal{U}(\bullet, t), \mathbf{y}\right] - E^{\omega}\left[\mathcal{D}\left[\mathcal{U}(\bullet, t), \mathbf{y}\right]\right], u_i(\bullet, t)\right\rangle\right\}\right] \\
&\quad = \frac{1}{2}\frac{\partial^2}{\partial y_i \partial y_j}\left[f_{\mathbf{Y}}\left\langle \Phi_r(\bullet, t), u_i(\bullet, t)\right\rangle\left\langle \Phi_r(\bullet, t), u_j(\bullet, t)\right\rangle\right]. \qquad (22)
\end{aligned}$$

Note, that

$$E^{\omega}\left[\mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \mathbf{Y}(t; \omega)\right]\right] = \int_{\mathbb{R}^s} f_{\mathbf{Y}}(\boldsymbol{\upsilon}, t)\mathcal{D}\left[\mathcal{U}(\mathbf{x}, t), \boldsymbol{\upsilon}\right]\mathrm{d}\boldsymbol{\upsilon}$$

and hence Eq. (19) follows. Equation for the mean field follows directly from the corresponding equation (13) and the zero-mean property of the Brownian motion. Finally, using Eq. (14) we obtain

$$\frac{\partial u_i(\mathbf{x},t)}{\partial t} = \boldsymbol{\Pi}_{\mathbf{V}_S^\perp}\left[E^\omega\left[\mathcal{D}\left[u(\mathbf{x},t;\omega)\right]Y_j(t;\omega)\right]\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)} + \boldsymbol{\Pi}_{\mathbf{V}_S^\perp}\left[\langle\Phi_r(\bullet,t),u_i(\bullet,t)\rangle\, E^\omega\left[\frac{\mathrm{d}W_r(t;\omega)}{\mathrm{d}t}Y_j(t;\omega)\right]\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)}.$$

The second term on the right hand side vanishes due to the non-anticipative property of Brownian motion [11]. Moreover,

$$E^\omega\left[\mathcal{D}\left[u(\mathbf{x},t;\omega)\right]Y_j(t;\omega)\right] = \int_{\mathbb{R}^s} \upsilon_j f_{\mathbf{Y}}(\boldsymbol{\upsilon},t)\mathcal{D}\left[\mathcal{U}(\mathbf{x},t),\boldsymbol{\upsilon}\right]\mathrm{d}\boldsymbol{\upsilon}.$$

Additionally, for the boundary conditions, we obtain from Theorem 1

$$\begin{aligned}\mathcal{B}\left[u_i(\boldsymbol{\xi},t)\right]|_{\boldsymbol{\xi}\in\partial D} &= E^\omega\left[Y_j(t;\omega)h_D(\boldsymbol{\xi},t)\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)}\\ &= h_D(\boldsymbol{\xi},t)E^\omega\left[Y_j(t;\omega)\right]\mathbf{C}^{-1}_{Y_i(t)Y_j(t)} = 0.\end{aligned}$$

Therefore, Eq. (21) follows. Finally the initial conditions are defined as in Theorem 1 with the stochastic vector $Y_i(t_0;\omega) = \langle u_0(\bullet;\omega) - \bar{u}_0(\bullet), u_{i0}(\bullet)\rangle$ described now by the associated probability density function $f_{\mathbf{Y}_0}(\mathbf{y})$. □

Note that a transport equation for the probability density function can also be obtained for the case of general time correlation structure for the excitation using recent results for stochastic dynamical systems [61,62].

4. Consistency with existing methodologies

The derivation of our new dynamically orthogonal field Eqs. (12)–(14) was based exclusively on the representation of the solution by the DO expansion. In what follows, we show that by imposing additional restrictions on the representation, either those of the PC or the POD expansion, we recover the set of equations that are obtained for each of these expansions. Therefore, the DO field Eqs. (12)–(14) can be considered as a general methodology that unifies two of the most important and widely used methods for evolving uncertainty in stochastic continuous systems governed by a SPDE.

4.1. Generalized polynomial chaos expansion

In the generalized PC method, introduced by Xiu and Karniadakis [54] the stochastic processes $\{Y_j(t;\omega)\}_{j=1}^s$ are chosen a priori and often fixed in time, based on the statistical characteristics of the system input process. Specifically, the stochastic processes are chosen to have the statistically time-independent form

$$Y_j(t;\omega) = \Phi_j(\boldsymbol{\zeta}(\omega)) \tag{23}$$

where Φ_j are orthogonal polynomials from the Askey scheme and $\boldsymbol{\zeta}(\omega)$ are given random variables [54]. In this case, the following orthogonality relation in the random space holds between the stochastic coefficients

$$E^\omega\left[\Phi_i(\boldsymbol{\zeta}(\omega))\Phi_j(\boldsymbol{\zeta}(\omega))\right] = E^\omega\left[\Phi_i(\boldsymbol{\zeta}(\omega))^2\right]\delta_{ij}.$$

The reduced order PC equations (e.g. [46,47,63,48,64]) are usually derived by substituting a representation as (7) but with the stochastic coefficients given by (23) to the SPDE (8) and then projecting it to the stochastic orthogonal basis functions $\Phi_j(\boldsymbol{\zeta}(\omega))$ using the inner product. Following these steps we obtain

$$E^\omega\left[\Phi_i(\boldsymbol{\zeta}(\omega))^2\right]\frac{\partial u_i(\mathbf{x},t;\omega)}{\partial t} = E^\omega\left[\mathcal{L}\left[u(\mathbf{x},t;\omega);\omega\right]\Phi_i(\boldsymbol{\zeta}(\omega))\right]. \tag{24}$$

To now show that the DO expansion can reduce to the PC expansion, we start from the DO field Eqs. (12)–(14) but we restrict them with (23). Then the equation for the stochastic coefficients $\{Y_j(t;\omega)\}_{j=1}^s$ is not used since those are chosen *a priori* in a classic PC equation. Then, our equation for the mean field (13) provides directly the equation in the set (24) that corresponds to $\Phi_i(\boldsymbol{\zeta}(\omega))$ being the constant polynomial. Finally, to obtain the remaining equations in (24), we start with the third of the DO field equations (14) in the form

$$\mathbf{C}_{Y_i(t)Y_j(t)}\frac{\partial u_i(\mathbf{x},t)}{\partial t} = E^\omega\left[\mathcal{L}\left[u(\mathbf{x},t;\omega);\omega\right]Y_j(t;\omega)\right] - \boldsymbol{\Pi}_{\mathbf{V}_S}\left[E^\omega\left[\mathcal{L}\left[u(\mathbf{x},t;\omega);\omega\right]Y_j(t;\omega)\right]\right]. \tag{25}$$

But, from (17), we have $E^\omega[\langle\mathcal{L}[u(\mathbf{x},t;\omega);\omega],u_k(\bullet,t)\rangle Y_j(t;\omega)] = \mathbf{C}_{\frac{\mathrm{d}Y_k(t)}{\mathrm{d}t}Y_j(t)} = 0$ since the stochastic characteristics of $\Phi_i(\boldsymbol{\zeta}(\omega))$ do not change with time. Therefore, we have $\boldsymbol{\Pi}_{\mathbf{V}_S}[E^\omega[\mathcal{L}[u(\mathbf{x},t;\omega);\omega]Y_j(t;\omega)]] = 0$ in (25). Hence, Eq. (25) and the mean equation (13) reduce to the family of PC equations (24).

4.2. Proper orthogonal decomposition

The POD method uses *a priori* chosen fields $\{u_j(\mathbf{x})\}_{j=1}^s$, generated either from an ensemble of experiments or from direct numerical simulations [35] and provides equations either for the stochastic or the deterministic coefficients $\{Y_j(t;\omega)\}_{j=1}^s$. In what follows we show how our DO equations reduce to the standard POD method (given the standard POD assumptions) for the stochastic case since the deterministic equations follow as a special case.

In a standard POD method, one chooses an expansion having the form

$$u(\mathbf{x},t;\omega) = \sum_{i=1}^{s} X_i(t;\omega)u_i(\mathbf{x}) \tag{26}$$

where $\{u_j(\mathbf{x})\}_{j=1}^s$ are fixed, orthonormal fields and $\{X_j(t;\omega)\}_{j=1}^s$ are stochastic processes (in general with non-zero mean). The reduced order POD evolutions equations are then usually obtained by Galerkin projection of the original SPDE (8) onto the orthonormal fields $u_j(\mathbf{x})$. In this way we obtain the set of equations

$$\frac{\mathrm{d}X_j(t;\omega)}{\mathrm{d}t} = \left\langle\mathcal{L}\left[u(\mathbf{x},t;\omega);\omega\right],u_j(\mathbf{x},t)\right\rangle. \tag{27}$$

To now show that the DO expansion can reduce to the POD method, we start from Theorem 1 and the DO field equations but we restrict them with (26). We consider just Eqs. (12) and (13) since $\{u_j(\mathbf{x})\}_{j=1}^s$ have already be imposed from the POD method. Moreover, we note that the coefficients $\{X_j(t;\omega)\}_{j=1}^s$ of the POD method are connected to the stochastic coefficients $\{Y_j(t;\omega)\}_{j=1}^s$ of Theorem 1 through the relation

$$X_j(t;\omega) = Y_j(t;\omega) + \left\langle\bar{u}(\mathbf{x},t),u_j(\mathbf{x})\right\rangle.$$

Then, by differentiating $X_j(t;\omega)$ and using Eqs. (12) and (13) we recover Eq. (27)

$$\begin{aligned}\frac{\mathrm{d}X_j(t;\omega)}{\mathrm{d}t} &= \frac{\mathrm{d}Y_j(t;\omega)}{\mathrm{d}t} + \left\langle\frac{\partial\bar{u}(\mathbf{x},t)}{\partial t},u_j(\mathbf{x},t)\right\rangle\\ &= \left\langle\mathcal{L}\left[u(\bullet,t;\omega);\omega\right] - E^\omega\left[\mathcal{L}\left[u(\bullet,t;\omega);\omega\right]\right],u_j(\bullet,t)\right\rangle\\ &\quad + \left\langle E^\omega\left[\mathcal{L}\left[u(\mathbf{x},t;\omega);\omega\right]\right],u_j(\mathbf{x},t)\right\rangle\\ &= \left\langle\mathcal{L}\left[u(\bullet,t;\omega);\omega\right],u_j(\bullet,t)\right\rangle.\end{aligned}$$

5. Dynamically orthogonal field equations for Navier–Stokes

In this section we illustrate how the derived DO field equations can be used for the solution of the stochastic, two-dimensional, Navier–Stokes equations. In what follows we consider incompressible flows in two different situations: a flow in a cavity and a flow past a circular cylinder with deterministic boundary conditions and the stochasticity introduced exclusively through the initial conditions of the problem.

5.1. Formulation of the field equations

We denote with $\mathbf{u}(\mathbf{x}, t; \omega) = (u(\mathbf{x}, t; \omega), v(\mathbf{x}, t; \omega))^{\mathrm{T}}$ and $p(\mathbf{x}, t; \omega)$ the random velocity field and the pressure field respectively. For two-dimensional Navier–Stokes flow the governing equations have the form

$$\frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = \frac{1}{\mathrm{Re}}\Delta u - \frac{\partial (u^2)}{\partial x} - \frac{\partial (uv)}{\partial y}$$
$$\frac{\partial v}{\partial t} + \frac{\partial p}{\partial y} = \frac{1}{\mathrm{Re}}\Delta v - \frac{\partial (uv)}{\partial x} - \frac{\partial (v^2)}{\partial y}$$
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$
$$\mathcal{B}\left[\mathbf{u}|_{\partial D}\right] = h_D(\boldsymbol{\xi}, t), \quad \boldsymbol{\xi} \in \partial D$$

where $\mathcal{B}$ is the linear operator representing the boundary conditions. Using representation (7) for the random field we will have

$$\begin{pmatrix} u(\mathbf{x}, t; \omega) \\ v(\mathbf{x}, t; \omega) \end{pmatrix} = \begin{pmatrix} \bar{u}(\mathbf{x}, t) \\ \bar{v}(\mathbf{x}, t) \end{pmatrix} + \sum_{i=1}^{s} Y_i(t; \omega) \begin{pmatrix} u_i(\mathbf{x}, t) \\ v_i(\mathbf{x}, t) \end{pmatrix}.$$

Moreover, the inner product will here have the form

$$\langle \mathbf{u}_1(\bullet, t; \omega), \mathbf{u}_2(\bullet, t; \omega) \rangle = \int_D u_1(\mathbf{x}, t; \omega) u_2(\mathbf{x}, t; \omega) \mathrm{d}\mathbf{x} + \int_D v_1(\mathbf{x}, t; \omega) v_2(\mathbf{x}, t; \omega) \mathrm{d}\mathbf{x}.$$

Inserting the above representation in the continuity equation we obtain

$$\nabla . \bar{\mathbf{u}}(\mathbf{x}, t) + \sum_{i=1}^{s} Y_i(t; \omega) \nabla \cdot \mathbf{u}_i(\mathbf{x}, t) = 0.$$

But since $Y_i(t; \omega)$ is random the above equation has the equivalent form

$$\nabla . \bar{\mathbf{u}}(\mathbf{x}, t) = 0 \tag{28a}$$
$$\nabla . \mathbf{u}_i(\mathbf{x}, t) = 0 \quad i = 1, \ldots, s. \tag{28b}$$

Then using the DO representation, we obtain the form of the evolution operator $\mathcal{L}$

$$\mathcal{L}_u\left[\mathbf{u}(\mathbf{x}, t; \omega); \omega\right] = -\frac{\partial p_0}{\partial x} + F_0 + Y_i(t; \omega)\left[-\frac{\partial p_i}{\partial x} + F_i\right] - Y_i(t; \omega) Y_j(t; \omega)\left[-\frac{\partial p_{ij}}{\partial x} + F_{ij}\right]$$
$$\mathcal{L}_v\left[\mathbf{u}(\mathbf{x}, t; \omega); \omega\right] = -\frac{\partial p_0}{\partial y} + G_0 + Y_i(t; \omega)\left[-\frac{\partial p_i}{\partial y} + G_i\right] - Y_i(t; \omega) Y_j(t; \omega)\left[-\frac{\partial p_{ij}}{\partial y} + G_{ij}\right]$$

where the definition of the fields on the right hand side is given in Appendix A.

5.2. Stochastic initial conditions

The initial conditions are assumed to consist of a mean field $\bar{\mathbf{u}}_0(\mathbf{x})$ that will be described later for every particular flow, and a stochastic part having the form $\sum_{i=1}^{s} Y_{i0}(\omega)\mathbf{u}_{i0}(\mathbf{x})$ where the random variables $Y_{i0}(\omega)$ are zero-mean, independent Gaussian and the fields $\mathbf{u}_{i0}(\mathbf{x})$ are taken to be the eigenfields of a given correlation operator $C(\mathbf{x}, \mathbf{y})$ having the form

$$\mathbf{C}(\mathbf{x}, \mathbf{y}) = \mathcal{M}(\mathbf{x}, \mathbf{y}) C(r)$$

where r is the Euclidean distance between the points $(\mathbf{x}, \mathbf{y})$, and $\mathcal{M}(\mathbf{x}, \mathbf{y})$ is a mollifier function which takes unit values away from the solid boundaries and vanishes smoothly close to them. By writing the correlation operator in this form we assure that initial states are consistent with the deterministic boundary conditions. In what follows we assume that $C(r)$ has the special form [65]

$$C(r) = (1 + br + b^2 r^2/3)\mathrm{e}^{-br}$$

where the constant b is taken to be equal to L^{-1}, with L being a characteristic length of the flow. The variance of the random variables is chosen based on the energy levels of the mean field so that it is comparable or larger in order to illustrate the potential of the method for larger energy stochastic perturbations.

5.3. Numerical solution of the evolution equations

The numerical discretization of the DO field equations can be performed using any method suitable for the deterministic Navier–Stokes equations. Here, for simplicity we employ a staggered grid combined with a donor-cell discretization scheme for the spatial derivatives. For the time discretization, we used Euler's method resulting in an explicit scheme for the velocities and an implicit scheme for the pressure (the full scheme is described in detail in [66]).

The numerical solution of the SDE for the processes $Y_i(t; \omega)$ was performed using a particle method [21] with 5×10^3 particles. Note that since the SDE has s dimensions (with $s = 5$ in the applications shown below) the computational cost for the evolution of this SDE is very small compared to the overall computational cost involving the Navier–Stokes-based equations for the mean and s basis fields. Moreover, the calculation of all field quantities that involve the mean value operator $E^{\omega}[\bullet]$ in Eqs. (13) and (14) can be done in terms of statistical moments of the stochastic process $Y_i(t; \omega)$ when we use the expressions for the evolution operator derived in the Appendix A and the linearity of the mean value operator $E^{\omega}[\bullet]$. For the Navier–Stokes system the equation for the mean field (Eq. (13)) requires only the computation of second order moments of $Y_i(t; \omega)$ while the calculation of the rhs for Eq. (14) requires also the third order moments of $Y_i(t; \omega)$.

5.4. Application results

In this section we present the results of the DO field equations applied to numerical simulations of two types of flows described by the Navier–Stokes equations. The stochasticity is introduced in both applications through the initial conditions which here also define the dimensionality s of the finite expansion (7) used in the DO equations. In the first application, we consider a lid driven cavity flow in a square domain with deterministic boundary conditions. As a second application, we simulate a two-dimensional flow past a circular cylinder with deterministic inflow velocity.

5.4.1. Cavity flow

As a first application we simulate a driven cavity flow in a square domain. The physical configuration (Fig. 1) consists of a square

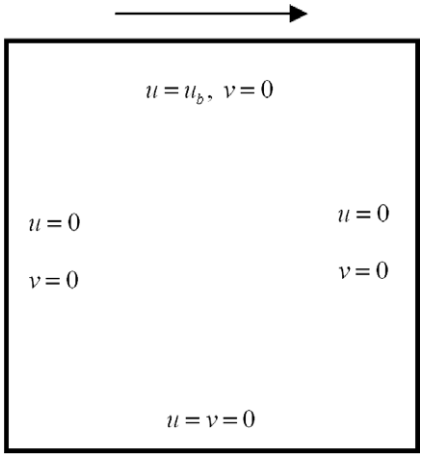

Fig. 1. Driven cavity flow, problem configuration.

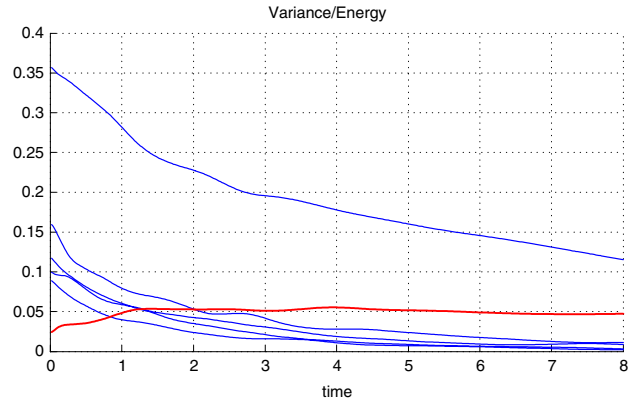

Fig. 3. Evolution of principal variances $\sigma_i^2(t),\ i = 1, \ldots, 5$ (blue curves) and mean field energy (red curve) for the flow in a cavity. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

container filled with a fluid. The lid of the contained moves at a given, constant velocity, thereby setting the fluid in motion. No-slip conditions are imposed on all four segments of the boundary with the exception of the upper boundary, along which the velocity u in the x-direction is set equal to the given lid velocity u_b to simulate the moving lid. The length of each side is $L = 1$ and the Reynolds number of the flow is taken to be $\mathrm{Re} = 1000$.

For the stochastic computation the lid velocity is taken to be $u_b = 1.5$ while in the DO expansion (7) we retain 5 modes which is equal to the stochastic dimension of the initial conditions. The flow fields associated with the initial conditions $u_0(\mathbf{x}; \omega)$ are shown in Fig. 2 in terms of the streamfunction.

By evolving all parameters of the system using the DO field equations we compute the complete five-dimensional probabilistic structure of the stochasticity inside V_S. In Fig. 3 we show the evolution of the principal variances $\sigma_i^2(t),\ i = 1, \ldots, 5$ which are the eigenvalues of the correlation operator $\mathbf{C}_{Y_i(t)Y_j(t)}$ (blue solid curves). They provide a direct measure of how the stochastic energy evolves with time. The red solid curve is associated with the deterministic kinetic energy of the mean flow field, i.e. the quantity $\langle \bar{u}(\bullet, t), \bar{u}(\bullet, t) \rangle$. We observe that the stochastic energy decays almost monotonically after some initial transient interactions, while the energy of the mean field slowly grows towards a steady limit. This is an expected behavior if we consider the fact that the deterministic cavity flow possess a stable attractor which is characterized by a steady velocity field. Therefore, in the absence of external stochastic excitation it is fully expected to have convergence of the system to this deterministic, one-dimensional attractor. The mean fields $\bar{\mathbf{u}}(\mathbf{x}, t)$ and orthonormal basis fields $\mathbf{u}_i(\mathbf{x}, t), i = 1, \ldots, 5$ are shown in Figs. 4 and 5 for two different time instances both in terms of the streamfunction and vorticity. For the same time instances we present three out of the five two-dimensional marginals associated with the stochastic processes $\{Y_j(t; \omega)\}_{j=1}^s$.

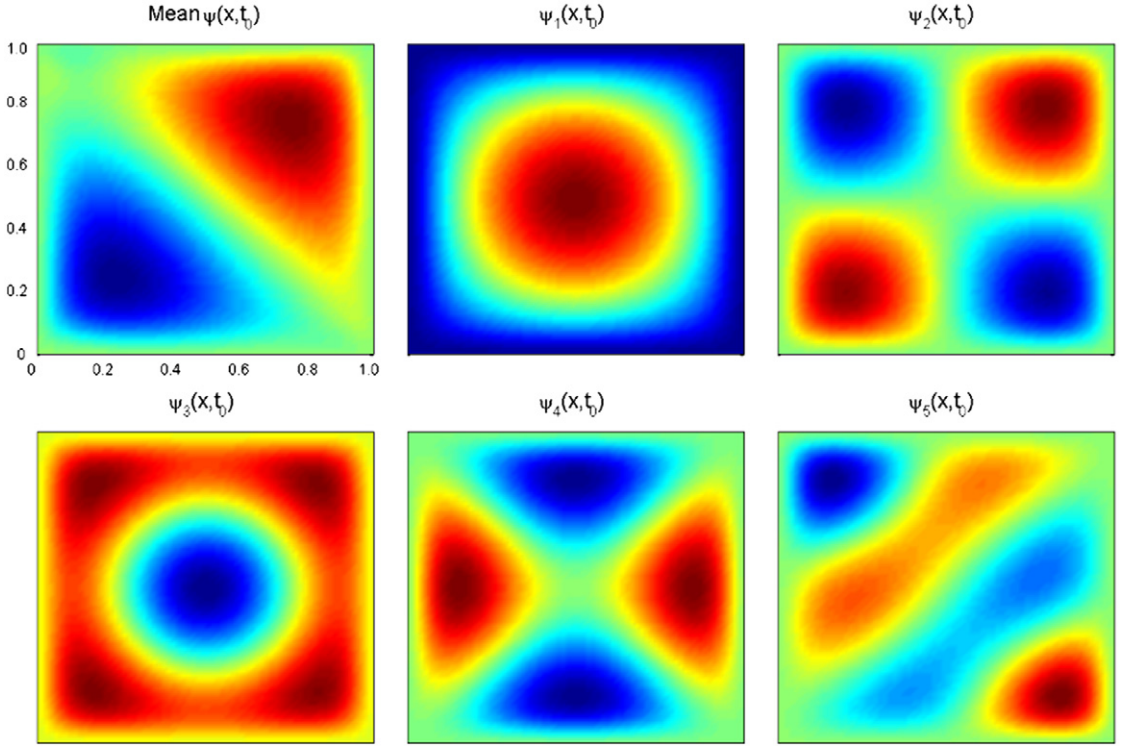

Fig. 2. Initial conditions for the mean and the basis of the stochastic subspace V_S in terms of the field streamfunction.

Fig. 4. Mean field and basis of the stochastic subspace V_S in terms of the streamfunction and vorticity field; two-dimensional marginals of the five-dimensional joint pdf $f(\mathbf{y}, t)$ at time $t = 2$.

Finally, in Fig. 6 we compare the mean streamfunction computed using the 5-modes DO method with the one obtained by Monte Carlo simulation initialized with the ESSE methodology and using 250 and 500 samples. We observe that as we increase the number of samples used for the Monte Carlo simulation we obtain better agreement with the DO mean estimate.

5.4.2. Flow past a circular disk

Here we consider the flow past a disk immersed in a channel. The inflow velocity at the left boundary has a parabolic profile with a maximum value $u = 1.5$; the disk measures $d = 1$ in diameter and is situated at a distance of 1.5 from the left and 1.6 from the upper boundary. It is well known that for two-dimensional flow past a circular cylinder, the first critical Reynolds number is around $\mathrm{Re} \sim 40$, where the flow bifurcates from steady state to periodic vortex shedding [67]. Here, we consider the case of $\mathrm{Re} = 100$. A typical realization for this case is shown in Fig. 7. The stochastic initial conditions are described by the mean field and the stochastic subspace basis fields. They are all shown in terms of the streamfunction in Fig. 8.

The principal variances $\sigma_i^2(t), i = 1, \ldots, 5$ (eigenvalues of $\mathbf{C}_{Y_i(t)Y_j(t)}$) (blue solid curves) and the kinetic energy of the mean flow field (red solid curve) are shown in Fig. 9. In this case, we find a more complex evolution of the stochastic energy characterized by oscillations and non-monotonic behavior. The evolution of the kinetic energy associated with the mean field is also more complex.

The mean fields $\bar{\mathbf{u}}(\mathbf{x}, t)$ and orthonormal basis fields $\mathbf{u}_i(\mathbf{x}, t), i = 1, \ldots, 5$ are shown in Figs. 10 and 11 for two different time instances in terms of the streamfunction. For the same time instances we also present four out of the five two-dimensional marginals associated with the stochastic processes $\{Y_j(t; \omega)\}_{j=1}^s$. As we can observe, the basis fields $\mathbf{u}_i(\mathbf{x}, t)$ are mainly distorted at locations close to the solid boundaries indicating that the main interaction of the stochastic subspace V_S and the mean flow is taking place close to these locations and especially the circular obstacle. This behavior has also been reported in previous work based on generalized PC method [47]. Larger interactions also occur where the mean vorticity is larger and where meanders and eddies form downstream.

Finally in Fig. 12 we compare the mean streamfunction computed using the presented method with the one obtained by