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A fully symmetric nonlinear biorthogonal decomposition theory for random fields

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ABSTRACT

We present a general approach for nonlinear biorthogonal decomposition of random fields. The mathematical theory is developed based on a fully symmetric operator framework that unifies different types of expansions and allows for a simple formulation of necessary and sufficient conditions for their completeness. The key idea of the method relies on an equivalence between nonlinear mappings of Hilbert spaces and local inner products, i.e. inner products that may be functionals of the random field being decomposed. This extends previous work on the subject and allows for an effective formulation of field-dependent and field-independent representations. The proposed new methodology can be applied in many areas of mathematical physics, for stochastic low-dimensional modelling of partial differential equations and dimensionality reduction of complex nonlinear phenomena. An application to a transient stochastic heat conduction problem in a one-dimensional infinite medium is presented and discussed.

1. Introduction

Random fields arise in many branches of mathematical physics including fluid dynamics, electrodynamics, transport theory, geophysics, quantum field theory and statistical physics. The general representation theory is rather technical [1–3] and, in a certain sense, it is closely connected to the representation theory of nonlinear functionals. Consider, as an example, a field equation where forcing terms, boundary conditions, physical parameters and/or initial conditions are set to be random. The solution to this problem (when it exists) is obviously a random field that can be conveniently thought of as an output of a nonlinear system whose input–output map is implicitly defined by the field equation itself. Such a map, which is often referred to as a "propagator" [4], connects suitable descriptors of the random input processes to the statistical properties of the solution. Therefore, according to this viewpoint, the representation of a random field reduces to the representation of a nonlinear system, i.e. nonlinear functional representation [5–7].

Historically, the first consistent theory characterizing nonlinear functionals of stochastic processes is due to Wiener [8] who pioneered a complete expansion [9] of any L^2-functional of the Brownian motion in terms Hermite polynomials. Subsequently, other authors extended Wiener's original ideas to arbitrary functionals of the Poisson process [10] and to more general independent increment processes [11] by using Itô's calculus. There were also attempts to construct Wiener–Hermite representations in terms of time-dependent bases [12–15], in order to refer the statistical description of a time-evolving stochastic system to an epoch that is not continuously escaping in the past (see [16] for a more recent account and [17] for an interesting alternative representation of time-evolving random spaces). All these pioneering contributions revealed a close connection between random input processes and orthogonal polynomial functionals [18]. However, the mathematical apparatus required to deal with these types of representations is rather complex and technical, mainly because of the infinite dimensionality of the stochastic processes involved. Significant mathematical simplifications are obtained if it is assumed that the random field can be represented in terms of a finite—though eventually large—number of random variables. In these cases, the functional representation theory reduces to the representation theory of multiparameter functions (see, e.g., [7] p. 13 or [5] p. 579). Based on this observation, many orthogonal representations of random fields have been constructed by using the standard theory of Hilbert spaces. Well known examples are generalized polynomial chaos [19–21] and Karhunen–Loève expansions.

The purpose of this paper is to develop a nonlinear extension of the biorthogonal decomposition method [22,23] that relies on an equivalence between nonlinear mappings of Hilbert spaces and *local inner products*, i.e. inner products that may be functionals of the random field being decomposed. This generalizes previous work on the subject [24–28] and yields a new methodology that can be employed in many areas of mathematical physics, for stochastic low-dimensional modelling of partial differential equations and dimensionality reduction of complex nonlinear phenomena. Following Aubry et al. [26,22,23], we will develop this decomposition theory based on a general operator framework that unifies different types of expansions and allows for a simple

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formulation of necessary and sufficient conditions for their completeness. As we will see, the apparent simplicity of this operatorial approach has its roots in the powerful theory of linear transformations acting on Hilbert spaces. Both field-dependent and field-independent representations will be discussed, with particular emphasis on field-dependent Galerkin modelling of stochastic partial differential equations. This is an attractive area of research. Indeed, several biorthogonal expansions have been recently proposed for low-dimensional modelling of incompressible random viscous flows [24,25] (see also [29]), thus extending the standard Galerkin framework [30–33] for stochastic variations of boundary conditions and other types of uncertainties. All these approaches will be essentially unified in the present paper. In this broader context we will see that, in principle, our theory allows us to construct reduced-order models of stochastic input processes and field equations having *minimal dimensionality*. This is of great interest in many areas of mathematical physics, e.g., when a reduced-order model is employed for control or optimization purposes [34,35], or for generating data-driven stochastic input models [36].

This paper is organized as follows. In Section 2 we develop the mathematical theory for a nonlinear biorthogonal decomposition of random fields. In Section 3 we discuss field-dependent and field-independent representations including generalized polynomial chaos [19,20], generalized spectral expansions [37] and proper generalized decompositions [38,39]. In Section 4 we present an application of the developed theory to a time-dependent stochastic heat conduction problem. Finally, the main findings and their implications are summarized in Section 5. We also include a brief Appendix where we recall some fundamental results of the spectral theory for symmetric operators acting on Hilbert spaces.

2. Nonlinear biorthogonal decomposition of random fields being functionals of a finite number of random variables

Let us introduce a suitable mathematical setting to study decomposition theories of continuous random fields that can be represented in terms of a finite—though eventually large—number of random variables.[1] To this end, let $(\Omega, \mathcal{S}, P)$ be a complete probability space, where Ω denotes the set of outcomes, $\mathcal{S}$ is the minimal σ-algebra of the subsets of Ω and $P : \mathcal{S} \to [0, 1]$ is the applicable probability measure. On this probability space we consider a finite-dimensional real random vector

$$\begin{aligned} &\xi : \Omega \to \mathbb{R}^n \\ &\omega \to \xi(\omega) \stackrel{\text{def}}{=} (\xi_1(\omega), \ldots, \xi_n(\omega)) \end{aligned} \tag{1}$$

characterizing the input uncertainties of the system. These are assumed to be statistically known. For any Borel function f depending on ξ, the expected value is defined as

$$\langle f \rangle \stackrel{\text{def}}{=} \int_\Omega f(\xi(\omega)) \, \mathrm{d}P(\omega) = \int_{\mathbb{R}^n} f(x) \mathrm{d}\mu_\xi(x), \tag{2}$$

where $\mu_\xi(x)$ is the distribution measure of (1), i.e.

$$\mu_\xi(\mathfrak{B}) \stackrel{\text{def}}{=} P\left(\xi^{-1}(\mathfrak{B})\right), \tag{3}$$

for any Borel set $\mathfrak{B} \subseteq \mathbb{R}^n$. We denote by $\Sigma = \xi(\Omega)$ the range space of ξ and we assume that it is a bounded subset of $\mathbb{R}^n$. If μ_ξ is absolutely continuous with respect to the Lebesgue measure then there exist a probability density function $w : \Sigma \to \mathbb{R}^+$, such that

$$\langle f \rangle = \int_\Sigma f(\xi) w(\xi) \, \mathrm{d}\Sigma, \tag{4}$$

where $\mathrm{d}\Sigma \stackrel{\text{def}}{=} \mathrm{d}\xi_1 \cdots \mathrm{d}\xi_n$.

A continuous scalar random field in a space–time domain is represented as a function

$$u : X \times T \times \Omega \to \mathbb{R}, \tag{5}$$

where $X \subseteq \mathbb{R}^d$ $(d = 1, 2, 3)$ denotes the spatial domain, $T \subseteq \mathbb{R}$ is the temporal domain and Ω is the sample space. If we consider $u(x, t; \omega)$ as an output of a certain nonlinear system, e.g., defined implicitly by a field equation, whose uncertainties are represented in terms of the finite-dimensional random vector (1), then in view of the Doob–Dynkin lemma (see, e.g., [40] p. 8 or [41] p. 7), $u(x, t; \omega)$ can be entirely described in terms of the same set of random variables, i.e. we have the identity

$$u(x, t; \omega) \equiv u(x, t; \xi(\omega)). \tag{6}$$

This fundamental result allows us to represent a random field as a *parametric* field in a Hilbert space $\mathcal{H}(X \times T \times \Sigma)$.

If $\mathcal{H}$ is separable, i.e. if it admits a countable orthonormal basis, then it can be obviously represented as tensor product of two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ [42, p. 51] as[2]

$$\mathcal{H} \simeq \mathcal{H}_1 \otimes \mathcal{H}_2, \tag{7}$$

where the symbol "$\simeq$" means *isomorphic*. Possible choices of $\mathcal{H}$, $\mathcal{H}_1$ and $\mathcal{H}_2$ are

$$L^2(X \times T \times \Sigma) \simeq L^2(X \times T) \otimes L^2(\Sigma), \tag{8}$$

$$\simeq L^2(T) \otimes L^2(X \times \Sigma), \tag{9}$$

$$\simeq L^2(T \times \Sigma) \otimes L^2(X). \tag{10}$$

These three different possibilities correspond to three different types of expansions first investigated by Venturi et al. [24] (form (9)) and Mathelin et al. [25] (form (10)). Generalized polynomial chaos [19,20] and generalized spectral expansions [37] are representations of type (8). We remark that other choices for $\mathcal{H}_1$ and $\mathcal{H}_2$ may be based on Sobolev spaces $\mathcal{W}^{k,2}$ [46, p. 40].

A representation of the random field (6) in the tensor product space (7) takes the general form

$$u = \sum_{i,j=1}^{\infty} a_{ij} \phi_i \psi_j, \quad \phi_i \in \mathcal{H}_1, \ \psi_j \in \mathcal{H}_2, \tag{11}$$

where ϕ_i and ψ_j are orthonormal[3] basis functions of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. According to a theorem of Schmidt [47], any representation of a tensor product of two Hilbert spaces is unitarily equivalent to a diagonal representation [48, p. 118]. This means that we can transform (11) into the equivalent expansion

$$u = \sum_{k=1}^{\infty} \mu_k \Phi_k \Psi_k, \quad \Phi_k \in \mathcal{H}_1, \ \Psi_k \in \mathcal{H}_2 \tag{12}$$

by means of unitary transformations in $\mathcal{H}_1$ and $\mathcal{H}_2$. We remark that such a diagonalization procedure cannot be extended, in general, to tensor products involving more than two Hilbert spaces. For

[1] As we have already seen, the choice to rely on a finite-dimensional random space avoids many technical difficulties and, at the same time, encompasses most practical applications.

[2] Let us recall that a separable Hilbert space is necessarily isomorphic with the Lebesgue space L^2 [43, p. 55]. For a rigorous definition of tensor products of Hilbert spaces see also [42] p. 51, [44] p. 27 or [45] p. 91.

[3] Orthonormality is clearly relative to specific choices of inner products in $\mathcal{H}_1$ and $\mathcal{H}_2$ (see the subsequent Section 2.1).

instance, if $\mathcal{H} \simeq \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ is a tensor product of three Hilbert spaces, then

$$u = \sum_{i,j,k=1}^{\infty} c_{ijk} \phi_i \psi_j \eta_k, \tag{13}$$

where $\phi_i \in \mathcal{H}_1$, $\psi_j \in \mathcal{H}_2$ and $\eta_k \in \mathcal{H}_3$, cannot be reduced to a *triorthogonal* expansion (see, e.g., [49,48,50]).

2.1. Local inner products

Let us introduce the notion of *local inner product* on $\mathcal{H}_1$ and $\mathcal{H}_2$, which is at the basis of the nonlinear decomposition technique developed in the paper. To this end we first consider the following two local bilinear forms[4] [51, p. 202]

$$\{\cdot,\cdot\}_u : \mathcal{H}_1 \times \mathcal{H}_1 \to \mathbb{R}, \tag{14}$$

$$(\cdot,\cdot)_u : \mathcal{H}_2 \times \mathcal{H}_2 \to \mathbb{R}, \tag{15}$$

where the subscripts "u" in both (14) and (15) emphasize the fact that such forms depend also and possibly in a nonlinear way on the random field u. We will also assume that (14) and (15) are nondegenerate and satisfy the requirements of symmetry and positive definiteness, i.e. they define two *local inner products* in $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. They key observation for the development of a nonlinear decomposition theory is that a local bilinear form can be reduced to a standard bilinear form operating on transformed fields, i.e. there exist two linear operators

$$A_u : \mathcal{H}_1 \to \mathcal{H}_1 \quad \text{and} \quad B_u : \mathcal{H}_2 \to \mathcal{H}_2, \tag{16}$$

depending nonlinearly on u, such that

$$\{\phi_1, \phi_2\}_u = \{A_u \phi_1, \phi_2\}, \quad \forall \phi_1, \phi_2 \in \mathcal{H}_1, \tag{17}$$

$$(\psi_1, \psi_2)_u = (B_u \psi_1, \psi_2), \quad \forall \psi_1, \psi_2 \in \mathcal{H}_2, \tag{18}$$

where at the right hand side there are global (eventually standard) inner products. This result is known as the *first representation theorem* [52, p. 322] and, as pointed out by Tonti [53] p. 1352, it is a rather general fact, i.e. the change in a bilinear functional is equivalent to a premultiplication by an operator. Moreover, the requirement that $\{\cdot,\cdot\}_u$ and $(\cdot,\cdot)_u$ are inner products implies that A_u and B_u are also bounded, symmetric and positive.

As an example, consider the following inner product (Einstein's summation convention on repeated indices is assumed)

$$(p, q) \stackrel{\text{def}}{=} \int_X g_{ij}(x) p^i(x) q^j(x) \mathrm{d}X \tag{19}$$

inducing a norm in the space of vector fields represented in a curvilinear coordinate system [54] with metric $g_{ij}(x)$. If we assume that g_{ij} is a possibly nonlinear functional of a field $u(x)$, then

$$(p, q)_u \stackrel{\text{def}}{=} \int_X g_{ij}(x; u)\, p^i(x) q^j(x) \mathrm{d}X \tag{20}$$

defines a *local inner product*, which is nondegenerate only if $g_{ij}(x; u)$ is nonsingular. A physical example may be the Lagrangian coordinate system of fluid mechanics where the metric field depends on the velocity that solves, e.g., the Navier–Stokes equations. It is clear that (20) can be reduced to a standard inner product by considering the following trivial linear operator

$$B_u p \stackrel{\text{def}}{=} g_{ij}(x; u)\, p^i(x). \tag{21}$$

This yields

$$(p, q)_u = (B_u p, q) = (p, B_u q). \tag{22}$$

We remark that local bilinear forms can also be defined in terms of operators associated with partial differential equations in a very similar way to the one used in the formulation of action functionals for non-potential operators [55,53,56,57]. Indeed, this type of approach has been recently adopted by Nouy et al. [37] for the construction of equation-dependent spectral representations of the random space. We will return to this important point in the subsequent Section 3.1.

2.2. The operators U, $U^\dagger$ and their spectral representation

It is convenient to develop the biorthogonal decomposition theory based on a general operator framework that unifies different types of expansions and allows for a simple formulation of necessary and sufficient conditions for their completeness. To this end, following Aubry et al. [26,22,23], we define the following linear operator

$$U : \mathcal{H}_1 \to \mathcal{H}_2 \tag{23}$$

such that

$$\forall \phi \in \mathcal{H}_1 \qquad U\phi \stackrel{\text{def}}{=} \{u, \phi\}_u, \tag{24}$$

where $\{\cdot,\cdot\}_u$ denotes a local inner product in $\mathcal{H}_1$. By using Eq. (17), we can transform (24) as

$$U\phi = \{u, A_u \phi\} = \left\{A_u \otimes I_{\mathcal{H}_2} u, \phi\right\}, \tag{25}$$

where $\{,\}$ is a global (eventually standard) inner product in $\mathcal{H}_1$ and $I_{\mathcal{H}_2}$ denotes the identity transformation in $\mathcal{H}_2$. In this paper we will always assume that U is *compact*[5] ([52] p. 260, [43] p. 172, [42] p. 198). The tensor product operator $A_u \otimes I_{\mathcal{H}_2}$ defines the following nonlinear mapping from $\mathcal{H}$ into $\mathcal{H}$

$$g_1(u) \stackrel{\text{def}}{=} A_u \otimes I_{\mathcal{H}_2} u. \tag{26}$$

This transformation can be obviously represented in $\mathcal{H}_1 \otimes \mathcal{H}_2$ as (see Eq. (11))

$$g_1(u) = \sum_{i,j=1}^{\infty} a_{ij} A_u \phi_i \psi_j. \tag{27}$$

The adjoint of U in the sense of operators acting between different Hilbert spaces (having different local inner products) satisfies (e.g., [59] p. 133)

$$(\psi, U\phi)_u = \{U^\dagger \psi, \phi\}_u, \quad \forall \phi \in \mathcal{H}_1, \ \forall \psi \in \mathcal{H}_2. \tag{28}$$

This implies that $U^\dagger$ is a linear operator from $\mathcal{H}_2$ into $\mathcal{H}_1$ [52, p. 256]

$$U^\dagger : \mathcal{H}_2 \to \mathcal{H}_1 \tag{29}$$

such that

$$\forall \psi \in \mathcal{H}_2, \quad U^\dagger \psi \stackrel{\text{def}}{=} (u, \psi)_u. \tag{30}$$

By using Eq. (18), we can transform (30) as

$$U^\dagger \phi = (u, B_u \psi) = \left(I_{\mathcal{H}_1} \otimes B_u u, \psi\right), \tag{31}$$

where $(\cdot,\cdot)$ is a global inner product in $\mathcal{H}_2$ and $I_{\mathcal{H}_1}$ denotes the identity transformation in $\mathcal{H}_1$. Similarly to Eq. (26), the tensor

[4] We recall that a local bilinear form on $\mathcal{H}_1$ is a map which attempts to correspond with every tern of vectors $\phi_1, \phi_2 \in \mathcal{H}_1$ and $u \in \mathcal{H}$ a real number $\{\phi_1, \phi_2\}_u$ in a bilinear way in ϕ_1 and ϕ_2.

[5] Generalizations to non-compact operators are useful and sometimes of primary importance. For instance, U may be unbounded and may have a continuous spectrum. The latter situation is discussed by Aubry et al. [58] in the context of turbulent flows.

product operator $I_{\mathcal{H}_1} \otimes B_u$ defines the following nonlinear mapping from $\mathcal{H}$ into $\mathcal{H}$

$$g_2(u) \stackrel{\text{def}}{=} I_{\mathcal{H}_1} \otimes B_u u, \tag{32}$$

which can be represented in $\mathcal{H}_1 \otimes \mathcal{H}_2$ as

$$g_2(u) = \sum_{i,j=1}^{\infty} a_{ij} \phi_i B_u \psi_j. \tag{33}$$

Now, the spectral decomposition of the compact operator U yields a representation of the random field u in the form (see [52] p. 261 or [22] p. 690)

$$u = \sum_{i=1}^{\infty} \mu_i \Phi_i \Psi_i, \quad \Phi_i \in \mathcal{H}_1, \ \Psi_i \in \mathcal{H}_2, \tag{34}$$

where the basis functions Φ_i and Ψ_i are *locally orthonormal* in their respective spaces, i.e. they satisfy

$$\{\Phi_i, \Phi_j\}_u = (\Psi_i, \Psi_j)_u = \delta_{ij}. \tag{35}$$

From Eqs. (34) and (35) we obtain the so-called *dispersion* relations

$$U\Phi_k = \mu_k \Psi_k, \tag{36}$$

$$U^\dagger \Psi_k = \mu_k \Phi_k, \tag{37}$$

coupling locally orthogonal sets of modes in $\mathcal{H}_1$ to those in $\mathcal{H}_2$. By applying $U^\dagger$ to (36) and U to (37) we finally obtain the eigenvalue problems

$$U^\dagger U \Phi_k = \mu_k^2 \Phi_k, \tag{38}$$

$$UU^\dagger \Psi_k = \mu_k^2 \Psi_k. \tag{39}$$

We notice that the operators $UU^\dagger$ and $U^\dagger U$ are compact,[6] symmetric and positive and they admit the following representation

$$U^\dagger U \Phi_k = \{k_{U^\dagger U}, \Phi_k\}_u, \tag{40}$$

$$UU^\dagger \Psi_k = (k_{UU^\dagger}, \Psi_k)_u, \tag{41}$$

where the kernel functions $k_{U^\dagger U}$ and $k_{UU^\dagger}$ are easily obtained as

$$k_{U^\dagger U} \stackrel{\text{def}}{=} \left(u, u'\right)_u = \sum_{k=1}^{\infty} \mu_k^2 \Phi_k \Phi_k', \tag{42}$$

$$k_{UU^\dagger} \stackrel{\text{def}}{=} \{u, u'\}_u = \sum_{k=1}^{\infty} \mu_k^2 \Psi_k \Psi_k'. \tag{43}$$

The apex notation denotes evaluation at a different point for those variables that are not integrated out by the inner products. For instance, if $\mathcal{H}_2 \equiv \mathcal{H}_2(T)$ then the kernel (43) is

$$k_{UU^\dagger}(t, t') = \left\{u(x, t; \xi), u(x, t'; \xi)\right\}_u = \sum_{k=1}^{\infty} \mu_k^2 \Psi_k(t) \Psi_k(t'). \tag{44}$$

In order to compute a nonlinear biorthogonal expansion of a random field u, we need to solve simultaneously (36) and (37). This problem is not equivalent to the solution of the eigenvalue problems (38) and (39) since the dispersion relations $\Phi_k \leftrightarrow \Psi_k$ may be lost. Indeed a solution to (36)–(37) is a solution to (38)–(39), but the converse is not necessarily true. Therefore, it is a common practice to solve one eigenvalue problem (either (38) or (39) and then use one dispersion relation to compute the other basis. It is useful to remark that the eigenfunctions of $UU^\dagger$ and $U^\dagger U$ define locally orthonormal bases of $\mathrm{N}(U)^\perp$ and $\mathrm{N}(U^\dagger)^\perp$, respectively, where N denotes the null space of an operator and the symbol "$\perp$" indicates the orthogonal complement [52, p. 252]. This means that, in general, these spectral bases will not be complete in $\mathcal{H}_1$ and $\mathcal{H}_2$. (See Appendix for further details). However, in the context of the representation of a specific random field u, the null space of the field-dependent operator U is not required since it does not obviously contribute to the representation of u.

2.3. The equivalence between local inner products and nonlinear mappings

From what has been said, it is clear that we can effectively determine a biorthogonal expansion of a random field in terms of locally orthogonal modes provided we select two local inner products in $\mathcal{H}_1$ and $\mathcal{H}_2$. This is equivalent to choosing two bounded, symmetric and positive linear operators A_u and B_u acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. In this section we would like show that a decomposition of a random field based on local inner products can be equivalently seen as a decomposition of a nonlinearly mapped field with respect to standard inner products. To this end let us first apply the so-called *second representation theorem* [52, p. 331] to (17) and (18)

$$\{\phi_1, \phi_2\}_u = \{A_u^{1/2}\phi_1, A_u^{1/2}\phi_2\}, \quad \forall \phi_1, \phi_2 \in \mathcal{H}_1, \tag{45}$$

$$(\psi_1, \psi_2)_u = (B_u^{1/2}\psi_1, B_u^{1/2}\psi_2), \quad \forall \psi_1, \psi_2 \in \mathcal{H}_2, \tag{46}$$

where $A_u^{1/2}$ and $B_u^{1/2}$ denote the (unique) square root operators corresponding to A_u and B_u, respectively.[7] The second representation theorem allows us to transform effectively locally orthogonal modes Φ_k and Ψ_k into globally orthogonal ones $\widetilde{\Phi}_k$ and $\widetilde{\Psi}_k$ through the mappings

$$\widetilde{\Phi}_k \stackrel{\text{def}}{=} A_u^{1/2}\Phi_k, \tag{47}$$

$$\widetilde{\Psi}_k \stackrel{\text{def}}{=} B_u^{1/2}\Psi_k. \tag{48}$$

In fact, from (35) and (45)–(48) it easily follows that

$$\{\Phi_i, \Phi_j\}_u = \{\widetilde{\Phi}_i, \widetilde{\Phi}_j\} = \delta_{ij}, \tag{49}$$

$$(\Psi_i, \Psi_j)_u = (\widetilde{\Psi}_i, \widetilde{\Psi}_j) = \delta_{ij}. \tag{50}$$

Now we can transform the biorthogonal expansion (34) in terms of globally orthogonal modes. To this end we simply apply the tensor product operator $A_u^{1/2} \otimes B_u^{1/2}$ to (34), to obtain the following new field

$$g(u) \stackrel{\text{def}}{=} \sum_{k=1}^{\infty} \mu_k A_u^{1/2}\Phi_k B_u^{1/2}\Psi_k = \sum_{k=1}^{\infty} \mu_k \widetilde{\Phi}_k \widetilde{\Psi}_k, \tag{51}$$

where g is a *nonlinear mapping* from $\mathcal{H}$ into $\mathcal{H}$ defined as

$$\begin{aligned} &g : \mathcal{H} \to \mathcal{H} \\ &u \to g(u) \stackrel{\text{def}}{=} A_u^{1/2} \otimes B_u^{1/2} u. \end{aligned} \tag{52}$$

Obviously, the nonlinearity of the mapping g is due to the nonlinear functional dependence of the linear operators $A_u^{1/2}$ and $B_u^{1/2}$ on u.

From (49)–(51) we obtain the following dispersion relations in terms of globally orthogonal modes and standard inner products

$$\{g(u), \widetilde{\Phi}_k\} = \mu_k \widetilde{\Psi}_k, \tag{53}$$

$$(g(u), \widetilde{\Psi}_k) = \mu_k \widetilde{\Phi}_k. \tag{54}$$

[6] We recall that if U is compact then $U^\dagger$ is compact and so are the operator products $UU^\dagger$ and $U^\dagger U$ (see, e.g., [52] pp. 158–159).

[7] Since the operators A_u and B_u are symmetric and positive they have a well defined unique symmetric square root [52, p. 281].

At this point it is convenient to define two operators $G : \mathcal{H}_1 \to \mathcal{H}_2$ and $G^\dagger : \mathcal{H}_2 \to \mathcal{H}_1$ such that

$$G\phi \stackrel{\text{def}}{=} \{g(u), \phi\}, \qquad G^\dagger \psi \stackrel{\text{def}}{=} (g(u), \psi). \tag{55}$$

This allows us to write (53) and (54) in the operatorial form

$$G\widetilde{\Phi}_k = \mu_k \widetilde{\Psi}_k, \tag{56}$$

$$G^\dagger \widetilde{\Psi}_k = \mu_k \widetilde{\Phi}_k. \tag{57}$$

A comparison between (56)–(57) and (36)–(37) shows that G and U are related by the following operatorial identities

$$GA_u^{1/2} = B_u^{1/2} U, \qquad G^\dagger B_u^{1/2} = A_u^{1/2} U^\dagger. \tag{58}$$

From (56) and (57) we also see that $\widetilde{\Phi}_k$ and $\widetilde{\Psi}_k$ are eigenfunctions of the symmetric eigenvalue problems

$$G^\dagger G\widetilde{\Phi}_k = \{k_{G^\dagger G}, \widetilde{\Phi}_k\} = \mu_k^2 \widetilde{\Phi}_k, \tag{59}$$

$$GG^\dagger \widetilde{\Psi}_k = (k_{GG^\dagger}, \widetilde{\Psi}_k) = \mu_k^2 \widetilde{\Psi}_k, \tag{60}$$

where the kernel functions $k_{G^\dagger G}$ and $k_{GG^\dagger}$ are

$$k_{G^\dagger G} \stackrel{\text{def}}{=} \left(g(u), g(u)'\right) = \sum_{k=1}^{\infty} \mu_k^2 \widetilde{\Phi}_k \widetilde{\Phi}_k', \tag{61}$$

$$k_{GG^\dagger} \stackrel{\text{def}}{=} \{g(u), g(u)'\} = \sum_{k=1}^{\infty} \mu_k^2 \widetilde{\Psi}_k \widetilde{\Psi}_k'. \tag{62}$$

Again, the apex notation here denotes evaluation at a different point for those variables that are not integrated out by the inner products (for an example, see Eq. (44)). Thus, a decomposition of a random field u based on local inner products can be equivalently seen as a decomposition of a nonlinearly mapped field $g(u)$ with respect to standard inner products. Is the converse statement true? In other words, if we arbitrarily select a nonlinear mapping from $\mathcal{H}$ into $\mathcal{H}$, will we be able determine two symmetric operators $A_u^{1/2}$ and $B_u^{1/2}$ defining two local inner products in $\mathcal{H}_1$ and $\mathcal{H}_2$ and such that (51) is satisfied? Unfortunately, the answer to this question is negative. In fact, there exist even linear transformations from $\mathcal{H}$ into $\mathcal{H}$ that cannot be represented in terms of tensor product operators. This means that we only have a partial equivalence between local inner products and nonlinear mappings. However, in the particular case where the operators $A_u^{1/2}$ and $B_u^{1/2}$ are *invertible* then the mapping $g(u)$ is invertible as well and there is a one-to-one correspondence between the operators U and G (see Eq. (58)). This implies that locally and globally orthogonal modes are in a one-to-one correspondence as well (see Eq. (47)–(48)).

2.4. An illustrative example

Let us assume that the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ appearing in the tensor product (7) are

$$\mathcal{H}_1 = L^2(X \times \Sigma), \tag{63}$$

$$\mathcal{H}_2 = L^2(T). \tag{64}$$

According to this choice, the random field u is represented as a superimposition of random spatial modes modulated by deterministic temporal modes, i.e.

$$u(x, t; \xi) = \sum_{k=1}^{\infty} \mu_k \Psi_k(t) \Phi_k(x; \xi). \tag{65}$$

This type of expansion has been studied by Venturi et al. [24] in the context of stochastic low-dimensional modelling of random fluid flows. In order to set up a nonlinear decomposition theory we need define two local inner products or, equivalently, two bounded symmetric transformations in $\mathcal{H}_1$ and $\mathcal{H}_2$. In this illustrative example we will examine the following simple choices

$$A_u^{1/2}\phi = \mathcal{A}_u^{1/2}(x; \xi)\, \phi(x; \xi), \tag{66}$$

$$B_u^{1/2}\psi = \mathcal{B}_u^{1/2}(t)\psi(t), \tag{67}$$

where $\mathcal{A}_u^{1/2}(x; \xi)$ and $\mathcal{B}_u^{1/2}(t)$ are real positive measures that are possibly nonlinear functionals of u. The associated local inner products are explicitly obtained as

$$\{\phi_1, \phi_2\}_u \stackrel{\text{def}}{=} \int_X \langle \phi_1(x; \xi)\phi_2(x; \xi)\mathcal{A}_u(x; \xi)\rangle \mathrm{d}X, \tag{68}$$

$$(\psi_1, \psi_2)_u \stackrel{\text{def}}{=} \int_T \psi_1(t)\psi_2(t)\mathcal{B}_u(t)\mathrm{d}t. \tag{69}$$

Correspondingly, the operators U and $U^\dagger$ (Eqs. (25) and (31)) are

$$U\phi = \int_X \langle u(x, t; \xi)\, \phi(x; \xi)\, \mathcal{A}_u(x; \xi)\rangle \mathrm{d}X, \tag{70}$$

$$U^\dagger \psi = \int_T u(x, t; \xi)\, \psi(x, t)\, \mathcal{B}_u(t)\mathrm{d}t. \tag{71}$$

This yields the following operator product

$$UU^\dagger\psi = \int_T \int_X \langle u(x, t; \xi)\, u\left(x, t'; \xi\right) \times \mathcal{A}_u(x; \xi)\rangle \mathcal{B}_u(t')\psi(t')\mathrm{d}X\mathrm{d}t'$$

whose eigenfunctions Ψ_j are locally orthonormal with respect to (69), i.e.

$$(\Psi_k, \Psi_j)_u = \delta_{kj}. \tag{72}$$

Once the modes Ψ_j are available, we can easily determine the corresponding modes Φ_k through the dispersion relation

$$\Phi_k(x; \xi) = \frac{1}{\mu_k} \int_T u(x, t; \xi)\, \Psi_k(t)\mathcal{B}_u(t)\mathrm{d}t. \tag{73}$$

This completes the computation of the biorthogonal decomposition of u in terms of locally orthogonal modes Ψ_j and Φ_k. Next, we examine the relation between local inner products and nonlinear mappings discussed in the previous subsection. To this end let us first notice that in this particular example the transformations $A_u^{1/2}$ and $B_u^{1/2}$ defined in (66) and (67) are invertible and their inverses are

$$A_u^{-1/2}\phi = \frac{\phi(x; \xi)}{\mathcal{A}_u^{1/2}(x; \xi)}, \qquad B_u^{-1/2}\psi = \frac{\psi(t)}{\mathcal{B}_u^{1/2}(t)}. \tag{74}$$

Therefore, we have a one-to-one correspondence between decomposition theories based on local inner products and decomposition theories based on the following nonlinearly mapped field

$$g(u)(x, t; \xi) \stackrel{\text{def}}{=} \mathcal{A}_u^{1/2}(x; \xi)\, \mathcal{B}_u^{1/2}(t) u(x, t; \xi) \tag{75}$$

with respect to standard inner products. This correspondence can be easily checked by a direct calculation. For instance, the dispersion relation

$$U\Phi_k = \int_X \langle u\Phi_k\mathcal{A}_u\rangle \mathrm{d}X = \mu_k \Psi_k, \tag{76}$$

can be equivalently written in the form (56) as

$$G\widetilde{\Phi}_k = \int_X \langle g(u)\widetilde{\Phi}_k\rangle \mathrm{d}X = \mu_k \widetilde{\Psi}_k, \tag{77}$$

where

$$\widetilde{\Phi}_k(x;\xi) = \mathcal{A}_u^{1/2}(x;\xi)\,\Phi_k(x;\xi)\,, \tag{78}$$

$$\widetilde{\Psi}_k(t) = \mathcal{B}_u^{1/2}(t)\Psi_k(t), \tag{79}$$

are globally orthogonal modes. We will see in Section 4.1 that suitable choices of field-dependent integration measures $\mathcal{A}_u$ and $\mathcal{B}_u$ could yield to biorthogonal representations converging faster than the classical stochastic proper orthogonal decomposition [24], which is obtained for $\mathcal{A}_u = 1$ and $\mathcal{B}_u = 1$ in the present example. The high convergence rate will be obviously in the new metric associated with the integration measures $\mathcal{A}_u$ and $\mathcal{B}_u$.

3. Field-dependent and field-independent decomposition theories

Field-dependent decomposition theories are based on random fields whose representation is already known, for instance in a polynomial chaos [60,19,20] or in a biorthogonal wavelet [61] basis. When we deal with field-dependent decompositions we are usually working *simultaneously* in both Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. In these cases we look for *another* representation of the random field satisfying various types of requirements. For example, several biorthogonal expansions converging optimally in the mean, in the second order moment and in the standard deviation sense have been recently proposed for low-dimensional modelling of random incompressible flows [24] and robust control of cylinder wakes [25]. These new approaches extend the standard Galerkin framework [30–33] for stochastic variations of boundary conditions and other types of uncertainties.

In a *field-independent* decomposition theory we are looking for a *complete* representation of either $\mathcal{H}_1$ or $\mathcal{H}_2$ by using information that are not dependent on any particular field. Therefore field-independent methods are well suited, e.g., for the representation of *unknown* solutions to stochastic field equations where physical parameters, boundary conditions, geometry and initial conditions are set to be random [62–64,24]. One of the most famous and widely employed type of field-independent representation is the generalized polynomial chaos expansion [19–21]. More recent approaches are based on high dimensional model representations [65,66], sparse grid adaptive stochastic collocation [67], generalized spectral decompositions [37,68] and proper generalized decompositions [38,39].

3.1. Orthogonal representations of random space

In this subsection we would like to discuss several alternatives to field-independent orthogonal representation of random space based on the spectral theory for symmetric operators. This topic lies somewhat out the paper's main line of development, but we would like to discuss it for completeness, especially in connection with recent results on reduced basis approximation of partial differential equations. To this end let us consider the tensor product space $\mathcal{H}_1(\Sigma) \otimes \mathcal{H}_2(X \times T)$ and look for an expansion of a random field in the form

$$u(x,t;\xi) = \sum_{k=1}^{\infty} \widehat{u}_k(x,t)\,\Gamma_k(\xi)\,, \tag{80}$$

where $\Gamma_k(\xi)$ is an orthonormal basis of $\mathcal{H}_1$ while $\widehat{u}_k$ are, in general, not-orthogonal space–time modes belonging to $\mathcal{H}_2$. The development (80) is based on the original ideas of Wiener [8], who pioneered a complete polynomial expansion [9,69] of any L^2 functional of the Brownian motion process.[8] In the context of spectral theory for symmetric operators, the basis functions Γ_k appearing in (80) can be obtained from the eigenvalue problem

$$\{\mathcal{K}, \Gamma_k\} = \gamma_k \Gamma_k, \tag{81}$$

where $\mathcal{K}(\xi,\xi')$ is a suitable symmetric kernel function. For example, if $\mathcal{H}_1(\Sigma) = L^2(\Sigma)$ then (81) takes the following explicit form

$$\int_{\Sigma} \mathcal{K}(\xi,\xi')\,\Gamma_k(\xi')\,w(\xi')\,\mathrm{d}\xi' = \gamma_k \Gamma_k(\xi)\,, \tag{82}$$

where $w(\xi)$ denotes the probability density function of the random input vector (1). It is interesting to note that multi-dimensional representations of a random space can be obtained directly from (81) or (82) without resorting to tensor products of one-dimensional bases. Indeed, given the kernel $\mathcal{K}$ the problem defined in (82) can also be seen as a multi-dimensional generalization of the singular value decomposition which has been extensively studied in the literature in the finite dimensional case (see, e.g., [71,72] and the reference therein). In that context it has been found that the construction of an optimal (separated) multi-dimensional basis $\Gamma_k(\xi)$ for a given tensor is not trivial and sometimes it is even an ill-posed problem [73,74]. Various algorithms have been recently proposed for the identification of tensor eigenfunctions (see, e.g., [75] and the references therein).

Obviously, the choice of the kernel and the bilinear form in (81) are fundamental in order to obtain a complete[9] and rapidly convergent expansion. A very important question therefore is how to select them *a priori*, i.e., without prior knowledge of the random field. Unfortunately, a general answer to this question is still lacking. Indeed, recent research activity of Nouy [76] (see also [37]) has focused in obtaining spectral expansions based on the weak formulation of the stochastic field equation itself rather than on its solution. In other words, he proposed an *equation-dependent* decomposition method for the resolution of stochastic problems that do not require prior knowledge of the random field. Other types of equation-dependent (separated) representations have been recently proposed for modelling high-dimensional physical phenomena. For instance, the so-called *proper generalized decomposition* [38] constitute an appealing technique for reducing drastically the number of degrees of freedom that functional approximations to stochastic partial differential equations involve [39].

We would like to remark that the generalized spectral decomposition approach resembles in several aspects a nonlinear biorthogonal decomposition method. In particular, it results in a nonlinear eigen-like problem for the basis functions through two dispersion-like relations (see Eqs. (9)–(12) of Nouy and Le Maître [37]). There are also several fundamental differences between the two methods which we would like to discuss hereafter. In the present work, a separated representation of a random field in a tensor product Hilbert space is searched such

[8] As it is well known, Brownian motion can be represented in terms of an infinite number of independent Gaussian random variables. This fact induced several researches to apply polynomial chaos expansions to finite dimensional random fields by using the statistical independence hypothesis as a fundamental requirement. However, this hypothesis is no longer needed in the case of finite dimensional random spaces. Indeed, polynomial chaos expansions for arbitrarily correlated random inputs were already proposed by Soize and Ghanem [70].

[9] In order for the representation to be complete, the null space of the operator defined at the left hand side of Eq. (81) has to be empty (see Appendix for further details). Moreover, every complete representation of $\mathcal{H}_1$ based on the eigenvalue problem (81) is *unitarily equivalent* to any other complete representation, i.e. there exists a suitable rotation of the function space that carries one representation into the other.

that it is optimal with respect to a metric which has a separation property. In [76,37] the metric is based on the weak form of the underlying field equation that describes the system and, in general, such a metric does not have a separation property. This is because the weak formulation of a nonlinear equation basically yields to *semilinear* forms instead of bilinear ones. Therefore the generalized spectral decomposition method in general leads to a non-classical (pseudo) eigenproblem whose mathematical framework is unfortunately still not well developed. When the metric arising from the generalized spectral decomposition method degenerates into a classical tensor product metric then the generalized spectral decomposition is equivalent to an orthogonal expansion with respect to two local inner products in Hilbert spaces.

Equation-dependent bilinear forms occupy a place of peculiar significance also in variational methods for non-potential operators [56]. For example, it has been shown by Magri [55] that every linear equation admits an *action functional* if the bilinear form is defined in terms of the linear operator associated with the equation itself. This has been subsequently extended by Tonti [53] to arbitrary nonlinear problems by considering bilinear forms defined in terms of Gâteaux derivatives [51,57]. Further research along this direction, i.e. spectral expansions generated through equation-dependent bilinear forms, could lead to breakthroughs in the representation theory of solutions to stochastic nonlinear problems.

3.2. Stochastic low-dimensional modelling of PDEs based on field-dependent orthogonal decompositions

Stochastic low-dimensional modelling of partial differential equations based on field-dependent decompositions is an attractive area of research. The main objective is to construct reduced order dynamical systems of manageable computational complexity to be employed, e.g., for control or optimization purposes [34,35]. Among different stochastic modelling techniques, Galerkin approaches are largely employed because of their versatility and ease of implementation. Dynamical equations are usually projected into a suitable set of orthogonal modes whose convergence rate plays a fundamental role in obtaining low-dimensional models that can be rapidly integrated. This explains why the majority of existing field-dependent methods rely on Karhunen–Loève expansions.

However, more efficient alternatives can be developed within the nonlinear biorthogonal framework. Indeed, for a given random field each reasonable choice of a field-dependent norm yields to different spectral expansions having different convergence rates, which are optimal in the metric associated with the chosen norm. The important question at this point is: *what is the desired metric*? This is equivalent to ask: how do we select the field-dependent operators A_u and B_u for the representation a given random field or for the Galerkin decomposition of a specific stochastic partial differential equation? Clearly, it is not easy to provide a general answer to this question since it is problem-dependent. For instance, in the context of data-driven stochastic input model generation [36], a useful metric may be learned from experimental measurements through well known techniques such as kernel principal component analysis[10] [77,78]. For other types of problems, e.g. low-dimensional Galerkin modelling of stochastic partial differential equations, the definition of a useful field-dependent metric may be not a trivial task.

Hereafter, we briefly outline a simple criterion to construct field-dependent operators A_u and B_u based on the minimization of the following *complementary energy functional*

$$\mathcal{F}_M[A_u, B_u] \stackrel{\text{def}}{=} \frac{E_c(M)}{E(\infty)}, \tag{83}$$

where $E(M)$ and $E_c(M)$ denote, respectively, the representation energy with M modes and its complementary, i.e.

$$E(M) \stackrel{\text{def}}{=} \sum_{k=1}^{M} \mu_k^2[A_u, B_u], \quad E_c(M) \stackrel{\text{def}}{=} \sum_{k=M+1}^{\infty} \mu_k^2[A_u, B_u]. \tag{84}$$

In Eq. (84) we have emphasized the fact that the eigenvalues μ_k^2 are considered as scalar functions of two operators A_u and B_u [52, p. 44]. Also, the quantity $E(\infty)$ coincides with the *trace* of $UU^\dagger$ (or $U^\dagger U$) and it can be conveniently calculated as a function of its kernel, i.e. without computing the whole spectrum (see, e.g., [29] Section 3.3). This allows us to rewrite the functional (83) in the following alternative form

$$\mathcal{F}_M[A_u, B_u] = 1 - \frac{E(M)}{\operatorname{tr}(UU^\dagger)}. \tag{85}$$

The advantage of this formulation relies on the fact that the calculation of low-order functionals, e.g., $\mathcal{F}_1$ and $\mathcal{F}_2$, requires only the first few largest eigenvalues. These can be computed efficiently even for large-dimensional problems by employing parallel eigenvalue solvers based on the Arnoldi method. Minimization of (85) for a prescribed M yields to the identification of two operators A_u and B_u and associated field-dependent inner products in $\mathcal{H}_1$ and $\mathcal{H}_2$ (see Eqs. (45) and (46)).

The basic idea behind the minimization of the complementary energy functional (85) is to look for field-dependent norms that maximize the representation energy of the random field for a selected number of expansion terms, i.e. try to inject as much energy as possible into the first few modes. This results in a series expansion that will be optimally convergent in the sense of these norms. At this point it is important to remark that when we deal with *functionals* of the random field, such as the second order moment or even more general nonlinear functionals (e.g. the residual of a stochastic partial differential equation), we have no guarantee that an expansion based on a specific field-dependent norm will be also optimal for the representation of the given functional. This is the case, for example, of the second order moment for which the standard Karhunen–Loève expansion provides the best convergence rate. Therefore, choosing a metric that minimizes the complementary energy functional may be not always a pertinent choice since it could lead to poor convergences with respect to other useful metrics.

4. An application to time-dependent stochastic heat conduction in a one-dimensional infinite medium

In this section we present a simple application of the nonlinear biorthogonal technique to a time-dependent stochastic heat conduction problem in a one-dimensional infinite medium. The main purpose of this application is provide a clear exposition of the theoretical apparatus developed in the paper rather than attempting to tackle complex problems. The field equation describing the physical phenomenon is

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \tag{86}$$

where $u(x, t)$ is the temperature field and α denotes the thermal diffusivity [79, p. 28]. For a given initial condition $u(x, 0)$ the analytical solution to (86) can be represented as [80, p. 227]

$$u(x, t) = \int_{-\infty}^{\infty} \mathcal{G}_\alpha(x, t|x', 0)\, u(x', 0)\, \mathrm{d}x', \tag{87}$$

where the Green function $\mathcal{G}_\alpha$ is

$$\mathcal{G}_\alpha(x, t|x', t') \stackrel{\text{def}}{=} \frac{1}{[4\pi\alpha(t - t')]^{1/2}} \exp\left[-\frac{(x - x')^2}{4\alpha(t - t')}\right]. \tag{88}$$

[10] The "feature space" in this case is defined by the mapping $g(u)$ of Section 2.3.

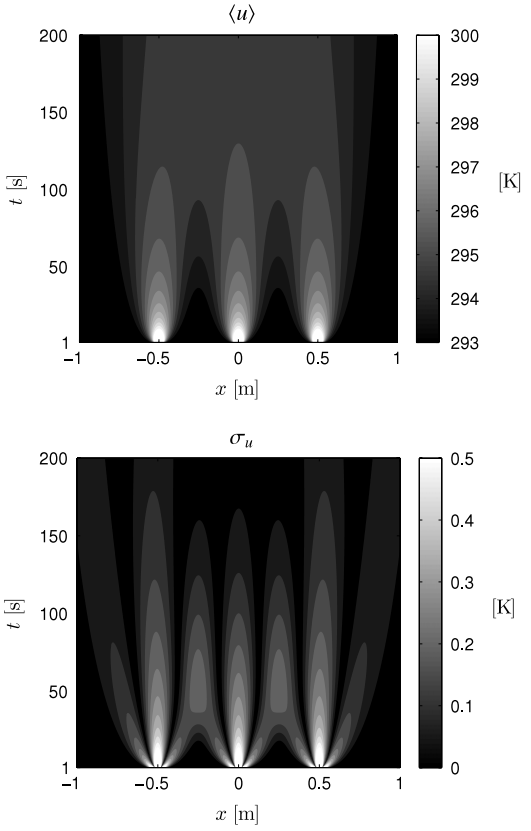

Fig. 1. Mean (top) and standard deviation (bottom) of the random temperature field corresponding to a random thermal diffusivity following a uniform probability distribution with mean $\langle\alpha\rangle = 16.56 \times 10^{-5}$ m^2/s and standard deviation approximately 17%$\langle\alpha\rangle$.

The subscript "α" in $\mathcal{G}_\alpha$ reminds us that this function depends also on the thermal diffusivity. The integral representation (87) allows us to determine the temperature transient corresponding to any initial condition. In particular, the response of the system to a set of N Dirac impulses in the form

$$u(x,0) = u_0 + \sum_{j=1}^{N} \delta(x - l_j) \tag{89}$$

is easily obtained as

$$u(x,t) = u_0 + \sum_{j=1}^{N} \mathcal{G}_\alpha\left(x, t | l_j, 0\right), \quad x \in \mathbb{R},\ t \geq 0. \tag{90}$$

In order to completely define the prototype heat conduction problem, we extract the following space–time subdomains

$$X \stackrel{\text{def}}{=} [-1, 1]\ \text{m}, \qquad T \stackrel{\text{def}}{=} [1, 200]\ \text{s} \tag{91}$$

and we consider $N = 3$ equally spaced Dirac impulses located at

$$l_j = -1 + \frac{j}{2}\ [\text{m}], \quad j = 1, \ldots, 3. \tag{92}$$

Also, we set $u_0 = 293$ K in Eqs. (89) and (90).

Next, we assume that the thermal diffusivity of the medium can be modelled as a random variable in the form

$$\alpha(\xi) \stackrel{\text{def}}{=} \langle\alpha\rangle\,(1 + \sigma\xi), \quad \sigma = 0.3, \tag{93}$$

where $\langle\alpha\rangle = 16.56 \times 10^{-5}$ m^2/s and ξ follows a uniform probability distribution in $[-1, 1]$. The selected mean thermal diffusivity corresponds to pure silver [79, p. 28]. Note also that the standard deviation of α is approximately[11] 17%$\langle\alpha\rangle$. The uncertainty in α induces a random Green function (88) and, correspondingly, a random temperature field, which is denoted as $u(x, t; \xi)$ in agreement with previous notation. In Fig. 1 we show the mean and the standard deviation of such a temperature field in the space–time domain of interest.

4.1. Nonlinear biorthogonal expansions based on field-dependent integration measures

In order to determine a nonlinear biorthogonal decomposition of the random temperature we consider the following *class* of local inner products

$$\{\phi_1, \phi_2\}_u \stackrel{\text{def}}{=} \int_\Sigma \phi_1(\xi)\,\phi_2(\xi)\,\mathcal{A}_u(\xi)\,\mathrm{d}\xi, \tag{94}$$

$$(\psi_1, \psi_2)_u \stackrel{\text{def}}{=} \int_X \int_T \psi_1(x,t)\,\psi_2(x,t)\,\mathcal{B}_u(x,t)\,\mathrm{d}x\mathrm{d}t, \tag{95}$$

where $\mathcal{A}_u(\xi)$ and $\mathcal{B}_u(x, t)$ are two continuous positive integration measures depending nonlinearly on u.[12] In this framework, every biorthogonal expansion of the random temperature

$$u(x, t; \xi) = u_0 + \sum_{k=1}^{\infty} \mu_k \Psi_k(x,t)\,\Phi_k(\xi) \tag{96}$$

is in a direct correspondence with a specific choice of $\mathcal{A}_u$ and $\mathcal{B}_u$. For instance, the standard Karhunen–Loève decomposition is obtained by selecting

$$\mathcal{A}_u(\xi) = w(\xi) \quad \text{and} \quad \mathcal{B}_u(x,t) = 1, \tag{97}$$

where $w(\xi) = 1/2$ is the uniform probability density of the random input variable ξ (Eq. (93)). At this point the question is: how do we select the integration measures $\mathcal{A}_u$ and $\mathcal{B}_u$? We have seen that a possible criterion is to maximize the representation energy for a prescribed number of modes, i.e. minimize the complementary energy functional defined in Eq. (85). As pointed out at the end of Section 3.2, this may not necessarily be a pertinent choice since it could lead to poor convergences when representing other useful functionals of the random field, such as the second order moment.

The minimization of the complementary energy can be done analytically,[13] provided one has available an analytical expression for the first few eigenvalues of $UU^\dagger$ or $U^\dagger U$, or numerically, through constrained iterative minimization algorithms. Here we follow the latter approach. To this end we employ (97) as a starting point for the optimization procedure and we minimize $\mathcal{F}_M[\mathcal{A}_u, \mathcal{B}_u]$ iteratively until a prescribed tolerance is achieved. The results of the minimization are shown in Fig. 2, where we plot the normalized spectrum

$$e_k \stackrel{\text{def}}{=} \frac{\mu_k^2}{E(\infty)} \tag{98}$$

[11] In fact, thanks to the statistical assumptions on the random variable ξ we have $\langle\xi^2\rangle = 1/3$ and therefore the standard deviation of α is $\langle\alpha\rangle\sigma/\sqrt{3}$, i.e. approximately 17%$\langle\alpha\rangle$ for $\sigma = 0.3$.

[12] Clearly, we have selected the following Hilbert spaces $\mathcal{H}_1 = L^2(\Sigma)$ and $\mathcal{H}_2 = L^2(X \times T)$ for the tensor product representation (7). Also, the operators A_u and B_u associated with the local inner products (95) and (94) are explicitly given as $A_u\phi = \mathcal{A}_u(\xi)\,\phi(\xi)$ and $B_u\psi = \mathcal{B}_u(x,t)\,\psi(x,t)$.

[13] We would like to remark that an analytical approach to nonlinear biorthogonal decomposition can be also developed within a variational framework if it is assumed that the modes Φ_k and Ψ_k are functionally dependent on the integration measures $\mathcal{A}_u$ and $\mathcal{B}_u$. Indeed, minimization of the distance between u and its biorthogonal representation (96) in a field-dependent norm yields to a nonlinear eigenvalue problem.

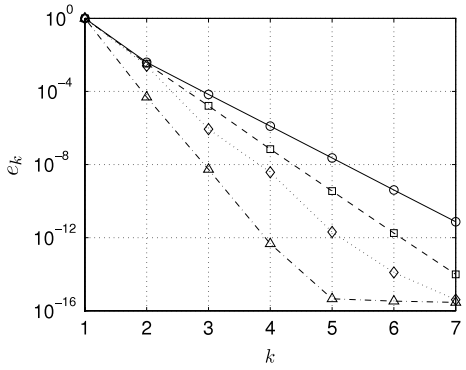

Fig. 2. Normalized spectral decay of polynomial chaos (○), Karhunen–Loève (□) and field-dependent nonlinear biorthogonal expansions based on integration measures minimizing the functionals $\mathcal{F}_2$ (◇) and $\mathcal{F}_1$ (△).

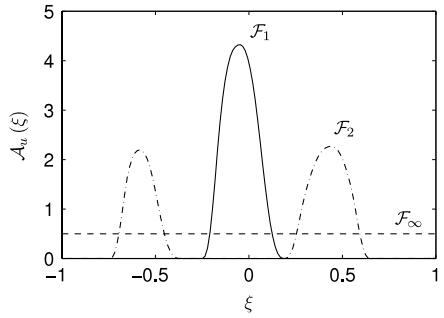

Fig. 3. Field-dependent integration measures (probability densities) $\mathcal{A}_u(\xi)$ minimizing $\mathcal{F}_1$ (−), $\mathcal{F}_2$ (− · −) and $\mathcal{F}_\infty$ (− − −).

corresponding to different optimal integration measures ($E(\infty)$ is defined in Eq. (84) and it coincides with the trace of $UU^\dagger$ or $U^\dagger U$). For the purpose of comparison we also include the spectral decay of Karhunen–Loève and generalized (Legendre) polynomial chaos expansions. In the latter case the spectrum is computed as a standard L^2 space–time norm of not-normalized chaos modes $\widehat{u}_k(x,t)$ (see Eq. (80)). Results of Fig. 2 clearly indicate that the best convergence rate is achieved for integration measures minimizing

$$\mathcal{F}_1[\mathcal{A}_u, \mathcal{B}_u] = 1 - \frac{\mu_1^2[\mathcal{A}_u, \mathcal{B}_u]}{\mathrm{tr}(UU^\dagger)}, \tag{99}$$

where μ_1^2 is the largest eigenvalue of the correlation operator $UU^\dagger$ (or $U^\dagger U$) and the trace is explicitly obtained as

$$\mathrm{tr}(UU^\dagger) = \int_X \int_T \int_\Sigma (u(x,t;\xi) - u_0)^2 \mathcal{A}_u(\xi)\, \mathcal{B}_u(x,t)\, \mathrm{d}\xi \mathrm{d}x \mathrm{d}t. \tag{100}$$

In Fig. 3 we compare different optimal integration measures[14] $\mathcal{A}_u(\xi)$ obtained by minimizing $\mathcal{F}_1$, $\mathcal{F}_2$ and $\mathcal{F}_\infty$. The latter case obviously corresponds to a measure which is coincident with the first guess (97). In fact, as is easily seen from Eq. (85), $\mathcal{F}_\infty$ is already at its absolute minimum, i.e. $\mathcal{F}_\infty \equiv 0$ for all $\mathcal{A}_u$ and $\mathcal{B}_u$. In general, for each specific choice of M the minimization of $\mathcal{F}_M$ allows us to identify a new probability density function $\mathcal{A}_u(\xi)$ having support within the range space of ξ. In other words, it allows us to construct a nonlinear mapping between the random input variable ξ and another random variable ζ which is capable

[14] We would like to remark that the obtained measures are always positive and greater than 10^{-2}. This is because we have implemented a constraint in the minimization algorithm for the complementary energy functional in order to avoid degenerated cases.

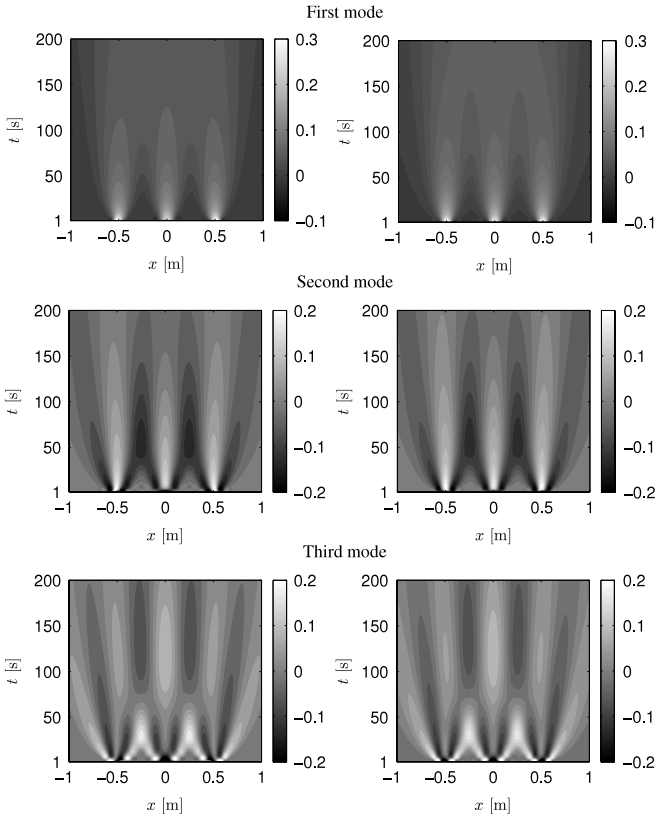

Fig. 4. Left column: Normalized space–time modes $\Psi_k(x,t)$ ($k = 1, 2, 3$) based on a decomposition theory with integration measures minimizing $\mathcal{F}_1$. Right column: Normalized Karhunen–Loève modes.

of significantly improving the converge rate of the underlying biorthogonal expansion. Indeed, from Figs. 2 and 3 we see that the highest convergence rate is based on a probability measure which is rather concentrated near zero.

In Fig. 4 we compare normalized space–time modes $\Psi_k(x,t)$ of a decomposition theory based on integration measures minimizing $\mathcal{F}_1$ with standard Karhunen–Loève modes. Clearly, normalization is relative to different space–time inner products. We see that there are very small differences between the two sets of modes. This is because $\mathcal{B}_u(x,t) \approx 1$. Similarly, in Fig. 5 we compare globally orthogonal modes $\widetilde{\Phi}_k(\xi)$ based on a decomposition theory with integration measures minimizing $\mathcal{F}_1$ with standard Karhunen–Loève modes. Global orthogonality is easily obtained by renormalizing $\Phi_k(\xi)$ relatively to the probability measure $w(\xi) = 1/2$. As we have seen in Section 2.3, this can be easily done by multiplying each locally orthogonal mode by $\mathcal{A}_u^{1/2}(\xi)/\sqrt{2}$. This implies that the modes shown in Fig. 5(a) and (b) are both orthonormal relatively to the same standard inner product.

5. Summary

We have presented a general approach for nonlinear biorthogonal representation of continuous random fields that are functionals of a finite number of random variables. This systematic procedure can be employed in many areas of mathematical physics, for stochastic low dimensional modelling of partial differential equations and dimensionality reduction of complex nonlinear phenomena. The mathematical theory at the basis of the proposed decomposition method relies on an equivalence between nonlinear mappings of Hilbert spaces and local inner products, i.e. inner products that may be functionals of the random field being decomposed. By employing a general operator framework, we

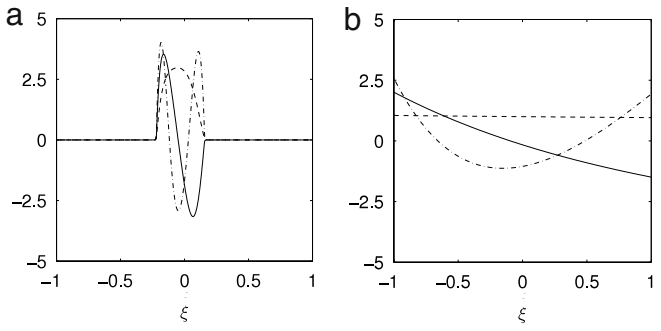

Fig. 5. (a) Gobally orthogonal modes $\widetilde{\Phi}_k(\xi)$ based on a decomposition theory with integration measures minimizing $\mathcal{F}_1$; (b) Karhunen–Loève modes. In both plots we show the first (– – –), the second (—) and the third (— · —) mode.

have unified different types of expansions and provided necessary and sufficient conditions for their completeness.

We have applied this new methodology to a simple time-dependent stochastic heat conduction problem in a one-dimensional infinite medium and we have shown how to construct simple field-dependent orthogonal representations of random space relatively to a metric that yields the fastest spectral decay for the correlation operators. We remark that such a metric may be not always a pertinent choice because it could lead to poor convergences with respect to other useful metrics. In fact, when we deal with *functionals* of the random field, such as the second order moment or even more general nonlinear functionals such as the residual of a stochastic partial differential equation, we have no guarantee that an expansion of the random field based on a specific local inner product will be also optimal for the representation of the given functional. This is the case, for example, of the second order moment for which the standard Karhunen–Loève expansion provides the best convergence rate.

In the context of *field-independent* spectral representations this naturally lead us to the following question: how do we select a metric for an optimal representation of the solution to a specific stochastic field equation? Unfortunately, a general answer to this question is still lacking. Indeed, several effective approaches for the representation of solutions to stochastic partial differential equations have been recently proposed by Nouy et al. [76,37,68,39] and Chinesta et al. [38] based on the weak formulation of the field equation itself. For linear equations it is easy to see that these approaches employ equation-dependent inner products in a very similar way to that one considered in the construction of action functionals for non-potential operators [55,53,56,57]. Further research is necessary in order to determine whether orthogonal expansions based on inner products depending on a specific equation are effective in representing its stochastic solution.

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Appendix. Completeness

Based on the notation of Section 2.2, in this Appendix we address the following question: which conditions on u, A_u and B_u have to be satisfied in order to obtain a complete decomposition of $\mathcal{H}$ by using a tensor product of $UU^\dagger$ and $U^\dagger U$ spectral projections? Intuitively, the answer is connected to the properties of u, A_u and B_u. But how?

We have seen that if U is compact then $U^\dagger$ is compact, and both $UU^\dagger$, $U^\dagger U$ are compact, symmetric and positive. The spectral theorem [52, p. 260] therefore guarantees that the operators $UU^\dagger$ and $U^\dagger U$ admit the following spectral representations

$$UU^\dagger = \sum_h \lambda_h^2 P_h, \quad P_h^\dagger = P_h, \tag{101}$$

$$U^\dagger U = \sum_h \lambda_h^2 Q_h, \quad Q_h^\dagger = Q_h, \tag{102}$$

where λ_k^2 are eigenvalues (counted with their multiplicity) of $UU^\dagger$ (or $U^\dagger U$) while P_h and Q_h are compact symmetric projections onto $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Convergence of (101) and (102) is in norm. Moreover, P_h and Q_h have a range of finite dimension and they constitute a complete orthogonal family *together* with the projections P_0 and Q_0 onto the null spaces of $UU^\dagger$ and $U^\dagger U$. This latter part of the spectral theorem is very important because the null spaces of $UU^\dagger$ or $U^\dagger U$ may be not empty sets, and therefore we may need to consider the associated pair of projections (P_0, Q_0) in order to complete the representation. Since every linear operator maps null elements onto null elements, the null space of $UU^\dagger$ coindices with that of $U^\dagger$, i.e.

$$\mathsf{N}\left(UU^\dagger\right) = \mathsf{N}\left(U^\dagger\right), \tag{103}$$

$$\mathsf{N}\left(U^\dagger U\right) = \mathsf{N}(U), \tag{104}$$

where N denotes the null space of an operator. Moreover, compact operators are necessarily bounded and this means that [52, p. 155]

$$\mathsf{N}\left(U^\dagger\right) = \mathsf{R}(U)^\perp \cap \mathcal{H}_2, \tag{105}$$

$$\mathsf{N}(U) = \mathsf{R}\left(U^\dagger\right)^\perp \cap \mathcal{H}_1, \tag{106}$$

where R denotes the range of an operator and the symbol "$\perp$" denotes the orthogonal complement [52, p. 252]. In the specific case of Eqs. (105) and (106) we have

$$\mathsf{R}(U)^\perp = \left[\psi \in \mathcal{H}_2 \mid (\psi, \widehat{\psi})_u = 0, \quad \forall \widehat{\psi} \in \mathsf{R}(U)\right],$$

$$\mathsf{R}\left(U^\dagger\right)^\perp = \left[\phi \in \mathcal{H}_1 \mid \{\phi, \widehat{\phi}\}_u = 0, \quad \forall \widehat{\phi} \in \mathsf{R}\left(U^\dagger\right)\right].$$

If we put together Eqs. (103)–(106), we obtain

$$\mathsf{N}\left(UU^\dagger\right) = \mathsf{R}(U)^\perp \cap \mathcal{H}_2, \tag{107}$$

$$\mathsf{N}\left(U^\dagger U\right) = \mathsf{R}\left(U^\dagger\right)^\perp \cap \mathcal{H}_1. \tag{108}$$

Now, if the null spaces (105) and (106) (or, equivalently, (107) and (108)) are *empty* then the spectral families of projectors (P_h, Q_h) obtained from the eigenvalue problems (38)–(39) or from the dispersion relations

$$UQ_h = \lambda_h P_h, \tag{109}$$

$$U^\dagger P_h = \lambda_h Q_h, \tag{110}$$

are sufficient for a complete representation of *any* $\mathcal{H}$-functional of the random field. On the contrary, if the null spaces (105) and (106) are not empty then we need to include the projections (P_0, Q_0) onto such nulls paces in order to complete the representation. We remark that it is often not an easy task to identify the null space of an operator and therefore the practical implementation of the completeness arguments just discussed may be not straightforward.

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