Real-Time Reduced-Order Modeling of Stochastic Partial Differential Equations via Time-Dependent Subspaces

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Abstract
We present a new methodology for the real-time reduced-order modeling of stochastic partial differential equations called the dynamically/bi-orthonormal (DBO) decomposition. In this method, the stochastic fields are approximated by a low-rank decomposition to spatial and stochastic subspaces. Each of these subspaces is represented by a set of orthonormal time-dependent modes. We derive exact evolution equations of these time-dependent modes and the evolution of the factorization of the reduced covariance matrix. We show that DBO is equivalent to the dynamically orthogonal (DO) \cite{1} and bi-orthogonal (BO) \cite{2} decompositions via linear and invertible transformation matrices that connect DBO to DO and BO. However, DBO shows several improvements compared to DO and BO: (i) DBO performs better than DO and BO for cases with ill-conditioned covariance matrix; (ii) In contrast to BO, the issue of eigenvalue crossing is not present in the DBO formulation; (iii) In contrast to DO, the stochastic modes are orthonormal, which leads to more accurate representation of the stochastic subspace. We study the convergence properties of the method and compare it to the DO and BO methods. For demonstration, we consider three cases: (i) stochastic linear advection equation, (ii) stochastic Burgers’ equation, and (iii) stochastic incompressible flow over a bump in a channel. Overall we observe improvements in the numerical accuracy of DBO compared against DO and BO.

Keywords: Uncertainty quantification, stochastic partial differential equation, reduced order model, time-dependent subspaces

1. Introduction
The pressing need of conducting verification and validation (V&V) for realistic simulations in scientific and engineering applications requires propagating uncertainty in these systems. These systems are often subject to uncertainty that may come from imperfectly known parameters — that can be modeled as random parameters — or random initial/boundary conditions, or by systems that are characterized by inherent stochastic dynamics, such as coarse grain models of multi-scale systems, in which the effects of unresolved scales are modeled as stochastic processes \cite{3}. Uncertainty quantification (UQ) in such systems can disentangle the effects of different uncertain sources on the quantities of interest and it can guide the decision making process and ultimately lead to more reliable predictions and designs.

One of the fundamental challenges in performing UQ in complex engineering and scientific systems is the computational cost associated with this task. These systems are often characterized by high-dimensional ordinary/partial differential equations, whose forward simulation can be computationally costly. There are a large number of techniques for performing UQ. These methods are primarily either sample based such as Monte Carlo (MC) method and its variants such as multi-level MC and quasi-MC (QMC) \cite{4–6}, or are based on polynomial chaos expansion (PCE) \cite{7–17}.

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While PCE performs well for nearly elliptic problems or flow at low Reynolds numbers, solving highly transient stochastic ordinary/partial differential equations (SODE/SPDE) is particularly challenging for this method. It was shown in [18] that for the one dimensional advection equation with a uniform random transport velocity the order of polynomial chaos must increase with time to maintain the error below a given value. PCE also loses its efficiency for nonlinear systems with intermittency and positive Lyapunov exponents [19].

Reduced order modeling approaches are popular tools for state prediction and control of deterministic evolutionary dynamical systems [20–27]. With the recent developments in data-fusion and specifically multi-fidelity modeling approaches [28–30], in which imperfect predictions can be effectively utilized when combined with high-fidelity data, reduced order modeling techniques will play a crucial role as a surrogate model that generates low-fidelity data at a low computational cost. In the context of SPDEs, the dynamically orthogonal decomposition (DO) was introduced [1] as a stochastic reduced order modeling technique, in which the stochastic field \( u(x, t; \omega) \) is approximated as:

\[
u(x, t; \omega) = \bar{u}(x, t) + \sum_{i=1}^{r} u_i(x, t)y_i(t; \omega),\]

where \( \bar{u}(x, t) \) is the mean, \( u_i(x, t) \) are a set of deterministic time-dependent orthonormal modes in the spatial domain and \( y_i(t; \omega) \) are zero-mean random processes in the stochastic domain and \( r \) is the reduction order. To remove the redundancy in time, the evolution of the spatial subspace, i.e. \( \partial u_i(x, t)/\partial t \), is chosen to be orthogonal to \( u_j(x, t) \). By enforcing the above constraints, one can derive closed-form evolution equations for \( \bar{u}(x, t) \), \( u_i(x, t) \) and \( y_i(t; \omega) \). The imposed conditions on the above decomposition are not unique. Bi-orthogonal (BO) decomposition is one such variant, in which the spatial basis are orthogonal and the stochastic basis are orthonormal [31]. Recently, a non-intrusive DO formulation was introduced [32] and it was shown that the DO evolution equations are the optimality conditions of a variational principle that seeks to minimize the distance between the rate of change of full-dimensional dynamics and that of the DO reduction. For linear parabolic SPDEs, the difference between the approximation error of \( r \)-term DO decomposition and \( r \)-term Karhunen-Loève (KL) decomposition can be bounded [33]. Independently and prior to the development of DO/BO, the idea of using time-dependent basis had been introduced in very different fields, namely chemistry and quantum mechanics for the approximation of the deterministic Schrödinger equations by the Multi Configuration Time Dependent Hartree (MCTDH) method [34, 35], and in deterministic settings [36].

It was shown in [37] that both DO and BO are equivalent: in both of these methods \( u_i(x, t) \) and \( y_i(t; \omega) \) span the same subspace and a linear invertible time-dependent matrix transforms one to the other. This matrix transformation amounts to an in-subspace rotation and stretching for \( u_i(x, t) \) modes and \( y_i(t; \omega) \) coefficients. In contrast to PCE, BO/DO decompositions allow the stochastic coefficients evolve with time as opposed to time-invariant polynomial chaos basis. This relaxation allows BO/DO decompositions to “follow” the transient dynamics. It was shown that in the limit of zero variance of \( y_i(t; \omega) \), the subspace of \( u_i(x, t) \) converges exponentially fast to the most unstable subspace of the dynamical system — associated with the \( r \) most dominant eigendirections of the Cauchy–Green tensor [38]. It was shown that the reduction based on the time-dependent basis and coefficients can capture the low-dimensional structure of the intermittent dynamics [39].

Although both DO and BO are mathematically equivalent, they exhibit different numerical performance. When the eigenvalues of the reduced covariance matrix are close or cross each other, the BO formulation becomes numerically unstable. On the other hand, the DO decomposition does not have the issue of eigenvalue crossing. However, when the eigenvalues of the reduced covariance matrix are not close, BO exhibits better numerical performance than DO [37]. This is mainly attributed to the orthonormality of \( y_i(t; \omega) \) coefficients in the BO formulation, which maintains a well-conditioned representation of the stochastic subspace at all times. However, in the DO decomposition, the stochastic coefficients \( y_i(t; \omega) \) could be highly correlated. This has inspired a hybrid DO/BO method where BO is the dominant solver, but near the eigenvalue crossing the solver switches to DO [40].
Both DO and BO decompositions perform poorly when the covariance matrix is singular or near singular. In the case of DO, the covariance matrix is full, while in the case of BO the covariance matrix is diagonal. In DO the inverse of the covariance matrix is required for the evolution of the spatial basis and in BO the inverse of the diagonal covariance matrix are needed for the evolution of the stochastic basis. The issue of singular covariance matrix can commonly occur in DO/BO decompositions, since one has to resolve the stochastic system up to a small threshold eigenvalue. This necessitates adaptive DO/BO where modes are added and removed at the threshold eigenvalue \[37\]. This issue has motivated using pseudo-inverse of the covariance matrix \[40\], where the eigenvalue of the singular or near-singular mode below a threshold value is replaced with a minimum tolerable value. This approach trades the stability of the DO/BO systems with introducing errors in the system of the order of the minimum tolerable value.

The motivation for this paper is to introduce a new decomposition that resolves the aforementioned challenges in using DO and BO. To this end, we present a new methodology in which: (i) the spatial and stochastic bases are represented by a set of time-dependent orthonormal modes; (ii) an additional equation for the evolution of a factorization of the covariance is derived; and (iii) the condition number of the decomposition is reduced to \[\sqrt{\lambda_{\text{max}}(t)/\lambda_{\text{min}}(t)}\], where \(\lambda_{\text{min}}(t)\) and \(\lambda_{\text{max}}(t)\) are the minimum and maximum eigenvalues of the covariance matrix, respectively.

The structure of the paper is as follows: In Section 2, we review the formulation of the DBO representation, its evolution equations and prove the equivalence of this method to the DO and BO methods. In Section 3, we compare the performance of the presented method with DO and BO via several benchmark problems: (i) Stochastic linear advection equation (ii) Stochastic Burgers’ equation; and (iii) 2D stochastic incompressible Navier-Stokes equation for flow over a bump. In Section 4, a brief summary of the present work is presented.

2. Methodology

2.1. Definitions and Notation

We denote a random vector field by \(u(x, t; \omega)\), where \(x \in D\) is the spatial coordinate in the physical domain \(D \subset \mathbb{R}^d\), where \(d=1,2\) or \(3\), and \(t > 0\) is time and \(\omega \in \Omega\) is the random event in the sample space \(\Omega\). The inner product in the spatial domain between two random fields \(u(x, t; \omega)\) and \(v(x, t; \omega)\) is then defined as:

\[
\langle u(x, t; \omega), v(x, t; \omega) \rangle = \int_D u(x, t; \omega)v(x, t; \omega)dx,
\]

and the \(L_2\) norm induced by the above inner product is:

\[
\|u(x, t; \omega)\|_2 = \left(\langle u(x, t; \omega), u(x, t; \omega) \rangle\right)^{1/2}.
\]

The expectation of the random field is defined as:

\[
\bar{u}(x, t) = \mathbb{E}[u(x, t, \omega)] = \int_{\Omega} u(x, t; \omega)\rho(\omega) d\omega,
\]

where \(\rho(\omega)\) is the probability density function. The inner product in the random space is defined as the correlation between two random fields:

\[
\mathbb{E}[u(x, t; \omega)v(x, t; \omega)] = \int_{\Omega} u(x, t; \omega)v(x, t; \omega)\rho(\omega) d\omega.
\]

The covariance operator between two random fields at time \(t\) is then obtained from:

\[
C(x, x', t) = \mathbb{E}[(u(x, t; \omega) - \bar{u}(x, t))(v(x', t; \omega) - \bar{v}(x', t))].
\]

We introduce the \textit{quasimatrix} notation as defined in \[41\], in which one of the dimensions is discrete as usual but the other dimension is continuous:

\[
U(x, t) = [u_1(x, t) \mid u_2(x, t) \mid \cdots \mid u_r(x, t)],
\]
\[ Y(t; \omega) = \begin{bmatrix} y_1(t; \omega) & y_2(t; \omega) & \cdots & y_r(t; \omega) \end{bmatrix}, \]

where \(U(x, t)\) and \(Y(t; \omega)\) are quasimatrices of size \(\infty \times r\). The inner product for two quasimatrices \(U(x, t) = \begin{bmatrix} u_1(x, t) & u_2(x, t) & \cdots & u_r(x, t) \end{bmatrix}\) and \(V(x, t) = \begin{bmatrix} v_1(x, t) & v_2(x, t) & \cdots & v_r(x, t) \end{bmatrix}\) is defined by a matrix \(A\) such that,

\[ A = \langle U(x, t), V(x, t) \rangle, \]

where

\[ A_{ij} = \langle u_i(x, t), v_j(x, t) \rangle, \quad i = 1, 2, \ldots, r_1, \quad j = 1, 2, \ldots, r_2. \quad (1) \]

\(A\) is a matrix of dimensions \(r_1 \times r_2\). In general, for the case of \(r_1 = r_2\), matrix \(A\) is not symmetric.

2.2. System of stochastic PDEs

We consider the following stochastic partial differential equation (SPDE), which defines the system evolution:

\[ \frac{\partial u(x, t; \omega)}{\partial t} = \mathcal{F}(u(x, t; \omega)), \quad x \in D, \omega \in \Omega, \quad (2a) \]
\[ u(x, t_0; \omega) = u_0(x; \omega), \quad x \in D, \omega \in \Omega, \quad (2b) \]
\[ \mathcal{B}(u(x, t; \omega)) = h(x, t), \quad x \in \partial D, \quad (2c) \]

where \(\mathcal{F}\) is, in general, a non-linear differential operator, and \(\mathcal{B}\) is, in general, a linear differential operator, and \(\partial D\) denotes the boundary of the domain \(D\). In this work we consider deterministic boundary conditions. For an algorithm to treat random boundary conditions for time-dependent subspaces, see reference [42].

2.3. Dynamically bi-orthonormal decomposition

We consider the following decomposition,

\[ u(x, t; \omega) = \bar{u}(x, t) + \sum_{j=1}^{r} \sum_{i=1}^{r} u_i(x, t) \Sigma_{ij}(t) y_j(\omega, t) + e(x, t; \omega), \quad (3) \]

which is referred to as the dynamically bi-orthonormal (DBO) decomposition. In the above expression \(u_i(x, t), i = 1, 2, \ldots, r\) are a set of orthonormal spatial modes:

\[ \langle u_i(x, t), u_j(x, t) \rangle = \delta_{ij}, \]

and they constitute the spatial basis for the DBO decomposition, and \(y_i(\omega, t), i = 1, 2, \ldots, r\) are a set of orthonormal stochastic modes:

\[ \mathbb{E}[y_i(t; \omega) y_j(t; \omega)] = \delta_{ij}, \]

that have zero mean i.e., \(\mathbb{E}[y_i(t; \omega)] = 0, i = 1, 2, \ldots, r\), and \(e(x, t; \omega)\) is the reduction error. Moreover, both the spatial and stochastic coefficients are dynamically orthogonal i.e., the rate of change of these subspaces is orthogonal to the space spanned by these modes:

\[ \frac{\partial U(x, t)}{\partial t} \perp U(x, t) \iff \left\langle \frac{\partial u_i(x, t)}{\partial t}, u_j(x, t) \right\rangle = 0 \quad i, j = 1, \ldots, r, \quad (4) \]
\[ \frac{dY(t; \omega)}{dt} \perp Y(t; \omega) \iff \mathbb{E} \left[ \frac{dy_i(t; \omega)}{dt} y_j(t; \omega) \right] = 0 \quad i, j = 1, \ldots, r. \quad (5) \]

If the spatial and stochastic modes are orthonormal at \(t = 0\), imposing the above constraints ensures the orthonormality of the two bases for all time since:

\[ \frac{d}{dt} \langle u_i(x, t), u_j(x, t) \rangle = \left\langle \frac{\partial u_i(x, t)}{\partial t}, u_j(x, t) \right\rangle + \left\langle u_j(x, t), \frac{\partial u_i(x, t)}{\partial t} \right\rangle = 0 \quad i, j = 1, \ldots, r. \quad (6) \]
The associated boundary conditions are given by:

\[ \mathcal{B}[\pi(x, t)] = h(x, t), \quad x \in \partial D, \quad (12a) \]
\[ \mathcal{B}[u(x, t)] = 0, \quad x \in \partial D. \quad (12b) \]

The proof for the above theorem is given in Appendix A.

We show in Section 2.7, that imposing the above constraints leads to a unique decomposition. The covariance operator is approximated from the DBO decomposition as in the following:

\[ C(x, x', t) = \mathbb{E}[u_i(x, t)\Sigma_{ij}(t)y_j(t; \omega)u_m(x', t)\Sigma_{mn}(t)y_n(t; \omega)] \]
\[ = u_i(x, t)u_m(x', t)\Sigma_{ij}(t)\Sigma_{mn}(t)\mathbb{E}[y_j(t; \omega)y_n(t; \omega)] \]
\[ = u_i(x, t)u_m(x', t)\Sigma_{ij}(t)\Sigma_{mn}(t)\delta_{jn} \]
\[ = u_i(x, t)u_m(x', t)\Sigma_{ij}(t)\Sigma_{mj}(t), \quad (8) \]

where we have used the orthonormality condition imposed on the stochastic basis. The matrix \( \Sigma(t) \in \mathbb{R}^{r \times r} \) is a factorization of the reduced covariance matrix \( C(t) \in \mathbb{R}^{r \times r} \) as in the following:

\[ C(t) = \Sigma(t)\Sigma(t)^T, \quad (9) \]

and it is related to the covariance matrix in the full-dimensional space with:

\[ C(x, x', t) = U(x, t)C(t)U^T(x', t). \quad (10) \]

2.4. DBO field equations

In this section we present closed-form evolution equations for \( \tilde{u}(x, t), \Sigma(t), Y(t; \omega) \) and \( U(x, t) \) for the DBO decomposition.

**Theorem 2.1.** Let Eq. (3) represent the DBO decomposition of the solution of SPDE given by Eq. (2). Then, under the assumptions of the DBO decomposition, the closed-form evolution equations for the mean, covariance factorization, stochastic and spatial bases are expressed by:

\[ \frac{\partial \tilde{u}(x, t)}{\partial t} = \mathbb{E}[\mathcal{F}(u(x, t; \omega))], \quad (11a) \]
\[ \frac{d\Sigma_{ij}(t)}{dt} = \left\langle u_i(x, t), \mathbb{E}[\tilde{\mathcal{F}}(u(x, t; \omega))y_j(t; \omega)] \right\rangle, \quad (11b) \]
\[ \frac{dy_i(t; \omega)}{dt} = \left[ \left\langle u_j(x, t), \tilde{\mathcal{F}}(u(x, t; \omega)) \right\rangle - \left\langle u_j(x, t), \mathbb{E}[\tilde{\mathcal{F}}(u(x, t; \omega))y_k(t; \omega)] \right\rangle y_k(t; \omega) \right] \Sigma_{ji}(t)^{-1}, \quad (11c) \]
\[ \frac{\partial u_i(x, t)}{\partial t} = \left[ \mathbb{E}[\tilde{\mathcal{F}}(u(x, t; \omega))y_j(t; \omega)] - u_k(x, t) \left\langle u_k(x, t), \mathbb{E}[\tilde{\mathcal{F}}(u(x, t; \omega))y_j(t; \omega)] \right\rangle \right] \Sigma_{ij}(t)^{-1}, \quad (11d) \]

where \( \tilde{\mathcal{F}}(u(x, t; \omega)) \) is a mean-subtracted quantity

\[ \tilde{\mathcal{F}}(u(x, t; \omega)) = \mathcal{F}(u(x, t; \omega)) - \mathbb{E}[\mathcal{F}(u(x, t; \omega))]. \]
2.5. Equivalence of DO, BO and DBO methods

Two decompositions are equivalent if they represent the same random fields for all times. The spatial subspaces of two equivalent decompositions are identical and therefore, one can find invertible transformation matrices that maps one subspace to the other. This amounts to an in-subspace rotation. The same is true for stochastic subspaces of two equivalent decompositions. The equivalence of DO and BO was first shown in [37]. In this section, we show that DBO is equivalent to DO and BO. We first show that DBO is equivalent to DO and BO and then derive the equivalence relations.

Lemma 2.1. Let DO and DBO be equivalent via the transformations: \( U_{DO} = U_{DBO} R_u \) and \( Y_{DO} = Y_{DBO} W_y \), where \( R_u \in \mathbb{R}^{r \times r} \) and \( W_y \in \mathbb{R}^{r \times r} \). Then: (i) \( R_u \) is an orthogonal matrix (ii) \( W_y = \Sigma_{DBO}^T R_u \), and (iii) \( \frac{dR_u}{dt} = 0 \).

The proof for Lemma (2.1) is given in Appendix B.

Theorem 2.2. Let \( U_{DO}(x,t), Y_{DO}(t;\omega) \) represent the DO decomposition of SPDE in Eq.(2) and let \( U_{DBO}(x,t), \Sigma_{DBO}(t) \) and \( Y_{DBO}(t;\omega) \) represent its DBO decomposition. Suppose that at \( t = 0 \) the two bases are equivalent i.e., \( U_{DO}(x,t_0) = U_{DBO}(x,t_0) R_u(t_0) \) and \( Y_{DO}(t_0;\omega) = Y_{DBO}(t_0;\omega) W_y(t_0) \). Then the two subspaces remain equivalent for all \( t > 0 \).

The proof for Theorem (2.2) is given in Appendix B.

Lemma 2.2. Let BO and DBO be equivalent via the transformations: \( U_{BO} = U_{DBO} W_u \) and \( Y_{BO} = Y_{DBO} R_y \), where \( R_u \in \mathbb{R}^{r \times r} \) and \( W_y \in \mathbb{R}^{r \times r} \). Then: (i) \( R_u \) is an orthogonal matrix (ii) \( W_u = \Sigma_{DBO} R_y \) (iii) \( \frac{dR_u}{dt} = 0 \).

The proof for Lemma (2.2) is given in Appendix C.

Theorem 2.3. Let \( U_{BO}(x,t), Y_{BO}(t;\omega) \) represent the BO decomposition of SPDE in Eq.(2) and let \( U_{DBO}(x,t), \Sigma_{DBO}(t) \) and \( Y_{DBO}(t;\omega) \) represent its DBO decomposition. Suppose that at \( t = 0 \) the two bases are equivalent i.e., \( U_{BO}(x,t_0) = U_{DBO}(x,t_0) W_u(t_0) \) and \( Y_{BO}(t_0;\omega) = Y_{DBO}(t_0;\omega) R_y(t_0) \). Then the two subspaces remain equivalent for all \( t > 0 \).

The proof for Theorem (2.3) is given in Appendix C.

In Fig.(1) we summarize the equivalence relations between DBO, DO and BO. The equivalence relations between BO and DO are taken from [37].

2.6. Mode ranking

In this section, we determine the ranking of the modes in the stochastic and spatial subspace of DBO as performed in [32]. In all the subsequent numerical examples, without the loss of generality, we consider the rotation matrices i.e., \( R_u \) and \( R_y \) to be identity matrices. The spatial DBO modes are ranked in the direction of the most energetic modes i.e., the modes are ranked based on the variance captured by each mode. To this end, we perform eigenvalue decomposition of the covariance matrix \( C_{DBO}(t) = \Sigma_{DBO}(t) \Sigma_{DBO}(t)^T \) given by:

\[
C_{DBO}(t) \Psi_{DBO}(t) = \Psi_{DBO}(t) \Lambda(t),
\]

where \( \Psi(t) \) are the eigenvectors and \( \Lambda(t) \) is a diagonal matrix of the eigenvalues of the covariance matrix. The eigenvalues are ranked such that \( \lambda_1(t) \geq \lambda_2(t) \geq \cdots \geq \lambda_r(t) \). The ranked DBO modes based on the variance i.e., \( \lambda_i(t) \), are obtained by an in-subspace rotation along the direction of the eigenvectors of the \( C_{DBO}(t) \) matrix obtained from DBO:

\[
\tilde{U}_{DBO}(t) = U_{DBO}(t) \Psi_{DBO}(t).
\]

For \( R_y = I \), the DBO stochastic modes are ranked in the direction of the most energetic directions.
The constraints imposed on the BO decomposition are as in the following: (i) The first set of leading to a fully determined unique decomposition. (ii) The second set of constraints are imposed by the orthogonality of the spatial coefficients. The total DOF is equal to the number of entries in matrix \( \Lambda \). In this simplification \( \Lambda \) can be considered as a discrete representation of the mean subtracted random field, where \( n \) is the number of discrete points in spatial domain and \( s \) is the number of samples of the random field. In this section, we determine the degrees of freedom and the number of constraints imposed by each decomposition, and we show that in BO, DO and DBO decompositions the total number of constraints is equal to the number of degrees of freedom — leading to unique decompositions. In the following analysis we drop the explicit dependence on \( t \) for brevity.

2.7. Redundancy in time

All three components of the DBO decomposition i.e., \( U(x, t) \), \( Y(x, t) \) and \( \Sigma(t) \) are time dependent. The issue of time redundancy also exists in both BO and DO decompositions. We present a simple but insightful and unifying approach to clarify the constraints and degrees of freedom (DOF) in devising new time-dependent decompositions. For simplicity, we consider a finite-dimensional example. In particular, we consider the full-dimensional decomposition of a time-dependent matrix \( A(t) \in \mathbb{R}^{n \times s} \). In this simplification \( A(t) \) can be considered as a discrete representation of the mean subtracted random field, where \( n \) is the number of discrete points in spatial domain and \( s \) is the number of samples of the random field. In this section, we determine the degrees of freedom and the number of constraints imposed by each decomposition, and we show that in BO, DO and DBO decompositions the total number of constraints is equal to the number of degrees of freedom — leading to unique decompositions. In the following analysis we drop the explicit dependence on \( t \) for brevity.

2.7.1. BO

We first consider the BO decomposition of matrix \( A \) given by: \( A = U Y^T \), where \( U \in \mathbb{R}^{n \times s} \) are the set of orthogonal spatial modes and \( Y \in \mathbb{R}^{n \times s} \) are the set of orthonormal stochastic coefficients. The total DOF is equal to the sum of number of entries in matrix \( U \) i.e., \( n \times s \) and entries in matrix \( Y \) i.e., \( s \times s \). Therefore, the total DOF is given by: \( N_{DOF} = n \times s + s \times s \). The constraints imposed on the BO decomposition are as in the following: (i) The first set of constraints are the compatibility conditions, where \( A_{ij} = U_{ik} Y_{jk} \), which imposes \( N_{c_1} = n \times s \) constraints. (ii) The second set of constraints are imposed by the orthogonality of the spatial modes \( \langle u_i, u_j \rangle = \delta_{ij} \lambda_i \), which impose \( N_{c_2} = s(s - 1)/2 \) independent constraints. We take into account the number of \( \langle u_i, u_j \rangle = 0 \), \( i = 1, 2, \ldots, s \) for \( j < i \). Note that for \( j > i \) the constraints are equivalent to those of \( i < j \), since \( \langle u_i, u_j \rangle = \langle u_j, u_i \rangle \), and therefore they are not independent constraints and thus not counted. (iii) The third set of constraints are imposed by the orthonormality of the stochastic coefficients: \( E[y_i y_j] = \delta_{ij}, i = 1, 2, \ldots, s \) and \( j \leq i \), which imposes \( N_{c_3} = s(s + 1)/2 \) independent constraints. Therefore, for the BO decomposition, the total number of constraints is equal to total DOF, i.e. \( N_{DOF} = N_{c_1} + N_{c_2} + N_{c_3} = n \times s + s \times s \), leading to a fully determined unique decomposition.
2.7.2. DO

The DO decomposition is given by: $A = U Y^T$, where the spatial modes are a set of orthonormal vectors and $Y$ are the stochastic coefficients. The total DOF of DO is the same as that of the BO for the same reasons mentioned above, $N_{DOF} = n \times s + s \times s$. The constraints imposed on the DO decomposition are as in the following: (i) Similar to the BO decomposition, there are $N_{c1} = n \times s$ constraints imposed by the compatibility equations $A_{ij} = U_{ik} Y_{jk}$. (ii) The orthonormality of the spatial modes ($\langle u_i, u_j \rangle = \delta_{ij}$) imposes $N_{c2} = s(s+1)/2$ independent constraints. (iii) The dynamically orthogonal condition $\langle \dot{u}_i, u_j \rangle = 0$, $i = 1, 2, \ldots, s$ and $j < i$ imposes $N_{c3} = s(s-1)/2$ independent constraints. Note that $\langle \dot{u}_i, u_i \rangle = 0$, $i = 1, 2, \ldots, s$ does not impose independent constraints as $\langle u_i, u_i \rangle = 1$ already enforces this condition. This can be seen by taking the time derivative of the orthonormality constraints:

$$\frac{d}{dt} \langle u_i, u_i \rangle = \langle \dot{u}_i, u_i \rangle + \langle u_i, \dot{u}_i \rangle = 2 \langle \dot{u}_i, u_i \rangle = 0.$$

Therefore, similar to BO, the DO decomposition leads to a fully determined decomposition as the total number of DOF and constraints are equal, i.e. $N_{DOF} = N_{c1} + N_{c2} + N_{c3} = n \times s + s \times s$.

2.7.3. DBO

Now, we consider the DBO decomposition, which is given by: $A = U Y^T$, where the spatial modes and stochastic modes are a set of orthonormal bases. The total DOF for DBO is given by the total number of elements in each of the matrices in the decomposition i.e., $n \times s$ entries in $U$ matrix, $s \times s$ entries in the $\Sigma$ matrix and $s \times s$ entries in the $Y$ matrix. Thus, the total DOF is: $N_{DOF} = n \times s + s \times s + s \times s$. The constraints imposed by the DBO decomposition are as in the following: (i) Similar to the BO and DO decompositions, there are $N_{c1} = n \times s$ constraints imposed by the compatibility conditions $A_{ij} = U_{ik} \Sigma_{km} Y_{jm}$. (ii) The orthonormality of stochastic and spatial modes ($\langle u_i, u_j \rangle = \delta_{ij}$ and $E[y_i y_j] = \delta_{ij}$) imposes $s(s+1)/2$ constraints each, which in total imposes $N_{c2} = s(s+1)$. (iii) The dynamically orthogonal constraints for spatial and stochastic modes ($\langle \dot{u}_i, u_j \rangle = 0$ and $E[y_i \dot{y}_j] = 0$) imposes $s(s-1)/2$ constraints each. Thus, the total constraints from the dynamically orthogonal condition are $N_{c3} = s(s-1)$.

The total number of constraints for the DBO decomposition is $n \times s + s(s+1) + s(s-1)$, which is equal to the number of degrees of freedom, and this results in a fully determined DBO decomposition for matrix $A$.

We conclude that to obtain a unique time-dependent decomposition, the number of degrees of freedom and the number of constraints need to be equal. The summary of the constraints and degrees of freedom for BO, DO and DBO are presented in Table 1. Introducing additional degrees of freedom requires additional constraints to keep the system fully determined and thus unique. In the light of the above analysis, DBO allows for $s \times s$ additional degrees of freedom compared to DO by adding the matrix $\Sigma$ to the decomposition. These additional constraints are then utilized to enforce the orthonormality and dynamically orthogonal conditions on the stochastic coefficients $Y$. The orthonormality of $Y$ coefficients in the DBO decomposition cannot be enforced in the DO decomposition. As we will demonstrate this loss of orthonormality of $Y$ in the DO decomposition can lead to degradation of accuracy in highly ill-conditioned problems.

2.8. Error Analysis

In Section 3, we compare the results of the DBO numerical solutions with the analytical solution using the following error calculations. To the end, we compute the $L_2$ norm of the error of the mean ($\epsilon_m(t)$) as in the following:

$$\epsilon_m(t) = \left( \int_D (\bar{u}(x,t) - \bar{u}_{DBO}(x,t))^2 dx \right)^{1/2},$$

where $\bar{u}(x,t)$ represents the mean of the analytical solution and $\bar{u}_{DBO}(x,t)$ represents the mean obtained from the DBO evolution equations. The error of the variance ($\epsilon_v(t)$) is calculated using
the $L_2$-norm in both the spatial and stochastic dimensions:

$$E(x, t; \omega) = u(x, t; \omega) - \bar{u}(x, t) - \sum_{j=1}^{r} \sum_{i=1}^{r} u_{\text{DBO}, i}(x, t) \Sigma_{\text{DBO}, i}(t) y_{\text{DBO}, i}(\omega, t),$$

$$\epsilon_v(t) = \left( \int_D E[E(x, t; \omega)^2] dx \right)^{1/2},$$

where $u(x, t; \omega)$ represents the analytical stochastic field, $\bar{u}(x, t)$ represents the mean of the analytical stochastic flow field, whereas $u_{\text{DBO}, i}(x, t)$, $\Sigma_{\text{DBO}, i}(t)$ and $y_{\text{DBO}, i}(\omega, t)$ represent the solutions of the components of the DBO decomposition obtained from the DBO evolution equations.

### 3. Demonstration cases

#### 3.1. Stochastic linear advection equation

We consider linear advection governed by:

$$\frac{\partial u}{\partial t} + V(\omega) \frac{\partial u}{\partial x} = 0, \quad x \in [0, 2\pi] \quad \text{and} \quad t \in [0, t_f],$$

$$u(x, 0) = \sin(x), \quad x \in [0, 2\pi],$$

with periodic boundary condition. The randomness in the system comes from the advection velocity $V(\omega)$. The random velocity is specified by $V(\omega) = \bar{v} + \sigma \xi(\omega)$, where $\bar{v} = 1.0$, $\sigma = 1.0$ and $\xi(\omega)$ is a uniform random variable in the interval of $\xi \sim U[-1, 1]$ with variance $1/3$. The physical domain is discretized using the Fourier spectral method with $N_s = 512$ Fourier modes. The random space is one dimensional and is discretized with the probabilistic collocation method (PCM) with $N_r = 256$ Legendre-Gauss points. The third-order Runge-Kutta scheme is used for the time integration with $\Delta t = 10^{-3}$. At $t = 0$, the stochastic fluctuations are zero, and therefore, the simulation is initialized at $t = \Delta t$ to avoid singularity of the covariance matrix. The system is numerically evolved till $t_f = 10$. The linear advection Eq.(15) has a closed-form solution as follows:

$$u(x, t; \omega) = g(x - V(\omega)t) = \sin(x - (\bar{v} + \sigma \xi(\omega))t).$$

This system can be expressed exactly with KL modes and the reduction order of $r = 2$ as follows:

$$u(x, t; \omega) = \bar{u}(x, t) + \sum_{i=1}^{r} \sqrt{\lambda_i(t)} u_i(x, t) y_i(t, \omega),$$
where,
\[
\bar{u}(x, t) = \sin(x - \bar{v}t) \frac{\sin(\sigma t)}{\sigma t}, \\
u_1(x, t) = \frac{1}{\sqrt{\pi}} \sin(x - \bar{v}t), \\
u_2(x, t) = -\frac{1}{\sqrt{\pi}} \cos(x - \bar{v}t), \\
y_1(t; \omega) = \frac{\sqrt{\pi}}{\sqrt{\lambda_1(t)}} \left( \cos(\sigma \xi t) - \frac{\sin(\sigma t)}{\sigma t} \right), \\
y_2(t; \omega) = \frac{\sqrt{\pi}}{\sqrt{\lambda_2(t)}} \sin(\sigma \xi t), \\
\lambda_1(t) = 1 - \frac{\sin(2\sigma t)}{2\sigma t}, \\
\lambda_2(t) = 1 + \frac{\sin(2\sigma t)}{2\sigma t} - \frac{2\sin^2(\sigma t)}{(\sigma t)^2}.
\]

The mean, spatial and stochastic bases of the DBO decomposition are initialized with KL modes given above. The covariance factorization is initialized by:
\[
\Sigma(t) = \begin{bmatrix} \sqrt{\lambda_1(t)} & 0 \\ 0 & \sqrt{\lambda_2(t)} \end{bmatrix}.
\]  

In Fig. (2a-2b), the $L_2$ error of the mean and variance for both DO and DBO methods are shown, respectively. Since the solution of this problem can be exactly expressed with two DBO modes, the errors in the mean and variance come from the temporal, spatial and the PCM discretization of the random space. To the end, we present mean and variance errors for two values of $\Delta t = 10^{-3}$ and $2 \times 10^{-4}$, in which the smaller $\Delta t$ shows smaller errors. We also refined the resolution for spatial and random discretizations, and we did not, however, observe noticeable change in the mean and variance errors. This demonstrates that the temporal discretization is the main source of error. For long time integration, the resolution of solving Eq. (11c) must increase in time i.e., higher number of samples of $\xi$, to maintain a desired level of accuracy as increasing time increases the wave number of $y_i(t; \omega)$ modes. However, in the DBO decomposition, the computational cost of increasing resolution in the random space is insignificant, as we solve the stochastic ODE of small order (here $r = 2$) given by Eq. (11c). This is in contrast to the PCM method, in which to maintain the desired level of accuracy the PCE order must increase with time, which results in solving larger system of PDEs. See reference [18] for detailed error analysis of the stochastic linear advection equation using PCM. The BO method for this case would diverge because of eigenvalue crossing. It is clear that both DBO and DO show similar errors as they are equivalent. However, the DBO shows slightly smaller errors in both mean and the variance.
3.2. Stochastic Burgers’ equation with manufactured solution

We consider the stochastic Burgers’ equation governed by:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + f(x, t; \omega), \quad x \in [0, 2\pi] \quad \text{and} \quad t \in [0, t_f]. \tag{18a}
\]

\[
u (x, 0; \omega) = g(x), \quad x \in [0, 2\pi]. \tag{18b}
\]

We consider the following manufactured solution expressed by the KL decomposition with \( r = 2 \) modes:

\[
\bar{u}(x, t) = \sin(x - t),
\]

\[
u_1(x, t) = \frac{1}{\sqrt{\pi}} \cos(x - t), \quad \nu_2(x, t) = \frac{1}{\sqrt{\pi}} \cos(2x - 3t),
\]

\[
\nu_3(t; \omega) = \sin(\pi \xi_1(\omega) - t), \quad \nu_4(t; \omega) = \cos(\pi \xi_2(\omega) - t),
\]

\[
\lambda_1(t) = (4.5 + \sin(t))^2, \quad \lambda_2(t) = \epsilon^2 \cdot (1.5 + \cos(3t))^2.
\]

We initialize the DBO systems with KL modes similar to the previous example. The stochastic forcing \( f(x, t; \omega) \) is calculated accordingly such that the above decomposition satisfies Eq.(18). In the above equation \( \nu = 0.05 \) and \( \xi_d \sim U[-1, 1] \). Here, \( d \) is the dimension of the random space, which for this case is taken to be \( d = 2 \). The parameter \( \epsilon \) scales the smaller eigenvalue i.e., \( \lambda_2(t) \), which in turn controls the condition number of the covariance matrix. The physical domain is considered to be periodic. We discretize the spatial domain using the Fourier spectral method with \( N_s = 128 \) modes. The random space is two-dimensional and is discretized with the ME-PCM (Multi-Element Probabilistic Collocation Method) [8] with 8 elements each containing 4 points in each random direction. Thus, the total points in every random direction is 32, which results in \( N_r = 1024 \). The third-order Runge-Kutta method is used for the time integration with \( \Delta t = 10^{-3} \). Since at \( t = 0 \) the stochasticity is zero, the numerical computation is started from \( t_s = 0.01 \). The system is numerically evolved till \( t_f = 3\pi \).

The purpose of this case is to compare the performance of DO, BO and DBO methods for cases with ill-conditioned covariance matrices. We also compare the performance of DBO with pseudo-inverse DO (PI-DO) [40], where the authors proposed using pseudo inverse in the presence of singular or near-singular covariance matrices. Two values of \( \epsilon \) are considered and the evolution of the system for DO, PI-DO, BO and the DBO methods are studied. We use the \( L_2 \) error for evaluation of the mean and variance errors i.e., Eq.(13) and Eq.(14) between the four methods.

In Fig.(3), the evolution of the eigenvalues, mean and variance error are shown for two values of \( \epsilon = 10^{-3} \) and \( \epsilon = 10^{-5} \). Fig.(3c) and Fig.(3d) show a comparison between the mean errors for \( \epsilon \) values \( 10^{-3} \) and \( 10^{-5} \), respectively. Similarly, Fig.(3e) and Fig.(3f) show the variance error for \( \epsilon \) values \( 10^{-3} \) and \( 10^{-5} \) respectively. The PI-DO case is studied only for the case with \( \epsilon = 10^{-5} \), since for the case with \( \epsilon = 10^{-3} \) the covariance matrix does not become singular. Two threshold values are used for the inversion of the covariance matrix in the PI-DO method: \( \sigma_{th} = 10^{-9} \) and \( \sigma_{th} = 10^{-10} \). See reference [40] for more details on the threshold values. As shown in [40], the choice of the threshold value can play a significant role in the performance of PI-DO. Based on the formulation of the eigenvalues, lower values of \( \epsilon \) creates an ill-conditioned covariance matrix for DO, BO as well as an ill-conditioned \( \Sigma \) matrix for DBO. However, in both DO and BO the condition number of the covariance matrix is \( \kappa_{DO,BO} = \lambda_1(t)/\lambda_2(t) \), which scales with \( 1/\epsilon^2 \), while the condition number of the \( \Sigma \) in the DBO decomposition is \( \kappa_{DBO} = \sqrt{\lambda_1(t)/\lambda_2(t)} \), which scales with \( 1/\epsilon \). Since DO, BO and DBO are equivalent, it is expected that they all perform similarly for the well-condition covariance matrix, i.e., \( \epsilon = 10^{-3} \). This can be seen in Fig.(3a), Fig.(3c) and Fig.(3e), where all three methods exhibit the same levels of error in mean and variance and the eigenvalues of the covariance matrix match well with the true eigenvalues. However, for the case with \( \epsilon = 10^{-5} \), it is expected that DBO performs better than BO and DO and this can be seen in Fig.(3b), Fig.(3d) and Fig.(3f). For this case neither DO, BO nor PI-DO can capture the smallest eigenvalue i.e., \( \lambda_2(t) \) correctly. As a result they introduce error of the order of \( \sqrt{\lambda_2(t)} \sim O(\epsilon) \), which can be observed in Fig.(3d) and Fig.(3f). As seen in Fig.(3d) and Fig.(3f),
the threshold value of $\sigma_{th} = 10^{-9}$ for pseudo-inverse introduces higher order errors than that of the $\sigma_{th} = 10^{-10}$. The pseudo-inverse method introduces $O(\sigma_{th})$ in the simulation whenever the lowest eigenvalue attains a value lower than the threshold $\sigma_{th}$.

We have also investigated the effect of the condition number of the system on the spatial and stochastic modes. In Fig.(4), the two spatial modes and the phase space i.e., $y_1(t;\omega)$ vs. $y_2(t;\omega)$, are shown for four different times: $t = 0, 1, 2, 3$ and $5.2$. At $t = 0$, the spatial modes and stochastic coefficients match well with those of the KL decomposition as shown in Fig.(4a-4c). However, as time progresses to $t = 1.2$ and $t = 3.2$ the ability of the BO, DO, and PI-DO to retain the near-singular mode deteriorate as shown in Fig.(4e-4f) and Fig.(4h-4i). At time $t = 5.2$, BO, DO, and PI-DO completely fail to capture the lowest variance mode. Moreover, for both DO and PI-DO, the inability to accurately resolve the low-variance mode adversely affects first mode. See Fig.(4g) and Fig.(4j).

### 3.3. Burgers’ equation with stochastic forcing

In this section, we consider Burgers’ equation subject to random forcing where a large number of modes are needed to resolve the system accurately due to nonlinear interaction between the modes. We investigate the effect of low eigenvalues on the accuracy of the solution and the effect of long time integration on the solution for both DO and the DBO methods. The governing equation is given by:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + \frac{(1 + \xi)}{2} \sin(2\pi t), \quad x \in [0, 2\pi] \quad \text{and} \quad t \in [0, t_f],
\]

\[
u u(x, 0; \omega) = g(x) \quad x \in [0, 2\pi],
\]

where $\nu = 0.04$ and $\xi \sim \mathcal{U}[-1,1]$ is a one-dimensional uniform random variable and the initial condition is taken to be:

\[
g(x) = 0.5(\exp(\cos(x)) - 1.5) \sin(x + 2\pi \cdot 0.37).
\]

We use the Fourier spectral method for space discretization with $N_x = 128$ Fourier modes, and PCM is used for the discretization of the one-dimensional random space $\xi$. We use $N_r = 64$ Legendre-Gauss collocation points. The third-order Runge-Kutta scheme is used for evolving the discrete systems in time with $\Delta t = 10^{-3}$. At $t = 0$ the system is deterministic, hence the covariance matrix is singular. Therefore, neither DO nor DBO decompositions can be initialized at $t = 0$. To this end, we evolve the stochastic systems up to $t_s = 2$ using PCM and the KL decomposition of the solution at this time is taken as the initial condition. This is in accordance to methodology presented in [43].

This case is used to study two properties of an ill-conditioned system on the overall accuracy of the mean and variance: (i) effect of low eigenvalues resulting in an ill-conditioned covariance matrix, (ii) effect of unresolved modes on long term integration. To study the effect of low eigenvalues we consider two reduction sizes of $r = 7$ and $r = 9$ and the system is evolved till $t_f = 3$. Fig.(5) shows the eigenvalues for this case as extracted from the PCM solution. It is observed that modes 8 and 9 (shown in red) have eigenvalues which are the order of $10^{-15}$, rendering the covariance matrix $C$ highly ill-conditioned. The mean error for reduction sizes $r = 7$ and $r = 9$ can be seen in Fig.(6a-6b), respectively. The variance error is plotted in Fig.(6c-6d). It can be seen that the lower modes affect the accuracy of the solution for DO. The error affects the solution of the higher modes and we observe an increased error for the DO method in case of reduction order $r = 9$. The DBO method, on the other hand, resolves the lower mode accurately without affecting the accuracy of the higher modes. In fact adding additional modes, improves the accuracy of the DBO solution as seen from the variance error plots in Fig.(6d).

The solutions for the long time integration case for the stochastic Burgers’ equation is shown in Fig.(7). Between $t = 2$ and $t = 3$, we observe that the DO has higher error as the lower modes affect the accuracy of the higher modes. This result is same as seen from the previous case Fig.(6). As the lower modes start gaining energy, the error from the unresolved modes dominates the error of the effect of lower modes and hence, we observe that the error for both the DO and the DBO methods is the same as time progresses.
$\epsilon = 10^{-3}$

$\epsilon = 10^{-5}$

Figure 3: Burgers’ equation with manufactured forcing: A comparison between two values of $\epsilon$, which controls the condition number of the system, is shown. The left column: (a), (c) and (e) correspond to the eigenvalues, mean error and variance error for the case with $\epsilon = 10^{-3}$, respectively. The right column: (b), (d) and (f) correspond to the eigenvalues, mean error and variance error for the case with $\epsilon = 10^{-5}$, respectively. It is observed that as the system becomes ill-conditioned for $\epsilon = 10^{-5}$, the errors for the DO, PI-DO and the BO method increase whereas the DBO maintains the same accuracy for both the $\epsilon$ values. The code used in this example is available on GitHub at https://github.com/ppatil1708/DBO.git
Figure 4: Burgers’ equation with manufactured forcing: The two physical modes and the phase space for the stochastic basis are shown at different times as the simulations progresses. The first row shows the modes and phase space at $t = 0.1$. All the methods start from the same initial condition. In the second row, the modes and phase space are shown for $t = 1.2$. The next rows show the system at $t = 3.2$ and $5.2$, respectively. It is observed that the low variance mode is affected first and subsequently as the evolution continues the higher variance mode loses its accuracy as well. The code used in this example is available on GitHub at https://github.com/ppatil1708/DBO.git.
Figure 5: Burgers’ equation with stochastic forcing: Growth in the eigenvalues as the system evolves. The modes shown in red dotted lines are the unresolved modes i.e., modes which are not included in the simulations. These eigenvalues are obtained by performing Karhunen-Loève decomposition on the instantaneous samples.

Figure 6: Burgers’ equation with stochastic forcing (effect of low variance modes on the accuracy of the solution): It is observed that effectively resolving the modes with lower variance improves the numerical accuracy of the solution. The DO method fails to resolve the lower eigenvalues and hence the error for DO is higher than that of the DBO method. The code used in this example is available on GitHub at https://github.com/ppatil1708/DBO.git
Figure 7: Burgers’ equation with stochastic forcing (long time integration effects): The 9 dominant modes are used to resolve the system. The mean error and variance error for DBO and DO as compared with PCM are shown in (a) and (b). It is observed that DBO performs better for short time (i.e., till 4 time units). After 4 time units the lower unresolved modes gain variance and the effect of these unresolved modes dominate the error which is equal for both DO and DBO methods. The code used in this example is available on GitHub at https://github.com/ppatil1708/DBO.git.

3.4. Stochastic incompressible Navier-Stokes: Flow over a bump

In this example, we apply the DO and DBO decompositions to solve stochastic incompressible Navier-Stokes equations. The governing equations are given by:

\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}, \quad (20a)
\]

\[
\nabla \cdot \mathbf{u} = 0. \quad (20b)
\]

where \( \mathbf{u} = (u_x, u_y) \) is the velocity vector field, \( \mathbf{f} = (f_x, f_y) = (1, 0) \) is the forcing and \( p \) is the pressure field. We solve the flow over a bump in a channel as shown in Fig.(8a), where flow is from left to right. Periodic boundary condition is imposed in the streamwise direction and no-slip boundary condition is imposed at the bottom and top walls. We consider \( \nu = 0.04 \) and \( \rho = 1 \) and the Reynolds number is based on the channel height and time-averaged centerline horizontal velocity which is roughly equal to \( Re = 1500 \). For these parameters the flow is not chaotic, but it is time dependent due to constant shedding of separated region behind the bump. The stochasticity is introduced in the flow via random initial conditions given by the following equation:

\[
\mathbf{u}(x, y, 0; \omega) = \mathbf{u}_0(x, y) + \sum_{i=1}^{d} \sigma \xi_i(\omega) \Phi_i(x, y), \quad (21)
\]

where \( \mathbf{u}_0(x, y) \) is the solution of a deterministic simulation at \( t = 50 \). The deterministic solution at this time has reached the statistically steady state. In the above initial condition \( \Phi_i = (\Phi_{x_i}, \Phi_{y_i}) \) are the Proper Orthogonal Decomposition (POD) modes obtained from the deterministic simulation of the flow over a bump at \( Re = 1500 \). We consider \( d = 2 \) and the \( \Phi_y \) component of the two corresponding POD modes are shown in Fig.(8b-8c). For the spatial discretization of the mean flow and the spatial basis, we use spectral/hp element method with quadrilateral elements for \( N_e = 1451 \) and polynomial order 5. The spectral element mesh is shown in Fig.(8a). A first-order time-splitting scheme is used for the evolution of mean and the spatial basis, in which the nonlinear terms are treated explicitly and the diffusion terms are treated implicitly. The time-integration step of \( \Delta t = 10^{-4} \) is used. The random space is two-dimensional and discretization of the stochastic coefficients in the random space is performed using ME-PCM with 4 elements in each random direction and 4 quadrature points in each element. Therefore,
the total number of quadrature points in every direction of the random space is 16 and hence, the total number of quadrature points in the two dimensional random space is \( N_r = 16^2 = 256 \). We solved both DO and DBO systems with identical discretization schemes as described above till \( t_f = 5 \), which amounts to 20 flow through periods.

To compare the performance of DO and DBO we performed simulations for two reduction sizes: \( r = 2 \) and \( r = 3 \). For the reference solution, we performed 256 non-intrusive direct numerical simulation (DNS) at the same ME-PCM quadrature points. We then performed KL decomposition of the 256 sample at each time step. The eigenvalues of the covariance matrix of DO, DBO for the case of \( r = 2 \) and the two largest KL eigenvalues are shown in Fig.(9a). It is clear that both methods perform well and match the two most energetic KL modes, although the eigenvalues of DBO are more accurate than that of the DO.

In the case of \( r = 3 \), the eigenvalue associated with the third mode has very small values. In fact at \( t = 0 \) the third eigenvalue is zero. This eigenvalue gradually grows due to nonlinearity of Navier-Stokes equations. To avoid an exact singularity, the DO and DBO simulations for \( r = 3 \) are initialized at \( t = 1 \) from the solution of the corresponding KL decomposition. The system is ill-conditioned for \( r = 3 \) due to the low variance of the third mode. At \( t = 1 \), the third eigenvalue is roughly equal to \( 10^{-10} \) as shown in Fig.(9b). The third eigenvalue of the DO decomposition deviates from the truth due to the near singularity and it eventually leads to the divergence of the DO system, while DBO performs accurately and all three eigenvalues match those of the KL.

Fig.(10) shows evolution of the \( u_y \) of the mean and three dominant spatial modes of the DBO and KL system at \( t = 1, 2 \) and 3. By visual comparison we can observe that the KL and DBO modes are similar at every time step. Mode 1 and 2 of the system are the POD modes we have used as an initialization for the stochastic random conditions, convected through the channel by the mean velocity, \( \bar{u}_x(x, y, t) \) of the flow. It is necessary to consider the lower eigenvalues into the flow field as we observe that over time the lower eigenvalues can gain energy and alter the system dynamics.

4. Summary

In this paper, we present a new real-time reduced order modeling methodology called the \textit{dynamically bi-orthonormal} (DBO) decomposition for solving stochastic partial differential equations. The presented method approximates a random field by decomposing it to a set of time-dependent orthonormal spatial basis, a set of time-dependent orthonormal stochastic basis and a low-rank factorization of the covariance matrix. We derived closed form evolution equations for above components of the decomposition as well as the time-dependent mean field.

We show that the presented method is equivalent to the dynamically orthogonal and bi-orthonormal decompositions via an invertible matrix transformation. We derive evolution equation for these transformation matrices. Although DBO is equivalent to both DO and BO decompositions, it exhibits superior numerical performance especially in highly ill-conditioned systems. In both BO and DO decompositions, the condition number of covariance matrix,
whether diagonal (BO) or full (DO), is \( \lambda_{\text{max}}(t)/\lambda_{\text{min}}(t) \), where \( \lambda_{\text{min}}(t) \) and \( \lambda_{\text{max}}(t) \) are the smallest and largest eigenvalues of the covariance matrix, respectively. However, in the DBO decomposition, a factorization of the covariance matrix \( \Sigma(t) \) is inverted, and \( \Sigma(t) \) has the condition number of \( \sqrt{\lambda_{\text{max}}(t)/\lambda_{\text{min}}(t)} \). The improvement in the condition number of the DBO systems compared with BO or DO is important for adaptive reduced order modeling as the newly added or removed mode has very small eigenvalues. The DBO decomposition tolerates significantly smaller eigenvalues compared to BO and DO without degrading the accuracy. Moreover, in comparison with BO, DBO does not become singular in the case of eigenvalue crossing, and in comparison with DO, the DBO stochastic coefficients are orthonormal, resulting in better-conditioned representation of the stochastic subspace compared to that of DO.

We demonstrated the DBO decomposition for several benchmark SPDEs: (i) linear advection equation (ii) Burgers’ equation with manufactured solution, (iii) and Burgers’ equation with random initial condition. We also applied DBO to stochastic incompressible Navier-Stokes equation. We compared the performance of DBO against BO and DO. We conclude that for well-conditioned cases, the numerical accuracy of all three decompositions are similar. However, for ill-conditioned systems, where BO and DO either diverge or show poor numerical performance, the DBO decomposition performs well.

We conclude by showing a limitation of the presented method. In particular we revisit the demonstration case for stochastic Navier-Stokes equation as presented in Section 3.4. We consider the same problem setup as the previous case of Reynolds number 1500 except that the kinematic viscosity is chosen to be \( \nu = 0.015 \) which changes the Reynolds number to \( Re = 5000 \). For this Reynolds number the flow is chaotic. To ensure that the flow is chaotic, we solved three deterministic cases by perturbing the horizontal forcing with three values \( f_x = 1 - \epsilon, 1 \) and \( 1 + \epsilon \) with \( \epsilon = 10^{-3} \). The resulting shear viscous force in the \( x \)-direction on the top and bottom walls is plotted in Fig.(11a). It is clear that difference between the three solutions due to the perturbation grows and after \( t > 116 \) becomes \( O(1) \) – verifying that the flow is chaotic. We consider DBO reduction with \( r = 2 \). The eigenvalues of the covariance of the DBO system and those of the KL decomposition are plotted in Fig.(11b). We observe that for the chaotic regime a fast decay of the eigenvalues is not observed, since the randomness in the initial condition quickly propagates on large number of independent dimensions in the phase space of the dynamical system due to strong non-linear interaction between the modes and fast growth of small perturbations. As a result, the effect of unresolved modes must be accounted for.
Figure 10: Flow over a bump in a channel flow: The spatial modes of DBO and KL for the stochastic flow in a channel with bump are visualized for comparison in the figure above. Column 1: The $\bar{u}_y(x, t)$ for different time instants. Column 2, 3 & 4: The three dominant spatial modes for the DBO and KL simulation. Rows 1 and 2 correspond to the DBO and KL spatial modes for $t = 1$ respectively. Rows 3 and 4 correspond to the DBO and KL spatial modes at $t = 2$ respectively. Finally, rows 5 and 6 correspond to the DBO and KL spatial modes at $t = 3$ respectively.
Figure 11: Dynamically bi-orthonormal decomposition for flow over a bump in a channel in chaotic regime: (a) The growth of the small perturbations in the forcing measured by the horizontal viscous shear force on the walls. The signals are observed to completely diverge after $t = 116$. (b) The growth in the eigenvalues of the DBO system with $r = 2$ and the eigenvalues of the Karhunen-Loève decomposition.

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A. Derivation of the DBO evolution equations

A.1. Proof of Theorem(2.1)

For the sake of brevity in notation, we denote $\pi(x,t)$ as $\pi$, $u_i(x,t)$ as $u_i$, $y_i(t;\omega)$ as $y_i$ and $\Sigma_{ij}(t)$ as $\Sigma_{ij}$. The complete stochastic field given by $u(x,t;\omega)$, will be denoted as $u$. To obtain the evolution equations of each of the DBO components, we first substitute the DBO decomposition, given by Eq.(3), into a general form of SPDE as given by Eq.(2a). This follows:

$$\frac{\partial \pi}{\partial t} + \frac{\partial u_i}{\partial t} \Sigma_{ij} y_j + u_i \frac{d \Sigma_{ij}}{dt} y_j + u_i \Sigma_{ij} \frac{dy_j}{dt} = \mathcal{F}(u)$$

(22)

We take expectation of the above equation:

$$\frac{\partial \pi}{\partial t} = \mathbb{E}[\mathcal{F}(u)],$$

(23)

where we have used $\mathbb{E}[y_i] = 0$ and $d\mathbb{E}[y_i]/dt = 0$. The above equation denotes the evolution of the mean field, which is given by the first equation in the theorem i.e, Eq.(11a). We proceed further by obtaining a mean subtracted form of the original SPDE, by subtracting the above mean evolution equation from Eq.(22). This follows:

$$\frac{\partial u_i}{\partial t} \Sigma_{ij} y_j + u_i \frac{d \Sigma_{ij}}{dt} y_j + u_i \Sigma_{ij} \frac{dy_j}{dt} = \tilde{\mathcal{F}}(u),$$

(24)

where $\tilde{\mathcal{F}}(u) = \mathcal{F}(u) - \mathbb{E}[\mathcal{F}(u)]$. We then project the mean-subtracted equation onto the stochastic modes $y_k$,

$$\frac{\partial u_i}{\partial t} \Sigma_{ij} \mathbb{E}[y_j y_k] + u_i \frac{d \Sigma_{ij}}{dt} \mathbb{E}[y_j y_k] + u_i \Sigma_{ij} \mathbb{E}[\frac{dy_j}{dt} y_k] = \mathbb{E}[\tilde{\mathcal{F}}(u) y_k].$$
The stochastic modes are orthonormal i.e., \( E[y_j y_k] = \delta_{jk} \) and dynamically orthogonal i.e., \( E[\frac{dy_j}{dt} y_k] = 0 \). Using these two conditions and changing index \( k \) to \( j \), the above equation simplifies to:

\[
\frac{\partial u_i}{\partial t} \Sigma_{ij} + u_i \frac{d\Sigma_{ij}}{dt} = E[\hat{F}(u) y_j].
\] (25)

We now project the above equation onto the spatial modes \( u_k \),

\[
\left\langle u_k, \frac{\partial u_i}{\partial t} \right\rangle \Sigma_{ij} + \left\langle u_k, u_i \right\rangle \frac{d\Sigma_{ij}}{dt} = \left\langle u_k, E[\hat{F}(u) y_j] \right\rangle.
\]

By enforcing the orthonormality property i.e., \( \left\langle u_k, u_i \right\rangle = \delta_{ki} \) and the dynamical orthogonality property i.e., \( \left\langle \frac{\partial u_k}{\partial t}, u_i \right\rangle = 0 \) of the spatial basis, we obtain the evolution equation of the \( \Sigma_{ij} \) corresponding to Eq.(11b):

\[
\frac{d\Sigma_{ij}}{dt} = \left\langle u_i, E[\hat{F}(u) y_j] \right\rangle.
\] (26)

To obtain the evolution equations for the spatial modes, we substitute Eq.(26) into Eq.(25) and we then multiply both sides by \( \Sigma_{ij}^{-1} \). This results in:

\[
\frac{\partial u_i}{\partial t} = \left[ E[\hat{F}(u) y_j] - u_k \left\langle u_k, E[\hat{F}(u) y_j] \right\rangle \right] \Sigma_{ij}^{-1}.
\]

Similarly, to obtain the evolution equation for the stochastic modes, we project Eq.(24) onto the spatial modes \( u_k \). This results in:

\[
\left\langle u_k, \frac{\partial u_i}{\partial t} \right\rangle \Sigma_{ij} y_j + \left\langle u_k, u_i \right\rangle \frac{d\Sigma_{ij}}{dt} y_j + \left\langle u_k, u_i \right\rangle \Sigma_{ij} \frac{dy_j}{dt} = \left\langle u_k, \hat{F}(u) \right\rangle.
\]

Once again we utilize the orthonormality and dynamical orthogonality of the spatial modes and substitute Eq.(26) into the above equation. We finally swap the indices \( j \) and \( i \) to get the form in Eq.(11c). The resulting equation is:

\[
\frac{dy_i}{dt} = \left[ \left\langle u_j, \hat{F}(u) \right\rangle - \left\langle u_j, E[\hat{F}(u) y_k] \right\rangle y_k \right] \Sigma_{ji}^{-1}.
\]

Since the boundary conditions are deterministic, the boundary conditions for the mean and the spatial modes are given by:

\[
\mathcal{B}[\pi(x,t)] = h(x,t), \quad x \in \partial D,
\]

\[
\mathcal{B}[u_i(x,t)] = 0, \quad x \in \partial D.
\]

The initial conditions for the mean are given by applying the mean value to the stochastic field at \( t = 0 \):

\[
\pi_0(x,t_0) = E[u_0(x; \omega)].
\]

This completes the proof.

**B. Equivalence of DO and DBO methods**

**B.1. Proof of Lemma (2.1)**

(i) The transformation matrix \( R_u \) can be obtained by projecting the equivalence relation \( U_{DO} = U_{DBO} R_a \) onto \( U_{DBO} \). This results in:

\[
U_{DO} = U_{DBO} R_a,
\]

\[
R_u = \langle U_{DBO}, U_{DO} \rangle,
\] (27)
where we have used the orthonormality property of $U_{DBO}$ basis: $\langle U_{DBO}, U_{DBO} \rangle = I$, where $I$ is the identity matrix. Similarly projecting the equivalence relation onto $U_{DO}$ basis and using the orthonormality property of the $U_{DO}$ basis: $\langle U_{DO}, U_{DO} \rangle = I$ we obtain,

$$
\langle U_{DO}, U_{DBO} \rangle R_u = I,
$$

$$
R_u^{-1} = \langle U_{DO}, U_{DBO} \rangle.
$$

It follows from the definition of inner product of quasimatrices i.e., Eq.(1), that the transpose of the inner product can be written as $\langle V(x, t), U(x, t) \rangle = \langle U(x, t), V(x, t) \rangle^T$. The above equation can be re-written as the transpose of inner product of quasimatrices in the following form:

$$
R_u^{-1} = (U_{DBO}, U_{DO})^T.
$$

Now, using the result from Eq.(27), the above equation can be written as,

$$
R_u^{-1} = R_u^T, \quad R_u^T R_u = I.
$$

This equation shows that $R_u^T$ is an inverse of $R_u$, which is a property of orthogonal matrices. Therefore, $R_u$ is an orthogonal matrix.

(ii) Since the two decompositions are equivalent, we have

$$
U_{DBO} \Sigma_{DBO} Y_{DBO}^T = U_{DO} Y_{DO}^T.
$$

Using the transformation definition $U_{DO} = U_{DBO} R_u$ and $Y_{DO} = Y_{DBO} W_y$, the DO decomposition can be expressed as:

$$
U_{DBO} \Sigma_{DBO} Y_{DBO}^T = U_{DBO} R_u W_y^T Y_{DBO}^T.
$$

Projecting the above equation on the $U_{DBO}$ basis and using the orthonormality property of the DBO basis i.e., $\langle U_{DBO}, U_{DBO} \rangle = I$, we get:

$$
\langle U_{DBO}, U_{DBO} \rangle \Sigma_{DBO} Y_{DBO}^T = \langle U_{DBO}, U_{DBO} \rangle R_u W_y^T Y_{DBO}^T.
$$

$$
\Sigma_{DBO} Y_{DBO}^T = R_u W_y^T Y_{DBO}^T.
$$

We now project the above equation on the stochastic DBO basis, i.e. $Y_{DBO}$:

$$
\Sigma_{DBO} \mathbb{E}[Y_{DBO}^T Y_{DBO}] = R_u W_y^T \mathbb{E}[Y_{DBO}^T Y_{DBO}].
$$

The stochastic basis of DBO are orthonormal i.e., $\mathbb{E}[Y_{DBO}^T Y_{DBO}] = I$. We apply this property to the above equation and simplify it further, which results in:

$$
\Sigma_{DBO} = R_u W_y^T.
$$

Multiplying the above equation by $R_u^T$ from left and using $R_u^T = R_u^{-1}$ and transposing the resulting equation yields:

$$
W_y = \Sigma_{DBO}^T R_u.
$$

(iii) We now prove that the $R_u$ matrix does not evolve in time. The evolution equation for $U_{DO}$ in a quasimatrix form can be written as:

$$
\frac{\partial U_{DO}}{\partial t} = \mathbb{E}[\hat{\mathcal{F}} Y_{DO}] - U_{DO} \mathbb{E} \left[ \langle U_{DO}, \hat{\mathcal{F}} \rangle Y_{DO} \right] C_{DO}^{-1}.
$$
Substituting the transformation \( U_{DO} = U_{DBO} R_u \) and \( Y_{DO} = Y_{DBO} W_y \) in the above equation results in:

\[
\frac{\partial U_{DBO}}{\partial t} R_u + U_{DBO} \frac{dR_u}{dt} = \left[ E[\hat{\mathcal{F}} Y_{DBO}] - U_{DBO} R_u R_u^T E[\langle U_{DBO}, \hat{\mathcal{F}} \rangle Y_{DBO}] \right] W_y C_{DO}^{-1}.
\]

Projecting the above equation on the \( U_{DBO} \) bases, using the dynamically orthogonal condition i.e., \( \langle U_{DBO}, U_{DBO} \rangle = 0 \), orthonormality property of DBO spatial modes i.e., \( \langle U_{DBO}, U_{DBO} \rangle = I \) and orthogonal matrix property i.e., \( R_u R_u^T = I \) on the previous equation results in:

\[
\frac{dR_u}{dt} = \left[ \langle U_{DBO}, E[\hat{\mathcal{F}} Y_{DBO}] \rangle - E[\langle U_{DBO}, \hat{\mathcal{F}} \rangle Y_{DBO}] \right] W_y C_{DO}^{-1}.
\]

The expectation operator and the spatial inner product operations commute, which results in:

\[
\frac{dR_u}{dt} = 0.
\]

This completes the proof.

**B.2. Proof of Theorem (2.2)**

In this section, we prove that the DO and DBO decompositions of SPDE in Eq. (2) remain equivalent for all time. We begin with the evolution equations for the stochastic and spatial DO bases in the quasimatrix form:

\[
\frac{\partial U_{DO}}{\partial t} = \left[ E[\hat{\mathcal{F}} Y_{DO}] - U_{DO} E[\langle U_{DO}, \hat{\mathcal{F}} \rangle Y_{DO}] \right] C_{DO}^{-1},\tag{28a}
\]

\[
\frac{dY_{DO}}{dt} = \langle \hat{\mathcal{F}}, U_{DO} \rangle .\tag{28b}
\]

We substitute the transformation \( U_{DO} = U_{DBO} R_u \) and \( Y_{DO} = Y_{DBO} W_y \) in the evolution equation for spatial DO modes i.e., Eq.(28a). The equation thus becomes:

\[
\frac{\partial U_{DBO}}{\partial t} R_u + U_{DBO} \frac{dR_u}{dt} = \left[ E[\hat{\mathcal{F}} Y_{DBO}] - U_{DBO} R_u R_u^T E[\langle U_{DBO}, \hat{\mathcal{F}} \rangle Y_{DBO}] \right] W_y C_{DO}^{-1}.
\]

Using the results of (i) and (iii) from Lemma (2.1), the above equation can be simplified as:

\[
\frac{\partial U_{DBO}}{\partial t} R_u = \left[ E[\hat{\mathcal{F}} Y_{DBO}] - U_{DBO} E[\langle U_{DBO}, \hat{\mathcal{F}} \rangle Y_{DBO}] \right] W_y C_{DO}^{-1} .\tag{29}
\]

The covariance matrix for DO is defined by the following equation:

\[
C_{DO} = E[Y_{DO}^T Y_{DO}] .\tag{30}
\]

We can simplify the above equation by using the transformation \( Y_{DO} = Y_{DBO} W_y \) and using the orthonormality of the DBO stochastic modes:

\[
C_{DO} = E[Y_{DO}^T Y_{DO}] ,
\]

\[
C_{DO} = W_y^T E[Y_{DBO}^T Y_{DBO}] W_y ,
\]

\[
C_{DO} = W_y^T W_y .
\]

Thus, \( C_{DO}^{-1} \) can be written as \( C_{DO}^{-1} = W_y^{-1} W_y^{-T} \). We now simplify the \( W_y C_{DO}^{-1} \) which appears in Eq.(29) and using inverse of \( W_y^T \) from the property (ii) from Lemma (2.1).

\[
W_y C_{DO}^{-1} = W_y W_y^{-1} W_y^{-T} ,
\]

\[
= \Sigma_{DBO}^{-1} R_u .
\]
Multiplying Eq.(29) by $R^T_u$ from right and using the value of $W_y C_{DO}^{-1}$ from the above equations and using the property of orthogonal matrix $R_u$ i.e., $R^T_u R_u = I$, the evolution equation simplifies to:

$$\frac{dU_{DBO}}{dt} = \left[ \mathbb{E} \left[ \hat{\mathcal{J}} Y_{DBO} \right] - U_{DBO} \mathbb{E} \left[ \left\langle U_{DBO} \hat{\mathcal{J}} \right\rangle Y_{DBO} \right] \right] \Sigma^{-1}_{DBO}.$$

The above equation is the evolution equation of the DBO spatial modes in quasimatrix form. Similarly, substituting the transformations $U_{DO} = U_{DBO} R_u$ and $Y_{DO} = Y_{DBO} W_y$ in the evolution equation for $Y_{DO}$, i.e. Eq.(28b), results in:

$$\frac{dY_{DBO}}{dt} W_y + Y_{DBO} \frac{dW_y}{dt} = \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle R_u.$$ (31)

From parts (ii) and (iii) of Lemma (2.1), we have: $\frac{dW_y}{dt} = \frac{d\Sigma_{DBO}^T}{dt} R_u$. Using this relation in Eq.(31):

$$\frac{dY_{DBO}}{dt} W_y + Y_{DBO} \frac{d\Sigma_{DBO}^T}{dt} R_u = \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle R_u,$$

$$\frac{dY_{DBO}}{dt} W_y = \left[ \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle - Y_{DBO} \mathbb{E} \left[ Y^T_{DBO} \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle \right] \right] R_u,$$

where evolution of $\Sigma_{DBO}^T$ given by: $\frac{d\Sigma_{DBO}^T}{dt} = \mathbb{E} \left[ Y^T_{DBO} \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle \right]$ is substituted in the above equation. Multiplying both sides of the equation by $W_y^{-1}$ from the right and using the result of part (ii) of Lemma (2.1), we get:

$$\frac{dY_{DBO}}{dt} = \left[ \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle - Y_{DBO} \mathbb{E} \left[ Y^T_{DBO} \left\langle \hat{\mathcal{J}}, U_{DBO} \right\rangle \right] \right] \Sigma_{DBO}^{-T}.$$ 

The above equation is the evolution equation of the DBO stochastic modes in the quasimatrix form. Thus, we see that the equivalence between the stochastic basis is maintained $\forall t > 0$. This completes the proof.

C. Equivalence of BO and DBO methods

C.1. Proof of Lemma (2.2)

(i) To obtain the properties of $R_y$ matrix, we begin with the orthonormality property of the stochastic BO modes and substitute the transformation $Y_{BO} = Y_{DBO} R_y$ in the equation for orthonormality of $Y_{BO}$ modes,

$$\mathbb{E} \left[ Y^T_{BO} Y_{BO} \right] = I,$$

$$R^T_y \mathbb{E} \left[ Y^T_{DBO} Y_{DBO} \right] R_y = I,$$

$$R^T_y R_y = I.$$

The last equation shows that $R^T_y$ is an inverse of the $R_y$ matrix, which is a property of an orthogonal matrix. Thus, $R_y$ is an orthogonal matrix.

(ii) From the equivalence of the decompositions we have:

$$U_{DBO} \Sigma_{DBO} Y^T_{DBO} = U_{BO} Y^T_{BO}.$$

Substituting the transformations $Y_{BO} = Y_{DBO} R_y$ and $U_{BO} = U_{DBO} W_u$ in the above equation results in:

$$U_{DBO} \Sigma_{DBO} Y^T_{DBO} = U_{DBO} W_u R^T_y Y^T_{DBO}.$$ 

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Projecting the above equation onto the $U_{DBO}$ basis and using orthonormality property of the DBO spatial basis, i.e. $\langle U_{DBO}, U_{DBO} \rangle = I$, results in

$$\langle U_{DBO}, U_{DBO} \rangle \Sigma_{DBO} Y^T_{DBO} = \langle U_{DBO}, U_{DBO} \rangle W_u R^T_y Y^T_{DBO},$$

$$\Sigma_{DBO} Y^T_{DBO} = W_u R^T_y Y^T_{DBO}.$$

Now projecting onto the stochastic basis $Y_{DBO}$ and using the orthonormality of the stochastic basis i.e., $E[ \dot{Y}^T_{DBO} Y_{DBO} ] = I$, results in:

$$\Sigma_{DBO} E[ Y^T_{DBO} Y_{DBO} ] = W_u R^T_y E[Y^T_{DBO} Y_{DBO}],$$

$$\Sigma_{DBO} = W_u R^T_y,$$

where we have used $R^T_y = R_y^{-1}$.

(iii) We now derive the evolution equation for $R_y$. We begin with the evolution equation for $U_{BO}$ in the quasimatrix form, which is written as:

$$\frac{\partial U_{BO}}{\partial t} = U_{BO} M + E[ \tilde{\mathbf{F}} Y_{DBO} ],$$

where,

$$M = E[ \frac{dY^T_{DBO}}{dt} Y_{DBO} ].$$

Simplifying the above equation for $M$ by using the transformation relation $Y_{BO} = Y_{DBO} R_y$ results in:

$$M = E \left[ \left( \frac{dR^T_y}{dt} Y^T_{DBO} + R^T_y \frac{dY^T_{DBO}}{dt} \right) Y_{DBO} R_y \right].$$

Using the dynamic orthogonality orthonormality of the DBO stochastic basis, i.e., $E[ \dot{Y}^T_{DBO} Y_{DBO} ] = 0$, and $E[ Y^T_{DBO} Y_{DBO} ] = I$, we can simplify the equation for $M$ as:

$$M = \frac{dR^T_y}{dt} R_y. \quad (32)$$

Now substituting the transformation $Y_{BO} = Y_{DBO} R_y$ and $U_{BO} = U_{DBO} W_u$ in the evolution equation of the BO spatial modes results in:

$$\frac{\partial U_{DBO}}{\partial t} W_u + U_{DBO} \frac{dW_u}{dt} = U_{DBO} W_u M + E[ \tilde{\mathbf{F}} Y_{DBO} ] R_y. \quad (33)$$

Substituting $M$ from Eq.(32) into Eq.(33):

$$\frac{\partial U_{DBO}}{\partial t} W_u + U_{DBO} \frac{dW_u}{dt} = U_{DBO} W_u \frac{dR^T_y}{dt} R_y + E[ \tilde{\mathbf{F}} Y_{DBO} ] R_y.$$

Projecting the above equation onto the DBO spatial basis and using the dynamic orthogonality and orthonormality of the $U_{DBO}$ basis:

$$\frac{dW_u}{dt} = W_u \frac{dR^T_y}{dt} R_y + \langle U_{DBO}, E[ \tilde{\mathbf{F}} Y_{DBO} ] \rangle R_y. \quad (34)$$

On the other hand, the evolution equation for $\Sigma_{DBO}$ is given by:

$$\frac{d\Sigma_{DBO}}{dt} = \langle U_{DBO}, E[ \tilde{\mathbf{F}} Y_{DBO} ] \rangle.$$
Substituting this value for the last term on the right hand side in Eq.(34), we get:

\[
dW_u \frac{dt}{t} = W_u \frac{dR^u}{dt} R_y + \frac{d\Sigma_{DBO}}{dt} R_y. \tag{35}
\]

Taking time derivative of relation in part (ii) of Lemma (2.2) results in:

\[
dW_u \frac{dt}{t} = \frac{d\Sigma_{DBO}}{dt} R_y + \Sigma_{DBO} \frac{dR_y}{dt}. \tag{35}
\]

Equating the definitions of \( \frac{dW_u}{dt} \) obtained from property (ii) of Lemma (2.2) and Eq.(35):

\[
\frac{d\Sigma_{DBO}}{dt} R_y + \Sigma_{DBO} \frac{dR_y}{dt} = W_u \frac{dR^T_y}{dt} R_y + \frac{d\Sigma_{DBO}}{dt} R_y,
\]

\[
\Sigma_{DBO} \frac{dR_y}{dt} = W_u \frac{dR^T_y}{dt} R_y.
\]

Since \( R_y \) is an orthogonal matrix:

\[
R^T_y R_y = I,
\]

\[
\frac{dR^T_y}{dt} R_y = -R^T_y \frac{dR_y}{dt}.
\]

\[
\Sigma_{DBO} \frac{dR_y}{dt} = -W_u R^T_y \frac{dR_y}{dt}.
\]

We know that \( W_u R^T_y = \Sigma_{DBO} \). The above equation thus, becomes

\[
\frac{dR_y}{dt} = 0.
\]

This completes the proof.

C.2. Proof of Theorem (2.3)

In this section, we prove that the equivalence relation is valid for all \( t > 0 \). We plug \( U_{BO} = U_{DBO} W_u \) and \( Y_{BO} = Y_{DBO} R_y \) into the BO evolution equations in quasimatrix form given by:

\[
\frac{\partial U_{BO}}{\partial t} = U_{BO} M + E[\mathcal{F} Y_{BO}], \tag{36a}
\]

\[
\frac{dY_{BO}}{dt} = \left( \left\langle \mathcal{F} , U_{BO} \right\rangle - E[Y_{BO} S] \right) \Lambda^{-1}, \tag{36b}
\]

where,

\[
M = E[\frac{dY_{BO}^T}{dt} Y_{BO}],
\]

\[
S = \left\langle \frac{\partial U_{BO}}{\partial t} , U_{BO} \right\rangle.
\]

We start with the evolution equations for spatial BO modes i.e., Eq.(36a) and apply the transformation \( U_{BO} = U_{DBO} W_u \) and \( Y_{BO} = Y_{DBO} R_y \):

\[
\frac{\partial U_{DBO}}{\partial t} W_u + U_{DBO} \frac{dW_u}{dt} = U_{DBO} W_u M + E[\mathcal{F} Y_{DBO}] R_y,
\]

\[
\frac{\partial U_{DBO}}{\partial t} W_u + U_{DBO} \frac{dW_u}{dt} = U_{DBO} W_u \left( \left( \frac{dR^T_y}{dt} Y_{DBO} + R^T_y \frac{dY_{DBO}}{dt} \right) Y_{DBO} R_y \right) + E[\mathcal{F} Y_{DBO}] R_y.
\]
Using the dynamical orthogonal property of the stochastic DBO modes and property (iii) of Lemma (2.2), above equation simplifies to:
\[
\frac{\partial U_{DBO}}{\partial t} W_u + U_{DBO} \frac{dW_u}{dt} = \mathbb{E}[\tilde{f} Y_{DBO}] R_y.
\]
Taking time derivative of property (ii) of Lemma (2.2), and using property (iii) to simplify we obtain \(\frac{dW_u}{dt} = \frac{\Sigma_{DBO}}{dt} R_y\). Substituting this equation in the above equation:
\[
\frac{\partial U_{DBO}}{\partial t} W_u = \mathbb{E}[\tilde{f} Y_{DBO}] R_y - U_{DBO} \frac{d\Sigma_{DBO}}{dt} R_y,
\]
\[
\frac{\partial U_{DBO}}{\partial t} = \left[ \mathbb{E}[\tilde{f} Y_{DBO}] - U_{DBO} \left( U_{DBO}, \mathbb{E}[\tilde{f} Y_{DBO}] \right) \right] R_y W_u^{-1},
\]
\[
\frac{\partial U_{DBO}}{\partial t} = \left[ \mathbb{E}[\tilde{f} Y_{DBO}] - U_{DBO} \left( U_{DBO}, \mathbb{E}[\tilde{f} Y_{DBO}] \right) \right] \Sigma_{DBO}^{-1}.
\]
This is the evolution equation for \(U_{DBO}\) in the quasimatrix form. Thus, the equivalence for the spatial modes is preserved \(\forall t > 0\). Similarly, substituting the transformation equations in the evolution equation for stochastic modes i.e., Eq.(36b):
\[
\frac{dY_{DBO}}{dt} R_y + Y_{DBO} \frac{dR_y}{dt} = \left[ \langle \tilde{f}, U_{DBO} \rangle W_u - \mathbb{E}[Y_{DBO} R_y S] \right] \Lambda^{-1}.
\]
Using property (iii) of Lemma (2.2) and the definition of \(S\) in the BO equations, we get:
\[
\frac{dY_{DBO}}{dt} R_y = \left[ \langle \tilde{f}, U_{DBO} \rangle W_u - \mathbb{E}[Y_{DBO} R_y S] \right] \Lambda^{-1}.
\]
Using the dynamical orthogonality condition and orthonormality condition for the spatial modes for DBO, we get:
\[
\frac{dY_{DBO}}{dt} R_y = \left[ \langle \tilde{f}, U_{DBO} \rangle W_u - Y_{DBO} \mathbb{E}[Y_{DBO} \tilde{f}, U_{DBO}] \right] W_u^{-1} \Lambda^{-1}.
\]
From property (ii) and (iii) of Lemma (2.2) we know that \(\frac{dW_u}{dt} = \frac{\Sigma_{DBO}}{dt} R_y\). Using this equation and the value of \(\Sigma_{DBO}\) evolution in the previous equation we get:
\[
\frac{dY_{DBO}}{dt} R_y = \left[ \langle \tilde{f}, U_{DBO} \rangle - Y_{DBO} \mathbb{E}[Y_{DBO} \tilde{f}, U_{DBO}] \right] W_u \Lambda^{-1}.
\]
Now, from the properties of BO spatial modes, we know that
\[
\langle U_{BO}, U_{BO} \rangle = \Lambda.
\]
Using the transformation and orthonormality of the DBO modes
\[
W_u^{T} \langle U_{DBO}, U_{DBO} \rangle W_u = \Lambda,
\]
\[
W_u^{T} W_u = \Lambda,
\]
\[
\Lambda^{-1} = W_u^{-1} W_u^{-T}.
\]
Using this definition of \(\Lambda^{-1}\) and using property (ii) of Lemma (2.2) in Eq.(37):
\[
\frac{dY_{DBO}}{dt} = \left[ \langle \tilde{f}, U_{DBO} \rangle - Y_{DBO} \mathbb{E}[Y_{DBO} \tilde{f}, U_{DBO}] \right] \Sigma_{DBO}^{T}.
\]
Thus, we obtain the evolution equation for the stochastic DBO modes in the quasimatrix form. This shows that the equivalence is preserved for all \(t\), given that the modes are equivalent at time \(t = 0\). This completes the proof.
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