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Transient response analysis of randomly parametrized finite element systems based on approximate balanced reduction

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Highlights

- We propose a model reduction technique for large scale stochastic finite element systems.
- The reduced basis spans the dominant eigenspace of the stochastic controllability Gramian.
- Computationally efficient iterative Arnoldi–Lyapunov basis building methods for large stochastic systems.
- Implicit restart scheme for Arnoldi–Lyapunov vector basis has been proposed.
- Transient response analysis of large dynamical systems illustrated with numerical examples.

Abstract

A model order reduction scheme of the transient response of large-scale randomly parametrized linear finite element system in state space form has been proposed. The reduced order model realization is aimed at preserving the invariant properties of the dynamic system model based on the dominant coupling characteristics of the specified system inputs and outputs. An *a-priori* model reduction strategy based on the balanced truncation method has been proposed in conjunction with the stochastic spectral Galerkin finite element method. Approximation of the dominant modes of the controllability Gramian has been performed with iterative Arnoldi scheme applied to Lyapunov equations. The reduced order representation of the randomly parametrized dynamical system has been obtained with Arnoldi–Lyapunov vector basis using an implicit time stepping algorithm. The performance and the computational efficacy of the proposed scheme has been illustrated with examples of randomly parametrized advection–diffusion–reaction problem under the action of transient external forcing functions. The convergence of the proposed reduced order scheme has been shown with a-posteriori error estimates.

Keywords: Stochastic transient response; Balanced truncation; Stochastic spectral Galerkin; Controllability Gramian

1. Introduction

Uncertainty in the mathematical modeling of engineering systems has been an active area of research over the past few decades which focuses on the statistical quantification of the effect of input uncertainty on the response quantities

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of interest. This resolution of the stochastic mathematical models and the propagation of uncertainty has called for efficient numerical methods to tackle these expensive problems which range from non-intrusive efficient Monte-Carlo and quasi-Monte Carlo techniques to the intrusive stochastic spectral Galerkin methods. Excellent review articles have summed up in the research in this domain [1,2]. It should be noted though that the above stochastic systems are different from the classical "stochastic differential equations". In the latter case, the random inputs are in the form of idealized processes (such as Wiener process, Poisson process, to name a few) and the stochastic calculus used for their study is a mature subject of active research [3]. In the present work we have considered the uncertain inputs to be in the form of random parameters associated with the system of governing partial differential equations describing the physical system to be studied.

Uncertainty in coupled multiphysics linear time-invariant (LTI) systems have been found to have a huge impact on their control performance [4]. The present work focuses on the resolution of the randomly parametrized LTI systems using efficient reduced order modeling techniques. Thus the first part of the article gives the key concepts employed in the description and quantification of the random parameters in stochastic partial differential equations (SPDE) and the incorporation of this description within the stochastic finite element setup. The solution techniques employed for the stochastic linear system can be broadly classified into two broad categories: (a) the non-intrusive stochastic sample based simulation techniques and (b) intrusive stochastic spectral Galerkin methods.

Various Monte Carlo Simulation (MCS) techniques belong to the class of non-intrusive methods and have been widely used. These methods have the virtue of easy implementation and trivial parallelization but the convergence of the solution statistics is slow with the mean value converging as $1/N_s$ where N_s is the number of random realizations. Sometimes the convergence can be accelerated by improved sampling techniques (such as the importance sampling, Latin hypercube sampling, orthogonal sampling, to name a few) such as the "variance reduction techniques" [5] or the response surface method or the experiment design method. The limitations of these techniques are generally dictated by the dimension of the input stochastic space.

Alternatives to MCS methods can provide us with an explicit functional relationship between the independent input random variables and hence can allow easy evaluation of functional statistics or probabilities. Non-statistical approaches based on a perturbation method [6], the Neumann expansion method [7,8] estimates the response surface in a parameter space. On the other hand the Galerkin-type methods [9–12] developed with differing choice of the approximation space, systematically lead to a high precision solution allowing the response to be expressed explicitly in terms of the basic random variables describing the uncertainties. Their principal drawback lies in the fact that the dimensionality of the resulting system of linear equations is huge. The difficulty to build efficient preconditioners and memory requirements induced by these techniques are still challenging and active areas of research.

The additional computational overhead associated with obtaining the response statistics of the randomly parametrized systems have motivated researchers to look into various model reduction techniques for the numerical solution of SPDE. A review of some of these techniques can be found in [13,14]. Some of these techniques attempt to perform a spectral (Hilbert Karhunen–Loève) decomposition of the stochastic solution to obtain the set of basis functions [15] or use a low-order Neumann expansion scheme to compute an estimation of the correlation structure of the response vector [11]. These belong to the class of *a-posteriori* model reduction since the optimal basis is calculated from a primary approximation of the statistics of the stochastic response. On the other hand the *a-priori* model reduction schemes in the context of Galerkin spectral stochastic methods evaluate the stochastic basis functions for approximating the solution using well defined optimality criterion. Methods belonging to this category are Generalized Spectral Decomposition [16] and the so called Reduced Basis methods [17].

On the other hand, the problem of reduced order modeling for linear time invariant systems (LTI) has been studied widely within the scope of control literature [18,19]. The foundation for the minimal realization of LTI systems using balanced truncation has been laid in [20] which is a principal components analysis of the LTI system using the concept of observability and controllability Gramians. Among the vast range of other model reduction techniques for LTI systems we refer to the singular value decomposition based approaches [21], the classical moment matching techniques [22] and singular perturbation technique [23] for the attention they have received. Model reduction for systems with random inputs modeled as stochastic processes have been studied in [24,25].

The objective of this study is to approach model reduction from a systems perspective where the complete information of the LTI system is available in the form of a finite element model obtained from applying the stochastic spectral Galerkin method to a randomly parametrized stochastic partial differential equation. These systems typically have very large dimension and it is a challenge to realize their transient response statistics with an appropriate

reduced order model. This has remained a sparsely studied topic in the model reduction literature for large dynamical systems and forms the focus of the present work. This belongs to a class of an *a-priori* model reduction technique. The motivation of the work is provided by the fact that the statistics of the dynamical response of the randomly parametrized LTI system can be approximated by retaining only the dominant dynamical coupling characteristics between the specified input and desired outputs of the system.

For this we have looked at the dominant eigencomponents of the symmetric, positive definite controllability Gramian of the randomly parametrized system. For a stable LTI system, the dominant eigenmodes of the stochastic controllability Gramian can provide a reduced subspace in which the solution can be approximated with good accuracy. The extension of the idea of dominant modes of the controllability Gramian to the spectral stochastic Galerkin framework classically employed for the propagation of the input parametric uncertainty to the system response would give the justification of using the method for large-scale randomly parametrized FE systems. The matrix Lyapunov equations involved in resolving the stochastic controllability Gramian can be quite expensive and hence alternative numerical schemes for approximate solutions of these equations have to be investigated.

The paper is organized as follows. In Section 2 we introduce the model reduction problem for the resolution of the time domain response of LTI systems and give an overview of some model reduction strategies. Following this we introduce the stochastic finite elements of randomly parametrized partial differential equations in Section 3. This section briefly describes the representation of the random field in a finite dimensional stochastic space and the spectral Galerkin method of resolution of the response of the stochastic linear systems. Section 4 gives the model reduction for technique for stochastic dynamical systems. It discusses the idea of the minimal realization of the dynamical system based on the principal modes of the controllability Gramian and discusses the numerical methods for evaluating the principal components of this Gramian based on Arnoldi's algorithm. Section 5 demonstrates the proposed method with numerical examples of a transient advection–diffusion–reaction system and a pure diffusion problem. Section 6 gives the summary and the principal contributions of this work.

2. Background of model order reduction for dynamical systems

We consider a dynamical system in the state space form obtained from the finite element model of a physical LTI system as

$$\mathbf{C}\dot{\mathbf{X}}(t) = \mathbf{A}\mathbf{X}(t) + \mathbf{B}\mathbf{f}(t) \tag{1}$$

where $\mathbf{X}(t) \in \mathbb{R}^n$ is the vector of the state variables, $\mathbf{A}, \mathbf{C} \in \mathbb{R}^{n\times n}$ is the system matrix and $\mathbf{B} \in \mathbb{R}^{n\times p}$ is the matrix associated with the locations of a finite number p of inputs $\mathbf{f}(t) = \{f_1(t), \ldots, f_p(t)\}$. It is assumed here that the system matrices $\mathbf{A}$ and $\mathbf{C}$ are large and sparse in nature, which is the case for finite element implementation with finite order piecewise polynomials. The objective of most model reduction techniques is to obtain a good low order approximation of the solution of Eq. (1) by identifying a dominant subspace in which the time varying response of the system exists.

Model reductions in the context of state space systems have been widely studied for many decades [19]. Classical control theory literature relies on two key concepts for a low order realization of the plant mode. These are the principal component analysis and the singular value decomposition. If we consider a set of outputs of an unsteady state space system at discrete points in time as $\bar{\mathbf{X}} = \{\mathbf{X}(t_1), \mathbf{X}(t_2), \ldots, \mathbf{X}(t_m)\}$ where $\bar{\mathbf{X}} \in \mathbb{R}^{n\times m}$ then using the concept of principal component analysis it is possible to construct an alternative set of basis vectors $\mathbf{U} = \{U_1, \ldots, U_q\}$ such that $\mathbf{U} \in \mathbb{R}^{n\times q}$ where $q \ll n$. The response vector can be expressed in these bases as $\mathbf{x} = \sum_{i=1}^{q} U_i x_i$ and its time derivative as $\dot{\mathbf{x}} = \sum_{i=1}^{q} U_i \dot{x}_i$. Using this, we can transform the equation in this reduced basis as

$$\mathbf{U}^T\mathbf{C}\,\mathbf{U}\dot{\mathbf{x}}(t) = \mathbf{U}^T\mathbf{A}\,\mathbf{U}\mathbf{x}(t) + \mathbf{U}^T\mathbf{B}\mathbf{f}(t) \tag{2}$$

where $\mathbf{x} = \{x_1, \ldots, x_q\} \in \mathbb{R}^q$ are the undetermined coefficients associated with the reduced basis. However, the solution vectors at discrete points in time are not known a-priori and hence it is not possible to ascertain the bases of a minimal order model directly. As a result we resort to the information available to us from the mathematical model of the dynamic LTI state space system.

2.1. Overview of the model reduction strategies

Model reduction schemes for large LTI systems based on balancing [25] aims to preserve invariant properties of the strong input–output dynamical coupling of the LTI system. This approach is of particular relevance in the present context and we briefly discuss the method here. We consider an LTI system as

$$\begin{cases} \dot{\mathbf{X}} = \mathbf{A}\mathbf{X} + \mathbf{B}\mathbf{f} \\ \mathbf{Y} = \mathbf{E}\mathbf{X} \end{cases} \tag{3}$$

with $\mathbf{A} \in \mathbb{R}^{n\times n}$, $\mathbf{B} \in \mathbb{R}^{n\times p}$, $\mathbf{E} \in \mathbb{R}^{m\times n}$ where p and m are the number of inputs and outputs respectively. The system is subjected to a sequence of p inputs in $\mathbf{f}(t) = \mathbf{e}_i\delta(t),\ 1 \leqslant i \leqslant p$ such that $\delta(t)$ are unit impulse functions and $\mathbf{e}_i$ is the ith column of the $p \times p$ identity matrix. We consider a set of such sequences of p inputs. If an impulse response matrix of the state space system is considered which consists of k response vectors denoted by $\bar{\mathbf{X}}(t) \in \mathbb{R}^{n\times k}$ with $k > p$, we can construct a Gramian of the state response as

$$\mathbf{P}^2 = \int_{t_1}^{t_2} \bar{\mathbf{X}}(t)\bar{\mathbf{X}}^T(t)dt. \tag{4}$$

Here $\mathbf{P}^2$ is a real symmetric matrix which is termed as the controllability Gramian for state space systems in the control literature [20]. It has been shown that the system is controllable if and only if the matrix $\mathbf{P}^2$ is a full rank matrix. Controllability in this context is defined as the ability to take the system from some initial state $\mathbf{X}(t_0)$ to a final state $\mathbf{X}(t_1)$ with an input signal. For controllable systems, $\mathbf{P}^2$ is a positive semi-definite matrix. An eigendecomposition of this Gramian $\mathbf{P}^2$ gives

$$\mathbf{P}^2 = \boldsymbol{\Phi}\Lambda^2\boldsymbol{\Phi}^T; \quad \boldsymbol{\Phi} \in \mathbb{R}^{n\times n},\ \Lambda^2 = \operatorname{diag}\left\{\lambda_1^2, \ldots, \lambda_n^2\right\} \tag{5}$$

where $\lambda_1^2 \geqslant \lambda_2^2 \geqslant \cdots \geqslant \lambda_n^2 \geqslant 0$ is a non-negative sequence of eigenvalues and $\boldsymbol{\Phi} = \{\phi_1, \ldots, \phi_n\}$ is a matrix of mutually orthogonal eigenvectors such that $\boldsymbol{\Phi}^T\boldsymbol{\Phi} = \mathbf{I}$. If we denote the set of k piecewise continuous input functions of $\mathbf{f}(t) \in \mathbb{R}^p,\ t \in [0, T]$ as $\{\mathbf{f}_1(t), \ldots, \mathbf{f}_k(t)\}$ within a unit circle such that $\left(\int_0^T \|f_i(t)\|^2\, dt\right)^{1/2} \leqslant 1,\ \forall i$ where $f_i(t)$ are the components of any $\mathbf{f}_j(t)$, and the set of state responses to these functions denoted as $\underline{\mathbf{U}}$ then

$$\underline{\mathbf{U}} = \left\{\mathbf{X}_j \in \mathbb{R}^n : \mathbf{X}_j = \int_0^T \boldsymbol{\psi}(t,\tau)\mathbf{B}\mathbf{f}_j(\tau)d\tau, \forall\ j = 1, \ldots, k\right\} \tag{6}$$

where $\boldsymbol{\psi}(t,\tau)$ is the state-transition matrix from τ to t. Referring back to Eq. (4) it can be shown that the components of $\underline{\mathbf{U}} \in \mathbb{R}^{n\times k}$ trace an ellipsoid whose principal axes are given by the eigenvectors of the controllability Gramian $\mathbf{P}^2$. For state space systems (as given in Eq. (1)), it can be seen that the state-transition matrix is given as $\psi(t,\tau) = \exp\{\mathbf{A}(t-\tau)\}$. For stable systems where the eigenvalues of the system matrix A lie on the left half plane, $\mathbf{P}^2$ converges to a steady state matrix as $t \to \infty$, i.e. the controllability Gramian is given as

$$\mathbf{P}^2 = \int_0^\infty \exp\{\mathbf{A}\,t\}\,\mathbf{B}\mathbf{B}^T \exp\left\{\mathbf{A}^T t\right\} dt \tag{7}$$

where $\mathbf{P}^2$ is a stable matrix. The Gramian $\mathbf{P}^2$ contains the strong coupling characteristics between the input and the output of the state space system. Hence the principal components of the matrix Gramian $\mathbf{P}^2$ would give a dominant subspace in which the solution of the state space system lies. And this idea can potentially be used for the model order reduction of the large transient dynamic systems.

Usually two Gramians of the state space system are considered while implementing the idea of balanced truncation. These are the controllability Gramian $\mathbf{P}^2$ and the observability Gramian $\mathbf{Q}^2$. These Gramians determine the observable and controllable characteristics of the system which are mathematical duals. For the continuous time LTI systems these Gramians can be resolved from the solution of the coupled *Lyapunov* equations as

$$\begin{cases} \mathbf{A}\mathbf{P}^2 + \mathbf{P}^2\mathbf{A}^T &= -\mathbf{B}\mathbf{B}^T \\ \mathbf{A}^T\mathbf{Q}^2 + \mathbf{Q}^2\mathbf{A} &= -\mathbf{E}^T\mathbf{E}. \end{cases} \tag{8}$$

Under the assumption of A being stable, the Gramians $\mathbf{P}^2$ and $\mathbf{Q}^2$ are positive semi-definite amenable to the factorization $\mathbf{P}^2 = \mathbf{P}_c^T\mathbf{P}_c$ and $\mathbf{Q}^2 = \mathbf{Q}_o^T\mathbf{Q}_o$ (which are referred to as the Cholesky factors of the Gramians). The *Hankel singular values* of the system are defined as

$$\mathbf{P}_c\mathbf{Q}_o^T = \begin{bmatrix}\mathbf{U}_1 & \mathbf{U}_2\end{bmatrix}\begin{bmatrix}\Sigma_1 & 0\\ 0 & \Sigma_2\end{bmatrix}\begin{bmatrix}\mathbf{V}_1^T\\ \mathbf{V}_2^T\end{bmatrix} \tag{9}$$

where the diagonal matrices Σ_1 and Σ_2 consist of descending order of singular values $\sigma_i > \sigma_{i+1}$ of the matrices $\mathbf{P}_c\mathbf{Q}_o^T$. If the number of Hankel singular values chosen to represent the reduced order system is restricted to r then the reduced order model can be realized with the r components of vectors $\mathbf{U}_r$ and $\mathbf{V}_r^T$. This leads to the concept of balanced truncation where the least controllable and observable states are rejected via a similarity transformation which balances the system. In other words, a state-space realization is sought so that the controllability and observability Gramians are diagonalized and equal to the Hankel singular values. The balanced truncation approach leads to a model reduction approach which captures the transient behavior of the system satisfactorily but fails to capture the steady state response with sufficient accuracy. To overcome this, the method of singular perturbation approximation expands the solution to have zero error under steady state condition [26,27]. But this approach is computationally expensive since it involves the solution of the matrix Lyapunov equations which involve a computational cost of $\mathscr{O}(n^3)$.

Another significant model reduction approach which has been the subject of rigorous research is based on the Krylov subspace approximation of the transfer functions of the state-space systems [22,28]. The primary aim of these model reduction schemes is to obtain a good approximation of the dynamical characteristics (transfer function) of the system over a wide frequency range of the problem. This is achieved by expanding the moments of the transfer function with respect to the Laplace variable (or the shifted Laplace variable) and matching at least the low order moments of this expansion. If we consider an LTI state space system in Eq. (3), its frequency domain input–output relationship is captured by the relationship $\hat{\mathbf{Y}}(s) = \mathbf{H}(s)\hat{\mathbf{F}}(s)$ where the transfer function $\mathbf{H}(s)$ is given by

$$\mathbf{H}(s) = \mathbf{E}\,(s\mathbf{I} - \mathbf{A})^{-1}\,\mathbf{B} \quad s \in \mathbb{C}. \tag{10}$$

Here $\mathbf{H}(s)$ is a rational function of the Laplace variable s. It is assumed that the pencil $(s\mathbf{I} - \mathbf{A})$ is regular [29]. The transfer function is expanded as moments of s (or multipoint expansions about $(s - s_i)$) and the objective is to match the first q moments using a projection $\mathcal{P} = \mathbf{U}\mathbf{W}^T \in \mathbb{R}^{n\times n}$ with $\mathbf{U}, \mathbf{W} \in \mathbb{R}^{n\times q}$ being biorthogonal matrices such that $\mathbf{W}^T\mathbf{U} = \mathbf{I}$. The reduced order model is hence obtained as the projection of the solution on $\mathbf{U}$ and the residual being orthogonal to the space spanned by $\mathbf{W}$ as

$$\begin{cases}\mathbf{W}^T\mathbf{U}\dot{\mathbf{x}} = \mathbf{W}^T\mathbf{A}\mathbf{U}\mathbf{x} + \mathbf{W}^T\mathbf{B}\mathbf{f}\\ \mathbf{Y} = \mathbf{E}\mathbf{U}\mathbf{x}\end{cases} \tag{11}$$

where the solution is given by $\mathbf{X} = \mathbf{U}\mathbf{x}$. The block Krylov subspace projection technique is utilized to evaluate $\mathbf{U}$ and $\mathbf{W}$ such that the first few moments of the solution are approximated accurately

$$\begin{aligned}&\text{colsp}\,[\mathbf{U}] = \mathcal{K}_q\,(\mathbf{A}, \mathbf{B})\\ &\text{colsp}\,[\mathbf{W}] = \mathcal{K}_q\left(\mathbf{A}^T, \mathbf{E}^T\right).\end{aligned} \tag{12}$$

The general proof of the moment matching properties of U and W has been provided in [22]. Asymptotic Waveform Evaluation (AWE) [30], Arnoldi based algorithm [31], Lanczos method [28], and Padé via Lanczos (PVL) [32] can perform single input single output system (SISO) reduction by matching the first few moments of the rational transfer function.

3. Brief overview of the stochastic finite element method

A random field α can be defined on a compact region $\mathscr{D} \subseteq \mathbb{R}^d$ and an associated probability space $(\Theta, \mathscr{F}, P)$, where $\theta \in \Theta$ is a sample point from the sampling space Θ, $\mathscr{F}$ is the complete Borel σ-algebra over the subsets of Θ and P is the probability measure. This leads to the representation of the random field as a measurable mapping as $\alpha : \mathscr{D} \times \Theta \to \mathbb{R}$. The random field at each point in the region has a certain degree of correlation with those at the

other points characterized by a representative geometrical dimension. This provides the necessary spatial description of the uncertain parameter within the framework of a stochastic partial differential equation as

$$\mathscr{L}_\alpha(u) = f \quad \text{on } \mathscr{D} \text{ with } G_i u = 0 \text{on } \partial\mathscr{D}_i \ \forall\, i = 1, 2, \ldots \tag{13}$$

where $\mathscr{D}$ is a bounded domain with $\partial\mathscr{D}_i$ denoting parts of the boundary $\forall\, i$. The parameter α is spatially varying random field in the probability space $(\Theta, \mathscr{F}, P)$. The representation of this random field in a finite dimensional random space which makes it feasible to incorporate this description in a numerical model is considered in the following section.

3.1. Discretization of random fields

The probabilistic description of the uncertain parameter is provided with a prescribed mean and a covariance function $cov[a] : \mathscr{D} \times \mathscr{D} \to \mathbb{R}$ defined on the open, bounded polygonal domain in $\mathscr{D}$. For second order random fields, there is a compact self-adjoint operator

$$\mathcal{T}_a v(\cdot) = \int_{\mathscr{D}} cov[a](\mathbf{r}, \cdot) v(\mathbf{r}) d\mathbf{r} \quad \forall v \in L^2(\mathscr{D}) \tag{14}$$

along with a sequence of non-negative eigenpairs $\{(\lambda_i, \varphi_i)\}_{i=1}^{\infty}$ which describes the eigenvalue problem as

$$\mathcal{T}_a \varphi_i = \lambda_i \varphi_i, \quad (\varphi_i, \varphi_j)_{L^2(\mathscr{D})} = \delta_{ij}. \tag{15}$$

Assuming that the eigenpairs $[\varphi_i, \lambda_i]$ are in descending order as $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, it is possible to give a truncated Karhunen–Loève (KL) expansion of the random field $a(\mathbf{r}, \theta)$ as

$$\hat{a}_m(\theta, \mathbf{r}) = E[a](\mathbf{r}) + \sum_{i=1}^{m} \sqrt{\lambda_i} \varphi_i(\mathbf{r}) \xi_i(\theta) \quad \forall m \in \mathbb{N}_+ \tag{16}$$

where $E[a](\mathbf{r})$ is the mean function, $\{\xi_i(\theta)\}_{i=1}^{m}$ are a set of mutually independent, uncorrelated standard Gaussian random variables with zero mean ($\mathrm{E}[\xi_i] = 0$) and unit variance ($\mathrm{E}\left[\xi_i^2\right] = 1$). The eigenfunctions $\varphi_i(\mathbf{r})$ can be assumed to have sufficient smoothness for smooth covariance functions. Thus practical engineering problems model the parametric uncertainty with a finite set of random variables $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_m) : \Theta \to \mathbb{R}^m$, using first few largest eigenpairs in the reduced probability space $\left(\Theta^{(m)}, \mathscr{F}^{(m)}, P^{(m)}\right)$, where $\Theta^{(m)} = \mathrm{Range}(\boldsymbol{\xi})$ is a subset of $\mathbb{R}^m$, $\mathscr{F}^{(m)}$ is the associated Borel σ-algebra and $P^{(m)}$ is the image probability measure. It must be pointed out that calculation of the KL Expansion for random fields on arbitrary domains is not always easy and approximate numerical methods have to be adopted for this purpose [33].

However, for arbitrary random field models, the random parameter can be expressed in a mean-square convergent series using the Wiener–Askey chaos expansion [34] where the stochastic process is discretized with a set of independent identically distributed (iid) random variables $\hat{\boldsymbol{\xi}}(\theta) = \{\hat{\xi}^{(1)}, \ldots, \hat{\xi}^{(n)}\}$ as

$$a(\mathbf{r}, \theta) = \sum_{i=0}^{p} \mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta)) a_i(\mathbf{r}) \tag{17}$$

where $\mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta))$ are the multivariate orthogonal polynomial functions with respect to the joint probability density function of the stochastic Hilbert space i.e. $\left\langle \mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta)), \mathscr{H}_j(\hat{\boldsymbol{\xi}}(\theta)) \right\rangle_{L^2(\Theta)} = \delta_{ij} \left\| \mathscr{H}_i^2(\hat{\boldsymbol{\xi}}(\theta)) \right\|_{L^2(\Theta)}$. Here $\langle \cdot, \cdot \rangle_{L^2(\Theta)}$ denotes the inner product in the stochastic Hilbert space with $\|\cdot\|_{L^2(\Theta)}$ being the associated norm. The undetermined coefficients $a_i(\mathbf{r})$ associated with the series expansion can be evaluated as

$$a_i(\mathbf{r}) = \frac{\left\langle a(\mathbf{r}, \theta), \mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta)) \right\rangle_{L^2(\Theta)}}{\left\| \mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta)) \right\|_{L^2(\Theta)}}. \tag{18}$$

The solution methodology presented in this paper is applicable to this kind of general decomposition of the random field. In the following section we describe the stochastic spectral Galerkin method which is used to give the stochastic

weak formulation of the problem for a discretized random field represented in a finite dimensional stochastic space with a set of iid random variables.

3.2. Stochastic spectral Galerkin method

Let us consider the spaces involved with the stochastic weak formulation of the randomly parametrized linear system given in Eq. (13). The spatial domain $\mathscr{D}$ is meshed with finite elements $\Delta(\mathscr{D})$ such that $\bigcup \Delta(\mathscr{D}) = \mathscr{D}$. For the standard deterministic finite elements, the weak form of the governing partial differential equations is stated as: $b(u(\mathbf{r}), v(\mathbf{r})) = l(v(\mathbf{r}))\ \forall v \in \mathcal{H}^p \subset L^2(\Delta(\mathscr{D}))$ where u is the solution that is sought, v consists of the test functions in the admissible space with b and l being the continuous bilinear and linear forms respectively on the spatial domain $\mathbf{r} \in \Delta(\mathscr{D})$. The space $\mathcal{H}^p$ consists of polynomial functions which are C^p-continuous within the element domain. Now we assume that the input randomness has been modeled in a finite M dimensional stochastic space $\Theta^{(M)}$ with a denumerable set of iid random variables, we define a tensor product space on the FE approximation space and the stochastic space as $S^{p,q}(\Delta(\mathscr{D}), \Theta^{(M)})$. It consists of polynomials which converge in the $L^2\left(\Theta^{(M)}, dP_{\boldsymbol{\xi}}; \Delta(\mathscr{D})\right)$ sense which is consistently defined with the norm of the FE approximating functions and the stochastic space [10]. Hence for the case of the weak form obtained with the stochastic spectral Galerkin framework, we can write the bilinear and linear forms for the above system as

$$\mathbf{b}(u, v) = \int_{\Theta^{(M)}} b(u(\mathbf{r}, \theta), v(\mathbf{r}, \theta)) dP_{\boldsymbol{\xi}}(\theta); \qquad \mathbf{l}(v) = \int_{\Theta^{(M)}} l(v(\mathbf{r}, \theta)) dP_{\boldsymbol{\xi}}(\theta) \tag{19a}$$

$$\text{so that} \quad \mathbf{b}(u, v) = \mathbf{l}(v). \tag{19b}$$

It can be seen that the stochastic linear $\mathbf{l}(v)$ and bilinear forms $\mathbf{b}(u, v)$ in the above equation consist of approximation of the system solution at FE nodal points with a set of spatial interpolation functions and a set of stochastic basis. We denote the approximate stochastic solution at the FE nodes by the vector $\mathbf{u}(\theta) \in \mathbb{R}^n$. The latter exists in $\mathbb{R}^n \otimes \Theta^{(M)}$, where $\Theta^{(M)}$ is a finite dimensional stochastic space for real-valued random variables $\hat{\boldsymbol{\xi}}(\theta) = \{\hat{\xi}^{(1)}, \ldots, \hat{\xi}^{(p)}\}$ as described in Section 3.1 (see [13,9]). For independent random components $\hat{\xi}^{(i)}$, $\Theta^{(M)}$ is a tensor product space $\Theta^1 \otimes \cdots \otimes \Theta^M$. According to this approximate basis building technique which focuses on expressing the solution vector using some finite order stochastic polynomial functions, the solution vector $\mathbf{u}(\theta)$ is expressed as

$$\mathbf{u}(\theta) = \sum_{i=0}^{p} \mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta)) \bar{\mathbf{u}}_i(\theta); \quad \bar{\mathbf{u}}_i(\theta) \in \mathbb{R}^n\ \forall i \tag{20}$$

where $\mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta))$ are the basis in $\Theta^{(M)}$, $\bar{\mathbf{u}}_i(\theta)$ are the set of p unknown coefficients. The form of the polynomial functions $\mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta))$ used in Eq. (20) varies according to the chosen solution approach, such as the stochastic spectral Galerkin approaches (polynomial chaos, generalized chaos) classically use orthogonal polynomial basis. The latter method poses the problem as: find $\mathbf{u}(\theta) \in \mathbb{R}^n \otimes \Theta^{(M)}$ such that

$$\sum_{i=0}^{p} \mathrm{E}\left[\mathbf{A}(\theta) \mathscr{H}_j(\hat{\boldsymbol{\xi}}(\theta)) \mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta))\right] \bar{\mathbf{u}}_i = \mathrm{E}\left[\mathscr{H}_j(\hat{\boldsymbol{\xi}}(\theta)) \mathbf{F}\right] \quad \forall\, j = 0, 1, \ldots, p \tag{21}$$

where the matrix $\mathbf{A}(\theta)\ \forall \theta \in \Theta^{(M)}$ and vector $\mathbf{F}$ are the linear system matrices obtained from the application of the classical FE approximation to the randomly parametrized system in Eq. (13). As a result of Eq. (21) we obtain a set of linear algebraic equations with $\bar{\mathbf{u}}_i$ as the unknown coefficients which can be written as $\overline{\mathbf{A}}\bar{\mathbf{u}} = \overline{\mathbf{F}}$. The coefficient matrix $\overline{\mathbf{A}}$ is a significantly large, block sparse matrix whose size is governed by the dimension of the stochastic space and the order of chaos chosen for the stochastic polynomial functions $\mathscr{H}_i(\hat{\boldsymbol{\xi}}(\theta))$.

This stochastic spectral Galerkin method has been applied widely for the resolution of the system response of various computational mechanics problems such as structural dynamics [35,36], fluid flow [37] to name a few. However, the computational cost associated with the solution of the linear system resulting from Eq. (21) can become prohibitive for systems with large dimensions and even for moderate values of variability of the input random field. Krylov-type solution techniques [38,39] have been established which take advantage of the sparsity of the system and employ a preconditioner to efficiently solve a given system. As a result model reduction in the context of uncertainty

propagation methods within the spectral Galerkin framework is a crucial field of research with the potential to offer a substantial improvement in the computational efficacy of these methods. The following section focuses on a model reduction technique for the resolution of the transient response of randomly parametrized dynamical systems.

4. Randomly parametrized linear time invariant system

We consider a bounded domain $\mathscr{D} \in \mathbb{R}^d$ with piecewise Lipschitz boundary $\partial\mathscr{D}$, where $d \leq 3$ is the spatial dimension and $t \in \mathbb{R}^+$ is the time. We consider here a linear stochastic dynamical system with parametric uncertainty as

$$\frac{\partial x(\mathbf{r}, t; \theta)}{\partial t} = \nabla \left(k(\mathbf{r}, \theta)\nabla x(\mathbf{r}, t; \theta)\right) + f(\mathbf{r}, t) \quad \mathbf{r} \in \mathscr{D},\ t = [0, T] \tag{22}$$

where the $k(\mathbf{r}, \theta) : \mathbb{R}^d \times \theta \to \mathbb{R}$ is a square integrable random field in the probability space $(\Theta, \mathscr{F}, P)$ and $f(\mathbf{r}, t) \in \mathbb{R}$ is the deterministic time varying external forcing function. The objective is to solve for the stochastic transient system response $x(\mathbf{r}, t; \theta)$ which exists in the tensor product Hilbert space $H(\mathscr{D} \times \Theta \times T)$. A finite element discretization of the spatial domain results in the set of elements $S_e = \{\Delta(\mathscr{D}_h) : \bigcup \Delta(\mathscr{D}_h) = \mathscr{D}\}$ where h is the mesh parameter size. The discretized stochastic field is expressed at the n_e nodal points within each element of the FE mesh as $\mathbf{k}^e(\theta) \in \mathbb{R}^{n_e}$ and is interpolated inside the element domain with the spatial basis function as

$$k^e(\mathbf{r}, \theta) = [N(\mathbf{r})]^T \mathbf{k}^e(\theta) = [N(\mathbf{r})]^T \sum_{i=0}^{p_k} \hat{\boldsymbol{k}}_i^e \mathscr{H}_i(\theta) \tag{23}$$

where $\hat{\boldsymbol{k}}^e \in \mathbb{R}^{n_e}\ \forall i = 1, \ldots, p_k$, $[N(\mathbf{r})]$ is the vector of FE shape functions belonging to the Sobolev space $S^{k,2} \subset L^2(\Delta(\mathscr{D}_h))$ which are C^k-continuous within the element domain, $k \geqslant 1$. Also, $\mathscr{H}(\boldsymbol{\xi}(\theta)) = \left\{\mathscr{H}_1(\boldsymbol{\xi}(\theta)), \ldots, \mathscr{H}_{p_k}(\boldsymbol{\xi}(\theta))\right\}$ are the orthogonal stochastic polynomials which model the input parametric uncertainty in the finite dimensional stochastic space. This leads to the stochastic finite element linear system as

$$\mathbf{C}\dot{\mathbf{X}}(t; \theta) = \mathbf{K}(\theta)\mathbf{X}(t; \theta) + \bar{\mathbf{B}}\mathbf{f}(t) \tag{24}$$

$$\text{or,} \quad \dot{\mathbf{X}}(t; \theta) = \mathbf{A}(\theta)\mathbf{X}(t; \theta) + \mathbf{B}\mathbf{f}(t). \tag{25}$$

We take the forcing function $\mathbf{f}(t)$ to be deterministic throughout this study. Here $\mathbf{K}(\theta)$ or $\mathbf{A}(\theta)$ are the system matrices for each stochastic sample realization $\theta \in \Theta^{(M)}$. The above equation is in the standard state-space form introduced in Eq. (1) and we have changed the descriptor form of the linear system in Eq. (24) to the standard form in Eq. (25) where $\mathbf{A}(\theta) = \mathbf{C}^{-1}\mathbf{K}(\theta)$ and $\mathbf{B} = \mathbf{C}^{-1}\bar{\mathbf{B}}$. Doing this has its disadvantages which might seriously affect the efficiency of the solver. However, we have used the standard form of Eq. (25) for the time being to facilitate ease of theoretical discussion without making the notation too complicated. We would include in the subsequent section the methods to deal with the descriptor systems within a completely generic framework (given in Section 4.4). Here $\bar{\mathbf{B}}$ is the input distribution array and hence $\mathbf{B} \in \mathbb{R}^{n \times p}$ is associated with the p inputs to the system. The inputs are modeled via $\mathbf{f}(t) = \left\{f_1(t), \ldots, f_p(t)\right\} \in \mathbb{R}^p$. The stochastic matrix and $K(\theta)$ are expressed in the series expansion form as

$$\mathbf{K}(\theta) = \mathbf{K}_0 + \sum_{i=i}^{P_k} \mathbf{K}_i \mathscr{H}_i(\boldsymbol{\xi}(\theta)) \tag{26}$$

where $\mathbf{K}_0 \in \mathbb{R}^{n \times n}$ is the matrix belonging to the baseline model (with the associated stochastic functions being equal to 1) while $\mathbf{K}_i$ are the perturbation matrices associated with the stochastic functions in $\mathscr{H}(\boldsymbol{\xi}(\theta))$. The input parametric uncertainty is modeled within the probabilistic framework with iid random variables $\boldsymbol{\xi}(\theta) \in \mathbb{R}^M$. Hence the global input stochastic space is a M dimensional hyperspace $\Theta^{(M)} \subset \Theta$.

4.1. Minimal realization of the randomly parametrized dynamical system

The state transition matrix $\boldsymbol{\Psi}(t, \tau; \theta)$ of the stochastic LTI system would incorporate the input parametric uncertainty in $\boldsymbol{\xi}(\theta) \in \mathbb{R}^M$. Hence $\boldsymbol{\Psi}(t, \tau; \theta) : \mathbf{X}(\tau; \theta) \mapsto \mathbf{X}(t; \theta)$ for each $\theta \in \Theta^{(M)}$. The concept of model reduction based on the eigendecomposition of the controllability Gramian (discussed in Eq. (5)) and the model order

reduction method based on balanced truncation detailed in Section 2.1 is invoked here. The controllability Gramian of this system $\mathbf{P}^2(\theta) \in \mathbb{R}^{n\times n}$ can be realized for each point in the M dimensional stochastic input space $\Theta^{(M)}$. Our aim here is to obtain the dominant stochastic modes of the controllability Gramian and the solution of the stochastic system would be projected on to these basis functions.

The stochastic controllability Gramian for the randomly parametrized LTI system in Eq. (25) obeys the Lyapunov equation for each sample θ as

$$\mathbf{A}(\theta)\mathbf{P}^2(\theta) + \mathbf{P}^2(\theta)\mathbf{A}^T(\theta) + \mathbf{B}\mathbf{B}^T = 0; \quad \text{where } \mathbf{P}^2(\theta) \in \mathbb{R}^{n\times n} \ \forall\ \theta \in \Theta^{(M)} \tag{27}$$

where the stochastic coefficient matrix $\mathbf{A}(\theta)$ can be written in the series expandable form as $\mathbf{A}(\theta) = \sum_{i\in\mathscr{I}_{\mathscr{H}}} \mathbf{A}_i\ \mathscr{H}_i(\boldsymbol{\xi}(\theta))$ with $\mathbf{A}_i \in \mathbb{R}^{n\times n}\ \forall i$. Hence the dominant modes of $\mathbf{P}^2(\theta)$ would be obtained in $\mathbb{R}^n$ for every random sample realization in $\Theta^{(M)}$. Here we take $\mathbf{X}(t;\theta) \in \mathbb{R}^n$ to denote the stochastic system solution for every random sample $\theta \in \Theta^{(M)}$ at all points in time $t \in [0, T]$. If we use a separable representation of this space in the form $H(T) \otimes H(\mathbb{R}^n \times \Theta^{(M)})$, the stochastic system response $\mathbf{X}(t,\theta) \in \mathbb{R}^n$ at time t can be represented as

$$\mathbf{X}(t;\theta) = \sum_{i=0}^{n_r} \alpha_i(t)U_i(\theta); \quad \text{such that } U_i(\theta) : \mathbb{R}^n \times \theta \to \mathbb{R}^n,\ \alpha_i : T \to \mathbb{R} \quad \forall i \tag{28}$$

where $\mathbf{U}(\theta) = \{U_0, \ldots, U_{n_r}\}$ are the n_r stochastic reduced basis of the linear system and $\alpha = \{\alpha_1, \ldots, \alpha_{n_r}\}$ is the map of the time dependent stochastic coefficients to n_r undetermined coefficients. The identification of the principal modes $\mathbf{U}$ can be performed from the spectral decomposition of the stochastic Gramian $\mathbf{P}^2(\theta)$ using methods such as stochastic sampling. The simplest sampling based technique is the Monte Carlo method where the principal modes of $\mathbf{P}^2(\theta)$ for each stochastic sample θ of an ensemble of N random samples in $\Theta^{(M)}$ is solved to obtain $\mathbf{U}_\theta \in \mathbb{R}^{n\times n_r}$ for each random realization θ. Assuming that these modes are associated with the most dominant spectral components, we can expand them with orthogonal polynomials spanning the stochastic Hilbert space as $U_i(\theta) = \sum_{j=0}^{p} U_{ij}\mathscr{H}_j(\boldsymbol{\xi}(\theta))$ such that

$$U_{ij} = \frac{\left\langle \mathscr{H}_j(\boldsymbol{\xi}(\theta)), U_i(\theta)\right\rangle_{L^2(\Theta^{(M)})}}{\left\| \mathscr{H}_j^2(\boldsymbol{\xi}(\theta))\right\|_{L^2(\Theta^{(M)})}}; \quad U_{ij} \in \mathbb{R}^n. \tag{29}$$

However, this method is not favorable since obtaining ensemble of $U_i(\theta)$ for every random realization θ is computationally quite expensive. It is possible to use efficient stochastic sampling based techniques or other surrogate modeling to improve the evaluation of these bases functions [40–42].

A closer look into the problem of identification of the dominant modes of the stochastic transient system reveals that it is necessary to evaluate a vector basis $\mathbf{U}^r = \left[U_1^r, \ldots, U_{n_r}^r\right]$ such that it captures the solution of the stochastic finite element system within the time interval $t = [0, T]$ with sufficient accuracy. Hence, if we start with a generic framework of decomposition of the tensor product Hilbert space in which the stochastic transient solution exists (considered in the context of Eq. (28)) with a set of basis functions, we can write

$$\mathbf{X}(t,\theta) = \sum_{i\in\mathscr{I}_\alpha}\sum_{j\in\mathscr{I}_{\mathscr{H}}} \alpha_i\mathscr{H}_j(\theta)U_{ij}^r \tag{30}$$

where $U_{ij}^r \in \mathbb{R}^n$ are the reduced basis functions on which the solution is projected, $\mathscr{I}_\alpha$ and $\mathscr{I}_{\mathscr{H}}$ are the cardinality of the sets consisting of the undetermined coefficients α and the orthogonal stochastic functions $\mathscr{H}_j(\theta)$ respectively. The residual $\mathbf{R}(t;\theta) \in \mathbb{R}^n,\ \forall\theta \in \Theta^{(M)}$ associated with the stochastic transient FE linear system (given in Eq. (24)) is given as

$$\mathbf{R}(t;\theta) = \mathbf{C}\dot{\mathbf{X}}(t;\theta) + \mathbf{K}(\theta)\mathbf{X}(t;\theta) - \bar{\mathbf{B}}\mathbf{f}(t). \tag{31}$$

Here we apply the stochastic Galerkin method where the residual is made orthogonal to the basis U^r in $\mathbb{R}^n$ and the finite order orthogonal basis functions $\mathscr{H}(\theta)$ spanning the stochastic subspace $\Theta^{(M)}$. This can be written as

$$\left\langle \mathscr{H}_i(\theta)U_j^r, \mathbf{R}(t,\theta)\right\rangle_{\mathbb{R}^n\times L^2(\theta^{(M)})} = 0 \quad \forall i \in \mathscr{I}_{\mathscr{H}},\ \forall j \in \mathscr{I}_\alpha,\ \text{and } \forall t \in [0, T] \tag{32}$$

where $\mathbf{R}(t,\theta) : \mathbb{R}^n \times \Theta^{(M)} \rightarrow \mathbb{R}^n$ is the residual of the linear system given in Eq. (31). The identification of the dominant basis U^r has to be determined which is the focus of the following sections.

4.2. Vectorization of stochastic Lyapunov matrix equations

To obtain the reduced basis as discussed in Eq. (30) we focus on the stochastic controllability Gramian considered in Eq. (27). The stochastic realizations of the Gramian of the stochastic time varying linear system satisfies Eq. (27). The random quantity $\mathbf{P}^2(\theta)$ can be expressed as a series expansion of finite order chaos expansion in the stochastic Hilbert space with orthogonal polynomials as

$$\mathbf{P}^2(\theta) = \sum_{i \in \mathscr{I}_{\mathscr{H}}} \mathbf{P}_i \mathscr{H}_i\left(\boldsymbol{\xi}(\theta)\right). \tag{33}$$

The Lyapunov equation involving this stochastic controllability Gramian $\mathbf{P}^2(\theta)$ can be solved with the Galerkin method using this expansion. Applying the Galerkin orthogonalization of the residual to the orthogonal stochastic basis we have

$$\left\langle \mathscr{H}_i(\boldsymbol{\xi}(\theta)), \left(\mathbf{A}(\theta)\mathbf{P}^2(\theta) - \mathbf{P}^2(\theta)\mathbf{A}^T(\theta) + \mathbf{B}\mathbf{B}^T\right)\right\rangle_{L^2(\theta^{(M)})} = 0; \quad \forall\, i \in \mathscr{I}_{\mathscr{H}}. \tag{34}$$

In order to facilitate the matrix equation (such as the one given in Eq. (27)) to be expressed as a set of linear equations, we use the linear map $vec(\cdot)$ which describes a one to one mapping a set of k column vectors in the $n \times k$-dimensional matrix to a vector in the nk-dimensional space and is expressed as $vec(\mathbf{V}_{n\times k}) = \left[V_{11}, \ldots, V_{n1}, \ldots, V_{1k}, \ldots, V_{nk}\right]$. Using this linear map and the associated identities i.e. $vec(\mathbf{AXB}) = (\mathbf{B}^T \otimes \mathbf{A})vec(\mathbf{X})$, we can write Eq. (27) as

$$\begin{aligned} &vec\left(\mathbf{A}(\theta)\mathbf{P}^2(\theta) + \mathbf{P}^2(\theta)\mathbf{A}^T(\theta) + \mathbf{B}\mathbf{B}^T\right) = 0 \\ &\text{or,} \quad [\mathbf{I}\otimes\mathbf{A}(\theta) + \mathbf{A}(\theta)\otimes\mathbf{I}]\, vec\left(\mathbf{P}^2(\theta)\right) = -vec\left(\mathbf{B}\mathbf{B}^T\right) \end{aligned} \tag{35}$$

where $\mathbf{I} \in \mathbb{R}^{n\times n}$ is the identity matrix. Using this we can transform the expansion of the stochastic Gramian in Eq. (33) to

$$vec(\mathbf{P}^2(\theta)) = \sum_{i \in \mathscr{I}_{\mathscr{H}}} vec(\mathbf{P}_i)\mathscr{H}_i(\boldsymbol{\xi}(\theta)). \tag{36}$$

This vector form of the equation is utilized in the Galerkin framework in an identical manner as shown in Eq. (34) which can be written as

$$\left\langle \mathscr{H}_i(\boldsymbol{\xi}(\theta)), \left(\mathbf{A}(\theta)\sum_{i\in\mathscr{I}_{\mathscr{H}}} vec(\mathbf{P}_i)\mathscr{H}_i(\boldsymbol{\xi}(\theta))\right)\right\rangle_{L^2(\theta^{(M)})} = -\left\langle \mathscr{H}_i(\boldsymbol{\xi}(\theta)), vec(\mathbf{B}\mathbf{B}^T)\right\rangle_{L^2(\theta^{(M)})}; \quad \forall\, i \in \mathscr{I}_{\mathscr{H}} \tag{37}$$

where $\mathbf{A}(\theta) = [\mathbf{I}\otimes A(\theta) + A(\theta)\otimes\mathbf{I}]$. This gives a linear system of the form

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \cdots & \mathbf{A}_{1p} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathbf{A}_{p1} & \cdots & \cdots & \mathbf{A}_{pp} \end{bmatrix} vec\left(\begin{bmatrix} \mathbf{P}_1 \\ \vdots \\ \vdots \\ \mathbf{P}_p \end{bmatrix}\right) = vec\left(\begin{bmatrix} -\mathbf{B}\mathbf{B}^T \\ 0 \\ \vdots \\ 0 \end{bmatrix}\right) \tag{38}$$

where the matrix blocks $\mathbf{A}_{ij} = \left\langle \mathscr{H}_i(\boldsymbol{\xi}(\theta)), [\mathbf{I}\otimes\mathbf{A}(\theta) + \mathbf{A}(\theta)\otimes\mathbf{I}]\, \mathscr{H}_j(\boldsymbol{\xi}(\theta))\right\rangle_{L^2(\theta^{(M)})}$ involve inner product of the set of stochastic polynomials in $\mathscr{H}(\boldsymbol{\xi}(\theta))$. $\mathbf{P}_i$ are block matrices as given in Eq. (33) and the right hand side of the equation has only its first block as nonzero, while the rest are zero since $\mathrm{E}\left[\mathscr{H}_i(\theta)\right] = 0\ \forall i \neq 0$. The above system of linear matrix equations can be solved using solvers based on matrix factorization or Krylov based methods. For example, the Bartels–Stewart method [43] or the Hammarling method [44] involves reducing the coefficient matrix

to a real Schur form which involves a computational cost of $\mathcal{O}(N^3)$ where N is the dimension of the linear system. In the vectorized form, as shown in Eqs. (35) and (38), the dimension of the linear system to be solved is given as $N = n^2 n_p$ where n_p is given by the dimension of the stochastic system M and order of chaos expansion chosen p as $n_p = \binom{M}{p}$. After solving for the vectorized Lyapunov Gramian, the Gramian matrix $\mathbf{P}^2(\theta)$ can be reconstructed using the inverse mapping of the linear map used in Eq. (36). Hence solving the full vectorized Lyapunov equation can become extremely expensive even for moderate dimensions of input stochastic space.

4.3. Approximating the stochastic Gramian of the random system response

A closer look at the stochastic Gramian matrix $\mathbf{P}^2(\theta)$ reveals that for every random sample θ it can be written in $t \in [0, \infty)$ as

$$\mathbf{P}^2(\theta) = \int_0^\infty \exp\{\mathbf{A}(\theta)\, t\}\, \mathbf{B}\mathbf{B}^T \exp\left\{\mathbf{A}^T(\theta)\, t\right\} dt. \tag{39}$$

Since the exponential term could be represented in a series expandable form with stochastic coefficients, a general representation of this stochastic Gramian can be written as $\mathbf{P}(\theta) = \sum_{i=0}^{n_a} \bar{\lambda}_i(\theta)\bar{\mathbf{P}}_i$ like the expression in Eq. (33). It is seen that the time domain solution of the randomly parametrized system in Eq. (25) exists in the tensor product space $\mathcal{S}^{n,\theta}$ given by

$$\mathcal{S}^{n,\theta} := \mathbb{R}^n \otimes L^2(\Theta^M) \tag{40}$$

where $\mathbb{R}^n$ contains the solution at the n finite element nodes and $L^2(\Theta^{(M)})$ is a function space of the M-dimensional stochastic space defined by the iid random variables used to model the input uncertainty. Assuming that we choose n_a stochastic basis functions spanning an n_a dimensional subspace of the stochastic functions space $L^2(\Theta^{(M)})$ as $\mathscr{H}(\boldsymbol{\xi}(\theta)) = \left\{\mathscr{H}_0(\boldsymbol{\xi}(\theta)), \ldots, \mathscr{H}_{n_a}(\boldsymbol{\xi}(\theta))\right\}$, we can express the solution vector at time t as

$$\begin{aligned} &\mathbf{X}(t,\theta) = \sum_{i=1}^{n}\sum_{j=0}^{n_a} \mathbf{e}_i \mathscr{H}_j(\boldsymbol{\xi}(\theta)) x_{i,j} \quad \text{where } \mathbf{e}_i \in \mathbb{R}^n \\ &\text{or,} \quad \mathbf{X}(t,\theta) = \underline{\mathbf{X}}(t)\mathscr{H}(\boldsymbol{\xi}(\theta)) \end{aligned} \tag{41}$$

where $\underline{\mathbf{X}} \in \mathbb{R}^{n \times n_a}$ is a second order tensor associated with the canonical bases $\mathbf{e}_i$ of the Euclidean space $\mathbb{R}^n$ and $\mathscr{H}(\boldsymbol{\xi}(\theta))$ is the basis of the stochastic subspace spanned by the polynomial function elements of it. Now we apply the stochastic Galerkin method where the residual of the linear system is made orthogonal to the stochastic basis functions. Thus from Eq. (25) we write

$$\begin{aligned} &\left\langle \mathscr{H}_i(\boldsymbol{\xi}(\theta)), \left\{\dot{\underline{\mathbf{X}}}(t)\mathscr{H}(\boldsymbol{\xi}(\theta)) - \mathbf{A}(\theta)\underline{\mathbf{X}}(t)\mathscr{H}(\boldsymbol{\xi}(\theta)) + \mathbf{B}\mathbf{f}(t)\right\}\right\rangle_{L^2(\theta)} = 0 \\ &\qquad \text{which gives,} \quad \dot{\mathcal{X}}(t) = \mathcal{A}\mathcal{X}(t) + \mathcal{B}\mathcal{F}(t) \end{aligned} \tag{42}$$

where $\mathcal{A} \in \mathbb{R}^{N_a \times N_a}$ is a block sparse finite element system obtained with the finite order chaos expansion with stochastic Galerkin method. The objective of the model reduction scheme is to identify a dominant basis for the second order tensor $\underline{\mathbf{X}}$ with which the solution can be accurately approximated with lesser computational effort.

If the second order tensor $\underline{\mathbf{X}}$ is vectorized as $X_{\text{vec}} = vec(\underline{\mathbf{X}}) \in \mathbb{R}^{N_a}$ (where $N_a = n.n_a$), then it is possible to construct a squared Gramian matrix $\overline{\mathbf{W}}^2$ for the solution approximated in the tensor product space $S^{n,\theta}$ as

$$\overline{\mathbf{W}}^2 = \int_0^T \left\{X_{\text{vec},1}(t), \ldots, X_{\text{vec},k}(t)\right\} \left\{X_{\text{vec},1}(t), \ldots, X_{\text{vec},k}(t)\right\}^T dt \tag{43}$$

where $\overline{\mathbf{W}}^2 \in \mathbb{R}^{N_a \times N_a}$ is a Gramian of the system in the tensor product space spanned by $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\} \otimes \mathscr{H}(\boldsymbol{\xi}(\theta))$ and $\left\{X_{\text{vec},1}(t), \ldots, X_{\text{vec},k}(t)\right\}$ is a collection of k vectors each of dimension N_a which represent solutions at time t. This follows from the discussion of the controllability Gramian presented in Section 2.1. From this discussion it is

clear that the stochastic Gramian $\overline{W}^2$ in Eq. (45) is exact for the chosen order of chaos in expressing the solution of the randomly parametrized system in the tensor product space denoted by $\mathcal{S}^{n,\theta}$ in Eq. (40). It is readily seen that the Gramian $\overline{\mathbf{W}}^2$ satisfies the Lyapunov equation

$$\mathcal{A}\overline{\mathbf{W}}^2 + \overline{\mathbf{W}}^2\mathcal{A}^T = \mathcal{B}\mathcal{B}^T. \tag{44}$$

The above is a matrix equation of dimension $N_a \times N_a$ which is significantly larger than the size of the baseline finite element system. The dimension increases exponentially with the order of chaos and the dimension of the input stochastic space. The solution of this matrix equations can be performed with the available Lyapunov equation solver [45]. However, these solvers are computationally expensive and does not take advantage of the sparsity of the system matrices which is always obtained for large FE systems.

The spectral decomposition of the $\overline{\mathbf{W}}^2$ would give the dominant eigenmodes which form the basis of the reduced subspace in which the solution is sought [46]. The stochastic system solution with a finite order chaos expansion in $t = [0, T]$ can be approximated with the dominant modes obtained from the eigen decomposition of $\overline{\mathbf{W}}^2$ such that

$$\overline{\mathbf{W}}^2 = \overline{\boldsymbol{\Phi}}\boldsymbol{\Lambda}\overline{\boldsymbol{\Phi}}^T. \tag{45}$$

Here $\overline{\boldsymbol{\Phi}} = \left\{\overline{\phi}_i : \overline{\phi}_i^T\overline{\phi}_j = \delta_{ij},\ \overline{\phi}_i \in \mathbb{R}^{N_a}\ \forall\ i, j = 1, \ldots, n_r\right\}$ where n_r denotes the reduced number of eigenmodes chosen from the eigenvalue decomposition of $\overline{\mathbf{W}}^2$. The eigenvectors $\overline{\phi}_i \in \mathbb{R}^{N_\alpha}$ can be transformed via the inverse vectorization operator to the matrix $\overline{\boldsymbol{\phi}}_{i,n_a} \in \mathbb{R}^{n\times n_a}$ as $\overline{\boldsymbol{\phi}}_{i,n_a} = vec^{-1}(\overline{\phi}_i)\ \forall\ 1 \leqslant i \leqslant n_r$ such that $\overline{\boldsymbol{\phi}}_{i,n_a} = \left[\overline{\phi}_{i,1}\cdots\overline{\phi}_{i,n_a}\right]$ where $\overline{\phi}_{i,j} \in \mathbb{R}^n\ \forall\ j = 1, \ldots, n_a$. These, when used as the basis in $\mathbb{R}^{n\times n} \times \Theta^{(M)}$ on which the solution $\mathbf{X}(t;\theta)$ is projected, give

$$\mathbf{X}(t,\theta) = \sum_{i=1}^{n_r}\alpha_i(t)\sum_{j=1}^{n_a}\overline{\phi}_{i,j}\mathscr{H}_j(\boldsymbol{\xi}(\theta)). \tag{46}$$

Here the coefficients α_i capture the time varying component of the solution. A careful observation shows that the reduced order model of the system response is based on identifying the principal modes on which the solution can be projected in the tensor product space $\mathcal{S}^{n,\theta}$ (as given in Eq. (40)). Increasing the order of the minimal realization, i.e. using a higher number of basis functions $\overline{\boldsymbol{\phi}}_{i,n_a}$ from the spectral decomposition of $\overline{\mathbf{W}}^2$ does not increase the order of chaos functions used in approximating the solution. It only provides a better approximation of the solution in the stochastic space in which the Gramian $\overline{W}^2$ has been conceived.

Now solving the eigenvalue problem to identify the principal modes of the solution can become quite expensive when dealing with large finite element systems and even a moderate dimensional stochastic space. The primary obstacle is the solution of the matrix Lyapunov equations followed by the solving for the dominant eigenmodes of the Gramian. This serves as the motivation to look for alternate techniques to identify the principal modes of the Gramian of the stochastic state space system [47].

It might be noted here that we do not actually require the estimate of the Gramian $\overline{\mathbf{W}}^2$, rather it is only necessary to obtain the principal modes of this Gramian. This motivates us to seek a low-rank approximation $\overline{\mathbf{W}}^2_*$ of the Gramian such that $\left\|\overline{\mathbf{W}}^2 - \overline{\mathbf{W}}^2_*\right\|_{\mathrm{F}}$ is minimized where $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius matrix norm. This has been looked at in the following section.

4.4. Arnoldi's method for decomposition of Gramian matrix

An eigenvalue decomposition of the matrix $\overline{\mathbf{W}}^2$ is given in Eq. (45) where the eigenvalues in the diagonal matrix Λ is assumed to be ordered as $|\lambda_1| \geqslant \cdots \geqslant |\lambda_{N_a}|$. If we choose only the first n_r modes from this set then the approximate Gramian is given as $\overline{\mathbf{W}}^2_* = \overline{\boldsymbol{\Phi}}_{n_r}\boldsymbol{\Lambda}_{n_r}\overline{\boldsymbol{\Phi}}_{n_r}$. If we choose a basis $\mathbf{U}_{n_r} \in \mathbb{R}^{N_a\times n_r}$ on which the Gramian $\overline{\mathbf{W}}^2$ is projected, we can write the Lyapunov equation in Eq. (44) as

$$\mathbf{U}_{n_r}^T\mathcal{A}\mathbf{U}_{n_r}\mathcal{W} + \mathcal{W}\mathbf{U}_{n_r}^T\mathcal{A}^T\mathbf{U}_{n_r} = -\mathbf{U}_{n_r}^T\mathcal{B}\mathcal{B}^T\mathbf{U}_{n_r}. \tag{47}$$

Using this, the approximate Gramian is given by $\overline{\mathbf{W}}_*^2 = \mathbf{U}_{n_r} \mathcal{W} \mathbf{U}_{n_r}^T$. The accuracy of the solution is governed by the selection of the basis $\mathbf{U}_{n_r}$ which should span the same n_r dimensional subspace as that spanned by the vectors in $\overline{\boldsymbol{\Phi}}_{n_r}$.

This motivates us to identify the subspace associated with the dominant modes of the stochastic system matrices present in the Lyapunov equations. We start with the m-dimensional Krylov subspace associated with the system matrices obtained after applying the stochastic Galerkin method as

$$\mathcal{K}_m \{\mathcal{A}, \mathcal{B}\} = \text{span} \left\{ \mathcal{B}, \mathcal{A}\mathcal{B}, \mathcal{A}^2\mathcal{B}, \ldots, \mathcal{A}^{m-1}\mathcal{B} \right\}. \tag{48}$$

For $\mathcal{B} \in \mathbb{R}^{n \times q}$ with q inputs, the block Krylov method would be considered where the dimension of the Krylov space would become $m \times q$. The block Arnoldi algorithm [48] is used to calculate the orthonormal basis Q spanning the m dimensional dominant eigenspace. This consists of the following steps

Estimation of the Arnoldi–Lyapunov bases for reduced order modeling of stochastic system

1. *Initialize* $\mathbf{Q} = [\mathbf{Q}_1]$ *such that* $\mathbf{Q}_1 \in \mathbb{R}^{n \times q}$ *with an orthogonal basis spanning the column space of* $\mathcal{B}$.
2. *Calculate the orthogonal bases spanning the* n_k *dimensional block Krylov space given by*

$$\mathcal{K}_{n_k}(\mathcal{A}, \mathcal{B}) = \text{span} \left\{ \mathcal{B}, \mathcal{A}\mathcal{B}, \mathcal{A}^2\mathcal{B}, \ldots, \mathcal{A}^{n_k-1}\mathcal{B} \right\}$$

   using a Gram–Schmidt process or a modified Gram–Schmidt process to get the set of orthogonal vector bases $\mathbf{Q} = \left\{ \mathbf{Q}_1, \mathbf{Q}_2, \ldots, \mathbf{Q}_{n_k} \right\}$ *where* $\mathbf{Q}_i \in \mathbb{R}^{n \times q}$ $\forall i = 1, \ldots, n_k$.
3. *To use an error indicator as a stopping criterion, use the following steps*
   (a) *Calculate the block upper Hessenberg matrix* $\mathcal{A}_{qn_k} \in \mathbb{R}^{qn_k \times qn_k}$ *such that* $\mathcal{A}_{qn_k} = \mathbf{Q}^T \mathcal{A} \mathbf{Q}$ *and denoting the residual of the Lyapunov equation as* $\mathcal{R}(\overline{\mathbf{W}}_*^2) = \mathcal{A}(\mathbf{Q}\overline{\mathbf{W}}_*^2\mathbf{Q}^T) + (\mathbf{Q}\overline{\mathbf{W}}_*^2\mathbf{Q}^T)\mathcal{A}^T + \mathcal{B}\mathcal{B}^T$ *we apply a Galerkin type orthogonalization of the residual to the Krylov space* $\mathcal{K}_{n_k}(\mathcal{A}, \mathcal{B})$ *to obtain the problem statement*

$$\text{find } \overline{\mathbf{W}}_*^2 \text{ such that } \mathbf{Q}^T \mathcal{R}(\overline{\mathbf{W}}_*^2)\mathbf{Q} = 0.$$

   This gives an estimate of the reduced Lyapunov solution vector $\overline{\mathbf{W}}_*^2$
   (b) *If the residual norm* $\left\| \mathcal{R}(\overline{\mathbf{W}}_*^2) \right\|_{\text{F}} > \epsilon$, *increase the value of* n_k *and include more Krylov bases from step 2 and repeat the previous steps.*
4. *Obtain the reduced order Lyapunov solution as* $\mathbf{Q}\overline{\mathbf{W}}_*^2\mathbf{Q}^T$.

It has been shown in [49] that the Galerkin type orthogonalization of the residual to the orthogonal basis $\mathbf{Q}$ as $\mathbf{Q}^T R(X_{qn_k})\mathbf{Q} = 0$ is satisfied if and only if $\overline{\mathbf{W}}_*^2$ satisfies the reduced Lyapunov equation

$$\mathcal{A}_{qn_k}\overline{\mathbf{W}}_*^2 + \overline{\mathbf{W}}_*^2\mathcal{A}_{qn_k}^T + \mathcal{B}_{qn_k}\mathcal{B}_{qn_k}^T = 0 \tag{49}$$

where $\mathcal{B}_{qn_k} = \mathbf{Q}^T\mathcal{B}$. The orthogonal basis $\mathbf{Q} \in \mathbb{R}^{n \times qn_k}$ spanning the Krylov subspace approximates the Gramian matrix $\overline{\mathbf{W}}^2$ as

$$\overline{\mathbf{W}}^2 = \mathbf{Q}\overline{\mathbf{W}}_*^2\mathbf{Q}^T. \tag{50}$$

We can use these orthogonal basis functions to approximate the solution of the linear system in Eq. (42). Approximating $\mathcal{X}(t) = \mathbf{Q}\mathcal{X}_{qn_k}(t)$ and $\dot{\mathcal{X}}(t) = \mathbf{Q}\dot{\mathcal{X}}_{qn_k}(t)$ we have the linear system as

$$\dot{\mathcal{X}}_{qn_k}(t) = \mathcal{A}_{qn_k}\mathcal{X}_{qn_k}(t) + \mathcal{B}_{qn_k}(t). \tag{51}$$

The above system can be resolved with any time integration scheme such as the explicit Runge–Kutta type methods or the implicit time stepping schemes (such as Euler's method).

The error estimation procedure which is used as a stopping criterion to restrict the Krylov space dimension to an optimum value is a computationally expensive procedure which has a computational complexity of $\mathcal{O}\left((qn_k)^3\right)$. Hence in the above discussed Arnoldi algorithm, the error estimation step is included not after every step of the block Krylov basis evaluation but only after certain manually chosen intervals to enhance the computational efficiency of the method.

For descriptor systems of the form given in Eq. (24) it is not always computationally advantageous to take the inverse of the $\mathcal{C}$ matrix and take the equation in standard form as given in Eq. (25). This makes the system lose its

sparsity pattern and hence the storage requirement for the matrix $\mathbf{A}$ in Eq. (42) becomes huge. This is especially disadvantageous when solving the randomly parametrized system with the stochastic Galerkin method which results in a block sparse coefficient matrix composed of the individual blocks of the system matrix. Hence the descriptor form is more suitable especially for FE linear systems. The Lyapunov theory for descriptor systems is available [50,51], but it requires extensive matrix–matrix products which destroys the desired sparsity of the system once again. Noting that the parametric uncertainty in the system is present in the form of the random diffusion coefficient only, it is readily seen that using the spectral Galerkin method we get a matrix $\mathcal{C}$ which is block diagonal in nature. The product of a block-diagonal matrix and another block-sparse matrix preserves the block sparse nature of the latter matrix. Thus storing the inverse of the matrix essentially requires the storing of just the deterministic baseline matrix as $\mathbf{C}^{-1}$ and the block diagonal inverse of the matrix $\mathcal{C}$ is given as $\left[\mathcal{C}^{-1}\right]_{ii} = \left(1/\left\langle \mathscr{H}_i \right\rangle^2\right) C^{-1}$ where $\left[\mathcal{C}^{-1}\right]_{ii}$ is the ith diagonal block of $\mathcal{C}^{-1}$. This is an advantageous situation for the implementation of the Krylov based methods. Hence the Krylov space can be formed such that the $\mathcal{C}$ matrix is used as a preconditioner, i.e.

$$\mathcal{K}_{n_k}\left(\mathcal{C}^{-1}\mathcal{K}, \mathcal{C}^{-1}\bar{\mathcal{B}}\right) = \text{span}\left\{\mathcal{C}^{-1}\bar{\mathcal{B}}, \left(\mathcal{C}^{-1}\mathcal{K}\right)\mathcal{C}^{-1}\bar{\mathcal{B}}, \left(\mathcal{C}^{-1}\mathcal{K}\right)^2\mathcal{C}^{-1}\bar{\mathcal{B}}, \ldots, \left(\mathcal{C}^{-1}\mathcal{K}\right)^{n_k}\mathcal{C}^{-1}\bar{\mathcal{B}}\right\}. \tag{52}$$

The modified Gram–Schmidt orthogonalization applied to these basis vectors would create an orthonormal basis $\mathbf{Q}_d$ which gives the upper Hessenberg matrix $\mathcal{A}_{qn_k} = \mathbf{Q}_d^T\left(\mathcal{C}^{-1}\mathcal{K}\right)\mathbf{Q}_d^T$. Thus the descriptor system, when solved with this vector basis gives

$$\mathcal{C}_{qn_k}\dot{\mathcal{X}}_{qn_k} = \mathcal{K}_{qn_k}\mathcal{X}_{qn_k}(t) + \bar{\mathcal{B}}_{qn_k}(t) \quad \text{where } \mathcal{C}_{qn_k} = \mathbf{Q}_d^T\mathcal{C}\mathbf{Q};\ \mathcal{K}_{qn_k} = \mathbf{Q}_d^T\mathcal{K}\mathbf{Q}. \tag{53}$$

The original solution is obtained using the transformation $\mathcal{X}(t) = \mathbf{Q}_d\mathcal{X}_{qn_k}(t)$. In the following section we discuss the method for updating the dominant subspace which involves a recalculation of the basis functions using a restarted Arnoldi algorithm.

4.5. Implicit restarting of Arnoldi–Lyapunov basis evaluation

The Arnoldi vectors derived using the Arnoldi–Lyapunov algorithm relies on the system solution of the LTI finite element system with a finite order chaos expansion using a time integration technique. An implicit time marching algorithm, such as Euler's central difference scheme relies on evaluating the forcing terms and the response quantities at the center of each time step. Let us consider a transient LTI diffusion system (in the descriptor form) with a random diffusion coefficient (given in Eq. (24)) expressed with finite order chaos expansion of the input random variables as

$$\mathcal{C}\dot{\mathcal{X}}(t) + \mathcal{K}\mathcal{X}(t) = \bar{\mathcal{B}}\mathcal{F}(t). \tag{54}$$

Solving this system with Euler's central difference scheme, we choose to divide the time domain of interest into a finite number of divisions. The time step size is governed by the dynamics of the system and is chosen such that it is within the characteristic time length of the dynamic system. The linear system giving the solution at $t = T_{n+1}$ is

$$\left([\mathcal{C}] + [\mathcal{K}]\frac{\Delta t}{2}\right)\mathcal{X}_{n+1} = F_{n+1}\left(\mathcal{F}(T_{n+1}), \mathcal{F}(T_n), \mathcal{X}_n, \mathcal{C}, \mathcal{K}, \bar{\mathcal{B}}\right) \tag{55}$$

where the forcing at the step T_{n+1} is given by a combination of the forcing at steps T_{n+1} and T_n along with the response at the previous step n given by $\mathcal{X}_n$. The Arnoldi–Lyapunov algorithm given in Section 4.4 starts with the matrices $\mathcal{C}$, $\mathcal{K}$ and $\bar{\mathcal{B}}$ to evaluate the dominant basis with which the LTI system solution can be approximated. However, as the time marching algorithm tries to capture long time integration response, it might occur for rapidly changing systems that the basis functions fail to capture the response with sufficient accuracy or the solution might diverge altogether. A recalculation of the Arnoldi bases under such conditions would avoid a breakdown of the proposed scheme in Section 4.4.

To implement this, we consider the right hand side of the linear system in Eq. (55) obtained with Euler's central difference scheme. Thus

$$\left([\mathcal{C}] + [\mathcal{K}]\frac{\Delta t}{2}\right)\mathcal{X}_{n+1} = \bar{\mathcal{B}}\left(\frac{\mathcal{F}_{n+1} + \mathcal{F}_n}{2}\right) + \bar{\mathcal{X}}_n \quad \text{where } \bar{\mathcal{X}}_n = \left([\mathcal{C}] + [\mathcal{K}]\frac{\Delta t}{2}\right)\mathcal{X}_n. \tag{56}$$

The Arnoldi–Lyapunov algorithm is initialized to evaluate the basis functions of the dominant Krylov subspace $\mathcal{K}_{n_k}\left(\mathcal{C}^{-1}\mathcal{K}, \mathcal{C}^{-1}\mathcal{B}\right)$. But additional information on the right side of Eq. (56) is available in the form of the vector $\bar{\mathcal{X}}_n$. This can be incorporated into the Arnoldi basis calculation to obtain a better estimate of reduced subspace in which the solution exists.

For the sake of simplicity, first we refer to the baseline LTI system in Eq. (3), in which, the state transition matrix, given as $\boldsymbol{\psi}(t,\tau)$, takes the form of $\exp\{\mathbf{A}(t-\tau)\}$. This is utilized to get the response of the system at time t subject to an initial condition $\mathbf{X}_0$ as $\mathbf{X}(t) = \boldsymbol{\psi}(t,t_0)\mathbf{X}_0$ with $t_0 = 0$. Hence the response of the LTI system at every $t \in [0,\infty)$ to the initial condition specified by $\mathbf{X}(t_0)$ and the forcing $\mathbf{Bf}(t)$ is given as

$$\mathbf{X}(t) = \boldsymbol{\psi}(t,t_0)\mathbf{X}_0 + \int_0^t \boldsymbol{\psi}(t,\tau)\mathbf{Bf}(\tau)d\tau. \tag{57}$$

In the absence of a forcing term, i.e. if $\mathbf{f}(\tau) = 0$, and with a prescribed initial condition $\mathbf{X}_0$, the response $\mathbf{X}(t)$ would only consist of $\mathbf{X}(t) = \mathbf{X}_0 \exp\{\mathbf{A}t\}$. Here we note the identity $(G * \delta) = G$ for any bounded function G and unit impulse (or delta) function δ, where '$*$' denotes the convolution operation. Using this the response $\mathbf{X}(t)$ in the above equation can be written as

$$\mathbf{X}(t) = \boldsymbol{\psi}(t,\tau) * (\mathbf{X}_0\delta(\tau) + \mathbf{Bf}(\tau)) = \boldsymbol{\psi}(t,\tau) * [\mathbf{X}_0 \;\; \mathbf{B}]\,[\delta(\tau) \;\; \mathbf{f}(\tau)]^T \tag{58}$$

where $\delta(t)$ is the delta distribution, $[\mathbf{X}_0 \;\; \mathbf{B}] \in \mathbb{R}^{n\times(q+1)}$ is the matrix combining the vector $\mathbf{X}_0 \in \mathbb{R}^n$ and matrix $\mathbf{B} \in \mathbb{R}^{n\times q}$, while $[\delta(\tau) \quad \mathbf{f}(\tau)] \in \mathbb{R}^{q+1}$ is the combined vector of the delta function and the q input functions. Assuming that the system is stable under the action of all piecewise continuous bounded functions in $[0, T]$, we can identify a modified Gramian matrix which satisfies the Lyapunov equations

$$\mathbf{A}\overline{\mathbf{W}}_m^2 + \overline{\mathbf{W}}_m^2\mathbf{A}^T + \mathbf{B}_x\mathbf{B}_x^T = 0 \tag{59}$$

where $\mathbf{B}_x = [\mathbf{X}_0 \;\; \mathbf{B}] \in \mathbb{R}^{n\times(q+1)}$. This form is particularly conducive for constructing (or restarting) the Arnoldi–Lyapunov algorithm discussed in Section 4.4. We can now incorporate the vector of the initial condition to the force locator matrix $\mathbf{B}$ which would be taken into account while constructing the block Krylov bases with the force locator matrix $\mathbf{B}_x$.

Extension of the above discussion to the randomly parametrized LTI system in Eq. (42) is straightforward. It is seen that the modified block Krylov algorithm restarted at an arbitrary time step t_{r+1} where the solution $\mathcal{X}_r = \mathcal{X}(t = t_r)$ at the step t_r is available would consider the matrix $\mathcal{B}_x = [\mathcal{X}_r \;\; \mathcal{B}]$ and form the Krylov bases as

$$\mathcal{K}_{n_k}^r(\mathcal{A}, \mathcal{B}_x) = \text{span}\left\{\mathcal{B}_x, \mathcal{A}\mathcal{B}_x, \mathcal{A}^2\mathcal{B}_x, \ldots, \mathcal{A}^{n_k-1}\mathcal{B}_x\right\}. \tag{60}$$

Additionally, when we start the Krylov basis evaluation with initial condition set to zero, the above Krylov space is equivalent to the one obtained with $\mathcal{K}_{n_k}(\mathcal{A}, \mathcal{B})$ as given in Section 4.4.

Thus the scheme of restarting the Arnoldi–Lyapunov vector estimation implicitly after finite intervals of time consists of the following steps

Implicit restarting of Arnoldi–Lyapunov basis evaluation for time integration

1. *Initialize the global error indicator ε_g, the Arnoldi–Lyapunov convergence criterion ϵ_{AL}, implement the prescribed initial condition $\mathcal{X}_r = \mathcal{X}_0$, initialize $r = 0$.*
2. *Set up the LTI system using the central difference the time marching algorithm (as per Eq. (55)) and implement the initial and boundary conditions. Begin evaluation of the Arnoldi vectors on which the solution would be projected as follows:*
   (a) *Set $\mathbf{Q} = \mathbf{Q}_1$ such that $\mathbf{Q}_1$ are the orthogonal basis spanning the column space of*
   $$\mathcal{B}_x = [\mathcal{X}_r \;\; \mathcal{B}] \in \mathbb{R}^{n\times(q+1)}. \tag{61}$$
   (b) *Initialize n_k and calculate the orthogonal bases spanning the n_k dimensional block Krylov space given by*
   $$\mathcal{K}_{n_k}(\mathcal{A}, \mathcal{B}_x) = \text{span}\left\{\mathcal{B}_x, \mathcal{A}\mathcal{B}_x, \mathcal{A}^2\mathcal{B}_x, \ldots, \mathcal{A}^{n_k-1}\mathcal{B}_x\right\}$$
   using a modified Gram–Schmidt process to get the set of orthogonal vector bases $\mathbf{Q} = \left\{\mathbf{Q}_1, \mathbf{Q}_2, \ldots, \mathbf{Q}_{n_k}\right\}$ where $\mathbf{Q}_i \in \mathbb{R}^{n\times q}\ \forall i = 1, \ldots, n_k$.

(c) *The error indicator to evaluate the optional Krylov space dimension is determined as*

i. *Evaluate block upper Hessenberg matrix* $\mathcal{A}_{qn_k} = \mathbf{Q}^T \mathcal{A} \mathbf{Q}$; $\mathcal{A}_{qn_k} \in \mathbb{R}^{qn_k \times qn_k}$ *along with the Lyapunov residual* $\mathcal{R}(\overline{\mathbf{W}}_*^2) = \mathcal{A}(\mathbf{Q}\overline{\mathbf{W}}_*^2\mathbf{Q}^T) + (\mathbf{Q}\overline{\mathbf{W}}_*^2\mathbf{Q}^T)\mathcal{A}^T + \mathcal{B}\mathcal{B}^T$.

ii. *Apply Galerkin type orthogonalization of the residual to the Krylov space* $\mathcal{K}_{n_k}(\mathcal{A}, \mathcal{B})$:

$$\text{find } \overline{\mathbf{W}}_*^2 \text{ such that } \mathbf{Q}^T \mathcal{R}(\overline{\mathbf{W}}_*^2)\mathbf{Q} = 0$$

This gives an estimate of the reduced Lyapunov solution vector $\overline{\mathbf{W}}_*^2$

iii. *If the residual norm* $\left\| \mathcal{R}(\overline{\mathbf{W}}_*^2) \right\|_{\mathrm{F}} > \epsilon_{AL}$, *increase the value of* n_k *and include more Krylov bases from step 3 and repeat the previous steps.*

(d) *Project the solution on the Arnoldi–Lyapunov vectors as* $\mathcal{X}(t) = \mathbf{Q}\mathcal{X}_{qn_k}(t)$ *and solve the LTI system using the central difference scheme at subsequent time steps as*

$$\mathbf{Q}^T \left([\mathcal{C}] + [\mathcal{K}] \frac{\Delta t}{2} \right) \mathbf{Q} \bar{\mathcal{X}}_{n+1} = \mathbf{Q}^T F_{n+1} \left(\mathcal{F}(T_{n+1}), \mathcal{F}(T_n), \mathbf{Q}\bar{\mathcal{X}}_n, \mathcal{C}, \mathcal{K}, \bar{\mathcal{B}} \right) \tag{62}$$

with the solution at discrete time steps given by $\mathcal{X}_{n+1} = \mathbf{Q}\bar{\mathcal{X}}_{n+1}$.

(e) *Calculate the* L^2 *norm of the residual vector of the LTI system at time step* T_{n+1} *given by*

$$\mathcal{R}_{n+1} = \left([\mathcal{C}] + [\mathcal{K}] \frac{\Delta t}{2} \right) \mathcal{X}_{n+1} - F_{n+1} \left(\mathcal{F}(T_{n+1}), \mathcal{F}(T_n), \mathbf{Q}\mathcal{X}_n, \mathcal{C}, \mathcal{K}, \bar{\mathcal{B}} \right) \tag{63}$$

as $\|\mathcal{R}_{n+1}\|_2$.

(f) *If* $\|\mathcal{R}_{n+1}\|_2 > \varepsilon_g$ *then go to step* 2 *of the algorithm and restart the calculation of the Arnoldi–Lyapunov basis evaluation with* $\mathcal{X}_r = \mathcal{X}_n$. *Otherwise if* $\|\mathcal{R}_{n+1}\|_2 \leqslant \varepsilon_g$, *goto step (d) and carry on with the time marching algorithm.*

3. *The solution vector at the discrete time steps* $i = 1, 2, \ldots, n$ *is given by the vectors* $\mathcal{X}_i$.

The above algorithm ensures that the accuracy of the solution of the randomly parametrized LTI system obtained at all time steps do not fall below the prescribed value ε_g. The check for the residual of the linear system for the implicit restarting can be performed after every few time steps as governed by the accuracy requirement of the problem and also the consideration for the additional cost associated with the residual evaluation. It might be pointed out the choice of the number of Arnoldi–Lyapunov basis functions and the frequency of restart are interrelated for stable time evolving systems. Choosing a large number of Arnoldi–Lyapunov bases can ensure good approximation accuracy of the solution over a long time integration, however, an additional cost is associated with it. On the other hand, evaluation of a revised set of Arnoldi–Lyapunov vectors also increases the computational overhead of the solver. Hence the choice of the number of Arnoldi–Lyapunov vector basis (i.e. the reduced subspace dimension) and the interval after which the Arnoldi–Lyapunov basis estimation is restarted are complimentary aspects of the numerical algorithm and has to be judiciously chosen to optimize the efficiency of the solver.

4.6. Computational complexity

The computational advantage of the proposed minimal realization technique for stochastic systems with Arnoldi–Lyapunov basis vectors is discussed here. Evaluation of the n_k Arnoldi–Lyapunov bases (each of dimension n) requires $n_k \mathcal{O}(n^2)$ floating point operations [52]. Additionally, the error estimator which is used as a stopping criterion for the Arnoldi–Lyapunov iterative method has a complexity of the order $\mathcal{O}\left((qn_k)^3\right)$ where q is the number of inputs in the stochastic LTI system. Since evaluating the error estimator is a computationally expensive operation, it is not repeated for every evaluation of the Arnoldi–Lyapunov basis vector. We assume here that the estimation of the error evaluation occurs at every n_{err} interval where $n_{\mathrm{err}} < n_k$. Hence the number of error estimations involved in evaluating n_k Arnoldi–Lyapunov bases is $\lfloor n_k/n_{\mathrm{err}} \rfloor$ where $\lfloor \bullet \rfloor$ denotes the floor function. Hence the total computational complexity for evaluating n_k Krylov bases with an error estimation performed at every n_{err} steps is $N_{\mathrm{comp}} = n_k \mathcal{O}(n^2) + \lfloor n_k/n_{\mathrm{err}} \rfloor \mathcal{O}\left((qn_k)^3\right)$.

Once the reduced number of Arnoldi–Lyapunov bases (n_k) has been calculated, the solution of the LTI stochastic system is projected on to these bases and a central difference time stepping algorithm is implemented. The resulting linear system has a dimension of $n_k \times n_k$. The computational complexity of evaluating the stochastic time domain

response at n_t time steps of a system is then $n_t \mathcal{O}(n_k^3)$, since the resolution of a linear system of dimension n_k is $\mathcal{O}(n^3)$. Hence the total cost of resolution of the stochastic LTI with reduced number of Arnoldi–Lyapunov vectors is

$$N_{AL} = n_k \mathcal{O}(n^2) + \lfloor n_k / n_{\text{err}} \rfloor \, \mathcal{O}\left((q n_k)^3\right) + n_t \mathcal{O}\left(n_k^3\right). \tag{64}$$

The restart points are judiciously chosen in order to keep the cost of evaluating the expensive error estimators at minimum.

In comparison, the resolution of the full stochastic LTI system without applying any model reduction technique is given as $n_t \mathcal{O}(n^3)$ where we assume that the cost of resolution of a $n \times n$ linear system is $\mathcal{O}(n^3)$. It has to be noted though that the latter estimation corresponds to the worst case scenario. Linear solvers based on Krylov methods can speed up the solution for sparse linear systems using optimal preconditioners. But, we choose $\mathcal{O}(n^3)$ as the baseline value against which we compare the efficiency of the proposed method. With the reduced n_k bases, the resolution of the transient response is for n_t time steps costs $n_t \mathcal{O}(n_k^3)$ compared to $n_t \mathcal{O}(n^3)$ without any model reduction. Here $n_k \ll n$, hence the cost of time integration of the reduced system is much less than that of the full system. The additional cost of evaluating the Arnoldi–Lyapunov bases is given by N_{comp} which depends on n as $n_k \mathcal{O}(n^2)$. Hence the cost for evaluating the reduced bases is less by about an order of (n/n_k) than the full system solution. The cost for restarting the solver is calculated by assuming that the solver is restarted at time steps $\{n_{t_1}, n_{t_2}, \ldots, n_{t_r}\}$, thus there are r restarts, and that the number of reduced Arnoldi–Lyapunov vectors used to calculate the response at each restart is $\{n_{k_0}, n_{t_1}, \ldots, n_{k_r}\}$. This results in the Arnoldi–Lyapunov vector basis calculation being repeated r times which entails a cost of

$$N_{AL_r} = \sum_{i=0}^{r} \left[n_{k_i} \mathcal{O}(n^2) + \lfloor n_{k_i} / n_{\text{err}} \rfloor \, \mathcal{O}\left(\left(q n_{k_i}\right)^3\right) + \left(n_{t_{i+1}} - n_{t_i}\right) \mathcal{O}\left(n_{k_i}^3\right) \right] \tag{65}$$

with $n_{t_0} = 0$ and $n_{t_{r+1}} = n_t$. From the above expression, it can be seen that the computational complexity is given as a square of the dimension of the full system n multiplied by the number of basis in each stage of the Arnoldi–Lyapunov calculation. This is less than the full system resolution by one order of n at each time step. Moreover, the dependence of the computational complexity on the square of the dimension of the full system (as in Eq. (64)) is weighted only by the number of reduced basis which is less than n_t. If we increase the number of time steps the Arnoldi–Lyapunov algorithm becomes more advantageous since the cost of the full system resolution increases linearly with the number of time steps weighted by the cube of the linear system dimension. On the other hand for the reduced order model, the computational cost also varies linearly with the number of time steps but is weighted by the cube of the dimension of the reduced system n_k only. Hence this offers a significant computational advantage.

5. Numerical results

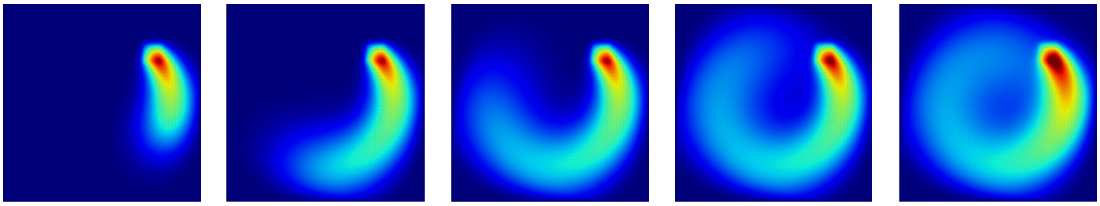
In this section we present the results obtained from the numerical simulation of the transient response of various randomly parametrized LTI dynamical systems whose solution has been obtained with the proposed reduced Arnoldi–Lyapunov basis vectors spanning a dominant subspace of the solution.

5.1. Advection-diffusion–reaction system

Here consider the finite element simulation of a large advection–diffusion–reaction system to demonstrate the applicability of the proposed Arnoldi–Lyapunov reduced basis for the resolution of its time domain response. We consider the geometrical properties of the advection–diffusion–reaction system as described in [53] such that the physical domain $\mathscr{D} \in \mathbb{R}^2$ is a square contained in $[0, 1] \times [0, 1]$ and the time domain of interest is $t = [0, 0.03]$. The coordinate axes are denoted by (r, s). The governing equation is given as

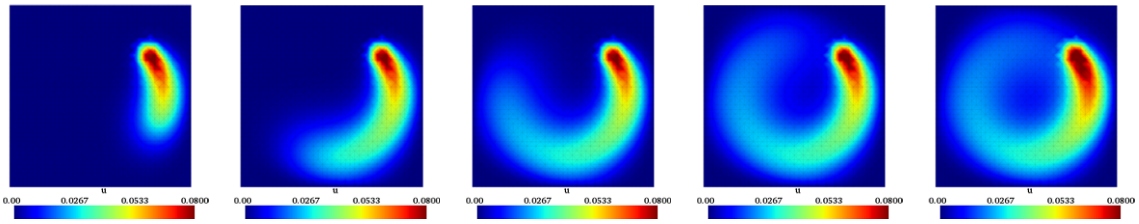
$$\begin{aligned} &\dot{x} - \nabla\left(k(\theta) \nabla x\right) + c \cdot \nabla x + \sigma x = f \\ &x = 0 \quad \text{on } \partial\mathscr{D} \times t \\ &x = 0 \quad \text{on } \mathscr{D} \times \{0\} \end{aligned} \tag{66}$$

where the diffusion coefficient has been modeled as a lognormal random field with mean value of 1.0 and standard deviation of 0.5. The constant c is chosen to be spatially varying as $c = 250\left(s - \frac{1}{2}, \frac{1}{2} - r\right)$ and $f(r, s, t) = 100$ on



(a) $t = 1T_{\text{tot}}/5$. (b) $t = 2T_{\text{tot}}/5$. (c) $t = 3T_{\text{tot}}/5$. (d) $t = 4T_{\text{tot}}/5$. (e) $t = 5T_{\text{tot}}/5$.

Fig. 1. Reference solution of the deterministic model of the advection–diffusion–reaction problem on a square domain.



(a) $t = 1T_{\text{tot}}/5$. (b) $t = 2T_{\text{tot}}/5$. (c) $t = 3T_{\text{tot}}/5$. (d) $t = 4T_{\text{tot}}/5$. (e) $t = 5T_{\text{tot}}/5$.

Fig. 2. Mean response of the stochastic model problem with a lognormal random diffusion coefficient using a 4th order polynomial chaos expansion.

the square sub-domain $[0.7, 0.8] \times [0.7, 0.8]$. This emulates a velocity field which rotates in the clockwise direction with its center at $\left(\frac{1}{2}, \frac{1}{2}\right)$. The physical domain has been meshed with isoparametric quadrangular elements of order 2 and the time range of interest $t = [0, 0.03]$ has been divided into 100 uniform intervals.

The random field $k(\theta)$ is characterized with an exponential covariance kernel. The finite dimensional representation of the random field is given with 4 iid random variables $\boldsymbol{\xi}(\theta) = \{\xi_1, \ldots, \xi_4\}$ with Hermite chaos. The finite element treatment of the stochastic dynamical system given in Eq. (66) results in system matrices of the form

$$\mathbf{C}\dot{\mathbf{X}}(t;\theta) + \mathbf{K}(\theta)\mathbf{X}(t;\theta) = \bar{\mathbf{B}} f(t) \tag{67}$$

where $\mathbf{K}(\theta) = \sum_{i=0}^{M} \mathbf{K}_i \mathscr{H}_i(\boldsymbol{\xi}(\theta))$ is the series representation of the system matrix with a random diffusion coefficient. A stochastic Galerkin projection of the solution on the orthogonal basis functions $\mathscr{H}(\boldsymbol{\xi}(\theta)) = \left\{\mathscr{H}_0(\boldsymbol{\xi}(\theta)), \ldots, \mathscr{H}_p(\boldsymbol{\xi}(\theta))\right\}$ leads to a block sparse system of equations as

$$\left\langle \mathscr{H}_i(\boldsymbol{\xi}(\theta)), \left(\mathbf{C}\dot{\mathbf{X}}(t,\theta) + \mathbf{K}(\theta)\mathbf{X}(t,\theta) - \bar{\mathbf{B}} f(t)\right)\right\rangle_{L^2(\theta)} = 0; \quad \forall i = 0, \ldots, p$$

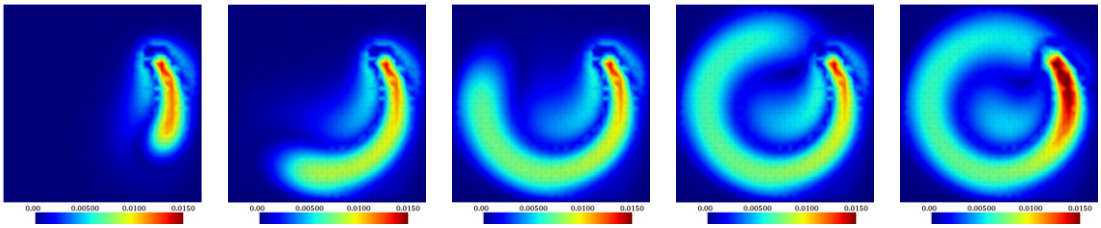
$$\text{which gives} \quad \mathcal{C}\dot{\mathcal{X}}(t) + \mathcal{K}\mathcal{X}(t) = \bar{\mathcal{B}} f(t) \tag{68}$$

where $\mathcal{C}$ is a block diagonal matrix, with $\mathcal{K}$ being a block sparse matrix and $\mathcal{X}(t)$ is a $n(p+1)$ vector denoting the stochastic system response, where n is the number of degrees of freedom associated with the finite element system. It can be seen from the above equations that the system given in Eq. (66) gives rise to an unsymmetrical coefficient matrix $\mathbf{K}(\theta)$ and hence $\mathcal{K}$. Here we have chosen 4th order stochastic Hermite polynomials basis with which the solution has been approximated.

Fig. 1 shows the response of the baseline (deterministic) dynamic advection–diffusion–reaction system subjected to deterministic external forcing as described in the context of Eq. (66) at 5 discrete points in time. The time domain response has been resolved with the central difference scheme.

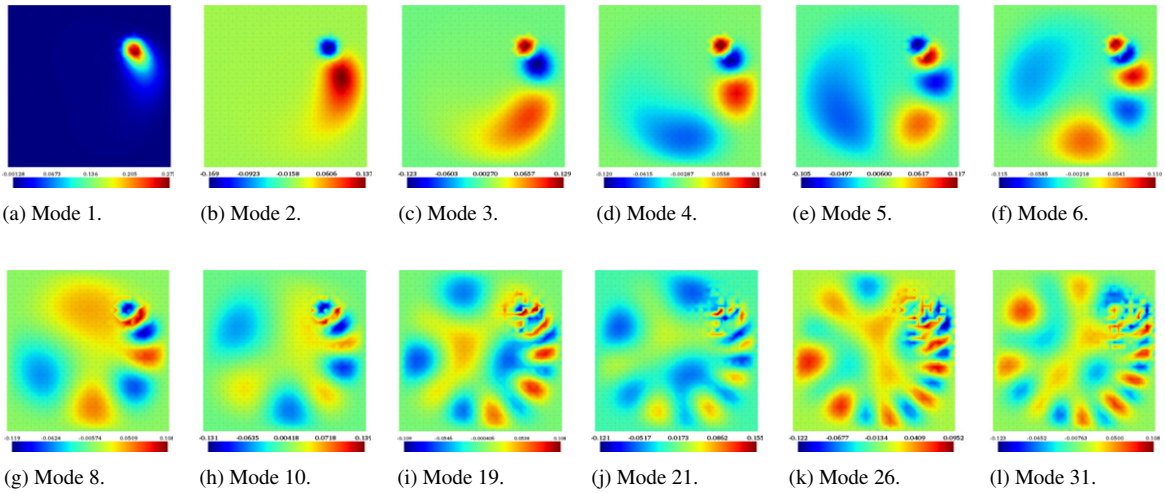
Figs. 2 and 3 shows the response statistics, i.e. the mean and the standard deviation respectively, of the response of the randomly parametrized system resolved with polynomial chaos expansion under the action of the deterministic external forcing. We have used 4th order Hermite chaos for a 4 dimensional input stochastic space represented with 4 independent identically distributed random variables.

Fig. 4 gives the first few eigenmodes of the controllability Gramian $\overline{\mathbf{W}}^2$ of the deterministic dynamical system. Here the estimation of the eigenvectors associated with the largest eigenvalues is exact since the Gramian has been calculated first following which we have performed an eigenvalue analysis of the deterministic Gramian. It can be



(a) $t = 1T_{\text{tot}}/5$. (b) $t = 2T_{\text{tot}}/5$. (c) $t = 3T_{\text{tot}}/5$. (d) $t = 4T_{\text{tot}}/5$. (e) $t = 5T_{\text{tot}}/5$.

Fig. 3. Standard deviation of the response of the stochastic model problem with a lognormal random diffusion coefficient using a 4th order polynomial chaos expansion.



(a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Mode 4. (e) Mode 5. (f) Mode 6.

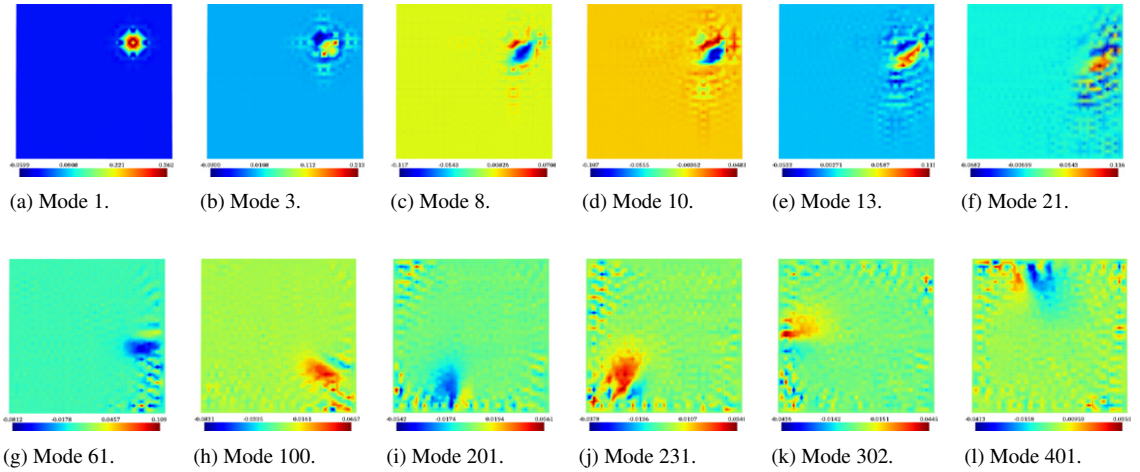
(g) Mode 8. (h) Mode 10. (i) Mode 19. (j) Mode 21. (k) Mode 26. (l) Mode 31.

Fig. 4. Various eigenmodes of the complete Gramian of the response of the baseline (deterministic) advection–diffusion–reaction system.

seen that the first eigenmode almost replicate the solution at the very early time steps. Gradually the modes become more complex and exhibit an anticlockwise rotation pattern. All the modes presented in this figure are orthogonal to each other and have been normalized.

We give the mean Arnoldi–Lyapunov basis vectors of the randomly parametrized dynamical system in Fig. 5 which have been calculated using the algorithm presented in Section 4.3. The basis vectors span the dominant eigenspace of the stochastic controllability Gramian matrix. These vectors are orthonormalized and are used to model the reduced order response of the dynamical system. It is seen that these modes are significantly different from the ones presented in Fig. 4. However, it is still apparent that a clockwise rotation pattern is exhibited as the mode number increases. The solution to the randomly parametrized advection–diffusion–reaction system is approximated with a subset of Arnoldi–Lyapunov basis vectors and the accuracy of the solution has been compared with respect to the dimension of the reduced space in which the solution is sought.

Fig. 6 gives the mean response of the stochastic LTI system calculated with the 4th order chaos expansion of the input iid random variables. The mean response has been evaluated with an increasing subset of Arnoldi–Lyapunov basis vectors and have been studied for their accuracy. Here the mean response with 4th order chaos has been approximated successively with 150, 300, 400 and 600 basis functions and Fig. 6(a)–(d) shows the improved accuracy of the solution as the number of Arnoldi–Lyapunov basis vectors are increased. These have been compared to the full system solution without a reduced subspace projection which has been shown in Fig. 6(e). The plots indicate that with fewer basis vectors, the solutions at early time steps are accurate but the time evolution of the solution stops altogether after a finite interval of time. For example the mean response calculated with 150 modes stops evolving in time from $t = 2T_{\text{tot}}/5$ onwards. When using a higher number of modes, say 300 the solution grows until $t = 3T_{\text{tot}}/5$ after which it becomes stagnant, while the response with 600 modes captures almost the entire time varying solution.



(a) Mode 1. (b) Mode 3. (c) Mode 8. (d) Mode 10. (e) Mode 13. (f) Mode 21.

(g) Mode 61. (h) Mode 100. (i) Mode 201. (j) Mode 231. (k) Mode 302. (l) Mode 401.

Fig. 5. Plots of the mean of the various basis functions spanning the dominant subspace of the stochastic controllability Gramian of the randomly parametrized linear system calculated with an iterative Krylov method implemented within the scope of Arnoldi's algorithm.

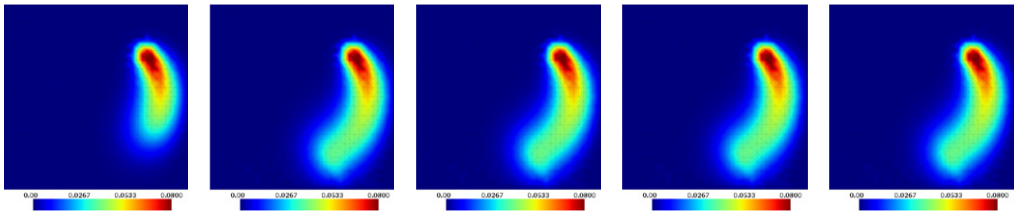
To quantify the approximation error in obtaining the transient response of the LTI system with a reduced number of Arnoldi–Lyapunov basis vectors, we construct a relative error indicator which is defined as follows

$$\varepsilon_n^m = \frac{\left\| \mathcal{X}_n^{\text{red},m} - \mathcal{X}_n^{\text{full}} \right\|_2}{\left\| \mathcal{X}_n^{\text{full}} \right\|_2} \tag{69}$$

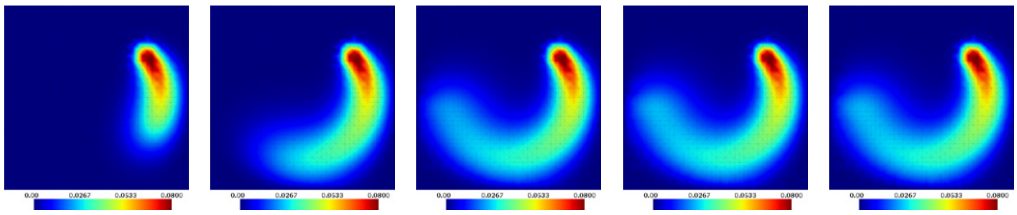
where $\mathcal{X}_n^{\text{full}}$ is the full system solution at time step n, $\mathcal{X}_n^{\text{red},m}$ is the approximate solution at time step n computed with m Arnoldi–Lyapunov vectors and $\|\cdot\|_2$ denotes the L^2 vector norm. Hence the relative error norm is a function of the dimension of the reduced subspace in which the solution is sought and varies with time.

Fig. 7 shows the plot of this relative error norm ε_n^m on the time range of interest $t = [0, 0.03]$ s with different orders of approximation of the response vector. Fig. 7(a) shows the error in approximating the deterministic solution with the Gramian of the deterministic transient response while Fig. 7(b) gives the same for the randomly parametrized system with the stochastic Gramian. Of course in the latter case the dimension of the linear system is significantly larger and hence a higher number of basis vectors are required to satisfactorily capture the system response over the entire time range. Additionally, it is seen that the approximation error obtained for the deterministic transient system is many orders of magnitude lower than that for the stochastic system. This is expected since the dimension of the stochastic linear system is much higher than the deterministic one. Hence the approximation error is comprised of the error in the tensor product of the finite dimensional stochastic subspace spanned by the orthogonal polynomial chaos functions and the vector space associated with the FE discretization. From Fig. 7 it is seen that the maximum approximation accuracy (of the order of 10^{-15}) is obtained at all time steps with approximately 400 modes while for the stochastic system the maximum approximation accuracy (of the order of 10^{-7}) is obtained with approximately 700 modes. This leads to a significant improvement in the computational efficacy of the time stepping algorithm since a good approximation of the stochastic response expressed with the finite order chaos expansion is obtained with only a few basis functions. For example, the finite element discretization of the advection–diffusion–reaction problem leads to a linear system of dimension ≈2000. With 4th order chaos expansion in 4 dimensional stochastic space, we have to solve a $\approx 1.4 \times 10^5$ dimensional block sparse linear system at each time step. In contrast, it is seen that 700 Arnoldi–Lyapunov vectors provide us with a solution of accuracy 10^{-7} at all time steps.

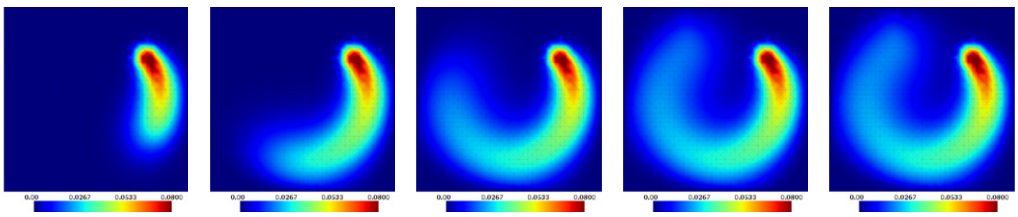
Fig. 8 gives the standard deviation of the response of the stochastic LTI system calculated with the 4th order chaos expansion of the input iid random variables. The response standard deviation has been evaluated with an increasing subset of Arnoldi–Lyapunov basis vectors (such as 150, 300, 400 and 600) and have been studied for their accuracy as given in Fig. 8(a)–(d). These show the improved accuracy of the solution as the number of basis vectors are increased. These have been compared to the full system solution without a reduced subspace projection which has been shown in Fig. 8(e). The plots indicate that with fewer basis functions, the solutions at early time steps are accurate but the time



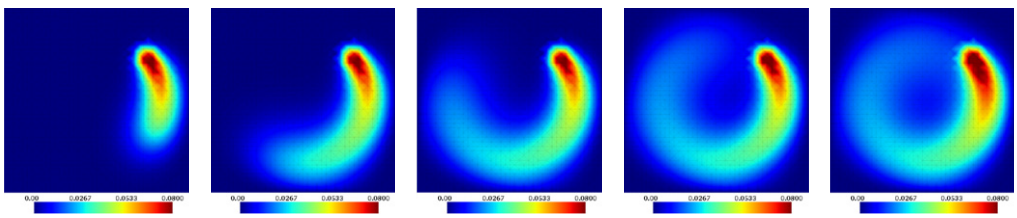
(a) Mean calculated with 150 PC basis.



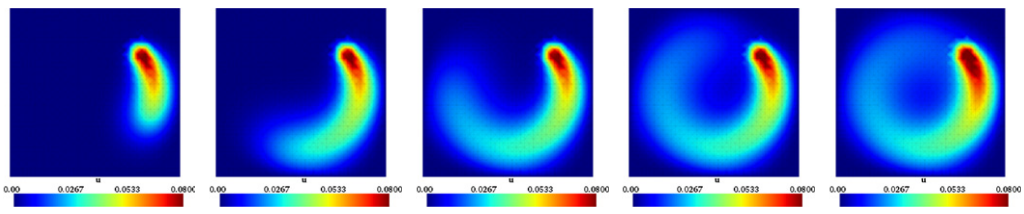
(b) Mean calculated with 300 PC basis.



(c) Mean calculated with 400 PC basis.



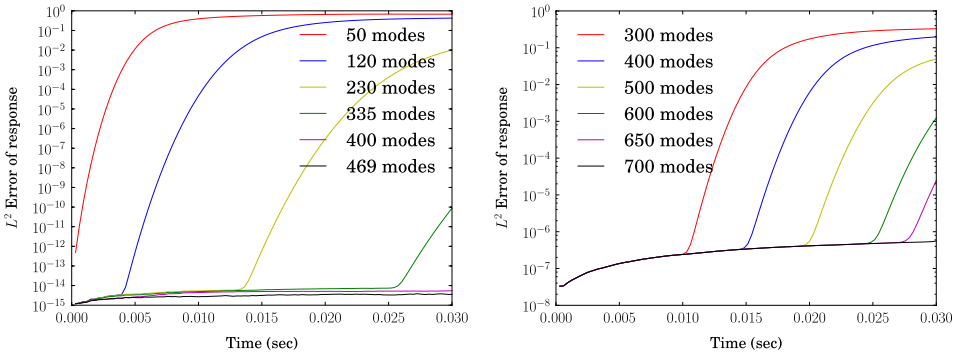
(d) Mean calculated with 600 PC basis.



(e) Mean of the full system PC solution.

Fig. 6. Approximate mean response calculated with various reduced number of Arnoldi–Lyapunov basis vectors spanning the dominant subspace associated with the stochastic Gramian of the randomly parametrized linear system. The basis functions were calculated with an iterative Krylov method implemented within the scope of Arnoldi's algorithm. The responses are shown at different instances of time $t = iT_{\text{tot}}/5$ with $i = 1, \ldots, 5$ along each row.

evolution of the solution stops altogether after a finite interval of time. This behavior is consistent and similar to that obtained for the mean response given in Fig. 6. For example the standard deviation of the response calculated with 150 modes is found to become stagnant from $t = 2T_{\text{tot}}/5$ onwards which is similar to the behavior of the mean response



(a) L^2 error, deterministic system. (b) L^2 error, stochastic system.

Fig. 7. Plots of the L^2 error of the reduced basis transient solution vector with respect to the complete solution obtained with a time marching algorithm for two different cases: deterministic system (a) without considering any parametric uncertainty and randomly parametrized system (b) with finite order chaos expansion of the solution vector.

of the system as shown in Fig. 6. Again, using a higher number of modes, say 300, the solution grows till $t = 3T_{\text{tot}}/5$ after which it becomes stagnant, while the response with 600 modes captures almost the entire time varying solution.

The results demonstrate the applicability of the proposed method for the reduced order realization of the stochastic system response using the principal Arnoldi–Lyapunov modes associated with the stochastic controllability Gramian. It should also be noted that the system being solved here (i.e. the linear system given in Eq. (68)) is unsymmetrical due to the presence of the non self-adjoint advection term. The numerical results of the approximation of the stochastic response with the reduced number of modes indicates that the method is not limited to symmetric systems but is also effective for unsymmetrical cases which are generally more complicated to handle.

5.2. *Pure diffusion with boundary terms*

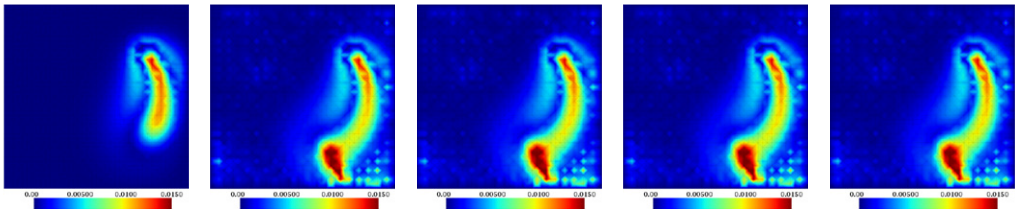
We study another example problem here which consists of a randomly parametrized unsteady diffusion system to demonstrate the applicability of the model reduction technique that has been proposed here. The physical configuration of the problem is defined on a circular arc-like domain which is shown in Fig. 9(a). The governing equation for this unsteady diffusion equation is given as

$$\begin{aligned} &c\dot{x}(t;\theta) - \nabla\left(k(\theta)\nabla x(t;\theta)\right) = 0 \quad \text{on } \mathscr{D}\ \forall\ t \in [0,T] \\ &\mathbf{n}_1.\nabla x(t;\theta) = f_1(t) \quad \text{on } \Gamma^1 \quad \text{and} \quad \mathbf{n}_2.\nabla x(t;\theta) = f_2(t) \quad \text{on } \Gamma^2\ \forall\ \theta \in \Theta \\ &\quad \text{and} \quad x(t=0;\theta) = x_0 \quad \text{on } \mathscr{D}\ \forall\ \theta \in \Theta \end{aligned} \tag{70}$$

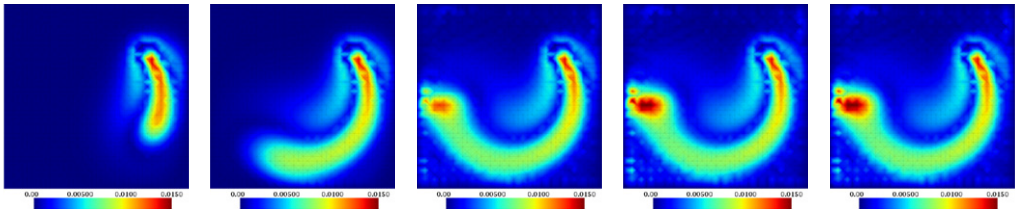
where Γ^1 is the 'red' part of the boundary in Fig. 9(a) which supplies the input flux to the system and Γ^2 denotes the 'green' portion of the boundary which dissipates energy. Thus this is a mixed boundary condition problem with the Γ^1 having a Neumann boundary while Γ^2 consists of Robin boundary conditions. The above equation indicates that the initial and boundary conditions are prescribed on the boundary for every sample realization of the randomly parametrized system. The time integration is carried out using the implicit Euler's central difference scheme with a time step size whose upper bound is governed by the dynamic characteristics of the transient system and has been chosen to be sufficiently small to ensure stability and convergence. The time range of interest for this problem is $t = [0, 500]$s. The boundary source term consists of an exponentially decaying flux modeled as $f_1(t) = \bar{f}_1 e^{-c_d t}$ where c_d is a positive constant while the dissipation boundary term has been modeled as $f_2(t) = \bar{f}_2(x(t;\theta) - x_\infty)$ where x_∞ is a constant. We have chosen the constants x_0 (the initial condition) and x_∞ to be equal to 273. This results in the linear system of equations

$$\mathbf{C}\dot{\mathbf{X}}(t;\theta) + \mathbf{K}(\theta)\mathbf{X}(t;\theta) + \mathbf{H}\mathbf{X}(t;\theta) = \bar{\mathbf{B}}\mathbf{f}(t) \tag{71}$$

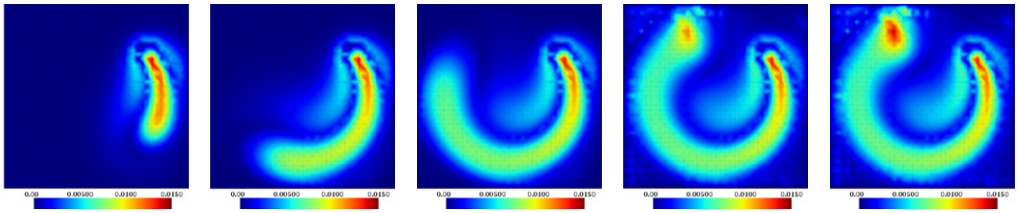
where $\bar{\mathbf{B}} \in \mathbb{R}^{n\times 2}$ is the locator matrix associated with the forcing vector $\mathbf{f}(t) = \{f_1(t),\ f_2(t)\}$ and $\mathbf{H}$ is a boundary contribution matrix obtained from the finite element method applied to the boundary term $\bar{f}_2(x(t;\theta))$ depending on



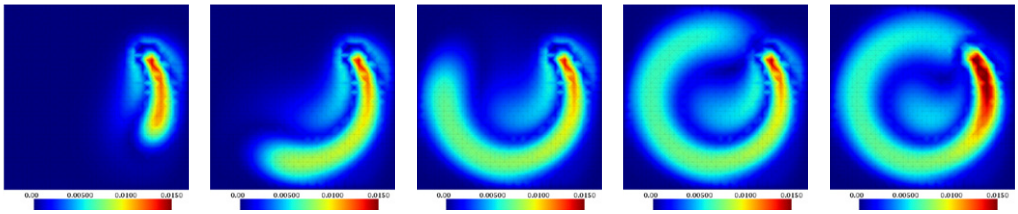
(a) Standard deviation calculated with 150 PC basis.



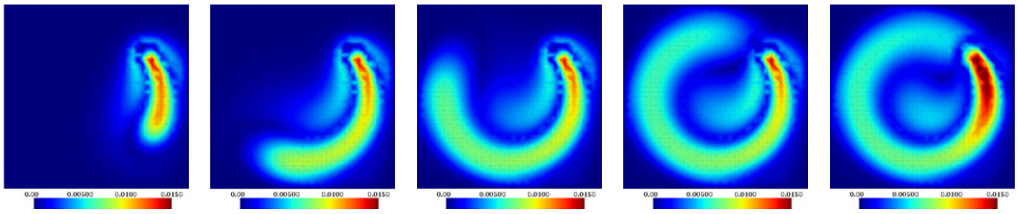
(b) Standard deviation calculated with 300 PC basis.



(c) Standard deviation calculated with 400 PC basis.



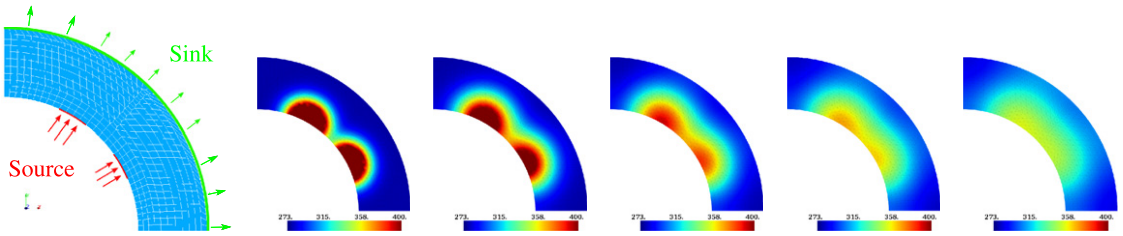
(d) Standard deviation calculated with 600 PC basis.



(e) Standard deviation of the full system PC solution.

Fig. 8. Approximation of the standard deviation of the response calculated with various reduced number of Arnoldi–Lyapunov basis vectors spanning the dominant subspace associated with the stochastic Gramian of the randomly parametrized linear system. The basis functions were calculated with an iterative Krylov method implemented within the scope of Arnoldi's algorithm. The responses are shown at different instances of time $t = iT_{\text{tot}}/5$ with $i = 1, \ldots, 5$ along each row.

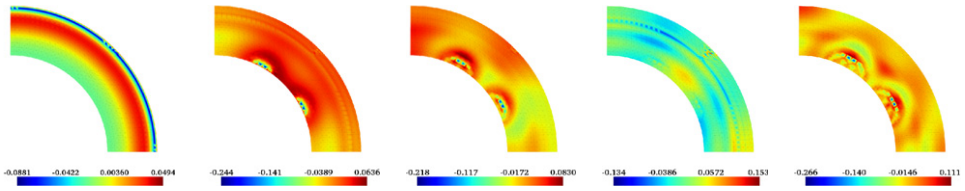
the field value $x(t, ; \theta)$ at the boundary. Hence the block Krylov method (as detailed in Section 4.4) of order n_k would consist of $2n_k$ vectors of length n where the latter is the number of degrees of freedom obtained from the FE discretization. After applying the stochastic Galerkin method with finite order chaos expansion of the stochastic



(a) Configuration of the transient system.

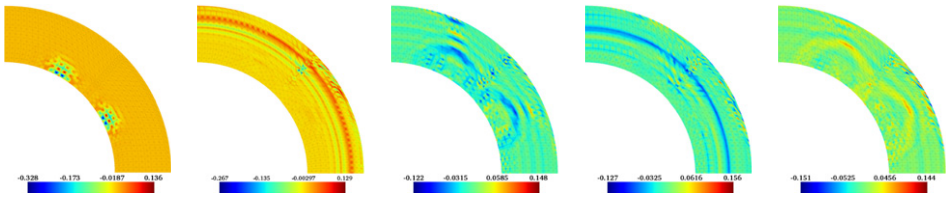
(b) Solution at five different instance of time $t = iT_{\text{tot}}/5$ where $i = 1, \ldots, 5$.

Fig. 9. Configuration of the LTI system under the action of external forcing functions along with the reference solution of the baseline (deterministic) model for the transient diffusion problem.



(a) Mode 03. (b) Mode 12. (c) Mode 20. (d) Mode 23. (e) Mode 28.

Fig. 10. Various eigenmodes of the complete controllability Gramian of the baseline (deterministic) diffusion system with boundary forcing terms.



(a) Mode 03. (b) Mode 40. (c) Mode 65. (d) Mode 69. (e) Mode 80.

Fig. 11. Various Arnoldi–Lyapunov eigenmodes of the controllability Gramian obtained with a block Krylov method applied to the baseline (deterministic) diffusion system with boundary forcing terms.

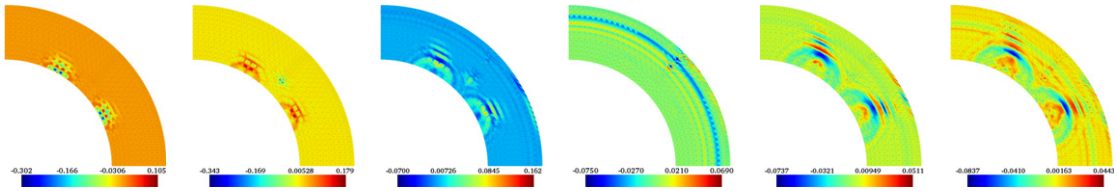
solution vector we obtain

$$\mathcal{C}\dot{\mathcal{X}}(t) + \mathcal{K}\mathcal{X}(t) + \mathcal{H}X(t) = \bar{\mathcal{B}}\mathcal{F}(t) \tag{72}$$

where $\mathcal{C}$ and $\mathcal{H}$ are block diagonal matrices, while $\mathcal{K}$ is a block sparse matrix. It might be noted here that the system matrices obtained are symmetric, which was not the case in the advection–diffusion–reaction problem given in Section 5.1.

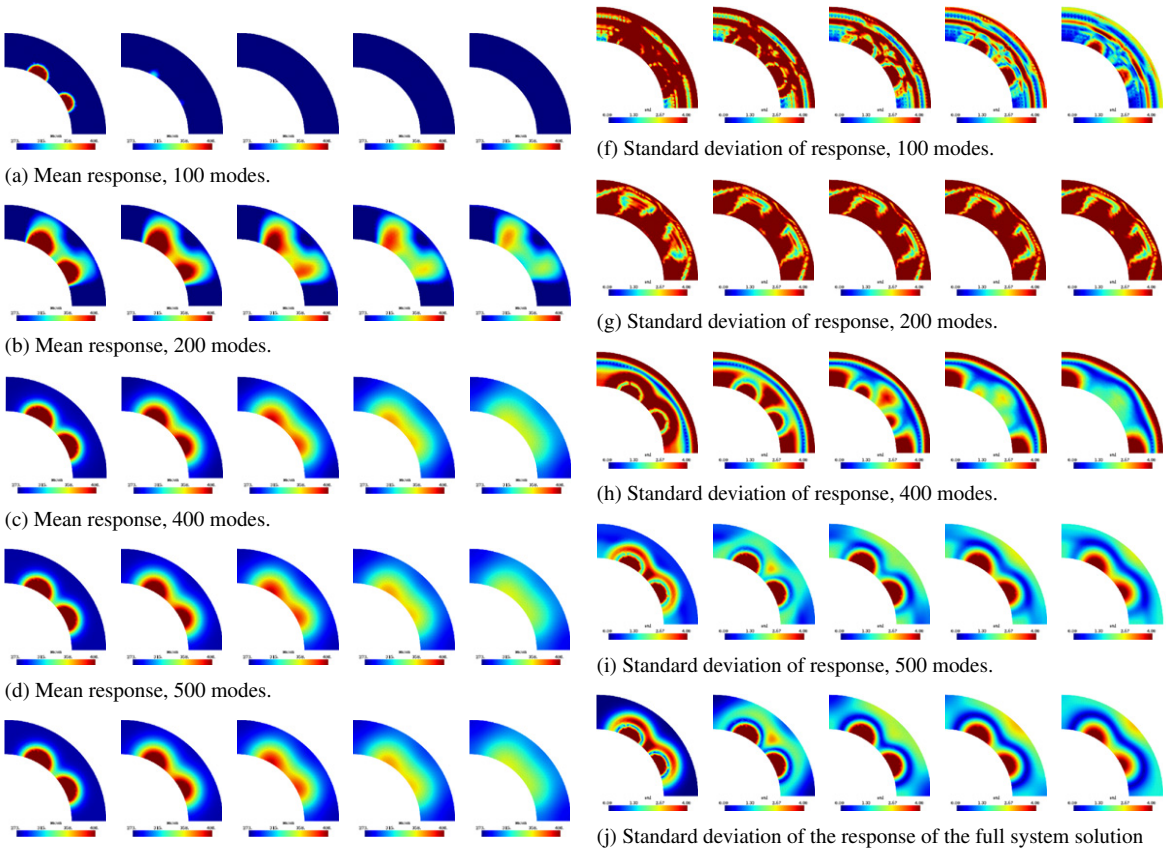
Fig. 9 gives the reference solution of the baseline (deterministic) model (schematic diagram shown in Fig. 9(a)) at 5 different instants of time which shows the energy input to the system at the two locations of the inner circumference gradually being dissipated via the outer circumferential edge. The various eigenmodes associated with the largest eigenvalues of the controllability Gramian of this deterministic model is shown in Fig. 10 which has been computed after the controllability Gramian matrix has been solved from the Lyapunov equation. Hence this method is extremely expensive and the dominant Arnoldi–Lyapunov eigenvectors have to be calculated from the block Krylov space using the algorithm detailed in Section 4.4. It can be seen that the block Krylov modes are generally not close to the eigenmodes of the controllability Gramian, but it is possible to intuitively relate the modeshapes in Fig. 11 to the impulse response behavior of the physical system.

Now, for the randomly parametrized diffusion system, calculating the controllability Gramian becomes prohibitively expensive and hence the dominant Arnoldi–Lyapunov vectors are calculated using Arnoldi's algorithm on the Lyapunov matrix equations in the tensor product space of the vector of finite element nodal degrees of freedom



(a) Mode 05. (b) Mode 12. (c) Mode 24. (d) Mode 46. (e) Mode 60. (f) Mode 70.

Fig. 12. Plots of the mean of the various Arnoldi–Lyapunov eigenmodes of the stochastic controllability Gramian approximated with finite order chaos expansion of the randomly parametrized diffusion system with boundary forcing terms.



(a) Mean response, 100 modes.

(b) Mean response, 200 modes.

(c) Mean response, 400 modes.

(d) Mean response, 500 modes.

(e) Mean response of the full system solution shown at five different instances of time $t = iT_{\text{tot}}/5$ where $i = 1, \ldots, 5$.

(f) Standard deviation of response, 100 modes.

(g) Standard deviation of response, 200 modes.

(h) Standard deviation of response, 400 modes.

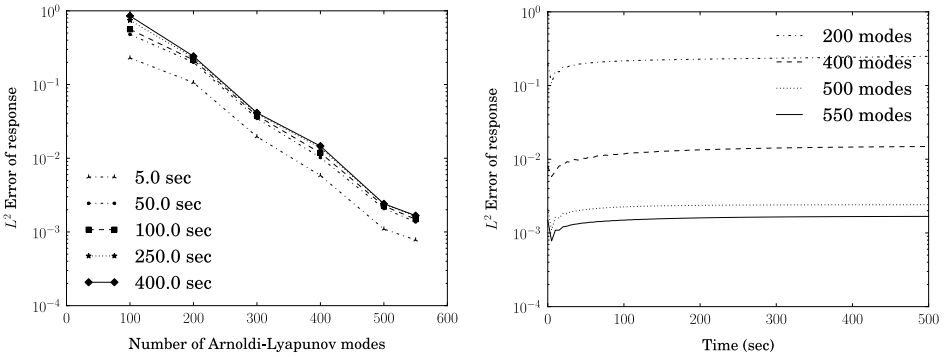
(i) Standard deviation of response, 500 modes.

(j) Standard deviation of the response of the full system solution shown at five different instances of time $t = iT_{\text{tot}}/5$ where $i = 1, ..., 5$.

Fig. 13. Plots of the mean (left column) and standard deviation (right column) of the response to the randomly parametrized diffusion system under the action of the boundary forcing terms. The statistics of the response obtained with various reduced order models (realized with the Arnoldi–Lyapunov eigenmodes) of the system is shown here. The bottom most row gives the mean and standard deviation of full system response which is treated as the benchmark solution. The stochastic solutions in all these cases have been approximated with a 4th order chaos expansion for a 4-dimensional input space.

and the finite order chaos expansion of the stochastic space. The mean of these eigenvectors is shown in Fig. 12 which again exhibits a similar pattern with respect to the forcing imposed at the boundary to those shown in Figs. 10–11.

The statistics of the solution of the transient diffusion system under the action of time varying boundary forcing terms is shown in Fig. 13 which compares the accuracy of the solution obtained with increasing the dimension of the reduced subspace in which the solution is sought, i.e. as the number of Arnoldi–Lyapunov basis vectors is increased. It can be seen that for low order approximations with only 100 eigenmodes, the solution fails to give any reasonable



(a) L^2 norm of the error of the stochastic solution vector specific values of t for increasing number of Arnoldi–Lyapunov modes.

(b) L^2 norm of the error of the stochastic solution vector at all t.

Fig. 14. Plots of the L^2 errors of the stochastic solution vector for various dimension of the reduced subspace in which the solution is approximated. The reduced subspace dimension is determined by the number of Arnoldi–Lyapunov basis functions used to approximate the controllability Gramian with finite order chaos expansion.

response statistics, while as more basis functions are included to construct the approximate solution the accuracy of the response increases. It can also be noted that as the higher order statistics of the solution are sought, it becomes necessary to incorporate additional modes into the reduced order model. It should however, be noted that increasing the number of Arnoldi–Lyapunov basis functions does not mean an increase in the degree of the stochastic chaos functions used to approximate the solution vector. It can be seen that even the low order approximations of the solution with the Arnoldi–Lyapunov basis vectors give the solution with the 4th order chaos expansion. However, the higher order statistics of the response necessitates additional terms associated with the 4th degree stochastic polynomial terms in order to obtain a good approximation of the response.

Fig. 14 gives the L^2 error of the approximate solution vector with respect to the full system solution (as described by Eq. (69)) when using a 4th order chaos expansion with different reduced order models of the randomly parametrized diffusion system. We present the convergence rate of the solution with the number of approximating Arnoldi–Lyapunov vectors at various instances in time (such as $t = [5, 50, 100, 250, 400]$ s) in Fig. 14(a) which shows a nearly exponential convergence. The L^2 error norm at all instances of time is shown in Fig. 14(b) which shows that the error increases slightly as the value of t increases. Thus, increasing the number of Arnoldi–Lyapunov modes leads to a rapid improvement in the solution accuracy.

6. Summary & conclusions

A computationally efficient scheme of resolution of the transient response of numerical models of large scale randomly parametrized dynamical systems has been proposed. The methodology relies on obtaining a minimal order realization of the linear time invariant system based on the idea of preserving the strong dynamical coupling of the specified input–output characteristics of the system. The uncertainty associated with the random input parameters is propagated to the system response using the established framework of stochastic spectral Galerkin method. The resulting linear system due to the application of this method is orders of magnitude larger than the baseline FE linear systems and model reduction techniques are very important in this context. The transient response of the randomly parametrized linear system has been approximated with a denumerable set of dominant dynamical modes obtained from the spectral decomposition of the stochastic controllability Gramian.

The controllability Gramian satisfies the stochastic Lyapunov equation which requires the resolution of a matrix equation of significant dimension. Different methods of resolution of this stochastic matrix equation using a stochastic sampling based technique to the series expansion of the stochastic Gramian matrix with orthogonal stochastic polynomials and applying the 'vec' transformation have been discussed. However, the computational cost associated with these methods becomes prohibitively large even for moderate dimensional systems. Hence an alternative method of approximating the stochastic controllability Gramian with a reduced number of Arnoldi–Lyapunov vector bases has been proposed. This approach avoids the full solution of the stochastic Lyapunov equation and

approximates the dominant invariant subspace associated with spectral components of the stochastic controllability Gramian. The algorithm approximating the transient stochastic response with the Arnoldi–Lyapunov basis vectors in conjunction with an implicit time stepping scheme has been detailed. Additionally, to enhance the stability and convergence properties of the time integration scheme further, especially for long time integration problems, a restarted Arnoldi–Lyapunov basis vector estimation has been proposed. The latter relies on reinitializing the reduced-order basis evaluation after finite intervals of time based on the solution of the dynamic system obtained at that time step. The theoretical justification for the implicit restarting of the basis evaluation has been discussed. Finally the steps of the algorithm have been detailed in an itemized algorithm. The proposed reduced order modeling of the randomly parametrized system with Arnoldi–Lyapunov vectors basis has been demonstrated with examples of an advection–diffusion–reaction problem on a regular square domain and a pure diffusion problem with boundary forcing terms on a circular arc-shaped domain. The numerical results demonstrate the applicability of the proposed methodology to large scale randomly parametrized finite element systems subjected to transient external forcing.

The salient features of the work presented here are

- A randomly parametrized large-scale linear time invariant finite element system has been considered and a computationally efficient minimal realization scheme to obtain the transient response of this system has been studied.
- The minimal realization of the LTI system has been obtained from the dominant spectral components of the stochastic controllability Gramian.
- The theoretical and implementational aspects of different methods of resolution of the principal modes of the stochastic controllability Gramian has been provided and analyzed for their computational overhead.
- To mitigate the cost associated with the solution of the large dimensional matrix equations, the Arnoldi–Lyapunov basis spanning the dominant space associated with the spectral components of the stochastic controllability Gramian has been investigated.
- The computationally efficient methodology to resolve the transient response of the LTI system with an Arnoldi–Lyapunov vector basis has been highlighted in an algorithm.
- An implicit scheme of restarting the determination of the Arnoldi–Lyapunov vector basis has been proposed and the theoretical justification for this has been detailed.
- The minimal realization of the dynamic characteristics of the randomly parametrized system has been illustrated with two stochastic finite element problems in conjunction with a spectral Galerkin approach which demonstrates the applicability of the reduced order evaluation of the transient response of large computational models.

Future work would aim to extend the reduced order modeling approach with Arnoldi–Lyapunov vectors to calculate the transient response of structural dynamic systems with input parametric uncertainty. Also, the theoretical development which can provide an a-priori knowledge of the accuracy of the transient response of the randomly parametrized system as a function of the number of Arnoldi–Lyapunov basis used in its calculation would be quite useful for the computational scheme presented here. This might lead to a unique global error indicator combining the residuals of the Lyapunov equation and the stochastic LTI system which can be used to decide the implicit restart points of the Arnoldi–Lyapunov basis evaluation algorithm. Lastly, investigation into the possibility of using efficient preconditioners for the Arnoldi–Lyapunov algorithm, which can give better convergence of the solution with fewer number of basis functions, would be important in the context of this study.

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