Stochastic Model Reduction of Allen-Cahn Phase Field Model with High Dimensional Random Forcing

by

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Abstract of "Stochastic Model Reduction of Allen-Cahn Phase Field Model with High Dimensional Random Forcing"

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The Karhunen-Loeve (KL) decomposition provides a low dimensional representation for square integrable stochastic fields as it is optimal in the mean square sense. Despite the success of these methods for many stochastic systems of practical interest, potential roadblock occurs in strongly time-dependent problems. Motivated by this limitation, Sapsis and Lermusiaux(2009), developed the dynamically orthogonal(DO) framework, which allows for the simultaneous evolution of both the spatial basis and stochastic basis. Using the framework of Dynamical Orthogonality(DO) condition, a coupled set of evolution equations are derived for Allen-Cahn phase field transport equation. The reduced order field equations (DO equations) consists of (i) the system of Partial Differential equations(PDEs) that describes the evolution of the mean field and the orthonormal spatial basis(modes) defining the stochastic subspace where uncertainty "lives" and (ii) the set of Stochastic Differential equations(SDEs) that describes the evolution of stochastic basis(coefficients) defining how the stochasticity will be evolved within the reduced order stochastic subspace. Numerical simulations are performed for time independent high dimensional stochastic forcing based on Karhunen-Loeve(KL) decomposition. The aim of the current work is to investigate dimension reduction in high dimensional random space by analyzing the number of DO modes required to resolve the transient stochastic Allen-Cahn equation.

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Chapter 1

Introduction

In recent years, there has been a growing interest in quantifying parametric uncertainties in physical and engineering problems through the probabilistic framework. Such problems are often governed by stochastic partial differential equations (SPDEs), and they arise in various fields of continuum mechanics such as fluid mechanics, solid mechanics, wave propagation, etc. The source of stochasticity in all the above cases includes uncertainty in physical parameters, initial and/or boundary conditions, etc. All these stochastic parameters can be characterized as random processes or random variables. Several methods have been developed to study SPDEs, including Monte Carlo (MC) method and its variants and, more recently, generalized polynomial chaos (gPC), multi-element generalized polynomial chaos (ME-gPC), probabilistic collocation method (PCM) , multi-element probabilistic collocation method (ME-PCM) and many other variants (see e.g. [2], [3], [4], [5], [6]).

Another aspect in uncertainty quantification is order-reduction schemes or reduced- order models (ROMs) for the simplification and analysis of high-dimensional complex systems across many physical and engineering disciplines. For many stochastic systems of practical interest, it has been known that the solution possess an inherent low-dimensional character. Many methods in ROMs have been developed in the context of deterministic framework such as proper orthogonal decomposition (POD) or principal component analysis (PCA) with applications to many disciplines such as turbulent fluid flows, structural vibration to name a few. However, there have been a few researches on ROMs in the context of stochastic framework.

1.1 Time Dependent Karhunen-Loeve (KL) type expansions

The Karhunen-Loeve (KL) type decomposition provides a low-dimensional representation for square integrable random processes as it is optimal in the mean square sense. It has been widely used in the context of the deterministic problems under the name of POD or PCA. In the stochastic framework, the KL expansion has been used mainly to represent the random processes of the input parameter with the solution or quantity of interest being often represented as gPC basis or to find a low-dimensional structure of the solution in the post-processing as it often requires to solve a large-scale eigenvalue problem.

Schemes based on ROMs are essentially relying on the projection of the original system into a "suitable" set of modes representing important and essential components of the dynamics. This projection can be performed either with respect to a spatially dependent basis or with respect to a stochastically-dependent basis. For both cases, various approaches and rules have been developed for the choice, computation, or improvement of these basis elements.

For the first family of methods (spatially-dependent basis) some of the most popular methods for the basis selection include empirical criteria such as energy based proper orthogonal decomposition (POD) (see for example [7], [8]). For the second family of methods (projection to a stochastic basis) one of the most popular approaches is the Gaussian closure (assumption that the solution has a Gaussian stochastic structure) which, however, has limited applicability for problems where the non-Gaussian character is inevitable. For this case the employment of a polynomial chaos basis and its variants may provide for many cases a reliable computational scheme [4], [5], [6].

Despite the success of these methods in many problems of practical interest there are important limitations associated with them. On the one hand, methods relying on the selection of a spatial basis present important limitations in problems with strongly time-dependent character where the basis employed may become irrelevant as time evolves. On the other hand, methods relying on a pre-selected stochastic structure suffer from important limitations especially in problems with highly non-Gaussian structure or with strongly transient stochastic characteristics.

Motivated by these limitations an alternative approach for the solution of stochastic systems that tracks the KL representation at a given time according to the evolution equations was proposed in [1]. The new method adopts a redundant representation where both the spatial and stochastic basis evolve in time unlike the traditional methods such as gPC and POD. By imposing the dynamical constraints on the spatial basis, called the dynamical orthogonality (DO) condition, the authors were able to derive the DO evolution equations for all the components involved - mean, the spatial basis and stochastic basis. These equations (DO evolution equations) consists of a deterministic PDE describing the evolution of the mean field, a set of deterministic PDEs describing the evolution of the spatiotemporally-dependent deterministic basis, and a set of stochastic differential equations describing the evolution of the stochastic basis.

Recently, [11], [12] adopted the same redundant representation used in [1]. By imposing static constraints on both the spatial and the stochastic basis, called the *bi-orthogonal* (BO) condition, an independent set of equations describing the evolution of all the quantities involved (DyBO or BO equations) was obtained. The precise mathematical relationship between the two methods was established rigorously in [9]; the methods are equivalent in the sense that one can be derived from the other through an invertible and linear transformation governed by an orthogonal matrix differential equation. Moreover, the BO becomes unstable when there is an eigenvalue crossing, while it preserves a diagonal covariance matrix for all times. The hybrid approach to tackle the singular limit of the DO equations was also established rigorously by [10] by combining Polynomial Chaos with DO based schemes. A robust and hybrid framework was further proposed by [13] as a reduced-order modeling approach by utilizing an invertible and linear transformation between the DO and BO and by employing a pseudo-inverse technique for inverting the covariance matrix.

1.2 Organization of the thesis

In Chapter 2, we provide brief introduction to the generalized representation of the stochastic fields. We introduce the generalized Karhunen-Loeve type expansions and discuss its advantages with Proper Orthogonal Decomposition (POD) and Polynomial Chaos (PC) type representations.

In Chapter 3, we introduce Dynamically Orthogonal methodology for Allen-Cahn phase field transport equation. We derive the set of evolution equations that consists of a system of deterministic PDEs for the mean and spatial basis and a system of stochastic ODEs for the stochastic basis for both one and two dimensional Allen-Cahn phase field model.

In Chapter 4, we provide the numerical illustrations for Stochastic Allen-Cahn equations. We discuss in detail the method of manufactured solutions for establishing time accuracy. Thereafter, we analyze the Stochastic Allen-Cahn equation under high dimensional random forcing.

Chapter 2

Representation of the Stochastic Fields

The Karhunen-Loeve expansion follows that every random field $\phi(x,t;\omega)$ at a given time t can be approximated by finite series expansion with N terms:

$$\phi(x,t;\omega) = \bar{\phi}(x,t) + \sum_{i=1}^{N} X_i(t;\omega)\phi_i(x,t)$$

For the random field $\phi(x,t;\omega)$, the expectation operator for ϕ is defined as

$$\bar{\phi}(x,t) \equiv \mathbb{E}[\phi(x,t;\omega)] = \int \phi(x,t;\omega)dP(\omega)$$

The set of all continuous and square integrable random fields, i.e., $\int \mathbb{E}[\phi(x,t;\omega)^T\phi(x,t;\omega)]dx$ is finite, where $\phi(x,t;\omega)$ is the transpose of ϕ, for all $t\epsilon T$ and the bi-linear form of the covariance operator

$$C_{\phi(.,t;\omega)\phi(.,s;\omega)}(x,y) = \mathbb{E}[(\phi(x,t;\omega) - \bar{\phi}(x,t))^T(\phi(x,s;\omega) - \bar{\phi}(x,s))]$$

form a Hilbert space. The spatial inner product is defined as

$$\langle\phi(\cdot,t;\omega),\phi(\cdot,s;\omega)\rangle = \int \phi(x,t;\omega),\phi(x,s;\omega)dx$$

Indeed, it is known that the KL decomposition is optimal in the mean square sense. In the context of numerical method to SPDEs, constraints are required to derive how the components in the above KL decomposition evolve in time.

We emphasize that through this approach, no assumptions are required for the spatial characteristics of uncertainty, such as homogeneity. Moreover, the non-Gaussian character of the random field is fully respected since this is expressed completely through the random evolution of the scalar coefficients.

This is not the case for other approaches used such as the Proper Orthogonal Decomposition (POD) method where the field is represented as

$$\phi(x,t;\omega) = \bar{\phi}(x) + \sum_{i=1}^{N} X_i(t;\omega)\phi_i(x)$$

or the polynomial-chaos method where the following representation is used

$$\phi(x,t;\omega) = \bar{\phi}(x,t) + \sum_{i=1}^{N} X_i(\omega)\phi_i(x)$$

In both of the above cases the lack of time dependence on either the deterministic fields or the stochastic coefficients restrict the representation capabilities. This is not the case for the generalized Karhunen-Loeve expansion where all quantities evolve with time, allowing for very efficient representation of any given field.

Chapter 3

Dynamically Orthogonal reduced order model

3.1 Dynamically Orthogonal(DO) representation

Using a time dependent generalization of the Karhunen-Loeve expansion, we have that every random field $\phi(x,t;\omega)$ at a given time t can be approximated by a finite series of the form

$$\phi(x,t;\omega) = \bar{\phi}(x,t) + \sum_{i=1}^{N} X_i(t;\omega)\phi_i(x,t) = \bar{\phi} + X_i\phi_i \tag{1}$$

where $\phi_i(x,t)$ are the eigenfunctions, and $X_i(t;\omega)$ are zero-mean stochastic processes whose variance $\mathbb{E}\left[X^2(t;\omega)\right]$is equal to the corresponding eigenvalue $\lambda_i(t)$ of the eigenvalue problem of the Karhunen-Loeve decomposition:

$$\int_D C_{\phi(\cdot,t)\phi(\cdot,t)}(x,y)\phi_i(x,t)dx = \lambda_i(t)\phi_i(y,t),\ \text{y} \in \text{D} \tag{2}$$

Defining the linear subspace $V_s = span\{\phi_i(x,t)\}_{i=1}^{N}$ as the linear subspace spanned by the N deterministic eigenfields associated with the N largest eigenvlaues.

3.2 DO field equations for Allen-Cahn

Governing equation for 1-D Allen-Cahn phase field model is as follows;

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = \gamma\left[\frac{\partial^2 \phi}{\partial x^2} - \frac{\phi^3-\phi}{\eta^2} + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int(\phi^3-\phi)dx\right] \tag{3}$$

All quantities $\bar{\phi}(x,t), \phi_i(x,t), X_i(t;\omega)$, $i = 1,\ldots,N$ in the representation (2) are time-dependent and hence there exists some redundancy in the representation. Therefore, additional constraints are needed to be imposed in order to formulate a well posed problem for the unknown quantities. A natural constraint to overcome redundancy is that the evolution of the basis $\{\phi_i(x,t)\}_{i=1}^N$ be *normal* to the space V_s; which can be expressed as following:

$$\frac{dV_s}{dt} \perp V_s \Longleftrightarrow \left\langle \frac{\partial \phi_i(x,t)}{\partial t}, \phi_j(x,t)\right\rangle = 0,\ i,j = 1,\ldots,N \tag{4}$$

This condition is referred to as the *dynamically orthogonal (DO) condition.* The DO condition preserves orthonormality of the basis $\{\phi_i(x,t)\}_{i=1}^N$ since

$$\frac{\partial}{\partial t}\langle \phi_i(\cdot,t), \phi_j(\cdot,t)\rangle = \left\langle \frac{\partial \phi_i(\cdot,t)}{\partial t}, \phi_j(x,t)\right\rangle + \left\langle \phi_i(\cdot,t), \frac{\partial \phi_j(\cdot,t)}{\partial t}\right\rangle = 0,\ i,j = 1,\ldots,N \tag{5}$$

and results in a set of independent and explicit evolution equations for all the unknown quantities. Furthermore, considering $u(x,t;\omega)$ as a random variable and using *DO* representation, $u(x,t;\omega)$ can be approximated as follows:

$$u(x,t;\omega) = \bar{u}(x,t) + \sum_{i=1}^{N} Y_i(t;\omega)u_i(x,t) = \bar{u} + Y_i u_i \tag{6}$$

Inserting DO representation into eq(1), we get;

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\bar{\phi}+X_i\phi_i\right)+\left(\bar{u}+Y_iu_i\right)\frac{\partial}{\partial x}\left(\bar{\phi}+X_i\phi_i\right)\\
=&\gamma\Bigg[\frac{\partial^2}{\partial x^2}\left(\bar{\phi}+X_i\phi_i\right)-\frac{1}{\eta^2}\Big\{\left(\bar{\phi}+X_i\phi_i\right)^3-\left(\bar{\phi}+X_i\phi_i\right)\Big\}\\
&+\frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\Big\{\left(\bar{\phi}+X_i\phi_i\right)^3-\left(\bar{\phi}+X_i\phi_i\right)\Big\}\,dx\Bigg]
\end{aligned}\tag{7}$$

The above equation can be expressed as follows;

$$\frac{\partial\bar{\phi}}{\partial t}+\phi_i\frac{dX_i}{dt}+X_i\frac{\partial\phi_i}{\partial t}=\mathcal{L}\left[\phi(\cdot,t;\omega)\right]=\mathcal{L}\left[\phi\right]\tag{8}$$

where,

$$\begin{aligned}
\mathcal{L}\left[\phi\right]=&-\bar{u}\frac{\partial\bar{\phi}}{\partial x}-\bar{u}X_i\frac{\partial\phi_i}{\partial x}+Y_iu_i\frac{\partial\bar{\phi}}{\partial x}-Y_iX_ju_i\frac{\partial\phi_j}{\partial x}\\
&+\gamma\Bigg[\frac{\partial^2\bar{\phi}}{\partial x^2}+X_i\frac{\partial^2\phi_i}{\partial x^2}-\frac{1}{\eta^2}\Bigg\{\bar{\phi}^3+3X_i\bar{\phi}^2\phi_i+3X_iX_j\bar{\phi}\phi_i\phi_j\\
&+X_iX_jX_k\phi_i\phi_j\phi_k-\bar{\phi}-X_i\phi_i\Bigg\}+\frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\Bigg\{\bar{\phi}^3+3X_i\bar{\phi}^2\phi_i\\
&+3X_iX_j\bar{\phi}\phi_i\phi_j+X_iX_jX_k\phi_i\phi_j\phi_k-\bar{\phi}-X_i\phi_i\Bigg\}dx\Bigg]
\end{aligned}$$

3.2.1 DO evolution equation for the mean

Considering the fact that $X_i(t;\omega), Y_i(t;\omega)$ are zero mean stochastic processes, the properties associated with the expectation operator are as follows:

$$\begin{aligned} &\mathbb{E}\left[X_i\right] = 0 \\ &\mathbb{E}\left[Y_i\right] = 0 \end{aligned} \tag{9}$$

By applying the expectation operator on both sides of eq(8) we obtain the evolution equation for the mean:

$$\boxed{\begin{aligned} \frac{\partial \bar{\phi}}{\partial t} &= \mathbb{E}\left[\mathcal{L}\left[\phi\right]\right] \\ &= -\bar{u}\frac{\partial \bar{\phi}}{\partial x} - S_{ij}u_i\frac{\partial \phi_j}{\partial x} + \gamma\left[\frac{\partial^2 \bar{\phi}}{\partial x^2} - \frac{1}{\eta^2}\left\{F_0 + F_1 + F_2\right\}\right. \\ &\quad \left. + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\left\{F_0 + F_1 + F_2\right\}dx\right] \end{aligned}} \tag{10}$$

where,

$$\boxed{\begin{aligned} &F_0 = \bar{\phi}^3 - \bar{\phi} \\ &F_1 = 3C_{ij}\bar{\phi}\phi_i\phi_j \\ &F_2 = C_{ijk}\phi_i\phi_j\phi_k \\ &C_{ij} = \mathbb{E}\left[X_iX_j\right] \\ &C_{ijk} = \mathbb{E}\left[X_iX_jX_k\right] \\ &S_{ij} = \mathbb{E}\left[Y_iX_j\right] \end{aligned}}$$

3.2.2 DO evolution equations for the stochastic basis(coefficients)

Subtracting eq(10) from eq(8) we get;

$$\phi_i \frac{dX_i}{dt} + X_i \frac{\partial \phi_i}{\partial t} = \mathcal{L}[\phi] - \mathbb{E}[\mathcal{L}[\phi]] \tag{11}$$

where,

$$\begin{aligned}
\mathcal{L}[\phi] - \mathbb{E}[\mathcal{L}[\phi]] = & -\bar{u} X_i \frac{\partial \phi_i}{\partial x} - Y_i u_i \frac{\partial \bar{\phi}}{\partial x} - Y_i X_j u_i \frac{\partial \phi_j}{\partial x} + S_{ij} u_i \frac{\partial \phi_j}{\partial x} \\
& + \gamma \Bigg[X_i \frac{\partial^2 \phi_i}{\partial x^2} - \frac{1}{\eta^2} \Bigg\{ 3X_i \bar{\phi}^2 \phi_i + 3X_i X_j \bar{\phi} \phi_i \phi_j \\
& - 3C_{ij} \bar{\phi} \phi_i \phi_j + X_i X_j X_k \phi_i \phi_j \phi_k - C_{ijk} \phi_i \phi_j \phi_k - X_i \phi_i \Bigg\} \\
& + \frac{1}{|\Omega_p|} \frac{1}{\eta^2} \int_{\Omega_p} \Bigg\{ 3X_i \bar{\phi}^2 \phi_i + 3X_i X_j \bar{\phi} \phi_i \phi_j \\
& - 3C_{ij} \bar{\phi} \phi_i \phi_j + X_i X_j X_k \phi_i \phi_j \phi_k - C_{ijk} \phi_i \phi_j \phi_k - X_i \phi_i \Bigg\} dx \Bigg]
\end{aligned}$$

By projecting eq(11) on the spatial basis we have,

$$\langle \phi_i, \phi_l \rangle \frac{dX_i}{dt} + X_i \left\langle \frac{\partial \phi_i}{\partial t}, \phi_l \right\rangle = \langle \mathcal{L}[\phi] - \mathbb{E}[\mathcal{L}[\phi]], \phi_l \rangle = \left\langle \tilde{\mathcal{L}}[\phi], \phi_l \right\rangle, \; l = 1, \dots, N \tag{12}$$

Now the first term on the LHS of eq(12) vanishes because of the orthonormality except one term for which $i = l$. Moreover, the dynamically orthogonal condition implies that the second term in the LHS vanishes completely. Therefore, we get evolution equations for the stochastic basis as,

$$\boxed{\begin{aligned}\frac{dX_l}{dt} &= \left\langle \tilde{\mathcal{L}}\left[\phi\right], \phi_l \right\rangle, \, l = 1, \ldots, N \\ &= -\bar{u}X_i \left\langle \frac{\partial \phi_i}{\partial x}, \phi_l \right\rangle - Y_i u_i \left\langle \frac{\partial \bar{\phi}}{\partial x}, \phi_l \right\rangle - R_{ij} u_i \left\langle \frac{\partial \phi_j}{\partial x}, \phi_l \right\rangle + \gamma \Bigg[X_i \left\langle \frac{\partial^2 \phi_i}{\partial x^2}, \phi_l \right\rangle \\ &\quad - \frac{1}{\eta^2} \Big\{ \langle G_0, \phi_l \rangle + \langle G_1, \phi_l \rangle + \langle G_2, \phi_l \rangle \Big\} + \frac{1}{|\Omega_p|} \frac{1}{\eta^2} \left\langle \int_{\Omega_p} \Big\{ G_0 + G_1 + G_2 \Big\} dx, \phi_l \right\rangle \Bigg]\end{aligned}} \tag{13}$$

where,

$$\boxed{\begin{aligned}&G_0 = X_i \phi_i (3\bar{\phi}^2 - 1) \\ &G_1 = 3 D_{ij} \bar{\phi} \phi_i \phi_j \\ &G_2 = D_{ijk} \phi_i \phi_j \phi_k \\ &D_{ij} = X_i X_j - C_{ij} \\ &D_{ijk} = X_i X_j X_k - C_{ijk} \\ &R_{ij} = Y_i X_j - S_{ij}\end{aligned}}$$

3.2.3 DO evolution equations for the spatial basis(modes)

Utilizing the linearity of the expectation operator and mean-zero property of the stochastic basis, we can deduce that;

$$\begin{aligned}
&\mathbb{E}\left[\tilde{\mathcal{L}}\left[\phi\right]\right] = \mathbb{E}\left[\mathcal{L}\left[\phi\right]\right] - \mathbb{E}\left[\mathbb{E}\left[\mathcal{L}\left[\phi\right]\right]\right] = 0 \\
&\mathbb{E}\left[\tilde{\mathcal{L}}\left[\phi\right] X_l\right] = \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right]
\end{aligned} \tag{14}$$

Multiplying eq(8) with X_l and applying the expectation operator we get

$$\mathbb{E}\left[\frac{dX_i}{dt} X_l\right] \phi_i + \mathbb{E}\left[X_i X_l\right] \frac{\partial \phi_i}{\partial t} = \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right] \tag{15}$$

By putting *DO* evolution equations for stochastic basis in eq(15) , and using the interchangeability of the inner product on the physical and stochastic domain, we have

$$\begin{aligned}
\mathbb{E}\left[X_i X_l\right] \frac{\partial \phi_i}{\partial t} &= \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right] - \mathbb{E}\left[\frac{dX_i}{dt} X_l\right] \phi_i \\
&= \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right] - \mathbb{E}\left[\left\langle \tilde{\mathcal{L}}\left[\phi\right], \phi_i \right\rangle X_l\right] \phi_i \\
&= \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right] - \mathbb{E}\left[\left\langle \tilde{\mathcal{L}}\left[\phi\right] X_l, \phi_i \right\rangle\right] \phi_i \\
&= \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right] - \left\langle \mathbb{E}\left[\tilde{\mathcal{L}}\left[\phi\right] X_l\right], \phi_i \right\rangle \phi_i \\
&= \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right] - \left\langle \mathbb{E}\left[\mathcal{L}\left[\phi\right] X_l\right], \phi_i \right\rangle \phi_i
\end{aligned} \tag{16}$$

Therefore evolution equations for the spatial basis can be written as

$$\boxed{\frac{\partial \phi_i}{\partial t} = \bigg(\mathbb{E}[\mathcal{L}[\phi]X_l] - \langle \mathbb{E}[\mathcal{L}[\phi]X_l], \phi_l \rangle \phi_l \bigg) C_{il}^{-1}, \; i = 1, \ldots, N} \tag{17}$$

where the expression for the first term on the RHS is given by,

$$\boxed{\begin{aligned} \mathbb{E}[\mathcal{L}[\phi]X_l] = & -C_{il}\bar{u}\frac{\partial \phi_i}{\partial x} - S_{il}u_i\frac{\partial \bar{\phi}}{\partial x} - S_{ijl}u_i\frac{\partial \phi_j}{\partial x} \\ & + \gamma\Bigg[C_{il}\frac{\partial^2 \phi_i}{\partial x^2} - \frac{1}{\eta^2}\Bigg\{C_{il}H_i + C_{ijl}H_{ij} + C_{ijkl}H_{ijk}\Bigg\} \\ & + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\Bigg\{C_{il}H_i + C_{ijl}H_{ij} + C_{ijkl}H_{ijk}\Bigg\}dx\Bigg] \end{aligned}}$$

and

$$\boxed{\begin{aligned} & H_i = \phi_i(3\bar{\phi}^2 - 1) \\ & H_{ij} = 3\bar{\phi}\phi_i\phi_j \\ & H_{ijk} = \phi_i\phi_j\phi_k \\ & C_{il} = \mathbb{E}\left[X_i X_l\right] \\ & C_{ijl} = \mathbb{E}\left[X_i X_j X_l\right] \\ & C_{ijkl} = \mathbb{E}\left[X_i X_j X_k X_l\right] \\ & S_{il} = \mathbb{E}\left[Y_i X_l\right] \\ & S_{ijl} = \mathbb{E}\left[Y_i X_j X_l\right] \end{aligned}}$$

Chapter 4

Numerical Illustrations

4.1 Numerics for manufactured solution

Considering $\gamma = 1$ and $\eta = 1$, we assume the exact solution to the stochastic partial differential eq(8) as,

$$\phi(x,t;\omega) = cos(\pi x)sin(\pi t) + cos(2\pi x)sin(2\xi t) + cos(4\pi x)sin(4\xi t) \tag{18}$$

where ξ is uniformly distributed random variable in $[-1, 1]$. In the DO representation, the solution can be expressed as,

$$\phi(x,t;\omega) = \bar{\phi}(x,t) + \sum_{i=1}^{2} \phi_i(x,t)X_i(t;\omega) \tag{19}$$

Therefore the exact formulas for $\bar{\phi}$, ϕ_i and X_i, utilizing the modes to be orthonormal and coefficients to be zero mean stochastic processes, we have

$$\bar{\phi}(x,t) = cos(\pi x)sin(\pi t)$$

$$\phi_1(x,t) = cos(2\pi x)$$

$$\phi_2(x,t) = cos(4\pi x)$$

$$X_1(t;\omega) = sin(2\xi t)$$

$$X_2(t;\omega) = sin(4\xi t)$$

The DO evolution equations $(10, 13, 17)$ involve numerical integration in physical space as well as in parametric space. We define the collocation points and weights for the physical space by $(x_k, w_k)_{k=1}^{N_s}$ and the parametric space by $(\xi_j, w_j)_{j=1}^{N_r}$. Two inner products are involved in DO equations:

- Inner product in the physical space

$$\langle h(x), g(x) \rangle = \int_D h(x)g(x)dx \approx \sum_{k=1}^{N_s} h(x_k) g_{x_k} w_k$$

- Inner product in random space, i.e., mean value operator

$$\mathbb{E}[h(\omega)g(\omega)] = \int_\Omega h(\omega)g(\omega)\rho(\omega)d\omega \approx \sum_{j=1}^{N_r} h(\xi_j)g(\xi_j)w_j$$

4.1.1 Numerical solution for evolution of mean

Analyzing evolution equation of the mean eq(10) with the aforementioned manufactured solution results in the following numerical algorithm:

- The Legendre spectral Galerkin scheme is used physical space. The second order derivative corresponding to diffusive term is evolved in time using second order Crank-Nicolson method whereas first order derivative corresponding to convection term is augmented using Adams-Bashforth time integration scheme. The non-linear term is treated as a source term and is numerically treated similar to convection term.

- The forcing term which is added in the evolution equation for the mean, as a result of manufactured solution, is treated as a source term and is calculated at discrete half time interval($t^{n+\frac{1}{2}}$).

- Since $X_i(t;\xi)$ corresponds to zero mean stochastic processes where $\xi(\omega)$ is uniformly distributed random variable, therefore the Stochastic collocation scheme is used in parametric space.

The spatial basis(modes) are chosen to be orthonormal whereas stochastic basis(coefficients) are chosen to be zero mean stochastic processes. The evolution equation for the mean is initially solved by passing the exact values of spatial and stochastic basis. The parameter chosen are as follows:

- $\Delta t = 0.0001$: Discrete time step.
- $t_f = 10.0$: Final time.
- $N = 2$: Number of terms in K-L expansion(number of modes).
- $Ns = 32$: Number of Legendre-Gauss-Lobatto quadrature points corresponding to the polynomials of degree less than or equal to Ns.
- $Nr = 32$: Number of Legendre-collocation points in parametric space.

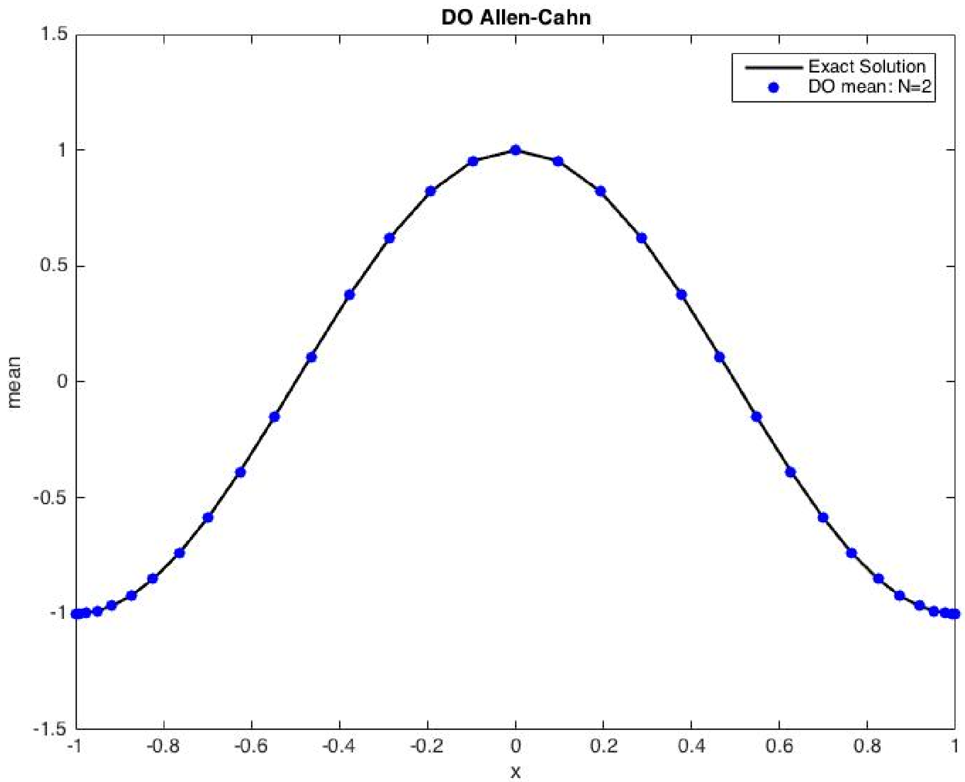

Figure 1: This figure illustrates mean of the DO solution for the Allen-Cahn equation at $t_f = 2.5$ with the initial condition corresponding to orthonormal spatial basis and zero mean stochastic basis. The parameters are $Ns = 32$, $Nr = 32$.

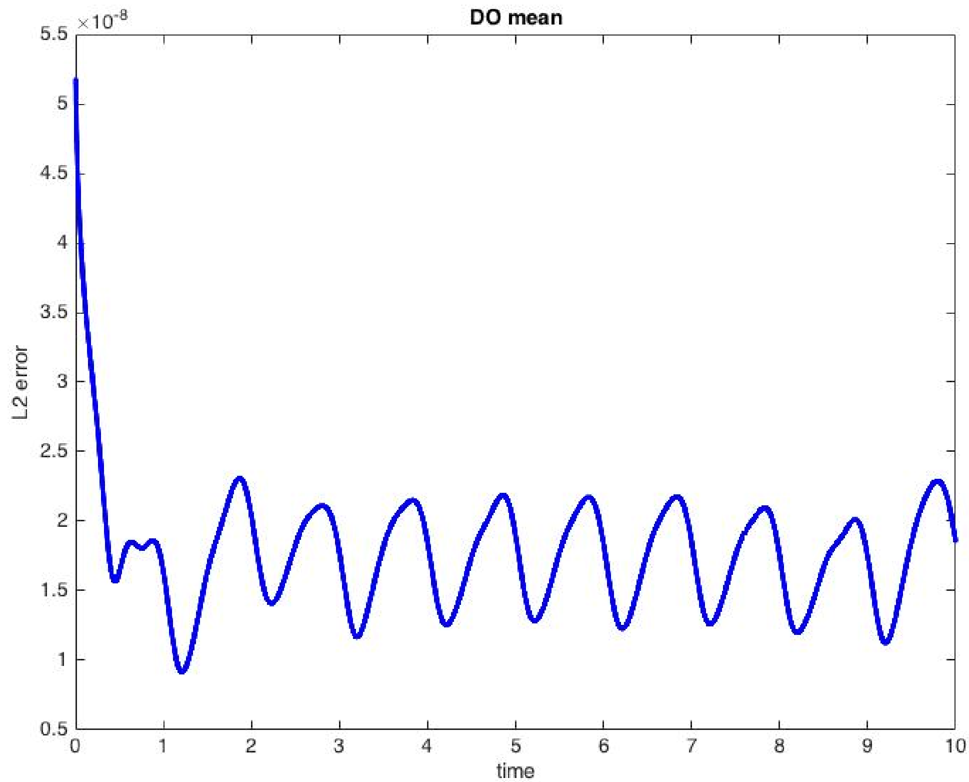

Figure 2: This figure illustrates the evolution of $L2$ error of the mean with time. The discrete time step is taken as $\Delta t = 0.0001$ and final time is $t_f = 10.0$. The parameters are $Ns = 32$, $Nr = 32$ The $L2$ error scales on $1.0e - 08$ demonstrating second order accuracy.

4.1.2 Numerical solution for evolution of stochastic basis

The probabilistic collocation method is used for discretization in parametric space. Fourth order Runge-Kutta scheme is used as a time integrator. The evolution equations for the stochastic basis is numerically computed by passing the exact values of mean and the modes(spatial basis). The parameter chosen are as follows:

- $\Delta t = 0.001$: Discrete time step.
- $t_f = 10.0$: Final time.
- $N = 2$: Number of terms in K-L expansion(number of modes).
- $Ns = 32$: Number of Legendre-Gauss-Lobatto quadrature points corresponding to the polynomials of degree less than or equal to Ns.
- $Nr = 32$: Number of Legendre-collocation points in parametric space.

As shown in Fig.3 the L2 error in stochastic basis initially increases with time. However, the error in two stochastic basis(coefficents) gets stabilized at different order, at higher time intervals.

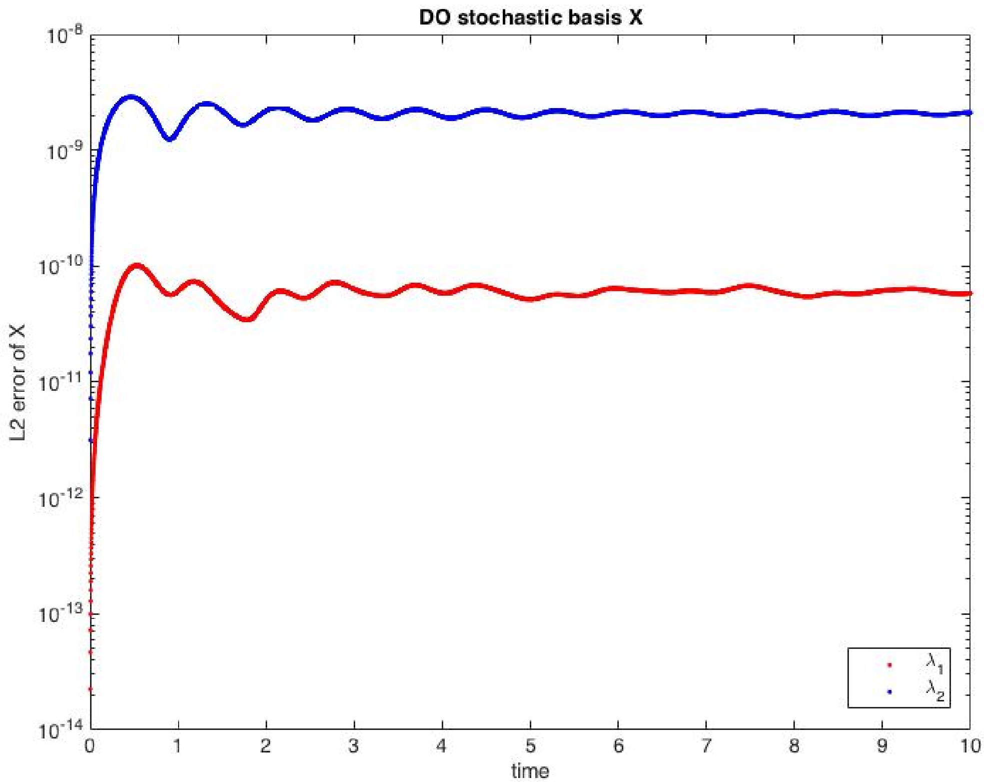

Figure 3: This figure illustrates the evolution of $L2$ error of the stochastic basis with time. The discrete time step is taken as $\Delta t = 0.001$ and final time is $t_f = 10.0$. The parameters are $Ns = 64$, $Nr = 64$. The error for X initially increases with time.

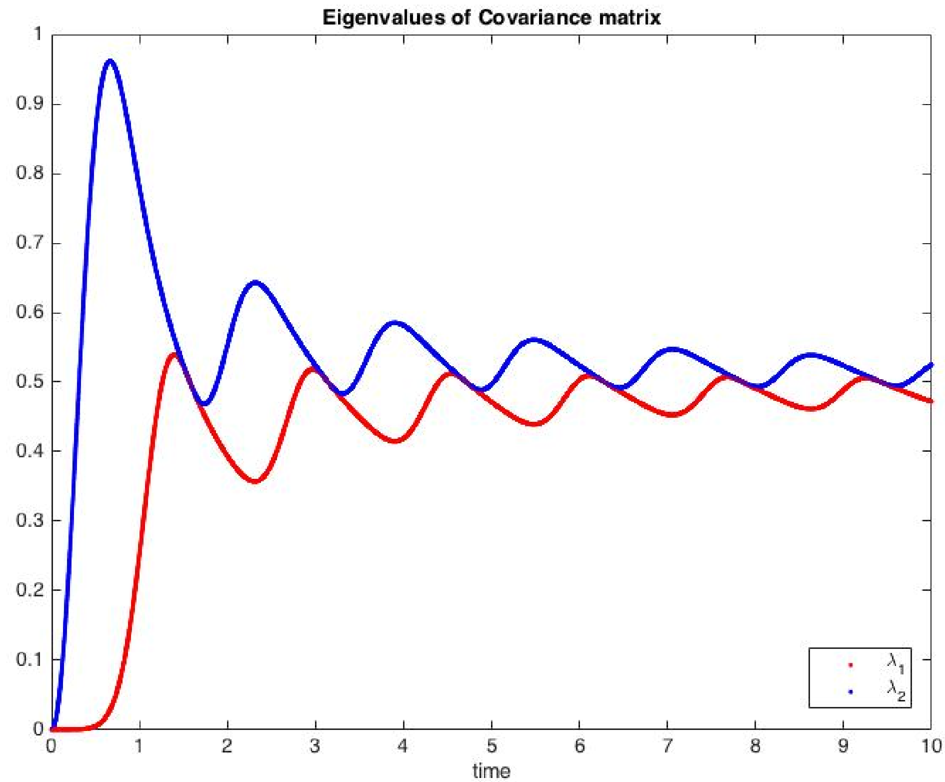

Figure 4: This figure illustrates the evolution of eigenvalues of the covariance matrix with time. The discrete time step is taken as $\Delta t = 0.001$ and final time is $t_f = 10.0$. The parameters are $Ns = 64$, $Nr = 64$.

4.1.3 Numerical solution for evolution of spatial basis

- The Legendre spectral Galerkin scheme is used physical space. The second order derivative corresponding to diffusive term is evolved in time using second order Crank-Nicolson method whereas first order derivative corresponding to convection term is augmented using Adams-Bashforth time integration scheme. The non-linear term is treated as a source term and is numerically treated similar to convection term.

- The forcing term which is added in the evolution equation for the mean, as a result of manufactured solution, is treated as a source term and is calculated at discrete half time interval($t^{n+\frac{1}{2}}$).

- Since $X_i(t;\xi)$ corresponds to zero mean stochastic processes where $\xi(\omega)$ is uniformly distributed random variable, therefore the Stochastic collocation scheme is used in parametric space.

The numerical integration is performed from second time step in order to avoid the covariance matrix becoming singular.

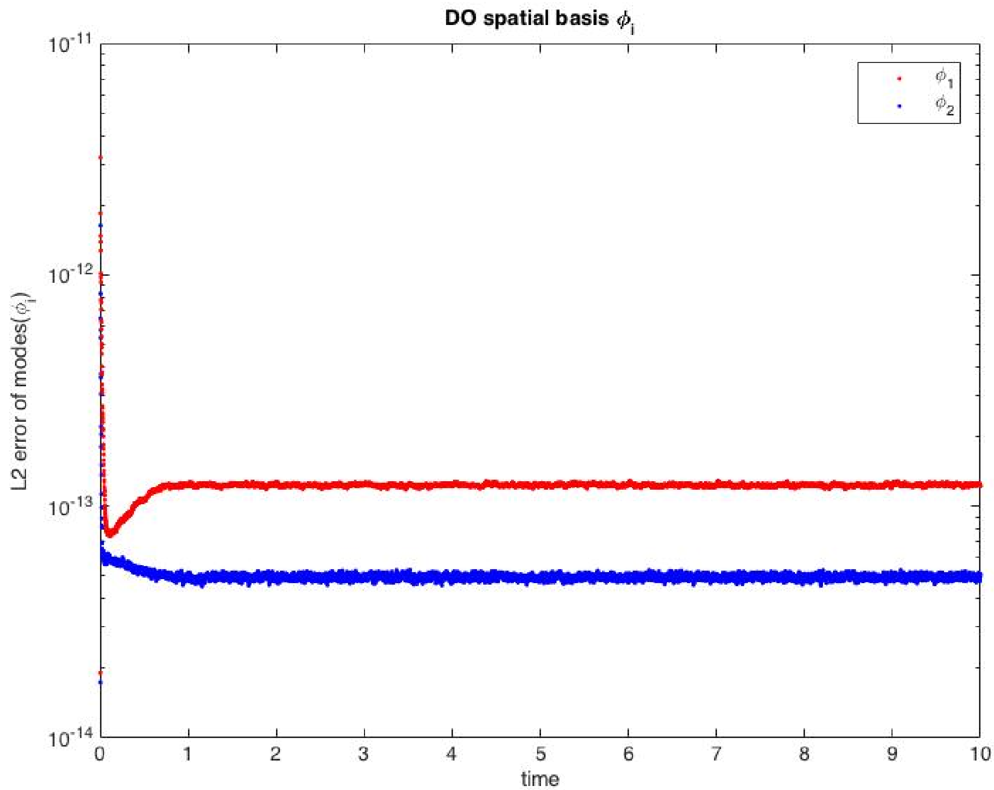

Figure 5: This figure illustrates the evolution of $L2$ error of the spatial basis with time. The discrete time step is taken as $\Delta t = 0.001$ and final time id $t_f = 10.0$. The parameters are $Ns = 127$, $Nr = 127$.

4.2 Numerics for high dimensional random forcing

Consider the stochastic Allen-Cahn phase field model with high dimensional random forcing. Here ξ_m are m independent and identically uniformly distributed(i.i.d) random variables.

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = \gamma\left[\frac{\partial^2 \phi}{\partial x^2} - \frac{\phi^3 - \phi}{\eta^2} + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int(\phi^3 - \phi)dx\right] + \sum_{m=1}^{M}\frac{\xi_m}{m^2}sin\left(\frac{m\pi x}{2}\right) \tag{20}$$

where $\xi_m \sim \mathbb{U}\left[-1, 1\right]$

and the initial condition is given as

$$\phi(x, 0, \omega) = cos(\pi x) + sin(2\pi\xi)cos(2\pi x) + sin(4\pi\xi)cos(4\pi x) \tag{21}$$

DO evolution field equations are solved numerically for above equation. In order to avoid curse of dimensionality, the stochastic ODE, governing the evolution of stochastic basis(coefficeints), are solved using Monte Carlo non intrusive sampling algorithm.

The following parameters are chosen

- $\Delta t = 10E-5$: Discrete time step.
- $t_f = 0.85$: Final time.
- $N = 2, 3, 4$: Number of modes
- $Ns = 128$: Number of Legendre-Gauss-Lobatto quadrature points corresponding to the polynomials of degree less than or equal to Ns.
- $Nr = 100000$: Number of Monte Carlo samples in parametric space.
- $M = 100$: Number of terms in stochastic forcing.

After inserting the DO representation in eq(44) we get the following necessary operators

$$
\begin{aligned}
\mathcal{L}\left[\phi\right] = & -\bar{u}\frac{\partial\bar{\phi}}{\partial x} - \bar{u}X_i\frac{\partial\phi_i}{\partial x} + Y_i u_i\frac{\partial\bar{\phi}}{\partial x} - Y_i X_j u_i\frac{\partial\phi_j}{\partial x} \\
& + \gamma\left[\frac{\partial^2\bar{\phi}}{\partial x^2} + X_i\frac{\partial^2\phi_i}{\partial x^2} - \frac{1}{\eta^2}\left\{\bar{\phi}^3 + 3X_i\bar{\phi}^2\phi_i + 3X_iX_j\bar{\phi}\phi_i\phi_j\right.\right. \\
& \left. + X_iX_jX_k\phi_i\phi_j\phi_k - \bar{\phi} - X_i\phi_i\right\} + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\left\{\bar{\phi}^3 + 3X_i\bar{\phi}^2\phi_i\right. \\
& \left.\left. + 3X_iX_j\bar{\phi}\phi_i\phi_j + X_iX_jX_k\phi_i\phi_j\phi_k - \bar{\phi} - X_i\phi_i\right\}dx\right] \\
& + \sum_{m=1}^{M}\frac{\xi_m}{m^2}sin\left(\frac{m\pi x}{2}\right)
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
\mathcal{L}\left[\phi\right]-\mathbb{E}\left[\mathcal{L}\left[\phi\right]\right]= & -\bar{u}X_i\frac{\partial\phi_i}{\partial x}-Y_iu_i\frac{\partial\bar{\phi}}{\partial x}-Y_iX_ju_i\frac{\partial\phi_j}{\partial x}+S_{ij}u_i\frac{\partial\phi_j}{\partial x}\\
& +\gamma\left[X_i\frac{\partial^2\phi_i}{\partial x^2}-\frac{1}{\eta^2}\left\{3X_i\bar{\phi}^2\phi_i+3X_iX_j\bar{\phi}\phi_i\phi_j\right.\right.\\
& \left.-3C_{ij}\bar{\phi}\phi_i\phi_j+X_iX_jX_k\phi_i\phi_j\phi_k-C_{ijk}\phi_i\phi_j\phi_k-X_i\phi_i\right\}\\
& +\frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\left\{3X_i\bar{\phi}^2\phi_i+3X_iX_j\bar{\phi}\phi_i\phi_j\right.\\
& \left.\left.-3C_{ij}\bar{\phi}\phi_i\phi_j+X_iX_jX_k\phi_i\phi_j\phi_k-C_{ijk}\phi_i\phi_j\phi_k-X_i\phi_i\right\}dx\right]\\
& +\sum_{m=1}^{M}\frac{\xi_m}{m^2}sin\left(\frac{m\pi x}{2}\right)
\end{aligned}
\tag{23}
$$

We have the following coupled DO evolution equations

$$\boxed{\begin{aligned}\frac{\partial \bar{\phi}}{\partial t} &= \mathbb{E}\left[\mathcal{L}\left[\phi\right]\right] \\ &= -\bar{u}\frac{\partial \bar{\phi}}{\partial x} - S_{ij}u_i\frac{\partial \phi_j}{\partial x} + \gamma\left[\frac{\partial^2 \bar{\phi}}{\partial x^2} - \frac{1}{\eta^2}\Big\{F_0 + F_1 + F_2\Big\}\right. \\ &\left. + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\Big\{F_0 + F_1 + F_2\Big\}dx\right]\end{aligned}} \tag{24}$$

where,

$$\boxed{\begin{aligned} &F_0 = \bar{\phi}^3 - \bar{\phi} \\ &F_1 = 3C_{ij}\bar{\phi}\phi_i\phi_j \\ &F_2 = C_{ijk}\phi_i\phi_j\phi_k \\ &C_{ij} = \mathbb{E}\left[X_iX_j\right] \\ &C_{ijk} = \mathbb{E}\left[X_iX_jX_k\right] \\ &S_{ij} = \mathbb{E}\left[Y_iX_j\right]\end{aligned}}$$

$$\boxed{\begin{aligned}\frac{dX_l}{dt} &= \left\langle \mathcal{L}\left[\phi\right] - \mathbb{E}\left[\mathcal{L}\left[\phi\right]\right], \phi_l \right\rangle,\ l = 1, \ldots, N \\ &= -\bar{u}X_i \left\langle \frac{\partial \phi_i}{\partial x}, \phi_l \right\rangle - Y_i u_i \left\langle \frac{\partial \bar{\phi}}{\partial x}, \phi_l \right\rangle - R_{ij} u_i \left\langle \frac{\partial \phi_j}{\partial x}, \phi_l \right\rangle + \gamma \Bigg[X_i \left\langle \frac{\partial^2 \phi_i}{\partial x^2}, \phi_l \right\rangle \\ &- \frac{1}{\eta^2}\Big\{ \langle G_0, \phi_l\rangle + \langle G_1, \phi_l\rangle + \langle G_2, \phi_l\rangle \Big\} + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\left\langle \int_{\Omega_p} \Big\{ G_0 + G_1 + G_2 \Big\} dx, \phi_l \right\rangle \Bigg] \\ &+ \sum_{m=1}^{M} \frac{\xi_m}{m^2} \left\langle sin\left(\frac{m\pi x}{2}\right), \phi_l \right\rangle \end{aligned}} \tag{25}$$

where,

$$\boxed{\begin{aligned} &G_0 = X_i \phi_i (3\bar{\phi}^2 - 1) \\ &G_1 = 3D_{ij}\bar{\phi}\phi_i\phi_j \\ &G_2 = D_{ijk}\phi_i\phi_j\phi_k \\ &D_{ij} = X_i X_j - C_{ij} \\ &D_{ijk} = X_i X_j X_k - C_{ijk} \\ &R_{ij} = Y_i X_j - S_{ij} \end{aligned}}$$

$$\boxed{\frac{\partial \phi_i}{\partial t} = \bigg(\mathbb{E}[\mathcal{L}[\phi]X_l] - \langle \mathbb{E}[\mathcal{L}[\phi]X_l], \phi_l\rangle\phi_l\bigg)C_{il}^{-1},\ i = 1, \ldots, N} \tag{26}$$

where the expression for the first term on the RHS is given by,

$$\boxed{\begin{aligned}\mathbb{E}[\mathcal{L}[\phi]X_l] = &-C_{il}\bar{u}\frac{\partial \phi_i}{\partial x} - S_{il}u_i\frac{\partial \bar{\phi}}{\partial x} - S_{ijl}u_i\frac{\partial \phi_j}{\partial x} \\ &+ \gamma\Bigg[C_{il}\frac{\partial^2 \phi_i}{\partial x^2} - \frac{1}{\eta^2}\Big\{C_{il}H_i + C_{ijl}H_{ij} + C_{ijkl}H_{ijk}\Big\} \\ &+ \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int_{\Omega_p}\Big\{C_{il}H_i + C_{ijl}H_{ij} + C_{ijkl}H_{ijk}\Big\}dx\Bigg] \\ &+ \sum_{m=1}^{M}\mathbb{E}\left[\xi_m X_l\right]\frac{1}{m^2}sin\left(\frac{m\pi x}{2}\right)\end{aligned}}$$

and

$$\boxed{\begin{aligned}&H_i = \phi_i(3\bar{\phi}^2 - 1) \\ &H_{ij} = 3\bar{\phi}\phi_i\phi_j \\ &H_{ijk} = \phi_i\phi_j\phi_k \\ &C_{il} = \mathbb{E}\left[X_iX_l\right] \\ &C_{ijl} = \mathbb{E}\left[X_iX_jX_l\right] \\ &C_{ijkl} = \mathbb{E}\left[X_iX_jX_kX_l\right] \\ &S_{il} = \mathbb{E}\left[Y_iX_l\right] \\ &S_{ijl} = \mathbb{E}\left[Y_iX_jX_l\right]\end{aligned}}$$

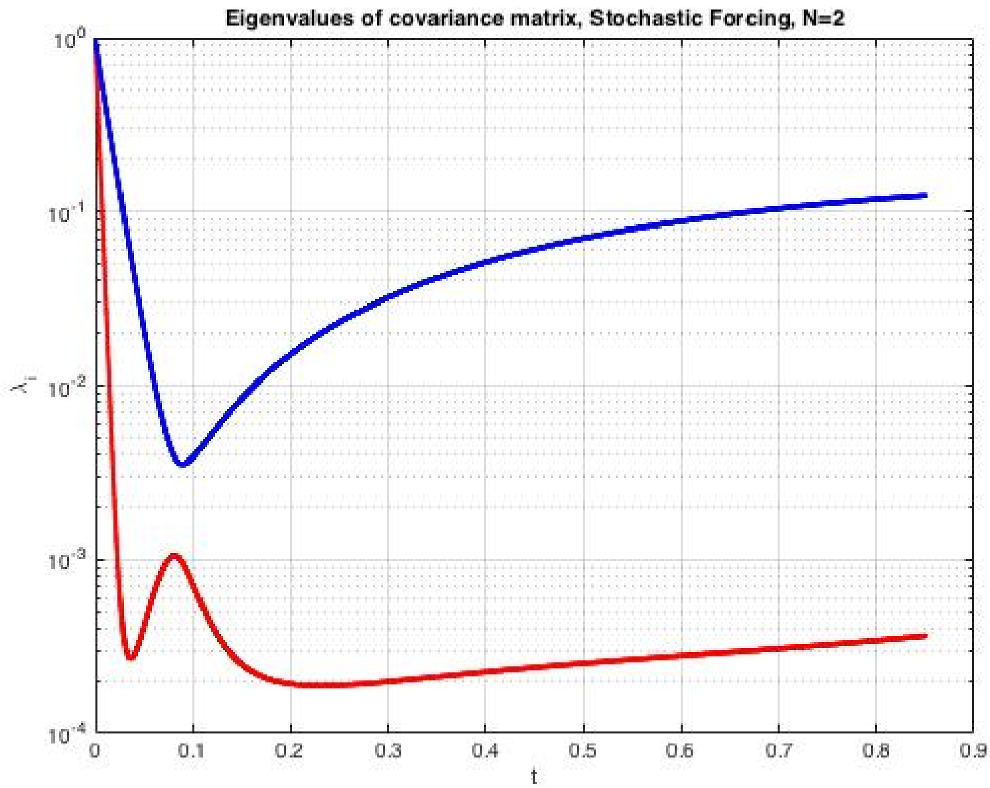

Figure 6: This figure illustrates the evolution of eigenvalues of the covariance matrix under high dimensional random forcing. The discrete time step is taken as $\Delta t = 1.0E-5$ and final time is $t_f = 0.85$. The parameters are $Ns = 128$, $Nr = 100000$, $N = 2$.

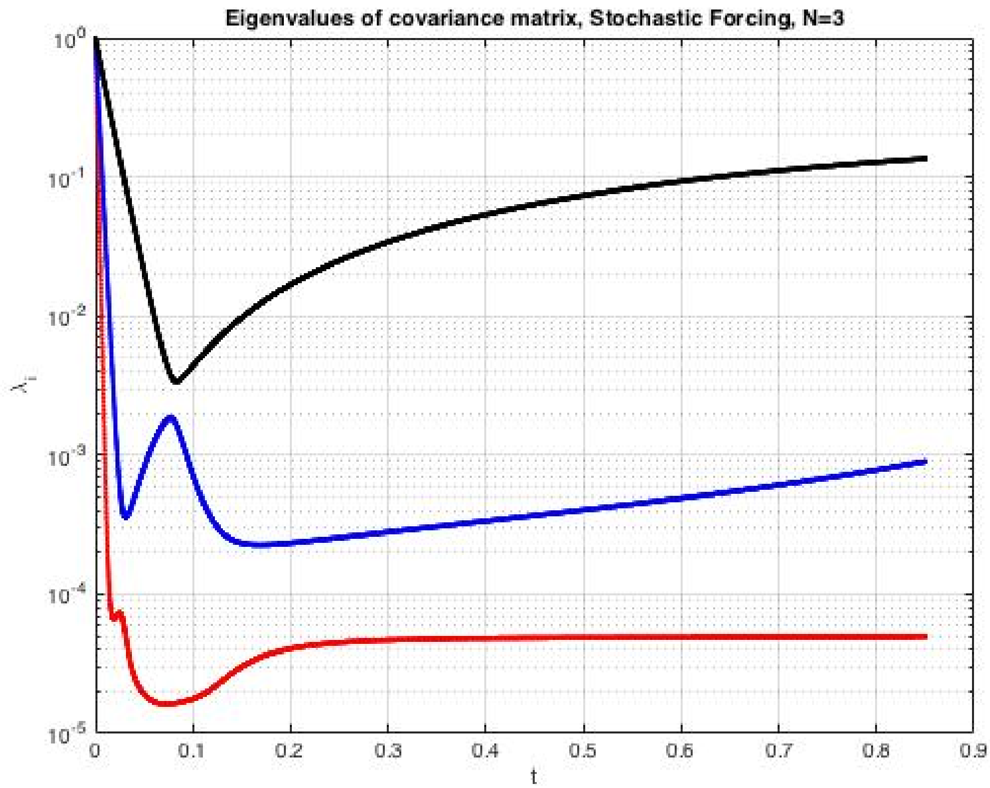

Figure 7: This figure illustrates the evolution of eigenvalues of the covariance matrix under high dimensional random forcing. The discrete time step is taken as $\Delta t = 1.0E-5$ and final time is $t_f = 0.85$. The parameters are $Ns = 128$, $Nr = 100000$, $N = 3$.

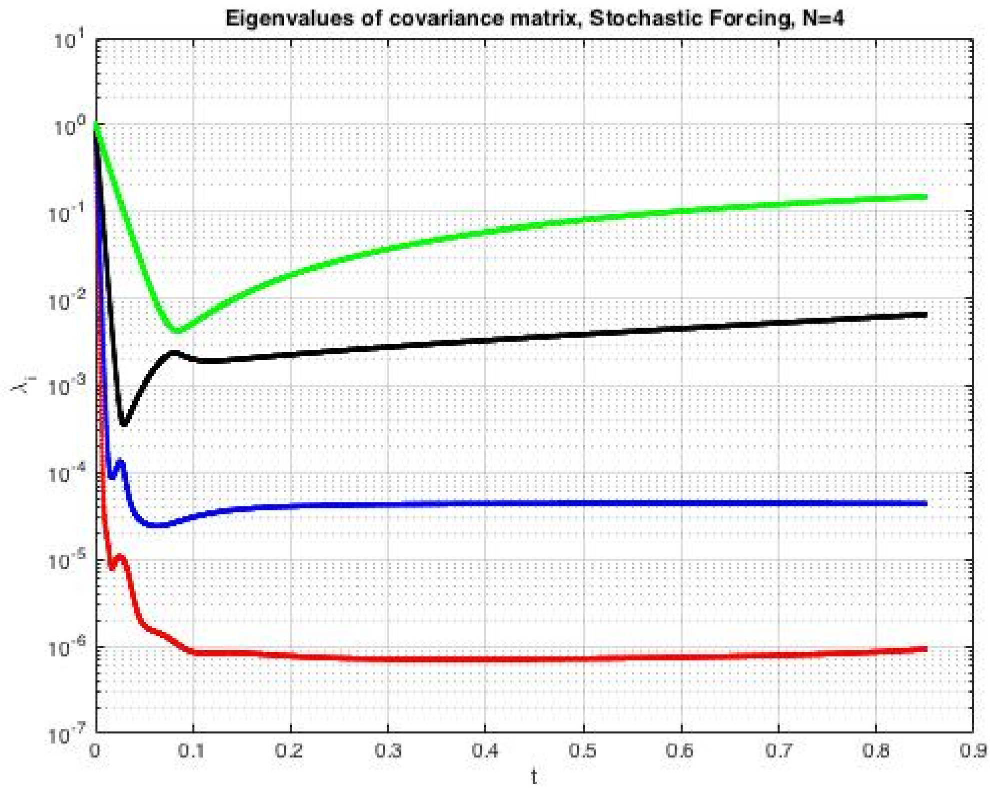

Figure 8: This figure illustrates the evolution of eigenvalues of the covariance matrix under high dimensional random forcing. The discrete time step is taken as $\Delta t = 1.0E-5$ and final time is $t_f = 0.85$. The parameters are $Ns = 128$, $Nr = 100000$, $N = 4$.

Chapter 5

Conclusions and Future Work

In this thesis, we have derived the closed set of Dynamically Orthogonal field equations that determine the evolution of continuous stochastic fields for Stochastic Allen-Cahn equation. Since the basis of the stochastic subspace is evolving according to the system SPDE, fewer modes are needed to capture most of the stochastic energy relative to the classic POD and Polynomial Chaos methods. This is demonstrated by solving Stochastic Allen-Cahn equation under high dimensional random forcing.

The Dynamically Orthogonal framework provides a good platform to investigate the interfacial instabilities in mixing layer by coupling the Stochastic Allen-Cahn equation with the Stochastic Navier-Stokes equation. Th rich flow physics can be understood by quantifying parametric uncertainties. Adaptive modeling and adaptive sampling are also promising future directions for devising robust and hybrid numerical schemes for Dynamically Orthogonal field equations.

Appendix

Mass fraction conservation in DO field equations

Analyzing the 1-D Allen-Cahn equation

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = \gamma\left[\frac{\partial^2 \phi}{\partial x^2} - \frac{\phi^3 - \phi}{\eta^2} + \frac{1}{|\Omega_p|}\frac{1}{\eta^2}\int(\phi^3 - \phi)dx\right]$$

The last term in the RHS of above equation is introduced as a nonlocal Lagrange multiplier to enforce the mass fraction conservation satisfying

$$\frac{d}{dt}\int_{\Omega_p} \phi dx = 0 \tag{27}$$

The aforementioned condition is satisfied in the deterministic Allen-Cahn equation by considering Neumann boundary condition for ϕ

$$\frac{\partial \phi}{\partial n} = 0 \tag{28}$$

Analyzing mass conservation issue for stochastic Allen-Cahn by substituting DO representation for ϕ in eq(31) we get

$$\frac{d}{dt}\int_{\Omega_p} \left(\bar{\phi} + X_i\phi_i\right) dx = 0 \tag{29}$$

Applying the expectation operator in eq(33) we get

$$\frac{d}{dt}\int_{\Omega_p} \left(\bar{\phi} + \mathbb{E}\left[X_i\right]\phi_i\right) dx = 0 \tag{30}$$

resulting in

$$\frac{d}{dt}\int_{\Omega_p} \bar{\phi} dx = 0 \tag{31}$$

as X_i are zero mean stochastic processes. Subtracting eq(35) from eq(33) we get

$$\frac{d}{dt}\int_{\Omega_p} X_i \phi_i dx = 0 \tag{32}$$

Since $X_i(t;\omega)$ is random the above equation tantamount to

$$\frac{d}{dt}\int_{\Omega_p} \phi_i dx = 0 \tag{33}$$

In order to preserve the mass conservation for DO field equations for mean and modes, the conditions from eq(35) and eq(37) has to be satisfied respectively. Assuming that DO mean and modes satisfy Neumann boundary condtions

$$\begin{aligned} \frac{\partial \bar{\phi}}{\partial n} &= 0 \\ \frac{\partial \phi_i}{\partial n} &= 0 \end{aligned} \tag{34}$$

After integrating DO evolution equation for the mean, discarding Lagrange multiplier term, over the physical domain and incorporating Neumann boundary conditions for mean and modes, we see that the terms having linear operator(linear in ϕ) vanishes. Considering the integrand corresponding to non linear operator

$$\mathcal{NL}[\phi] = \left(\bar{\phi} + X_i\phi_i\right)^3 = \bar{\phi}^3 + 3X_i\bar{\phi}^2\phi_i + 3X_iX_j\bar{\phi}\phi_i\phi_j + X_iX_jX_k\phi_i\phi_j\phi_k \tag{35}$$

Applying the expectation operator in the above equation we get

$$\mathbb{E}\left[\mathcal{N}\mathcal{L}\left[\phi\right]\right] = \bar{\phi}^3 + 3\mathbb{E}\left[X_i X_j\right]\bar{\phi}\phi_i\phi_j + \mathbb{E}\left[X_i X_j X_k\right]\phi_i\phi_j\phi_k \tag{36}$$

Hence, the Lagrange multiplier term introduced in the DO evolution equation for the mean, eq(10), satisfies the mass conservation property. Multiplying eq(39) by X_l and taking expectation we have

$$\mathbb{E}\left[\mathcal{N}\mathcal{L}\left[\phi\right]X_l\right] = 3\mathbb{E}\left[X_i X_l\right]\bar{\phi}^2\phi_i + 3\mathbb{E}\left[X_i X_j X_l\right]\bar{\phi}\phi_i\phi_j + \mathbb{E}\left[X_i X_j X_k X_l\right]\phi_i\phi_j\phi_k \tag{37}$$

Taking the projection of eq(41) on the spatial basis we have

$$\begin{aligned}\left\langle \mathbb{E}\left[\mathcal{N}\mathcal{L}\left[\phi\right]X_l\right], \phi_l\right\rangle &= \mathbb{E}\left[X_i X_l\right]\left\langle 3\bar{\phi}^2\phi_i, \phi_l\right\rangle \\ &+ \mathbb{E}\left[X_i X_j X_l\right]\left\langle 3\bar{\phi}\phi_i\phi_j, \phi_l\right\rangle \\ &+ \mathbb{E}\left[X_i X_j X_k X_l\right]\left\langle \phi_i\phi_j\phi_k, \phi_l\right\rangle\end{aligned} \tag{38}$$

Therefore, we can see that the Lagrange multiplier term that is added in the DO evolution equation of the modes takes into account the projection of the non-linear onto the spatial basis.

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