Chaotic Modeling and Simulation (CMSIM) 4: 615–623, 2013

Stochastic Model Reduction for Polynomial Chaos Expansion Using Proper Orthogonal Decomposition

Mehrdad Raisee[1], Dinesh Kumar[2] and Chris Lacor[2⋆]

[1] Center of Excellence in Design and Optimization of Energy Systems (CEDOES) School of Mechanical Engineering, College of Engineering, University of Tehran, P.O.Box: 11155-4563, Tehran, IRAN
(E-mail: mraisee@ut.ac.ir)

[2] Fluid Mechanics and Thermodynamics Research Group, Department of Mechanical Engineering, Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussels, BELGIUM
(E-mail: dkumar@vub.ac.be, chris.lacor@vub.ac.be)

Abstract. In this paper, a non-intrusive stochastic model reduction scheme is developed for polynomial chaos representation using proper orthogonal decomposition. The main idea is to extract the optimal orthogonal basis via inexpensive calculations on a coarse mesh and then use them for the fine discretization analysis. The developed reduced-order model is implemented to the stochastic steady-state heat diffusion equation. The random conductivity field is approximated via the Karhunen-Loeve (KL) expansion. Input random variables are uniformly distributed so that the Gauss-Legendre quadrature scheme is utilized for the numerical integration. The numerical results showed that the non-intrusive model reduction scheme is able to accurately reproduce mean and variance fields. It is found that the computation-time of the reduced-order model is lower than that of the full-order model.
Keywords: Uncertainty Quantification, Polynomial Chaos, Reduced-order Model.

1 Introduction

In many engineering applications, uncertainty in physical properties, input data and model parameters result in uncertainties in the system output. A representative practical example is design of turbomachineries where uncertainties in flow conditions and small variations in structural parameters of components(e.g. blade profile) can have a significant impact on the performance. For design refinement of such complex mechanical devices, it is necessary to include all uncertainty information in the output results using uncertainty quantification (UQ) schemes. However, many complex applications require a fine 3D

⋆ Corresponding Author

Received: 2 April 2013 / Accepted: 26 September 2013

ISSN 2241-0503

computational mesh, small time-step and high-dimensional space for stochastic analysis. This dramatically increases the computational cost which is not desirable for design proposes. Thus, it is necessary to employ efficient numerical schemes for stochastic analysis of complex industrial flows. A variety of different uncertainty quantification methods such as Monte Carlo approach, sensitivity method, perturbation method, regression method and polynomial chaos have been proposed for uncertainty quantification. All of these techniques have positive and negative features, and no single technique is optimum for all situations. Following our previous work on UQ (Dinescu *et al.* [1] and Wang *et al.* [7]), here we employed Polynomial Chaos (PC) approach to model uncertainty propagation. Polynomial chaos methods have been successfully applied to solid mechanics problems by several researches (See for example Ghanem and Spanos [3] and Doostan *et al.* [2]). PC schemes have also been employed for a number of fluid mechanics problems by a number of researchers such as: Walters and Huyse [6], Mathelin *et al.* [4] and Dinescu *et al.* [1]. The polynomial chaos representation can be used for different Probability Density Functions (PDFs) and can be implemented through either intrusive or non-intrusive methods. The intrusive approach requires the modification of the CFD codes and this may be difficult, expensive, and time consuming for many CFD problems. Moreover, the source codes of most commercial CFD softwares are not accessible and thus it is impossible to implement the intrusive PC approach to such softwares. For these reasons, here we focused on non-intrusive PC methodology with uniform PDF for uncertainty quantification. The main shortcoming of all PC methods is the *curse of dimensionality*. Developing efficient reduced-order models for shortening the computational cost associated with the stochastic analysis is of great interest for prediction of complex industrial flows with large number of uncertain parameters. In recent years, several model reduction techniques have been proposed for uncertainty quantification. Two informative examples of such works are: Nouy [5] and Doostan *et al.* [2]. In Nouy [5] a Generalize Spectral Decomposition (GSD) was proposed that gives the reduced basis independent of the stochastic discretization scheme. The GSD implementation to a class of Stochastic Partial Differential Equations (SPDE) leads to drastic computational saving though does not circumvent the curse of dimensionality. Doostan *et al.* [2] proposed an intrusive model reduction technique for chaos representation of a SPDE to tackle the curse of dimensionality. A 2D test case from solid mechanics is chosen to illustrate the accuracy and convergence of the model.

In this work, a non-intrusive reduced-order technique is developed and applied to the 2D steady-state stochastic heat diffusion equation. This paper is organized as follows. In Section 2 we present the details of mathematical formulation and problem under investigation. In Section 3, the model reduction methodology is described. Finally, in Section 4 the numerical results are presented and discussed.

2 Mathematical Formulation

To demonstrate the non-intrusive stochastic model reduction algorithm, 2D steady-state stochastic heat conduction in a square plate of side $2a$ is considered (see Figure 1). The 2D heat diffusion with random thermal conductivity is described by the following SPDE:

$$\frac{\partial}{\partial x}(k(x,y;\boldsymbol{\zeta})\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k(x,y;\boldsymbol{\zeta})\frac{\partial T}{\partial y}) = 0 \tag{1}$$

As shown in Figure (1), the top boundary of the plate is at hot temperature

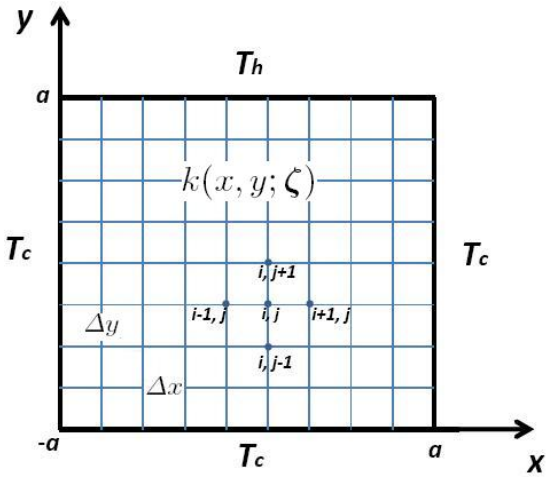

Fig. 1. Schematic of computational domain.

T_h whilst the side and bottom boundaries of the plate are at cold temperature T_c. The thermal conductivity of the plate, $k(x,y;\boldsymbol{\zeta})$, is assumed to be a two-dimensional homogeneous random process with known mean $\bar{k}(x,y)$ and known covariance function:

$$R(x_1,y_1;x_2,y_2) = {\sigma_k}^2 e^{-|x_1-x_2|/b_x - |y_1-y_2|/b_y} \tag{2}$$

where b_x and b_y are the correlation lengths in x and y directions, respectively, and σ_k is the standard deviation on the thermal conductivity.
A key ingredient here is the representation of stochastic thermal conductivity field as a Karhunen-Loeve (KL) expansion, a type of Fourier expansion for random functions, which amounts to a discretization in the space of random events. According to the KL expansion, the eigenvalues and eigenfunctions are obtained by solving the following 2D integral equation:

$$\int_D R(x_1,y_1;x_2,y_2)\phi_n(x_2,y_2)dx_2dy_2 = \lambda_n\phi_n(x_1,y_1) \tag{3}$$

Separation of kernel (2) as $R(x_1,y_1;x_2,y_2) = {\sigma_k}^2 e^{-|x_1-x_2|/b_x}.e^{-|y_1-y_2|/b_y}$ and substitution in (3) leads to two identical 1D integral eigenvalue equations in

x and y directions. Solution of the integral equations give eigenvalues (i.e. $\lambda_i^{(x)}$ and $\lambda_j^{(y)}$) and their corresponding eigenfunctions (i.e. $\phi_i^{(x)}$ and $\phi_j^{(y)}$). As described in Ghanem and Spanos [3], the complete form of KL expansion for random process $k(x, y; \boldsymbol{\zeta})$ is:

$$k(x,y;\boldsymbol{\zeta}) = \bar{k}(x,y) + \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\left\{\sqrt{\lambda_i^{(x)}\lambda_j^{(y)}}\zeta_{i,j}\frac{1}{\sqrt{2}}[\phi_i^{(x)}(x)\phi_j^{(y)}(y) + \phi_j^{(x)}(x)\phi_i^{(y)}(y)]\right\} \tag{4}$$

Having obtained an analytical expression for the thermal conductivity, the SPDE (Equation (1)) is discretized using an explicit central differencing scheme in a uniform grid ($\Delta x = \Delta y$), see Figure 1. Thus, for any set of $\boldsymbol{\zeta} \equiv \{\zeta_i\}_{i=1}^n$, first thermal conductivity is calculated in the computational domain using KL expression (Equation (4)). Then, the new temperature T^{n+1} at grid node (i, j) is obtained from old nodal temperature T^n of neighbouring nodes. The solution is converged when the maximum error between the old and new temperature values is sufficiently small($\epsilon \simeq 10^{-9}$).

3 Model Reduction Methodology

In the classical polynomial chaos expansion, the random temperature field $T(x, y; \boldsymbol{\zeta})$ can be decomposed into deterministic and stochastic components. The PC representation of temperature field of order p for n random variable $\boldsymbol{\zeta} \equiv \{\zeta_i\}_{i=1}^n$ can be written as:

$$T(x,y;\boldsymbol{\zeta}) - < T(x,y) > = \sum_{i=1}^{P} T_i(x,y)\psi_i(\boldsymbol{\zeta}) \tag{5}$$

where the total number of terms are $P + 1 = (p + n)!/p!n!$ and the mean value of $T(x, y; \boldsymbol{\zeta})$ is expressed as:

$$< T(x,y) > = \int_{\omega} T(x,y;\boldsymbol{\zeta}) f(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \tag{6}$$

In the above equation, f is Probability Density Function (PDF). Here we assumed random variables are uniformly distributed over interval [-1,1] and thus the PDF is $f = 1/2^n$ for n random variables $\{\zeta_i\}_{i=1}^n$. The non-intrusive method uses spectral projection to find the PC expansion coefficients $T_i(x, y)$ in Equation (5). Projecting Equation (5) onto the k^{th} basis and use of orthogonality gives:

$$T_i(x,y) = \frac{1}{< \psi_i^2(\boldsymbol{\zeta}) >} \int_{\omega} T(x,y;\boldsymbol{\zeta})\psi_i(\boldsymbol{\zeta}) f(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \tag{7}$$

The objective of the spectral projection method is to compute the polynomial coefficients by evaluating numerator in Equation (7) numerically, while the

dominator can be computed analytically for multi-variant orthogonal polynomials. Here we used the n-dimensional *Gauss-Legendre quadrature* to compute the projection integrals in Equation (7) as:

$$T_i(x,y) = \frac{1}{<\psi_i^2(\boldsymbol{\zeta})>} \sum_{i_1=1}^{q} ... \sum_{i_n=1}^{q} (w_1^{i_1} \otimes ... \otimes w_n^{i_n}) T(x,y;\zeta_1^{i_1},..,\zeta_n^{i_n}) \psi_i(\zeta_1^{i_1},..,\zeta_n^{i_n}) f(\zeta_1^{i_1},..,\zeta_n^{i_n}) \quad (8)$$

where $(\boldsymbol{\zeta}^k, \boldsymbol{w}^k)$, $k = 1,2,..,q$ are the one-dimensional (1D) Gauss-Legendre integration points and weights.

The above classical expansion dose not represent an optimal PC representation of $T(x,y,\boldsymbol{\zeta})$. To find the optimal PC expansion one can consider the fact that spatial discretization errors and random discretization errors may be decoupled. Therefore, one can minimize the random discretization errors on the coarse grid and then solve the real physical problem on a fine mesh by using limited number of optimal random basis $\{z_i\}_{i=1}^m$ (obtained in the coarse grid analysis) where m is the number of dominated eigenvalues. The first step in the model reduction scheme is to find optimal PC basis using POD; a well-known procedure for extracting a basis for a model decomposition from an ensemble of realizations. To this end, suppose in a coarse grid, expression (9) represents an optimal PC expansion of the stochastic temperature field $T(x,y,\boldsymbol{\zeta})$;

$$T(x,y;\boldsymbol{\zeta}) - < T(x,y) > = \sum_{i=1}^{m} T^i(x,y) z_i(\boldsymbol{\zeta}) \quad (9)$$

Now in the coarse grid, the covariance function $C(x_1,y_1;x_2,y_2)$ of temperature field can be obtained from:

$$C(x_1,y_1;x_2,y_2) = \sum_{i=1}^{P} T_i(x_1,y_1) T_i(x_2,y_2) < \psi_i^2 > \quad (10)$$

The corresponding eigenvalues ν_i and eigenfunctions $\phi_i(x,y)$ are the solution of the following eigenvalue problem:

$$\int_D C(x_1,y_1;x_2,y_2)\phi_i(x_2,y_2)dx_2dy_2 = \nu_i\phi_i(x_1,y_1) \quad (11)$$

The upper limit m in the Equation (9) can be found by the size of dominant eigenspace (10) such that $\sum_{i=1}^m \nu_i / \sum_i \nu_i \geq 0.99$.

Having obtained $T_i(x,y)$ from classical PC on the coarse grid and eigenfunctions $\phi_i(x,y)$ from the solution of eigenvalue problem (11), the set of optimal basis $\{z_i\}_{i=1}^m$ can be now represented as a linear combination of the set of classical polynomial chaos; $\{\psi_i\}_{i=1}^P$ using the following scalar product:

$$z_i(\boldsymbol{\zeta}) = [T(x,y;\boldsymbol{\zeta}) - < T(x,y) >, \phi_i(x,y)] = \sum_{j=1}^{P} \alpha_{ij}\psi_j(\boldsymbol{\zeta}) \quad (12)$$

The scalar product of functions v and w is defined as: $[v,w] = \int_x v.wdx$.

where coefficient α_{lj} are obtained via the scalar product:

$$\alpha_{ij} = \int_R T_j(x,y)\phi_i(x,y)d\overrightarrow{x}\,d\overrightarrow{y} \tag{13}$$

One now dose the classical polynomial chaos on a fine mesh, where z_i are used instead of ψ_i. For $1 \leq i \leq m$, the coefficients in expansion (9) are obtained from:

$$T^i(x,y) = \frac{< T(x,y;\zeta), z_i >}{< z_i, z_i >} = \frac{1}{\nu_i}\sum_{j=1}^{P} \alpha_{ij} < T(x,y;\boldsymbol{\zeta}), \psi_j > \tag{14}$$

4 Results and Discussion

We now examine the performance of the reduced-order model by analyzing the 2D steady-state heat conduction equation. It is assumed that the top wall is at $T_h = 300°C$ and side and bottom walls at $T_c = 100°C$. First, a 2D KL expansion is performed using the exponential kernel with a standard deviation of $\sigma_k = 1.0\ W/m.K$ and correlation lengths of $b_x = b_y = 10.0\ m$. The mean thermal conductivity is assumed to be $\bar{k} = 5.0\ W/m.K$. The first six largest terms in the KL expansions are chosen for further analysis.

Figures 2 and 3 respectively show the distributions of eigenvalues and $\mid \alpha_{ij} \mid$ coefficients obtained from the coarse discretization analysis on a 5×5 mesh when a second-order Legendre polynomial ($p = 2$) is employed. From these figures it can be concluded that only two ($m = 2$) basis functions (i.e. z_1 and z_2) are adequate for the fine discretization analysis. Thus, fine discretization analysis is performed using the new z_1 and z_2 basis functions on a 41×41 mesh. The computed mean and variance fields using full- and reduced-order models are compared in Figure 4. It is visible the fine grid computations via reduced- and full-order models resulted in identical results for the mean temperature field. Moreover, full- and reduced-order analysis on the fine mesh produced very similar variance fields. In Figure 4(f), regions of high absolute relative error (about 10%) are visible in the top corners of the domain. This error can be reduced by considering more basis functions (e.g. z_3) in the PC expansion but the reduced-order computational cost will also increase.

The ratio of computation-time for the reduced-order analysis to the time needed for the full-order calculation using five fine meshes of 21×21, 26×26, 31×31, 36×36 and 41×41 is shown in Figure 5. A coarse mesh with 10×10 grid nodes is used for the coarse grid analysis. This figure shows that for the present problem with six random variables, the reduced-order model is less expensive than the full-order model when a 21×21 mesh is used. By increasing the size of the fine mesh to 26×26 the advantage of the reduced-order model over the standard PC becomes more evident. It is seen that with the reduced-order model about 20% saving in CPU-time can be obtained when a mesh with 41×41 nodes is used for the fine scale discretization. Further saving in the CPU-time may be achieved by combination of the current reduced-order model with other efficient numerical schemes such as for example sparse sampling schemes for the stochastic discretization and multi-grid methods for the spatial discretization.

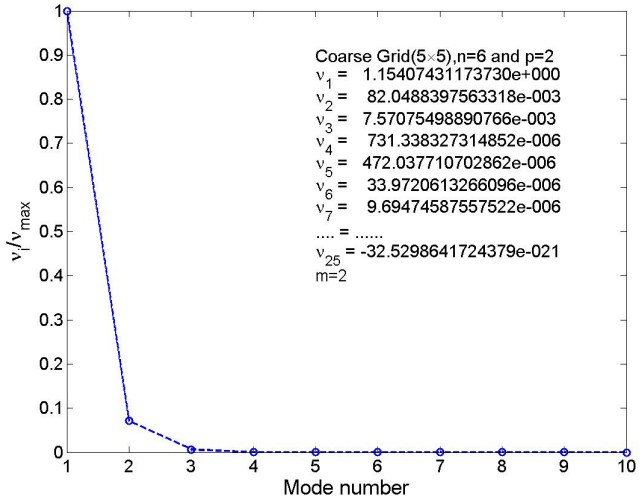

Fig. 2. Computed eigenvalues using coarse discretization analysis.

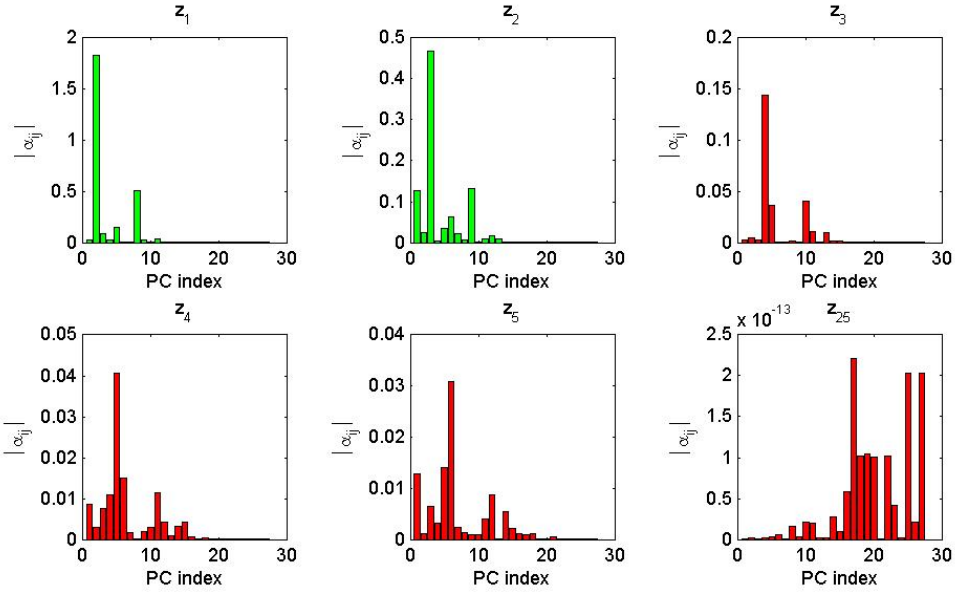

Fig. 3. Computed $| \alpha_{ij} |$ using coarse discretization analysis.

Conclusion

In this paper, a non-intrusive model reduction technique for PC expansion is presented and discussed. The reduced-order model is applied to the 2D steady-state heat diffusion equation. Distributions of mean and variance obtained from the reduced-order model are compared with those of full-order model. The numerical results show that the developed reduced-order model is able to

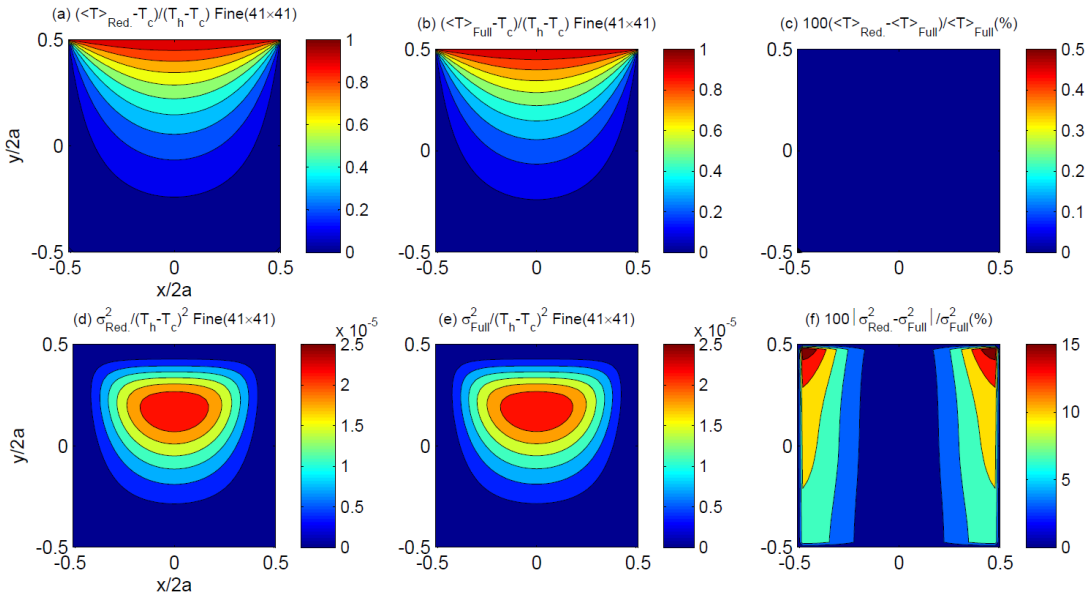

Fig. 4. Comparison of mean and variance fields.

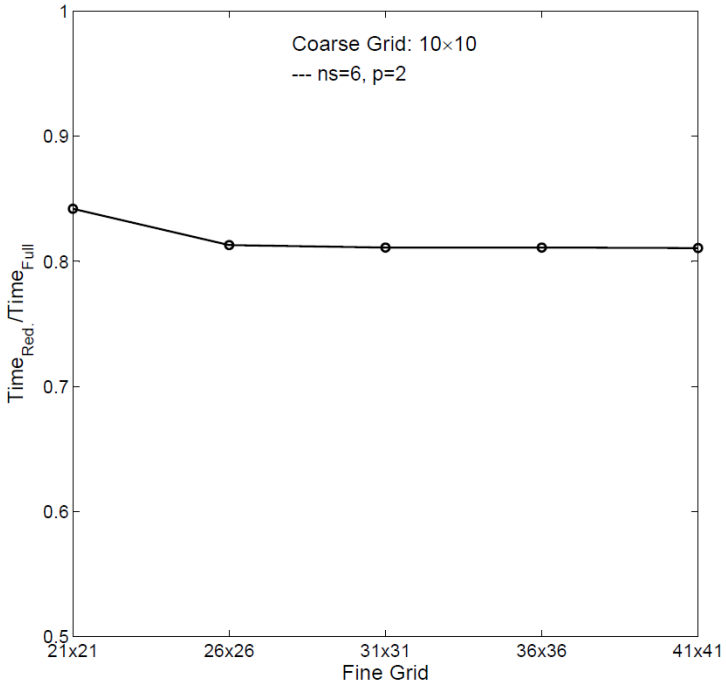

Fig. 5. Ratio of reduced-order computation-time to the full-order computation-time.

produce acceptable results for such statistical quantities. Computation-time of the reduced-order model is found to be lower than that of the full-order model.

Acknowledgment

The authors wish to thank Vrije Universiteit Brussel (VUB) and University of Tehran (UT) for providing financial support of this work.

References

1.C. Dinescu, S. Smirnov, Ch. Hirsch, and C. Lacor. Assessment of intrusive and non-intrusive non-deterministic CFD methodologies based on polynomial chaos expansions. *Int. J. of Eng. Systems Modeling and Simulation*, 2:87-98, 2010.
2.A. Doostan, R. Ghanem, and J. Red-Horse. Stochastic model reduction for chaos representations. *Comp. Meth. in Appl. Mech. and Eng.*, 196:3951-3966, 2007.
3.R. Ghanem, and O. Spanos. Stochastic Finite Elements: A Spectral Approach, 1991, Springer Verlag.
4.L. Mathelin, M. Y. Hussaini, and T. A. Zang. Stochastic approaches to uncertainty quantification in CFD simulations. *Numer. Algorithms*, 38:209-236, 2007.
5.A. Nouy. A generalized spectral decomposition technique to solve a class of linear stochastic partial differential equations. *Comp. Meth. in Appl. Mech. and Eng.*, 196:4521-4537, 2007.
6.R. W. Walters, and L. Huyse. Uncertainty analysis for fluid mechanics with applications. NASA/CR 2002-211449.
7.X. Wang, Ch. Hirsch, Z. Liu, S. Kang, and C. Lacor. Uncertainty-based robust aerodynamic optimization of rotor blades. *Int. J. Numer. Meth. Eng.*, 94:111-127, 2013.