EFFICIENT UNCERTAINTY QUANTIFICATION USING A TWO-STEP APPROACH WITH CHAOS COLLOCATION

Alex Loeven*, Jeroen Witteveen*, and Hester Bijl*

*Delft University of Technology, Faculty of Aerospace Engineering Kluyverweg 1, 2629 HS Delft, The Netherlands † e-mail: G.J.A.Loeven@TUDelft.nl

Key words: Computational Fluid Dynamics, Fluid-Structure Interaction, Non-Intrusive, Polynomial Chaos, Stochastic Collocation, Uncertainty Quantification

Abstract. In this paper a Two Step approach with Chaos Collocation for efficient uncertainty quantification in computational fluid-structure interactions is followed. In Step I, a Sensitivity Analysis is used to efficiently narrow the problem down from multiple uncertain parameters to one parameter which has the largest influence on the solution. In Step II, for this most important parameter the Chaos Collocation method is employed to obtain the stochastic response of the solution. The Chaos Collocation method is presented in this paper, since a previous study showed that no efficient method was available for arbitrary probability distributions. The Chaos Collocation method is compared on efficiency with Monte Carlo simulation, the Polynomial Chaos method, and the Stochastic Collocation method. The Chaos Collocation method is non-intrusive and shows exponential convergence with respect to the polynomial order for arbitrary parameter distributions. Finally, the efficiency of the Two Step approach with Chaos Collocation is demonstrated for the linear piston problem with an unsteady boundary condition. A speed-up of a factor of 100 is obtained compared to a full uncertainty analysis for all parameters.

1 INTRODUCTION

There is an increasing interest in uncertainty analysis applied to computational fluid-structure interactions, since the influence of inherent physical uncertainties can no longer be neglected. In the past decades numerical errors have been decreased due to more accurate algorithms and more powerful computing facilities to such an extent, that uncertainties are now the limiting factor in obtaining reliable results. When fluid-structure interaction is concerned, small uncertainties in the input parameters can lead to unreliable solutions after long time integration. Therefore, to obtain more reliable results, uncertainty quantification is necessary.

Deterministic computations for fluid-structure interaction problems are already computationally intensive due to the dynamic coupling between the fluid and structure. Uncertainty quantification requires an additional method to obtain the stochastic properties.

This leads to an increase in the computational work compared to the deterministic case. Especially for multiple uncertain parameters the amount of work increases rapidly. Efficiency of the uncertainty quantification is, therefore, of great importance.

In this paper the efficiency of uncertainty quantification for multiple uncertain parameters is increased by following a Two Step approach⁹ with Chaos Collocation. In Step I, a Sensitivity Analysis is employed to identify the most important parameter¹ of the problem. In Step II, the stochastic response of the solution is obtained for the most important parameter using the Chaos Collocation method. Since computational fluid-structure interaction problems are computationally intensive, the second step has to be performed as efficiently as possible.

Sensitivity Analysis is an efficient way to identify the most important uncertain parameter of the problem. Sensitivity Analysis compares the scaled sensitivity derivatives. Only the standard deviations of the uncertain parameters are taken into account, which is a good measure of the uncertainty. Sensitivity derivatives give the sensitivity of the solution with respect to a parameter. They are computed using the continuous sensitivity equations. The parameter with the largest scaled sensitivity derivatives has the largest influence on the solution and is identified to be the most important parameter of the problem.

A previous study⁹ showed that there was no method available which is most efficient for arbitrarily distributed uncertain parameters to be applied in Step II. Therefore, the Chaos Collocation method is introduced in this paper. It is a non-intrusive method which shows exponential convergence with respect to the polynomial order for arbitrarily distributed input parameters. The Chaos Collocation method consists of a Lagrange-Chaos interpolation between the collocation points. The collocation points coincide with the quadrature points used in the Gauss-Chaos quadrature for integrating the Chaos Collocation approximation to obtain high order approximations of the mean and variance.

The efficiency of the Chaos Collocation method is compared to the Monte Carlo method, the Polynomial Chaos method, and the Stochastic Collocation method. The efficiency of the methods is compared by looking at the error convergence with respect to the computational work. The computational work is expressed in the number of times a deterministic system is solved. The methods are compared for short and long time integration with uniformly, exponentially, and normally distributed input parameters.

Finally, the Two Step approach with Chaos Collocation is demonstrated for the linear piston with an unsteady boundary condition. First a Sensitivity Analysis is performed for the four uncertain parameters of the test problem. For the most important parameter the Chaos Collocation method is used to find to probability distribution of the piston position. A speed-up factor of 100 is found compared to a full uncertainty analysis for all four parameters.

2 TWO STEP APPROACH FOR EFFICIENT UNCERTAINTY QUANTIFICATION

Since the propagation of probability distributions for multiple uncertain parameters is computationally intensive a two step approach is followed. The first step consists of a Sensitivity Analysis, which is performed to identify the most important parameter of the problem. After that in the second step the uncertainty of the identified parameter is propagated using the Chaos Collocation method which results in the stochastic response of the solution based on the input distribution of the uncertain parameter. The Chaos Collocation method is introduced in this paper. It is compared on efficiency with Monte Carlo simulation, the Polynomial Chaos method, and the Stochastic Collocation method. In section 4 the efficiency of these methods is compared.

In this section the methods are explained using the following general differential equation

$$\mathcal{L}u(\mathbf{x}, t, \theta) = S(\mathbf{x}, t, \theta),\tag{1}$$

where $u(\mathbf{x}, t, \theta)$ is the solution and \mathcal{L} is a differential operator which contains space and time differentiation and can be nonlinear. For example $\mathcal{L} = \partial/\partial t + u\partial/\partial x$ results in $\mathcal{L}u = u_t + uu_x$. The solution $u(\mathbf{x}, t, \theta)$ is a function of space \mathbf{x} , time t and the random event $\theta \in [0, 1]$. $S(\mathbf{x}, t, \theta)$ is a space and time dependent source term which can also depend on the random event θ . The random event θ is introduced by an uncertain parameter $p(\theta)$.

2.1 Step I: Sensitivity Analysis to obtain the most important parameter

Sensitivity Analysis is based on the sensitivity derivative. In this paper sensitivity derivatives¹¹ are used to identify the most important uncertain parameter in a particular physical system. Sensitivity is used here as an efficient way of reducing the amount of uncertain parameters.

The sensitivity derivative of the solution $u(\mathbf{x}, t, \theta)$ with respect to the uncertain parameter $p(\theta)$ is defined as

$$u_p = \frac{\partial u(\mathbf{x}, t, \theta)}{\partial p(\theta)}.$$
 (2)

Here the continuous sensitivity equation approach¹¹ is used to compute the sensitivity derivative since the implementation is straightforward and the solution is exact. The continuous sensitivity equation solves for the sensitivity derivatives directly, it is the derivative of the original equation with respect to the uncertain parameter. Two equations have to be solved, namely

$$\mathcal{L}u(\mathbf{x}, t, \theta; \mu_p) = S(\mathbf{x}, t, \theta; \mu_p)$$
(3)

$$\frac{\partial}{\partial p} \left\{ \mathcal{L}u(\mathbf{x}, t, \theta; p(\theta)) = S(\mathbf{x}, t, \theta; p(\theta)) \right\} \bigg|_{p(\theta) = \mu_p}, \tag{4}$$

where μ_p is the mean of the parameter $p(\theta)$. The first is the original differential equation of the problem (1) using μ_p for $p(\theta)$. The second equation (4) is called the continuous sensitivity equation.

When more parameters are involved in the problem the sensitivity derivative with respect to each parameter is calculated. By scaling the sensitivity derivatives with the standard deviation of the parameters all sensitivity derivatives have the dimension of $u(\mathbf{x}, t, \theta)$ and can be compared. The standard deviation is used for scaling since this is a good measure of the amount of uncertainty of the parameter. If the solution depends on N parameters, the most important parameter is

$$\max \{ u_{p_1} \sigma_{p_1} , u_{p_2} \sigma_{p_2} , \dots, u_{p_N} \sigma_{p_N} \}.$$
 (5)

Once the most important parameter is obtained by Eq. (5) the stochastic response of the solution can be computed based on the input distribution of the uncertain parameter.

2.2 Step II: Uncertainty quantification methods to obtain the stochastic response of the solution

In Step II only methods are used which result in the complete probability distribution function of the solution. The methods for Step II increase the amount of work with respect to deterministic computations. Therefore, in case of the computationally intensive fluid-structure interactions, the method which is used to obtain the stochastic response also has to be efficient. Different method exist, here Monte Carlo simulation, the Polynomial Chaos method, and the Stochastic Collocation method are compared on efficiency with the Chaos Collocation method, which is introduced in section 3.

2.2.1 Monte Carlo simulation

Monte Carlo simulation is the most natural way to obtain the stochastic response. Monte Carlo simulation works as follows:

- 1. Take a value from the domain [0,1], this is called sampling;
- 2. Calculate the corresponding value for the random variable using its distribution function;
- 3. Solve the problem like a deterministic problem;
- 4. Repeat this many (M) times and analyze the statistical properties of the set of solutions.

Typically in the order of thousands of samples are required to obtain reasonable accuracy. Techniques exist to minimize the number of samples, like stratified sampling (Latin Hypercube) or variance reduction. The original Monte Carlo simulation uses random

sampling, with a convergence rate of $\mathcal{O}(M^{-1/2})$. Here stratified or Latin Hypercube sampling is used, the convergence is improved, but to $\mathcal{O}(M^{-1})$ only. An advantage of Monte Carlo simulation is that the method is non-intrusive, a disadvantage is the amount of computational work.

2.2.2 Polynomial Chaos

The Polynomial Chaos method results in a spectral representation of the stochastic response of the solution and high order approximations of the mean and variance. Based on the Homogeneous Chaos theory of Wiener¹³ the original Polynomial Chaos method was developed by Ghanem and Spanos.⁴ This framework was extended by Xiu and Karniadakis¹⁶ to the Askey Polynomial Chaos. Due to the chaos representation the input uncertainties can be expressed in two terms only. The Askey Polynomial Chaos has been successfully applied to several problems, among others fluid-structure interactions. Recently, the Polynomial Chaos framework has been extended to obtain exponential convergence for arbitrary distributions^{12,14} using numerical techniques to construct an optimal set of orthogonal polynomials. An advantage of the Polynomial Chaos method is the exponential convergence with respect to the polynomial order, a disadvantage is the intrusiveness due to the coupled system of equations that has to be solved. A lot of research to non-intrusive polynomial chaos⁶ methods is done to simplify the implementation using existing solvers.

The Polynomial Chaos method starts with the polynomial chaos expansion of the solution $u(\mathbf{x}, t, \theta)$ and all uncertain parameters, with the infinite sum truncated at a finite number of P+1 terms:

$$u(\mathbf{x}, t, \theta) \approx \sum_{i=0}^{P} u_i(\mathbf{x}, t) \Psi_i(\zeta(\theta)).$$
 (6)

This expansion is a spectral expansion in the vector of random variables $\zeta(\theta)$ with the random trial basis $\{\Psi_i\}$. Equation (6) divides the random variable $u(\mathbf{x}, t, \theta)$ into a deterministic part, the coefficients $u_i(\mathbf{x}, t)$ and a stochastic part, the polynomials $\Psi_i(\zeta(\theta))$. The total number of expansion terms is P+1, which is determined by the dimension n of the vector of random variables $\zeta(\theta)$ (i.e. the number of uncertain parameters) and the highest order p of the polynomials $\{\Psi_i\}$

$$P + 1 = \frac{(n+p)!}{n!p!}. (7)$$

Substituting the polynomial chaos expansion (6) into the differential equation (1) results in

$$\mathcal{L}\sum_{i=0}^{P} u_i(\mathbf{x}, t) \mathbf{\Psi}_i(\boldsymbol{\zeta}(\theta)) \approx S(\mathbf{x}, t, \theta).$$
 (8)

Here, the source term S has to be expanded as well, however for convenience in this notation it is omitted. To ensure that the truncation error is orthogonal to the functional space spanned by $\{\Psi_i\}$ a Galerkin projection on each basis $\{\Psi_k\}$ is applied

$$\left\langle \mathcal{L} \sum_{i=0}^{P} u_i(\mathbf{x}, t) \mathbf{\Psi}_i, \mathbf{\Psi}_k \right\rangle = \left\langle S, \mathbf{\Psi}_k \right\rangle, \qquad k = 0, 1, \dots, P.$$
 (9)

This deterministic set of P+1 coupled equations can be solved using standard numerical techniques. Here a Block-Gauss-Seidel iterative method is employed to obtain the coefficients of the expansion. Since some iterations are required, the amount of work increases to several times P+1. From Eq. (9) the coefficients $u_i(\mathbf{x},t)$ are calculated and the stochastic solution $u(\mathbf{x},t,\theta)$ is reconstructed using Eq. (6). The mean μ_u and the variance σ_u^2 of the stochastic solution can be determined using:

$$\mu_u = u_0, \tag{10}$$

$$\sigma_u^2 = \sum_{i=1}^P u_i(\mathbf{x}, t)^2 \left\langle \mathbf{\Psi}_i^2 \right\rangle. \tag{11}$$

These expressions follow from the definition of the mean and variance.

2.2.3 Stochastic Collocation

A different spectral approach is the Stochastic Collocation method. It was developed by Mathelin and Hussaini¹⁰ to reduce the costs of the Askey Polynomial Chaos method in case of nonlinear equations. The method is successfully applied to a quasi-1D nozzle with uncertain inlet conditions and nozzle shape. Mathelin and Hussaini showed a substantial decrease of computing time using the Stochastic Collocation method compared to the Polynomial Chaos method. For each collocation point the problem is solved deterministically. The distribution function of the solution is reconstructed using global polynomial interpolation. The mean and variance are obtained using Gaussian quadrature. In case of the Stochastic Collocation method the distribution function of the random variable is projected from [0,1] on the domain [-1,1], which is called the α domain, by the linear transformation

$$\mathcal{F}_{\tilde{u}}(\tilde{u}) = 2F_u(u) - 1 \quad \text{or} \quad \alpha = 2\theta - 1,$$
 (12)

where $\mathcal{F}_{\tilde{u}}(\tilde{u})$ is the projected distribution function on the α domain [-1,1] and $F_u(u)$ the distribution function on $\theta \in [0,1]$. The projected solution is $\tilde{u}(\mathbf{x},t,\alpha)$. The α domain is a stochastic space which is defined according to a standard domain of orthogonal polynomials [-1,1]. From the α domain N_p collocation points α_i are taken. The method proposed by Mathelin and Hussaini¹⁰ uses N_p Gauss-Legendre quadrature points and Lagrange interpolating polynomials of order $N_p - 1$ for the function approximation. The

projected stochastic solution $\tilde{u}(\mathbf{x},t,\alpha)$ is approximated by the following expansion

$$\tilde{u}(\mathbf{x}, t, \alpha) \approx \sum_{i=1}^{N_p} \tilde{u}_i(\mathbf{x}, t) h_i(\alpha),$$
(13)

with $\tilde{u}_i(\mathbf{x}, t)$ the values of $\tilde{u}(\mathbf{x}, t, \alpha)$ in the collocation points α_i and $h_i(\alpha)$ interpolating polynomials of degree $N_p - 1$, with $h_i(\alpha_j) = \delta_{ij}$. Transformation (12) is applied to the differential equation (1) after which expansion (13) is substituted. A Galerkin projection on each basis $\{h_l\}$ is applied to ensure that the error is orthogonal to the functions basis spanned by $\{h_i\}$:

$$\left\langle \mathcal{L} \sum_{i=1}^{N_p} \tilde{u}_i(\mathbf{x}, t) h_i, h_l \right\rangle = \left\langle S, h_l \right\rangle, \qquad l = 1, \dots, N_p.$$
 (14)

The Galerkin projection (14) is approximated using Gaussian quadrature. For a general inner product $\langle f(\alpha), g(\alpha) \rangle$ of two functions $f(\alpha)$ and $g(\alpha)$ Gaussian quadrature results in:

$$\langle f(\alpha), g(\alpha) \rangle = \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_p} f_i g_j h_i(\alpha_l) h_j(\alpha_l) w_l,$$

$$= \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_p} f_i g_j \delta_{il} \delta_{jl} w_l,$$

$$= \sum_{l=1}^{N_p} f_l g_l w_l,$$
(15)

where w_l are the quadrature weights corresponding to the collocation points α_l . The resulting set of equations is fully decoupled. The mean μ_u and the variance σ_u^2 of the stochastic solution can be determined using:

$$\mu_u = \sum_{i=1}^{N_p} \frac{1}{2} u_i(\mathbf{x}, t) w_i, \tag{16}$$

$$\sigma_u^2 = \sum_{i=1}^{N_p} \frac{1}{2} (u_i(\mathbf{x}, t))^2 w_i - \left(\sum_{i=1}^{N_p} \frac{1}{2} u_i(\mathbf{x}, t) w_i\right)^2, \tag{17}$$

where w_i are the weights corresponding to the collocation points α_i . These relations are derived from the definition of the mean and variance.

3 CHAOS COLLOCATION

The Chaos Collocation method is based on the idea of a chaos transformation which is also used in the Polynomial Chaos methods. Exponential convergence of the Chaos Collocation is shown in section 4 for three standard distributions. The Chaos Collocation method converges exponentially for arbitrary probability distributions. In the Chaos Collocation method first Lagrange-Chaos interpolation is used for the distribution function approximation. With Lagrange-Chaos interpolation it is possible to describe the input distribution with two collocation points only. Just as for the Polynomial Chaos method, where two polynomial coefficients describe the input distribution. Secondly, Gauss-Chaos quadrature is used to compute the Galerkin projection and the integration of the approximation of the distribution function. Like ordinary Gauss quadrature is able to integrate polynomials exactly, the Gauss-Chaos quadrature integrates polynomial chaoses exactly. By using Gauss-Chaos quadrature a decoupled set of equations and a higher order approximation of the mean and variance are obtained.

Chaos Collocation expansion with Lagrange-Chaos interpolation

Each variable depending on the uncertain input parameter is expanded as follows:

$$u(\mathbf{x}, t, \theta) = \sum_{i=0}^{P} u_i(\mathbf{x}, t) h_i(\xi(\theta)), \qquad (18)$$

where $u_i(\mathbf{x}, t)$ is the solution $u(\mathbf{x}, t, \theta)$ at the collocation point θ_i and h_i is the Lagrange interpolating polynomial chaos corresponding to the collocation points θ_i . P is the order of the interpolating polynomial chaos. The difference with ordinary Lagrange interpolation is that here a polynomial chaos is used instead of ordinary polynomials. The Lagrange interpolating polynomial is a function in terms of the random variable $\xi(\theta)$. The random variable $\xi(\theta)$ is chosen on the standard domains [-1,1], $[0,\infty)$ or $(-\infty,\infty)$, such that the uncertain input parameter $p(\theta)$ is a linear transformation of $\xi(\theta)$:

$$p(\theta) = \frac{p(\theta_1)\xi(\theta_0) - p(\theta_0)\xi(\theta_1)}{\xi(\theta_0) - \xi(\theta_1)} + \frac{p(\theta_0) - p(\theta_1)}{\xi(\theta_0) - \xi(\theta_1)}\xi(\theta) = \tilde{p}_0 + \tilde{p}_1\xi(\theta), \tag{19}$$

which follows from the expansion of $p(\theta)$ similar to equation (18). The Lagrange interpolating polynomial chaos is the polynomial chaos $h(\xi(\theta))$ of order P that passes through the P+1 collocation points. It is given by:

$$h_i(\xi(\theta)) = \prod_{\substack{k=0\\k\neq j}}^{P} \frac{\xi(\theta) - \xi(\theta_k)}{\xi(\theta_i) - \xi(\theta_k)},$$
(20)

with $h_i(\xi(\theta_j)) = \delta_{ij}$. The collocation points are chosen such that they correspond to the Gauss-Chaos quadrature points used to integrate the function $u(\mathbf{x}, t, \theta)$ in the θ domain.

The solution has to be integrated in order to obtain for instance the mean or variance. To find the Gauss-Chaos quadrature points and weights the procedure below is followed.

Computing Gauss-Chaos quadrature points with corresponding weights

A powerful method to compute Gaussian quadrature rules is by means of the Golub-Welsch algorithm.⁵ This algorithm requires the recurrence coefficients³ of polynomials which are orthogonal with respect to the weighting function of the integration. Exponential convergence for arbitrary probability distributions is obtained when the polynomials are orthogonal with respect to the probability density function of ξ , so $w(\xi) = f_{\xi}(\xi)$. The recurrence coefficients are computed using the discretized Stieltjes procedure,² which is a stable method for arbitrary distribution functions. For convenience of notation the argument θ is omitted from here on.

First the recurrence coefficients have to be computed. Orthogonal polynomials satisfy the three-term recurrence relation:

$$\pi_{i+1}(\xi) = (\xi - \alpha_i)\pi_i(\xi) - \beta_i\pi_{i-1} \qquad i = 0, 1, \dots, P,$$

$$\pi_{-1}(\xi) = 0, \ \pi_0(\xi) = 1, \tag{21}$$

where α_i and β_i are the recurrence coefficients determined by the weighting function $w(\xi)$ and $\{\pi_i(\xi)\}_{i=0}^P$ is a set of (monic) orthogonal polynomials with $\pi_i(\xi) = \xi^i + \mathcal{O}(\xi^{i-1}), i = 0, 1, \ldots, P$. The recurrence coefficients are given by the Darboux's formulae:³

$$\alpha_{i} = \frac{(\xi \pi_{i}, \pi_{i})}{(\pi_{i}, \pi_{i})} \qquad i = 0, 1, \dots, P,$$

$$\beta_{i} = \frac{(\pi_{i}, \pi_{i})}{(\pi_{i-1}, \pi_{i-1})} \qquad i = 1, 2, \dots, P,$$
(22)

where (\cdot, \cdot) denotes an inner product. The first coefficient β_0 is given by (π_0, π_0) . Gander and Karp² showed that discretizing the weighting function leads to a stable algorithm. Therefore the discretized Stieltjes procedure is used to obtain the recurrence coefficients. Hereto, first the weighting $w(\xi)$ is discretized by

$$w_N(\xi) = \sum_{j=1}^N w_j \delta(\xi - \xi_j),$$
 $w_j > 0,$ (23)

where δ is the Dirac delta function. Stieltjes' procedure starts with i = 0. With (22) the first coefficient α_0 is computed, $\beta_0 = \sum_{j=1}^N w_j$. Now $\pi_1(\xi)$ is computed by (21) using α_0 and β_0 . This is repeated for i = 1, 2, ..., P. When continuous weighting functions are considered $P \ll N$, for discrete measures $P \leq N$. The inner product is defined as

$$(p(\xi), q(\xi)) = \int_{S} p(\xi)q(\xi)w_{N}(\xi)d\xi = \sum_{j=1}^{N} w_{j}p(\xi_{j})q(\xi_{j}),$$
(24)

for two functions $p(\xi)$ and $q(\xi)$.

From the recurrence coefficients α_i and β_i , i = 0, 1, ..., P, the collocation points ξ_i and corresponding weights w_i are computed using the Golub-Welsch algorithm.⁵ With the recurrence coefficients the following matrix is constructed:

$$J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \emptyset & & \\ & \sqrt{\beta_2} & \alpha_3 & \sqrt{\beta_3} & & & & \\ & & \ddots & \ddots & \ddots & & \\ & \emptyset & & \sqrt{\beta_{P-1}} & \alpha_{P-1} & \sqrt{\beta_P} & & \\ & & \sqrt{\beta_P} & \alpha_P & & & \end{bmatrix}.$$
 (25)

The eigenvalues of J are the collocation points ξ_i , i = 0, ..., P, which are the roots of the polynomial of order P+1 from the set of the constructed orthogonal polynomials. The weights are found by $w_i = \beta_0 v_{1,i}^2$, i = 0, ..., P, where $v_{1,i}$ is the first component of the normalized eigenvector corresponding to eigenvalue ξ_i .

Now the collocation points ξ_i in the ξ -domain are known. They are mapped to the θ -domain using the distribution function of ξ . The chaos collocation points θ_i are found by

$$\theta_i = F_{\xi}(\xi_i), \qquad i = 0, \dots, P. \tag{26}$$

For a uniformly distributed parameter the Chaos Collocation method results in the original Stochastic Collocation method, ¹⁰ if $\xi(\theta)$ is chosen to be U(-1,1) distributed.

Application to a general differential equation

Substitute expansion (18) into the general differential equation (1). A Galerkin projection on each basis $\{h_k(\xi(\theta))\}$ is applied:

$$\left\langle \mathcal{L} \sum_{i=1}^{P} u_i(\mathbf{x}, t) h_i, h_k \right\rangle = \left\langle S, h_k \right\rangle, \qquad k = 1, \dots, P.$$
 (27)

This projection is approximated using Gauss-Chaos quadrature. The result is a deterministic system of equations which is fully decoupled. The mean and variance of the solution are found by equations (16) and (17), but here with $u_i(\mathbf{x}, t)$ the solution at the collocation point $u(\mathbf{x}, t, \theta_i)$ and w_i the weight correspondent with collocation point θ_i .

The presented Chaos Collocation method has one disadvantage compared to the Polynomial Chaos method. The number of required collocation points increases rapidly with the number of uncertain parameters. When the number of uncertain parameters increases, the collocation points are generally found using tensor products of one-dimensional polynomials. Improvements in this area have been performed by Xiu and Hesthaven¹⁵ for the Stochastic Collocation method. An extension to the Chaos Collocation method will be investigated in the near future.

4 EFFICIENCY OF THE CHAOS COLLOCATION METHOD

The efficiency of the Chaos Collocation method is investigated for a simple fluidstructure interaction problem, a linear piston problem. Here the spring stiffness k is assumed to be uncertain with a uniform, exponential, and normal probability distribution function, respectively. These three distributions are chosen since they represent a different parameter domain: finite [a,b], semi-infinite $[a,\infty)$, and infinite $(-\infty,\infty)$. For all three distributions the same mean and variance are used for an equal comparison. The method is compared with Monte Carlo simulation, the Polynomial Chaos method, and the Stochastic Collocation method. The error convergence with respect to the amount of computational work is used. The work is expressed as the number of times a deterministic problem needs to be solved. For the Polynomial Chaos method the amount of work is I*(P+1) where P is the order of the approximation and I the number of Block-Gauss-Seidel iterations required to obtain the polynomial coefficients with an accuracy of 10⁻⁸. For the following computations about 3-5 iterations were required. The Stochastic Collocation and Chaos Collocation method both use one deterministic computation for every collocation point. As Lin et al.⁸ stated the performance of the Polynomial Chaos method strongly depends on the length of the time integration. Therefore, the efficiency of all methods is investigated for both short and long time integration.

4.1 The linear piston problem

The test problem is the linear piston problem indicated in Figure 1. The linear piston is chosen since it is a test problem which is easily evaluated, but still has all aspects of fluid-structure interaction problems. It consists of a one-dimensional fluid domain on

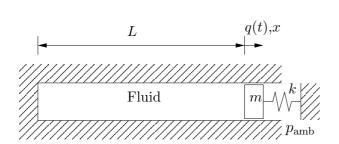


Figure 1: Linear piston problem.

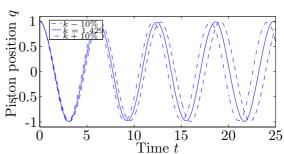


Figure 2: Realizations using different values for the spring stiffness k of the linear piston problem for $k = \mu_k = 1.429$ and $k = \mu_k \pm 10\%$.

one side bounded by a mass which is attached to a spring. The fluid is modeled using the linearized isentropic Euler equations. The piston position q(t) and velocity $\dot{q}(t)$ are determined by the mass of the piston m, the spring stiffness k, the length of the fluid domain L, the fluid state $U = (\rho, \rho u)^T$ and the ambient pressure $p_{\rm amb}$. A second-order central finite volume discretization is used for the flow. The time integration is performed

using an ESDIRK-4 scheme.¹⁷ The complete and equations can be found in Reference [9].

4.2 Efficiency for short time integration

In this section short time integration is considered. The piston position is evaluated till T=10 which corresponds to approximately 1.5 period. The error convergence is considered of the relative error of the mean of the piston position q, which is defined as

$$\varepsilon_q(T) = \frac{\mu_q(T) - \mu_{q, \text{reference}}(T)}{\mu_{q, \text{reference}}(T)}.$$
(28)

The reference solution is computed using a 20th order Polynomial Chaos approximation. The relative error of the mean with respect to the amount of computational work is indicated in Figures 3(a) till (c). From the figures the following can be concluded.

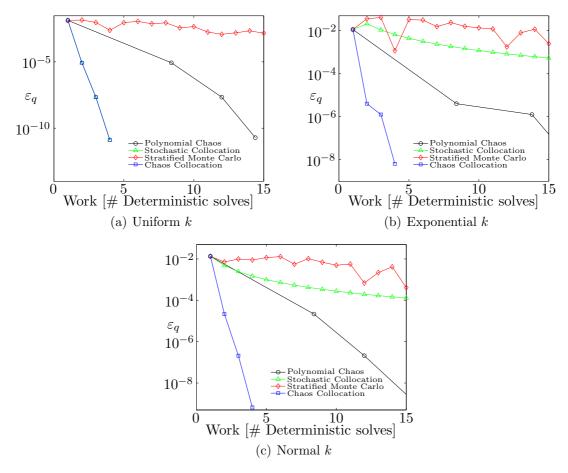


Figure 3: Error convergence of the mean of the piston position μ_q at T=10 (approximately 1.5 period) with respect to the amount of computational work, expressed in the number of times a deterministic system has to be solved.

For all distributions the Chaos Collocation method is the most efficient method. Only for the uniform distribution the Chaos Collocation method is the same as the Stochastic Collocation method. The Chaos Collocation method converges just as the Polynomial Chaos method exponentially with respect to the polynomial order. Due to the decoupled system of equations that has to be solved the amount of work decreased with a factor 3–5, since no iterations are required to obtain the polynomial coefficients.

4.3 Efficiency for long time integration

The long time integration is investigated by evaluating the piston position till T = 100, which corresponds to approximately 15 periods. The reference solution for this case is computed using Monte Carlo simulation with 10^6 samples. Figures 4(a) till (c) show the convergence of the relative error of the mean of the piston position q with respect to the amount of work.

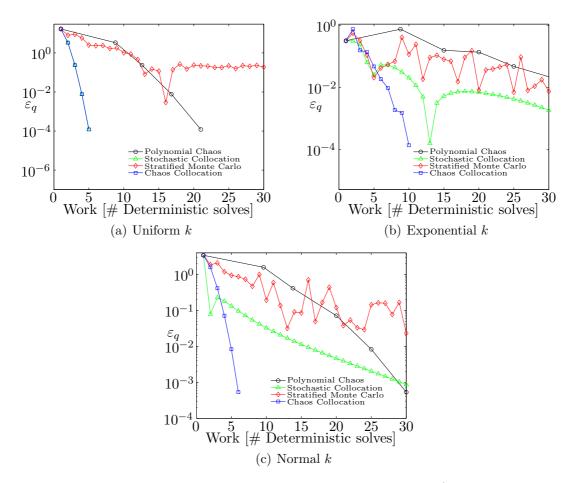


Figure 4: Error convergence of the mean of the piston position μ_q at T=100 (approximately 15 periods) with respect to the amount of computational work, expressed in the number of times a deterministic system has to be solved.

For long time integration the convergence does not show a nice convergence behavior anymore. However, the Chaos Collocation method is by far the most efficient method for all distribution types. This is due to the exponential convergence and the low amount of collocation points.

The results for short and long time integration show that the Chaos Collocation method is the most efficient in all cases. The results hold for arbitrary distributions, since the Chaos Collocation method is capable of approximating arbitrary distributions efficiently by obtaining the optimal Gauss-Chaos quadrature points and weights numerically. For the Polynomial Chaos method one has to use for example Gram-Schmidt orthogonalization¹⁴ to generate an orthogonal polynomial basis to obtain exponential convergence as well. Due to the low amount of collocation points, the Chaos Collocation method will always be more efficient than a Galerkin based Polynomial Chaos method, which requires several iterations to solve for the polynomial coefficients.

5 DEMONSTRATION OF THE TWO STEP APPROACH WITH CHAOS COLLOCATION FOR THE LINEAR PISTON PROBLEM

To demonstrate the Two Step approach with Chaos Collocation for uncertainty quantification, the linear piston problem is used with a moving wall at the left boundary, see Figure 5. The forcing is assumed to be harmonic according $f(t) = A\sin(\omega t)$, with A the forcing amplitude and ω the forcing frequency. The parameters are set to

$$k = 1$$
 $m = 1$ $A = 0.1$ $\omega = 0.8$.

These four parameters are assumed to be uncertain, and uniformly distributed according $U(\mu-10\%,\mu+10\%)$. The forcing frequency is set here to $\omega=0.8$ since the solution is not diverging for this value. Taking ω close to 1 leads to a diverging oscillation.

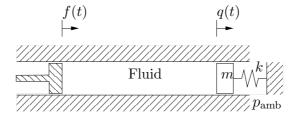
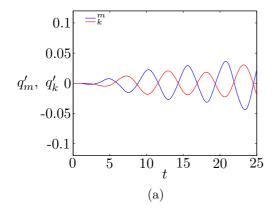


Figure 5: Linear piston with an unsteady forcing f(t) at the left wall.

5.1 Step I: Identifying the most important parameter for the piston problem using Sensitivity Analysis

A Sensitivity Analysis is performed for the four uncertain parameters. Figures 6(a) and (b) show the scaled sensitivity derivatives with respect to each parameter. The

sensitivity derivatives with respect to m, k and ω diverge, which means they have an increasing influence on the solution. For this testcase, however, clearly the sensitivity derivative with respect to ω diverges much faster than the others. The forcing frequency ω is the most important parameter. Therefore the next section presents the results for the uncertainty quantification for an uncertain forcing frequency ω . The computational cost of this first step is equal to 5 deterministic solves.



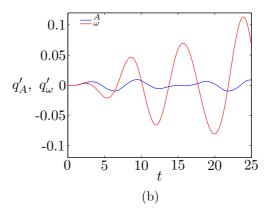


Figure 6: Sensitivity derivatives of the piston position with respect to all dependent parameters. (a) the structure parameters, piston mass m and spring stiffness k. (b) the boundary condition parameters, the forcing amplitude A and the forcing frequency ω .

5.2 Step II: Obtaining the stochastic response of the piston position q using the Chaos Collocation method

The forcing frequency is uniformly distributed by $U(\mu_{\omega} - 10\%, \mu_{\omega} + 10\%)$ with mean $\mu_{\omega} = 0.8$, resulting in a variation around the mean of 10 percent. Since ω occurs in non-polynomial terms in the equations as for instance $\omega \cos(\omega t)$ the Polynomial Chaos method is not straightforward. The previous sections showed that for a uniformly distributed parameter the Chaos Collocation method and the Stochastic Collocation method are the most efficient method for both short and long time integration. The non-polynomial terms are not a problem for both methods. To obtain more general results, the Chaos Collocation method is used. When the forcing frequency had a different probability distribution, the Chaos Collocation method would have been the most efficient, since the Chaos Collocation method converges exponentially for arbitrary probability distributions.

Figures 7 and 8 make clear that deterministic computations can be unreliable when uncertainties in the input parameters are present. Furthermore it is shown that computing only the mean and variance of the solution is not sufficient, even for an interval approximation. Figure 7 shows the response of the piston position q for $t \in [0, 50]$. The deterministic solution with $\omega = \mu_{\omega}$ is included as well as the results for a Monte Carlo

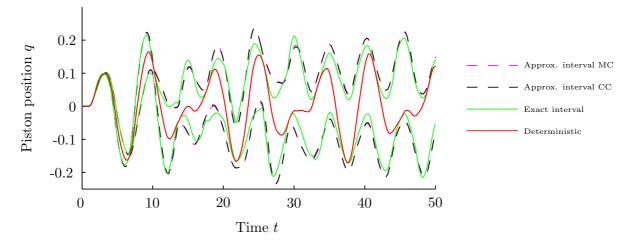


Figure 7: The piston position response for t=[0,50]. The deterministic response for $\omega=\mu_{\omega}$ is included as well as the approximated interval $[\mu_q-\sqrt{3}\sigma_q,\mu_q+\sqrt{3}\sigma_q]$ based on a uniformly distributed random variable computed using the Chaos Collocation method and Monte Carlo simulation. The exact interval obtained from Monte Carlo simulation is also shown.

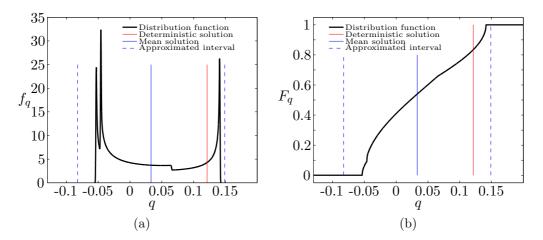


Figure 8: The stochastic properties of the piston position q at t=50. The probability density function $f_q(q)$ (a) and the probability distribution function $F_q(q)$ (b). The deterministic result for $\omega = \mu_{\omega}$ and an approximated interval $[\mu_q - \sqrt{3}\sigma_q, \mu_q + \sqrt{3}\sigma_q]$ based a uniformly distributed random variable are included.

simulation using 500 samples. A 7th order approximation is obtained efficiently using 8 collocation points for the Chaos Collocation method. A 7th order approximation has the same order of accuracy as the used temporal and spatial discretizations of the deterministic solver. The exact interval which contains all possible values for the piston position q is obtained from the Monte Carlo simulation. The interval is approximated assuming a uniform distribution, using the mean and standard deviation the interval is $[\mu_q - \sqrt{3}\sigma_q, \mu_q + \sqrt{3}\sigma_q]$. However, due to the non-linear dependence of the solution with respect to the uncertain parameter the distribution is not uniform and not even symmetric anymore. The approximated interval is symmetric, that is why in Figure 7 at some points the real interval is outside the approximated interval. When the mean and variance are used to approximate an interval based on the input distribution, the resulting interval can differ significantly from the real interval. This can best be seen in Figure 7, at t = 27 the interval is too conservative, while at t = 30 the approximated interval is too small.

To stress the importance of computing the complete distribution function instead of just the mean and variance figure 8 shows the probability distribution of the piston position q at t=50 resulting from a uniformly distributed forcing frequency ω . Figure 8(a) shows the probability density function $f_q(q)$ and Figure 8(b) shows the probability distribution function $F_q(q)$ of the piston position q. The figure perfectly shows the importance of computing the distribution function $F_q(q)$ instead of only the mean and variance. The mean value has a small probability to occur, just as the deterministic solution. From Figure 8(a), it can be seen that the probability of the mean is equal to the probability of the deterministic solution for this case. The highest probability of the solution is at the edges of the domain. The piston position at t=50 is most likely to be q(50)=-0.04 or q(50)=0.14 at the peaks of the probability density function $f_q(q)$. This is a huge difference with both the mean and the deterministic solution. This result perfectly illustrates the importance of uncertainty quantification.

5.3 Efficiency of the Two Step approach with Chaos Collocation

The use of the Two Step approach increases the efficiency of the uncertainty quantification significantly. Table 1 shows an overview of the amount of computational work required to obtain the stochastic response of the piston position q based on the four uncertain input parameters. When the stochastic response is computed for all uncertain parameters, the Polynomial Chaos method is the most efficient method. However, it still requires 1320 deterministic solves. This is unacceptable, since deterministic computational fluid-structure interaction computations are extremely computationally demanding. The Two Step approach requires 5 deterministic solves to identify the most important parameter using Sensitivity Analysis, after which the Chaos Collocation method provides a 7th order approximation of the stochastic response of the piston position requiring 8 deterministic solves. Consequently, the Two Step approach uses only 13 deterministic solves in total. When the Polynomial Chaos method was used for Step II, 37 deterministic solves were required. This is due to the fact that 4 Block-Gauss-Seidel iterations were necessary

to obtain the polynomial coefficients with an accuracy of 10^{-8} .

Compared to the Polynomial Chaos method for four uncertain parameters, the Two Step approach with Chaos Collocation results in a speed-up factor of 100. Here, one must be aware that including all four parameters in the uncertainty quantification provides more information about the solution and combined effects of uncertain parameters. However, the amount of work required for a full four parameter uncertainty quantification is unacceptable for computational fluid-structure interaction problems.

Table 1: Overview of the amount of computational work expressed in the number of times a deterministic system is solved for the linear piston problem with an unsteady boundary condition. Four parameters are assumed to be uniformly distributed.

Approach	(Step II) Method	Sensitivity	Obtain stoch.	Total
		Analysis	response of q	Work
		[det. solves]	[det. solves]	[det. solves]
All four	7 th order Chaos Collocation	-	8^{4}	4096
parameters	7 th order Polynomial Chaos	-	$(4+7)!/(7!4!) \cdot 4$	1320
Two Step	7 th order Chaos Collocation	5	8	13
approach	7 th order Polynomial Chaos	5	$8 \cdot 4 = 32$	37

6 CONCLUSIONS

In this paper a Two Step approach with Chaos Collocation is followed for efficient uncertainty quantification in computational fluid-structure interaction problems with multiple uncertain parameters. The first step consists of a Sensitivity Analysis to identify the most important parameter of the problem. This is an efficient way to reduce the problem to one uncertain parameter. In the second step the Chaos Collocation method is employed to obtain the stochastic response based on the probability distribution of the uncertain input parameter.

Since there was no method available which was most efficient for arbitrary input distributions, the Chaos Collocation method was introduced. The Chaos Collocation method combines the non-intrusiveness and ability to handle non-linearities easily of the Stochastic Collocation method with the exponential convergence for arbitrary probability distributions of the Polynomial Chaos method. The Chaos Collocation method was compared on efficiency with Monte Carlo simulation, the Polynomial Chaos method, and the Stochastic Collocation method. Both short and long time integration were considered for three input distributions: uniform, exponential, and normal. The comparison showed that the Chaos Collocation method is the most efficient method for all cases. A big advantage of the

Chaos Collocation method is that it is non-intrusive, which means existing deterministic solvers can be used. Furthermore non-linearities are not a problem and only P+1 collocation points are required for a P^{th} order approximation. A disadvantage is the rapid increase in the required amount of collocation points when the number of uncertain parameters increases. But since the Two Step approach reduces the problem to a problem with only one uncertain parameter the Chaos Collocation is the most efficient method for this approach.

The Two Step approach with Chaos Collocation has been demonstrated for the linear piston problem with an unsteady boundary condition. First in Step I Sensitivity Analysis identified the forcing frequency ω as the most important parameter for this case. A 7th order Chaos Collocation approximation is computed with 8 collocation points. The results show how uncertainty quantification is used to obtain reliable results. Also the importance has been made clear why the complete stochastic response of the solution is required and not only approximations of the mean and variance. The amount of work significantly decreased using the Two Step approach: only 13 deterministic solves were required for the 7th order approximation. When all four parameters would have been taken into account, the Polynomial Chaos method is most efficient, requiring 1320 deterministic solves. As a result, the Two Step approach shows a reduction factor of 100 compared to the full uncertainty analysis of all uncertainty quantification for all parameter, the gain in efficiency means the difference between feasible and non-feasible uncertainty quantification for computationally intensive problems.

REFERENCES

- [1] Bose, D., Wright, M., and Gökçen, T., Uncertainty and Sensitivity Analysis of Thermochemical Modeling for Titan Atmospheric Entry, AIAA paper 2004-2455, *Proc. of the 37th AIAA Thermophysics Conference*, Portland, June, (2004).
- [2] Gander, M.J. and Karp, A.H., Stable Computation of High Order Gauss Quadrature Rules using Discretization for Measures in Radiation Transfer, *Journal of Quantitative Spectroscopy Radiative Transfer*, **68**, pp. 213–223, (2001).
- [3] Gautschi, W., Orthogonal Polynomials (in Matlab), Journal of Computational and Applied Mathematics, 178, pp. 215–234, (2005).
- [4] Ghanem, R.G. and Spanos, P., Stochastic Finite Elements: A Spectral Approach, Springer-Verlag, New York, (1991).
- [5] Golub, G.H. and Welsch, J.H., Calculation of Gauss Quadrature Rules, *Mathematics of Computation*, **23**(106), pp. 221–230, (1969).

- [6] Hosder, S., Walters, R.W., and Perez, R., A Non-Intrusive Polynomial Chaos Method for Uncertainty Propagation in CFD Simulations, AIAA paper 2006-891, *Proc. of the* 44th AIAA Aerospace Sciences Meeting and Exhibit, Reno, January, (2006).
- [7] Kleiber, M. and Hien, T.D., The Stochastic Finite Element Method, Wiley, (1992).
- [8] Lin, G., Su, C.H., and Karniadakis, G.E., The Stochastic Piston Problem, *Proc. Nat. Acad. Sciences*, **101**(45), pp. 15840–15845, (2004).
- [9] Loeven, G.J.A., Witteveen, J.A.S., and Bijl, H., Efficient Uncertainty Quantification in Computational Fluid-Structure Interaction, AIAA paper 2006-1634, *Proc. of the* 8th AIAA Non-Deterministic Approaches Conference, Newport, May, (2006).
- [10] Mathelin, L. and Hussaini, M.Y., A Stochastic Collocation Algorithm for Uncertainty Analysis, NASA/CR-2003-212153, (2003).
- [11] Turgeon, É., Pelletier, D., and Borggaard, J., Applications of Continuous Sensitivity Equations to Flows with Temperature-dependent Properties, *Numerical Heat Transfer*, *Part A*, **44**, pp. 611–624, (2003).
- [12] Wan, X. and Karniadakis, G.E., Beyond Wiener-Askey Expansions: Handling Arbitrary PDFs, J. Sci. Comput., Published online: December 23, (2005).
- [13] Wiener, N., The Homogeneous Chaos, Amer. J. Math., 60, pp. 897–936, (1938).
- [14] Witteveen, J.A.S. and Bijl, H., Modeling Arbitrary Uncertainties Using Gram-Schmidt Polynomial Chaos, AIAA paper 2006-896, *Proc. of the 44th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, January, (2006).
- [15] Xiu, D. and Hesthaven, J.S., High-Order Collocation Methods for Differential Equations with Random Inputs, SIAM J. Sci. Comput., 27(3), pp. 1118–1139, (2005).
- [16] Xiu, D. and Karniadakis, G.E., The Wiener-Askey Polynomial Chaos for Stochastic Differential Equations, SIAM J. Sci. Comput., 24(2), pp. 619–644, (2002).
- [17] van Zuijlen, A.H. and Bijl, H., Implicit and Explicit Higher Order Time Integration Schemes for Structural Dynamics and Fluid-Structure Interaction Computations, Computers and Structures, 83, pp. 93–105, (2005).