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D4.5: Uncertainty Quantification, sensitivity analysis and optimization: Final public report (WP4)

Executive summary

This report provides an overview of several uncertainty quantification methods, including Monte Carlo, Quasi Monte Carlo, Latin Hypercube Sampling, Method of Moments, Stochastic Collocation, and Polynomial Chaos Expansion. Continuous adjoint method is presented, as an alternative to non-intrusive approaches combined with stochastic optimization methods, in order to mitigate the increased computational cost associated with uncertainties.

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Table of Contents

List of abbreviations

EC	European Commission
CFD	Computational Fluid Dynamics
QoI	Quantities of Interest
UQ	Uncertainty Quantification
PCE	Polynomial Chaos Expansion
MC	Monte-Carlo
PCE	Polynomial Chaos Expansion
niPCE	Non-intrusive PCE
PDF	Probability Density Functions

1 Introduction

1.1 Uncertainty Quantification

Computational Fluid Dynamics (CFD) methods have a strong track record of accurate predictions in applications where the stochastic nature of real-world fluid mechanics problems is not considered. CFD codes can reliably predict flows with deterministic input parameters and compute quantities of interest (QoI) for engineers, such as the drag coefficient of an airfoil under infinite flow conditions. However, there are cases where uncertainties in system behavior are quantifiable and significant. For example, a slight change in a compressor's inlet flow angle can have a profound effect on its performance. In such cases, the engineer needs to consider the probability distribution of the boundary condition for the inlet flow angle and determine the corresponding probability distribution of the QoI. This process of propagating input uncertainties to output quantities is known as Uncertainty Quantification (UQ), and there are various UQ methods available for achieving this goal.

The Monte Carlo technique is widely recognized as the most precise and accurate method for UQ. It involves sampling by solving the deterministic problem multiple times, randomly selecting stochastic inputs according to their respective probability distributions. This allows for determining the distribution of the QoI. However, while the standard Monte Carlo method is accurate, it is often cost-prohibitive in real-world applications due to the considerable time required for each CFD evaluation, which can take hours to complete. Additionally, the convergence rate of the method is inversely proportional to the square root of the number of samples $1/\sqrt{N}$, further adding to the computational expense. The Quasi Monte Carlo method is an alternative approach that utilizes quasi-random sequences of uncertain inputs, which share some properties of random sequences used in standard Monte Carlo. This results in a convergence rate proportional to $(logN)^8/N$, (Morokoff & Caflisch, 1995). McKay developed another sampling technique called Latin Hypercube Sampling, as mentioned in (McKay, 1992). In this method, the samples taken must satisfy specific constraints, which allows for sampling to be independent of the number of uncertain variables. Despite these improvements, stochastic sampling techniques, including Latin Hypercube Sampling, are still not considered cost-effective for CFD applications and are primarily limited to other fields such as computational finance.

The Method of Moments, also known as the Perturbation method, is an approach that approximates the QoI by employing its Taylor Expansion in terms of the uncertain input variables, around their mean values (Xiu, 2010). Typically, the expansion is truncated up to the second order, and the moments of the QoI are approximated directly from the moments of the truncated expansion. This method is valid for small input and output variations. However, a higher order truncation scheme can be applied (Papoutsis-Kiachagias, Papadimitriou, & Giannakoglou, 2012), and the statistical moments of the outputs are expressed as functions of their derivatives with respect to the uncertain variables, allowing for a more accurate approximation of the QoI in the presence of larger input and output variations.

Stochastic Collocation methods rely on interpolation schemes to compute stochastic quantities. Various types of interpolation schemes, such as piecewise linear or Lagrange interpolation, have been adopted for approximating the QoI (Ganapathysubramanian & Zabaras, 2007; Eldred, 2009; Xiu, 2009). The interpolation is constructed by sampling the QoI at a set of nodes in the stochastic space of the uncertain variables. The crucial aspect in this approach is the selection of nodes, as they need to be carefully chosen to ensure that the obtained approximation is accurate enough, while keeping the number of samples manageable in terms of computational cost.

In spectral methods, the QoI is approximated using basis functions that capture the spectral characteristics of the uncertain inputs. The Polynomial Chaos Expansion (PCE) is a spectral method that utilizes orthogonal polynomial bases to represent the dependence of the evaluation model's outputs on the uncertain variables (Pettersson, Iaccarino, & Nordström, 2015; Knio, Najm, Ghanem, et al., 2001; Debusschere et al., 2004). This concept was initially introduced by Wiener in (Wiener, 1938) for Gaussian processes in (Xiu & Karniadakis, 2003). PCE methods can be implemented in either an intrusive or non-intrusive manner, depending on whether software programming is required or not. Non-intrusive

Polynomial Chaos Expansion (niPCE) offers the advantage of not modifying the CFD code. Instead, the truncated spectral representation of the QoI is utilized, and the coefficients of the basis functions of the PCE are determined using existing software as a "black box" approach. This allows for a more seamless integration of PCE into existing CFD simulations without requiring modifications to the underlying code. The orthogonal polynomial basis in PCE allows for the computation of PCE coefficients in terms of integrals involving the QoI. These integrals are evaluated at Gaussian nodes, resulting in an efficient method for UQ compared to other methods (Ghisu & Shahpar, 2017). The theoretical background of PCE has been well-established (Cuneo, Traverso, & Shahpar, 2017) and applied in various studies (Emory, Iaccarino, & Laskowski, 2016). However, the "Curse of Dimensionality" remains a challenge, as the number of samples increases exponentially with the number of uncertain variables.

The niPCE method is similar to stochastic collocation, but differs in the choice of basis, which depends on the Probability Density Functions (PDFs) of the uncertain inputs, as the chosen polynomial basis is orthogonal with respect to those PDFs. A comparison between niPCE and Stochastic Collocation can be found in (Eldred & Burkardt, 2009). The curse of dimensionality, which is a main drawback of niPCE and Stochastic Collocation, has been addressed through various techniques, such as Gauss Quadrature with sparse Smolyak (Smolyak, 1963) nodes for computing integrals, or a least squares approach to reduce the number of required samples.

1.2 Robust Design Optimization

The objective function or QoI under uncertainties in the operating/environmental conditions of a system. The goal of robust design is to create systems that are not significantly affected by expected changes in the environment, ensuring reliable performance in the presence of uncertainties. While conventional design/optimization processes aim to minimize the objective function or QoI, robust design optimization takes into account the uncertainties and seeks to optimize the performance of the system under these uncertainties.

$$F = \mu_F + \sigma_F \ , \quad k \ \epsilon \ \mathbb{R} \tag{1}$$

where μ_F represents the mean value and σ_F represents the variance of the QoI, and k is a user-defined weight.

Indeed, in the context of Robust Design optimization, stochastic methods such as evolutionary algorithms can be combined with UQ methods to effectively account for uncertainties in the system's performance. The niPCE method, as mentioned in (Liatsikouras, Asouti, Giannakoglou, Pierrot, & Megahed, 2017), can be used as a UQ tool without requiring any software development. The niPCE can be used to evaluate the objective function or QoI with uncertainties, as represented by Eq. 1, and integrated with the evolutionary algorithm for shape optimization of systems such as airfoils. Similar approaches combining UQ methods and stochastic optimization have been presented in other references such as (Duvigneau, 2007; Papoutsis-Kiachagias et al., 2012; Vigouroux et al., 2021; Ho & Yang, 2012).

Adjoint-based techniques have been developed as an alternative to non-intrusive approaches combined with stochastic optimization methods, in order to mitigate the increased computational cost associated with uncertainties. In non-intrusive approaches, a single evaluation of the QoI/objective function can be more expensive due to the uncertainties involved, and the cost of stochastic optimization methods is often higher compared to gradient-based methods. Adjoint-based techniques enable the calculation of gradients that are needed for optimization and/or UQ purposes, which can potentially reduce the computational cost of the overall process.

2 Methodology

2.1 niPCE Variants

2.1.1 Multidimensional niPCE

Assuming the QoI, J, depends on the vector of uncertain variables $c_i, i \in [1, M]$. According to niPCE, J can be approximated as

$$J(\vec{c}) \approx \sum_{i=0}^{\infty} J_i H_i(\vec{c}) \tag{2}$$

where $H_i(\vec{c})$ present multivariate orthogonal polynomials of the uncertain variables and J_i are their corresponding weights. The orthogonality property of the base polynomials $H_i(\vec{c})$ in the niPCE method means that the following holds for any given pair H_i and H_j of the multivariate orthogonal polynomials of the uncertain variables

$$\langle H_i(\vec{c}), H_j(\vec{c})\rangle_W = \int \cdots \int H_i(\vec{c}) H_j(\vec{c}) W(\vec{c}) d\vec{c} = \langle H_i(\vec{c}), H_i(\vec{c})\rangle_W \, \delta_{ij} \tag{3}$$

where

$$W(\vec{c}) = \prod_{i=1}^{M} w_i\,(c_i) = w_1\,(c_1)\, w_2\,(c_2) \cdots w_M\,(c_M) \tag{4}$$

is the product of the Probability Density Functions (PDF) $w_i, i \in [1, M]$ of the uncertain variables and δ_{ij} is the Kronecker symbol.

For practical applications, the infinite sum in Eq. 2 is truncated and only a finite number of polynomials is used. Assuming that the largest polynomial degree maintained is k, then Eq. 2 is rewritten as

$$J(\vec{c}) \approx \sum_{i=0}^{Q-1} J_i H_i(\vec{c}) \tag{5}$$

where $Q = \frac{(M+k)!}{M!k!}$. A multidimensional polynomial $H_i(\vec{c})$ of degree m can be defined as the product of univariate polynomials $p_{i_l}(c_l)$ with a sum of degrees equal to m. Mathematically, this can be expressed as:

$$H(\vec{c}, m) = \prod_{l=1}^{M} p_{i_l}\,(c_l) \tag{6}$$

$$\sum_{l=1}^{M} i_l = m \tag{7}$$

It's important to note that there are multiple multivariate polynomials of degree m that can be constructed. Specifically, there are $\frac{(m+M-1)!}{m!-(M-1)!}$ different combinations that can lead to a multivariate polynomial of degree m. When all these polynomials are combined up to the maximum degree k, it results in the Q polynomials as retained in Eq. 2. The choice of univariate orthogonal polynomials p depends on the statistical distribution of the uncertain variables and is typically selected from the Wiener-Askey family (Xiu & Karniadakis, 2003).

2.2 Continuous adjoint equations

The governing equations of the flow problems solved in the steady- state, incompressible Navier-Stokes equations coupled with the Spalart-Allmaras turbulence model (Spalart & Allmaras, 1992). Excluding heat transfer, these are written as,

$$R^p = -\frac{\partial v_j}{\partial x_j} = 0 \tag{8}$$

$$R_i^v = v_j \frac{\partial v_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu +) \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right] + \frac{\partial p}{\partial x_i} = 0\,, \qquad i = 1, 2(, 3) \tag{9}$$

$$R^{\tilde{\nu}} = v_j \frac{\partial \tilde{\nu}}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\tilde{\nu}}{\sigma}\right) \frac{\partial \tilde{\nu}}{\partial x_j}\right] - \frac{c_{b2}}{\sigma}\left(\frac{\partial \tilde{\nu}}{\partial x_j}\right)^2 - \tilde{\nu}\, P(\tilde{\nu}) + \tilde{\nu}\, D(\tilde{\nu}) = 0 \tag{10}$$

where v_i are the velocity components, p is the static pressure divided by the constant fluid density, $\tau_{ij} = (\nu + \nu_t)\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$ and ν and $\nu_t = \tilde{\nu} f_{v_1}$ are the constant bulk and turbulent viscosities. Eq. 10 is solved for $\tilde{\nu}$ and terms $P(\tilde{\nu})$ & $D(\tilde{\nu})$ stand for the production and destruction terms, respectively, while the rest of terms in Eq. 10 are explained in (Spalart & Allmaras, 1992). The above-mentioned mean flow equations along with the turbulence model equations and their boundary conditions are referred to as the primal (or state) equations of the optimization problem. The vector of primal variables, U, contains v_i, p and the turbulence model variables.

2.2.1 Introduction of the Adjoint Variables

For the formulation of adjoint method, the starting point is to define augmented function F_{aug}, which is defined by adding the volume integrals of the state equations, multiplied by the adjoint variables, to J, namely,

$$F_{aug} = J + \int_{\Omega} \left(u_i R_i^v + q R^p + \tilde{\nu}_a R^{\tilde{\nu}}\right) d\Omega \tag{11}$$

where is the computational domain. In Eq. 11, u_i stand for the adjoint to the primal velocity components v_i whereas q is the adjoint pressure. The adjoint variables can also be seen as Lagrange multipliers. Since the residuals of the primal equations must be zero, the value of F_{aug} is identical to that of J. The derivatives of L with respect to (w.r.t.) the design variables b_n, $n \in [1, N]$, yields

$$\frac{\delta F_{aug}}{\delta b_n} = \frac{\delta J}{\delta b_n} + \int_{\Omega} \left(u_i \frac{\delta R_i^v}{\delta b_n} + q \frac{\delta R^p}{\delta b_n} + \tilde{\nu_a} \frac{\delta R^{\tilde{\nu}}}{\delta b_n}\right) d\Omega \tag{12}$$

$\delta\Phi/\delta b_n$ is used to denote the total (or material) derivative of an arbitrary quantity Φ (which can be any of the flow variables or even the residual of the state equations) and represents the total change in Φ by varying b_n.

$$\frac{\delta \Phi}{\delta b_n} = \frac{\partial \Phi}{\partial b_n} + \frac{\partial \Phi}{\partial x_k}\frac{\delta x_k}{\delta b_n} \tag{13}$$

The partial derivative $\frac{\partial \Phi}{\partial b_n}$ represents only the variation in Φ caused due to changes in the design and flow variables, by neglecting space deformations.

In order to formulate the adjoint equations, the total derivatives of the primal equations have to be developed. Since the shape and discretization of Ω depends on b_n, the total and spatial derivatives symbols do not permute but are related through (?, ?),

$$\frac{\delta}{\delta b_n}\left(\frac{\partial (.)}{\partial x_j}\right) = \frac{\partial}{\partial x_j}\left(\frac{\delta (.)}{\delta b_n}\right) - \frac{\partial (.)}{\partial x_k}\frac{\partial}{\partial x_j}\left(\frac{\delta x_k}{\delta b_n}\right) \tag{14}$$

A detailed application of Eq. 14 to the incompressible Navier-Stokes equations for laminar flows is presented in (Kavvadias, Papoutsis-Kiachagias, & Giannakoglou, 2015).

2.2.2 Objective Function Expression and its Differentiation

In this section, two commonly used objective functions are differentiated. The first is the force exerted on a solid body, projected onto the r_i direction (force type objective function), where $r_i$are the components of a user-defined unit vector. This objective function is defined as

$$J^F = \int_{S_W} \left[\left(p\delta_i^j - \tau_{ij} \right) r_j \right] n_i dS \tag{15}$$

where S_W is the part of the wall surface where the objective function is defined and δ_i^j is the Kronecker symbol. In external aerodynamics, if r_i is aligned with the farfield flow velocity, Eq.15 represents the drag force. J_F may also represent lift by appropriately defining r_i.

In general, any objective function defined along S can be expressed as

$$J_F = \int_S j_S dS = \int_S j_{S,i} n_i dS \tag{16}$$

where j_S is the boundary integrand. Differentiating J w.r.t. b_n gives

$$\frac{\delta J_F}{\delta b_n} = \int_S \frac{\delta j_{S,i}}{\delta b_n} n_i dS + \int_S j_{S,i} \frac{\delta (n_i dS)}{\delta b_n} \tag{17}$$

Since $j_{S,i} = j_{S,i}(v_k, p, \tau_{kj})$, for Eq.15 using the chain rule to develop $\delta j_{S,i}/\delta b_n$ yields

$$\frac{\delta J_F}{\delta b_n} = \int_S \frac{\partial j_{S,i}}{\partial v_k} n_i \frac{\delta v_k}{\delta b_n} dS + \int_S \frac{\partial j_{S,i}}{\partial p} n_i \frac{\delta p}{\delta b_n} dS + \int_S \frac{\partial j_{S,i}}{\partial \tau_{kj}} n_i \frac{\delta \tau_{kj}}{\delta b_n} dS + \int_S j_{S,i} \frac{\delta (n_i dS)}{\delta b_n} \tag{18}$$

Computing the variations of the flow quantities w.r.t. b_n appearing in Eq.18 would lead to a method with a cost scaling with N. To avoid this, the adjoint approach is developed.

2.2.3 Sensitivity derivatives

After formulating the adjoint PDEs and their boundary conditions, the remaining terms originating from Eq. 14, along with the last term Eq. 18 and additional terms emerging during the derivation of the adjoint boundary conditions, give rise to the SD expression, namely

$$\begin{aligned}
\frac{\delta F}{\delta b_n} = & \int_{S_W, i} \frac{\delta (n_i dS)}{\delta b_n} + \left(-u_i v_j \frac{\partial v_i}{\partial x_k} - u_j \frac{\partial p}{\partial x_k} - \tau_{ij}^a \frac{\partial v_i}{\partial x_k} + u_i \frac{\partial \tau_{ij}}{\partial x_k} + q \frac{\partial v_j}{\partial x_k} \right) \frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) d \\
& - \int_{S_W} \left(-u_k n_k + \frac{\partial j_{S_W,k}}{\partial \tau_{lz}} n_k n_l n_z \right) \tau_{ij} \frac{\delta (n_i n_j)}{\delta b_n} dS \\
& - \int_{S_W} \frac{\partial j_{S_W,k}}{\partial \tau_{lz}} n_k lz \tau_{ij} \frac{\delta (ij)}{\delta b_n} dS \\
& - \int_{S_W} \frac{\partial j_{S_W,k}}{\partial \tau_{lz}} n_k lz \tau_{ij} \frac{\delta (ij)}{\delta b_n} dS \\
& - \int_{S_W} \left[\frac{\partial j_{S_W,k}}{\partial \tau_{lz}} n_k (lz + lz) \right] \tau_{ij} \frac{\delta (ij)}{\delta b_n} dS
\end{aligned} \tag{19}$$

where $j_{S_W,i}$ is the part of $j_{S,i}$ defined along S_W, and $\mathbf{t}^{\mathrm{I}}, \mathbf{t}^{\mathrm{II}}$ are the two tangential unit vectors along S_W, forming a local Frenet system with $\mathbf{n}$. In shape optimization, depending on the parameterization used, $\frac{\partial x_k}{\partial b_n}$ can analytically be computed by differentiating the parameterization equation(s). The first term is the field integral that includes the grid sensitivities $(\frac{\partial x_k}{\partial b_n})$. This term corresponds to the displacement of the internal nodes of the computational grid due to variations in b_n. The computational cost of this term is potentially very high, as it scales linearly with the number of design variables, n .

3 Results and conclusion

The report highlighted the importance of UQ methods and Robust Design Optimization in addressing the inherent uncertainties. Two approaches, niPCE and continuous adjoint, were discussed as potential solutions to mitigate the computational cost associated with UQ and optimization. niPCE was presented as a UQ tool that can be used in combination with stochastic optimization methods. niPCE approximates the QoI using multivariate orthogonal polynomials of uncertain variables, allowing for efficient evaluation of the objective function in optimization without requiring software development. However, it was noted that niPCE may have increased computational cost compared to optimization without uncertainties, as each evaluation of the QoI can be expensive. Continuous adjoint was highlighted as an alternative approach that allows for the calculation of gradients necessary for optimization and/or UQ purposes. This method involves the use of adjoint equations to compute sensitivities of the objective function with respect to design variables, enabling efficient optimization with reduced computational cost compared to stochastic optimization methods. Continuous adjoint is particularly suitable for gradient-based methods, which are typically less computationally expensive compared to stochastic optimization methods. Erfan Farhikhteh (ESR5) combined PCE with an the OpenFOAM-based continuous adjoint solver, where the QoI is the axial moment of wind turbine blade and the objective function of the optimization problem is a weighted sum of its mean value and variance, UQ is carried out based on niPCE. The results presented that the optimized blade objective function increased by 8% with respect to the baseline design.

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