Semi-intrusive and non-intrusive stochastic methods for aerospace applications

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Abstract

In this work we present semi-intrusive and non-intrusive techniques for uncertainties quantification (UQ) in the context of the solution of partial differential equations, with a specific application to aerodynamics problems. These methods has been applied successfully to a supersonic nozzle flow and the analysis of an inviscid transonic flow over a RAE 2822 airfoil. In this case, we consider three uncertainties, on the Mach number, the angle of attack and the heat coefficient ratio and the numerical results are compared with experimental data.

1. Introduction

In the last decades strong effort was devoted to the development of accurate deterministic numerical algorithms. An open question concerns how to quantify the confidence level of numerical simulations by considering that the physical system is affected by several sources of uncertainty. To establish the quality of a numerical simulation Verification & Validation have been introduced [2]. Verification aims to quantify the errors associated to the numerical resolution of the given system of equations, while Validation aims to identify whether system of equation is a correct representation of physics. At the state of the art two kind of methodologies exist: intrusive and non-intrusive. The intrusive technique consist to write an ad-hoc code by modifying an existing deterministic ones to compute the statistics of interest. On the contrary a non-intrusive approach uses a deterministic code as a black-box without any other modifications. In this work a semi-intrusive scheme is proposed. We can call it semi-intrusive because it needs only a small number of modifications in order to be implemented in a deterministic code. In particular the number of partial differential equations (PDEs) is left unchanged in this scheme in contrast with conventional intrusive polynomial chaos (PC) methods. These methods are then applied to compute statistics for a supersonic nozzle flow and for the inviscid transonic flow over a RAE 2822 airfoil. In this case, three uncertainties have been taken into account at the same time. The paper is organized as follows: Section §2 describes in some details the SI method; §3 reviews the non-intrusive PC approach employed in this work; §4 is devoted to the description of the test case and the analysis of the results. Conclusions and work perspective are furnished in the closing section §5.

2. Semi-intrusive scheme for UQ

In this section we first introduce the mathematical setting of the problem §2.1 and then we present the semi-intrusive scheme §2.2.

2.1 Problem setting

Consider the following problem for an output of interest $u(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega))^*$:

$$\mathcal{L}(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega); u(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega))) = \mathcal{S}(\boldsymbol{x}, t, \boldsymbol{\xi}(\omega)), \tag{1}$$

*In the following the exposition is made for a scalar output variable (u) for brevity, but the extension to the multidimensional output case is straightforward where the operator $\mathcal{L}$ can be either an algebraic or a differential operator (in this case we need appropriate initial and boundary conditions). The operator $\mathcal{L}$ and the source term $\mathcal{S}$ are defined on the domain $D \times T \times \Xi$, where $\boldsymbol{x} \in D \subset \mathbb{R}^{n_d}$, with $n_d \in \{1, 2, 3\}$, and $t \in T$ are the spatial and temporal dimensions. Randomness is introduced in (1) and its initial and boundary conditions in term of d second order random parameters $\boldsymbol{\xi}(\boldsymbol{\omega}) = \{\xi_1(\omega_1), \ldots, \xi_d(\omega_d)\} \in \Xi$ with parameter space $\Xi \subset \mathbb{R}^d$. The symbol $\boldsymbol{\omega} = \{\omega_1, \ldots, \omega_d\} \in \Omega \subset \mathbb{R}$ denotes realizations in a complete probability space $(\Omega, \mathcal{F}, P)$. Here Ω is the set of outcomes, $\mathcal{F} \subset 2^{\Omega}$ is the σ-algebra of events and $P : \mathcal{F} \to [0, 1]$ is a probability measure. In our case the random variables $\boldsymbol{\omega}$ are by definition standard uniformly $\mathcal{U}(0, 1)$ distributed. Random parameters $\boldsymbol{\xi}(\boldsymbol{\omega})$ can have any arbitrary probability density function $p(\boldsymbol{\xi}(\boldsymbol{\omega}))$, in this way $p(\boldsymbol{\xi}(\boldsymbol{\omega})) > 0$ for all $\boldsymbol{\xi}(\boldsymbol{\omega}) \in \Xi$ and $p(\boldsymbol{\xi}(\boldsymbol{\omega})) = 0$ for all $\boldsymbol{\xi}(\boldsymbol{\omega}) \notin \Xi$; we can now drop the argument $\boldsymbol{\omega}$ for brevity. The probability density function $p(\boldsymbol{\xi}(\boldsymbol{\omega}))$ is defined as a joint probability density function from the independent probability function of each variable: $p(\boldsymbol{\xi}(\boldsymbol{\omega})) = \prod_{i=1}^{d} p_i(\xi_i)$. This assumption allows to an independent polynomial representation for every direction in the probabilistic space with the possibility to recover the multidimensional representation by tensorization. The aim is to find the statistical moments of the solution $u(\boldsymbol{\xi})$.

2.2 Semi-intrusive scheme

Let us introduce SI method for the quasi-1D Euler equations modelling the compressible flows in nozzle geometries

$$\begin{cases} \dfrac{\partial \mathbf{u}}{\partial t} + \dfrac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \mathbf{s}(x) & t > 0, x \in [0, L] \\ \\ \text{initial and boundary conditions} & , \end{cases} \tag{2}$$

where $\mathbf{u} = (\rho A, \rho u A, E A)^T$ with ρ the density, u the velocity, $e^{\text{tot}} = \rho e + \frac{\rho}{2} u^2$ the total energy with e the specific internal energy, $A(x)$ is the known nozzle section area distribution. The physical flux reads $\mathbf{f}(\mathbf{u}) = (\rho u A, \rho u^2 A + pA, huA)^T$ with p the pressure and $h = e^{\text{tot}} + p$ the total enthalpy. The source term is given by $\mathbf{s}(x) = (0, p\, dA/dx, 0)$. System (2) is closed by the equation of state $p = p(\rho, e)$; for the perfect gas flows considered in this study, $p = (\gamma - 1)\rho e$ with γ the ratio of specific heats. The test-cases considered in this work will solve (2) either with $dA/dx \neq 0$ and γ considered as a random variable (stochastic nozzle flow).

We consider a spatial discretisation for (2) with node points $x_i = i\Delta x$ where i belongs to some subset of $\mathbb{Z}$, a time step $\Delta t > 0$ and set $t_n = n\Delta t$, $n \in \mathbb{N}$. The control volumes are as usual the intervals $C_i = [x_{i-1/2}, x_{i+1/2}]$ with $x_{i+1/2} = \frac{x_i + x_{i+1}}{2}$. We start from a finite volume scheme, and for the simplicity of exposure, we only consider a first order in time and space scheme. The generalisation to more accurate scheme is obvious. Thus we define the *deterministic scheme* as

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n - \frac{\Delta t}{\Delta x}\Big(\mathbf{F}(\mathbf{u}_{i+1}^n, \mathbf{u}_i^n) - \mathbf{F}(\mathbf{u}_i^n, \mathbf{u}_{i-1}^n)\Big) \tag{3}$$

with $\mathbf{u}_i^0$ being an approximation of $\int_{C_i} \mathbf{u}_0(x) \mathrm{d}x/\Delta x$ and $\mathbf{F}$ a consistent approximation of the continuous flux $\mathbf{f}$. In all what follows, $\mathbf{F}$ is the Roe flux.

When $\mathbf{u}_0$ or the flux $\mathbf{f}$ depends on a random variable ξ, we propose the following modifications. First the set $\Xi \subset \mathbb{R}^d$ is subdivided into non overlapping subset Ξ_j, $j = 1, \ldots, n_p$ and the variables are represented by their conditional expectancies in the Ξ_j subsets. More precisely, our set of variables is

$$\mathbf{u}_{i,j}^n \approx \frac{\mathcal{E}(\int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{u}(x, t_n, \xi(\omega)) \mathrm{d}x \,|\, \omega \in \Xi_j)}{\Delta x P(\Xi_j)}.$$

where expectancy, of a generic function $g = g(\xi)$ is equal to

$$\mathcal{E}(g(\xi)) = \int_{\Xi} g(\xi) \mathrm{d}\xi$$

where $\mathrm{d}\xi$ may or may not have a density. The scheme evolves as

$$\mathbf{u}_{i,j}^{n+1} = \mathbf{u}_{i,j}^n - \frac{\Delta x}{\Delta t}\Big(\mathcal{E}(\mathbf{F}(\mathbf{u}_{i+1}^n, \mathbf{u}_i^n)|\Xi_j) - \mathcal{E}(\mathbf{F}(\mathbf{u}_i^n, \mathbf{u}_{i-1}^n)|\Xi_j)\Big).$$

The scheme is fully defined provided the "flux" $\mathcal{E}(\mathbf{F}(\mathbf{u}_{l+1}^n, \mathbf{u}_l^n)|\Xi_k)$ can be evaluated for any l and k.

2.2.1 Some numerical remarks

In the case of a nozzle flow, the problem is steady, so that an implicit scheme is used to achieve faster convergence to a steady-state. The *deterministic* scheme is a linearized implicit one: we look for the solution on the cell C_i as the limit of a sequence U_i^n when $n \to +\infty$. In the example we consider, the iteration for cell C_i is defined by

$$\frac{\Delta x}{\Delta t}\delta \mathbf{u}_i^n - A_{i-1/2}^{-}\delta \mathbf{u}_{i-1}^n - A_i \delta \mathbf{u}_i - A_{i+1/2}^{+}\delta \mathbf{u}_{i+1}^n = \mathbf{F}(\mathbf{u}_{i+1}^n, \mathbf{u}_i^n) - \mathbf{F}(\mathbf{u}_i^n, \mathbf{u}_{i-1}^n) - \mathbf{s}(\mathbf{u}_i)^n. \tag{4}$$

where $\delta \mathbf{u}_i^n = \mathbf{u}_i^{n+1} - \mathbf{u}_i^n$, $\mathbf{F}$ is the Roe flux, $A_{i+1/2}$ is the Roe matrix between states $\mathbf{u}_i$ and $\mathbf{u}_{i+1}$ at t_n, and A^+ (resp. A^-) is the positive (resp. negative) part of A. For the sake of simplicity, the boundary conditions are omitted in the description. System (4) is solved by Gauss Seidel iteration with a CFL number (hence time-step Δt) increased after each iteration. To summarize, the state vector $\mathbf{u}^{n+1} = (\mathbf{u}_1^{n+1}, \dots, \mathbf{u}_i^{n+1}, \dots, \mathbf{u}_{i_{max}}^{n+1})^T$ is obtained by

$$\mathbf{u}^{n+1} = \mathcal{G}(\mathbf{u}^n)$$

where the operator $\mathcal{G}$ gathers the implicit phase, the flux formulation and the boundary conditions.

If some parameter is random, the iteration writes

$$\mathbf{u}^{n+1} = \mathcal{G}(\mathbf{u}^n, \xi(\omega))$$

and we can apply the same procedure as before, *i.e.* evolve the conditional expectancies

$$\mathbf{u}_{i,j}^n \approx \frac{\mathcal{E}(\int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{u}(x, t_n, \xi(\omega))\mathrm{d}x \,|\, \omega \in \Xi_j)}{\Delta x P(\Xi_j)}.$$

via the "scheme"

$$\mathbf{u}_{i,j}^{n+1} = \mathcal{E}(\mathcal{G}(\mathbf{u}^n, \xi(\omega)),$$

We arrive exactly at the same problem, namely, given a set of constant values $\{\mathbf{u}_{j=0}, \dots, \mathbf{u}_{j=n_p}\}$ that are interpreted as the conditional expectancies of a function $\mathbf{u}$ in Ξ_j,

$$\mathbf{u}_j = \frac{\mathcal{E}(\mathbf{u} \,|\, \Xi_j)}{P(\Xi_j)}$$

and a measurable function f, find an accurate approximation of $\mathcal{E}(f(\mathbf{u}) \,|\, \Xi_j)$ for any j.

3. Non-intrusive Polynomial Chaos technique

In this section we briefly sketch the non-intrusive PC technique first introduced by Wiener [4] . In this work we used the framework of the so-called generalized Polynomial Chaos (gPC) [3] in which the correct set of polynomials is chosen as an optimal basis for different (continuous) probability distribution types. First a sampling method is chosen to generate a discrete parameter space $\boldsymbol{\xi}_i \in \overline{\Xi} \subset \Xi$ with $i = 1, \dots, N$ in which the model equation (1) is evaluated by a deterministic code determining a set of solution $u_i = u(\boldsymbol{\xi}_i)$. Finally it is necessary to reconstruct the variable $u(\boldsymbol{\xi})$ as a polynomial expansion in which the coefficients are computed evaluating d-dimensional integrals with an opportune quadrature techniques in which the u_i values are needed.

3.1 Generalized Polynomial Chaos expansion

We can employ the orthogonal basis reported in the Askey scheme [3] to approximate the functional form between each random inputs and the stochastic response. The chaos (truncated) expansion reads

$$u(\boldsymbol{\xi}) = \tilde{u}(\boldsymbol{\xi}) + O_T = \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}) + O_T, \tag{5}$$

where Ψ_k are the polynomials of total order n_o which form an Hilbert basis of $L_2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$ and the number of terms in the expansion (5) is

$$N_{tot} = \frac{(n_o + d)!}{n_o! \, d!} = P + 1. \tag{6}$$

Recalling the definition of the inner product, the determination of the PC coefficients of the output expansion reduces to the evaluation of N_{tot} d-dimensional integrals

$$\beta_k = \frac{\int_\Xi u(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}}{\langle \Psi_k \Psi_k \rangle}, \tag{7}$$

The stochastic solution $u(\boldsymbol{\xi})$ is now reconstructed as $\tilde{u}(\boldsymbol{\xi})$ from which we can compute the expected value $\mathcal{E}(u)$ and the variance $\sigma^2(u)$:

$$\mathcal{E}(\tilde{u}) = \beta_0 \tag{8}$$

$$\sigma^2(\tilde{u}) = \sum_{k=1}^{P} \beta_k^2 \langle \Psi_k^2(\boldsymbol{\xi}) \rangle. \tag{9}$$

From ANOVA theory, for uniformly distributed inputs, the variance $\sigma^2(u)$ can be decomposed as

$$\sigma^2 = \sum_{s=1}^{d} \sum_{j_1<..<j_s}^{d} \sigma^2\left(u_{j_1 \ldots j_s}\right) \tag{10}$$

where

$$\sigma^2\left(u_{j_1 \ldots j_s}\right) = \int u^2_{j_1 \ldots j_s} d\xi. \tag{11}$$

Then, it is possible to compute the contribution of each uncertainty and interaction effects.

4. UQ for the transonic flow over the RAE 2822 airfoil

In this section numerical results obtained by the SI scheme are compared with the PC ones for a supersonic nozzle flow and a transonic flow over RAE2822 airfoil.

4.1 Supersonic nozzle flow

Let us consider to compute statistic solutions of a supersonic nozzle by means of SI and a non-intrusive polynomial chaos method [8]. The outlet pressure is chosen in order to have a compression shock in the divergent part of the nozzle, exactly located at $x = 0.75$. The flow is characterized by an isentropic region of increasing speed or Mach number between $x = 0$ and the mean shock location in the divergent (the flow becoming supersonic at the nozzle throat located in $x = 0$). The mean γ is 1.4, and a maximal variation of 5% is considered. A uniform pdf is used for γ, in order to compare SI and PC. A preliminary convergence study with respect to the stochastic estimation has been realized, by using an increasing refinement of the probabilistic space discretization in the case of the SI method, and an increasing polynomial order in the case of PC method. The deterministic flow solver is an in-house code, based on finite volume formulation (for more details see [8]). The mean solutions computed by the two methods are coincident. The same trend is obtained if a Gaussian pdf is considered for γ (the figure is not reported for brevity). In Figure 1, the standard deviation of the Mach is reported along the nozzle for an uniform pdf (5th polynomial order for PC and 5 points in the probability space for SI). The standard deviation distributions computed by means of SI and PC are nearly coincident, except in the shock region, where there is a difference of 5% in the maximal standard deviation. The stochastic estimation remains globally very similar for the newly proposed SI approach and the well-established PC method, both similar to Monte Carlo results, which allows to validate the SI method results for the case of a uniform pdf.

4.2 Transonic flow over RAE 2822 airfoil

The inviscid flow over a RAE 2822 airfoil has been taken into account. A flow with Mach number $M = 0.729$, angle-of-attack $\alpha = 2.31^\circ$ and the heat capacity ratio for a diatomic gas $\gamma = c_p/c_v = 1.4$ (where c_p and c_v ahre the heat capacities at constant pressure and volume respectively) is considered, that is a classical test-case for a transonic regime. By using these conditions, the flow is characterized by a shock wave on the upper surface, located approximately at $x/c = 0.55$,

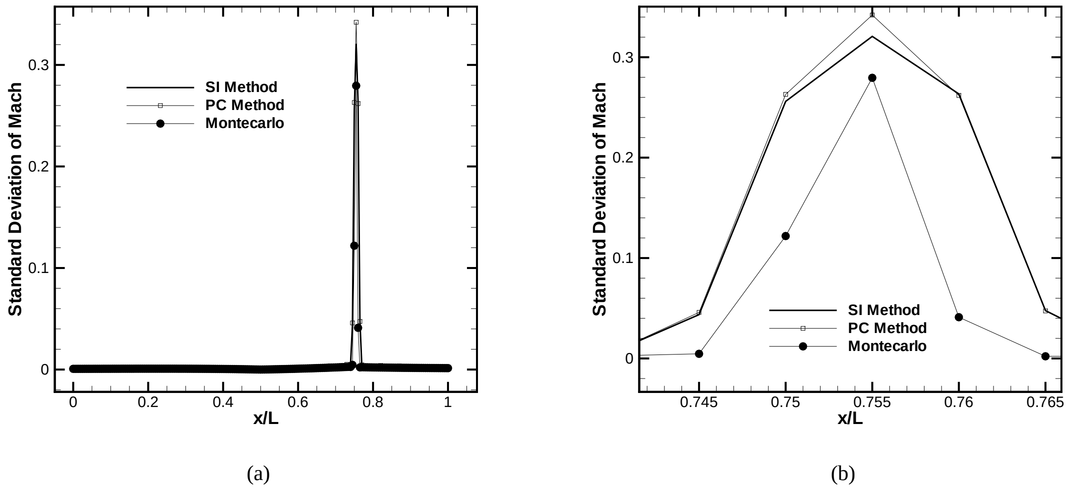


Figure 1: Nozzle flow with uncertain γ (uniform pdf). Standard deviation for the Mach number distribution: global view (a) and close-up on the shock region (b).

as shown from the experimental data of NASA [1], when the same conditions for M, α have been used. In this work we considered three sources of uncertainties, associated to the Mach number, the angle of attack and the polytropic coefficient γ. A uniform pdf with a maximal variation of ±3% with respect to the reference value have been taken into account. In the table 1 the bounds values are reported for each uncertainty.

Table 1: Bounds for the stochastic variables

Variable	Min	Max	Reference
M	0.70713	0.75087	0.729
α	2.3793	2.2407	2.31
γ	1.3580	1.4420	1.4

Computational fluid-dynamics (CFD) solver is based on FluidBox Platform and the SCOTCH [10] library has been used to obtain the domain decompositions in order to perform parallel computing. Residual distribution (RD) schemes have been used for discretization on nodal solutions. For steady problems, they consists in evaluating the local cell residual and distribute it to the nodes of the element. The nodal solution is then updated in order to bring the cell residual to zero [9].

First we performed a mesh convergence study by using meshes of increasing density (described in table 2). We used an unstructured mesh based on triangles. In the table 2, the number of triangles and the first size of the meshes are reported. This study is necessary in order to choose a mesh ensuring at the same time a good accuracy and a low computational cost because of stronger computational effort demanded by a stochastic computation with respect to a deterministic one. In figure 2, pressure coefficient alog the profile, defined as $C_P = 2(p - p_\infty)/(\rho_\infty V_\infty^2)$ where the subscript ∞ indicates freestream conditions, has been reported for each mesh. As shown in this figure, medium and fine meshes display very slight differences, that motivates the choice of the medium grid for stochastic computations.

Table 2: Mesh convergence

Mesh	Triangles	First mesh size
Coarse	4 800	4E-3
Medium	19 200	2E-3
Fine	76 800	1E-3

First, the CFD solver has been coupled with the non-intrusive PC method in order to take into account the three uncertainties (Tab. 1) on Mach number, α and γ. Full tensorization has been used for the discretization of the stochastic space, then a number equal to $(p + 1)^3$ of deterministic computations have been performed, where p is the polynomial

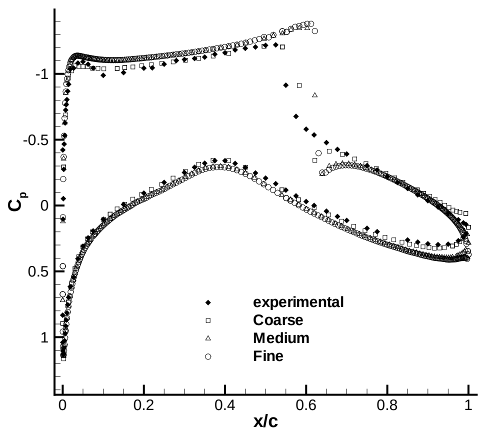
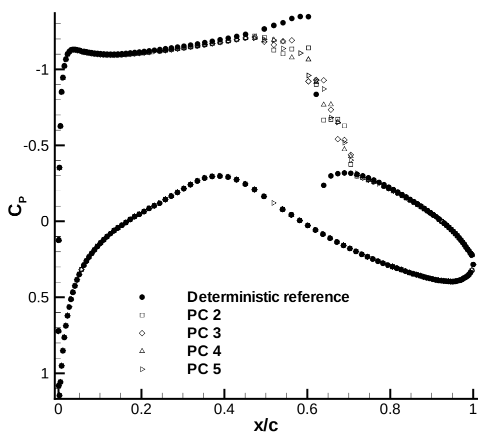


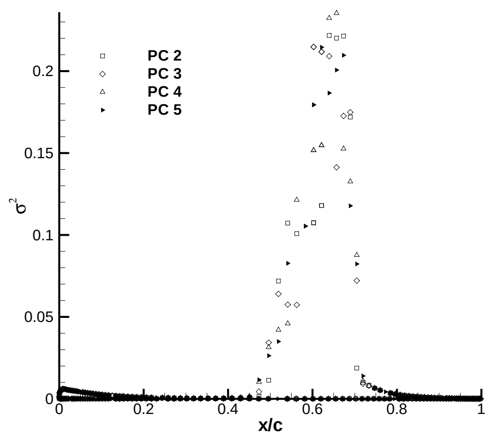
Figure 2: Mesh convergence for the deterministic scheme

order. Convergence of PC stochastic method has been assessed by comparing several stochastic solutions for different orders p.

In figure 3, pressure coefficient mean (3(a)) and variance (3(b)) have been reported for different polynomial orders with the deterministic solution. It can be observed that mean solutions are more smooth with respect to the deterministic solution, and the variance is concentrated as expected near the shock (then on the upper-side of the airfoil). Seeing the oscillation in the peak variance (Fig. 3(b)), it seems necessary to use an high polynomial order (5th) for obtaining a converged stochastic solution.



(a)

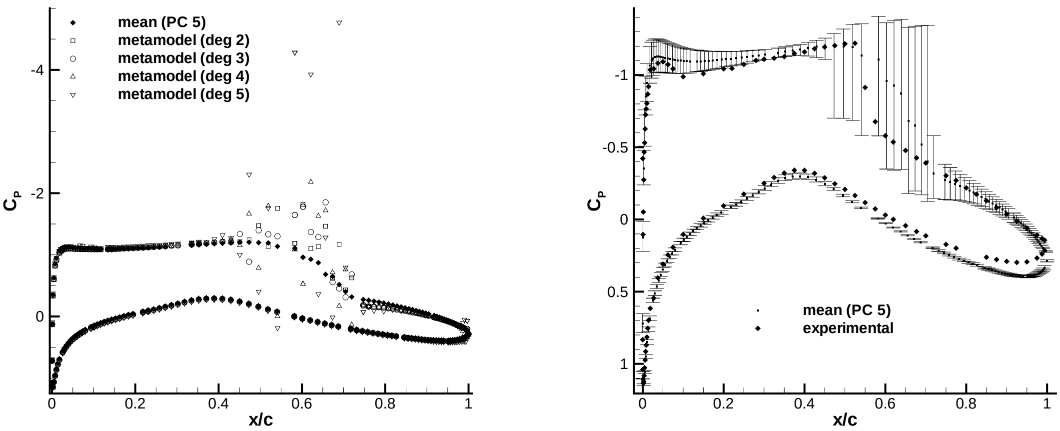


(b)

Figure 3: Mean (a) and variance (b) solutions along the profile for the pressure coefficient C_p by means of PC method.

The correctness of the polynomial representation in the shock region is one of the major issue of the PC technique. The polynomial expansion described in Eq. 5 is a representation of the output as a function of the stochastic space. Then, it can be used as a substitute function for the output statistics. In order to show some problems of PC method near the shock, pressure coefficient statistics have been computed by performing a Monte Carlo computation (10 000 individuals with a quasi-Monte Carlo Sobol sequence) basing on Eq. 5. Then, solutions obtained for different polynomial order p have been reported in figure 4(a). It is evident that with an increasing degree of the polynomial representation spurious oscillations appear near the shock region, while in the smoother region of the presssure coefficient solution the convergence is achieved quickly. This shows an hard convergence of the polynomial reconstruction even for high polynomial orders.

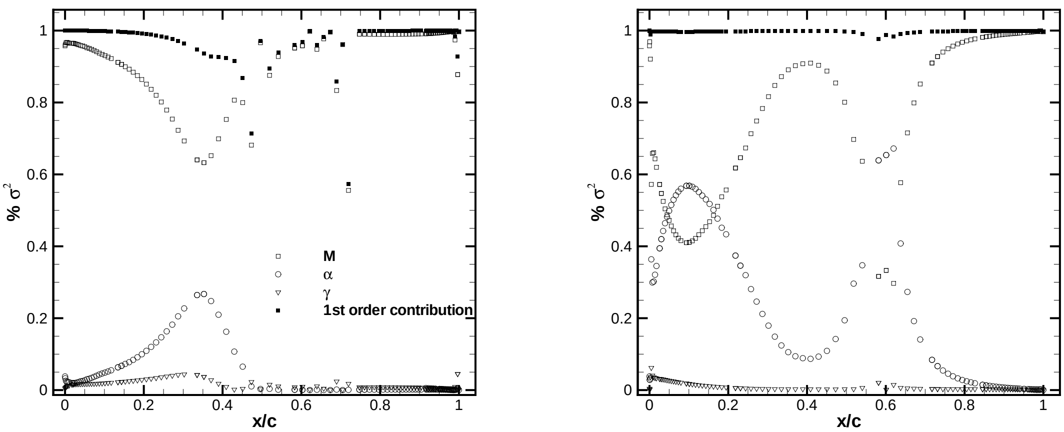
If polynomial expansion is used, it is possible easily to compute the probability density function for each output. In this case, we can compute for example the error bars ensuring that there is a 95% of probability for the solution to be in these intervals. In the figure 4(b) the mean solution with these error bars is reported. This shows the great potentiality of the stochastic analysis, allowing to compare numerical and experimental error bars.



(a) (b)

Figure 4: (a) Convergence for PC with increasing degrees. (b) Mean solution and confidence intervals

An ANOVA analysis has been applied on the pressure coefficient variance in order to compute the hierarchy of most influent uncertainties. Then, the global variance has been decomposed by computing linear contribution of each uncertainty and interaction mixed effects. In figure 5, first-order contributions of the global variance and of each uncertainty has been reported for the upper-side (Figure 5(a) and the lower-side (Figure 5(a)) of the airfoil. It is evident that first-order contributions are predominant seeing that they explain the 99% of the variance along the profile. Moreover, Mach number and α are the most important parameters, on the contrary γ can be neglected in the stochastic analysis (at least for what concerns pressure coefficient statistics).



(a) (b)

Figure 5: ANOVA analysis applied to the pressure coefficient C_p along the profile, on the upper-side (a) and lower-side (b).

5. Conclusions

Stochastic CFD simulations have a great interest in order to improve the predictivity of numerical simulation. In this paper, two numerical techniques for stochastic analysis have been presented, the classical non-intrusive PC method and a semi-intrusive method. Performances of these two methods have been tested on a supersonic nozzle flow and a transonic flow over a RAE2822 airfoil. PC method shows a great flexibility with respect to the coupling with a CFD code and efficiency even if presents some issues in shock-dominated flows. Semi-intrusive method demands an effort for implementation but displays an interesting potentiality in order to consider a whatever form of pdf.

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