

## A SIMPLE SEMI-INTRUSIVE METHOD FOR UNCERTAINTY QUANTIFICATION OF SHOCKED FLOWS, COMPARISON WITH A NON-INTRUSIVE POLYNOMIAL CHAOS METHOD

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**Abstract.** *The purpose of this paper is to provide a description and a comparison of a method already described in [1] with more standard UQ tools.*

### 1 INTRODUCTION

This paper is devoted to the comparison of two methods of uncertainty quantification (UQ) in the context of compressible inviscid flows. More specifically, we aim at comparing a well documented non-intrusive Polynomial Chaos (PC) method with a newly developed approach [1] offering the potential advantage of being less dependent on the probability distribution functions (pdf) of the random variables of the problem. This new approach is said semi-intrusive (SI) because it requires only a limited amount of modification in a deterministic flow solver to quantify the uncertainty on the flow state when the flow solver includes uncertain variables; in particular, the number of partial differential equations to solve is left unchanged with respect to the deterministic case (in contrast with conventional intrusive method such as PC), with these PDEs solved on an extended computational domain including the random space variables. The SI and PC methods will be first compared by computing the compressible flow of perfect gas in a nozzle, using the quasi-1D Euler model, with uncertainty on the heat coefficient ratio  $\gamma$ . This test-problem has been retained because it encompasses the essential features of compressible flows with a reduced computational cost allowing an extensive comparison of the UQ strategies, including convergence studies on the polynomial order for the PC approach and on the refinement level of the stochastic space discretization for the newly proposed approach. To allow further comparison with existing PC techniques described in [12], we also compute shock-tube problems governed by the 1D Euler equations where the uncertainty is injected in the initial conditions, namely on the location of the interface between the light and

heavy fluid initially at rest. The paper is organized as follows : Section 2 describes in some details the method recently proposed in [1]; Section 3 reviews the non-intrusive Polynomial Chaos approach also employed in this study as a reference method; Section 4 describes the test-cases retained for assessing the performances of both UQ approaches and analyzes the results with emphasis on the choice of the pdf for the uncertain variables. Conclusions are drawn and work perspectives given in a closing section.

## 2 A FLEXIBLE SEMI-INTRUSIVE METHOD

### 2.1 A GENERAL STRATEGY

Let us start from a PDE of the type

$$\mathcal{L}(u, \omega) = 0 \tag{1}$$

defined in a domain  $K$  of  $\mathbb{R}^d$ , subjected to boundary conditions. Since the discussion of this section is formal, we put the different boundary conditions of the problem in the symbol  $\mathcal{L}$ . The operator  $\mathcal{L}$  may depend on some random variables  $X$  depending themselves on a random parameter  $\omega$ , *i.e.* an element of a set  $\Omega$  equipped with a probability measure  $d\mu$ . We assume, using abuse of notations, that the measure is such that  $\Omega$  can be identified to a subset of  $\mathbb{R}^d$ , still denoted by  $\Omega$ , for some  $d$ , and the expectancy of any  $d\mu$  measurable function  $\Psi(X)$  is

$$\mathcal{E}(\Psi(X)) = \int_{\Omega} \Psi(x) d\mu(x)$$

where  $d\mu$  may or may not have a density. In (1), the uncertainty is weakly coupled with the PDE, *i.e.* the random variable  $X$  does not depend on any space variables. However, the measure  $d\mu$  may depend on some space variable. The examples we have in mind are such that for a given realisation  $\omega_0 \in \Omega$ ,  $\mathcal{L}(u, X(\omega_0)) = 0$  is a “standard” PDE, such as the Laplace equation, Burgers equation, the Navier Stokes equations, etc. To make things even clearer let us consider the quasi-1D Euler equations modelling the compressible flows in nozzle geometries :

$$\left\{ \begin{array}{l} \frac{\partial U}{\partial t} + \frac{\partial f(U)}{\partial x} = S(x) \quad t > 0, x \in [0, L] \\ \text{initial and boundary conditions} \end{array} \right. \tag{2}$$

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

(stochastic nozzle flow) or with  $A = cst$ ,  $\gamma$  fixed to 1.4 but uncertain initial conditions (stochastic shock-tube problem taken from [12]).

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  $\mathcal{C}_i = [x_{i-1/2}, x_{i+1/2}]$  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

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} \left( F(U_{i+1}^n, U_i^n) - F(U_i^n, U_{i-1}^n) \right) \quad (3)$$

with  $U_i^0$  being an approximation of  $\int_{\mathcal{C}_i} U_0(x) dx / \Delta x$  and  $F$  a consistent approximation of the continuous flux  $f$ . In all what follows,  $F$  is the Roe flux.

When  $U_0$  or the flux  $f$  depends on a random variable  $X$ , we propose the following modifications. First the set  $\Omega \subset \mathbb{R}^d$  is subdivided into non overlapping subset  $\Omega_j$ ,  $j = 1, \dots, n_p$  and the variables are represented by their conditional expectancies in the  $\Omega_j$  subsets. More precisely, our set of variables is

$$U_{i,j}^n \approx \frac{\mathcal{E}(\int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t_n, X(\omega)) | \omega \in \Omega_j)}{\Delta x P(\Omega_j)}.$$

which evolves as

$$U_{i,j}^{n+1} = U_{i,j}^n - \frac{\Delta x}{\Delta t} \left( \mathcal{E}(F(U_{i+1}^n, U_i^n) | \Omega_j) - \mathcal{E}(F(U_i^n, U_{i-1}^n) | \Omega_j) \right).$$

The scheme is fully defined provided the “flux”  $\mathcal{E}(F(U_{l+1}^n, U_l^n) | \Omega_k)$  can be evaluated for any  $l$  and  $k$ . This will be the topic of a further section. The choice of the time step also has to be discussed.

## 2.2 CASE OF A NOZZLE FLOW

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  $\mathcal{C}_i$  as the limit of a sequence  $U_i^n$  when  $n \rightarrow +\infty$ . In the example we consider, the iteration for cell  $\mathcal{C}_i$  is defined by

$$\frac{\Delta x}{\Delta t} \delta U_i^n - A_{i-1/2}^- \delta U_{i-1}^n - A_i \delta U_i - A_{i+1/2}^+ \delta U_{i+1}^n = F(U_{i+1}^n, U_i^n) - F(U_i^n, U_{i-1}^n) - S(U_i)^n. \quad (4)$$

where  $\delta U_i^n = U_i^{n+1} - U_i^n$ ,  $F$  is the Roe flux,  $A_{i+1/2}$  is the Roe matrix between states  $U_i$  and  $U_{i+1}$  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. In the test case we have considered (shocked nozzle), the inlet and outlet boundary conditions are subsonic and approximated via a characteristic approach. System (4) is solved by Gauss Seidel iteration with a CFL number (hence time-step  $\Delta t$ ) increased after each iteration. To summarize, the state vector  $U^{n+1} = (U_1^{n+1}, \dots, U_i^{n+1}, \dots, U_{max}^{n+1})^T$  is obtained by

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

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

If some parameter is random, the iteration writes

$$U^{n+1} = \mathcal{G}(U^n, X(\omega))$$

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

$$U_{i,j}^n \approx \frac{\mathcal{E}(\int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t_n, X(\omega)) | \omega \in \Omega_j)}{\Delta x P(\Omega_j)}.$$

via the “scheme”

$$U_{i,j}^{n+1} = \mathcal{E}(\mathcal{G}(U^n, X(\omega))),$$

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

$$U_j = \frac{\mathcal{E}(U | \Omega_j)}{P(\Omega_j)}$$

and a measurable function  $f$ , find an accurate approximation of  $E(f(U) | \Omega_j)$  for any  $j$ . A solution to this problem is described in the next section.

### 2.3 SOME COMPUTATIONAL REMARKS

Let  $d\mu$  be a probability measure and  $X$  be a random variable defined on the probability space  $(\Omega, d\mu)$ . Assume we have a decomposition of  $\Omega$  by non overlapping subsets  $\Omega_i$ ,  $i = 1, N$  of strictly positive measure:

$$\Omega = \cup_{i=1}^N \Omega_i.$$

We are given the conditional expectancies  $E(X | \Omega_i)$ . Can we estimate for a given  $f$ ,  $E(f(X))$ ? Assuming  $X = (X_1, \dots, X_n)$ , the idea is the following : for each  $\Omega_i$ , we wish to evaluate a polynomial  $P_i \in \mathbb{R}^n[x_1, \dots, x_n]$  of degree  $n$  such that

$$E(X | \Omega_j) = \frac{\int_{\mathbb{R}^n} 1_{\Omega_j}(x_1, \dots, x_n) P(x_1, \dots, x_n) d\tilde{\mu}}{\mu(\Omega_i)} \quad \text{for } j \in \mathcal{S}_i \quad (5)$$

where  $d\tilde{\mu}$  is the image of  $d\mu$  and  $\mathcal{S}_i$  is a stencil associated to  $\Omega_i$ .<sup>1</sup>

This problem is reminiscent of what is done in finite volume schemes to compute a polynomial reconstruction in order to increase the accuracy of the flux evaluation thanks to the MUSCL extrapolation. Among the many references that have dealt with this problem, with the Lebesgue measure  $dx_1 \dots dx_n$ , one may quote [2] and for general meshes [6, 3]. A systematic method for computing the solution of problem (5) is given in [4].

Assume that the stencil  $\mathcal{S}_i$  is defined, the technical condition that ensures a unique solution to problem (5) is that the Vandermonde-like determinant (given here for one random variable for the sake of simplicity)

$$\Delta_i = \det \left( E(x^l | \Omega_j) \right)_{0 \leq l \leq n, j \in \mathcal{S}_i}. \quad (6)$$

is non zero. In the case of several random variable, the exponent  $l$  in (6) is replaced by a multi-index.

Once the solution of (5) is known, we can estimate

$$E(f(X)) \approx \sum_{j=1}^N \int_{\mathbb{R}^n} 1_{\Omega_j}(x_1, \dots, x_n) f(P(x_1, \dots, x_n)) d\tilde{\mu}.$$

The following approximation results hold : if  $f \in C^p(\mathbb{R}^n)$  with  $p \geq n$  then

$$\left| E(f(X)) - \sum_{j=1}^N \int_{\mathbb{R}^n} 1_{\Omega_j}(x_1, \dots, x_n) f(P(x_1, \dots, x_n)) d\tilde{\mu} \right| \leq C(\mathcal{S}) \max_j [\mu(\Omega_j)^{\frac{p+1}{p}}]$$

for a set of regular stencil; the proof is a straightforward generalization of the approximation results contained in [5].

In all the following practical illustrations, we will use only one or two sources of uncertainty even though the method can be used for any number of uncertain parameters - a large number of uncertain parameters leads however to other known problems such as the so-called curse of dimensionality. The space  $\Omega$  is subdivided into non overlapping measurable subsets. In the case of one source of uncertainty, the subsets can be identified, via the measure  $d\mu$ , to  $N$  intervals of  $\mathbb{R}$  which are denoted by  $[\omega_j, \omega_{j+1}]$ . The case of multiple sources can be considered by tensorisation of the probabilistic mesh. This formalism enables to consider correlated random variables.

Let us describe in details what is done for a single source of uncertainties. In the cell  $[\omega_j, \omega_{j+1}]$ , the polynomial  $P_{i+1/2}$  is fully described by a stencil  $\mathcal{S}_{i+1/2} = \{i + 1/2, i_1 +$

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<sup>1</sup>For example,  $d\mu$  is the sum of a Gaussian and a Dirac at  $x_0$ ,

$$\int_{\mathbb{R}^n} P(x) d\tilde{\mu} = \alpha \frac{1}{\sqrt{2\pi\sigma}} \int_{\mathbb{R}} P(x) e^{-\frac{(x-m)^2}{2\sigma}} dx + (1 - \alpha) P(x_0)$$

$1/2, \dots\}$  such that in the cell  $[\omega_j, \omega_{j+1}]$  with  $j + 1/2 \in \mathcal{S}_{i+1/2}$  we have

$$E(P_{i+1/2} | [\omega_j, \omega_{j+1}]) = E(u | [\omega_j, \omega_{j+1}]).$$

It is easy to see that there is a unique solution to that problem provided that the elements of  $\{[\omega_j, \omega_{j+1}]\}_{j+1/2 \in \mathcal{S}_{i+1/2}}$  do not overlap, which is the case. In the numerical examples, we consider three reconstruction mechanisms :

- a first order reconstruction: we simply take  $\mathcal{S}_{i+1/2} = \{i+1/2\}$  and the reconstruction is piecewise constant,
- a centered reconstruction: the stencil is  $\mathcal{S}_{i+1/2} = \{i-1/2, i+1/2, i+3/2\}$  and the reconstruction is piecewise quadratic. At the boundary of  $\Omega$ , we use the reduced stencils  $\mathcal{S}_{1/2} = \{1/2, 3/2\}$  for the first cell  $[\omega_0, \omega_1]$  and  $\mathcal{S}_{N-1/2} = \{N-1/2, N-3/2\}$  for the last cell  $[\omega_{N-1}, \omega_N]$ , *i.e.* we use a linear reconstruction at the boundaries.
- An ENO reconstruction : for the cell  $[\omega_i, \omega_{i+1}]$ , we first evaluate two polynomials of degree 1. The first one,  $p_i^-$ , is constructed using the cells  $\{[\omega_{i-1}, \omega_i], [\omega_i, \omega_{i+1}]\}$  and the second one,  $p_i^+$ , on  $\{[\omega_i, \omega_{i+1}], [\omega_{i+1}, \omega_{i+2}]\}$ . We can write (with  $\omega_{i+1/2} = \frac{\omega_i + \omega_{i+1}}{2}$ )

$$p_i^+(\xi) = a_i^+(\xi - \omega_{i+1/2}) + b_i^+ \text{ and } p_i^-(\xi) = a_i^-(\xi - \omega_{i+1/2}) + b_i^-.$$

We choose the least oscillatory one, *i.e.* the one which realises the oscillation  $\min(|a_i^+|, |a_i^-|)$ . In that case, we take a first order reconstruction on the boundary of  $\Omega$ .

Other choices are possible such as WENO-like interpolants. Again, the case of multiple source of uncertainties can be handled by tensorisation.

### 3 POLYNOMIAL CHAOS METHOD

Polynomial Chaos (PC) expansions are derived from the original theory of Wiener on spectral representation of stochastic processes using Gaussian random variables. PC expansions have been used for UQ by Ghanem and Spanos [7] and extended by Xiu and Karniadakis [8] to non-Gaussian processes. Any well-behaved process  $y$  (e.g. a second-order process) can be expanded in a convergent (in the mean square sense, see Cameron and Martin [9]) series of the form :

$$y(x, t, \xi) = \sum_{\alpha} y_{\alpha}(x, t) \Psi_{\alpha}(\xi) \tag{7}$$

where  $\xi$  is a set of  $nx$  independent random variables  $\xi = (\xi_1, \xi_2, \dots, \xi_n)$  and  $\alpha$  a multi-index  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$  with each component  $\alpha_i = 0, 1, \dots$ . The multivariate polynomial function  $\Psi_{\alpha}$  is defined by a product of orthogonal polynomials  $\Phi_i^{\alpha_i}(\xi_i)$  in relation to the probability density of the random variable  $\xi_i$ , namely  $\Psi_{\alpha}(\xi) = \prod_{i=1}^{nx} \Phi_i^{\alpha_i}(\xi_i)$ . A one-to-one correspondence exists between the choice of stochastic variable  $\xi_i$  and the

polynomials  $\Phi_i^{\alpha_i}(\xi_i)$  of degree  $\alpha_i$ . For instance if  $\xi_i$  is a normal/uniform variable, the corresponding  $\Phi_i^{\alpha_i}(\xi_i)$  are Hermite/Legendre polynomials of degree  $\alpha_i$ ; the degree of  $\Psi_\alpha$  is  $|\alpha|_1 = \sum_{i=1}^{nx} \alpha_i$ . The multivariate polynomial functions  $\Psi_\alpha$  are orthogonal with respect to the probability distribution function of the vector  $\xi$  of standard independent random variables  $\xi_i, i = 1, 2, \dots, nx$ . Coefficients  $y_\alpha(x, t)$  are the PC coefficients or stochastic modes of the random process  $y$ . Defining the scalar product by the expectation operator yields :

$$y_\alpha(x, t) = \langle y(x, t), \Psi_\alpha \rangle \|\Psi_\alpha\|^{-2} \quad (8)$$

For practical use, the PC expansions have to be truncated in term of degree polynomial  $no$  :

$$y(x, t, \xi) = \sum_{|\alpha|_1 \leq no} y_\alpha(x, t) \Psi_\alpha(\xi) \quad (9)$$

The number of multivariate polynomials  $\Psi_\alpha$ , that is the dimension of the expansion basis, is related to the stochastic dimension  $nx$  and the degree  $no$  of polynomials and is given by the formula  $(nx + no)! / (nx! no!)$ . Several approaches can be used to estimate PC coefficients. The first approach is based on a Galerkin projection of the model equations; it leads to a set of coupled equations and requires an adaptation of the deterministic code in order to be applied. Alternative non-intrusive approaches are based on Monte Carlo simulations or quadrature formulae to evaluate PC coefficients (see for instance [10]). When the number  $d$  of variables is large, quadrature formulae based on tensor product of a 1D formula require too many numerical evaluations and Sparse Grids integration based on Smolyak's construction [11] are preferred. For these non intrusive approaches, PC coefficients are therefore evaluated from a set of points and weights  $(\xi_i, \omega_i)$  by formulae of the form :

$$y_\alpha(x, t) = \|\Psi_\alpha\|^{-2} \sum_{i=1}^n y(x, t, \xi_i) \Psi_\alpha(\xi_i) \omega_i \quad (10)$$

From the PC expansion (9), it is easy to derive the mean  $E$  and variance  $V$  of the random process. To simplify notations, an orthonormal basis is chosen,  $\|\Psi_\alpha\| = 1 \forall \alpha$ ; the following equalities hold in that case :

$$E(y(x, t)) = y_0(x, t) \quad (11)$$

$$V(y(x, t)) = \sum_{\alpha} y_\alpha^2(x, t) \quad (12)$$

## 4 APPLICATION

Two test-cases are considered in this section to assess the performance of the semi-intrusive method described in Section 2 :

- the steady shocked flow in a convergent-divergent nozzle, of fixed (deterministic) geometry :

$$A(x) = \begin{cases} 1 + 6(x - \frac{1}{2})^2 & \text{for } 0 < x \leq \frac{1}{2} \\ 1 + 2(x - \frac{1}{2})^2 & \text{for } \frac{1}{2} < x \leq 1 \end{cases}$$

with fixed (deterministic) boundary conditions (subsonic inlet flow with a stagnation pressure  $p_0 = 2$  bar and a stagnation temperature  $T_0 = 300$  K, subsonic outlet flow with  $p_e = 1.6529$  bar yielding an exact shock position at  $x = 0.75$  in the nozzle divergent) but an uncertain heat coefficient ratio  $\gamma$ . The random parameter  $\omega = \gamma$  varies within the range  $[1.33, 1.47]$ , following various choices of pdf (uniform, Gaussian and discontinuous) described below.

- the Sod shock tube ( $x \in [0, 1]$ ) with fixed heavy and light fluid properties (deterministic initial states), a fixed heat coefficient ratio  $\gamma = 1.4$  in the perfect gas equation of state but an uncertain position  $x_d$  of the diaphragm initially separating the heavy and light fluids :

$$\begin{pmatrix} \rho^0(x) \\ \rho^0(x)u^0(x) \\ E^0(x) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 2.5 \end{pmatrix} \text{ if } x \leq x_d, \quad \begin{pmatrix} \rho^0(x) \\ \rho^0(x)u^0(x) \\ E^0(x) \end{pmatrix} = \begin{pmatrix} 0.125 \\ 0 \\ 0.25 \end{pmatrix} \text{ otherwise}$$

The initial position of the diaphragm is such that  $x_d = 0.5 + 0.05\omega$  where the stochastic parameter  $\omega \in [-1, 1]$  is described by various pdf (uniform, Gaussian, discontinuous).

- The random parameter  $\omega$  (defining either the heat ratio or the diaphragm initial position) ranges between  $\omega_{min}$  and  $\omega_{max}$ ; the interval  $[\omega_{min}, \omega_{max}]$  is mapped onto  $[a, b]$  by a linear transformation and the pdf on  $[a, b]$  is either :
  - uniform with  $\omega \in [a, b] = [0, 1]$ ,
  - “Gaussian”, with the density given by  $f(x) = \frac{1}{M}e^{-\frac{\omega^2}{2}}1_{[-2,2]}$ , the constant  $M$  chosen so as to normalize the density and  $[a, b] = [-2, 2]$ .
  - discontinuous on  $[a, b] = [0, 1]$  with a density defined by :

$$f(\gamma) = \frac{1}{M} \times \begin{cases} \frac{1 + \cos(\pi x)}{2} & \text{if } x \in [0.5, 1] \\ 10 + \frac{1 + \cos(\pi x)}{2} & \text{if } x \in [0, 0.5] \\ 0 & \text{else} \end{cases} \quad (13)$$

and  $M = \frac{11}{2}$  to ensure normalization.

#### 4.1 Nozzle flow with uncertain $\gamma$

The two stochastic methods previously described, SI (semi-intrusive) and PC (Polynomial Chaos) are used to compute statistic solutions of a supersonic nozzle. 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 mean  $\gamma$  is 1.4, and a maximal variation of 5% is considered.

Different pdf are used for  $\gamma$ , *i.e.* uniform and Gaussian in order to compare SI and PC, and the discontinuous pdf (13) to demonstrate the flexibility offered by the SI method. After a study on the grid convergence, the 1D physical space is divided in 201 points (with the normalized geometric domain that varies from 0 to 1). 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 probabilistic space discretization varies from 5 to 160 points (5, 10, 20, 40, 80, 160), while the polynomial order varies from 2 to 5. Next, the stochastic solutions are compared computing the mean and the variance of the Mach number and pressure distributions along the nozzle using various choices of pdf for  $\gamma$ . Finally, a comparison in terms of computational cost is performed. In Figure 1, the mean solutions of Mach number and the pressure along the 1D nozzle are reported, where the mean stochastic solutions are computed with the SI method using 160 points in the probabilistic space and the PC method using a 5th order polynomial, with  $\gamma$  described by a uniform pdf ( $\gamma$  varying between 1.33 and 1.47). As can be observed in figure 1, the mean 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  $x = 0.5$ ), followed by a subsonic flow behind the shock with decreasing speed. The mean solutions computed by the two UQ methods are coincident. The same trend is obtained if a Gaussian pdf is considered for  $\gamma$  (the figure is not reported for brevity). Next the standard deviation of the Mach num-

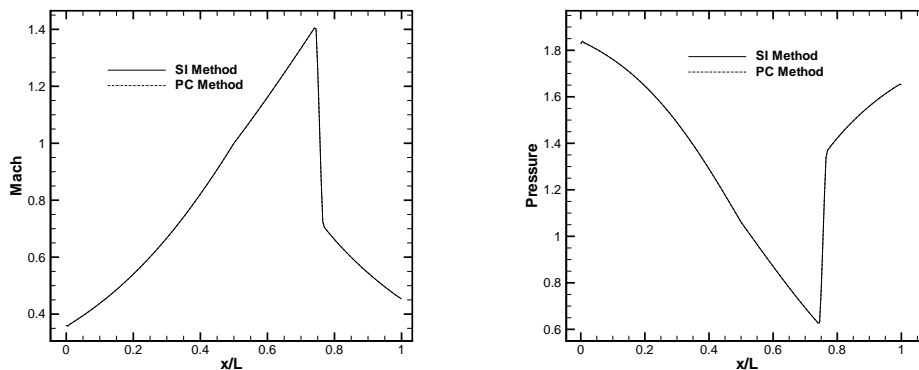


Figure 1: Nozzle flow with uncertain  $\gamma$  (uniform pdf). Computed mean distribution for the Mach number (left) and the static pressure (right) using the semi-intrusive method with 160 points in the probabilistic space and the PC method with a 5th order polynomial.

ber is computed along the nozzle by using different refinement levels for the probabilistic space in the case of the SI method (Figure 2) and different polynomial order in the case of the PC method (Figure 3), always keeping a uniform pdf for  $\gamma$ . In Figure 2, it is shown

that a 10-point discretization of the probabilistic space is sufficient to obtain a converged solution. A close-up on the shock region indicates very small differences between a 10-point and a 40-point discretization but a perfect match between this latter and the finest 160-point discretization. When analyzing the PC method in Figure 3, the solutions seem very similar for different polynomial orders; however, a closer observation of the shock region leads to conclude the maximal standard deviation is not properly estimated as long as the highest-order (here 5th order) polynomial is used. In Figure 4 and Figure

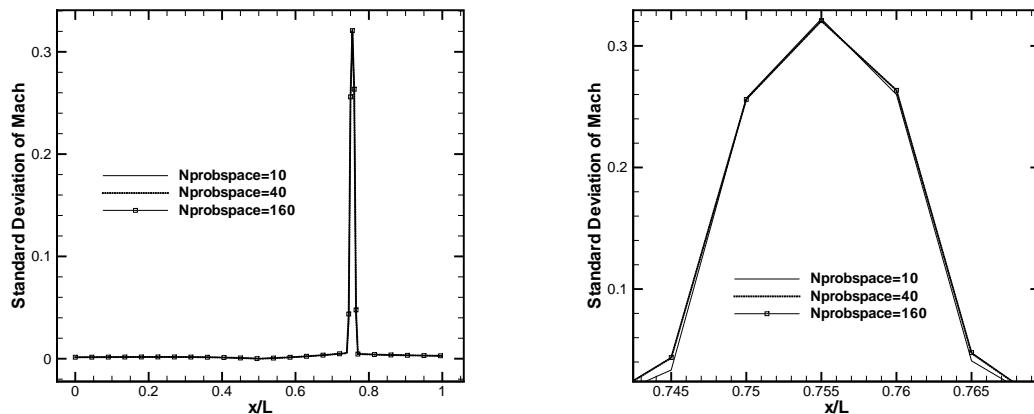


Figure 2: Nozzle flow with uncertain  $\gamma$  (uniform pdf). Convergence study for the standard deviation on the Mach number distribution computed using the semi-intrusive method.

5, the standard deviation of the Mach is reported along the nozzle for an uniform pdf and a Gaussian pdf respectively. For what concerns the uniform pdf, 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. If a Gaussian pdf is considered (Figure 5), there is a stronger variation near the shock and the difference in the maximal standard deviation increases up to 12%. The stochastic estimation remains globally very similar for the newly proposed SI approach and the well-established PC method, which allows to validate the SI method results for the case of a uniform and Gaussian pdf on  $\gamma$ . It is interesting to show the kind of innovative contribution the SI method can bring with respect to the PC method. To this end, in figure 6 the standard deviation of Mach is reported along the nozzle when the discontinuous pdf (13) is considered. Note that choosing (13) to describe the random variable  $\gamma$  introduces no change whatsoever in the application of the SI method (while the PC method can no longer be used). The standard deviation of the Mach number distribution computed for this discontinuous pdf is plotted in Fig. 6 for several levels of discretization refinement in the probabilistic space : here again the result can be considered as almost converged with

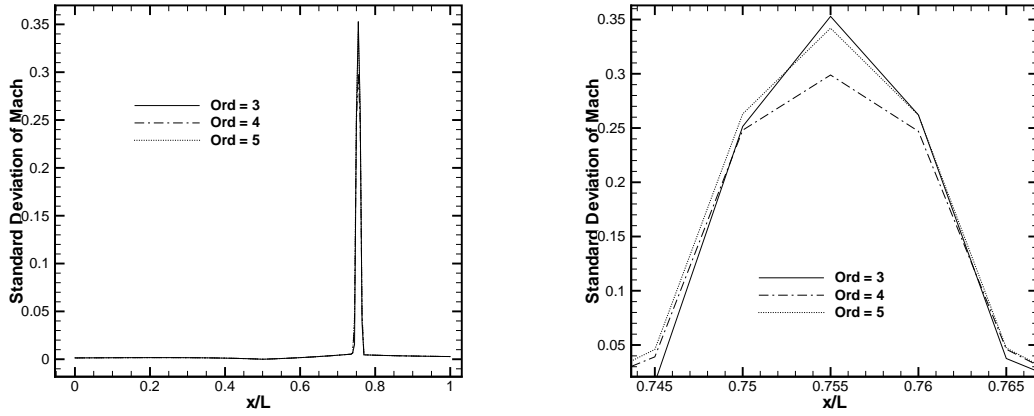


Figure 3: Nozzle flow with uncertain  $\gamma$  (uniform pdf). Convergence study for the standard deviation on the Mach number distribution computed using the NIP method.

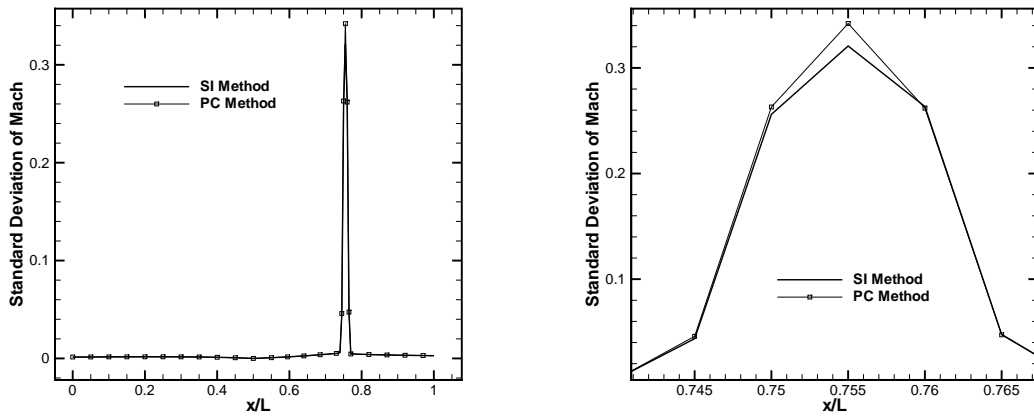


Figure 4: Nozzle flow with uncertain  $\gamma$  (uniform pdf). Standard deviation for the Mach number distribution. Left : global view; right : close-up on the shock region.

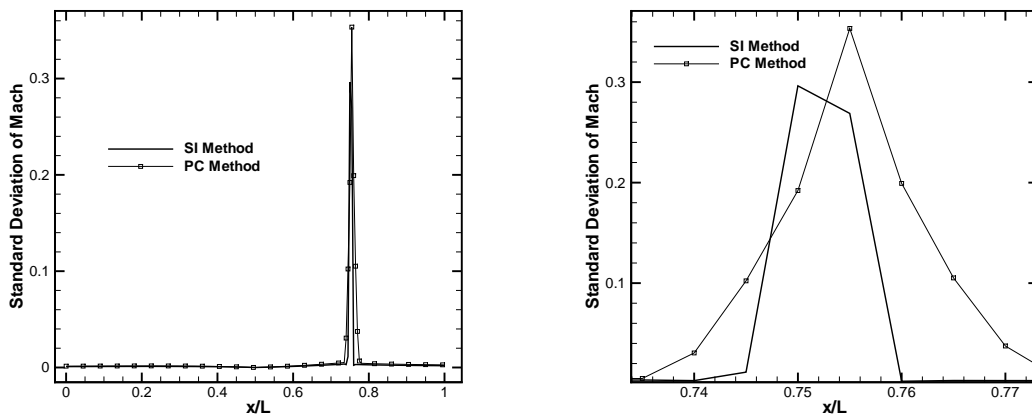


Figure 5: Nozzle flow with uncertain  $\gamma$  (Gaussian pdf). Standard deviation for the Mach number distribution. Left : global view; right : close-up on the shock region.

no more than a 10-point discretization and fully converged with a 40-point discretization. To conclude this first comparison, let us estimate the respective computational cost of the

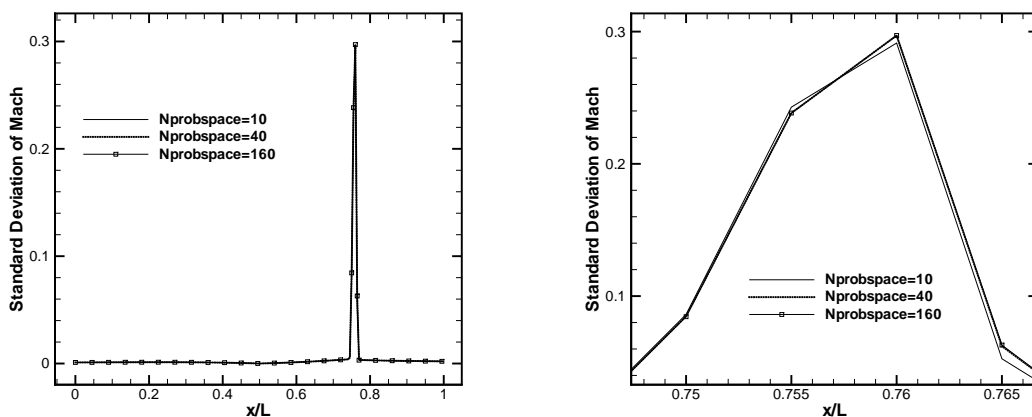


Figure 6: Nozzle flow with uncertain  $\gamma$  (discontinuous pdf). Convergence study for the standard deviation on the Mach number distribution computed using the semi-intrusive method.

SI and PC methods. The computational cost of a single classical deterministic simulation is supposed to be equal to unity. Since, for the PC method, it is necessary to perform  $(order + 1)$  deterministic simulations (in the case of 1 uncertainty), the resulting cost for a 5th order polynomial - required to achieve a converged value of the variance in the shock

region- is 6. With the SI method the computational cost is estimated as nearly two times the number of points discretizing the probabilistic space. Since 10 points are found to be sufficient in order to obtain a converged solution, the cost of the SI method can be estimated as 20 for the problem studied. In conclusion, for the nozzle case, the cost of the SI method is about three times the cost of the PC method. It should be pointed out again, however, the use of the SI method is not restricted to specific choices of pdf for the random variable.

## 4.2 UNCERTAIN SHOCK TUBE

The uncertain Sod shock tube previously described has been analyzed in [12] with a 200-point discretization in the physical space and an intrusive PC method using a 11th-order polynomial; the random parameter  $\omega$  defining the uncertain diaphragm position is described by a uniform pdf. Figure 7 is taken from reference [12] (page 2463, figure 15) and displays the computed distributions for the mean density and its variance. The scale on the left (resp. on the right) corresponds to the mean density (resp. the density variance); hence the density variance  $\sigma$  varies in the range  $[0, 0.014]$ . This same problem

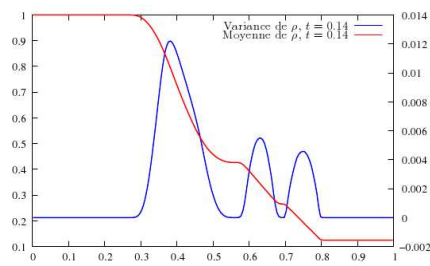


Figure 7: Mean and standard deviation for the uncertain interface problem. Figure taken from [12], page 2463. The mean scale is on the left, the deviation scale is on the right.

has been computed with the SI method, using also 200 points in the physical space and a uniform distribution with 5, 10, 20, 40 and 80 regularly spaced points in the random space so as to analyze the convergence of the method. The scheme relies on a Roe solver with flux limiting and a superbee limiter; the random reconstruction uses the ENO-like procedure described in Section 2. The results are displayed in Figure 8 : the computed mean distribution and its variance can be considered as converged when 20 points are used in the random space. The results are in very good agreement with those obtained in [12] and displayed in Fig.7. A detailed comparison in term of costs is hard to perform because a rather sophisticated solver is used in [12], whose unit cost remains unknown (but is probably larger than the unit cost of the Roe scheme with superbee limiter and ENO-like procedure used in the SI approach). An upper bound can be however estimated assuming the same unit cost for a deterministic calculation and proceeding as in the previous uncertain nozzle flow : with a 11th-order polynomial the cost of the PC approach

is at least 12 while the cost of the SI approach would be  $2 \times 20 = 40$ . A factor 3 (at most) exists between the SI method and the (intrusive) PC method. The great advantage of the proposed SI approach is its ability to deal with general pdf in a highly flexible way : therefore, keeping numerical ingredients unchanged, we proceed to analyze the uncertain shock tube problem with a Gaussian pdf and a discontinuous pdf. The random

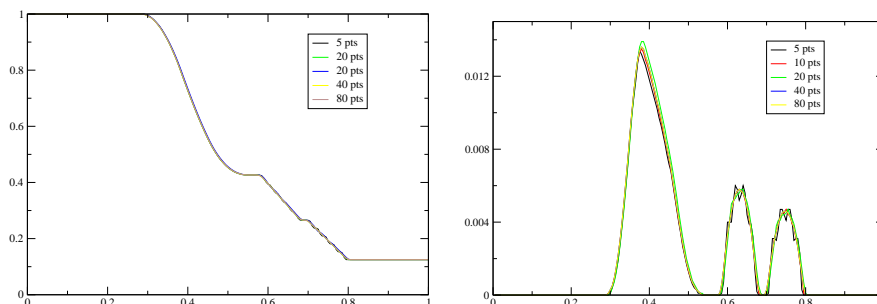


Figure 8: Shock tube with uncertain initial membrane position described by a uniform pdf. Convergence study for the mean density distribution (left) and the standard deviation of the density distribution (right) computed using the semi-intrusive method.

variable  $\omega$  is now described by a Gaussian pdf with 0 mean and variance equal to unity. The convergence of the method is again quite fast, with results that can be considered as converged when 20 points are used to discretize the random space. The use of the

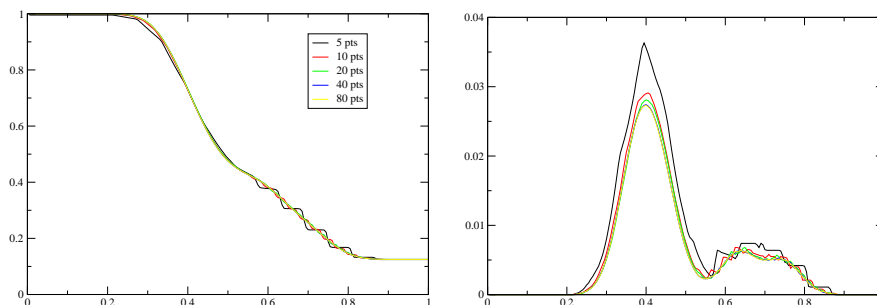


Figure 9: Shock tube with uncertain initial membrane position described by a Gaussian pdf. Convergence study for the mean density distribution (left) and the standard deviation of the density distribution (right) computed using the semi-intrusive method.

discontinuous pdf (13) yields the results displayed in Fig. 10 which, again, illustrate the fast convergence of the method. We have also computed and plotted the solution  $U(x, t, \omega)$  for each case. With moving discontinuities and because of the tensorisation, the reconstruction on the random variable crosses zones where the solution is discontinuous; a centered reconstruction would not allow in that case to get correct values and the ENO

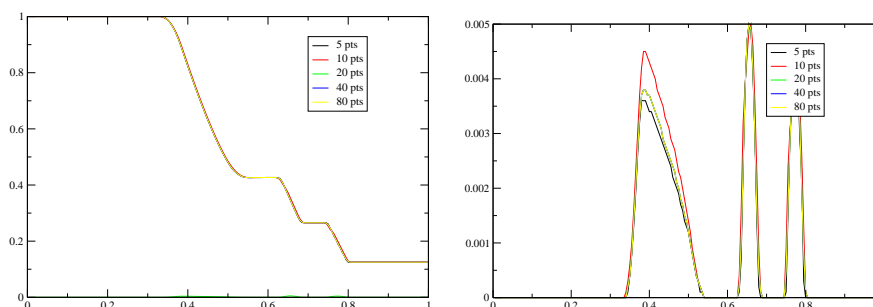


Figure 10: Shock tube with uncertain initial membrane position described by a discontinuous pdf. Convergence study for the mean density distribution (left) and the standard deviation of the density distribution (right) computed using the semi-intrusive method.

reconstruction is essential to obtain an accurate solution. An example of plot for  $U(x, t, \omega)$  is displayed in Figure 11

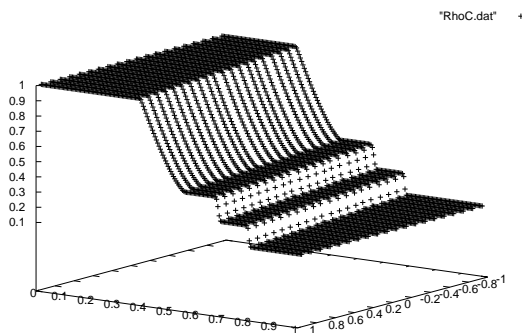


Figure 11: Response surface for the density of the Sod shock tube problem with uniform distribution on the initial diaphragm position.

## 5 CONCLUSION AND FUTURE WORK

We have compared well-established non-intrusive and intrusive PC methods with an original semi-intrusive method inspired by standard reconstruction methods used in the context of finite volume methods. The test cases selected for comparison are a steady nozzle flow problem and a shock tube, respectively described by the quasi-1D or 1D Euler equations. Several choices of pdf have been investigated for the single random parameter retained at this stage. In both cases, SI and PC methods yield results which are very similar if not identical.

The main difference between the SI and PC methods is on the type of pdf that can be

handled. The PC methods need the knowledge of the Gaussian points associated to the multivariate polynomials  $\Psi_\alpha$ ; it is not easy to get that information in general. The SI method can handle *a priori* any type of pdf at the expense of a generally higher computational cost.

The demonstration of interest of the SI method having been successfully performed, our efforts shall focus on the computational cost issue. In this paper, the SI method uses a uniform discretization of the random space. The cost can certainly be diminished by using sparse grid methods, but they need to be adapted to this SI technique. Extensions to multidimensional problems and to problems involving more uncertainties is under way. We also wish to apply the method to flow problems where the real experimental data are described by arbitrary pdf in order to fully exploit the remarkable flexibility of the proposed SI approach.

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