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Numerical investigation on the Total Sensitivity Index influence in the solution of stochastic partial differential equations

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Numerical investigation on the Total Sensitivity Index influence in the solution of stochastic partial differential equations

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Abstract: In the present work a criterion on the reduction of the stochastic dimensions has been investigated in the context of the stochastic partial differential equations. Three different types of equations have been analyzed: elliptical, parabolic and an hyperbolic. For each equation, both mean and variance have been computed on some scalar output of interest. The complete and the reduced models have been compared in terms of statistical moments. The validity and the efficiency of a criterion based on TSI index has been investigated, and an error correlation has been found between the error on the variance and the TSI, that will be validated in a future work for more complex equations.

Key-words: ANOVA analysis, PDE, uncertainty, TSI, stochastic dimensions reduction

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Analyse et étude de l'influence du "Total Sensitivity Index" dans la solutions des équations stochastiques aux dérivées partielles

Résumé : Dans ce rapport nous avons étudié un critère pour la réduction des dimensions stochastiques dans le contexte des équations aux dérivées partielles. On a pris en compte trois types différentes d'équations : elliptiques, paraboliques et hyperboliques. Pour chaque équation, la moyenne et la variance des quelques outputs spécifiques ont été calculées. Les modèles complétés et réduits ont été comparés en terme de moments statistiques. On a estimé la précision et l'efficacité de ce critère basé sur le TSI, et on a trouvé une corrélation sur l'erreur permettant de lier l'erreur sur la variance et le TSI, ce qui sera validé dans le futur sur des équations plus complexes.

Mots-clés : analyse ANOVA, EDP, incertitude, TSI, réduction des dimensions stochastiques

Contents

1	Introduction	5
2	ANOVA decomposition and Sobol indices	5
2.1	Sobol sensitivity indices	6
2.2	TSI computation from PC expansion	6
3	Problem setting	7
4	Numerical results	8
4.1	Elliptic	8
4.2	Parabolic	11
4.3	Hyperbolic	13
5	Conclusions	13
6	Perspectives	13
7	Acknowledgements	14
A	Geometry description of the nozzle	16

List of Figures

1	Errors for the mean and variance for the elliptic problem	10
2	Errors for the mean and variance for the parabolic problem	12
3	Errors for the mean and variance for the hyperbolic problem	14

List of Tables

1	Bounds for the stochastic variables in the elliptic problem	9
2	TSI values for the elliptical complete problem	9
3	Bounds for the stochastic variables in the parabolic problem	11
4	TSI values for the parabolic complete problem	12
5	Bounds for the stochastic variables in the hyperbolic problem	13
6	TSI values for the hyperbolic complete problem	13

1 Introduction

In the last years the interest in the uncertainty quantification (UQ) has motivated an increasing effort in the analysis of stochastic partial differential equations (sPDEs) [1]. The common requirement of the analysis of sPDEs with a large number of parameters has motivated a series of approaches for an efficient reduction of the stochastic dimension of the problems. In this context the major effort has been devoted in the so-called ANOVA decomposition [2] and related techniques. However even if efficient techniques exist for the computation of the ANOVA decomposition terms an open question, related to the choice of most important parameters, remains. Recently Hestaven has proposed a strategy for the dimensional reduction of ordinary differential equations based on the so-called total sensitivity index (TSI) of the variables. The TSI of a given variable measures the contribution of this variable to the variance, including all the interactions with the other variables. The idea proposed by Hestaven is to freeze (replacing with their mean value) all the variables with a TSI inferior to a prescribed threshold. After an extensive experimental campaign, the Hestaven criterion has been calibrated to two percent for ordinary differential equations.

The aim of the present work is to investigate numerically the possibility to extend this criterion to sPDEs. Moreover, the idea is to set up a strategy in order to estimate the error associated to the statistical moments when only the reduced model is used, *i.e.* when all the non-important parameters are frozen, computed with respect to the references values of the complete model.

2 ANOVA decomposition and Sobol indices

Let us consider to have a given equation, or a systems of equations, to solve and to have an output of interest $f = f(\boldsymbol{\xi})$. The output of the system is dependent by d uncertainties parameters ξ_i assumed so that $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_d\} \in \Xi \subset \mathbb{R}^d$. In this work we assume independent distributed random variables $\xi_i \in \Xi_i$ and, consequently, the space Ξ can be obtained by tensorization of their monodimensional spaces, *i.e.* $\Xi_i \subset \mathbb{R}$, $\Xi = \Xi_1 \times \dots \times \Xi_d$.

From the independence of the random variables follows directly $p(\boldsymbol{\xi}) = \prod_i p(\xi_i)$. Assuming $f(\boldsymbol{\xi}) \in L^2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$ then a Sobol unique functional decomposition exists:

$$f(\boldsymbol{\xi}) = \sum_{\mathbf{u} \subseteq \{1, \dots, d\}} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) \quad (1)$$

where \mathbf{u} is a set of integers with cardinality $v = |\mathbf{u}|$ and $\boldsymbol{\xi}_{\mathbf{u}} = \{\xi_{u_1}, \dots, \xi_{u_v}\}$. Each function $f_{\mathbf{u}}$ is computed by the relation[3]:

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \int_{\Xi_{\bar{\mathbf{u}}}} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}_{\bar{\mathbf{u}}}) d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - \sum_{\mathbf{w} \subset \mathbf{u}} f_{\mathbf{w}}(\boldsymbol{\xi}_{\mathbf{w}}) \quad (2)$$

where $\Xi_{\bar{\mathbf{u}}}$ is the space Ξ without the dimensions contained in \mathbf{u} and $\boldsymbol{\xi}_{\bar{\mathbf{u}}}$ is the vector $\boldsymbol{\xi}$ without the variables in \mathbf{u} .

By definition

$$f_0 = \int_{\Xi} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} \quad (3)$$

is the mean of the function $f(\boldsymbol{\xi})$. This functional decomposition is called ANOVA if each of the 2^d elements of the decomposition, except f_0 , verifies for every ξ_i :

$$\int_{\Xi_i} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) p(\xi_i) d\xi_i = 0, \quad \forall i \in \mathbf{u} \quad (4)$$

Directly from eq. 4 follows the orthogonality:

$$\int_{\Xi} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) f_{\mathbf{w}}(\boldsymbol{\xi}_{\mathbf{w}}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \mathbf{u} \neq \mathbf{w} \quad (5)$$

2.1 Sobol sensitivity indices

We are interested in the reduction of the stochastic problem, i.e. computing statistical moments of the function $f = f(\boldsymbol{\xi})$ by reducing the computational cost as much as possible. We propose to identify the important stochastic variables, that must be retained in the stochastic analysis, by means of the so-called total sensitivity indices (TSI) for every random variable ξ_i . Further details on the choice of this criterion will be discussed in the next session.

Employing the ANOVA decomposition it is possible to decompose the variance of $f = f(\boldsymbol{\xi})$:

$$\sigma^2(f) = \sum_{\substack{\mathbf{u} \subseteq \{1, \dots, d\} \\ \mathbf{u} \neq \emptyset}} \sigma_{\mathbf{u}}^2(f_{\mathbf{u}}) \quad (6)$$

where

$$\sigma_{\mathbf{u}}^2(f_{\mathbf{u}}) = \int_{\Xi_{\mathbf{u}}} f_{\mathbf{u}}^2(\boldsymbol{\xi}_{\mathbf{u}}) p(\boldsymbol{\xi}_{\mathbf{u}}) d\boldsymbol{\xi}_{\mathbf{u}} \quad (7)$$

and $\Xi_{\mathbf{u}} = \Xi_{u_1} \times \dots \times \Xi_{u_v}$.

The Sobol sensitivity indices (SI), are defined as:

$$S_{\mathbf{u}} = \frac{\sigma_{\mathbf{u}}^2}{\sigma^2} \quad (8)$$

measuring the sensitivity of the variance due to the v -order ($v = |\mathbf{u}|$) interaction between the variables in $\boldsymbol{\xi}_{\mathbf{u}}$. It is evident that the summation of the $2^d - 1$ Sobol indices is equal to one. The total sensitivity indices measure the sensitivity of each variable (or group of variables) to the overall variance:

$$\text{TSI}_j = \sum_{j \in \mathbf{u}} S_{\mathbf{u}}. \quad (9)$$

2.2 TSI computation from PC expansion

The computation of the Sobol indices is possible using every sample stochastic method (Monte Carlo, quasi-Monte Carlo) but can be done in a very efficient way when a polynomial expansion of the solution is adopted. The idea is to compute the expansion of the solution (truncated) and compute the Sobol indices from the expansion instead of computing them on the real function. Remember the polynomial expansion:

$$f(\boldsymbol{\xi}) = \tilde{f}(\boldsymbol{\xi}) + \mathcal{O}_T = \sum_{k=0}^P \beta_k \Psi_k(\boldsymbol{\xi}) + \mathcal{O}_T, \quad (10)$$

with a number of terms related to the maximum degree of the polynomial reconstruction n_o and the dimension of the system d : $P + 1 = \frac{(n_o+d)!}{n_o!d!}$. For further details on the polynomial chaos techniques see [4]. Each element $f_{\mathbf{u}}$ of the functional decomposition of $f(\boldsymbol{\xi})$ is approximated by the relative term $\tilde{f}_{\mathbf{u}}$:

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) \approx \tilde{f}_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \sum_{k \in K_{\mathbf{u}}} \beta_k \Psi_k(\boldsymbol{\xi}_{\mathbf{u}}), \quad (11)$$

where the set of indices $K_{\mathbf{u}}$ is given by

$$K_{\mathbf{u}} = \left\{ k \in \{1, \dots, P\} \mid \Psi_k(\boldsymbol{\xi}_{\mathbf{u}}) = \prod_{i=1}^{|\mathbf{u}|} \phi_{\alpha_i^k}(\xi_{u_i}), \alpha_i^k > 0 \right\} \quad (12)$$

and $\phi_{\alpha_i^k}(\xi_{u_i})$ are the monodimensional polynomials for every direction ξ_i of degree k chosen with respect to the so-called Wiener-Askey scheme [5].

Thanks to the orthogonality it is possible to obtain directly the variance $\tilde{\sigma}^2(f) = \sigma^2(\tilde{f}) \approx \sigma^2(f)$ and the conditional variance $\tilde{\sigma}_{\mathbf{u}}^2(f_{\mathbf{u}}) = \sigma_{\mathbf{u}}^2(\tilde{f}_{\mathbf{u}}) \approx \sigma_{\mathbf{u}}^2(f_{\mathbf{u}})$ from the following relations:

$$\begin{aligned} \tilde{\sigma}^2(f) &= \sum_{k=1}^P \beta_k^2 \langle \Psi_k, \Psi_k \rangle \\ \tilde{\sigma}_{\mathbf{u}}^2(f_{\mathbf{u}}) &= \sum_{k \in K_{\mathbf{u}}} \beta_k^2 \langle \Psi_k, \Psi_k \rangle. \end{aligned} \quad (13)$$

Sobol sensitivity indices follows directly from eq. 13:

$$S_{\mathbf{u}} \approx \tilde{S}_{\mathbf{u}} = \frac{\tilde{\sigma}_{\mathbf{u}}^2(f_{\mathbf{u}})}{\tilde{\sigma}^2(f)} = \frac{\sum_{k \in K_{\mathbf{u}}} \beta_k^2 \langle \Psi_k, \Psi_k \rangle}{\sum_{k=1}^P \beta_k^2 \langle \Psi_k, \Psi_k \rangle} \quad (14)$$

and the total sensitivity index is always defined by the equation 9.

3 Problem setting

In the framework of the PDEs, a generic second order equations, for a scalar variable $u(x, t)$ defined on $[a, b] \times [0, T] \mapsto \mathbb{R}$, reads

$$\omega \frac{\partial u}{\partial t} - \frac{d}{dx} \left(\nu \frac{du}{dx} \right) + \tau \frac{du}{dx} + \sigma u = f(x, t), \quad (15)$$

correlated by the oportune boundary and initial conditions. For the sake of simplicity, in the following, only Dirichlet boundary conditions are adopted

$$\begin{cases} u(a, t) &= \alpha \\ u(b, t) &= \beta \\ u(x, 0) &= u_0(x), \end{cases} \quad (16)$$

while the initial condition is a polynomial function of x .

In this work all the types of PDE have been investigated. For the elliptic and parabolic equation we solved the scalar equations obtained directly from 20

choosing opportunely the coefficients and setting the boundary, i.e. minimum and maximum values allowed, for the remaining parameters, while for the hyperbolic equation we solved the compressible nozzle flow problem. In the first two cases the output of the system is identified as

$$F(T) = \frac{\int_a^b u(x, T) dx}{\int_a^b dx} \quad (17)$$

while in the third case, the hyperbolic one, the output of the system is chosen as the shock position in the divergent part of the nozzle.

For the output $F(T)$ the expected value and its variance is then computed by the following relations

$$\begin{aligned} \mathcal{E}(T) &= \int_{\Xi} F(T) d\Xi \\ \text{Var}(T) &= \int_{\Xi} (F(T) - \mathcal{E})^2 d\Xi. \end{aligned} \quad (18)$$

In the numerical section §4 the error with respect to the complete problem will be computed according to the following definitions:

$$\begin{aligned} \text{err}_{\text{mean}} &= \frac{|\mathcal{E} - \mathcal{E}^r|}{\mathcal{E}} 100 \\ \text{err}_{\text{variance}} &= \frac{|\text{Var} - \text{Var}^r|}{\text{Var}} 100, \end{aligned}$$

where the symbol $()^r$ represents the reduced problem.

4 Numerical results

In this section we present the numerical results obtained for three sPDEs. In this work only uniform pdf are taken into account. Anyway, remark that the proposed analysis can be easily extended to a pdf of whatever form. First the complete problem, *i.e.* considering all the stochastic dimensions, is analyzed with a quasi-Monte Carlo method with 400000 deterministic runs: this solution is assumed to be the reference solution. The Sobol indices have been then computed, as explained in §2, with PC. Proceeding progressively, the problem is reduced freezing the unimportant variables until the monodimensional problem. For every reduced problem the error on the expected value and the variance is computed and correlated to the total amount of TSI relatively to the non-frozen stochastic dimensions.

4.1 Elliptic

The elliptic equation is obtained from 17 setting

$$\omega = 0, \quad \nu = 1, \quad \tau = 1, \quad a = 0 \quad \text{and} \quad b = 1. \quad (19)$$

If we indicate with the symbol $'$ the derivative with respect to x the equation reads:

$$u'' + \sigma u = f(x) = \gamma \cos \delta x$$

with the boundary conditions

$$\begin{cases} u(0) = \alpha \\ u(1) = \beta \end{cases} \quad (20)$$

For this equation the exact solution can be expressed as

$$u(x) = c_1 e^{-\sqrt{\sigma}x} + c_2 e^{\sqrt{\sigma}x} + \frac{\gamma}{\delta^2 + \sigma} \cos \delta x$$

and the coefficient can be computed imposing the boundary conditions and resolving the linear system

$$\begin{bmatrix} 1 & 1 \\ e^{-\sqrt{\sigma}} & e^{\sqrt{\sigma}} \end{bmatrix} \begin{Bmatrix} c_1 \\ c_2 \end{Bmatrix} = \begin{Bmatrix} \alpha - \frac{\gamma}{\delta^2 + \sigma} \\ \beta - \frac{\gamma}{\delta^2 + \sigma} \cos \delta \end{Bmatrix}.$$

In the table 1 the bounds for the stochastic parameters are reported.

Variable	Min	Max	Mean	Uncertainty
σ	0.01	0.05	0.03	$\pm 66.67\%$
γ	8	12	10	$\pm 20\%$
δ	0.5	1.5	1.0	$\pm 50\%$
α	0.0	5.0	2.5	$\pm 66.67\%$
β	3.0	8.0	5.5	$\pm 45.55\%$

Table 1: Bounds for the stochastic variables in the elliptic problem

In the table 2 the values for the total sensitivity index, calculated as shown in §2, are reported for the complete problem.

Variable	TSI
σ	2.276639e-05
γ	6.223883e-03
δ	4.134716e-03
α	4.948589e-01
β	4.948210e-01

Table 2: TSI values for the elliptical complete problem

It is evident from the table 2 that the boundary values (α and β) are the most important sources of uncertainties, while σ is the less influent parameter. If we proceed freezing, in the order, σ , δ , γ and β we can compute the errors, for the expected value and for the variance, with respect to the complete problem.

The total amount of TSI for each uncertainty in the reduced problem, is then computed as a percentage of the total amount of TSI (of the complete problem):

$$\%T SI = \frac{\sum_i T SI_i}{\sum_j T SI_j} 100, \quad (21)$$

where the index i runs on the non-frozen variables, while j runs on all the variables of the complete problem.

For all the problems, 400000 deterministic runs have been employed. In the figure 1 the errors for the expected value (a) and variance (b) are reported.

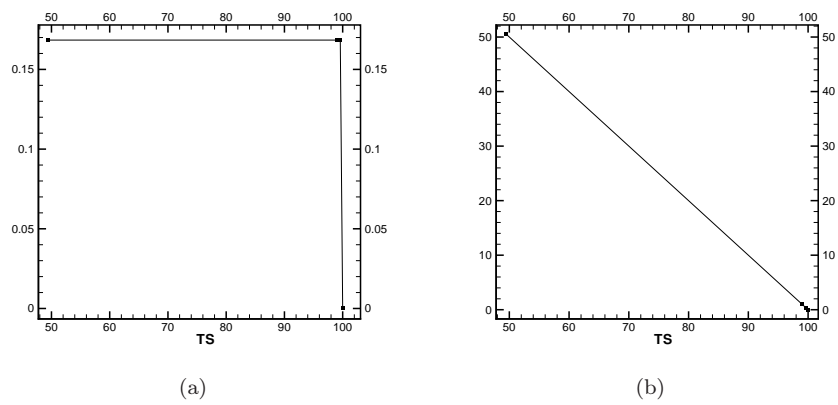


Figure 1: Errors for the mean (a) and variance (b) as function of the total amount of TSI with respect to the complete elliptic problem.

4.2 Parabolic

The parabolic equation is obtained from 17 setting

$$\omega = 1, \quad \sigma = 0, \quad \tau = 0, \quad a = 0 \quad \text{and} \quad b = \gamma, \quad (22)$$

with the source term $f(x, t) = 0$. The final equation becomes, for $x \in [0, \gamma]$ and $t \in [0, T]$,

$$\frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial x^2} = 0,$$

with boundary and initial conditions:

$$\begin{cases} u(0, t) &= 0 \\ u(\gamma, t) &= 0 \\ u_0(x, t) &= Ax^2 + Bx + C. \end{cases} \quad (23)$$

In the following results the final time is chosen as $T = 0.1$. The equation 23 can be solved employing a modal solution:

$$u(x, t) = \sqrt{\frac{2}{\gamma}} \sum_{i=1}^{+\infty} C_i \sin\left(\frac{\pi x i}{\gamma}\right) e^{-\frac{\pi^2 i^2 \nu t}{\gamma^2}}$$

with the coefficients C_i obtained after imposing the initial conditions:

$$C_i = \sqrt{\frac{2}{\gamma}} \int_0^\gamma \sin\left(\frac{\pi x i}{\gamma}\right) u_0(x) dx.$$

In the present work, the series is truncated and a preliminary study of convergence has been performed, not reported here for brevity, in order to asset the modal convergence of the solution.

In the table 3 the bounds for the five stochastic parameters are reported.

Variable	Min	Max	Mean	Uncertainty
ν	0.02	0.08	0.05	$\pm 60\%$
γ	0.7	1.3	1.0	$\pm 30\%$
A	2.0	4.0	3.0	$\pm 33.33\%$
B	-3.0	-1.0	-2.0	$\pm 50\%$
C	0.0	2.0	1.0	$\pm 100\%$

Table 3: Bounds for the stochastic variables in the parabolic problem

The complete problem has been solved with 400000 deterministic runs and the Sobol indices have been computed as reported in §2. In the table 4 TSI indices are reported for the complete problem.

The parameter ν is nearly not influent, while C is the most influent. Note that a variable with a narrow variability can be more influent than a variable with a larger one. In this case we proceeded freezing in the order ν , A , γ and B .

In the figure 2 the errors for the expected value (a) and variance (b) are reported.

Variable	TSI
ν	4.675377e-03
γ	9.337960e-02
A	8.078432e-02
B	1.751148e-01
C	6.650567e-01

Table 4: TSI values for the parabolic complete problem

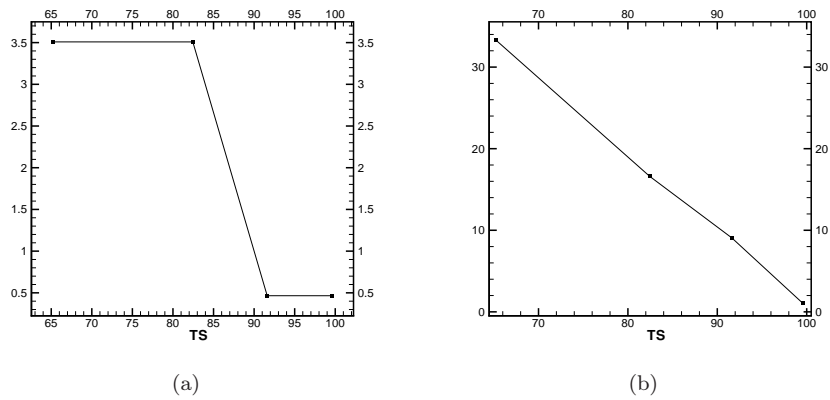


Figure 2: Errors for the mean (a) and variance (b) as function of the total amount of TSI with respect to the complete parabolic problem.

4.3 Hyperbolic

For the hyperbolic case we considered a nozzle problem, for which an analytical solution is possible.

The five parameters in this case are the polytropic coefficient of the gas γ , the ratio between the external pressure and the reservoir pressure P_e/P_0 , the ratio of the exit and throat area A_e/A_t and two coefficients used in the geometrical representation of the nozzle shape α and β . A complete description of the nozzle shape parametrization is given in Appendix A.

In the table 5 the bounds for the five stochastic parameters are reported.

Variable	Min	Max	Mean	Uncertainty
γ	1.3	1.5	1.4	$\pm 7.142\%$
P_e/P_0	0.8181855	0.8347145	0.8264500	$\pm 1.0\%$
A_e/A_t	1.4	1.6	1.5	$\pm 6.667\%$
α	0.00	0.01	0.005	$\pm 100\%$
β	0.4	0.6	0.5	$\pm 20\%$

Table 5: Bounds for the stochastic variables in the hyperbolic problem

In this case the TSI for the five parameters are reported in the table 6.

Variable	TSI
γ	1.701168e-01
P_e/P_0	1.813889e-01
A_e/A_t	5.359230e-01
α	6.193598e-03
β	1.240211e-01

Table 6: TSI values for the hyperbolic complete problem

The non-important parameter in this case is α while the most influent is the ratio A_e/A_t . We proceed freezing progressively α , β , γ e P_e/P_0 obtaining the errors for the expected value and variance, reported in figure 3.

5 Conclusions

In all the configurations that we studied, the error on the expected value is always inferior to the error on the variance. Moreover, we remark that the error on the variance is roughly a linear function of the $\%TSI$. This result can be used to obtain a confidence estimation when a reduced model is used in order to reduce an high-dimensional stochastic problem.

6 Perspectives

This work, focused on the analysis of a TSI criterion for a stochastic dimensional reduction, is part of a wider research that aims to develop efficient strategy for the robust optimization under uncertainties. We hope to apply soon this study to more complex configurations.

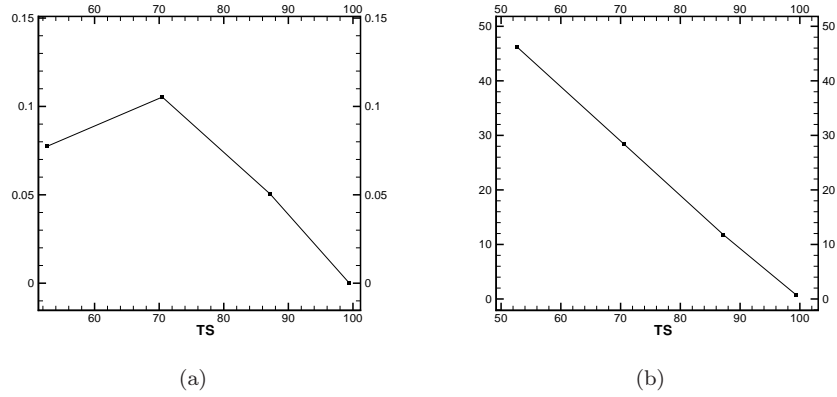


Figure 3: Errors for the mean (a) and variance (b) as function of the total amount of TSI with respect to the complete hyperbolic problem.

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A Geometry description of the nozzle

We report here the equations used for the geometrical description of the nozzle. The nozzle is a classical de Laval configuration.

$$\begin{aligned}y_c &= 1 + 0.75x^2 \\y_d &= 1 + \alpha x + \beta x^2 + \gamma_d x^3 \quad \text{with} \quad \gamma_d = A_e/A_t - 1 - \alpha - \beta\end{aligned}$$



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