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NUMERICAL METHODS FOR UNCERTAINTY PROPAGATION IN HIGH SPEED FLOWS

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Abstract. *Shock-dominated flows are strongly sensitive to uncertainties and exhibit highly non-linear responses to perturbations. We study two classical problems in unsteady compressible fluid dynamics: the Riemann problem and the Woodward-Colella forward step flow. Assuming that uncertainties are present in the initial and boundary conditions, the objective is to characterize their effect on the solution. The problem is formulated in a probabilistic setting and stochastic expansion methods are used. We show that high-order expansions are required to capture the correct statistical moments of the solution because convergence is hindered by the presence of sharp flow field structures. We also show how both intrusive and non-intrusive versions of the stochastic expansion method suffer from this slow convergence behavior.*

1 INTRODUCTION

The characterization of uncertainties in high speed shock-dominated flows is challenging because of the presence of sharp features and strongly non-linear system responses. Limited variability in the operating conditions can lead to sharp changes in the output, with distinctly modified physical behavior and vastly different flow fields. Consider for example the supersonic inviscid flow over a ramp; a small change in the Mach number can *transition* the system from an attached oblique shock scenario to a detached normal shock one if the critical turning angle is exceeded [2].

Uncertainty quantification (UQ) aims at determining rigorously the impact of limited knowledge and variability in the problem definition on selected quantities of interest. We consider a probabilistic framework, in which the input uncertainties are represented as random variables, and the objective of the UQ analysis is to determine the probability distributions (or some statistical moments) of the output. From a mathematical perspective the original (deterministic) mathematical problem is cast in a stochastic framework.

Sampling methods such as Monte Carlo have been traditionally applied to solve such stochastic problems; realizations are drawn from input probabilistic distributions and the ensemble of the corresponding solutions is interpreted as an empirical distribution of the random solution allowing to generate statistical outputs [1]. The flexibility and simplicity of this approach has led to its wide use, but its slow convergence limits its applicability for large-scale problems, motivating research in other methodologies.

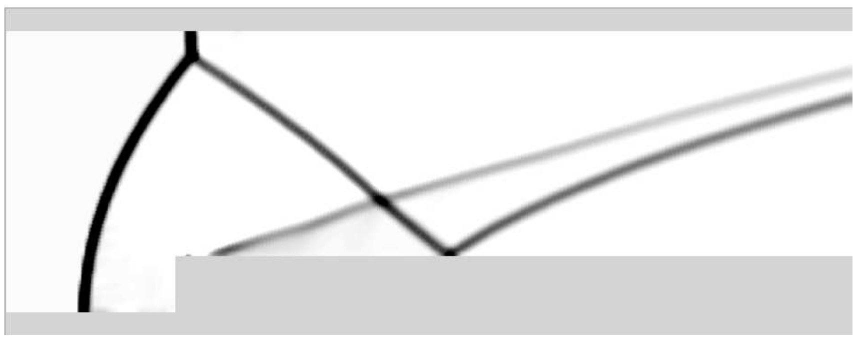

Figure 1: Woodward and Colella [8] forward facing step problem. Velocity divergence field. Nominal (deterministic) solution corresponding to Mach = 2.75.

Recently several approaches based on stochastic expansions of the solution in the space spanned by the uncertain variables have been introduced [6]. Polynomial chaos methods are particularly attractive because they allow for a reformulation of the stochastic problem as a set of (coupled) deterministic problems that are amenable to analysis [10, 11]. On the other hand, this approach requires modification of the existing computational tool: is an intrusive approach. An alternative class of methods, namely stochastic collocation approaches, share a similar mathematical structure but allow for reuse of existing deterministic codes [5]

Stochastic expansion methods exhibit exponential convergence and, therefore, can be extremely effective when compared to Monte-Carlo-type approaches. This advantage is a direct consequence of the expected *smoothness* of the system response with respect to variability of the input quantities [10, 5]. As mentioned before it is clear that in problems characterized by highly non-linear responses and sharp transitions, stochastic expansions methods can experience difficulties. In this paper, we explore the application of such methods to unsteady high-speed compressible flow problems governed by the Burgers and Euler equations. We illustrate how the presence of shock waves hinders the convergence of the approach, and discuss why both intrusive and non-intrusive formulations suffer from this problem.

2 UNCERTAINTY IN SHOCK-DOMINATED FLOW

Consider the supersonic flow over a forward step in a channel, the classical Woodward-Colella test [8]. The objective is to characterize the position of the shock waves at a particular instant of time after the impulsive start of the channel. In Fig. 1 the nominal solution obtained for an inflow Mach number of 2.75, at time $t = 2$ on a grid consisting of $\approx 16,000$ elements is reported. The numerical solution is obtained using a second-order spatial discretization and an explicit Runge-Kutta integration [9]. The velocity divergence is used as a scalar field indicator to expose the shock location.

We assume that the inflow Mach number is uncertain, specified as a uniform random variable defined over the interval $[2.5, 3.0]$. In the UQ analysis, we will consider the output of interest to be the statistical average (mean) of the velocity divergence.

A straightforward application of Monte Carlo (MC) method leads to the results shown in Fig.2, an ensemble averaging of 1000 solutions obtained for randomly chosen Mach numbers in the above mentioned interval.

Figure 2: Woodward and Colella [8] forward facing step problem. Mean velocity divergence field. corresponding to an uncertain input Mach number [2.5 : 3.0]. Monte Carlo sampling based on 1000 realizations.

It is obvious from the comparison of Fig. 1 and 2 that the mean effect of the uncertainty in the inflow conditions is to smear the shock wave, an observation reported previously in the literature [7].

In order to simplify the description of the spectral expansion methods, we will discuss now a simplified shock dynamics problem governed by the Burgers equations.

3 A MODEL PROBLEM

We consider the one-dimensional viscous Burgers equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \tag{1}$$

The viscosity is assumed to be small ($\nu = 0.02$) and we are interested in the time-dependent behavior that includes the formation of shocks (or, more precisely, very sharp gradients). The initial conditions are uncertain and assumed to be:

$$u(x,t=0,\xi) = 3\xi exp\left[-\frac{(x-x_0)^2}{30w^2}\right] sin(\beta x) + \alpha\left[tanh\left(\frac{x_0-x}{2w}\right)\right] \quad (2)$$

where $\beta = 5.3$, $w = 0.03$ and $x_0 = 0.5$. The uncertainty is characterized by additive noise described by a single random variable $\xi \in [-1:1]$, distributed non-uniformly in the domain ($x \in [0:1]$). The mean and variance of the initial conditions are reported in Fig. 3. In the absence of uncertainty, $\alpha = 1$ correspond to an initial condition that leads to a shock , while $\alpha = -1$ leads to a smooth solution (expansion fan).

4 STOCHASTIC GALERKIN METHOD

We assume that the solution can be expressed accurately as a Fourier expansion of orthogonal polynomials truncated after $(M+1)$ terms:

$$u(x,t,\xi) \approx u_M(x,t,\xi) = \sum_{i=0}^{M} u_i(x,t)\pi_i(\xi) \quad (3)$$

where π_i are the polynomial basis functions, in this case univariate Legendre polynomials, and u_i are the *unknown* coefficients.

The choice of the Legendre polynomial basis is optimal with respect to a uniform weight function, which corresponds to the uniform random variable ξ [6]. The statistics of the solution are easily computed from the expansion, for example the expectation (mean) is

$$\mathbb{E}[u] \approx \mathbb{E}[u_M] = \langle\sum_{i=0}^{M} u_i\pi_i\rangle = u_0\langle\pi_0\rangle + \sum_{i=1}^{M} u_i\langle\pi_i\rangle = u_0 \quad (4)$$

from the orthogonality of the polynomial basis. The variance is computed as:

$$v = var[u] \approx var[u_M] = \langle(u_M - \mathbb{E}[u_M])^2\rangle = \langle\left(\left(\sum_{i=0}^{M} u_i\pi_i\right) - u_0\right)^2\rangle = \sum_{i=1}^{M} u_i^2 C_i \quad (5)$$

where $\langle\pi_i\pi_j\rangle = C_i\delta_{ij}$ and C_i is only a function of the polynomial basis selected.

The coefficients u_i are computed by inserting the expression (3) in the governing equation:

$$\sum_{i=0}^{M} \frac{\partial u_i}{\partial t}\pi_i + \left(\sum_{j=0}^{M} u_j\pi_j\right)\left(\sum_{i=0}^{M} \frac{\partial u_i}{\partial x}\pi_i\right) = \nu\sum_{i=0}^{M} \frac{\partial^2 u_i}{\partial x^2}\pi_i$$

Multiplying by π_k and integrating over the probability space - Galerkin projection - we obtain a system of $M+1$ coupled and deterministic equations for the coefficients u_k:

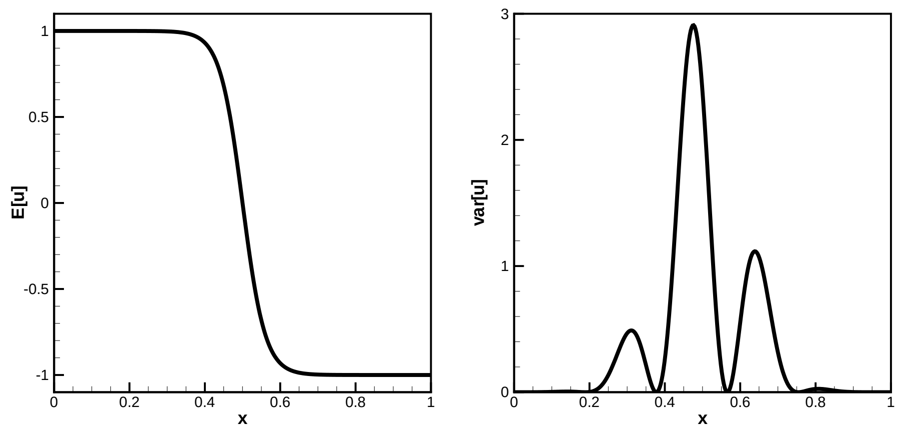

Figure 3: Initial conditions for the uncertain Burgers equation ($\alpha = 1$ in Eq. 2).

$$\frac{\partial u_k}{\partial t} + \sum_{i=0}^{M}\sum_{j=0}^{M} u_i \frac{\partial u_j}{\partial x} C_{ijk} = \nu \frac{\partial^2 u_k}{\partial x^2} \qquad \text{for } k = 0, 1, ..., M. \tag{6}$$

where $\langle \pi_i \pi_j \pi_k \rangle = C_{ijk}$ is only a function of the polynomial basis selected. A similar projection applied to the initial conditions leads to

$$\begin{aligned} u_0(x, t = 0, \xi) &= tanh\left[\frac{x_0 - x}{2w}\right] \\ u_1(x, t = 0, \xi) &= 3exp\left[-\frac{(x - x_0)^2}{30w^2}\right] sin(\beta x) \\ u_k(x, t = 0, \xi) &= 0 \qquad \text{for } k = 2, ..., M. \end{aligned} \tag{7}$$

For the numerical solution of the Eq. 6, we consider a straightforward spatial discretization and an explicit time integration based on a three-step Runge-Kutta scheme. For the ℓ-th node of a spatial grid, the semi-discrete finite difference stencil is written as:

$$\left(\frac{du_k}{dt}\right)^{\ell} = -\sum_{i=0}^{M}\sum_{j=0}^{M} \frac{1}{3}\left(u_i^{\ell-1} + u_i^{\ell} + u_i^{\ell+1}\right)\left(\frac{u_j^{\ell+1} - u_j^{\ell-1}}{x^{\ell+1} - x^{\ell-1}}\right) C_{ijk} + \nu \left(\frac{d^2 u_k}{dx^2}\right)^{\ell} \tag{8}$$

In the following, the approach illustrated above is referred to as polynomial chaos (PC) [6]. It is difficult to determine *a priori* the order of truncation M required to achieve a specified accuracy. One of the objectives of the following examples is to show how the formation of shock waves leads to large approximation errors.

5 STOCHASTIC COLLOCATION APPROACH

An alternative approach that we compare to the PC approach is the stochastic collocation (SC) method [5]. The starting point is the observation that the statistical moments of the uncertain solution are *simply* integrals over the space spanned by the random inputs. It is therefore possible to compute them very effectively using Gauss quadrature. For example the solution mean is:

$$\mathbb{E}[u] = \int_{-1}^{1} u(x,t,\xi) f_\xi d\xi \approx \sum_{i=0}^{M} u(x,t,\xi_i)\omega_i \tag{9}$$

where the abscissa ξ_i are the zeros of the Legendre polynomial of order $M+1$ and the weights ω_i are the integrals of Lagrange polynomials defined at the abscissas. The variance can be computed in a similar way. Again, the choice of the Legendre polynomials is optimal with respect to the uniform measure defined by the input uncertainty ξ.

The advantage of both the MC and the SC approaches is their inherent simplicity; they just require successive solutions of the deterministic problem for fixed values of ξ; this is obviously not the case in the PC approach that requires the development of a modified solution methodology.

It is worth mentioning that both the PC and SC approaches use the Legendre polynomials as a building block and aim at forming an interpolant in the space spanned by the uncertain variables, although in the SC approach this interpolant is never used. The connections between the two approaches – and formal equivalence for linear problems – is explored in detail in [4].

6 COMPUTATIONAL STUDY

The predicted time evolution of the solution statistics for the problem described in Section 3 are compared in Fig. 4-6 for the PC, SC and Monte Carlo methods. Fig. 4 shows that the PC and SC approaches produce *largely equivalent* results independently of the order of expansion, and eventually reproduce the statistics obtained using Monte Carlo sampling (obtained using 10,000 samples). It is worth noting that even with $M = 22$, differences remain noticeable especially in the variance profile. More importantly with low-order expansions (e.g. $M = 3$ and $M = 8$) considerable qualitative discrepancies with respect to the MC results are present.

The shock formation process induces the slow convergence, as illustrated in Fig. 7 where a different initial condition ($\alpha = -1$ in Eq. 2) is considered. In this case, an expansion truncated at $M = 3$ leads to accurate predictions of both the expectation and the variance of the solution.

To investigate in more details the accuracy of PC expansions, we report the time evolution of the mean solution with different polynomial order in Fig. 8. The low-order stochastic expansion ($M = 3$) leads to the emergence of several shocks which mimic the formation of discontinuities in the deterministic problem. On the other hand the solution

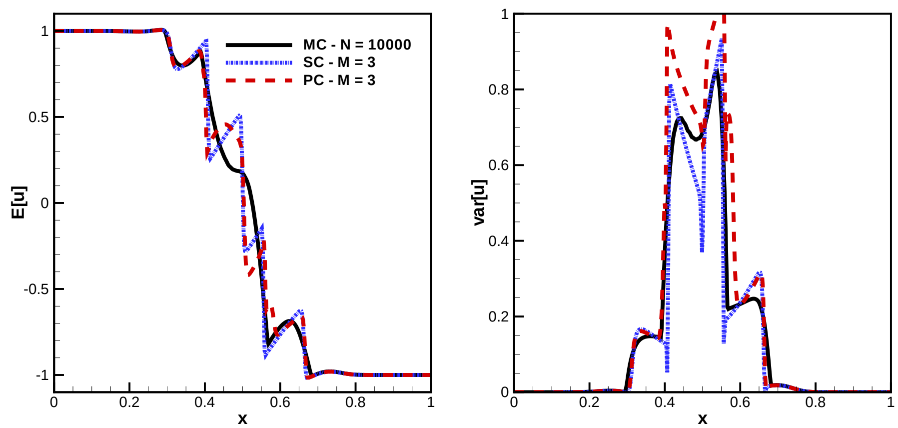

Figure 4: Expected solution and variance of the uncertain Burgers equation, obtained at $t = 0.012$ using Monte Carlo (MC), stochastic collocation (SC) and polynomial chaos (PC). $\alpha = 1$ in Eq. 2. Both PC and SC methods are based on $M = 3$

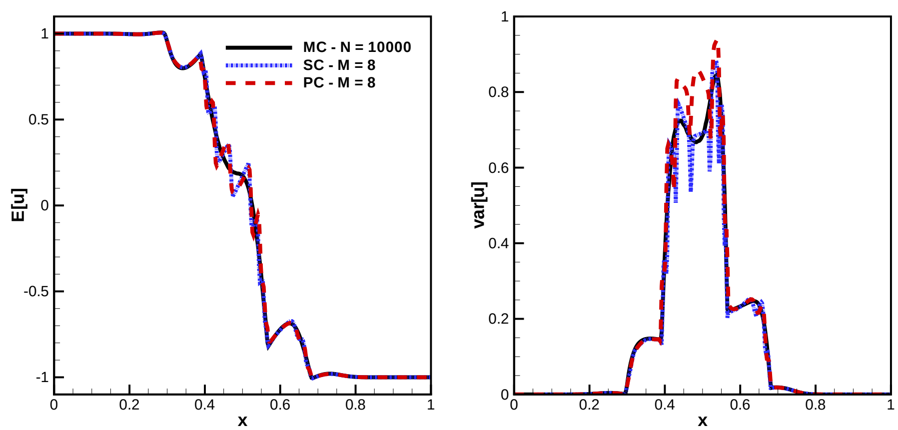

Figure 5: Expected solution and variance of the uncertain Burgers equation, obtained at $t = 0.012$ using Monte Carlo (MC), stochastic collocation (SC) and polynomial chaos (PC). $\alpha = 1$ in Eq. 2. Both PC and SC methods are based on $M = 8$

obtained with the high-order expansion, in accordance to the Monte Carlo computation, remains *smooth*. The explanation of the observed error is related to the approximation introduced to represent the solution. The polynomial chaos order determines the governing equations (6) for the modes of the expansion; specifically the truncation order M determines the size of the linear system and therefore the number of characteristics [11].

Additional insights into the error introduced by the PC truncation can be extracted from Fig. 9, in which the L_∞ error of the mean solution (computed with respect to the

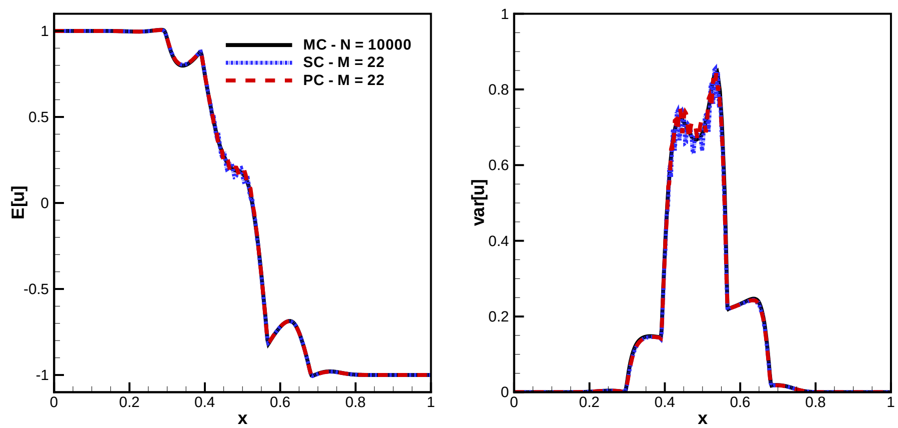

Figure 6: Expected solution and variance of the uncertain Burgers equation, obtained at $t = 0.012$ using Monte Carlo (MC), stochastic collocation (SC) and polynomial chaos (PC). $\alpha = 1$ in Eq. 2. Both PC and SC methods are based on $M = 22$

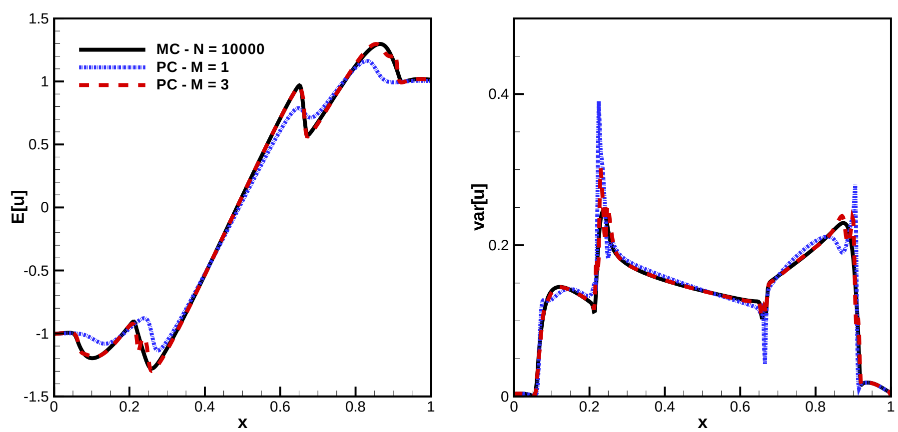

Figure 7: Expected solution and variance of the uncertain Burgers equation, obtained at $t = 0.012$ using Monte Carlo (MC) and polynomial chaos (PC). $\alpha = -1$ in Eq. 2

MC solution obtained using 10,000 realizations) is reported. The comparison between $M = 3$ and $M = 22$ shows that the error reduction is *only* about one order of magnitude!

7 DISCUSSION

The simple example illustrated above outlines the difficulties associated with low-order PC expansions in high speed flows. It is useful to point out that the phenomena observed is not directly connected to the well-known Gibbs phenomenon associated to polynomial

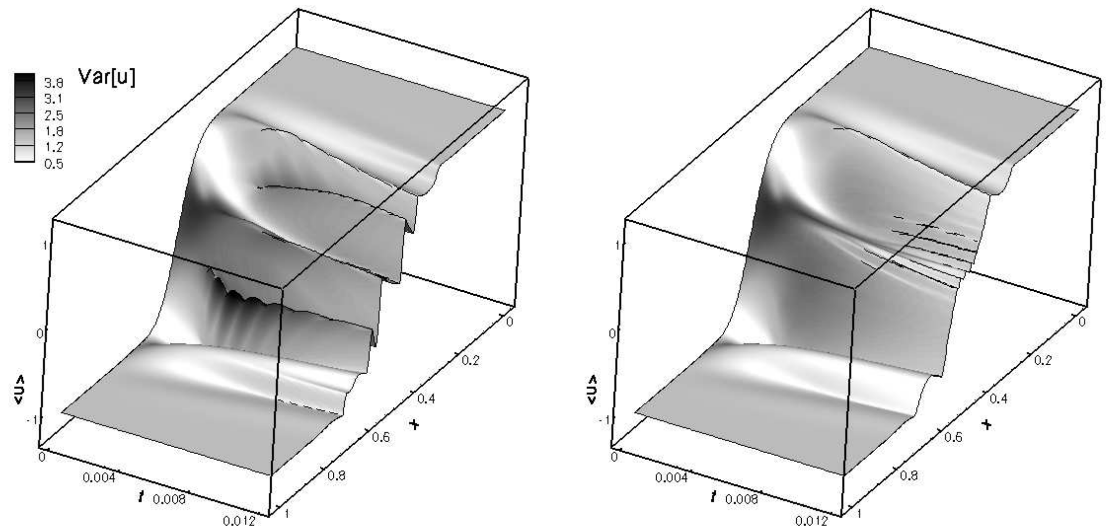

Figure 8: Time evolution of the expected solution obtained using PC expansions with $M = 3$ (left) and $M = 22$ (right). The surface is colored with the solution variance. $\alpha = 1$ in Eq. 2.

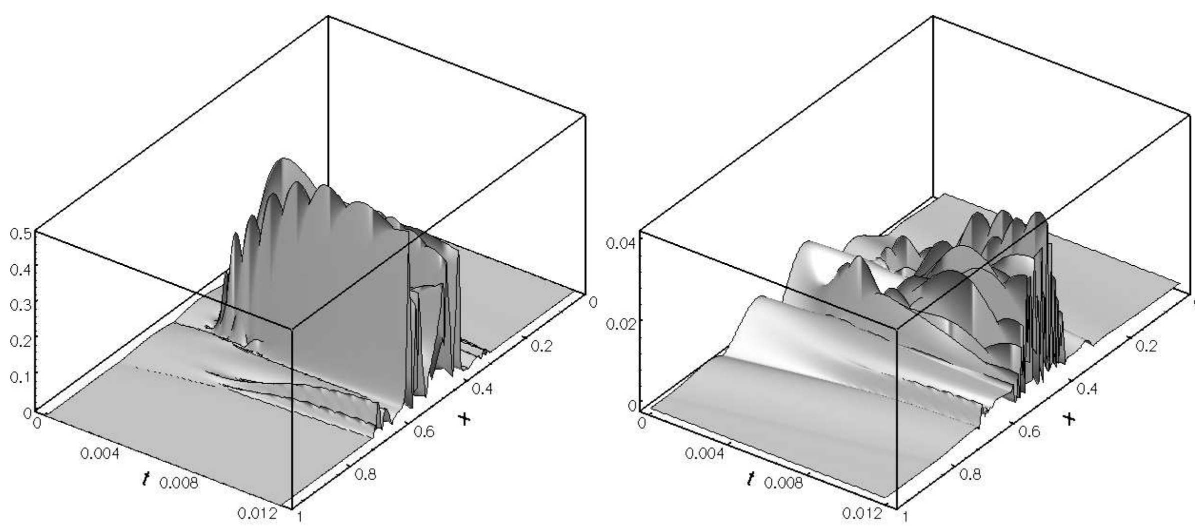

Figure 9: Time evolution of the error defined as the difference between the expected solution obtained using PC expansions and Monte Carlo sampling. PC expansions with $M = 3$ (left) and $M = 22$ (right). $\alpha = 1$ in Eq. 2.

interpolations of discontinuous functions [3]. In the present setting, the shocks are sharp features smeared over multiple grid cells, and the moments of the solutions are not polluted by strong oscillations. The features we observe in Fig. 4 are associated to the series truncation and the limited number of characteristics representing the ensemble behavior of the system. In the Monte Carlo results, on the other hand, the large sample might correspond to an extremely large number of characteristics which could be said to give rise to a *diffusion* of the deterministic shock structure. This conjecture seems to be confirmed by the results obtained by using stochastic collocation to solve the uncertain Woodward-Colella step problem introduced earlier, are reported in Fig. 10. As expected, the increase of the expansion order leads to smoother system response. This observation leads to the conjecture that low-order polynomial chaos expansions can be effectively used if an appropriate *diffusive* model for the truncation error in the stochastic expansion is included. Further work is required to verify if this approach can be a viable alternative to high-order expansions.

In conclusion, we have illustrated how stochastic expansion approaches have limited capabilities in capturing uncertainty propagation in shock-dominated fluid flow problems. For the simple Burgers equation example the observed reduction in convergence rate could be completely eliminated by changing the initial deterministic state from a compression to an expansion. This demonstrates that the problem with low-order expansion is directly associated to the limited set of characteristics that can be captured.

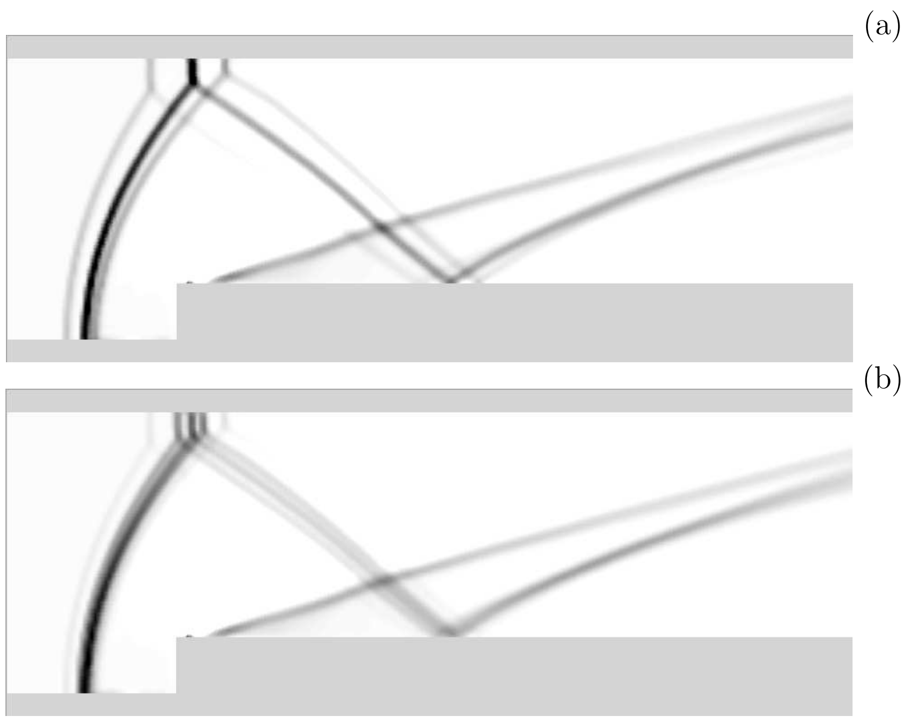

Figure 10: Woodward and Colella [8] forward facing step problem. Mean velocity divergence field corresponding to an uncertain input Mach number [2.5 : 3.0]. Stochastic collocation based on $M = 3$ (a) and $M = 5$ (b).

REFERENCES

[1] J. S. Liu, Monte Carlo Strategies in Scientific Computing, Springer Series in Statistics, 2001.

[2] J.D. Anderson, Fundamental of Aerodynamics, McGraw-Hill, 2001.

[3] T. Chantrasmi, A. Doostan, G. Iaccarino, Pade-Legendre Approximants for Uncertainty Analysis with Discontinuous Response Surfaces. *J. Comput. Phys.*, Vol. **228** (19), pp. 71597180, 2009.

[4] P.G. Constantine, D. F. Gleich, Iaccarino G. Spectral Methods for Parameterized Matrix Equations. submitted to *SIMAX* 2009.

[5] D. Xiu, J.S. Hesthaven, High order collocation methods for the differential equations with random inputs, *SIAM J. Sci. Comput.* Vol. **27**, pp. 1118-1139, 2005.

[6] R. Ghanem,P. Spanos, Stochastic Finite Elements: A Spectral Approach, Springer-Verlag, New York, 1991.

[7] J.A.S. Witteveen, H. Bijl, A TVD uncertainty quantification method with bounded error applied to transonic airfoil flutter *Commun. Comput. Phys.* Vol. **6** pp. 406-432, 2009.

[8] P. Woodward, P. Colella The numerical simulation of two-dimensional fluid flow with strong shocks *Journal of Computational Physics* Vol **54**, pp. 115-173, 1984.

[9] R. Pecnik, P. Constantine, F. Ham, G. Iaccarino, A probabilistic framework for high-speed flow simulations. *CTR Annual Research Brief*, pp. 3-17, 2008.

[10] F. Nobile, R. Tempone and C.G. Webster. A sparse grid stochastic collocation method for partial differential equations with random input data. Report number: TRITA-NA 2007:07. To appear SINUM.

[11] P. Pettersson, G. Iaccarino, J. Nordstroem, Numerical analysis of the Burgers equation in the presence of uncertainty *J. Comput. Phys.*, Vol. **228** (19), pp. 7159-7180, 2009.