Non-Intrusive Polynomial Chaos Methods for Stochastic CFD – Theory and Applications

Serhat Hosder
Department of Mechanical and Aerospace Engineering
205 ME Building, University of Missouri-Rolla
Rolla, Missouri, 65409-0500, USA

hosders@umr.edu

Robert W. Walters
Vice President for Research
301 Burruss Hall, Virginia Tech
Blacksburg, Virginia, 24061, USA

rwalters@vt.edu

ABSTRACT

This paper gives the theory behind non-intrusive polynomial chaos (NIPC) used for uncertainty propagation in computational simulations with the emphasis on the Point-Collocation NIPC technique, which has been recently developed by the authors. The application of Point-Collocation NIPC to stochastic CFD is demonstrated with two examples: (1) stochastic expansion wave problem with an uncertain deflection angle (geometric uncertainty) and (2) stochastic transonic wing case with uncertain free-stream Mach number and angle of attack. For each problem, input uncertainties are propagated both with the NIPC method and Monte Carlo techniques to obtain the statistics of various output quantities. Confidence intervals for Monte Carlo statistics are calculated using the Bootstrap method. For the expansion wave problem, a 4th degree polynomial chaos expansion, which requires 5 deterministic CFD evaluations, has been sufficient to predict the statistics within the confidence interval of 10,000 crude Monte Carlo simulations. In the transonic wing case, for various output quantities of interest, it has been shown that a 5th degree Point-Collocation NIPC expansion obtained with Hammersley sampling was capable of estimating the statistics at an accuracy level of 1,000 Latin Hypercube Monte Carlo simulations with a significantly lower computational cost. Overall, the examples demonstrate that the non-intrusive polynomial chaos has a promising potential as an effective and computationally efficient uncertainty propagation technique for stochastic CFD simulations.

1.0 INTRODUCTION

A deterministic computational fluid dynamics (CFD) simulation gives a single solution for a certain set of input parameters (the geometry, free-stream flow conditions, angle of attack etc.). In real life, these parameters are mostly uncertain and the variability associated with them can have substantial impact on the final result. Stochastic CFD simulations are needed to assess the uncertainty in the solution and to achieve a certain level of robustness or reliability in the final aerodynamic design. Development of credible stochastic aerodynamic simulation tools require effective and efficient methods to model and propagate the input

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uncertainties, and sufficient testing on various fluid dynamics problems. In this paper, we give the theory behind the non-intrusive polynomial chaos (NIPC) techniques used for uncertainty propagation and demonstrate the application of a NIPC method to selected stochastic CFD problems.

Several methods have been used to model and propagate uncertainty in stochastic computational simulations. Interval analysis, propagation of uncertainty using sensitivity derivatives, Monte Carlo simulations, moment methods and polynomial chaos are among the main approaches implemented in CFD simulations. Detailed description and analysis of each method for selected fluid dynamics problems can be found in Walters and Huyse [1]. In this paper we focus on uncertainty propagation with the polynomial chaos (PC) method, which is based on the spectral representation of the uncertainty. Several researchers have studied and implemented the PC approach for a wide range of problems. Ghanem and Spanos (1990, [2]) and Ghanem (1999, [3], [4]) applied the PC method to several problems of interest to the structures community. Mathelin et al. [5] studied uncertainty propagation for a turbulent, compressible nozzle flow by this technique. Xiu and Karniadakis [6] analyzed the flow past a circular cylinder and incompressible channel flow by the PC method and extended the method beyond the original formulation of Wiener [7] to include a variety of basis functions. In 2003, Walters [8] applied the PC method to a two-dimensional steady-state heat conduction problem for representing geometric uncertainty. Following this effort, an implicit compact PC formulation was implemented for the stochastic Euler equations (Perez and Walters [9]).

The Polynomial chaos (PC) method for the propagation of uncertainty in computational simulations involves the substitution of uncertain variables and parameters in the governing equations with the polynomial expansions. In general, an intrusive approach will calculate the unknown polynomial coefficients by projecting the resulting equations onto basis functions (orthogonal polynomials) for different modes. As its name suggests, the intrusive approach requires the modification of the deterministic code and this may be difficult, expensive, and time consuming for many complex computational problems such as the full Navier-Stokes simulation of 3-D, viscous, turbulent flows around realistic aerospace vehicles, chemically reacting flows, numerical modeling of planetary atmospheres, or multi-system level simulations which include the interaction of many different codes from different disciplines. To overcome such inconveniences associated with the intrusive approach, non-intrusive polynomial chaos formulations have been developed for uncertainty propagation. Most of the NIPC approaches in the literature are based on *sampling* (Debusschere et al., [10] Reagan et. al.,[11] and Isukapalli [12]) or *quadrature* methods (Debusschere et al. [10] and Mathelin et al. [13]) to determine the projected polynomial coefficients. Recently, Hosder and Walters [14] applied a Point-Collocation NIPC to selected stochastic Computational Fluid Dynamics (CFD) problems and Loeven et al. [15] introduced a non-intrusive Probabilistic Collocation approach for efficient propagation of arbitrarily distributed parametric uncertainties.

In the following section, the theory of non-intrusive polynomial chaos is described with particular emphasis on the Point-Collocation NIPC technique. Next, the application of Point-Collocation NIPC to stochastic CFD simulations is demonstrated with two examples: (1) stochastic expansion wave problem with geometric uncertainty and (2) stochastic transonic wing case with uncertain free-stream Mach number and angle of attack. For each problem, input uncertainties are propagated both with the NIPC method and Monte Carlo techniques to obtain the statistics of various output quantities and a detailed analysis of results are presented. The conclusions are given in Section IV.

2.0 THEORY OF NON-INTRUSIVE POLYNOMIAL CHAOS

The polynomial chaos is a stochastic method, which is based on the spectral representation of the uncertainty. An important aspect of spectral representation of uncertainty is that one may decompose a random function (or variable) into separable deterministic and stochastic components. For example, for any random variable (i.e., α^*) such as velocity, density or pressure in a stochastic fluid dynamics problem, we can write,

$$\alpha^*(\vec{x},\vec{\xi}) = \sum_{i=0}^{P} \alpha_i(\vec{x})\,\Psi_i(\vec{\xi}), \tag{1}$$

where $\alpha_i(\vec{x})$ is the deterministic component and $\Psi_i(\vec{\xi})$ is the random basis function corresponding to the i^{th} mode. Here we assume α^* to be a function of deterministic independent variable vector $\vec{x}$ and the n-dimensional random variable vector $\vec{\xi} = (\xi_1,...,\xi_n)$, which has a specific probability distribution. The discrete sum is taken over the number of output modes,

$$P+1 = \frac{(n+p)!}{n!\,p!}, \tag{2}$$

which is a function of the order of polynomial chaos (p) and the number of random dimensions (n). The basis function ideally takes the form of multi-dimensional Hermite Polynomial to span the n-dimensional random space when the input uncertainty is Gaussian (unbounded), which was first used by Wiener ([7], [16]) in his original work of polynomial chaos. Legendre (Jacobi) and Laguerre polynomials are optimal basis functions for bounded (uniform) and semi-bounded (exponential) input uncertainty distributions respectively in terms of the convergence of the statistics. Different basis functions can be used with different input uncertainty distributions (See Xiu and Karniadakis [6] for a detailed description), however the convergence may be affected depending on the basis function used [17]. The detailed information about polynomial chaos expansions can be found in Walters and Huyse [1] and Hosder et al. [14].

To model the uncertainty propagation in computational simulations via polynomial chaos with the intrusive approach, all dependent variables and random parameters in the governing equations are replaced with their polynomial chaos expansions. Taking the inner product of the equations, (or projecting each equation onto k^{th} basis) yield $P + 1$ times the number of deterministic equations which can be solved by the same numerical methods applied to the original deterministic system. Although straightforward in theory, an intrusive formulation for complex problems can be relatively difficult, expensive, and time consuming to implement. To overcome such inconveniences associated with the intrusive approach, non-intrusive polynomial chaos formulations have been considered for uncertainty propagation.

The objective of the non-intrusive polynomial chaos methods is to obtain approximations of the polynomial coefficients without making any modifications to the deterministic code. Main approaches for non-intrusive polynomial chaos are sampling based, collocation based, and quadrature methods. To find the polynomial coefficients $\alpha_k = \alpha_k(\vec{x}),\ (k = 0,1,...,P)$ in Equation 1 using sampling based and quadrature methods, the equation is projected onto kth basis:

$$\left\langle \alpha^*(x,\vec{\xi}),\, \Psi_k(\vec{\xi}) \right\rangle = \left\langle \sum_{i=0}^{P} \alpha_i \Psi_i(\vec{\xi}),\, \Psi_k(\vec{\xi}) \right\rangle, \tag{3}$$

where the inner product of two functions $f(\vec{\xi})$ and $g(\vec{\xi})$ is defined by

$$\left\langle f(\vec{\xi}),\, g(\vec{\xi}) \right\rangle = \int_R f(\vec{\xi}) g(\vec{\xi}) p_N(\vec{\xi})\, d\vec{\xi}. \tag{4}$$

Here the weight function $p_N(\vec{\xi})$ is the probability density function of $\vec{\xi}$ and the integral is evaluated on the support (R) region of this weight function. Using the orthogonality of the basis functions,

$$\left\langle \alpha^*(x,\vec{\xi}),\, \Psi_k(\vec{\xi}) \right\rangle = \alpha_k \left\langle \Psi_k^2(\vec{\xi}) \right\rangle \tag{5}$$

we can obtain

$$\alpha_k = \frac{\left\langle \alpha^*(x,\vec{\xi}),\, \Psi_k(\vec{\xi}) \right\rangle}{\left\langle \Psi_k^2(\vec{\xi}) \right\rangle}. \tag{6}$$

In sampling based methods, the main strategy is to compute $\alpha^*(x,\vec{\xi})\Psi_k(\vec{\xi})$ for a number of samples ($\vec{\xi}_i$ values) and perform averaging to determine the estimate of the inner product $\left\langle \alpha^*(x,\vec{\xi}),\, \Psi_k(\vec{\xi}) \right\rangle$. Quadrature methods calculate the same term, which is an integral over the support of the weight function $p_N(\vec{\xi})$, using numerical quadrature. Once this term is evaluated, both methods (sampling based and quadrature) use Equation 6 to estimate the projected polynomial coefficients for each mode.

II.1. Point-Collocation Non-Intrusive Polynomial Chaos

The collocation based NIPC method starts with replacing the uncertain variables of interest with their polynomial expansions given by Equation 1. Then, *P+1* vectors ($\vec{\xi}_i = \{\xi_1,\xi_2,...,\xi_n\}_k,\ k = 0,1,2,...,P$) are chosen in random space for a given PC expansion with *P +1* modes and the deterministic code is evaluated at these points. With the left hand side of Equation 1 known from the solutions of deterministic evaluations at the chosen random points, a linear system of equations can be obtained:

$$\begin{bmatrix} \Psi_0(\vec{\xi}_0) & \Psi_1(\vec{\xi}_0) & \cdots & \Psi_P(\vec{\xi}_0) \\ \Psi_0(\vec{\xi}_1) & \Psi_1(\vec{\xi}_1) & \cdots & \Psi_P(\vec{\xi}_1) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_0(\vec{\xi}_P) & \Psi_1(\vec{\xi}_P) & \cdots & \Psi_P(\vec{\xi}_P) \end{bmatrix} \begin{Bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_P \end{Bmatrix} = \begin{Bmatrix} \alpha^*(\vec{\xi}_0) \\ \alpha^*(\vec{\xi}_1) \\ \vdots \\ \alpha^*(\vec{\xi}_P) \end{Bmatrix} \tag{7}$$

The spectral modes (α_k) of the random variable α^* are obtained by solving the linear system of equations given above. Using these, mean (μ_{α^*}) and the variance ($\sigma^2_{\alpha^*}$) of the solution can be obtained by

$$\begin{aligned} \mu_{\alpha^*} &= \alpha_0 \\ \sigma^2_{\alpha^*} &= \sum_{i=1}^{P} \alpha_i^2 \left\langle \Psi_i^2(\vec{\xi}) \right\rangle \end{aligned} \tag{8}$$

The Point-Collocation approach was first introduced by Walters [8] to approximate the polynomial chaos coefficients of the metric terms, which are required as input stochastic variables for the intrusive polynomial chaos representation of a stochastic heat transfer problem with geometric uncertainty. In 2006, Hosder et. al. [14] applied this Point-Collocation NIPC method to stochastic fluid dynamics problems with geometric uncertainty. They demonstrated the efficiency and the accuracy of the NIPC method in terms of modelling and propagation of an input uncertainty and the quantification of the variation in an output variable. That study included a single random input variable, and the collocation locations were equally spaced in the random space. Following that work, Hosder et. al. [18] applied the Point-Collocation NIPC to model stochastic problems with multiple uncertain input variables having uniform probability distributions and investigated different sampling techniques (Random, Latin Hypercube, and Hammersley) to select the optimum collocation points. The results of the stochastic model problems showed that all three sampling methods exhibit a similar performance in terms of the accuracy and the computational efficiency of the chaos expansions. However, the convergence of the Point-Collocation NIPC statistics obtained with Hammersley and Latin Hypercube sampling exhibit a much smoother (monotonic) convergence compared to the cases obtained with random sampling.

The solution of linear problem given by Equation 7 requires $P+1$ deterministic function evaluations. If more than $P+1$ samples are chosen, then the over-determined system of equations can be solved using the Least Squares method. Hosder et. al. [18] investigated this option by increasing the number of collocation points in a systematic way through the introduction of a parameter n_p defined as

$$n_p = \frac{number\ of\ samples}{P+1}. \tag{9}$$

In the solution of stochastic model problems with multiple uncertain variables, they have used $n_p = 1, 2, 3,$ and 4 to study the effect of the number of collocation points (samples) on the accuracy of the polynomial chaos expansions. Their results showed that using a number of collocation points that is twice more than the minimum number required ($n_p=2$) gives a better approximation to the statistics at each polynomial degree. This improvement can be related to the increase of the accuracy of the polynomial coefficients due to the use of more information (collocation points) in their calculation. The results of the stochastic model problems also indicated that for problems with multiple random variables, improving the accuracy of polynomial chaos coefficients in NIPC approaches may reduce the computational expense by achieving the same accuracy level with a lower order polynomial expansion.

2.1.1 Computational Cost

Figure 1 shows the computational cost associated with the Point-Collocation and the numerical quadrature NIPC. For the point collocation, the number of function evaluations is equal to $n_p \times (P+1)$ where $P+1$ is the number of output modes for a given polynomial degree and number of random variables (n) (See Equation 2). The number of function evaluations for the numerical quadrature is n^{nq} where nq is the number of quadrature points in each random dimension. For a single random variable, the number of function evaluations for each method is comparable. However, as the number of random variables increase, the computational cost of the numerical quadrature grows significantly. One may think of using an optimum number of quadrature points to reduce the cost, but for a general stochastic function or problem, considerable number of quadrature points may be required to evaluate the integration with desired accuracy as shown by Huyse et al. [17]. For both methods, the computational cost becomes formidable with the increase of the polynomial degree and the number of random variables. It should be noted that in Figure 1 the limits of the number of function evaluations are extended to very large numbers to show the general trend. In reality, especially for large-scale stochastic computations, one can afford only a certain number of deterministic runs to the produce the output values at the selected collocation or quadrature points. This emphasizes the necessity of the implementation of innovative methods in large-scale stochastic problems to model and propagate multiple input uncertainties with desired accuracy and efficiency.

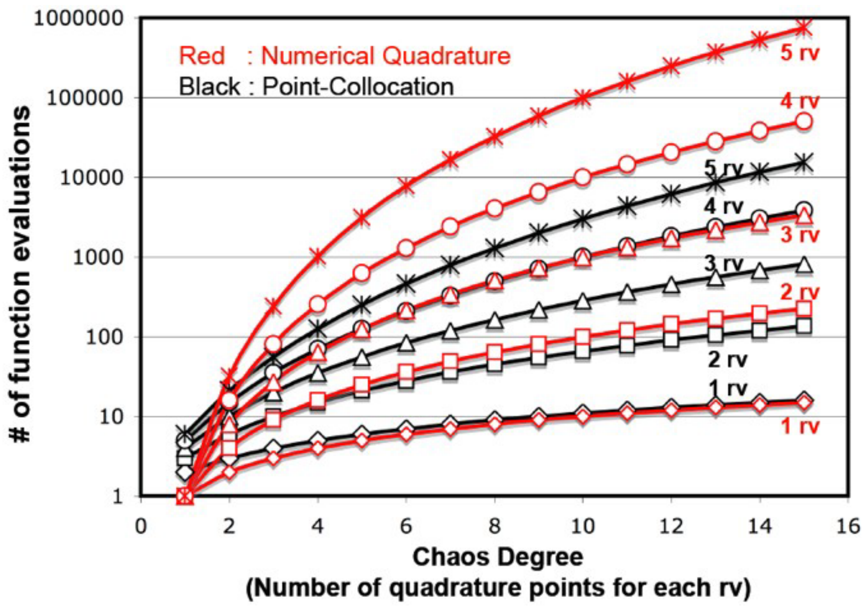

Figure 1: The number of function evaluations for the Point-Collocation and (n_p=1) and the numerical quadrature NIPC for different number of random variables

3.0 APPLICATION EXAMPLES

3.1 Stochastic Expansion Wave Problem

To analyze the stochastic expansion wave problem, we consider inviscid, steady, two-dimensional, supersonic flow of a calorically perfect gas over a convex corner. Under these conditions, a centered expansion fan originates from the sharp convex corner as shown in Figure 2. The static pressure, which is the output quantity of interest for this problem, decreases continuously across the expansion fan and remains constant in the region downstream of the rearward Mach line. The deterministic problem involves the solution of the supersonic flow field for a given free stream Mach number (M_{ref}), specific heat ratio (γ), and the deflection angle (θ).

To solve the deterministic problem, one may use the Prandtl-Meyer relations to calculate the Mach number at any increment of deflection angle across the expansion fan. Once the Mach number is known, the pressure drop (P/P_{ref}) can be calculated using the isentropic relations for a perfect gas. The details of the Prandtl-Meyer solution can be found in Anderson [19]. In our study, we solved the deterministic problem numerically using the CFL3D code of NASA Langley Research Center to demonstrate the application of the Point-Collocation NIPC method to CFD simulations. CFL3D is a three-dimensional, finite-volume, Navier-Stokes code capable of solving steady or time-dependent aerodynamic flows ranging from subsonic to supersonic speeds [20].

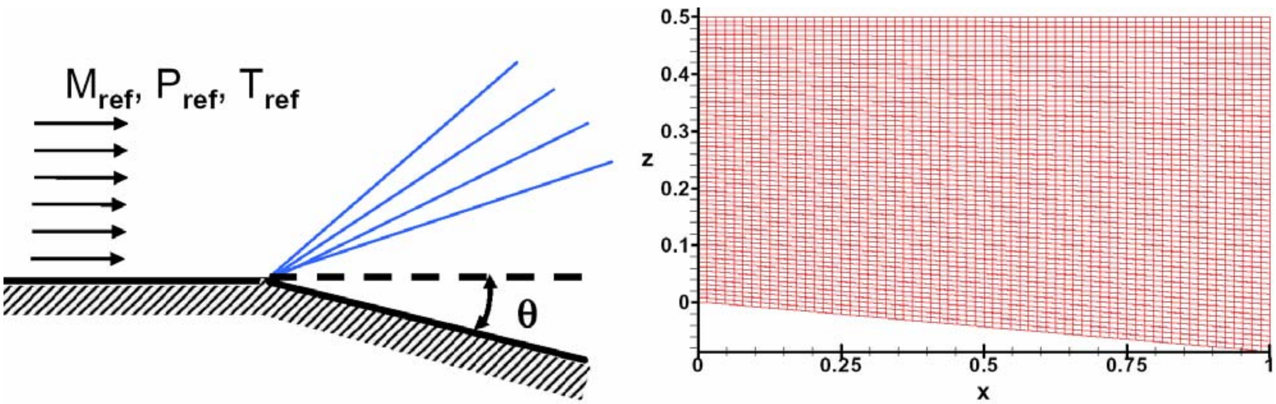

Figure 2: Description of the supersonic, inviscid flow over a convex corner with a turn angle of θ. On the right, the mean grid (65x65) used in Euler computations is shown. The mean deflection angle (θ_{mean}) is 5.0 degrees.

We used CFL3D to solve the Euler equations, which are a subset of Navier-Stokes equations and govern the inviscid, compressible flow of a fluid. Both NIPC and Monte Carlo methods used the deterministic solutions from Euler calculations in their implementation. The computations were performed on grids, which have 65 grid points in both x- and z-directions. Figure 2 shows the grid with the mean deflection angle, θ_{mean}. The equations were integrated in time using an implicit approximate factorization scheme to reach the steady state. A full multigrid (multigrid+mesh sequencing) method was used for convergence acceleration. The free-steam Mach number was chosen as M_{ref} = 3.0 and the angle of attack was set to zero degrees. The inviscid fluxes on the cell-faces were calculated using Roe flux difference splitting and the primitive variables on the cell faces were obtained using an upwind-bias 3rd-order accurate scheme with the MinMod limiter.

The stochastic expansion wave problem was formulated by introducing a geometric uncertainty through the deflection angle (θ) that was uncertain and described by a Gaussian distribution:

$$\theta(\xi) = \theta_{mean} + \xi\sigma \tag{10}$$

The mean deflection angle was 5 degrees and the coefficient of variation was 10%. Here ξ is a normally distributed random variable with zero mean and unit variance ($\xi = N[0,1]$). Uncertainty propagation in supersonic expansion flow has been modeled using crude Monte Carlo and the Point-Collocation NIPC methods. In Monte Carlo simulations, 10,000 grids were created using 10,000 samples from the $\theta(\xi)$ distribution. The Euler Equations were solved on each grid using the CFL3D code. A fourth order polynomial expansion was chosen to model the uncertainty propagation with the NIPC method. To obtain the polynomial coefficients, five deterministic solutions were evaluated on five grids with deflection angles that correspond to $\xi_0 = 0.0$, $\xi_1 = 1.0$, $\xi_2 = -1.0$, $\xi_3 = 2.0$, and $\xi_4 = -2.0$ (i.e., the collocation locations are equally spaced in the random space). It should be noted that each deterministic solution that corresponds to a specific value of ($\theta(\xi)$) was obtained on a different grid, which has different cell center locations. Each deterministic solution was interpolated to the mean grid to calculate the Monte Carlo statistics at the cell center locations of the mean grid. Similarly, the polynomial chaos expansions for the pressure were calculated at the mean grid cell center locations using five deterministic solutions that were obtained from the interpolation of the original $\theta(\xi_i)$ $(i = 0,...,4)$ results to the mean grid.

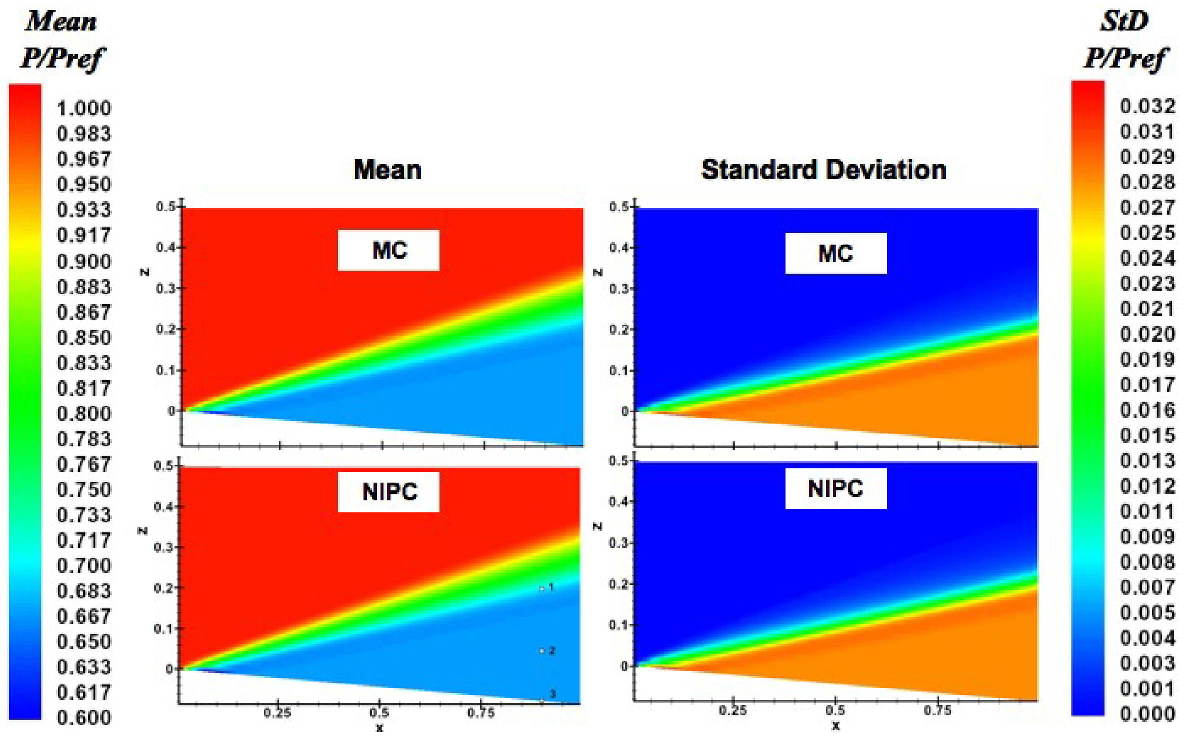

Figure 3: Mean and standard deviation distributions of pressure (*P/P_{ref}*) obtained from MC simulations and Point-Collocation NIPC for the supersonic expansion wave problem. The three locations showed in the mean polynomial chaos plot designate the points where the quantitative analyses were performed.

Figure 3 gives the mean and standard deviation contours of pressure for the NIPC method and the Monte Carlo simulations. The qualitative agreement between the results of the two methods is good. Across the expansion wave, a smooth mean pressure drop is observed. The standard deviation increases smoothly across the expansion wave for all cases. To analyze the statistics of the Monte Carlo and NIPC methods quantitatively, we have picked three locations in the flow field. All three are on the same streamwise station, but they are at different distances from the wall (Figure 3). Location 1 ($x = 0.8984$, $z = 0.1978$) is in the expansion fan towards the rearward Mach line, Location 2 ($x = 0.8984$, $z = 0.0445$) is downstream of the expansion fan, and Location 3 ($x = 0.8984$, $z = -0.0772$) is a point on the wall downstream of the expansion fan. The static pressure histograms at these locations are shown in Figure 4. At all locations, the histograms of the non-intrusive polynomial chaos method are in good agreement with the ones obtained with the Monte Carlo simulations. The distribution at location 1 (expansion fan) is slightly skewed to the right, whereas the histograms at locations 2 and 3 follow the Gaussian distribution closely. For location 1, it can be seen that a fourth-order polynomial expansion is sufficient to model the non-Gaussian contributions observed at this region of the flow. Table 1 gives the mean and the standard deviation of the pressure at the three stations depicted above. For each statistical quantity obtained with the Monte Carlo Simulations, a 95% confidence interval is also presented. We use the bootstrap method to compute the confidence intervals as well as the standard error estimate of each statistical quantity. The advantage of this method is that it is not restricted to a specific distribution, e.g. a Gaussian. It is easy and efficient to implement and can be completely automated to any estimator, such as the mean or the variance. In practice, one takes 25–200 bootstrap samples to obtain a standard error estimate. In our computations, we used 500 bootstrap samples. Note that each sample consisted of 10,000 observations selected randomly from the original Monte Carlo simulations by giving equal probability (1/10,000) to each observation. For all three locations, the mean and standard deviation values obtained with the NIPC method fall within the 95% confidence intervals that were calculated for the statistics of Monte Carlo simulations. The standard deviation at location 1 is approximately 2.5 times less than the ones obtained at locations 2 and 3 for both orders of spatial accuracy. These results can also be detected visually from the histogram plots.

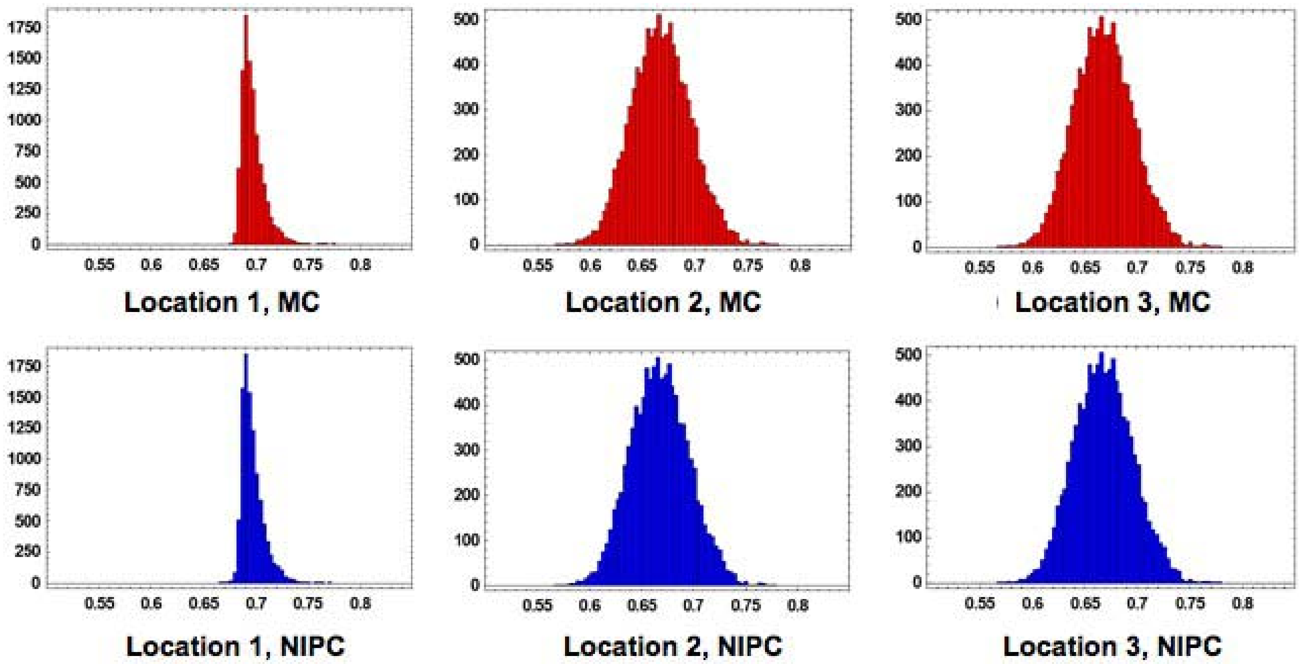

Figure 4: Static pressure histograms obtained at three locations for the supersonic expansion wave problem using MC and Point-Collocation NIPC methods.

Table 1: Mean and standard deviation (StD) distributions of pressure (P/P_{ref}) obtained with MC and Point-Collocation NIPC methods at three selected locations for the supersonic expansion wave problem. The 95% confidence intervals for the MC statistics are calculated using the Bootstrap method.

Statistics	Location	NIPC	MC	95% Confidence Interval
Mean	1	0.697085	0.697122	[0.696907, 0.697336]
	2	0.668056	0.668065	[0.667515, 0.668629]
	3	0.668071	0.668070	[0.667519, 0.668633]
StD	1	0.0107491	0.0107470	[0.0104820, 0.0110103]
	2	0.0280358	0.0280317	[0.0276231, 0.0284082]
	3	0.0280277	0.0280260	[0.0276174, 0.0284027]

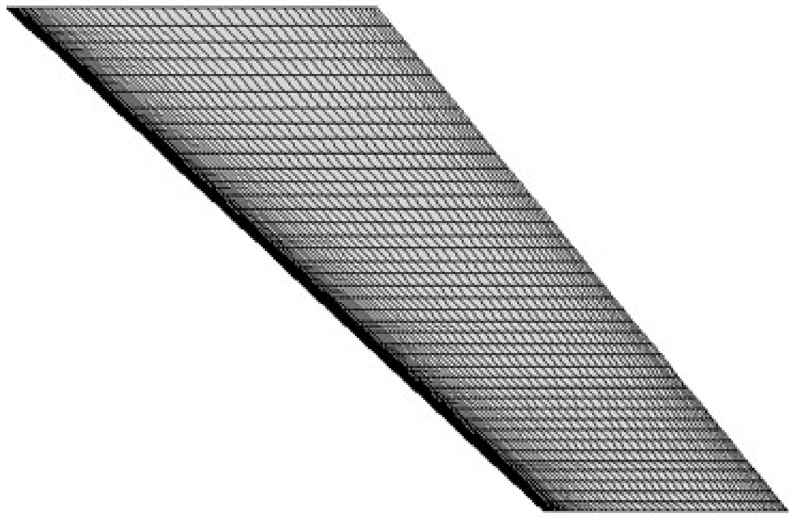

Figure 5: AGARD 445.6 Wing and the surface grid

3.2 Stochastic Transonic Wing Problem

To demonstrate the application of Point-Collocation NIPC to an aerospace problem with multiple uncertain input variables, a stochastic computational aerodynamics problem, which includes the numerical simulation of steady, inviscid, transonic flow over a three-dimensional wing has been selected. The wing geometry is the AGARD 445.6 Aeroelastic Wing [21] (Figure 5), which has been extensively used to validate computational aeroelasticity tools especially in the determination of flutter boundary at various transonic Mach numbers. The wing has a quarter-chord sweep angle of 45 deg., a panel aspect ratio of 1.65, a taper ratio of 0.66, and a NACA 65A004 airfoil section. The current study includes the aerodynamic simulations with the rigid wing assumption, which can be thought as a preliminary investigation before the application of the NIPC to a stochastic computational aeroelasticity problem involving the same geometry. As in the expansion wave problem, we used CFL3D code to solve the steady Euler equations numerically. The computational grid has a C-H topology with $193 \times 65 \times 42$ points.

For the stochastic aerodynamics problem, the free-stream Mach number (M_∞) and the angle of attack (α) are treated as uncertain variables. The Mach number is modeled as a uniform random variable between $M_\infty(\xi_1) = 0.8$ and $M_\infty(\xi_1) = 1.1$, and the angle of attack is defined as a uniform random variable between $\alpha(\xi_2) = -2.0$ and $\alpha(\xi_2) = 2.0$ degrees. Note that here each component of the random variable vector $\vec{\xi} = \{\xi_1, \xi_2\}$ is a uniform random variable defined in the interval [-1,1]. Therefore, in our NIPC calculations, we have used multi-dimensional Legendre polynomials that are orthogonal in the interval [-1,1] for each random dimension. Stochastic solutions to the problem were obtained with two approaches: Latin Hypercube Monte Carlo with 1000 samples and Point-Collocation NIPC. Based on the observations from the stochastic model problems studied [18], Hammersley Sampling with $n_p = 2$ has been used for the selection of collocation points for the NIPC approach. The chaos expansions were obtained up to a polynomial degree of 5. Table 2 gives the computational cost associated with each stochastic approach. As can be seen from this table, on the same computer (SGI Origin 3800 with 64 processors used), it took 46.6 hours to finish the Monte Carlo simulations whereas the computational time was approximately 2 hours for the Point Collocation NIPC with a polynomial degree of 5.

Table 2: The computational cost for the evaluation of Latin Hypercube Monte Carlo simulations and the Point-Collocation NIPC for the stochastic transonic wing problem. (p is the degree of polynomial chaos)

	Monte Carlo	NIPC				
		p = 1	*p = 2*	*p = 3*	*p = 4*	*p = 5*
Number of CFD runs	1,000	6	12	20	30	42
Wall clock time (hours)	46.6	0.28	0.56	0.94	1.4	1.96

Table 3: The Latin Hypercube Monte Carlo statistics for C_L and C_D. The 95% confidence intervals for the MC statistics were calculated using the Bootstrap Method

	Mean	95% CI of Mean	StD	95% CI of StD
CL	0.000169661	[-0.005324476, 0.005058219]	0.084082119	[0.081239769, 0.08641931]
CD	0.002538528	[0.002414416, 0.002655811]	0.002164797	[0.002075901, 0.002234283]

Table 3 gives the statistics and the 95% confidence intervals of the lift (C_L) and drag (C_D) coefficient obtained with the Latin Hypercube Monte Carlo simulations. In Figure 6, the convergence of C_L and C_D statistics obtained with the Point-Collocation NIPC is presented. For all polynomial degrees, the NIPC approximations to the mean and the standard deviation of the lift coefficient stays within the 95% confidence interval of the Monte Carlo statistics. The mean of the drag coefficient falls within the confidence interval at a polynomial degree of 3 whereas the standard deviation enters the interval with a polynomial degree of 4. The histogram of the drag coefficient obtained with the NIPC approach gets very similar to the histogram shape of the Monte Carlo simulations at a polynomial degree of 5 (Figure 7). The mean and the standard deviation distributions of the pressure coefficient (Cp) on the wing upper surface is given in Figure 8. The Monte Carlo and the NIPC statistics are in a good qualitative agreement in most regions of the wing. Overall, this computational example shows that a 5th degree Point-Collocation NIPC expansion obtained with Hammersley sampling and $n_p = 2$ is capable of estimating the statistics at an accuracy level of 1000 Latin Hypercube Monte Carlo simulations with a significantly lower computational cost.

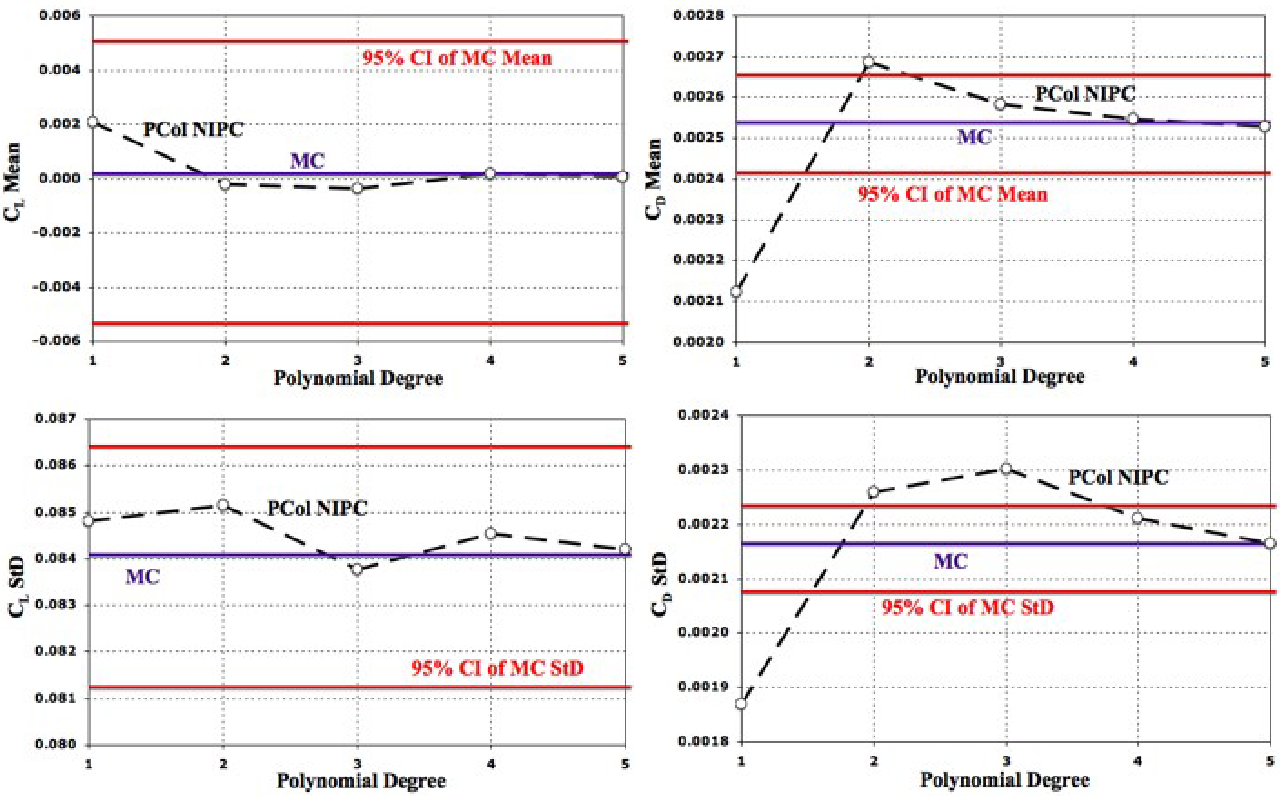

Figure 6: Mean and standard deviation of C_L and C_D obtained with Point-Collocation NIPC and Latin Hypercube Monte Carlo

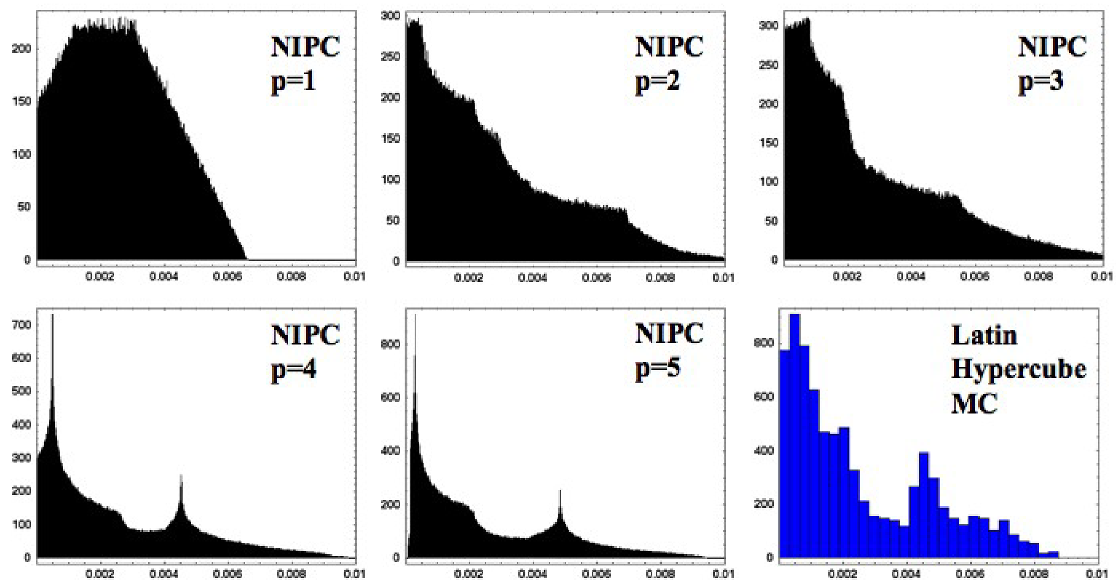

Figure 7: The histograms of C_D obtained with the Latin Hypercube Monte Carlo (MC) and NIPC

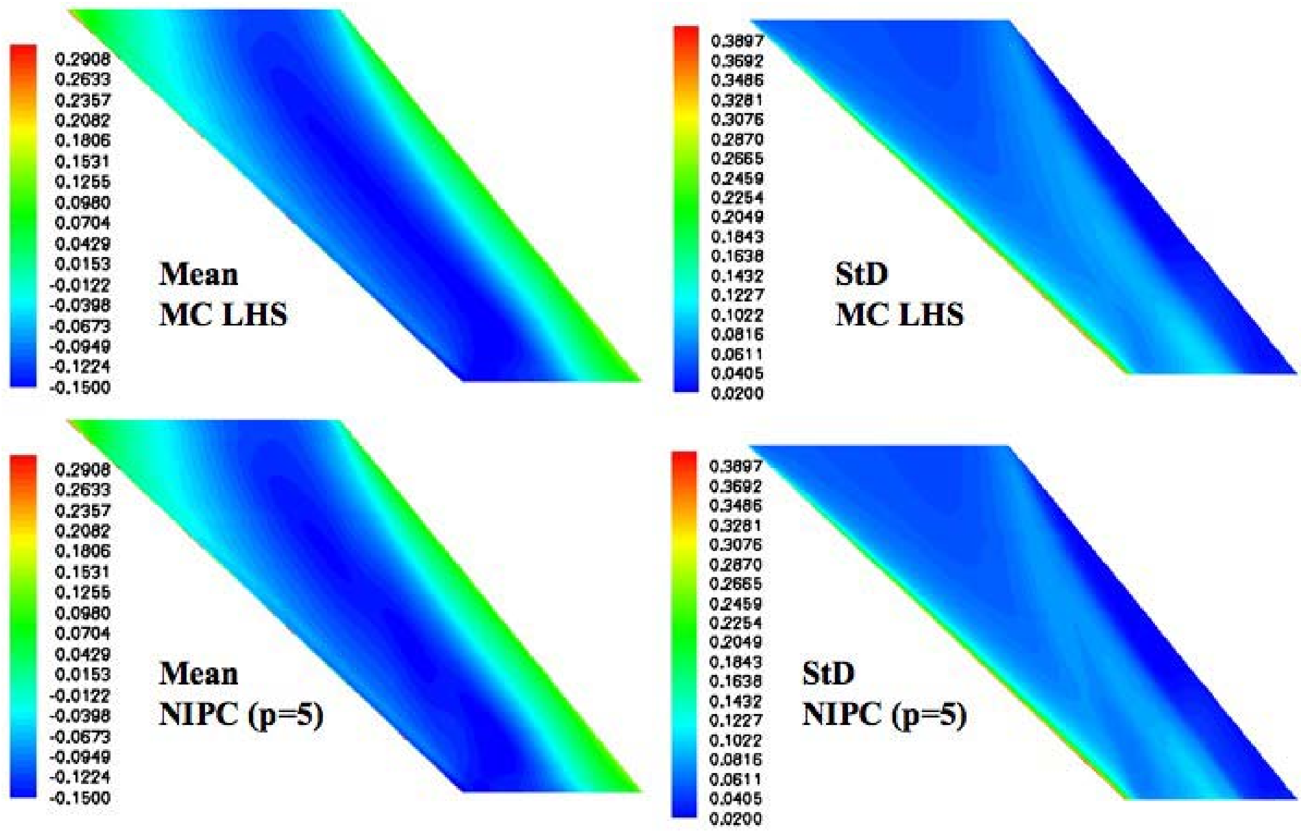

Figure 8: Mean and standard deviation of pressure coefficient (*Cp*) on the upper surface of the AGARD 445.6 Wing. The Point-Collocation NIPC results are obtained with 5th degree chaos expansions.

Using the NIPC expansions, one can also efficiently obtain the complete probability distribution (histogram) of any flow quantity at any point in the flow field. This information is especially important for the surface pressure distributions, which are often used for comparison with the experimental data in CFD validation studies. With the complete probability distribution information, it is possible to calculate the confidence intervals for the CFD results, which may be uncertain due to the variations in various input parameters such as the free-stream Mach number or the angle of attack studied in the present stochastic transonic wing study. Figure 9 shows the uncertainty bars for the upper surface *Cp* distributions on the AGARD 445.6 Wing at three spanwise stations. These uncertainty bars include the *Cp* values within 95% confidence intervals obtained with the Point-Collocation NIPC Method. As can also be seen from the contour plot of the standard deviation, the largest uncertainty in pressure is located in the leading edge region towards the tip of the wing.

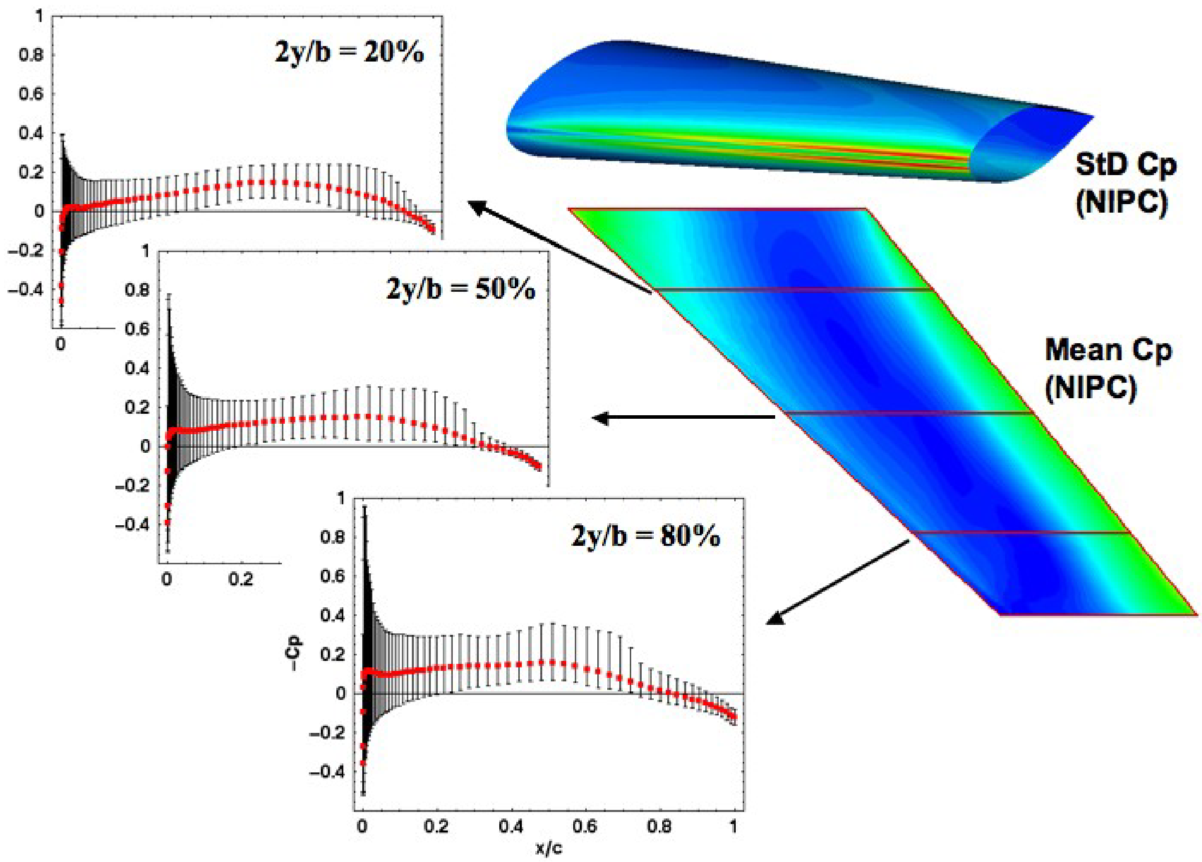

Figure 9: Uncertainty bars for the upper surface *Cp* distributions of the AGARD 445.6 Wing at three spanwise stations. The uncertainty bars include *Cp* values within 95% confidence intervals obtained with the Point-Collocation NIPC method.

4.0 CONCLUSIONS

In this paper, we have discussed the theory behind some of the non-intrusive polynomial chaos (NIPC) methods used for uncertainty modeling and propagation in computational simulations. Our particular emphasis was on the Point-Collocation NIPC, which has been recently developed by the authors. We have demonstrated the application of Point-Collocation NIPC to stochastic CFD with two examples: (1) stochastic expansion wave problem with an uncertain deflection angle (geometric uncertainty) and (2) stochastic transonic wing case with uncertain free-stream Mach number and angle of attack. For both cases, various statistics were computed both with the NIPC method and Monte Carlo techniques. Confidence intervals for Monte Carlo statistics were calculated using the Bootstrap method. For the expansion wave problem, a 4^{th} degree polynomial chaos expansion, which required 5 deterministic evaluations was sufficient to predict the statistics within the confidence interval of 10,000 crude Monte Carlo simulations. In the transonic wing case, for various output quantities of interest, it has been shown that a 5^{th} degree Point-Collocation NIPC expansion obtained with Hammersley sampling was capable of estimating the statistics at an accuracy level of 1,000 Latin Hypercube Monte Carlo simulations with a significantly lower computational cost. Overall, the examples demonstrated that the non-intrusive polynomial chaos has a promising potential as an effective and computationally efficient uncertainty propagation technique in stochastic CFD problems. Our current research focus on further improvement of the accuracy and computational efficiency of the Point-Collocation NIPC technique by the investigation and implementation of optimum basis functions for arbitrary input uncertainty distributions, adaptive strategies for the determination of optimum polynomial degree, and importance sampling for the selection of optimum collocation points. In addition to stochastic CFD, our efforts also include the application of NIPC method to various large-scale computational simulations involving the uncertainty quantification of Martian atmosphere, robust design of aerospace vehicles, and stochastic multidisciplinary design and optimization.

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Paper No. 47

Discusser's Name: D. Bose

Question: (1) How does the cost of your technique go up with the number of uncertain parameters? (2) Is there a breakeven point in the number of uncertain variables beyond which the polynomial chaos approach offers no advantage?

Author's Reply: (1) For the point-collocation non-intrusive polynomial chaos method, the number of deterministic runs should be at least $(n+p)!/\,n!\,p!$ where n = number of random variables and p = the order of the polynomial chaos. For a least-squares approach, this number will increase by a factor of two (optimum n_p factor described in the paper). (2) As described in the previous question, when the number of deterministic runs (samples) becomes comparable to the typical numbers used in MC simulations, the advantage of computational efficiency may degrade. However, the accuracy of statistics may still be better than the ones obtained with MC with the same number of samples.

Discusser's Name: W. Oberkampf

Question: Is the convergence rate of non-intrusive polynomial chaos expansion dependent on (a) the number of random variables that are uncertain and (b) the variance of the random variables?

Author's Reply: The authors of the paper have not yet investigated the questions asked about the convergence of the point-collocation non-intrusive polynomial chaos. However, these points will definitely be addressed during the further study of the method.