Evaluation of discontinuity treatment in intrusive polynomial chaos for uncertainty quantification of a nozzle flow in CFD

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Abstract
Stochastic flow simulation methods based on the polynomial chaos expansion (PCE) are developed and verified to quantify the propagation of a geometric uncertainty of a quasi-one dimensional flow in a supersonic wind tunnel. The effect of uncertainty in the area of diffuser throat, i.e. second throat, on the wind tunnel starting problem is focused on, where a slight change in the area can cause a large jump of the shock wave resulting in a breakdown of the supersonic test conditions. Two major numerical techniques in our intrusive PCE are the multi-wavelet (MW) basis and the multi-element (ME) PCE, in order to properly deal with discontinuous responses of output variables, which are caused by the shock wave and its jump at started/unstarted mode change. Single-element spectral PCE using Legendre basis and the Haar-wavelet are also included as special cases of the MW, and the methods are all compared with Monte-Carlo Simulations (MCS) executed by the deterministic code. Response surfaces of the pressure by the employed PCEs qualitatively agree with the result of MCS except the spectral PCE. Furthermore, from quantitative evaluations by the probability density function (PDF) of the output on a rather complicated response surface with several discontinuities, the ME-PCE best agrees with the MCS at much lower computation costs.

Keywords : Uncertainty quantification, Computational fluid dynamics, Polynomial chaos, Wavelet, Shock wave

1. Introduction

In recent years, research on uncertainty quantification (UQ) that evaluates the propagation of input uncertainties to output values attracts attention in the field of computational fluid dynamics (CFD). It is expected as a new role of numerical simulations and a mean to improve the reliability of simulations. Various methods are roughly divided into two: a non-intrusive method typified by the MCS that obtain output statistics from many analysis results of the original or deterministic code, and an intrusive method that requires new codes to solve extended governing equations in which unknown variables are expressed as functions of random variables standing for the input uncertainty.

Since the non-intrusive method can handle an analysis program as a black box, it can be applied to any complicated simulations such as aero-elasticity coupled analysis or combustion flow analysis, but the high calculation cost due to many runs is an apparent drawback. On the other hand, the intrusive method aims at reducing the total cost of UQ by solving extended equations. The representative method is the PCE that originates from Spectrum approach by Ghanem and Spanos (1991), and has been generalized to deal with uncertainties of a PDF other than the normal distribution (Xiu and Karniadakis, 2002; Xiu and Karniadakis, 2003). In the method, variables with uncertainties are all expanded using the orthogonal basis that is determined according to the input PDF. UQ is carried out by a single execution of the program and there is no concern about sample-point selection methods and number of samples points, which are important factors in the non-intrusive method. The above generalized PCE is a very effective method for UQ whose output changes smoothly against the deviation of input, and also the characteristics of spectral convergence of errors.
with respect to the polynomial order of basis function have been verified (Xiu and Karniadakis, 2003). Despite the merits, the intrusive PCE is not a generally established method. One of the reasons for the difficulty is that it is necessary to expand the reciprocal and square roots of variables with the basis function of the random variable, depending on the selection of the variable to be expanded. The formulation is complicated and has arbitrariness. In this research, we use the Roe variable transformation proposed by Pettersson et al. (2014) to extend the compressible flow equations to the stochastic space. As a result, all unknowns, flux vectors and source terms in this study are expressed in a quadratic form of the Roe variables (Roe, 1981), and the formulation of the intrusive problem is clarified.

Another problem, or a disadvantage of PCE, is that the response of the solution can not be properly expressed by a linear combination of orthogonal polynomials spanning the whole probability space when the output shows abrupt changes with respect to a change in input. A remedy is to use localized basis function instead of globally continuous basis used in the classical or spectral PCE. The localization is realized by two methods, one is using wavelets for the basis and another is using the ME-PCE (Wan and Karniadakis, 2006). As for the wavelet, we use the MW by Alpert (1993), the application of which to UQ is first proposed by Le Maitre et al. (2004a, 2004b). Legendre polynomials of the spectral PCE for inputs with uniform PDF, and Haar wavelet are both included as special cases of the MW. As for the ME-PCE, stochastic space is divided into several intervals and orthogonal polynomials basis and the PDF are respectively redefined in each interval. We term all the methods introduced above as PCE and its extensions, and investigate the most suitable method for a problem with strongly discontinuous response both in the physical and stochastic space.

In this research, we specifically focus on the problem of uncertainty in the geometry of a supersonic wind tunnel, which is modeled by a quasi-one-dimensional compressible flow. The wind tunnel is composed of a nozzle throat, test section and diffuser with a second throat. Depending on the height (area) of the second throat, a supersonic flow is started in the test section, or it is broken down by a large jump of the shock wave upstream. A problem of geometric uncertainty by the intrusive PCE is first introduced by Walters (2003) but most studies from then are dealt with non-intrusive methods possibly due to the versatility of the non-intrusive method and increased complexity in the intrusive method. In this study, extended governing equations are derived based on the Roe variables reviewed above, but it must be modified to take into account the cubic products of the stochastic variables. The resulting form becomes clear and concise again.

2. PCE and its extension

In the PCE, variables with uncertainty are expanded by orthogonal basis polynomials of random variables. The following form is then assumed,

\[ u(t, x, \xi) = \sum_{i=0}^{N_p} u_i(t, x) \psi_i(\xi) \]  

where \( u_i(t, x) \) is an expansion coefficient as a functions of time \( t \) and space \( x \), \( \psi_i(\xi) \) is a basis function in terms of a random variable \( \xi \) with a specific probability distribution, the subscript \( i \) is a mode and \( N_p \) is the maximum polynomial degree considered. The basis functions are orthogonal to each other, and if they are further normalized, the inner product defined in the following equation satisfies

\[ < \psi_i|\psi_j> = \int_\xi \psi_i(\xi) \psi_j(\xi) p(\xi) d\xi = \delta_{ij}, \]  

where \( \delta_{ij} \) is a Kronecker delta, \( p(\xi) \) is a PDF which the input uncertainty \( \xi \) follows, and \( R \) is the range of definition of \( \xi \). The average and variance of the dependent variable \( u \) are easily obtained from the expansion coefficients as,

\[ \bar{u} = E[u] = u_0(t, x) \]  

\[ \text{Var}[u] = \sum_{i=1}^{N_p} u_i^2(t, x). \]
In this paper, input geometric uncertainty is assumed to follow a uniform PDF. For the classical or spectral PCE with a globally continuous polynomial basis, the corresponding orthogonal basis is Legendre polynomials, the normalized version of which for $\xi \in [-1, 1]$ up to $N_p=2$ are written as,

$$
\begin{align*}
\psi_0 &= \frac{1}{\sqrt{2}}, \\
\psi_1 &= \frac{3}{2} \xi, \\
\psi_2 &= \frac{5}{2} \xi^2 - 1.
\end{align*}
$$

(5)

2. 1 MW basis for PCE

In order to improve the accuracy and robustness of uncertainty analysis of flows including discontinuities, we use wavelets as basis functions. Wavelets are localized waves and they are considered to be more suitable for expressing steep gradient or discontinuous changes than global basis functions. For UQ in CFD, the Haar wavelet is first used for a stable/unstable bifurcation problem of Rayleigh-Benard convection (Le Maitre et al., 2004a). The method is then extended (Le Maitre et al., 2004b) to improve smooth variations as well using localized piecewise polynomial wavelets called MW, briefly described below. A set of mother wavelet is defined in the range $\xi \in [-1, 1]$ as,

$$
\psi^n_i (\xi) =
\begin{cases}
  f_i(\xi) & 0 \leq \xi \leq 1 \\
  (-1)^{i+N_p} f_i(-\xi), & -1 \leq \xi < 0 \\
  0 & \text{otherwise}
\end{cases}
$$

(6)

where $f_i(\xi)$ is an $N_p$-th order polynomial that satisfies the following two properties of vanishing moments (Eq. (7)) and orthonormality (Eq. (8)),

$$
\begin{align*}
\langle \psi^n_i, x^j \rangle &= 0, \quad 0 \leq i, j \leq N_p \\
\langle \psi^n_i, \psi^n_j \rangle &= \delta_{ij}.
\end{align*}
$$

(7)

(8)

For detailed procedure to satisfy Eqs. (7) and (8), see the article by Alpert (1993). The formulae for $N_p=2$ actually used in this study are given below,

$$
\begin{align*}
f_0 &= \frac{1}{\sqrt{2}} \left(30\xi^2 - 24\xi + 1\right), \\
f_1 &= \frac{1}{\sqrt{2}} \left(15\xi^2 + 1\right), \\
f_2 &= \frac{1}{\sqrt{2}} \left(12\xi^2 - 15\xi + 4\right).
\end{align*}
$$

(9)

Mother wavelets for the piecewise constant ($N_p=0$), i.e. Haar wavelet, and the MW of Eq. (9) are compared in Figs. 1 (a) and (b).
Wavelet family are then defined by translation (index $k$ below) and dilation (indexed $j$ below) of the mother wavelets as follows,

$$
\psi_{i,j,k}^{\eta}(\xi) = 2^{j/2} \psi_{i}^{\eta}(2^j \xi - k), \quad i = 0, 1, \cdots, N_p; \quad j = 0, 1, \cdots, N_r; \quad k = 0, 1, \cdots, 2^j - 1,
$$

(10)

where $N_r$ is the maximum resolution level. The complete MW bases are constructed using Legendre polynomials for the resolution level 0, and the MW Eq. (6) for the resolution level 1 or higher. Any random variable is expanded by the MW basis, in the common form as Eq. (1),

$$
u(t, x, \xi) = \sum_{m=0}^{P} u_m(t, x) \psi_m^\eta(\xi), \quad P = (N_p + 1)2^{N_r} - 1,
$$

(11)

where $\psi_m^\eta(\xi)$ for $0 \leq m \leq N_p$ denote Legendre polynomials up to order $N_p$, and $\psi_m^\eta(\xi)$ for $N_p < m \leq P$ denote the MW with the index $m$ defined as,

$$
m = (N_p + 1)(2^j + k) + i, \quad i = 0, 1, \cdots, N_p; \quad j = 0, 1, \cdots, N_r; \quad k = 0, 1, \cdots, 2^j - 1.
$$

(12)

As written above, a special case of $N_p=0$ corresponds to the spectral PCE with Legendre polynomials basis, and $N_p=0$ corresponds to the Haar wavelet, which are to be compared in the later section.

2.2 ME-PCE

A trouble of PCE for discontinuous problems in the stochastic space is also remedied by the ME method (Wan and Karniadakis, 2006). The stochastic space is divided into multiple elements and the results of independently analyzed PCE in each element are connected to represent the complicated response surface of output. The PCE analysis needs to be carried out for the number of intervals, but the calculation cost is essentially lower than that of MCS. The following procedure redefines both the PDF for each interval and the corresponding local orthogonal basis. First, the interval $[a, b]$ of the random variable $\xi$ is mapped to the new interval $[-1, 1]$ of the random variable $\tau$, and then the PDF $\bar{\rho}$ is obtained by the following equation:

$$
\bar{\xi} = \frac{b-a}{2} \tau + \frac{a+b}{2}
$$

(13)

$$
\bar{\rho} = \det \left[ \frac{\partial \bar{\xi}}{\partial \tau} \right] \frac{\bar{\rho}(\bar{\xi}(\tau))}{W(b) - W(a)}
$$

(14)

where $W(\bar{\xi})$ is a cumulative distribution function of $\bar{\rho}$. Next, a new basis function $\eta$ is obtained using the following recurrence formula which any orthogonal polynomial satisfies,

$$
\eta_{i+1}(\tau) = (\tau - \alpha_i)\eta_i(\tau) - \beta_i \eta_{i+1}(\tau), \quad i = 0, 1, \cdots
$$

(15)

$$
\eta_1(\tau) = 1, \quad \eta_0(\tau) = 0
$$

(16)

$$
\alpha_i = \frac{\langle \eta_i, \eta_i \rangle}{\langle \eta_0, \eta_i \rangle}, \quad i = 0, 1, \cdots
$$

(17)

$$
\beta_i = \frac{\langle \eta_i, \eta_i \rangle}{\langle \eta_{i+1}, \eta_{i+1} \rangle}, \quad i = 1, 2, \cdots
$$

(18)

The analyses of PCE in each interval are independent and can be run in parallel.

3. Governing equations

In this study, we quantify the effect of geometric uncertainty of the flow in a supersonic wind tunnel. It is modeled
by the inviscid, quasi-one-dimensional compressible flow equations as follows,

$$\frac{\partial (QC)}{\partial t} + \frac{\partial (FC)}{\partial x} = S,$$

(19)

where \( t \) is time, \( x \) is the spatial coordinate in the flow direction, \( Q \) is a conservative variables vector, \( F \) is a flux vector, \( S \) is a source term vector and \( C \) is the cross sectional area. As proposed by Petterson et al. (2014), unknown variables are first transformed from the conservative variables to ‘Roe variables’ (Roe, 2010a) \( \psi_i \) \((i=1, 2, 3)\) defined below,

$$\begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix} = \begin{bmatrix} \rho^{1/2} & \rho^{1/2}u & \rho^{1/2}H \end{bmatrix},$$

(20)

where \( \rho \) is the density, \( u \) is the velocity and \( H \) is the total enthalpy per unit mass. Components of the vectors \( Q, F \) and \( S \) in terms of Roe variables are written as follows,

$$\begin{align*}
Q &= \begin{bmatrix} w_1^2 & w_1w_2 & \frac{1}{2}w_1^2 + \frac{\gamma+1}{2\gamma}w_3^2 \\
   & w_2^2 & w_3^2 
\end{bmatrix}, \\
F &= \begin{bmatrix} w_1w_2 & w_2^2 & \frac{w_1}{\gamma}w_2 + \frac{\gamma+1}{2\gamma}w_3^2 \\
   & w_3^2 & w_3w_2 
\end{bmatrix}, \\
S &= \begin{bmatrix} 0 & 0 \\
   & \gamma \frac{w_1}{\gamma}w_3 + \frac{\gamma+1}{2\gamma}w_3^2 \frac{\partial C}{\partial x} & 0 
\end{bmatrix},
\end{align*}$$

(21)

where \( \gamma \) is the ratio of specific heats. In the intrusive PCE, all variables affected by the assumed uncertainties must be expanded by the basis function of the input random variable as in Eq. (11). If the initial or boundary conditions are the only sources of uncertainties, only unknown variables (Roe variables) need to be expanded. However, the present study extends it to include the cubic products of stochastic variables, the final form of the new components of the governing equations Eq. (19) are concisely written as follows,

$$\begin{align*}
CC &= \begin{bmatrix} A(C, \psi_i)w_i & A(C, \psi_j)w_j \\
   & A(C, \psi_k)w_k 
\end{bmatrix}, \\
CF &= \begin{bmatrix} \frac{\gamma-1}{\gamma}A(C, \psi_i)w_i + \frac{\gamma+1}{2\gamma}A(C, \psi_j)w_j \\
   & A(C, \psi_k)w_k 
\end{bmatrix}, \\
S &= \begin{bmatrix} 0 & 0 \\
   & \frac{\gamma-1}{\gamma} \frac{\partial C}{\partial x} w_3 + \frac{\gamma+1}{2\gamma}A(C, \psi_j)w_j 
\end{bmatrix},
\end{align*}$$

(23)

where bold faces denote the vectors of expansion coefficients, namely, \( \psi_i = [\psi_{i,0}, \psi_{i,1}, \ldots, \psi_{i,P}] \) \((i=1, 2, 3)\) and \( C = [C_1, C_2, \ldots, C_p] \), and the definition of \((P+1) \times (P+1)\) matrix \( A \) is written as,

$$[A(C, w_n)]_j = \left< \psi_i \psi_j \sum_l C_l \psi_l \sum_m w_m \psi_m \right>_i = \sum_i \sum_l w_m C_l \left< \psi_i \psi_j \psi_l \psi_i \right> \quad m=1, 2, 3$$

(24)
The system of governing equations is now comprised of $3 \times (P + 1)$ equations for the same number of unknowns $w_i$.

4. Numerical computation method

Finite volume method is used for the spatial discretization of Eq. (19). Roe’s flux difference splitting scheme is used for the numerical flux and MUSCL interpolation is used for the third-order spatial accuracy, detailed as follows.

The expansion coefficients of Roe variables $w_i$ ($i=1\sim3$) are interpolated to the cell interface by MUSCL, and then the flux Jacobian matrix necessary for the upwind scheme is defined as the derivatives of the new flux vector $CF$ in Eq. (23) with respect to the coefficients of Roe variables $w_i$. As in the deterministic equation, the flux Jacobian matrix are calculated with ‘Roe average’ values, which are arithmetic averages of $w_i$ on both sides of the cell interface, because all the elements of $CF$ are quadratic forms of the elements of $w_i$ (Roe, 1981). The eigen values and eigen vectors of the flux Jacobian matrix are calculated by the Intel MKL in this study. As for the time integration, two-step Runge-Kutta scheme is used to obtain steady state solutions.

The fourth-order tensors $<\psi_1/\psi_2/\psi_3/\psi_4>$ in Eq. (24) are pre-computed numerically by Gaussian quadrature and stored.

5. Results and discussion

The wind tunnel geometry in the flow direction $x$ is defined by the following formulae,

$$C(x) = \begin{cases} a - b \cdot \exp\{-\ln 2 \cdot x^2\} & 0 \leq x \leq 4 \\ a - (a-h) \cdot \exp\{-\ln 2 \cdot (x-8)^2\} & 4 \leq x \leq 8 \\ 1 - (1-h) \cdot \exp\{-\ln 2 \cdot (x-8)^2\} & 8 \leq x \leq 12 \end{cases}$$

where $h$ is the cross sectional area of the second throat explained below. The first throat is at the inlet ($x=0$) and the choking condition (flow Mach number 1) is fixed there. The nozzle expands till $x=4$ and the diffuser follows. The second throat of the diffuser is at $x=8$ to decelerate the supersonic flow in the test section and it serves to reduce the inlet-to-exit total pressure ratio in the operating condition. The area $h$ in Eq. (25) is assumed to have an uncertainty of a uniform PDF in the range $h \in [0.4, 0.5]$, and then it is expressed as a linear function of the standard random variable $\xi \in [-1,1]$ along with the average $\mu=0.45$ and the width $\Delta h = 0.5-0.4 = 0.1$ as follows,

$$h = \mu + \Delta h/2 \cdot \xi.$$ (26)

The expansion coefficients $C_{n}(x)$ in Eq. (22) for the respective orthonormal bases in Chapter 2 are obtained from Eq. (26).

Computational grids are composed of equally divided 150 cells in the domain $0 \leq x \leq 12$. Flow variables are non-dimensionalized by the inlet values. The density and pressure for the sonic flow at the inlet are $p_{\text{in}} = 1$ and $p_{\text{atm}} = 1/\gamma$ respectively. The initial condition of the computation is a uniform flow with the same values as the inlet. At the flow exit of $x=12$, the inlet-to-exit total pressure ratio is fixed at $p_{0,\text{in}}/p_{0,\text{out}} = 1.41$ and other variables are extrapolated from the interior. For the condition, the shock wave always exists between the second throat and the exit for the assumed range of $h$.

Figure 2 shows Mach number distributions of three computational results by the deterministic code for the nominal condition $h=\mu$, and other conditions $h = \mu \pm 0.05 \Delta h$. It also shows the corresponding geometries. Supersonic and subsonic regions are clearly distinguished by the Mach number. At the nominal condition, the flow expands to reach Mach number of 1.92 at $x=4$, and it is then isentropically compressed till the shock wave behind the second throat around $x=8.52$. A slightly wider second throat of $h = \mu + 0.05 \Delta h$ has little effect on the resulting flow. These two cases are ‘started’ states of the wind tunnel where a design Mach number is established in the test section at the end of nozzle. On the other hand, a slightly narrow second throat of $h = \mu - 0.05 \Delta h$ causes a drastic change in the result. The shock wave jumps far upstream to $x=2.36$. The supersonic flow at the test section has broken down and it is called ‘unstarted’ state. The subsonic flow behind the first shock wave is accelerated in the contraction part and it chokes again at the second throat, resulting in a second shock wave at $x=8.28$ behind the second throat.
Fig. 2  Wind tunnel geometries (bottom lines and the right ordinate) for the nominal, slightly wider and narrow second throat area, and corresponding Mach number distributions (upper lines and the left ordinate) by the deterministic code.

Table 1 lists the stochastic simulation methods in this study. MCS is regarded as the correct solution of UQ, and the others are PCE and its extensions described in Chapter 2.

| Abbreviation of the method | Notes |
|----------------------------|-------|
| 1. MCS                     | 400 runs of the deterministic code |
| 2. Legendre               | Single-element, spectral PCE (N_r=0, N_p=2) |
| 3. Haar                   | Haar-wavelet (N_r=3, N_p=0) |
| 4. MW                     | Multi-wavelet basis of N_r=3, N_p=2 |
| 5. ME                     | Equally divided N_r=2^3 elements (N_p=2) |

Figure 3 (a) shows pressure distributions on the x-ξ plane by MCS. It means the response surface of the pressure with respect to the change in the uncertainty input. It is colored in the range 0.27 ≤ p/p_{in} ≤ 1.35. As shown in Fig. 2, the response surface drastically changes depending on the started/unstarted states. Precise observation indicates that the boundary of the two states is at ξ=0.045, i.e. h=0.448. Figures 3 (b)-(e) are the results of PCEs listed in Table 1. The Legendre-spectral PCE in Fig. 3 (b) shows quite different tendencies from that of MCS. The result shows inability of globally continuous basis function to represent discontinuous responses. On the other hand, Figures 3 (c)-(e) qualitatively reproduce the complicated response surface of MCS. The Haar wavelet in Fig. 3 (c) is much better than Fig. 3 (b), but piecewise constant basis function in the stochastic space results in non-smooth and stair-like pressure distributions. The MW in Fig. 3 (d) and ME in Fig. 3 (e) recover the smooth contours also, but locally second order polynomials in the stochastic space cause some singular distributions near ξ=0.045. In Fig. 3 (e), stochastic space ξ [-1, 1] is divided equally into eight elements for the same resolution as the Haar and MW. Despite the independent analysis in each element, the resulting contour lines are smoothly connected at the element interfaces.

The average and standard deviation of the pressure along the flow directions are shown in Figs. 4 (a) and (b). Consistent with Figs. 3 (a)-(e), the Legendre-spectral PCE obviously differs from other results, while the other PCE’s follows MCS reasonably.

Other statistics in the flow sections are next investigated for more quantitative assessment of the employed methods. Figure 5 compares the pressure responses at x=4 with respect to the change in ξ. The Legendre-spectral PCE expresses the variation as a globally quadratic function of ξ. The stair-like variation by the Haar wavelet is suitable to represent discontinuous changes, although insufficient resolution of N_r=3 predicts the discontinuity at slightly different location of ξ=0. Both the MW and ME show localized quadratic variations in each of equally divided 2^3 sections in this study and the predicted responses are almost identical in Fig. 5. Figures 6 (a)-(e) show the PDF of pressure at the same location x=4. The PDF by the MW and ME in Figs. 6 (d) and (e), respectively, are close to Fig. 6 (a) despite the discrepancy near the discontinuity in Fig. 5.

Similarly, the pressure responses at x=8.44 and the PDF are shown in Fig. 7 and Figs. 8 (a)-(e). As shown in Fig. 7, the profile by the MCS shows rapid increases in the pressure in both negative and positive regions of ξ, in addition to
Fig. 3  Response surfaces of the streamwise pressure with respect to the geometry uncertainty of the wind tunnel.

Fig. 4  Average and standard deviation of the pressure along the flow direction $x$. 
Fig. 5  Response of the pressure with respect to the stochastic variable $\zeta$ at $x=4$.

Fig. 6  PDF of the pressure at $x=4$. 
Fig. 7  Response of the pressure with respect to the stochastic variable $\zeta$ at $x=8.44$.

Fig. 8  PDF of the pressure at $x=8.44$. 
the sudden decrease at $\xi=0.045$ observed in Fig. 5 as well. Two rapid increases are due to gradual traverse of the shock wave standing behind the second throat independent of the started/unstarted states, and the sudden decrease is due to a mode change from unstarted to started states. Tendencies of results by respective PCE’s are similar to Fig. 5, but the overshoot/undershoot of the pressure by the MW are more distinctively observed for the complicated profile at this flow section. The result of ME best agrees with the MCS. It is also true for the PDF in Figs. 8 (a)-(e). The ME predicts the four peaks and their location (frequently occurring pressure values) observed in the PDF of MCS, although one of the peaks at the highest pressure around $p/p_{\infty}=1.14$ is not distinctive. The other PCE results are rather different from the MCS.

The differences of the PDF of PCE’s from that of MCS, or errors, are quantitatively evaluated in the L1- and L2-norm as follows, for both results in Figs. 6 and 8.

$$L1 = \int_{p_{\text{min}}}^{p_{\text{max}}} |\text{PDF}_{\text{PCE}} - \text{PDF}_{\text{MCS}}| \Delta p \approx \sum_{n=1}^{N} (\text{PDF}_{\text{PCE},n} - \text{PDF}_{\text{MCS},n}) \Delta \tilde{p}$$

$$L2 = \sqrt{\int_{p_{\text{min}}}^{p_{\text{max}}} (\text{PDF}_{\text{PCE}} - \text{PDF}_{\text{MCS}})^2 \Delta p} = \sqrt{\sum_{n=1}^{N} (\text{PDF}_{\text{PCE},n} - \text{PDF}_{\text{MCS},n})^2 \Delta \tilde{p}}$$

where $\hat{p} = p/p_{\infty}$, the subscript PCE denotes one of the PCE methods, the overline $\overline{\text{PDF}}_{(\cdot),n}$ denotes the average of PDF in the small interval between $\hat{p}_{\text{min}} + (n-1)\Delta \hat{p}$ and $\hat{p}_{\text{min}} + n\Delta \hat{p}$, and $N = (\hat{p}_{\text{max}} - \hat{p}_{\text{min}})/\Delta \hat{p}$ with $\hat{p}_{\text{min}} = 0$, $\hat{p}_{\text{max}} = 1.6$ and $\Delta \hat{p} = 0.032$. The results are listed in Table 2. The errors of the ME are the smallest at both locations and both norms.

| PCE method | $x=4$, $L1 \times 10^{-2}$ | $x=4$, $L2 \times 10^{-2}$ | $x=8.44$, $L1 \times 10^{-2}$ | $x=8.44$, $L2 \times 10^{-2}$ |
|------------|-----------------|-----------------|-----------------|-----------------|
| Legendre   | 4.72            | 9.45            | 3.16            | 4.85            |
| Haar       | 1.58            | 3.13            | 4.61            | 6.54            |
| MW         | 0.69            | 1.29            | 3.25            | 4.67            |
| ME         | 0.69            | 1.27            | 1.19            | 1.95            |

6. Conclusion

Flow simulation methods to quantify the effect of input uncertainty using PCE and its extensions are developed and verified for quasi-one-dimensional compressible flows. The starting problem of a supersonic wind tunnel to establish a design flow condition is focused on. Governing equations for the intrusive PCE are derived to include a geometric uncertainty in a concise form. Following the approach of Roe variable transformation by Petterson et al. (2014), our equations uniformly includes fourth-order tensor that is pre-computed and stored in the simulations.

The starting problem includes strong discontinuities in the physical and stochastic space due to a shock wave and its sudden jump at the critical condition. We used two methods to handle the discontinuities, one is the PCE with MW basis and another is the ME-PCE, both localizing the basis function in the stochastic space. The Legendre polynomial basis, which has superior characters for smooth outputs, and Haar wavelet basis were also used and compared. The ME-PCE outperforms the other methods in terms of various statistic values and best predicts the result of MCS at much lower calculation costs. The improved performance of ME-PCE against the UQ problem with discontinuous outputs is not limited to the present study but a general result, and it will be used for future studies to try spatially multi-dimensional problem where the execution of the MCS is prohibitively high calculation cost.

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