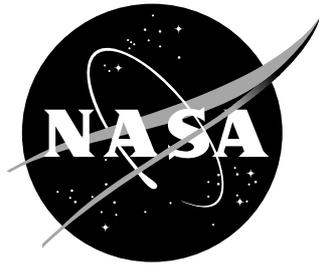


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A Stochastic Collocation Algorithm for Uncertainty Analysis

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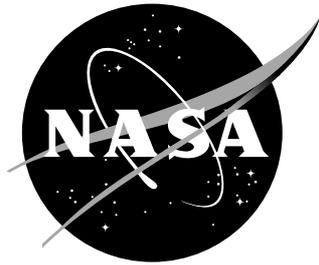
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Abstract

This report describes a stochastic collocation method to adequately handle a physically intrinsic uncertainty in the variables of a numerical simulation. For instance, while the standard Galerkin approach to Polynomial Chaos requires multi-dimensional summations over the stochastic basis functions, the stochastic collocation method enables to collapse those summations to a one-dimensional summation only. This report furnishes the essential algorithmic details of the new stochastic collocation method and provides as a numerical example the solution of the Riemann problem with the stochastic collocation method used for the discretization of the stochastic parameters.

1 Background

With the continuous development and improvement of both CFD simulations reliability and accuracy, further developments toward physically relevant results raise the need to account for more realistic operating conditions. Past simulations used deterministic parameters such as for the boundary conditions, initial conditions, geometry of the problem, physical properties, etc. Meanwhile, the actual conditions are not known precisely and one must account for a certain level in uncertainty in the simulations. In a more general framework, it is indeed of critical importance to quantify uncertainty (*e.g.* [9, 1, 17]) and establish a confidence interval for the simulation-based predictions or design ([3]). Unlike reliability analysis which deals with rare but catastrophic events, uncertainty analysis is concerned with the probabilistic aspects of the simulations due to the stochastic nature of physical parameters, initial and boundary conditions. Some sources of uncertainty identified in numerical simulations include:

- inaccuracy / indeterminacy of initial conditions (experimental data, variability of operating environment),
- bias in physical models (turbulence model),
- approximations in mathematical model (due to linearization or assumptions that neglect some physical effects such as temperature and/or pressure dependence of relevant physical parameters),
- uncertainty in describing the physical reality (errors in geometry, roughness, boundary conditions),
- discretization errors (numerical diffusion, round-off, algorithmic errors due to incomplete iteration process, etc.).

See [1] or [4] for a more complete review.

One crucial issue is to accurately propagate uncertainty from, say, the boundary conditions to the bulk field and finally to the output of the simulation. Several techniques have been proposed in the past. Among these, the currently most commonly used is the so-called perturbation technique that basically involves expanding the variables of the problem in terms of Taylor series around their mean value (*e.g.* [11]). Though effective, this technique is limited to Gaussian or weakly non-Gaussian processes due to the difficulty in incorporating terms of order higher than two. Still, this technique allows for a quick estimation of the low order statistics.

When one wants to get access to the full statistics, one can make use of the Monte Carlo technique. It is considered as an “exact” method for accounting for uncertainty in the sense that it does not require any approximations nor assumptions. The main advantages are that its convergence rate does not depend on the number of independent random variables and that its application is straightforward. However, it becomes intractable for large problems as it requires to carry thousands of simulations which results in prohibitive CPU time. Indeed, the resulting approximated variance of a σ^2 -variance random process is $\sigma_{MC}^2 = \sigma^2/n$ where n is the number of independent samples. Despite some techniques which improve the convergence

rate (Latin Hypercube, importance sampling, etc.), this last point prevents its use for most of the practical problems currently studied by CFD.

Another possibly viable approach consists in deriving the inverse of the stochastic operator (that represents the governing equations) by expanding it in a Neumann series. Meanwhile, the derivation of the Neumann series may however become difficult, if not impossible, for complex problems.

An alternative, and more effective, approach is the Polynomial Chaos. Originating in the work of Wiener (1938) and mainly applied in the field of structural mechanics, this technique is now making its way in the fluid mechanics community ([15, 16, 12, 14]). The basic idea is to project the variables of the problem onto a stochastic space spanned by a set of complete orthogonal polynomials Ψ that are functions of a random variable $\xi(\theta)$, where θ is a random event. The terms of the polynomials are functions of $\xi(\theta)$ and are thus functionals. Many random variables can be used: for example, $\xi(\theta)$ can be a Gaussian variable associated with Hermite polynomials. This is the original form of the Wiener work and is called homogeneous chaos. Other expansions are possible: Laguerre polynomials with a Gamma distributed variable, Jacobi polynomials with Beta distribution, etc. Obviously, the convergence rate, and thus the number of terms required for a given accuracy, depends both on the random process to be approximated and on the random variable used. This aspect was illustrated by [15].

Using this approach, each variable of the problem to simulate is expanded as, say for the velocity u :

$$u(\mathbf{x}, t, \theta) = \sum_{i=0}^{\infty} u_i(\mathbf{x}, t) \Psi_i(\xi(\theta)) . \quad (1)$$

For practical simulations, the series has to be truncated to a finite number of terms, hereafter denoted N_{PC} . This framework remains valid also for partially, or non-, correlated variables. In that case, the variables of the problem are functions of several independent random variables and ξ is now a vector. The general expression for the Hermite polynomial H is

$$H_p(\xi_{i_1}, \dots, \xi_{i_n}) = (-1)^p e^{\frac{1}{2} \xi^T \xi} \frac{\partial^p}{\partial \xi_{i_1} \dots \partial \xi_{i_n}} e^{-\frac{1}{2} \xi^T \xi} . \quad (2)$$

As discussed in [2], there is a one-to-one correspondence between functions $H_p(\xi_{i_1}, \dots, \xi_{i_n})$ and $\Psi_j(\xi(\theta))$.

The general expression for the Hermite Chaos is finally given by

$$u(\mathbf{x}, t, \theta) = \sum_{i=0}^{N_{PC}} u_i(\mathbf{x}, t) \Psi_i(\xi(\theta)) , \quad (3)$$

with the number of terms N_{PC} determined from

$$N_{PC} + 1 = \frac{(n_{pc} + p_{pc})!}{n_{pc}! p_{pc}!} , \quad (4)$$

where p_{pc} is the order of the expansion and n_{pc} the dimensionality. It follows that N_{PC} grows very quickly with the dimension and the order of the decomposition. As an example, for a second order, 2-D Hermite polynomial expansion, we get

$$u(\mathbf{x}, t, \theta) = u_0(\mathbf{x}, t) + u_1(\mathbf{x}, t) \xi_1(\theta) + u_2(\mathbf{x}, t) \xi_2(\theta) + u_3(\mathbf{x}, t) (\xi_1^2(\theta) - 1) + u_4(\mathbf{x}, t) \xi_1(\theta) \xi_2(\theta) + u_5(\mathbf{x}, t) (\xi_2^2(\theta) - 1) \quad (5)$$

where $\xi_1(\theta)$ and $\xi_2(\theta)$ are two independent random variables.

In the case of the Hermite polynomials, the *zeroth* order represents the mean value and the first order the Gaussian part while higher orders account for non-Gaussian contributions. The Hermite polynomials span a complete orthogonal set of basis functions in the stochastic space. The inner product is expressed as

$$\langle f_1(\boldsymbol{\xi}) f_2(\boldsymbol{\xi}) \rangle = \int_{-\infty}^{\infty} f_1(\boldsymbol{\xi}) f_2(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad (6)$$

where the weight function $w(\boldsymbol{\xi})$ is the n_{pc} -D normal distribution:

$$w(\boldsymbol{\xi}) = \frac{1}{\sqrt{(2\pi)^{n_{pc}}}} e^{-\frac{1}{2} \boldsymbol{\xi}^T \boldsymbol{\xi}}. \quad (7)$$

In the L_2 norm space, we thus get

$$\langle \Psi_i \Psi_j \rangle = \langle \Psi_i^2 \rangle \delta_{ij}, \quad (8)$$

where δ is the Kronecker operator.

2 Full Spectral Approach for Quasi 1-D Nozzle Flow

To illustrate the Polynomial Chaos approach and highlight the computational burden of the multidimensional stochastic summations, the Polynomial Chaos technique is derived here for a quasi 1-D nozzle flow. Mathelin and Hussaini ([7]) have presented results for inviscid quasi 1-D nozzle flow solutions using Polynomial Chaos.

The system of compressible Euler equations in conservative form is

$$\mathbf{Q}_t + \mathbf{F}_x = \mathbf{S}, \quad (9)$$

where

$$\mathbf{Q} = \begin{pmatrix} \rho A \\ \rho u A \\ \rho E A \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} \rho u A \\ \rho u^2 A + P A \\ \rho u E A + P u A \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} 0 \\ P \partial A / \partial x \\ 0 \end{pmatrix}, \quad (10)$$

with ρ the density, u the velocity, A the cross-section area, P the static pressure and E the total energy.

The pressure can be removed from the above equations making use of the following equation:

$$E = \frac{P}{(\gamma - 1)\rho} + \frac{1}{2} u^2. \quad (11)$$

Equation (9) thus becomes

$$\mathbf{Q} = \begin{pmatrix} \rho A \\ \rho u A \\ \rho E A \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} \rho u A \\ \frac{3-\gamma}{2} \rho u^2 A + (\gamma - 1) \rho E A \\ \gamma \rho u E A - \frac{\gamma-1}{2} \rho u^3 A \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} 0 \\ (\gamma - 1) \left[\rho E - \frac{\rho u^2}{2} \right] \partial A / \partial x \\ 0 \end{pmatrix}. \quad (12)$$

The Euler equations are discretized in space using the spectral element method. This spatial discretization is consistent with the spectral expansion involved in the Polynomial Chaos technique. Equation (9) is projected onto a spectral and stochastic basis and the Galerkin technique is applied. The spectral space is spanned by Chebyshev polynomials on points (in local coordinates $\bar{x} \in [-1, 1]$):

$$\bar{x}_n = \cos\left(\frac{\pi n}{N}\right) \quad \forall n \in [0; N] \subset \mathbb{N}, \quad (13)$$

where N is the number of points within each element. The interpolants of variables, say u , in spectral space read as

$$u(\bar{x}, t) = \sum_{n=0}^N u_n(t) h_n(\bar{x}). \quad (14)$$

where

$$h_n(\bar{x}) = \frac{2}{N} \sum_{m=0}^N \frac{1}{\bar{c}_n \bar{c}_m} T_m(\bar{x}_n) T_m(\bar{x}), \quad (15)$$

with T_m the Chebyshev polynomials and \bar{c}_i such as

$$\bar{c}_i = 2 \quad i \in \{0; N\} \quad (16)$$

$$\bar{c}_i = 1 \quad i \in]0; N[\subset \mathbb{N}. \quad (17)$$

Similarly, in the stochastic space,

$$u(\theta, x, t) = \sum_{i=0}^{N_{PC}} u_i(x, t) \Psi_i(\xi(\theta)). \quad (18)$$

After rearrangement, it finally follows:

$$\mathbf{Q} = \left(\begin{array}{c} \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{n=0}^N \rho_{i,n} A_j \langle \Psi_i \Psi_j \Psi_l \rangle (h_n, h_p) \\ \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \rho_{i,n} u_{j,m} A_k \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle (h_n, h_m, h_p) \\ \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \rho_{i,n} E_{j,m} A_k \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle (h_n, h_m, h_p) \end{array} \right) \quad \forall \{l \in [0; N_{PC}], p \in [0; N]\} \subset \mathbb{N} \quad (19)$$

$$\mathbf{S} = \left(\begin{array}{c} 0 \\ (\gamma - 1) \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \rho_{i,n} E_{j,m} \frac{\partial A_k}{\partial x} \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle (h_n, h_m, h_p) \\ -\frac{\gamma - 1}{2} \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{r=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \sum_{o=0}^N \rho_{i,n} u_{j,m} u_{k,o} \frac{\partial A_r}{\partial x} \langle \Psi_i \Psi_j \Psi_k \Psi_r \Psi_l \rangle (h_n, h_m, h_o, h_p) \\ 0 \end{array} \right) \quad (20)$$

$$\frac{\partial \mathbf{F}}{\partial x} = \left(\begin{aligned}
& \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \rho_{i,n} u_{j,m} \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle \left[(h_n, h_m, h_p) \frac{\partial A_k}{\partial x} + A_k \left(\left(\frac{\partial h_n}{\partial x}, h_m, h_p \right) + \left(h_n, \frac{\partial h_m}{\partial x}, h_p \right) \right) \right] \\
& \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{r=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \sum_{o=0}^N \frac{3-\gamma}{2} \rho_{i,n} u_{j,m} u_{k,o} \langle \Psi_i \Psi_j \Psi_k \Psi_r \Psi_l \rangle \left[(h_n, h_m, h_o, h_p) \frac{\partial A_k}{\partial x} + A_k \left(\left(\frac{\partial h_n}{\partial x}, h_m, h_o, h_p \right) + \left(h_n, \frac{\partial h_m}{\partial x}, h_o, h_p \right) + \left(h_n, h_m, \frac{\partial h_o}{\partial x}, h_p \right) \right) \right] + \\
& (\gamma - 1) \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \rho_{i,n} E_{j,m} \langle \Psi_i \Psi_j \Psi_k \Psi_l \rangle \left[(h_n, h_m, h_p) \frac{\partial A_k}{\partial x} + A_k \left(\left(\frac{\partial h_n}{\partial x}, h_m, h_p \right) + \left(h_n, \frac{\partial h_m}{\partial x}, h_p \right) \right) \right] \\
& \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{r=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \sum_{o=0}^N \gamma \rho_{i,n} u_{j,m} E_{k,o} \langle \Psi_i \Psi_j \Psi_k \Psi_r \Psi_l \rangle \left[(h_n, h_m, h_o, h_p) \frac{\partial A_k}{\partial x} + A_k \left(\left(\frac{\partial h_n}{\partial x}, h_m, h_o, h_p \right) + \left(h_n, \frac{\partial h_m}{\partial x}, h_o, h_p \right) + \left(h_n, h_m, \frac{\partial h_o}{\partial x}, h_p \right) \right) \right] - \\
& \frac{\gamma - 1}{2} \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} \sum_{k=0}^{N_{PC}} \sum_{r=0}^{N_{PC}} \sum_{s=0}^{N_{PC}} \sum_{n=0}^N \sum_{m=0}^N \sum_{o=0}^N \sum_{q=0}^N \rho_{i,n} u_{j,m} u_{k,o} u_{r,q} \langle \Psi_i \Psi_j \Psi_k \Psi_r \Psi_s \Psi_l \rangle \\
& \left[(h_n, h_m, h_o, h_q, h_p) \frac{\partial A_k}{\partial x} + A_k \left(\left(\frac{\partial h_n}{\partial x}, h_m, h_o, h_q, h_p \right) + \left(h_n, \frac{\partial h_m}{\partial x}, h_o, h_q, h_p \right) + \left(h_n, h_m, \frac{\partial h_o}{\partial x}, h_q, h_p \right) + \left(h_n, h_m, h_o, \frac{\partial h_q}{\partial x}, h_p \right) \right) \right]
\end{aligned} \right) \quad (21)$$

where γ is the specific heat ratio ($\gamma = 1.4$ for diatomic gas).

The scalar products in the spectral space are defined by, say for (h_n, h_m, h_o)

$$\begin{aligned}
(h_n, h_m, h_o) &= \int_{-1}^1 h_n(\bar{x}) h_m(\bar{x}) h_o(\bar{x}) d\bar{x} \\
&= \frac{8}{N^3} \sum_{a=0}^N \sum_{b=0}^N \sum_{c=0}^N \frac{T_a(\bar{x}_n) T_b(\bar{x}_m) T_c(\bar{x}_o)}{\bar{c}_a \bar{c}_b \bar{c}_c \bar{c}_n \bar{c}_m \bar{c}_o} \int_{-1}^1 T_a(\bar{x}) T_b(\bar{x}) T_c(\bar{x}) d\bar{x}.
\end{aligned} \quad (22)$$

The nonlinearity in the inviscid momentum flux results in a 9-dimensional summation in Eq. (21). Five of these sums are due to the Polynomial Chaos expansion, and would remain even for a simple finite difference spatial discretization. For the extension of this problem to turbulent, viscous flow (see Mathelin, *et al.* [8]), the corresponding equation for the turbulent kinetic energy contains a 12-dimensional sum, with seven of these due to the Polynomial Chaos terms.

For this problem all the nonlinearities are of polynomial type. For the Riemann problem, a fundamental component of many modern algorithms for solving Euler and Navier-Stokes equations, the nonlinearities are more complex. The appropriate approach to this for Polynomial Chaos methods is not obvious.

3 Stochastic Collocation Method

The stochastic collocation method was developed to enable application to Spectral Discontinuous Galerkin Methods (for which solution of the Riemann problem is a necessity) as well as to reduce the cost of Polynomial Chaos methods for more classical discretizations, such as described above for quasi 1-D nozzle flow.

Let a and b be two independent random variables. In the Polynomial Chaos method, the infinite series for each variable would be expressed as, say, for a ,

$$a = \sum_{i=0}^{\infty} a_i \Psi_i(\xi), \quad (23)$$

and the product ab would be

$$ab = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_i b_j \Psi_i(\xi) \Psi_j(\xi). \quad (24)$$

(Here we drop any dependence upon x and t and concentrate on just the random variable ξ without reference to the random event parameter θ .)

The finite series for a is then

$$a = \sum_{i=0}^{N_{PC}} a_i \Psi_i(\xi). \quad (25)$$

The usual Galerkin truncation yields for the expansion coefficients of the product $c = ab$

$$(ab)_k = \sum_{i=0}^{N_{PC}} \sum_{j=0}^{N_{PC}} a_i b_j \langle \Psi_i \Psi_j \Psi_k \rangle \quad \forall k \in [0; N_{PC}] \subset \mathbb{N}. \quad (26)$$

Therefore, computing the $N_{PC} + 1$ coefficients of the product ab takes of order N_{PC}^3 operations. The complexity is even greater for cubic products. Moreover, for non-polynomial nonlinearities, such as those that arise in the Riemann problem, the Galerkin truncation is not obvious.

For traditional deterministic problems, these difficulties are often treated by resorting to a collocation method instead of the Galerkin method. The usual spatial collocation approach consists of projecting the equations into the physical space (\bar{x}). But a “physical space” corresponding to the random variable ξ has limited physical meaning, and the spatial scheme cannot be directly transformed. To deal with this problem, we define a new stochastic space whose properties are known.

In the stochastic collocation method (SCM) one lets the Probability Density Function (PDF) of the random variable ξ serve as the basis for the transformation between the physical random variable ξ and its artificial stochastic space. We use α to denote a point in this artificial stochastic space. The range of the corresponding Cumulative Distribution Function (CDF) is $[0,1]$, and provided that the underlying PDF is non-zero in the interior of its domain, the CDF is strictly monotonic and therefore this transformation is bijective. Denote the CDF of ξ by $\mathcal{F}_\xi(\xi)$. We prefer to map the CDF to the standard domain $[-1,1]$ of orthogonal polynomials, and so we define

$$F_\xi(\xi) = 2\mathcal{F}_\xi(\xi) - 1. \quad (27)$$

Finally, denote the inverse of F_ξ by G_ξ . Let α be a point in the domain $[-1,1]$ of G . This is the new, known stochastic space that is the foundation of the SCM. We have then

$$\alpha = F_\xi(\xi) = 2\mathcal{F}_\xi(\xi) - 1 \quad (28)$$

and

$$\xi = G_\xi(\alpha). \quad (29)$$

The SCM utilizes collocation points $\alpha_i, i = 0, \dots, N_q$, in $[-1,1]$. These have associated quadrature weights w_i , chosen to give the best approximation to inner products on $[-1,1]$. In the present work we make the

particular choice of the Gauss-Legendre points and weights. The collocation points in the stochastic space are associated with the points $\xi_i, i = 0, \dots, N_q$, in random variable space according to (29).

Let us return now to the example of evaluating the product of two random variables a and b . First we construct the appropriate mapping functions, F_a and F_b (and also their inverses G_a and G_b), from the PDFs of a and b . Second, we evaluate a and b at the points α_i , obtaining

$$\begin{aligned} a_i &= G_a(\alpha_i) \quad i = 0, \dots, N_q \\ b_i &= G_b(\alpha_i) \quad i = 0, \dots, N_q. \end{aligned} \quad (30)$$

These functions are then approximated in α -space by their interpolating polynomials, as for example,

$$a^{N_q}(\alpha) = \sum_{j=0}^{N_q} a_j h_j(\alpha), \quad (31)$$

where the functions h_i are the classical Lagrange interpolants based on the $N_q + 1$ collocation points, i.e., h_j is a polynomial of degree N_q and $h_j(\alpha_i) = \delta_{ij}$.

The representation of the product $c = ab$ associated with a Galerkin method would be

$$\langle a^{N_q} b^{N_q} h_k \rangle = \sum_{i=0}^{N_q} \sum_{j=0}^{N_q} a_i b_j \langle h_i h_j h_k \rangle. \quad (32)$$

But in the SCM we resort to the quadrature rule to approximate this as

$$\begin{aligned} \langle a^{N_q} b^{N_q} h_k \rangle &\simeq \sum_{l=0}^{N_q} \sum_{i=0}^{N_q} \sum_{j=0}^{N_q} a_i b_j h_i(\alpha_l) h_j(\alpha_l) h_k(\alpha_l) w_l \\ &= \sum_{l=0}^{N_q} \sum_{i=0}^{N_q} \sum_{j=0}^{N_q} a_i b_j \delta_{il} \delta_{jl} \delta_{kl} w_l \\ &= a_k b_k w_k. \end{aligned} \quad (33)$$

So, the representation of the product is just

$$G_c(\alpha) \equiv c^{N_q}(\alpha) = \sum_{k=0}^{N_q} (a_k b_k w_k) h_k(\alpha). \quad (34)$$

The last step is to map this result back into the random variable space to obtain the approximate CDF of $c = ab$. Recall that (34) gives the representation in α -space of the random variable c . We now need to back out the CDF of c from the transformation rules (28) and (29). (In these equations we make the appropriate identification $\xi = c$.) We have, finally, for the CDF, \mathcal{F}_c , of c

$$\begin{aligned} \mathcal{F}_c(c) &= \frac{1}{2} (F_c(c) + 1) \\ &= \frac{1}{2} (G_c^{-1}(\alpha) + 1), \end{aligned} \quad (35)$$

recalling that F_c is the inverse function of G_c . The PDF of c is then readily obtained by differentiation of (35).

In our present implementation of the SCM we use standard interpolation methods for the mappings (28) and (35). For the forward mapping we start with a uniform distribution of the ξ_i (a_i in our example) for representing the PDF of ξ . We base the interpolant for the inverse mapping on the collocation points α_i , in which case we have

$$G_c(\alpha_i) = a_i b_i w_i \quad i = 0, \dots, N_q, \quad (36)$$

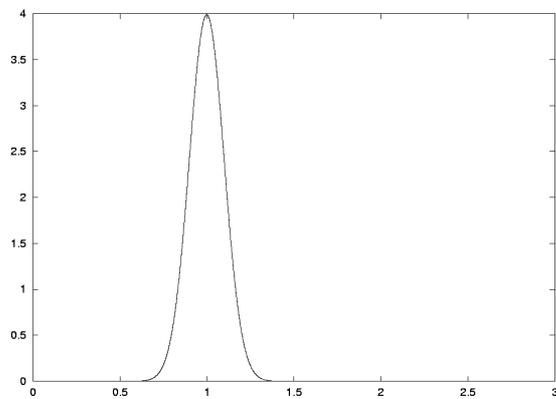
since $h_k(\alpha_i) = \delta_{ik}$.

The complexity of this implementation of the SCM in one dimension is N_q , regardless of the form of the nonlinearity. In contrast the Galerkin method already scales as N_{PC}^3 for a simple quadratic nonlinearity. The quadrature in the stochastic collocation method does introduce additional errors compared with those of the Galerkin method, but these are reduced as N_q increases. This is usually not a major issue since the collocation scheme allows for dramatic speed-up compared to full Galerkin approach and a relatively high value for N_q is affordable.

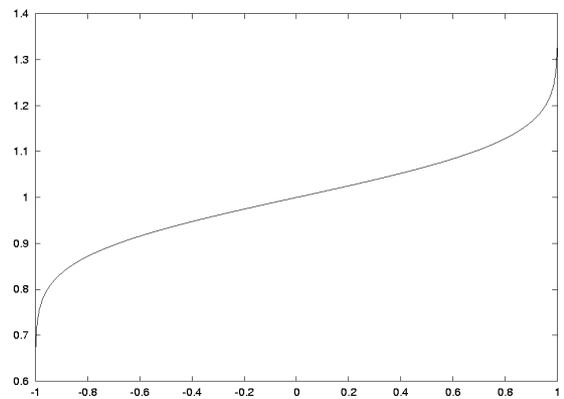
As an example of this process, consider the cubic equation

$$f(u) = u^3, \quad (37)$$

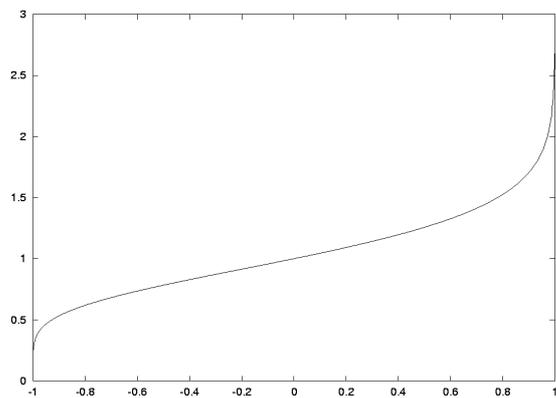
where u is a Gaussian random variable, with mean 1.0 and standard deviation of $1/(2\sqrt{\pi})$. Figure 1 shows the PDF of u , the α -representation of u , the α -representation of $f(u) = u^3$, and the corresponding PDF of $f(u)$.



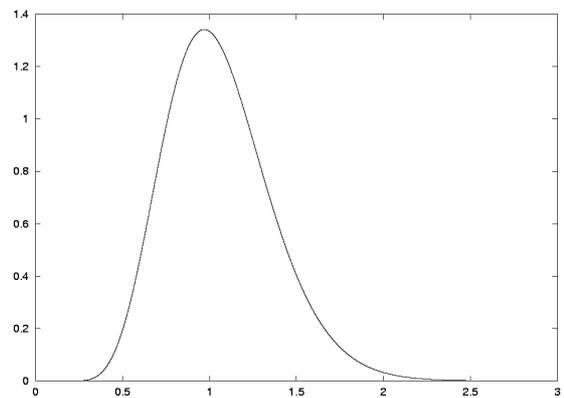
(a) PDF of input function u .



(b) Projection of the input function into the α -space.



(c) Output function $f(u)$ in the α -space



(d) PDF of output function $f(u)$.

Figure 1: Illustration of stochastic collocation for $f(u) = u^3$.

4 Application to Stochastic Riemann Solver

To illustrate the applicability of the above method, the stochastic Riemann problem is considered here. The field variables are assumed to be discontinuous at a time t and this leads to the generation of shock wave, rarefaction and expansion fan. See Landau & Lifshitz ([5]) or Liepmann & Roshko ([6]) for a review of the physical phenomena involved. To compute the resulting state for later times, one can make use of the algorithm proposed by Sod ([10]). It produces strongly non-linear equations including rational powers and conditional expressions. While straightforward in a deterministic space, the application of such an algorithm becomes very tricky with a stochastic approach. For example, two expressions are to be applied depending on the pressure ratio: if $P^*/P > 1$, then use equation (a) and if $P^*/P < 1$, then use equation (b). But when both pressures are non-deterministic, what does $P^*/P > 1$ or $P^*/P < 1$ mean ?

Using the collocation scheme, the pressure ratio now has a deterministic expression in the α -space and it is possible to determine the resulting state. Figures 2 through 4 show the propagation of the stochastic description of the state across the discontinuity, *i.e.*, the stochastic collocation solution of the stochastic Riemann problem. In these computations $N_q = 200$.

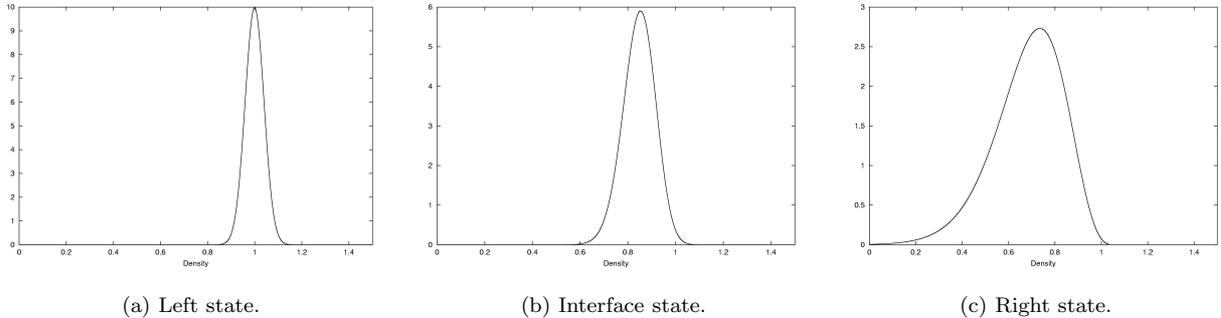


Figure 2: Density PDF evolution throughout a discontinuity.

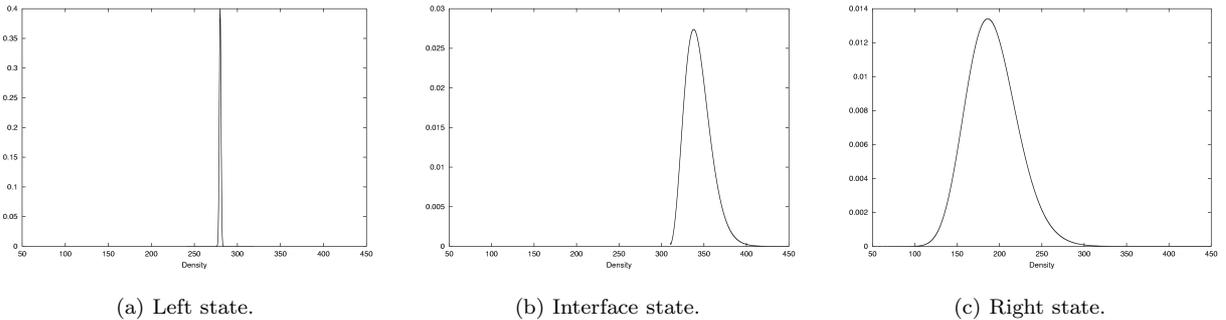


Figure 3: Velocity PDF evolution throughout a discontinuity.

Preliminary results from Mathelin, *et al.* ([8]) indicate that substantial CPU savings have been achieved by the stochastic collocation method in Polynomial Chaos solutions of quasi 1-D nozzle flow. In their simplest case, Euler flow, the computational time was reduced by a factor of 4. The computational savings is strongly dependent upon the discretization parameters. More details are available in [8].

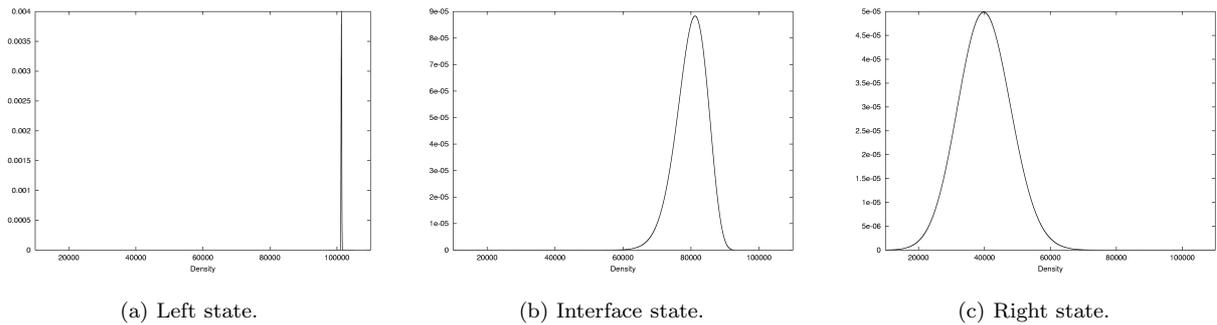


Figure 4: Pressure PDF evolution throughout a discontinuity.

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References

- [1] H. W. COLEMAN AND F. STERN, *Uncertainties and CFD code validation*, J. Fluids Eng., 119 (1997), pp. 795–803.
- [2] R. G. GHANEM AND P. D. SPANOS, *Stochastic finite elements: a spectral approach*, Springer-Verlag, New-York, 1991.
- [3] L. HUYSE, *Free-form airfoil shape optimization under uncertainty using maximum expected value and second-order second-moment strategies*, ICASE Report No. 2001–18, 2001.
- [4] U. B. MEHTA, *Some aspects of uncertainty in computational fluid dynamics results*, J. Fluids Eng., 113 (1991), pp. 538–543.
- [5] L. D. LANDAU AND E. M. LIFSHITZ, *Course of theoretical physics. Vol.6. Fluid mechanics*, Pergamon press, Oxford, 1982.
- [6] H. W. LIEPMANN AND A. ROSHKO, *Elements of gas dynamics*, Wiley, New-York, 1957.
- [7] L. MATHELIN AND M. Y. HUSSAINI, *Uncertainty quantification in CFD simulations: a stochastic spectral approach*, 2nd International Conference on Computational Fluid Dynamics, Sydney, Australia, July 15-19, 2002.
- [8] L. MATHELIN, M. Y. HUSSAINI, T. A. ZANG AND F. BATAILLE, *Uncertainty propagation for turbulent, compressible flow in a quasi-1D nozzle using polynomial chaos*, AIAA-2003-4240, 16th AIAA CFD Conference, Orlando, FL, June 23-26, 2003.
- [9] P.J. ROACHE, *Perspective: a method for uniform reporting of grid refinements studies*, J. Fluids Eng., 116 (1994), pp. 405–413.
- [10] G. A. SOD, *A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws*, J. Comput. Phys., 27 (1978), pp. 1–31.
- [11] A. C. TAYLOR, L. L. GREEN, P. A. NEWMAN AND M. M. PUTKO, *Some advanced concepts in discrete aerodynamic sensitivity analysis*, AIAA-2001-2529, 2001.

- [12] R. W. WALTERS AND L. HUYSE, *Uncertainty analysis for fluid mechanics with applications*, ICASE Report No. 2002-1, 2002.
- [13] N. WIENER, *The homogeneous chaos*, Amer. J. Math., 60 (1938), pp. 897–936.
- [14] D. XIU, D. LUCOR, C.-H. SU AND G. EM. KARNIADAKIS, *Stochastic modeling of flow-structure interactions using generalized polynomial chaos*, J. Fluids Eng., 124(1) (2002), pp. 51–59.
- [15] D. XIU AND G. EM. KARNIADAKIS, *The Wiener-Askey polynomial chaos for stochastic differential equations*, SIAM J. Sci. Comput. 24(2), (2002), pp. 619–644.
- [16] D. XIU D. AND G. EM. KARNIADAKIS, *Modeling uncertainty in flow simulations via generalized polynomial chaos*, J. Comput. Phys. (2002), to appear.
- [17] H. C. YEE AND P. K. SWEBY, *Aspects of numerical uncertainties in time marching to steady-state numerical solutions*, AIAA J., 36(5) (1998), pp. 712–724.

