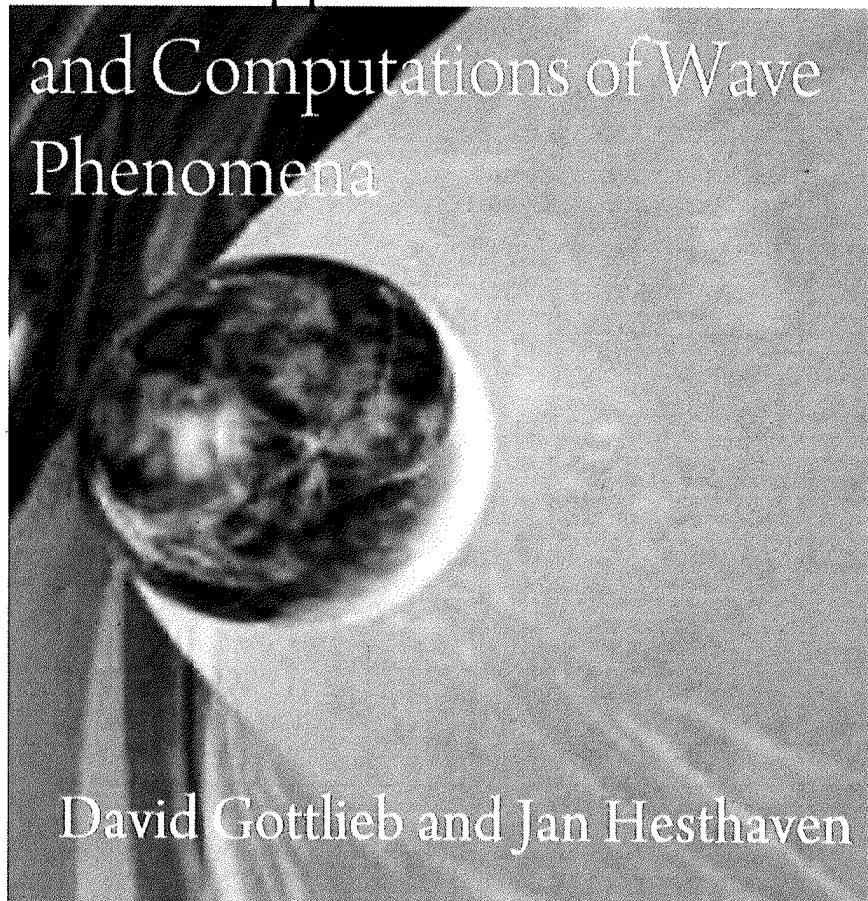


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Novel Approaches to the Modeling and Computations of Wave Phenomena



David Gottlieb and Jan Hesthaven

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Final Technical Report

Abstract

The aim of this project was to develop and study numerical methods for the solutions of hyperbolic equations that include uncertainties. In particular application to electromagnetics waves have been considered. The following results were obtained during this research: 1. The nature of the deterministic systems resulting from applying the polynomial chaos method to an hyperbolic system was clarified, and in particular the role of the boundary conditions. 2. The evolution of the probability density functions of uncertainties in problems described by hyperbolic systems was found, and an application to the Maxwells equations of electromagnetics had been carried out. 3. Reduced basis methods have been applied to several wave propagation problems.

1 Galerkin Method for Wave Equations with Uncertainty

In [10] the polynomial chaos method applied to wave problems have been considered. In recent years there is a growing interests in studying efficient numerical methods for solving differential equations with random inputs. Many approaches can be employed, among which the Polynomial Chaos (PC) based methods have received intensive attention. The original PC method was developed by R. Ghanem and was inspired by the Wiener chaos expansion which uses Hermite polynomials of Gaussian random variables to represent random processes. Later the approach was extended to generalized Polynomial Chaos (gPC) where general orthogonal polynomials are adopted for improved representations of more general random processes. With PC/gPC serving as a complete basis to represent random processes, a stochastic Galerkin projection can be used to transform the (stochastic) governing equations to a set of deterministic equations that can be readily discretized via standard numerical techniques. Although such a Galerkin approach is effective in many problems, its application to hyperbolic problems is limited. The primary reason is because the properties of the resulting system of equations from a Galerkin projection is not fully understood. When uncertainty does not change the direction of the characteristics, the Galerkin system can be shown to be hyperbolic and solved in a straightforward manner.

We studied the application of the gPC Galerkin method to the simulations of hyperbolic systems that contain uncertainties. In general these uncertainties may enter through initial conditions, boundary conditions or through uncertainties in the coefficients of the problem. In solving numerically the Maxwell's equations of electromagnetics, for example, one often faces uncertain material properties or small scales

that can not be resolved and have to be modeled statistically. Here we deal with the case that the coefficients are functions of random variables. In particular we use a scale wave equation as a model and study the situation in which the inflow-outflow conditions change as a function of a random variable.

We have shown that the deterministic system is a symmetric hyperbolic system with positive as well negative eigenvalues. A consistent and stable method of imposing the boundary conditions is outlined. The boundary conditions are not satisfied exactly at the boundaries but rather to the order of the scheme. Convergence of the scheme is established.

A simple scalar equation that illustrates the difficulties in applying the (generalized) Polynomial Chaos to hyperbolic equations is:

$$\frac{\partial u(x, t, y)}{\partial t} = c(y) \frac{\partial u(x, t, y)}{\partial x}, \quad x \in (-1, 1), \quad t > 0, \quad (1)$$

where $c(y)$ is a random transport velocity of a random variable $y \in \Omega$ in a properly defined complete random space with event space Ω and probability distribution function $\rho(y)$. With this the expectation of a given function is $\mathbb{E}[f(y)] = \int f(y)\rho(y)dy$.

The initial condition is given by

$$u(x, 0, y) = u_0(x, y). \quad (2)$$

The boundary conditions are more complicated as they depend on the sign of the random transport velocity $c(y)$. A well posed set of boundary conditions is given by:

$$\begin{aligned} u(1, t, y) &= u_R(t, y) & c(y) > 0, \\ u(-1, t, y) &= u_L(t, y) & c(y) < 0. \end{aligned}$$

Equations (1)–(3) complete the setup of the problem.

For simplicity we will discuss the case of random variable y with beta distribution in $(-1, 1)$ (upon proper scaling). In this case the expansion functions P_k are the (normalized) Jacobi polynomials. (Note this includes the special case of Legendre polynomials with uniformly distributed random variable y .)

In the gPC Galerkin method we seek an approximation to the true solution via a finite-term gPC expansion

$$v(x, t, y) = \sum_{k=0}^N \hat{v}_k(x, t) P_k(y) \quad (3)$$

and project

$$\frac{\partial v(x, t, y)}{\partial t} - c(y) \frac{\partial v(x, t, y)}{\partial x} = 0$$

onto the subspace spanned by the first $(N + 1)$ gPC basis polynomials and obtain the following system

$$\frac{\partial \hat{v}_j(x, t)}{\partial t} = \sum_{k=0}^N a_{j,k} \frac{\partial \hat{v}_k(x, t)}{\partial x}, \quad j = 0, \dots, N. \quad (4)$$

If we denote by $\mathbf{A}$ the $(N + 1) \times (N + 1)$ matrix whose entries are $\{a_{j,k}\}_{0 \leq j,k \leq N}$ and $\mathbf{v} = (\hat{v}_0, \dots, \hat{v}_N)^T$ a vector of length $(N + 1)$, then system (4) can be written as

$$\frac{\partial \mathbf{v}(x, t)}{\partial t} = \mathbf{A} \frac{\partial \mathbf{v}(x, t)}{\partial x}. \quad (5)$$

Note that from the definition $a_{jk} = a_{kj}$, i.e., $\mathbf{A} = \mathbf{A}^T$, the system (5) is therefore *symmetric hyperbolic*, this is consistent with the fact that the original equation (1) is hyperbolic for each realization of y .

A less trivial question is the nature of the inflow-outflow boundary conditions. The boundary conditions for the original scalar equation (1) depend on the particular realization of the random variable y (see (3)). However upon the Galerkin projection in the random dimension the deterministic system (5) is independent of y . In Theorem 1 we investigate how the inflow-outflow conditions are reflected in the system (5).

Theorem 1:

Consider the deterministic system (5) where the coefficients a_{jk} are defined. Then if $c(y) \geq 0$ (reps. $c(y) \leq 0$) for all y , then the eigenvalues of $\mathbf{A}$ are all non-negative (reps. non-positive); if $c(y)$ changes sign, i.e., $c(y) > 0$ for some y and $c(y) < 0$ for some other y , then $\mathbf{A}$ has both positive and negative eigenvalues.

Based on Theorem 1 have developed a stable way of employing boundary conditions for the GPC method for hyperbolic systems of equations. A detailed discussion is presented in [10]

2 Evolution of PDF for Hyperbolic Equations with Uncertainties

In [12] the evolution of the probability density function was considered for PDEs that simulate wave phenomena containing uncertainties .

Hyperbolic equations (such that the Euler equations of gas dynamics or the Maxwell's equations of electromagnetics) may contain uncertainties in the coefficients of the equations or in the data (initial or boundary conditions). One way of treating these uncertainties is to model them by random variables with some known distributions. However, even if the initial distributions are known, the probabilistic properties of the solution changes in time. We propose to study this behavior in order to understand the time development of the solutions.

In [12] the cumulative (or probability) distribution function (CDF) of the output solutions of some one-dimensional wave equations fluctuating by the random changes in the media parameters was computed. We will review here this work.

The numerical tool to handle randomness, we employ the technique of the so-called *polynomial chaos (PC) expansions*. The main advantage of the PC expansions is that we separate the deterministic and the non-deterministic parts in the functions u so that we can compute numerically each PC mode $u_k(x, t)$; we only have to compute the PC modes once instead of evaluating the output solution for each ξ^i .

We work with both the exact solutions and the numerical ones of the one-dimensional problems. We then compare the statistics for both solutions (e.g. PDF, CDF, mean, variance and moment generating function, e.t.c.).

Although in general the explicit solutions of PDE are not available or of some complicated forms, some known solutions can validate the numerical (or experimental) solutions. Furthermore, we can derive explicitly the probability distribution/density functions of output solutions and we can then trace down how the randomness in the input data affects the output. We also derive the moment generating function, mean and variance.

We considered the 1-D Maxwell equations for $(u, v)^T = (u^\xi(x, t), v^\xi(x, t))^T$ in $\Omega =$

$(-\infty, \infty) \times (0, \infty)$:

$$\begin{cases} \begin{pmatrix} u \\ v \end{pmatrix}_t = \begin{pmatrix} 0 & \frac{1}{\mu} \\ \frac{1}{\epsilon} & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}_x \text{ in } \Omega, \\ u(x, 0) = h_1(x), \\ v(x, 0) = h_2(x), \end{cases} \quad (2.1)$$

where (permeability, permittivity) = $(\mu, \epsilon) = (\mu_1, \epsilon_1)$ for $x \leq \xi$ and $= (\mu_2, \epsilon_2)$ for $x > \xi$, $\mu_1, \mu_2, \epsilon_1, \epsilon_2 > 0$, ξ is a random variable and has a uniform PDF $g(\xi) = \frac{1}{2}\chi_{[-1,1]}(\xi)$. Let $c = 1/\sqrt{\epsilon\mu}$, $c_1 = 1/\sqrt{\epsilon_1\mu_1}$ and $c_2 = 1/\sqrt{\epsilon_2\mu_2}$ with $c_1 \neq c_2$.

We found the distribution function $F(s)$ for the output u . By definition, we have

$$F(s) = P(u \leq s) = \sum_{j=0}^3 P(u \leq s, (x, t) \in \Omega_j). \quad (2.2)$$

We can deduce the distribution function F . For example, if $h_1(x) = x$, $h_2(x) = 2x$, $\mu_1 = \epsilon_1 = 1$, $\mu_2 = \epsilon_2 = 1/3$ (thus $c_1 = 1$, $c_2 = 3$), we then find the solutions:

$$u = \begin{cases} x + 2t & \text{in } \Omega_0, \\ 4x + 5t - 3\xi & \text{in } \Omega_1, \\ \frac{4}{3}x + 5t - \frac{1}{3}\xi & \text{in } \Omega_2, \\ x + 6t & \text{in } \Omega_3. \end{cases} \quad (2.3)$$

At the point, e.g. $(x, t) = (0, 1)$, since $P(2 \leq s, \xi > 1) = P(6 \leq s, \xi < -3) = 0$, we deduce:

$$F(s) = P(5 - 3\xi \leq s, 0 < \xi < 1) + P(5 - \frac{\xi}{3} \leq s, -3 < \xi < 0) \quad (2.4)$$

$$= \left\{ \begin{array}{ll} 0 & \text{if } s < 2 \\ \frac{s-2}{6} & \text{if } 2 \leq s < 5 \\ \frac{1}{2} & \text{if } s \geq 5 \end{array} \right\} + \left\{ \begin{array}{ll} 0 & \text{if } s < 5 \\ \frac{3(s-5)}{2} & \text{if } 5 \leq s < \frac{16}{3} \\ \frac{1}{2} & \text{if } s \geq \frac{16}{3} \end{array} \right\} \quad (2.5)$$

We can define the moment generating function for u , $m(t)$, and apply the Monte Carlo integration too.

$$m(t) = \int_{-\infty}^{\infty} e^{tu} f(u) du \sim \frac{1}{M} \sum_{i=1}^M e^{tu^i}. \quad (2.6)$$

Then the n th moment is:

$$m^{(n)}(0^+) \sim \frac{1}{M} \sum_{i=1}^M (u^i)^n. \quad (2.7)$$

The mean and variance can be evaluated as follows.

$$E(u) = m'(0^+) \sim \frac{1}{M} \sum_{i=1}^M u^i, \quad (2.8a)$$

$$Var(u) = m''(0^+) - (E(u))^2 \sim \frac{1}{M} \sum_{i=1}^M (u^i)^2 - (E(u))^2. \quad (2.8b)$$

3 Certified Reduced Basis Methods

In [1] we proposed certified reduced basis methods to enable the efficient and reliable evaluation of a general output that is implicitly connected to a given parameterized input through the harmonic Maxwell's equations. The truth approximation and the development of the reduced basis through a greedy approach is based on discontinuous Galerkin approximations of the linear partial differential equation. The development allows the use of different approximation spaces for solving the primal and the dual truth approximation problems to respect the characteristics of both problem types, leading to an overall reduction in the off-line computational effort.

The main features of the method are: i) rapid convergence on the entire set of parameters, ii) rigorous a posteriori error estimators for the output and iii) a parameter independent off-line phase and a computationally very efficient on-line strategy to enable the rapid solution of many query problems arising in control, optimization, and design. The versatility and the performance of this approach is shown through some numerical experiments, illustrating the modeling of material variations, problems with resonant behavior, and applications related to radar scattering prediction.

In [2] A Galerkin approach was combined with a reduced basis method for the evaluation of outputs of interest implicitly depending on a given input via the resolution of a PDE issue from a harmonic wave propagation problem. The main features of the method are: i) rapid convergence on the entire set of parameters, ii) a posteriori error estimators for the output and iii) an off-line (parameter independent) on-line (very fast) computational strategy. In the present paper we allow the use of different approximation spaces for solving the primal and dual *truth approximation* problems reducing the off-line computational effort.

In [3] In a posteriori error analysis of reduced basis approximations to affinely parameterized partial differential equations, the construction of the lower bounds for coercivity and inf-sup stability constants is required. In [1] the authors presented an

efficient method compatible with an off-line/on-line strategy, where the online computation is reduced to minimizing a linear functional (assuming the affine dependence on the parameters) under a few linear constraints reflecting stability information. These constraints depend on nested sets of parameters obtained iteratively using a greedy algorithm. In the paper, we improved this method so that it becomes more efficient and have a nice property, namely, the computed lower bound is monotonically increasing with respect to the nested sets. The new method is applied to the construction of the inf-sub stability constant of an electromagnetic cavity problem, providing good lower bounds and capturing the resonance lines very efficiently and accurately.

4 Problems with random inputs

In [5] we proposed a way of accounting for the lack of detailed knowledge about material shapes in computational time-domain electromagnetics. We use Legendre-Gauss-Lobatto, Stroud-2 and Stroud-3 quadrature formulae to solve the resulting stochastic equation and we show the efficiency of the proposed method over statistical Monte-Carlo simulations. We also show how the radar-cross-section in scattering is affected by the uncertainty in shape of the objects and by the direction of the incident field.

In CHL we discuss computationally efficient ways of accounting for the impact of uncertainty, e.g., lack of detailed knowledge about sources, materials, shapes, etc., in computational time-domain electromagnetics. In contrast to classic statistical Monte Carlo-based methods, we explore a probabilistic approach based on high-order accurate expansions of general stochastic processes. We show this to be highly efficient and accurate on both one- and two-dimensional examples, enabling the computation of global sensitivities of measures of interest, e.g., radar-cross-sections (RCS) in scattering applications, for a variety of types of uncertainties.

In [7] Recently there has been a growing interest in designing efficient methods for solutions of ordinary/partial differential equations with random input. The thisend, Stochastic Galerkin (SG) methods appear to be superior to other non-sampling methods, and in many cases, to several sampling methods. However, when the governing equations take complicated forms, numerical implementations of SG methods can become non-trivial and care is needed to design robust and efficient solvers for the resulting equations. On the other hand, the traditional sampling methods, e.g., Monte Carlo methods, are straightforward to implement, but they do not offer convergence

as fast as stochastic Galerkin methods. In this paper, a high-order Stochastic collocation approach is proposed. Similar to SG methods, the collocation methods also take advantage of the smoothness assumption of the solutions in random space to achieve fast convergence. On the other hand, the numerical implementation of the stochastic collocation is trivial as it only requires repetitive runs of an existing deterministic solver, similar to Monte Carlo methods. The computational cost of the collocation methods depends on the choice of the collocation points and we present several feasible constructions. One particular choice, based on sparse grids, depends weakly on the dimensionality of the random space and is more suitable for high accuracy computations of practical applications with large dimensional random input. Numerical examples are presented to demonstrate the accuracy and efficiency of the stochastic collocation methods.

In [8] It is well known that the steady state of an isentropic flow in a dual-throat nozzle with equal throat areas is not unique. In particular there is a possibility that the flow contains a shock wave, whose location is determined solely by the initial condition. In this paper, we consider cases with uncertainty in this initial condition and use generalized polynomial chaos methods to study the steady-state solutions for stochastic initial conditions. Special interest is given to the statistics of the shock location. The polynomial chaos (PC) expansion modes are shown to be smooth functions of the spatial variable x , although each solution realization is discontinuous in the spatial variable x . When the variance of the initial condition is small, the probability density function (PDF) of the shock location is computed with high accuracy. Otherwise, many terms are needed in the PC expansion to produce reasonable results due to the slow convergence of the PC expansion, caused by non-smoothness in random space.

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- [12] C. Jung "Evolution of probability distribution in time for solutions of hyperbolic equations" to appear in JSC.

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1. J.S. Hesthaven and T. Warburton, "Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications". Springer Texts in Applied Mathematics 54, Springer Verlag, New York. 478 pages. To appear Dec 2007.
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8. David Gottlieb and Dongbin Xiu, "Galerkin Method for Wave Equations with Uncertain Coefficients" to appear.
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Honors & Awards Received

David Gottlieb received the NASA group achievement award in 1992. He was given the Ford Foundation chair at Brown University in 1993. He received an honorary doctorate from the university of Paris 1994 and from the university of Uppsala, Sweden in 1996. He has been elected to the National Academy of Sciences in 2007.

Jan Hesthaven Received the BSF Postdoctoral Fellowship in 1995, the Sloan Fellowship in 2000. He was Manning Assistant Professor at Brown U. in 2001, got the CAREER award of BSF in 2002 and in 2004 he received the Phillip J. Bray award for Teaching Excellence Brown University.