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Abstract

A method is developed in this paper to accelerate the convergence in computing the solution of stochastic algebraic systems of equations. The method is based on computing, via statistical sampling, a polynomial chaos decomposition of a stochastic preconditioner to the system of equations. This preconditioner can subsequently be used in conjunction with either Chaos representations of the solution or with approaches based on Monte Carlo sampling. In addition to presenting the supporting theory, the paper also presents a convergence analysis and an example to demonstrate the significance of the proposed algorithm.

Introduction

In many problems of science and engineering the quest for accuracy in predicting the behavior of the associated physical systems has motivated the adoption of stochastic equations as viable representative models (Ghanem and Spanos, 1991; Soize, 2001; Soize, 2003). In many of these models, the governing equations take the form of partial differential equations with coefficients represented as stochastic processes or variables (Ghanem and Spanos, 1991). In discretizing these equations, linear algebraic systems ensue with entries that consist of generally correlated random variables (Ghanem and Spanos, 1991; Soize and Ghanem, 2003). A general and standard approach for estimating the solution of these stochastic equations is obtained through a Monte Carlo simulation logic that involves solving the full equations once for each realization in a statistical sample associated with the random system, and thus synthesizing a corresponding sample of the random solution (Schueller, 2001). The iterative solution of these equations would normally involve developing a different conditioner for each of the samples. Consequently, if the number of samples is large and/or there are additional computational loops such as a frequency loop, a time loop, an equilibrium iteration loop for non linear problems, then the numerical effort associated with the construction of the conditioners can become prohibitive. The main idea of this paper is to propose, as an initial step (outside the principal loops), the construction of an algebraic representation of a random conditioner, called the stochastic conditioner. Since the conditioner is a random matrix which depends on the random parameters in the original matrix of the problem, this algebraic representation is chosen as the chaos decomposition of the random conditioner. Once constructed, this conditioner can then be

used either in accelerating the convergence of Monte Carlo sampling of in producing computationally efficient estimates of the Chaos decomposition of the solution (Ghanem and Spanos, 1991). The present paper deals with problem where the linear algebraic system to be solved is frequency-dependent as would be the case in many dynamics problems. After describing the mathematical setting for the discretized problem in the next next section, the stochastic conditioners are introduced and a construction algorithm is described for their computation. An algorithm for estimating a solution of the stochastic equations is then presented followed by a convergence analysis. A numerical example is then used to expand on and demonstrate the various steps in building the conditioner.

Discretized equations in the frequency domain

Consider the algebraic problem associated with solving the following linear system of equations,

$$A(\omega, \xi)X(\omega) = F(\omega, \xi)\,, \quad \omega \in B, \tag{1}$$

in which ω is a real parameter such as frequency, ξ is an R^n-valued second-order random variable whose components are independent normalized Gaussian random variables, $A(\omega, \xi)$ is a random symmetric $(m \times m)$ complex matrix, $F(\omega, \xi)$ is a C^m-valued second-order random variable and $X(\omega)$ is a C^m-valued random variable. The objective is to develop an acceleration procedure for the solution of Eq. (1) when either chaos developments or Monte Carlo Simulation (MCS) method is used in its resolution (Ghanem and Spanos, 1991; Ghanem and Red-Horse, 1999). In the case of the MCS method, a chaos decomposition is used. The proposed acceleration procedure relies on the development of stochastic conditioners.

Introducing stochastic conditioners

For a given stochastic conditioner $C(\omega, \xi)$, introduce the conditioned stochastic matrix of the system $A^{\mathrm{cond}}(\omega, \xi) = A(\omega, \xi)C(\omega, \xi)$. The stochastic solution to problem (1) is then obtained as

$$X(\omega) = C(\omega, \xi)Y(\omega)\,, \quad A^{\mathrm{cond}}(\omega, \xi)Y(\omega) = F(\omega, \xi)\,, \quad \omega \in B\,. \tag{2}$$

Certain properties are imposed on matrix $C(\omega, \xi)$ in order to maintain some desirable properties of the solution process: (1) $X(\omega) \in L^2(\Omega, R^m)\,, \quad \forall \omega \in B$, (2) $C(\omega, \xi)$ is a.s. invertible for every $\omega \in B$, (3) in general $C(\omega, \xi)$ is a full matrix. Consequently, $A^{\mathrm{cond}}(\omega, \xi)$ is also full and such an approach would lead us to a prohibitive numerical effort for solving the resulting algebraic problem. A constraint on $C(\omega, \xi)$ should therefore be introduced to reduce this cost by maintaining a sparse representation of $A^{\mathrm{cond}}(\omega, \xi)$.

Construction of stochastic conditioner

Any approximation of $A(\omega, \xi)^{-1}$ satisfying the above properties is an acceptable conditioner. From a design perspective, a compromise must be made between proximity to $A(\omega, \xi)^{-1}$ and the numerical effort associated with constructing the approximation. We present a conditioner based on the stochastic incomplete LU factorization of the stochastic system matrix. The construction of the stochastic incomplete LU factorization (Golub

and Loan, 1991) of stochastic system matrix $A(\omega, \xi)$ is an independent initial step in the construction of the stochastic solution of equation Eq. (1). Since for each $\omega \in B$, matrix $A(\omega, \xi)$ is invertible a.s., for each $\omega \in B$, it admits an incomplete factorization

$$L^{\mathrm{inc}}(\omega, \xi) U^{\mathrm{inc}}(\omega, \xi) = L^{\mathrm{inc}}(\omega, \xi) D^{\mathrm{inc}}(\omega, \xi) L^{\mathrm{inc}}(\omega, \xi)^T \quad , \quad \text{a.s.} \tag{3}$$

In this factorization, $L^{\mathrm{inc}}(\omega, \xi)$ is a random sparse triangular complex matrix having 1 on its diagonal and $D^{\mathrm{inc}}(\omega, \xi)$ is a random diagonal complex matrix. Stochastic representations of $L^{\mathrm{inc}}(\omega, \xi)$ and $D^{\mathrm{inc}}(\omega, \xi)$ in terms of their respective chaos decompositions are given as

$$L^{\mathrm{inc}}(\omega, \xi) = \sum_{|\alpha|=0}^{P_1} L_\alpha^{\mathrm{inc}}(\omega) \Psi_\alpha(\xi) \,, \qquad D^{\mathrm{inc}}(\omega, \xi) = \sum_{|\alpha|=0}^{P_1} D_\alpha^{\mathrm{inc}}(\omega) \Psi_\alpha(\xi) \,, \tag{4}$$

in which $L_\alpha^{\mathrm{inc}}(\omega)$ and $D_\alpha^{\mathrm{inc}}(\omega)$ are complex matrices with the same sparsity structure as $L^{\mathrm{inc}}(\omega, \xi)$ and $D^{\mathrm{inc}}(\omega, \xi)$ respectively, and are explicitly given by

$$L_\alpha^{\mathrm{inc}}(\omega) = \frac{\langle L^{\mathrm{inc}}(\omega, \xi) \Psi_\alpha(\xi) \rangle}{\langle \Psi_\alpha(\xi)^2 \rangle} \,, \qquad D_\alpha^{\mathrm{inc}}(\omega) = \frac{\langle D^{\mathrm{inc}}(\omega, \xi) \Psi_\alpha(\xi) \rangle}{\langle \Psi_\alpha(\xi)^2 \rangle} \,. \tag{5}$$

Throughout this paper, for a multi-index $\alpha = (\alpha_1, \ldots, \alpha_n)$ of length $|\alpha| = \alpha_1 + \ldots + \alpha_n$, each term in the sum $\sum_{|\alpha|=0}^{P}$ is itself the summation over all multi-indices of a given length. Once the incomplete factorization of $A(\omega, \xi)$ has been computed as described above, the stochastic conditioner can then be explicitly written as

$$C(\omega, \xi) = \left(L^{\mathrm{inc}}(\omega, \xi) D^{\mathrm{inc}}(\omega, \xi) L^{\mathrm{inc}}(\omega, \xi)^T \right)^{-1} \quad , \tag{6}$$

in which L^{inc} and D^{inc} are given by Eq. (4). It should be noted that the stochastic conditioner $C(\omega, \xi)$ is never constructed explicitly using Eq. (6) because the inversion of sparse matrices in that equation leads to a full matrix for $C(\omega, \xi)$. An implicit procedure for implementing the conditioning is next described.

Solution of the stochastic system

The intermediate solution $Y(\omega, \xi)$ is first obtained as the solution to a conditioned system by using an iterative algorithm, followed by the evaluation of $X(\omega, \xi)$ using Eq. (2).

Constructing the solution of the conditioned system. For each sample $\xi^{(r)}$ of ξ and using an iterative algorithm, the solution $Y^{(r)}(\omega)$ of the conditioned deterministic matrix equation $Y^{(r)}(\omega) = F(\omega, \xi^{(r)})$, must be computed. As previously explained, sample $C(\omega, \xi^{(r)})$ of stochastic conditioner $C(\omega, \xi)$ is not explicitly computed. Rather, an iterative procedure involving $C^{-1}(\omega, \xi^{(r)})$ is utilized for solving the previous equation. In such a procedure, expressions of the form $W = A^{\mathrm{cond}}(\omega, \xi^{(r)})V$, have to be calculated. Using Eqs. (2) and (6), complex vector W is given by $W = A(\omega, \xi^{(r)})R$ in which R is the solution of the linear system $C(\omega, \xi^{(r)})^{-1}R = V$ which can be rewritten as $L^{\mathrm{inc}}(\omega, \xi^{(r)}) D^{\mathrm{inc}}(\omega, \xi^{(r)}) L^{\mathrm{inc}}(\omega, \xi^{(r)})^T R = V$. The chaos decompositions of $L^{\mathrm{inc}}(\omega, \xi)$ and $D^{\mathrm{inc}}(\omega, \xi)$, given by Eq. (4) are utilized in this equation. Given the lower triangular structure of $L^{\mathrm{inc}}(\omega, \xi^{(r)})$, the solution is readily obtained using two back-substitutions. This process is very efficient due to the very sparse nature of $L^{\mathrm{inc}}(\omega, \xi)$.

Constructing a representation of stochastic solution $X(\omega, \xi)$. A truncated decomposition of stochastic solution $X(\omega, \xi)$ is written as $X_{P_2}(\omega, \xi) = \sum_{|\alpha|=0}^{P_2} X_\alpha(\omega) \Psi_\alpha(\xi)$, in which $X_\alpha(\omega)$ is given by $X_\alpha(\omega) = \langle X(\omega, \xi) \Psi_\alpha(\xi) \rangle / \langle \Psi_\alpha^2(\xi) \rangle$. Moreover, the first of Eq. (2) is rewritten as $C^{-1}(\omega, \xi) X(\omega, \xi) = Y(\omega, \xi)$ or, using Eq. (6), $L^{\text{inc}}(\omega, \xi) D^{\text{inc}}(\omega, \xi) L^{\text{inc}}(\omega, \xi)^T X(\omega, \xi) = Y(\omega, \xi)$. The solution $X(\omega, \xi)$ is then obtained mainly using two very sparse back-substitutions.

Numerical example

Definition of the mechanical system with random uncertainties. Below, we consider a static problem which is then independent of the frequency parameter ω. The stochastic system is a fixed structure constituted of an isotropic non homogeneous linear elastic medium occupying a three-dimensional bounded domain Ω with boundary $\partial \Omega$, defined in Fig. 1.
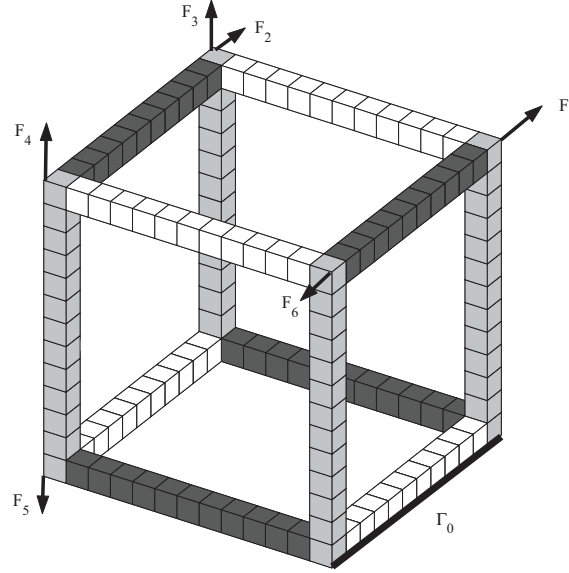

Figure 1. Geometrical definition and finite element mesh of the structural domain Ω and of the three subdomains Ω_1 (gray), Ω_2 (dark gray) and Ω_3 (white). The external applied forces are indicated with arrows. Boundary Γ_0 is indicated by the thick dark solid line.

The structure is fixed on the part Γ_0 for which the displacement field is zero (see Fig. 1). Domain Ω is the union of the three subdomains, Ω_1, Ω_2 and Ω_3, as indicated in the figure. For $k = 1, 2, 3$, subdomain Ω_k is occupied by a homogeneous medium whose Young modulus is E_k and Poisson coefficient is ν_k such that $\nu_k = 0.3$. The uncertainties concern only the Young moduli which are modeled by independent second-order random variables whose mean values $\bar{E}_k = \langle E_k \rangle$ are such that $\bar{E}_1 = 2.1 \times 10^{10}$, $\bar{E}_2 = 2\bar{E}_1$ and $\bar{E}_3 = \bar{E}_1/2$. For fixed k, random variable E_k is written as $E_k = \left(1 - \frac{\delta_k}{\sqrt{2}}\right) \bar{E}_k + \frac{\delta_k \bar{E}_k}{\sqrt{2}} \xi_k^2$. In this equation, ξ_k is a normalized Gaussian random variable (centered with variance equal to 1) and $\delta_k \in [0, \sqrt{2}[$, which is defined by $\delta_k = \sigma_k / \bar{E}_k$, $\sigma_k^2 = \langle E_k^2 \rangle - \bar{E}_k^2$, permits the control of the dispersion of random variable E_k. It should be noted that the above construction results in $E_k > 0$ almost surely. For the numerical calculations, the values of the dispersions parameters are $\delta_1 = 0$, $\delta_2 = 0.6$ and $\delta_3 = 0.8$ which means that subdomain Ω_1 has no uncertainties (deterministic medium). The externally applied forces are constituted of 6 point forces denoted as $f_1, \ldots, f_6$, defined in Fig. 1, the magnitudes of which are such

that $|f_2| = |f_5| = |f_6|$ and $|f_1| = |f_3| = |f_4| = 2|f_2|$. The finite element mesh of the mechanical system is defined in Fig. 1 and is constituted of 8-nodes isoparametric 3D solid finite elements. The number of DOFs is $m = 1500$.

Efficiency of the stochastic conditioner. In this section, we compare the numerical costs of the stochastic solution construction of Eq. (1) using the stochastic conditioner and using the usual conditioner for the following conditions: the number N_1 of realizations used for calculating Eq. (5) is 4500, the number N_2 of realizations used for calculating $X_\alpha(\omega)$ is 1800, $P_1 = 2$ and $P_2 = 4$. The numerical cost for the construction of the stochastic conditioner is denoted by $C_1(\ell)$ and depends on its bandwidth ℓ. The numerical cost for the construction of the stochastic solution using the stochastic conditioner without including $C_1(\ell)$ is denoted by $C_2(\ell)$. Finally, the numerical cost for constructing the stochastic solution using the usual conditioner is denoted by $C_3(\ell)$. It should be noted that the construction of the stochastic conditioner is presented separately because its construction can generally be performed in an initial step. In addition, we present normalized numerical costs with respect to the total cost for the construction of the stochastic solution, that is to say, (1) the normalized numerical cost $\mathrm{eff}_1(\ell) = C_1(\ell)/C_3(\ell)$ for the construction of the stochastic conditioner, and (2) the normalized numerical cost $\mathrm{eff}_2(\ell) = C_2(\ell)/C_3(\ell)$ for the construction of the stochastic solution using the stochastic conditioner. Figure 2 displays the graph of function $\ell \mapsto \mathrm{eff}_1(\ell)$.
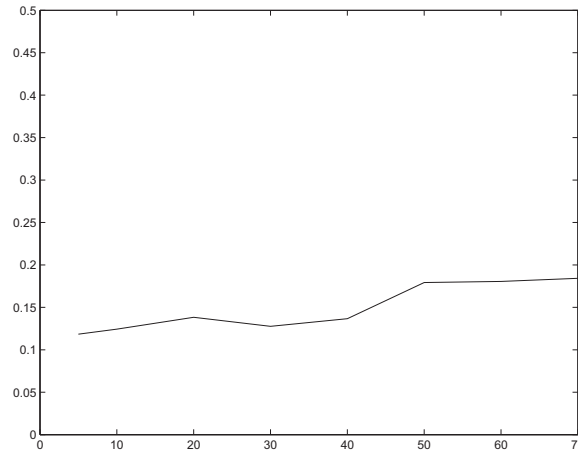

Figure 2. Normalized numerical cost for the construction of the stochastic conditioner as a function of its bandwith ℓ: graph of $\ell \mapsto \mathbf{eff}_1(\ell)$; $N_1 = 4500$, $N_2 = 1800$; $P_1 = 2$, $P_2 = 4$.

It can be seen that, as expected, this normalized cost increases with the bandwidth. Figure 3 displays the graph of function $\ell \mapsto \mathrm{eff}_2(\ell)$ which shows that the gain increases with the bandwidth (that is also understandable). Comparing Figs. 2 and 3, it can be seen that the gain corresponds to the cost of the usual conditioner which is, with the stochastic conditioner, constructed in an initial step, outside the loops related to the samples. It is clear from this argument that the proposed stochastic conditioning is particularly suitable for problems in which the construction of the stochastic conditioner can be performed outside the main loops of the problem under consideration such as the time loop for an evolution problem, the equilibrium iterative loop for a nonlinear problem, etc. Moreover, it should be noted that, the greater the number of samples in the MCS method, the greater the efficiency.
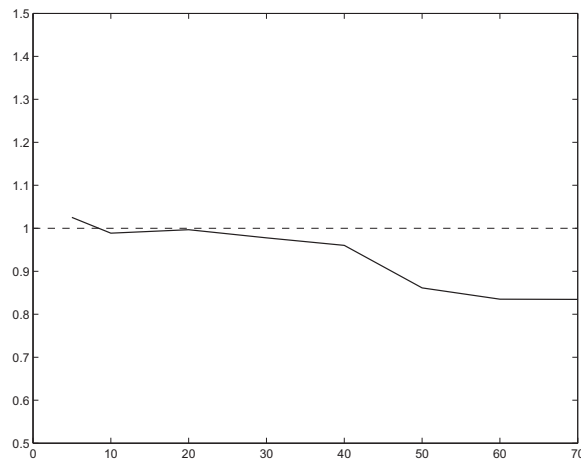
Figure 3. **Efficiency analysis for the construction of the stochastic solution using the stochastic conditioner as a function of its bandwidth ℓ: graph of $\ell \mapsto \mathbf{eff}_2(\ell)$ (solid line). The dashed line represents the normalized reference numerical cost corresponding to $C_3(\ell)$.**

Conclusions

The construction of a stochastic conditioner using the chaos decomposition is proposed. The convergence properties of this stochastic conditioner are studied through a numerical example which shows that a significant gain is obtained. In addition, for the treated example, it has been seen that, the convergence of the chaos decompositions of the diagonal and triangular parts of the stochastic conditioner is reached for different values of the decomposition chaos order. This property allows the numerical effort associated with the construction of the stochastic conditioner to be further decreased. The persistence of this very useful property merits further investigation in connection with a broader classes of random matrices.

References

Ghanem, R., and Red-Horse, J. 1999. Propagation of uncertainty in complex physical systems using a stochastic finite element approach. *Physica D*, **133**(1–4), 137–144.

Ghanem, R., and Spanos, P. 1991. *Stochastic Finite Elements: A Spectral Approach*. Springer-Verlag.

Golub, G.H., and Loan, C.F. Van. 1991. *Matrix Computation*. The John Hopkins University Press.

Schueller, G. 2001. Computational stochastic mechanics - recent advances. *Computers and Structures*, **79**, 2225–2234.

Soize, C. 2001. Maximum entropy approach for modeling random uncertainties in transient elastodynamics. *J. Acoust. Soc. Am.*, **109**(5), 1979–1996.

Soize, C. 2003. Random matrix theory and non-parametric model of random *Journal of Sound and Vibration*, **263**, 893–916.

Soize, C., and Ghanem, R. 2003. Physical Systems with Random Uncertainties: Chaos representations with arbitrary probability measure. *SIAM Journal of Scientific Computing*.