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GENERATING SIMULATED RESPONSES FOR STOCHASTIC SYSTEMS USING POLYNOMIAL CHAOS AND WICK PRODUCTS

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ABSTRACT

The development of parameter estimation techniques is often based upon testing using simulated measurements corrupted with noise. For deterministic systems, producing sample noisy signals is relatively easy. For stochastic systems, particularly if several parameters are stochastic, the cost of the usual Monte Carlo calculations can be prohibitive. The paper discusses the use of polynomial chaos and Wick products for efficiently generating sample signals.

INTRODUCTION

Parameter estimation techniques can be characterized by their approaches: A) parameters that are constant or deterministic in form. For example, assuming that the modulus of elasticity, E, is given by $E(T) = a_0 + a_1 f_1(T) + a_2 f_2(T)$ where T is temperature and $f_1(T)$ and $f_2(T)$ are prescribed functions of temperature. B) the parameters sought are functions of time, for example the time variation of the surface heat flux. C) cases where the parameters represent physical properties that are stochastic in nature, e.g., the permeability of a media, or stochastic boundary conditions. Good descriptions of methods appropriate to A) and B) are given by Beck [1, 2] and Vogel [3]. Many examples of these methods can be found in several recent conferences [4-5]. For C) a common approach for estimating the parameters is that of Kalman filtering with stochastic "plant noise" [6,7,8]

The efficiency and accuracy of the methods are usually demonstrated by applying them to measured responses of systems with known values of the parameters. These measured responses are typically taken as the simulated responses corrupted by noise. The noise is almost always of zero mean and with constant standard deviation, that is *homogeneous* or *wide sense stationary* noise. Relatively few examples exist of the application of these methods to experimental measurements, particularly in the field of heat transfer. Part of the reason is that in many heat transfer experiments the boundary conditions are hard to specify with exactness. For example, maintaining a prescribed temperature at the boundary is difficult to do, surface convection coefficients are generally variable in space and time, particularly for turbulent flows, and most thermal properties are functions of temperature, e.g., conductivity and specific heat capacity, or of surface conditions, e.g., surface emissivity or nucleate boiling conditions. Thus many experimentalists are content to make estimates by curve or least squares fitting and to state results in the form $\pm x\%$. A major need is to convince the community that inverse parameter estimation methods should be applied by demonstrating that they are accurate and reasonable to apply.

For the deterministic system, while the computation of the response may be difficult and expensive, once obtained, the corruption of the signal by noise can be easily done and the behavior of the estimation method easily checked. For example, consider the transient behavior of an object cooling by convection to ambient air. For a high conductivity the lumped capacity response is given by

$$\rho c V \frac{dT}{dt} = hA(T_\infty - T) \qquad (1)$$

where ρcV represents the capacitance, T_∞ is the ambient temperature, and hA is the product of surface heat transfer coefficient and the

surface area. For a constant ambient temperature, the equation can be non- dimensionalized to the form

$$\frac{d\Theta}{dt} = -C\Theta \quad 0 \le t \le T \tag{2}$$

where $\Theta = (T - T_\infty)/(T(0) - T_\infty)$ and $C = hA/\rho cV$. The solution, $\Theta(t) = exp(-Ct)$, with $C = 1$ will be taken as our base case in the discussion of the development of simulated responses.

The value of C can be obtained by the usual parameter estimation techniques based upon a one term Taylor series approach using the equations

$$\begin{aligned} \Theta(t) - \Theta(C_0) =& \frac{\partial \Theta(t)}{\partial C}|_{C_0}(C - C_0) \\ \equiv& A(t)(C - C_0) \qquad (3a) \\ \sigma^{-2}(C) =& A^T\Sigma^{-1}A \qquad (3b) \\ C = C_0 + \sigma^2\Sigma^{-1}A^T&(\Theta(t) - \Theta(C_0)) \qquad (3c) \end{aligned}$$

where Σ is the covariance matrix of the noise and C_0 is an initial guess for C and the process is iterated to convergence. In many papers discussing the development of methods, the testing has been done using only a few sample realizations. This is unfortunate because the demonstration of the robustness of the method should be based upon a large number of tests. Figure 1a shows typical realizations for a zero mean noise with $\sigma = 0.05$ and Figure 1b illustrates the resulting estimates of C. Although the standard deviation of the estimated values of C, $\sigma(C) = 0.0359$ agrees well with that predicted from Eq. 3b, 0.0387, the figure clearly shows that one cannot judge the method using only one or two realizations to test it.

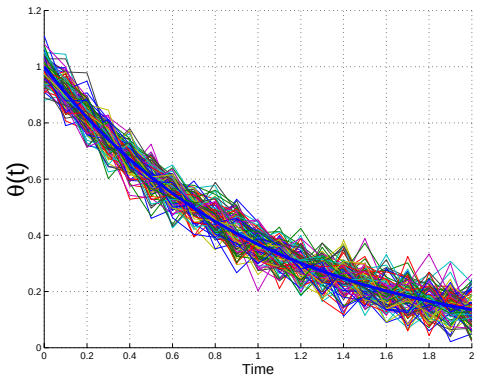

Figure 1a. Realizations of Noisy Responses for Eq. 2 with σ =0.05

Stochastic equations can be conveniently classified by

1 stochastic boundary conditions with deterministic properties
2 stochastic source terms with deterministic properties
3 properties that are random variables
4 properties that are stochastic processes

Solutions to types 1 and 2 are basically deterministic in form and are discussed in detail by Soong [9] and other than numerical concerns pose no substantial problems. Types 3 and 4 are of interest here.

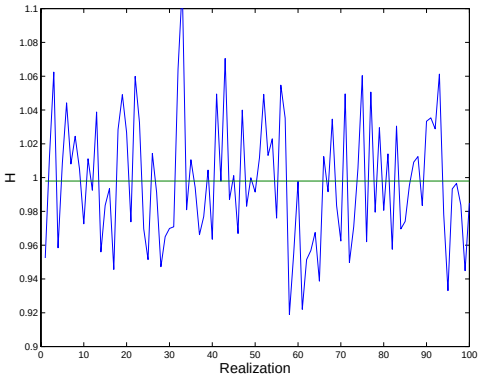

Figure 1b. Estimates of C for σ =0.05 (the line represents the mean value of C)

Let the parameter C be either a) a constant with respect to time and equal to $\overline{C}$, or b) corrupted by white noise and given by $\overline{C} + \alpha w$ where w represents a white noise process in time. Testing parameter estimation methods requires generating simulated realizations. For a) this means computing many deterministic solutions by Monte Carlo or using simpler techniques based upon 1st or 2nd order approximations. The first is computationally expensive, the second is limited in the noise that can be considered [10, 11]. For b) there is really little choice other than Monte Carlo simulations in which random white noise processes are generated over the time period of interest and the equations integrated over time. Most stochastic equations are viewed from Ito's point of view and good descriptions of numerical methods are given by Gard [12] and Kloeden [13].

Figures 2a and 2b depict typical realizations of $\Theta(t)$ and estimates of C for $\alpha/\overline{C}$=0.05. While the estimates of C using Eq. 3 are very good, the computational expense of generating the realizations is high.

Probably more interesting is how the standard deviation of the response varies with time as shown on Figure 2c. Whatever method we are going to use to generate realizations more efficiently than Monte Carlo must accurately reproduce the exact time history.

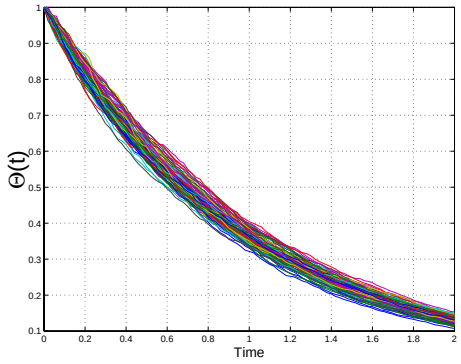

Figure 2a. Realizations of Responses for Eq. 2 with $C = 1 + \alpha w$ with α =0.05

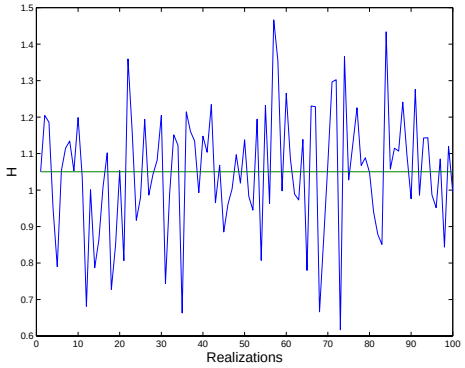

Figure 2b. Estimates of C for α =0.05 (the line represents the mean value of C

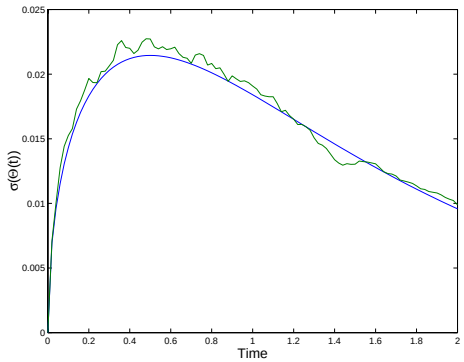

Figure 2c. Standard Deviation of $\Theta(t)$ with $C = 1 + \alpha w$ with α =0.05 (solid line = exact, ragged = Monte Carlo

Let us first carefully differentiate between the use of the terms random variables, random fields, and stochastic processes in this paper.

Consider a probability space (Ω, A, P) where Ω represents all possible events, and A represents the events actually occurring. P represents a measure of the probability, i.e. $P(A)$ is the probability that A occurred. A stochastic process, $X(x, \omega)$, is formally defined as a set of random variables where x represents a dimension of the problem, i.e., time, space, or time and space, and ω represents a specific realization, i.e. an event. For a specific value of x, say x_i, $X(x_i, \omega)$ represents a random variable or random vector in the probability space. For each fixed ω, say ω_j, $X(x, \omega_j)$ represents a real valued function over the x dimension space.

We reserve the term 'random variable' for the case when C is constant with respect to t in solving Eq. 2. If its mean and standard deviation vary with t in a fixed and deterministic manner, it is termed a 'random field'. If, on the other hand, $C(t)$ is represented as $\overline{C} + \sigma w$ where w is white noise we term it as a 'stochastic process' which will be taken to be homogeneous, i.e., of constant standard deviation and mean, over all t.

Methods of solving stochastic problems generally involve two steps:

1 representing a random field in terms of uncorrelated random variables
2 converting all random variables into Gaussian variables.

Inasmuch as lack of correlation does not imply independence, the second step is necessary for both practical and theoretical reasons since uncorrelated Gaussian random variables are independent. The following sections on Polynomial Chaos and Wick products describe methods for achieving the desired conversions.

Our **goal** is to represent the realizations in the form

$$\Theta(t) = \Theta_0 + \sum_{i=1}^{N_\Theta} \Theta_i(C(\omega)) f_i(t) \qquad (4)$$

where $f_1(t), f_2(t)$ are relatively easy to evaluate so that by choosing specific values of $C(\omega)$ we can construct a realization $\Theta(t)$ without integrating Eq. 2.

POLYNOMIAL CHAOS EXPANSIONS FOR RANDOM VARIABLES

In Weiner's study of the kinetic theory of gases and other homogeneous structures, he showed that a random variable, $X(x,\omega)$, with any probability density distribution could be represented as a nonlinear function of a standard Gaussian random variable ξ, i.e. one with zero mean and unit standard deviation, by expressing it in the form

$$C = \sum_{i=0}^{\infty} C_i h_i(\xi) \qquad (5a)$$

where $h_i(\xi)$ are Hermite polynomials given by

$$h_i(\xi) = -(1)^i e^{\xi^2/2} \frac{d^i}{d\xi^i} e^{-\xi^2/2} \qquad (5b)$$

This representation is referred to as homogeneous chaos. The $h_i(\xi)$ are orthonormal with respect to the weight function $e^{-\xi^2/2}/\sqrt{2\pi}$ over the range $-\infty \le x < \infty$ and the first several are shown in Column 2 of Table 1.

Table 1
Chaos Polynomials

Order	One Random Variable	Two Random Variables
i	h_i	$\Psi(\xi_1,\xi_2)$
0^{th}	1	1
1^{st}	ξ	ξ_1
		ξ_2
2^{nd}	ξ^2-1	ξ_1^2-1
		$\xi_1\xi_2$
		ξ_2^2-1

Note that since $h_1(\xi) = \xi$, the first two terms of the series are the standard representation of a Gaussian random variable with $C_0 = E(C)$ and $C_1 = \sigma(C)$. Expressing $\Theta(t)$ as

$$\Theta(t) = \sum_{i=0}^{\infty} \Theta_i h_i(\xi) \qquad (6)$$

and substituting into Eq. 2, with C represented by Eq. 5a, multiplying by $h_j(\xi)$ and integrating with respect to the weight function, the coefficients $\Theta_i(t)$ satisfy

$$\frac{d\Theta_i(t)}{dt} = -\sum_{k=0}^{N_C}\sum_{j=0}^{N_\Theta} \frac{c_{ijk}}{E(h_k^2)} C_j \Theta_k(t) \qquad (7a)$$

where

$$E(h_k^2(\xi) = k! \qquad (7b)$$

$$c_{ijk} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} h_i(\xi) h_j(\xi) h_k(\xi) e^{-\xi^2/2} d\xi \qquad (7c)$$

In Eq. 7a, we have truncated the series for C and for Θ at N_C and N_Θ respectively.

The results of this representation of $\Theta(t)$ in terms of the series expansion is the set of coupled equations for $\Theta_0, \Theta_1, ...\Theta_{N_\Theta}$ shown in Table 2.

Table 2
Equations for Polynomial Chaos

Equations
$d\Theta_0/dt = -\Theta_0 - \alpha\Theta_1$
$d\Theta_1/dt = -\Theta_1 - \alpha\Theta_0 - 2\alpha\Theta_2$
$d\Theta_2/dt = -\Theta_2 - \alpha\Theta_1 - 3\alpha\Theta_3$
$d\Theta_3/dt = -\Theta_3 - \alpha\Theta_2 - 4\alpha\Theta_4$

Figure 3 compares the exact solution with solutions of Eq. 7a for $N_\Theta = 1, 2,$ and 3.

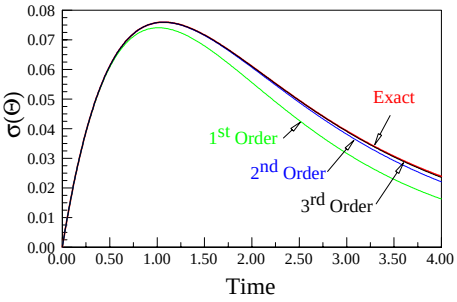

Figure 3. Convergence of Eq. 6 to the exact value for C being a random variable

Even for this relatively small number of terms, the agreement is very acceptable. Unfortunately, the simultaneous equations are coupled as shown in Table 2.

One of the problems with treating C as a random variable is the need to restrict the coefficient of variation to ensure that the property is reasonable. For example, for a Gaussian distribution this means limiting $\sigma(C)$ such that $\overline{C} - 3\sigma(C) > 0$ to ensure its positivity. A common representation of C that ensures positivity is $C = exp(\xi)$, i.e. a log-normal distribution. For $\alpha \le 0.5$ it takes approximately 3 terms in the expansion in terms of Hermite polynomials, Eq. 5, for a reasonably accurate representation

of C, leading to a minimum of 3 terms in the expansion of $\Theta(t)$ and thus requiring the solution of 3 coupled equations for a single random variable, ξ.

RANDOM FIELDS AND KARHUNEN-LOEVE EXPANSION

When $C(t)$ is a stochastic process, $C(t)$ is a random field, not a random variable. This is handled by subdividing the space $0 \leq t < T$ into small increments, and assigning different values of $C(t)$ to each subdivision when integrating with respect to t. How to choose the value of C appropriate to the increment t to $t + \delta t$ is an open question [14]. Common choices are the midpoint value or some spatial average over the increment. In general, midpoint values tend to over predict the variability in $\Theta(t)$ and spatial averaging under predicts the variability. Regardless of the choice, the numerical solution of Eq. 2 causes no conceptual difficulties, but it means that each solution is unique and that drawing general conclusions is not possible.

Suppose that the random field is homogeneous, i.e., its mean and standard deviation are constant with respect to t, but that the properties are spatially correlated, $E(C(t_i), C(t_j)) = \Sigma_C(C_i, C_j)$. Let V be a vector of $C(t_1)....C(t_n)$ that characterizes the random field. Then because the covariance matrix Σ_C is symmetric and positive definite, there is a transformation from V to Ξ for which Σ_Ξ is diagonal, i.e., the components of the new vector Ξ are uncorrelated. In the multi-variate statistical literature, these new random variables are referred to as *principal components*. In the transformation $V = U\Xi$, the matrix U is formed from the eigenvectors of Σ_C. Note that while uncorrelated, the new random variables are not independent.

If instead of discrete values of C, a continuous distribution is used, then the approach described above leads to the Karhunen-Loeve expansion in terms of continuous eigenfunctions (see Ghanem and Spanos [15] for details). Inasmuch as only a few such eigenfunctions are known analytically, one generally resorts to numerical evaluation, often using the finite element approach, which is then the equivalent of the discrete process described above.

If C is a Gaussian random field, then lack of correlation implies independence. The resulting random field in terms of ξ is now composed of as many independent vectors, whose components are the values of C to be associated with each increment of t, as there are increments in t.

The Karhunen-Loeve (K-L) expansion of white noise is given by

$$w(t) = \sum_{i=1}^{KL=\infty} \xi_i \sqrt{\frac{2}{T}} \frac{cos((2i-1)\pi t)}{2T} \qquad (8)$$

where ξ_i are standard Gaussian random variables. When using a finite number KL in the series, just as for the eigenvectors described above, the magnitudes of ξ_i must be adjusted to yield the correct variance of the field. Tests of solving Eq. 2 over the interval $0 \leq t \leq 2$ have shown that five (5) values of ξ_i are sufficient to adequately represent the time history of $\sigma(\Theta(t))$ shown in Figure 3c.

Our problem now has KL random variables, not one, and the expansion of Eq. 6, must be modified. Ghanem and Spanos [15] have extended Weiner's concept of homogenous chaos to represent multiple random variables in terms of standard Gaussian random variables by expanding in a series of generalized chaos polynomials

$$d\Theta(t) = \sum_{i=0}^{\infty} \Theta_i(t) H_i(\xi) \qquad (9)$$

where now

$$H_k(\xi_1^{i_1}, \xi_2^{i_2}, ...\xi_n^{i_n}) = (-1)^k e^{\xi^2/2} \frac{d^k}{d\xi_1^{i_1} \xi_2^{i_2}} e^{-\xi^2/2} \qquad (10a)$$

with

$$\xi^2 = \xi_1^2 + \xi_2^2 + ...\xi_n^2 \qquad (10b)$$

and i_j represents the number of times that ξ_j appears in H_k and $i_1 + i_2 + ...i_n = k$. For any given order of the chaos polynomial $H_k(\xi_1^{i_1}, \xi_2^{i_2}, ...\xi_n^{i_n})$, there are several unique polynomials, e.g. for H_2, we have $H_2(\xi_1, \xi_2)$, $H_2(\xi_1, \xi_3)$, $H_2(\xi_1, \xi_n)$ et seq. For each unique polynomial there is an associated coefficient in the series, Eq. 9. Following Ghanem and Spanos, we represent Eq. 9 in terms of these unique polynomials as a truncated series

$$\Theta(t) = \sum_{i=0}^{P} \Theta_i(t)\Psi_i(\xi) \qquad (11)$$

For two random variables ξ_1 and ξ_2, the expressions for $\Psi_0, \Psi_1$and Ψ_2 are shown in column 3 of Table 1. Ghanem and Spanos termed this extension of homogeneous chaos, polynomial chaos, and the technique has been used in solving multi-random variable problems in structures, heteregeneous media, and ground water analysis [16, 17].

The total number of terms, P, is

$$P = \frac{(N_\Theta + N_\xi)!}{N_\Theta! N_\xi!} \qquad (12)$$

Thus even though the expansion, Eq. 9, is limited to a relatively low order polynomial Ψ_k, the number of coefficients of Θ_k that must be evaluated increases at exceptional speed. For example, using a 3rd order polynomial with 2 random variables leads to solving 10 coupled equations for each value of Θ.

For the case where C is represented by white noise, Eq. 2 was solved in two ways. First, the range of t was subdivided into N_ξ equally sized intervals and assuming that ξ_i in each interval was an independent Gaussian random variable. Expanding $\Theta(t)$ using 1st order Hermite polynomials,

$$\Theta(t) = \Theta_0 + \sum_{i=1}^{N_\xi} \Theta_i h_1(\xi_i) \qquad (13)$$

with $N_\xi = 40$ gives the results shown in Figure 5. The solution of the coupled equations was obtained using a 4th order Runge Kutta method over each of the equally sized intervals N_t. In this approach good results required that integration interval, Δt matched the random variable interval, $N_\xi = N_t$. Use of fewer values of ξ_i led to unacceptable results. If the K-L expansion was used, good results were obtained with a reduced number of terms as shown. In the first approach we have 41 coupled equations to solve, in the second, $KL + 1$. The results based upon the one term expansion, $N_\Theta = 1$, i.e. a Gaussian expansion, are in good agreement with the exact solution and there is no need to employ higher order hermite polynomials in the expansion for $\Theta(t)$. However, for $C(t)$ given by other than Gaussian white noise, higher order expansions will generally be needed.

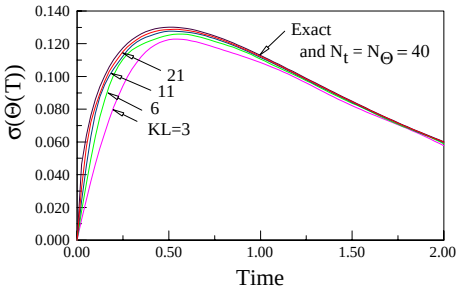

Figure 5. Illustrating the Convergence of the K-L Approach to solving Eq. 2 for white noise

STOCHASTIC WHITE NOISE PROCESSES AND WICK PRODUCTS

When the correlation length is large, then only a few vectors must be considered, but if it is small, then many must be and in the limit as the field approaches white noise as many vectors as there are increments in t must be considered as described above. If the properties constitute a random field, that is their statistics are known, then solving by using the expansion in terms of Ξ is unrealistically expensive and one is limited to solutions that are unique to the specific random field considered.

However if $C(t)$ is a mean value $\overline{C}$ modified by white noise, a different approach has been described by Holden et al. [18]. This approach is based upon the Wick product. Consider two stochastic processes, F and G, and let each be represented by an expansion in chaos polynomials

$$F = \sum f_i H_i \qquad G = \sum g_j H_j \qquad (14a)$$

then the Wick product is defined as

$$F \diamond G = \sum f_i g_i H_{i+j} \qquad (14b)$$

Wick products have several valuable features. They are associative, distributive, and commutative. They can be differentiated and integrated according to the usual rules of calculus. Probably most important are the relations

$$E(F \diamond G) = E(F)E(G) \quad \text{if} F \neq G \qquad (15a)$$

$$F^{\diamond k} = F \diamond F^{\diamond(k-1)} \quad \text{with } F^{\diamond 0} = 1 \qquad (15b)$$

$$E(e^{\diamond X}) = e^{E(X)} \qquad (15c)$$

$$\text{if} \quad P(F) = \sum_{n=0}^{N} a_n F,$$

$$P^{\diamond}(F) = \sum_{n=0}^{N} a_n F^{\diamond n} \qquad (15d)$$

Following Holden, one simply writes the original equation as

$$\frac{d\Theta(t)}{dt} = -C(\omega) \diamond \Theta(t) \tag{16}$$

and integrates as though it were an ordinary differential equation to obtain

$$\Theta(t) = e^{\diamond -C(\omega)t} \tag{17}$$

Using Eq. 23c, we find the expected value of $\Theta(t)$

$$E(\Theta(t)) = e^{-E(k)t} = e^{-\overline{C}t} \tag{18a}$$

To find the standard deviation of $\Theta(t)$ we cannot use Eq. 15a since $F = \Theta$ and $G = \Theta$. Instead, we can show that

$$E(\Theta^2) = e^{\alpha^2 t} E(\Theta \diamond \Theta) \tag{18b}$$

and thus

$$\sigma^2(\Theta) = e^{-2\overline{C}t}\left(e^{\alpha^2 t} - 1\right) \tag{18c}$$

in agreement with the exact solution. *Note the term* $\alpha^2 t$. If the equation is not nondimensionalized, the units of this product are clearly inconsistent. For a Brownian process, $B(t)$, $\sigma^2(B) = t$ and it is for this reason, that one must be careful to use Eq. 2, not Eq. 1.

When an analytical relationship between $E(\Theta \diamond \Theta)$ and $E(\Theta^2)$ is not available, then one must expand the solution and the noise in series, Eq. 14a, and project the solution onto the space, similar to the method used for polynomial chaos. An important point is that the expected value of the solution is simply the first term in the series which corresponds to the deterministic solution based upon average values of the parameters. The equations for the other coefficients in the series are coupled to the first and to the preceding terms, but not to subsequent terms. Thus the solution can be obtained in a straightforward recursive way. Figure 6 illustrates the solution to Eq. 2.

One must also realize that the use of Wick products is not without questions. Kesse [19] points out the expected value is independent of the statistics of the process, contrary to some Monte Carlo simulation results. Benth and Theting [20] note that the validity of the Wick product needs to be confirmed mathematically and physically for each application.

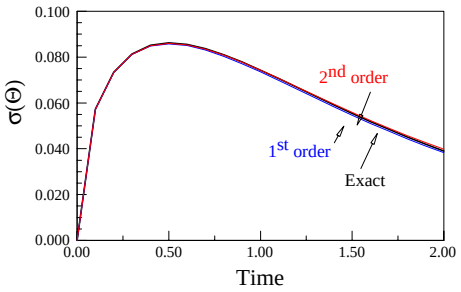

Figure 6. Convergence of the Wick solution of Eq. 2 for white noise

Following Holden, one can easily compute different realizations and obtain estimates of the relevant statistics by noting that Eq. 17 can be written for $\overline{C} = 1$ to first order (i.e. Gaussian) as (see Exercise 2-15 of Holden)

$$\Theta(t) = e^{-t}(1 + \alpha B(t) \tag{19}$$

where $B(t)$ is a Brownian process whose increments are Gaussian white noise. One simply creates a $NxMC$ array of standard random variables and substitutes into Eq. 19 to create MC realizations.

Unfortunately one cannot always find the analytical relationship between $E(\Theta \diamond \Theta)$ and $E(\Theta^2)$ comparable to Eqs. 18a and 19. Instead we use the series expansion and judge the results by comparison to the Monte Carlo solution. As seen in Figure 6, the agreement is acceptable.

CONCLUSIONS

Both the polynomial chaos and the Wick product approach yield equations of the form of Eq. 4 that we desired. Once Θ_i are computed, then one simply samples values of the independent random variables, ξ_i, and evaluates the realization, $\Theta(t)$ without the need to re-solve Eq. 2. In essence one has reduced the $N_t xMC$ problem to a MC sized problem, thus achieving substantial reductions in computing time. The reason for preferring the Wick approach is that the equation for Θ_0 is uncoupled from Θ_i as contrasted to the polynomial chaos set of equations. Theting has used the Wick method to generate realizations for flow through porous media. Of particular note is the simplification when positivity of C is achieved, for example by using $C(t) = exp(w)$. A correlation of $C(t)$ to better represent reality can be introduced

by using a smoothed white noise, w_ϕ, as described by Holden who gives a simple relationship between $exp \diamond w_\phi$ and $exp \diamond w$ that enables a straightforward solution to Eq. 2 using the Wick calculus. The polynomial chaos approach requires several terms in the expansion, Eq. 6, to represent $C(t)$, increasing the number of coupled equations to be solved, which that for Θ_0, the mean response, is dependent upon the remaining equations, leading to high computing expense.

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