STOCHASTIC FINITE ELEMENTS WITH MULTIPLE RANDOM NON-GAUSSIAN PROPERTIES

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ABSTRACT: The spectral formulation of the stochastic finite-element method is applied to the problem of heat conduction in a random medium. Specifically, the conductivity of the medium, as well as its heat capacity are treated as uncorrelated random processes with spatial random fluctuations. Using the spectral stochastic finite-element method, this paper analyzes the sensitivity of heat conduction problems to probabilistic models of random data. In particular, both the thermal conductivity and the heat capacity of the medium are assumed to be uncertain. The implementation of the method is demonstrated for both Gaussian and lognormal material properties, modeled either as random variables or random processes.

INTRODUCTION

Mathematical models of physical systems, be they in the form of partial differential equations or in some other algorithmic form, are essentially abstract representations of our observations regarding these systems. One important usage of these models derives from their ability to predict the behavior of the systems in response to their environment and thus allow for the mitigation against extreme conditions under which these systems may fail to fulfill their intended function. With the recent technological advances in materials and computational science, the expected accuracy of these models is being continually pushed to its limits. The engineering of materials at the nanoscale level, for example, requires tolerances that are vanishingly small. Also, given the capabilities of today's computers, and even more so the extrapolation of these capabilities into the near future, ever more sophisticated models of physical systems can be solved numerically, thus providing higher accuracy on the behavior of these systems and significantly extending their operational boundaries.

It is therefore clear that the drive for more accurate models is justified both by the need for the added accuracy from such models as well as by the ability to solve numerically the corresponding complex equations. One way to achieve this higher accuracy is to improve the fidelity of the parameters of the analytical model. In many cases, the accuracy in estimating these parameters can indeed be tightly controlled. The high costs associated with such a control, however, make it very desirable to be able to assess a priori the sensitivity of the predictions with respect to specific parameters, so as to guide future experimental investigations according to a rational cost-effective strategy.

In this paper, these sensitivities are investigated by casting the problem in a probabilistic context, thus providing a rigorous framework in which to characterize the uncertainties in the data, to propagate them through the mathematical model, and to study their effect on predicted field variables. A number of papers and books have been devoted to analyzing the propagation of uncertainty as described above (Shinozuka and Lenoe 1976; Beck et al. 1985; Der Kiureghian and Liu 1986; Liu et al. 1986, 1987; Shinozuka 1987; Deodatis and Shinozuka 1989; Spanos and Ghanem 1989; Deodatis 1991; Ghanem and Spanos 1991; Li and Der Kiureghian 1993; Fadale and Emery 1994; Ghanem and Brzkala 1996). The framework set forth in this paper views the random nature of the problem as contributing a new dimension to the problem along which approximation techniques, such as the weighted residual method, are applied. The details of this technique have been published elsewhere (Ghanem and Spanos 1991), and a brief review is included here for the sake of completeness.

In this paper an uncertain property of a medium will be expanded according to

$$\mathbf{k}(\mathbf{x}, \theta) = \sum_i \xi_i(\theta)\mathbf{k}_i(\mathbf{x}) \tag{1}$$

where θ denotes the random dimension; $\mathbf{k}_i$ represents a certain scale of fluctuation of the property $\mathbf{k}$; while ξ_i represents its random magnitude and hence the random contribution of that particular scale to the overall property. Both the property and its various scales are global quantities and depend on the spatial position $\mathbf{x}$; they can also be multivariate quantities. The random medium, acting as a nonlinear filter, will couple the uncertainties from the various scales. Thus, the solution sought in this paper, is a multidimensional nonlinear function of the set $\{\xi_i\}$ and will be assumed to have the following generic form:

$$T(\mathbf{x}, t, \theta) \equiv T(\{\xi_i(\theta)\}) = \sum_{i=0}^{\infty} T_i(\mathbf{x}, t)\psi_i(\theta) \tag{2}$$

where $\{T_i(\mathbf{x}, t)\}$ = deterministic quantities to be calculated; and $\{\psi_i(\theta)\}$ is a basis in the space of random variables. This basis will be taken to be the set of multidimensional Hermite polynomials in the quantities $\{\xi_i(\theta)\}$. This basis will be referred to as the polynomial chaos (Wiener 1938). The Monte Carlo simulation procedure is a special case of the preceding representation, with

$$\psi_i(\theta) = \delta(\theta - \theta_i) \tag{3}$$

where θ_i is a particular outcome; and δ denotes the Kronecker delta function. In this case, the nonlinear filter action of the porous medium is eliminated by virtue of the property of the delta functions. Higher order interactions between the various scales are therefore nonexistent in this case, and the scales associated with a Monte Carlo simulation are independent. This is as expected, since in this case, these scales represent independent realizations of the random property of the medium. It is clear, therefore, that Monte Carlo simulation provides a collocation approximation along the random dimension. This paper will present the framework that generalizes this concept. Of course, for the approximation associated with (3), the deterministic quantities $T_i(\mathbf{x}, t)$ represent individual realizations of the solution process that are associated with the random abscissa θ_i. Moreover, in a Monte Carlo setting, the equations for $T_i(\mathbf{x}, t)$ are uncoupled. More generally, the equations for the $T_i(\mathbf{x}, t)$ will be coupled, and they must be solved

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for simultaneously, thus requiring additional computational effort. However the number of terms required in the series representation will depend on the particular basis chosen. A balance can thus be reached between the size of the final system and the level of coupling between its components.

In addition to providing insight into the propagation of uncertainty with respect to scales of fluctuation of the random material properties, a format of the solution as given by (2) has an important appeal. Specifically, having distilled the uncertainty out of the spatial dimension through a representation that is reminiscent of the method of separation of variables, it becomes possible to perform a number of analytical operations on the solution process. These may be needed to determine, among others, the optimal sampling locations for both material properties and field variable. The details of these calculations, however, are not pursued further in this paper since the emphasis here is on developing the framework for characterizing the solution process itself.

In the next section, the discretization of random processes in terms of a finite number of random variables is presented. Emphasis is placed on two expansions, namely the Karhunen-Loève and the polynomial chaos expansions.

In the next section, random variables and stochastic processes are briefly reviewed with emphasis on their representation in computationally tractable forms. Following that, the nondimensional equations governing heat conduction in a randomly heterogeneous medium are reviewed. Next, the discretization with respect to the spatial variables is implemented via the finite-elements formalism, resulting in a set of nonlinear ordinary differential equations with respect to the time variable. In view of the randomness of the material properties of the material, the unknowns at this stage consist of vectors of random variables representing the temperature at the nodes. After that, the Karhunen-Loève and the polynomial chaos expansions are used to obtain an ordinary differential equation with deterministic coefficients. Finally, the formalism is exemplified by its application to a one-dimensional (1D) problem, and the significance of the results is discussed.

REPRESENTATION OF RANDOM VARIABLES AND STOCHASTIC PROCESSES

The development presented in this paper hinges on the definition of random variables as ''measurable functions'' from the space of elementary events to the real line. As functions, approximation theory, as developed for deterministic functions, will be applied to random variables. The main question to be addressed, already raised in the Introduction, is the characterization of the solution to a physical problem where some parameters of the model have been modeled as stochastic processes. The answer to this question lies in the realization that in the deterministic finite-element method, as well as most other numerical analysis techniques, a solution to a deterministic problem is known once its projection on a basis in an appropriate function space has been evaluated. It often happens, in deterministic analysis, that the coefficients in such a representation have an immediate physical meaning, which distracts from the mathematical significance of the solution. Carrying this argument over to the case involving stochastic processes, the solution to the problem will be identified with its projection on a set of appropriately chosen basis functions. A random variable will thus be reviewed as a function of a single variable, θ, that refers to the space of elementary events. A stochastic process, or field, E is then a function of $n + 1$ variables where n is the physical dimension of the space over which each realization of the process is defined. As already mentioned in the Introduction, Monte Carlo simulation can be viewed as a collocation along this θ dimension. Other approximations along this dimension are possible and are explored in this section. This theoretical development is consistent with the identification of the space of second-order random variables as a Hilbert space with the inner product on it defined as the mathematical expectation operation (Loève 1977). Second-order random variables are those random variables with finite variance; they are mathematically similar to deterministic functions with finite energy.

Karhunen-Loève Expansion

The Karhunen-Loève expansion (Loève 1977) of a stochastic process $E(\mathbf{x}, \theta)$ is based on the spectral expansion of its covariance function $R_{EE}(\mathbf{x}, \mathbf{y})$. Here, $\mathbf{x}$ and $\mathbf{y}$ are used to denote spatial coordinates, while the argument θ indicates the random nature of the corresponding quantity. The covariance function being symmetrical and positive definite, by definition has all of its eigenfunctions mutually orthogonal, and they form a complete set spanning the function space to which $E(\mathbf{x}, \theta)$ belongs. It can be shown that if this deterministic set is used to represent the process $E(\mathbf{x}, \theta)$, then the random coefficients used in the expansion are also orthogonal. The expansion then takes the following form:

$$E(\mathbf{x}, \theta) = \bar{E}(\mathbf{x}) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}\xi_i(\theta)\phi_i(\mathbf{x}) \tag{4}$$

where $\bar{E}(\mathbf{x})$ denotes the mean of the stochastic process; and $\{\xi_i(\theta)\}$ forms a set of orthogonal random variables. Furthermore, $\{\phi_i(\mathbf{x})\}$ are the eigenfunctions and $\{\lambda_i\}$ are the eigenvalues, of the covariance kernel, and can be evaluated as the solution to the following integral equation

$$\int_D R_{EE}(\mathbf{x}, \mathbf{y})\phi_i(\mathbf{y})\, d\mathbf{y} = \lambda_i\phi_i(\mathbf{x}) \tag{5}$$

where D denotes the spatial domain over which the process $E(\mathbf{x}, \theta)$ is defined. The most important aspect of this spectral representation is that the spatial random fluctuations have been decomposed into a set of deterministic functions in the spatial variables multiplying random coefficients that are independent of these variables. If the random process being expanded, $E(\mathbf{x}, \theta)$, is Gaussian, then the random variables $\{\xi_i\}$ form an orthonormal Gaussian vector. The Karhunen-Loève expansion is mean-square convergent irrespective of the probabilistic structure of the process being expanded, provided it has a finite variance (Loève 1977). Moreover, the closer a process is to white noise, the more terms are required in its expansion, while at the other limit, a random variable can be represented by a single term. In physical systems, it can be expected that material properties vary smoothly at the scales of interest in most applications, and therefore only few terms in the Karhunen-Loève expansion can capture most of the uncertainty in the process.

Polynomial Chaos Expansion

The covariance function of the solution process is not known a priori, and hence the Karhunen-Loève expansion cannot be used to represent it. Since the solution process is a function of the material properties, nodal temperatures $T(\theta)$ can be formally expressed as some nonlinear functional of the set $\{\xi_i(\theta)\}$ used to represent the material stochasticity. It has been shown (Cameron and Martin 1947) that this functional dependence can be expanded in terms of polynomials in Gaussian random variables, referred to as polynomial chaoses. Namely

$$T(\theta) = a_0\Gamma_0 + \sum_{i_1=1}^{\infty} a_{i_1}\Gamma_1(\xi_{i_1}(\theta)) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Gamma_2(\xi_{i_1}(\theta), \xi_{i_2}(\theta)) + \cdots \tag{6}$$

In this equation, the symbol $\Gamma_n(\xi_{i_1}, \ldots, \xi_{i_n})$ denotes the polynomial chaos (Wiener 1938; Kallianpur 1980) of order n in the variables $(\xi_{i_1}, \ldots, \xi_{i_n})$. These are generalizations of the multidimensional Hermite polynomials to the case where the independent variables are functions measurable with respect to the Wiener measure. Eq. (6) has been shown (Cameron 1947) to be a mean-square convergent representation for second-order random variables. This validity of the covergence of this expansion is irrespective of the constitutive mechanistic behavior of the material, and it merely states that a general random variable, with unknown probabilistic behavior, can be expanded as a polynomial in Gaussian variables according to the expansion given by (6). It should also be noted that other expansions in terms of polynomials of non-Gaussian variables are not guaranteed to converge. Introducing a one-to-one mapping to a set with ordered indices denoted by $\{\psi_i(\theta)\}$ and truncating the polynomial chaos expansion after the pth term, (6) can be rewritten as

$$T(\theta) = \sum_{j=0}^{P} T_j\psi_j(\theta) \tag{7}$$

These polynomials are orthogonal in the sense that their inner product $\langle\psi_j\psi_k\rangle$, which is defined as the statistical average of their product, is equal to zero for $j \neq k$. Moreover, they can be shown to form a complete basis in the space of second-order random variables. A complete probabilistic characterization of the process $T(\theta)$ is obtained once the deterministic coefficients T_j have been calculated. A given truncated series can be refined along the random dimension either by adding more random variables to the set $\{\xi_i\}$ or by increasing the maximum order of polynomials included in the polynomial chaos expansion. The first refinement takes into account higher frequency random fluctuations of the underlying stochastic process, while the second refinement captures strong nonlinear dependence of the solution process on this underlying process.

It should be noted at this point that the polynomial chaos expansion can be used to represent, in addition to the solution process, stochastic processes that model non-Gaussian material properties. The processes representing the material properties are thus expressed as the output of a nonlinear system to a Gaussian input.

GOVERNING EQUATIONS

Since it will be assumed in the foregoing that the material properties of the medium are spatially varying, it will be necessary to carefully develop the nondimensional form of the heat conduction equations. The heat equation for a spatially varying medium is given by

$$c\frac{\partial T}{\partial t} - \boldsymbol{\nabla}\cdot\mathbf{k}\boldsymbol{\nabla}T = 0, \quad \mathbf{x} \in \Omega \tag{8}$$

subjected to the following initial and boundary conditions

$$T(0, \mathbf{x}) = T_0 \tag{9a}$$

$$T(t, \mathbf{x}) = T_b, \quad \mathbf{x} \in \Gamma_1 \tag{9b}$$

$$-\mathbf{k}\frac{\partial T}{\partial n} = q_b, \quad \mathbf{x} \in \Gamma_2 \tag{9c}$$

In these equations, Ω denotes the spatial domain of definition of the problem, Γ_1 denotes a subset of its boundary along which essential boundary conditions are applied, while Γ_2 denotes that portion of the boundary along which natural conditions are applied and $\mathbf{x}$. Moreover, $\mathbf{k}$ and c denote, respectively, the conductivity tensor and the volumetric heat capacity of the medium which will be assumed to be a spatially varying random process. Let

$$\mathbf{k} = [\mathbf{k}_{ij}] = \bar{k}_{11}[\mathbf{a}_{ij}] \tag{10}$$

where $\mathbf{a}$ = anisotropy tensor, equal to the identity tensor for a homogeneous and isotropic material; and k_{11} denotes the mean of the conductivity tensor in direction 11. Moreover, we introduce the following nondimensional space and time variables

$$\boldsymbol{\zeta} = \frac{\mathbf{x}}{L}; \quad t^+ = \frac{t}{t^*} \tag{11a,b}$$

where L = some representative spatial scale; and t^* = representative time scale, and let the new nondimensional temperature be given by

$$T^+ = \frac{T - T_0}{q_b L/k_{11}} \tag{12}$$

The governing equation can then be rewritten as

$$\frac{c}{t^*}\frac{\partial T^+}{\partial t^+} - \frac{\bar{k}_{11}}{L^2}\boldsymbol{\nabla}\cdot\mathbf{a}\boldsymbol{\nabla}T^+ = 0 \tag{13}$$

or

$$\frac{cL^2}{k_{11}t^*}\frac{\partial T^+}{\partial t^+} - \boldsymbol{\nabla}\cdot\mathbf{a}\boldsymbol{\nabla}T^+ = 0 \tag{14}$$

Denoting by α the diffusivity of the medium

$$\alpha = \frac{\bar{k}_{11}}{\bar{c}} \tag{15}$$

the governing equation can be rewritten as

$$\frac{cL^2}{\bar{c}\alpha t^*}\frac{\partial T^+}{\partial t^+} - \boldsymbol{\nabla}\cdot\mathbf{a}\boldsymbol{\nabla}T^+ = 0 \tag{16}$$

Choosing the representative time scale according to

$$t^* = \frac{L^2}{\alpha}; \quad t^+ = \frac{\alpha t}{L^2} \tag{17a,b}$$

results in the final form of the governing equation

$$d\frac{\partial T^+}{\partial t^+} - \boldsymbol{\nabla}\cdot\mathbf{a}\boldsymbol{\nabla}T^+ = 0 \tag{18}$$

where

$$d = \frac{c}{\bar{c}} \tag{19}$$

The initial and boundary conditions, associated with the new nondimensional variables are given by

$$T^+(0, \boldsymbol{\zeta}) = 0 \tag{20a}$$

$$T^+(t, \boldsymbol{\zeta}) = \frac{T_b - T_0}{q_b L k_{11}}, \quad \boldsymbol{\zeta} \in \Gamma_1 \tag{20b}$$

$$-\mathbf{a}\frac{\partial T}{\partial n} = 1, \quad \boldsymbol{\zeta} \in \Gamma_2 \tag{20c}$$

Following the presentation in the second section of this paper, the conductivity tensor and the volumetric heat capacity

can be represented using their Karhunen-Loève expansions in the form

$$d(\zeta) = 1 + \sum_{i=1}^{N_c} \xi_i d_i(\zeta) = \sum_{i=0}^{N_c} \xi_i d_i(\zeta) \tag{21}$$

and

$$\mathbf{a}(\zeta) = \mathbf{I} + \sum_{i=1}^{N_k} \xi_i \mathbf{a}_i(\zeta) = \sum_{i=0}^{N_k} \xi_i \mathbf{a}_i(\zeta) \tag{22}$$

Assuming that the processes $\mathbf{a}$ and d are independent, the random variables ξ_i appearing in their respective expansions are also independent. Statistical independence in this context reflects the more basic assumption that the randomness in the thermal conductivity and the heat capacity are introduced by two different phenomena at the microstructure level. This assumption may need to be revised once enough studies have been conducted to explain the propagation of uncertainty from microscale processes to the macroscale coefficients appearing in the differential equations.

Thus, denoting

$$N = N_c + N_k \tag{23}$$

(21) and (22) can be rewritten as

$$d(\zeta) = 1 + \sum_{i=1}^{N} \xi_i d_i(\zeta), \quad d_i = 0, \quad i > N_c \tag{24}$$

and

$$\mathbf{a}(\zeta) = \mathbf{I} + \sum_{i=1}^{N} \xi_i \mathbf{a}_i(\zeta), \quad \mathbf{a}_i = 0, \quad i \leq N_c \tag{25}$$

Substituting these two expansions into the governing equation yields

$$\left(1 + \sum_{i=1}^{N} \xi_i d_i(\zeta)\right) \frac{\partial T}{\partial t^+} - \nabla \cdot \left(1 + \sum_{i=1}^{N} \xi_i \mathbf{a}_i(\zeta)\right) \nabla T = 0 \tag{26}$$

It is emphasized at this point that the representations given by (24) and (25) should not be construed as constitutive relations for the material behavior. They merely represent a mathematically concise and consistent description of the spatial fluctuations of the material property. In the next section, the finite-element method will be implemented to reduce this partial differential equation into an algebraic system of equations while taking proper consideration of the randomness of all quantities involved.

STOCHASTIC FINITE ELEMENT

In the spirit of the finite-element method, this last equation is projected onto a basis consisting of test function, which is taken here to be the set of local polynomials. This results in the following integral equation:

$$\sum_{i=0}^{N} \int_{\Omega} \xi_i d_i(\zeta) \frac{\partial T^+}{\partial t^+} \mathbf{H}(\zeta)\, d\zeta - \int_{\Omega} \nabla \cdot \left(\sum_{i=0}^{N} \xi_i \mathbf{a}_i(\zeta)\right) \nabla T^+ \mathbf{H}(\zeta)\, d\zeta = 0 \tag{27}$$

where $\mathbf{H}$ = traditional finite-element shape function vector. Applying Stokes' theorem to the second integral results in

$$\sum_{i=0}^{N} \xi_i \int_{\Omega} d_i(\zeta)\mathbf{H}(\zeta) \frac{\partial T^+}{\partial t^+}\, d\zeta + \sum_{i=0}^{N} \xi_i \int_{\Omega} \nabla \mathbf{H}(\zeta)\mathbf{a}_i(\zeta)\nabla T^+\, d\zeta = -\sum_{i=0}^{N} \xi_i \int_{\Gamma} \mathbf{a}_i(\zeta) \frac{\partial T^+}{\partial n}\, d\Gamma \tag{28}$$

The integral on the right-hand side of this equation can be rewritten as

$$-\int_{\Gamma} \mathbf{a}(\zeta) \frac{\partial T^+}{\partial n}\, d\Gamma = -\int_{\Gamma_1} \mathbf{a}(\zeta) \frac{\partial T^+}{\partial n}\, d\Gamma + -\int_{\Gamma_2} \mathbf{a}(\zeta) \frac{\partial T^+}{\partial n}\, d\Gamma = \int_{\Gamma_2} q(\zeta)\, d\Gamma - \int_{\Gamma_1} \mathbf{a}(\zeta) \frac{\partial T^+}{\partial n}\, d\Gamma$$

It is important to note in this last equation that the natural boundary condition is applied with probability 1 to the boundary Γ_2. The final finite-element equation can be obtained upon carrying out the Galerkin procedure. This results in the following system of algebraic equations:

$$\sum_{i=0}^{N} \xi_i \mathbf{C}_i \dot{\mathbf{T}} + \sum_{i=0}^{N} \xi_i \mathbf{K}_i \mathbf{T} = \mathbf{q} \tag{29}$$

where the matrices $\mathbf{C}_i$ and $\mathbf{K}_i$ are obtained by assembling the elemental matrices given by

$$\mathbf{C}_i^{(e)} = \int_{\Omega^{(e)}} d_i(\zeta)\mathbf{H}(\zeta)\mathbf{H}^T(\zeta)\, d(\zeta) \tag{30}$$

and

$$\mathbf{K}_i^{(e)} = \int_{\Omega^{(e)}} \nabla \mathbf{H}^T(\zeta)\mathbf{a}_i(\zeta)\nabla \mathbf{H}(\zeta)\, d(\zeta) \tag{31}$$

and the right-hand side of vector is obtained by assembling the following elemental vectors

$$\mathbf{q}^{(e)} = \int_{\Gamma^{(e)}} \mathbf{H}(\zeta)\, d\Gamma \tag{32}$$

The essential boundary conditions can then be implemented according to standard finite-element procedures, assuming they are to be imposed with probability 1. For each realization of the random variables ξ_i, the preceding equations can be solved for a corresponding realization of the temperature $\mathbf{T}$ throughout the domain. Next, a procedure is developed that implements the concepts developed in the second section of this paper. Specifically, the temperature field $\mathbf{T}$ is represented as

$$\mathbf{T} = \sum_{i=0}^{M} \psi_j \mathbf{T}_j \tag{33}$$

and a framework is developed for evaluating the deterministic coefficients $\mathbf{T}_j$ in this expansion. Substituting this expansion in (29) yields

$$\sum_{j=0}^{M} \sum_{i=0}^{N} \xi_i \psi_j \mathbf{C}_i \dot{\mathbf{T}}_j + \sum_{j=0}^{M} \sum_{i=0}^{N} \xi_i \psi_j \mathbf{K}_i \mathbf{T}_j = \mathbf{q} \tag{34}$$

Multiplying this last equation by each of the ψ_k and taking the ensemble average results in the following equation:

$$\sum_{j=0}^{M} \sum_{i=0}^{N} \langle \xi_i \psi_j \psi_k \rangle \mathbf{C}_i \dot{\mathbf{T}}_j + \sum_{j=0}^{M} \sum_{i=0}^{N} \langle \xi_i \psi_j \psi_k \rangle \mathbf{K}_i \mathbf{T}_j = \langle \mathbf{q} \psi_k \rangle, \quad k = 1, \ldots, M \tag{35}$$

This last procedure is mathematically equivalent to forcing the error in the approximation for the temperature to be orthogonal to the approximating space as defined by the basis $\{\psi_i\}$. Finally, denoting $\langle \xi_i \psi_j \psi_k \rangle$ by d_{ijk}, and $\langle \mathbf{q} \psi_k \rangle$ by $\mathbf{q}_k$, this last equation becomes

$$\sum_{j=0}^{M} \sum_{i=0}^{N} d_{ijk} \mathbf{C}_i \dot{\mathbf{T}}_j + \sum_{j=0}^{M} \sum_{i=0}^{N} d_{ijk} \mathbf{K}_i \mathbf{T}_j = \mathbf{q}_k, \quad k = 1, \ldots, M \tag{36}$$

This is a deterministic equation that can be solved for the unknown coefficients $\mathbf{C}_i$. Values for the coefficients d_{ijk} can be calculated ahead of time and tabulated. Table 1 shows one such table for the 1D case where a single random variable ξ_1 is used to characterize the randomness of the problem; this would correspond to the case where only one property is modeled as a random variable.

Once the coefficients in the expansion of the solution process have been evaluated, the variance of the solution can be readily obtained. Noting that the polynomial chaos basis is orthogonal, a simple expression for the covariance matrix of the solution process is given by

$$\mathbf{R}_{TT} = \sum_{i=1}^{N} \mathbf{T}_i \mathbf{T}_i^T \langle \psi_i^2 \rangle \tag{37}$$

The variance of the solution at any modal point is then obtained as the diagonal elements of $\mathbf{R}_{TT}$. Of course, additional information is contained in the expansion coefficients $\mathbf{T}_i$, beyond this second-order characterization. Indeed, a complete probabilistic characterization is condensed in these coefficients. Simulated realizations of the solution can be simply obtained by generating a set of random variables ξ_i from which the polynomial chaoses are formed and used in the expansion of the temperature field. The coefficients of the first-order expansion (those multiplying the first-order polynomials, ξ_1, ξ_2, ξ_3, ξ_4) can be viewed as the first-order sensitivity coefficients

TABLE 1. Nonzero Values of d_{ijk} for $M = 1$; 1D Polynomials

$i+1$ (1)	$j+1$ (2)	$k+1$ (3)	d_{ijk} (4)
1	1	1	1
1	2	2	1
1	3	3	2
1	4	4	6
1	5	5	24
2	1	2	1
2	2	1	1
2	2	3	2
2	3	2	2
2	3	4	6
2	4	3	6
2	4	5	24
2	5	4	24
3	1	3	2
3	2	2	2
3	2	4	6
3	3	1	2
3	3	3	8
3	3	5	24
3	4	2	6
3	4	4	36
3	5	3	24
3	5	5	192
4	1	4	6
4	2	3	6
4	2	5	24
4	3	2	6
4	3	4	36
4	4	1	6
4	4	3	36
4	4	5	216
4	5	2	24
4	5	4	216
5	1	5	24
5	2	4	24
5	3	3	24
5	3	5	192
5	4	2	24
5	4	4	216
5	5	1	24
5	5	3	192
5	5	5	1,728

similar to those obtained from a perturbation-based analysis of the problem (Fadale and Emery 1994).

IMPLEMENTATION DETAILS

The stochastic finite-element method presented in this paper can be readily integrated into an existing deterministic finite-element program. The necessary steps for doing so are as follows:

1. Decompose the random material properties into their basic scales of fluctuation using the Karhunen-Loève expansion. For the case of a random variable, these reduce to a single scale of constant value.
2. Construct the capacitance and conductance matrices using, in turn, each of these scales as the material property. Denote each of the matrices by $\mathbf{C}_i$ and $\mathbf{K}_i$ corresponding to scale i.
3. Construct a large matrix of dimension $n \times N$ where n denotes the number of degrees-of-freedom in a deter-

TABLE 2. $\psi_i(\eta)$ Used in Evaluating Polynomial Chaos Coefficients of Lognormal Process

$\psi_i(\xi)$ (1)	$\psi_i(\eta)$ (2)	$\langle \psi_i(\eta) \rangle$ (3)
ξ_i	$\eta_i + g_i$	g_i
$\xi_i\xi_j - \delta_{ij}$	$(\eta_i + g_i)(\eta_j + g_j) - \delta_{ij}$	$g_i g_j$
$\xi_i\xi_j\xi_k - \xi_i\delta_{jk} - \xi_j\delta_{ik} - \xi_k\delta_{ij}$	$(\eta_i + g_i)(\eta_i + g_j)(\eta_j + g_k) - g_i\delta_{jk} - g_j\delta_{ik} - g_k\delta_{ij}$	$g_i g_j g_k$

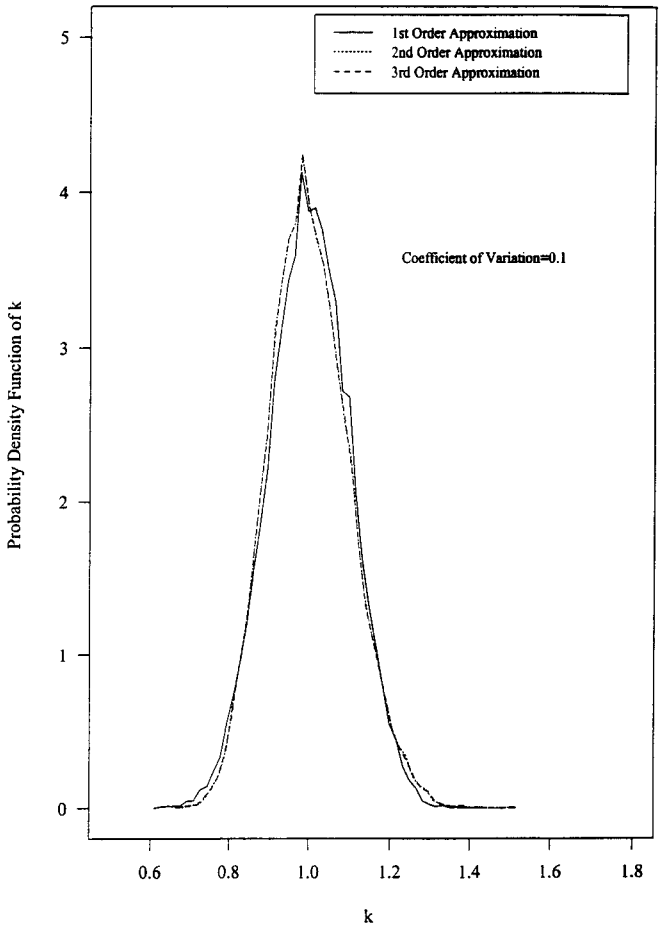

FIG. 1. Approximation of Lognormal Variables by Successive Polynomial Chaos; COV = 0.1

ministic problem, and N denotes the number of terms retained in the random expansion. Index the submatrices by j and k.

4. Multiply each $\mathbf{C}_i$ and $\mathbf{K}_i$ by the coefficient d_{ijk} for each j and k and add the product thus obtained to the j-k submatrix in the large matrix.
5. Only the first block of the right-hand side vector is nonzero and is equal to its deterministic value. This of course is only true under the assumption that the applied fluxes are deterministic, and the procedure must be modified accordingly for random fluxes.
6. Essential boundary conditions are applied to the nodes associated with the mean term in the expansion (the first block). Homogeneous boundary conditions of the same type applied to the first block are applied to all of the other blocks. This will ensure that the boundary conditions are satisfied with probability one.
7. The large system of equations is solved for the coefficients in the expansion for the temperature field.
8. The variance of the temperature can be evaluated using (39).

The framework presented in the previous sections is now applied to a simple example. Consider a 1D domain defined over $\zeta \in [0, 1]$, with both random heat capacity and random conductivity. Assume each of these two random quantities to be specified, in a probabilistic sense, by its mean value and its correlation function. Note that in the case of a random variable, this mean value would be a constant, and the correlation function would be equal to the variance of the random variable. The two random processes can then be represented in the following form:

$$\mathbf{C} = \bar{\mathbf{C}} + \xi_1 \mathbf{C}_1 \tag{38}$$

and

$$\mathbf{K} = \bar{\mathbf{K}} + \xi_1 \mathbf{K}_1 + \xi_2 \mathbf{K}_2 + \xi_3 \mathbf{K}_3 \tag{39}$$

where the random variables ξ_i appearing in both expansions are orthogonal. The inclusion of two terms in the representation of the heat capacity reflects the hypothesis that it varies slowly over space, while the inclusion of four terms in the representation for the conductivity corresponds to the hypothesis that this property varies more significantly over space. To combine both expansions in the same computational framework, it is expedient to rewrite them as follows:

$$\mathbf{C} = \bar{\mathbf{C}} + \xi_1 \mathbf{0} + \xi_2 \mathbf{0} + \xi_3 \mathbf{0} + \xi_4 \mathbf{C}_4 = \sum_{i=0}^{4} \xi_i \mathbf{C}_i \tag{40}$$

and

$$\mathbf{K} = \bar{\mathbf{K}} + \xi_1 \mathbf{K}_1 + \xi_2 \mathbf{K}_2 + \xi_3 \mathbf{K}_3 + \xi_4 \mathbf{0} = \sum_{i=0}^{4} \xi_i \mathbf{K}_i \tag{41}$$

Moreover, an expansion of the temperature field will be sought in the form

$$\mathbf{T} = \bar{\mathbf{T}} + \xi_1 \mathbf{T}_1 + \xi_2 \mathbf{T}_2 + \xi_3 \mathbf{T}_3 + \xi_4 \mathbf{T}_4 + (\xi_1^2 - 1)\mathbf{T}_5 + (\xi_1 \xi_2)\mathbf{T}_6 + (\xi_1 \xi_3)\mathbf{T}_7 + (\xi_1 \xi_4)\mathbf{T}_8 + (\xi_2^2 - 1)\mathbf{T}_9 + (\xi_2 \xi_3)\mathbf{T}_{10} + (\xi_2 \xi_4)\mathbf{T}_{11} + (\xi_3^2 - 1)\mathbf{T}_{12} + (\xi_3 \xi_4)\mathbf{T}_{13} + (\xi_4^2 - 1)\mathbf{T}_{14} = \sum_{i=0}^{14} \psi_i \mathbf{T}_i \tag{42}$$

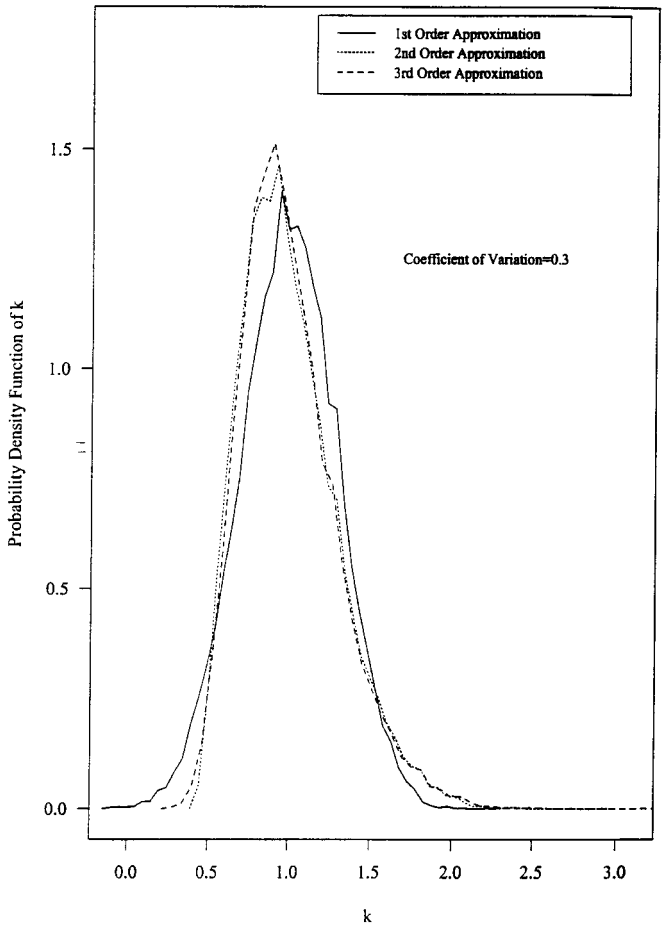

FIG. 2. Approximation of Lognormal Variables by Successive Polynomial Chaos; COV = 0.3

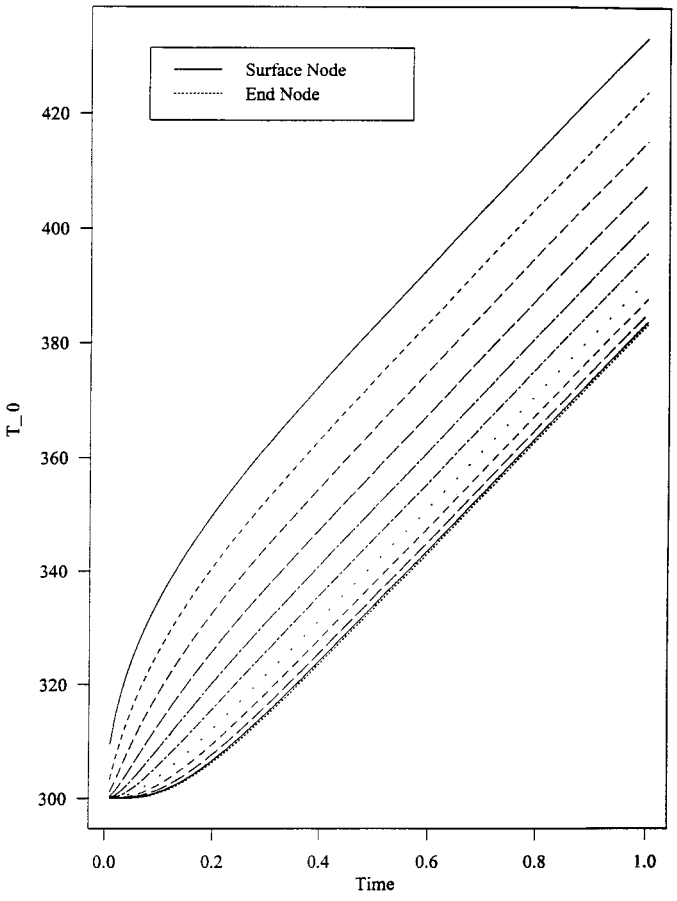

FIG. 3. Coefficients in Expansion of Temperature. Deterministic Parameters

This expansion includes all of the second-order terms in the four variables ξ_i defining the material properties and thus serves as an approximation of the temperature field as a surface in the space defined by these variables (recall that $\xi_0 \equiv 1$ and is thus not considered as one of the basic variables). The indexing on the coefficients in all of the preceding expansions is compatible with a four-dimensional (4D) expansion. For lower dimensional expansion, the same indexing can still be used with only the coefficients referencing the active ξ_i variables not equal to zero. For higher order expansions, on the other hand, the indexing scheme must be modified to insert the polynomials with respect to the new variables at their appropriate location. The significance of the various terms in (42) is of great relevance in applications. In particular, to the extent that each ξ_i represents the contribution of the ith scale of fluctuation of a specific material property, the coefficients of the first-order terms in the expansion of the temperature field (i.e., those terms multiplying the first-order polynomials), represent the first-order sensitivity of the temperature with respect to that specific scale. The first-order sensitivity of the temperature with respect to the overall property is obtained by adding the contribution from all scales making up that property. The resolution of the sensitivity at the levels of individual scales, however, is of great significance in itself. Indeed, it permits the identification of the significant scales of the property, thus indicating a preferred strategy for the experimental estimation of that property. Through a judicious spacing of measurements along a specimen, a specific scale of fluctuation of the material property can be evaluated. The higher order terms in the expansion can be used to refine the estimated values of these sensitivities to within target accuracy.

NON-GAUSSIAN MATERIAL PROPERTIES

For non-Gaussian material properties the method presented in this paper is still applicable, provided the polynomial chaos expansion is used to represent the material property instead of the Karhunen-Loève expansion. Assume, for example that the conductivity process k_{11} is a lognormal process and is thus obtained as the exponential of a Gaussian process g defined as

$$g = \bar{g} + \xi_1 g_1 + \xi_2 g_2 + \xi_3 g_3 \tag{43}$$

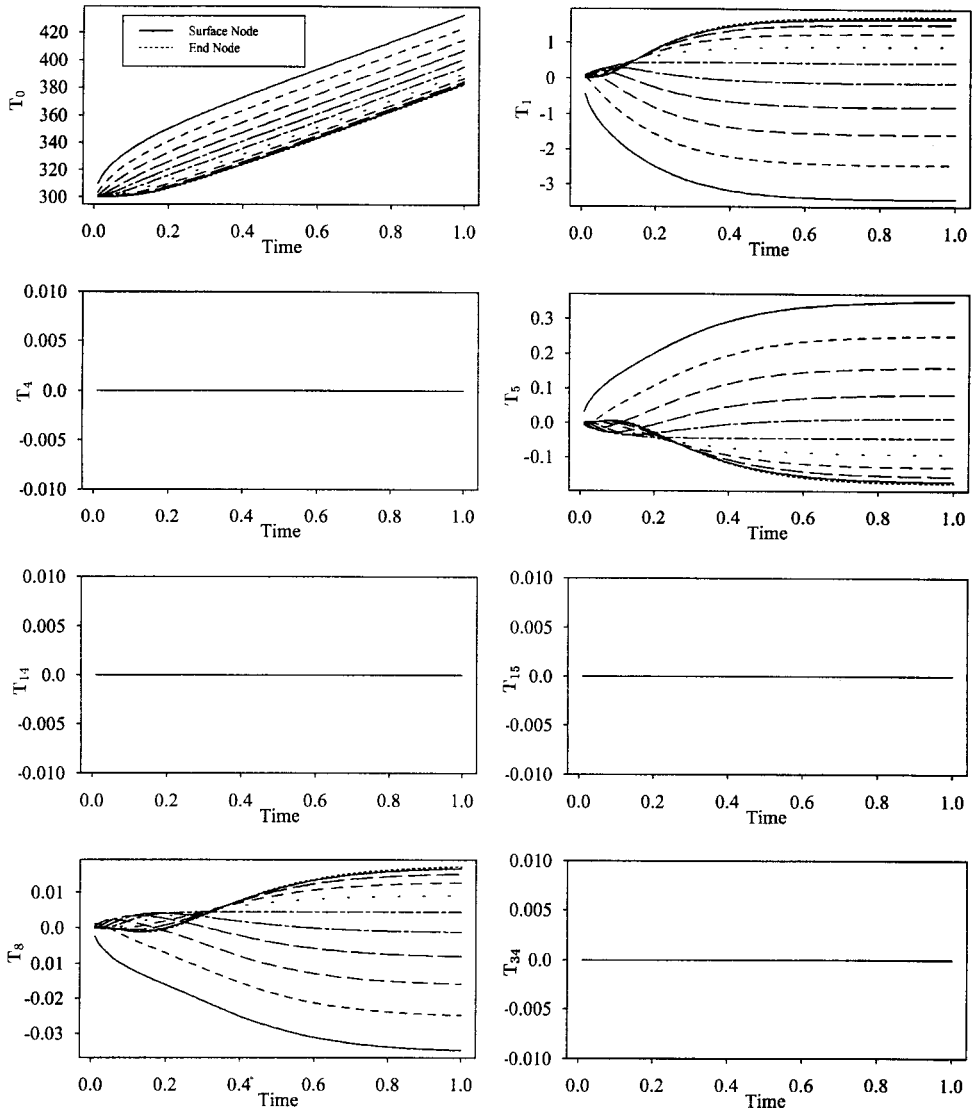

FIG. 4. Coefficients in Expansion of Temperature. Gaussian Conductivity; COV Conductivity = 0.1; COV Heat Capacity = 0

Then k_{11} can be written as a polynomial in the three variables, ξ_1, ξ_2, and ξ_3. In particular, a form is sought in terms of the polynomial chaos polynomials, resulting in the following relation:

$$k_{11} = e^g = \sum_{i=0}^{N} k_i \psi_i \tag{44}$$

In view of the orthogonality of the ψ_i variables, the coefficients k_i can be obtained as

$$k_i = \frac{\langle \psi_i e^g \rangle}{\langle \psi_i^2 \rangle} \tag{45}$$

The denominator in this last equation is easy to calculate and tabulate. The numerator, on the other hand, requires special treatment (Ghanem, unpublished paper, 1997). Specifically, it can be rewritten as

$$\langle \psi e^g \rangle = \int_{-\infty}^{\infty} \psi(\boldsymbol{\xi}) \exp\left[g - \frac{1}{2} \boldsymbol{\xi}^T \boldsymbol{\xi} \right] d\boldsymbol{\xi} \tag{46}$$

This integral can be evaluated in closed form resulting in

$$k_i = \frac{\langle \psi_i(\boldsymbol{\eta}) \rangle}{\langle \psi_i^2 \rangle} \exp\left[\bar{g} + \frac{1}{2} \sum_{j=1}^{N} g_j^2 \right] \tag{47}$$

with $\psi_i(\boldsymbol{\eta})$ given in Table 2. For the case where the process g is reduced to a random variable, thus resulting in a single term in its expansion, the lognormal variable k can then be written as a 1D polynomial in this Gaussian variable according to

$$k = \exp\left[\bar{g} + \frac{\sigma_g^2}{2} \right] \sum_{j=0}^{\infty} \frac{\sigma_g^j}{j!} \psi_j \tag{48}$$

Figs. 1 and 2 show the probability density function of a lognormal variable being approximated in this fashion. Fig. 1 corresponds to a coefficient of variation (COV) of the lognormal variable equal to 0.1 while Fig. 2 corresponds to a COV equal to 0.3. Each of these figures shows the probability density function associated with successively higher levels of approximation, with the first level being equal to the Gaussian approximation.

If the random process for the heat capacity c is also non-

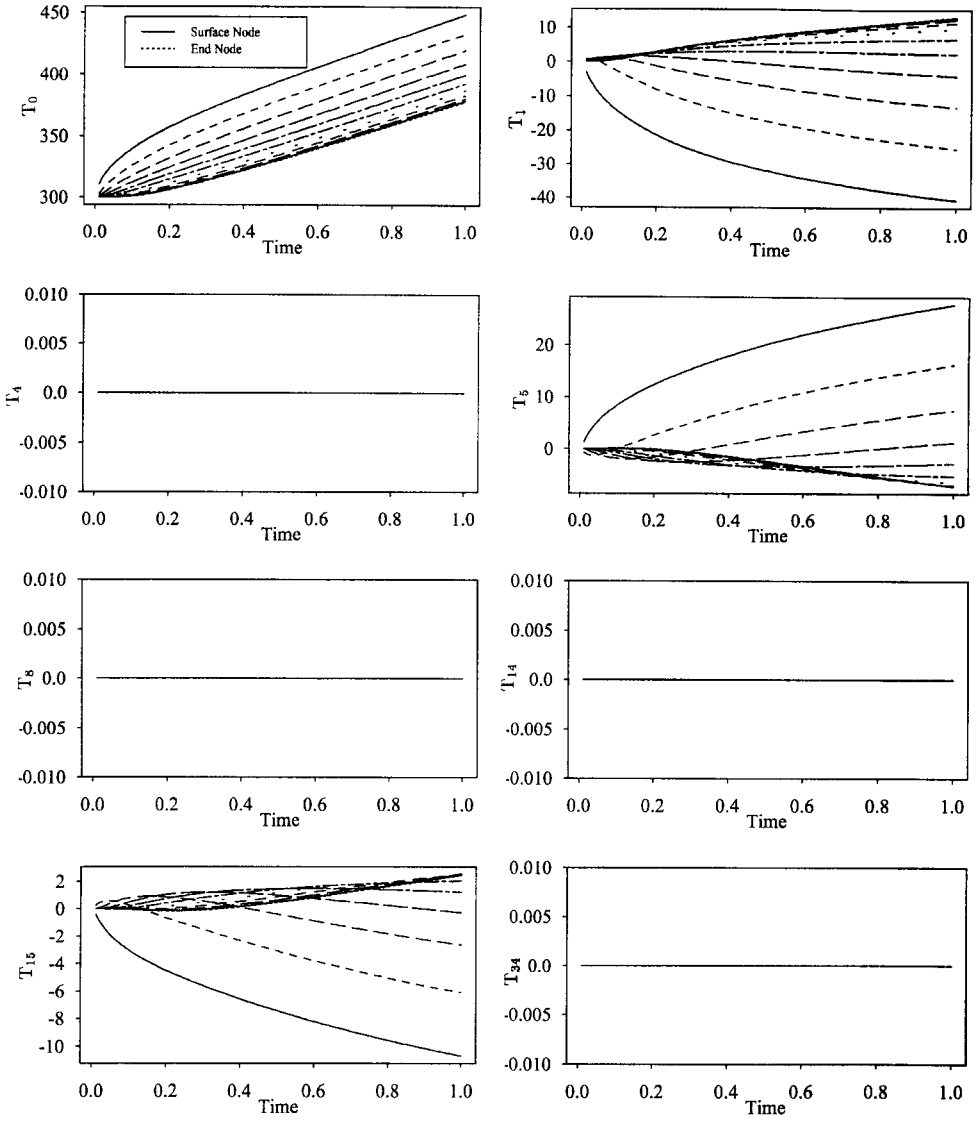

FIG. 5. Coefficients in Expansion of Temperature. Gaussian Conductivity; COV Conductivity = 0.4; COV Heat Capacity = 0

Gaussian and is also represented as a polynomial in a Gaussian variable ξ_4 then the preceding equations for the capacitance matrix **C** and, and the conductivity matrix **K**, are replaced by the following two equations:

$$\mathbf{C} = \bar{\mathbf{C}} + \xi_1\mathbf{0} + \xi_2\mathbf{0} + \xi_3\mathbf{0} + \xi_4\mathbf{C}_4 + (\xi_1^2 - 1)\mathbf{0} + (\xi_1\xi_2)\mathbf{0} + (\xi_1\xi_3)\mathbf{0} + (\xi_1\xi_4)\mathbf{0} + (\xi_2^2 - 1)\mathbf{0} + (\xi_2\xi_3)\mathbf{0} + (\xi_2\xi_4)\mathbf{0} + (\xi_3^2 - 1)\mathbf{0} + (\xi_3\xi_4)\mathbf{0} + (\xi_4^2 - 1)\mathbf{C}_14 = \sum_{i=0}^{14} \psi_i\mathbf{C}_i \quad (49)$$

and

$$\mathbf{K} = \bar{\mathbf{K}} + \xi_1\mathbf{K}_1 + \xi_2\mathbf{K}_2 + \xi_3\mathbf{K}_3 + \xi_4\mathbf{0} + (\xi_1^2 - 1)\mathbf{K}_5 + (\xi_1\xi_2)\mathbf{K}_6 + (\xi_1\xi_3)\mathbf{K}_7 + (\xi_1\xi_4)\mathbf{K}_8 + (\xi_2^2 - 1)\mathbf{K}_9 + (\xi_2\xi_3)\mathbf{K}_{10} + (\xi_2\xi_4)\mathbf{K}_{11} + (\xi_3^2 - 1)\mathbf{K}_{12} + (\xi_3\xi_4)\mathbf{K}_{13} + (\xi_4^2 - 1)\mathbf{0} = \sum_{i=0}^{14} \psi_i\mathbf{K}_i \quad (50)$$

The expansion for the temperature field remains unchanged. In the case of either the conductivity or the heat capacity being modeled as a random variable as opposed to a random process, the preceding expansions simplify by restricting them to a single variable ξ_i and all of its 1D polynomials. This is consistent with the notion that a random variable is a limiting case of a stochastic process as its correlation length becomes very large, thus allowing one term in its Karhunen-Loève expansion to substantially dominate over all others.

Obviously, the coefficients d_{ijk} associated with the 4D expansions in this example must be obtained from a table similar to Table 1 developed specifically for the 4D (or higher) case. Such tables can be readily developed using any of the readily available symbolic manipulation packages such as Macsyma or Mathematica.

NUMERICAL EXAMPLE

The method described earlier is now exemplified by its application to a simple problem. Consider a 1D domain of unit length subjected to a constant heat flux, $q_b = 1$, at one end and perfectly insulated at the other end. Let the initial temperature

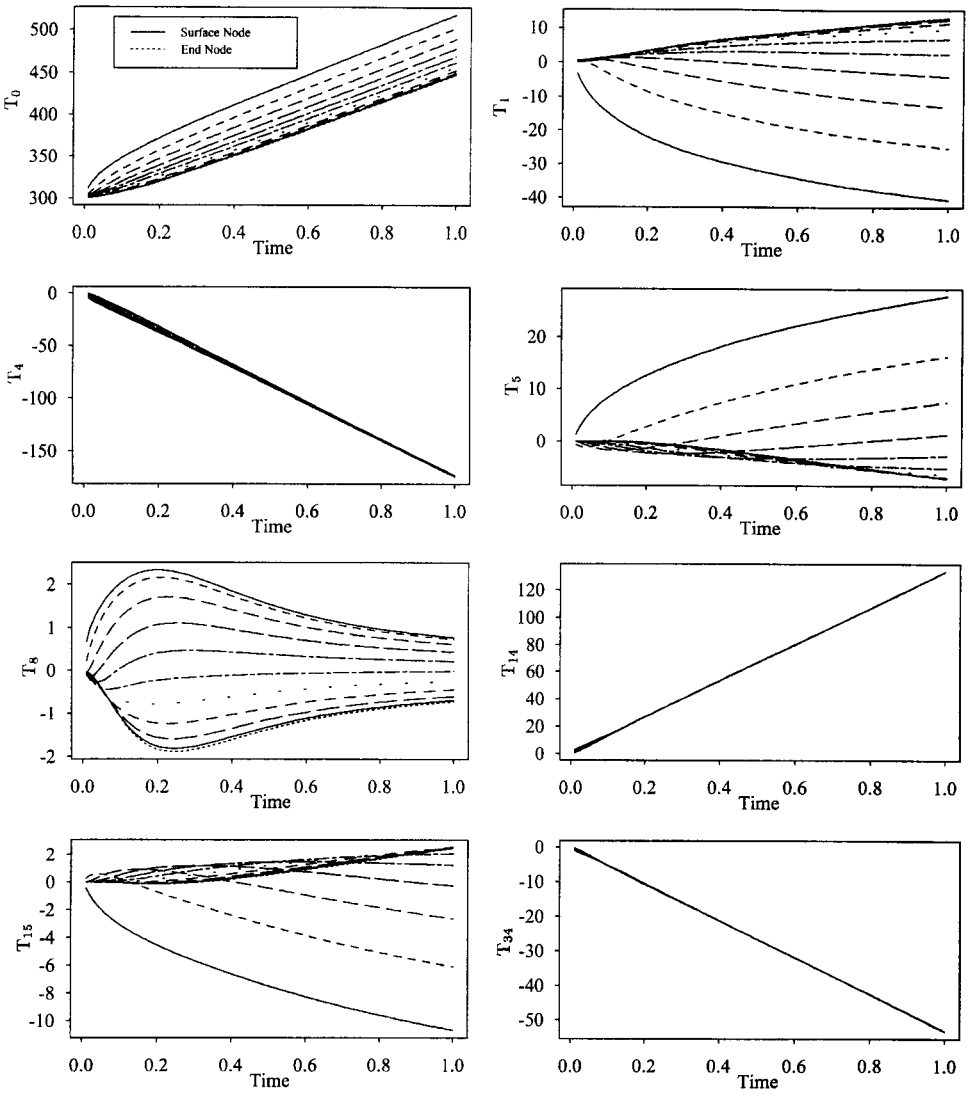

FIG. 6. Coefficients in Expansion of Temperature. Gaussian Conductivity and Heat Capacity; COV Conductivity = 0.4; COV Heat Capacity = 0.4

of the domain be at 300°C. The spatial domain is divided into a uniform mesh of 10 elements. Fig. 3 shows the evolution with time of the temperature at various nodal points in the domain under the assumption of a homogeneous medium. The remaining figures show the results associated with the thermal conductivity and the heat capacity having nonzero COV. In all of the following cases, the material will be assumed to be isotropic with random fluctuations having an exponentially decaying correlation function. Figs. 4 and 5 correspond to a random conductivity with COVs = 0.1 and 0.4, respectively. Fig. 6 corresponds to the case where both the conductivity and the heat capacity are random with each of their COVs = 0.4. The subscript on the temperature in all the figures refers to the expansion given in (44). In the case where only one of the properties is random, the coefficients of the other property, as given in (43) and (44), are automatically set to zero since they are proportional to the COV of the property. This explains the zero value of some of the coefficients in the figures whenever one of the properties is deterministic. Both material properties have thus far been assumed to have a Gaussian distribution.

Fig. 7 shows results associated with the conductivity having a lognormal distribution with a COV = 0.4. It is observed that the effect of non-Gaussian material randomness increases substantially with the level of random fluctuations as described by the COV. In Fig. 7 the heat capacity is assumed to be deterministic, and three terms are used in expanding the lognormal conductivity [four terms in (50) including the mean]. This corresponds to the terms $\mathbf{K}_0$, $\mathbf{K}_1$, $\mathbf{K}_5$ and $\mathbf{K}_{15}$ in (52) being nonzero. Note that the terms $\mathbf{T}_{15}$ and $\mathbf{T}_{34}$ are not shown in (44). They refer to the third-order term in the expansion of the conductivity and the third-order term in the expansion of the heat capacity, and their associated polynomials have the form $\psi_{15} = \xi_1^3 - 3\xi_1$ and $\psi_{34} = \xi_4^3 - 3\xi_4$.

In all of the aforementioned results, the correlation length of the conductivity process is taken to be very large (10,000), and a single term is included in its expansion. Figs. 8 and 9 show results similar to those in Figs. 4 and 5 except now the correlation length of the conductivity process is taken to be equal to 0.2, and two terms are included in the expansion of the process. These results correspond to the case of a Gaussian

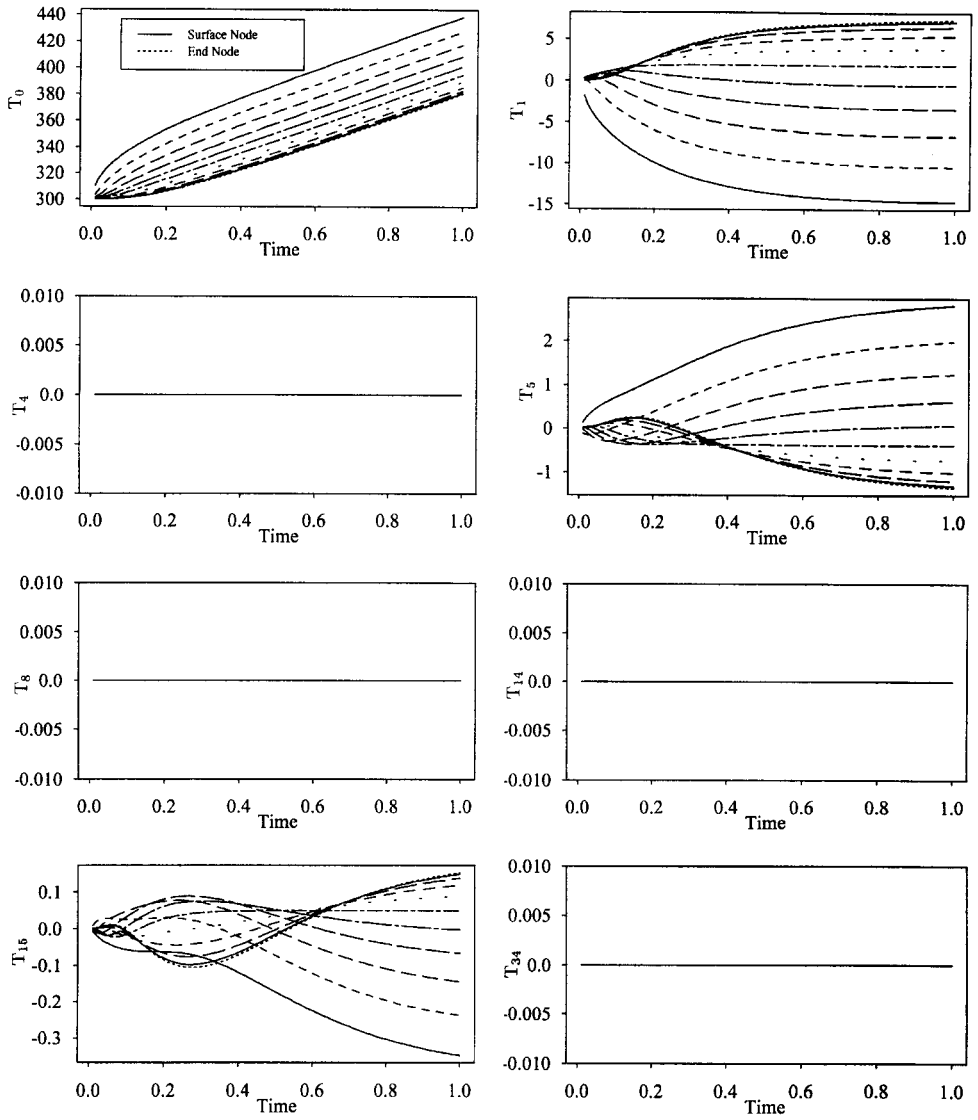

FIG. 7. Coefficients in Expansion of Temperature. Lognormal Conductivity; COV Conductivity = 0.4; COV Heat Capacity = 0

conductivity process. This implies that the terms multiplying the polynomials in ξ_1 and ξ_2 are now activated. The first-order sensitivity, captured by the terms multiplying ξ_1 and ξ_2, is now resolved with respect to each of these scales. Given the short correlation length used in this example, the contribution from the two scales is of the same order of magnitude. The scales of fluctuation represent the frequencies of fluctuation of the data at which the contributions to the overall property are uncorrelated. It is clear from these results that the sensitivity of the temperature field with respect to the uncertainties in the conductivity depends greatly on these scales of fluctuation, and it seems that modeling thermal conductivity as a stochastic process as opposed to a random variable can provide much toward meaningful experiment design. Give the simple character of the problem used in this example, the specific conclusions drawn here cannot, obviously, be generalized. The qualitative nature of these conclusions, however, are adequately supported by this 1D example. Figs. 10 and 11 finally show results associated with the distribution, along the domain, of the values of coefficients $\mathbf{T}_i$. Fig. 10 corresponds to the case of a random variable conductivity, while Fig. 11 corresponds to the case of a stochastic conductivity process with correlation length equal to 0.2. In both cases, the COV of the conductivity is 0.4, and the heat capacity is assumed to be a random variable with a COV also equal to 0.4. It is clear from Figs. 10 and 11 that different spatial locations within the domain feature different levels of sensitivity to fluctuations in the thermal properties of the medium. This information is again very valuable for devising an experimental program aimed at measuring the mean and variability in these properties.

It is clear from the results presented in this section that the temperature distribution throughout the domain is much more sensitive to variations in the heat capacity than to variations in the conductivity. Moreover, for larger values of COVs of the heat capacity, second-order effects, as captured by the coefficients T_{14} and T_{34}, have the same order of magnitude as the first-order sensitivity coefficient T_4. It should be noted, however, that the uncertainty in the value of the heat capacity is likely to be much smaller than the uncertainty in the value of thermal conductivity.

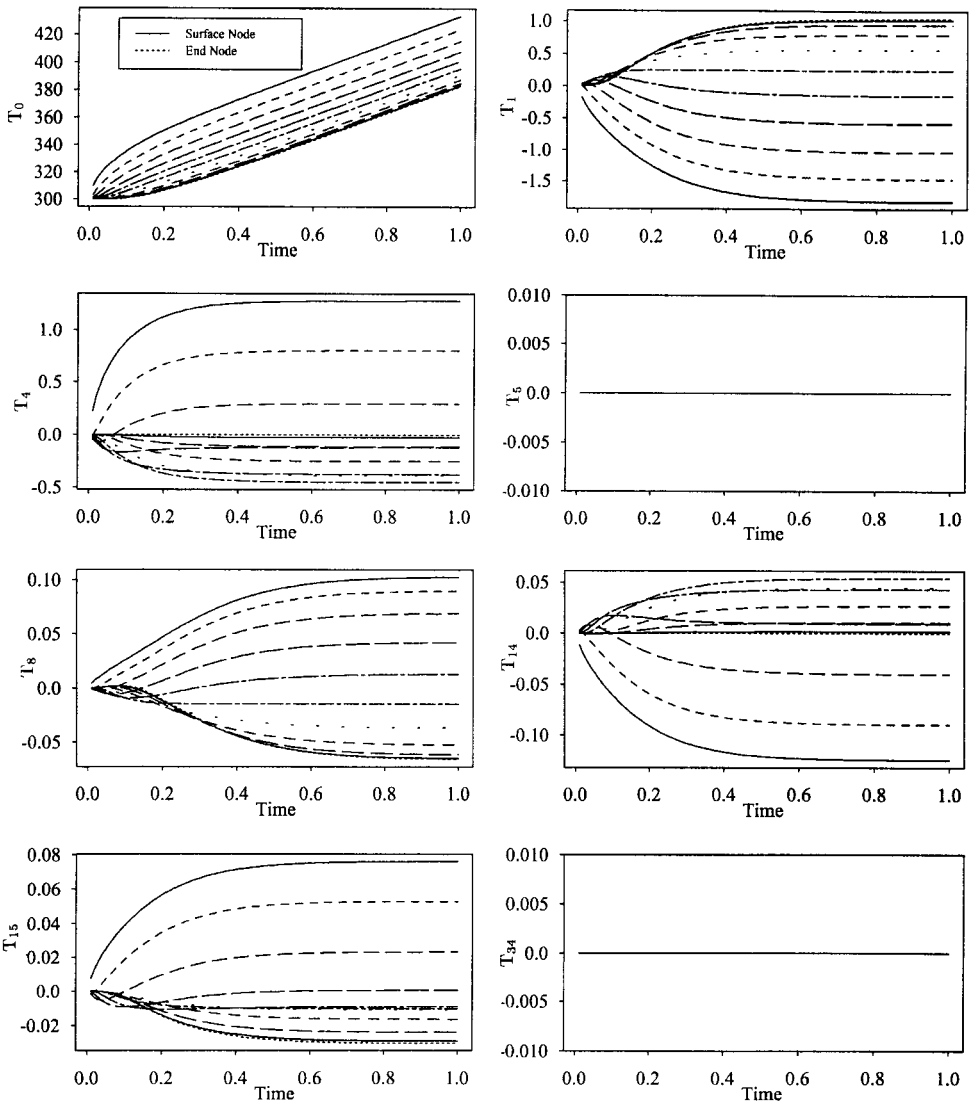

FIG. 8. Coefficients in Expansion of Temperature. Gaussian Conductivity Process; COV Conductivity = 0.1; Correlation Length = 0.2; Two Terms in Karhunen-Loève Expansion

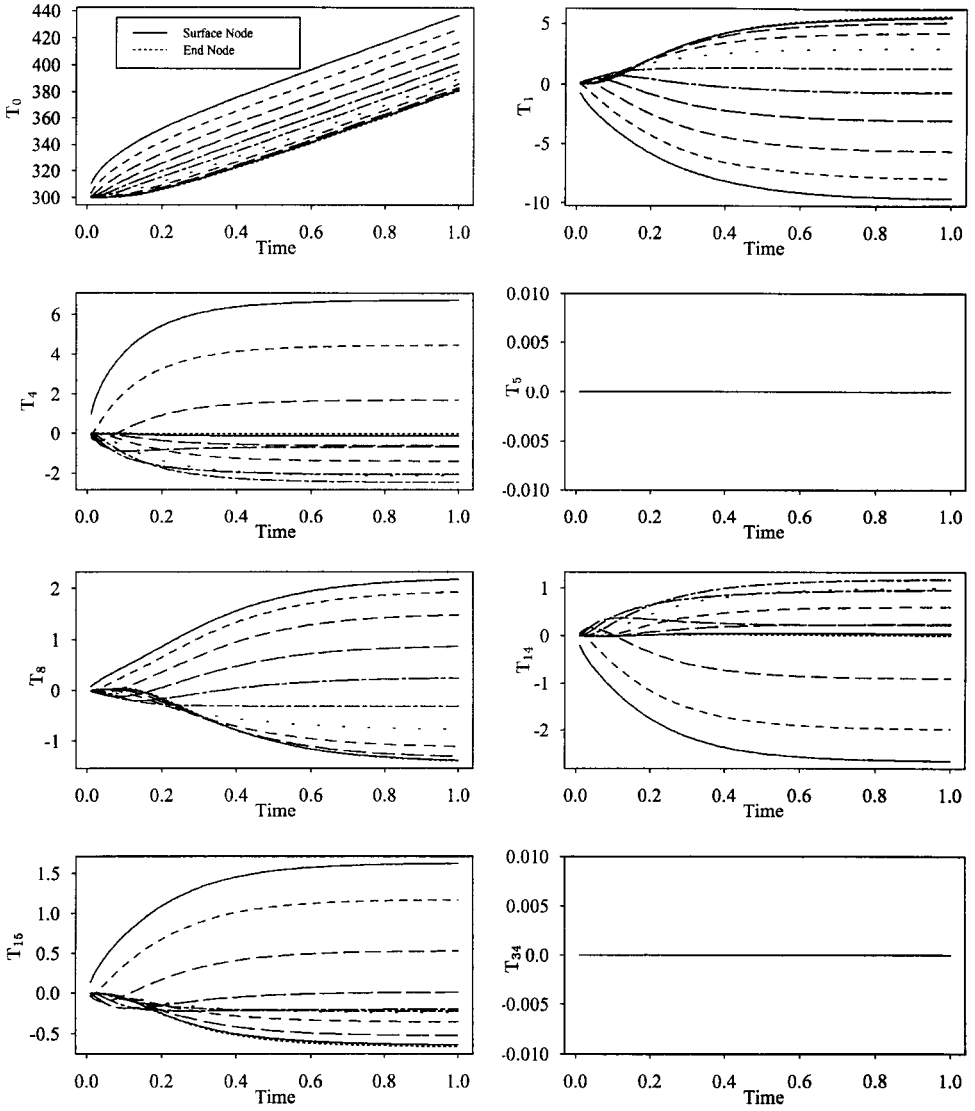

FIG. 9. Coefficients in Expansion of Temperature. Gaussian Conductivity Process; COV Conductivity = 0.4; Correlation Length = 0.2; Two Terms in Karhunen-Loève Expansion

CONCLUSIONS

A method has been presented that is capable of addressing in great generality heat conduction problems involving random media. The method is based on treating the random aspect of the problem as a new dimension along which a spectral expansion is carried out. The method has been exemplified by its application to a simple problem. Material properties modeled as stochastic processes are handled just as easily as those modeled as random variables, and multiple heterogeneities can be included simultaneously. Moreover, the method is not restricted in its applicability to Gaussian material properties as demonstrated by the application. This method, however, results in an extended system of equations that is larger than the associated deterministic finite-element system. This increase in size is commensurate with the addition of a new dimension to the problem and should be viewed as the cost of added accuracy. Techniques are being developed that capitalize on the peculiar structure of the final large matrix (Ghanem and Kruger 1996). This peculiarity stems from the fact that each of its submatrices has an identical nonzero structure. It has been observed from the results presented in this paper that great value is to be gained from modeling the material properties as stochastic processes as opposed to modeling them as random variable.

An important value of the procedure presented in this paper is that it provides the solution in the form of a convergent expansion; thus a reliable characterization for the propagation of uncertainty from the thermal properties values to the predicted values of the temperature can be obtained.

It should be noted that the uncertainty in the coefficients of a differential equation, which have been represented by means of their respective Karhunen-Loève expansions, derives from the more basic uncertainty present at the microstructural level of the material. The macroscale coefficients, referring to the coefficients in the governing differential equation, typically are obtained from the microstructure through an averaging process over a representative volume. The outcome of this process implicitly generates a spatially fluctuating averaged quantity (by taking adjacent representative volumes), thus leading the

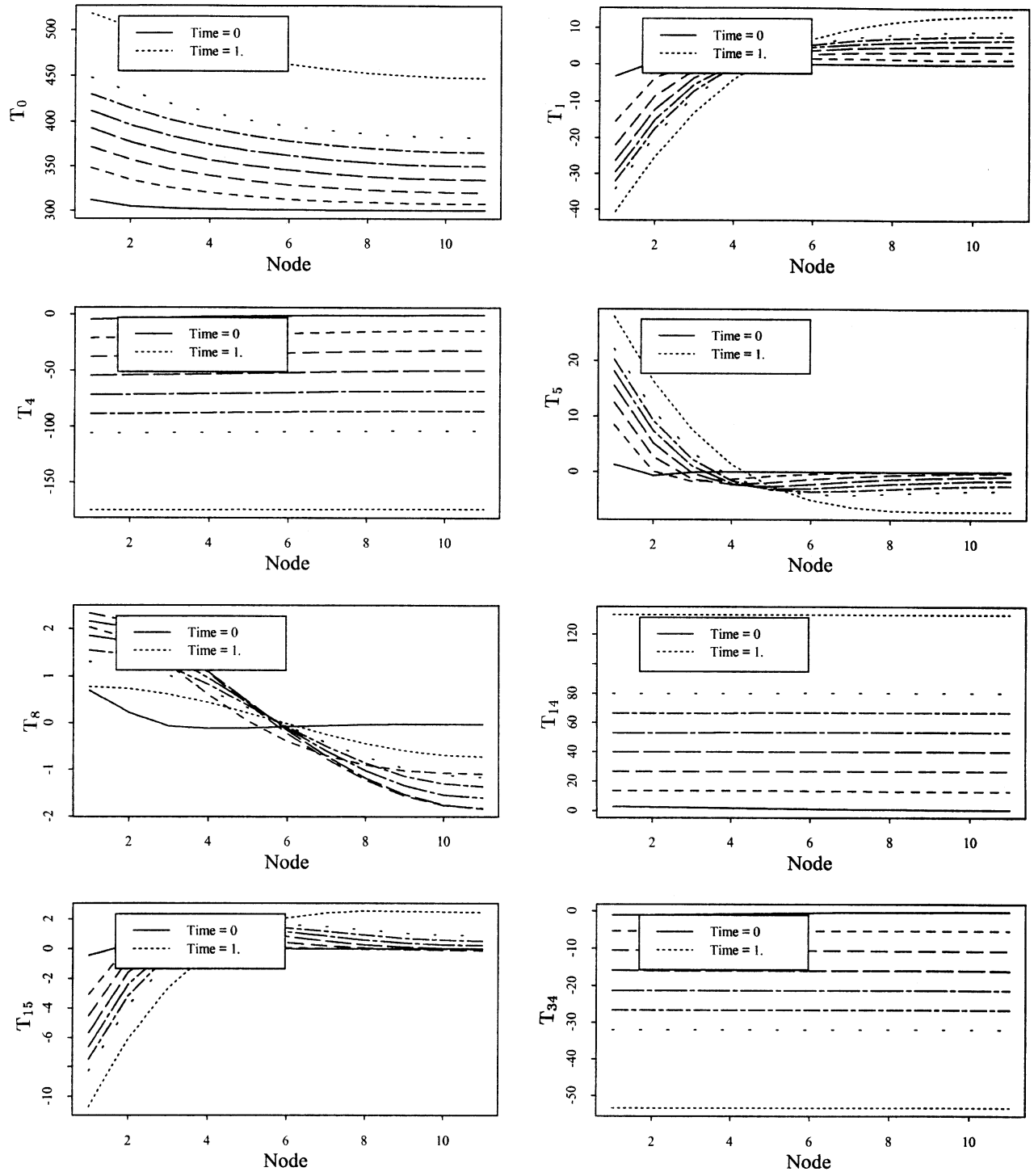

FIG. 10. Coefficients in Expansion of Temperature. Gaussian Conductivity and Heat Capacity; COV Conductivity = 0.4; COV Heat Capacity = 0.4

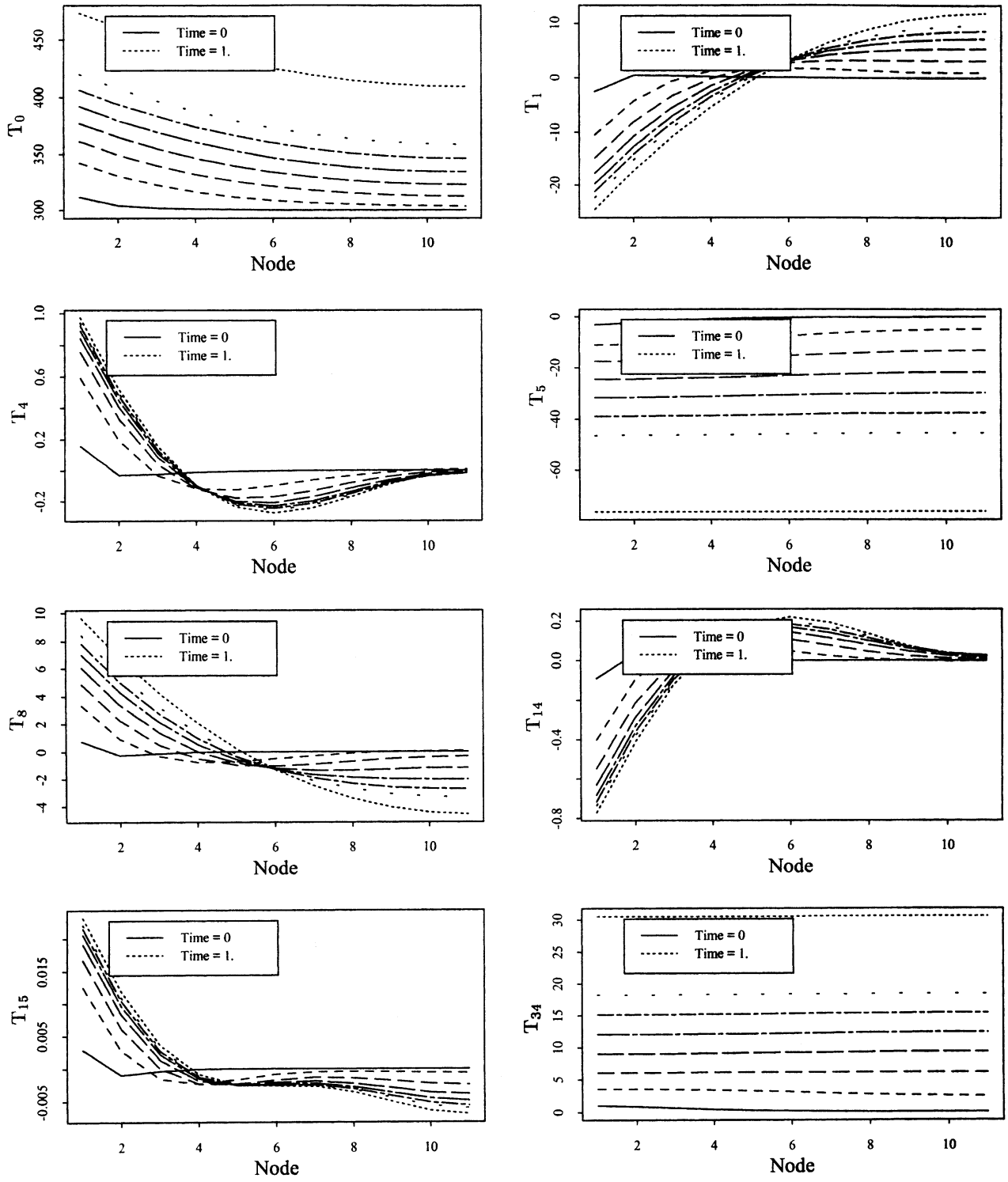

FIG. 11. Coefficients in Expansion of Temperature. Gaussian Conductivity Process; Gaussian Heat Capacity Variable; COV Conductivity = 0.4; COV Heat Capacity = 0.4; Correlation Length = 0.2; Two Terms in Karhunen-Loève Expansion

way to the spatial fluctuations which are modeled as a stochastic process. It should also be stressed that, by varying the correlation length of the stochastic process both slowly and rapidly, fluctuating processes can be modeled. An important outcome of the present study is the identification of those scales of fluctuation that are important for enhancing the predictive capability of the differential equation model. This should assist researchers in microstructure modeling to tailor their experiments toward detecting and quantifying those scales.

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