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Variability response functions for apparent material properties

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ABSTRACT

The computation of apparent material properties for a random heterogeneous material requires the assumption of a solution field on a finite domain over which the apparent properties are to be computed. In this paper the assumed solution field is taken to be that defined by the shape functions that underpin the finite element method and it is shown that the variance of the apparent properties calculated using the shape functions to define the solution field can be expressed in terms of a variability response function (VRF) that is independent of the marginal distribution and spectral density function of the underlying random heterogeneous material property field. The variance of apparent material properties can be an important consideration in problems where the domain over which the apparent properties are computed is smaller than the representative volume element and the approach introduced here provides an efficient means of calculating that variance and performing sensitivity studies with respect to the characteristics of the material property field. The approach is illustrated using examples involving heat transfer problems and finite elements with linear and nonlinear shape functions and in one and two dimensions. Features of the VRF are described, including dependency on shape and scale of the finite element and the order of the shape functions.

1. Introduction

In the practical analysis of engineering problems using continuum approaches, apparent, effective, or homogenized material properties must be computed to apply the governing equations of continuum mechanics. When an apparent material property is computed in a given domain from an underlying random field model for a spatially varying material property the result is a random quantity that is no longer spatially variable. For example, apparent elastic modulus or thermal conductivity are random variables that are spatially constant over the problem domain as opposed to the underlying spatially varying random fields. As the volume of the domain increases, the variance of the apparent properties decreases until it becomes negligible, at which point one is said to have reached the representative volume element (RVE). For many structural and mechanical systems, assumption of an RVE is appropriate, but for many others residual uncertainty in the apparent properties should be considered. This situation has, to some extent, been characterized as involving the statistical volume element (SVE) [1–3] and addressed using Monte Carlo based finite element approaches [4–6]. This paper describes a method for computing the variability of apparent material properties—specifically the thermal conductivity—using variability response functions (VRFs) that have the advantage of being analytically rather than numerically derived and provide a method for computing the variance of the apparent property that is independent of the distribution and spectrum of the underlying material property field. In the context of this paper, the VRF formulation is developed by imposing the shape functions of the finite element formulation on the problem domain and computing apparent properties based on equivalence of the finite element characteristic matrices for the heterogeneous and homogeneous versions of the problem.

One of the challenges present in any approach to computing apparent properties is that the apparent property obtained depends on the boundary conditions applied to the heterogeneous version of the problem in obtaining the apparent property [7,8]. Using the shape functions of a finite element formulation does not remove this boundary condition dependence, but does allow the obtained apparent properties to be, in a sense, consistent with the formulation used in further finite element analysis of the problem. Other approaches commonly used include the imposition of periodic boundary conditions [9].

The VRF approach to uncertainty quantification was developed in the context of computing the variance of the displacement response of structural systems with spatially varying, random material properties [10–12]. It has since been extended to the problem

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of computing the variance of apparent elastic material properties for statically determinate, indeterminate, and continuum systems [8,13,14]. Here, those approaches are combined with the seminal approach to the stochastic finite element method that computes the variability of the nodal displacements in a finite element model based on an underlying stochastic field of material properties [12].

The remainder of the paper is organized as follows: First a problem statement is given that defines more precisely the notion of the apparent material property and the residual uncertainty associated with the apparent property. Next the general approach to computing VRFs for the apparent material properties in a finite element context is introduced for the heat conduction problem. Examples are then given for the linear and quadratic one dimensional elements and the linear triangular element. Finally, comments are provided on how this version of assessing the uncertainty of apparent properties may find a place in a multi-scale analysis context.

2. Problem statement

Let $\Omega \subset \mathbb{R}^n$ define a solid body occupied by a material with properties defined by the spatially varying and random (heterogeneous) matrix $\mathbf{c}(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^n$ and subject to Neumann and Dirichlet boundary conditions on the boundary segments $\partial\Omega_{neumann}$ and $\partial\Omega_{dirichlet}$ respectively. Consider now the case in which this body, subject to the same boundary conditions, is occupied by a material with properties defined by the spatially invariant (homogeneous) matrix $\bar{\mathbf{c}}$. The definition of an apparent property depends on choosing $\bar{\mathbf{c}}$ such that

$$g(\phi_{het}(\mathbf{x})) = g(\phi_{hom}(\mathbf{x})) \tag{1}$$

where $\phi_{het}(\mathbf{x})$ and $\phi_{hom}(\mathbf{x})$ are solution fields in the heterogeneous and homogeneous bodies respectively and $g(\cdot)$ represents a function of those solution fields that is usually chosen to have some physical meaning. In elasticity problems the strain energy is often chosen to act as $g(\cdot)$ so that the energetics of the heterogeneous and homogeneous versions of the problem are equivalent. Other rational choices, however, can be made. For example, in a heat transfer problem $g(\cdot)$ could be chosen to be the temperature at a particular point of importance in the problem, and similarly in an elasticity problem a key displacement could be selected. The matrix $\bar{\mathbf{c}}$ of apparent material properties is itself stochastic, unless Ω is a representative volume element (RVE) but not spatially varying. The primary interest in this paper is computation of the uncertainty associated with $\bar{\mathbf{c}}$, when the problem domain is a finite volume smaller than the RVE. Beyond the fact that the solution $\bar{\mathbf{c}}$ to Eq. (1) is itself stochastic, that solution depends on the specific boundary conditions applied in computing $\phi_{het}(\mathbf{x})$ and $\phi_{hom}(\mathbf{x})$. This dependence of apparent material properties on boundary conditions represents a significant challenge to developing consistent and widely applicable definitions of apparent properties. Most currently available approaches involve assumption of periodic boundary conditions or the assumption of a form for the solution field. In this paper, the second approach is taken, but in a novel way involving the use of the shape functions associated with finite elements used to solve practical problems numerically.

In this paper, a stochastic scheme for computing apparent properties is proposed for the scalar field problem of heat conduction in one, two, or three spatial dimensions with a single material property defining a constitutive matrix that is physically isotropic and is also statistically homogeneous and isotropic. That is, the solution field is the temperature $\phi(\mathbf{x}) = t(\mathbf{x})$ and the material property is the thermal conductivity $\mathbf{c}(\mathbf{x}) = \lambda(\mathbf{x})$. The randomness in the problem can be modeled as $\lambda(\mathbf{x}) = \lambda(\mathbf{x})\lambda^*$ in which $\lambda(\mathbf{x}) = \lambda_0(1 + f(\mathbf{x}))$ is a random field composed of a mean value λ_0 and a random part $f(\mathbf{x})$, a mean zero, statistically homogeneous and isotropic random field characterized by its spectral density $S_{ff}(\boldsymbol{\kappa})$, $\boldsymbol{\kappa} \in \mathbb{R}^n$ where $\boldsymbol{\kappa}$ is a vector of wave numbers. For the case of heat conduction, the constitutive matrix of the homogeneous problem is $\bar{\lambda} = \bar{\lambda}\lambda^*$ and the goal of this paper is to evaluate the uncertainty in $\bar{\lambda}$ by developing efficient means of computing var$[\bar{\lambda}]$. Specifically, the goal is to develop a variability response function for var$[\bar{\lambda}]$ such that

$$\mathrm{var}[\bar{\lambda}] = \int_{[-\infty,\infty]^n} \mathrm{VRF}_{\bar{\lambda}}(\boldsymbol{\kappa}) S_{ff}(\boldsymbol{\kappa})\, d\boldsymbol{\kappa} \tag{2}$$

where $\mathrm{VRF}_{\bar{\lambda}}(\boldsymbol{\kappa})$ is a VRF for the apparent conductivity that is independent of the distribution and spectrum of $f(\mathbf{x})$.

3. Finite element based VRFs for apparent conductivity

A finite element is defined by its geometry and the shape functions used to interpolate the solution field within the element domain. In this paper the element domain is $\Omega \subset \mathbb{R}^n$ and the shape functions are denoted by $\mathbf{N} = [N_1(\mathbf{x}), \ldots, N_m(\mathbf{x})]$ where m is the number of nodes the element possesses. In the case of the scalar field heat transfer problem, m is also the total number of degrees of freedom in the element. The gradients of the shape functions are denoted by $\mathbf{B}$, an $n \times m$ matrix with components $B_{ij} = \partial N_j(\mathbf{x})/\partial x_i$ for the heat transfer problem. The conductivity matrix for the heterogeneous version of the problem is $\lambda(\mathbf{x}) = \lambda_0(1 + f(\mathbf{x}))\mathbf{I}$ where I is the $n \times n$ identity matrix, and the conductivity matrix of the homogeneous version of the problem is $\lambda = \bar{\lambda}\mathbf{I}$.

Given these definitions, and further defining $\mathbf{B}^* = \mathbf{B}^T\mathbf{B}$ for compactness of notation, the characteristic matrices of the homogeneous and heterogeneous versions of the problem can be defined as

$$\mathbf{k}_{hom} = \bar{\lambda} \int_\Omega \mathbf{B}^*(\mathbf{u})\, d\mathbf{u} \tag{3}$$

$$\mathbf{k}_{het} = \lambda_0 \int_\Omega \mathbf{B}^*(\mathbf{u})(1 + f(\mathbf{u}))\, d\mathbf{u}. \tag{4}$$

Except in the case where $\mathbf{B}^*$ is a constant matrix—corresponding to linear shape functions—it is not possible to define a single value of $\bar{\lambda}$ using $\mathbf{k}_{het} = \mathbf{k}_{hom}$. Therefore a matrix of apparent conductivities $\bar{\lambda}$ such that

$$\bar{\lambda}_{ij} = \frac{\lambda_0}{\int_\Omega B^*_{ij}(\mathbf{u})\, d\mathbf{u}} \times \int_\Omega B^*_{ij}(\mathbf{u})(1 + f(\mathbf{u}))\, d\mathbf{u} \tag{5}$$

defines the components of a matrix that contains a set of apparent material properties.

The mean of $\bar{\lambda}_{ij}$ is obtained by

$$E[\bar{\lambda}_{ij}] = \frac{\lambda_0}{\int_\Omega B^*_{ij}(\mathbf{u})\, d\mathbf{u}} \times E\left[\int_\Omega B^*_{ij}(\mathbf{u})(1 + f(\mathbf{u}))\, d\mathbf{u}\right] \tag{6}$$

$$E[\bar{\lambda}_{ij}] = \frac{\lambda_0}{\int_\Omega B^*_{ij}(\mathbf{u})\, d\mathbf{u}} \times \int_\Omega B^*_{ij}(\mathbf{u}) E[(1 + f(\mathbf{u}))]\, d\mathbf{u} \tag{7}$$

$$E[\bar{\lambda}_{ij}] = \lambda_0 \tag{8}$$

since $E[f(\mathbf{u})] = 0$ and $B^*_{ij}(\mathbf{u})$ is deterministic. The variance is $\mathrm{var}[\bar{\lambda}_{ij}] = E[\bar{\lambda}_{ij}^2] - E[\bar{\lambda}_{ij}]^2$. Calculation of the second moment $E[\bar{\lambda}_{ij}^2]$, the remaining quantity needed to calculate the variance, begins with