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A relaxation approach to modeling the stochastic behavior of elastic materials

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ABSTRACT

Even in the simple linear elastic range, the material behavior is not deterministic, but fluctuates randomly around some expectation values. The knowledge about this characteristic is obviously trivial from an experimentalist's point of view. However, it is not considered in the vast majority of material models in which "only" deterministic behavior is taken into account.

One very promising approach to the inclusion of stochastic effects in modeling of materials is provided by the so-called Chaos Polynomial Expansion. It has been used, for example, to derive the so-called stochastic finite element method. This method yields results that are exactly of the desired kind, but unfortunately at increased numerical costs.

This contribution aims to propose a new ansatz that is also based on a stochastic series expansion along with an appropriate relaxation procedure at the Gauβ point level. Energy relaxation provides a synthesized (deterministic) stress measure, while simultaneously offering stochastic properties such as the variance. The total procedure only needs negligibly more computation effort than a simple elastic calculation.

1. Introduction

Modern engineering aims to reduce the amount of materials to save resources both during manufacturing and operation. However, this goal also provokes a secondary effect: a shift of the stress state closer to the limit state. This implies that buffers before tolerances are hurt become smaller. On the other hand, all materials show a stochastic behavior, which is caused, for example, by small deviations at the microscale. This stochastic property can be described mathematically by parameters as the expectation value and the standard deviation. If the buffer between tolerances and standard deviations now tends to become zero or even negative, the sustainability cannot be adequately described by material models that rely solely on the deterministic behavior.

This issue can be taken into account by employing different strategies, of which the Karhunen-Loève Expansion (Karhunen, 1947; Loève, 1978) and the Chaos Polynomial Expansion (or Wiener Chaos Expansion) (Wiener, 1938) are quite promising. The idea of a stochastic expansion has been applied to various problems, including sensitivity analysis (Crestaux et al., 2009), nonlinear random vibration (Li and Ghanem, 1998) for the Chaos Polynomial expansion and the analysis of human faces (Kirby and Sirovich, 1990), cosmology (Tegmark et al., 1997), and selection and ordering (Fukunaga and Koontz, 1970) for the Karhunen-Loève expansion, which shows the respective "universal" applicability. The expansions have also been used in a context of structural mechanics yielding to the famous stochastic finite element method. For example, we refer to the works in (Deb et al., 2001; Frauenfelder et al., 2005; Matthies and Keese, 2005; Dasgupta, 2008; Matthies, 2008; Bieri and Schwab, 2009). Comparable approaches to model reduction have been presented, e.g., by (Meyer and Matthies, 2003).

The two expansions are applied to both the input parameters, e.g. the elastic constants, and the output parameters, e.g. the displacement field. Whereas the stochastic coefficients of the input parameters can be determined from experiments and calculated employing the covariance matrix, the stochastic coefficients of the output parameters are unknowns that have to be found in addition to the expectation values. This increased number of unknowns naturally increases the necessary computational effort. More precisely, in the context of stochastic finite elements, this means that the number of *nodal* unknowns is significantly increased, which in turn increases the computation time drastically.

A different method is the stochastic perturbation method, cf. (Kamiński and Kleiber, 2000; Sakata et al., 2008; Kamiński, 2013), which is based on a (direct) Taylor series expansion of the stochastic field variables. It has successfully been used also for highly non-linear

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problems, e.g. geometrically non-linear plasticity in (Kamiński, 2010). Furthermore, it has been proven beneficial for the computation of effective elastic constants for materials with stochastic inclusions, see e.g. (Kamiński and Kleiber, 2000; Sakata et al., 2008; Kamiński, 2013) or (Gao et al., 2011) using a mixed perturbation Monte-Carlo method. This strategy allows for a resolution of the topology of the inclusions at the expense of a finite element treatment: the inclusion and the matrix material in a representative volume element (RVE) are discretized by finite elements and subjected to some average strain. Periodic boundary conditions allow for the computation of the effective elastic constants at the *macroscale*, which are determined by the stochastic interaction of matrix and inclusion material at the (resolved) *microscale*. This general procedure is adopted from the so-called FE^2 method. Here, a RVE simulation is performed for every single material (= integration) point, which -once again- increases the numerical effort to a large degree.

In this work, we aim at contributing to the computation of the effective material point behavior for microstructures with stochastic fluctuations by using "ingredients", which have been proposed both for the derivation of the stochastic finite element method and the RVE treatment. However, we do not apply any (stochastic) finite element or FE^2 (RVE) method directly but use relaxation strategies for the derivation of effective stochastic elastic constants *and* the effective stochastic strain. These effective stochastic quantities allow for the computation of the effective stochastic stresses. To this end, we apply the very same idea of the stochastic expansion as used by the stochastic finite elements. However, in contrast to the stochastic finite element method, the stochastic degrees of freedom are not added to the nodal quantities at the macroscale but to the material (= Gauβ) point quantities at the microscale, i.e. strains and material parameters. From the FE^2 (RVE), we take the idea to consider some microstructure *within* a material point and compute effective quantities. In our approach, we use this idea in a much more "homogenized" way as in classical FE^2 (RVE) strategies. Therefore, one drawback of our approach is that at the present stage, we need to neglect any spatial information. To be more precise, the gradient interactions between stochastic distributions at different Gauβ points as well as the spatial distribution of random elastic constants within the material point cannot be taken directly into account. On the other hand, we obtain explicit formulas for the expectation and standard deviation of the stress, with only marginally increased computation times as compared to the purely deterministic elastic simulation. The stochastic expansion can also be applied for very general probability distribution functions of the elastic properties, for example, we do not need to assume the fluctuations to be Gaussian. Finally, there is no need to compute eigenvalue expansions of the random fields – our results are formulated in terms of stochastic moments of the original material properties, which may be estimated experimentally. In other words, no stochastic expansion is present in the final formulas.

We begin with the physical modeling concept, which sets the fundamental mathematical problem. Subsequently, a small review of the Karhunen-Loève expansion is presented. For convenience, we also give a brief review on the stochastic finite element method, which eases a later comparison between our new method and the established one. We also discuss how to model the effective stochastic behavior of a material point. This procedure enables the investigation of the stochastic behavior of the effective elastic constants, the effective strains, and the effective stress. For convenience, we collect all final results in one section. Before we conclude, we also present first numerical results.

2. The stochastic material point behavior

There exists various ways for modeling the stochastic material behavior, e.g., the stochastic finite element method. However, as will be shown in Section 4, application of the stochastic finite element method increases numerical costs by a remarkable degree. The same argument of highly increased numerical effort is true for other modern upscaling methods as, e.g. the so-called FE^2 method, which solves a finite element problem at the microscale providing the average quantities as stress and stiffness within a representative volume element (RVE) for the finite element procedure at the macroscale. This procedure has been proven to be very powerful to account for microstructural properties that influence the macroscopic behavior of the construction part. An important aspect is how to construct RVEs such that they are statistically representative if stochastic effects play an important role at the microscale, see e.g. (Ostoja-Starzewski, 2006; Soize, 2008). An application of the stochastic finite element method in the context of the FE^2 method would also be possible in general but at numerical costs that can hardly be invested. In (Sakata et al., 2008; Gao et al., 2011), a stochastic homogenization was performed using the perturbation method and Monte-Carlo approaches at a scale which corresponds to the lower scale in a FE^2 setting: precise assumptions on the geometry at this low scale and employing periodic boundary conditions result in effective elastic constants. This approach, however, would have to be performed at each integration point in a complete FE^2 treatment.

For a new point of view, which synthesizes both worlds and also improves the numerical performance, we propose a novel strategy that relies on the stochastic expansions, as also the stochastic finite elements, and homogenization strategies, as also the FE^2 (RVE) treatment, and thus provides an effective material point result for the stochastic elastic constants, stochastic strains, and stochastic stresses. Compared to the stochastic finite element method, our approach operates at a different level, precisely on the material point level or equivalently on the Gauβ point level (= integration point level). In contrast to finite element-based homogenization methods as in (Kamiński and Kleiber, 2000; Sakata et al., 2008), we present analytical formulas for the effective, stochastic stress, which, of course, do not account for geometrical aspects as it would be possible for the approach in (Kamiński and Kleiber, 2000; Sakata et al., 2008; Gao et al., 2011). On the other hand, our modeling does not modify the finite element method at the macroscopic level and thus increases numerical efforts only to a very limited extent.

For the purpose of shifting the evaluation of the stochastic material behavior from the displacement field (operating at the nodes) to the material point level (operating at the Gauβ point level), the material point has to be equipped with an additional "degree of freedom" that takes account of the stochastic information. In a comparable way to the stochastic finite element method, each material point has to be enabled to display the stochastic material behavior at a "spatial" level. We thus divide each material point into n domains for which we assume a uniform distribution that yields $1/n$ as the volume fraction of each domain in the respective material point. For metallic materials, these domains may be identified, e.g., as the crystallographic grains. The "microscale" of the material point is described in terms of the microscale "spatial" coordinate χ (whereas $\boldsymbol{x}$ denotes the spatial coordinate at the macroscale). A schematic plot is given in Fig. 1 for a one-dimensional domain space, for simplicity, but the results are not restricted to this case. A geometrical resolution of χ would be provided by the FE^2 (RVE) treatment, as performed, e.g. in (Sakata et al., 2008), such that our approach might be interpreted as an "emulated" RVE. After this "spatial" discretization by means of χ, we apply some (energetic) relaxation approach yielding the effective material point quantities, as it has also be used for upscaling in a FE^2 (RVE) setting.

Each domain is indicated by the index i and thus serves as spatial discretization of the microscale within the material point. This increase in the degrees of freedom allows for a stochastic material behavior in each domain. For now, we restrict ourselves to the linear-elastic case, implying that the elastic constants are the only material parameters entering the model. They can be expanded by employing a stochastic expansion as

$$\mathbb{E}(\chi, \xi) = \mathbb{E}_0(\chi) + \sum_{k=1}^{k_{\max}} \xi_k \, \mathbb{E}_k(\chi), \tag{1}$$

see also (14). This series expansion is adopted from the stochastic finite element method. Complete details and mathematical foundations are presented in Section 3 while the modeling idea is outlined in this