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A model-reduction approach in micromechanics of materials preserving the variational structure of constitutive relations

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ABSTRACT

In 2003 the authors proposed a model-reduction technique, called the Nonuniform Transformation Field Analysis (NTFA), based on a decomposition of the local fields of internal variables on a reduced basis of modes, to analyze the effective response of composite materials. The present study extends and improves on this approach in different directions. It is first shown that when the constitutive relations of the constituents derive from two potentials, this structure is passed to the NTFA model. Another structure-preserving model, the hybrid NTFA model of Fritzen and Leuschner, is analyzed and found to differ (slightly) from the primal NTFA model (it does not exhibit the same variational upper bound character). To avoid the "on-line" computation of local fields required by the hybrid model, new reduced evolution equations for the reduced variables are proposed, based on an expansion to second order (TSO) of the potential of the hybrid model. The coarse dynamics can then be entirely expressed in terms of quantities which can be pre-computed once for all. Roughly speaking, these pre-computed quantities depend only on the average and fluctuations per phase of the modes and of the associated stress fields. The accuracy of the new NTFA-TSO model is assessed by comparison with full-field simulations. The acceleration provided by the new coarse dynamics over the full-field computations (and over the hybrid model) is then spectacular, larger by three orders of magnitude than the acceleration due to the sole reduction of unknowns.

1. Introduction

A common engineering practice in the analysis of composite structures is to use *effective* or *homogenized* material properties instead of taking into account all details of the individual phase properties and geometrical arrangement.

The homogenization of *linear* properties of composites is now a rather well-documented subject, supported by significant theoretical advances. The reader is referred to Milton (2002) for a state-of-the art of the subject. Provided that the length scales are well separated (i.e. when the typical length scale of the heterogeneities is small compared to the typical length scale of the structure), the linear effective properties of a composite can be completely determined by solving once for all a finite number of unit-cell problems (six in general). Then the analysis of a structure composed of such a composite material can be performed using these pre-computed effective linear properties. In summary, the analysis of a linear

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composite structure consists of two totally independent steps, first an homogenization step at the unit-cell level only, and second a standard structural analysis performed at the structure level only.

The situation is more complicated when the composite is made of individual constituents governed by two potentials, free-energy and dissipation potential, accounting for reversible and irreversible processes respectively and even worse when one of these potentials (or both) is non-quadratic. The most common examples of such materials are viscoelastic or elasto-viscoplastic materials. The overall response of the composite is history-dependent and this includes the history of local fields. It has long been recognized by Rice (1970), Mandel (1972) or Suquet (1985), that the exact description of the effective constitutive relations of such composites requires the determination of all microscopic plastic strains *at the unit-cell level*. For structural computations, the consequence of this theoretical result is that the two levels of computation, the level of the structure and the level of the unit-cell, remain intimately coupled. With the increase in computational power, numerical FEM^2 strategies for solving these coupled problems have been proposed (see Feyel and Chaboche, 2000; Terada and Kikuchi, 2001, for instance) but are so far limited by the formidable size of the corresponding problems.

A common practice to avoid these coupled computations is to investigate the response of representative volume elements by full-field methods and to use the response of these simulations to calibrate postulated phenomenological macroscopic models. There is however a considerable arbitrariness in the choice of the macroscopic model and most of the huge information generated by the full-field simulations is lost, or discarded.

An alternative line of thought consists in viewing the equations for the local plastic field as a system of ordinary differential equations (an infinite number of them, or a large number after discretization) at each integration point of the structure. It is therefore quite natural to resort to *model-reduction techniques* to reduce the complexity of the local plastic strain fields. Reduced-order models aim at achieving a compromise between analytical approaches, which are costless but often very limited by nonlinearity, and full-field simulations which resolve all complex details of the exact solutions, even though they are not always essential to the understanding of the problem, but come at a very high cost. Model-reduction has a long history in Fluid Mechanics (see Sirovich, 1987; Holmes et al., 1996, for instance) and in many other fields of computational physics (Lucia et al., 2004). Its use in Solid Mechanics is more recent (see Ryckelynck and Benziane, 2010; Chinesta and Cueto, 2014, and the references herein).

One of the earliest, and pioneering, attempt to reduce the complexity of the plastic strain fields in micromechanics of materials is the Transformation Field Analysis (TFA) of Dvorak (1992) which assumes uniformity of the plastic strain in the phases or in subdomains. It has been further developed in Dvorak et al. (1994), extended to periodic composites by Fish et al. (1997) and has been incorporated successfully in structural computations (Dvorak et al., 1994; Fish and Yu, 2002; Kattan and Voyiadjis, 1993). However, the assumption of uniform plastic strain fields is far from reality and in order to reproduce accurately the actual effective behavior of the composite, it is essential to capture correctly the heterogeneity of the plastic strain field which requires a large number of subdomains.

This last observation has motivated the introduction in Michel et al. (2000) and Michel and Suquet (2003) of the Nonuniform Transformation Field Analysis (NTFA) where the (visco)plastic strain field within each phase is decomposed on a finite set of plastic modes which can present large deviations from uniformity. The reduced variables are the components of the (visco)plastic strain field on the (visco)plastic modes. Approximate evolution laws for these variables have been proposed (Michel and Suquet, 2003, 2009). A significant advantage of the NTFA is that it provides localization rules allowing for the reconstruction of local fields which are used to predict local phenomena such as the distribution of stresses or the plastic dissipation at the microscopic scale (Michel and Suquet, 2009). This model, which will be called the *original* NTFA model, was first applied to two-dimensional situations by Michel and Suquet (2003, 2004, 2009). It has subsequently been applied to three-dimensional problems by Fritzen and Böhlke (2010) and extended to phases with transformation strains by Largenton et al. (2014). A step towards a more rational derivation of the evolution equation for the reduced variables has been achieved by Fritzen and Leuschner (2013), who proposed a hybrid form of the incremental variational principles for materials governed by two potentials. Their extension of the original NTFA model is discussed in the present paper (Section 5) and has motivated some of the developments here, as will be explained.

The NTFA model consists of two main steps:

1. In a first step, common to all reduced-order models, a *reduced basis* has to be selected (the element of this basis are called modes). However, by contrast with most other model-reduction techniques (see Radermacher and Reese, 2014, for instance), the natural variables for the decomposition are the internal variables and not the displacement (or velocity) field. Several methods are available to construct this basis, in which the modes are either identified once for all, or are enriched "on-the-fly". The selection of modes is not our main purpose here and it will be assumed that these modes have been identified separately, in a preliminary step of the reduced-order model. The snapshot Proper Orthogonal Decomposition (POD) will be used in the present study. The reduced variables are the components of the fine variables, which are the fields of internal variables, on these modes.
2. In a second step, *reduced evolution equations* (evolution equations for the reduced variables) have to be derived, a problem which can be alternatively described as defining the "coarse dynamics" from the "fine dynamics". Actually in several reduced-order models this step is omitted (and not even mentioned) and the coarse dynamics is simply obtained by computing the fine variables and applying the fine dynamics to them. This requires the "on-line" evaluation of the fine variables (in the course of the computation of the coarse variables) and can be very costly, at least in the micromechanical problems that we have in mind. The hybrid model of Fritzen and Leuschner (2013) belongs to this category and requires