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High-performance model reduction techniques in computational multiscale homogenization

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Abstract

A novel model-order reduction technique for the solution of the fine-scale equilibrium problem appearing in computational homogenization is presented. The reduced set of empirical shape functions is obtained using a partitioned version — that accounts for the elastic/inelastic character of the solution — of the Proper Orthogonal Decomposition (POD). On the other hand, it is shown that the standard approach of replacing the nonaffine term by an interpolant constructed using only POD modes leads to ill-posed formulations. We demonstrate that this ill-posedness can be avoided by enriching the approximation space with the span of the gradient of the empirical shape functions. Furthermore, interpolation points are chosen guided, not only by accuracy requirements, but also by stability considerations. The approach is assessed in the homogenization of a highly complex porous metal material. Computed results show that computational complexity is independent of the size and geometrical complexity of the Representative Volume Element. The speedup factor is over three orders of magnitude — as compared with finite element analysis — whereas the maximum error in stresses is less than 10%.

Keywords: Multiscale; Homogenization; Model reduction; High-performance reduced-order model; Hyperreduction; POD

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1. Introduction

1.1. Motivation and goal

The major challenge in the macro-scale continuum description of heterogeneous materials such as composites and polycrystalline metals (that exhibit a clear *heterogeneous* composition at the micro-, or meso-, scale, but that can be regarded, for practical purposes, as *homogeneous* at the macro-scale) lies in the determination of a constitutive connection, between macro-stresses and macro-strains, that accurately reflects the properties and geometrical arrangement of the distinct phases at the finer scale. It is well-known [34] that, under the hypotheses of either *periodicity or statistical homogeneity*, on the one hand; and *scale separation*, on the other hand, this constitutive link can be systematically established by solving, for *each* point at the coarse scale, a boundary value problem (BVP) on a certain representative microscopic subdomain. In a strain-driven formulation of this BVP, the macro-strain at a given point acts as "loading parameter", in the form of appropriate essential boundary conditions, whereas the associated macro-stress is obtained through volume averaging — i.e., *homogenization* — of the corresponding micro-stress field.

Methods dealing with the solution of this BVP range from purely analytical approaches to *direct computational methods*, such as the two-level, Finite Element (FE^2) method [29]. Analytical approaches are computationally inexpensive, but only valid for certain types of geometrically and constitutively simple micro-structures. By contrast, direct computational methods have no other limitation in scope than the imposed by the aforementioned hypotheses of statistical homogeneity and scale separation — in these methods, the microscopic BVP at each coarse-scale point is attacked using no other approximation than the spatial discretization of the pertinent solution strategy, thus, circumventing the need for introducing *ad-hoc*, simplifying assumptions regarding the topological arrangement of the micro-phases and/or their collective constitutive behavior. Needless to say, the versatility of direct computational homogenization comes at a significant price: its enormous computational cost.

Between these two extremes (purely analytical and direct computational methods), there are homogenization strategies that can be termed *semi-analytical*, since they combine analytical results with numerical computations. Such is the case of the *Transformation Field Analysis* (TFA) [25] and variants thereof [48,49,55,30], which are based on the *pre-computation* of certain characteristic operators (strain localization and influence tensors) using the information obtained from solving a carefully chosen battery of fine-scale BPVs. Although these methods have notably widen the scope of classical analytical approaches — while maintaining their low computational cost — they are still predicated, to a lesser or greater extent, on ad-hoc assumptions connected with the constitutive description of the involved phases. Consideration of new materials with unstudied compositions using semi-analytical approaches, thus, requires additional research efforts by specialists in the field and eventual modifications of the corresponding mathematical and numerical formulations — in contrast to direct computational homogenization approaches, such as the FE^2 method, in which the formulation is "material-independent", and hence more versatile.

The current state of affairs in the field of two-scale homogenization seems to call, thus, for a unified homogenization approach that combines somewhat the advantages of direct computational homogenization and analytical and semi-analytical techniques. It would be desirable to have a homogenization method with a computational cost virtually *independent of the geometric complexity* of the considered representative volume, as in analytical and semi-analytical techniques. At the same time, it would be also interesting to arrive at a method whose mathematical formulation dispenses with *ad-hoc*, simplifying assumptions related with the composition of the heterogeneous material; i.e., one enjoying the versatility, unrestricted applicability and "user-friendliness" — insofar as it would totally relieve the modeler from the often exceedingly difficult task of visualizing such assumptions — of direct computational homogenization methods. The goal of the present paper is to show that these desirable attributes can be achieved, for arbitrarily complex heterogeneous materials *well into the inelastic range*, by using the so-called [46] *reduced-basis* (RB) *approximation* in the solution of the fine-scale BVPs.