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A stochastic approximation approach to improve the convergence behavior of hierarchical atomistic-to-continuum multiscale models

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ABSTRACT

The aim of this work is to provide an improved information exchange in hierarchical atomistic-to-continuum settings by applying stochastic approximation methods. For this purpose a typical model belonging to this class is chosen and enhanced. On the macroscale of this particular two-scale model, the balance equations of continuum mechanics are solved using a nonlinear finite element formulation. The microscale, on which a canonical ensemble of statistical mechanics is simulated using molecular dynamics, replaces a classic material formulation. The constitutive behavior is computed on the microscale by computing time averages. However, these time averages are thermal noise-corrupted as the microscale may practically not be tracked for a sufficiently long period of time due to limited computational resources. This noise prevents the model from a classical convergence behavior and creates a setting that shows remarkable resemblance to iteration schemes known from stochastic approximation. This resemblance justifies the use of two averaging strategies known to improve the convergence behavior in stochastic approximation schemes under certain, fairly general, conditions. To demonstrate the effectiveness of the proposed strategies, three numerical examples are studied.

1. Introduction

The macroscopic behavior of solid material as well as most failure mechanisms such as fatigue or crack propagation is governed by processes at an atomistic level. While purely phenomenological material models using continuum mechanics are without doubt very powerful and efficient, much effort has been put into the incorporation of atomic scale mechanics in order to go beyond the phenomenological approach and obtain more natural models.

The atomistic modeling of macroscopic bodies is still beyond every computational capacity and will remain so in the near future, considering the predicted computational power growth (Lim et al., 2015). Multiscale models that combine continuum mechanics on a macroscale with molecular mechanics on a microscale avoid a full atomistic treatment and have been studied mostly in the last two decades. These models can be roughly divided into concurrent (also partitioned-domain) and hierarchical (also sequential) models.

Concurrent atomistic-to-continuum models incorporate the microscale in critical areas like crack tips or in close distance to nanoindentation, while the majority of the domain is handled by the macroscopic formulation. Coupling both scales at

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the interface is a challenging task. A variety of models have been proposed, which can be categorized *e.g.* by their governing formulation, coupling boundary conditions and the presence or absence of a "handshake" region. One of the most successful representatives of this category is the quasicontinuum (QC) method (Tadmor et al., 1996; Miller and Tadmor, 2009). In its original formulation, the QC method is static, *i.e.* it aims at finding an equilibrium configuration by minimizing a given potential energy at zero temperature. Hot-QC was later proposed by Tadmor et al. (2013) and Dupuy et al. (2005) to incorporate finite temperature. Recently, Kim et al. (2014) combined hot-QC with hyperdynamics in order to overcome the short accessible time lengths, known as hyper-QC. Other interesting models are the bridging domain method (BDM) (Xiao and Belytschko, 2004), the coarse-grained molecular dynamics method (CGMD) (Rudd and Broughton, 1998), the coupled atomistic and discrete dislocation (CADD) method (Shilkrot et al., 2002; Miller et al., 2004), the multiscale non-equilibrium molecular dynamics (MS-NEMD) model (Liu and Li, 2007; Li and Sheng, 2010) and multiscale methods extending Andersen–Parrinello–Rahman molecular dynamics (Li and Tong, 2015; Tong and Li, 2015). For detailed reviews and benchmark of the most common concurrent-type models see Miller and Tadmor (2009), Zeng and Li (2010), Tadmor et al. (2012), and Davydov et al. (2014).

Hierarchical atomistic-to-continuum models make use of both scales in the entire domain. The entire body is treated as a continuum and *e.g.* discretized by finite elements, while the microscale is introduced locally using appropriate representative volume elements (RVE). These methods are computationally powerful as there is no direct coupling between the scales. While concurrent models and possible applications are studied to a considerable extent, there is little coverage of hierarchical models in the literature (Tadmor et al., 2000; Liu et al., 2004). In hierarchical models, the atomic behavior should be related to the macroscopic deformation according to the Cauchy–Born rule (Ericksen, 2008), hence, homogeneous lattice deformation is assumed. Chung and Namburu (2003) and Clayton and Chung (2006) proposed a two-scale method that is able to incorporate a number of periodic defect arrangements (vacancies, dislocations, and misorientation boundaries) and computes the macroscopic mechanical properties predicted upon a static representation (*i.e.* at zero temperature). The generalized mathematical homogenization (GMH) method (Fish et al., 2007; Fish and Fan, 2008; Li et al., 2008) is a bottom-up approach in which the microscale is used to systematically upscale the macroscopic equations (coupled thermo-mechanical continuum).

In most hierarchical models, the microscale is used to supply the local constitutive behavior for the macroscopic calculations. In this data estimation process, the microscopic boundary conditions and constraints are dictated by the macroscale. In finite temperature simulations, the microscale is tracked for some time and the constitutive quantities are subsequently computed through spatial and time averaging. Herein lies one of the key challenges in hierarchical modeling. Inappropriately chosen RVEs and/or too short periods of time for data estimation lead to poor accuracy on the macroscale. Furthermore, choosing large RVEs and sufficiently sampling the microscopic quantities results in excessive computational cost for any practical problem. Therefore, the estimated data and hence the macroscopic solution fields will be erroneous in practical calculations. This means that data estimation can be thought of as a measurement process, in which the measured value is noise-corrupted. Naturally, one should always strive to reduce this error as far as possible. In a classical way, this can only be achieved by using larger RVEs and increased computational time on the microscale, both of which result in an increased computational burden.

This paper discusses strategies for reducing the error without introducing further computational cost using stochastic approximation (Kushner and Yin, 2003; Spall, 2003). Stochastic approximation (SA) is generally concerned with finding roots or extrema of noise-corrupted functions and is used in different areas in science and economics. A great deal of focus is placed on machine learning algorithms (Benaim, 1993; Cheng and Titterington, 1994; López-Rubio and Luque-Baena, 2011). But there are also fields of application in classical engineering, *e.g.* in the optimization of shape designs (El Alem et al., 2011; Seyedpoor et al., 2011), for estimating the thermal conductivity in boreholes (Wen-Long et al., 2012) or damping approximation (Sultan, 2010). In order to improve convergence of SA iteration schemes, the two strategies "averaging of the iterates" and "averaging of the iterates and observations" are known. As their names imply, both strategies aim at effectively reducing the noise by using averaged quantities. Hierarchical atomistic-to-continuum models exhibit strong similarities to SA schemes, which justifies the use of those two averaging strategies to reduce the error in the macroscopic solution fields.

This paper is organized as follows. In Section 2, the selected hierarchical model will be discussed in detail. Section 3 gives a short introduction to stochastic approximation and the averaging strategies. The implementation details of the two averaging strategies applied to the selected model will be given in Section 4. Section 5 uses three numerical examples to demonstrate the performance of the proposed strategies. Finally, a conclusion closes the paper.

2. Multiscale model

This section introduces a multiscale method coupling molecular dynamics and the finite element method. It will serve as a framework to test the performance of standard methods in stochastic approximation. On the macroscale of this model, a standard nonlinear finite element formulation is employed. The microscale is incorporated at each integration point of the macroscopic domain in the shape of a MD cell. Each MD cell contains N atoms arranged in a perfect (defect-free) crystal and shows periodic boundary conditions.