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Coupling the finite element method and molecular dynamics in the framework of the heterogeneous multiscale method for quasi-static isothermal problems

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ABSTRACT

Multiscale models are designed to handle problems with different length scales and time scales in a suitable and efficient manner. Such problems include inelastic deformation or failure of materials. In particular, hierarchical multiscale methods are computationally powerful as no direct coupling between the scales is given. This paper proposes a hierarchical two-scale setting appropriate for isothermal quasi-static problems: a macroscale treated by continuum mechanics and the finite element method and a microscale modelled by a canonical ensemble of statistical mechanics solved with molecular dynamics. This model will be implemented into the framework of the heterogeneous multiscale method. The focus is laid on an efficient coupling of the macro- and micro-solvers. An iterative solution algorithm presents the macroscopic solver, which invokes for each iteration an atomistic computation. As the microscopic computation is considered to be very time consuming, two optimisation strategies are proposed. Firstly, the macroscopic solver is chosen to reduce the number of required iterations to a minimum. Secondly, the number of time steps used for the time average on the microscale will be increased with each iteration. As a result, the molecular dynamics cell will be allowed to reach its state of thermodynamic equilibrium only in the last macroscopic iteration step. In the preceding iteration steps, the molecular dynamics cell will reach a state close to equilibrium by using considerably fewer microscopic time steps. This adapted number of microsteps will result in an accelerated algorithm (aFE-MD-HMM) obtaining the same accuracy of results at significantly reduced computational cost. Numerical examples demonstrate the performance of the proposed scheme.

1. Introduction

Many problems in nature show a multiscale character in space and time. Inelastic deformation, failure of materials, micro- and nano electro-mechanical systems are just a few examples. These problems may result from material inhomogeneities or complex mechanical processes. Multiscale models are able to incorporate the physics of the involved scales in a suitable and efficient manner. In particular, two-scale methods employing a continuum-on-atomistic setting have recently become popular in the literature. The information exchange between these scales in a numerical simulation permits a classification into two groups: hierarchical (or serial) and concurrent (or simultaneous) methods.

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The continuum-on-atomistic setting is extensively debated in the literature in a concurrent coupling of scales (Curtin and Miller, 2003; Miller and Tadmor, 2009; Zeng and Li, 2010). One or a few critical regions of the system are atomistically modelled (*e.g.* to resolve local defects or singularities) and directly coupled with the surrounding continuum regions. The quasi-continuum (QC) method (Tadmor et al., 1996; Miller and Tadmor, 2009) is one of the most successful models in concurrent coupling. It is based on standard finite elements and constitutive equations derived from atomistic interactions. Next to that, there are the bridging-scale method (Liu et al., 2007) and the multiscale continuum field theory (Zeng et al., 2011). The coarse-grained molecular dynamics (CGMD) (Rudd and Broughton, 1998, 2000) approach produces equations of motion for the nodal fields of a finite element model, which are derived from an underlying atomistic model at thermodynamic equilibrium. Furthermore, the atomic-scale finite element method (AFEM) (Liu et al., 2004a, 2005; Xu and Liu, 2014) extends the finite element method to the atomic scale. A seamless multiscale method suitable for large scale static problems may be achieved by combining AFEM with continuum FEM elements. Another attractive method is the so-called perfectly matched multiscale simulation (PMMS) (To and Li, 2005; Li et al., 2006), which was initially derived to reduce spurious phonon reflections at the multiscale interface. Besides, a computational multiscale method to couple thermomechanical equations at the coarse scale with nonequilibrium molecular dynamics at the fine scale was developed (Liu and Li, 2007; Li et al., 2008b; Li and Sheng, 2010; Li and Tong).

In contrast, a hierarchical continuum-on-atomistic coupling (*e.g.* to supply constitutive relations at the macroscale) is not extensively investigated in the literature (Tadmor et al., 2000; Liu et al., 2004b). The hierarchical two-scale method first develops a microscale model in the shape of an appropriately chosen representative volume element (RVE) that comprises all the various microstructural heterogeneities, and then deduces the macroscale constitutive laws and state variables, such as stress and heat flux, from the microscopic behaviour by an averaging procedure (Hill, 1972). As no direct coupling between the two scales is given, this method is computationally powerful. This procedure is known as homogenisation in the literature and is usually used in a continuum-on-continuum setting (Geers et al., 2010). Hierarchical continuum-on-atomistic models are sparse in the literature, even when the numerical implementation may be considered to be straightforward (E and Engquist, 2005; E et al., 2005; Abdulle et al., 2012). Chung and Namburu (2003) and Clayton and Chung (2006) developed an approach to embed atomistic physics into a continuum formulation for large-scale systems. This was achieved by applying the Cauchy–Born rule to the atomic scale and superposing perturbation displacements at each load increment to the microscale. A bottom-up approach denotes the generalised mathematical homogenisation (GMH) method (Fish et al., 2007; Fish and Fan, 2008; Li et al., 2008a), which evolves a continuum model by advancing a sequence of fine scale atomistic models in representative volumes placed at the quadrature points of the discretised continuum model. However, the modelling of the representative volumes gives a molecular dynamics-like problem and is not integrated for the full atomistic motion. A framework that combines the serial and concurrent coupling in the generalised mathematical homogenisation method is given by Fish et al. (2010). Chockalingam and Wellford (2011) give a homogenisation procedure with an emphasis on thermal problems. It is based on a uniform weighted residual approximation method to consistently model the interaction of the continuum and atomistic scale. A coarse-grained molecular dynamics model for solid systems based on the Mori–Zwanzig projection method is described by Li (2010), while an atomistic-continuum coupled model for thermo-mechanics of materials in micro-nano scales is presented by Xiang et al. (2012). Furthermore, the remarkable heterogeneous multiscale method (described in Section 2) is ageneral top-down approach to design multiscale algorithms. While this method is mainly used for concurrent coupling schemes in the literature, the proposed methodology also applies to a hierarchical coupling.

Let us assume that in a two-scale continuum-on-atomistic setting the macroscopic solver and the microscopic solver are chosen according to the problem at hand. Furthermore, let us assume that both solvers are optimised on their own scale. On the macroscale this could be the type of the solver, the number of integration points or the number of elements. On the microscale this could be the type of the solver, the size of the microscopic time step or the number of atoms in a molecular dynamics cell. Next to this separate optimisation, there is potential for improving the model's efficiency in the coupling of solvers, which is not extensively exploited in the literature so far. The purpose of this paper is to investigate the possibility of enhancing the coupling of a macroscopic iterative solver with a microscopic one. Firstly, the macroscopic solver could be chosen to invoke the microscopic computation as rarely as possible, if the atomistic simulation is identified as the computationally most intensive factor. Secondly, if an iterative macroscopic solver is chosen, the number of microscopic steps could be adjusted in the iterations to give the same accuracy of the converged result faster. The obtained accelerated algorithm (we will call it aFE-MD-HMM) will yield the same accuracy of the results at significantly reduced computational cost.

The paper is organised as follows. Section 2 presents the heterogeneous multiscale method and its seamless derivate. Then, Section 3 gives the proposed two-scale continuum-on-atomistic model suitable for quasi-static isothermal problems. Section 4 demonstrates the performance of the proposed scheme on classical problems in elasticity. Finally, a conclusion closes the paper.

2. The HMM framework

The heterogeneous multiscale method (HMM) (E and Engquist, 2003; Li and E, 2005; E et al., 2007; Abdulle and Nonnenmacher, 2009; Abdulle et al., 2012) provides a top-down approach in modelling multiscale problems. The