Comparison of several staggered atomistic-to-continuum concurrent coupling strategies

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Abstract

In this contribution several staggered schemes used to couple continuum mechanics (CM) and molecular mechanics (MM) are proposed. The described approaches are based on the atomistic-to-continuum correspondence, obtained by spatial averaging in the spirit of Irving and Kirkwood, and Noll. Similarities between this and other concurrent coupling schemes are indicated, thus providing a broad overview of different approaches in the field. The schemes considered here are decomposed into the surface-type (displacement or traction boundary conditions) and the volume-type. The latter restricts the continuum displacement field (and possibly its gradient) in some sense to the atomistic (discrete) displacements using Lagrange multipliers. A large-strain CM formulation incorporating Lagrange multipliers and a strategy to solve the resulting coupled linear system using an iterative solver is presented.

Finally, the described coupling methods are numerically examined using two examples: uniaxial deformation and a plate with a hole relaxed under surface tension. Accuracy and convergence rates of each method are reported. It was found that the displacement (surface) coupling scheme and the Lagrangian (volume) scheme based on either discrete displacements or the H_1 norm derived from continuous displacement fields provide the best performance.

1. Introduction

In recent decades there has been a growth of interest regarding approaches to couple the description of matter at different scales, namely continuum mechanics (CM), molecular mechanics (MM), and quantum mechanics (QM). Some approaches couple the description in a sequential manner, that is to say the output from a fine scale is directly used in a coarse scale. Usually a more challenging approach is to perform concurrent coupling, in which principally different descriptions are used simultaneously for different parts of the domain. Concurrent coupling methods can

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be categorized by factors [1] such as the continuum model used, the presence or absence of a "handshake" region, coupling boundary conditions and the governing formulation. Often concurrent methods are tailored for use in a particular type of problem, such as dynamic zero-temperature problems at both continuum and atomistic sides [2–4] or a quasi-static continuum with either zero [5–7] or finite [8] temperature atomistic simulations. Very rarely are concurrent coupling schemes applied to solid amorphous materials [9,10]. Finally, there are methods that bridge continuum and quantum descriptions [11–14]. For a general overview we refer the reader to [15,16,1].

It is important to note that concurrent methods may require an iterative approach to reach the solution; see for example the Bridging Scale Method (BSM) [6]. Alternatively, there are methods that are formulated in a monolithic manner such as the Quasi-Continuum (QC) [17–19], the Bridging Domain Method (BDM) [20] and the Arlequin method [21,22].

Many of the coupling methods directly or indirectly postulate a procedure to compute continuum fields from atomistic simulations which are then used to define the total Hamiltonian and/or constraints on primary (displacements or velocity) fields. In many cases these can be considered as specializations of the theoretical link established by Irving and Kirkwood [23], and Noll [24]. For example, in [25,26] the authors explicitly use results of the atomistic-to-continuum correspondence in conjunction with the delta-function as an averaging kernel to calculate cell-integrated quantities which are then used in the coupling procedure. Monolithic methods which use a handshake interface between atomistic and continuum domains [21,22,20] require the localization of the potential energy to a spatial point in order to define the total Hamiltonian for the system.

Although monolithic concurrent coupling schemes such as the QC, BDM or Arlequin methods are, in general, computationally faster than staggered coupling schemes, there are several reasons why utilizing the latter may be desirable. First, if one considers a thermo-mechanical quasi-static problem, there is a clear time-scale separation between the two descriptions. This often leads to a definition of the temperature field in terms of time-averaged atomistic fluctuations. In such a case there is, it seems, no other choice but to solve the two problems independently while coupling using staggered approaches. This is partly due to the fact that it is the free-energy which is considered in CM. This quantity is not immediately available from MM[1] and thus blending the two to derive a variational formulation is not trivial. As an example, one of the extensions of the QC method to finite temperatures [27] effectively leads to a staggered solution approach. Alternatively, one can construct effective (coarse-grained) thermodynamic potentials based on the principle of maximum entropy. Using this approach coupling at non-uniform temperatures can be achieved in a monolithic manner using, for example, another extension of the QC method [28,29].

Staggered schemes may be applied not only to couple MM and CM, but also CM and QM [11,12]. In the latter case, the principal differences between governing equations[2] lead to staggered approaches being widely adopted. Note that the QM Hamiltonian is defined for the system as a whole, as opposed to the MM Hamiltonian which is attributed to collections of, at most, four particles.

The blending of CM and MM Hamiltonians is relatively simple when the systems considered on the MM side consist of two-point (pair) potentials. In such a case the energy attributed to each bond is situated at the geometric center of particle pairs and is blended with the CM Hamiltonian according to a chosen weighting function. This, however, becomes much more complicated and not unique for cases when three- and four-point potentials are considered. To the best of our knowledge, coupling methods based on the blending of Hamiltonians have not been applied to such cases. Even for pair-potentials, bonds can be weighted in different ways; see the discussion in [20,5] and the references therein. The issue is principally similar to that of localizing the potential energy of a particle system in order to obtain the balance of energy in terms of atomistic quantities [30]. One further method to localize the potential energy for the purpose of coupling atomistic and continuum models is proposed in [5].

Finally, staggered schemes are easier to implement in a non-intrusive fashion when utilizing third-party finite-element (FE) and molecular dynamics (MD) codes.

Staggered methods do not need to define the total Hamiltonian in order to derive the governing equations for the system as a whole from a variational principle. Even though this is the case, constraints between the corresponding kinematic and/or kinetic quantities have to be introduced. In the most simple case, such constraints can be imposed

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[1] There are a few methods that describe how to obtain the free-energy macroscopically, such as the integration of stresses with respect to the applied deformation gradient while keeping the temperature fixed.

[2] The Kohn–Sham equations of the density functional theory on the QM side lead to a general eigenvalue problem as opposed to the partial differential equations on the CM side.