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Bridging Methods for Atomistic-to-Continuum Coupling and Their Implementation

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Abstract. Several issues connected with bridging methods for atomistic-to-continuum (AtC) coupling are examined. Different coupling approaches using various energy blending models are studied as well as the influence that model parameters, blending functions, and grids have on simulation results. We use the Lagrange multiplier method for enforcing constraints on the atomistic and continuum displacements in the bridge region. We also show that continuum models are not appropriate for dealing with problems with singular loads, whereas AtC bridging methods yield correct results, thus justifying the need for a multiscale method. We investigate models that involve multiple-neighbor interactions in the atomistic region, particularly focusing on a comparison of several approaches for dealing with Dirichlet boundary conditions.

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1 Introduction

Atomistic models such as molecular dynamics are an accepted approach for accurately describing material processes that occur at the microscopic level. Unfortunately, many systems of interest involve too many particles to be feasibly treated using such methods. As a result, approximations to atomistic models that are more efficient yet have sufficient accuracy are of interest. Several approaches have been proposed in that sense; a particular ambitious approach, called MAAD ("macroatomistic *ab initio* dynamics"), that attempts to couple continuum to statistical to quantum mechanics is described in [11]. In general, the methods described in the literature attempt to couple between two scales (e.g., micron- and nano-scales). Some of the methods apply domain decomposition using

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the same physical description, i.e., the same type of equations, on the whole domain; this is the case of the quasi-continuum method [10, 13, 14]. Other methods implement domain decomposition using different models in different domains, applying some sort of coupling mechanism between them; some examples of this type of approach are found in [1–4, 8, 15–17]. For a review of multiscale material methods, the reader is referred to [18–20].

In atomistic-to-continuum (AtC) coupling techniques, an atomistic model is used in regions where microscale resolution is necessary but elsewhere, a (discretized) continuum model is applied. Several methods were proposed in the manner; for a comparison of different multiscale methods for the coupling of atomistic and continuum models see [9]. The central question in AtC coupling methods is how to couple the models, taking into account their different natures. In [1, 2, 4], a force-based blending model is applied to couple atomistic and continuum models. Blending is effected in a *bridge region* (also called *interface* or *blending* or *overlap region*) over which the atomistic displacement is constrained by the interpolation of the continuum displacement. Seemingly, such an approach over-constrains the system and causes the computational solution to deviate from what is expected.

Instead, we follow a similar approach to that in [3] and use a Lagrange multiplier method to enforce constraints, thus reducing the number of constraints. The focus in [3] is on a comparison between overlapping and non-overlapping domain decomposition methods, whereas we examine several components of overlapping domain decomposition methods (also called "handshake" models [12]) featuring two different blending schemes; we also study issues related to the implementation of those methods. In contrast to [1], where coupling is implemented at the force level, we blend the models at the energy level and use the minimization of the blended potential energy to determine the equilibrium configuration of the system; an approach, called the Arlequin method, for which the energy of the system is assumed to be shared between co-existent models was studied in [5–7]. This paper focuses on implementation details and difficulties of AtC coupling methods. In particular, we study several issues related to the application of an augmented Lagrange multiplier method, including the effects of nonuniformity of the Lagrange multiplier grid and the value chosen for the penalty parameter.

Another issue of interest is the application of boundary conditions. In physical systems, long–range interactions are the general case; therefore, multiple-neighbor interactions have to be implemented. Thus, an appropriate treatment is needed to correctly describe system interactions near the boundary where only a few atoms are available for interaction. In this paper, several different approaches for the case of Dirichlet, i.e., displacement, boundary conditions, in the context of multiple-neighbor interactions, are discussed and compared in Section 7.

The outline of this paper is as follows. In Section 2, we present the general framework of the AtC coupling method, as well as its implementation in one dimension. We describe the different components of the model as well as a physical interpretation for the energy blending technique. In Section 3, we introduce the quantitative tools implemented in the