Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 279 (2014) 29–45
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Energy-based atomistic-to-continuum coupling without ghost forces

C. Ortner[a], L. Zhang[b,*]

[a] *Mathematics Institute, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK*
[b] *Department of Mathematics, Institute of Natural Sciences, and MOE Key Lab in Scientific and Engineering Computing, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China*

Received 18 January 2014; received in revised form 12 May 2014; accepted 10 June 2014
Available online 24 June 2014

Abstract

We present a practical implementation of an energy-based atomistic-to-continuum (a/c) coupling scheme without ghost forces, and numerical tests evaluating its accuracy relative to other types of a/c coupling schemes.

Keywords: Atomistic/continuum coupling; Quasicontinuum; Quasi-nonlocal; Error analysis

1. Introduction

Atomistic-to-continuum coupling methods (a/c methods) are a class of computational multiscale schemes that combine the accuracy of atomistic models of defects with the computational efficiency of continuum models of elastic far-fields [1–5]. In the present article, we present the first successful implementation of a practical *patch test consistent* energy based a/c coupling scheme. Previously such schemes were only available for 2-body interactions [6,7].

In recent years a numerical analysis theory of a/c methods has emerged; we refer to [8] for a review. This theory has identified three prototypical classes of a/c schemes: patch test consistent energy-based coupling, force-based coupling (including force-based blending), and energy-based blending. The classical numerical analysis concepts of consistency and stability are applied to precisely quantify the errors committed in these schemes, and clear guidelines are established for their practical implementation including optimisation of approximation parameters. The results in [9,10,8,11,12] indicate that patch test consistent a/c couplings observe (quasi-)optimal error estimates in the energy-norm. However, to this date, no general construction and implementation of such schemes has been presented. Instead, one normally compromises by either turning to patch test consistent force-based schemes [13–15,1] or to blending schemes [3,16] which have some control over the consistency error. Quasi-optimal implementations of such schemes are described in [16,15].

* Corresponding author. Tel.: +86 2154742994; fax: +86 2154747161.
E-mail addresses: christoph.ortner@warwick.ac.uk (C. Ortner), lzhang2012@sjtu.edu.cn, mail4lei@gmail.com, lzhang@sjtu.edu.cn (L. Zhang).

http://dx.doi.org/10.1016/j.cma.2014.06.019
0045-7825/

Existing patch test consistent schemes are restricted in their range of validity: [4] is only consistent for flat a/c interfaces and short-ranged interactions, [17] extends the idea to arbitrary range and [12] to domains with corners (but restricting again to nearest-neighbour interaction). On the other hand, the schemes presented in [6,7,18] are valid for general interaction range and a/c interfaces with corners, but are restricted to pair interactions.

In the present article, we shall present a generalisation of the geometric reconstruction technique [4,17,12], which we subsequently denote GRAC. Briefly, the idea is that, instead of evaluating the interatomic potential near the a/c interface with atom positions obtained by interpolating the continuum description, one extrapolates atom positions from those in the atomistic region (geometric reconstruction). This idea is somewhat analogous to the implementation of Neumann boundary conditions for finite difference schemes. There is substantial freedom in how this reconstruction is achieved, leading to a number of *free parameters*. One then determines these *reconstruction parameters* by solving the "geometric consistency equations" [17], which encode a form of patch test consistency and lead to a first-order consistent coupling scheme [11].

The works [17,12,11] have demonstrated that GRAC is a promising approach, but also indicate that explicit analytical determination of the reconstruction parameters for general a/c interface geometries with general interaction range may be impractical. Instead we propose to compute the reconstruction parameters in a preprocessing step. Although this is a natural idea it has not been pursued to the best of our knowledge.

A number of challenges must be overcome to obtain a robust numerical scheme in this way. The two key issues we will discuss are:

(A) If the geometric consistency equations have a solution then it is not unique. The consistency analysis [11] suggests that a solution is best selected through ℓ^1-minimisation of the coefficients. Indeed, we shall demonstrate that the least squares solution leads to prohibitively large errors.
(B) In [19] we proved that there exists no universally stable a/c coupling of geometric reconstruction type. We will see that this is in fact of practical concern and demonstrate that the stabilisation mechanism proposed in [19] appears to resolve this issue.

In the remainder of the paper we present a complete description of a practical implementation of the GRAC method (Section 2) and numerical experiments focused primarily on investigating approximation errors (Section 3). We will comment on open issues and possible improvements in Section 4, which are primarily concerned with the computational cost of determining the reconstruction coefficients.

2. Formulation of the GRAC method

In formulating the GRAC scheme, we adopt the point of view of [20], where the computational domain and boundary conditions are considered part of the approximation. This setting is convenient to assess approximation errors. Adaptions of the coupling mechanism to other problems are straightforward.

We first present a brief review, ignoring some technical details, of a model for crystal defects in an infinite lattice from [20], and some results concerning their structure (Section 2.1). In Section 2.2 we present a generic form of a/c coupling schemes, which we then specialise to the GRAC scheme in Section 2.3. In Section 2.3 and in Section 2.4 we address, respectively, the two key issues (A) and (B) mentioned in the introduction.

For the sake of simplicity of presentation, and to emphasise the algorithmic aspects of the GRAC method, we restrict the presentation to relatively simple settings such as point defects and microcracks as in [16,15]. The concepts required to generalise the presentation to problems involving dislocations can be found in [20].

2.1. Atomistic model

Let $d \in \{2, 3\}$ denote the problem dimension. Fix a non-singular $\mathsf{A} \in \mathbb{R}^{d\times d}$ to define a Bravais lattice $\mathsf{A}\mathbb{Z}^d$. Let $\Lambda \subset \mathbb{R}^d$ be a discrete reference configuration of a crystal, possibly with a local defect: for some compact domain $\Omega^{\rm def}$ we assume that $\Lambda \setminus \Omega^{\rm def} = \mathsf{A}\mathbb{Z}^d \setminus \Omega^{\rm def}$ and $\Lambda \cap \Omega^{\rm def}$ is finite. It can be readily seen [20], that certain point defects (e.g., interstitials, vacancies; see Fig. 1) can be enforced that way.

To avoid minor technical difficulties, we prescribe a maximal interaction neighbourhood in the reference configuration. This is a restriction that can be lifted with little additional work [20, Remark 2.1]. For each $\ell \in \Lambda$ we denote this neighbourhood by $\mathcal{N}(\ell) := \{\ell' \in \Lambda \mid |\ell' - \ell| \le r_{\rm cut}\}$, for some specified cut-off radius $r_{\rm cut}$. (Note that