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A Posteriori Error Estimate and Adaptive Mesh Refinement Algorithm for Atomistic/Continuum Coupling with Finite Range Interactions in Two Dimensions

Mingjie Liao[1], Ping Lin[2] and Lei Zhang[3,*]

[1] *School of Mathematics and Physics, University of Science and Technology Beijing, Beijing 100083, P.R. China.*
[2] *Department of Mathematics, University of Dundee, Dundee, DD1 4HN, Scotland, United Kingdom.*
[3] *School of Mathematical Sciences, Institute of Natural Sciences and MOE-LSC, Shanghai Jiao Tong University, Shanghai 200240, P.R. China.*

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Abstract. In this paper, we develop the residual based a posteriori error estimates and the corresponding adaptive mesh refinement algorithm for atomistic/continuum (a/c) coupling with finite range interactions in two dimensions. We have systematically derived a new explicitly computable stress tensor formula for finite range interactions. In particular, we use the geometric reconstruction based consistent atomistic/continuum (GRAC) coupling scheme, which is quasi-optimal if the continuum model is discretized by P^1 finite elements. The numerical results of the adaptive mesh refinement algorithm is consistent with the quasi-optimal a priori error estimates.

AMS subject classifications: 65N12, 65N15, 70C20, 82D25

Key words: Atomistic models, coarse graining, atomistic-to-continuum coupling, quasicontinuum method, a posteriori error estimate.

1 Introduction

Atomistic/continuum (a/c) coupling methods are a class of computational multiscale methods for crystalline solids with defects that aim to optimally balance the accuracy of the atomistic model and the efficiency of the continuum model [12,19,36]. The construction and analysis of different a/c coupling methods have attracted considerable attention in the research community in recent years. Rigorous a prior analysis and systematic

*Corresponding author. *Email addresses:* mliao@xs.ustb.edu.cn (M. Liao), plin@maths.dundee.ac.uk (P. Lin), lzhang2012@sjtu.edu.cn (L. Zhang)

benchmark has been done in, for example, [13–15,23,29,30]. We refer readers to [16,18] for a review. The study of a/c coupling methods has not only provided an analytical framework for the prototypical problems [9], but also opened avenue for coupling schemes in more complicated physical situations [3,4,10].

Like many multiscale methods dealing with defects or singularities, adaptivity is the key for the efficient implementation of a/c coupling methods. In contrast to the a priori analysis, the development of a posteriori analysis for a/c coupling methods are still lagging behind. Although heuristic methods have been proposed in the engineering literature [33,36,40]. Previous mathematical justifications are largely limited to one dimension cases [1,2,33]. In particular, the residual based a posteriori error bounds for a/c coupling schemes are first derived in [20,25,27] by Ortner et al. in one dimension.

In [41], we carried out a rigorous a posteriori analysis of the residual, the stability constant, and the error bound, for a consistent atomistic/continuum coupling method [28] with nearest neighbor interactions in two dimensions. Corresponding adaptive mesh refinement algorithm was designed and implemented based on the a posteriori error estimates, and the convergence rate with respect to degrees of freedom is the same as quasi-optimal a priori error estimates. This is the first rigorous a posteriori analysis for a/c coupling method in two dimensions. With the a posteriori error estimates and the adaptive algorithm, we can not only automatically move the a/c interface and adjust the discretization of the continuum region, but also change the size of the computational domain. We have also introduced the so-called "stress tensor correction" technique, which distinguish the essential difference of high dimensional results compared with previous one dimensional results.

In this paper, we treat the more general case of a/c coupling with finite range interactions, which is physically more relevant and algorithmically more involved. The a priori analysis of GRAC scheme has been extended from nearest neighbor case in [28] to finite range interactions in [29]. ℓ^1-minimization is introduced to resolve the issue of non-uniqueness of reconstruction parameters, and a stabilisation mechanism is proposed in [24] to reduce the stability gap between the a/c coupling scheme and the original atomistic model.

The analytical framework for both a priori analysis and a posteriori analysis of a/c coupling methods strongly relies on the stress based formulation. In [21,26], an explicit formulation of stress tensor is proposed based on a mollified version of line measure supported on the interaction bonds, thence one can obtain an integral representation of finite differences to further derive an integral representation of the first variation of the interaction energy. This representation greatly simplifies the expression of the stress tensor and plays a significant role in the a priori analysis. However, the obtained stress tensor is a function of the continuous space variable, therefore it is difficult to compute in practice, and not suitable for the a posteriori estimates and adaptive computation.

In this paper, we derive a novel expression of the stress tensor for finite range interactions, which is new to the best of our knowledge. The stress tensor is piecewise constant and only depends on a local neighborhood, therefore it is computable and the assembly