Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.OA-2017-0094

Vol. **12**, No. 1, pp. 233-264
February 2019

# A Posteriori Error Control for Three Typical Force-Based Atomistic-to-Continuum Coupling Methods for an Atomistic Chain

Hao Wang[1,*], Shaohui Liu[2] and Feng Yang[3]

[1] *School of Mathematics, Sichuan University, No. 24 South Section One, Chengdu, 610065, China*
[2] *Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, New York, 11794-3600, U.S*
[3] *College of Mathematical Science, Beijing University, Zhongguancun Road 1, Beijing, 100000, China*

Received 28 July 2017; Accepted (in revised version) 28 April 2018

**Abstract.** We consider the problem of a posteriori error estimates and adaptivity for three typical force-based atomistic-to-continuum coupling methods. Combining the residual and the stability estimates, we derive computable a posteriori error estimators for the three methods in the energy norm and formulate adaptive algorithms using these estimators. Our numerical experiments show optimal convergence rates of these algorithms. The efficiency of the estimators are also demonstrated numerically.

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

**Key words**: Atomistic-to-continuum coupling, a posteriori error estimate, adaptivity, force based method.

## 1. Introduction

Atomistic-to-continuum (a/c) coupling methods, also known as quasicontinuum (QC) methods, are a class of of multiscale methods for coupling an atomistic model of a solid with a continuum model which is often obtained by the Cauchy-Born approximation. The atomistic model is used in certain regions of interest, such as crystal defects and their neighbourhoods, to gain a good accuracy while a continuum model is applied to reduce the cost of the computation in the elastic far fields. We refer to [25, 26, 32] for perfect reviews for such methods.

There are two major types of a/c coupling methods, namely the energy-based methods and the force-based methods. The energy-based methods approximate the energy of the atomistic system by a coupling energy and essentially solve energy minimization problems

*Corresponding author. *Email addresses:* wangh@scu.edu.cn (H. Wang), shaohui.liu@stonybrook.edu (S. H. Liu), yang_feng@pku.edu.cn (F. Yang)

 

[12, 17–20, 30, 35, 38, 40]. However, the original energy-based (QCE) method, despite its simple formulation, exhibits spurious force at the coupling interface which reduces the accuracy of computing the deformation and the lattice stability [7, 8, 28, 33] while the improved energy-based methods have the difficulty of the reconstruction of the energy of the interface atoms [35, 36, 38, 39]. On the other hand, the force-based methods directly solve equilibrium equations of the coupling forces at each degree of freedom [6, 14, 23] and possess better accuracy with simple constructions. However the original force-based (QCF) method has certain stability issues which make the determination of the lattice stability challenging. The stability is then improved by blending the atomistic force with the continuum force in certain regions so that the blended equation becomes positive definite [16] which gives the blended QCF (BQCF) method. Such improvement is also achieved by changing the formulation of the problem to a stress-based variational formulation which gives the stress-based a/c (SAC) method [23].

Considerable efforts have been devoted to the *a priori* analysis of the force-based methods [4, 6, 10, 14, 16, 22, 24, 27], especially the (in-)stability of these methods as mentioned earlier. Meanwhile, comparatively little research has been carried out to the *a posteriori* error estimates and adaptivity of the force-based methods. The existing literature, to the best knowledge of the authors, only consider energy-based methods [1–3, 34, 37, 41, 42].

The current work aims to provide a first step for the a posteriori error estimates and adaptivity of the force-based methods. We derive the residual based error estimators for three prototype force-based methods, namely the QCF, the SAC and the BQCF methods, following the framework provided in [34]. We consider a 1D periodic next-nearest-neighbour multi-body interaction atomistic system and its force-based approximations. Though in a 1D setting, the system we consider and the numerical experiments we do preserve many important aspects in higher dimensions which we believe are valuable contributions to this field.

The outline of the paper is listed below.

In Section 2, we introduce the atomistic model problem, the three force-based a/c coupling methods and the notation that will be used throughout the paper. We note that some of the setting and notation follows from [23].

In Section 3, we derive the residual estimates for the three methods in a discrete negative Sobolev norm. We see that the residual estimate of the QCF method can be given as a special case of the BQCF method.

In Section 4, we give the a posteriori stability analysis through a different approach compared with that in [34]. In Section 5, we combine the residual estimates and the stability to give a posteriori error estimators for the deformation gradient.

In Section 6, we develop adaptive algorithms according to the error estimators and present numerical examples to illustrate the performances. In particular, we consider what we call the model adaptivity problem using the residual approach.

We note that we will use a/c (short name for atomistic-to-continuum) and QC (short name for quasicontinuum) liberally since they have the same meaning at least in the present work.