Comput. Methods Appl. Mech. Engrg. 268 (2014) 763–781

Contents lists available at ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma

Theory-based benchmarking of the blended force-based quasicontinuum method ☆

Xingjie Helen Li [a], Mitchell Luskin [b,*], Christoph Ortner [c], Alexander V. Shapeev [b]

[a] Department of Applied Mathematics, Brown University, 182 George St., Providence, RI 02912, USA
[b] School of Mathematics, University of Minnesota, 206 Church St. SE, Minneapolis, MN 55455, USA
[c] Mathematics Institute, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK

ARTICLE INFO

Article history:
Received 5 April 2013
Received in revised form 27 August 2013
Accepted 7 October 2013
Available online 28 October 2013

Keywords:
Quasicontinuum
Error analysis
Atomistic to continuum
Embedded atom model
Quasi-nonlocal

ABSTRACT

We formulate an atomistic-to-continuum coupling method based on blending atomistic and continuum forces. Our precise choice of blending mechanism is informed by theoretical predictions. We present a range of numerical experiments studying the accuracy of the scheme, focusing in particular on its stability. These experiments confirm and extend the theoretical predictions, and demonstrate a superior accuracy of B-QCF over energy-based blending schemes.

1. Introduction

Atomistic-to-continuum coupling methods (a/c methods) have been proposed to increase the computational efficiency of atomistic computations involving the interaction between local crystal defects with long-range elastic fields [7,22,29,40,15,30,6,18]; see [26] for a recent review of a/c coupling methods and their numerical analysis. Energy-based methods in this class, such as the quasicontinuum model (denoted QCE [41]), exhibit spurious interfacial forces ("ghost forces") even under uniform strain [39,8]. The effect of the ghost force on the error in computing the deformation and the lattice stability by the QCE approximation has been analyzed in [8,9,31,10], where lattice stability refers to the positive definiteness of the Hessian matrix of the total potential energy. The development of more accurate energy-based a/c methods is an ongoing process [40,15,37,38,20,34,5].

An alternative approach to a/c coupling is the force-based quasicontinuum (QCF) approximation [11,12,7,29,25], but the non-conservative and indefinite equilibrium equations make the iterative solution and the determination of lattice stability more challenging [13,12,14]. Indeed, it is an open problem whether the (sharp-interface) QCF method is stable in dimension greater than one. Although some recent results in this direction exist [24], it is still unclear to what extent they can be extended for general atomistic domains and in the presence of defects.

Many blended a/c coupling methods have been proposed in the literature, e.g., [4,2,23,1,36,16,35,3,42]. In [21], we formulated a blended force-based quasicontinuum (B-QCF) method, similar to the method proposed in [25], which smoothly

☆ This work was supported in part by the NSF PIRE Grant OISE-0967140, DOE Award DE-SC0002085, and AFOSR Award FA9550-12-1-0187. CO was supported by EPSRC Grant EP/H003096 "Analysis of atomistic-to-continuum coupling methods."

* Corresponding author. Tel.: +1 612 625 6565; fax: +1 612 626 2017.
E-mail addresses: xingjieli@brown.edu (X.H. Li), luskin@umn.edu (M. Luskin), christoph.ortner@warwick.ac.uk (C. Ortner), alexander@shapeev.com (A.V. Shapeev).

0045-7825/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cma.2013.10.007

blends the forces of the atomistic and continuum model instead of the sharp transition in the QCF method. Under the simplifying assumption that deformation is homogeneous, we established sharp conditions under which a linearized B-QCF operator is positive definite, which effectively guarantees stability of the numerical scheme. Surprisingly, the required blending width to ensure positive definiteness of the linearized B-QCF operator is *asymptotically* small (however typical prefactors in the relative size of the blending region are not predicted by the theory). The one-dimensional theory developed in [21] is complete and agrees with the numerical experiments. However, the two-dimensional theory was based on a conjecture that has been proved only in a particular case (see Remark 3.1 for more details) and therefore requires numerical validation.

In the present paper, we present focused numerical experiments to validate and extend the theoretical conclusions in [21,19]. In particular, we study (i) whether stability of the B-QCF method in 2D can be systematically improved with increasing the blending width, (ii) whether a relatively narrow blending, as suggested by the theory, is enough in practice, and (iii) whether using the quintic spline (that has the regularity assumed in the theory) has advantages over the cubic spline. In addition we provide accuracy benchmarks similar to those in [27]. Our numerical benchmarks demonstrate that the B-QCF scheme is a practical a/c coupling mechanism with performance (accuracy versus computational cost) superior to energy-based blending schemes.

1.1. Summary

In Section 2, we introduce the B-QCF model for a 1D atomistic chain. We state the asymptotically optimal condition on the blending size in Theorem 2.1 and apply a uniform expansion to the atomistic chain in subSection 2.2. The critical strain errors between the atomistic and B-QCF models with different blending size are computed in this subsection. The numerical results perfectly match the analytic prediction, that is, the errors decay polynomially in terms of the blending size.

In Section 3, we establish the B-QCF model for a 2D hexagonal lattice. We state sufficient and necessary conditions on the blending width under which the B-QCF operator is positive definite. To numerically investigate the positive-definiteness of the B-QCF operators in 2D, we apply three different classes of deformations to the perfect lattice, which are the uniform expansion, two types of shear deformation, and a general class of homogeneous deformations. The results of 2D uniform expansion are similar to those of the 1D example, and they agree with the theoretical conclusions well.

The stability regions of the different models under homogeneous deformations are consistent with the analytic prediction. By using a small blending region, the 2D B-QCF operator becomes almost as stable as the atomistic model, compared to the fact that the stability region of the force-based quasicontinuum (QCF) method, i.e., the B-QCF method without blending region, is a proper subset of the fully atomistic model [13,12,14]. However, the stability error under shear deformation for the B-QCF operator seems to only depend linearly on the system size, which is observed from the numerical experiments.

In Section 4, we implement the B-QCF method from a *practical* point of view. We briefly review the accuracy results in terms of computational cost, i.e., the total number of degrees of freedom DoF, and then include some numerical experiments for a di-vacancy and microcrack to demonstrate the superior accuracy of B-QCF over other a/c coupling schemes that we have investigated previously in [27].

2. The B-QCF operator in 1D

2.1. Notation

We denote the scaled reference lattice by $\epsilon\mathbb{Z} := \{\epsilon\ell : \ell \in \mathbb{Z}\}$. We apply a macroscopic strain $F > 0$ to the lattice, which yields

$$\mathbf{y}_F := F\epsilon\mathbb{Z} = (F\epsilon\ell)_{\ell\in\mathbb{Z}}.$$

The space $\mathcal{U}$ of $2N$-periodic zero mean displacements $\mathbf{u} = (u_\ell)_{\ell\in\mathbb{Z}}$ from $\mathbf{y}_F$ is given by

$$\mathcal{U} := \left\{ \mathbf{u} : u_{\ell+2N} = u_\ell \text{ for } \ell \in \mathbb{Z}, \text{ and } \sum_{\ell=-N+1}^{N} u_\ell = 0 \right\}$$

and we thus admit deformations $\mathbf{y}$ from the space

$$\mathcal{Y}_F := \{\mathbf{y} : \mathbf{y} = \mathbf{y}_F + \mathbf{u} \text{ for some } \mathbf{u} \in \mathcal{U}\}.$$

We set $\epsilon = 1/N$ throughout so that the reference length of the computational cell remains fixed.

We define the discrete differentiation operator, $D\mathbf{u}$, on periodic displacements by

$$(D\mathbf{u})_\ell := \frac{u_\ell - u_{\ell-1}}{\epsilon}, \quad -\infty < \ell < \infty.$$

We note that $(D\mathbf{u})_\ell$ is also $2N$-periodic in ℓ and satisfies the zero mean condition. We will often denote $(D\mathbf{u})_\ell$ by Du_ℓ. We then define $\left(D^{(2)}\mathbf{u}\right)_\ell$ and $\left(D^{(3)}\mathbf{u}\right)_\ell$ for $-\infty < \ell < \infty$ by