Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2020-0107

Vol. **29**, No. 4, pp. 1246-1272
April 2021

Blended Ghost Force Correction Method for 3D Crystalline Defects

Lidong Fang[1] and Lei Zhang[1,*]

[1] *School of Mathematical Sciences, Institute of Natural Sciences, and MOE-LSC, Shanghai Jiao Tong University, Shanghai, 200240, China.*

Received 10 June 2020; Accepted (in revised version) 11 August 2020

Abstract. Atomistic/continuum coupling method is a class of multiscale computational method for the efficient simulation of crystalline defects. The recently developed blended ghost force correction (BGFC) method combines the efficiency of blending methods and the accuracy of quasi-nonlocal (QNL) type methods. BGFC method can be applied to multi-body interaction potentials and general interfaces. In this paper, we present the formulation, implementation and analysis of the BGFC method in three dimensions. In particular, we focus on the difference and connection with other blending variants, such as energy based blended quasi-continuum method (BQCE) and force based blended quasi-continuum method (BQCF). The theoretical results are justified by a few benchmark numerical experiments with point defects and microcrack in the three dimensional face-centered cubic (FCC) lattice.

AMS subject classifications: 65N12, 65N50, 70C20, 74G65, 82D25

Key words: Multiscale computational method, atomistic/continuum coupling, crystalline defects, blending method, ghost force correction, many-body interaction potential.

1 Introduction

Atomistic/continuum (a/c) coupling method is a class of computational multiscale methods [36] that aim to combine the accuracy of fine scale models and the efficiency of coarse scale models for crystalline defects. Namely, fine scale models can be applied in a small neighborhood of the localized defects such as vacancies and dislocations, while coarse scale models can be employed away from the defect cores where elastic deformation occurs.

In the past two decades, a/c methods have attracted great attention from both the engineering community and the mathematical community [1, 2, 13, 18, 22, 24, 32, 35, 36].

*Corresponding author. *Email addresses:* ldfang.sjtu@gmail.com (L. Fang), lzhang2012@sjtu.edu.cn (L. Zhang)

On one hand, predictive simulations for materials defects such as point defects and dislocations are essential to underpin the elastic and plastic deformation mechanism of materials [28]; on the other hand, the quantitative estimates of the approximation error for a/c methods as a representative concurrent multiscale method help elucidate open questions and establish an analytical framework for similar multiscale computational methods [3,7,12,29].

For a/c coupling methods, fine scale models are usually empirical interaction potentials, while coarse scale models are coarse-grained continuum elastic models. Energy based methods and force based methods are two major classes of a/c coupling methods, we refer to [18,22,36] for reviews of many existing a/c methods. Energy based methods construct a hybrid energy functional as a weighted combination of atomistic and continuum energy functional, and one of the major challenges for energy based methods is to eliminate the so-called "ghost forces" [22] near the atomistic/continuum interface. Force based methods compute the equilibrium of atomistic and continuum forces from corresponding energies, see [6,16,17,21,23] for recent advances. In practice, force based methods can remove ghost forces, and seem to be optimal in terms of coupling error. However, they are not conservative, namely, there is no associated energy functional, and it is usually difficult to establish the stability of the force operator.

Blending type energy based a/c coupling methods [15, 19, 37] smear out the a/c interface and thus propose a weighted energy functional by a blending function. It is easy to implement, however, it does not eliminate the ghost forces as consistent methods do, and only has suboptimal convergence rate [15].

Quasi-nonlocal (QNL) type energy based a/c coupling methods aim to eliminate the ghost force. Therefore, they are referred to as consistent coupling methods. QNL type methods have been well developed in 1D and 2D for multi-body interactions and general interfaces [8,26,33]. However, in three dimensions, QNL type methods are only available for pair interactions [20,30,31], and the construction for multi-body interactions remains open.

In [27], we constructed the blended ghost force correction (BGFC) scheme by integrating two popular ideas: blending [37] and ghost force correction [32]. The BGFC scheme combines the efficiency of the blending methods as well as the accuracy of the QNL type consistent methods. It is quasi-optimal in the sense that it yields the same convergence rate as the force based a/c coupling schemes [14–16]. In fact, it is most instructive to derive the scheme through a modification of the site energies, which can be regarded as a prediction-correction scheme.

For simplicity, the implementation of the BGFC method in [27] is restricted in two dimensions. In this paper, we extend the BGFC scheme to three dimensions. This extension is highly nontrivial since the lattice structure, the partition of the graded mesh, and the implementation of the finite element method are much more complicated in three dimensions. We implement the 3D BGFC method for the FCC lattice and a second-nearest-neighbor multi-body interaction potential, and test a few prototypical benchmark examples such as the single-vacancy, separated-vacancy, and microcrack.