Commun. Comput. Phys.
doi: 10.4208/cicp.250213.270813a

Vol. **15**, No. 3, pp. 647-676
March 2014

On the Effect of Ghost Force in the Quasicontinuum Method: Dynamic Problems in One Dimension

Xiantao Li[1] and Pingbing Ming[2,*]

[1] *Department of Mathematics, the Pennsylvania State University, University Park, Pennsylvania, 16802, USA.*
[2] *LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, AMSS, Chinese Academy of Sciences, No. 55, East Road Zhong-Guan-Cun, Beijing, 100190, P.R. China.*

Received 25 February 2013; Accepted (in revised version) 27 August 2013

Communicated by Weinan E

Abstract. Numerical error caused by "ghost forces" in a quasicontinuum method is studied in the context of dynamic problems. The error in the discrete $W^{1,\infty}$ norm is analyzed for the time scale $\mathcal{O}(\varepsilon)$ and the time scale $\mathcal{O}(1)$ with ε being the lattice spacing.

AMS subject classifications: 65N15, 74G15, 70E55

Key words: Quasicontinuum methods, ghost force, dynamic problems.

1 Introduction

The present paper is concerned with the error caused by ghost forces in quasicontinuum (QC) type of multiscale coupling methods for crystalline solids. In these methods, one reduces the degrees of freedom of an atomic level description by replacing part of the system with continuum mechanics models [2,15,25,38,39]. Such integrated methods have been very useful in studying mechanical properties of solids. It allows one to simulate a relatively large system while still able to keep the atomistic description around the critical areas, such as crack tips and dislocation cores. These methods have also drawn much attention from numerical analysts. We refer to [6, 7, 11, 12, 21, 27, 30, 36] and references therein for a list of representative works. Nevertheless, many challenges in the analysis of these methods still remain. Examples include full three-dimensional problems, systems with line or wall defects, and problems with bifurcation. We refer to [22, 31] for a review

---

[*] Corresponding author. *Email addresses:* `xli@math.psu.edu` (X. Li), `mpb@lsec.cc.ac.cn` (P. B. Ming)

of the recent progress in this area. A critical issue that arises in the numerical analysis is *ghost forces*, which is the non-zero forces on the atoms near the atomistic/continuum interface at an equilibrium state [38]. For statics problems, the removal of ghost forces is a necessary ingredient to achieve uniform accuracy [11,30]. For one-dimensional models, the influence of ghost forces has been explicitly characterized in [6, 26, 27]. They found that the ghost force induces a negligible error on the solution, which is usually as small as the lattice spacing. But it may lead to an $\mathcal{O}(1)$ error on the gradient of the solution at the interface, which decays to $\mathcal{O}(\varepsilon)$ at distance $\mathcal{O}(\varepsilon|\ln\varepsilon|)$ from the interface with ε being the lattice spacing. The influence of the ghost force for a two-dimensional model and a three-dimensional model with a planar interface has recently been studied in [4,5]. It was found that the ghost forces still lead to an $\mathcal{O}(\varepsilon)$ error on the solution, while the gradient of the error is $\mathcal{O}(1)$, which decays from the interface to $\mathcal{O}(\varepsilon)$ over a distance at most $\mathcal{O}(\sqrt{\varepsilon})$. The decay rates seem to be much smaller than that of the one-dimensional problems.

The QC method can be extended to dynamic problems using the coarse-grained energy and the Hamilton's principle [33,37]. The dynamic QC method couples an elastodynamics model with a molecular dynamics model. Many dynamic coupling methods with similar goals have recently been developed, see [1, 2, 8–10, 17, 18, 20, 32, 35, 40, 41, 43–45]. However, very little has been done to study the stability and accuracy of these methods. Most numerical studies have been focused on the artificial reflections at the interface. The reflection is caused by the drastic change in the dispersion relation across the interface, which is often due to the difference between the mesh size in the continuum region and the lattice spacing in the molecular dynamics model. The reflection can be studied by considering an incident wave packet traveling toward the interface and examine the amplitude of the reflected waves [8,19]. The issue of ghost forces for the dynamic problems, however, has not yet been addressed.

The purpose of this paper is to study the effect of ghost forces in the context of *dynamic problems*. To focus primarily on the issue of ghost forces, we consider the dynamic models in [33, 37] derived from the original QC method when the mesh size coincides with the lattice spacing. In addition, the initial displacement is given by a uniform deformation. This allows us to compute the error caused only by the ghost forces. The error will be studied in the discrete $W^{1,\infty}$-norm as done for static problems [4,6,26,27]. The maximum norm for the gradient of the error is particularly suited for the ghost force issue because it controls the pointwise accuracy, while the error measured in the discrete $W^{1,p}$ norm or in the discrete L^p norm with $1<p<\infty$ is often insufficient because it cannot fully reflect the local oscillatory nature of the ghost force. From a practical viewpoint, the discrete gradient measures the relative atomic displacement. Therefore, a pointwise measure is more indicative of the local lattice distortion and it is extremely useful for understanding how the error influences the structures of local defects. Our study shows that the error, which is initially zero, grows dramatically quickly, and already becomes $\mathcal{O}(1)$ at the $\mathcal{O}(\varepsilon)$ time scale. The error exhibits fast oscillations, with amplitude of the order of ε. On the $\mathcal{O}(1)$ time scale, which is typically the time scale of interest, the amplitude of the oscillations grows, and it is bounded by an $\mathcal{O}(\sqrt{\varepsilon})$ quantity. The average of the oscillations has a