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GHOST FORCE INFLUENCE OF A QUASICONTINUUM METHOD IN TWO DIMENSION*

Jingrun Chen
South Hall 6705, Mathematics Department, University of California, Santa Barbara, CA93106, USA
ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China
Email: chenjr@lsec.cc.ac.cn
Pingbing Ming
LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China
Email: mpb@lsec.cc.ac.cn

Abstract

The error caused by the ghost force is studied for a quasicontinuum method with planar interface in two dimension. For a special case, we derive an analytical expression of the error, which is exploited to prove that the ghost force may lead to a finite size error for the gradient of the solution. The pointwise estimate of the error shows that the error decays algebraically away from the interface, which is much slower than that of the one-dimensional problem, for which the error decays exponentially away from the interface.

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Key words: Quasicontinuum method, Ghost force, Interfacial layer.

1. Introduction

Multiscale methods have been developed to simulate mechanical behaviors of solids for several decades [18]. Combination of models at different scales greatly enhances the dimension of problems that computers can deal with. However, problems regarding the consistency, stability and convergence of the multiscale methods may arise from the coupling procedure [3]. Taking the quasicontinuum (QC) method [13, 24] for example, one of the main issues is the so called ghost force problem [22], which is the artificial non-zero force that the atoms experience at the equilibrium state. In the language of numerical analysis, the scheme lacks consistency at the interface between the atomistic region and the continuum region [4]. For the one-dimensional problem, it has been shown in [2, 20] that the ghost force may lead to a finite size error for the gradient of the solution. The error decays exponentially away from the interface.

To understand the influence of the ghost force for high dimensional problems, we study a two-dimensional triangular lattice model with a QC approximation. This QC method couples the Cauchy-Born elasticity model [1] and the atomistic model with a planar interface. Numerical results show that the ghost force may lead to a finite size error for the gradient of the solution as the one-dimensional problem. The error profile exhibits a layer-like structure. Outside the layer, the error decays algebraically.

To further characterize the influence of the ghost force, we introduce a square lattice model with a QC approximation. Compared to the triangular lattice model, this model can be solved

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analytically and the error profile exhibits a clear layer-like structure. Based on the analytical solution, we prove the error committed by the ghost force for the gradient of the solution is $\mathcal{O}(1)$ and the error decays away from the interface to $\mathcal{O}(\varepsilon)$ at distance $\mathcal{O}(\sqrt{\varepsilon}\,)$, where ε is the equilibrium bond length. These are also confirmed by the numerical results. We note that there are some recent efforts devoted to the convergence analysis for ghost force free multiscale coupling methods in high dimension, we refer to [16, 21] and the references therein.

The paper is organized as follows. Numerical results for the triangular lattice model and the square lattice model with QC approximations are presented in § 2 and § 3, respectively. We derive an analytical expression of the solution of the square lattice model with a QC approximation in § 4. The pointwise estimate of the solution is proved in § 5.

2. A QC Method for Triangular Lattice

2.1. Atomistic and continuum models

We consider the triangular lattice $\mathbb{L}$, which can be written as

$$\mathbb{L} = \Big\{ x \in \mathbb{R}^2 \mid x = ma_1 + na_2,\ m, n \in \mathbb{Z} \Big\}$$

with the basis vectors $a_1 = (1, 0), a_2 = (1/2, \sqrt{3}/2)$. Define the unit cell of $\mathbb{L}$ as

$$\Gamma = \Big\{ x \in \mathbb{R}^2 \mid x = c_1 a_1 + c_2 a_2,\ -1/2 \le c_1, c_2 < 1/2 \Big\}.$$

We shall consider lattice system $\varepsilon\mathbb{L}$ inside the domain $\Omega = \Gamma$, and denote $\Omega_\varepsilon = \Omega \cap \varepsilon\mathbb{L}$, where ε is the equilibrium bond length. Assume that the atoms are interacted with the potential function, which is usually a highly nonlinear function, e.g., the Lennard-Jones potential [15]. Denote by $\mathcal{S}_1$ and $\mathcal{S}_2$ the first and the second neighborhood interaction ranges; see Fig. 2.1. In particular, we have

$$\begin{aligned}
&\mathcal{S}_1 = \cup_{i=1}^{6} s_i = \{a_1, a_2, -a_1 + a_2, -a_1, -a_2, a_1 - a_2\},\\
&\mathcal{S}_2 = \cup_{i=7}^{12} s_i = \{a_1 + a_2, -a_1 + 2a_2, -2a_1 + a_2, -a_1 - a_2, a_1 - 2a_2, 2a_1 - a_2\}.
\end{aligned}$$

For $\mu \in \mathbb{Z}^2$, the translation operator T_ε^μ is defined for any lattice function $z : \mathbb{L} \to \mathbb{R}^2$ as

$$(T_\varepsilon^\mu z)(x) = z(x + \varepsilon\mu_1 a_1 + \varepsilon\mu_2 a_2) \quad \text{for } x \in \mathbb{L}.$$

We define the forward and backward discrete gradient operators as

$$D_s^+ = \varepsilon^{-1}(T_\varepsilon^\mu - I) \qquad \text{and} \qquad D_s^- = \varepsilon^{-1}(I - T_\varepsilon^\mu),$$

where $s = \mu_1 a_1 + \mu_2 a_2$ and I is the identity operator. We shall also use the short-hand

$$Dz = (D_1^+ z, D_2^+ z) = (D_{s_1}^+ z, D_{s_2}^+ z).$$

In what follows, we denote $z(x)$ as the deformed positions of the atoms.

Consider an atomic system posed on Ω_ε. The total energy is given by

$$E_{\text{at}}^{\text{tot}} = \frac{1}{2} \sum_{x \in \Omega_\varepsilon} \sum_{s \in \mathcal{S}_1 \cup \mathcal{S}_2} V\left(|D_s^+ z(x)|\right), \tag{2.1}$$