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Analysis of Geometrically Consistent Schemes with Finite Range Interaction

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Abstract. We analyze the geometrically consistent schemes proposed by E. Lu and Yang [6] for one-dimensional problem with finite range interaction. The existence of the reconstruction coefficients is proved, and optimal error estimate is derived under sharp stability condition. Numerical experiments are performed to confirm the theoretical results.

AMS subject classifications: 65N15, 65N30

Key words: Quasicontinuum method, atomic-to-continuum coupling, stability, finite range interactions.

1 Introduction

The main motivation for the multiscale coupling method is that the macroscale model is sufficiently accurate except the isolated regions in which the microscale model is required to resolve the details of the local events take place in these regions. The quasicontinuum (QC) method [31] is one of the earliest multiscale coupling method for modeling the mechanical deformation of crystalline solids. There are two class methods in QC: the energy-based method and the force-based method. In this paper we focus on the energy-based method, and refer to [16] and [14,15] for a review on the force-based method and its recent progress. We list several representatives of the energy-based QC method: the dead load force correction method [29]; the quasinonlocal method (QNL) [30] and the

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generalized QNL [12, 27, 28]; the geometrically consistent scheme (GCS) [6] and its generalization [24, 25]; and the blended QC [1, 26, 32]. The essential difference among these methods are the strategies to deal with the energy of the atoms inside the atomistic-to-continuum (a/c) interface. It is worthwhile to mention that there are also some other a/c energy-based coupling methods such as the optimization-based coupling method [19].

In this study we shall focus on GCS proposed by E. Lu and Yang. This scheme depends only on the lattice structure of the system and works for all existing empirical potentials with an arbitrary interaction range. It generalizes QNL proposed in [30]. New variants of GCS have recently been proposed in [24, 25], which have been proven to be first-order consistent. A reflection method in the spirit of GCS was constructed in [21]. Though there seems no straightforward extension of this method to 2d/3d, the authors proved the first-order accuracy of the reflection method in 1d under sharp stability condition. A set of coefficients has to be precomputed in the implementation of GCS. Such coefficients (we call GCS coefficients) for various lattice structures with different interaction ranges have been charted in [6], while its existence for problems with arbitrary interaction range interaction remains unproved. Progress in this direction has been made in [24] in 2d. We prove the existence of GCS coefficients in 1d, and hope it may provide certain insights for 2d/3d.

Ming and Yang [17] analyzed GCS for an atomic chain with second neighboring interaction. Uniformly first-order accuracy has been proved in the discrete $W^{1,\infty}$ norm. However, the stability condition is suboptimal, and their analysis is confined to second neighboring interaction. This motivates our study on GCS for finite range interaction, which is particularly important when van der Waals type interactions play an essential role. For example, we are interested in modeling the mechanical interaction between atom clusters. We firstly prove that the GCS coefficients indeed exist for 1d chain with finite range interaction, while it is not unique. Next we derive a special symmetric solution, which essentially coincides with that in [6] for the interaction range less than five. Motivated by [24,25], we propose a minimizing algorithm to obtain new sets of GCS coefficients. Numerical evidence suggests that GCS with such coefficients may have smaller error. We establish an identity for GCS coefficients, upon which we prove the first-order consistency of GCS in a negative Sobolev norm. Using this identity, a discrete Wirtinger inequality and a generalized polarization identity, we prove that GCS with finite range interaction is stable under the sharp stability condition for Dirichlet boundary value problem. The stability condition is sharp in the sense that the difference between the stability condition of GCS and that of the atomic model is of $\mathcal{O}(\varepsilon^2)$, where ε is the lattice spacing. We test the accuracy of GCS by a set of numerical examples, which show that GCS has optimal convergence rate in the discrete $W^{1,p}$ norm for $2 \leq p \leq \infty$. The analysis is carried out for the pairwise potential for brevity, which can be extended for many-body potential by combining the techniques from [7] and [11, 16].

The paper is organized as follows. In Section 1, we introduce the setup of the problem and the geometrical consistent scheme. In Section 2, we propose a condition under which GCS coefficients exist. A special set of GCS coefficients is explicitly derived, and