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THERE IS NO POINTWISE CONSISTENT QUASICONTINUUM ENERGY

MATTHEW DOBSON

Abstract. Much work has gone into the construction of quasicontinuum energies that reduce the coupling error along the interface between atomistic and continuum regions. The largest consistency errors are typically pointwise $O(\frac{1}{\varepsilon})$ errors, and in some cases this has been reduced to pointwise $O(1)$ errors. In this paper we show that one cannot create a coupling method using a finite-range coupling interface that has o(1)-consistency in the interface, and we use this to give an upper bound on the order of convergence in discrete $w^{1,p}$-norms in 1D.

1. Introduction

Atomistic to continuum coupling schemes attempt to provide the high accuracy of an atomistic simulation while also providing the computational savings of a coarse-grained continuum approximation. Such simulations are used in the study of localized defects that interact with a long-range elastic field, such as crack tips, voids, and interstitials. The quasicontinuum method directly couples an atomistic region, where each atom interacts with every other atom within a cut-off radius, to a continuum region, whose strain energy density is computed by assuming Cauchy-Born kinematics (locally uniform deformation gradients). Many variants of the scheme exist that differ on how to couple the regions together.

One can classify quasicontinuum methods based on whether they create a total energy or directly couple forces in such a way that there does not exist a total energy. The original formulation of the quasicontinuum method [21, 15] creates a total energy by defining an energy for each degree of freedom (atom or finite element) and using a weighted sum. Unfortunately, the model contains spurious forces at the atomistic to continuum interface called ghost forces [17]. These forces are a pointwise $O(\frac{1}{\varepsilon})$ consistency error in the linearized scheme and reduce the order of convergence with respect to the interatomic spacing parameter ε [4]. Subsequent methods such as the quasinonlocal quasicontinuum method [20] or the geometrical reconstruction scheme [7] removed some ghost forces, but were restricted on the number of neighbors or to specific interface geometry in 2D and 3D. Recently, the ECC and ACC quasicontinuum variants have been proposed in 1D and 2D , and these schemes are free of ghost forces for the case of pair-potential interactions [18]. A related method, derived as an extension of QNL, is formulated in 1D in [11].

An alternative approach to consistency is the use of the force-based quasicontinuum method [2, 3, 14], which assigns forces to any degree of freedom, atomistic or continuum, as though the entire model were of the same type. Since the continuum model and atomistic model are $o(1)$-consistent and there are no special force laws in the atomistic-to-continuum interface, this creates a globally point-wise consistent scheme for any geometry. However, this method is more difficult to analyze since it does not derive from an energy [5, 6]. Solutions to the force-based equations can be approximated by employing the ghost-force correction scheme [19, 3].

Here we ask the question of whether it is possible to create a quasicontinuum energy which is globally $o(1)$-pointwise consistent. We will find in Section 3 that even in the case of a linear, 1-D model it is impossible to make an $o(1)$ consistent blending of the atomistic and continuum region for any finite-sized interface region. While such a finiteness assumption is common, a quasicontinuum force coupling with growing interfaces is treated in [13]. In Section 4, we will

show how this leads to a bound on the maximal order of convergence in discrete $w^{1,p}$-norms in 1D. Convergence analysis for related quasicontinuum schemes include [12, 8, 1, 10].

2. Models

We denote the positions of a periodic atomistic chain by

$$y \in \mathbb{R}^N = \{\mathbb{R}^{\mathbb{Z}} \ : \ y_{\ell+N} = y_\ell + F \text{ for all } \ell \in \mathbb{Z}\},$$

where F denotes the macroscopic deformation gradient for the periodic length and $N \in \mathbb{Z}_{\geq 0}$ denotes the number of atoms in the periodic cell. We scale the reference length of the the interatomic spacing by $\varepsilon = \frac{1}{N}$ in order to have a well-defined continuum limit. We denote the displacements from the uniformly deformed position by $u_i = y_i - F\varepsilon i$ for all $i \in \mathbb{Z}$. We define the backward difference quotient

$$D_r u_i = \frac{u_i - u_{i-r}}{r\varepsilon} \qquad r \in \mathbb{Z}^{>0},$$

where we will write Du_i to denote $D_1 u_i$. We will write the vector of such differences as Du. We likewise define the centered second-difference quotient

$$D_r^2 u_i = \frac{u_{i+r} - 2u_i + u_{i-r}}{r^2\varepsilon^2} \qquad r \in \mathbb{Z}^{>0}.$$

2.1. **Atomistic and continuum models.** We consider the atomistic energy composed of pairwise interactions with the nearest R neighbors, given by

$$\mathcal{E}_\varepsilon^a(u) = \sum_{r=1}^{R}\sum_{i=1}^{N} \varepsilon\phi(rF + rD_r u_i), \tag{1}$$

where ϕ denotes the interatomic interaction potential and R denotes the finite-range cut-off. The energy is scaled by the lattice spacing ε so that there is a finite energy in the limit $N \to \infty$. The continuum approximation uses the same pair potential and approximates the total energy by

$$\mathcal{E}_\varepsilon^c(u) = \sum_{r=1}^{R}\sum_{i=1}^{N} \varepsilon\phi(rF + rDu_i). \tag{2}$$

That is, interactions of the form $\phi\Big(\frac{y_i - y_{i-r}}{\varepsilon}\Big)$ are replaced by $\phi\Big(r\frac{y_i - y_{i-1}}{\varepsilon}\Big)$. The continuum energy is an accurate approximation when y_i is smooth. In practical applications, the cost of computing the continuum energy is reduced by computing the energy as a sum over the nodes in a piecewise linear mesh rather than a sum over all atoms.

Expanding the pairwise interactions, we have

$$\phi(rF + D_r u_i) \approx \phi(rF) + \phi'(rF)D_r u_i + \frac{1}{2}\phi''(rF)(D_r u_i)^2 + \cdots \qquad \text{for } r \in \mathbb{Z}^{>0}.$$

For the atomistic model, the (scaled) forces on the atoms are

$$(L_\varepsilon^a u)_i = -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}^a(u)}{\partial u_i} = -\sum_{r=1}^{R} r^2\phi''(rF)D_r^2 u_i, \tag{3}$$

and for the continuum model, the (scaled) forces on the nodes are

$$(L_\varepsilon^c u)_i = -\frac{1}{\varepsilon}\frac{\partial \mathcal{E}^c(u)}{\partial u_i} = -\sum_{r=1}^{R} r^2\phi''(rF)D^2 u_i. \tag{4}$$

2.2. **Quasicontinuum coupling.** A quasicontinuum energy couples the atomistic and continuum energies, by partitioning the chain into an atomistic region $\mathcal{A}$ and a continuum region $\mathcal{C}$ that satisfy

$$\mathcal{A} \cup \mathcal{C} = (0,1] \quad \text{and} \quad \mathcal{A} \cap \mathcal{C} = \emptyset. \tag{5}$$

We assume that $\mathcal{A}$ is a finite union of intervals. An atom i is in the atomistic region if $\varepsilon i \in \mathcal{A}$. Away from the boundary of these regions, the energy is computed using the energy contributions $\mathcal{E}_i^a$ or $\mathcal{E}_i^c$. Near the interface between the regions, there can exist special interfacial energies that we assume are finite range and which do not change in form with ε. Note that the interfacial interactions may be longer-ranged than the atomistic ones.

The above assumptions imply that away from the atomistic to continuum interface and for sufficiently large N, the atoms in the continuum region only feel continuum forces (4) and the atoms in the atomistic region only feel atomistic forces (3). We define $\widehat{\mathcal{A}}_\varepsilon$ and $\widehat{\mathcal{C}}_\varepsilon$ as the interior portions of the atomistic and continuum region that only feel interactions from within their specific region. We define the interface region $\mathcal{I}_\varepsilon = [0,1] \setminus (\widehat{\mathcal{A}}_\varepsilon \cup \widehat{\mathcal{C}}_\varepsilon)$. In the following, we will focus on a single interface between the atomistic and continuum regions.

3. Consistency at the Interface

We say that a family of operators L_ε is $o(1)$-consistent with the atomistic operator L^a if

$$\lim_{\varepsilon \to 0} \|L_\varepsilon u - L_\varepsilon^a u\|_{\ell_\varepsilon^\infty} = 0 \tag{6}$$

for every $u \in C^2_{per}(\overline{\Omega})$, where for every N, $u \in C^2_{per}(\overline{\Omega})$ defines a vector $u \in \mathbb{R}^N$ by $u_i = u(i/N)$. Equivalently, we have the local consistency requirement that the equations are consistent if

$$(L_\varepsilon u - L_\varepsilon^a u) = 0 \qquad \text{for the three vectors } u_j = 1, j, j^2. \tag{7}$$

We note that the continuum operator L_ε^c is consistent with the atomistic operator. In the following, we show that one cannot satisfy these consistency equations for a quasicontinuum energy even in the simplified case of second-neighbor interactions in a 1-D chain with harmonic pair potentials.

We now restrict ourselves to the second-neighbor ($R = 2$) case for the atomistic and continuum energies. We write the quasicontinuum operator in terms of its first and second-neighbor contributions

$$L_\varepsilon^{qc} = \frac{1}{\varepsilon^2}(\phi''(F) L_1^{qc} + \phi''(2F) L_2^{qc}), \tag{8}$$

where the operators L_1^{qc} and L_2^{qc} are independent of ϕ and ε. This form is possible when we assume that the corresponding energy is a function of the "strains" $D_r u$ only. We then consider possible choices for quasicontinuum energies. Since the first neighbor term for both atomistic and continuum operator are identical, it is standard to take the same operator for the first neighbor term of a quasicontinuum energy. This gives $(L_1^{qc} u)_j = -\varepsilon^2 D^2 u_j$. The second neighbor term is a symmetric operator satisfying

$$(L_2^{qc} u)_i = \begin{cases} -u_{j+2} + 2u_j - u_{j-2} = -4\varepsilon^2 D_2^2 u_i & \varepsilon i \in \widehat{\mathcal{A}}_\varepsilon, \\ -4u_{j+1} + 8u_j - 4u_{j-1} = -4\varepsilon^2 D^2 u_i & \varepsilon i \in \widehat{\mathcal{C}}_\varepsilon, \end{cases} \tag{9}$$

where we have not yet specified the interaction law in the interface $\mathcal{I}_\varepsilon$. We now consider one boundary between atomistic and continuum regions. Let m denote the number of atoms in the interval of the atomistic to continuum interface $\mathcal{I}_\varepsilon$ surrounding the boundary between the regions. This is represented in the operator L_2^{qc} by an $m \times m$ set of coefficients, $(L_2^{qc})_{ij}$ for

$1 \le i, j \le m$. We have labeled the interface starting at $j = 1$ and will assume without loss of generality that $(L_2^{qc} u)_j$ is continuum for $j < 1$ and atomistic for $j > m$.

Proposition 3.1. *There is no symmetric linear quasicontinuum operator L_ε^{qc} satisfying* (7).

Proof. We suppose toward contradiction that L^{qc} satisfies (7). Then, for all i, we have that

$$\sum_j (L_{ij}^{qc} - L_{ij}^a) j = 0 \qquad \text{and} \qquad \sum_j (L_{ij}^{qc} - L_{ij}^a) j^2 = 0, \tag{10}$$

where j runs over all indices for our periodic chain, though due to the limited range of interactions outside the interface, we may restrict $j = -1, \dots, m+2$. Now, we will sum the equations above for $i = 1, \dots, m$, pre-multiplying by i^2 and i, respectively, in order to cancel out the interface variables in the interior. We note that by symmetry, $L_{ij}^{qc} = L_{ij}^c$ for $j < 1$ and $L_{ij}^{qc} = L_{ij}^a$ for $j > m$. We have

$$\begin{aligned}
0 &= \sum_{i=1}^m \sum_{j=-1}^{m+2} i^2 (L_{ij}^{qc} - L_{ij}^a) j - \sum_{i=1}^m \sum_{j=-1}^{m+2} i (L_{ij}^{qc} - L_{ij}^a) j^2, \\
&= \sum_{i=1}^m \sum_{j=1}^m (L_{ij}^{qc} - L_{ij}^a)(i^2 j - i j^2) + \sum_{i=1}^m \sum_{j \in \{-1,0\}} (L_{ij}^c - L_{ij}^a)(i^2 j - i j^2) \\
&\quad + \sum_{i=1}^m \sum_{j \in \{m+1, m+2\}} (L_{ij}^a - L_{ij}^a)(i^2 j - i j^2)
\end{aligned}$$

We cancel the first summation by the symmetry of both L_ε^{qc} and L^a, and the third summation cancels identically. The second summation has a single non-zero term $i = 1, j = -1$, so that we have

$$\begin{aligned}
0 &= \sum_{i=1}^m \sum_{j \in \{-1,0\}} (L_{ij}^c - L_{ij}^a)(i^2 j - i j^2) \\
&= 1(-1 - 1) = -2.
\end{aligned}$$

We have arrived at a contradiction to our assumption that L^{qc} was consistent (10). □

4. Global convergence error

The result above shows that any linear quasicontinuum scheme must have at least O(1) consistency error in the ℓ^∞ norm. We can use the above bound on interfacial consistency error to give an upper bound on the order of convergence for any quasicontinuum energy. We recall the definitions of the discrete ℓ_ε^p-norms on $\mathbb{R}^N$,

$$\begin{aligned}
\|u\|_{\ell_\varepsilon^p} &:= \left(\varepsilon \sum_{j=1}^N |u_j|^p \right)^{1/p}, \qquad 1 \le p < \infty, \\
\|u\|_{\ell_\varepsilon^\infty} &:= \max_{1 \le j \le N} |u_j|.
\end{aligned}$$

Provided that L_ε^{qc} is shift-invariant, that is, it satisfies (7) for $v_j = 1$, we can write the operator in terms of differences,

$$L_\varepsilon^{qc} u = \widetilde{L}_\varepsilon^{qc} D u,$$

where we note that the coefficients of $\varepsilon \widetilde{L}_\varepsilon^{qc}$ are bounded independently from ε. We have the following lower bound for the error.

Corollary 4.1. *There exists $u \in C^2_{per}(\overline{\Omega})$ such that for $L^{qc}_\varepsilon u_{qc} = L^a_\varepsilon u$ the error $e = u - u_{qc}$ satisfies*

$$\|De\|_{\ell^p_\varepsilon} \geq C\varepsilon^{1+1/p}$$

for $1 \leq p \leq \infty$.

Proof. Since the coefficients of $\varepsilon \widetilde{L}^{qc}_\varepsilon$ are bounded, we have the inequality $\|L^{qc}v\|_{\ell^\infty_\varepsilon} \leq \frac{C}{\varepsilon}\|Dv\|_{\ell^\infty_\varepsilon}$. Using the fact that the operator is not o(1)-consistent, we choose $u \in C^2_{per}$ such that

$$\lim_{\varepsilon\to 0} \|(L^a_\varepsilon - L^{qc}_\varepsilon)u\|_{\ell^\infty_\varepsilon} \geq c.$$

We then write

$$c \leq \|(L^a_\varepsilon - L^{qc}_\varepsilon)u\|_{\ell^\infty_\varepsilon} = \|L^{qc}_\varepsilon e\|_{\ell^\infty_\varepsilon} \leq \frac{C}{\varepsilon}\|De\|_{\ell^\infty_\varepsilon}.$$

Which implies $\|De\|_{\ell^\infty_\varepsilon} \geq C\varepsilon$. The estimate for other norms follows from the equivalence estimates for ℓ^p norms, $\|De\|_{\ell^p_\varepsilon} \geq \varepsilon^{1/p}\|De\|_{\ell^\infty_\varepsilon} \geq C\varepsilon^{1+1/p}$. □

This result implies that the rates of convergence obtained in 1D for the quasinonlocal quasicontinuum method in [4, 16] are asymptotically optimal among all possible quasicontinuum energies with finite-range interface interactions.

5. Conclusion

There is much past and ongoing work to create consistent atomistic-to-continuum coupling schemes, and a major obstacle are the $O(\frac{1}{\varepsilon})$-ghost forces common in such models. Quasicontinuum energies that are O(1)-consistent have been constructed in 1D and 2D, at least for the case of pair-potential interactions. In this work we have shown the impossibility of improving the asymptotic truncation error for a linear quasicontinuum energy in 1D. Since a higher dimensional problems can behave like a 1D configuration due to the geometry (such as simple uniaxial strain applied parallel to a planar atomistic-to-continuum interface), this implies that it is impossible to make a general o(1)-consistent coupling energy in higher dimensions as well. The effect on the rate of convergence shows that in 1D the quasinonlocal quasicontinuum energy and its generalizations are asymptotically optimal among quasicontinuum energies with respect to $w^{1,p}$-norm convergence. However, for other quantities of interest, such as the critical strain for dislocation movement [9], such a method may not be asymptotically optimal.

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