About an analytical verification of quasi-continuum methods with $\Gamma$-convergence techniques

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ABSTRACT

Quasi-continuum (QC) methods are computational techniques, which reduce the complexity of atomistic simulations in a static setting while keeping information on small-scale structures and effects. The main idea is to couple atomistic and continuum models and thus to obtain quite detailed but still not too expensive numerical simulations.

We aim at a mathematically rigorous verification of QC methods by means of discrete to continuum limits. In this article we present our first results for the so-called quasi-nonlocal QC method in the context of fracture mechanics. To this end we start from a one-dimensional chain of atoms with nearest and next-to-nearest neighbour interactions of Lennard-Jones type. This is considered as a fully atomistic model of which the $\Gamma$-limits (of zeroth and first order) for an infinite number of atoms are known [7].

The QC models we construct are equal to this fully atomistic model in the atomistic region; in the continuum regime we approximate the next-to-nearest neighbour interactions by some nearest neighbour potential which is related to the so-called Cauchy-Born rule. Further we choose certain representative atoms in order to coarsen the mesh in the continuum region. It turns out that the selection of the representative atoms is crucial and influences the $\Gamma$-limits.

We regard a QC model as good if the $\Gamma$-limits of zeroth and first order or at least their minimal values and minimizers are the same as those of the fully atomistic model. Our analysis shows that, while in an elastic regime only the size of the atomistic region matters, in the case of fracture a proper choice of the representative atoms is an essential ingredient.

INTRODUCTION

Quasi-continuum (or QC) methods are computational techniques, which couple atomistic and continuum descriptions of crystalline solids. Applications include nano-indentations, defects and fracture mechanics. There exist various types of QC-methods: Some are formulated in an energy based framework, some in a force based framework; further there exist different couplings between the atomistic and continuum regions, see [4, 9] for recent overviews, in particular on the large numerical literature including work on error analysis.

Here we are interested in an analytical approach in order to verify the QC methods from a more fundamental point of view by a discrete to continuum limit. Up to our knowledge, only two works on related analytical investigations of QC methods are available: In [5] quasi-continuum approximations are studied in an elastic higher-dimensional regime. In [1] a one-dimensional setting with nearest neighbour interactions is studied. While the corresponding atomistic/continuum coupling does not create difficulties in the case of convex interaction potentials, Lennard-Jones potentials firstly lead to an unwanted behaviour since the location of fracture is more favourable in the continuum than in the atomistic part. In [1] this is overcome by introducing ad hoc a specific scaling of the continuum energy. We aim for a further understanding of this and choose the perspective of $\Gamma$-convergence, which is an appropriate notion for the convergence of variational problems, see the beginning of the next section. We include fracture in our analysis and start with a one-dimensional atomistic model problem, which takes nearest and next-to-nearest neighbour interaction into
account. The limiting behaviour of the corresponding discrete model was analyzed by means of \(\Gamma\)-convergence techniques in [7] for a large number of atoms.

From the fully atomistic model we construct a QC-approximation which is based on the well-known quasi-nonlocal quasi-continuum method, cf. [4,6] and references therein. This is an energy based QC-method which has a special coupling at the interface between the atomistic and continuum regions to eliminate so-called ghost-forces. It keeps the nearest and next-to-nearest neighbour interactions in the atomistic (nonlocal) region and approximates the next-to-nearest neighbour interactions in the continuum (local) region as outlined below. Furthermore the set of admissible functions is changed by fixing certain representative atoms. This leads to a reduction of the degrees of freedom. We investigate the limiting behaviour of the so obtained quasi-continuum energy functional by deriving the \(\Gamma\)-limits of zeroth and first order in the theorems of this article. We compare this with the limiting results of the original fully atomistic model. In Corollary 6 we study the minimal values of the limiting energies and obtain that the choice of the representative atoms as well as of the atomistic region is crucial in order to have defined an appropriate quasi-continuum model problem which has the same limiting properties as the fully atomistic model.

This article is an abridged version of our work [8] under preparation, in which we consider more general settings and discuss the impact of these analytical observations on QC methods further.

**BACKGROUND AND SETTING OF THE PROBLEM**

The main tool of this work is the so called \(\Gamma\)-convergence of which we quickly recall the definition and main properties, see e.g. [2] for details and references.

**Definition 1.** Let \(X\) be a metric space and let \(H_\varepsilon : X \to [-\infty, +\infty]\). Then \(H_\varepsilon\) \(\Gamma\)-converges to \(H_0\) as \(\varepsilon \to 0\) if for all \(x \in X\):

(i) \(\forall x_\varepsilon \to x \in X\) there holds \(H_0(x) \leq \liminf_{\varepsilon \to 0} H_\varepsilon(x_\varepsilon)\),

(ii) \(\exists x_\varepsilon \to x \) such that \(H_0(x) = \lim_{\varepsilon \to 0} H_\varepsilon(x_\varepsilon)\).

We then write \(H_\varepsilon \rightrightarrows H_0\) as shorthand. If \((H_\varepsilon)\) additionally satisfies some coercivity conditions, then

\[
\inf H_\varepsilon \to \min H_0
\]

and minimizers of \(H_\varepsilon\) converge, up to subsequences, to minimizers of \(H_0\). Moreover, we say that \((H_\varepsilon)\) \(\Gamma\)-converges of first order to \(H_1\) if

\[
\frac{H_\varepsilon - \min H_0}{\varepsilon} \rightrightarrows H_1.
\]

The \(\Gamma\)-limit of first order yields a finer approximation of \(H_\varepsilon\). Indeed, under some conditions on \((H_\varepsilon)\),

\[
\inf H_\varepsilon = \min H_0 + \varepsilon \min H_1 + o(\varepsilon).
\]

Next we present the atomistic model problem. This coincides with the discrete system considered in [7], to which we refer to for further details. For sake of simplicity let \(J_1, J_2\) be Lennard-Jones potentials, i.e., for \(z > 0\) set \(J_i(z) = \frac{k_1^i}{z^6} + \frac{k_2^i}{z^{12}}\) with \(k_1^i, k_2^i > 0\) and \(i = 1, 2\). We set \(\lambda_n = \frac{1}{n}\) and consider the reference configuration \(\lambda_n \mathbb{Z} \cap [0, 1]\). We denote by \(u : \lambda_n \mathbb{Z} \cap [0, 1] \to \mathbb{R}\) the deformation of the atoms from their reference configuration, write \(u^i\) as shorthand for \(u(i\lambda_n)\) and identify \(u \in \mathcal{A}_n(0, 1)\) with the piecewise affine interpolation of the \(u^i\)s with \(0 \leq i \leq n\). For given parameters \(\ell, u_0^{(1)}, u_1^{(1)} > 0\), we consider the boundary conditions

\[
u^0 = 0, \ u^1 = \lambda_n u_0^{(1)}, \ u^{n-1} = \ell - \lambda_n u_1^{(1)}, \ u^n = \ell,
\]
i.e., we fix the deformation of the first two and last two atoms. The corresponding energy is now defined as the sum of all nearest and next-to-nearest neighbour interactions with a canonical scaling. We set

\[ H^\ell_n(u) = \sum_{i=0}^{n-1} \lambda_n J_1 \left( \frac{u^{i+1} - u^i}{\lambda_n} \right) + \sum_{i=0}^{n-2} \lambda_n J_2 \left( \frac{u^{i+2} - u^i}{2\lambda_n} \right). \]

if \( u \) satisfies the boundary conditions, and infinity else. We are interested in solving the minimization problem

\[ \min_{u \in A_n(0,1)} H^\ell_n(u), \]

which is studied in terms of \( \Gamma \)-convergence of zeroth and first order in [7].

As mentioned above, here we consider the so-called quasi-nonlocal quasi-continuum method. The approximation of \( H^\ell_n \) is obtained in two steps:

(a) Replace second neighbour interactions by certain nearest neighbour interactions,

(b) Reduce the degrees of freedom by choosing a smaller set \( B_n \subset A_n(0,1) \) for the set of admissible functions.

To obtain (a) the next-to-nearest neighbour interactions are approximated as

\[ J_2 \left( \frac{u^{i+2} - u^i}{2\lambda_n} \right) \approx \frac{1}{2} J_2 \left( \frac{u^{i+1} - u^i}{\lambda_n} \right) + J_2 \left( \frac{u^{i+2} - u^{i+1}}{\lambda_n} \right). \]

While this approximation turns out to be appropriate in the bulk, this is not the case close to surfaces. We therefore construct the QC-model accordingly: For given \( n \in \mathbb{N} \) let \( k^1_n \) and \( k^2_n \) be integers with \( 0 < k^1_n < k^2_n \leq n - 2 \). We define the energy \( H^\ell QC_n \) as the functional which arises by using the above approximation for \( k^1_n \leq i \leq k^2_n - 2 \) and by keeping the atomistic description elsewhere. After several elementary calculations, this leads to the following energy functional

\[ H^\ell QC_n(u) = \frac{\lambda_n}{2} J_1 \left( u_0^{(1)} \right) + \sum_{i=0}^{k^1_n-1} \lambda_n \mathcal{E}^i(u) + \int_{\lambda_n(k^1_n-\frac{1}{2})}^{\lambda_n(k^1_n+\frac{1}{2})} J_{CB}(u'(x))dx + \sum_{i=k^1_n-1}^{n-2} \lambda_n \mathcal{E}^i(u) \]

where \( \mathcal{E}^i(u) = J_2 \left( \frac{u^{i+2} - u^i}{2\lambda_n} \right) + \frac{1}{2} \left( J_1 \left( \frac{u^{i+1} - u^i}{\lambda_n} \right) + J_1 \left( \frac{u^{i+2} - u^{i+1}}{\lambda_n} \right) \right) \) and \( J_{CB}(z) = J_1(z) + J_2(z) \).

Another important step to reduce the computational cost is to reduce the degrees of freedom, which corresponds to (b). Instead of every atom in the chain we consider just a proper choice of representative atoms (repatoms). Let \( 0 = t^0_n < t^1_n < \cdots < t^{r_n}_n = n \), with \( r_n \leq n \). Then the set of repatoms is defined as \( T_n = \{ t^0_n, ..., t^{r_n}_n \} \). By defining the energy \( H^\ell QC_{\mathcal{T}_n} \) as

\[ H^\ell QC_{\mathcal{T}_n}(u) = \left\{ \begin{array}{ll} H^\ell QC_n(u) & \text{if } u \in A_{\mathcal{T}_n}(0,1), \\ +\infty & \text{else,} \end{array} \right. \]

we reduce the set of admissible deformations to \( A_{\mathcal{T}_n}(0,1) \) which are the piecewise affine interpolations of the \( u^i \)'s with \( i \in T_n \). In the continuum region this corresponds to using finite elements with linear shape functions. In this work we always assume that there exists a sequence \( (h_n) \) such that \( \lambda_n h_n \to 0 \) as \( n \to \infty \) and

\[ \sup_{n \geq 0} \max_{0 \leq i \leq r_n} (t^i_{n+1} - t^i_n) \leq h_n. \]  

This ensures that the mesh size of \( T_n \) shrinks to zero as \( n \) tends to infinity, possibly at a different order than the atomistic lattice spacing.
CONVERGENCE RESULTS

The aim of this section is to present some Γ-convergence results for the fully atomistic model as well as for the QC-approximations. We then compare the limits and derive conclusions on appropriate definitions of QC-models, see Corollary 6. For the proofs of the results of this section we refer to [7,8]. The Γ-limit of the functionals $H_{n}^{\ell}$ and $H_{n}^{\ell, QC, T_{n}}$ involves the convexification $J_{0}^{\ast}$ of the effective potential

$$J_{0}(z) = J_{2}(z) + \frac{1}{2} \inf \{ J_{1}(z_{1}) + J_{1}(z_{2}) : z_{1} + z_{2} = 2z \}.$$ 

In the following we always assume that the Lennard-Jones potentials $J_{1}, J_{2}$ are such that $J_{0}$ has a unique minimizer $\gamma$ and $J_{CB}(z) = J_{0}(z)$ for $0 < z \leq \gamma$, (2) which implies $J_{CB}^{\ast} \equiv J_{0}^{\ast}$.

**Theorem 2.** Let $J_{1}, J_{2}$ satisfy (2) and let $T = (T_{n})$ satisfy (1). Then the Γ-limits of $H_{n}^{\ell}$ and $H_{n}^{\ell, QC, T_{n}}$ with respect to the $L^{1}(0,1)$-topology exist. They coincide and are given on $L^{1}(0,1)$ by

$$H_{0}^{\ell}(u) = \int_{0}^{1} J_{CB}^{\ast}(u'(x)) \, dx$$

if $u \in BV(0,1)$ with $u(0) = 0, u(1) = \ell$, and infinity else.

By Jensen’s inequality we have $\min_{\nu} H_{0}^{\ell}(u) = J_{CB}^{\ast}(\ell)$. The Γ-limit of zeroth order does not contain boundary layers and gives no information about the number and location of possible cracks, which is captured by the first order Γ-limit. To this end we introduce new energies $H_{1,n}^{\ell}$ and $H_{1,n}^{\ell, QC, T_{n}}$ as follows

$$H_{1,n}^{\ell}(u) = H_{n}^{\ell}(u) - \min_{\lambda_{n}} H_{0}^{\ell}, \quad H_{1,n}^{\ell, QC, T_{n}}(u) = \frac{H_{n}^{\ell, QC, T_{n}}(u) - \min_{\lambda_{n}} H_{0}^{\ell}}{\lambda_{n}}$$

and denote their Γ-limits by $H_{1}^{\ell}$ and $H_{1}^{\ell, QC, T}$, respectively, where $T = (T_{n})$. A similar compactness result as obtained for $H_{1,n}^{\ell}$ in [7] exists for the functional $H_{1,n}^{\ell, QC, T_{n}}$. According to the prescribed deformation $\ell$ of the last atom we have two regimes: elastic deformation ($0 < \ell \leq \gamma$) or fracture ($\ell > \gamma$).

We state the Γ-limit results for both cases separately. In the elastic regime the limiting behavior of $H_{1,n}^{\ell}$ and $H_{1,n}^{\ell, QC, T_{n}}$ coincides in terms of Γ-convergence under assumptions on the choices of the atomistic region and the repatoms, see Theorem 3.

**Theorem 3.** Let $J_{1}, J_{2}$ satisfy (2) and let $T = (T_{n})$ satisfy (1). Let $0 < \ell \leq \gamma$, $u_{0}^{(1)}, u_{1}^{(1)} > 0$ and $(k_{1}^{n}), (k_{2}^{n})$ be sequences of integers such that

$$\lim_{n \to \infty} \frac{k_{1}^{n}}{\log(n)} = +\infty \text{ and } \lim_{n \to \infty} \frac{n - k_{1}^{n}}{\log(n)} = +\infty.$$ 

Moreover, let $T_{n} \subset \{0, 1, \ldots, n\}$ be such that $\{0, \ldots, k_{1}^{n}\} \cup \{k_{2}^{n}, \ldots, n\} \subset T_{n}$. Then $H_{1,n}^{\ell}$ and $H_{1,n}^{\ell, QC, T_{n}}$ Γ-converge with respect to the $L^{\infty}(0,1)$-topology to the functional $H_{1}^{\ell}$ defined by

$$H_{1}^{\ell}(u) = B\left(u_{0}^{(1)}, \ell\right) + B\left(u_{1}^{(1)}, \ell\right) - J_{CB}(\ell) - (J_{CB}^{\ast})(\ell) \left(\frac{u_{0}^{(1)} + u_{1}^{(1)}}{2} - \ell\right)$$

if $u(t) = \ell t$ for $t \in [0,1]$, and infinity else, where the boundary layer energy $B(\theta, \ell)$ is defined as
\[ B(\theta, \ell) = \inf_{N \in \mathbb{N}} \min \left\{ \frac{1}{2} J_1(\theta) + \sum_{i=0}^{k} \mathcal{J}_2 \left( \frac{v^{i+2} - v^i}{2} \right) + \frac{1}{2} \left( J_1(\ell) - J_C(\ell) \right) \right\}, \]

where \( v^i = \theta, \) if \( i \geq N \).

Theorem 3 implies that in the elastic case, i.e., \( \ell \leq \gamma \), the limiting behaviour of the original problem and of the QC approximations coincide for quite general choices of the atomistic region. If we denote by \( N_A \) the number of atoms in the atomistic region and by \( N = n + 1 \) the number of all atoms, then the limits coincide for every choice of \( p \geq 1 \) such that \( N_A^p \sim N \).

The case \( \ell > \gamma \) leads to fracture. Each crack costs a certain amount of fracture energy. In regions where second neighbour interactions are considered the crack opening leads to boundary layer energies which depend on whether the cracks occur at the boundary or in interior of the system, see [7]. A crack at the boundary leads to a boundary layer energy of the form

\[ B_b(\theta) = \inf_{k \in \mathbb{N}} \min \left\{ \frac{1}{2} J_1(\theta) + \sum_{i=0}^{k} \mathcal{J}_2 \left( \frac{v^{i+2} - v^i}{2} \right) + \frac{1}{2} \left( J_1(\theta) - J_C(\theta) \right) \right\}, \]

The boundary layer energy of a free surface reads

\[ B(\gamma) = \inf_{N \in \mathbb{N}} \min \left\{ \frac{1}{2} J_1(\gamma) + \sum_{i=0}^{k} \mathcal{J}_2 \left( \frac{v^{i+2} - v^i}{2} \right) + \frac{1}{2} \left( J_1(\gamma) - J_C(\gamma) \right) \right\}, \]

The \( \Gamma \)-limit of \( H_{1,n}^r \) is calculated in [7] and reads

**Theorem 4.** Let \( \ell > \gamma \) and \( u^{(0)}, u^{(1)} > 0 \), let \( J_1, J_2 \) are potentials of Lennard-Jones type. Then the \( \Gamma \)-limit of \( H_{1,n}^r \) with respect to the \( L^1(0,1) \)-topology is given by \( H_1^r \) on \( L^1(0,1) \), defined as

\[ H_1^r(u) = B(u^{(0)}, \gamma) \left( 1 - \#(S_u \cap \{0\}) \right) + B(u^{(1)}, \gamma) \left( 1 - \#(S_u \cap \{1\}) \right) - J_C(\gamma), \]

if \( u \in SBV \) with \( u(0-) = 0, u(1+) = \ell \), \( 0 < \#S_u < \infty \), \( \|u\| > 0 \) on \( S_u \) and \( u' = \gamma \) a.e., and infinity else, where

\[ B_{B} (\theta) = \frac{1}{2} J_1(\theta) + B(\gamma) + B_b(\theta) - 2J_0(\gamma), \]

\[ B_{IJ} = 2B(\gamma) - 2J_0(\gamma). \]

To state the corresponding result for \( H_{1,n}^{r, QC_T} \) we introduce some quantities related to the limiting behaviour of \( (T_n) \). For \( x \in (0,1) \) we define

\[ B(x, T) = \lim \inf_{n \to \infty} \{ t_n^{i+1} - t_n^i, k_n^1 < t_n^i < t_n^{i+1} < k_n^2, t_n^i, t_n^{i+1} \in T_n, \lim_{n \to \infty} \lambda_n t_n^i = x \}, \]

\[ \alpha(T) = \lim \inf_{n \to \infty} \{|q_n - k_n^1|, q_n \in T_n, q_n > k_n^1 \}, \]

\[ \beta(T) = \lim \inf_{n \to \infty} \{|q_n - k_n^2|, q_n \in T_n, q_n < k_n^2 \}. \]

Roughly speaking, \( B(x, T) \) measures the mesh density at some macroscopic point \( x \) in the continuum region and \( \alpha(T) \) and \( \beta(T) \) quantify the atomic distance between the atomistic/continuum interface and the nearest representative atom in the continuum region. Finally we define the boundary layer energy, which corresponds to fracture in the atomistic region but is close to the interface. For \( m \in \mathbb{N} \) we set
Theorem 5. We can now state the Corollary 6. where it is assumed, without loss of generality, that

\[ \text{Let } v: \mathbb{N} \to \mathbb{R}, v^0 = 0, v^{i+1} - v^i = v^{i+2} - v^{i+1} \forall k \leq i < k + m - 1. \]

Note that \( m \) corresponds to the distance between the first representative atom in the continuum region and the atomistic/continuum interface.

We can now state the \( \Gamma \)-limit result for \( H_{1,n}^{\ell,\text{QC},\mathcal{T}} \).

**Theorem 5.** Let \( \ell > \gamma \) and \( u_0^{(1)}, u_1^{(1)} > 0 \), and let \( J_1, J_2 \) satisfy (2). Let \( \mathcal{T} = (\mathcal{T}_n) \) be such that (1) holds and \((k_n^1), (k_n^2)\) be sequences with

\[ \lim_{n \to \infty} k_n^1 \lambda_n = \xi_1, \quad \lim_{n \to \infty} k_n^2 \lambda_n = \xi_2 \quad \text{such that } 0 < \xi_1 < \xi_2 < 1. \] (3)

Then \( H_{1,n}^{\ell,\text{QC},\mathcal{T}} \) \( \Gamma \)-converges with respect to the \( L^1(0,1) \)-topology to the functional \( H_1^{\ell,\text{QC},\mathcal{T}} \) defined as

\[ H_1^{\ell,\text{QC},\mathcal{T}} (u) = H_1^\ell (u) - B_{1f} (S_u \cap \{\xi_1, \xi_2\}) + B_{1f} (\alpha (\mathcal{T}), \xi_1) + B_{1f} (\beta (\mathcal{T}), \xi_2) - B(x, \mathcal{T}) \]

where \( \alpha (\mathcal{T}), \beta (\mathcal{T}) \) are functions such that

\[ \alpha (\mathcal{T}) = \xi_1, \quad \beta (\mathcal{T}) = \xi_2 \].

if \( u \in SBV(0,1) \) with \( u(0-) = 0, u(1+) = \ell, 0 < |S_u| < \infty, |u| > 0 \) on \( S_u \) and \( u' = \gamma \) a.e., and infinity else, where

\[ B_{1f} (n, z) = \min \{ B_{A1f} (n), -B(z, \mathcal{T}) J_{CB} (y), B(y) - (n + 1) J_{CB} (y) \} \]

with

\[ B_{A1f} (n) = B_{1f} (n - 1) + B(\gamma) - 2J_{CB} (y) \] for \( n \in \mathbb{N} \) and \( B_{A1f} (+\infty) = B_{1f} \).

The assumptions (3) on \( k_n^1, k_n^2 \) imply that the atomistic region is of the same order as the continuum region, which is not the case in applications. We mention that in many cases this assumption can be relaxed to the same assumption as in Theorem 4, see [8]. Theorem 5 implies that the \( \Gamma \)-limits \( H_1^\ell \) and \( H_1^{\ell,\text{QC},\mathcal{T}} \) do not coincide except in the trivial case when the continuum region vanishes, i.e., \( \xi_1 = \xi_2 \). However we also obtain some insight into the quality of the QC approximation if \( \xi_1 \neq \xi_2 \). To this end we study the minimal values and minimizers of the limit functional and compare the behaviour for different choices of \( \mathcal{T}_n \) and a special choice of the boundary conditions.

**Corollary 6.** Let \( J_1, J_2 \) satisfy (2). Let \( \ell > \gamma \), \( u_0^{(1)} = \delta_1 := \arg \min J_1 (z) \) and \( u_1^{(1)} = \gamma \).

Moreover, define \( \mathcal{T}_n^1 = (\mathcal{T}_n^1) \) and \( \mathcal{T}_n^2 = (\mathcal{T}_n^2) \) as

\[ \mathcal{T}_n^1 = \{0, \ldots, n\} \text{ and } \mathcal{T}_n^2 = \{0, \ldots, k_n^1, k_n^1 + m, k_n^1 + 2m, \ldots, k_n^2 - m, k_n^2, \ldots, n\}, m \geq 2, \]

where it is assumed, without loss of generality, that \( m \) divides \((k_n^2 - k_n^1)\) for all \( n \). Then

(1) min \( H_1^\ell = B_{1f} (\delta_1) + B(\gamma, \gamma) \) and the jump appears in 0,

(2) min \( H_1^{\ell,\text{QC},\mathcal{T}_n^1} = B(\delta_1, \gamma) + B(\gamma, \gamma) - J_{CB} (y) \) and the jump appears indifferently in \( [\xi_1, \xi_2] \),

(3) min \( H_1^{\ell,\text{QC},\mathcal{T}_n^2} = \min H_1^\ell \) and the jump appears in 0.

Let \( \mathcal{T} = (\mathcal{T}_n) \) satisfy (1), such that \( \{0, \ldots, n\} \cup \{k_n^1, \ldots, n\} \subset \mathcal{T}_n \) and such that there exists a sequence \( (Q_n) \) with \( \lim_{n \to \infty} Q_n = +\infty \) such that \( Q_n \leq |t_n^{i+1} - t_n| \). \( \forall t_n^{i+1}, t_n^i \in \mathcal{T}_n, k_n^1 < t_n^i < t_n^{i+1} < k_n^2. \) Then

\[ H_1^{\ell,\text{QC},\mathcal{T}} (u) = \begin{cases} H_1^\ell (u) & \text{if } S_u \cap (\xi_1, \xi_2) = \emptyset, \\ +\infty & \text{else}. \end{cases} \]
An example of a $\mathcal{T} = (\mathcal{T}_n)$ having the properties of the last statement of Corollary 6 is
$$\mathcal{T}_n = \{0, \ldots, k_n^1, k_n^2 + \sqrt{n}, k_n^2, \ldots, \sqrt{n}, k_n^2, \ldots, n\},$$
where we assume that $\sqrt{n}$ divides $(k_n^2 - k_n^1)$ for all $n$. This choice implies that the finite element mesh size and the atomistic lattice spacing shrink to zero in different orders.

**CONCLUSIONS**

In this article we compare the limiting behaviour of a one-dimensional atomistic model problem that allows for the occurrence of cracks and its quasi-nonlocal quasi-continuum approximation as the number of particles tends to infinity. Depending on the boundary conditions, the limiting process, which is based on $\Gamma$-convergence techniques, leads to two different cases either elastic behaviour or fracture. In the elastic case the original and the approximated energy have the same $\Gamma$-limit under some general assumptions on the interaction potentials and the representative atoms.

In the case of fracture it turns out that choosing the representative atoms such that one has a coarse mesh in the continuum region is crucial. Corollary 6 yields that a very coarse grid at the interface and in the continuum region lead to the right limiting behaviour in the sense that a crack is energetically more favourable to take place in the atomistic region than in the continuum one, as desired. Moreover, the energy needed to create a crack is the same for this QC model as for the fully atomistic model. On the other hand, if one considers a QC approximation without choosing a coarser mesh, Corollary 6 shows that this can lead to a completely different limiting behaviour. Hence the $\Gamma$-convergence techniques applied yield some analytical insight into appropriate quasi-continuum modelling. We will investigate this further in future work [8]. Moreover, we will include general defects and external forces into the model.

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