

STRESS-BASED ATOMISTIC/CONTINUUM COUPLING: A NEW VARIANT OF THE QUASICONTINUUM APPROXIMATION

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ABSTRACT. The force-based quasicontinuum (QCF) approximation is the principle that lies behind the most commonly used atomistic/continuum hybrid models for crystalline solids. Recent analyses have shown some potential pitfalls of the QCF method, particularly the lack of positive definiteness of the linearized QCF operator and the lack of uniform stability as the number of atoms tends to infinity. We derive a weak variational representation of the QCF operator and identify the origin of these difficulties as the lack of an interface condition on the stresses. This leads us to propose an improved variant of the QCF method that can be understood as a coupling mechanism based on stresses rather than forces.

1. INTRODUCTION

Atomistic/continuum (A/C) coupling methods, such as the quasicontinuum (QC) method [12, 13, 16], are important tools in modern materials simulations since they enable, in principle, the accurate description of phenomena that are accessible neither to pure atomistic nor pure continuum models. However, difficult open problems remain for the formulation of accurate and reliable energy-based coupling mechanism [8, 17].

The force-based quasicontinuum (QCF) approximation [10, 16, 2, 6] is the only known atomistic/continuum (A/C) coupling scheme for general interaction potentials and general A/C interface geometries, that does not exhibit spurious ghost forces at the interface. Moreover, it is the underlying principle behind the most commonly used quasicontinuum software (www.qcmethod.com).

Over the past year, considerable progress has been made on the analysis of the QCF method [2, 6, 5, 4, 11]. These references have shown several interesting and unexpected analytical structures. In particular, if the QCF operator is written in a weak variational form, then certain interface terms appear that are the cause of some undesirable (in-)stability properties of the method. For example, it can be shown that the linearized QCF operator is almost never positive definite [6, Thm. 1], which has, for example, severe consequences for the solution of the nonlinear QCF system [4].

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In this article, we first present a formulation of the QCF method for a 1D periodic chain with second-neighbour pair interactions and coarse-graining by a P1-finite element scheme (Section 2). We then derive the weak form of the QCF equations, where we will provide a physical interpretation of the interface terms in terms of an atomistic stress function (Section 3.1). Next, we review the aforementioned instability results and extend the result showing lack of positive definiteness to the coarse-grained case (Section 3.2). Guided by these motivations we then define, in Section 4, a new force-based A/C method that is based on coupling stresses as opposed to forces. We will review some error estimates for this method that we have derived in [11], and prove that the linearization of the new method is typically positive definite. We show that this leads to optimal error estimates in discrete $W^{1,p}$ -norms that do not hold for the classical QCF method.

2. THE FORCE-BASED QUASICONTINUUM METHOD

2.1. Notation for discrete functions. Our models will be formulated for infinite chains, hence we introduce some notation for functions defined on \mathbb{Z} , which we will denote $v = (v_\xi)_{\xi \in \mathbb{Z}} \in \mathbb{R}^{\mathbb{Z}}$. The space of $2N$ -periodic functions is denoted by $\mathbb{R}_\#^{\mathbb{Z}}$. We will normally work on a particular period, which we denote

$$\mathcal{L} = \{-N+1, \dots, N\}.$$

Throughout, we define $\varepsilon = 1/N$. This will later be the atomistic spacing in non-dimensional variables.

For any set $\mathcal{K} \subset \mathbb{R}^{\mathbb{Z}}$, for any $p \in [1, \infty)$, and for any function $v \in \mathbb{R}^{\mathbb{Z}}$, we define the norms

$$\|v\|_{\ell_\varepsilon^p(\mathcal{K})} = \left(\varepsilon \sum_{\xi \in \mathcal{K}} |v_\xi|^p \right)^{1/p}, \quad \text{and} \quad \|v\|_{\ell_\varepsilon^\infty(\mathcal{K})} = \|v\|_{\ell^\infty(\mathcal{K})} = \max_{\xi \in \mathcal{K}} |v_\xi|.$$

If the set (\mathcal{K}) is omitted from the above notation, then it is assumed that $\mathcal{K} = \mathcal{L}$. For $p = 2$ and $\mathcal{K} = \mathcal{L}$ the associated inner product is

$$(v, w)_\varepsilon = \varepsilon \sum_{\xi \in \mathcal{L}} v_\xi w_\xi \quad \text{for } v, w \in \mathbb{R}^{\mathbb{Z}}.$$

Using the notation $1 = (1)_{\xi \in \mathbb{Z}}$, the set of periodic functions with mean zero is denoted by

$$\mathcal{U} = \{v \in \mathbb{R}_\#^{\mathbb{Z}} : (v, 1)_\varepsilon = 1\}. \quad (1)$$

For $v \in \mathbb{R}^{\mathbb{Z}}$ we define $v' = (v'_\xi)_{\xi \in \mathbb{Z}}$, $v'' = (v''_\xi)_{\xi \in \mathbb{Z}}$, and $v''' = (v'''_\xi)_{\xi \in \mathbb{Z}}$ as follows:

$$v'_\xi = \frac{v_\xi - v_{\xi-1}}{\varepsilon}, \quad v''_\xi = \frac{v_{\xi+1} - 2v_\xi + v_{\xi-1}}{\varepsilon^2}, \quad \text{and} \quad v'''_\xi = \frac{v_{\xi+1} - 3v_\xi + 3v_{\xi-1} - v_{\xi-2}}{\varepsilon^3}.$$

2.2. Atomistic model problem. We wish to present our ideas in the simplest possible setting. To that end we focus on a one-dimensional periodic chain, thus ignoring difficult questions associated with boundaries, defects, or complicated lattice geometries in 2D/3D. We define the set of admissible deformations as

$$\mathcal{Y} = \mathbf{B}x + \mathcal{U} = \{\mathbf{B}x + u : u \in \mathcal{U}\}, \quad (2)$$

where \mathcal{U} is the *displacement space* defined in (1). We note that $2N$ denotes the number of atoms per period, and $\varepsilon = 1/N$ is the atomic spacing in non-dimensional coordinates. We define a reference lattice

$$x = (x_\xi)_{\xi \in \mathbb{Z}} = (\varepsilon \xi)_{\xi \in \mathbb{Z}}.$$

The constant $B > 0$ can be thought of as a macroscopic strain. Thus, the admissible deformations are the periodic displacements with zero mean from the homogeneous lattice Bx . For future reference, we also define

$$\mathcal{Y}^+ = \{y \in \mathcal{Y} : y'_\xi > 0 \text{ for all } \xi \in \mathbb{Z}\}.$$

For simplicity, we assume that each atom interacts only with its next and next-nearest neighbours through a pair potential $\phi \in C^3(0, +\infty)$, such as a Lennard–Jones or Morse potential. The *internal stored energy* of a deformation $y \in \mathcal{Y}$ is then given by

$$\Phi^a(y) = \varepsilon \sum_{\xi \in \mathcal{L}} \phi(y'_\xi) + \varepsilon \sum_{\xi \in \mathcal{L}} \phi(y'_\xi + y'_{\xi+1}).$$

Assuming that all external forces are dead loads, collected into a function $g \in \mathcal{U}$, the *total energy* of a deformation y is given by

$$\Phi_{\text{tot}}^a(y) = \Phi^a(y) - (g, y)_\varepsilon.$$

The problem we wish to solve is to find a local minimizer of Φ_{tot}^a in \mathcal{Y} :

$$\text{Find } y^a \in \operatorname{argmin} \Phi_{\text{tot}}^a(\mathcal{Y}). \quad (3)$$

2.3. The local QC approximation. It can be shown (see, e.g., [1, 6, 9, 14]) that in regions of the domain \mathcal{L} where the atomistic deformation is smooth (by which we mean that y'_ξ varies slowly) one can replace the atomistic model by the Cauchy–Born approximation

$$\Phi^c(y) = \int_{-1}^1 W(y') \, dx,$$

where $W(t) = \phi(t) + \phi(2t)$ is the Cauchy–Born stored energy function. The P1-finite element discretization of Φ^c is sometimes also called the so-called *local quasicontinuum (QCL) approximation*. (The QCL method is derived, in reverse order, by first coarse-graining the atomistic model and then applying the Cauchy–Born rule in each finite element. [12, 13])

To formulate this, we partition the domain by choosing a finite number of *repatoms*

$$\mathcal{L}_{\text{rep}} = \{\xi_1, \dots, \xi_M\} \subset \mathcal{L},$$

where $M \ll N$ and $\xi_1 < \xi_2 < \dots < \xi_M$. The grid is extended periodically, that is, we define $\xi_{m+M} = \xi_m + 2N$ for all $m \in \mathbb{Z}$. The position of the repatoms are $X_m = x_{\xi_m} = \varepsilon \xi_m$. The mesh size functions for elements and for nodes are

$$h_m = X_m - X_{m-1} \quad \text{and} \quad H_m = \frac{1}{2}(X_{m+1} - X_{m-1}), \quad \text{for } m \in \mathbb{Z}.$$

Moreover, we define the mesh-dependent inner product

$$(v, w)_h = \sum_{m=1}^M H_m v_{\xi_m} w_{\xi_m} \quad \text{for } v, w \in \mathbb{R}^{\mathbb{Z}}.$$

We denote by \mathcal{S}_h^1 the space of *piecewise linear functions* with respect to the grid $(X_m)_{m \in \mathbb{Z}}$. If $v_h \in \mathcal{S}_h^1$ then we denote its nodal values by $V_m = v_h(X_m) = v_{h,\xi_m}$, and its gradient in the interval (X_{m-1}, X_m) by $V'_m = (V_m - V_{m-1})/h_m$, that is,

$$v_{h,\xi} = V_{m-1} + V'_m(x_\xi - X_{m-1}) \quad \text{for } \xi = \xi_{m-1}, \dots, \xi_m.$$

Finally, we define the finite element deformation and displacement spaces associated with \mathcal{Y} and \mathcal{U} , respectively, as

$$\mathcal{U}_h = \{u_h \in \mathcal{S}_h^1 \cap \mathbb{R}_{\#}^{\mathbb{Z}} : (u_h, 1)_h = 0\} \quad \text{and} \quad \mathcal{Y}_h = \mathbf{B}x + \mathcal{U}_h.$$

For future reference, we also define $\mathcal{Y}_h^+ = \{y_h \in \mathcal{Y}_h : y'_{h,\xi} > 0 \text{ for all } \xi \in \mathbb{Z}\}$.

The total energy functional for the QCL method is given by

$$\Phi_{\text{tot}}^c(y) = \Phi^c(y) - (g, y)_h \quad \text{for } y \in \mathcal{Y},$$

where we have approximated the inner product $(\cdot, \cdot)_\varepsilon$ by $(\cdot, \cdot)_h$, which can be computed with complexity $O(K)$. If $y_h \in \mathcal{Y}_h$ (with vector of nodal values Y) then the functional can be written as

$$\Phi_{\text{tot}}^c(y_h) = \sum_{m=1}^M h_m W(Y'_m) - \sum_{m=1}^M H_m g_{\xi_m} Y_m. \quad (4)$$

In the QCL method, we aim to find a local minimizer of Φ_{tot}^c in \mathcal{Y}_h , that is:

$$\text{Find } y_h^c \in \arg\min \Phi_{\text{tot}}^c(\mathcal{Y}_h). \quad (5)$$

2.4. The force-based QC approximation. If y^a is a solution of (3) then it satisfies the first-order criticality condition

$$(f^a(y) + g, v)_\varepsilon = 0 \quad \forall v \in \mathcal{U}, \quad (6)$$

where the (scaled) force vector $f^a = (f_\xi^a)_{\xi \in \mathbb{Z}}$ is defined as

$$f_\xi^a(y) := -\frac{1}{\varepsilon} \frac{\partial \Phi^a(y)}{\partial y_\xi}, \quad \text{for } \xi \in \mathbb{Z}.$$

Similarly, if $y_h^c \in \mathcal{Y}_h$ is a solution of (5) then it satisfies

$$(F^c(y_h^c) + g, v_h)_h = 0 \quad \forall v_h \in \mathcal{U}_h, \quad (7)$$

where the generalized forces $F^c = (F_m^c)_{m \in \mathbb{Z}}$ are given by

$$F_m^c(y_h) = -\frac{1}{H_m} \frac{\partial \Phi^c(y_h)}{\partial Y_m} \quad \text{for } m \in \mathbb{Z}.$$

We remark that we could equally formulate (6) and (7) pointwise (e.g., $f_\xi^a(y) + g_\xi = 0$ for $\xi \in \mathbb{Z}$), however, it was shown in [6, 11] that this is problematic for the QCF method, which we define next.

To construct the QCF method, we partition the set of repatoms $\mathcal{L}_{\text{rep}} = \mathcal{L}_a \cup \mathcal{L}_c$ into the degrees of freedom for which we require atomistic accuracy, \mathcal{L}_a , and those for which the accuracy of the continuum model is sufficient, \mathcal{L}_c . For simplicity, we assume throughout that, for some constant $\kappa \in \mathbb{N}$,

$$\mathcal{L}_a = \{-\kappa, \dots, \kappa\}, \quad \text{and that} \quad \{-\kappa - 2, \dots, \kappa + 2\} \subset \mathcal{L}_{\text{rep}}. \quad (8)$$

The first condition is only to simplify the notation and is needed neither for the formulation nor the analysis of the two A/C methods that we discuss in this paper. The second condition is not strictly necessary either but does considerably simplify both the analysis and the implementation of the QCF method and stress-based method that we define in Section 4.

Upon defining the QCF force vector

$$F^{\text{qc}}(y) = (F_m^{\text{qc}}(y))_{m \in \mathbb{Z}} \quad \text{where} \quad F_m^{\text{qc}}(y) = \begin{cases} f_{\xi_m}^{\text{a}}(y), & \text{if } \xi_m \in \mathcal{L}_{\text{a}}, \\ F_m^{\text{c}}(y), & \text{if } \xi_m \in \mathcal{L}_{\text{c}}, \end{cases}$$

extended periodically for $m \in \mathbb{Z}$, the QCF method is defined by the following non-linear variational problem:

$$\text{Find } y_h^{\text{qc}} \in \mathcal{Y}_h \text{ s.t.} \quad (F^{\text{qc}}(y_h^{\text{qc}}) + g, v_h)_h = 0 \quad \forall v_h \in \mathcal{U}_h. \quad (9)$$

3. ANALYSIS OF THE QCF METHOD

In this section we summarize a number of recent results from [5, 6, 11]. We begin by deriving the weak variational forms of (6), (7) and (9), which are crucial to the analysis of the QCF method.

3.1. Stress functions and weak variational forms. A straightforward and standard calculation, starting from (4), gives the following representation of the first variation of Φ^{c} , which is the most convenient form for finite element analysis:

$$-(F^{\text{c}}(y_h), v_h)_h = \sum_{m=1}^M h_m \Sigma_m^{\text{c}}(y_h) V_m' \quad \text{for all } v_h \in \mathcal{U}_h, \quad (10)$$

where $\Sigma_m^{\text{c}}(y_h) = DW(Y_m')$. We note, moreover, that

$$F_m^{\text{c}}(y_h) = H_m^{-1} [\Sigma_{m+1}^{\text{c}}(y_h) - \Sigma_m^{\text{c}}(y_h)]. \quad (11)$$

While continuum models are usually formulated in terms of stresses as in (10), atomistic models are almost exclusively formulated in terms of forces as in (6). However, it was seen in [5, 6, 11, 14, 15] that, in order to understand the consistency and stability of coupling mechanisms, it is crucial to understand the weak forms of the atomistic and quasicontinuum models. Hence, in [11], we derive a stress function for the atomistic model:

Proposition 1. *Let $y \in \mathcal{Y}^+$ then*

$$-(f^{\text{a}}(y), v)_{\varepsilon} = \varepsilon \sum_{\xi \in \mathcal{L}} \Sigma_{\xi}^{\text{a}}(y) v_{\xi}' \quad \text{for all } v \in \mathcal{U}, \quad (12)$$

where the atomistic stress function $\Sigma_{\xi}^{\text{a}}(y)$ is given by

$$\Sigma_{\xi}^{\text{a}}(y) = \phi'(y_{\xi}') + \phi(y_{\xi-1}' + y_{\xi}') + \phi(y_{\xi}' + y_{\xi+1}'). \quad (13)$$

Moreover, the atomistic forces and stresses are related by the formula

$$f_{\xi}^{\text{a}}(y) = \varepsilon^{-1} [\Sigma_{\xi+1}^{\text{a}}(y) - \Sigma_{\xi}^{\text{a}}(y)]. \quad (14)$$

Proof. The first result follows immediately upon noticing that

$$\Sigma_\xi^a(y) = \frac{1}{\varepsilon} \frac{\partial \Phi^a(y)}{\partial y'_\xi}.$$

The formula (14) can be verified by a direct computation. \square

Before we state the weak variational form of the QCF method, we need some additional notation. We denote the indices of the degrees of freedom corresponding to the interface atoms $-\kappa, \kappa$ by $\underline{K}, \overline{K} \in \{1, \dots, M\}$, that is,

$$\xi_{\overline{K}} = \kappa, \quad \text{and} \quad \xi_{\underline{K}} = -\kappa.$$

The set of indices of finite elements (X_{m-1}, X_m) that belong, respectively, to the atomistic and continuum regions are defined as $\mathcal{M}_a = \{\underline{K}, \dots, \overline{K} + 1\}$ and $\mathcal{M}_c = \{1, \dots, M\} \setminus \mathcal{M}_a$. We think of the interface elements $(X_{\underline{K}-1}, X_{\underline{K}})$ and $(X_{\overline{K}}, X_{\overline{K}+1})$ as belonging to the atomistic region. To simplify the notation, we will also use the convention $\Sigma_m^a(y_h) = \Sigma_{\xi_m}^a(y_h)$ for $y_h \in \mathcal{Y}_h^+$ and for $m \in \mathcal{M}_a$.

With this notation, we can insert (11) and (14) into (15) and perform summation by parts separately in the atomistic and continuum regions, and collect the boundary terms in a convenient way, to arrive at the following result [11, Sec. 4.1].

Proposition 2. *Let $y_h \in \mathcal{Y}_h^+$ and $\Sigma_m^{a/c} = \Sigma_m^{a/c}(y_h)$; then, for all $v_h \in \mathcal{U}_h$,*

$$\begin{aligned} -(F^{\text{qc}}(y_h), v_h)_h = & \sum_{m \in \mathcal{M}_a} \varepsilon V'_m \Sigma_m^a + \sum_{m \in \mathcal{M}_c} h_m V'_m \Sigma_m^c \\ & - V_{\underline{K}-1}(\Sigma_{\underline{K}}^c - \Sigma_{\underline{K}}^a) + V_{\overline{K}+1}(\Sigma_{\overline{K}+1}^c - \Sigma_{\overline{K}+1}^a). \end{aligned} \quad (15)$$

We see from Proposition 2 that the QCF method does not satisfy the common principle in continuum multiphysics modelling of equality of the normal components of the stresses at an interface. Indeed, weakly imposing this condition is equivalent to dropping the interface terms in the second line of (15). We will explain next that these interface terms are the origin of a number of undesirable properties of the QCF method.

3.2. Consequences of the interface terms. In this section we cite two unexpected results from [5, 6] concerning the stability of the QCF method.

3.2.1. Lack of positive definiteness. The simplest, and possibly most important notion of stability for energy minimization problems is positive definiteness of the Hessian matrix. For example, if y^a is a local minimizer then $D^2\Phi^a(y^a) \geq 0$, and usually one even has strict positive definiteness. The same is true for the local QC energy. However, for the QCF method, we have the following result.

Proposition 3. *Suppose that \mathbf{B} is chosen so that $\phi''(2\mathbf{B}) \neq 0$; then there exist positive constants C_1, C_2 such that, for N sufficiently large and for $2 \leq \kappa \leq N/2$,*

$$-C_1 N^{1/2} \leq \inf_{\substack{u_h \in \mathcal{U}_h \\ \|u_h\|_{\ell_\varepsilon^2} = 1}} (-DF^{\text{qc}}(\mathbf{B}x)u_h, u_h)_h \leq -C_2 N^{1/2}.$$

Proof. Without coarse-graining, i.e., with $\mathcal{U}_h = \mathcal{U}$, this result is given in [5, Thm. 4.1]. The main idea of the proof presented there was to find a test function that is constant in the atomistic region, piecewise affine in the continuum region, and has oscillations of order $\varepsilon^{1/2}$ in the interface region. These oscillations ensure that the interface terms dominate.

For the present case it is sufficient to note that the test function constructed in the proof of [5, Thm. 4.1] is affine in the continuum region and thus, after shifting it by a constant value, belongs to \mathcal{U}_h for any choice of finite element grid. \square

This result has a number of undesirable consequences:

1. Positive definiteness of the linearization is the simplest way to establish stability of a numerical scheme and its absence makes the analysis of the QCF method in higher dimensions a formidable challenge.
2. It is shown in [4] that the lack of positive definiteness implies that certain commonly used nonlinear iterative solvers for the QCF method are unstable.
3. If we could have shown that DF^{qc} is positive definite if and only if $D^2\Phi^a$ is positive definite up to a controllable error (such a result holds, e.g., for the quasinonlocal coupling scheme [3, 14]), then we could use this property to decide whether a given computed QCF solution corresponds to a minimum, maximum or saddle point. In view of Proposition 3, we do not have this possibility. Alternative notions of stability were suggested in [5] but require further investigation.

3.2.2. Instability in various Sobolev spaces. In the absence of positive definiteness, one needs to prove invertibility and boundedness of the inverse of the linearized operator directly. It turns out, however, that for most natural choices of (discrete) function spaces no uniform bounds on the inverse operator hold. For the case $\mathcal{U} = \mathcal{U}_h$, i.e., $\mathcal{L}_{\text{rep}} = \{-N + 1, \dots, N\}$, it was shown in [5, Thm. 4.3] that, if $DF^{\text{qc}}(\mathbf{B}x)$ is invertible and if $\phi''(2\mathbf{B}) \neq 0$, then

$$\|DF^{\text{qc}}(\mathbf{B}x)^{-1}\|_{L(\mathcal{U}^{-1,p}, \mathcal{U}^{1,p})} \gtrsim N^{1/p},$$

where $\mathcal{U}^{\pm 1,p}$ are discrete variants of the Sobolev spaces $W_{\#}^{\pm 1,p}(-1, 1)$ of periodic functions. In the same way as Proposition 3, this result is again established by constructing test functions for which the interface terms dominate.

Since it is quite tedious to generalize this result to arbitrary discretizations we will not give a rigorous statement of this kind for the coarse-grained case. However, it seems that the proof carries over with only minor modifications, and hence we strongly expect that a similar (negative) result will remain true.

We note that it is in fact possible to prove sharp stability results in higher order discrete Sobolev spaces $\mathcal{U}^{2,p}$, $p \in [2, \infty]$ (see [5] for the case $p = \infty$ and [7] for the general case). However, experience from regularity theory for elliptic PDE, and numerical experiments [7] clearly show that these stability results hold only at smooth deformations but fail in the presence of defects, or even if the deformation at which F^{qc} is linearized is not globally smooth. Hence, these results are only of limited value for the analysis of the QCF method.

3.2.3. Stability in the space of Lipschitz functions and error estimates. The space of Lipschitz functions is the only suitable function space identified so far that allows a rigorous error analysis of the QCF method under reasonably general conditions. In [11] we establish stability and consistency estimates in $\mathcal{U}^{1,\infty}$, which allow a rigorous error analysis that is valid for large and non-smooth deformations. However, it is again due to the interface terms that our stability estimates do not hold up to bifurcation points.

4. STRESS-BASED A/C COUPLING

If we take the point of view, as is usually done in finite element analysis, that the weak variational forms (10) and (12) are the most natural representations of the atomistic and continuum models then it is reasonable to consider a *stress-based* atomistic/continuum (SAC) coupling mechanism. We define the SAC operator $S^{\text{qc}} : \mathcal{Y}_h \rightarrow \mathcal{U}_h^*$, in variational form, via

$$(S^{\text{qc}}(y_h), v_h)_h = \sum_{m \in \mathcal{M}_a} \varepsilon V'_m \Sigma_m^a(y_h) + \sum_{m \in \mathcal{M}_c} h_m V'_m \Sigma_m^c(y_h), \quad (16)$$

where we recall that $\Sigma_m^a = \Sigma_{\xi_m}^a$ is defined in (13), and $\Sigma_m^c(y_h) = DW(Y'_m)$ is defined in (10). The resulting nonlinear system is

$$\text{Find } y_h \in \mathcal{Y}_h \text{ s.t. } (S^{\text{qc}}(y_h), v_h)_h = (g, v_h)_h \quad \forall v_h \in \mathcal{U}_h. \quad (17)$$

We can immediately make the following interesting observation: The variational form of the SAC operator is identical to the weak variational form of the QCF operator (15) after dropping the interface terms

$$-V_{\underline{K}-1}(\Sigma_{\underline{K}}^c - \Sigma_{\underline{K}}^a) + V_{\overline{K}+1}(\Sigma_{\overline{K}+1}^c - \Sigma_{\overline{K}+1}^a).$$

Hence, we see that this new method can also be understood as as a force-based QC method, in which equality of the normal components of the stresses at the atomistic/continuum interface is imposed weakly.

Since the SAC method does not have the problematic interface terms, we expect that it will have superior stability properties compared to the QCF method. In the remainder of the section, we first summarize the error estimates proven for the SAC method in [11]. We will then prove that the linearized SAC operator is positive definite, however, not necessarily up to bifurcation points. Finally, we will show that the linearized QCS operator is stable in a range of discrete Sobolev spaces up to a simple bifurcation point, uniformly in N and κ .

4.1. A priori error estimates. Before we can embark on the analysis of the SAC method, we need to briefly define a modified nodal interpolant. The problem is that the standard nodal interpolant does not map \mathcal{U} to \mathcal{U}_h . Hence, in [11, Sec. 2.6.1] we define an interpolant $I_h : \mathcal{U} \rightarrow \mathcal{U}_h$ via

$$(I_h u)_{\xi_m} = u_{\xi_m} + C \text{ for all } m = 1, \dots, M, \quad \text{with } C \text{ s.t. } (I_h u, 1)_h = 0.$$

With slight abuse of notation, we also define the nodal interpolation operator on \mathcal{Y} , as

$$I_h(Bx + u) = Bx + I_h u. \quad (18)$$

From [15, Thm. A.4, Eq. (74)], we obtain the following interpolation error estimate:

$$\|I_h y' - y'\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m\})} \leq \frac{1}{2} h_m \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})}. \quad (19)$$

As the first crucial step for the error analysis we establishing an inf-sup stability result. The following result shows that if $y_h \in \mathcal{Y}_h^+$ and $\gamma_s(y_h) > 0$ then the operator $DS^{\text{qc}}(y_h)$ is invertible with an explicit bound on the inverse.

Lemma 4 (Stability). *Let $y_h \in \mathcal{Y}_h^+$; then*

$$\inf_{\substack{u_h \in \mathcal{U}_h \\ \|u'_h\|_{\ell^\infty} = 1}} \sup_{\substack{v_h \in \mathcal{U}_h \\ \|v_h\|_{\ell^1} = 1}} (DS^{\text{qc}}(y_h)u_h, v_h)_h \geq \gamma_s(y_h), \quad \text{where}$$

$$\gamma_s(y_h) = \frac{1}{2} \min \left\{ \min_{m \in \mathcal{M}_c} D^2 W(Y'_m), \right.$$

$$\left. \min_{m \in \mathcal{M}_a} \left(\phi''(y'_{h,\xi}) - 2|\phi''(y'_{h,\xi_m} + y'_{h,\xi_{m+1}})| - 2|\phi''(y'_{h,\xi_{m-1}} + y'_{h,\xi_m})| \right) \right\}.$$

Proof. It is easy to see that S^{qc} is differentiable in \mathcal{Y}_h^+ . Defining $(\mathcal{J}_{m,n})_{m,n=1}^M$ as

$$\mathcal{J}_{m,m} = D^2 W(Y'_m) \quad \text{for } m \in \mathcal{M}_c,$$

and

$$\mathcal{J}_{m,n} = \phi''(y'_{h,\xi}) + \begin{cases} \phi''(y'_{h,\xi_m} + y'_{h,\xi_{m-1}}), & m \in \mathcal{M}_a, n = m-1, \\ \phi''(y'_{h,\xi_m} + y'_{h,\xi_{m-1}}) + \phi''(y'_{h,\xi_m} + y'_{h,\xi_{m+1}}), & m \in \mathcal{M}_a, n = m, \\ \phi''(y'_{h,\xi_m} + y'_{h,\xi_{m+1}}), & m \in \mathcal{M}_a, n = m+1, \end{cases}$$

and $\mathcal{J}_{m,n} = 0$ otherwise, we obtain

$$(DS^{\text{qc}}(y_h)u_h, v_h)_h = \sum_{m,n=1}^M h_m \mathcal{J}_{mn} V'_m U'_n.$$

The result follows by applying the abstract inf-sup estimate [11, Lemma 7]. \square

The main strength of this stability estimate is that it is valid up to bifurcation points. For example, if we consider the purely homogeneous deformation $y = \mathbf{B}x$ (if $g = 0$), then it is shown in [3], under the assumptions $\phi''(\mathbf{B}) > 0$ and $\phi''(2\mathbf{B}) \leq 0$, that this is a stable equilibrium of the atomistic model if and only if

$$\phi''(\mathbf{B}) + 4\phi''(2\mathbf{B}) + O(\varepsilon^2) > 0.$$

Under the same conditions, Lemma 4 shows that

$$\gamma_s(\mathbf{B}x) > 0 \quad \text{iff.} \quad \phi''(\mathbf{B}) + 4\phi''(2\mathbf{B}) > 0,$$

that is, the SAC method is stable to within an $O(\varepsilon^2)$ error of the critical strain \mathbf{B} at which the homogeneous deformation $y = \mathbf{B}x$ becomes unstable.

The second fundamental ingredient is a consistency error estimate.

Lemma 5 (Consistency). *Let $y \in \mathcal{Y}^+$ then*

$$\sup_{\substack{u_h \in \mathcal{U}_h \\ \|u_h\|_{\ell_\varepsilon^1} = 1}} \left| (S^{\text{qc}}(I_h y), u_h)_h + (f^{\text{a}}(y), u_h)_\varepsilon \right| \leq \mathcal{E}_{\text{approx}}^{\text{s}}(y) + \mathcal{E}_{\text{model}}^{\text{s}}(y),$$

where the approximation error $\mathcal{E}_{\text{approx}}$ and model error $\mathcal{E}_{\text{model}}$ are, respectively,

$$\mathcal{E}_{\text{approx}} = C_1 \max_{m \in \mathcal{M}_c} h_m^2 \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})}^2, \quad \text{and} \quad (20)$$

$$\mathcal{E}_{\text{model}} = C_2 \varepsilon^2 \left\{ \|y''\|_{\ell^\infty(\mathcal{L}_c)}^2 + \|y'''\|_{\ell^\infty(\mathcal{L}_c^{\text{b}})} \right\}, \quad (21)$$

and where the constants C_1, C_2 depend on $\min_{\xi \in \mathcal{L}_c^{\text{b}}} y'_\xi$ and on the interaction potential, and $\mathcal{L}_c^{\text{b}} = \{-N+1, \dots, N\} \setminus \{-\kappa, \dots, \kappa+1\}$ is modification of the set \mathcal{L}_c that takes into account bonds as opposed to atoms.

Proof. The proof of this lemma is contained in [11, Sec. 3,5], however, for the purpose of illustration we give a brief sketch.

We begin by writing out $(S^{\text{qc}}(I_h y), u_h)_h + (f^{\text{a}}(y), u_h)_\varepsilon$, using the weak form (12):

$$\begin{aligned} (S^{\text{qc}}(I_h y), u_h)_h + (f^{\text{a}}(y), u_h)_\varepsilon &= \sum_{m \in \mathcal{M}_a} h_m \Sigma_m^{\text{a}}(I_h y) U'_m + \sum_{m \in \mathcal{M}_c} h_m \Sigma_m^{\text{c}}(I_h y) U'_m \\ &\quad - \sum_{\xi \in \mathcal{L}} \varepsilon \Sigma_\xi^{\text{a}}(y) u'_{h,\xi}. \end{aligned}$$

Since $I_h y$ and y differ only by a constant in the atomistic region the contributions in the atomistic region from the SAC and the atomistic models are the same, so that we are left with

$$\begin{aligned} (S^{\text{qc}}(I_h y), u_h)_h + (f^{\text{a}}(y), u_h)_\varepsilon &= \sum_{\xi \in \mathcal{L}_c^{\text{b}}} \varepsilon (DW((I_h y)'_\xi) - \Sigma_\xi^{\text{a}}(y)) u'_{h,\xi} \\ &= \sum_{\xi \in \mathcal{L}_c^{\text{b}}} \varepsilon (DW((I_h y)'_\xi) - DW(y'_\xi)) u'_{h,\xi} + \sum_{\xi \in \mathcal{L}_c^{\text{b}}} \varepsilon (DW(y'_\xi) - \Sigma_\xi^{\text{a}}(y)) u'_{h,\xi}. \end{aligned}$$

Estimating the first group in the above representation is a classical superconvergence estimate (see [11, Sec. 4,5] for the full details), using the interpolation error estimate (19), and leads directly to the $\mathcal{E}_{\text{approx}}$ term.

To estimate the second group we use a consistency error estimate between the atomistic and continuum stresses (see [11, Sec. 3] for a more general result),

$$|\Sigma_\xi^{\text{a}}(y) - DW(y'_\xi)| \leq C_3 \varepsilon^2 \left\{ |y'''_\xi| + \frac{1}{2} (|y''_\xi|^2 + |y''_{\xi-1}|^2) \right\}, \quad (22)$$

where C_3 depends only on $\min y'_\xi$. This contribution leads to the term $\mathcal{E}_{\text{model}}$ in the consistency error estimate. \square

Finally, before we state the main error estimate, we need to estimate the effect of approximating $(\cdot, \cdot)_\varepsilon$ by $(\cdot, \cdot)_h$. A minor modification of [11, Sec. 4] (see also [15]) gives the following result.

Lemma 6 (Consistency of External Forces). *The consistency error for the external forces is bounded by*

$$\sup_{\substack{v_h \in \mathcal{U}_h \\ \|v'_h\|_{\ell_\varepsilon^1} = 1}} |(g, v_h)_\varepsilon - (g, v_h)_h| \leq \mathcal{E}_{\text{ext}}, \quad \text{where}$$

$$\mathcal{E}_{\text{ext}} = \max_{m \in \mathcal{M}_c} h_m^2 \left[\|g''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})} + 4\|g'\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m\})} \right].$$

We are now in a position to formulate the main result of [11, Sec. 5]. Its proof is technical but straightforward once the stability and consistency results of this section are established. The theorem essentially states that, *if y^a is a stable critical point of the atomistic model, and if both y^a and g are sufficiently smooth in the continuum region, then there exists a (locally unique) solution y_h^{qc} of the SAC method (16) in a neighbourhood of y^a such that quasi-optimal error estimates hold.*

Theorem 7. *Let $y^a \in \mathcal{Y}^+$ be a critical point of the atomistic energy Φ_{tot}^a , and suppose that $\gamma_s(y^a) > 0$.*

There exists a constant $\delta > 0$, which depends only on $\min(y^a)'$ and on $\gamma_s(y^a)$, such that, if

$$\mathcal{E}_{\text{model}}(y^a) + \mathcal{E}_{\text{approx}}(y^a) + \mathcal{E}_{\text{ext}} < \delta, \quad (23)$$

then there exists a locally unique solution $y_h^{\text{qc}} \in \mathcal{Y}_h^+$ of the SAC method (17) satisfying

$$\begin{aligned} \|(y_h^{\text{qc}} - y^a)'\|_{\ell^\infty} &\leq \max_{m \in \mathcal{M}_c} \frac{1}{2} h_m \|(y^a)''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})} \\ &\quad + 4\gamma_s(y^a)^{-1} (\mathcal{E}_{\text{model}}^s(y^a) + \mathcal{E}_{\text{approx}}^s(y^a) + \mathcal{E}_{\text{ext}}). \end{aligned} \quad (24)$$

Moreover, we have the superconvergence result

$$\|(y_h^{\text{qc}} - y^a)'\|_{\ell^\infty} \leq 4\gamma_s(y^a)^{-1} (\mathcal{E}_{\text{model}}^s(y^a) + \mathcal{E}_{\text{approx}}^s(y^a) + \mathcal{E}_{\text{ext}}). \quad (25)$$

4.2. Positive definiteness of the SAC method. Recall from Section 3.2 that one of our main motivations for formulating the SAC method was the lack of positive definiteness of the linearized QCF operator. We will now show that the SAC method does preserve positive definiteness, however, not necessarily up to bifurcation points. For simplicity we consider only the case $y = Bx$, which was introduced in [3] as a model problem, however, our arguments are easily extended to large deformations.

Proposition 8. *Let $B > 0$ such that $\phi''(B) > 0$ and $\phi''(2B) \leq 0$, then*

$$\phi''(B) + 4.5\phi''(2B) \leq \inf_{\substack{u_h \in \mathcal{U}_h \\ \|u'_h\|_{\ell_\varepsilon^2} = 1}} (S^{\text{qc}}(Bx)u_h, u_h)_h \leq \phi''(B) + 4.11\phi''(B).$$

Proof. For $y = \mathbf{B}x$ we obtain from the proof of Lemma 4 that

$$(DS^{\text{qc}}(\mathbf{B}x)u_h, u_h) = \sum_{m,n=1}^M h_m \mathcal{J}_{mn} U'_m U'_n,$$

where

$$\mathcal{J}_{mn} = \begin{cases} \phi''(\mathbf{B}) + 4\phi''(2\mathbf{B}), & m \in \mathcal{M}_c, n = m, \\ \phi''(\mathbf{B}) + 2\phi''(2\mathbf{B}), & m \in \mathcal{M}_a, n = m, \\ \phi''(2\mathbf{B}), & m \in \mathcal{M}_a, n = m \pm 1, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, we can explicitly write

$$\begin{aligned} (DS^{\text{qc}}(\mathbf{B}x)u_h, u_h) &= \sum_{m=1}^{\underline{K}-1} h_m (\phi''(\mathbf{B}) + 4\phi''(2\mathbf{B})) |U'_m|^2 + \sum_{m=\overline{K}+2}^M h_m (\phi''(\mathbf{B}) + 4\phi''(2\mathbf{B})) |U'_m|^2 \\ &\quad + \sum_{m=\underline{K}}^{\overline{K}+1} h_m \left\{ (\phi''(\mathbf{B}) + 2\phi''(2\mathbf{B})) |U'_m|^2 + \phi''(\mathbf{B}) (U'_{m-1} U'_m + U'_{m+1} U'_m) \right\}. \end{aligned} \tag{26}$$

We estimate the mixed terms from below by

$$U'_{m\pm 1} U'_m \geq -\frac{1}{2} |U'_{m\pm 1}|^2 - \frac{1}{2} |U'_m|^2.$$

A straightforward calculation, using the fact that $\phi''(2\mathbf{B}) \leq 0$, shows that

$$\begin{aligned} (DS^{\text{qc}}(\mathbf{B}x)u_h, u_h) &\geq \sum_{m=1}^M h_m (\phi''(\mathbf{B}) + 4\phi''(2\mathbf{B})) |U'_m|^2 \\ &\quad - \frac{1}{2} \phi''(2\mathbf{B}) \varepsilon (|U'_{\underline{K}}|^2 + |U'_{\overline{K}+1}|^2) + \frac{1}{2} \phi''(2\mathbf{B}) \varepsilon (|U'_{\underline{K}-1}|^2 + |U'_{\overline{K}+2}|^2). \end{aligned}$$

Estimating the terms with positive coefficients in the second row below by zero yields the stated lower bound.

To obtain an upper bound, we construct an explicit test function, similarly as in [4, Lemma 2]. For positive constants α, β , there exists a unique test function $\hat{u}_h \in \mathcal{U}_h$ such that

$$\hat{U}'_m = \begin{cases} -(\alpha\varepsilon)^{-1}, & m = \underline{K} - 1, \\ -(\beta\varepsilon)^{-1}, & m = \underline{K}, \\ (\beta\varepsilon)^{-1}, & m = \overline{K} + 1, \\ (\alpha\varepsilon)^{-1}, & m = \overline{K} + 2, \\ 0, & \text{otherwise.} \end{cases}$$

Moreover, if $2/\alpha + 2/\beta = 1$ then this test function has norm $\|\hat{u}'_h\|_{\ell_\varepsilon^2} = 1$. Inserting it into (26), after a short calculation, we obtain

$$(DS^{\text{qc}}(\mathbf{B}x)\hat{u}_h, \hat{u}_h)_h = \phi''_{\mathbf{B}} + 4\phi''_{2\mathbf{B}} + \phi''_{2\mathbf{B}} \left(\frac{2}{\sqrt{\alpha\beta}} - \frac{4}{\beta} \right).$$

Clearly, we can choose α, β so that the term in brackets becomes positive, and thus obtain an upper bound that gives a constant worse than 4. Numerically optimizing

over α, β , suggests the choice

$$\alpha = 2.11, \quad \beta = \frac{2\alpha}{\alpha - 2} = 38.3636.$$

Inserting these numerical values, we obtain

$$(DS^{\text{qc}}(\mathbf{B}x)\hat{u}_h, \hat{u}_h)_h \leq \phi''(\mathbf{B}) + (4 + 0.11)\phi''(2\mathbf{B}),$$

which is precisely the stated upper bound. \square

This result, and its obvious generalizations to large deformations, shows that the linearized SAC operator is indeed positive definite. This will considerably simplify the stability analysis in higher dimensions. However, we have also obtained an upper bound on the coercivity constant, which shows that there exist homogeneous deformations $y = \mathbf{B}x$ which are stable in both the atomistic and continuum model, but for which $DS^{\text{qc}}(\mathbf{B}x)$ is not positive definite. The gap is relatively small, however, and could be considered acceptable. This question deserves further investigation.

4.3. Error estimates in other norms. We conclude with a brief comment on error estimates in other Sobolev norms. We will not give a rigorous analysis, but only a brief outline of the main arguments.

Suppose that we are in the situation of Theorem 7, that is, we have guaranteed the existence of a stable atomistic equilibrium y^a and of an SAC solution y_h^{qc} in a neighbourhood. If y^a contains singularities (in 2D/3D, e.g., a crack tip singularity or the elastic field generated by a dislocation) then error estimates in ℓ^∞ may be too restrictive, especially in view of the fact that error estimates in ℓ_ε^2 correspond more closely to errors in the energy.

Suppose now that the SAC operator is positive definite in a neighbourhood of the solutions y^a, y_h^{qc} (we have shown in the previous section that this can be expected), then we can deduce from Theorem 7 and a simple generalization of Lemma 5, for simplicity assuming that \mathcal{E}_{ext} vanishes, that

$$\|(I_h y^a - y_h^{\text{qc}})'\|_{\ell_\varepsilon^2} \leq C \left\{ \left(\sum_{m \in \mathcal{M}_c} h_m^4 \|(y^a)''\|_{\ell_\varepsilon^2(\{\xi_{m-1}+1, \dots, \xi_m-1\})}^4 \right)^{1/2} + \varepsilon^2 \|(y^a)'''\|_{\ell_\varepsilon^2(\mathcal{L}_c^b)} \right\}.$$

where C depends on $\min(y^a)'_\xi$, on the interaction potential, and on the coercivity constant. Moreover, using the Riesz–Thorin interpolation theorem, one can interpolate between the error estimates in ℓ^∞ and ℓ_ε^2 and obtain error estimates in all ℓ_ε^p -norms, $2 \leq p \leq \infty$,

$$\|(I_h y^a - y_h^{\text{qc}})'\|_{\ell_\varepsilon^p} \leq C \left\{ \left(\sum_{m \in \mathcal{M}_c} h_m^{2p} \|(y^a)''\|_{\ell_\varepsilon^{2p}(\{\xi_{m-1}+1, \dots, \xi_m-1\})}^{2p} \right)^{1/p} + \varepsilon^2 \|(y^a)'''\|_{\ell_\varepsilon^p(\mathcal{L}_c^b)} \right\}.$$

We note that these quasi-optimal error estimates in ℓ_ε^p norms are not valid for the original QCF method, and we therefore expect that in the presence of strong singularities the SAC method may be superior. A careful investigation of this claim for 2D/3D examples is still open.

CONCLUSION

We have formulated the force-based quasicontinuum method for a 1D periodic chain with second-neighbour pair interactions. We have shown that this method has some potential pitfalls for both the analysis and practical applications. The origin of these difficulties are interface terms that appear only in the weak variational form, and hence, we suggested a new force-based coupling scheme, based on coupling stresses (SAC method), that circumvents many problems of the QCF method. We gave a preliminary error and stability analysis of this new method.

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