

Numerical Methods for Multilattices

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Abstract

Among the efficient numerical methods based on atomistic models, the quasicontinuum (QC) method has attracted growing interest in recent years. The QC method was first developed for crystalline materials with Bravais lattice and was later extended to multilattices (Tadmor et al, 1999). Another existing numerical approach to modeling multilattices is homogenization. In the present paper we review the existing numerical methods for multilattices and propose another concurrent macro-to-micro method in the homogenization framework. We give a unified mathematical formulation of the new and the existing methods and show their equivalence. We then consider extensions of the proposed method to time-dependent problems and to random materials.

Keywords: atomistic model, quasicontinuum method, multilattice, homogenization, multiscale method,
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1 Introduction

In some applications of solid mechanics, such as modeling cracks, structural defects, or nanoelectromechanical systems, the classical continuum description is not suitable, and it is required to utilize an atomistic description of materials. However, full atomistic simulations are prohibitively expensive, hence one needs to coarse-grain the problem. The quasicontinuum (QC) method [39] is one of the most efficient methods of coarse-graining the atomistic statics. The idea behind QC is to introduce a piecewise affine constraints for the atoms in regions with smooth deformation and use the Cauchy-Born rule to define the energy of the corresponding groups of constrained atoms. To formulate the QC method for multilattice crystals one must account for relative shifts of Bravais lattices which the multilattice is comprised of [40].

The QC method is a multiscale method capable of coupling atomistic and continuum description of materials. It is intended to model an atomistic material in a continuum manner in the regions where the deformation is smooth and use the fully atomistic model only in the small neighborhood of defects, thus effectively reducing the degrees of freedom of the system. Originally, the QC method was developed for crystalline materials with a (single) Bravais lattice [39] and the convergence of a few variants of the method has been analyzed under some practical assumptions (see, e.g., [16, 17, 19, 29, 30, 31, 34, 35]). The QC method is based on the so-called Cauchy-Born rule

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(see, e.g., [9, 20, 23, 25]) which states that the energy of a certain volume of a material can be approximated through the deformation energy density, which is computed for a representative atom assuming that the neighboring atoms follow a uniform deformation. Later, QC was extended to multilattices [40] (a multilattice is a union of a number of Bravais lattices) based on the improved Cauchy-Born rule [38] which accounts for relative shifts between the Bravais lattices. Examples of such materials include diamond cubic Si, HCP metals (stacking two simple hexagonal lattices with a shift vector) like Zr, ferroelectric materials, salts like Sodium Chloride, and intermetallics like NiAl. More recent developments of QC for multilattices also include adaptive choice of representative cell of multilattices [15]. It appears that no rigorous analysis is available so far for the multilattice QC.

In the present work we propose a treatment of multilattices within the framework of numerical homogenization. Homogenization techniques for partial differential equations (PDEs) with multiscale coefficients are known to be successful for obtaining effective equations with coefficients properly averaged out [8]. Finite element methods based on homogenization theory have been pioneered by Babuška [5] and have attracted growing attention these past few years (see [1, 18, 21, 26] for textbooks or review papers). Following the ideas of [8], we use homogenization techniques to describe the coarse-graining of multilattices and based on that, propose a macro-to-micro numerical algorithm which we call the *homogenized QC (HQC)* method. We give a unified mathematical description and establish equivalence between the homogenized QC, the multilattice QC of [40], and the finite element method applied to the continuously homogenized equations (see [4, 24] and references therein for homogenization of atomistic media).

Despite the formal equivalence of these numerical methods for the multilattices, we find several benefits of the homogenization framework. First, in this framework the connection to the well-developed theory of continuum homogenization and related numerical methods becomes more apparent. This allows us to apply the numerical analysis techniques developed for continuum homogenization [1, 18] to the multilattice QC method (see the preprint [4] for an example of such application). Second, homogenization theory can be used to upscale the atomistic model in both, time and space, which makes it promising for modeling and especially analyzing zero temperature and finite temperature motion of atomistic materials [18, 24, 33]. In this work we demonstrate such an application of HQC to zero-temperature dynamics (Section 8). Also, homogenization can be applied to “stochastic” materials, atomistic counterparts of which include polymers [7] and glasses (we give an example of such application in Section 7). Last, for the finite temperature simulations, when materials are modeled with static atoms interacting with effective temperature-dependent potentials, the discrete homogenization (Section 4.3) may serve as a rigorous instrument to derive such potentials. We note that the idea of applying homogenization to atomistic media has appeared in the literature before [7, 11, 13, 14, 24].

The paper is organized as follows. We present the atomistic model in Section 2, and the quasicontinuum method in Section 3. In Section 4 we present the technique of homogenization applied to the atomistic equations. In Section 5 we present the HQC method—a concurrent macro-to-micro algorithm based on the discrete homogenization. The method is formulated in such a way that it allows for a straightforward extension to non-crystalline materials if the microstructure is known; an example of such extension is given in Section 7. Section 6 is devoted to showing the equivalence of the following four methods: the HQC method, the multilattice QC, the finite element method applied to continuously homogenized equations, and the QC method applied to the discretely homogenized equations. In Section 8 we apply the proposed macro-to-micro method to a long-wave unsteady evolution of a 1D multilattice crystal. Concluding remarks are given in

Section 9. The commonly used notations are collected in the appendix.

2 Problem Formulation

The focus of the present study is on correct treatment of atomistic materials with spatially oscillating or inhomogeneous local properties.

2.1 Equations of Equilibrium

We describe the formulation of the problem of finding an equilibrium of an atomistic material in the periodic setting. We consider the periodic boundary conditions for simplicity, in order to avoid difficulties arising from presence of the boundary of the atomistic material. Nevertheless, it should be noted that the numerical method and the algorithm proposed in the present work can be applied to Dirichlet, Neumann, or other boundary conditions.

2.1.1 Deformation

Consider an atomistic material occupying a region $\Omega = (0, 1]^d$ in its reference (i.e., undeformed) configuration and extended periodically outside of Ω . The set of positions of atoms in the reference configurations are

$$\mathcal{M} = \Omega \cap \bigcup_{\alpha=0}^{m-1} (\epsilon\mathbb{Z}^d + \epsilon p_\alpha),$$

where $p_\alpha \in [0, 1]^d$ is a shift vector of α -th species of atoms in the reference configuration; in total we have m species of atoms. We assume that $p_\alpha \neq p_\beta$ for $\alpha \neq \beta$ and, for convenience, $p_0 = 0$.

We collect these shift vectors into the set $\mathcal{P} := \{p_\alpha : \alpha = 0, \dots, m-1\}$. Thus, if we denote a Bravais lattice in Ω as

$$\mathcal{L} = \Omega \cap \epsilon\mathbb{Z}^d,$$

then we can write $\mathcal{M} = \mathcal{L} + \epsilon\mathcal{P}$. We will call \mathcal{M} a multilattice.

When the material experiences a deformation the atom positions become $x + u(x)$, where $u(x)$ is the displacement. We assume that $u(x)$ is periodic, i.e., $u(x+a) = u(x)$ for all $a \in \mathbb{Z}^d$. The space of all periodic displacements is denoted as $\mathcal{U}_{\text{per}}(\mathcal{M})$. Since we only consider the systems invariant w.r.t. translation in space, we will also need the space of displacements with zero average, $\mathcal{U}_{\#}(\mathcal{M})$ (see Appendix A.1 for the precise definitions).

2.1.2 Interaction

We assume the most general form of interaction (finite-range, multi-body) between atoms. For each atom $x \in \mathcal{M}$ we introduce its “interaction neighborhood” — a set of vectors $\mathcal{R}_\epsilon(x)$ such that $\{x + \epsilon r : r \in \mathcal{R}_\epsilon(x)\}$ are the atoms that x interacts with. The energy of an atom $x \in \mathcal{M}$ is denoted as $V_\epsilon(D_{\mathcal{R}_\epsilon(x)}u(x); x)$, where $D_{\mathcal{R}_\epsilon}u = (D_r u)_{r \in \mathcal{R}_\epsilon}$ (see Appendix A.3) is a collection of discrete directional derivatives of u corresponding to the set of neighbors \mathcal{R}_ϵ (these notations were first introduced in [28]). The discrete derivative in direction r of u evaluated at $x \in \mathcal{M}$ is defined as $D_r u(x) := \frac{u(x+\epsilon r) - u(x)}{\epsilon}$. The needed properties and definitions of discrete directional derivatives

can be found in Appendix A.2, and more details on discrete directional derivatives — in Appendix A.3.

Thus, the interaction energy of the displacement u is given by the interaction potential V_ϵ as

$$E(u) = \frac{1}{\#\mathcal{M}} \sum_{x \in \mathcal{M}} V_\epsilon(D_{\mathcal{R}_\epsilon(x)}u(x); x) = \langle V_\epsilon(D_{\mathcal{R}_\epsilon}u) \rangle_{\mathcal{M}},$$

where $\langle g \rangle_S$ denotes the average value of a function g defined on a discrete set S .

The subscript ϵ in V_ϵ and \mathcal{R}_ϵ indicates that these objects depend non-smoothly on x : indeed, the interaction energy and the interaction neighborhood may depend on the species of atoms α for $x \in \mathcal{L} + \epsilon p_\alpha$. For instance, we can consider a Lennard-Jones potentials with atom-dependent parameters:

$$V(D_{\mathcal{R}_\epsilon}u; x) = \sum_{r \in \mathcal{R}_\epsilon} s_{x, x+\epsilon r} \left(-2 \left(\frac{|r+D_r u|}{\ell_{x, x+\epsilon r}} \right)^{-6} + \left(\frac{|r+D_r u|}{\ell_{x, x+\epsilon r}} \right)^{-12} \right), \quad (2.1)$$

where $s_{x, x+\epsilon r}$ and $\ell_{x, x+\epsilon r}$ are, respectively, the strength and the equilibrium distance of interaction of atoms x and $x + \epsilon r$.

We assume that the interaction neighborhood $\mathcal{R}_\epsilon(x + \epsilon p_\alpha)$, and the interaction potential $V_\epsilon(\bullet, x + \epsilon p_\alpha)$, for $x \in \mathcal{L}$ depends only on α , the particular species of atoms, but does not depend on x ; we therefore write $\mathcal{R}_\epsilon(x + \epsilon p_\alpha) =: \mathcal{R}_{\epsilon, \alpha}$ and $V_\epsilon(\bullet, x + \epsilon p_\alpha) =: V_{\epsilon, \alpha}$. Then, we can use the following form of the energy:

$$\begin{aligned} E(u) &= \left\langle \frac{1}{m} \sum_{\alpha=0}^{m-1} V_\epsilon(D_{\mathcal{R}_\epsilon(x+\epsilon p_\alpha)}u(x + \epsilon p_\alpha); x + \epsilon p_\alpha) \right\rangle_{x \in \mathcal{L}} \\ &= \left\langle \frac{1}{m} \sum_{\alpha=0}^{m-1} V_{\epsilon, \alpha}(D_{\mathcal{R}_{\epsilon, \alpha}}u(x + \epsilon p_\alpha)) \right\rangle_{x \in \mathcal{L}}, \end{aligned} \quad (2.2)$$

where we used a more verbose notation for averaging of a function g defined on a discrete set S , $\langle g \rangle_S =: \langle g(x) \rangle_{x \in S}$. This expression for the energy will be used to write down the energy of the multilattice QC method in a familiar way (see (3.5)).

The latter form of the energy will be used whenever we need periodicity of interaction (for the Cauchy-Born rule and for the homogenization). However we stress that the formulation of the proposed numerical method (Section 5) requires neither periodicity of \mathcal{M} nor periodicity of interaction.

2.1.3 External Force

The potential energy of the external force $f = f(x)$ is

$$-F(u) = -\langle f, u \rangle_{\mathcal{M}},$$

where by $\langle w, v \rangle_{\mathcal{M}} := \langle w \cdot v \rangle_{\mathcal{M}}$ we denote a scalar product of $w, v \in \mathcal{U}_{\text{per}}(\mathcal{M})$. (To be precise, it is an inner product on $\mathcal{U}_{\#}(\mathcal{M})$ and a semi-inner product on $\mathcal{U}_{\text{per}}(\mathcal{M})$.) The forces $f = f(x)$ are applied as “dead loads”, i.e., they are independent of actual atom positions $x + u$. For the problem to be well-posed, the sum of all forces per period is assumed to be zero, i.e., $\langle f \rangle_{\mathcal{M}} = 0$.

2.1.4 Equation of Equilibrium

We denote the total potential energy of the atomistic system as

$$\Pi(u) = E(u) - F(u).$$

A displacement $u \in \mathcal{U}_\#(\mathcal{M})$ is a stable equilibrium if it is a local minimizer of Π , which implies that u is a critical point of Π :

$$\langle \delta\Pi(u), v \rangle_{\mathcal{M}} := \frac{d}{dt} \Pi(u + tv) \Big|_{t=0} = 0 \quad \forall v \in \mathcal{U}_\#(\mathcal{M}). \quad (2.3)$$

We assume that the function $\Pi(u)$ is smooth enough and hence $\langle \delta\Pi(u), v \rangle_{\mathcal{M}}$ is a linear functional w.r.t. $v \in \mathcal{U}_\#(\mathcal{M})$, which justifies identification of $\delta\Pi(u)$ with an element of $\mathcal{U}_\#$. Alternatively, the problem of finding the equilibrium configuration of atoms can formally be written as

$$\frac{\partial \Pi}{\partial u(x)} = 0 \quad \forall x \in \mathcal{M},$$

if we consider Π as a function of finite number of variables $u(x)$, $x \in \mathcal{M}$.

For the equations (2.3) to have a unique solution, we must additionally require that the average of u is zero:

$$\langle u \rangle_{\mathcal{M}} = 0. \quad (2.4)$$

The equilibrium equations (2.3) together with the additional condition (2.4) can be written in variational form: find $u \in \mathcal{U}_{\text{per}}(\mathcal{M})$ such that

$$\langle \delta E(u), v \rangle_{\mathcal{M}} = F(v) \quad \forall v \in \mathcal{U}_{\text{per}}(\mathcal{M}) \quad (2.5a)$$

$$\langle u \rangle_{\mathcal{M}} = 0, \quad (2.5b)$$

where the functional derivative $\delta E : \mathcal{U}_{\text{per}}(\mathcal{M}) \rightarrow \mathcal{U}_{\text{per}}(\mathcal{M})$ is computed as

$$\langle \delta E(u), v \rangle_{\mathcal{M}} = \left\langle \sum_{r \in \mathcal{R}_\epsilon} V'_{\epsilon,r}(D_{\mathcal{R}_\epsilon} u), D_r v \right\rangle_{\mathcal{M}}, \quad (2.6)$$

and $V'_{\epsilon,r}(D_{\mathcal{R}_\epsilon} u)$ denotes, effectively, the gradient of a scalar function V_ϵ w.r.t. its vector-valued variable $D_r u$ (note the difference with $V_{\epsilon,\beta}$ introduced in (2.2)). Here and in what follows, with a slight abuse of notations, we keep the sign of summation over $r \in \mathcal{R}_\epsilon$ inside the triangular brackets of the scalar product.

2.2 Example: a Simplified Model

The following simplified model will be useful in illustrating the numerical methods presented in this paper.

Assume one space dimension, $d = 1$; the domain $\Omega = (0, 1]$, the shift vectors in fixed configuration

$$\mathcal{P} = \left\{ 0, \frac{1}{m}, \dots, \frac{(m-1)}{m} \right\}, \quad (2.7)$$

the multilattice

$$\mathcal{M} = \bigcup_{\alpha=0}^{m-1} (\epsilon\mathbb{Z} + \epsilon \frac{\alpha}{m}) \cap \Omega = \frac{\epsilon}{m} \mathbb{Z} \cap \Omega,$$



Figure 1: Illustration of a simplified atomistic model

and the basic lattice $\mathcal{L} = \epsilon\mathbb{Z} \cap \Omega$. We further assume $\mathcal{R} = \{\frac{1}{m}\}$ (nearest neighbor interaction only) and consider the “linear spring model” with the atomistic potential

$$V_\epsilon(D_r u; x) = \psi_\epsilon(x) \frac{(D_r u)^2}{2}, \quad (2.8)$$

with $r = \frac{1}{m}$. Such system can be interpreted as a system of masses located at positions $x + u$ and connected with ideal springs with spring constants $k = \psi_\epsilon(x)/\epsilon$, as illustrated in Figure 1.

The equilibrium equation then becomes

$$\langle \psi_\epsilon D_r u, D_r v \rangle_{\mathcal{M}} = \langle f, v \rangle_{\mathcal{M}} \quad (2.9)$$

3 Quasicontinuum (QC) Method

Traditionally, numerical methods such as the finite element method (FEM) are applied to continuum equations which can then be solved on a computer. The characteristic feature of atomistic models we are discussing in the paper is their discreteness, with a number of degrees of freedom often too large to keep track of each individual atom. Therefore, similarly to FEM, the ideas of reducing the number of degrees of freedom are used for atomistic models as well. The difference is now that the reduction is done from a large but finite number of degrees of freedom to a smaller number of degrees of freedom. The QC method is a representative of such methods. We first present its simple-lattice version. The QC method consists in reducing the number of degrees of freedom of the atomistic system by choosing a coarse mesh of nodal atoms and assuming that the positions of the other atoms can be reconstructed by a linear interpolation.

It should be noted that we discuss here only the *local* version of QC which is equivalent to applying FEM to the Cauchy-Born continuum model of elasticity. We are not considering coupling the continuum and discrete models in this paper.

3.1 Notations

Assume a partition \mathcal{T}_h of the domain Ω into simplicial elements T , which we will conveniently refer to as the *mesh*. Normally, $\#(\mathcal{T}_h) \ll \#(\mathcal{L})$ (recall that by $\#(\bullet)$ we denote the number of elements in a set). By $|T|$ we denote the Lebesgue measure of T . The QC solution will be denoted as u^h .

The space of piecewise linear discrete vector-functions is denoted as

$$\mathcal{U}_{\text{per}}^h = \{u^h \in (W_{\text{per}}^{1,\infty}(\Omega))^d : u^h|_T \in P_1(T) \forall T \in \mathcal{T}_h\}, \quad (3.1)$$

and the space of piecewise constant vector-functions as

$$\mathcal{Q}_{\text{per}}^h = \{q^h \in (L_{\text{per}}^\infty(\Omega))^d : q^h|_T \in P_0(T) \forall T \in \mathcal{T}_h\}.$$

3.2 QC for simple lattice

In this (and only this) subsection we make the simple lattice assumption. That is, we assume that $m = 1$ and hence $\mathcal{M} = \mathcal{L}$. In particular, in this subsection we write $V_\epsilon(D_{\mathcal{R}}u; x) = V(D_{\mathcal{R}}u)$ and $\mathcal{R}_\epsilon(x) = \mathcal{R}$ as they no longer depend on x .

The QC method [39] aims at finding a minimizer of

$$\Pi(u^h) = \langle V(D_{\mathcal{R}}u^h) \rangle_{\mathcal{L}} - F(u^h)$$

in $\mathcal{U}_{\text{per}}^h$. Minimizing $\Pi(u^h)$ in $\mathcal{U}_{\text{per}}^h$ indeed reduces the number of degrees of freedom of the system from $O(\#\mathcal{M})$ to $O(\#\mathcal{T}_h)$ (recall that $\#\mathcal{T}_h \ll \#\mathcal{M}$). However, one must still spend $O(\#\mathcal{M})$ operations to compute the effective forces on the reduced degrees of freedom. In order to have an efficient numerical method (i.e., a method with $O(\#\mathcal{T}_h)$ operations) one introduces an approximation to $\Pi(u^h)$ which is called the *local QC method* [39] (hereinafter referred to as the QC method).

The local QC method first approximates $D_r u^h$ with $\nabla_r u^h$ within each T (hence the name of the method: the nonlocal finite difference $D_r u^h$ is approximated with the “local” directional derivative $\nabla_r u^h$). Then for each $x \in T$ one has

$$V(D_{\mathcal{R}}u^h) \approx V(\nabla_{\mathcal{R}}u^h) = W(\nabla u^h|_T),$$

where $W(F) := V(F\mathcal{R})$ is the Cauchy-Born energy density associated with a displacement gradient F (see (A.4) to obtain the precise definition of $F\mathcal{R}$). Second, the local QC method changes the sum over $x \in \mathcal{L}$ effectively to integration over Ω , i.e.,

$$E^{\text{qc}}(u^h) := \int_{\Omega} W(\nabla u^h) dx = \sum_{T \in \mathcal{T}_h} |T| W(\nabla u^h|_T).$$

The variational formulation of the QC method is thus

$$\int_{\Omega} \sum_{r \in \mathcal{R}} \delta W(\nabla_r u^h) : \nabla_r v^h dx = F^h(v^h) \quad \forall v \in \mathcal{U}_{\text{per}}^h, \quad (3.2)$$

where δW denotes the derivative of W and the semicolon denotes the inner product of matrices. For uniqueness of solution we should restrict ourselves to $u^h \in \mathcal{U}_{\#}^h$.

3.3 Multilattice QC

Approximating the exact minimizer of $\Pi(u)$ with a piecewise linear $u^h \in \mathcal{U}_{\text{per}}^h$ may be accurate enough for the case when the interatomic interaction $V_\epsilon(\bullet, x)$ varies smoothly with x (more precisely, if the mesh \mathcal{T}_h resolves well the variations in $V_\epsilon(\bullet, x)$). However, for materials with multilattice structure (examples of such materials were given in the introduction) the piecewise linear approximation of the displacement u cannot be accurate.

In this subsection we present the Multilattice QC (MQC) method first introduced in [40] which is designed to handle the multilattice microstructure.

Define the space of QC deformations of the multilattice

$$\mathcal{U}^{h,q} = \left\{ u^h + \sum_{\alpha=1}^{m-1} q_\alpha^h w_\alpha : u^h \in \mathcal{U}_{\text{per}}^h, q_\alpha^h \in \mathcal{Q}_{\text{per}}^h, \alpha = 1, \dots, m-1 \right\}, \quad (3.3)$$

where q_α^h are the deformed shift vectors (recall that p_α are the undeformed shift vectors) and

$$w_\alpha|_{\mathcal{L}+\epsilon p_\beta} = \delta_{\alpha\beta} \quad (\alpha, \beta = 0, \dots, m-1), \quad (3.4)$$

are the associated basis functions, with $\delta_{\alpha\beta}$ denoting the Kronecker delta. For a more detailed introduction of the space of QC deformations, refer to [4]. In each element $T \in \mathcal{T}_h$ we have $m-1$ nonzero shift vectors q_α^h and we set $q_0^h := 0$. We denote

$$\mathbf{q}^h := (q_1^h, \dots, q_{m-1}^h) \in (\mathcal{Q}_{\text{per}}^h)^{m-1}.$$

Next, form the interaction energy $E(u)$ with $u = u^h + \sum_{\alpha=1}^{m-1} q_\alpha^h w_\alpha \in \mathcal{U}^{h,q}$:

$$\begin{aligned} E(u) &= E\left(u^h + \sum_{\alpha=1}^{m-1} q_\alpha^h w_\alpha\right) \\ &= \left\langle V_\epsilon \left(D_{\mathcal{R}_\epsilon(x)} \left(u^h(x) + \sum_{\alpha=1}^{m-1} D_r q_\alpha^h(x) w_\alpha(x) \right); x \right) \right\rangle_{x \in \mathcal{M}} \\ &= \left\langle \frac{1}{m} \sum_{\beta=0}^{m-1} V_\epsilon \left(D_{\mathcal{R}_\epsilon(x+\epsilon p_\beta)} \left(u^h(x+\epsilon p_\beta) + \sum_{\alpha=1}^{m-1} q_\alpha^h(x+\epsilon p_\beta) w_\alpha(x+\epsilon p_\beta) \right); x+\epsilon p_\beta \right) \right\rangle_{x \in \mathcal{L}} \\ &= \left\langle \frac{1}{m} \sum_{\beta=0}^{m-1} V_{\epsilon,\beta} \left(D_{\mathcal{R}_{\epsilon,\beta}} u^h(x+\epsilon p_\beta) + \sum_{\alpha=1}^{m-1} D_{\mathcal{R}_{\epsilon,\beta}} q_\alpha^h(x+\epsilon p_\beta) w_\alpha(\epsilon p_\beta) \right) \right\rangle_{x \in \mathcal{L}} \end{aligned}$$

where we used periodicity of V_ϵ (see (2.2)) and w_α (which follows directly from the definitions of w_α and \mathcal{M}). Similarly to the simple-lattice QC, we perform a local quasicontinuum approximation which consists in: (i) assuming that the energy associated with each T depends on the displacement gradient and shift vectors only in T , and (ii) changing the summation over $x \in \mathcal{L}$ to the integration over Ω :

$$\begin{aligned} E(u) &\approx \int_\Omega \frac{1}{m} \sum_{\beta=0}^{m-1} V_{\epsilon,\beta} \left(\nabla_{\mathcal{R}_{\epsilon,\beta}} u^h + \sum_{\alpha=1}^{m-1} q_\alpha^h D_{\mathcal{R}_{\epsilon,\beta}} w_\alpha(\epsilon p_\beta) \right) dx \\ &= \sum_{T \in \mathcal{T}_h} |T| \frac{1}{m} \sum_{\beta=0}^{m-1} V_{\epsilon,\beta} \left((\nabla u^h|_T) \mathcal{R}_{\epsilon,\beta} + \sum_{\alpha=1}^{m-1} (q_\alpha^h|_T) D_{\mathcal{R}_{\epsilon,\beta}} w_\alpha(\epsilon p_\beta) \right) =: \tilde{E}^{\text{mqc}}(u^h, \mathbf{q}^h), \end{aligned}$$

where we used the identity $\nabla_{\mathcal{R}_{\epsilon,\beta}} u^h|_T = (\nabla u^h|_T) \mathcal{R}_{\epsilon,\beta}$, cf. (A.4).

Remark 3.1. *The expression for $\tilde{E}^{\text{mqc}}(u^h, \{q_\alpha^h\})$ can be further simplified by denoting the species of atoms $\epsilon\beta + \mathcal{R}$ as $\mathcal{A}_{\epsilon,\beta}$ (formally $\mathcal{A}_{\epsilon,\beta} := (a_{\beta,r})_{r \in \mathcal{R}_{\epsilon,\beta}}$ where $a_{\beta,r} \in \{0, \dots, m-1\}$ is defined so that $p_{a_{\beta,r}} \in p_\beta + r + \mathbb{Z}$). Then the sum in \tilde{E}^{mqc} can be simplified as the difference between the shift vectors of interacting atoms:*

$$\begin{aligned} \sum_{\alpha=1}^{m-1} (q_\alpha^h|_T) D_{\mathcal{R}_{\epsilon,\beta}} w_\alpha(\epsilon p_\beta) &= \left(\sum_{\alpha=1}^{m-1} (q_\alpha^h|_T) D_r w_\alpha(\epsilon p_\beta) \right)_{r \in \mathcal{R}_{\epsilon,\beta}} \\ &= \left((q_{a_{\beta,r}}^h|_T) (w_\alpha(\epsilon p_{a_{\beta,r}}) - w_\alpha(\epsilon p_\beta)) \right)_{r \in \mathcal{R}_{\epsilon,\beta}} = \left((q_{a_{\beta,r}}^h|_T) - (q_\beta^h|_T) \right)_{r \in \mathcal{R}_{\epsilon,\beta}} \end{aligned}$$

This yields

$$\tilde{E}^{\text{mqc}}(u^h, \{q_\alpha^h\}) = \sum_{T \in \mathcal{T}_h} |T| \frac{1}{m} \sum_{\beta=0}^{m-1} V_{\epsilon, \beta} \left((\nabla_{\mathcal{R}_{\epsilon, \beta}} u^h + q_{\mathcal{A}_{\epsilon, \beta}}^h - q_\beta^h)|_T \right). \quad (3.5)$$

In the next step, the shift vectors q_α are eliminated from (3.3) by requiring the variation of $\tilde{E}^{\text{mqc}}(u^h, \{q_\alpha\})$ w.r.t. q_γ in each triangle be zero:

$$\frac{1}{m} \sum_{\beta=0}^{m-1} \sum_{r \in \mathcal{R}_\beta} V'_{\epsilon, \beta, r} \left((\nabla u^h|_T) \mathcal{R}_{\epsilon, \beta} + \sum_{\alpha=1}^{m-1} (q_\alpha^h|_T) D_{\mathcal{R}_{\epsilon, \beta}} w_\alpha(\epsilon p_\beta) \right) D_r w_\gamma(\epsilon p_\beta) = 0 \quad (3.6)$$

$$(\gamma = 1, 2, \dots, m-1).$$

The equations (3.6) form a system of $m-1$ equations for $m-1$ unknowns $(q_\alpha)_{\alpha=1}^{m-1}$ in each T , from where under some stability assumptions (see, e.g., [20]) it is possible to determine the shift vectors q_α depending (as a rule, nonlinearly) only on the displacement gradient:

$$\mathbf{q}^h|_T = \mathbf{q}(\nabla u^h|_T).$$

Note that the function $\mathbf{q}(\mathbf{F})$ does not depend on T , unless different periodic materials are considered in different elements T .

We now form a QC energy with q_α eliminated:

$$E^{\text{mqc}}(u^h) := \tilde{E}^{\text{mqc}}(u^h, \mathbf{q}(\nabla u^h)). \quad (3.7)$$

The QC equation of equilibrium now reads: find $u^h \in \mathcal{U}_{\text{per}}^h$ such that

$$\langle \delta E^{\text{mqc}}(u^h), v^h \rangle_\Omega = F^h(v^h) \quad \forall v^h \in \mathcal{U}_{\text{per}}^h.$$

The function u^h gives a macroscopic displacement of the material, and one needs to compute $u^h + \sum_{\alpha=1}^{m-1} q_\alpha^h w_\alpha$ for the microstructure. We note that since q_α were found from letting the variation of $\tilde{E}^{\text{mqc}}(u^h, q_\alpha)$ w.r.t. q_α be zero, we have

$$\delta E^{\text{mqc}}(u^h) = \delta_{u^h} \tilde{E}^{\text{mqc}}(u^h, \mathbf{q}(\nabla u^h)). \quad (3.8)$$

Remark 3.2. *Instead of eliminating $\mathbf{q}^h = \mathbf{q}(\nabla u^h)$, one could also look for a critical point (or a minimizer) of the energy $\tilde{E}^{\text{mqc}}(u^h, \mathbf{q}^h)$ w.r.t. both u^h and \mathbf{q}^h . In [37] the latter approach is reported to be more efficient.*

3.4 Application of QC to the Simplified Model

We illustrate an application of QC to the simplified 1D model (2.8) for two species of atoms (i.e., $m = 2$), $\psi_\epsilon(0) = \psi_1$, $\psi_\epsilon(\frac{\epsilon}{2}) = \psi_2$.

If we approximate the exact solution with $u^h \in \mathcal{U}_{\text{per}}^h$ as it is done in the simple-lattice QC (cf. Section 3.2) then we will find the approximate energy

$$\sum_{T \in \mathcal{T}_h} |T| \frac{1}{2} \left[\psi_1 \frac{(\nabla_r u^h)^2}{2} + \psi_2 \frac{(\nabla_r u^h)^2}{2} \right] = \sum_{T \in \mathcal{T}_h} |T| \frac{\psi_1 + \psi_2}{2} \frac{(\nabla_r u^h)^2}{2}.$$

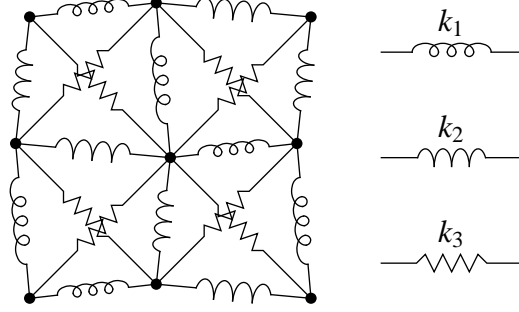


Figure 2: Illustration of a 2D model problem with heterogeneous interaction.

Here $\tilde{\psi}^0 = \frac{\psi_1 + \psi_2}{2}$ is the wrong effective spring constant, since if the two springs in series are replaced with two identical springs with the effective spring constant ψ_0 then $\psi_0 = \frac{2\psi_1\psi_2}{\psi_1 + \psi_2}$ (see, e.g., [11]).

If instead we allow for nonzero shift vector q_1 then the corresponding MQC energy (3.5) is

$$\tilde{E}^{\text{mqc}}(u^h, q_1^h) = \sum_{T \in \mathcal{T}_h} |T| \frac{1}{2} \left[\psi_1 \frac{(\nabla_r u^h + q_1^h)^2}{2} + \psi_2 \frac{(\nabla_r u^h - q_1^h)^2}{2} \right]$$

with $r = \frac{1}{2}$. The strong form of (3.6) in this case can be obtained by differentiating the above expression w.r.t. q_1^h in each T :

$$\psi_1 ((\nabla_r u^h + q_1^h)|_T) - \psi_2 ((\nabla_r u^h - q_1^h)|_T) = 0,$$

from where we find

$$q_1^h|_T = \frac{\psi_2 - \psi_1}{\psi_1 + \psi_2} (\nabla_r u^h|_T).$$

Substituting this back to the MQC energy (cf. (3.7)) yields

$$\begin{aligned} E^{\text{mqc}}(u^h) &= \sum_{T \in \mathcal{T}_h} |T| \frac{1}{2} \left[\psi_1 \frac{1}{2} \left(\frac{2\psi_2}{\psi_1 + \psi_2} (\nabla_r u^h|_T) \right)^2 + \psi_2 \frac{1}{2} \left(\frac{2\psi_1}{\psi_1 + \psi_2} (\nabla_r u^h|_T) \right)^2 \right] \\ &= \sum_{T \in \mathcal{T}_h} |T| \frac{2\psi_1\psi_2}{\psi_1 + \psi_2} \frac{(\nabla_r u^h|_T)^2}{2}, \end{aligned}$$

where the effective spring constant is now computed correctly.

4 Homogenization of Atomistic Media

We now present another coarse graining strategy based on homogenization. We derive below the homogenized model of the atomistic material which will be the basis for formulating and analyzing a quasicontinuum method for multilattices. We will first present the “classical” approach of upscaling the atomistic equations to a continuum model and in Section 4.3 we will outline a strategy where the multilattice atomistic model is upscaled to the simple lattice model.

We note that the first works concerned with upscaling atomistic equations are [11, 12, 24]. In the present section we derive the upscaled equations for a general model of interaction in many dimensions as opposed to the pairwise interaction in 1D assumed in the upscaled equations [11, 12, 24]. The upscaled equations are derived using a formal asymptotic expansion. Rigorous error bounds for the homogenized equations can be found in the preprint [4] for the case of the 1D nearest neighbor interaction and in [3] for the case of a 1D finite-range nonlinear interaction.

4.1 Asymptotic expansion

In order to take into account the local variation of the atomistic interaction we think of the displacement as depending on a fast and a slow scale $u(x) \sim u(x, x/\epsilon)$. We define $x \in \mathbb{R}^d$, the macro (“slow”) variable, and $y = x/\epsilon \in \mathbb{Z}^d + \mathcal{P}$, the micro (“fast”) variable, and consider a series of functions $u^n : \mathbb{R}^d \times (\mathbb{Z}^d + \mathcal{P}) \rightarrow \mathbb{R}^d$ indexed by $n = 0, 1, 2, \dots$. As we consider the local structure and interaction to be periodic, we assume that the functions u^n are \mathcal{P} -periodic in the fast variable, i.e., they satisfy for all $(x, y) \in \Omega \times \mathcal{P}$

$$u^n(x, y + j) = u^n(x, y), \quad \forall j \in \mathbb{Z}^d$$

while the behavior w.r.t. x is similar as considered in the previous sections

$$u^n(x + i, y) = u^n(x, y), \quad \forall i \in \mathbb{Z}^d.$$

We then consider the asymptotic expansion

$$u(x) \sim (u^0(x) + \epsilon u^1(x, y) + \epsilon^2 u^2(x, y) + \dots) \Big|_{y=x/\epsilon} \quad \forall x \in \mathcal{M}. \quad (4.1)$$

Notice that we directly assume that the homogenized solution, u^0 , does not depend on y .

We now proceed as in the “classical homogenization” [6, 8, 36] and plug the ansatz (4.1) into (2.5):

$$\left\langle \left(\sum_{r \in \mathcal{R}_\epsilon} V'_{\epsilon, r} (D_{x, \mathcal{R}_\epsilon} u^0 + \epsilon D_{x, \mathcal{R}_\epsilon} T_{y, \mathcal{R}_\epsilon} u^1 + D_{y, \mathcal{R}_\epsilon} u^1 + \dots) \right. \right. \\ \left. \left. , D_{x, r} T_{y, r} v + \epsilon^{-1} D_{y, r} v \right) \Big|_{y=x/\epsilon} \right\rangle_{\mathcal{M}} = \langle f, v \rangle_{\mathcal{M}},$$

where the test functions $v = v(x, y)$ are continuous and smooth in $x \in \Omega$ and discrete in $y \in \mathcal{P}$. Here we used the relation (A.3) to expand the full derivative D_r through partial derivatives $D_{x, r}$, $D_{y, r}$, and the translation operator $T_{y, r}$, and used the collection-of-derivatives notation $D_{\mathcal{R}}$ (see Appendix A.3 for more details).

We then extend the equation on the entire $\mathcal{M} \times \mathcal{P}$:

$$\left\langle \sum_{r \in \mathcal{R}_\epsilon} V'_{\epsilon, r} (D_{x, \mathcal{R}_\epsilon} u^0 + \epsilon D_{x, \mathcal{R}_\epsilon} T_{y, \mathcal{R}_\epsilon} u^1 + D_{y, \mathcal{R}_\epsilon} u^1 + \dots) \right. \\ \left. , D_{x, r} T_{y, r} v + \epsilon^{-1} D_{y, r} v \right\rangle_{\mathcal{M} \times \mathcal{P}} = \langle f, v \rangle_{\mathcal{M} \times \mathcal{P}}. \quad (4.2)$$

We now expand this equation in powers of ϵ . For that, we use the approximation $D_{x, r} \approx \nabla_{x, r}$ (i.e., we essentially use Taylor series to expand $D_{x, r}$), and the notations $V_\epsilon(\bullet; x) = V(\bullet; y)$ and

$\mathcal{R}_\epsilon(x) = \mathcal{R}(y)$, and change a sum over \mathcal{M} to an integral:

$$\left\langle \sum_{r \in \mathcal{R}} V'_r(\nabla_{x, \mathcal{R}} u^0 + \epsilon \nabla_{x, \mathcal{R}} T_{y, \mathcal{R}} u^1 + D_{y, \mathcal{R}} u^1 + \dots) \right. \\ \left. , \nabla_{x, r} T_{y, r} v + \epsilon^{-1} D_{y, r} v \right\rangle_{\Omega \times \mathcal{P}} = \langle f, v \rangle_{\Omega \times \mathcal{P}}, \quad (4.3)$$

where $\langle \bullet \rangle_{\Omega, \mathcal{P}}$ is a short-hand for $\int_{\Omega} \langle \bullet \rangle_{\mathcal{P}} dx$.

We first collect the $O(\epsilon^{-1})$ terms in (4.3):

$$\left\langle \sum_{r \in \mathcal{R}} V'_r(\nabla_{x, \mathcal{R}} u^0 + D_{y, \mathcal{R}} u^1), D_{y, r} v \right\rangle_{\Omega \times \mathcal{P}} = 0.$$

As usual in homogenization we write the solution of this equation (of course, equipped with the zero-average boundary conditions) as $u^1(x, y) = \chi(\nabla_x u^0(x); y) + \bar{u}^1(x)$, where $\chi = \chi(\mathbf{F}; y) : \mathbb{R}^{d \times d} \times \mathcal{P} \rightarrow \mathbb{R}^d$ solves

$$\text{find } \chi(\mathbf{F}, \bullet) \in \mathcal{U}_{\#}(\mathcal{P}) \text{ s.t. } \left\langle \sum_{r \in \mathcal{R}} V'_r(\mathbf{F}\mathcal{R} + D_{y, \mathcal{R}} \chi(\mathbf{F})), D_{y, r} \sigma \right\rangle_{\mathcal{P}} = 0 \quad \forall \sigma \in \mathcal{U}_{\#}(\mathcal{P}). \quad (4.4)$$

To obtain the equation for the homogenized solution $u^0(x)$, we collect the $O(\epsilon^0)$ terms in (4.3) and use the test function \bar{v} of x only:

$$\left\langle \sum_{r \in \mathcal{R}} V'_r(\nabla_{x, \mathcal{R}} u^0 + D_{y, \mathcal{R}} u^1), \nabla_{x, r} \bar{v} \right\rangle_{\Omega \times \mathcal{P}} = \langle f, \bar{v} \rangle_{\Omega \times \mathcal{P}}.$$

This leads to the homogenized equation

$$\langle \delta\Phi^0(\nabla_x u^0), \nabla_x \bar{v} \rangle_{\Omega} = \langle f, \bar{v} \rangle_{\Omega}, \quad (4.5)$$

or equivalently in the strong form $-\nabla_x \cdot \delta\Phi^0(\nabla_x u^0) = f(x)$, where $\delta\Phi^0 : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}^{d \times d}$ satisfies

$$\delta\Phi^0(\mathbf{F}) = \left\langle \sum_{r \in \mathcal{R}(y)} V'_r(\mathbf{F}\mathcal{R} + D_{y, \mathcal{R}} \chi(\mathbf{F})) r^{\top} \right\rangle_{y \in \mathcal{P}}. \quad (4.6)$$

Thus, we obtained the equation for the homogenized displacement u^0 with the homogenized tensor $\delta\Phi^0$. For the equation (4.5) to have a unique solution, it has to be supplemented with boundary conditions, for instance by requiring that u^0 is periodic and has zero average.

As an illustrative example, in the case of 1D with a pair interaction potential we can write $V(D_{\mathcal{R}(y)} u; y) = \sum_{r \in \mathcal{R}(y)} \Phi_r(D_r u; y)$ (cf. the Lennard-Jones potential in (2.1)), consequently,

$$\delta\Phi^0(F) = \left\langle \sum_{r \in \mathcal{R}(y)} \Phi'_r(Fr + D_{y, r} \chi(F)) r \right\rangle_{y \in \mathcal{P}},$$

where the derivative of Φ_r is with respect to F .

Remark 4.1. *In the above formal arguments we assumed, for simplicity, that the external force f is a continuous function of x and moreover does not depend on y , i.e., $f = f(x)$, $x \in \Omega$. We emphasize that oscillatory external forces could also be considered. The homogenized equation would then depend on a proper average of the external forces. The assumption that f is a function of the continuous variable x can later be relaxed once the homogenized equations are discretized on a finite element mesh.*

4.1.1 Underlying Homogenized Energy

It is useful to highlight one more feature of the homogenized equations.

Proposition 4.1. *The function $\delta\Phi^0(\mathbf{F})$ defined by (4.6) is the derivative of the following function*

$$\Phi^0(\mathbf{F}) := \langle V(\mathbf{F}\mathcal{R} + D_{y,\mathcal{R}}\chi(\mathbf{F})) \rangle_{y \in \mathcal{P}} \quad (4.7)$$

w.r.t. \mathbf{F} .

Proof. Compute the variation of (4.7) w.r.t. \mathbf{F} :

$$\delta\Phi^0(\mathbf{F}) : \mathbf{G} = \left\langle \sum_{r \in \mathcal{R}} V'_r(\mathbf{F}\mathcal{R} + D_{y,\mathcal{R}}\chi(\mathbf{F})) \cdot (\mathbf{G}r + D_{y,\mathcal{R}}\delta\chi(\mathbf{F}) : \mathbf{G}) \right\rangle_{y \in \mathcal{P}}. \quad (4.8)$$

Since $\delta\chi(\mathbf{F}) : \mathbf{G} \in \mathcal{U}_{\#}(\mathcal{P})$, the second term in (4.8) drops due to (4.4) and we have

$$\delta\Phi^0(\mathbf{F}) : \mathbf{G} = \left\langle \sum_{r \in \mathcal{R}} V'_r(\mathbf{F}\mathcal{R} + D_{y,\mathcal{R}}\chi(\mathbf{F})) \cdot \mathbf{G}r \right\rangle_{y \in \mathcal{P}} = \left\langle \sum_{r \in \mathcal{R}} V'_r(\mathbf{F}\mathcal{R} + D_{y,\mathcal{R}}\chi(\mathbf{F})) r^\top : \mathbf{G} \right\rangle_{y \in \mathcal{P}},$$

which is consistent with (4.6). \square

Corollary 4.2. *The equations (4.5) can be written as*

$$\langle \delta E^0(u^0), v \rangle_\Omega = \langle f, v \rangle_\Omega,$$

where

$$E^0(u^0) := \int_\Omega \Phi^0(\nabla u^0) dx. \quad (4.9)$$

The fact that the homogenized equations have an underlying energy may be important in some applications where, for instance, one chooses to use nonlinear conjugate gradient algorithms or needs to check for stability of numerical solutions.

4.2 Application of Homogenization to the Simplified Model

For the simplified model described in Section 2.2, the cell problem (4.4) in the strong form reads

$$D_{y,-r}(\psi(Fr + D_{y,r}\chi(F))) = 0.$$

where $r = \frac{1}{m}$ and $\psi(y) := \psi_\epsilon(\epsilon y)$. Its solution can be written as

$$D_{y,r}\chi(F) = \frac{C}{\psi} - Fr. \quad (4.10)$$

with $C = Fr \langle 1/\psi \rangle_{\mathcal{P}}$, and \mathcal{P} given by (2.7). The homogenized energy density is therefore

$$\Phi^0 = \langle \psi \frac{1}{2} (Fr + D_{y,r}\chi)^2 \rangle_{\mathcal{P}} = \left\langle \psi \frac{1}{2} \left(Fr + \frac{C}{\psi} - Fr \right)^2 \right\rangle_{\mathcal{P}} = \frac{1}{2} \frac{C^2}{\langle 1/\psi \rangle_{\mathcal{P}}} = \langle 1/\psi \rangle_{\mathcal{P}}^{-1} \frac{(Fr)^2}{2}, \quad (4.11)$$

which yields the homogenized energy

$$E^0(u^0) = \int_0^1 \langle 1/\psi \rangle_{\mathcal{P}}^{-1} \frac{(\nabla_r u^0)^2}{2} dx,$$

with the correct form of the effective spring constant $\psi^0 = \langle 1/\psi \rangle_{\mathcal{P}}^{-1}$.

We emphasize that this procedure and the obtained results are well-known for PDEs [8, Chap. 1], and are in agreement with the equations obtained using the multilattice CB rule (Section 3.3).

4.3 Discrete Homogenization

Homogenization effectively upscales the discrete problem with microstructure to a continuous problem of nonlinear elasticity. One can, however consider another approach where the upscaled model is a discrete model with no microstructure.

For that, one assumes that x is discrete, $x \in \mathcal{L}$, and approximates $D_{x,r}\bullet \approx (D_x\bullet)r$ in (4.2), where $D_x u(x) \in \mathbb{R}^{d \times d}$ is the discrete gradient of $u \in \mathcal{U}_{\text{per}}(\mathcal{L})$ at the point $x \in \mathcal{L}$ defined as $(D_x u(x))e_k = D_{x,e_k} u(x)$, $k = 1, \dots, d$. Following the above procedure of asymptotic expansion one gets the upscaled equation

$$\langle \delta\Phi^0(D_x u^0), D_x v \rangle_{\mathcal{L}} = \langle f, v \rangle_{\mathcal{L}} \quad \forall v \in \mathcal{U}_{\#}(\mathcal{L}), \quad (4.12)$$

where $\delta\Phi^0$ is defined by (4.6), the same equation as for the continuum homogenization.

Thus, we obtained the equation for the homogenized displacement u^0 with the homogenized tensor $\delta\Phi^0$. The homogenized tensor $\delta\Phi^0$ no longer depends on the fast variable y and therefore we can apply the standard QC method to the homogenized equation (4.12). Again, to ensure a unique solution for (4.12) we search for $u^0 \in \mathcal{U}_{\#}(\mathcal{L})$ (see the preprint [4] for more details).

One of the advantages of the discrete homogenization is that it is not required to assume a continuous force f . Another advantage is that the discrete homogenization can potentially be helpful in deriving effective interaction potentials, for instance by averaging over the temperature-related oscillations of atoms around their equilibrium positions.

5 Homogenized QC

We formulate a numerical macro-to-micro method for treating multilattices, which we call the homogenized quasicontinuum method (HQC). We introduce HQC in the framework of numerical homogenization. For the case of materials with known periodic structure (i.e., crystalline materials) the HQC method will be shown to be equivalent to applying finite elements to the homogenized equations (see Theorem 6.1).

Nevertheless, we argue that HQC can be applied to non-crystalline materials and to time-dependent zero-temperature and, possibly, finite-temperature problems. Indeed, in Section 7 we give an application of HQC to a stochastic material and in Section 8 we present an application of HQC to a 1D time-dependent zero-temperature evolution. In addition, the HQC serves a convenient framework for the error analysis [3, 4].

We present the HQC algorithm assuming that the microstructure is a function of the macroscopic displacement. A reformulation analogous to the concurrent coupling of [37] is also possible (cf. also Remark 3.2).

5.1 HQC Method

The method will be presented using macro-to-micro framework as used in some numerical homogenization procedures [1, 18, 26, 32, 41]. We present the method for the case when the external force $f = f_\epsilon$ may be microstructure-dependent.

5.1.1 Macroscopic affine displacement

We again assume a partition \mathcal{T}_h of the domain Ω into simplicial elements T , recall the definition of the space $\mathcal{U}_{\text{per}}^h$, (3.1), and introduce its subspace of zero-mean functions $\mathcal{U}_{\#}^h \subset \mathcal{U}_{\text{per}}^h$.

5.1.2 Sampling Domains

We choose a representative position $x_T^{\text{rep}} \in \mathcal{L}$ and a sampling domain $S_T^{\text{rep}} := x_T^{\text{rep}} + \epsilon\mathcal{P}$ associated with each $T \in \mathcal{T}_h$. The sampling domain is normally chosen inside T (the mesh can be highly refined in certain regions and therefore some sampling domains S_T^{rep} may be bigger than T). However, in the problems of coupling fully atomistic and coarse-grained equations, the mesh may be non-uniform and some $T \in \mathcal{T}_h$ may be too small to accommodate a sampling domain fully inside T .

The sampling domains have the associated operator of averaging over the sampling domain, $\langle \bullet \rangle_{x \in S_T^{\text{rep}}}$ and the functional space $\mathcal{U}_{\#}(S_T^{\text{rep}}) = \mathcal{U}_{\#}(\epsilon\mathcal{P})$ (see (A.1) for the precise definition).

5.1.3 Energy and Macro Nonlinear Form

Define the atomistic interaction energy of the HQC method

$$E^{\text{hqc}}(u^h) := \sum_{T \in \mathcal{T}_h} |T| \langle V_{\epsilon}(D_{\mathcal{R}_{\epsilon}} R_T(u^h)) \rangle_{x \in S_T^{\text{rep}}}, \quad (5.1)$$

where $R_T(u^h)$, defined by (5.3), is the microfunction constrained by u^h in the sampling domain S_T^{rep} .

The functional derivative of the above energy reads

$$\langle \delta E^{\text{hqc}}(u^h), v^h \rangle_{\Omega} = \sum_{T \in \mathcal{T}_h} |T| \left\langle \sum_{r \in \mathcal{R}_{\epsilon}} V'_{\epsilon,r}(D_{\mathcal{R}_{\epsilon}} R_T(u^h)), D_r \delta R_T(u^h) v^h \right\rangle_{x \in S_T^{\text{rep}}}, \quad (5.2)$$

where $\delta R_T(u^h)$ is the functional derivative of the reconstruction $R_T(u^h)$ defined below.

5.1.4 Microproblem

Given a function $u^h \in \mathcal{U}_{\text{per}}^h$, $R_T(u^h)$ is a function such that $R_T(u^h) - u_{\text{lin}}^h \in \mathcal{U}_{\#}(S_T^{\text{rep}})$ and

$$\left\langle \sum_{r \in \mathcal{R}_{\epsilon}} V'_{\epsilon,r}(D_{\mathcal{R}_{\epsilon}} R_T(u^h)), D_r s \right\rangle_{x \in S_T^{\text{rep}}} = 0 \quad \forall s \in \mathcal{U}_{\#}(S_T^{\text{rep}}), \quad (5.3)$$

where u_{lin}^h is an affine extrapolation of $u^h|_T$ over the entire \mathbb{R}^d . If $S_T^{\text{rep}} \subset T$ then u_{lin}^h can be substituted with u^h .

Remark 5.1. *When modeling essentially nonlinear phenomena (e.g., martensite-austenite phase transformation), one should require that the microstructure corresponds to a stable equilibrium. That is, one should require, in addition to (5.3), that $w = R_T(u^h) - u_{\text{lin}}^h \in \mathcal{U}_{\#}(S_T^{\text{rep}})$ is a local minimum of $\langle V_{\epsilon}(D_{\mathcal{R}_{\epsilon}}(u_{\text{lin}}^h + w)) \rangle_{x \in S_T^{\text{rep}}}$ [40, p. 238].*

Remark 5.2. *In the case of linear interaction, the reconstruction R_T is a linear function and hence $\delta R_T(u^h) v^h = R_T(v^h)$, which makes the derivative of the HQC energy (5.2) take the form*

$$\langle \delta E^{\text{hqc}}(u^h), v^h \rangle_{\Omega} = \sum_{T \in \mathcal{T}_h} |T| \left\langle \sum_{r \in \mathcal{R}_{\epsilon}} V'_{\epsilon,r}(D_{\mathcal{R}_{\epsilon}} R_T(u^h)), D_r R_T(v^h) \right\rangle_{x \in S_T^{\text{rep}}}.$$

Remark 5.3. *The functional derivative of the HQC energy (5.2) can equivalently be written as*

$$\langle \delta E^{\text{hqc}}(u^h), v^h \rangle_\Omega = \sum_{T \in \mathcal{T}_h} |T| \left\langle \sum_{r \in \mathcal{R}_\epsilon} V'_{\epsilon,r}(D_{\mathcal{R}_\epsilon} R_T(u^h)), (\nabla_r v^h|_T) \right\rangle_{x \in S_T^{\text{rep}}}, \quad (5.4)$$

by noting that $D_r \delta R_T(u^h) v^h = D_r v_{\text{lin}}^h + (D_r \delta R_T(u^h) v^h - D_r v_{\text{lin}}^h)$, that

$$\sum_{r \in \mathcal{R}_\epsilon} \langle V'_{\epsilon,r}(D_{\mathcal{R}_\epsilon} R_T(u^h)), (D_r \delta R_T(u^h) v^h - D_r v_{\text{lin}}^h) \rangle_{x \in S_T^{\text{rep}}} = 0,$$

in view of (5.3), and that $D_r v_{\text{lin}}^h = \nabla_r v^h$ on each T . Here we used the fact that $\delta R_T(u^h) v^h - v_{\text{lin}}^h \in \mathcal{U}_\#(S_T^{\text{rep}})$ which follows from taking the functional derivative of $R_T(u^h) - u_{\text{lin}}^h \in \mathcal{U}_\#(S_T^{\text{rep}})$.

5.1.5 Reconstruction

The functions $R_T(u^h)$ describe the microstructure of the solution inside each S_T^{rep} . One can reconstruct the solution describing the microstructure, $u^{h,c}$, from the homogenized solution u^h by combining $R_T(u^h)$ into a single function defined on entire atomistic lattice \mathcal{M} :

$$u^{h,c}(x) = R_T(u^h)(x) \quad (x \in T \cap \mathcal{M}). \quad (5.5)$$

That is, we effectively extend $R_T(u^h)$ periodically on each T . It should be noted that (5.5) does not uniquely determine $u^{h,c}(x)$ if $x \in \partial T$ for some $T \in \mathcal{T}_h$.

5.1.6 Variational Problem

We define the homogenized quasicontinuum approximation as the solution $u^h \in \mathcal{U}_\#^h$ of

$$\langle \delta E^{\text{hqc}}(u^h), v^h \rangle_\Omega = F^{\text{hqc}}(v^h) \quad \forall v^h \in \mathcal{U}_\#^h \quad (5.6)$$

where

$$F^{\text{hqc}}(v^h) = \sum_{T \in \mathcal{T}_h} |T| \langle f_\epsilon, v^h \rangle_{x \in S_T^{\text{rep}}}. \quad (5.7)$$

If the external force is smooth, it could instead be evaluated for a single representative atom.

In the case of linear nearest-neighbor 1D interaction it can be shown that (5.7) is well-posed and that the homogenized quasicontinuum solution u^h approximates the solution u of the original equations only in the L_2 -norm. To get a good approximation in the H^1 -norm, the reconstructed solution $u^{H,c}$ should instead be considered. We will report the analysis for the nonlinear case in a separate paper (see the preprint [4, Theorems 4 and 5] for the analysis of a linear model).

5.2 HQC Algorithm

The problem (5.6) is nonlinear and its practical implementation is usually done by the Newton's method. We briefly sketch below an algorithm for solving (5.6).

For the Newton's method we need to compute the second derivative of the energy (5.1):

$$\langle \delta^2 E^{\text{hqc}}(u^h) w^h, v^h \rangle_\Omega = \sum_{T \in \mathcal{T}_h} |T| \left\langle \sum_{r,\rho \in \mathcal{R}_\epsilon} V''_{\epsilon,r,\rho}(D_{\mathcal{R}_\epsilon} R_T(u^h)) D_\rho \delta R_T(u^h) w^h, D_r \delta R_T(u^h) v^h \right\rangle_{x \in S_T^{\text{rep}}}. \quad (5.8)$$

5.2.1 Newton's Iterations for the Macroproblem

The algorithm based on the Newton's method consists in choosing an initial guess $u^{h,(0)} \in U_{\#}^h$ and performing iterations

$$\langle \delta^2 E^{\text{hqc}}(u^{h,(n)})(u^{h,(n+1)} - u^{h,(n)}), v^h \rangle_{\Omega} = F^{\text{hqc}}(v^h) \quad \forall v^h \in \mathcal{U}_{\#}^h, \quad (5.9)$$

until $u^{h,(n+1)}$ becomes close to $u^{h,(n)}$ in a chosen norm.

To solve the linear system (5.9) for $u^{h,(n+1)} - u^{h,(n)} \in \mathcal{U}_{\#}^h$, we choose a nodal basis w_k^h ($1 \leq k \leq K$) of $\mathcal{U}_{\text{per}}^h$. One way to satisfy the condition $\langle u^h \rangle_{\Omega} = 0$ would be to perform all the computations with one basis function eliminated (e.g., to consider w_k^h for $2 \leq k \leq K$), and post-process the final solution as $u^h - \langle u^h \rangle_{\Omega}$.

The stiffness matrix of the system (5.9) will thus be

$$A_{lm} = \langle \delta^2 E^{\text{hqc}}(u^{h,(n)})w_l^h, w_m^h \rangle_{\Omega}$$

and the load vector will be

$$b_m = F^{\text{hqc}}(w_m^h).$$

As given by the formula (5.8) we need to compute the solution of microproblem $R_T(u^{h,(n)})$ on each sampling domain S_T^{rep} as well as its derivative $\delta R_T(u^{h,(n)})w_l^h$.

5.2.2 Solution of the Microproblem

The microproblem (5.3) can also be solved with Newton's method. For that, in each T one needs to choose an initial guess $u^{(n,0)}$ to $R_T(u^{h,(n)})$, for instance $u^{(n,0)}(x) := u^{h,(n)}(x)$ and solve

$$\left\langle \sum_{r \in \mathcal{R}_{\epsilon}} V'_{\epsilon,r}(D_{\mathcal{R}_{\epsilon}} u^{(n,\nu)}) + \sum_{r,\rho \in \mathcal{R}_{\epsilon}} V''_{\epsilon,r,\rho}(D_{\mathcal{R}_{\epsilon}} u^{(n,\nu)}) D_{\rho}(u^{(n,\nu+1)} - u^{(n,\nu)}), D_r s \right\rangle_{x \in S_T^{\text{rep}}} = 0$$

$$\forall s \in \mathcal{U}_{\#}(S_T^{\text{rep}}),$$

with respect to $u^{(n,\nu+1)}$ constrained by $u^{(n,\nu+1)} - u_{\text{lin}}^{h,(n)} \in \mathcal{U}_{\#}(S_T^{\text{rep}})$, until the difference between $u^{(n,\nu+1)}$ and $u^{(n,\nu)}$ is small in a chosen norm.

After that, we can compute $\delta R_T w_l^h = \delta R_T(u^{h,(n)})w_l^h$ by solving

$$\left\langle \sum_{r,\rho \in \mathcal{R}_{\epsilon}} V''_{\epsilon,r,\rho}(D_{\mathcal{R}_{\epsilon}} u^{(n,\nu)}) D_{\rho}(\delta R_T w_l^h), D_r s \right\rangle_{x \in S_T^{\text{rep}}} = 0 \quad \forall s \in \mathcal{U}_{\#}(S_T^{\text{rep}}) \quad (5.10)$$

constrained by $\delta R_T w_l^h - (w_l^h)_{\text{lin}} \in \mathcal{U}_{\#}(S_T^{\text{rep}})$. Notice that the gradient of all but $d+1$ basis functions $D_r(w_l^h)_{\text{lin}}$ inside T are zero, which implies that we essentially need to solve the problem (5.10) $d+1$ times.

Also observe that when computing $\delta R_T(u^{h,(n)})w_l^h$, we need to invert the same linear operator as in the final Newton's iteration, which allows for some additional optimization.

5.2.3 Possible Modifications of the Algorithm

First, notice that when solving for $u^{h,(n+1)}$ we could linearize the problem on the previous iteration $u^{h,(n)}$. In that case we would have linear cell problems and thus we would need only outer Newton's iteration, but it would be required to keep the values of the micro-solution $R_T(u^{h,(n)})$ from the previous iteration. We notice however that for a practical implementation of the above algorithm it may also be required to keep the values of the micro-solution: one needs these values to initialize the inner Newton iterations; depending on the initial guess for the microproblem the iterations may converge to a wrong microstructure.

Another modification could be to compute the contribution of the external force f_ϵ in (5.7) for a single atom in the case of no oscillations in f_ϵ .

In the case of linear interaction, the algorithm becomes simpler: one does not need to do Newton iterations. Nevertheless, the algorithm in Section 5.2 is applicable to the linear problem where it converges in just one iteration.

6 Equivalence of Numerical Methods for Multilattices

In this section we show the equivalence of three different methods for computing equilibrium of multilattice crystals, namely (1) the proposed HQC method, (2) finite element discretization of continuum homogenization, and (3) multilattice QC. We assume that in all four methods the external force f is approximated by the same function f^h .

Below we specify the four methods that we compare. It should be noted that given the macroscopic displacement u^h we cannot guarantee uniqueness of the energy as there may be several solutions to the micro-problems corresponding to different phases of a multilattice crystal. To address such non-uniqueness, we treat the energy and all the respective microfunctions as multi-valued (i.e., set-valued) functions of $u^h \in \mathcal{U}_\#^h$ and prove that these multi-valued functions coincide on each $u^h \in \mathcal{U}_{\text{per}}^h$.

Method 1. (HQC) We define the energy of the HQC method, $E^{\text{hqc}}(u^h)$, by (5.1), where $R_T(u^h)$ is the set of all solutions of (5.3).

Method 2. (FEM for homogenized equations) The energy of FEM discretization of the homogenized energy is $E^0(u^h)$ given by (4.9), and (4.7), and $\chi = \chi(\mathbf{F}; y)$ is a set of all solutions of (4.4).

Method 3. (Multilattice QC) $E^{\text{mqc}}(u^h)$ is defined by (3.7) and $\mathbf{q}^h = \mathbf{q}(\nabla u^h)$ by (3.6).

Theorem 6.1. $E^{\text{hqc}}(u^h) = E^0(u^h) = E^{\text{mqc}}(u^h)$ for any $u^h \in \mathcal{U}_{\text{per}}^h$.

Proof. Part 1, $E^{\text{hqc}}(u^h) = E^0(u^h)$. First, we show that the micro-functions of Methods 1 and 2, R_T and χ , are related through

$$(R_T(u^h))(x) = u_{\text{lin}}^h(x) + \epsilon \chi(\nabla u^h|_T; \frac{x}{\epsilon}). \quad (6.1)$$

Indeed, denote $\mathbf{F} = \nabla u^h|_T$ and compute $D_r R_T(u^h)$:

$$D_r R_T(u^h) = D_r u_{\text{lin}}^h + \epsilon D_r \chi(\mathbf{F}; \frac{x}{\epsilon}) = \mathbf{F}r + D_{y,r} \chi(\mathbf{F}; \frac{x}{\epsilon}). \quad (6.2)$$

The following calculation shows that the left-hand sides of (5.3) and (4.4) coincide up to a factor ϵ^{-1} :

$$\begin{aligned} \left\langle \sum_{r \in \mathcal{R}} V'_{\epsilon, r}(D_{\mathcal{R}_\epsilon} R_T(u^h); x), D_r s(x) \right\rangle_{x \in S_T^{\text{rep}}} &= \left\langle \sum_{r \in \mathcal{R}} V'_r(D_{\mathcal{R}(y)} R_T(u^h); y), \epsilon^{-1} D_{y, r} s(\epsilon y) \right\rangle_{y \in \mathcal{P}} \\ &= \epsilon^{-1} \left\langle \sum_{r \in \mathcal{R}} V'_r(\mathbf{F}\mathcal{R} + D_{y, \mathcal{R}} \chi(\mathbf{F}; y); y), D_{y, r} \sigma(y) \right\rangle_{y \in \mathcal{P}} \end{aligned}$$

where we do the change of the independent variable $y = \frac{x}{\epsilon}$, and of the test function $\sigma(y) = s(\epsilon y)$. Hence (6.1) indeed relates the set of solutions of (5.3) and (4.4) with $\mathbf{F} = \nabla u^h|_T$.

The following straightforward calculation concludes the proof of $E^{\text{hqc}}(u^h) = E^0(u^h)$:

$$\begin{aligned} E^{\text{hqc}}(u^h) &= \sum_{T \in \mathcal{T}_h} |T| \langle V_\epsilon(D_{\mathcal{R}_\epsilon} R_T(u^h)) \rangle_{x \in S_T^{\text{rep}}} \\ &= \sum_{T \in \mathcal{T}_h} |T| \langle V_\epsilon((\nabla u^h|_T) \mathcal{R}_\epsilon + D_{y, \mathcal{R}_\epsilon} \chi(\nabla u^h|_T; \frac{x}{\epsilon})) \rangle_{x \in S_T^{\text{rep}}} \\ &= \sum_{T \in \mathcal{T}_h} |T| \langle V((\nabla u^h|_T) \mathcal{R} + D_{y, \mathcal{R}} \chi(\nabla u^h|_T; y)) \rangle_{y \in \mathcal{P}} \\ &= \sum_{T \in \mathcal{T}_h} |T| \Phi^0(\nabla u^h|_T) = E^0(u^h), \end{aligned}$$

where we used (6.2) in the first step of this calculation.

Part 2, $E^{\text{hqc}}(u^h) = E^{\text{mqc}}(u^h)$. The main component of the proof consists in fixing $T \in \mathcal{T}_h$ and showing that $q_\alpha^h|_T$ and $R_T(u^h)$ are related through

$$q_\alpha^h|_T = U(\epsilon p_\alpha) - U(0), \quad \alpha = 0, \dots, m-1, \quad (6.3)$$

where $U := R_T(u^h) - u_{\text{lin}}^h \in \mathcal{U}_\#(S_T^{\text{rep}})$.

First, we define $\tilde{q}_\alpha^h|_T := U(\epsilon p_\alpha) - U(0)$. Notice that due to $\epsilon\mathcal{P}$ -periodicity of U , we can write

$$U(x) = \sum_{\alpha=0}^{m-1} U(\epsilon p_\alpha) w_\alpha(x),$$

subtracting the constant $U(0)$ and applying D_r yields

$$\begin{aligned} D_r U(x) &= D_r \left(-U(0) + \sum_{\alpha=0}^{m-1} U(\epsilon p_\alpha) w_\alpha(x) \right) \\ &= D_r \left(\sum_{\alpha=1}^{m-1} U(\epsilon p_\alpha) w_\alpha(x) \right) \\ &= D_r \sum_{\alpha=1}^{m-1} (\tilde{q}_\alpha^h|_T) w_\alpha(x), \end{aligned}$$

where we used the identity $\sum_{\alpha=0}^{m-1} w_\alpha(x) = 1$ for all $x \in \mathcal{M}$.

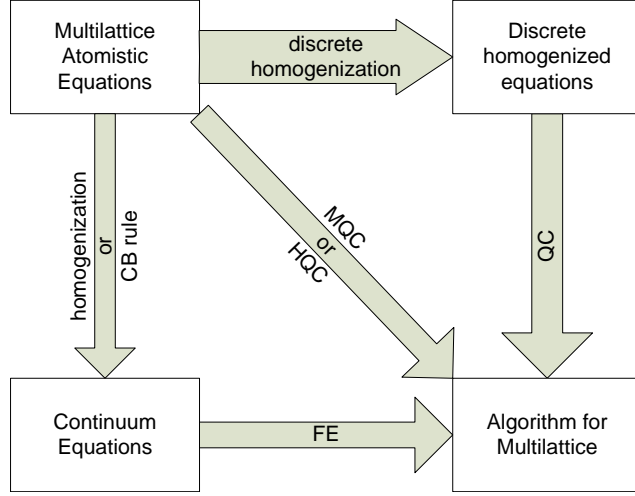


Figure 3: Equivalence of different methods

We then substitute $q_\alpha^h|_T = \tilde{q}_\alpha^h|_T$ into (3.6). The argument of V_ϵ in (3.6) can be written as

$$\begin{aligned} (\nabla u^h|_T)\mathcal{R}_{\epsilon,\beta} + \sum_{\alpha=1}^{m-1} (\tilde{q}_\alpha^h|_T)D_{\mathcal{R}_{\epsilon,\beta}}w_\alpha(\epsilon p_\beta) &= D_{\mathcal{R}_{\epsilon,\beta}}\left(u_{\text{lin}}^h + \sum_{\alpha=1}^{m-1} (\tilde{q}_\alpha^h|_T)w_\alpha(\epsilon p_\beta)\right) \\ &= D_{\mathcal{R}_{\epsilon,\beta}}\left(u_{\text{lin}}^h + U(\epsilon p_\beta)\right) = D_{\mathcal{R}_{\epsilon}(x)}R_T(u^h)(x)|_{x=\epsilon p_\beta} \end{aligned} \quad (6.4)$$

and therefore, upon noticing that summations over $x = \epsilon p_\beta$ and over $x \in S_T^{\text{rep}}$ coincide for the $\epsilon\mathcal{P}$ -periodic functions, we conclude that the left-hand sides of (3.6) and (5.3) coincide when $s(x)$ is chosen as $s(x) = w_\gamma(x) - \langle w_\gamma(x) \rangle_{x \in \epsilon\mathcal{P}}$, $\gamma = 1 \dots, m-1$ (then $D_r s = D_r w_\gamma$). This proves that $\tilde{q}_\alpha^h|_T$ satisfies (3.6), i.e., $q_\alpha^h|_T \supset \tilde{q}_\alpha^h|_T = U(\epsilon p_\alpha) - U(0)$ (in the sense of the sets of solutions).

To show the converse we notice that (5.3) holds with the function $s(x) = w_\gamma(x)$, $\gamma = 1 \dots, m-1$ and, obviously, with the function $s(x) = 1$. These functions form a basis of $\mathcal{U}_{\text{per}}(\mathcal{P}) = \mathcal{U}_{\text{per}}(S_T^{\text{rep}})$, therefore (5.3) holds with any $s \in \mathcal{U}_\#(S_T^{\text{rep}}) \subset \mathcal{U}_{\text{per}}(S_T^{\text{rep}})$. Hence, $q_\alpha^h|_T \subset U(\epsilon p_\alpha) - U(0)$, which concludes the proof of (6.3).

The stated identity $E^{\text{mqc}}(u^h) = E^{\text{hqc}}(u^h)$ follows directly from (6.4). \square

Remark 6.1. *One can consider yet another approach to coarse-graining multilattices, namely consider the discretely homogenized method (4.12) and apply the standard QC method (see Section 3.2) to it. As a result we will obtain energy of $\langle \Phi^0(\nabla u^h) \rangle_\Omega$ which obviously coincides with the energy of FEM applied to the continuously homogenized equations.*

As a corollary of Theorem 6.1 and Remark 6.1, the solutions corresponding to the different methods considered, being critical points of the energy, also coincide (of course, provided that the external force is treated in the same way for these methods). The Theorem 6.1 is graphically summarized in Fig. 3.

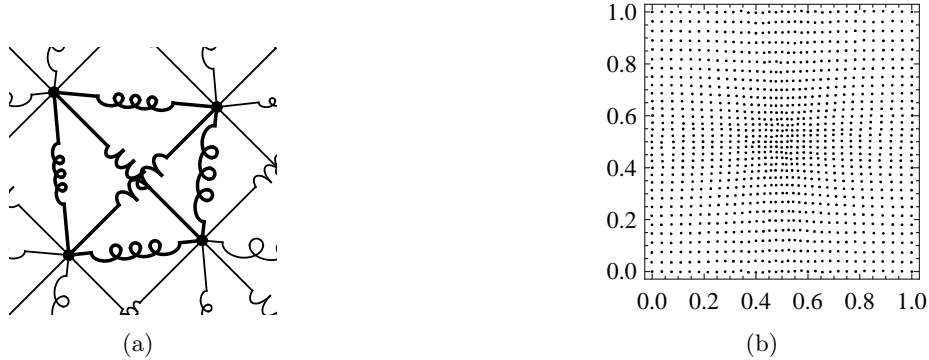


Figure 4: Stochastic atomistic model: An illustration of the model (left) and an exact solution for 32×32 atoms (right).

7 Application of HQC to Stochastic Materials

The HQC method can readily be generalized for non-crystalline materials such as glasses or complex metallic alloys. For that, lacking the period of the microstructure \mathcal{P} , one only needs to take S_T^{rep} large enough to accurately represent the material's microstructure. In this section we present an example of such computation.

Additionally to taking S_T^{rep} large enough, one could also average over an ensemble of samples of different microstructures for a given macroscopic displacement gradient $\nabla u^h|_T$ in each element T ; however, we do not pursue this in the present work. We refer to [10, 27] and references therein for theoretical studies of stochastic homogenization of lattice energies.

We take an atomistic system of 2048×2048 atoms. The atomistic bonds are chosen to have quadratic interaction energy,

$$E(u) = \left\langle \sum_{r \in \mathcal{R}} \frac{1}{2} \psi_{\epsilon, r}(x) (D_r u)^2 \right\rangle_{x \in \mathcal{M}}$$

with $\mathcal{R} = \{(1, 0), (0, 1), (1, 1), (-1, 1)\}$, as illustrated on Fig. 4(a). The bonds' strengths $\psi_{\epsilon, r}$ are randomly generated with a uniform distribution between 0.5 and 10 for $r = (1, 0)$ and $r = (0, 1)$ (i.e., vertical and horizontal bonds) and between 0.1 and 5 for $r = (1, 1)$ and $r = (-1, 1)$ (i.e., diagonal bonds). The external force is chosen as

$$f(x_1, x_2) = 10e^{-\cos(\pi x_1)^2 - \cos(\pi x_2)^2} \begin{pmatrix} \sin(2\pi x_1) \\ \sin(2\pi x_2) \end{pmatrix} - \bar{f},$$

where \bar{f} is determined so that the average of f is zero. The equilibrium configuration for a system with 32×32 atoms is illustrated on Fig. 4(b).

We then apply the HQC algorithm to that system. For the microproblem we choose a subsystem of $N_{\text{rep}} \times N_{\text{rep}}$ atoms and precompute the effective elasticity tensor. We then compute the HQC solution and compare it to the exact solution of the problem. A structured triangular uniform mesh with right-angled triangular elements with the leg size $h = \frac{1}{4}, \frac{1}{8}, \dots$ is used.

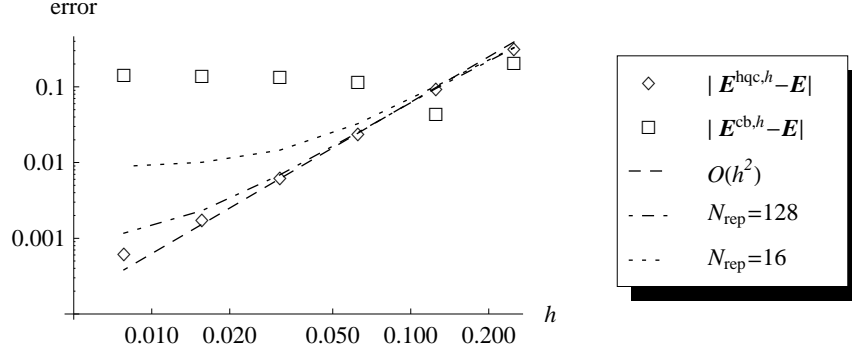


Figure 5: Dependence of relative error of computing the energy with HQC and a straightforward application of the Cauchy-Born rule. The squares and diamonds correspond to $N_{\text{rep}} = 2048$ (i.e., when the microproblem coincides with the entire system). A second-order convergence of HQC is observed whereas the Cauchy-Born rule solution does not converge. The dot-dashed and dotted curves are $|E^{\text{hqc}} - E|$ for $N_{\text{rep}} = 128$ and $N_{\text{rep}} = 16$ respectively.

For comparison, we also produce the results of calculation with (a straightforward application of) the Cauchy-Born rule for computing the effective elasticity tensor; i.e., when atoms are not allowed to relax to equilibrium when an external displacement gradient F is applied.

The relative errors of the interaction energy of HQC and CB solutions (E^{hqc} and E^{cb} , respectively) as compared to the energy of the exact solution E , are plotted in Fig. 5 for different mesh size h and different sampling domain size N_{rep} . A second-order convergence of HQC and absence of convergence of the solution computed according to the Cauchy-Born rule can be observed. One can also see that with $N_{\text{rep}} = 128$ (and even with $N_{\text{rep}} = 16$) one can get a rather accurate numerical solution.

8 Application of HQC to Time-dependent Problems

We apply the proposed HQC method to the 1D zero-temperature evolution of a multilattice, described by the following equations

$$\langle M^\epsilon \ddot{u}, v \rangle_{\mathcal{M}} = \langle \delta E(u), v \rangle_{\mathcal{M}} \quad \forall v \in \mathcal{U}_{\text{per}}(\mathcal{M}) \quad (8.1a)$$

$$u|_{t=0} = u^0 \quad (8.1b)$$

$$\dot{u}|_{t=0} = 0. \quad (8.1c)$$

where $u = u(t, x) \in C^2([0, T]; \mathcal{U}_{\text{per}}(\mathcal{M}))$ is the time-dependent displacement of atom x , $u^0 = u^0(x) \in \mathcal{U}_{\text{per}}(\mathcal{M})$ is the initial displacement, $M^\epsilon(x) = M(\frac{x}{\epsilon})$ is the mass of atom x , $\dot{u} = \frac{d}{dt}u$, $\ddot{u} = \frac{d^2}{dt^2}u$. We assume no external forces.

One can, assuming no fast oscillations in time of the microstructure, perform the two-scale expansion procedure for the time-depend case (which closely follows the continuum case [8])

$$\langle M^0 \ddot{u}, v \rangle_{\mathcal{M}} = \langle \delta E^0(u), v \rangle_{\mathcal{M}} \quad \forall v \in \mathcal{U}_{\text{per}}(\mathcal{M}),$$

where $E^0(u)$ is given by (4.9), and $M^0 = \langle M \rangle_{\mathcal{P}}$ and likewise formulate the macro-to-micro discretization [2, 22]

$$\langle M^0 \ddot{u}^h, v^h \rangle_{\mathcal{M}} = \langle \delta E^{\text{hqc}}(u^h), v^h \rangle_{\mathcal{M}} \quad \forall v \in \mathcal{U}_{\text{per}}^h.$$

For the numerical test we take the same lattices as for the simplified model with $m = 2$ (see Section 2.2). The atoms interact with the Lennard-Jones potential (2.1) with

$$s_{x, x+\epsilon r} = \begin{cases} 0.4 & \frac{x}{\epsilon} \text{ is half-integer} \\ 1.6 & \frac{x}{\epsilon} \text{ is integer,} \end{cases} \quad \ell_{x, x+\epsilon r} = \begin{cases} 1.01 & \frac{x}{\epsilon} \text{ is half-integer} \\ 0.99 & \frac{x}{\epsilon} \text{ is integer,} \end{cases}$$

and the cut-off distance $R = 3$. The masses of atoms are

$$M^\epsilon(x) = \begin{cases} 1 & \frac{x}{\epsilon} \text{ is half-integer} \\ 2 & \frac{x}{\epsilon} \text{ is integer.} \end{cases}$$

The atomistic system contains $\#(\mathcal{M}) = 2^{14}$ atoms.

The initial displacement is chosen in the following way: First, we compute an equilibrium displacement u , i.e., such that $\langle \delta E(u), v \rangle_{\mathcal{M}} = 0 \quad \forall v \in \mathcal{U}_{\text{per}}(\mathcal{M})$. Second, we compute an eigenvector of $\delta^2 E(u)$, u_1 , corresponding to the mode oscillating most slowly. Then, the initial displacement is taken to be $u^0 = u + 0.01 \frac{u_1}{\|Du_1\|_{L^\infty}}$. With such an initial displacement, the solution remains smooth (i.e., most of energy of the solution is contained in long wavelength modes) for times comparable to the oscillation period, and one can compare a QC approximation of the solution with the exact solution.

We compare the reconstructed solution obtained by the HQC discretization in space with the reference solution obtained in the full atomistic computation. The reconstruction of the HQC solution is performed similarly as described in Section 5.1.5. The HQC discretization is performed on a sequence of meshes with $h = \frac{1}{4}, \frac{1}{8}, \dots$. For the time integration, we use the Verlet method with the timestep $\tau = \frac{1}{20}h$ for the HQC solution and $\tau = \frac{1}{20}\epsilon$ for the reference atomistic solution. We run the computation until $T = \frac{1}{20}$, which corresponds to about a quarter of a period of oscillation of the solution.

The errors in (the discrete analogs of) $L^\infty([0, T]; L^2(\Omega))$ and $L^2([0, T]; H^1(\Omega))$ are presented in Fig. 6. One can clearly observe for relatively large h a second order convergence in the $L^2(\Omega)$ -norm and a first order convergence in the $H^1(\Omega)$ -norm, and the convergence seems to stagnate as h is further reduced.

9 Summary and Concluding Remarks

We have considered the problem of equilibrium of multilattice crystalline materials and discussed the application of the (local) QC method [40] for such materials. We then have proposed a homogenization framework and based on it proposed a numerical macro-to-micro method which we called HQC. We have shown that the four methods, namely the HQC method, the QC method applied to the discretely homogenized equations, the multilattice QC, and the finite element method applied to continuously homogenized equations, are equivalent.

Despite equivalence of the methods for statics of multilattice, we argue that the homogenization framework developed in this paper has several advantages. First, it contributes to a better

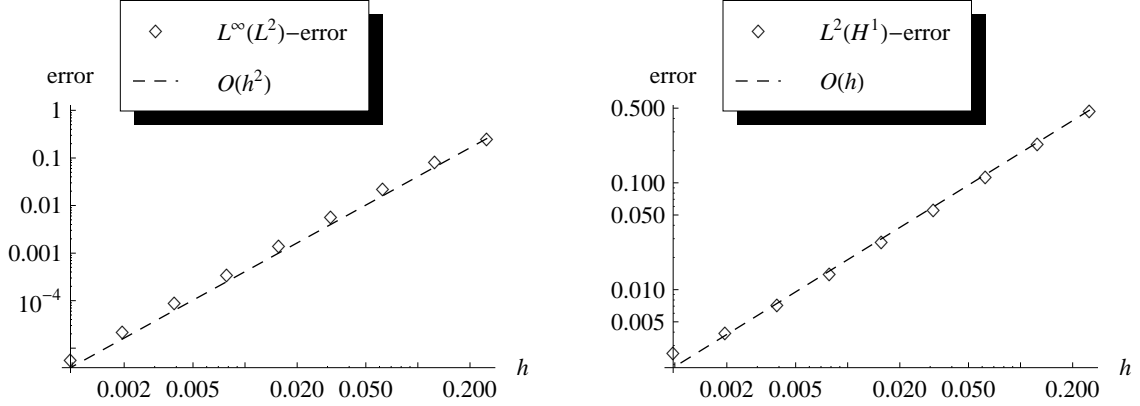


Figure 6: Error of time-dependent solution in (the discrete analogs of) the norms $L^\infty([0, T]; L^2(\Omega))$ (left) and $L^2([0, T]; H^1(\Omega))$ (right).

understanding of the multilattice QC method and provides a link to the existing theory of homogenization of PDEs. In particular, we have generalized and applied the HQC method to the case of random materials and to the unsteady case, numerically demonstrating convergence of the proposed numerical method. Second, the developed homogenization framework allows for application of analytical techniques available in the homogenization theory and thus seems most promising for convergence analysis of numerical methods for multilattices. We refer to our preprint [4] and an ongoing work [3] for an example of such analysis. We also note that the extension of the homogenization technique proposed in this paper to atomistic materials at finite temperature is of high interest.

A Notations

In this appendix we gather the frequently used notations.

A.1 Function spaces

For any finite set $S \subset \mathbb{R}^d$, we define the discrete averaging (integration) operator $\langle \bullet \rangle_S$ by

$$\langle u \rangle_S := \frac{1}{\#(S)} \sum_{x \in S} u(x),$$

and sometimes, more verbosely, as $\langle u(x) \rangle_{x \in S}$. Here $\#(S)$ is the number of elements in the set S .

We consider discrete periodic functions (e.g., displacements or external forces) with the periodic cell $\Omega = (0, 1]^d$ ($d \in \mathbb{N}$), and the lattice (being, actually, the discrete periodic cell) $S \subset \Omega$ ($S = \mathcal{L}, \mathcal{M}$) containing a finite number of points: $\#(S) < \infty$. The periodic extension of the lattice is denoted as $S_{\text{per}} = S + \mathbb{Z}^d$. Such space of periodic functions is denoted as

$$\mathcal{U}_{\text{per}}(S) = \{u : S_{\text{per}} \rightarrow \mathbb{R} : u(x + a) = u(x) \ \forall x \in S, \ \forall a \in \mathbb{Z}^d\}, \quad (\text{A.1})$$

and the space of periodic functions with zero average:

$$\mathcal{U}_{\#}(S) = \{u \in \mathcal{U}_{\text{per}}(S) : \langle u \rangle_S = 0\}.$$

We do not have separate notations for scalar and vector-valued functions and explicitly state whether the function is scalar or vector-valued when it may cause ambiguity.

Similarly to the discrete averaging, we also use continuum averaging notation $\langle u \rangle_{\Omega} := \int_{\Omega} u(x) dx$, and for functions of two variables we write $\langle v \rangle_{S_1 \times S_2} := \langle \langle v \rangle_{S_2} \rangle_{S_1}$, where each S_i ($i = 1, 2$) can be either continuous or discrete.

For vector-valued $u = u(x)$ and $v = v(x)$ we denote the pointwise scalar product as $u \cdot v$ (i.e., $(u \cdot v)(x) = u(x) \cdot v(x)$) and the semi-inner product in $\mathcal{U}_{\text{per}}(\mathcal{L})$ as

$$\langle u, v \rangle_{\mathcal{L}} = \langle u \cdot v \rangle_{\mathcal{L}} = \frac{1}{\#(\mathcal{L})} \sum_{x \in \mathcal{L}} u(x) \cdot v(x).$$

(It is a proper inner product only in $\mathcal{U}_{\#}(\mathcal{L})$.) We similarly define the pointwise scalar product and the (semi-)inner product for functions of continuum variable and for functions of several continuum or discrete variables.

A.2 Operators

For $u : S \rightarrow \mathbb{R}^d$ ($S = \mathcal{L}, \mathcal{M}$) we introduce the finite difference $D_{x,r}u$

$$D_{x,r}u(x) := \frac{u(x + \epsilon r) - u(x)}{\epsilon} \quad (\text{for } x \in S, r \in \mathbb{R}^d \text{ such that } x + \epsilon r \in S).$$

In addition to differentiation operators, we define for $u \in \mathcal{U}_{\text{per}}(\mathcal{L}_1)$, the translation operator $T_x u \in \mathcal{U}_{\text{per}}(\mathcal{L}_1)$

$$T_{x,r}u(x) := u(x + \epsilon r) \quad (\text{for } x \in S, r \in \mathbb{R}^d \text{ such that } x + \epsilon r \in S).$$

The definitions of the discrete derivative and translation generalize to functions of two variables by considering the partial discrete derivative and translation operators, i.e., $D_{x,r}, T_{x,r}$ applied to $u(\bullet, y)$ and $D_{y,r}, T_{y,r}$ applied to $u(x, \bullet)$.

In homogenization we consider “traces on diagonal” of function of two variables, $v = v(x, \frac{x}{\epsilon})$. For such functions we introduce full translation and full derivative operators $T_r := T_{x,r}T_{y,r}$, $D_r := \frac{1}{\epsilon}(T_r - I)$ so that

$$(T_r u)|_{y=\frac{x}{\epsilon}} = T_{x,r} \left(u|_{y=\frac{x}{\epsilon}} \right), \quad \text{and} \quad (D_r u)|_{y=\frac{x}{\epsilon}} = D_{x,r} \left(u|_{y=\frac{x}{\epsilon}} \right). \quad (\text{A.2})$$

The following relates the partial and the full translations and derivatives:

$$T_r = T_{x,r}T_{y,r} \quad \text{and} \quad D_r = D_{x,r}T_{y,r} + \frac{1}{\epsilon}D_{y,r}. \quad (\text{A.3})$$

Notice that the variables x and y are not symmetric in the definition of full derivative. If a function does not depend on y then the full derivative coincides with the derivative in x (likewise for the translation). Hence, for functions of x only, we sometimes omit the subscript x in the operators $D_{x,r}$ and $T_{x,r}$.

For continuous functions we denote ∇u a gradient of u and $\nabla_r u = (\nabla u) \cdot r$ a directional derivative. For a vector-valued function u , the directional derivative, $\nabla_r u$ is defined componentwise and the gradient ∇u is a matrix such that $\nabla_r u = (\nabla u)r$.

A.3 Functions of Vector-indexed Variables

We consider a general form of interaction, where an energy of each atom depends arbitrarily on relative displacements of all the nearby atoms. Namely, for the “interaction neighborhood” $\mathcal{R} = \{r_1, \dots, r_k\}$ we consider functions

$$V(D_{r_1}u, D_{r_2}u, \dots, D_{r_k}u).$$

Since the interaction neighborhood may be different for different atoms (recall that we consider multilattices) and contain different number of neighbors k , we index derivatives directly with $r \in \mathcal{R}$. That is, we use the following notation for tuples α indexed with $r \in \mathcal{R}$:

$$(\alpha_r)_{r \in \mathcal{R}} := (\alpha_{r_1}, \dots, \alpha_{r_k}) \quad \text{for } \mathcal{R} = \{r_1, \dots, r_k\}$$

and define

$$D_{\mathcal{R}}u := (D_r u)_{r \in \mathcal{R}}, \quad \nabla_{\mathcal{R}}u := (\nabla_r u)_{r \in \mathcal{R}}.$$

Thus, for the functions of \mathcal{R} -indexed tuples we write

$$V(D_{\mathcal{R}}u) := V(D_{r_1}u, D_{r_2}u, \dots, D_{r_k}u).$$

The common algebraic operations on \mathcal{R} -indexed tuples are taken componentwise, e.g.:

$$D_{\mathcal{R}}u + D_{\mathcal{R}}v = (D_r u + D_r v)_{r \in \mathcal{R}}, \quad F_{\mathcal{R}} = (F_r)_{r \in \mathcal{R}} \quad \text{etc.}, \quad (\text{A.4})$$

which is fully analogous to the algebraic operations on k -dimensional vectors.

A partial derivative of $V(D_{\mathcal{R}}u)$ w.r.t. $D_r u$ ($r \in \mathcal{R}$) is denoted as $V'_r(D_{\mathcal{R}}u)$.

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