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ANALYSIS OF MULTISCALE METHODS *[1)]

Wei-nan E
(*Department of Mathematics and PACM, Princeton University, USA*)
(*School of Mathematics, Peking University, Beijing 100871, China*)
(*E-mail: weinan@Princeton.EDU*)

Ping-bing Ming
(*LSEC, ICMSEC, Academy of Mathematics and System Sciences, Chinese Academy of Sciences, Beijing 100080, China*)
(*E-mail: mpb@lsec.cc.ac.cn*)

Dedicated to Professor Zhong-ci Shi on the occasion of his 70th birthday

Abstract

The heterogeneous multiscale method gives a general framework for the analysis of multiscale methods. In this paper, we demonstrate this by applying this framework to two canonical problems: The elliptic problem with multiscale coefficients and the quasicontinuum method.

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1. Introduction

In recent years we have seen a tremendous growth of activity on multiscale modelling and computation. Many of these problems and numerical algorithms involve multi-physics [16], i.e. the models at different scales are of very different nature, for example, molecular dynamics at the microscale and continuum mechanics at the macroscale. By coupling the macro-scale and micro-scale models, one hopes to obtain numerical algorithms that have the accuracy of microscale models at a cost comparable to the macroscale models. Many methods have been developed along these lines, including the Car-Parrinello method [12], the quasicontinuum method [39, 27] and more recently the heterogeneous multiscale method (HMM) [15].

The analysis of multiscale methods presents new challenges in numerical analysis. This is particularly true when multi-physics is involved. First of all, there is the issue of what one should take as the "exact solution" that the numerical solution should be compared with. Since multiscale methods typically involve several different components, the error also has several different contributions. Therefore one important point in the analysis of these methods is to be able to separate out these different contributions.

The framework of the heterogeneous multiscale method provides a general strategy both for the design and the analysis of multiscale methods. In this article we will discuss the application of HMM to two different problems. The first is the elliptic PDE with multiscale coefficients. The second is the quasicontinuum method for crystalline solids. We will focus on the analysis of these methods. For other applications and analysis of HMM, we refer to [32].

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2. General Strategy for the Analysis of Multiscale Methods

A general principle for analyzing HMM has been established in [15] and later elaborated in [17, 19, 34] on a variety of homogenization problems, ODEs [14] and stochastic ODEs [18, 41], and on quasicontinuum methods [21]. The common feature of all these problems is that there exists a closed macroscopic model, which may not be explicitly available or are very inefficient to use directly in numerical computations. We can then design multiscale methods using the microscale model and known qualitative features of the macroscale process in order to capture efficiently the macroscale behavior.

There are two main ingredients in HMM: An overall macroscopic scheme for the macroscopic state variable U, and estimating the missing macroscopic data by the microscopic model. Even though the HMM procedure is far more general, rigorous error estimates can only be expected in cases for which a lot is known about the macroscale model, even though it is not explicitly used in the numerical methods.

To analyze HMM, we begin by defining a macroscopic approximation method with the same macroscopic solver as that in HMM. The error between this approximate solution and the macroscopic solution can be analyzed using standard numerical analysis techniques (see [13] for finite element methods, [37] for finite difference methods, [24] for finite volume methods, and [1] for discontinuous Galerkin methods). Next we estimate the error between the HMM solution and the approximate solution of the macroscopic model, due to the fact some of the macroscopic data are estimated using the microscopic model, instead of being given by the macroscopic model itself, this gives us a general statement of the following type:

$$\|U - U_{\mathrm{HMM}}\| \leq C\big(H^k + e(\mathrm{HMM})\big), \tag{2.1}$$

where U_{HMM} is the HMM solution, U is the exact solution of the macroscopic model, k is the order of the macroscopic solver, and H is the step size of the macroscale numerical grid. The norm $\|\cdot\|$ should be chosen according to the specific problem at hand. The second term $e(\mathrm{HMM})$ is the new source of error due to the data estimation. Typically, the error $e(\mathrm{HMM})$ depends on the rate of relaxation of the microscopic state to the local equilibrium, the accuracy of the microscopic solver, and the accuracy of the data-processing step.

Observe that (2.1) bears some similarity to *Strang's Lemma* in finite element methods [13].

3. Application to the Elliptic Homogenization Problem

Consider the classical elliptic problem

$$\begin{cases} -\operatorname{div}\big(a^\varepsilon(x)\nabla u^\varepsilon(x)\big) = f(x) & x \in D \subset \mathbb{R}^d, \\ u^\varepsilon(x) = 0 & x \in \partial D. \end{cases} \tag{3.1}$$

Here ε is a small parameter that signifies the multiscale nature of the coefficient $a^\varepsilon(x)$. Several classical multiscale methodologies have been developed for the numerical solution of (3.1), the most well-known among which is the multigrid technique [10]. These classical multiscale methods are designed to resolve the details of the fine scale problem and are applicable for general problems, i.e., no special assumptions are required for the coefficient $a^\varepsilon(x)$. In contrast modern multiscale methods are designed specifically for recovering partial information about u^ε at a sublinear cost, i.e. the total cost grows sublinearly with the cost of solving the fine scale problem [16]. This is only possible by exploring the special features that $a^\varepsilon(x)$ might have, such as scale separation or self-similarity. The simplest example is when $a^\varepsilon(x) = a(x, x/\varepsilon)$, where $a(x, y)$ can either be periodic in y, in which case we assume the period to be $I = [-1/2, 1/2]^d$, or random but stationary under shifts in y, for each fixed $x \in D$. In both cases, it has been shown that [5, 36]

$$\|u^\varepsilon(x) - U(x)\|_{L^2(D)} \to 0, \tag{3.2}$$

where $U(x)$ is the solution of a homogenized equation:

$$\begin{cases} -\operatorname{div}\big(\mathcal{A}(x)\nabla U(x)\big) &= f(x) & x \in D, \\ U(x) &= 0 & x \in \partial D. \end{cases} \tag{3.3}$$

The homogenized coefficient $\mathcal{A}(x)$ can be obtained from the solutions of the so-called cell problem. In general, there are no explicit formulas for $\mathcal{A}(x)$, except in one dimension.

For (3.1) the macroscopic solver can be chosen as a conventional $\mathcal{P}_k$ finite element method on a triangulation $\mathcal{T}_H$ of element size H. The missing data is the effective stiffness matrix at this scale. This stiffness matrix can be estimated as follows. Assuming that the effective coefficient at this scale is $\mathcal{A}_H(x)$, we approximate $\big(\nabla V \cdot \mathcal{A}_H \nabla V\big)(x_\ell)$ for any $V \in X_H$ by solving the problem:

$$\begin{cases} -\operatorname{div}\big(a^\varepsilon(x)\nabla v_\ell^\varepsilon(x)\big) &= 0 & \text{in } I_\delta(x_\ell), \\ v_\ell^\varepsilon(x) &= V_\ell(x) & \text{on } \partial I_\delta(x_\ell), \end{cases} \tag{3.4}$$

where $I_\delta(x_\ell)$ is a cube of size δ centered at x_ℓ, and V_ℓ is the linear approximation of V at x_ℓ. We then let

$$\big(\nabla V \cdot \mathcal{A}_H \nabla V\big)(x_\ell) \simeq \frac{1}{\delta^d} \int_{I_\delta(x_\ell)} \nabla v_\ell^\varepsilon(x) \cdot a^\varepsilon(x) \nabla v_\ell^\varepsilon(x)\, dx. \tag{3.5}$$

The above two gives the approximate stiffness matrix at the scale H. For convenience, we define the corresponding bilinear form: For any $V, W \in X_H$

$$A_H(V,W) := \sum_{K \in \mathcal{T}_H} \frac{|K|}{\delta^d} \int_{I_\delta(x_\ell)} \nabla v_\ell^\varepsilon(x) \cdot a^\varepsilon(x) \nabla w_\ell^\varepsilon(x)\, dx,$$

where w_ℓ^ε is defined for $W \in X_H$ in the same way as v_ℓ^ε in (3.4) was defined for V.

We used Dirichlet boundary condition in (3.4). Other boundary conditions are possible, such as Neumann and periodic boundary conditions. In order to reduce the effect of the imposed boundary condition on $\partial I_\delta(x_\ell)$, we may choose a smaller cell $I_{\delta'}(x_\ell)$ with $\delta' < \delta$ in order to compute the averages in (3.5). For example, we may choose $\delta' = \delta/2$.

In practice, x_ℓ are the quadrature points of appropriate order (see Figure 1 and (3.7) below), and (3.4) is solved for the basis functions in the finite element space. In addition, $I_\delta(x_\ell)$ does not have to be a cube and does not have to have the same sizes at different locations.

So far the algorithm is completely general. The savings compared with solving the full fine scale problem comes from the fact that we can choose $I_\delta(x_\ell)$ to be smaller than K. The size of $I_\delta(x_\ell)$ is determined by many factors, including the accuracy and cost requirement, the degree of scale separation, and the microstructure in $a^\varepsilon(x)$. If $a^\varepsilon(x) = a(x, x/\varepsilon)$ and $a(x,y)$ is periodic in y, we can simply choose $I_\delta(x_\ell)$ to be $x_\ell + \varepsilon I$, i.e., $\delta = \varepsilon$. If $a(x,y)$ is random, then δ should be a few times larger than the local correlation length of a^ε. In the former case, the total cost is independent of ε. In the latter case, the total cost depends only weakly on ε [33].

The final problem is to solve

$$\min_{V \in X_H} \frac{1}{2} A_H(V,V) - (f,V). \tag{3.6}$$

We introduce the following accuracy conditions for kth-order numerical quadrature scheme [13]:

$$\int_K p(x)\, dx = \sum_{\ell=1}^{L} \omega_\ell |K| p(x_\ell) \quad \forall p(x) \in \mathcal{P}_{2k-2}. \tag{3.7}$$

Here $\omega_\ell > 0$ for $\ell = 1, \cdots, L$ are the weights. For $k = 1$, we assume the above formula to be exact for $p \in \mathcal{P}_1$.

Our main results for the linear problem are as follows. Similar results with some modifications hold for the nonlinear homogenization problems, we refer to [19, §5] for details.

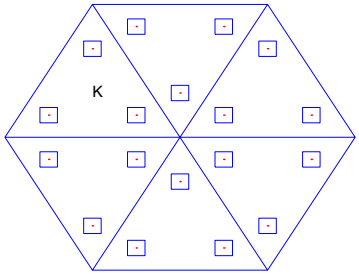

Figure 1: Illustration of HMM for solving (3.1). The dots are the quadrature points. The squares are the microcell $I_\delta(x_\ell)$.

Theorem 3.1. *[19, Theorem 1.1] Denote by U and U_{HMM} the solution of (3.3) and the HMM solution, respectively. Let*

$$e(HMM) = \max_{\substack{x_\ell \in K \\ K \in \mathcal{T}_H}} \|\mathcal{A}(x_\ell) - \mathcal{A}_H(x_\ell)\|,$$

where $\|\cdot\|$ is the Euclidean norm. If U is sufficiently smooth, a^ε is symmetric and uniformly elliptic, and (3.7) holds, then there exists a constant C independent of ε, δ and H, such that

$$\|U - U_{HMM}\|_{H^1(D)} \le C\big(H^k + e(HMM)\big), \tag{3.8}$$

$$\|U - U_{HMM}\|_{L^2(D)} \le C\big(H^{k+1} + e(HMM)\big). \tag{3.9}$$

If there exits a constant C_0 such that $e(HMM)|\ln H| < C_0$, then there exists a constant H_0 such that for all $H \le H_0$,

$$\|U - U_{HMM}\|_{W^{1,\infty}(D)} \le C\big(H^k + e(HMM)\big)|\ln H|. \tag{3.10}$$

At this stage, no assumption on the form of $a^\varepsilon(x)$ is necessary. U can be the solution of an arbitrary macroscopic equation with the same right-hand side as in (3.1). If U_{HMM} were to converge to U, i.e., $e(\mathrm{HMM}) \to 0$, U must be chosen as the solution of the homogenized equation, which we now assume exist [32]. To obtain quantitative estimates on $e(\mathrm{HMM})$, we must restrict ourselves to more specific cases.

Theorem 3.2. *[19, Theorem 1.2] For the periodic homogenization problem, we have*

$$e(HMM) \le \begin{cases} C\varepsilon & \text{if } I_\delta(x_\ell) = x_\ell + \varepsilon I, \\ C\Big(\dfrac{\varepsilon}{\delta} + \delta\Big) & \text{otherwise.} \end{cases}$$

In the first case, we should replace the boundary condition in (3.4) by a periodic boundary condition: $v_\ell^\varepsilon - V_\ell$ is periodic with period εI. For the second case we do not need to assume that the period of $a(x,\cdot)$ is a cube: In fact it can be of arbitrary shape as long as its translation tiles up the whole space.

To discuss the random case, we will use the set-up in [36] and [42]. First we introduce the mixing condition [25]. Let B be a domain in $\mathbb{R}^d$. Denote by $\mathcal{F}(B)$ the $\sigma-$algebra generated by $\{a(y,\omega), y \in B\}$. Let ξ, η be two random variables that are measurable with respect to $\mathcal{F}(B_1)$ and $\mathcal{F}(B_2)$, respectively, then

$$\frac{|\mathbb{E}\xi\eta - \mathbb{E}\xi\mathbb{E}\eta|}{(\mathbb{E}\xi^2)^{1/2}(\mathbb{E}\eta^2)^{1/2}} \le e^{-\lambda q}, \tag{\textbf{A}}$$

where $q = \mathrm{dist}(B_1, B_2)$, $\lambda > 0$ is a fixed constant.

Theorem 3.3. *[19, Theorem 1.3] For the random homogenization problem, assuming that the mixing condition* (**A**) *holds, then we have*

$$\mathbb{E}\, e(HMM) \le \begin{cases} C(\kappa)\Big(\dfrac{\varepsilon}{\delta}\Big)^{\kappa}, & d=3 \\ \textit{remains open}, & d=2 \\ C(\kappa)\Big(\dfrac{\varepsilon}{\delta}\Big)^{1/2}, & d=1 \end{cases}$$

where

$$\kappa = \frac{6-12\gamma}{25-8\gamma}$$

for any $0<\gamma<1/2$. *By choosing* γ *small,* κ *can be arbitrarily close to* $6/25$.

To prove this result, we assume that the cell size in (3.5) is $\delta' = \delta/2$.

In many applications, the microstructure information in $u^\varepsilon(x)$ is very important. $U_{\rm HMM}$ by itself does not give this information. However, this information can be recovered using a simple post-processing technique. For the general case, having $U_{\rm HMM}$, one can obtain locally the microstructural information using an idea in [35]. Assume that we are interested in recovering u^ε and ∇u^ε only in the subdomain $\Omega \subset D$. Consider the following auxiliary problem:

$$\begin{cases} -\operatorname{div}\big(a^\varepsilon(x)\nabla \tilde{u}^{\,\varepsilon}(x)\big) &= f(x) & x\in\Omega_\eta, \\ \tilde{u}^{\,\varepsilon}(x) &= U_{\rm HMM}(x) & x\in\partial\Omega_\eta, \end{cases} \tag{3.11}$$

where Ω_η satisfies $\Omega\subset\Omega_\eta\subset D$ and $\operatorname{dist}(\partial\Omega,\partial\Omega_\eta)=\eta$. We then have

Theorem 3.4. *[19, Theorem 1.4] There exists a constant* C *such that*

$$\Big(\fint_\Omega |\nabla(u^\varepsilon-\tilde{u}^{\,\varepsilon})|^2\,dx\Big)^{1/2} \le \frac{C}{\eta}\big(\|U-U_{HMM}\|_{L^\infty(\Omega_\eta)} + \|u^\varepsilon - U\|_{L^\infty(\Omega_\eta)}\big). \tag{3.12}$$

For the random problem, the last term was estimated in [42].

A much simpler procedure exists for the periodic homogenization problem. Consider the case when $k=1$ and choose $I_\delta = x_K + \varepsilon I$, where x_K is the barycenter of K. Here we have assumed that the quadrature point is at x_K.

Let $\tilde{u}^{\,\varepsilon}$ be defined piecewise as follows:

1. $\tilde{u}^{\,\varepsilon}|_{I_\delta} = v_K^\varepsilon$, where v_K^ε is the solution of (3.4) with the boundary condition that $v_K^\varepsilon - U_{\rm HMM}$ is periodic with period εI and $\int_{I_\delta}(\tilde{u}^{\,\varepsilon}-U_{\rm HMM})(x)\,dx = 0$.
2. $\big(\tilde{u}^{\,\varepsilon}-U_{\rm HMM}\big)|_K$ is periodic with period εI.

For this case, we can prove

Theorem 3.5. *[19, Theorem 1.5] Let* $\tilde{u}^{\,\varepsilon}$ *be defined as above, then*

$$\Big(\sum_{K\in\mathcal{T}_H} \|\nabla(u^\varepsilon-\tilde{u}^{\,\varepsilon})\|_{0,K}^2\Big)^{1/2} \le C(\sqrt{\varepsilon}+H). \tag{3.13}$$

Several other numerical methods have been developed to deal specifically with the case when $a(x,y)$ is periodic in y [2, 3, 8]. An alternative proposal for more general problems but with higher cost is found in [26, 22]. For a more thorough discussion of the different multiscale methods for this classical multiscale problem, we refer to [33].

4. Application to Quasicontinuum Method

In the continuum theory of nonlinear elasticity, we are interested in the displacement field U which minimizes some variational problem of the form

$$\int_D W(\nabla v)\,dx - \int_D f(v)\,dx \tag{4.1}$$

subject to certain boundary condition. Here f is the potential for the external force, and W is the stored energy functional of the material. An important problem is how to get W. It is customary in variational methods to take for granted that W is explicitly given, while in reality the way of getting W is quite empirical and sometimes even crude.

A different approach is quasicontinuum method (QC) proposed in [39, 27] for the analysis of the crystalline solids. It starts with an atomistic model of the type:

$$E\{x_1, \cdots, x_N\} = \sum_{i,j=1}^{N} V_0(r_{ij}) - \sum_{j=1}^{N} f(x_j), \tag{4.2}$$

where V_0 is the interaction potential between atoms, f is again the external potential for the applied force, x_j and y_j are respectively the deformed and undeformed position of the j-th atom, $r_{ij} = |x_i - x_j|$. More general types of atomistic models can be used (see [20] for such examples). But we will write (4.2) to keep the presentation simple.

Let $\mathcal{T}_H$ be again a finite element triangulation of D, and X_H be the vector-valued piecewise linear finite element space on $\mathcal{T}_H$. For any $V \in X_H$, the energy associated with the trial displacement field V is computed as follows. For each element K in $\mathcal{T}_H$, denote by $E_K(V)$ the energy of a unit cell in the crystal, deformed according to the constant deformation gradient $F = \nabla V|_K$, that is:

$$E_K(V) = \frac{\sum_{x_i, x_j \in \cap B_r(x_K)} V_0(r_{ij})}{n_r(x_K)/2},$$

where x_K is an interior point of K, for example, the barycenter of K; $B_r(x_K)$ is a small region around x_K, usually a ball centered at x_K with radius r. $n_r(x_K)$ is the number of unit cells in $B_r(x_K)$. In this formula, the positions of the atoms x_j are obtained from uniformly deforming the equilibrium lattice with deformation gradient F.

Let n_K be a proper weighting factor, which is roughly equal to the number of the unit cells inside the element K times the volume of deformed unit cell. Denote by B_ε the unit cell. The QC approximation to the total energy associated with V is given by:

$$E(V) = \sum_{K \in \mathcal{T}_H} n_K \int_{B_\varepsilon} E_K(V) - \int_D f(V)\, dx. \tag{4.3}$$

The QC solution U_{QC} is obtained by minimizing E in X_H.

This is the nonlocal version of QC, formulated by Knap and Ortiz [27]. It uses a cluster-based summation rule (this is the role of the $B_r(x_K)$) instead of the Cauchy-Born rule to define $E_K(V)$.

It is worth mentioning that similar ideas are used in [11] for searching the global minimizers of certain lattice models.

The only existing work on the error analysis of QC seems to be that of P. Lin [29] in which QC in the absence of external forces (hence no deformation) was analyzed. When deformation is present, the situation becomes quite different. Naively one might expect to prove a result stating that the global minimizers of the atomistic model (4.2) under applied force can be approximated to good accuracy by the QC solutions. Such a result is in general false, as can be seen from an argument similar to the one below. The best we can do is to show that QC solutions do indeed approximate some local minimizers of the full atomistic model to a good accuracy. Such local minimizers are physically relevant.

To understand QC, we go back to the question: How is W obtained? One common proposal is to use the Cauchy-Born rule [38, 7, 23]:

$$W_{\mathrm{CB}}(F) = \sum_{\alpha \in \varepsilon\ell \cap B_\varepsilon} V_0(F \cdot \alpha)/|B_\varepsilon|, \tag{4.4}$$

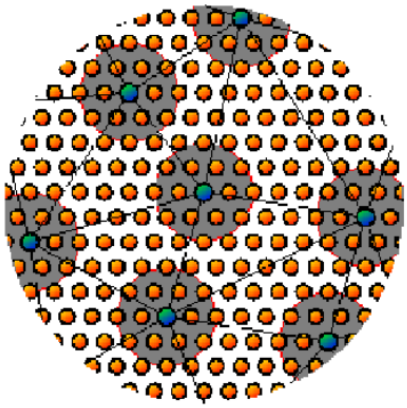

Figure 2: Schematic illustration of QC (courtesy of M. Ortiz). Only the atoms in the small cluster need to be visited during the computation

where ε is the lattice constant, ℓ is the periodic crystal lattice, and V_0 is the interaction potential between atoms.

An obvious mathematical difficulty with this approach is that (4.1) with W given by (4.4) gives a variational problem that seems to be badly behaved [4]. Indeed, it was proved in [6, Proposition 7] that $W(F)$ is not rank-one convex. Even more disturbing is the following observation for the full atomistic model.

Let us consider a one-dimension chain of atoms. Denote by l the length of the specimen, and $\{x_i\}_{i=0}^N$ the locations of the atoms in the reference configuration. Let $\{u_i\}_{i=0}^N$ be the displacement of the i^{th} atom, and $\dot{u}_i := (u_i - u_{i-1})/\lambda_N$ the relative elongation of the i^{th} atom, where $\lambda_N = l/N$ is the bond length. We write the strain energy as

$$E(u) = \sum_{i=1}^{N} \lambda_N \big(V_0(1+\dot{u}_i) - V_0(1+d/l)\big),$$

where the potential V_0 is Lennard-Jones potential [28]. d enters in the boundary condition: $u_0 = 0$ and $u_N = d$.

It is easy to check that the uniformly deformed state with $u_i = id/N$ is a local minimizer of E if $0 < d/l < \sqrt[6]{13/7} - 1$. The total energy of this state is $E(u) = 0$. But there is another state with a crack given by $u_i = 0$ for $1 \le i \le N-1$ and $u_N = d$, whose total energy is

$$E(u) = \lambda_N \big(V_0(1+Nd/l) - NV_0(1+d/l)\big).$$

It is clear that $V_0(1+Nd/l) \ll NV_0(1+d/l)$ if N is large enough, and if V_0 is bounded at large distance as is typically the case. This phenomenon, namely that the fractured state has less energy than the uniformly deformed state, is already known in the literature [40, 9].

The reason that crystals do not always crack when pulled is that the energy barrier for breaking a large set of chemical bonds is huge. Nevertheless this example implies that we have to think about local minimizers of the atomistic model in order to discuss coherent elastic deformation of crystals. In light of this, the following result becomes completely natural. To state the results, we make the following assumption:

Assumption A. For any domain D, there exists a constant K_D such that for the undeformed

configuration u and any $\varphi \in u + W_0^{1,\infty}(D)$ with $\|\varphi - u\|_{W^{1,\infty}(D)} \le K_D$,

$$\int_D W_{\mathrm{CB}}(\varphi)\,dx \ge \int_D W_{\mathrm{CB}}(u)\,dx.$$

Theorem 4.1. *If Assumption* **A** *holds, then there exists a constant κ such that for any $p > d$, if $\|\nabla f\|_{L^p(D)} \le \kappa$, then there exists a $W^{1,\infty}$-local minimizer U_{CB} of (4.1) with the stored energy W given by (4.4). Moreover, the full atomistic model has a local minimizer $\{x_j\}$ such that*

$$\Big(\sum_{j=1}^{N} \frac{1}{N}|U_{CB}(y_j) - u_j|^2\Big)^{1/2} \le C\varepsilon, \tag{4.5}$$

where $u_j = x_j - y_j$ is the displacement of $j-$th atom.

Here and in the following we use Dirichlet boundary condition.

The condition on the external forcing is necessary since at large enough forcing the elastically deformed state cease to be even a local minimizer.

Define

$$e_{\mathrm{QC}} := \max_{K\in\mathcal{T}_H} \left| n_r(x_K) - n_K \frac{|B_r(x_K)|}{|K|} \right|. \tag{4.6}$$

In the same spirit as in (2.1), and analogous to Theorem 3.1, we have the following error estimate for QC.

Theorem 4.2. *If Assumption* **A** *holds, there exist constants κ and H_0 such that for any $p > d$, if $\|\nabla f\|_{L^p(D)} \le \kappa$ and $0 < H < H_0$, then there exists U_{CB} and U_{QC}, which are respectively the $W^{1,\infty}$-local minimizers of (4.1) and (4.3), satisfying*

$$\|U_{CB} - U_{QC}\|_{H^1(D)} \le C\big(H + e(QC)\big). \tag{4.7}$$

$$\|U_{CB} - U_{QC}\|_{W^{1,\infty}(D)} \le C\big(H + e(QC)|\ln H|\big). \tag{4.8}$$

Similar to Theorem 3.2 and Theorem 3.3, we have

Theorem 4.3. *If $\mathcal{T}_H$ is* quasi-uniform*, then there exists a constant C such that*

$$e(QC) \le \begin{cases} C\dfrac{\varepsilon}{H} & \textit{Local QC [39]} \\[2ex] C\dfrac{\varepsilon}{r} & \textit{Nonlocal QC [27].} \end{cases}$$

Theorems 4.2 and 4.1 are valid under **Assumption A**, we have verified such assumption in [20] for several commonly used two-body potentials. Similar results with minor modification hold for complex lattice with many-body potentials, we refer to [20] for more details.

References

[1] D. N. Arnold, F. Brezzi, B. Cockburn and L. D. Marini, Unified analysis of discontinuous Galerkin methods for elliptic problems, *SIAM J. Numer. Anal.*, **39** (2002), 1749–1779.

[2] I. Babuska, Homogenization and its applications, mathematical and computational problems, Numerical Solutions of Partial Differential Equations-III, (SYNSPADE 1975, College Park MD, May 1975), (B. Hubbard eds.), Academic Press, New York, 1976, 89–116.

[3] I. Babuska, Solution of interface by homogenization I, II, III, *SIAM J. Math. Anal.*, **7** (1976), 603–634, 635–645, **8** (1977), 923–937.

[4] J. M. Ball and R. D. James, Proposed experimental tests of a theory of fine microstructure and the two-well problem, *Phil. Trans. R. Soc. Lond, A.*, **338** (1992), 389–450.

[5] A. Benssousan, J. L. Lions and G. Papanicolaou, Asymptotic Analysis of Periodic Structures, North-Holland, 1978.

[6] X. Blanc, C. Le Bris and P. L. Lions, From molecular models to continuum mechanics, *Arch. Rational Mech. Anal.*, **164** (2002), 341–381.

[7] M. Born and K. Huang, Dynamical Theory of Crystal Lattices, Oxford University Press, 1954.

[8] J. F. Bourgat, Numerical experiments of the homogenization method for operators with periodic coefficients, *Lecture Notes in Mathematics*, Vol 707. 330–356.

[9] A. Braides, G. Dal Maso and A. Garroni, Variational formulation of softening phenomena in fracture mechanics: The one-dimensional case, *Arch. Rational Mech. Anal.*, **146** (1999), 23–58.

[10] A. Brandt, Multi-level adaptive solutions to boundary-value problems, *Math. Comp.*, **31** (1977), 333-390.

[11] A. Brandt, Multigrid methods in lattice field computations, *Nuclear Physics B (Proc. Suppl.)*, **26** (1992), 137–180.

[12] R. Car and M. Parrinnello, Unified approach for molecular dynamics and density-functional theory, *Phys. Rev. Lett.*, **55** (1985), 2471–2474.

[13] P. G. Ciarlet, The Finite Element Method for the Elliptic Problems, North-Holland, Amsterdam, 1978.

[14] W. E, Analysis of the heterogeneous multiscale methods for ordinray differential equations, *Comm. Math. Sci.*, **1** (2003), 423–436.

[15] W. E and B. Engquist, The heterogeneous multiscale methods, *Comm. Math. Sci.*, **1** (2003), 87-132.

[16] W. E and B. Engquist, Multiscale modeling and computation, *Notices of the AMS*, **50** (2003), 1062–1070.

[17] W. E and B. Engquist, The heterogeneous multi-scale method for homogenization problems, preprint, submitted to MMS, 2002.

[18] W. E, X. T. Li and E. Vanden-Eijnden, Some recent progress in multiscale modelling, preprint, 2003.

[19] W. E, P. Ming and P. Zhang, Analysis of the heterogeneous multiscale method for elliptic homogenization problems, preprint, submitted to J. AMS, 2002.

[20] W. E and P. Ming, Atomistic and continuum theory of solids I, preprint, 2003.

[21] W. E and P. Ming, Analysis of quasicontinuum methods, preorint, 2003.

[22] Y. R. Efendiev, T. Y. Hou and X. Wu, Convergence of a nonconforming multiscale finite element method, *SIAM J. Numer. Anal.*, **37** (2000), 888-910.

[23] J. L. Ericksen, The Cauchy and Born hypotheses for crystals, In: Phases Transformations and Materials Instabilities in Solids, (M. Gurtin eds.), Academic Press, 1984, 61–77.

[24] R. Eymard, T. Gallouët and R. Herbin, Finite Volume Methods, In: Handbook for Numerical Analysis, (P. G. Ciarlet and J. L. Lions ed), Vol VII, North-Holland, Amsterdam, 2000, 715–1022.

[25] M. Freidlin, Functional Integration and Partial Differential Equations, Princeton, NJ, 1985.

[26] T. Hou and X. Wu, A multiscale finite element method for elliptic problems in composite materials and porous media, *J. Comput. Phys.*, **134** (1997), 169–189.

[27] J. Knap and M. Ortiz, An analysis of the quasicontinuum method, *J. Mech. Phys. Solids.*, **49** (2001), 1899–1923.

[28] J. E. Lennard-Jones and A. F. Devonshire, Critical and cooperative phenomena, III. A theory of melting and the structure of liquids, *Proc. Roy. Soc. Lond A.*, **169** (1939), 317–338.

[29] P. Lin, Theoretical and numerical analysis for the quasi-continuum approximation of a material particle model, *Math. Comp.*, **72** (2003), 657–675.

[30] A. M. Matache and C. Schwab, Two-scale finite element for homogenization problems, *M2AN.*, **36** (2002), 537-572.

[31] R. Miller and E. B. Tadmor, The Quasicontinuum method: overview, applications and current directions, *J. of Computer-Aided Material Design*, **9** (2002), 203–239.

[32] P. Ming, Analysis of Multiscale Methods: overview and perspective, to appear, 2004.

[33] P. Ming and X. Y. Yue, Numerical methods for multiscale elliptic problems, preprint, 2003.

[34] P. Ming and P. Zhang, Analysis of the heterogeneous multiscale methods for parabolic homogenization problem, preprint, 2003.

[35] J.T. Oden and K.S. Vemaganti, Estimation of local modelling error and global-oriented adaptive modeling of heterogeneous materials: error estimates and adaptive algorithms, *J. Comp. Phys.*, **164** (2000), 22–47.

[36] G. Papanicolaou and S. R. S. Varadhan, Boundary value problems with rapidly oscillating random coefficients, at Proceedings of conference on Random Fields, Esztergom, Hungary, 1979, published in Seria Colloquia Mathematica Societatis Janos Bolyai, North-Holland, **27** (1981), 835–873.

[37] R. D. Richtmyer and K. W. Morton, Difference Methods for Initial Value Problems, 2nd ed, Interscience, New York, 1967.

[38] I. Stakgold, The Cauchy relations in a molecular theory of elasticity, *Quart. Appl. Math.*, **8** (1950), 169–186.

[39] E. B. Tadmor, M. Ortiz and R. Phillips, Quasicontinuum analysis of defects in solids, *Phil. Mag.*, **A73** (1996), 1529–1563.

[40] L. Truskinovsky, Fracture as a phase transition, In Contemporary Research in the Mechanics and Mathematics of Materials (R. C. Batra and M. F. Beatty ed.), CIMNE, Barcelona, 1996, 322–332.

[41] E. Vanden-Eijden, Numerical techniques for multiscale dynamical systems with stochastic effects, *Comm. Math. Sci.*, **1** (2003), 385–391.

[42] V. V. Yurinskii, Averaging of symmetric diffusion in random media, Sibirsk. Mat. Zh., **23** (1982), no. 2, 176–188; English transl. in Siberian Math J., **27** (1986), 603–613.