Theoretical and numerical analysis for the quasi-continuum approximation of a material particle model

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Published in:
Mathematics of Computation

DOI:
10.1090/S0025-5718-02-01456-4

Publication date:
2003

Theoretical and numerical analysis of a material particle model

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Revised version (May 2001)

Abstract

In many applications materials are modeled by a large number of particles (or atoms) where any one of particles interacts with all others. Near or nearest neighbor interaction is expected to be a good simplification of the full interaction in engineering community. In this paper we shall analyze the approximate error between the solution of the simplified problem and that of the full-interaction problem so as to answer the question mathematically for a one dimensional model. A few numerical methods have been designed in engineering literatures for the simplified model. Recently much attention has been paid to a finite-element-like quasicontinuum (QC) method which is a mixed atomistic/continuum approximation model. No numerical analysis has been done yet. In the paper we shall estimate the error of the QC method for this one dimensional model. Possible ill-posedness of the method and its modification are discussed as well.

Descriptive title: Analysis of a material particle model.
Keywords. Lattice statics, particle motion, Lennard-Jones potential, global minimization, finite element method, error estimation, ill-posedness, quasi-continuum approximation, material modeling.
AMS(MOS) subject classifications. 65C20, 65K10, 65M15, 65M60, 73S10, 73V20.

1 Introduction

The analysis of the structure of material defects such as dislocations or fractures has to consider the effects at the scale of lattice. Directly solving the whole system (e.g. in the lattice statics and the molecular dynamics model) provides a powerful and accurate tool of analysis at this scale. However, because the number of particles (or atoms) in a material is huge, it is often impossible to solve the whole system under the existing computer power. The problem is often simplified by only considering the interaction of one particle with its nearby particles (or even its nearest neighbors). It is believed that the simplified problem is a good approximation to the original problem. But there is no mathematical proof available. On the other hand, even for the simplified problem the system is still huge and impossible to be solved directly. Recently a method called quasicontinuum (QC) approximation gains noticeable attention in engineering literatures (cf. [4, 1, 7]). The idea is that in the region where no defect occurs the material is modeled at the macroscopic scale and the theory of continuum elasticity may apply. It is incorporated with the finite element method and is expected to be an approximation of the full lattice-scale model. Numerical analysis to this approximation method is in its infancy. The

model is a system of a large number of material particles. Unlike usual physical problems the discrete subdomain of the approximation method is not treated as one small body but as a composition of a number of particles. As pointed out in [5] the presence of microstructure has motivated the development of numerical methods that can capture macroscopic information without resolving the microstructure on the physical length scale. The QC method seems to be such an example. As an initial theoretical study of the QC method we consider a typical one dimensional crystal material (an atomistic chain where interacting energy of any two atoms is the Lennard-Jones potential [3, 6]). Study of similar models can also be found in [2] and in [6] with emphasis on wave propagation and on nearest neighbor interaction under simpler potential functions which lead to a linearization of the mathematical problem. In this paper we shall consider the equilibrium configuration of these material particles where the pairwise potential is the more realistic Lennard-Jones potential and where the nearest neighbor interaction is not assumed in discussion. We shall estimate the error of the QC approximation.

Consider a one-dimensional crystal material where N atoms are distributed on a straight line. Let $u_i, i = 0, 1, \cdots, N$, denote the position of the ith atom and $W_{ij}(u_{ij})$ denote the embedding and interacting energy of atoms i and j, where $u_{ij} = |u_i - u_j|$. We assume that the energy functions W_{ij} between any two atoms are all same and denote it as W. Following Frank and vander Merwe we adopt the so called Lennard-Jones potential [3]

$$W(\alpha) = -(\frac{\sigma}{\alpha})^6 + (\frac{\sigma}{\alpha})^{12} \tag{1}$$

for the one-dimensional lattice. $\sigma > 0$ is something like the lattice scale. Also see Figure 1 for what the function looks like. Note that for α near zero the graphs of the function W and its derivatives are too high or too low to be shown in the figure. Obviously $\gamma = \sqrt[6]{2}\sigma$ is the

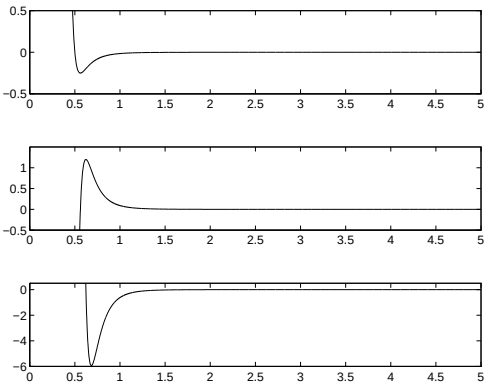

Figure 1: The functions $W(\alpha)$, $W'(\alpha)$ and $W''(\alpha)$ with $\sigma = 0.5$

minimum point of the function $W(\alpha)$. We thus can write down the total potential energy of the material $\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0,j\neq i}^{N} W(u_{ij})$. Stable configurations of the crystal material is identified by the minimizers of the potential energy subject to a stress free boundary condition (i.e. the force acting on the boundary atoms is zero). For the sake of determination, we fix the left-end atom, say, $u_0 = 0$ and let $u = (u_1, \cdots, u_N)^T$. Without loss of generality we let $u_i > u_{i-1},\ i = 1, \cdots, N$. So the problem in the full lattice scale is: find $\hat{u}$ such that

$$E(\hat{u}) = \min_u E(u) = \min_u \frac{1}{2}\sum_{i=0}^{N}\sum_{j=0,j\neq i}^{N} W(|u_j - u_i|) = \min_u \sum_{i=0}^{N}\sum_{j=i+1}^{N} W(u_j - u_i). \tag{2}$$

If we make a variable transformation $r_i = u_i - u_{i-1}$, $i = 1, 2, \cdots, N$, then we can write (2) in terms of $r = (r_1, \cdots, r_N)^T$:

$$\bar{E}(\hat{r}) = \min_r \bar{E}(r), \tag{3}$$

where

$$\bar{E}(r) = \sum_{i=1}^{N} W(r_i) + \sum_{i=1}^{N-1} W(r_i + r_{i+1}) + \cdots + W(\sum_{j=1}^{N} r_j) = \sum_{j=1}^{N} \sum_{i=1}^{N+1-j} W(\sum_{k=i}^{i+j-1} r_k). \tag{4}$$

Existence, uniqueness and conditioning of the problem will be discussed in §2 based on a solution estimate

$$\frac{4}{5}\sigma < r_i \leq \gamma. \tag{5}$$

The proof of (5) is not trivial but it is a key to obtain all results throughout the paper. Also in §2 we find that the problem in terms of the distance r has better conditioning than that in terms of the position u.

From the shape of the function $W(\alpha)$ the interaction of particles is weaker as their distance becomes larger. Hence the potential energy generated by one particle, say the ith particle, may count only the interaction with its nearby particles within a distance $\rho_c(\delta)$, where $\delta = |W(\rho_c)|$ is small and $\rho_c(\delta)$ is called a cut-off radius. $(u_i - \rho_c, u_i + \rho_c)$ is called a cut-off interval. Apparently we should let $\rho_c > \gamma$ since $W(\alpha)$ is not ignorable for $\alpha \leq \gamma$. The original full interaction model is largely simplified by this interaction cut-off. To analyze the error we introduce a cut-off fraction

$$F_c = \frac{\rho_c(\delta)}{\sigma} > 1. \tag{6}$$

Obviously as F_c grows the cut-off radius grows and the simplified system approaches the original system. In §3 we shall discuss the properties of the simplified problem and prove the error estimates

$$\|r - r^c\| \leq K F_c^{-5} \sigma \quad \text{or} \quad \|u - u^c\| \leq K(N\sigma) F_c^{-5}, \tag{7}$$

where K is a generic constant and r (or u) and r^c (or u^c) are the solution of the original problem and the simplified problem, respectively. $\|\cdot\|$ denotes $\|\cdot\|_\infty$ or $\frac{1}{\sqrt{N}}\|\cdot\|_2$ and $N\sigma = O(1)$ if the material has finite length.

In §4 we apply the idea of quasicontinuum (QC) approximation combined with the finite element method to the simplified problem. The finite element setting is a little different from the usual one. The independent variable is the index set of the particles $i = \{0, \cdots, N\}$. For this one-dimensional crystal material we only need a local QC model which assumes that each element contains a whole cut-off interval (cf. [7]). That is, the number of particles in one element $l > 2i_c(\delta)$, where $i_c(\delta)$ is the maximal number of particles in a half of a cut-off interval. We will see that the analysis is already fairly complicated for the local QC approximation. Through the problem in terms of the distance r and using a linear shape function for the finite element method we shall prove that for $l \geq 4i_c$

$$\|R_{i_k} - R^c_{i_k}\| \leq K(N\sigma) \max\{\frac{\eta}{N}, \frac{F_c^{-6}}{m}\} \tag{8}$$

and

$$\|U_{i_k} - u^c_{i_k}\| \le K(N\sigma)\max\{\frac{\eta}{4}F_c^{-1}, F_c^{-6}\}, \tag{9}$$

where $\|\cdot\|$ is either $\|\cdot\|_\infty$ or $\frac{1}{\sqrt{m}}\|\cdot\|_2$, $\eta = 2W'(\frac{8}{5}\sigma)\sigma/15 \approx 0.027$, m is the number of elements, R_{i_k} (or U_{i_k}) is the solution of the QC approximation at the kth element, $u^c_{i_k}$ is the i_kth component of the solution of the simplified problem and $R^c_{i_k} = u^c_{i_k} - u^c_{i_{k-1}}$. Then the error between the local QC solution and the full-lattice solution can be immediately obtained by combining (7)-(9). Here we write the error estimate in terms of F_c in order to avoid complicated notations. More precise results and their proof will be given in §4 Again $N\sigma = O(1)$ if the material has a finite length. Here we write the error estimates in terms of F_c for avoiding complicated notations and for seeing convergence directly as F_c grows. More precise results (including those for $l \le 4i_c$) and their proof will be given in §4 (See (49)-(51)). Better approximation can be obtained if we use higher order polynomial shape functions.

2 Analysis of the model problem and its solution

We analyze the one-dimensional crystal material model (2) or (3). If we only consider nearest neighbor interaction then the problem is trivial. In this case $\bar{E}(r) = \sum_{i=1}^N W(r_i)$. The minimum is $r_i = \gamma$, where γ is the minimum point of the function $W(\alpha)$. We shall study the problem without the nearest-neighbor-interaction assumption. There are several fundamental problems to be considered. They are boundedness, uniqueness and existence of the solution of problem (2) or (3). The existence of the solution is obvious since the function W, and then E or $\bar{E}$, is bounded below.

Theorem 1 *At a (local or global) minimum or (local or global) maximum of $E(u) = \bar{E}(r)$, $r_i = u_i - u_{i-1} \le \gamma$ for any $i = 1, 2, \cdots, N$, where $\gamma = 2^{\frac{1}{6}}\sigma \approx 1.12\sigma$.*

Proof: Suppose that we have two adjacent atoms such that $|u_{i_0} - u_{i_0-1}| > \gamma$. We can group all the atoms into two parts. Part I includes atoms $u_i, i = 0, 1, \cdots, i_0 - 1$ and part II includes atoms $u_i, i = i_0, \cdots, N$. It is easy to verify that $W(\alpha)$ increases if $\alpha > \gamma$. If we fix the relative distance of any two atoms in each group and shift all atoms in part II towards part I by a tiny distance, then the energy E will decrease a bit since the distance between atoms in part I and part II decreases and larger than γ. Similarly if we shift all atoms in part II away from part I by a tiny distance, the energy E will increase a bit. So E is not possible to reach the maximum or minimum at the current configuration. This proves the theorem. ∎

From the result, we know that the solution of problem (2) or (3) is bounded by $N\gamma$ or the length of thematerial is of $O(N\sigma)$. Next we give a lower bound for r_i.

Theorem 2 *At the global minimum of the energy $E(u) = \bar{E}(r)$, the distance of any two adjacent particles should be away from zero, say, $r_i = u_i - u_{i-1} > \frac{4}{5}\sigma$, $i = 1, 2, \cdots, N$.*

Proof: We assume that at the minimum configuration $u^* = (u^*_1, \cdots, u^*_N)$ there exists an i_0, $1 \le i_0 \le N$, such that $u^*_{i_0} - u^*_{i_0-1} \le \frac{4}{5}\sigma$ and for all $i < i_0$, $u^*_i - u^*_{i-1} > \frac{4}{5}\sigma$. We want to derive a contradiction out of the assumption, i.e. $E(u^*) \le E(u)$ for all u. The idea of the proof is to consider a specific configuration $u' = (u^*_1, \cdots, u^*_{i_0-1}, u'_{i_0}, \cdots, u'_N)$, where $u'_j = u^*_j + [\gamma - (u^*_{i_0} - u^*_{i_0-1})]$ for $j = i_0, \cdots, N$ (cf. Fig. 2).

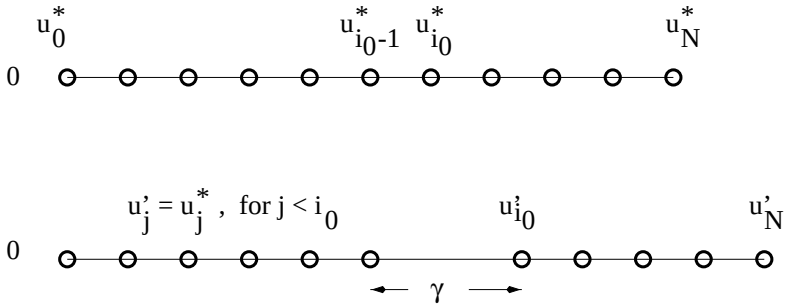

Figure 2: Configurations u^* and u'

From $E(u^*) \le E(u')$ we first show that there exists an interval with length γ which includes 5 particles in it. In fact, if this is not true then every interval with length γ at most includes 4 particles. Write down an equivalent total energy expression of (2):

$$E(u') = \sum_{i=0}^{N} E_i(u'), \quad \text{where } E_i(u') = \sum_{j=i+1}^{N} W(u'_j - u'_i). \tag{10}$$

We scale the axis according to the length γ starting from $u^*_{i_0}$ towards the right. Then in each length-γ interval $[u^*_{i_0} + (k-1)\gamma, u^*_{i_0} + k\gamma]$, $k = 1, 2, \cdots$, there are at most 4 atoms. We now compare $E(u')$ and $E(u^*)$.

$$\begin{aligned} E_0(u') &= \sum_{j=1}^{i_0-1} W(u^*_j - u^*_0) + \sum_{j=i_0}^{N} W(u'_j - u^*_0) \\ &= E_0(u^*) - \sum_{j=i_0}^{N} W(u^*_j - u^*_0) + \sum_{j=i_0}^{N} W(u'_j - u^*_0). \end{aligned}$$

Obviously $u'_j - u^*_0 \ge \gamma$ for $j \ge i_0$ since $u'_{i_0} - u^*_{i_0-1} = \gamma$. So we have $\sum_{j=i_0}^{N} W(u'_j - u^*_0) < 0$. For the other sum we have

$$-\sum_{j=i_0}^{N} W(u^*_j - u^*_0) \le -4W((i_0-1)\frac{4}{5}\sigma) - 4\sum_{j=1}^{\infty} W((i_0-1)\frac{4}{5}\sigma + j\gamma).$$

Note that if $i_0 = 1$ there is no $-4W((i_0-1)\frac{4}{5}\sigma)$ in above inequality. This gives

$$E_0(u') \le E_0(u^*) - 4W((i_0-1)\frac{4}{5}\sigma) - 4\sum_{j=1}^{\infty} W((i_0-1)\frac{4}{5}\sigma + j\gamma).$$

Similarly, for $l = 1, \cdots, i_0 - 3$, we have

$$\begin{aligned} E_l(u') &= E_l(u^*) - \sum_{j=i_0}^{N} W(u^*_j - u^*_l) + \sum_{j=i_0}^{N} W(u'_j - u^*_l) \\ &\le E_l(u^*) - 4W((i_0-l-1)\frac{4}{5}\sigma) - 4\sum_{j=1}^{\infty} W((i_0-l-1)\frac{4}{5}\sigma + j\gamma). \end{aligned}$$

For $l = i_0 - 2$ and $l = i_0 - 1$,

$$E_{i_0-2}(u') \le E_{i_0-2}(u^*) - 4W(\gamma) - 4\sum_{j=1}^{\infty} W(\frac{4}{5}\sigma + j\gamma),$$

$$E_{i_0-1}(u') \le E_{i_0-1}(u^*) - W(u^*_{i_0} - u^*_{i_0-1}) - 4W(\gamma) - 4\sum_{j=1}^{\infty} W(j\gamma).$$

From $r_{i_0} \le \frac{4}{5}\sigma$ we have $-W(u^*_{i_0} - u^*_{i_0-1}) \le -W(\frac{4}{5}\sigma) \approx -10.74$. Also, by the construction of u', $E_j(u') = E_j(u^*)$ for all $j \ge i_0$. We thus obtain

$$\begin{aligned} E(u') &\le E(u^*) - 10.74 - 2 \cdot 4W(\gamma) - 4\sum_{l=0}^{i_0-3} W((i_0 - l - 1)\frac{4}{5}\sigma) - 4\sum_{l=0}^{i_0-1}\sum_{j=1}^{\infty} W((i_0 - l - 1)\frac{4}{5}\sigma + j\gamma) \\ &\le E(u^*) - 10.74 - 8W(\gamma) - 8\sum_{l'=1}^{[(i_0-3)/2]} W(l'\gamma) - 8\sum_{l'=0}^{[(i_0-1)/2]}\sum_{j=1}^{\infty} W(l'\gamma + j\gamma), \end{aligned} \tag{11}$$

where we have used the facts that $-W((i_0 - l - 1)\frac{4}{5}\sigma) \le -W(\frac{i_0-l-1}{2}\gamma)$ for $l = 0, \cdots, i_0 - 3$ and $-W((i_0 - l - 1)\frac{4}{5}\sigma + j\gamma) \le -W(\frac{i_0-l-1}{2}\gamma + j\gamma)$ for $l = 0, \cdots, i_0 - 1$ and $j \ge 1$. We also have

$$-\sum_{j=1}^{\infty} W(j\gamma) = -\sum_{j=1}^{3} W(j\gamma) - \sum_{j=4}^{\infty} W(j\gamma) \le 0.2585 + \frac{1}{2}\int_3^{\infty} \frac{1}{j^6}\, dj \approx 0.2593,$$

where we have used $(\frac{\sigma}{\gamma})^6 = \frac{1}{2}$ and $1 - (\frac{\sigma}{j\gamma})^6 \le 1$;

$$\begin{aligned} &-\sum_{j=1}^{\infty} W(\gamma + j\gamma) = -\sum_{j=1}^{\infty} W(j\gamma) + W(\gamma) \le 0.0093; \\ &-\sum_{j=1}^{\infty} W(2\gamma + j\gamma) = -\sum_{j=2}^{\infty} W(j\gamma) + W(2\gamma) \le 0.0016; \\ &-\sum_{l'=3}^{\infty}\sum_{j=1}^{\infty} W(l'\gamma + j\gamma) \le \frac{1}{2}\sum_{l'=3}^{\infty}\sum_{j=l'+1}^{\infty} \frac{1}{j^6} \le \frac{1}{2}\int_2^{\infty}\int_{j=l'+1}^{\infty} \frac{1}{j^6} dj dl' \approx 0.0016. \end{aligned}$$

Hence,

$$E(u') \le E(u^*) - 10.74 + 8 \cdot 0.2593 + 8 \cdot 0.25 + 8 \cdot 0.2718 = E(u^*) - 4.4912 < E(u^*).$$

This shows that $E(u^*)$ is not the minimum. This contradiction implies that there exists at least an interval with length γ which includes 5 particles. Then there must be two adjacent particles, say, $u^*_{i_1-1}$, $u^*_{i_1}$, such that $u^*_{i_1} - u^*_{i_1-1} \le \frac{\gamma}{4}$. Therefore, we can assume that there exists an i_1 such that

$$u^*_{i_1} - u^*_{i_1-1} \le \frac{\gamma}{4}, \quad \text{but} \quad u^*_i - u^*_{i-1} > \frac{\gamma}{4} \quad \text{for all} \quad i < i_1.$$

Note that $W(u^*_{i_1} - u^*_{i_1-1}) \ge W(\frac{1}{4}\gamma) = 4^{11}(1 - (\frac{4}{\sqrt[6]{2}})^{-6}) \approx 4^{11}$.

Similarly to the previous argument and from $E(u^*) \le E(u')$ we can obtain (ignoring many algebraic operations) that there exists an interval of length γ including $4^2 + 1$ particles. In other words, there must be two adjacent particles, say, $u^*_{i_2-1}$, $u^*_{i_2}$, such that $u^*_{i_2} - u^*_{i_2-1} \le \frac{1}{4^2}\gamma$.

Repeating this argument we can conclude that there exists an interval of length γ which includes as many particles as you want if $E(u^*)$ is the minimum. This is a contradiction to the finite number of particles or atoms. This completes the proof of the theorem. ∎

Theorems 1 and 2 show that (5) holds. From (5) we can obtain the uniqueness of the solution of (2) or (3).

Theorem 3 *The (local) maximum and (local) minimum of the energy $\bar{E}(r) = E(u)$ is unique in the region* $\mathbf{R}$: $\frac{4}{5}\sigma \le r_i \le \gamma,\ i = 1, 2, \cdots, N$.

Proof: At the maximum or minimum of $\bar{E}(r)$ (cf. (4)), r should satisfy

$$\frac{\partial \bar{E}}{\partial r_i} = W'(r_i) + \sum_{j=(i-1)\vee 1}^{i\wedge(N-1)} W'(r_j + r_{j+1}) + \sum_{j=(i-2)\vee 1}^{i\wedge(N-2)} W'(\sum_{k=0}^{2} r_{j+k}) + \cdots + W'(\sum_{j=1}^{N} r_j) = 0, \quad (12)$$

where $a \vee b$ and $a \wedge b$ represents $max(a, b)$ and $min(a, b)$, respectively.

If the Hessian matrix of $\bar{E}(r)$ is diagonally dominant in the region $\mathbf{R}$ then the matrix is nonsingular in the region. We thus prove that the system (12) has a unique solution in the region (i.e. the minimum of $\bar{E}(r)$ is unique). So we only need to show that the Hessian matrix of $\bar{E}(r)$ is diagonally dominant in the region $\mathbf{R}$. The diagonal element of the Hessian matrix of $\bar{E}(r)$ is

$$\frac{\partial^2 \bar{E}}{\partial r_i^2} = W''(r_i) + \sum_{j=(i-1)\vee 1}^{i\wedge(N-1)} W''(r_j + r_{j+1}) + \sum_{j=(i-2)\vee 1}^{i\wedge(N-2)} W''(\sum_{k=0}^{2} r_{j+k}) + \cdots + W''(\sum_{j=1}^{N} r_j). \quad (13)$$

In the region $\mathbf{R}$, $r_i \le \gamma$. Hence, $W''(r_i) \ge W''(\gamma) \approx 15/\sigma^2$ since $W''(\alpha)$ decreases when $\alpha \le \gamma$. We also have

$$r_j + r_{j+1} > 2(\frac{4}{5}\sigma) > \gamma,\ r_j + r_{j+1} + r_{j+2} > 3(\frac{4}{5}\sigma), \cdots. \quad (14)$$

Hence, from the monotone property of $W''(\alpha)$, all other terms in the right hand side of (13) except $W''(r_i)$ are negative and the sum of them is larger than $A = 2W''(\frac{8}{5}\sigma) + 3W''(\frac{12}{5}\sigma) + \cdots$. Noting that $W''(\frac{8}{5}\sigma) \approx -0.7614/\sigma^2$, $W''(\frac{12}{5}\sigma) \approx -0.0375/\sigma^2$, $W''(\frac{16}{5}\sigma) \approx -0.0038/\sigma^2$, $\cdots$, we have

$$0 \ge A = \sum_{j=2}^{4} jW''(j\frac{4}{5}\sigma) + \sum_{j=5}^{N} jW''(j\frac{4}{5}\sigma) > -1.6505/\sigma^2 - 7(\frac{5}{4})^8 \int_4^\infty \frac{6}{x^7}\, dx/\sigma^2 \ge -1.7/\sigma^2.$$

At the same time we can calculate off-diagonal elements:

$$\begin{aligned}
\frac{\partial^2 \bar{E}}{\partial r_i \partial r_{i-1}} &= W''(r_{i-1} + r_i) + \sum_{j=(i-2)\vee 1}^{(i-1)\wedge(N-2)} W''(r_j + r_{j+1} + r_{j+2}) + \cdots + W''(\sum_{j=1}^{N} r_j), \\
\frac{\partial^2 \bar{E}}{\partial r_i \partial r_{i+1}} &= W''(r_i + r_{i+1}) + \sum_{j=(i-1)\vee 1}^{i\wedge(N-2)} W''(r_j + r_{j+1} + r_{j+2}) + \cdots + W''(\sum_{j=1}^{N} r_j), \\
\frac{\partial^2 \bar{E}}{\partial r_i \partial r_{i-2}} &= W''(r_{i-2} + r_{i-1} + r_i) + \sum_{j=(i-3)\vee 1}^{(i-2)\wedge(N-3)} W''(\sum_{k=0}^{3} r_{j+k}) + \cdots + W''(\sum_{j=1}^{N} r_j), \\
\frac{\partial^2 \bar{E}}{\partial r_i \partial r_{i+2}} &= W''(r_i + r_{i+1} + r_{i+2}) + \sum_{j=(i-1)\vee 1}^{i\wedge(N-3)} W''(\sum_{k=0}^{3} r_{j+k}) + \cdots + W''(\sum_{j=1}^{N} r_j), \\
&\cdots\ \cdots.
\end{aligned}$$

We can estimate all these off diagonal elements using (14). Hence, the sum of absolute values of all off diagonal elements of the Hessian matrix of $\bar{E}(r)$ is less than

$$\begin{aligned} B &\leq -2W''(2\cdot\frac{4}{5}\sigma) - 6W''(3\cdot\frac{4}{5}\sigma) - 12W''(4\cdot\frac{4}{5}\sigma) - \sum_{j=5}^{\infty} j(j-1)W''(j\cdot\frac{4}{5}\sigma) \\ &\leq 1.7934/\sigma^2 + 7(\frac{5}{4})^8 \int_4^{\infty} \frac{x-1}{x^7}\, dx/\sigma^2 \leq 1.8/\sigma^2 \end{aligned}$$

So the diagonal element is larger than $15/\sigma^2 - |A| \geq 13.7/\sigma^2 > B$. Therefore, each row of the Hessian matrix of $\bar{E}(r)$ is diagonally dominant in the region $\mathbf{R}$. We thus complete the proof. ∎

Because the global minimum of $\bar{E}(r) = E(u)$ exists these theorems imply that the global minimum of $\bar{E}(r)$ is located in the region $\mathbf{R}$ and the last theorem implies that $\bar{E}(r)$ has no other critical values in the region $\mathbf{R}$. Hence, the global minimum is unique in the region $\mathbf{R}$ since a global minimum can be a local minimum of a slightly larger region and Theorem 3 holds in the slightly larger region as well.

Remark 1 *The second derivative (Hessian matrix) $\bigtriangledown_r^2 \bar{E}(r)$ of $\bar{E}(r)$ with respect to r is symmetric. In the above theorem we have shown that $\bigtriangledown_r^2 \bar{E}(r)$ is diagonally dominant and the diagonal elements are all positive in the region $\mathbf{R}$. The eigenvalues of the Hessian matrix are thus all positive by Gershgorin's theorem. This implies that $\bigtriangledown_r^2 \bar{E}(r)$ is positive definite in the region $\mathbf{R}$. Using Gershgorin's theorem and the off-diagonal sum we calculated earlier we can actually have a lower bound of the eigenvalues (say, $\lambda_i,\ i = 1, \cdots, N$) of the Hessian matrix, i.e. $\lambda_i \geq (15-1.7-1.8)/\sigma^2 = 11.5/\sigma^2$. Similarly we can also have $\lambda_i \leq (15+1.7+1.8)/\sigma^2 = 17.5/\sigma^2$. So problem (3) is well-posed.*

Corollary 1 *$E(u)$ has a unique minimum and in the region $\mathbf{R}$ its second derivative is positive definite too. Hence, it has no any other critical values in the region $\mathbf{R}$.*

Proof: $r_i = u_i - u_{i-1},\ i = 1, \cdots, N$. So $r = Tu$, where $T = \begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & ... & ... & & \\ & & -1 & 1 & \\ & & & -1 & 1 \end{pmatrix}$. It is not difficult to verify that

$$\bigtriangledown_u^2 E(u) = T^T \bigtriangledown_r^2 E(r) T. \tag{15}$$

So in the region $\mathbf{R}$, $\bigtriangledown_u^2 E(u)$ is positive definite since $\bigtriangledown_r^2 E(r)$ is. This fact also shows that in the region $\mathbf{R}$ $E(u)$ has only one minimum and there are no any other critical values. ∎

Lemma 1 *The smallest and the largest eigenvalues of the matrix $\bigtriangledown_u^2 E(u)$ are of $O(1/(N\sigma)^2$ and $O(1/\sigma^2)$, respectively.*

Proof: The smallest and largest eigenvalues of a symmetric positive definite matrix B can be expressed as

$$\lambda_{min} = \min_{x \neq 0} \frac{x^T B x}{x^T x},\ \lambda_{max} = \max_{x \neq 0} \frac{x^T B x}{x^T x}. \tag{16}$$

From (15) $x^T \bigtriangledown_u^2 E(u)x = x^T T^T \bigtriangledown_r^2 E(r)Tx$. Using Remark 1 we thus have

$$x^T \bigtriangledown_u^2 E(u)x = (Tx)^T \bigtriangledown_r^2 E(r)(Tx) = O(\frac{1}{\sigma^2})(Tx)^T(Tx) = O(\frac{1}{\sigma^2})x^T T^T Tx, \tag{17}$$

where $x^T T^T Tx = x_1^2 + \sum_{i=1}^{N-1}(x_{i+1} - x_i)^2 \leq 4x^T x$. We can choose a special $x_s = (1, 0, \cdots, 0)^T$ such that $x_s^T T^T Tx_s = 2x_s^T x_s$. So from (16) the largest eigenvalue of $\bigtriangledown_u^2 E(u)$ is of $O(1/\sigma^2)$.

Now we consider the smallest eigenvalue. Assume $x_{i_0} = \max_i |x_i|$. Hence, $x^T x \leq N x_{i_0}^2$. Let $y_i = \frac{x_i}{x_{i_0}}$, $i = 1, 2, \cdots, N$. We have (noting that $|y_i| \leq 1$)

$$\begin{aligned} \frac{x^T T^T Tx}{x^T x} &\geq \frac{1}{N}((y_N - y_{N-1})^2 + \cdots + (y_{i_0+1} - 1)^2 + (1 - y_{i_0-1})^2 + \cdots + (y_2 - y_1)^2 + y_1^2) \\ &= \frac{1}{N} f(y), \quad \text{where } y = (y_1, \cdots, y_{i_0-1}, y_{i_0+1}, \cdots, y_N)^T. \end{aligned}$$

The minimum of $f(y)$ is $\frac{1}{i_0}$. Hence, $x^T T^T Tx \geq \frac{1}{N} \cdot \frac{1}{i_0} x^T x \geq \frac{1}{N^2} x^T x$. Also, we can choose a vector $x_p = (1, 2, \cdots, N)^T$ such that $\frac{x_p^T T^T Tx_p}{x_p^T x_p} = \frac{6}{(N+1)(2N+1)} = O(1/N^2)$. From (16) and (17) we obtain that the smallest eigenvalue of $\bigtriangledown_u^2 E(u)$ is of $O(1/(N\sigma)^2)$. ∎

Remark 2 *The above lemma implies that the problem (2) is ill-posed when N is large since the condition number of its Hessian matrix $\frac{\lambda_{max}}{\lambda_{min}}$ is $O(N^2)$.*

3 Cut-off — a simplification of the model

From the shape of the potential $W(\alpha)$ it may be good enough to consider only the interaction of one particle with its nearby particles within the cut-off radius ρ_c. In this section we shall prove error estimates (7) of such simplication in terms of the cut-off fraction F_c (See (6). We have shown that $\frac{4}{5}\sigma < r_i \leq \gamma = \sqrt[6]{2}\sigma$. We can then obtain

$$\frac{1}{\sqrt[6]{2}} F_c \leq i_c(\delta) \leq \frac{5}{4} F_c. \tag{18}$$

We can also verify that roughly

$$|W(i_c \frac{4}{5}\sigma)| \approx \delta \approx F_c^{-6}. \tag{19}$$

The total energy after the cut-off:

$$E_c(u^c) = \frac{1}{2} \sum_{i=0}^{N} \sum_{j=i-i_c(\delta) j \neq i}^{i+i_c(\delta)} W(|u_j^c - u_i^c|), \tag{20}$$

or in terms of r

$$\begin{aligned} \bar{E}_c(r) &= \sum_{i=1}^{N} W(r_i^c) + \sum_{i=1}^{N-1} W(r_i^c + r_{i+1}^c) + \cdots + \sum_{i=1}^{N-i_c+1} W(r_i^c + r_{i+1}^c + \cdots + r_{i+i_c-1}^c) \\ &= \sum_{j=1}^{i_c} \sum_{i=1}^{N+1-j} W(\sum_{k=i}^{i+j-1} r_k), \end{aligned} \tag{21}$$

where $u^c = (u_1^c, u_2^c, \cdots, u_N^c)^T$, $u_0^c = 0$ and $r^c = (r_1^c, \cdots, r_N^c)^T$, $r_i^c = u_i^c - u_{i-1}^c$. Hence the simplified problem of (2) or (3) is finding $\hat{r}^c$ such that

$$\bar{E}_c(\hat{r}^c) = min_{r^c} \bar{E}_c(r^c). \tag{22}$$

(In terms of u^c, the problem is $E_c(\hat{u}^c) = min_{u^c} E_c(u^c)$.)

Problem (22) is not same as the original problem (3). Obviously, Theorem 1 is no longer true for all local minimums or maximums. The distance of two adjacent particles may be larger than γ at some local minimum or maximum. For example, we could have $r_i^c > \rho_c$ for some i and the system is divided into two independent sub-systems at this i. There is no interaction between these two subsystems. So the problem (22) could have many local minimums which are not the minimum of the original system since $r_i^c \leq \gamma$ is not satisfied. However, we will prove that there exists a unique solution of problem (22) in the region $\mathbf{R}_c$ where the distance of any two adjacent particles is strictly less than the cut-off radius ρ_c, i.e.

$$\mathbf{R}_c = \{r^c : \ r_i^c < \rho_c, \ i = 1, 2, \cdots, N\}. \tag{23}$$

Once we have the existence of the minimum solution in the region $\mathbf{R}_c$ then it should be the global minimum of the problem (22) for any r^c since the minimum of the sub-system is larger than the minimum of the whole system.

Theorem 4 *If r^c or $u^c \in \mathbf{R}_c$ then, at the minimum of the energy $\bar{E}_c(r^c)$ or $E_c(u^c)$, the distance of any two adjacent particles should satisfy $\gamma > r_i^c = u_i^c - u_{i-1}^c > \frac{4}{5}\sigma$ for $i = 1, 2, \cdots, N$.*

Proof: The proof is just the same as that for Theorems 1 and 2 except restricting u^c in $\mathbf{R}_c$ in proving the first part of the inequality. ∎

Theorem 5 *The problem (22) has a unique solution for $r^c \in \mathbf{R}_c$.*

Proof: The existence of the global minimum of (22) is obvious since each term in the expression of $\bar{E}_c$ has a lower bound. Following the idea of the proof in Theorem 1, the global minimum must be in $\mathbf{R}_c$. From the previous theorem we thus have $r^c \in \mathbf{R}$. Following the proof of Theorem 3 step-by-step we can obtain that the Hessian matrix is symmetric positive definite in the region $\mathbf{R}$. Hence, the solution is unique. ∎

From Lemma 1 of the previous section the condition number of problem (2) is worse than that of problem (3) although they are mathematically equivalent. So it is better to solve problem (3). Next we prove the error estimate (7) for $r - r^c$ and then give the corresponding results (7) for $u - u^c$ using the relation $r - r^c = T(u - u^c)$.

Theorem 6 *Let r^c be the solution of (22) and r be the solution of (3). We have the first estimate of (7).*

Proof: The solution of (22) satisfies

$$\frac{\partial \bar{E}_c}{\partial r_i^c} = W'(r_i^c) + \sum_{j=(i-1)\vee 1}^{i\wedge(N-1)} W'(r_j^c + r_{j+1}^c) + \cdots + \sum_{j=(i-i_c)\vee 1}^{i\wedge(N-i_c)} W'(\sum_{k=0}^{i_c-1} r_{j+k}^c) = 0. \tag{24}$$

for $i = 1, 2, \cdots, N$. The solution of (3) satisfies (12). Subtracting (24) from (12) and applying the Taylor's theorem we have

$$H_c(\psi)(r - r^c) = g, \tag{25}$$

where $\psi = \theta r + (1-\theta) r^c$, $0 < \theta < 1$, $H_c(\psi) = \nabla^2_{r^c} \bar{E}_c(\psi)$ (cf. (13)) and $g = (g_1, \cdots, g_N)^T$, where

$$|g_i| = \sum_{j=(i-i_c-1)\vee 1}^{i\wedge(N-i_c-1)} W'(r_j + \cdots + r_{j+i_c}) + \cdots + W'(r_1 + \cdots + r_N). \tag{26}$$

Note that r and r^c both belong to the region $\mathbf{R}$. So $\psi \in \mathbf{R}$. Similarly to the proof of Theorem 3 we can have that $H_c(\psi)$ is strictly diagonally dominant and its diagonal elements (say, d_i) are larger than $11.5/\sigma^2$. Write $H_c = D + F = D(I + D^{-1}F)$ where $D = (d_i)$ is the diagonal part of H_c and F is the off-diagonal part of H_c. Strictly Diagonal dominance of H_c gives $\|D^{-1}F\|_\infty < 1$. Therefore

$$\|H_c^{-1}\|_\infty = \|(I + D^{-1}F)^{-1}D^{-1}\|_\infty \le \frac{\|D^{-1}\|_\infty}{1 - \|D^{-1}F\|_\infty} \le K\sigma^2.$$

Now we estimate g.

$$\begin{aligned} |g_i| &\le (i_c+1)W'((i_c+1)\frac{4}{5}\sigma) + (i_c+2)W'((i_c+2)\frac{4}{5}\sigma) + \cdots = \sum_{j=i_c+1}^{\infty} jW'(j\frac{4}{5}\sigma) \\ &\le \frac{1}{\sigma}(\frac{4}{5})^7 \int_{i_c}^{\infty} \frac{6}{j^6}\, dj = \frac{6}{5}(\frac{4}{5})^7 \frac{1}{\sigma}\frac{1}{i_c^5} \le \frac{48}{25} i_c |W(i_c\frac{4}{5}\sigma)| \le KF_c^{-5}/\sigma, \end{aligned}$$

where we have used (18) and (19). This completes the proof of the theorem under the norm $\|\cdot\|_\infty$. The result under the norm $\frac{1}{N}\|\cdot\|_2$ follows immediately. ∎

Remark 3 *Since $r = Tu$ and $r^c = Tu^c$ we have $u - u^c = T^{-1}(r - r^c)$. From the proof of* Lemma 1 *we have $x^T TT^T x \ge \frac{1}{N^2} x^T x$. This implies that $\|T^{-1}\|_2 \le N$. Furthermore we can actually find T^{-1} which is an lower triangular matrix where all lower triangular elements are* 1. *That means $\|T^{-1}\|_\infty = N$. Hence we have the second estimate of (7). Note that $N\sigma = O(1)$ if we assume the material is of finite length.* ∎

4 The quasicontinuum approximation and its error estimates

To further reduce the size of the problem we consider the local QC approximation combined with a finite-element-like idea for the problem (22) in this section. For simplicity, we partition the 1-D material into m parts (elements) such that there are l particles in each part. So the total number of particles is $N = ml$. If the number of particles is not equal in each element our argument can still be used without much difficulty. A middle atom of each element is a finite element node. We denote its position as U_{i_k}, $k = 1, \cdots, m$. We assume that the deformation of atoms between any two adjacent nodes (i.e. $(U_{i_{k-1}}, U_{i_k})$, $k = 2, \cdots, m$) is homogeneous, that is, the distance of any two adjacent particles in an interval $(U_{i_{k-1}}, U_{i_k})$ is same. For the 1-D material we consider in this paper there is no inhomogeneous effects. Local QC approximation is thus suggested (cf. [7]), that is, we assume $l > 2i_c(\delta)$. We will see later from the error estimate that the local approximation is good enough for our problem.

A more precise description is the following. Applying the finite element idea to the index set $\{i = 0, \cdots, N\}$ of a large number of points (or positions of particles) we write

$$U_i = \sum_{k=1}^{m} U_{i_k} \phi_k(i), \tag{27}$$

where ϕ_k are shape functions of i, U_{i_k}, $k = 1, \cdots, m$, is the position of the kth node particle in the kth element. Now if we use linear shape functions, then

$$\phi_k = \begin{cases} 0 & \text{if } i \le i_{k-1},\ i \ge i_{k+1} \\ \frac{i - i_{k-1}}{a_k} & \text{if } i_{k-1} \le i \le i_k \\ \frac{i_{k+1} - i}{a_{k+1}} & \text{if } i_k \le i \le i_{k+1} \end{cases} \tag{28}$$

and

$$U_j - U_{i_k} = \begin{cases} \frac{i_k - j}{a_k}(U_{i_k} - U_{i_{k-1}}) & \text{if } j < i_k \\ \frac{j - i_k}{a_{k+1}}(U_{i_{k+1}} - U_{i_k}) & \text{if } j > i_k, \end{cases} \tag{29}$$

where U_j is in the kth element, $a_k = i_k - i_{k-1}$, $k = 1, \cdots, m+1$. Under our assumption we simply have $a_k = [\frac{l}{2}]$ for $k = 1, m+1$ and $a_k = l$ for other k. If we make another approximation that the potential energy generated by every particle in one element is equal we are then able to write down the approximate total energy of the material. But in each element, say the kth, the deformation gradient $S_k = \frac{U_{i_k} - U_{i_{k-1}}}{a_k}$ in $[i_k - \frac{a_k}{2}, i_k]$ is different from the deformation gradient $S_{k+1} = \frac{U_{i_{k+1}} - U_{i_k}}{a_{k+1}}$ in the other part $[i_k, i_k + \frac{a_{k+1}}{2}]$ of the element. To make the approximate solution more smooth in each element some kind of average is suggested in [7]. One way is to average two deformation gradients in each element and the potential of the jth and the i_kth particles is calculated as $W(\frac{S_k + S_{k+1}}{2}(j - i_k))$. The other is to average the energies in two parts of each element using those two deformation gradients. The former should not be used since it allows one particle to cross the other, which is not physical. Figure 3 is an example of ten particles to show that the average of deformation gradients allows such an unphysical crossing, while the latter way does not. So we use the latter (i.e. energy average form) and the approximate total

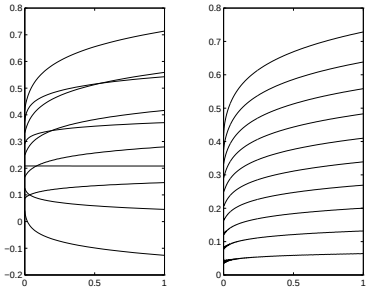

Figure 3: The deformation gradient average and the energy average solutions of $\frac{du}{dt} = \bigtriangledown E(u)$

energy can be written as

$$\begin{aligned} \tilde{E}^r &= l \sum_{k=1}^{m} \sum_{j = i_k - i_c(\sigma),\ j \ne i_k}^{i_k + i_c(\sigma)} W(|U_j - U_{i_k}|) \\ &= \frac{l}{2} \sum_{k=1}^{m} \Big(\sum_{j = i_k - i_c}^{i_k - 1} W(\frac{i_k - j}{a_k} R_{i_k}) + \sum_{j = i_k + 1}^{i_k + i_c} W(\frac{j - i_k}{a_{k+1}} R_{i_{k+1}}) \Big), \end{aligned} \tag{30}$$

where $R_{i_k} = U_{i_k} - U_{i_{k-1}}$ for $k = 1, 2, \cdots, m$ and denote $R = (R_{i_1}, \cdots, R_{i_m})^T$. For particles numbered in $[i_m, N]$ the deformation gradient is assumed to be the same as S_m or $\frac{R_{i_{m+1}}}{a_{m+1}} = \frac{R_{i_m}}{a_m}$

for simplicity. The approximate problem is to find $\hat{R}$ such that

$$\tilde{E}^r(\hat{R}) = \min_R \tilde{E}^r(R). \tag{31}$$

Similarly to the discussion for (22) the problem (31) may have unphysical solution as well if $U_j - U_{j-1} = R_{i_k}/a_k > \rho_c.$, In this case the problem is broken into two sub-problems for nodes $\{U_{i_1}, \cdots, U_{i_{k-1}}\}$ and $\{U_{i_k}, \cdots, U_{i_m}\}$. We thus can have one solution of (31) by solving the sub-problems. But the solution is not what we want since $U_j - U_{j-1} \gg \gamma$ in the kth element. As we did for (22) we consider a region

$$\mathbf{R}_{qc} = \{R_{i_k} : \ R_{i_k}/a_k < \rho_c, \ k = 1, 2, \cdots, m.\}. \tag{32}$$

If $\{R_{i_k}\}_{k=1}^m \in \mathbf{R}_{qc}$ then $\{R_j = U_j - U_{j-1}\}_{j=1}^N \in \mathbf{R}_c$. Using the technique in proving Theorems *1*, *2* and *4* we can prove that the solution of (31) in the region $\mathbf{R}_{qc}$ satisfies

$$\frac{4}{5}\sigma \le U_j - U_{j-1} = R_{i_k}/a_k \le \gamma \ \text{ for all } \ k, \tag{33}$$

where the integer $j \in (i_{k-1}, i_k]$. From the estimates of the solution we are able to prove the uniqueness and existence of the solution of (31) in the region $\mathbf{R}_{qc}$ similarly to previous arguments. However we shall focus on error estimates.

The solution R_{i_k} should satisfy

$$\begin{aligned} \frac{\partial \tilde{E}^r}{\partial R_{i_k}} &= \frac{1}{2}\Big(\sum_{j=i_k-i_c}^{i_k-1} W'\Big(\frac{i_k - j}{a_k} R_{i_k}\Big)(i_k - j) + \sum_{j=i_{k-1}+1}^{i_{k-1}+i_c} W'\Big(\frac{j - i_{k-1}}{a_k} R_{i_k}\Big)(j - i_{k-1})\Big) \\ &= \sum_{j=i_k-i_c}^{i_k-1} W'\Big(\frac{i_k - j}{a_k} R_{i_k}\Big)(i_k - j) = 0. \end{aligned} \tag{34}$$

for $k = 2, \cdots, m-1$. We can easily verify that the last equality of (34) also holds for $k = 1$ and $k = m$. So we have (34) for all $k = 1, \cdots, m$. The total energy after the cut-off can be written as

$$\bar{E}_c = \frac{1}{2}\sum_{i=0}^{N}\Big(\sum_{j=i-i_c\vee 1}^{i-1} W(r_i^c + \cdots + r_{j+1}^c) + \sum_{j=i+1}^{i+i_c\wedge N} W(r_j^c + \cdots + r_{i+1}^c)\Big), \tag{35}$$

where we have used $u_j^c - u_i^c = r_i^c + \cdots + r_{j+1}^c$ for $j > i$ and $u_i^c - u_j^c = r_j^c + \cdots + r_{i+1}^c$ for $j < i$.

We now estimate the error of the solution of this minimization problem (31) to that of (35) or (22). From error estimates for R_{i_k} we can then obtain those for U_{i_k}. The solution r_i^c that minimizes $\bar{E}_c$ should satisfy

$$\frac{\partial \bar{E}_c}{\partial r_i^c} = \frac{1}{2}\sum_{p=0}^{i_c-1}\sum_{j=i-i_c+p}^{i-1} W'(r_{i+p}^c + \cdots + r_{j+1}^c) + \frac{1}{2}\sum_{p=1}^{i_c}\sum_{j=i}^{i+i_c-p} W'(r_j^c + \cdots + r_{i-p+1}^c) = 0. \tag{36}$$

Let $R_{i_k}^c = u_{i_k}^c - u_{i_{k-1}}^c$ and $\bar{r}_i^c = R_{i_k}^c/a_k$ for all $i \in (i_{k-1}, i_k)$. To estimate the error between the solutions of (34) and (36) we need to replace R_{i_k} in the right hand side of (34) by $R_{i_k}^c$ and estimate its residue. For this purpose let $i = i_k$ in (36) and do Taylor's expansion at $R_{i_k}^c/a_k$ for each component of r^c involved. We then obtain

$$\sum_{j=i_k-i_c}^{i_k-1} (i_k - j) W'\Big(\frac{i_k - j}{a_k} R_{i_k}^c\Big) = h_{i_k}, \tag{37}$$

where

$$h_{i_k} = \frac{1}{2}\sum_{p=0}^{i_c-1}\sum_{j=i_k-i_c+p}^{i_k-1} W''(\psi_j^1)(r^c_{i_k+p}+\cdots+r^c_{j+1}-(i_k+p-j)R^c_{i_k}/a_k)$$
$$+\frac{1}{2}\sum_{p=1}^{i_c}\sum_{j=i_k}^{i_k+i_c-p} W''(\psi_j^2)(r^c_j+\cdots+r^c_{i_k-p+1}-(j-i_k+p)R^c_{i_k}/a_k).$$

Here $\psi_j^1 = \theta_1(r^c_{i+k}+\cdots+r^c_{j+1})+(1-\theta_1)(i_k+p-j)R^c_{i_k}/a_k$ and $\psi_j^2 = \theta_2(r^c_j+\cdots+r^c_{i-k+1})+(1-\theta_2)((j-i_k+p)R^c_{i_k}/a_k)$. Note that $\frac{4}{5}\sigma < r_i^c < \gamma$ for all i. So does $R^c_{i_k}/a_k$ for all k. Hence

$$(i_k+p-j)\frac{4}{5}\sigma < \psi_j^1 < (i_k+p-j)\gamma \ \ (j<i_k),\ (j-i_k+p)\frac{4}{5}\sigma < \psi_j^2 < (j-i_k+p)\gamma \ \ (j>i_k).$$

We thus have

$$h_{i_k} \le (|W''(\frac{4}{5}\sigma)|+2^2|W''(2\frac{4}{5}\sigma)|+\cdots+i_c^2|W''(i_c\frac{4}{5}\sigma)|)\Delta r_{i_k}^{max} \le 20\frac{\Delta r_{i_k}^{max}}{\sigma^2}, \tag{38}$$

where $\Delta r_{i_k}^{max} = \max_{j\in[i_k-i_c,i_k+i_c]}|r_j^c - R^c_{i_k}/a_k|$. Subtracting (37) from (34) and using Taylor's theorem we can obtain

$$\sum_{j=i_k-i_c}^{i_k-1}(i_k-j)^2W''((i_k-j)\psi)(R_{i_k}-R^c_{i_k})/a_k \le 20\frac{\Delta r_{i_k}^{max}}{\sigma^2}. \tag{39}$$

Here $\frac{4}{5}\sigma < \psi = (\theta R_{i_k}+(1-\theta)R^c_{i_k})/a_k < \gamma$ (where $0<\theta<1$). Noting that

$$\sum_{j=i_k-i_c}^{i_k-1}(i_k-j)^2W''((i_k-j)\psi) \ge W''(\gamma)+\sum_{j=2}^{4}j^2W''(j\frac{4}{5}\sigma)+\sum_{j=5}^{i_c(\delta)}j^2W''(j\frac{4}{5}\sigma) \ge 10/\sigma^2$$

and $a_k \le l$ we have:

$$|R_{i_k}-R^c_{i_k}| \le 2l\ \max_k\ \Delta r_{i_k}^{max}. \tag{40}$$

Now we estimate $\Delta r_{i_k}^{max}$ for the solution r^c of (22). From $\frac{4}{5}\sigma < r_i^c < \gamma \approx 1.12\sigma$ we immediately have $\Delta r_{i_k}^{max} \le (1.12-\frac{4}{5})\sigma = 0.32\sigma$. However, we can do better. From (24) we have (for all $i \ne j$):

$$|W'(r_i^c)-W'(r_j^c)| \le |W'(2\cdot\frac{4}{5}\sigma)-W'(2\gamma)|+W'(2\cdot\frac{4}{5}\sigma)+(|W'(3\cdot\frac{4}{5}\sigma)-W'(3\gamma)|)+$$
$$2W'(3\cdot\frac{4}{5}\sigma)+\cdots \approx 2W'(2\cdot\frac{4}{5}\sigma)$$

because $W'(\alpha)$ decreases dramatically as α increases. Noting that $|W'(r_i^c)-W'(r_j^c)| \ge W''(\gamma)|r_i^c-r_j^c| \ge 15|r_i^c-r_j^c|/\sigma^2$ we obtain $|r_i^c-r_j^c| \le (2W'(2\cdot\frac{4}{5}\sigma)/15)\sigma^2 = \eta\sigma$. Hence,

$$\Delta r_{i_k}^{max} \le \eta\sigma. \tag{41}$$

Next we treat (24) more carefully to obtain a much better estimate than (41). Subtracting the equations of (24) for $i=2$ and $i=j+1$ $(j\ge 2)$ we have (noting that $W''(2\cdot\frac{4}{5}\sigma)2W'(2\cdot\frac{4}{5}\sigma) \le O(3W'(3\cdot\frac{4}{5}\sigma))$)

$$\begin{aligned}|W'(r_2^c)-W'(r_{j+1}^c)| &\le |W''(2\cdot\frac{4}{5}\sigma)|(|r_1^c-r_j^c|+2|r_2^c-r_{j+1}^c|+|r_3^c-r_{j+2}^c|)+O(3W'(3\cdot\frac{4}{5}\sigma))\\ &\le 2|W''(2\cdot\frac{4}{5}\sigma)||r_2^c-r_{j+1}^c|+|W''(2\cdot\frac{4}{5}\sigma)||r_3^c-r_{j+2}^c|+O(3W'(3\cdot\frac{4}{5}\sigma)).\end{aligned}$$

Similarly to the above we have

$$|r_2^c - r_{j+1}^c| \leq O(|W''(2\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_3^c - r_{j+2}^c| + O(3W'(3\cdot\frac{4}{5}\sigma)/15)\sigma^2. \quad (42)$$

Subtracting the equations of (24) for $i = 3$ and $i = j+2$ ($j \geq 2$) we have

$$\begin{aligned}|W'(r_3^c) - W'(r_{j+2}^c)| \quad \leq \quad & |W''(2\cdot\frac{4}{5}\sigma)|(|r_2^c - r_{j+1}^c| + 2|r_3^c - r_{j+2}^c| + |r_4^c - r_{j+3}^c|) + \\ & |W''(3\cdot\frac{4}{5}\sigma)|(|r_1^c - r_j^c| + 2|r_2^c - r_{j+1}^c| + 3|r_3^c - r_{j+2}^c| + 2|r_4^c - r_{j+3}^c|) + \\ & |r_5^c - r_{j+4}^c|) + O(4W'(4\cdot\frac{4}{5}\sigma))\end{aligned}$$

We can verify that both $O(|W''(2\cdot\frac{4}{5}\sigma)|W'(3\cdot\frac{4}{5}\sigma)/15)$ and $O(|W''(3\cdot\frac{4}{5}\sigma)|W'(2\cdot\frac{4}{5}\sigma)/15) \leq O(4W'(4\cdot\frac{4}{5}\sigma))$. We thus have

$$\begin{aligned}&|r_3^c - r_{j+2}^c| \leq O(|W''(2\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_4^c - r_{j+3}^c| + O(|W''(3\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_5^c - r_{j+4}^c| \\ &+O(4W'(4\cdot\frac{4}{5}\sigma)/15)\sigma^2. \quad (43)\end{aligned}$$

Similarly we can obtain

$$\begin{aligned}&|r_i^c - r_{j+i-1}^c| \leq O(|W''(2\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_{i+1}^c - r_{j+i}^c| + O(|W''(3\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_{i+2}^c - r_{j+i+1}^c| \\ &+\cdots + O(|W''((i\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_{2i-1}^c - r_{j+2i-2}^c| + O(i|W''(i\cdot\frac{4}{5}\sigma)|/15)\sigma^2. \quad (44)\end{aligned}$$

for $1 \leq i \leq i_c$. For $i_c + 1 \leq i \leq [\frac{N}{2}]$ we have

$$\begin{aligned}&|r_i^c - r_{j+i-1}^c| \leq O(|W''(2\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_{i+1}^c - r_{j+i}^c| + O(|W''(3\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_{i+2}^c - r_{j+i+1}^c| \\ &+\cdots + O(|W''((i_c\cdot\frac{4}{5}\sigma)|/15)\sigma^2|r_{i+i_c-1}^c - r_{j+i+i_c-2}^c| + O(i_c|W''(i_c\cdot\frac{4}{5}\sigma)|/15)\sigma^2. \quad (45)\end{aligned}$$

Substituting (43) into (42) and then applying (41) we can dramatically reduce the first term (since $|W''(j\cdot\frac{4}{5}\sigma)| \ll 1$ for $j \geq 2$) and obtain $|r_2^c - r_{j+1}^c| \leq O(3W'(3\cdot\frac{4}{5}\sigma)/15)\sigma^2$. Similarly if we substitute (44) for $i = 4, 5, \cdots$ into (43) we will dramatically reduce the first and the second terms and obtain $|r_3^c - r_{j+2}^c| \leq O(4W'(4\cdot\frac{4}{5}\sigma)/15)\sigma^2$. Repeating this procedure we can obtain $|r_i^c - r_{j+i-1}^c| \leq O(iW'(i\cdot\frac{4}{5}\sigma)/15)\sigma^2$ for $1 \leq i \leq i_c$ and $|r_i^c - r_{j+i-1}^c| \leq O(i_cW'(i_c\cdot\frac{4}{5}\sigma)/15)\sigma^2$ for $i_c + 1 \leq i \leq [\frac{N}{2}]$. For $[\frac{N}{2}] \leq i \leq N$ we can start from $i = N$ and obtain the same estimates accordingly. Therefore, for $k = 1$ and $i_1 - i_c \geq i_c$

$$\begin{aligned}&\Delta r_{i_k}^{max} \leq \max_{i\in[i_k - i_c, i_k + i_c]} \sum_{j=i_{k-1}}^{i_k} |r_j^c - r_i^c|/a_k \leq \frac{1}{l}\sum_{j=2}^{i_c} jW'(j\frac{4}{5}\sigma)\sigma^2/15 + \frac{l-i_c}{l}i_cW'(i_c\frac{4}{5}\sigma)\sigma^2 \\ &\leq K(\frac{\eta}{l} + \frac{l-i_c}{l}\delta)\sigma. \quad (46)\end{aligned}$$

For $k=1$ and $i_1 - i_c < i_c$ (noting that $i_1 = [\frac{l}{2}]$) we have

$$\begin{aligned}
\Delta r_{i_k}^{max} &\leq \max_{i\in[i_k-i_c,i_k+i_c]} \sum_{j=i_{k-1}}^{i_k} |r_j^c - r_i^c|/l \\
&\leq \frac{1}{l}\sum_{j=2}^{i_1-i_c} j|W'(j\frac{4}{5}\sigma)|\sigma^2/15 + \frac{l-(i_1-i_c)}{l}(i_1-i_c)|W'((i_1-i_c)\frac{4}{5}\sigma)|\sigma^2 \\
&\leq K(\frac{\eta}{l} + \frac{[\frac{l}{2}]+1+i_c}{l}|W'(([\frac{l}{2}]-i_c)\frac{4}{5}\sigma)|\sigma)\sigma, \qquad (47)
\end{aligned}$$

For $1 < k < [\frac{m}{2}]$ we can have

$$\Delta r_{i_k}^{max} \leq K\delta\sigma. \qquad (48)$$

For $k \geq [\frac{m}{2}]$ the result is accordingly the same as (46)-(48). Therefore

$$\|R_{i_k} - R_{i_k}^c\| \leq \begin{cases} K\max\{\eta + (l-i_c)\delta, l\delta\}\sigma & \text{if } [\frac{l}{2}] - i_c \geq i_c \\ K\max\{\eta + ([\frac{l}{2}]+1+i_c)|W'(([\frac{l}{2}]-i_c)\frac{4}{5}\sigma)|\sigma, l\delta\}\sigma & \text{if } [\frac{l}{2}] - i_c < i_c \end{cases} \qquad (49)$$

where $\|\cdot\|$ can be $\|\cdot\|_\infty$ or $\frac{1}{\sqrt{m}}\|\cdot\|_2$. The first part of (49) shows (8) from (19) and $N = ml$. From the definition of R_{i_k} and $U_{i_0} = 0$ we can calculate

$$U_{i_1} = R_{i_1},\ U_{i_k} = \sum_{j=1}^{k} R_{i_j},\ \text{for}\ \ k = 1, 2, \cdots m.$$

Similarly $u_{i_k}^c = \sum_{j=1}^{k} R_{i_j}^c$. Thus the error between U_{i_k} and $u_{i_k}^c$ is:

$$\|U_{i_k} - u_{i_k}^c\| \leq \begin{cases} Km\max\{\eta + (l-i_c)\delta, l\delta\}\sigma & \text{if } [\frac{l}{2}] - i_c \geq i_c \\ Km\max\{\eta + ([\frac{l}{2}]+1+i_c)|W'(([\frac{l}{2}]-i_c)\frac{4}{5}\sigma)|\sigma, l\delta\}\sigma & \text{if } [\frac{l}{2}] - i_c < i_c \end{cases} \qquad (50)$$

The first part of (50) shows (9) from (19) and $N = ml$. Note that the length of our material problem is of $O(N\sigma)$. So for a material with finite length we have $ml\sigma = N\sigma = O(1)$.

Combining the error estimate (50) with (7) we obtain the error between the QC approximate solution U_{i_k} and the full lattice-scale solution u_{i_k}:

$$\|U_{i_k} - u_{i_k}\|_\infty \leq \begin{cases} K(N\sigma)(\max\{\frac{\eta}{l} + \frac{l-i_c}{l}\delta, \delta\} + i_c\delta) & \text{if } [\frac{l}{2}] - i_c \geq i_c \\ K(N\sigma)(\max\{\frac{\eta}{l} + \frac{[\frac{l}{2}]+1+i_c}{l}|W'(([\frac{l}{2}]-i_c)\frac{4}{5}\sigma)|\sigma, \delta\} + i_c\delta) & \text{if } [\frac{l}{2}] - i_c < i_c \end{cases} \qquad (51)$$

All notations used in estimates (49)-(51) have been explained in §1. These results not only prove the estimates mentioned in the introduction but also give error estimates for other choices of l. Better approximation is expected if we use higher order polynomial shape functions in (28). The method we have used to analyze this model may apply to other material particle problems and our results may also be useful to study dynamic features.

Acknowledgment The author would like to thank Professor A. Stuart for bringing him into this area and for many stimulating discussions and to thank Professors K. Cho and H. Gao for many discussions on the physical background.

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