Reliability of Atomistic-Continuum Modeling Simulations for Problems in Molecular Statics

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ABSTRACT

The goal-oriented error estimation and adaptivity methodology is extended to problems of molecular statics within the framework of the quasicontinuum approximation for the simulation of a nanoindentation problem. Computable error estimates are developed with respect to a physical quantity of interest, namely the force under the indenter. An adaptive scheme based upon these error estimates is also proposed to control the errors in the nanoindentation simulation within some user-supplied error tolerance. The results are compared with a highly resolved solution of the problem that is considered exact for the purposes of this work. It is shown that the proposed goal-oriented adaptive strategy successfully controls the error in the QCM approximation and allows one to obtain an accurate computation of the quantity of interest.

Keywords: multi-scale modeling, adaptive modeling, goal-oriented error estimation, quasicontinuum method, nanoindentation

1 INTRODUCTION

The quasicontinuum method (QCM) introduced by Tadmor, Ortiz, and Phillips [10], [8], [3] has been at the forefront of research in multi-scale methods. The methodology has been applied to problems in fracture [2], [4], grain boundary interaction [7], and nanoindentation [11], [9]. The objectives of the method are essentially twofold:

1. To dramatically reduce the number of degrees of freedom from $N \times d$.
2. To substantially lower the cost in the calculation of the potential energy by computing energies only at selected sites.

The approach becomes very efficient if one considers an adaptive scheme to automatically select the degrees of freedom that allow one to capture the critical deformations of the lattice. However, due to the various approximations in the method, the produced solution inevitably contains errors that need to be controlled.

We propose here to use the goal-oriented adaptive modeling algorithm based upon the work of Oden and Prudhomme [5] in order to demonstrate the applicability and effectiveness of this approach to QCM type problems. The idea is that there exists a mathematical model of a physical event that is believed to capture the essential features of the phenomenon, but is too expensive to compute, while, on the other hand, it is often the case that one can construct simplified models that are computable, but are known to be invalid under certain circumstances. For example, a molecular statics model with full fidelity is needed to capture the defects of the material in the vicinity of the indentation, while, in the far field, a "coarser model" will suffice. Goal-oriented adaptive techniques are attractive in the sense that the model selection can be automatically controlled by error estimates in a quantity of interest so that the quantity of interest is computed to within a user-specified tolerance. Thus, there are two key aspects of the goal-oriented approach: estimation of the error in a quantity of interest and the model selection algorithm. Our methodology has been implemented in a serial code of the QCM algorithm that has been made available on the internet (http://www.qcmethod.com).

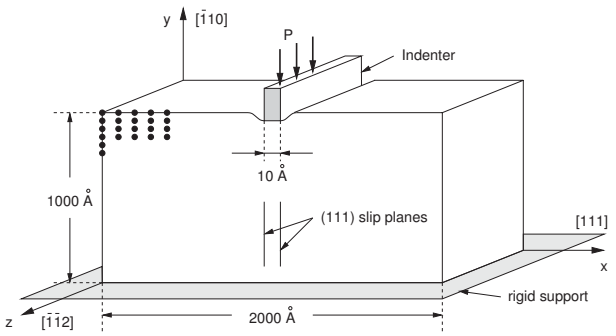

Figure 1: Geometrical setup of the nanoindentation problem

2 PROBLEM SETUP

Here we study the nanoindentation problem included in the QCM software package. Specifically, a thin Aluminum crystal is loaded by a rigid, rectangular indenter, see Figure 1. The indenter is 10Å wide in the plane and infinitely long out-of-plane. The dimensions of the

crystalline block are $2000\mathring{A} \times 1000\mathring{A}$ in the [111] and $[\bar{1}10]$ directions, respectively. The displacements are constrained in the $y = 0$ plane while the displacements for the atoms under the indenter are prescribed (and the force calculated subsequently). The indenter is moved down into the material in $2\mathring{A}$ steps and a total of 30 load steps are considered. Quasistatic steps are used for the solution of the displacements. The goal (quantity of interest) of this simulation is the force under the indenter.

3 ERROR ESTIMATION

Here, we briefly summarize the results for the error estimates in the force. Detailed explanations can be found in [6]. The molecular statics problem can be written mathematically as a constrained minimization problem:

$$E(\boldsymbol{u}) = \min_{\boldsymbol{v}\in V} E(\boldsymbol{v}) \tag{1}$$

where $V = \left(\mathbb{R}^d\right)^N$, $d = 2$ or 3, N is the number of atoms in the lattice, and

$$E(\boldsymbol{u}) = -\sum_{i=1}^{N} \boldsymbol{f}_i \cdot \boldsymbol{u}_i + \sum_{k=1}^{N} E_k(\boldsymbol{u}) \tag{2}$$

where $\boldsymbol{f}_i$ is the external load applied to an interior atom i and $E_k(\boldsymbol{u})$ is the energy of atom k determined from the Embedded Atom Method [1]. Here, $\boldsymbol{u}$ denotes the collection of displacement vectors $\boldsymbol{u}_i$ associated with each atom i. This problem can be rewritten into a variational statement given by

$$\begin{aligned} &\textit{Find } \boldsymbol{u} \in V \textit{ such that} \\ &\qquad B(\boldsymbol{u};\boldsymbol{v}) = F(\boldsymbol{v}), \quad \forall \boldsymbol{v} \in V_0 \end{aligned} \tag{3}$$

where $V_0 = \left(\mathbb{R}^d\right)^{N_a}$, N_a is the number of atoms in the interior of the lattice and

$$\begin{aligned} B(\boldsymbol{u};\boldsymbol{v}) &= \sum_{i=1}^{N_a} \left[\sum_{k=1}^{N} \frac{\partial E_k}{\partial \boldsymbol{u}_i}(\boldsymbol{u})\right] \cdot \boldsymbol{v}_i \\ F(\boldsymbol{v}) &= \sum_{i=1}^{N_a} \boldsymbol{f}_i \cdot \boldsymbol{v}_i \end{aligned} \tag{4}$$

with Dirichlet boundary conditions prescribed at the boundaries. Corresponding to this *primal problem* is the *dual problem* whose solution is the so-called *influence function* or *dual solution*. The dual problem is

$$\begin{aligned} &\textit{Find } \boldsymbol{p} \in V_0 \textit{ such that} \\ &\qquad B'(\boldsymbol{u};\boldsymbol{v},\boldsymbol{p}) = Q'(\boldsymbol{u};\boldsymbol{v}), \quad \forall \boldsymbol{v} \in V_0 \end{aligned} \tag{5}$$

where in this case

$$\begin{aligned} B'(\boldsymbol{u};\boldsymbol{v},\boldsymbol{p}) &= \sum_{j=1}^{N_a}\sum_{i=1}^{N_a} \boldsymbol{v}_j \cdot \left[\sum_{k=1}^{N} \frac{\partial^2 E_k}{\partial \boldsymbol{u}_j \partial \boldsymbol{u}_i}(\boldsymbol{u})\right] \cdot \boldsymbol{p}_i \\ Q'(\boldsymbol{u};\boldsymbol{v}) &= -\sum_{j=1}^{N_a} \boldsymbol{v}_j \cdot \left[\sum_{i=1}^{M} \frac{\partial^2 E_i}{\partial \boldsymbol{u}_j \partial u_{y,i}}(\boldsymbol{u})\right] \end{aligned} \tag{6}$$

where $(\cdot)'$ represents the Gâteaux derivative and $Q(\boldsymbol{u})$ is the quantity of interest (the force under the indenter), which is given by

$$Q(\boldsymbol{u}) = -\sum_{i=1}^{M} f_{y,i} = -\sum_{i=1}^{M} \frac{\partial E_i}{\partial u_{y,i}}(\boldsymbol{u}) \tag{7}$$

M being the number of atoms in contact with the lower surface of the indenter. These problems are the *base models* that are intractable due to size. In the QCM, the dimension of the problem is reduced to a set of representative atoms, the so-called "repatoms", and the calculation of site energies are considerably simplified in the regions where deformation gradients are quasi-uniform; see [3]. These approximations constitute the approximate or *surrogate* model that is solved for $\boldsymbol{u}_0$. Let R be the number of repatoms, $R << N$, and $W = (\mathbb{R}^d)^R$, $W_0 = (\mathbb{R}^d)^{R_a}$. The surrogate problem is then

$$\begin{aligned} &\textit{Find } \boldsymbol{u}_0 \in W \textit{ such that} \\ &\qquad B_0(\boldsymbol{u}_0;\boldsymbol{v}) = F_0(\boldsymbol{v}), \quad \forall \boldsymbol{v} \in W_0 \end{aligned} \tag{8}$$

The subscript zero denotes the surrogate model, obtained here by the quasicontinuum method. For the dual problem, we need to consider $\tilde{N}$ repatoms, $R < \tilde{N} < N$. Hence the surrogate dual problem is

$$\begin{aligned} &\textit{Find } \tilde{\boldsymbol{p}} \in \tilde{V} \textit{ such that} \\ &\qquad \tilde{B}'(\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0;\tilde{\boldsymbol{v}},\tilde{\boldsymbol{p}}) = \tilde{Q}'(\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0;\tilde{\boldsymbol{v}}), \quad \forall \tilde{\boldsymbol{v}} \in \tilde{V} \end{aligned} \tag{9}$$

where $\tilde{V} = (\mathbb{R}^d)^{\tilde{N}}$ and $\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0$ is an extension of $\boldsymbol{u}_0$ to $\tilde{V}$ (here, the extension is linear interpolation). With the primal and dual solutions, the error estimates in the quantity of interest can be computed as (see [5]):

$$\begin{aligned} &Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0) \approx \eta \\ &\eta = \tilde{R}(\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0;\tilde{\boldsymbol{p}}) = \sum_{i=1}^{\tilde{N}_a} \tilde{\boldsymbol{r}}_i(\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0) \cdot \tilde{\boldsymbol{p}}_i \end{aligned} \tag{10}$$

where $\boldsymbol{u}_0$ is a solution of (8), $\tilde{\boldsymbol{p}}_i$ are obtained from (9) and the $\tilde{\boldsymbol{r}}_i$ are the residuals which reflect the force imbalance at each atom i, $1 \le i \le \tilde{N}$.

4 ADAPTIVE ALGORITHM

With the computable error estimator in hand, we use the QCM software to compute the primal solution $\boldsymbol{u}_0$ and dual solution $\tilde{\boldsymbol{p}}$ and adapt the mesh so as to reduce the error $Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0)$. The adaptive algorithm then proceeds as follows:

1. Initialize the load step s = 0. Input user-tolerance γ.
2. s = s+1.
3. Solve the primal and dual problems.

4. Compute the error estimate according to (10).

5. Check: $|\eta| > \gamma|Q(\boldsymbol{u}_0)|$. If false: s=s+1, goto 2. If true: mark those elements with $|\eta^e(\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0, \tilde{\boldsymbol{p}})| > \alpha \max_e |\eta^e(\tilde{\boldsymbol{\pi}}\boldsymbol{u}_0, \tilde{\boldsymbol{p}})|$, where α is a user-supplied number between 0 and 1 and $\sum_e \eta^e = \eta$.

6. Refine flagged elements. Goto 3.

5 RESULTS

The results of numerical tests are shown comparing the accuracy to which QCM and the goal-oriented approach resolve the force under the indenter (in the goal-oriented solution, the error tolerance was set to 5%). The comparison is made with respect to a highly resolved solution ("overkill solution") that uses up to 42000 atoms. Figures 2 and 4 show the primal and dual solution, respectively, at the beginning of dislocation nucleation for the overkill solution while Figures 3 and 5 show the corresponding primal and dual solutions for the goal-oriented simulation.

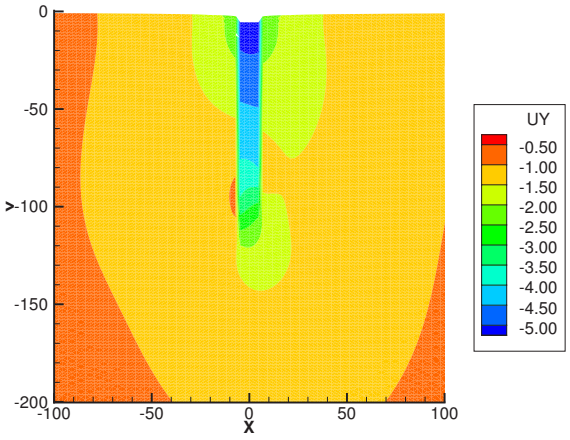

Figure 2: Displacement of atoms in the overkill solution at the beginning of dislocation nucleation

In the QC algorithm, a total of approximately 1600 atoms are used to obtain the solution. The goal-oriented solution used approximately 3200 atoms. Figure 6 shows the force-displacement curve comparing these solutions with the overkill solution. Notice how the QCM solution is stiffer than the overkill solution and the dislocations nucleate one load step too early while the goal-oriented adaptivity gives an accurate representation of the force. Figure 7 shows the relative exact error and the relative error estimate. It can be seen that the estimates are reasonably accurate, but do overestimate the error present in the quantity of interest.

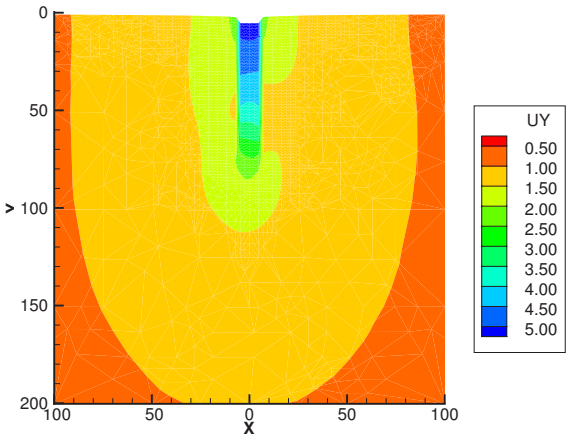

Figure 3: Displacement of atoms in the goal-oriented solution at the beginning of dislocation nucleation

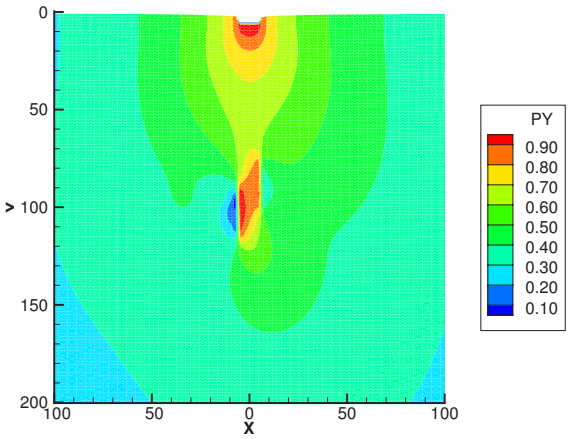

Figure 4: The influence function of the overkill solution at the beginning of dislocation nucleation

6 CONCLUSIONS

We have presented the implementation of the goal-oriented adaptive modeling methodology using the quasicontinuum method as a surrogate model to the molecular statics problem in an effort to demonstrate the applicability and effectiveness of the framework to multi-scale problems. Numerical simulations have been performed on a nanoindentation problem supplied with the QCM software package. Results show that the error estimator provides accurate estimates of the error in the force under the indenter with a reasonable number of degrees of freedom and that the proposed scheme allows one to automatically adapt the simulation in order to control the error to within some prescribed tolerance.

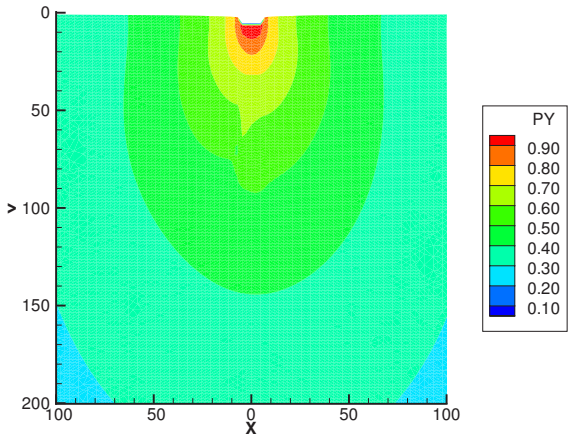

Figure 5: The influence function of the goal-oriented solution at the beginning of dislocation nucleation

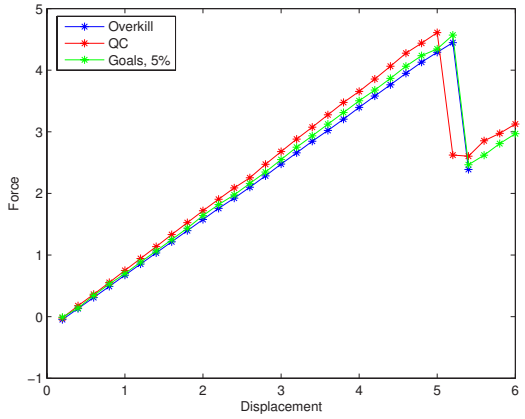

Figure 6: Comparison of force-displacement curves computed by the QCM and Goals to a highly resolved solution

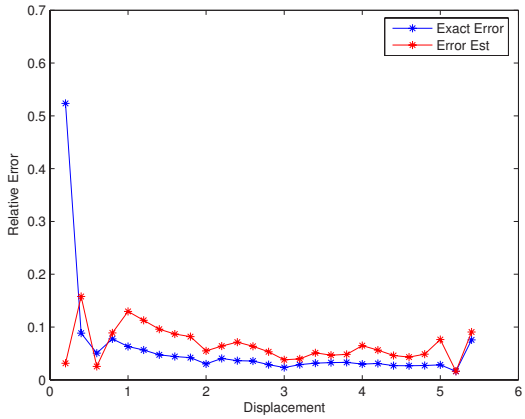

Figure 7: Comparison of the exact relative error to the estimated relative error

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