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# MESH OPTIMIZATION FOR THE QUASICONTINUUM METHOD: A GENERALIZATION OF VALE

J. Knap, J. Marian and M. Ortiz
*Division of Engineering and Applied Science*
*California Institute of Technology*
*Pasadena, CA 91125*

*Summary* The current formulation of the quasicontinuum (QC) method relies on a static triangulation of the reference crystal configuration. This computational mesh needs to encompass a wide range of spatial resolutions, from fully atomistic at defect cores, to continuum-like in defect-free regions. Moreover, it must continuously adapt to the structure of the deformation field, so as to return the least possible potential energy for a fixed number of nodes. In the implementations of the QC method to date, the mesh adaption procedure has been based on empirical indicators. We present a variational adaption Lagrangian-Eulerian (VALE) method for the QC method. In this approach, the computational mesh is factored directly into the description of the energetics of the crystal. Therefore, the energy minimizer determines not only the equilibrium configuration of the crystal, but also the optimal configuration of the computational mesh. We apply the VALE-QC method to the investigation of a wide array of problems, from nanoindentation to crack tips.

## PROBLEM FORMULATION

We consider a set of $N$ atoms occupying a subset of simple $d$-dimensional Bravais lattice spanned by lattice vectors $\boldsymbol{a}_i, i = 1, \ldots, d$. The coordinates of atoms in the reference configuration of the crystal are:

$$\boldsymbol{X}(\boldsymbol{l}) = \sum_{i=1}^{d} l^i \boldsymbol{a}_i, \quad \boldsymbol{l} \in \mathcal{L} \subset \mathbb{Z}^d, \tag{1}$$

$\boldsymbol{l}$ denotes the lattice coordinates and $\mathbb{Z}$ is the set of integer numbers. The corresponding atomic coordinates in the current configuration may be conveniently collected in an array $\boldsymbol{x} = \{\boldsymbol{x}(\boldsymbol{l}), \boldsymbol{l} \in \mathcal{L}\} \in X$. The linear space $X \equiv R^{Nd}$ may be referred to as the 'configuration' space of the crystal.

The energy of the crystal is assumed to expressible as a function of the atomic coordinates, i.e. $E(\boldsymbol{x})$. Moreover, any applied loads are considered conservative and to derive from an external potential $\Phi^{\text{ext}}(\boldsymbol{x})$. Therefore, the total potential energy of the crystal is:

$$\Phi(\boldsymbol{x}) = E(\boldsymbol{x}) + \Phi^{\text{ext}}(\boldsymbol{x}). \tag{2}$$

The stable equilibrium configurations of interest are the minimizers of $\Phi(\boldsymbol{x})$ over the space $X$, i. e., the solutions of the variational problem

$$\min_{\boldsymbol{x} \in X} \Phi(\boldsymbol{x}). \tag{3}$$

## A NEW FORM OF QC REDUCTION

The quasicontinuum theory strives to replace Eq. (3) with a reduced problem of finding the total potential energy minimizers over a subspace $X_h$ of $X$. Within the framework of the 'classical' quasicontinuum [2, 3, 1], a set of atoms, also referred to as 'representative atoms', is introduced to form a basis of $X_h$. Here instead, we construct $X_h$ by interpolation from an *arbitrary* set $T_h$ of $N_h \ll N$ points, or nodes, not necessarily coincident with atomic sites. Thus, let $\boldsymbol{Q}_h = \{\boldsymbol{Q}_h(i_h), i_h \in T_h\}$ denote an array of nodal coordinates in the reference configuration of the crystal, or referential nodal coordinates. Additionally, let $\mathcal{T}_h$ be a triangulation of $T_h$ and suppose that the crystal lattice $\mathcal{L}$ is contained within the polytope of $T_h$. The triangulation $\mathcal{T}_h$ supports a collection of shape functions, $\varphi_h(\boldsymbol{l}|i_h), i_h \in T_h$. The positions of all atoms in $\mathcal{L}$ can then be determined by interpolation of the coordinates of all nodes in the set $T_h$, namely,

$$\boldsymbol{x}_h(\boldsymbol{l}) = \sum_{i_h \in T_h} \varphi_h(\boldsymbol{l}|i_h) \boldsymbol{q}_h(i_h), \tag{4}$$

where $\boldsymbol{q}_h = \{\boldsymbol{q}_h(i_h), i_h \in T_h\}$ is an array containing the nodal coordinates in the current configuration of the crystal, or spatial nodal coordinates, i. e., an element of a linear space $X_h$ of dimension $N_h d$ (c.f. Knap and Ortiz [1]).

## REDUCED PROBLEM

Tadmor *et al.* [2, 3] define the reduced counterpart of (3) as

$$\min_{\boldsymbol{q}_h \in X_h} \Phi(\boldsymbol{q}_h). \tag{5}$$

Evidently, the energy minimizers of the reduced problem implicitly depend on the choice of the triangulation $\mathcal{T}_h$ through subspace $X_h$. As noted by Thoutireddy and Ortiz [4], the *optimal triangulation* is that which delivers the least minimum potential energy. This leads to a reduced problem of the form

$$\min_{\boldsymbol{q}_h, \boldsymbol{Q}_h} \Phi(\boldsymbol{q}_h, \boldsymbol{Q}_h). \tag{6}$$

in which the energy is minimized with respect to *both* spatial and referential nodal coordinates. The stationarity of the total potential energy yields the reduced equilibrium equations

$$\boldsymbol{f}_h(i_h) \quad = \quad \sum_{\boldsymbol{l}\in\mathcal{L}} \boldsymbol{f}(\boldsymbol{l}|\boldsymbol{x}_h)\varphi_h(\boldsymbol{l}|i_h) = \boldsymbol{0}, \tag{7}$$

$$\boldsymbol{F}_h(i_h) \quad = \quad \sum_{\boldsymbol{l}\in\mathcal{L}} \boldsymbol{f}(\boldsymbol{l}|\boldsymbol{x}_h) \sum_{j_h\in T_h} \frac{\partial\varphi_h(\boldsymbol{l}|j_h)}{\partial \boldsymbol{Q}_h(i_h)} \boldsymbol{q}_h(j_h) = \boldsymbol{0}. \tag{8}$$

Here,

$$\boldsymbol{f}(\boldsymbol{x}) = \Phi_{,\boldsymbol{x}}(\boldsymbol{x}) \tag{9}$$

are the forces corresponding to $\boldsymbol{x}$ and $\boldsymbol{f}(\boldsymbol{l}|\boldsymbol{x})$ is the value of $\boldsymbol{f}(\boldsymbol{x})$ at site $\boldsymbol{l}$. The system of equations (7) imposes the mechanical equilibrium of the crystal, whereas the system (8) imposes the configurational equilibrium of the nodes.

As noted by Tadmor *et al.* [2, 3], the practicality of the method requires the application of lattice summations rules in order to circumvent the calculation of the full atomistic force array $\boldsymbol{f}$. Following Knap and Ortiz [1], we employ cluster summation rules, albeit based on a slightly modified definition of the cluster. Specifically, the cluster of lattice sites located within a sphere of radius $r(i_h)$ centered on the node $i_h$ is defined as $\mathcal{C}(i_h) = \{l : |\boldsymbol{X}(\boldsymbol{l}) - \boldsymbol{Q}_h(i_h)| \le r(i_h)\}$. The application of these summation rules to the reduced equilibrium equations gives

$$\boldsymbol{f}_h(i_h) \quad \approx \quad \sum_{i'_h\in T_h} n_h(i'_h) \left[ \sum_{\boldsymbol{l}\in\mathcal{C}(i'_h)} \boldsymbol{f}(\boldsymbol{l}|\boldsymbol{x}_h)\varphi_h(\boldsymbol{l}|i_h) \right] = \boldsymbol{0}, \tag{10}$$

$$\boldsymbol{F}_h(i_h) \quad \approx \quad \sum_{i'_h\in T_h} n_h(i'_h) \left[ \sum_{\boldsymbol{l}\in\mathcal{C}(i'_h)} \boldsymbol{f}(\boldsymbol{l}|\boldsymbol{x}_h) \sum_{j_h\in T_h} \frac{\partial\varphi_h(\boldsymbol{l}|j_h)}{\partial \boldsymbol{Q}_h(i_h)} \boldsymbol{q}_h(j_h) \right] = \boldsymbol{0}. \tag{11}$$

where $n(i_h), i_h \in T_h$ are the cluster weights, computed, as before, by requiring that the summation rules be exact for all shape functions.

## CONCLUSIONS

We have developed a new formulation of the quasicontinuum method that generalizes the original description of Tadmor *et al.* [2]. The method now incorporates a variational technique [4] that leads to a natural coupling of mechanical and configurational force systems. In this manner, any arbitrariness associated with the initial choice of the reference configuration is removed, and the equilibrium configurations of interest are calculated on an optimal reference mesh. The new formulation results in enhanced computational efficiency and effectively removes *ad hoc* elements from previous implementations of the QC method. Calculations concerned with nano-indentation, straight dislocation cores and crack tips are presented which illustrate the performance and versatility of the method.

## References

[1] J. Knap and M. Ortiz. An analysis of the quasicontinuum method. *Journal of the Mechanics and Physics of Solids*, 49(9):1899–1923, 2001.

[2] E.B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. *Philos. Mag. A*, 73:1529–1563, 1996.

[3] E.B. Tadmor, R. Phillips, and M. Ortiz. Mixed atomistic and continuum models of deformation in solids. *Langmuir*, 12(19):4529–4534, 1996.

[4] P. Thoutireddy and M. Ortiz. A variational r-adaption and shape-optimization for finite-deformation elasticity. *International Journal for Numerical Methods in Engineering*, 2004.