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Nano-to-Micro Scale-Bridging by a Seamless Atomistic-Continuum Coupling Method

• Motivation

A key question addressing the length scale problem in atomistic simulations is a challenge for mechanics, mathematics and computer science:

"How to develop an atomistic-continuum coupling method that combines atomistic accuracy with continuum effectivity?"

• **Building blocks** of the present version of an atomistic-continuum (a-c) coupling method at $T = 0\,\mathrm{K}$: the **C**luster **Q**uasi-**C**ontinuum Method (QC) based on **E**nergy sampling, **CQC-E**, [2, 3, 4] which draws on the seminal work in [1].

(I) Coarse-Graining by Finite-Element Discretization

In regions of purely elastic deformations it is sufficient to consider the movement of some judiciously selected, representative atoms, which are the nodes in a finite element triangulation. Only these atoms keep their independent degrees of freedom, whereas all other atoms are kinematically determined by the motion of the mesh nodes, see Fig. 1 (left).

Fully atomistic resolution is chosen in regions of inelastic deformation like at crack tips, at disclocation sites etc.

(II) Summation Rules: Energy Sampling in Clusters

Even after coarse-graining the total potential still depends on the energy $E_{\boldsymbol{k}}$ of each atom $\boldsymbol{k}$: $E^{\mathrm{tot,h}} = \sum_{\boldsymbol{k}\in\mathscr{L}} E_{\boldsymbol{k}}$. Therefore, energy is calculated only in sampling clusters $\mathscr{C}_{\boldsymbol{i}}$. For a spherical cluster around mesh node $\boldsymbol{i}$, $\mathscr{C}_{\boldsymbol{i}} = \{\boldsymbol{k} : |\boldsymbol{X}_{\boldsymbol{k}} - \boldsymbol{X}_{\boldsymbol{i}}| \le R_c(\boldsymbol{i})\}$, the corresponding cluster summation rule yields the approximated total energy

$$E^{\mathrm{CQC-E}} = \sum_{\boldsymbol{i}\in\mathscr{L}_h} n_{\boldsymbol{i}} \sum_{\boldsymbol{k}\in\mathcal{C}_{\boldsymbol{i}}} E_{\boldsymbol{k}}\,.$$

The weighting factor $n_{\boldsymbol{i}}$ accounts for the energy contribution of non-cluster atoms that a attributed to the cluster $\mathscr{C}_{\boldsymbol{i}}$.

Equilibrium configurations at $T = 0\mathrm{K}$ are minimizers of the total energy $E^{\mathrm{CQC-E}}$, i.e. solutions of the variational problem:

$$\min_{\{\boldsymbol{x}_{\boldsymbol{a}}\}} E^{\mathrm{CQC-E}} \quad \rightarrow \quad \boldsymbol{f}_{\boldsymbol{a}}^{\mathrm{CQC-E}} = -\frac{\partial E^{\mathrm{CQC-E}}}{\partial \boldsymbol{x}_{\boldsymbol{a}}} = \boldsymbol{0} \;\forall\, \boldsymbol{a} \in \mathscr{L}_h.$$

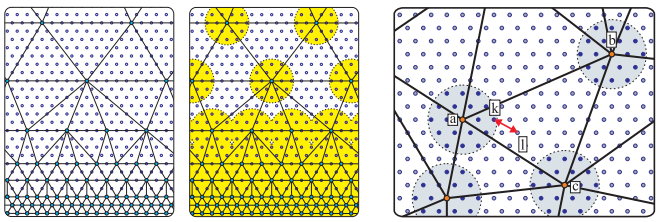

Fig. 1. Crystal subject to FE-discretization (left) and with cluster-atoms for energy sampling (centre). The method is fully nonlocal including interactions across clusters (right).

• **Nanoindentation into FCC Aluminum.** Since plastic deformation is confined to a small volume embedded in a much larger volume undergoing purely elastic deformation, nanoindentation is a paradigmatic problem for a-c coupling. The present CQC-E simulation results are in quantitative agreement with fully atomistic Molecular Statics (MS) but for a tiny fraction of the computation time.

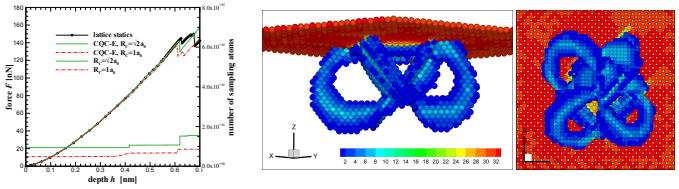

Fig. 2. Force-displacement curves show quantitative agreement of CQC-E with MS in both the elastic branch and the force-drop indicating discloation nucleation (left). Dislocation microstructure (centre and right) below the indenter in agreement with MS.

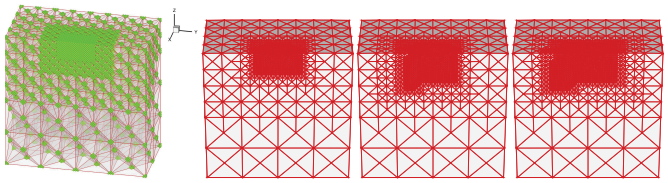

Fig. 3. Initial mesh with sampling clusters around mesh nodes (left). Adaptive mesh refinement, which is directed by the 2nd invariant of the Green strain tensor, enables an unbiased dislocation evolution by fully atomistic resolution in regions involved.

• Conclusions

The present atomistic-continuum coupling method, CQC-E based on energy sampling, exhibits a (i) variational structure, (ii) is fully nonlocal with atomic potentials as the only 'constitutive' input and enables a (iii) seamless scale transition from atomistic resolution to a coarse-grained description, [2].

In the simulations of nanoindentation the method proves its promising capacity to effectively reduce the prohibitive computational expense of fully atomistic resolution while faithfully simulating the materials response in significant details.

Acknowledgements

Financial support by the DFG through the Heisenberg programme (grant no. EI 453/2-1).

References

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