Center for Computational Sciences and Simulation CCSS

UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Seamless Nano-to-Micro Scale-Bridging by a Variationally Consistent Multiscale Method

Motivation

A key question addressing the length scale problem in atomistic simulations is equally a challenging task for engineering, maths 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 Cluster Quasi-continuum Method (QC) based on Energy sampling – **CQC-E**:

(I) Coarse-Graining by Finite-Element Discretization

In regions of purely elastic deformation 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.

Fully atomistic resolution is chosen in regions of inelastic deformation like at crack tips or at disclocation sites, grain boundaries and alike.

(II) Summation Rules: Energy Sampling in Clusters

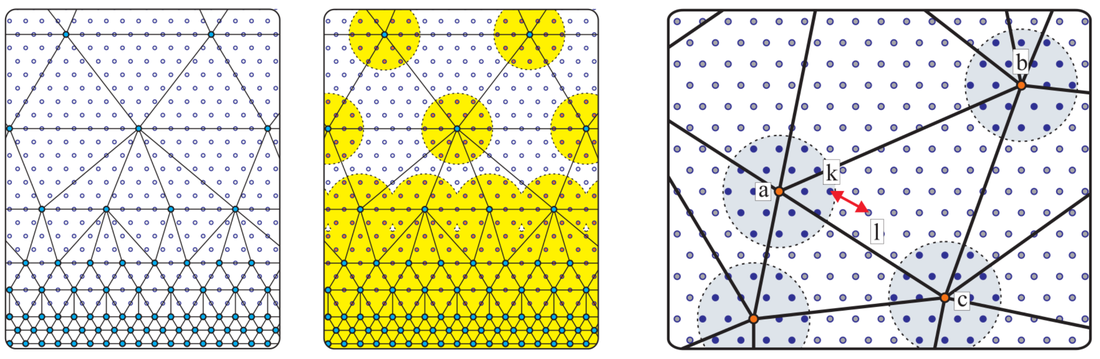
Even after coarse-graining the total potential still depends on the energy $E_{\boldsymbol{k}}$ of each atom $\boldsymbol{k}$: $E^{tot,h} = \sum_{\boldsymbol{k}\in L} E_{\boldsymbol{k}}$. Therefore, energy is calculated only in sampling clusters $C_{\boldsymbol{i}}$. For spherical clusters around mesh nodes, $C_{\boldsymbol{i}} = \{\boldsymbol{k} : |\boldsymbol{X_k} - \boldsymbol{X_i}| \leq R_c(\boldsymbol{i})\}$, the corresponding cluster summation rule reads

$$E^{\mathrm{CQC-E}} = \sum_{\boldsymbol{i}\in L_h} n_{\boldsymbol{i}} \sum_{\boldsymbol{k}\in C_{\boldsymbol{i}}} E_{\boldsymbol{k}}\,.$$

Therein, the weighting factor $n_{\boldsymbol{i}}$ accounts for the energy contribution of non-cluster atoms that a attributed to the cluster $C_{\boldsymbol{i}}$.

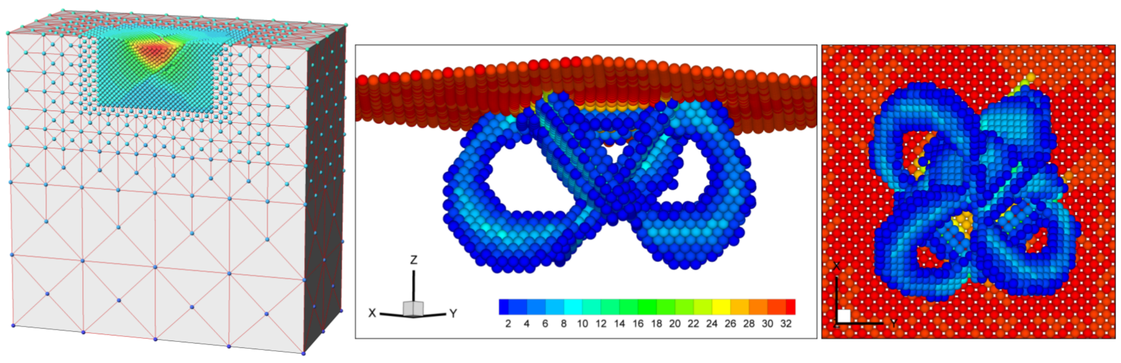
Equilibrium configurations at $T = 0\mathrm{K}$ are minimizers of the total energy $E^{\mathrm{CQC-E}}$, i.e. the solutions of the variational problem:

$$\min_{\{\boldsymbol{x_a}\}} E^{\mathrm{CQC-E}} \quad \rightarrow \quad \boldsymbol{f}_{\boldsymbol{a}}^{\mathrm{CQC-E}} = -\frac{\partial E^{\mathrm{CQC-E}}}{\partial \boldsymbol{x_a}} = \boldsymbol{0}\ \forall\, \boldsymbol{a} \in L_h.$$



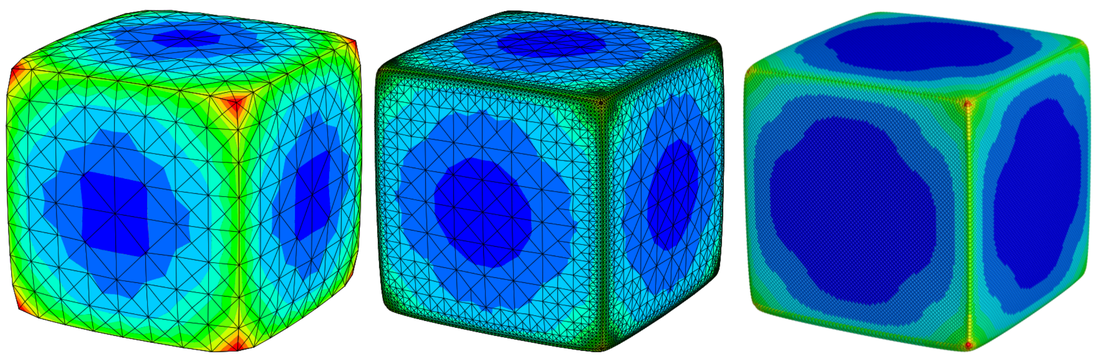
Crystal subject to FE-discretization (left) and with clusters around mesh-nodes for energy sampling (right). The method accounts for nonolocal atomic interactions everywhere.

• **Nanoindentation into FCC Aluminum.** Since plastic deformation is confined to a small area 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 MS but for a tiny fraction of the fully atomistic computation time.



Fully atomistic resolution right below the indenter (left) for dislocation nucleation and microstructure evolution (centre and right), which is embedded in a halfspace (coarser finite element discretiziation) undergoing purely elastic deformation.

• **Surface Relaxation of an FCC Cu Cube.** An fcc single-crystalline cube made of Cu is analyzed for surface relaxations. The CQC-E results based on adaptive mesh refinement according to strain concentrations exhibit quantitative agreement with MS for a small portion of the computational costs.



The contour plot of displacements $u_r = \sqrt{(u_x^2 + u_y^2 + u_z^2)}\,[\text{Å}]$ reveals quantitative agreement (left and centre: adaptively refined FE meshes) of CQC-E results with (right) MS.

Conclusions

In the simulations the present multiscale 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.

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References

[1] J.Knap, M.Ortiz, *J. Mech. Phys. Solids* 49, 1899–1923 (2001).
[2] B. Eidel, A. Stukowski, *J. Mech. Phys. Solids* 56, 87–106 (2009).
[3] B. Eidel, *Int. J. Mat. Res.* 100(11), 1503–1512 (2009).
[4] B. Eidel, *Habilitation Thesis*, University Duisburg-Essen (2011).

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