Mixed continuum/atomistic models: The quasi-continuum method

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Au (111) nanoindentation – MD analysis

Objective: One model which bridges atomistic and continuum descriptions seamlessly, i.e., contains atomistic and continuum limits as special cases.

All physics should be defined at the fundamental (atomistic) level (e.g., empirical potentials, DFT).

Coarse-graining should not introduce additional physics or assumptions (e.g., random noise, viscosity, thermostats, thermodynamic equilibrium…).

Coarsening/refinement should be:
- Inhomogeneous (e.g., full atomistics within defect cores, continuum-like behavior away from defects)
- Adaptive, i.e., local resolution should be provided by the method itself as part of the solution.
The quasicontinuum (QC) method, T=0

Lattice statics – Problem definition

- Reference configuration: Atoms arranged as a subset of a simple Bravais lattice.

- \( \mathcal{L} \subset \mathbb{R}^3 \equiv \) Enumeration of atoms in ensemble.

- Atom positions in reference configuration:
  \[
  X(l) = l^i a_i, \quad l \in \mathcal{L}
  \]

- Positions of atoms after deformation:
  \[
  q = \{q(l), \; l \in \mathcal{L}\} \in \mathbb{R}^{3N} \equiv X
  \]

- \( X \equiv Configuration \ space \ of \ ensemble. \)
Lattice statics - Problem definition

- We wish to determine the equilibrium configurations of the ensemble at zero temperature.

- Total energy: \( E(q), \quad q \in X, \quad t \in \mathbb{R} \)

- Problem:

\[
\inf_{q \in X} E(q)
\]

- Difficulties:
  
  i) \( N \) very large \( \sim 10^{23} \)

  ii) \( E(q) \) highly nonconvex \( \Rightarrow \) lattice defects, defect structures.
QC - Reduction

- Representative atoms: \( \mathcal{L}_h \subset \mathcal{L} \)
  \[ N_h = \text{card}(\mathcal{L}_h) \ll N \]
- Introduce triangulation \( \mathcal{T}_h \) of \( \mathcal{L}_h \)
- Basis functions: For \( l_h \in \mathcal{L}_h \),
  i) \( \varphi_h(X|l_h) \) continuous.
  ii) Linear over simplices \( K \in \mathcal{T}_h \)
  iii) \( \varphi_h(X(l_h)|l'_h) = \begin{cases} 1, & \text{if } l_h = l'_h \\ 0, & \text{otherwise} \end{cases} \)
QC - Reduction

- Interpolation: Let $\varphi_h(l|l_h) = \varphi_h(X(l)|l_h)$. Then

$$q_h(l) = \sum_{l_h \in \mathcal{L}_h} \varphi_h(l|l_h)q_h(l_h)$$

- For each triangulation $\mathcal{T}_h$, the collection of all interpolated configurations $q_h$ defines a linear subspace $X_h$ of $X$ of dimension $3N_h$. 

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Reduce problem:  \[ \inf_{q \in X_h} E(q) \]

- Reduced equilibrium equations:
  \[ f_h(l_h|q_h) = \sum_{l \in L} f(l|q_h) \varphi_h(l|l_h) = 0 \]
  where:  \[ f(l|q_h) = \frac{\partial E}{\partial q(l)}(q_h) \]

- Number of equilibrium equations = 3N_h = \text{dim}(X_h)
- But: Calculation of \( f_h(l_h|q_h) \) entails sum over entire lattice \( L \)!
QC - Reduction

\[ f_h(l_h|q_h) \]

\[ f(l|q_h) \]
QC – Lattice summation rules

- Problem: Approximate lattice sum \( S = \sum_{l \in \mathcal{L}} f(l) \)

- Summation rule: Let \( S_h \subset \mathcal{L} \). Then
  \[
  S \approx S_h = \sum_{l \in S_h} n_h(l) f(l)
  \]

- Example: Node-based summation rules, \( S_h = \mathcal{L}_h \), weights chosen such that \( \varphi(l | l_h) \) summed exactly for all \( l_h \in \mathcal{L}_h \).

- Monatomic chain: \( n_h(l_h) = \begin{cases} 
  h, & \text{if } l_h \text{ interior} \\
  (h + 1)/2, & \text{otherwise}
\end{cases} \)
QC – Reduced equations

- Combine interpolation and lattice summation rule:

\[
f_h(l_h|q_h) = \sum_{l \in S_h} n_h(l) f(l|q_h) \varphi_h(l|l_h) = 0
\]

- All operations are now \(O(N_h)\) provided \(\text{card}(S_h)\) is \(O(N_h)\).

- Example: For node-based summation rule,

\[
f_h(l_h|q_h) = \sum_{l'_h \in \mathcal{L}_h} n_h(l'_h) f(l'_h|q_h) \varphi_h(l'_h|l_h) = 0
\]

- Questions: Convergence, accuracy?

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Lattice summation rules - Stability

- Node-based summation rule *undersamples* the ensemble and is *unstable*.

Zero-energy mode of 32x32 Lennard-Jones fcc cluster resulting from node-based summation rule.
Cluster-based lattice summation rules

- \( C_h(l_h) \equiv \) Cluster of lattice sites centered at \( l_h \)

- Cluster summation rule:

\[
S_h = \sum_{l_h \in \mathcal{L}_h} n_h(l_h) \left\{ \sum_{l \in \mathcal{C}(l_h)} f(l) \right\}
\]

- \( n_h(l_h) \) s. t. \( \varphi(l|l_h) \) summed exactly.

- Monatomic chain: \( n_h(l_h) = h/(1 + 2r) \)
Cluster-based lattice summation rules

\[ \mathcal{L}_h \to \mathcal{L} \Rightarrow X_h \to X \text{ and } \inf E_h \to \inf E \]
Cluster sums - Effect of cluster size

Effect of cluster size on energy error for $0.1\sigma$ indentation of 64x64x64 fcc cell sample of Lennard-Jones crystal.
Convergence of energy error under regular refinement of fcc cell sample of Lennard-Jones crystal under point load.

\[ O(N_h^{-0.39}) \]

clusters overlap

\[ O(N_h^{-0.55}) \]

fully-resolved limit

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QC - Adaptivity

- $E(K) \equiv$ Lagrangian strain in simplex $K \in \mathcal{T}_h$

- Refinement criterion: Bisect $K$ if $|E(K)| \geq \text{TOL} \frac{b}{h(K)}$

Longest-edge bisection of tetrahedron (1,2,a,b) along longest edge (a,b) and of ring of tetrahedra incident on (a,b)

- General statement: $\inf_{q \in X_h, \mathcal{T}_h} E(q, \mathcal{T}_h)$

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Nanoindentation of [001] Au

(Kiely and Houston, Phys Rev B, 1998)
Nanoindentation of [001] Au

- Nanoindentation of [001] Au, 2x2x1 micrometers
- Spherical indentor, R=7 and 70 nm
- Johnson EAM potential
- Total number of atoms ~ 0.25 $10^{12}$
- Initial number of nodes ~ 10,000
- Final number of nodes ~ 100,000

Detail of initial computational mesh (Knap and Ortiz, 2002)
Nanoindentation - [001] Au

7 nm indenter, depth = 0.92 nm
Nanoindentation - [001] Au

7 nm indenter, depth = 0.92 nm
Nanoindentation - [001] Au

70 nm indenter, depth = 0.75 nm
Nanoindentation - [001] Au

70 nm indenter, depth = 0.75 nm

(Movie)
QC extensions: Complex lattices

Ag-Au nanoindentation
(Kovalewsky and Ortiz, 2003)
QC extensions: Charge redistribution

- Charge interpolation:
  \[ Q^A_h(l) = \sum_{l_h \in \mathcal{L}^A_h} \phi^A_h(l|l_h)Q^A_h(l_h) \]
  \[ Q^B_h(l) = \sum_{l_h \in \mathcal{L}^B_h} \phi^B_h(l|l_h)Q^B_h(l_h) \]

- Constrained minimization:
  \[ \min \{ (q^A_h, Q^A_h), (q^B_h, Q^B_h) \} \in X_h \]
  \[ E((q^A_h, Q^A_h), (q^B_h, Q^B_h)) \]

QC extensions - Dynamics

- Action integral: \[ I[q] = \int_a^b \left\{ \frac{m}{2} |\ddot{q}|^2 - E(q) \right\} dt \]

- Hamilton’s principle: \[ \delta I[q] = 0 \]

- Galerkin reduction: \[ X \rightarrow X_h, \quad M_h \ddot{q}_h + f_h(q_h) = 0 \]

- Limitations:
  
  i) Thermal component is wiped out.
  
  ii) Internal reflections (need absorbing boundaries).

Shenoy, Ortiz and Phillips (unpublished)

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QC extensions – Finite temperature

- Einstein model (Shenoy and Phillips, 1999):
  \[ F_h = E_h + \sum_{K \in T_h} n_h(K) 3k_B T \log \left( \frac{h D^{1/6}(K)}{k_B T} \right) \]

- Langevin: \( M_h \ddot{q}_h + \tau^{-1} M_h \dot{q}_h = f_h(q_h) + R_h(t) \)
  \[ \langle R_h(t) \otimes R_h(t) \rangle = \frac{2k_B T}{\tau \Delta t} M_h \]

- WKB (Kulkarni and Ortiz, 2003): \( X = X_h \oplus X'_h \)

\[ L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q(t), \dot{q}(t)) \, dt \]

\( q'_h(t) \), piecewise linear
QC extensions – Coupling to OFDFT

Structure: fcc Al crystal
Size: 2\(\mu\)m x 2\(\mu\)m x 1\(\mu\)m single crystal
Indenter radius: 0.75\(\mu\)m
Mesh: 105 elements \(\Rightarrow\) 420 OFDFT calculations

E.A. Carter, M. Fago, R. Hayes, M. Ortiz, 2002
Concluding remarks

- Continuum/atomistic methods are useful for:
  - Overcoming the size and time limitations of straight molecular dynamics
  - Building atomistic realism and fidelity into continuum boundary value problems

- Outstanding issues:
  - Mathematical analysis
  - Mesh optimization
  - Finite temperature
  - Transport properties:
    - Mass
    - Viscosity
    - Heat conduction
  - Dislocation dynamics

Nanovoid cavitation
Marian, Knap and Ortiz (2003)