Mixed continuum/atomistic models: The quasi-continuum method

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AHPCRC Workshop on the Mechanical Behavior of Materials from Atoms to Structures
AHCRC, UMN, November 5, 2003
Limits of discrete models

- First-principles calculations: Dislocation cores, dipoles, quadrupoles... $\sim 10^3$ atoms (T. Arias ´00)
- Molecular dynamics: Empirical potentials... $\sim 10^9$ atoms (F. Abraham ´03)
- Linear elasticity: Dislocation dynamics, $L \sim 10^6b$, $\varepsilon \sim 1\%$ (Bulatov et al. ´03)

Ta quadrupole (T. Arias ´00)

FCC ductile fracture (F.F. Abraham ´03)

FCC dislocation dynamics (M. Rhee et al. ´02)
Au (111) nanoindentation – MD analysis

- Early stages of indentation mediated by a defects → Need atomistics
- But elastic (long range) field important → large cells
- Indenter sizes ~ 70 nm, film thickness ~ 1 µm → large cells
- The vast majority of atoms in MD calculations move according to smooth elastic fields → MD wasteful!
- Mixed continuum/ atomistic description.

Multiscale continuum/atomistic models

- 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.

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

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

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

- \( X \equiv \) 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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QC - Reduction

- Reduced problem: \( \inf_{q \in X_h} E(q) \)

- Reduced equilibrium equations:

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

where: \( f(l | q_h) = \frac{\partial E}{\partial q(l)}(q_h) \)

- Number of equilibrium equations = 3 \( N_h = \dim(X_h) \)

- But: Calculation of \( f_h(l_h | q_h) \) entails sum over entire lattice \( \mathcal{L} \)!
QC - Reduction

\[ f_h(l_h \mid q_h) \]

\[ f(l \mid q_h) \]
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,

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

- Questions: Convergence, accuracy?
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

- $\mathcal{L}_h \rightarrow \mathcal{L} \Rightarrow X_h \rightarrow X$ and $\inf E_h \rightarrow \inf E$

Truncation scheme for overlapping clusters
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
QC - Adaptivity

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

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

Longest-edge bisection of tetrahedron \((1,4,a,b)\)
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)
Example - Nanoindentation of [001] Au

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

Detail of initial computational mesh

(Knap and Ortiz, *PRL* 90 2002-226102)
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
Nanovoid cavitation in Al

- 72x72x72 cell sample
- Initial radius $R=2a$
- Total number of atoms $\sim 16 \times 10^6$
- Initial number of nodes $\sim 34,000$

(Marian, Knap and Ortiz ´03)
Nanovoid cavitation in Al

Dislocation activity surging from the void
Nanovoid cavitation in Al

Formation of SFT-like structures following regular patterns
Nanovoid cavitation in Al

Detail of Lomer-Cottrell junction (locking point)
Nanovoid cavitation in Al

\{111\} facets

\frac{1}{6}\langle112\rangle

Shockley-type partials

\frac{1}{6}\langle110\rangle

Stair-rod type dislocations

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Nanovoid cavitation in Al

2\textsuperscript{nd} yield point: (being investigated)

Hardening regime: dislocation locking

1\textsuperscript{st} yield point

Initial elastic regime, following the interatomic potential’s shape

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Complex lattices

- Approach: Interpolate each sublattice independently.
- $\text{BaTiO}_3$: 5 sublattices, meshes, $\text{Ba, Ti, Ox, Oy, Oz}$.
Complex lattices

- Kinematics:
  \[ q_h^A(l) = \sum_{l_h \in \mathcal{L}_h^A} \phi_h^A(l|l_h) q_h^A(l_h) \]
  \[ q_h^B(l) = \sum_{l_h \in \mathcal{L}_h^B} \phi_h^B(l|l_h) q_h^B(l_h) \]

- Constrained minimization:
  \[
  \min_{(q_h^A, q_h^B) \in X_h} E(q_h^A, q_h^B)
  \]

- Cluster summation rules:
  \[
  E(q_h^A, q_h^B) \approx \sum_{l_h \in \mathcal{L}_h^A \cup \mathcal{L}_h^B} n_h(l_h) \left( \sum_{l \in \mathcal{C}(l_h)} E(l|q_h^A, q_h^B) \right)
  \]
Charge redistribution

- Charge interpolation:
  \[ Q_h^A(l) = \sum_{l_h \in \mathcal{L}_h^A} \phi_h^A(l|l_h)Q_h^A(l_h) \]
  \[ Q_h^B(l) = \sum_{l_h \in \mathcal{L}_h^B} \phi_h^B(l|l_h)Q_h^B(l_h) \]

- Constrained minimization:
  \[ \min \{ E((q_h^A, Q_h^A), (q_h^B, Q_h^B)) \mid ((q_h^A, Q_h^A), (q_h^B, Q_h^B)) \in X_h \} \]

BaTiO$_3$ – 180° wall

- Polarization in X-direction
- Nominal number of atoms $\sim 11 \times 10^6$
- 65x65x513 unit cells
- Atomistic resolution: 9 cells
- Goddard et al. polarizable Reax FF

(Kowalesky, Knap and Ortiz ´03)
BaTiO$_3$ – 180° wall

180°-wall: Displacements (close up)
BaTiO$_3$ – Tetragonal crack

Homogeneous tetragonal phase

33x65x11 unit cells

Crack

Crack tip

Mode I loading

Polarization
BaTiO$_3$ – Tetragonal crack

- Polarization field after three loading steps, showing domains and 90° walls
- Domain switching under cyclic loading?
- Misfit strains under cyclic loading?
- Bond breaking (Reax FF), crack growth?
- Crack-growth rates?
Dynamics

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

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

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

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

- Einstein model (Shenoy and Phillips, 1999):

\[ F_h = E_h + \sum_{K \in \mathcal{T}_h} n_h(K) 3k_B T \log \left( \frac{hD^{1/6}(K)}{k_BT} \right) \]

- Weak convergence + separation of time scales (Bornemann ’97):

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

\[ q_h(t), \text{ piecewise linear} \]

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Finite temperature

- Langevin dynamics (Marian, Knap and Ortiz ’03):

\[ M_h \ddot{q}_h + \tau^{-1} M_h \dot{q}_h = f_h(q_h) + R_h(t) \]

\[ R_h(l_h, t) = \sum_{l \in \mathcal{L}} R(l, t) \varphi_h(l|l_h) \]

\[ \langle R(l, t) \rangle = 0, \quad \langle R(l, 0) \otimes R(l, t) \rangle = 2 \frac{m^2}{\tau} k_B T I \delta(t) \]
Coupling to quantum mechanics

CB rule: Smith, Tadmor and Kaxiras, *PRL* 84, 2000, p. 1260)

Structure: fcc Al crystal
Size: 2μm x 2μm x 1μm single crystal
Indenter radius: 0.75μm
Mesh: 105 elements \(\Rightarrow\) 420 QM calculations
Total # QM calculations: \(\Rightarrow\) 8 million

E.A. Carter, M. Fago, R. Hayes, M. Ortiz ’03
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 ´03)