Atomistic-to-Continuum Coupling Methods for Crystalline Solids

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Approximation $\mathcal{E}^a(y)$ of the QM potential, Continuum approximation of atomistic model, Atomistic-to-continuum model coupling, Coarse-graining in the continuum region, Far-field and surface boundary conditions, and Accelerated dynamics are required for problems with defects and long-range elastic interactions.
Low energy local mimina (or dynamically metastable states) of $\mathcal{E}^a(y)$ have a lattice structure deformed by highly localized defects:
Point defects (vacancies, interstitials)
Line defects (dislocations)
Surface defects (grain boundaries).

Mathematical challenge to describe, analyze, and compute the multiscale energy landscape.

Energy

$w=$dislocation dipole separation
Consider interaction potentials $\mathcal{E}^a(y)$ whose energy-minimizing state is a (Bravais) lattice

$$A\mathbb{Z}^3 = \left\{ \sum_{i=1}^{3} m_i A_i \in \mathbb{R}^3 \text{ for } m \in \mathbb{Z}^3 \right\}$$

where $A = (A_1, A_2, A_3)$ for $A_i \in \mathbb{R}^3$ are reference lattice basis vectors.

Face-Centered Cubic Lattice:

$$A_1 = a_0 (1, 1, 0), \quad A_2 = a_0 (1, 0, 1), \quad A_3 = a_0 (0, 1, 1).$$
The atomistic reference domain is a subset of the lattice points satisfying

$$\Omega := \{ \xi_1, \ldots, \xi_M \} \subset \mathbb{AZ}^3.$$ 

Define the space of admissible deformations $y(\xi) : \Omega \to \mathbb{R}^3$ by

$$\mathcal{V} := \{ y(\xi) : \text{boundary conditions on } \partial \Omega \}$$

and compute local minima of

$$\arg \min_{y \in \mathcal{V}} \varepsilon^a(y).$$

Dislocations are admissible deformations for atomistic models, but have infinite energy for continuum models.
Choose a subset of $\Omega$ to be representative atoms with reference positions

$$\Omega^{rep} := \{\xi_{j_1}, \ldots, \xi_{j_N}\} \subset \Omega$$

where $N \ll M$ and construct a triangular finite element mesh $T \in \mathcal{T}$ with vertices, $\xi_{j_\ell}$ for $j = 1, \ldots, N$.

Denote the continuous, piecewise linear functions with respect to the mesh $\mathcal{T}$ by $P_1(\mathcal{T})$ and the corresponding piecewise linear approximation space by

$$\tilde{\mathcal{V}} := \mathcal{V} \cap P_1(\mathcal{T}).$$

The degrees of freedom of $Y \in \tilde{\mathcal{V}}$ are $\xi_{j_\ell}$ for $j = 1, \ldots, N$. 
Approximate

\[ \text{arg local min } E^a(y) \quad \text{by} \quad \text{arg local min } E^a(Y), \]

Identical to continuum piecewise linear finite element approximation except:

Reference domain is a lattice instead of a continuum.

Defects have finite energy and can be directly computed (they have infinite energy for continuum models such as the Volterra solutions).

Error: Displacement field constrained to be linear within each element.
Approximate

$$\arg \min_{y \in \mathcal{Y}} \mathcal{E}^a(y) \quad \text{by} \quad \arg \min_{Y \in \mathcal{\hat{Y}}} \mathcal{E}^a(Y).$$

Degrees of freedom reduced to $N << M$.
Must still compute $O(M)$ atomistic interactions because of nonlocal interactions.
Still need further approximation. Remedies:


or

Approximate by quadrature (sampling) of atomistic energy.
The Cauchy-Born continuum strain energy density is equal to the atomistic energy density for uniform strain \( y^F(\xi) := F\xi : \)

\[
W(F) := \frac{1}{\det A} \varepsilon^a_\ell (y^F) = \frac{1}{\det A} \left\{ \frac{1}{2} \sum_{m \in \mathbb{Z}^3} \phi (|m_i FA_i|) \right. \\
+ G \left( \sum_{m \in \mathbb{Z}^3} \rho (|m_i FA_i|) \right) \right\},
\]

where \( \det A \) is the volume of the reference unit cell and the sum is restricted by \( |m_i FA_i| \leq r_{cut} \).
Approximate FEM-A, $\mathcal{E}^a(Y)$, by FEM-C:

$$
\mathcal{E}^c(Y) = \sum_{T \in \mathcal{T}} \nu_T W(\nabla Y|_{T}) = \int_{\Omega} W(\nabla Y(x)) \, dx
$$

where $\nu_T$ is the volume of element $T$ and $W(\nabla Y|_{T})$ is the continuum strain energy density.

The work to compute the energy or forces has now been reduced to $\dim(\tilde{V}) = N$.

Modeling error introduced.
Motivation for Atomistic Modeling Near Defects

\[ \mathcal{E}^a(y) - \mathcal{E}^c(y) = 0 \left( \varepsilon^2 \int_\Omega |D^2y(x)|^2 + |D^3y(x)| \, dx \right) \]

where \( \varepsilon \) is the scaled lattice spacing (Blanc, Le Bris, & Lions). Second-order Cauchy-Born for multilattices: Van Koten & Ortner.

Deformation near a dislocation has singularity

\[ D^2y(x_1, x_2, x_3) = \mathcal{O} \left( \frac{1}{r^2} \right) \]

where \( r \) is the distance to the dislocation. The singularity is cut-off at \( r = \mathcal{O}(\varepsilon) \), so

\[ \mathcal{E}^a(y) - \mathcal{E}^c(y) = \mathcal{O}(1)! \]

For accuracy, keep atomistic interactions where the strain varies on the atomistic scale.
Energy-based Quasicontinuum Approximation (QCE)

For accuracy, use atomistic interactions for repatoms where the deformation gradient varies on the atomistic scale.

For efficiency, use strain energy density where the deformation gradient is sufficiently uniform.

\[ E_{\text{QCE}}(Y) = \sum_{\text{atomistic}} E_{a,j}(Y) + \sum_{T \in \mathcal{T}} \nu_T W(\nabla Y |_T) \]
\[ = \sum_{\text{atomistic}} E_{a,j}(Y) + \int_{\Omega_c} W(\nabla Y(x)) \, dx. \]

QCE energy of Tadmor, Ortiz, and Phillips conserves energy for uniform strain and has direct implementation with no special interfacial calculations by modifying \( \nu_T \) for triangles that border the interface.
Coupling Error for Uniform Deformation: The Patch Test

\[ \varepsilon^{QCE}(Y) = \sum_\text{atomistic} \varepsilon^a_j(Y) + \sum_{T \in T} \nu_T W(\nabla Y|_T) \]
\[ = \sum_\text{atomistic} \varepsilon^a_j(Y) + \int_{\Omega_c} W(\nabla Y(x)) \, dx. \]

Uniformly strained deformation \( y^F(\xi) := F\xi \).

By symmetry, \( \delta \varepsilon^a(y^F) = \delta \varepsilon^c(y^F) = 0 \).

QCE energy does not satisfy the patch test: there are nonzero “ghost” forces in the a/c interface under uniform strain (Tadmor, et. al.)

\[ \frac{\partial \varepsilon^{QCE}}{\partial y_m}(y^F) \neq 0 \]

for \( y_m \in r_{\text{cut-width}} \) neighborhood of the a/c interface.
Accuracy near lattice instabilities requires that \( \delta^2 \varepsilon^{QC}(y^{qc}) \) is positive definite iff (to first order error) \( \delta^2 \varepsilon^{a}(y^{qc}) \) is positive definite. \( \varepsilon^{QCE}(y) \) has \( O(1) \) critical strain error (Dobson, Luskin & Ortner).
## Comparison of BQCE and Other Coupled Energies

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<th>Ghost Force</th>
<th>Implementation</th>
<th>Model</th>
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<tr>
<td>QCE</td>
<td>Yes</td>
<td>Medium</td>
<td>Multi-body, 3D</td>
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<tr>
<td>Tadmor, Ortiz, &amp; Phillips</td>
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<tr>
<td>BQCE</td>
<td>Controllable</td>
<td>Medium +</td>
<td>Multi-body, 3D</td>
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<td>Van Koten, Luskin &amp; Ortner</td>
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<tr>
<td>Quasinonlocal</td>
<td>Corners &amp; Coarsening</td>
<td>Hard</td>
<td>Multi-body, 3D short-range</td>
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<td>Geom Reconstr</td>
<td>Corners &amp; Coarsening</td>
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<td>GR-AC</td>
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<td>Very Hard</td>
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<tr>
<td>Shapeev</td>
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<td>Hard</td>
<td>Pair interaction 2D, finite range</td>
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<td>Shapeev, Li &amp; Luskin in 1D</td>
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Force-Based Quasicontinuum Method (QCF):

\[ \mathcal{F}_{j}^{QCF}(Y) = \begin{cases} 
\mathcal{F}_{j}^{a}(Y) &= -\frac{\partial \mathcal{E}^{a}(Y)}{\partial Y_{j}} 
& \text{if } Y_{j} \text{ is atomistic}, \\
\mathcal{F}_{j}^{c}(Y) &= -\frac{\partial \mathcal{E}^{c}(Y)}{\partial Y_{j}} 
& \text{if } Y_{j} \text{ is continuum}. 
\end{cases} \]

Most popular method to couple multiphysics models generally, such as molecular mechanics to quantum mechanics.

QCF is the only known patch test consistent scheme with \( O(N) \) work to evaluate all of the forces, but is nonconservative and INDEFINITE (Dobson, Luskin & Ortner).
Blended Force-Based Methods

QCF is patch test consistent for many-body potentials, multilattices, 3D, but is not conservative and not positive definite. Blended QCF needs small interface width to be efficient.

Blended QCF is positive definite if and only if the atomistic model is positive definite and the blending width $K \gg N^{1/5}$ in atomistic scale or $O(\varepsilon^{4/5})$ blending width in the continuum scale) (Xingjie Helen Li, Luskin, & Ortner).

Lu & Ming have proven that a blended force-based method is stable in $w^{2,2}$ if the blending width $K = O(N)$ (or $O(1)$ blending width in the continuum scale).
References


