A Γ-Convergence Analysis of the Quasicontinuum Method

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The Quasicontinuum Method and Applications

Knap & Ortiz, 2003
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   - Atomistic Model
   - The Quasicontinuum Model

4. Numerical Examples

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We want to find the equilibrium configuration of the crystal, that is, we want to solve

$$\min_{u \in \mathcal{X}} F(u),$$

where the potential energy of the system is defined as

$$F(u) = \sum_{l \in \mathbb{Z}^n} \Phi(l, u)$$

where $u(l) = x(l) - q(l)$ is the displacement corresponding to the atom $l$, and $\Phi$ is the interatomic potential.
The Quasicontinuum Method

QC: A computational scheme for seamlessly bridging the atomistic and continuum description of materials.

- QC: Tadmor et al., 1996; Shennoy et al., 1998; Miller et al., 1998; Rodney-Philipps, 1999; Tadmor et al., 1999
We want to solve

$$\min_{u \in X} F(u)$$

**Energy-based QC:**

- **Interpolation Schemes:** coarse-graining of fully atomistic resolution via kinematic constraints.

  $$\min_{u \in X} F(u) \text{ is replaced by } \min_{u \in X_h} F(u)$$

- **Summation Rules:** approximation of the energy/forces via summation rules.

  $$\min_{u \in X_h} F(u) \text{ is replaced by } \min_{u \in X_h} F_h(u)$$
Interpolation Schemes

\[ X_h = \{ u : \mathbb{Z}^n \rightarrow \bar{\mathbb{R}}, \quad u(l) = \sum_{\alpha \in I} u_{\alpha} \varphi_{\alpha}(l) \} \]

Examples

- **FEM**

- **Max-Ent** (Arroyo-Ortiz 2006)
Summation Rules

\[ S = \sum_{l \in \mathbb{Z}^n} g(l) \approx \sum_{l \in \mathbb{Z}^n} w_h(l) g(l) = S_h, \]

Examples

- **Uniform Summation Rules**
  \[ w_h(l) = \begin{cases} 
  h, & \text{if } l \in h\mathbb{Z}; \\
  0, & \text{otherwise}. 
\end{cases} \]

- **Cluster Summation Rules** (Knap-Ortiz 2002)
  \[ w_h(l) = \begin{cases} 
  \frac{h}{1+2r}, & \text{if } l \in [h\mathbb{Z} - r, h\mathbb{Z} + r]; \\
  0, & \text{otherwise}. 
\end{cases} \]

- **Quadrature Rules** (Gunzburger-Zhang 2010)
  \[ w_h(l) = \begin{cases} 
  1, & \text{if } l \in h\mathbb{Z}; \\
  (h - 1)/2, & \text{if } l \in h\mathbb{Z} + h/3 \text{ or } l \in h\mathbb{Z} + 2h/3; \\
  0, & \text{otherwise}. 
\end{cases} \]
$$E_{\min} = \min_u E_0(u)$$

and a sequence of variational problems

$$E_{\min,\epsilon} = \min_{u_\epsilon} E_\epsilon(u_\epsilon).$$
The Problem Quasicontinuum model \( \Gamma \)-Convergence Numerical Examples Conclusions and Future Work

\( \Gamma \)-Convergence

We have

\[
E_{\text{min}} = \min_u E_0(u)
\]

and a sequence of variational problems

\[
E_{\text{min},\epsilon} = \min_{u_{\epsilon}} E_{\epsilon}(u_{\epsilon}).
\]

\( \Gamma \)-Convergence + Equicoercivity = Convergence of minimizers

\underline{Definition}

Let \( E_\epsilon : X \to \mathbb{R} \) with \( \epsilon > 0 \). We say that the sequence \( \{E_\epsilon\} \) \( \Gamma \)-converges to \( E_0 : X \to \mathbb{R} \), and we write \( \Gamma - \lim E_\epsilon = E_0 \), if

- (lower bound inequality) for every \( u \in X \) and every sequence \( \{u_\epsilon\} \) such that \( u_\epsilon \to u \in X \), \( E_0(u) \leq \liminf_{\epsilon \to 0} E_\epsilon(u_\epsilon) \);

- (Existence of recovery sequence) for every \( u \in X \), there exists a sequence \( \{u_\epsilon\} \) such that \( u_\epsilon \to u \in X \) and \( E_0(u) = \lim_{\epsilon \to 0} E_\epsilon(u_\epsilon) \).

Dal Maso, Introduction to Gamma convergence, Birkhauser (1993)

Harmonic Lattice

We consider the harmonic lattice where the potential energy is defined by

\[
F(u) = \frac{1}{\Omega} \sum_{l \in \mathbb{Z}^n} \frac{1}{2} \langle \Phi \ast u(l), u(l) \rangle - \Omega \sum_{l \in \mathbb{Z}^n} \langle f(l), u(l) \rangle,
\]

where \( \Phi \) is the force-constant field of the lattice, and \( f : \mathbb{Z}^n \to \mathbb{R}^n \) is an applied force field, which can also be written using the Fourier transform as

\[
F(u) = \frac{1}{(2\pi)^n} \int_B \frac{1}{2} \langle D(k) \hat{u}(k), \hat{u}^*(k) \rangle \, dk - \frac{1}{(2\pi)^n} \int_B \langle \hat{f}(k), \hat{u}(k) \rangle \, dk,
\]

where \( B \) is the Brioullin zone of the reciprocal lattice and

\[
D(k) = \frac{1}{\Omega^2} \hat{\Phi}(k)
\]

is the dynamical matrix of the lattice.
The Continuum Limit

- Sequence of scaled functions

\[ f_\epsilon(x) = \epsilon^2 f(\epsilon x) \]

of decreasing variation on the scale of the lattice.

- Sequence of scaled potential energy functions

\[ F_\epsilon(u) = \epsilon^{n-2} (E(u) - \langle f_\epsilon, u \rangle) \]
The sequence of scaled potential energy functions can also be defined as

\[ F_\epsilon(u) = E_\epsilon(u) - \langle f, u \rangle, \]

where the sequence of functionals \( E_\epsilon : H^1(\mathbb{R}^n) \to \mathbb{R} \) is defined as

\[
E_\epsilon(u) = \begin{cases} 
\frac{1}{(2\pi)^n} \int_{B/\epsilon} \frac{1}{2} \langle \epsilon^{-2} D(\epsilon k) \hat{u}(k), \hat{u}(k) \rangle \, dk, & \text{if } \text{supp}(\hat{u}) \in B/\epsilon \\
+\infty, & \text{otherwise}
\end{cases}
\]
Theorem (Ariza-Ortiz 2005)

Suppose that:

i) For every $\zeta \in \mathbb{C}^n$ the function $\langle D(\cdot)\zeta, \zeta \rangle$ is measurable on $B$.

ii) There is a constant $\tilde{C}$ such that

$$0 \leq \langle D(k)\zeta, \zeta \rangle \leq \tilde{C}|k|^2|\zeta|^2$$

for a.e. $k \in B$ and for every $\zeta \in \mathbb{C}^n$.

iii) For every $\zeta \in \mathbb{C}^n$, the functions $\epsilon^{-2}\langle D(\epsilon k)\zeta, \zeta \rangle$ converge for a.e. $k$ to $\langle D_0(k)\zeta, \zeta \rangle$.

Then, $\Gamma\lim_{\epsilon \to 0} E_\epsilon = \frac{1}{(2\pi)^n} \int \langle D_0(k)\hat{u}(k), \hat{u}^*(k) \rangle \, dk$, in the weak topology of $H^1(\mathbb{R})$. 
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$\Gamma$-convergence + Equicoercivity = Convergence of minimizers
We approximate

\[ E(u) = \frac{1}{\Omega} \sum_{l \in \mathbb{Z}^n} \frac{1}{2} \langle (\Phi \ast u)(l), u(l) \rangle \]

by

\[ E_h(u) = \frac{1}{\Omega} \sum_{l \in \mathbb{Z}^n} w_h(l) \frac{1}{2} \langle (\Phi \ast u)(l), u(l) \rangle, \]

or equivalently

\[ E_h(u) = \frac{1}{(2\pi)^n} \int_B \int_B \frac{1}{2} G_h(k - k') \langle D(k) \hat{u}(k), \hat{u}^*(k') \rangle \, dk' \, dk, \]

where

\[ G_h(k) = \hat{w}_h(k). \]
Continuum Limit: Scaling

If we define
- $X_{h,\epsilon}$: Given by scaled shape functions $\varphi_{\alpha, \epsilon}(x) = \varphi_{\alpha}(x/\epsilon)$.
- $G_{h,\epsilon}(k) = \epsilon^n G(\epsilon k)$.

Then, the sequence of scaled potential energy functionals is defined by

$$F_{h,\epsilon}(u) = \tilde{E}_{h,\epsilon}(u) - \langle f, u \rangle,$$

where

$$\tilde{E}_{h,\epsilon}(u) = \begin{cases} E_{h,\epsilon}(u) & \text{if } u \in X_{h,\epsilon} \\ +\infty, & \text{otherwise} \end{cases}$$

with

$$E_{h,\epsilon} = \frac{1}{(2\pi)^{2n}} \int_{B/\epsilon} \int_{B/\epsilon} \frac{1}{2} G_{h,\epsilon}(k-k') \langle \epsilon^{-2} D(\epsilon k') \hat{u}(k'), \hat{u}^*(k) \rangle \, dk \, dk'$$
Theorem

Let $X_{h,\epsilon}$ be a dense sequence of sets in $H^1(\mathbb{R}^n)$. Suppose that the assumptions over $D(k)$ still hold and that:

i) $G_h(k) - \delta(k) \in L^\infty$.

ii) There is a constant $\tilde{C}$ such that

$$0 \leq \int_B G(k - k') \langle D(k)\zeta, \zeta \rangle \, dk' \leq \tilde{C} |k|^2 |\zeta|^2.$$  \hspace{1cm} (1)

Then,

$$\Gamma-\lim_{\epsilon \to 0} \tilde{E}_{h,\epsilon}(u) = E_0(u)$$ \hspace{1cm} (2)

in the weak topology of $H^1(\mathbb{R}^n)$. 
Theorem

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i) $G_h(k) - \delta(k) \in L^\infty$.

ii) There is a constant $\tilde{C}$ such that

$$0 \leq \int_{B} G(k - k') \langle D(k)\zeta, \zeta \rangle dk' \leq \tilde{C}|k|^2|\zeta|^2. \quad (1)$$

Then,

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in the weak topology of $H^1(\mathbb{R}^n)$.

$\Gamma$-convergence + Equicoercivity = Convergence of minimizers
Numerical Examples: 2D

- Lennard-Jones Potential
- \( f_n = a n^2 |\sin(n\pi x/L)||\sin(n\pi y/L)| \)
- Max-Ent (Bompadre-Schmidt-Ortiz, submitted)
- Cluster summation rule
Numerical Examples: 3D

- Finnes-Sinclair Potential
- $f_n = a_n^2 |\sin(n\pi x / L)| |\sin(n\pi y / L)| |\sin(n\pi z / L)|$
- Max-Ent
- Cluster summation rule

![Graphs and images of numerical examples](image-url)
Summary and forthcoming

- Proposed a convergence approach
- Obtained sufficient conditions on interpolation schemes and summation rules
- Showed in numerical examples the convergence
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- Proposed a convergence approach
- Obtained sufficient conditions on interpolation schemes and summation rules
- Showed in numerical examples the convergence
- Defects
  - Dislocations: Dilute Limit (Ariza-Ortiz 2005)
  - Fracture (Braides-Lew-Ortiz 2006)