A Γ-Convergence Analysis of the Quasicontinuum Method

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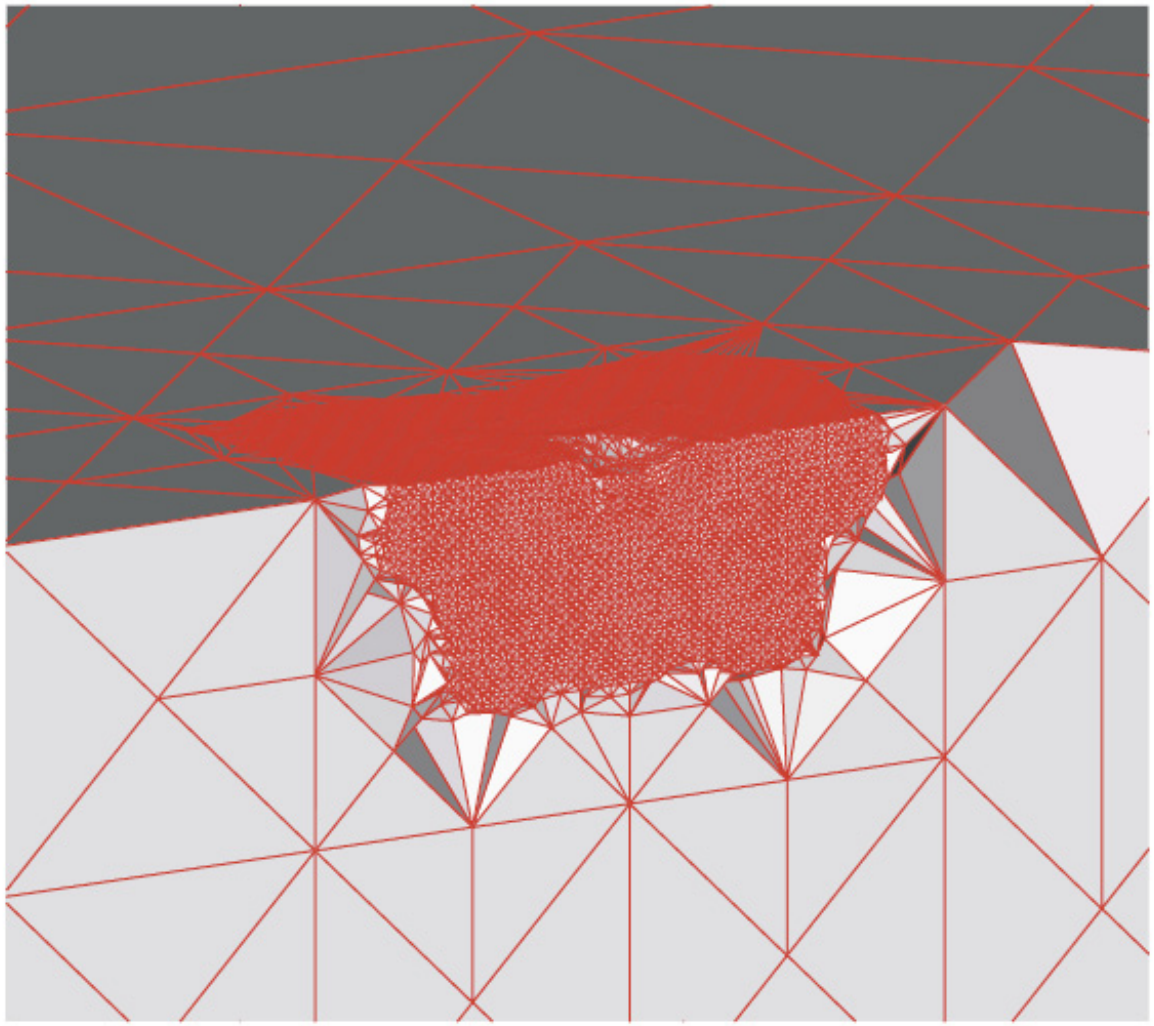
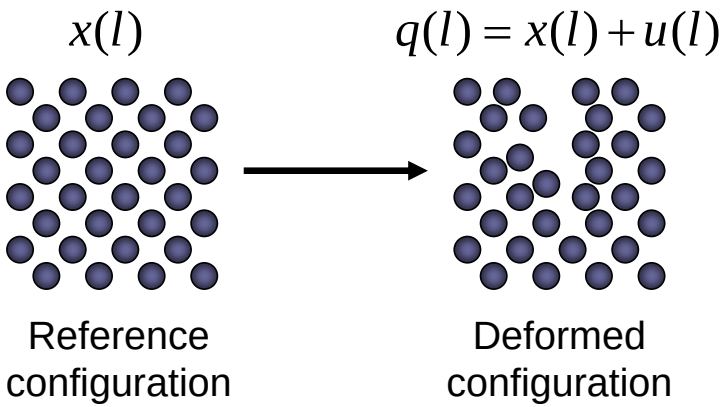
The Quasicontinuum Method and Applications



Knap & Ortiz, 2003

Outline

Atomistic Model



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

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

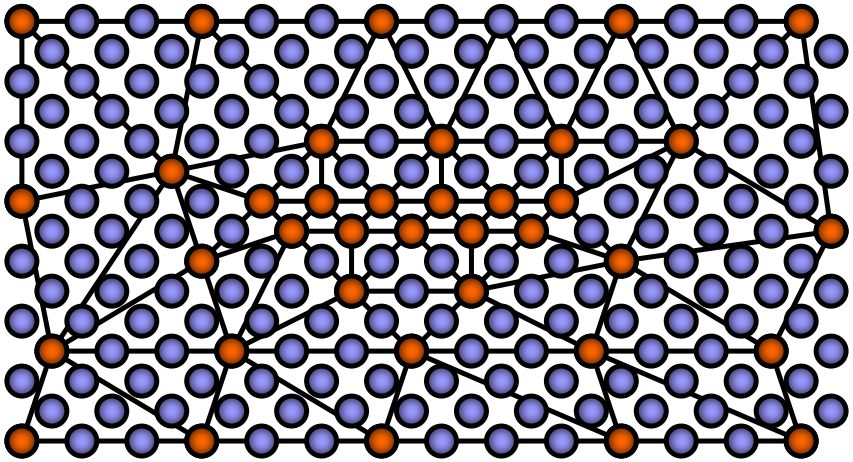
where the potential energy of the system is defined as

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

where $u(l) = x(l) - q(l)$ is the displacemente corresponding to the atom l, and Φ 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
- Numerical Analysis QC: Lin 2003; Dobson-Luskin-Ortner 2006-2011

The Quasicontinuum Method

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.

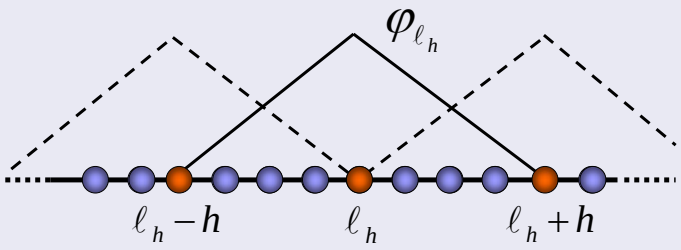
$$\min_{u \in X_h} F(u) \text{ is replaced by } \min_{u \in X_h} F_h(u)$$

Interpolation Schemes

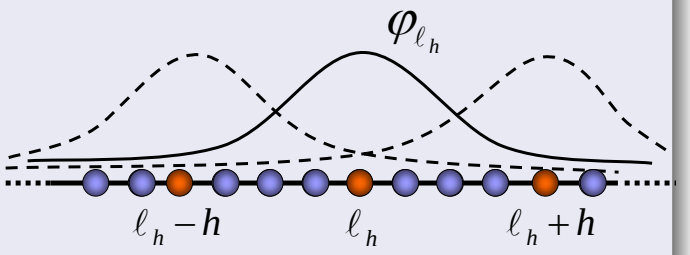
$$X_h = \{u : \mathbb{Z}^n \to \bar{\mathbb{R}}, \quad u(l) = \sum_{\alpha \in I} u_\alpha \varphi_\alpha(l)\}$$

Examples

- **FEM**



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



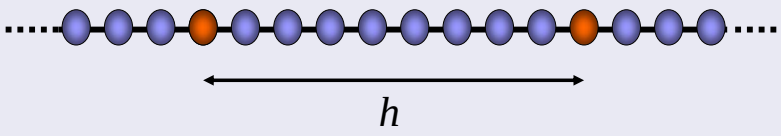
Summation Rules

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

Examples

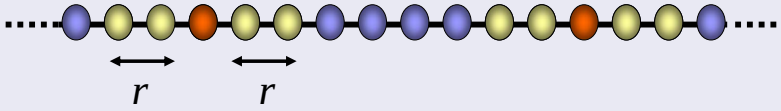
- **Uniform Summation Rules**

$$w_h(l) = \begin{cases} h, & \text{if } l \in h\mathbb{Z}; \\ 0, & \text{otherwise.} \end{cases}$$

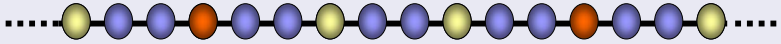


- **Cluster Summation Rules** (Knap-Ortiz 2002)

$$w_h(l) = \begin{cases} \frac{h}{1+2r}, & \text{if } l \in [h\mathbb{Z} - r, h\mathbb{Z} + r]; \\ 0, & \text{otherwise.} \end{cases}$$



- **Quadrature Rules** (Gunzburger-Zhang 2010)



$$w_h(l) = \begin{cases} 1, & \text{if } l \in h\mathbb{Z}; \\ (h-1)/2, & \text{if } l \in h\mathbb{Z} + h/3 \text{ or } l \in h\mathbb{Z} + 2h/3; \\ 0, & \text{otherwise.} \end{cases}$$

Γ-Convergence

We have

$$E_{min} = \min_{u} E_0(u)$$

and a sequence of variational problems

$$E_{min,\epsilon} = \min_{u_\epsilon} E_\epsilon(u_\epsilon).$$

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Γ-Convergence + Equicoercivity = Convergence of minimizers

Definition

Let $E_\epsilon : X \to \mathbb{R}$ with $\epsilon > 0$. We say that the sequence $\{E_\epsilon\}$ Γ-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)
- Braides, Gamma-convergence for beginners, vol. 22, Oxford (2002)

Harmonic Lattice

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

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

where Φ 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

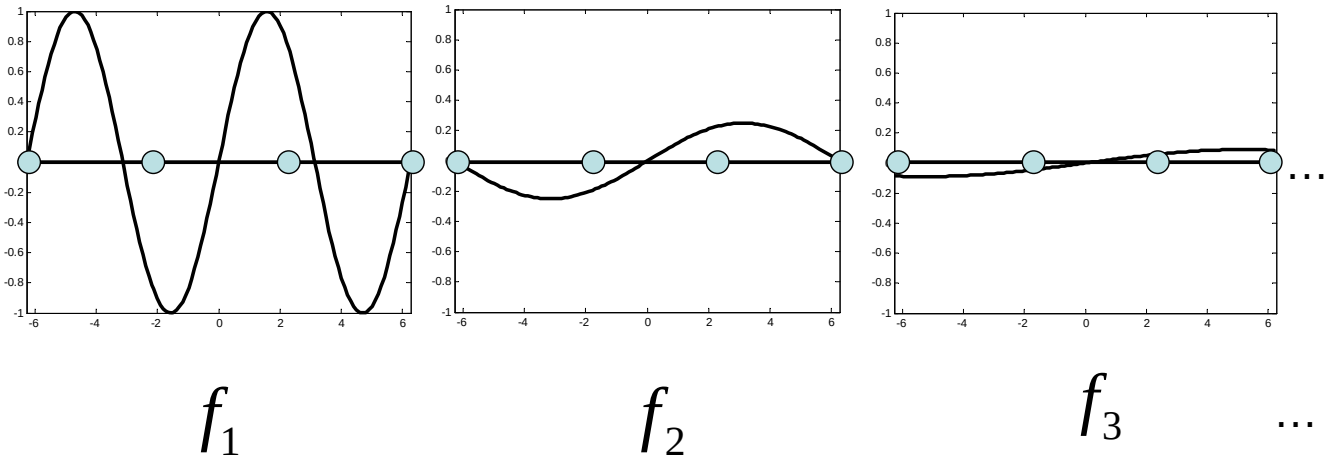
$$F(u) = \frac{1}{(2\pi)^n} \int_B \frac{1}{2} \langle D(k)\hat{u}(k), \hat{u}^*(k) \rangle \, dk - \frac{1}{(2\pi)^n} \int_B \langle \hat{f}(k), \hat{u}(k) \rangle \, dk,$$

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

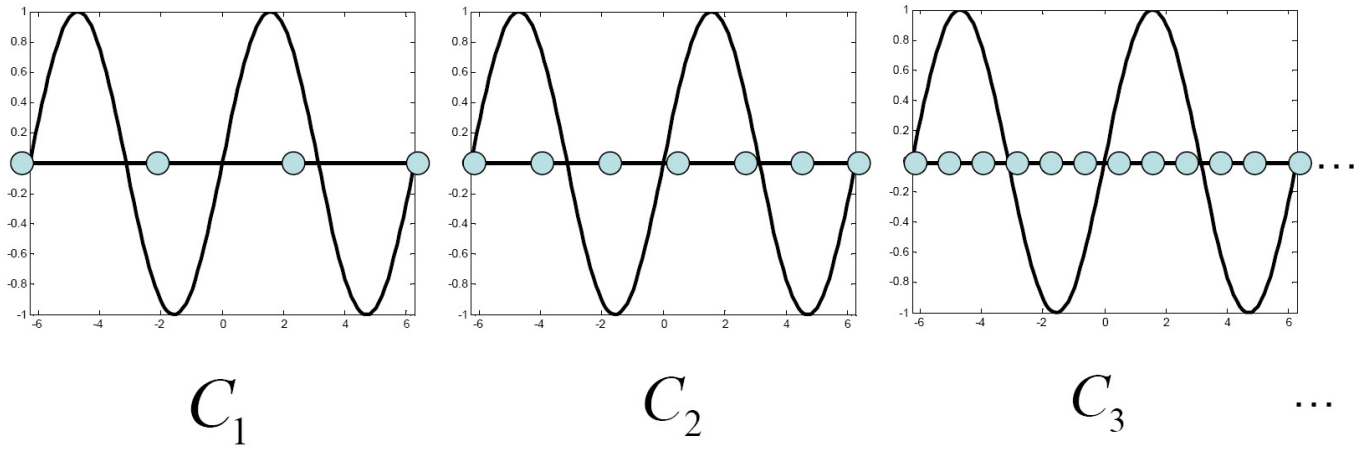
$$f_\epsilon(x) = \epsilon^2 f(\epsilon x)$$

of decreasing variation on the scale of the lattice.

- Sequence of scaled potential energy functions

$$F_\epsilon(u) = \epsilon^{n-2}\left(E(u) - \langle f_\epsilon, u\rangle\right)$$

The Continuum Limit - A different view



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 $E_\epsilon : H^1(\mathbb{R}^n) \to \bar{\mathbb{R}}$ is defined as

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

Continuum Limit (Cont.)

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, $\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon = \frac{1}{(2\pi)^n}\int \langle D_0(k)\hat{u}(k), \hat{u}^*(k)\rangle\, dk$, *in the weak topology of* $H^1(\mathbb{R})$.

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Γ-convergence + Equicoercivity = Convergence of minimizers

QC Scheme: Fourier Representation

We approximate

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

by

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

or equivalently

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

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

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

Continuum Limit (Cont.)

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*

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

Then,

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

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

Continuum Limit (Cont.)

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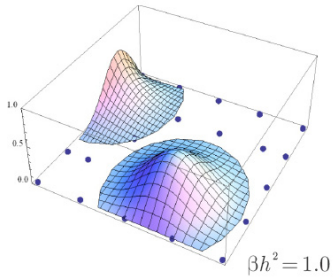
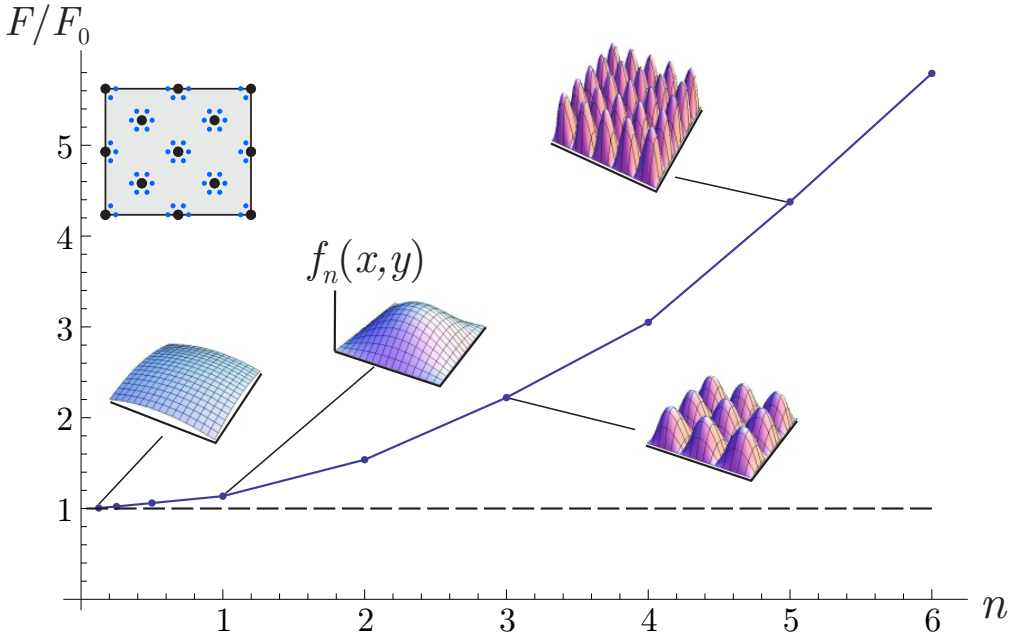
Γ-convergence + Equicoercivity = Convergence of minimizers

Numerical Examples: 2D

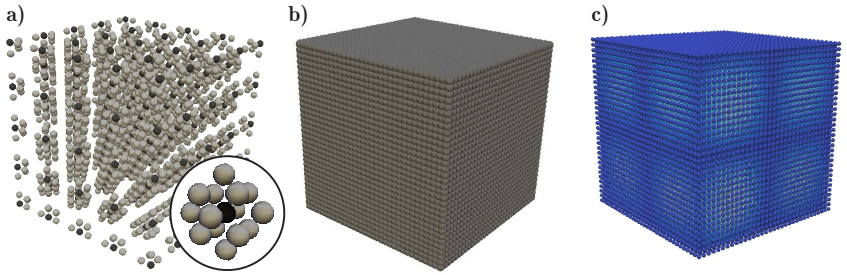
- Lennard-Jones Potential
- $f_n = an^2 |sin(n\pi x/L)||sin(n\pi y/L)|$
- Max-Ent (Bompadre-Schmidt-Ortiz, submitted)
- Cluster summation rule

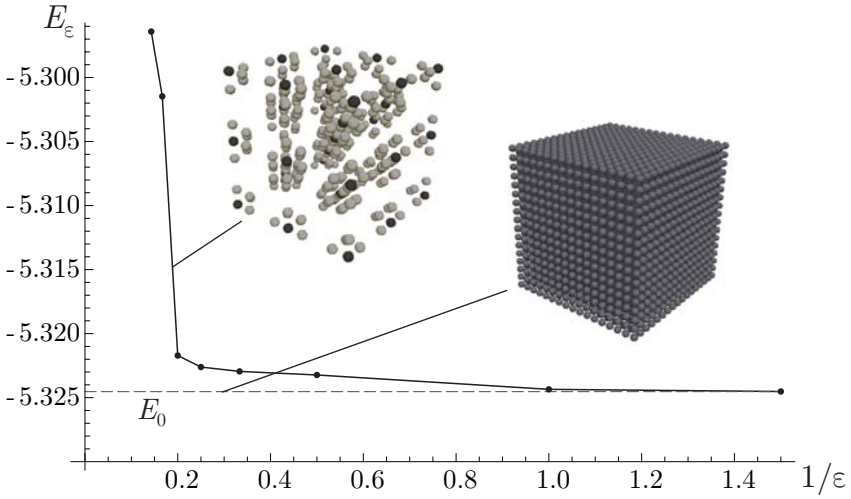


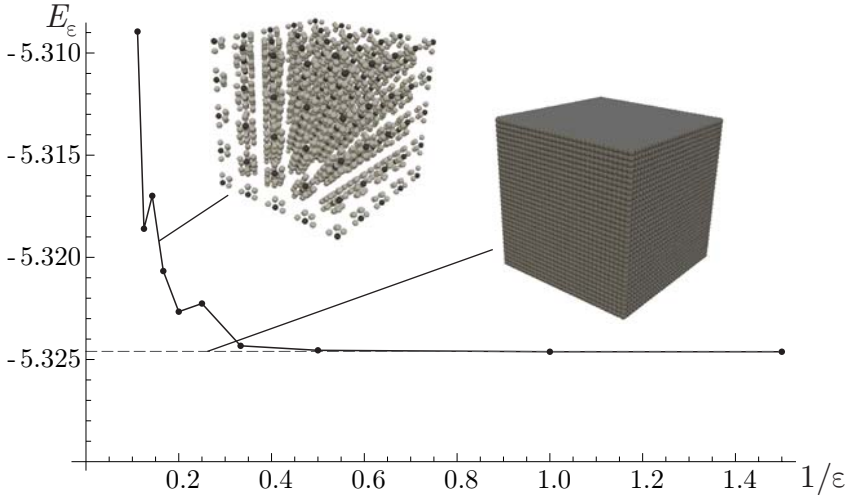


Numerical Examples: 3D

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

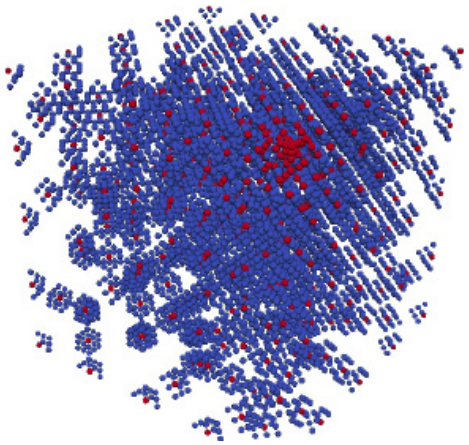






Summary and forthcoming

- Proposed a convergence approach
- Obtained sufficient conditions on interpolation schemes and summation rules
- Showed in numerical examples the convergence



Summary and forthcoming

- 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)