Theory Based Construction of Atomistic/Continuum (A/C) Coupling Methods

Lei Zhang 张镭 (Shanghai Jiao Tong University)
with Christoph Ortner (Warwick) and Alexander Shapeev (Moskow)

National University of Singapore, Singapore, Feb 13, 2015

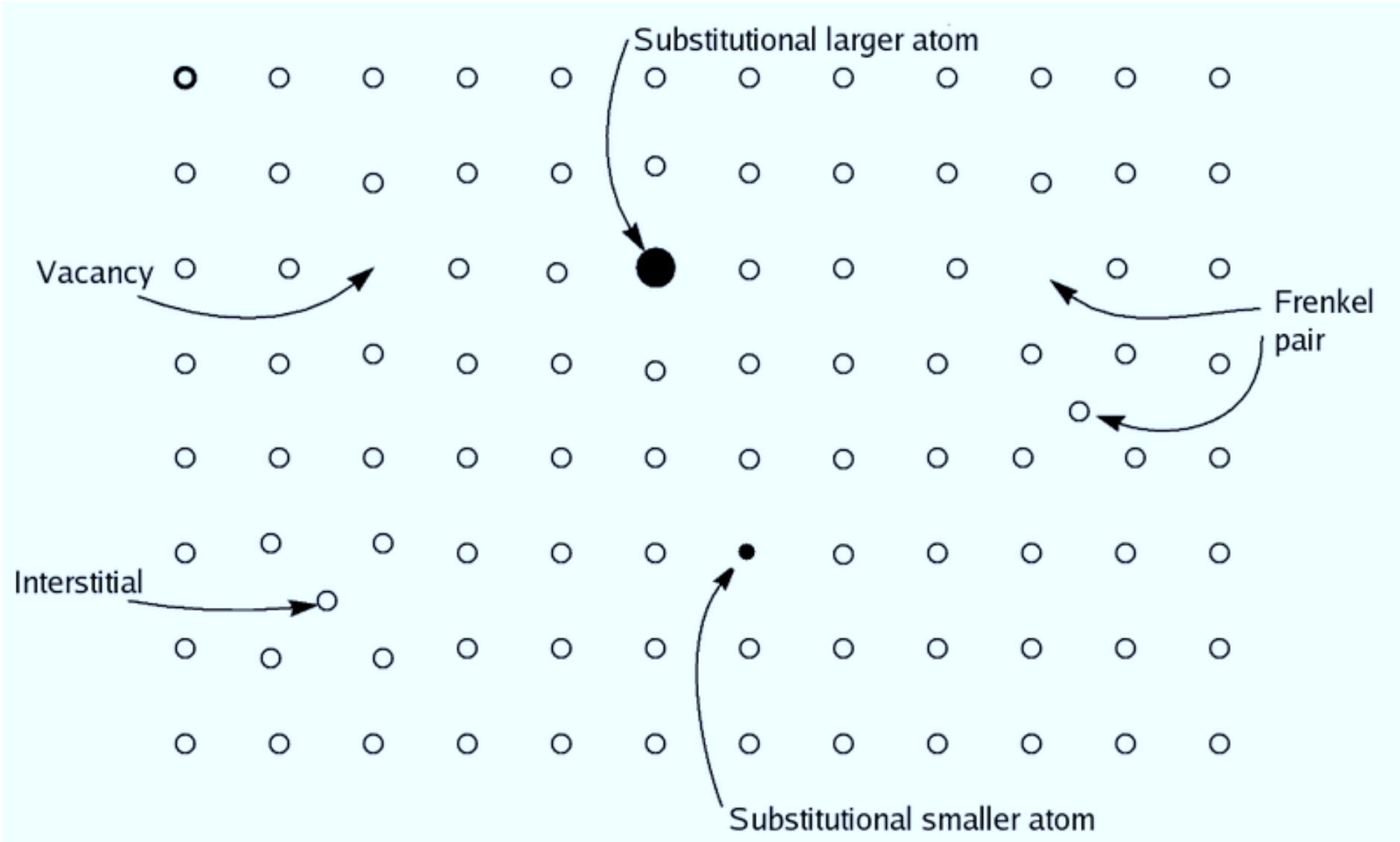
Outline

Focus: Multiscale methods for 2D/3D point defects at 0T, e.g., the coupling of length scales.

- Introduction
  - Atomistic/Continuum Coupling: Setup and Issues
- Construction and Analysis of Consistent Energy Based Method
  - Consistency: Ghost force removal (patch test Consistency).
  - Stability: Stability gap and stabilization.
  - Convergence: Balance of coupling, truncation and coarsening errors.
- Beyond Consistent Methods
  - Atomistic/Continuum blending with ghost force correction.
- Outlook

CO: Christoph Ortner, AS: Alexander Shapeev
CO & LZ, arXiv:1110.0168, 50(6), SINUM 2012, 2d nearest neighbor construction;
CO, AS & LZ, arXiv:1308.3894, SIAM MMS 2014, stability of consistent method;
CO & LZ, arXiv:1312.6814, CMAME 2014, optimal implementation for general cases;
CO & LZ, arXiv:1407.0053, blending with ghost force correction

Point Defects in 2D



[Wikipedia]

Atomistic Mechanics (0T statics)

- **Atomistic lattice functions**: $\mathcal{U} := \{v : \mathcal{L} \to \mathbb{R}^m\}$, Bravais lattice $\mathcal{L} = \mathrm{B}\mathbb{Z}^d$, $d = 2, 3$, $m = 1, 2, 3$. $\bar{v}$ is the nodal P_1 interpolation of v.

$$\mathcal{U}^{1,2} := \{u \in \mathcal{U} | \nabla \bar{u} \in L^2\}$$

- **Total energy** of configuration y:

$$\mathcal{E}_{\mathrm{a}}^{\mathrm{tot}}(y) := \mathcal{E}^{\mathrm{a}}(y) + \mathcal{P}_{\mathrm{a}}(y)$$

where $\mathcal{E}^{\mathrm{a}}$ = interaction energy, $\mathcal{P}_{\mathrm{a}}$ = potential of external forces, V is multi-body interaction potential,

$$\mathcal{E}^{\mathrm{a}}(y) = \sum_{x \in \mathcal{L}} V_x\big(D_\rho y(x); \rho \in \mathcal{R}\big)$$

where $D_\rho y(x) := y(x + \rho) - y(x)$.

- **Goal**: Find

$$y^{\mathrm{a}} \in \mathrm{argmin}\{\mathcal{E}_{\mathrm{a}}^{\mathrm{tot}}(\mathrm{y}) | \mathrm{y} \in \mathcal{Y}\}$$

where $\mathcal{Y} := \{y \in \mathcal{U} | y = y_0 + u$ for some $u \in \mathcal{U}^{1,2}\}$ and y_0 a proper reference deformation which imposes a far-field boundary condition.

Atomistic Mechanics (0T statics)

- **Assumptions**:
  - regularity of V, C^4 (no accumulation of atoms).
  - homogeneity of V, $V_x = V^{\rm hom}$ for x outside the defect.
  - finite interaction range $\mathcal{R}$, with cut-off radius $r_{\rm cut}$.
  - symmetry of V and $\mathcal{R}$, $-\mathcal{R} = \mathcal{R}$, and $V(\mathbf{g}) = \mathbf{V}(\mathbf{h})$, if $g_\rho = -h_{-\rho}$.
  - atomic spacing of $\mathcal{L}$ is 1.
- **Energy difference functional**: redefine

$$\mathcal{E}^{\rm a}(y) := \sum_{x\in\mathcal{L}} V(Dy(x)) - V(Dy_0(x))$$

  which is well defined if $y - y_0 \in \mathcal{U}^c$.
- We look for $y^{\rm a}$ with **Strong stability**

$$\langle \delta^2 \mathcal{E}^{\rm tot}_{\rm a}(y^{\rm a})v, v\rangle \geq \gamma^a \|\nabla \bar{v}\|^2_{L^2}, \forall v \in \mathcal{U}^c$$

  where $\mathcal{U}^c := \{u \in \mathcal{U} | {\rm supp}(u) \text{ is compact}\}$

Atomistic Mechanics (0T statics)

- **Regularity of the strongly stable equilibrium** away from the defect core: Given existence of the strong stable equilibrium, which is due to the property of the lattice and interatomic potential, $\exists c > 0$, such that [Ehrlacher et. al, 2013]

$$|\nabla^j \tilde{u}^{\mathrm{a}}(x)| \leq \begin{cases} c|x|^{1-d-j}, & \text{case point defect} \\ c|x|^{-j-1}\log|x|, & \text{case straight screw dislocation}, d = 2 \end{cases}$$

  where $\tilde{u}$ is smooth interpolant of u.

- Now we are in the position to consider the **finite dimension approximation** of this infinite dimensional problem (nonlinear, nonconvex)...

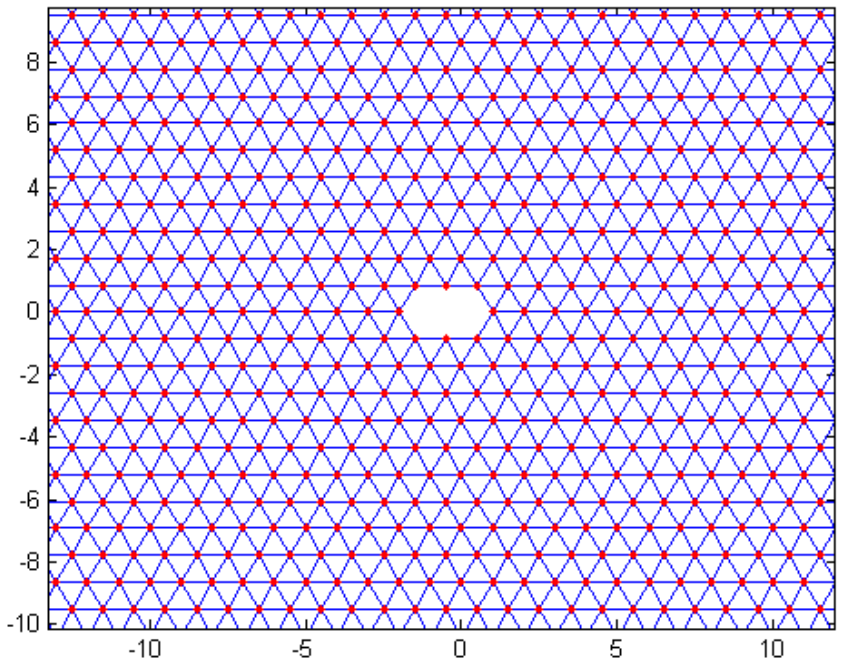
Why Do We Need Multiscale Method?

Microcrack in triangular lattice under macroscopic shear/stretch, EAM potential

$$V(g) := \sum_{\rho\in\mathcal{R}} \phi(|g_\rho|) + G\left(\sum_{\rho\in\mathcal{R}} \psi(|g_\rho|)\right), \quad \text{where}$$

$$\phi(s) := e^{-2A(s-1)} - 2e^{-A(s-1)}, \psi(s) := e^{-Bs},$$

$$\text{and } G(s) := C\left((s-s_0)^2 + (s-s_0)^4\right).$$



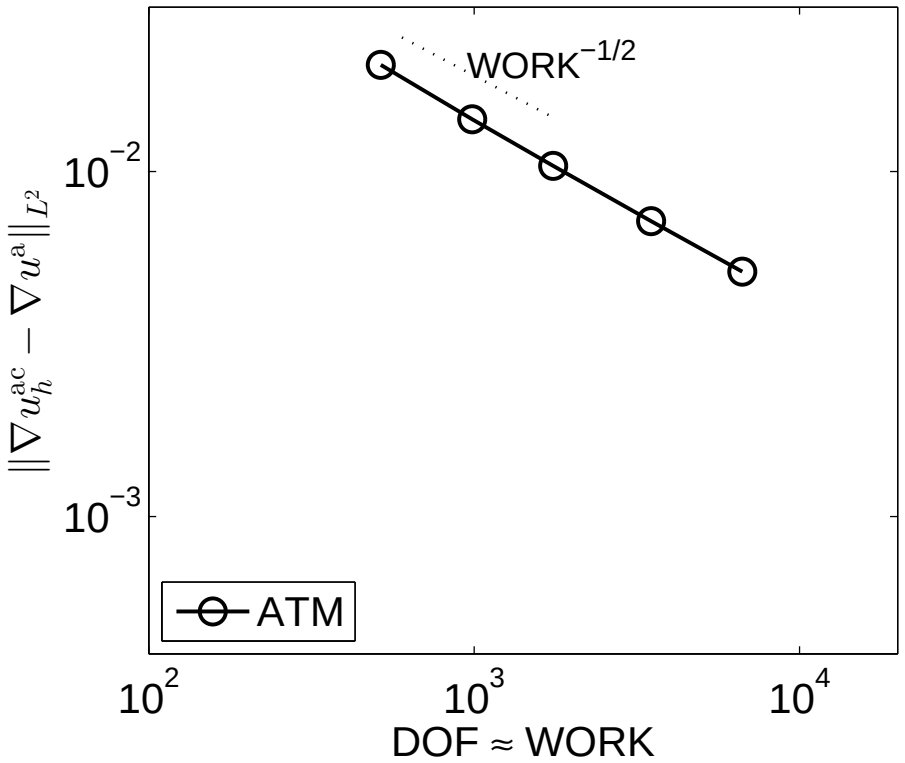
Why Do We Need Multiscale Method?

Microcrack in triangular lattice under macroscopic shear/stretch, EAM potential

$$V(g) := \sum_{\rho\in\mathcal{R}} \phi(|g_\rho|) + G\left(\sum_{\rho\in\mathcal{R}} \psi(|g_\rho|)\right), \quad \text{where}$$

$$\phi(s) := e^{-2A(s-1)} - 2e^{-A(s-1)}, \psi(s) := e^{-Bs},$$

$$\text{and } G(s) := C\left((s-s_0)^2 + (s-s_0)^4\right).$$



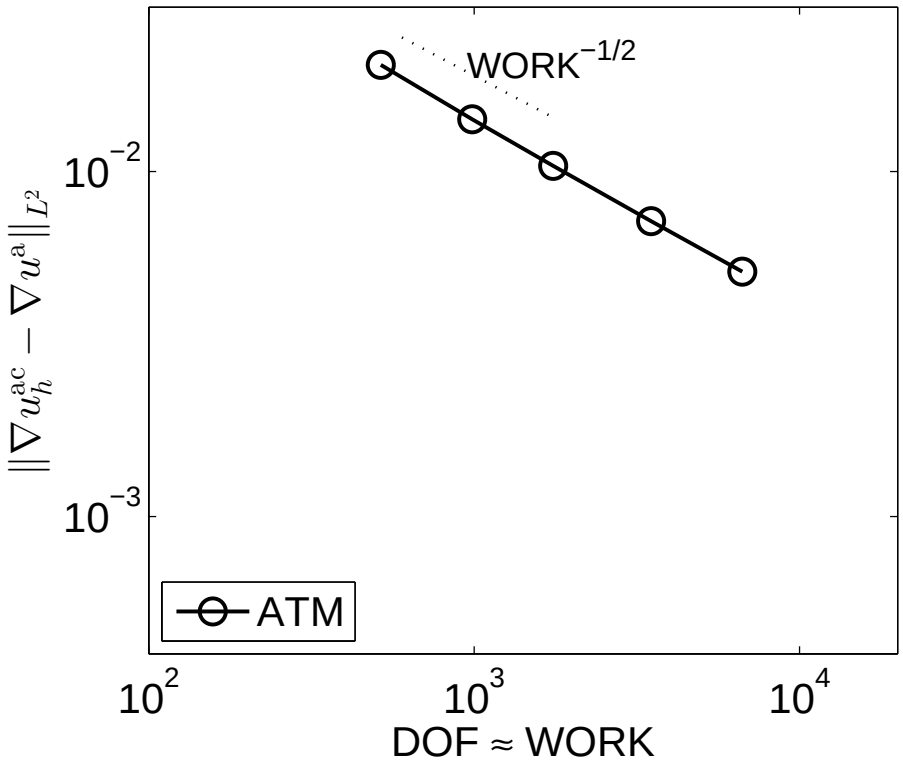
Why Do We Need Multiscale Method?

Microcrack in triangular lattice under macroscopic shear/stretch, EAM potential

$$V(g) := \sum_{\rho\in\mathcal{R}} \phi(|g_\rho|) + G\Big(\sum_{\rho\in\mathcal{R}} \psi(|g_\rho|)\Big), \quad \text{where}$$

$$\phi(s) := e^{-2A(s-1)} - 2e^{-A(s-1)}, \psi(s) := e^{-Bs},$$

$$\text{and } G(s) := C\big((s-s_0)^2 + (s-s_0)^4\big).$$



ATM (truncated atomistic simulation) error is controlled by the truncation error

$$\begin{aligned}\textbf{Err} &\le \|\nabla u\|_{\mathbb{R}^d\setminus\Omega_R} \\ &\le \Big(\int_R^\infty (r^{-d})^2 r^{d-1}\mathrm{dr}\Big)^{\frac{1}{2}} \\ &\le R^{-\frac{d}{2}} \simeq N^{-\frac{1}{2}}\end{aligned}$$

Note: decay of ∇u is r^{-d} in the far field.

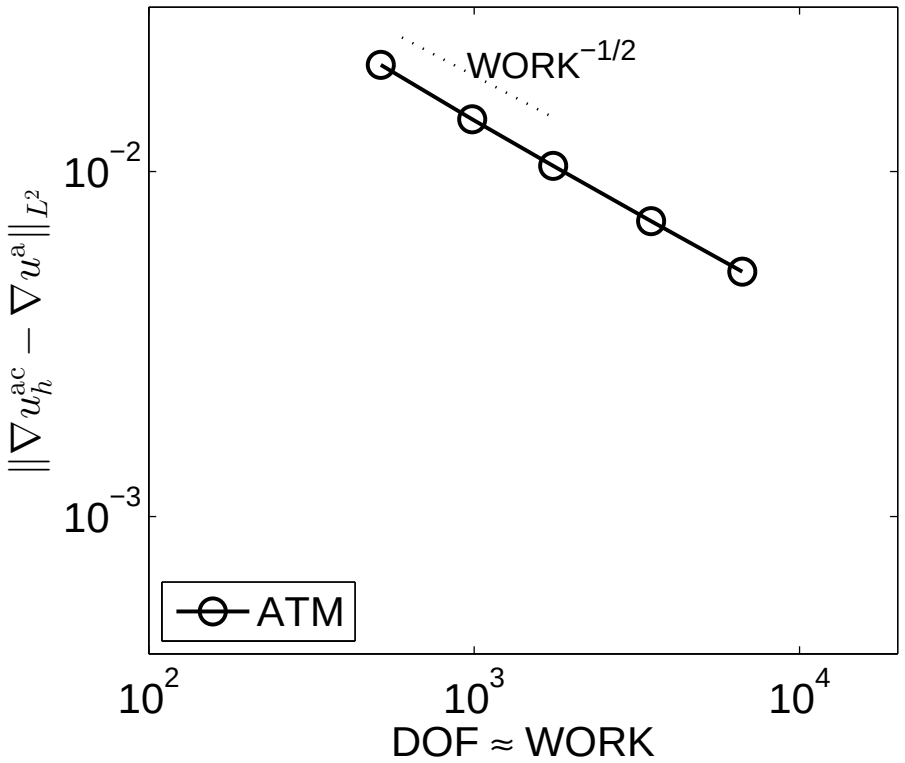
Why Do We Need Multiscale Method?

Microcrack in triangular lattice under macroscopic shear/stretch, EAM potential

$$V(g) := \sum_{\rho\in\mathcal{R}} \phi(|g_\rho|) + G\left(\sum_{\rho\in\mathcal{R}} \psi(|g_\rho|)\right), \quad \text{where}$$

$$\phi(s) := e^{-2A(s-1)} - 2e^{-A(s-1)}, \psi(s) := e^{-Bs},$$

$$\text{and } G(s) := C\left((s-s_0)^2 + (s-s_0)^4\right).$$

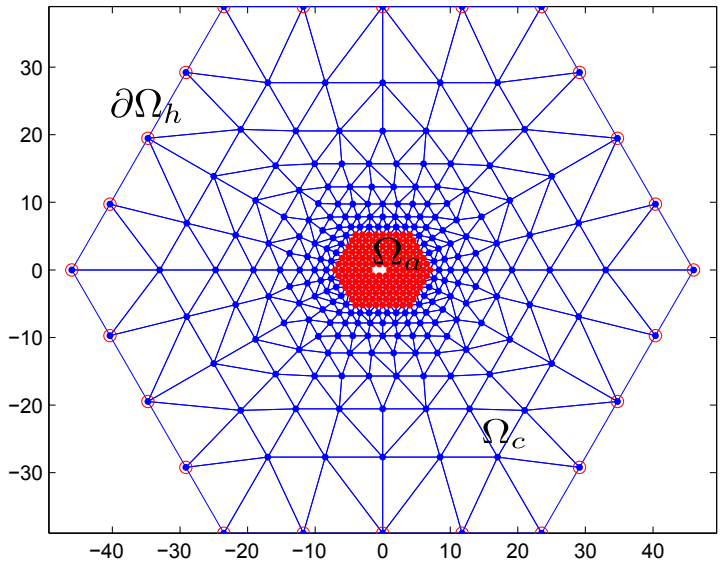


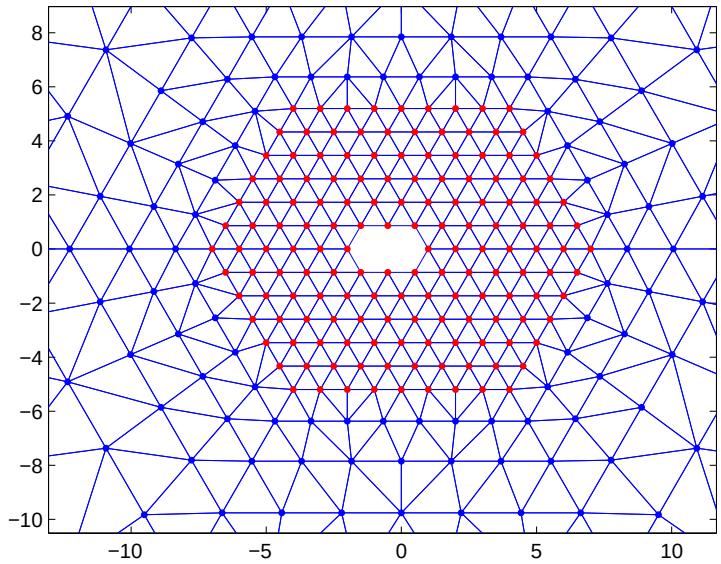
Can we find a better method, e.g., accuracy scales $O(N^{-1})$?

Idea:

- Coarse grainning the DoF.

Coarse Graining: Adaptive FEM





- Molecular statics: Find $y_a \in \boxed{\operatorname{argmin}\mathcal{E}^{\mathrm{a}}(\mathcal{Y})}$
- Coarse grained problem: Find $y_h \in \boxed{\operatorname{argmin}\mathcal{E}^{\mathrm{a}}(\mathcal{Y}_{\mathrm{h}})}$ where $\mathscr{T}_h$ resolves the defect, and $\mathcal{Y}_h = \mathcal{Y} \cap \mathrm{P}_1(\mathscr{T}_h)$
- $\|\nabla y_a - \nabla y_h\| \leq \|h\nabla^2 y_a\|_{\Omega\setminus\Omega_{\mathrm{a}}}$ [Lin, Ortner/Süli, Lin/Shapeev, ...]

But cost to evaluate $\mathcal{E}^{\mathrm{a}}|_{\mathcal{Y}_h}$, $\delta\mathcal{E}^{\mathrm{a}}|_{\mathcal{Y}_h}$ still $\simeq$ atomisitic dof in Ω_h.

Coarse Graining: Cauchy–Born Approximation

Atomistic Stored Energy:

$$\mathcal{E}^{\mathrm{a}}(y) = \sum_{x \in \mathcal{L}} V\big(y(x+\rho) - y(x); \rho \in \mathcal{R}\big)$$

Cauchy–Born Stored Energy:

$$\mathcal{E}^{\mathrm{c}}(y) = \int_{\Omega} W(\nabla y)\,\mathrm{dV}, \quad \text{where } W(\mathsf{F}) = V(\{\mathsf{F}\rho; \rho \in \mathcal{R}\}).$$

Theorem:

Let $y_{\mathrm{a}} \in \operatorname{argmin} \mathcal{E}^{\mathrm{tot}}_{\mathrm{a}}$ be "sufficiently smooth and strongly stable", then $\exists\ y_{\mathrm{c}} \in \operatorname{argmin} \mathcal{E}^{\mathrm{tot}}_{\mathrm{c}}$ such that

$$\|\nabla y_{\mathrm{a}} - \nabla y_{\mathrm{c}}\|_{\mathrm{L}^2} \lesssim C\big(\|\nabla^3 y_{\mathrm{a}}\|_{\mathrm{L}^2} + \|\nabla^2 y_{\mathrm{a}}\|^2_{\mathrm{L}^4}\big)$$

If the lattice spacing is ε, the RHS is $O(\varepsilon^2)$.
E & Ming (2007), Makridakis & Süli (2013), Ortner & Theil (2013)

Coarse Graining: Cauchy–Born Approximation

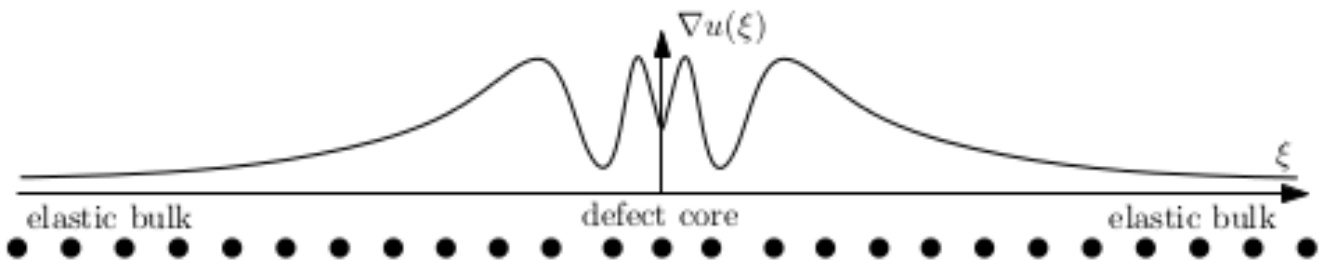
Atomistic Stored Energy:

$$\mathcal{E}^{\mathrm{a}}(y) = \sum_{x \in \mathcal{L}} V\big(y(x+\rho) - y(x); \rho \in \mathcal{R}\big)$$

Cauchy–Born Stored Energy:

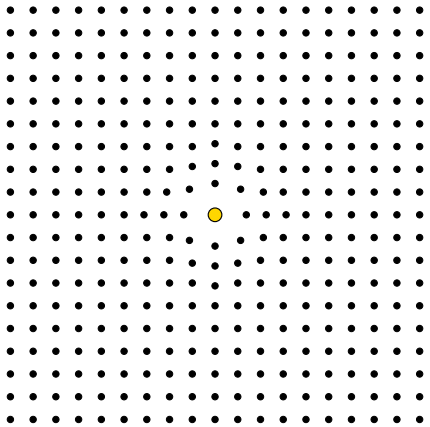
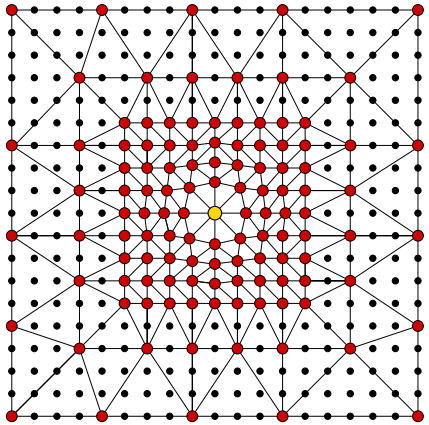
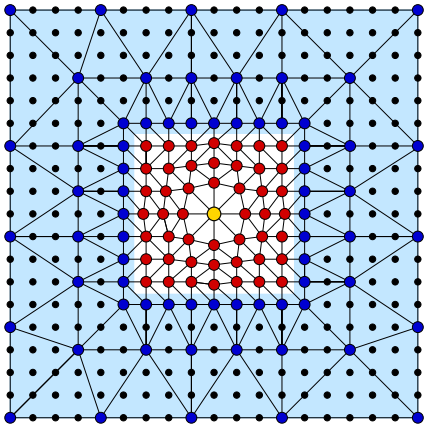
$$\mathcal{E}^{\mathrm{c}}(y) = \int_{\Omega} W(\nabla y)\,\mathrm{dV}, \quad \text{where } W(\mathsf{F}) = V(\{\mathsf{F}\rho; \rho \in \mathcal{R}\}).$$

- If there are no defects, then the Cauchy–Born model is a highly accurate continuum approximation.
- If there are defects (dislocation), then the Cauchy-Born model has $O(1)$ error.



[2012, Ortner & Luskin]

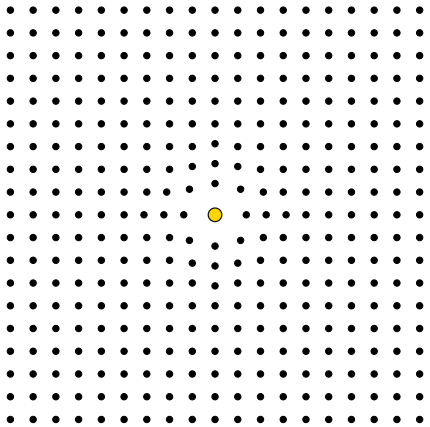
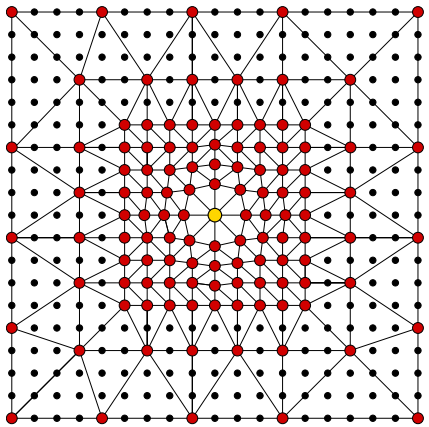
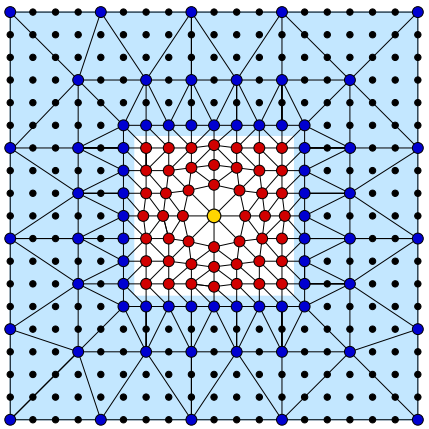
Atomistic/Continuum Coupling: First Attempt

$$\mathcal{E}^{\mathrm{a}}(y_h) \approx \mathcal{E}^{\mathrm{qce}}(y_h) := \sum_{x \in \mathcal{L}_{\mathrm{a}}} \omega_x V_x + \int_{\Omega_{\mathrm{c}}} W(\nabla y_h)\,\mathrm{d}x$$

Tadmor, Ortiz, Philips (1996)

Atomistic/Continuum Coupling: First Attempt

$$\mathcal{E}^{\mathrm{a}}(y_h) \approx \mathcal{E}^{\mathrm{qce}}(y_h) := \sum_{x \in \mathcal{L}_{\mathrm{a}}} \omega_x V_x + \int_{\Omega_{\mathrm{c}}} W(\nabla y_h)\,\mathrm{d}x$$

Tadmor, Ortiz, Philips (1996)

Fails the **patch test** (**ghost force**):

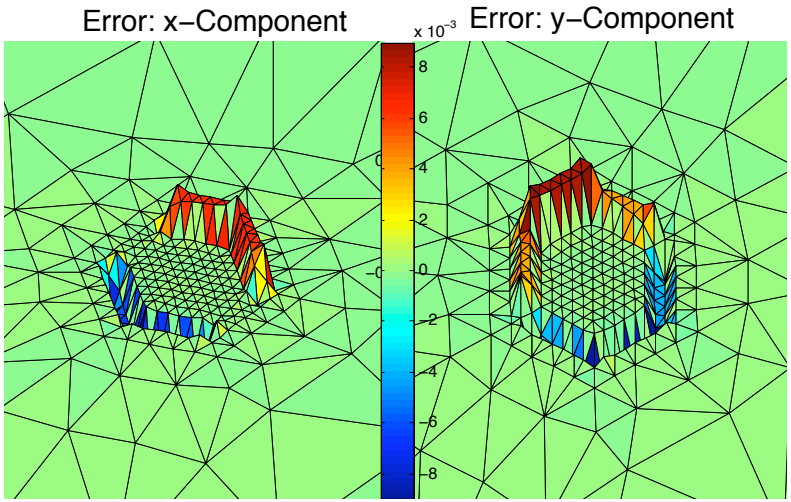
$$\delta\mathcal{E}^{\mathrm{a}}(y_{\mathsf{F}}) = 0$$

and

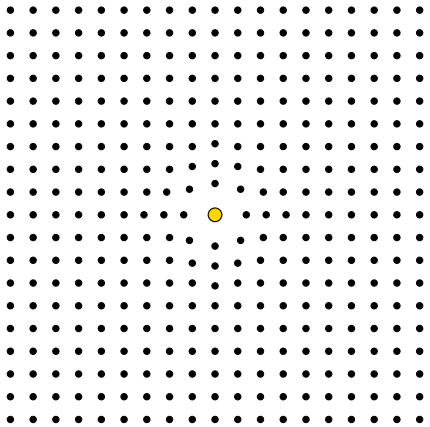
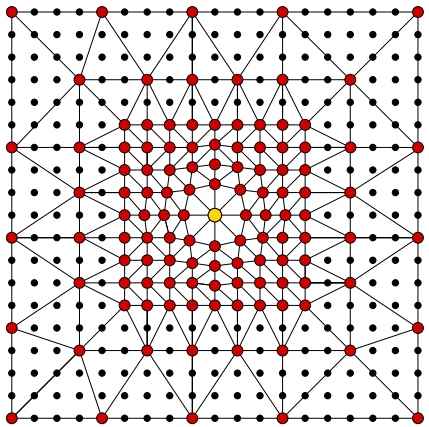
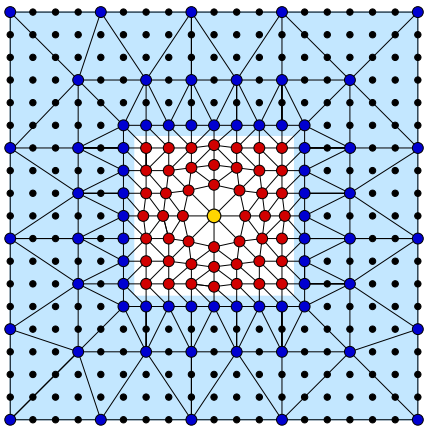
$$\delta\mathcal{E}^{\mathrm{c}}(y_{\mathsf{F}}) = 0,$$

but

$$\delta\mathcal{E}^{\mathrm{qce}}(y_{\mathsf{F}}) \neq 0 \ !$$



Atomistic/Continuum Coupling: First Attempt

$$\mathcal{E}^{\mathrm{a}}(y_h) \approx \mathcal{E}^{\mathrm{qce}}(y_h) := \sum_{x \in \mathcal{L}_{\mathrm{a}}} \omega_x V_x + \int_{\Omega_{\mathrm{c}}} W(\nabla y_h)\,\mathrm{d}x$$

Tadmor, Ortiz, Philips (1996)

Fails the **patch test** (**ghost force**):

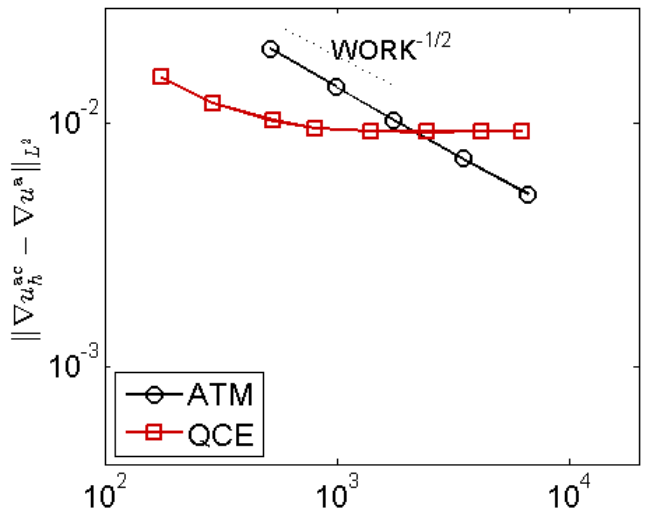
$$\delta\mathcal{E}^{\mathrm{a}}(y_{\mathsf{F}}) = 0$$

and

$$\delta\mathcal{E}^{\mathrm{c}}(y_{\mathsf{F}}) = 0,$$

but

$$\delta\mathcal{E}^{\mathrm{qce}}(y_{\mathsf{F}}) \neq 0 \ \textbf{!}$$



A 1D Model Problem

- Periodic displacements:

$$\mathcal{U} = \{\mathbf{u} = (u_n)_{n\in\mathbb{Z}} : u_{n+N} = u_n, \sum_{n=1}^{N} u_n = 0\},$$

$$\mathcal{Y} = \{\mathbf{y} = (y_n)_{n\in\mathbb{Z}} : y_n = x_n + u_n \text{ where } \mathbf{u} \in \mathcal{U}\}.$$

- Atomistic energy: (next-nearest neighbor pair interactions)

$$\mathcal{E}^{\mathrm{a}}(y) = \sum_{n=1}^{N} \phi(y'_n) + \sum_{n=1}^{N} \phi(y'_n + y'_{n+1}) = \sum_{n=1}^{N} \mathcal{E}^{\mathrm{a}}_n(y)$$

where $\mathcal{E}^{\mathrm{a}}_n(y) = \frac{1}{2}\{\phi(y'_{n-1} + y'_n) + \phi(y'_n) + \phi(y'_{n+1}) + \phi(y'_n + y'_{n+1})\}$

- Continuum finite element model

$$\mathcal{E}^{\mathrm{c}}(y) = \sum_{n=1}^{N} \{\phi(y'_n) + \phi(2y'_n)\} = \sum_{n=1}^{N} \mathcal{E}^{\mathrm{c}}_n(y)$$

where $\mathcal{E}^{\mathrm{c}}_n(y) = \frac{1}{2}\{\phi(2y'_n) + \phi(y'_n) + \phi(y'_{n+1}) + \phi(2y'_{n+1})\}$

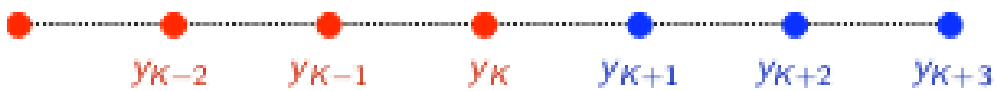
The Energy-Based Quasicontinuum Method

- Choose atomistic and continuum regions:

$$\mathcal{N}^{\mathrm{a}} \cup \mathcal{N}^{\mathrm{c}} = 1, \ldots, N$$

- Define a/c hybrid energy

$$\mathcal{E}^{\mathrm{qce}}(y) = \sum_{n \in \mathcal{N}^{\mathrm{a}}} \mathcal{E}_n^{\mathrm{a}}(y) + \underbrace{\sum_{n \in \mathcal{N}^{\mathrm{c}}} \mathcal{E}_n^{\mathrm{c}}(y)}_{\int_{\Omega^{\mathrm{c}}} W(Dy)\,\mathrm{d}x} - \langle g, y \rangle$$



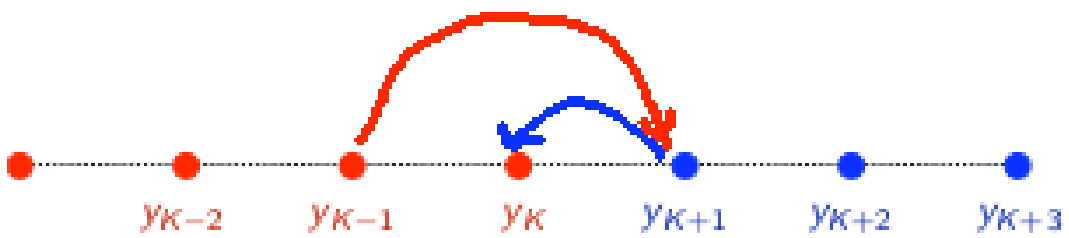
Ghost Forces

Solutions for $\mathcal{E}^{\mathrm{a}}$ and $\mathcal{E}^{\mathrm{c}}$:

$$\nabla \mathcal{E}^{\mathrm{a}}(x) = 0 \qquad \text{and} \qquad \nabla \mathcal{E}^{\mathrm{c}}(x) = 0$$

Insert $y_a = x$ into $\nabla \mathcal{E}^{\mathrm{qce}}$

$$\frac{\partial \mathcal{E}^{\mathrm{qce}}}{\partial y_n}\Big|_{y=x} = \frac{\phi'(2)}{2} \times \begin{cases} 0, & n = \ldots, K-2 \\ 1, & n = K-1 \\ -1, & n = K \\ -1, & n = K+1 \\ 1, & n = K+2 \\ 0, & n = K+3, \ldots \end{cases}$$



Alternative Approaches

1. **Energy-based coupling: Interface Correction**
2. **Force-based coupling:**
   - FeAt: Kohlhoff, Schmauder, Gumbsch (1989, 1991)
   - Dead-load GF removal: Shenoy, Miller, Rodney, Tadmor, Phillips, Ortiz (1999)
   - CADD: Shilkrot, Curtin, Miller (2002, . . .)
   - . . .
3. **Blending methods:** $E = \beta E_a + (1 - \beta) E_c$
   - Belytschko & Xiao (2004)
   - Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2008)
   - . . .

Consistent Energy-Based Coupling

Goal: Construct consistent A/C energy $\mathcal{E}^{\rm ac}$ by interface correction

$$\mathcal{E}^{\rm ac}(y) = \sum_{x\in\mathcal{L}_{\rm a}} V_x + \sum_{x\in\mathcal{L}_{\rm i}} \tilde{V}_x + \int_{\Omega_{\rm c}} W(Dy)\,{\rm d}x$$

find $\tilde{V}$ s.t. patch test consistency holds: $\delta\mathcal{E}^{\rm ac}(y_{\rm F}) = 0$ for all $\mathrm{F}\in\mathbb{R}^{d\times d}$.

1d, Shimokawa, et al (2004), E et al (2006),
For pair interaction, 2d/3d, Shapeev (2011,2012), Makridakis(2013)

Questions:

1. Does patch test consistency implies accuracy? A priori analysis?
2. How to construct consistent coupling method and optimal implementation?

Theory: A Priori Error Analysis

Framework: Let $y_{\mathrm{a}} \in \operatorname{argmin} \mathcal{E}_{\mathrm{a}}^{\mathrm{tot}}$, $y_{\mathrm{ac}} \in \operatorname{argmin} \mathcal{E}_{\mathrm{ac}}^{\mathrm{tot}}$, then

$$\|\nabla(y_{\mathrm{a}} - y_{\mathrm{ac}})\|_{\mathrm{L}^2} \approx \frac{\mathit{CONSISTENCY}}{\mathit{STABILITY}} = \frac{\|\delta\mathcal{E}^{\mathrm{a}}(y_{\mathrm{a}}) - \delta\mathcal{E}^{\mathrm{ac}}(y_{\mathrm{a}})\|_{\mathrm{H}^{-1}}}{\inf_{\|\nabla u\|_{\mathrm{L}^2}=1} \langle \delta^2\mathcal{E}^{\mathrm{ac}}(y_{\mathrm{a}})u, u\rangle}$$

3 Steps:

1. CONSISTENCY: $\langle \delta\mathcal{E}^{\mathrm{ac}}(y_{\mathrm{a}}) - \delta\mathcal{E}^{\mathrm{a}}(y_{\mathrm{a}}), u_h\rangle \lesssim h\|\nabla^2 y_{\mathrm{a}}\|_{\mathrm{L}^2(\Omega_{\mathrm{c}})}\|\nabla u_h\|_{L^2}$
2. STABILITY: $\langle \delta^2\mathcal{E}^{\mathrm{ac}}(y_{\mathrm{a}})u, u\rangle \geq C_{\mathrm{stab}}\|\nabla u\|_{\mathrm{L}^2}^2$
3. Error Estimate: Existence of A/C minimizer by inverse function theorem, convergence rate by decay estimate of defect

Theory: Convergence Estimates of A/C Coupling

$$\begin{aligned}\left\|\nabla(y_{\mathrm{a}}-y_{\mathrm{ac}})\right\|_{\mathrm{L}^2} \leq & \text{Consistency Err} + \text{Coarsening Err} + \text{Truncation Err} \\ \leq & \text{Consistency Err} + \underbrace{\|h\nabla^2\tilde{u}_a\|_{L^2(\Omega_c)}}_{P_1 \text{ FEM is used in } \Omega_c} + \|\nabla\bar{u}_a\|_{L^2(\mathbb{R}^d\setminus B_{R_c/2})} \\ \leq & \text{Consistency Err} + N^{-1/2-1/d} + N^{-1/2-1/d}\end{aligned}$$

for point defect ($|\nabla^j\tilde{u}_a(x)| \lesssim |x|^{-d+1-j}$), those parameters are (quasi-)optimal,

- R_a: radius of atomistic domain,
- $R_c \sim R_a^2$: radius of whole computational domain,
- $N \sim R_a^2$: total degree of freedom,
- $h(x) \sim (\frac{|x|}{R_a})^{3/2}$.

Patch Test Consistency $\Rightarrow$ First-order Consistency

If $\mathcal{E}^{\rm ac}$ is patch test consistent (no ghost force for homogeneous deformation):

$$\delta\mathcal{E}^{\rm ac}(y_{\rm F}) = 0 \qquad \forall {\rm F} \in \mathbb{R}^{d\times d}$$

"Theorem:" [First-order Consistency]

Suppose $\delta\mathcal{E}^{\rm ac}$ passes the patch test, V finite range multi-body potential + technical conditions +

- $d = 1$; or
- $d = 2$, $\Omega_{\rm a}$ connected; [Ortner, 2012] or
- $d = 3$, $\Omega_{\rm a}$ connected [in progress]

then

$$\begin{aligned}\left\langle \delta\mathcal{E}^{\rm ac}(y) - \delta\mathcal{E}^{\rm a}(y), u_h \right\rangle &= \sum_{T\in\mathcal{T}} (\Sigma_{\rm ac}(y;T) - \Sigma_{\rm a}(y;T)) : \nabla u_h \\ &\lesssim \|h\nabla^2 y\|_{{\rm L}^2(\Omega_{\rm c}\cup\Omega_{\rm i})} \|\nabla u_h\|_{{\rm L}^2}\end{aligned}$$

With the assumption of stability, $\Rightarrow \|\nabla u_{\rm a} - \nabla u_{\rm ac}\| \sim N^{-1}$.

Consequence of Patch Test Consistency

If an A/C energy $\mathcal{E}^{\mathrm{ac}}$ satisfies patch test consistency,

$$0 = \langle \delta\mathcal{E}^{\mathrm{ac}}(y_{\mathsf{F}}), u\rangle = \sum_{T\in\mathcal{T}} |T|\Sigma_{\mathrm{ac}}(y_{\mathsf{F}}; T) : \nabla_T u$$

then Σ_{ac} is discrete divergence free.

Lemma:

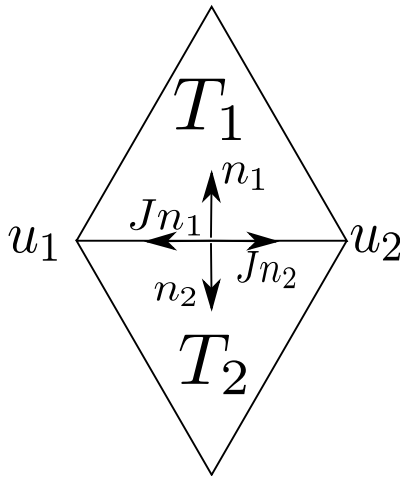
$\exists$ a function $\psi(\mathsf{F}, T) \in \mathrm{N}_1(\mathcal{T})^2$, such that

$$\Sigma_{\mathrm{ac}}(y_{\mathsf{F}}; T) = \partial W(\mathsf{F}) + J\nabla\psi(\mathsf{F}; T)$$

$\mathrm{N}_1(\mathcal{T})$ is Crouzeix–Raviart finite element space,

J is the counter-clockwise rotation by $\pi/2$.

$J\nabla\psi(\mathsf{F}; T)$ is divergence free piecewise constant tensor field [Arnold/Falk, Polthier/Preuß].



Construction of Consistent A/C Schemes

$$\mathcal{E}^{\rm ac}(y_h) = \sum_{x\in\mathcal{L}_{\rm a}} V_x + \sum_{x\in\mathcal{L}_{\rm i}} \tilde{V}_x + \sum_{x\in\mathcal{L}_{\rm c}} V_x^c$$

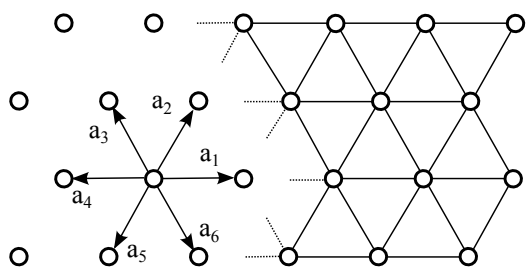
Construct $\tilde{V}$ s.t. $\delta\mathcal{E}^{\rm ac}(y_{\rm F}) = 0$ for all $\mathrm{F} \in \mathbb{R}^{d\times d}$.

General Construction: [1D, Shimokawa et al, 2004; E/Lu/Yang, 2006]

$$\tilde{V}_x = V\big(\tilde{g}_{x,r}; r \in \mathcal{R}\big)$$
$$\tilde{g}_{x,r} = \textstyle\sum_{s\in\mathcal{R}_x} C_{x,r,s} g_s$$

$\rightarrow$ Find $C_{x,r,s}$ s.t. $\delta\mathcal{E}^{\rm ac}(y_{\rm F}) = 0 \quad \forall \mathrm{F}$

$\rightarrow$ geometric conditions only!



2d, NN, multibody potential, triagular lattice

- Explicit constructions for 2D general interface
- **In general: compute $C_{x,r,s}$ numerically in preprocessing**

Construction of Consistent A/C Schemes

$$\mathcal{E}^{\rm ac}(y_h) = \sum_{x\in\mathcal{L}_{\rm a}} V_x + \sum_{x\in\mathcal{L}_{\rm i}} \tilde{V}_x + \sum_{x\in\mathcal{L}_{\rm c}} V_x^c$$

Construct $\tilde{V}$ s.t. $\delta\mathcal{E}^{\rm ac}(y_{\rm F}) = 0$ for all $\mathrm{F} \in \mathbb{R}^{d\times d}$.

General Construction: [1D, Shimokawa et al, 2004; E/Lu/Yang, 2006]

$$\tilde{V}_x = V\big(\tilde{g}_{x,r}; r\in\mathcal{R}\big)$$
$$\tilde{g}_{x,r} = \textstyle\sum_{s\in\mathcal{R}_x} C_{x,r,s} g_s$$

$\to$ Find $C_{x,r,s}$ s.t. $\delta\mathcal{E}^{\rm ac}(y_{\rm F}) = 0 \quad \forall \mathrm{F}$

$\to$ geometric conditions only!

1. Local Energy Consistency $\tilde{V}(y_{\rm F}) = V(y_{\rm F})$

2. Patch Test Consistency

$$\begin{aligned} 0 =& \langle \delta\mathcal{E}^{\rm ac}(y_{\rm F}), u\rangle \\ =& \sum_{x\in\mathcal{L}}\sum_{r\in\mathcal{R}} V_{{\rm F},r} \sum_{s\in\mathcal{R}} C_{x,r,s} D_s u \\ =& \sum_{x\in\mathcal{L}}\sum_{r\in\mathcal{R}}\sum_{s\in\mathcal{R}} (C_{x-a_s,r,s} V_{{\rm F},r} - C_{x,r,s} D_r V_{{\rm F},r}) u(x) \end{aligned}$$

$$\Rightarrow r = \sum_{s\in\mathcal{R}_x} C_{x,r,s} s. \qquad (a)$$

$$\Rightarrow \sum_{r\in\mathcal{R}}\sum_{s\in\mathcal{R}} (C_{x-s,r,s} V_{{\rm F},r} - C_{x,r,s} V_{{\rm F},r}) = 0. \qquad (b)$$

Solve (a) + (b) + B.C. in $\mathcal{L}_{\rm a}$ and $\mathcal{L}_{\rm c}$ to obtain $C_{x,r,s}$ for $x \in \mathcal{L}_{\rm i}$.

unknowns: $|\mathcal{I}||\mathcal{R}|^2$, eqns: $\le 5|\mathcal{I}||\mathcal{R}|$.

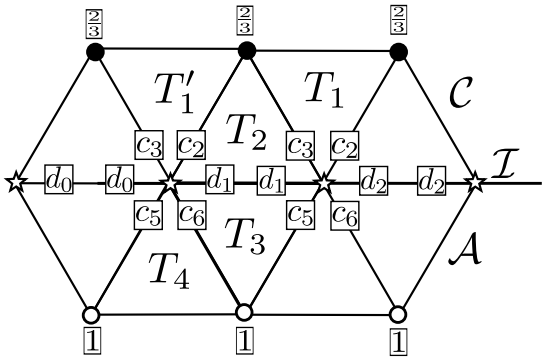
Construction of Consistent A/C Schemes

$$\mathcal{E}^{\mathrm{ac}}(y_h) = \sum_{x\in\mathcal{L}_{\mathrm{a}}} V_x + \sum_{x\in\mathcal{L}_{\mathrm{i}}} \tilde{V}_x + \sum_{x\in\mathcal{L}_{\mathrm{c}}} V_x^c$$

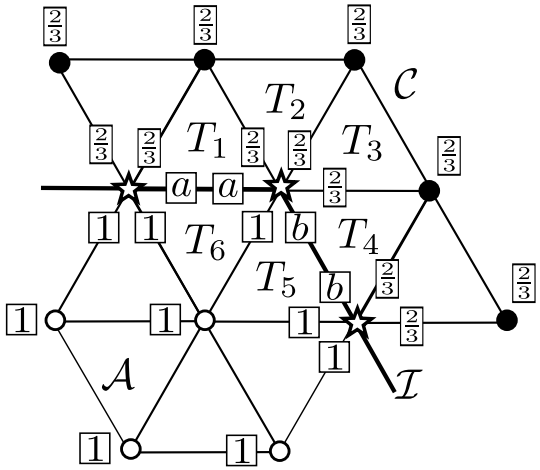
Construct $\tilde{V}$ s.t. $\delta\mathcal{E}^{\mathrm{ac}}(y_{\mathsf{F}}) = 0$ for all $\mathsf{F} \in \mathbb{R}^{d\times d}$.

General Construction:

Flat interface



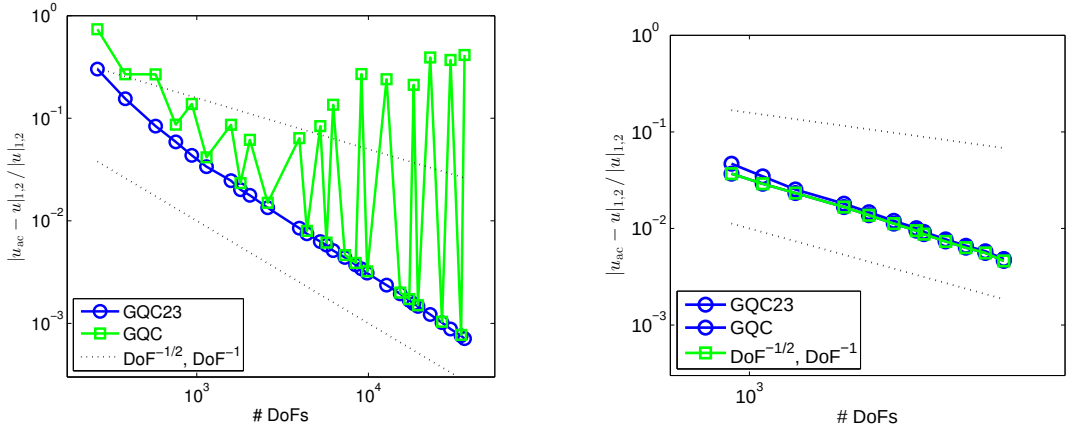
Interface with corner



$C_{x,r,r}$ for NN interaction, multibody potential, one-sided construction.

1. works for general interface in 2d
2. preprocessing for longer interaction range, coefficients are not unique, can be optimized by minimizing the consistency error.

Minimizing the Consistency Error



Left: H^1 Error with coefficients from least norm solution
Right: H^1 Error with coefficients from L^1 minimization

- Consistency Error Estimate

$$\left\langle \delta\mathcal{E}^{\mathrm{ac}}(y) - \delta\mathcal{E}^{\mathrm{a}}(y), u_h \right\rangle = \sum_{T\in\mathcal{T}} (\Sigma_{\mathrm{ac}}(y;T) - \Sigma_{\mathrm{a}}(y;T)) : \nabla u_h$$
$$\leq C \|h\nabla^2 y\|_{\mathrm{L}^2(\Omega_{\mathrm{c}}\cup\Omega_{\mathrm{i}})} \|\nabla u_h\|_{\mathrm{L}^2}$$

  The constant C is controled by $\max_{x\in\mathcal{I}} |\sum_{r\in\mathbb{R}} \sum_{s\in\mathbb{R}} |r||s| C_{x,r,s}|$.
- The coefficients needs to be pre-computed for longer range interactions, can be optimized for optimal accuracy.
- The coefficients can be obtained by solving a constrained L^1 minimization problem.

Stability of Consistent A/C Coupling Method

- Study the Hessians

$$\langle H^{\mathrm{a}}_{Dy} v, v\rangle := \langle \delta^2 \mathcal{E}^{\mathrm{a}}(y)v, v\rangle := \sum_{\xi\in\mathbb{Z}} \sum_{\xi,\varsigma\in\mathcal{R}} V_{\rho\varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)$$

$$\langle H^{\mathrm{ac}}_{Dy} v, v\rangle := \langle \delta^2 \mathcal{E}^{\mathrm{ac}}(y)v, v\rangle := \sum_{\xi\in\mathbb{Z}} \sum_{\xi,\varsigma\in\mathcal{R}} \tilde{V}_{\rho\varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)$$

Stability of Consistent A/C Coupling Method

- Study the Hessians

$$\langle H^{\mathrm{a}}_{Dy} v, v\rangle := \langle \delta^2 \mathcal{E}^{\mathrm{a}}(y)v, v\rangle := \sum_{\xi\in\mathbb{Z}} \sum_{\xi,\varsigma\in\mathcal{R}} V_{\rho\varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)$$

$$\langle H^{\mathrm{ac}}_{Dy} v, v\rangle := \langle \delta^2 \mathcal{E}^{\mathrm{ac}}(y)v, v\rangle := \sum_{\xi\in\mathbb{Z}} \sum_{\xi,\varsigma\in\mathcal{R}} \tilde{V}_{\rho\varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)$$

- Stability constant:

$$\gamma(H) := \inf_{\substack{u\in\mathcal{W}_0 \\ \|\nabla u\|_{L^2}=1}} \langle Hu, u\rangle.$$

We say that H is stable if $\gamma(H) > 0$.

Stability of Consistent A/C Coupling Method

- Study the Hessians

$$\langle H^{\mathrm{a}}_{Dy} v, v\rangle := \langle \delta^2 \mathcal{E}^{\mathrm{a}}(y)v, v\rangle := \sum_{\xi\in\mathbb{Z}} \sum_{\xi,\varsigma\in\mathcal{R}} V_{\rho\varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)$$

$$\langle H^{\mathrm{ac}}_{Dy} v, v\rangle := \langle \delta^2 \mathcal{E}^{\mathrm{ac}}(y)v, v\rangle := \sum_{\xi\in\mathbb{Z}} \sum_{\xi,\varsigma\in\mathcal{R}} \tilde{V}_{\rho\varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)$$

- Stability constant:

$$\gamma(H) := \inf_{\substack{u\in\mathcal{W}_0 \\ \|\nabla u\|_{L^2}=1}} \langle Hu, u\rangle.$$

  We say that H is stable if $\gamma(H) > 0$.

- For homogenous deformation y_{F},
  - $\gamma(H^{\mathrm{ac}}_{\mathrm{F}}) \le \gamma(H^{\mathrm{a}}_{\mathrm{F}})$ for all $\mathrm{F} > 0$.
  - $\gamma(H^{\mathrm{c}}_{\mathrm{F}}) = W''(\mathrm{F}) \ge \gamma(H^{\mathrm{a}}_{\mathrm{F}})$ for all $\det(\mathrm{F}) > 0$.

Universally Stable Method

Question: For any potential V, can we find such a A/C scheme, such that $\gamma_{\mathrm{F}}^{\mathrm{ac}} > 0$ if an only if $\gamma_{\mathrm{F}}^{\mathrm{a}} > 0$? If exists, such method is called univerally stable.

- universally stable method in 1D

$$z^* := \begin{cases} z(\xi), & \xi \le 0, \\ 2z(0) - z(-\xi), & \xi > 0. \end{cases}$$

$$\mathcal{E}^{\mathrm{rfl}}(y) := \mathcal{E}^*(y) + \int_0^\infty W(\nabla y)\,\mathrm{d}x, \qquad \text{where}$$

$$\mathcal{E}^*(y) := \sum_{\xi=-\infty}^{-1} \big[V(Dy^*(\xi)) - V(\mathrm{F}\mathcal{R})\big] + \tfrac{1}{2}\big[V(Dy^*(0)) - V(\mathrm{F}\mathcal{R})\big].$$

Universally Stable Method

Question: For any potential V, can we find such a A/C scheme, such that $\gamma_{\mathrm{F}}^{\mathrm{ac}} > 0$ if an only if $\gamma_{\mathrm{F}}^{\mathrm{a}} > 0$? If exists, such method is called univerally stable.

- universally stable method in 1D

$$z^* := \begin{cases} z(\xi), & \xi \le 0, \\ 2z(0) - z(-\xi), & \xi > 0. \end{cases}$$

$$\mathcal{E}^{\mathrm{rfl}}(y) := \mathcal{E}^*(y) + \int_0^\infty W(\nabla y)\,\mathrm{d}x, \qquad \text{where}$$

$$\mathcal{E}^*(y) := \sum_{\xi=-\infty}^{-1} \big[V(Dy^*(\xi)) - V(\mathrm{F}\mathcal{R})\big] + \tfrac{1}{2}\big[V(Dy^*(0)) - V(\mathrm{F}\mathcal{R})\big].$$

- Nonexistence of universally stable method in 2D, even for flat interface.

Stability Gap and Stabilization

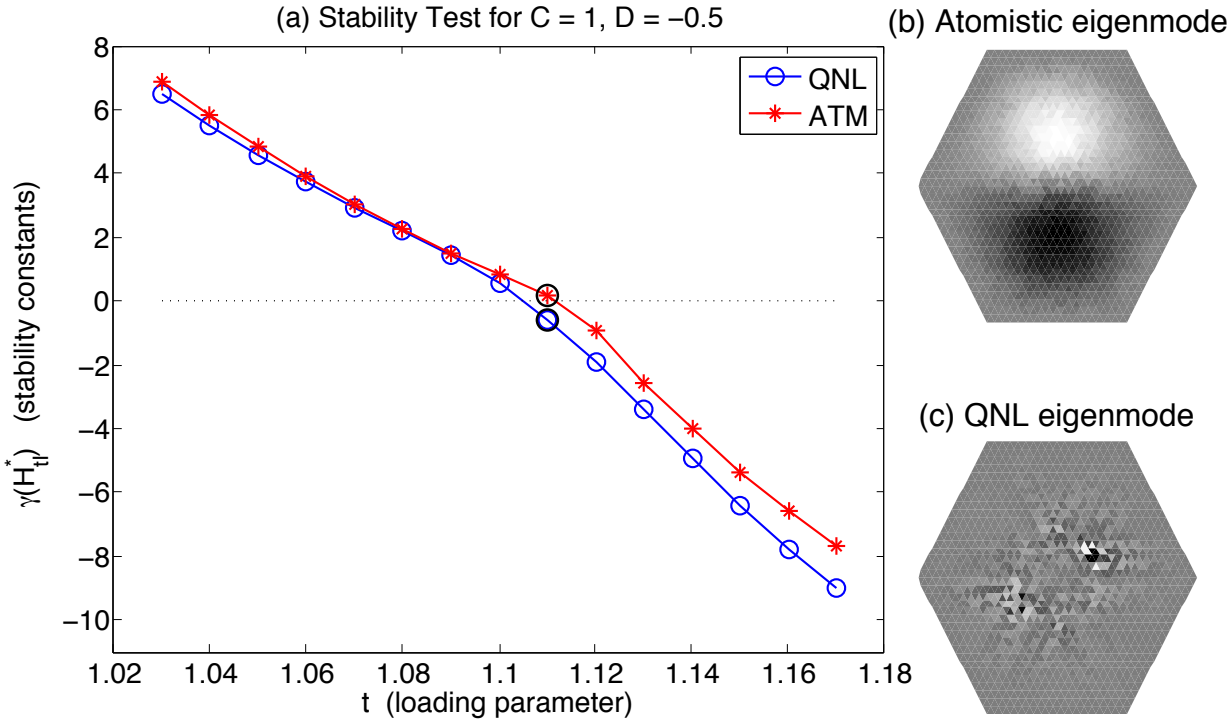


Figure: Stability test for $C = 1, D = -0.5$. The black circles indicate which eigenmodes (u_1-component) are plotted in (b, c).

$$V(g) := \sum_{\rho \in \mathcal{R}} \phi(|g_\rho|) + G\Big(\sum_{\rho \in \mathcal{R}} \psi(|g_\rho|)\Big) + D \sum_{j=1}^{6} (r_j \cdot r_{j+1} - 1/2)^2,$$

where $\phi(s) := e^{-2A(s-1)} - 2e^{-A(s-1)}$, $\psi(s) := e^{-Bs}$, and $G(s) := C\Big((s-s_0)^2 + (s-s_0)^4\Big)$

Stability Gap and Stabilization

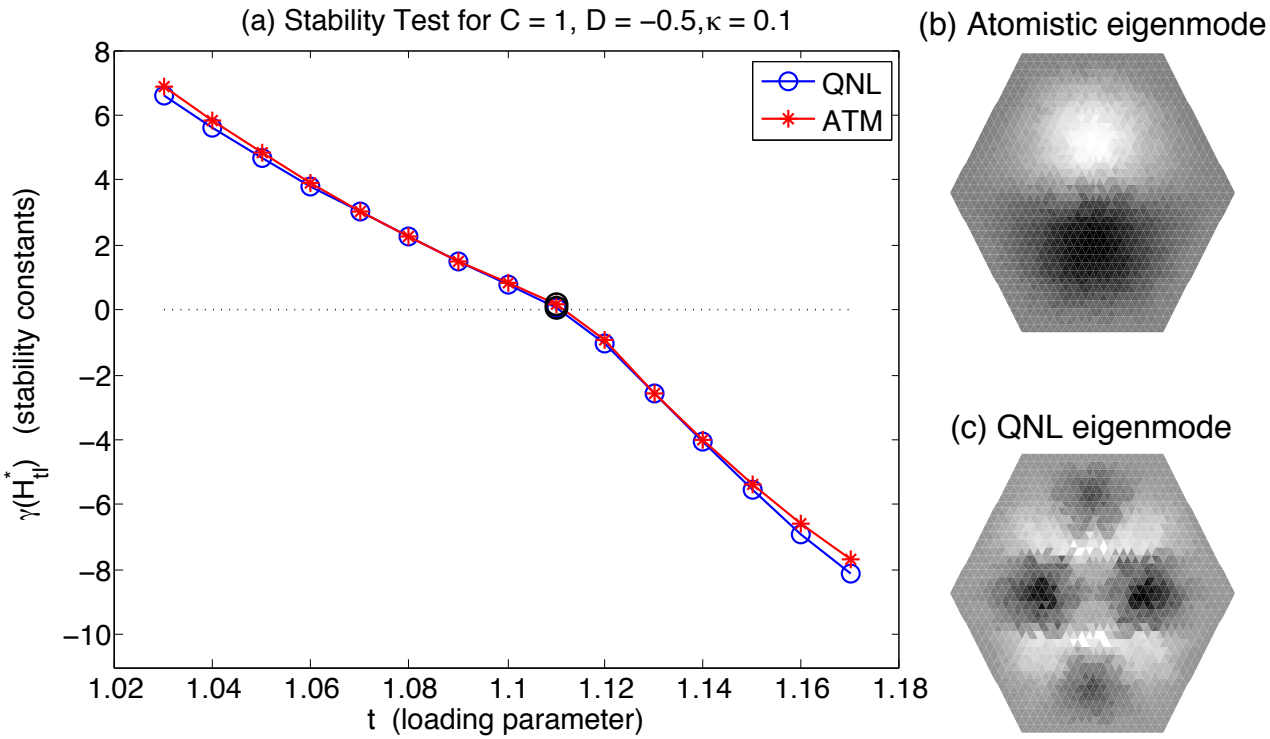


Figure: Stability test for $C = 1, D = -0.5, \kappa = 0.1$. The black circles indicate which eigenmodes (u_1-component) are plotted in (b, c).

$$\mathcal{E}^{\mathrm{stab}}(y) := \mathcal{E}^{\mathrm{ac}}(y) + \kappa \langle Su, u \rangle, \qquad \text{for } y = \mathsf{F}x + u, u \in \mathcal{W}_0,$$

where

$$\langle Su, u \rangle := \sum_{\xi \in \mathcal{L}^{(0)}} |D^2 u(\xi)|^2,$$

Stability Gap and Stabilization

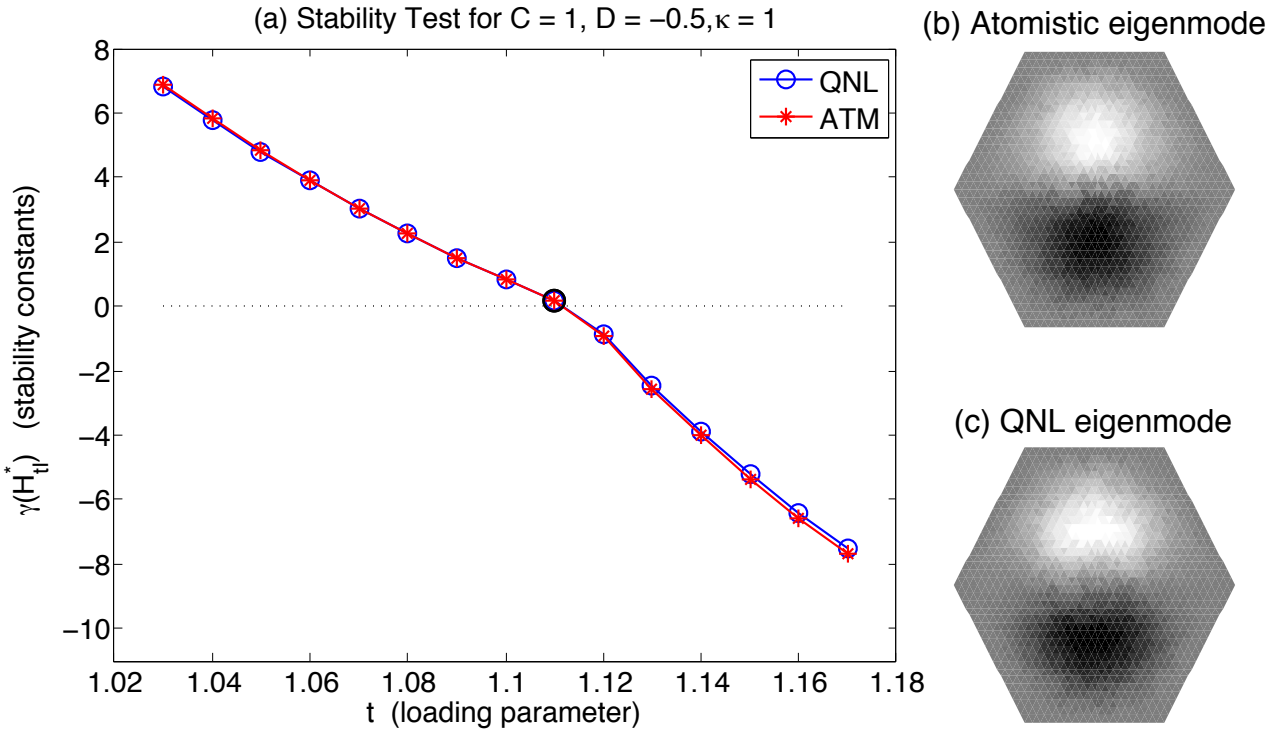


Figure: Stability test for $C = 1, D = -0.5, \kappa = 1$. The black circles indicate which eigenmodes (u_1-component) are plotted in (b, c).

$$\mathcal{E}^{\mathrm{stab}}(y) := \mathcal{E}^{\mathrm{ac}}(y) + \kappa \langle Su, u \rangle, \qquad \text{for } y = \mathsf{F}x + u, u \in \mathcal{W}_0,$$

where

$$\langle Su, u \rangle := \sum_{\xi \in \mathcal{L}^{(0)}} |D^2 u(\xi)|^2,$$

Tradeoff of Stabilization: Consistency vs. Stability

"Theorem:" [Critical Strain for Stablized A/C Coupling]

Let V have hexagonal symmetry, $\mathsf{F} \propto \mathsf{I}$, $V_{i,i+2} = V_{i,i+3} \equiv 0$, and $\tilde{c}_1^{(1)} - \tilde{c}_1^{(-1)} \neq 0$; then there exists constants $c_1, c_2 > 0$ such that

$$\gamma(H_{\mathsf{F}}^{\mathrm{a}}) - \frac{c_1}{\kappa^2} \leq \gamma(H_{\mathsf{F}}^{\mathrm{ac}} + \kappa S) \leq \gamma(H_{\mathsf{F}}^{\mathrm{a}}) - \frac{c_2}{\kappa^2}.$$

- existence of a critical loading parameter $t_*^\kappa \in [t_0, t_*]$ for which $\gamma(H_{t_\kappa^* \mathsf{I}}^{\mathrm{ac}} + \kappa S) = 0$ and such that

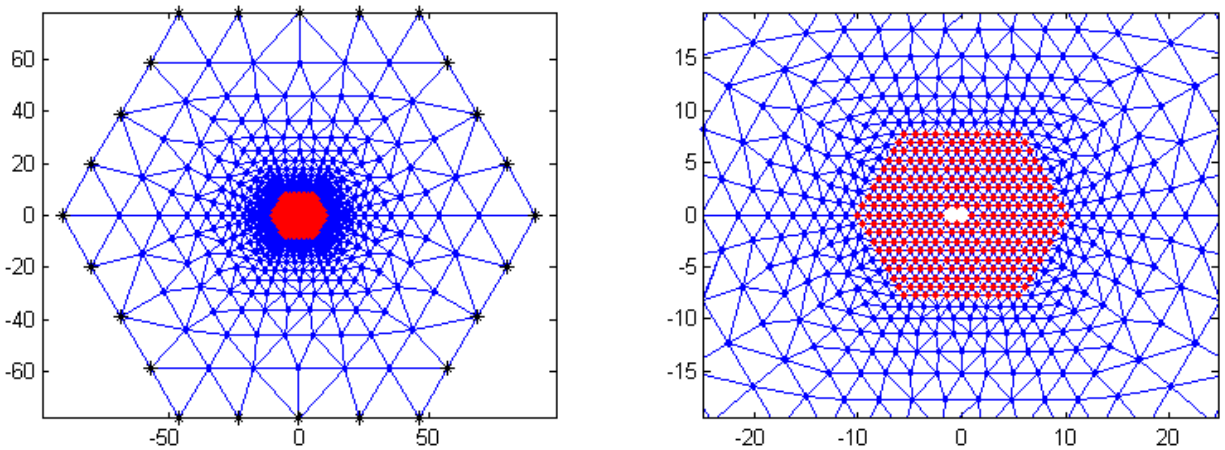
$$|t_*^\kappa - t_*| \approx \frac{1}{\kappa^2}.$$

- Therefore, if we wish to admit at most an $O(N^{-1})$ error in the critical strain, then we must accordingly choose $\kappa = O(N^{1/2})$. Unfortunately, this has a consequence for the consistency error of the stabilised A/C method, which will accordingly scale like $O(N^{1/2})$.

Numerical Experiment

Test Problem: microcrack in the triangular lattice, EAM multi-body potential, next nearest neighbor interaction

$$V = F_\alpha \left(\sum_{i \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{i \neq i} \phi_{\alpha\beta}(r_{ij})$$

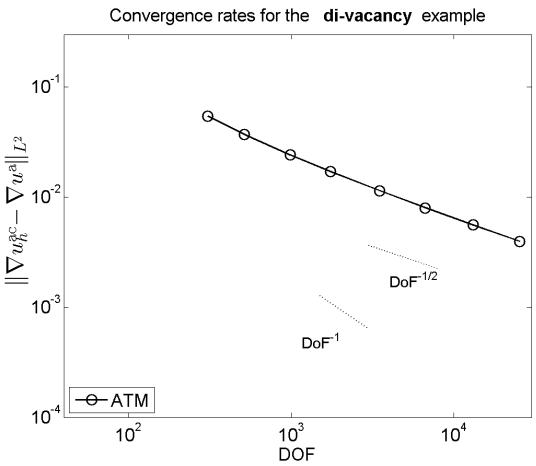


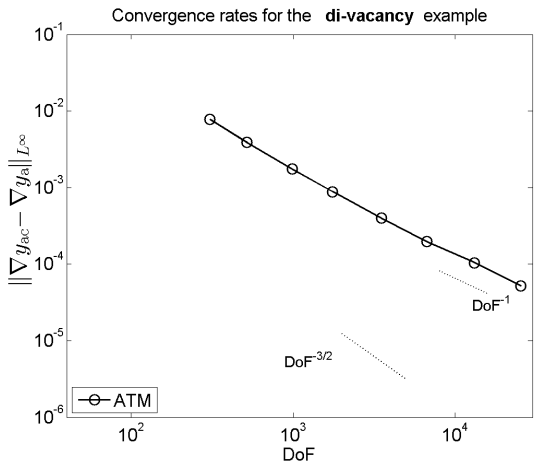
Apply 3% isotropic stretch and 3% shear loading

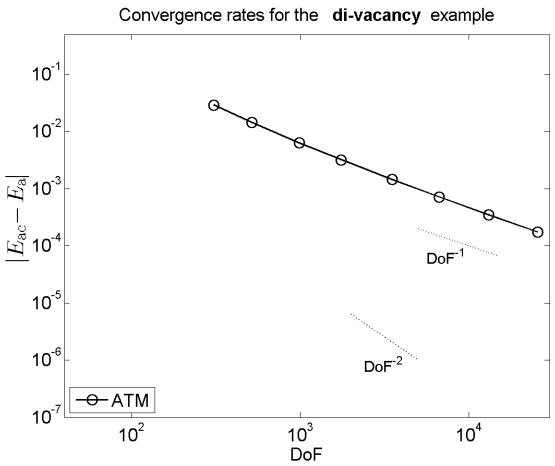
$$\mathrm{B} := \begin{pmatrix} 1+s & \gamma_{\mathrm{II}} \\ 0 & 1+s \end{pmatrix} \cdot \mathrm{F}_0.$$

where $\mathrm{F}_0 \propto I$ minimizes W, $s = \gamma_{\mathrm{II}} = 0.03$.

Numerical Experiment

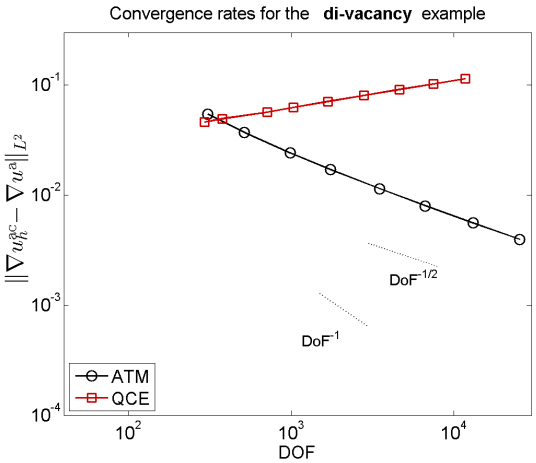


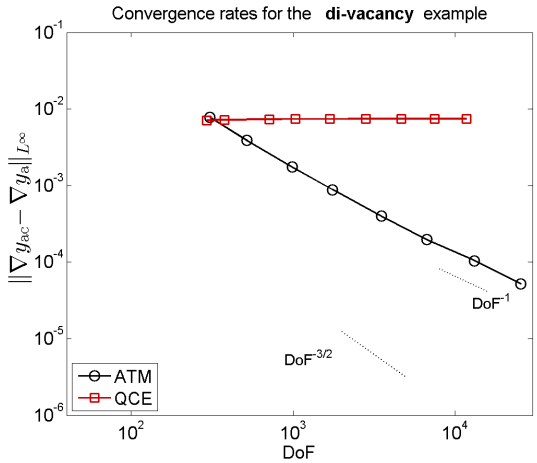


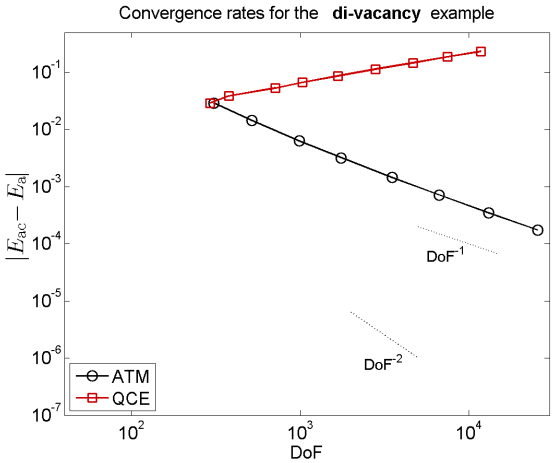


ATM: full atomistic model is minimized with the constraint $y = y_B$ in $\mathcal{L} \setminus \Omega$

Numerical Experiment

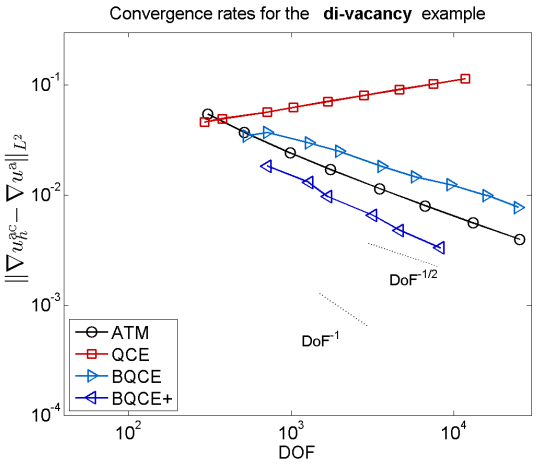


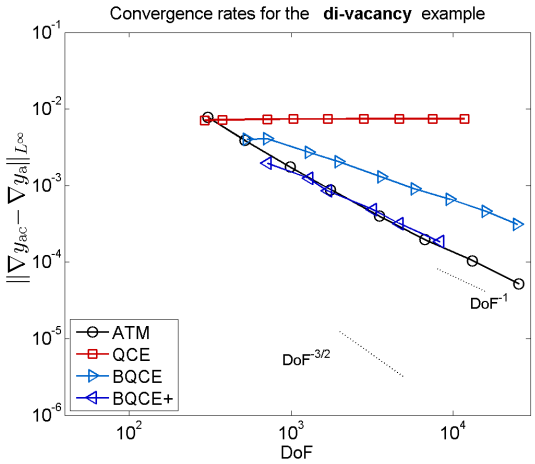


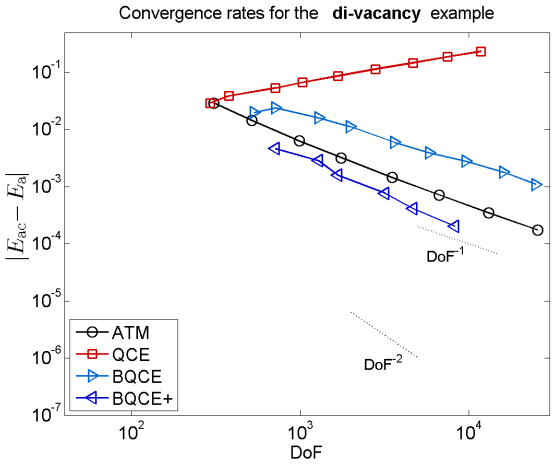


QCE: original quasicontinuum method without ghost-force correction, Tadmor, Ortiz, Philips, (1996).

Numerical Experiment

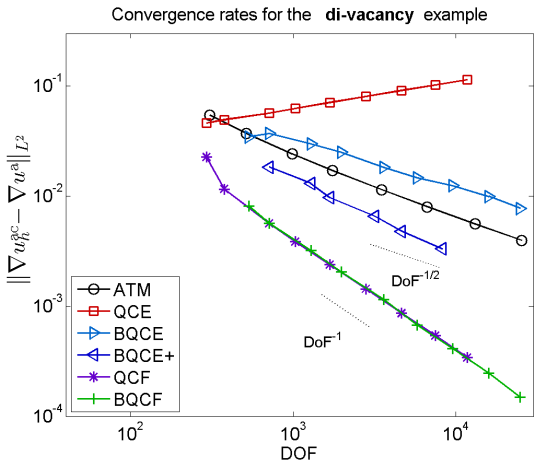


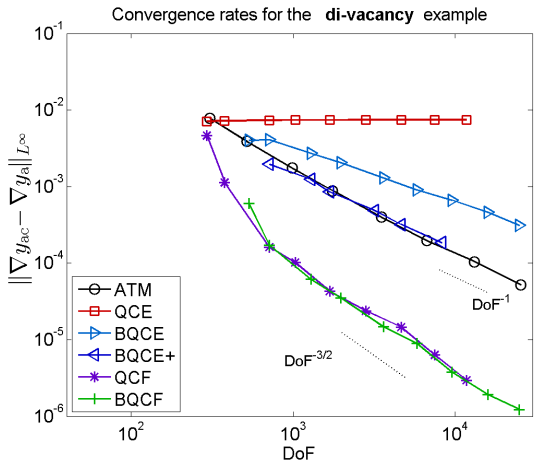


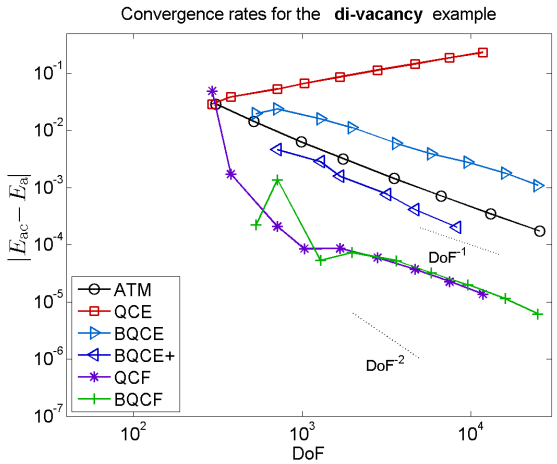


B-QCE, B-QCE+: blended quasicontinuum method, B-QCE+ is a variant with highly optimised approximation parameters Luskin et. al., (2012).

Numerical Experiment



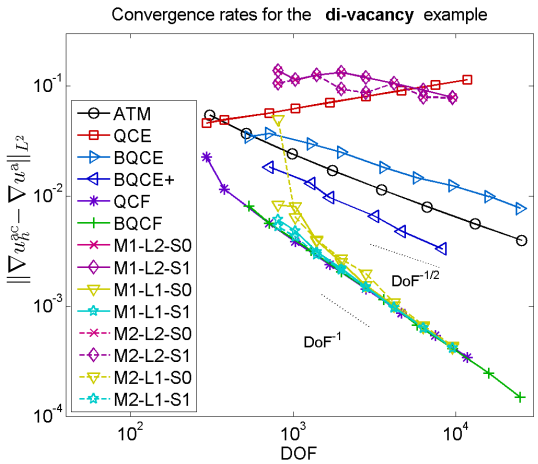


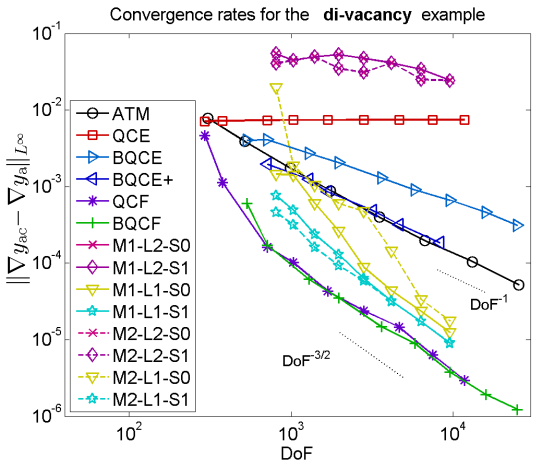


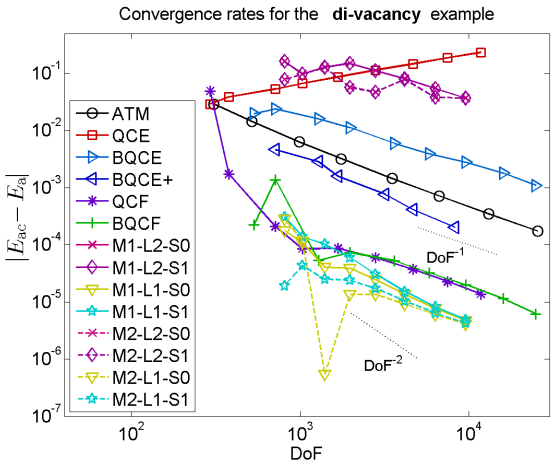
QCF: sharp-interface force-based a/c coupling Dobson et. al. (2009), formally equivalent to the quasi-continuum method with ghost-force correction Shenoy et. al., (1999).

B-QCF: blended force-based a/c coupling, as described in Li et. al, (2013).

Numerical Experiment







GRAC: two variants METHOD 1, METHOD 2 with both least squares solution and ℓ^1-minimisation to solve for the reconstruction parameters, and with stabilisation parameters $\kappa = 0, 1$. The resulting methods are denoted by $\mathtt{M}i\text{–}\mathtt{L}p\text{–}\mathtt{S}\kappa$, where $i \in \{1, 2\}$, $p \in \{2, 1\}$, $\kappa \in \{0, 1\}$

Blending with Ghost Force Correction (BGFC)

Energy-difference functional is well-defined.

$$\mathcal{E}^{\mathrm{a}}(u) := \sum_{a \in \mathcal{L}} V_a'(u), \qquad \text{where } V_a'(u) := V_a(x+u) - V_a(x),$$

where $\mathcal{L}$ be the lattice with defects.

Blending with Ghost Force Correction (BGFC)

Energy-difference functional is well-defined.

$$\mathcal{E}^{\mathrm{a}}(u) := \sum_{a\in\mathcal{L}} V_a'(u), \qquad \text{where } V_a'(u) := V_a(x+u) - V_a(x),$$

where $\mathcal{L}$ be the lattice with defects.
Let $\mathcal{L}^{\mathrm{hom}}$ be the homogenous reference lattice, V_a^{hom} be a globally homogeneous site potential,

$$\mathcal{E}^{\mathrm{a}}(u) = \sum_{a\in\mathcal{L}} V_a'(u) - \underbrace{\sum_{a\in\mathcal{L}^{\mathrm{hom}}} \langle \delta V_a^{\mathrm{hom}}(x), u\rangle}_{=0}$$

$$= \sum_{a\in\mathcal{L}} V_a''(u) + \langle \mathcal{L}^{\mathrm{ren}}, u\rangle,$$

where

$$V_a''(u) := V_a(x+u) - V_a(x) - \langle \delta V_a(x), u\rangle,$$

$$\langle \mathcal{L}^{\mathrm{ren}}, u\rangle := \sum_{a\in\mathcal{L}_{\mathrm{def}}} \langle \delta V_a(x), u\rangle - \sum_{a\in\mathcal{L}_{\mathrm{def}}^{\mathrm{hom}}} \langle \delta V_a^{\mathrm{hom}}(x), u\rangle.$$

BQCE Energy Functional

Define the BQCE energy functional

$$\mathcal{E}^{\mathrm{b}}(u_h) := \sum_{a \in \mathcal{L} \cap \Omega_h} (1 - \beta(a)) V_a'(u) + \int_{\Omega_h} Q_h \big[\beta W'(\nabla u_h)\big].$$

where $\beta \in C^{2,1}(\mathbb{R}^d)$, $\beta = 0$ in $B_{R^{\mathrm{a}}}$ with $R^{\mathrm{def}} \leq R^{\mathrm{a}} < R^{\mathrm{c}}$ and $\beta = 1$ in $\mathbb{R}^d \setminus B_{R_b}$, where R_b is the blending width.
The BQCE problem is to compute

$$u_h^{\mathrm{b}} \in \arg\min \left\{ \mathcal{E}^{\mathrm{b}}(v_h) \,\middle|\, v_h \in \mathcal{U}_h \right\}. \tag{1}$$

BQCE Energy Functional

Define the BQCE energy functional

$$\mathcal{E}^{\mathrm{b}}(u_h) := \sum_{a \in \mathcal{L} \cap \Omega_h} (1 - \beta(a)) V_a'(u) + \int_{\Omega_h} Q_h \big[\beta W'(\nabla u_h)\big].$$

where $\beta \in C^{2,1}(\mathbb{R}^d)$, $\beta = 0$ in $B_{R^{\mathrm{a}}}$ with $R^{\mathrm{def}} \le R^{\mathrm{a}} < R^{\mathrm{c}}$ and $\beta = 1$ in $\mathbb{R}^d \setminus B_{R_b}$, where R_b is the blending width.
The BQCE problem is to compute

$$u_h^{\mathrm{b}} \in \arg\min \left\{ \mathcal{E}^{\mathrm{b}}(v_h) \,\middle|\, v_h \in \mathcal{U}_h \right\}. \tag{1}$$

BQCE error is, cf. Li, Ortner, Shapeev, Van Koten, (2014)

$$\|\nabla u_h^{\mathrm{b}} - \nabla \overline{u^{\mathrm{a}}}\|_{L^2} \le C_1 \underbrace{\|\nabla^2 \beta\|_{L^2}}_{\text{due to ghost forces}} + C_2 \Big(\underbrace{\|\beta h \nabla^2 \tilde{u}^{\mathrm{a}}\|_{L^2(\Omega_h)}}_{\text{FEM coarsening error}} + \underbrace{\|\nabla \tilde{u}^{\mathrm{a}}\|_{L^2(\mathbb{R}^d \setminus B_{R^{\mathrm{c}}/2})}}_{\text{truncation error}} \Big) + .$$

$$\le C_1 N^{\frac{1}{2} - \frac{2}{d}} + C_2 N^{-\frac{1}{2} - \frac{1}{d}} \le C_1 N^{\frac{1}{2} - \frac{2}{d}}$$

by choosing $R_b \simeq R_a$.

BGFC Formulation

The BGFC energy is defined as

$$\mathcal{E}^{\mathrm{bg}}(u_h) := \sum_{a\in\mathcal{L}\cap\Omega_h} (1-\beta(a))V_a''(u_h) + \int_{\Omega_h} Q_h\big[\beta W''(\nabla u_h)\big] + \langle \mathcal{L}^{\mathrm{ren}}, u_h\rangle,$$

Apply the error analysis of BQCE to BGFC, the new constant C_1''

$$C_1'' \lesssim C\big\|\nabla \bar{u}^{\mathrm{a}}\big\|_{L^\infty(\mathbb{R}^d\setminus B_{R^{\mathrm{a}}-2r_{\mathrm{cut}}})} \lesssim (R^{\mathrm{a}})^{-d}.$$

and the ghost force error becomes

$$C_1''\|\nabla^2\beta\|_{L^2} \lesssim N^{-\frac{1}{2}-\frac{2}{d}}$$

best approximation error

$$\|\beta h\nabla^2\tilde{u}^{\mathrm{a}}\|_{L^2(\Omega_h)} + \|\nabla\tilde{u}^{\mathrm{a}}\|_{L^2(\mathbb{R}^d\setminus B_{R^{\mathrm{c}}/2})} \lesssim N^{-\frac{1}{2}-\frac{1}{d}}$$

Error of BGFC scheme is therefore (P1 FEM in the coarse graining region)

$$\boxed{\|\nabla u_h^{\mathrm{bg}} - \nabla\bar{u}^{\mathrm{a}}\|_{L^2} \lesssim N^{-\frac{1}{2}-\frac{1}{d}}.}$$

BGFC Formulation

The BGFC energy is defined as

$$\mathcal{E}^{\mathrm{bg}}(u_h) := \sum_{a\in\mathcal{L}\cap\Omega_h} (1-\beta(a))V_a''(u_h) + \int_{\Omega_h} Q_h\big[\beta W''(\nabla u_h)\big] + \langle \mathcal{L}^{\mathrm{ren}}, u_h\rangle,$$

Apply the error analysis of BQCE to BGFC, the new constant C_1''

$$C_1'' \lesssim C\big\|\nabla \bar{u}^{\mathrm{a}}\big\|_{L^\infty(\mathbb{R}^d\setminus B_{R^{\mathrm{a}}-2r_{\mathrm{cut}}})} \lesssim (R^{\mathrm{a}})^{-d}.$$

and the ghost force error becomes

$$C_1''\|\nabla^2\beta\|_{L^2} \lesssim N^{-\frac{1}{2}-\frac{2}{d}}$$

Using P2 FEM in the coarse graining region, the best approximation error

$$\|h^2\nabla^3\tilde{u}^{\mathrm{a}}\|_{L^2(\Omega_h\setminus B_{R^{\mathrm{a}}})} + \|\nabla\tilde{u}^{\mathrm{a}}\|_{L^2(\mathbb{R}^d\setminus B_{R^{\mathrm{c}}/2})}$$

can be balanced with ghost force error.
Optimal error estimate can be achieved by taking $R^{\mathrm{c}} \simeq (R^{\mathrm{a}})^{1+\frac{4}{d}}$.

$$\boxed{\|\nabla u^{\mathrm{bg,P2}} - \nabla\bar{u}^{\mathrm{a}}\|_{L^2} \lesssim N^{-\frac{1}{2}-\frac{2}{d}}.}$$

Connection to Ghost-Force Correction

We have

$$\begin{aligned}\mathcal{E}^{\mathrm{bg}}(u_h) &= \mathcal{E}^{\mathrm{b}}(u_h) - \sum_{a\in\mathcal{L}}(1-\beta(a))\langle \delta V_a(0), u_h\rangle - \int_{\mathbb{R}^d} Q_h\big[\beta\partial W(0) : \nabla u_h\big]\,\mathrm{d}x \\ &= \mathcal{E}^{\mathrm{b}}(u_h) - \langle \delta\mathcal{E}^{\mathrm{b}}(0), u_h\rangle \\ &= \mathcal{E}^{\mathrm{b}}(u_h) - \langle \delta\mathcal{E}^{\mathrm{b}}(0) - \mathcal{F}^{\mathrm{bqcf}}(0), u_h\rangle,\end{aligned}$$

The renormalisation step $V_a' \rightsquigarrow V''$ is equivalent to the ghost-force correction scheme of Shenoy et al (1999) , applied for a blended coupling formulation and in the reference configuration.

Connection to Ghost-Force Correction

We have

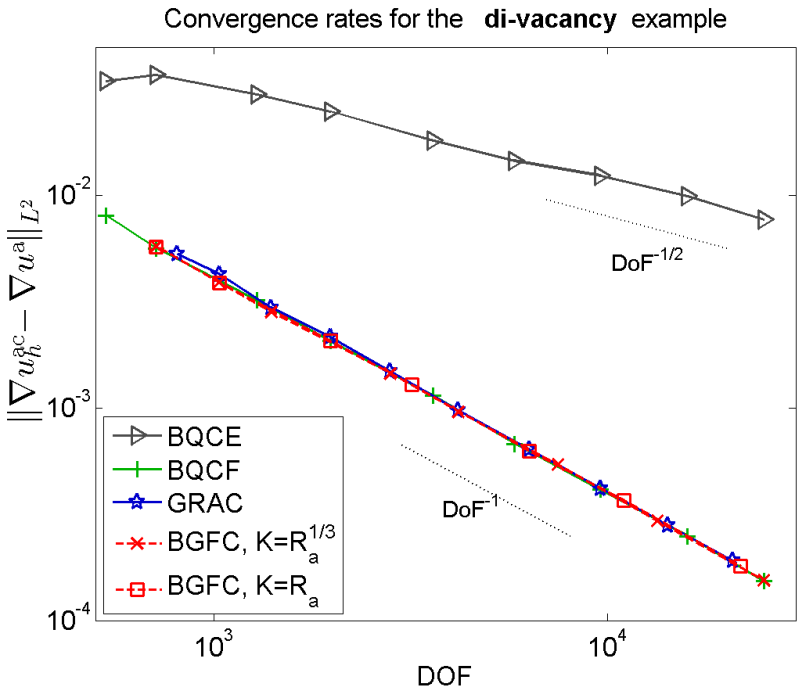
$$\begin{aligned}\mathcal{E}^{\mathrm{bg}}(u_h) &= \mathcal{E}^{\mathrm{b}}(u_h) - \sum_{a\in\mathcal{L}}(1-\beta(a))\langle \delta V_a(0), u_h\rangle - \int_{\mathbb{R}^d} Q_h\big[\beta\partial W(0) : \nabla u_h\big]\,\mathrm{d}x \\ &= \mathcal{E}^{\mathrm{b}}(u_h) - \langle \delta\mathcal{E}^{\mathrm{b}}(0), u_h\rangle \\ &= \mathcal{E}^{\mathrm{b}}(u_h) - \langle \delta\mathcal{E}^{\mathrm{b}}(0) - \mathcal{F}^{\mathrm{bqcf}}(0), u_h\rangle,\end{aligned}$$

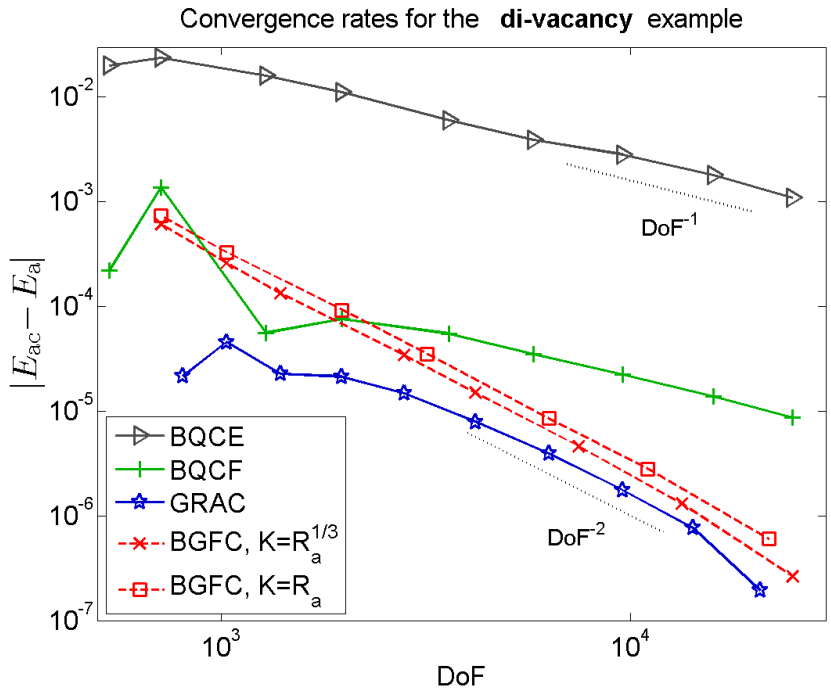
The renormalisation step $V_a' \rightsquigarrow V''$ is equivalent to the ghost-force correction scheme of Shenoy et al (1999) , applied for a blended coupling formulation and in the reference configuration.

The BGFC scheme can be generalized by choosing a suitable reference configuration (predictor) $\hat{u}_h$.

$$\mathcal{E}^{\mathrm{bg}}(u_h) := \mathcal{E}^{\mathrm{b}}(u_h) - \big\langle \delta\mathcal{E}^{\mathrm{b}}(\hat{u}_h) - \mathcal{F}^{\mathrm{bqcf}}(\hat{u}_h), u_h - \hat{u}_h\big\rangle,$$

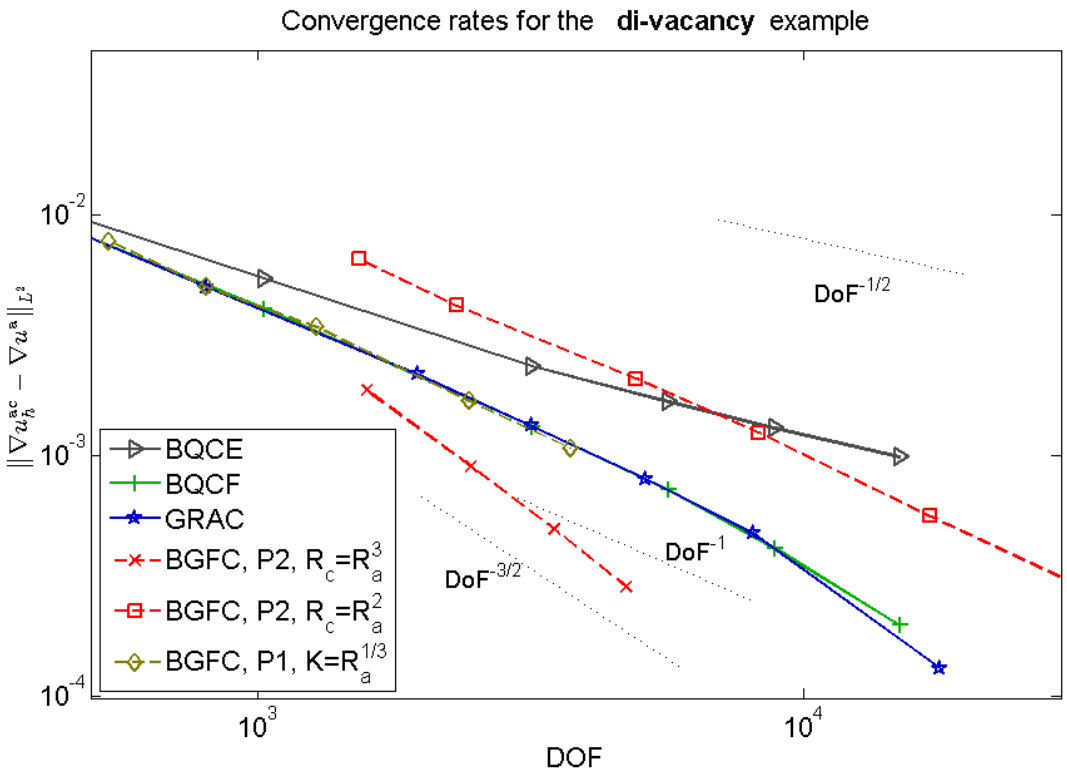
Numerical Results with BGFC





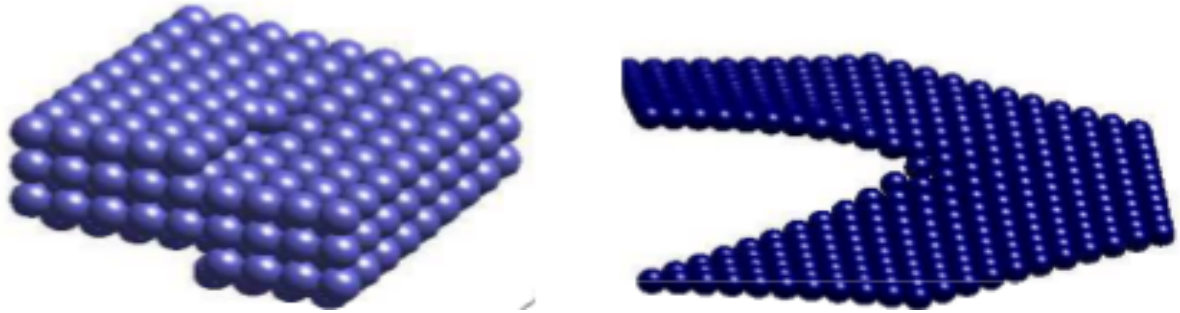
BGFC with P1 FEM

Numerical Results with BGFC



BGFC with P2 FEM

Anti-Plane Model for Screw Dislocation

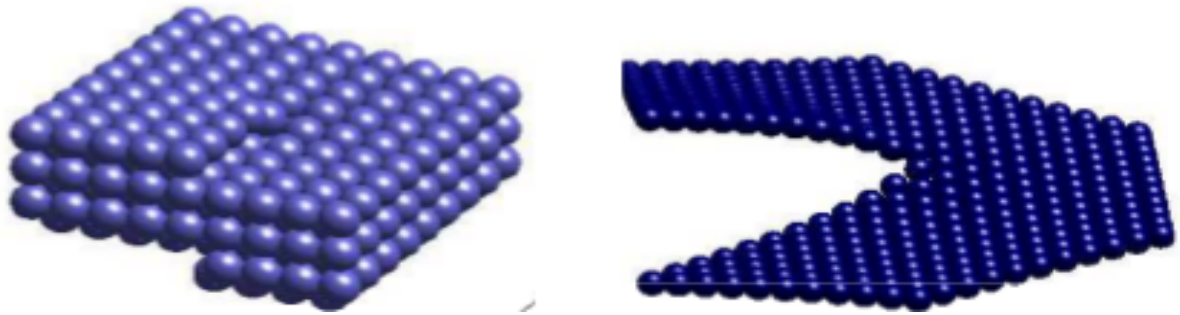


linear elasticity solution $y^{\mathrm{lin}}(a) = \frac{1}{2\pi}\arg(a - \hat{a})$

- Renormalized potential:
  $V^1(u) = V(y^{\mathrm{lin}} + u) - V(y^{\mathrm{lin}})$
  Apply consistent (cs) method to V^1,

$$\|\nabla u^a - \nabla u^{cs}\|_{L^2} \leq N^{-3/4}$$

Anti-Plane Model for Screw Dislocation



linear elasticity solution $y^{\mathrm{lin}}(a) = \frac{1}{2\pi}\arg(a - \hat{a})$

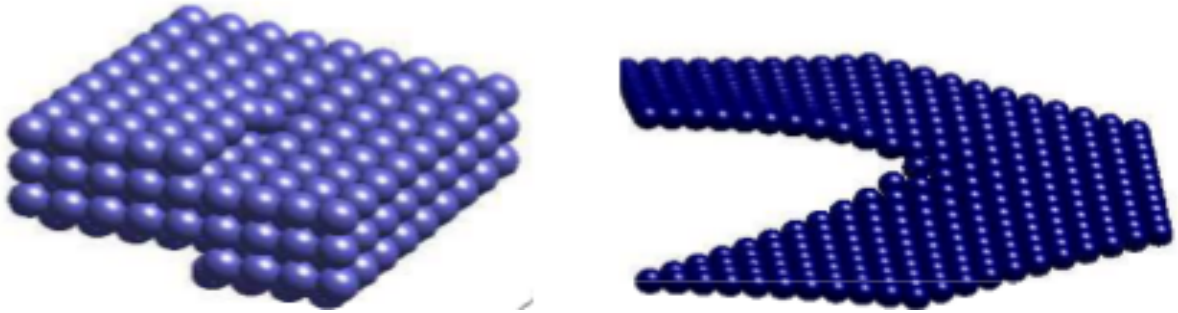
- Renormalized potential:
  $V^1(u) = V(y^{\mathrm{lin}} + u) - V(y^{\mathrm{lin}})$
  Apply consistent (cs) method to V^1,

$$\|\nabla u^a - \nabla u^{cs}\|_{L^2} \leq N^{-3/4}$$

- Another Renormalized potential:
  $V^2(u) = V(y^{\mathrm{lin}} + u) - V(y^{\mathrm{lin}}) - \langle \delta V(0), u \rangle$
  Apply blending (bg) method to V^2,

$$\|\nabla u^a - \nabla u^{bg}\|_{L^2} \leq N^{-1}(\log N)^{\frac{1}{2}}$$

Anti-Plane Model for Screw Dislocation



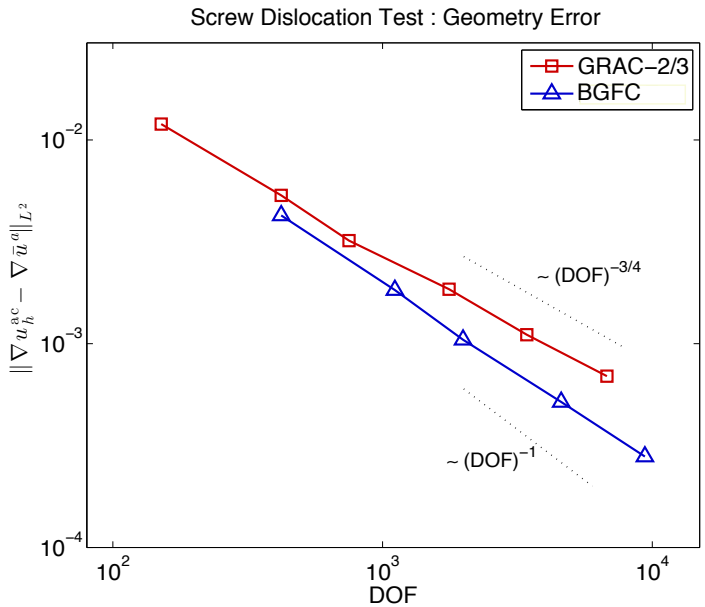
linear elasticity solution $y^{\mathrm{lin}}(a) = \frac{1}{2\pi}\arg(a - \hat{a})$

- Renormalized potential:
  $V^1(u) = V(y^{\mathrm{lin}} + u) - V(y^{\mathrm{lin}})$
  Apply consistent (cs) method to V^1,

$$\|\nabla u^a - \nabla u^{cs}\|_{L^2} \leq N^{-3/4}$$

- Another Renormalized potential:
  $V^2(u) = V(y^{\mathrm{lin}} + u) - V(y^{\mathrm{lin}}) - \langle \delta V(0), u \rangle$
  Apply blending (bg) method to V^2,

$$\|\nabla u^a - \nabla u^{bg}\|_{L^2} \leq N^{-1}(\log N)^{\frac{1}{2}}$$



Outlook

Summary

- Consistent energy coupling has optimal accuracy $O(N^{-1})$,
- Construction of consistent method with optimized consistency error,
- Stability and stabilization,
- Beyond consistent methods: the key is to find good 'predictor'.

Outlook

Summary

- Consistent energy coupling has optimal accuracy $O(N^{-1})$,
- Construction of consistent method with optimized consistency error,
- Stability and stabilization,
- Beyond consistent methods: the key is to find good 'predictor'.

Ongoing Work

- 3D arbitrary crystal,
- a posteriori error estimate and adaptive methods,
- dislocation, cracks, nano-indentation, ...
- Implementation, benchmarks, applications

Outlook

Summary

- Consistent energy coupling has optimal accuracy $O(N^{-1})$,
- Construction of consistent method with optimized consistency error,
- Stability and stabilization,
- Beyond consistent methods: the key is to find good 'predictor'.

Ongoing Work

- 3D arbitrary crystal,
- a posteriori error estimate and adaptive methods,
- dislocation, cracks, nano-indentation, ...
- Implementation, benchmarks, applications

Major Open Problems

- A/C methods for multi-lattices
- A/C methods for Coulomb interaction, e.g. charged crystal
- A/C methods for electronic structure models
- A/C methods at finite temperature (equilibrium and non-equilibrium)

Thanks for Your Attention!