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

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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 & 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

- Substitutional larger atom
- Vacancy
- Interstitial
- Substitutional smaller atom
- Frenkel pair

[Wikipedia]

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Atomistic Mechanics (0T statics)

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

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

- **Total energy** of configuration \( y \):

\[
\mathcal{E}_{\text{tot}}^a(y) := \mathcal{E}^a(y) + \mathcal{P}_a(y)
\]

where \( \mathcal{E}^a \) = interaction energy, \( \mathcal{P}_a \) = potential of external forces, \( V \) is multi-body interaction potential,

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

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

- **Goal**: Find

\[
y^a \in \arg\min \{ \mathcal{E}_{\text{tot}}^a(y) | y \in \mathcal{Y} \}
\]

where \( \mathcal{Y} := \{ y \in \mathcal{U} | y = y_0 + u \text{ for some } u \in \mathcal{U}^{1,2} \} \) 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 $V$, $V_x = V^{\text{hom}}$ for $x$ outside the defect.
  - finite interaction range $\mathcal{R}$, with cut-off radius $r_{\text{cut}}$.
  - symmetry of $V$ and $\mathcal{R}$, $-\mathcal{R} = \mathcal{R}$, and $V(g) = V(h)$, if $g_\rho = -h_{-\rho}$.
  - atomic spacing of $\mathcal{L}$ is 1.

- **Energy difference functional:** redefine
  \[
  \mathcal{E}^a(y) := \sum_{x \in \mathcal{L}} V(Dy(x)) - V(Dy_0(x))
  \]
  which is well defined if $y - y_0 \in \mathcal{U}^c$.

- We look for $y^a$ with **Strong stability**
  \[
  \langle \delta^2 \mathcal{E}_a^{\text{tot}}(y^a), \nu \rangle \geq \gamma^a \| \nabla \bar{\nu} \|_{L^2}^2, \forall \nu \in \mathcal{U}^c
  \]
  where $\mathcal{U}^c := \{ u \in \mathcal{U} | \text{supp}(u) \text{ is compact} \}$.
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 [Ehrlicher et. al, 2013]

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

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

\[ V(g) := \sum_{\rho \in \mathcal{R}} \phi(|g|) + G\left(\sum_{\rho \in \mathcal{R}} \psi(|g|)\right) \]

where

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

and \[ G(s) := C\left((s - s_0)^2 + (s - s_0)^4\right). \]
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ATM (truncated atomistic simulation) error is controlled by the truncation error

\[ \text{Err} \leq \|\nabla u\|_{\mathbb{R}^d \setminus \Omega_R} \]

\[ \leq \left(\int_R^\infty (r^{-d})^2 r^{d-1} \, dr\right)^{1/2} \]

\[ \leq R^{-\frac{d}{2}} \approx N^{-\frac{1}{2}} \]

Note: decay of \( \nabla u \) is \( r^{-d} \) in the far field.
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and \[ G(s) := C((s - s_0)^2 + (s - s_0)^4). \]

Can we find a better method, e.g.,

\[ \text{accuracy scales } O(N^{-1})? \]

Idea:

- Coarse grainning the DoF.
Coarse Graining: Adaptive FEM

- Molecular statics: Find $y_a \in \text{argmin} E^a(Y)$
- Coarse grained problem: Find $y_h \in \text{argmin} E^a(Y_h)$ where $T_h$ resolves the defect, and $Y_h = Y \cap P_1(T_h)$
  \[ \| \nabla y_a - \nabla y_h \| \leq \| h \nabla^2 y_a \|_{\Omega \setminus \Omega_a} \]
  [Lin, Ortner/Süli, Lin/Shapeev, ...]

But cost to evaluate $E^a|_{Y_h}$, $\delta E^a|_{Y_h}$ still $\approx$ atomisitic dof in $\Omega_h$. 

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Coarse Graining: Cauchy–Born Approximation

Atomistic Stored Energy:

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

Cauchy–Born Stored Energy:

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

Theorem:

Let \( y_a \in \arg\min \mathcal{E}^\text{tot}_a \) be “sufficiently smooth and strongly stable”, then \( \exists \ y_c \in \arg\min \mathcal{E}^\text{tot}_c \) such that

\[ \| \nabla y_a - \nabla y_c \|_{L^2} \lesssim C (\| \nabla^3 y_a \|_{L^2} + \| \nabla^2 y_a \|_{L^4}^2) \]

If the lattice spacing is \( \varepsilon \), the RHS is \( O(\varepsilon^2) \).

Coarse Graining: Cauchy–Born Approximation

Atomistic Stored Energy:

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

Cauchy–Born Stored Energy:

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

- 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

\[ \mathcal{E}^a(y_h) \approx \mathcal{E}^{qce}(y_h) := \sum_{x \in \mathcal{L}_a} \omega_x V_x + \int_{\Omega_c} W(\nabla y_h) \, dx \]

Tadmor, Ortiz, Philips (1996)
Atomistic/Continuum Coupling: First Attempt

\[ E^a(y_h) \approx E^{qc}(y_h) := \sum_{x \in L_a} \omega_x V_x + \int_{\Omega_c} W(\nabla y_h) \, dx \]

Tadmor, Ortiz, Philips (1996)

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

\[ \delta E^a(y_F) = 0 \]

and

\[ \delta E^c(y_F) = 0, \]

but

\[ \delta E^{qc}(y_F) \neq 0! \]
Atomistic/Continuum Coupling: First Attempt

\[ \mathcal{E}^a(y_h) \approx \mathcal{E}^{qce}(y_h) := \sum_{x \in \mathcal{L}_a} \omega_x V_x + \int_{\Omega_c} W(\nabla y_h) \, dx \]

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

\[ \delta \mathcal{E}^a(y_F) = 0 \]

and

\[ \delta \mathcal{E}^c(y_F) = 0, \]

but

\[ \delta \mathcal{E}^{qce}(y_F) \neq 0! \]
**A 1D Model Problem**

- Periodic displacements:

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

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

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

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

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

- Continuum finite element model

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

where \( \mathcal{E}^c_n(y) = \frac{1}{2} \{ \phi(2y'_n) + \phi(y'_n) + \phi(y'_{n+1}) + \phi(2y'_{n+1}) \} \)
The Energy-Based Quasicontinuum Method

- Choose atomistic and continuum regions:
  \[ N^a \cup N^c = 1, \ldots, N \]

- Define a/c hybrid energy
  \[
  \mathcal{E}^{qce}(y) = \sum_{n \in N^a} \mathcal{E}_n^a(y) + \sum_{n \in N^c} \mathcal{E}_n^c(y) - \langle g, y \rangle
  \]
  \[
  \int_{\Omega^c} W(Dy) \, dx
  \]
Ghost Forces

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

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

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

$$\left. \frac{\partial \mathcal{E}^{qce}}{\partial y_n} \right|_{y=x} = \frac{\phi'(2)}{2} \times \begin{cases} 
0, & n = \ldots, K - 2 \\
1, & n = K - 1 \\
-1, & n = K \\
1, & n = K + 1 \\
0, & n = K + 3, \ldots
\end{cases}$$
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:** $E = \beta E_a + (1 - \beta) E_c$
   - Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2008)
   - ...
Consistent Energy-Based Coupling

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

$$
\mathcal{E}^{ac}(y) = \sum_{x \in \mathcal{L}_a} V_x + \sum_{x \in \mathcal{L}_i} \tilde{V}_x + \int_{\Omega_c} W(Dy) \, dx
$$

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

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 $y_a \in \arg\min \mathcal{E}_{a}^{\text{tot}}$, $y_{ac} \in \arg\min \mathcal{E}_{ac}^{\text{tot}}$, then

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

3 Steps:

1. **CONSISTENCY:** $\langle \delta\mathcal{E}^{ac}(y_a) - \delta\mathcal{E}^a(y_a), u_h \rangle \lesssim h\|\nabla^2 y_a\|_{L^2(\Omega_c)}\|\nabla u_h\|_{L^2}$

2. **STABILITY:** $\langle \delta^2\mathcal{E}^{ac}(y_a)u, u \rangle \geq C_{\text{stab}}\|\nabla u\|_{L^2}^2$

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

\[ \| \nabla (y_a - y_{ac}) \|_{L^2} \leq \text{Consistency Err} + \text{Coarsening Err} + \text{Truncation Err} \]

\[ \leq \text{Consistency Err} + \| h \nabla^2 \tilde{u}_a \|_{L^2(\Omega_c)} + \| \nabla \tilde{u}_a \|_{L^2(\mathbb{R}^d \setminus B_{R_c/2})} \]

\[ \leq \text{Consistency Err} + N^{-1/2-1/d} + N^{-1/2-1/d} \]

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,
- \( h(x) \sim \left( \frac{|x|}{R_a} \right)^{3/2} \).
Patch Test Consistency $\Rightarrow$ First-order Consistency

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

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

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

- $d = 1$; or
- $d = 2$, $\Omega_a$ connected; [Ortner, 2012] or
- $d = 3$, $\Omega_a$ connected [in progress]

then

$$\langle \delta \mathcal{E}^{ac}(y) - \delta \mathcal{E}^{a}(y), u_h \rangle = \sum_{T \in T} (\Sigma^{ac}(y; T) - \Sigma^{a}(y; T)) : \nabla u_h$$

$$\lesssim \| h \nabla^2 y \|_{L^2(\Omega_c \cup \Omega_i)} \| \nabla u_h \|_{L^2}$$

With the assumption of stability, $\Rightarrow \| \nabla u_a - \nabla u_{ac} \| \sim N^{-1}.$
**Consequence of Patch Test Consistency**

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

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

then $\Sigma_{ac}$ is discrete divergence free.

**Lemma:**

∃ a function $\psi(F, T) \in N_1(\mathcal{T})^2$, such that

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

$N_1(\mathcal{T})$ is Crouzeix–Raviart finite element space,

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

$J \nabla \psi(F; T)$ is divergence free piecewise constant tensor field [Arnold/Falk, Polthier/Preuß].
Construction of Consistent A/C Schemes

\[ \mathcal{E}^{ac}(y_h) = \sum_{x \in L_a} V_x + \sum_{x \in L_i} \tilde{V}_x + \sum_{x \in L_c} V_x^c \]

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

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

\[ \tilde{V}_x = V(\tilde{g}_{x,r}; r \in \mathcal{R}) \]

\[ \tilde{g}_{x,r} = \sum_{s \in \mathcal{R}_x} C_{x,r,s} g_s \]

→ Find \( C_{x,r,s} \) s.t. \( \delta \mathcal{E}^{ac}(y_F) = 0 \) \( \forall F \)
→ geometric conditions only!

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

2d, NN, multibody potential, triangular lattice
Construction of Consistent A/C Schemes

$$\mathcal{E}^{ac}(y_h) = \sum_{x \in \mathcal{L}_a} V_x + \sum_{x \in \mathcal{L}_i} \tilde{V}_x + \sum_{x \in \mathcal{L}_c} V^c_x$$

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

General Construction: \cite{1D, Shimokawa et al, 2004; E/Lu/Yang, 2006}

1. Local Energy Consistency
   $$\tilde{V}(y_F) = V(y_F)$$

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

2. Patch Test Consistency
   $$0 = \langle \delta \mathcal{E}^{ac}(y_F), u \rangle$$
   $$= \sum_{x \in \mathcal{L}} \sum_{r \in \mathcal{R}} \sum_{s \in \mathcal{R}} V_{F,r} \sum_{s \in \mathcal{R}} C_{x,r,s} D_s u$$
   $$= \sum_{x \in \mathcal{L}} \sum_{r \in \mathcal{R}} \sum_{s \in \mathcal{R}} \sum_{s \in \mathcal{R}} (C_{x-a,s,r,s} V_{F,r} - C_{x,a,s} D_r V_{F,r}) u(x)$$

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

Solve $(a) + (b) + \text{B.C.}$ in $\mathcal{L}_a$ and $\mathcal{L}_c$ to obtain $C_{x,r,s}$ for $x \in \mathcal{L}_i$.

unknowns: $|I||\mathcal{R}|^2$, eqns: $\leq 5|I||\mathcal{R}|.$
Construction of Consistent A/C Schemes

\[ \mathcal{E}^{ac}(y_h) = \sum_{x \in \mathcal{L}_a} V_x + \sum_{x \in \mathcal{L}_i} \tilde{V}_x + \sum_{x \in \mathcal{L}_c} V^c_x \]

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

**General Construction:**

- **Flat interface**
- **Interface with corner**

\[ C_{x,r,r} \text{ for NN interaction, multibody potential, one-sided construction.} \]
  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

$$\langle \delta \mathcal{E}^{ac}(y) - \delta \mathcal{E}^{a}(y), u_h \rangle = \sum_{T \in \mathcal{T}} (\Sigma_{ac}(y; T) - \Sigma_{a}(y; T)) : \nabla u_h$$

$$\leq C \| h \nabla^2 y \|_{L^2(\Omega_c \cup \Omega_i)} \| \nabla u_h \|_{L^2}$$

The constant $C$ is controlled by $\max_{x \in \mathcal{I}} \left| \sum_{r \in \mathbb{R}} \sum_{s \in \mathbb{R}} |r| |s| C_{x,r,s} \right|$.  
- The coefficients need 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

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

\[
\langle H^{ac}_{Dy} v, v \rangle := \langle \delta^2 \mathcal{E}^{ac}(y) v, v \rangle := \sum_{\xi \in \mathbb{Z}} \sum_{\xi, \varsigma \in \mathcal{R}} \tilde{V}_{\rho \varsigma}(Dy(\xi)) \cdot D_\rho v(\xi) D_\varsigma v(\xi)
\]
Stability of Consistent A/C Coupling Method

- Study the Hessians

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

- Stability constant:

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

We say that $H$ is stable if $\gamma(H) > 0$. 
Stability of Consistent A/C Coupling Method

- Study the Hessians

\[
\langle H_{D_y}^a v, v \rangle := \langle \delta^2 E^a(y) \rangle v, v \rangle := \sum_{\xi \in \mathbb{Z}} \sum_{\xi, \varsigma \in \mathbb{R}} V_{\rho \varsigma}(D\varphi(\xi)) \cdot D\varphi(v)(\xi) D\varsigma(v)(\xi)
\]

\[
\langle H_{D_y}^{ac} v, v \rangle := \langle \delta^2 E^{ac}(y) \rangle v, v \rangle := \sum_{\xi \in \mathbb{Z}} \sum_{\xi, \varsigma \in \mathbb{R}} \tilde{V}_{\rho \varsigma}(D\varphi(\xi)) \cdot D\varphi(v)(\xi) D\varsigma(v)(\xi)
\]

- Stability constant:

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

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

- For homogenous deformation \( y_F \),
  - \( \gamma(H_F^{ac}) \leq \gamma(H_F^a) \) for all \( F > 0 \).
  - \( \gamma(H_F^c) = W''(F) \geq \gamma(H_F^a) \) for all \( \text{det}(F) > 0 \).
Universally Stable Method

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

- universally stable method in 1D

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

$$\mathcal{E}^{\text{fl}}(y) := \mathcal{E}^*(y) + \int_0^\infty W(\nabla y) \, dx,$$

where

$$\mathcal{E}^*(y) := \sum_{\xi = -\infty}^{-1} \left[ V(Dy^*(\xi)) - V(FR) \right] + \frac{1}{2} \left[ V(Dy^*(0)) - V(FR) \right].$$
Universally Stable Method

Question: For any potential $V$, can we find such a A/C scheme, such that $\gamma^\text{ac}_F > 0$ if and only if $\gamma^\text{a}_F > 0$? If exists, such method is called universally stable.

- universally stable method in 1D

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

\[ \mathcal{E}^{\text{rfl}}(y) := \mathcal{E}^*(y) + \int_0^\infty W(\nabla y) \, dx, \quad \text{where} \]

\[ \mathcal{E}^*(y) := \sum_{\xi = -\infty}^{-1} \left[ V(Dy^*(\xi)) - V(FR) \right] + \frac{1}{2} \left[ V(Dy^*(0)) - V(FR) \right]. \]

- 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).

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

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

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Singapore, Feb 13, 2015
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).

$$\mathcal{E}^{stab}(y) := \mathcal{E}^{ac}(y) + \kappa \langle Su, u \rangle,$$

for $y = Fx + u, u \in \mathcal{W}_0'$, where

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

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Tradeoff of Stabilization: Consistency vs. Stability

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

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

$$
\gamma(H^a_F) - \frac{c_1}{\kappa^2} \leq \gamma(H^{ac}_F + \kappa S) \leq \gamma(H^a_F) - \frac{c_2}{\kappa^2}.
$$

- existence of a critical loading parameter $t_{\kappa}^* \in [t_0, t_*)$ for which $\gamma(H^{ac}_{t_{\kappa}^* I} + \kappa S) = 0$ 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

\[ B := \begin{pmatrix} 1 + s & \gamma_{II} \\ 0 & 1 + s \end{pmatrix} \cdot F_0. \]

where \( F_0 \propto I \) minimizes \( W \), \( s = \gamma_{II} = 0.03. \)
Numerical Experiment

ATM: full atomistic model is minimized with the constraint $y = y_B$ in $\mathcal{L} \setminus \Omega$
**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)*.
GRAC: two variants METHOD 1, METHOD 2 with both least squares solution and $\ell^1$-minimisation to solve for the reconstruction parameters, and with stabilisation parameters $\kappa = 0, 1$. The resulting methods are denoted by $M_i-L_p-S_\kappa$, 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.

\[ E^a(u) := \sum_{a \in \mathcal{L}} V'_a(u), \]

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)

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

\[ \mathcal{E}^a(u) = \sum_{a \in \mathcal{L}} V'_a(u) - \sum_{a \in \mathcal{L}^\text{hom}} \langle \delta V_a^\text{hom}(x), u \rangle \]

\[ = \sum_{a \in \mathcal{L}} V''_a(u) + \langle \mathcal{L}^\text{ren}, u \rangle, \]

where

\[ V''_a(u) := V_a(x + u) - V_a(x) - \langle \delta V_a(x), u \rangle, \]

\[ \langle \mathcal{L}^\text{ren}, u \rangle := \sum_{a \in \mathcal{L}^\text{def}} \langle \delta V_a(x), u \rangle - \sum_{a \in \mathcal{L}^\text{hom}_\text{def}} \langle \delta V_a^\text{hom}(x), u \rangle. \]
Define the BQCE energy functional

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

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

The BQCE problem is to compute

\[ u^b_h \in \arg \min \{ E^b(v_h) \mid v_h \in U_h \}. \quad (1) \]
**BQCE Energy Functional**

Define the BQCE energy functional

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\mathcal{E}^b(u_h) := \sum_{a \in \mathcal{L} \cap \Omega_h} (1 - \beta(a)) V'_a(u) + \int_{\Omega_h} Q_h [\beta W'(\nabla u_h)].
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The BQCE problem is to compute

\[
u^b_h \in \arg \min \{ \mathcal{E}^b(v_h) \mid v_h \in \mathcal{U}_h \}. \tag{1}
\]

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

\[
\| \nabla u^b_h - \nabla \tilde{u}^a \|_{L^2} \leq C_1 \| \nabla^2 \beta \|_{L^2} + C_2 \left( \| \beta h \nabla^2 \tilde{u}^a \|_{L^2(\Omega_h)} + \| \nabla \tilde{u}^a \|_{L^2(\mathbb{R}^d \setminus B_{R^c/2})} \right) + \ldots
\]

\[
\leq C_1 N^{\frac{1}{2} - \frac{2}{d}} + C_2 N^{-\frac{1}{2} - \frac{1}{d}} \leq C_1 N^{\frac{1}{2} - \frac{2}{d}}
\]

by choosing \( R_b \simeq R_a \).
BGFC Formulation

The BGFC energy is defined as

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

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

\[ C_1'' \lesssim C \| \nabla \tilde{u}^a \|_{L^\infty(\mathbb{R}^d \setminus B_{R^a - 2r_{\text{cut}}})} \lesssim (R^a)^{-d}. \]

and the ghost force error becomes

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

best approximation error

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

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

\[ \| \nabla u_{h}^{\text{bg}} - \nabla \tilde{u}^a \|_{L^2} \lesssim N^{-\frac{1}{2} - \frac{1}{d}}. \]
BGFC Formulation

The BGFC energy is defined as

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

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

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

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

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

can be balanced with ghost force error.

Optimal error estimate can be achieved by taking \( R^c \approx (R^a)^{1 + \frac{4}{d}}. \)

\[ \| \nabla u^{bg, P2} - \nabla \bar{u}^a \|_{L^2} \lesssim N^{-\frac{1}{2} - \frac{2}{d}}. \]
Connection to Ghost-Force Correction

We have

\[ \mathcal{E}^{bg}(u_h) = \mathcal{E}^b(u_h) - \sum_{a \in \mathcal{L}} (1 - \beta(a)) \langle \delta V_a(0), u_h \rangle - \int_{\mathbb{R}^d} Q_h [\beta \partial W(0) : \nabla u_h] \, dx \]

\[ = \mathcal{E}^b(u_h) - \langle \delta \mathcal{E}^b(0), u_h \rangle \]

\[ = \mathcal{E}^b(u_h) - \langle \delta \mathcal{E}^b(0) - \mathcal{F}^{bqcf}(0), u_h \rangle, \]

The renormalisation step \( V'_a \leadsto V'' \) 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

$$ E^{bg}(u_h) = E^b(u_h) - \sum_{a \in \mathcal{L}} (1 - \beta(a)) \langle \delta V_a(0), u_h \rangle - \int_{\mathbb{R}^d} Q_h [\beta \partial W(0) : \nabla u_h] \, dx $$

$$ = E^b(u_h) - \langle \delta E^b(0), u_h \rangle $$

$$ = E^b(u_h) - \langle \delta E^b(0) - \mathcal{F}^{bqcf}(0), u_h \rangle, $$

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) $\hat{u}_h$.

$$ E^{bg}(u_h) := E^b(u_h) - \langle \delta E^b(\hat{u}_h) - \mathcal{F}^{bqcf}(\hat{u}_h), u_h - \hat{u}_h \rangle, $$
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 $y^{\text{lin}}(a) = \frac{1}{2\pi} \text{arg}(a - \hat{a})$

- Renormalized potential:
  $$V^1(u) = V(y^{\text{lin}} + u) - V(y^{\text{lin}})$$
  Apply consistent (cs) method to $V^1$, 
  $$\|\nabla u^a - \nabla u^{cs}\|_{L^2} \leq N^{-3/4}$$
linear elasticity solution \( y^{\text{lin}}(a) = \frac{1}{2\pi} \arg(a - \hat{a}) \)

- **Renormalized potential:**
  \[ V^1(u) = V(y^{\text{lin}} + u) - V(y^{\text{lin}}) \]

  Apply consistent (cs) method to \( V^1 \),

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

- **Another Renormalized potential:**
  \[ V^2(u) = V(y^{\text{lin}} + u) - V(y^{\text{lin}}) - \langle \delta V(0), u \rangle \]

  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 \( y^{\text{lin}}(a) = \frac{1}{2\pi} \arg(a - \hat{a}) \)

- Renormalized potential:
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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'.
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- Consistent energy coupling has optimal accuracy \( O(N^{-1}) \),
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Ongoing Work

- 3D arbitrary crystal,
- a posteriori error estimate and adaptive methods,
- dislocation, cracks, nano-indentation, ...
- Implementation, benchmarks, applications
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- Consistent energy coupling has optimal accuracy $O(N^{-1})$,
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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!