Construction and Analysis of Consistent Atomistic/Continuum Coupling Methods

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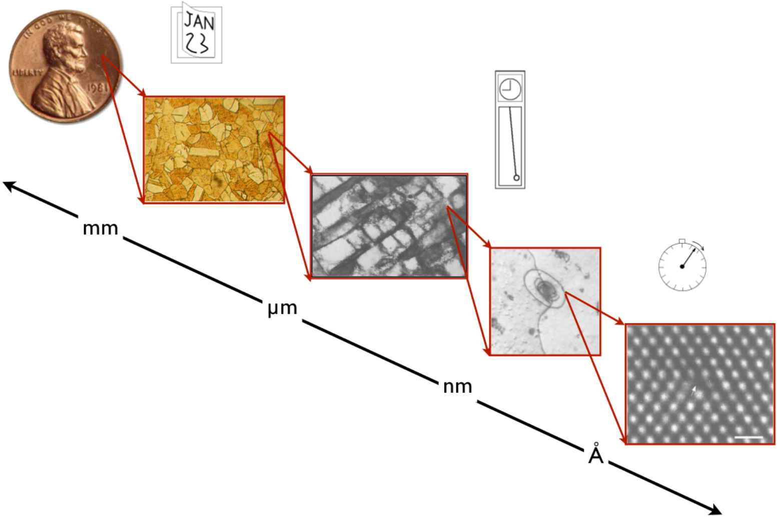
Outline

In this talk, we will focus on multiscale methods for 2D/3D point defects at 0T, namely, the coupling of length scales.

- Introduction
  - Multiscales in Materials & Crystalline Defects
  - Atomistic Simulation & Its Continuum Coarse Graining
  - Atomistic/Continuum Coupling
  - Issue of Patch Test Consistent (Ghost Force)
- Construction of Consistent Method
  - Overview
  - First Order Consistency
  - Construction
  - Numerical Experiment
  - Optimized construction
- Stability
  - Overview
  - Universally Stable Method
  - Stability Gap and Stabilization
  - Balance between Consistency and Stability
- Outlook

Multiple Scales in Materials



[Modeling Materials, Tadmor & Miller 2012]

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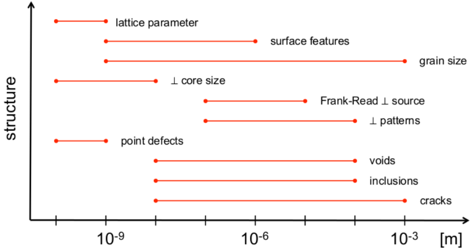
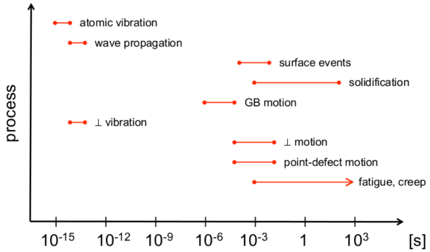




Structural features:

- range in size from 10^{-10} to 10^{-3} m
- interact atomistically at short distances and over long distances via long-range elastic stress fields.

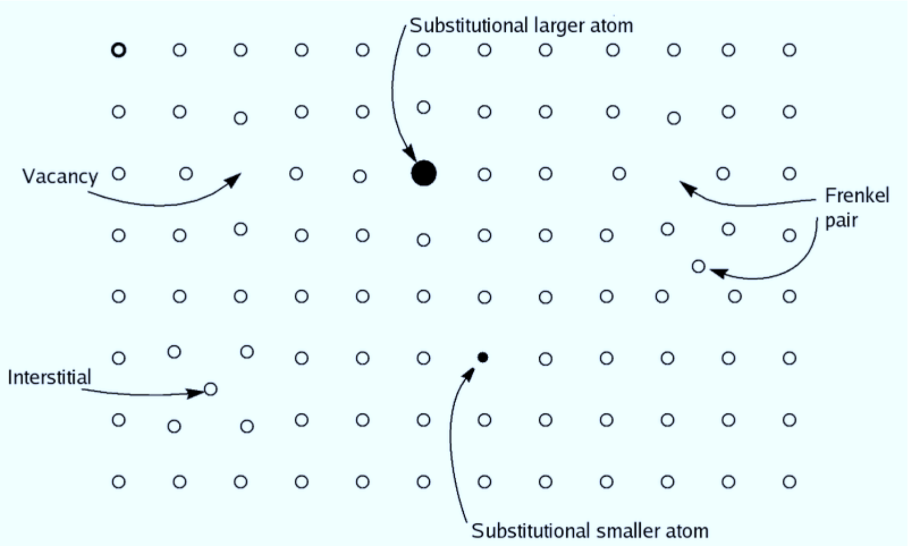
Materials processes:

- occur over time scales ranging from 10^{-15} to years.
- this broad range can sometimes be an asset when scale separation occurs.

Modeling material behavior requires methods able to span across length and time scales.

[Modeling Materials, Tadmor & Miller 2012]

Point Defects in 2D



[Wikipedia]

Atomistic Mechanics (0T statics)

- **Atomistic body**: N atoms at positions $y = (y_n)_{n=1}^N \in \mathbb{R}^{d\times N}$
- **Total energy** of configuration y:

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

  - $\mathcal{E}^{\rm a}$ = interaction energy, $\mathscr{P}_{\rm a}$ = potential of external frcs, V = multi-body interaction potential

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

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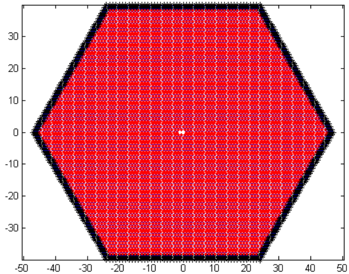
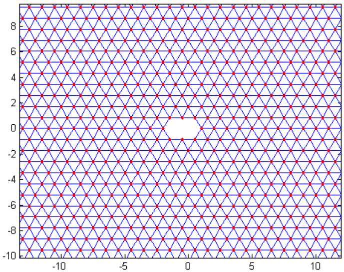




Example: microcrack

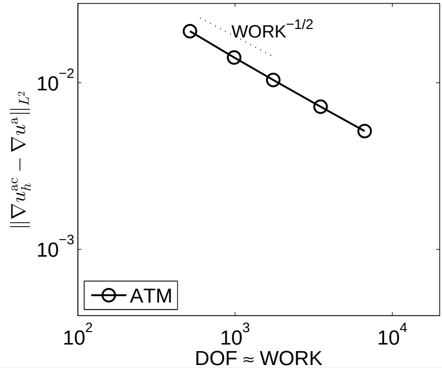
Atomistic Simulation

microcrack under macroscopic shear/stretch, EAM potential

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

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

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



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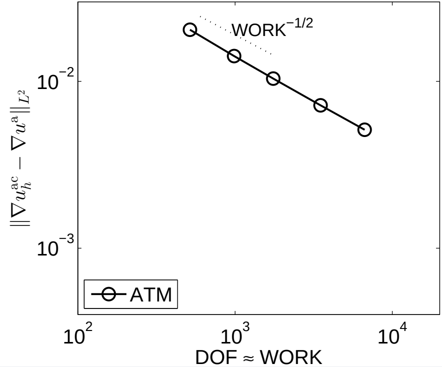

Can we find a better method, e.g., accuracy scales $O(N^{-1})$?

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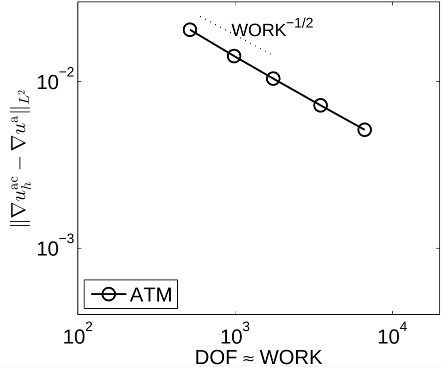

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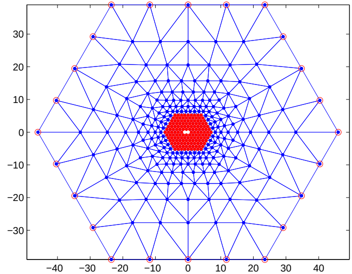
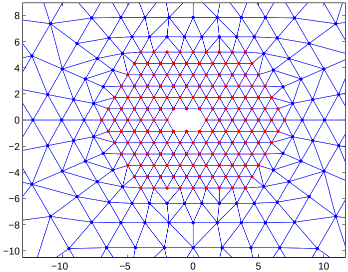
Idea

- Coarse grainning the DoF.

Coarse Graining: Adaptive FEM





- $\|\nabla y_a - \nabla y_h \leq \|h\nabla^2 y_a\|_{\Omega\setminus\Omega_{\mathrm{a}}}$ [Lin, Ortner/Süli, Lin/Shapeev, . . .]

But complexity to evaluate $\mathcal{E}^{\mathrm{a}}|_{\mathscr{Y}_h}$, $\delta\mathcal{E}^{\mathrm{a}}|_{\mathscr{Y}_h}$ is still $O(N)$!

Coarse Graining: Cauchy–Born Approximation

Atomistic Stored Energy:

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

Cauchy–Born Stored Energy:

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

Theorem: [2007, E/Ming]

Let $y_{\rm a} \in \operatorname{argmin} \mathcal{E}_{\rm a}^{\rm tot}$ be "sufficiently smooth globally", then there exists $y_{\rm c} \in \operatorname{argmin} \mathcal{E}_{\rm c}^{\rm tot}$ such that

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

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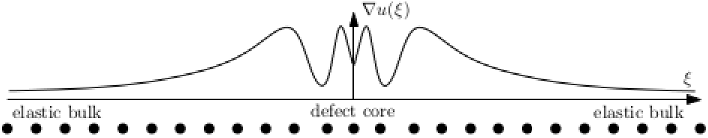
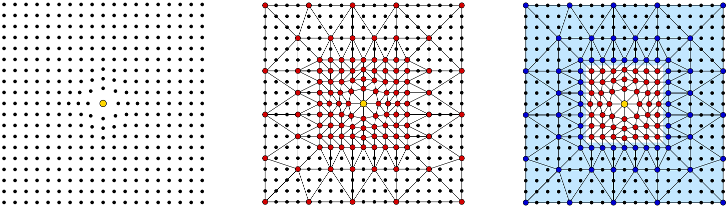
- If there are no defects, then the Cauchy–Born model is a highly accurate continuum approximation, $\|y_{\mathrm{a}} - y_{\mathrm{c}}\|_{H^1} \sim N^{-2}$.
- If there are defects, then the Cauchy-Born model has $O(1)$ error.



[2012, Ortner & Luskin]

Atomistic/Continuum Coupling: First Attempt



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

[Tadmor, Ortiz, Philips 1996]

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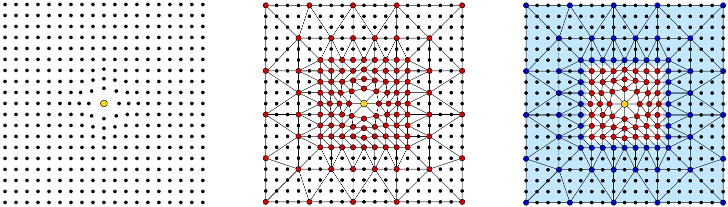

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[Tadmor, Ortiz, Philips 1996]

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

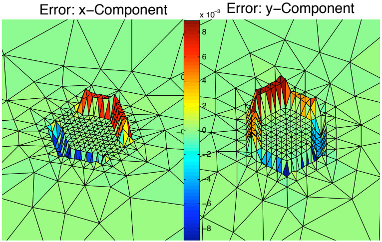
$$\delta\mathcal{E}^{\mathrm{a}}(y_{\mathsf{F}}) = 0$$

and

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

but

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



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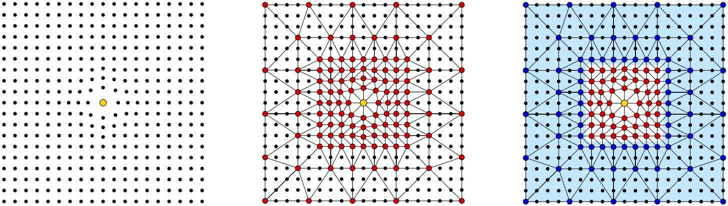

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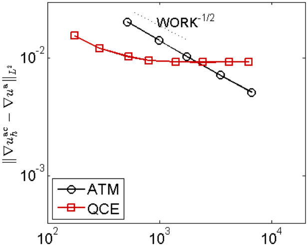


A 1D Model Problem

- Periodic displacements:

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

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

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

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

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

- Continuum finite element model

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

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

The Energy-Based Quasicontinuum Method

- Choose atomistic and continuum regions:

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

- Define a/c hybrid energy

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

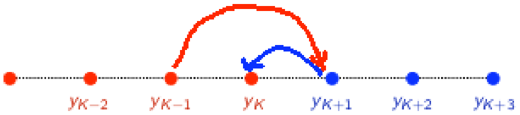
Ghost Forces

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:** $E = \chi E_a + (1 - \chi)E_c$
   - Belytschko & Xiao (2004)
   - Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2008)
   - . . .
4. **Quadrature approaches**
   - Knapp, Ortiz, Gunzburger, . . .

Consistent Energy-Based Coupling

Problem: "... the disadvantage of the energy based approach is that it is extremely difficult to eliminate the non-physical side effects of the coupled energy functional, dubbed 'ghost forces'."

– Tadmor & Miller, 2009

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

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

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

Questions:

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

A Priori Error Analysis

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

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

3 Steps:

1. CONSISTENCY: $\langle\delta\mathcal{E}^{\rm ac}(y_a) - \delta\mathcal{E}^{\rm a}(y_a), u_h\rangle \lesssim h\|\nabla^2 y_{\rm a}\|_{\rm L^2(\Omega_c)}\|\nabla u_h\|_{L^2}$
2. STABILITY: $\langle\delta^2\mathcal{E}^{\rm ac}(y)u, u\rangle \geq C_{\rm stab}\|\nabla u\|_{\rm L^2}^2$
3. REGULARITY: bounds on $\nabla^2 y_{\rm a}$, note that r^{-a} for defects ($a = 2$ dislocations, $a = 3$ vacancy)

Numerical Analysis Literature on A/C Coupling

cf 'Atomistic-to-Continuum Coupling', Acta Numerica (2013), Luskin/Ortner

Analysis for Energy-Based Coupling:

- 1D
  - NN, variational analysis: [Blanc/LeBris/Legoll, 2005]
  - Error estimates for QCE and QNL: [Dobson/Luskin, 2009], [Ming/Yang, 2010], [Ortner, 2010], [Ortner/Wang, 2011], [Li/Luskin, 2011
  - Sharp Stability Analysis, Linear Regime: [Dobson/Luskin/Ortner, 2010]
  - blending methods: [Luskin/van Koten, 2012]
- 2D, pair interactions, defects: [Ortner/Shapeev, 2012]
- 2D, first order consistency for general finite-range interactions: [Ortner, 2012]
- 3D, pair interactions: [Shapeev, 2012]
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Analysis for Force-based Coupling:

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Analysis for Multi-Lattices:

Dobson/Elliott/Luskin/Tadmor (2007); Abdulle/Lin/Shapeev (2011, 2012)

Patch Test Consistency implies First-order Consistency?

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

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

"Theorem:" [First-order Consistency]

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

- $d = 1$; or
- $d = 2$, Ω_{a} connected; [Ortner, 2012] or
- $d = 3$, Ω_{a} connected [LZ, 2013]

then

$$\langle \delta\mathcal{E}^{\mathrm{ac}}(y) - \delta\mathcal{E}^{\mathrm{a}}(y), u_h \rangle \lesssim \| h\nabla^2 y\|_{\mathrm{L}^2(\Omega_{\mathrm{c}}\cup\Omega_{\mathrm{i}})} \|\nabla u_h\|_{\mathrm{L}^2}$$

With the assumption of stability, $\|y_{\mathrm{a}} - y_{\mathrm{ac}}\| \sim N^{-1}$.

Consequence of Patch Test Consistency

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

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

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

Lemma:

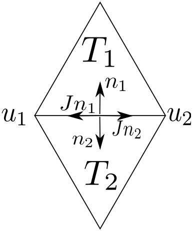
$\exists$ a function $\psi({\sf F}, T) \in {\rm N}_1(\mathscr{T})^2$, such that

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

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

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

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



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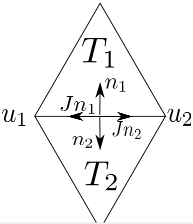
- For general deformation y, deformation gradient average for patch $\omega_f = (T_1 \cup T_2)$, $\mathsf{F}_f(y) = ⨍_{\omega_f} \nabla y \, \mathrm{d}x$,
  Corrector function: $\hat{\psi}(y; \cdot) = \sum_{f\in\mathscr{F}} \psi\big(\mathsf{F}_f(y); m_f\big)\zeta_f$
- Define the 'modified' stress function,

$$\widehat{\Sigma}_{\mathrm{ac}}(y; T) := \Sigma_{\mathrm{ac}}(y; T) - \mathsf{J}\nabla\hat{\psi}(y; T), \qquad \text{for } T \in \mathscr{T}.$$

  - $\widehat{\Sigma}_{\mathrm{ac}}(y_{\mathsf{F}}; T) = \partial W(\mathsf{F}) = \Sigma_{\mathrm{a}}(y_{\mathsf{F}}; T)$



Construction of Consistent A/C Schemes

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

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

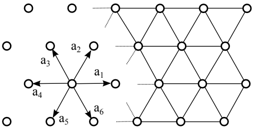
General Construction: [1D, Shimokawa et al, 2004; E/Lu/Yang, 2006]

$$\tilde V_x = V\big(\tilde g_{x,r}; r \in \mathscr{R}\big)$$

$$\tilde g_{x,r} = \textstyle\sum_{s\in\mathscr{R}_x} C_{x,r,s} g_s$$

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

→ geometric conditions only!



2d, NN, multibody potential, triagular lattice

- Explicit constructions for 2D general interface: [Ortner/LZ; SINUM, 2012]
- **In general: compute $C_{x,r,s}$ numerically in preprocessing**

Construction of Consistent A/C Schemes

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

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

→ geometric conditions only!

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

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

2. Patch Test Consistency

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

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

Solve (a) + (b) + B.C. in $\mathscr{L}_{\rm a}$ and $\mathscr{L}_{\rm c}$ to obtain $C_{x,r,s}$ for $x \in \mathscr{L}_{\rm i}$.
unknowns: $|\mathscr{L}_{\mathcal{I}}||\mathscr{R}|^2$, eqns: $|\mathscr{L}_{\mathcal{I}}|(2|\mathscr{R}|+3)$.

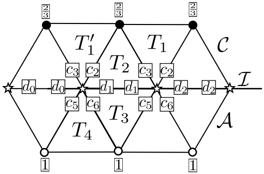
Construction of Consistent A/C Schemes

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

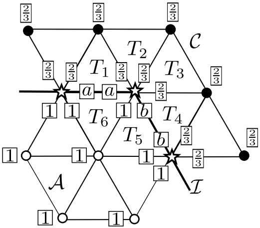
Construct $\tilde{V}$ s.t. $\delta\mathcal{E}^{\rm ac}(y_{\mathsf{F}}) = 0$ for all $\mathsf{F} \in \mathbb{R}^{d\times d}$.

General Construction:

Flat interface



Interface with corner



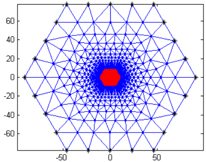
$C_{x,r,r}$ for NN interaction, multibody potential, one-sided construction.

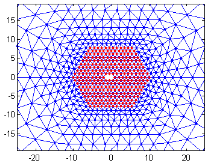
1. works for general interface in 2d
2. preprocessing for longer interaction range

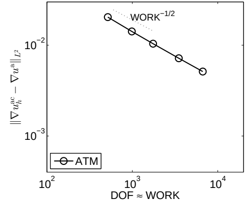
Numerical Experiment

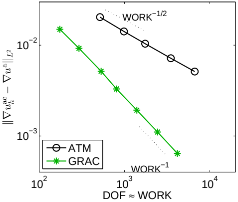
Test Problem: microcrack in the triangular lattice, EAM multi-body potential

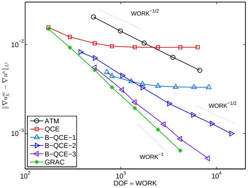
$$V = F_\alpha\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}(r_{ij})$$





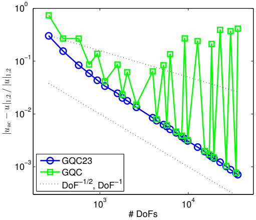


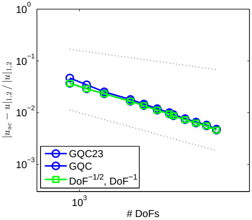




Optimization of the Reconstruction Coefficients

[Ortner/LZ, 2013]



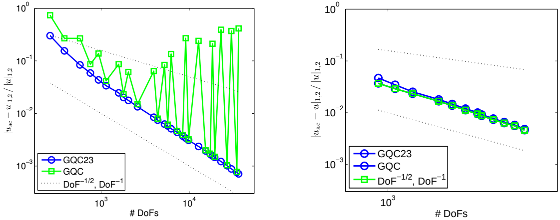


Left: H^1 Error with coefficients from least square solution
Right: H^1 Error with coefficients from L^1 minimization

- The coefficients needs to be pre-computed for longer range interactions, also needs to be optimized for better accuracy.

Optimization of the Reconstruction Coefficients

[Ortner/LZ, 2013]



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

- Consistency Error Estimate

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

$$\leq C \|h\nabla^2 y\|_{\mathrm{L}^2(\Omega_{\mathrm{c}}\cup\Omega_{\mathrm{i}})} \|\nabla u_h\|_{\mathrm{L}^2}$$

  The constant C is controled by $\sum_{r\in\mathbb{R}} \sum_{s\in\mathbb{R}} |r||s| C_{x,r,s}$.
- The coefficients can be obtained by solving a constrained L^1 minimization problem.

Stability of Consistent A/C Coupling Method

[Ortner/Shapeev/LZ, 2013]

- Study the Hessians

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

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- Stability constant:

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

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

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

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

Universally Stable Method

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

- universally stable method in 1D

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

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

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

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

Stability Gap and Stabilization

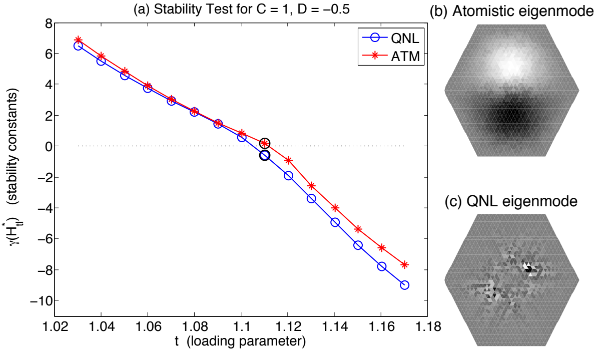

Figure : Stability test for $C = 1, D = -0.5$. The black circles indicate which eigenmodes (u_1-component) are plotted in (b, c).

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

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

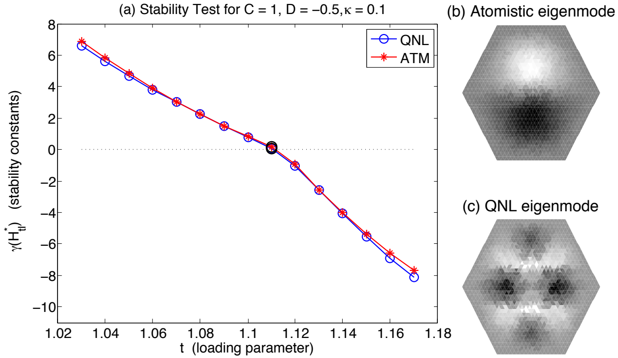

Figure : Stability test for $C = 1, D = -0.5, \kappa = 0.1$. The black circles indicate which eigenmodes (u_1-component) are plotted in (b, c).

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

where

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

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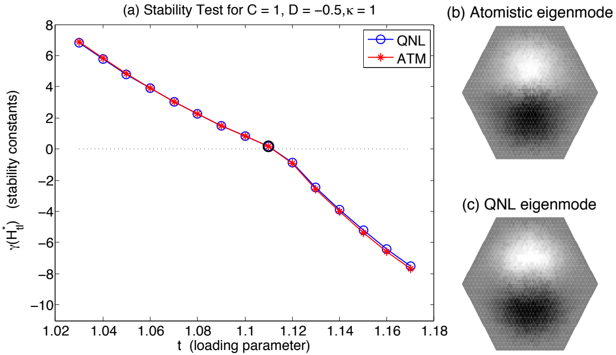

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Stablization: Consistency vs. Stability

"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

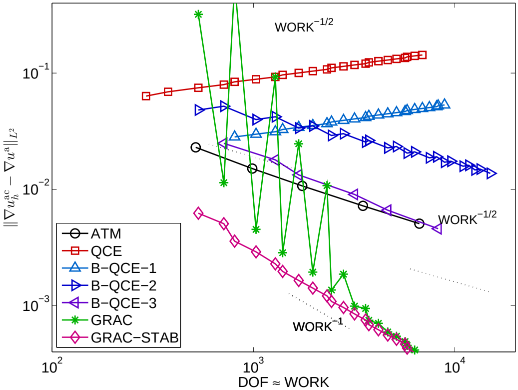
$$\gamma(H_{\mathsf{F}}^{\mathrm{a}}) - \frac{c_1}{\kappa^2} \leq \gamma(H_{\mathsf{F}}^{\mathrm{ac}} + \kappa S) \leq \gamma(H_{\mathsf{F}}^{\mathrm{a}}) - \frac{c_2}{\kappa^2}.$$

- 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 $O(N^{1/2})$.

Recipe for General Interaction Range



GRAC-STAB =

Geometric Reconstruction +

L^1 Minimization +

Stabilization

2nd nearest neighbor EAM potential

Outlook

Summary

- Consistent energy based method has accuracy $O(N^{-1})$
- Construction of consistent energy-based a/c methods
- Stability of consistent energy-based a/c methods

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- 3D
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Major Open Problems

- A/C methods for multi-lattices
- A/C methods for Coulomb interaction
- A/C methods for electronic structure models
- A/C methods for molecular dynamics

Thanks for Your Attention!

The Force-based Approach

A possible solution are **force-based a/c methods:**

- Dead-load GF removal: Shenoy, Miller, Rodney, Tadmor, Phillips, Ortiz (1999)
- FeAt: Kohlhoff, Schmauder, Gumbsch (1989, 1991)
- AtC: Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2007, . . .)
- CADD: Shilkrot & Curtin & Miller (2002, . . .)
- Adaptive Resolution MD: Delle Site et al. (2007, . . .)
- Brutal Force Mixing: Bernstein, Csanyi et al. (2007, . . .)
- . . . . . .
- Analysis: Dobson & Luskin (2008); Ming (2009); Dobson & Luskin & Ortner (2009, 2010, 2010); Makridakis & Ortner & Süli (2010, preprint); Dobson & Ortner & Shapeev (preprint), Lu & Ming (manuscript)

Consistency

Numerical Analysis Literature on Energy-Based Coupling:

- 1D, NN, variational analysis: [Blanc/LeBris/Legoll, 2005]
- 1D, Error estimates for QCE and QNL: [Dobson/Luskin, 2009], [Ming/Yang, 2010], [Ortner, 2010], [Ortner/Wang, 2011]
- 1D, Sharp Stability Analysis, Linear Regime: [Dobson/Luskin/Ortner, 2010]
- 1D, finite range: [Li/Luskin, preprint]
- 1D, EAM potentials: [Li/Luskin, 2011]
- 1D, blending methods: [Luskin/van Koten, preprint]
- 2D, pair interactions, defects: [Ortner/Shapeev, preprint]
- 2D, NN interactions: [Ortner/Zhang, manuscript]
- 2D, consistency for general finite-range interactions: [Ortner, preprint]

Cauchy–Born Approximation

Atomistic Stored Energy:

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

Cauchy–Born Stored Energy:

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

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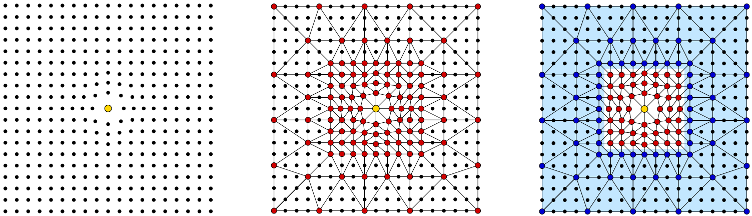
Theorem: [Similar to result by E/Ming; 2007]

Let $y_{\rm a} \in \operatorname{argmin} \mathcal{E}_{\rm a}^{\rm tot}$ be "sufficiently smooth globally", then there exists $y_{\rm c} \in \operatorname{argmin} \mathcal{E}_{\rm c}^{\rm tot}$ such that

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

If there are no defects, then the Cauchy–Born model is a highly accurate continuum approximation.

Atomistic/Continuum Coupling: First Attempt



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

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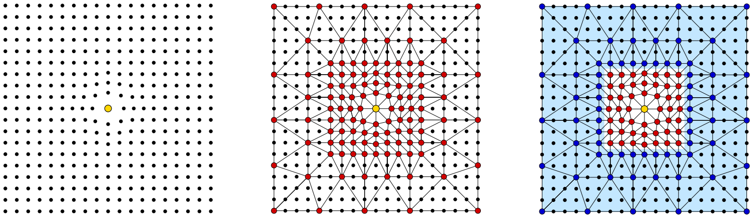

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Fails the **patch test**:

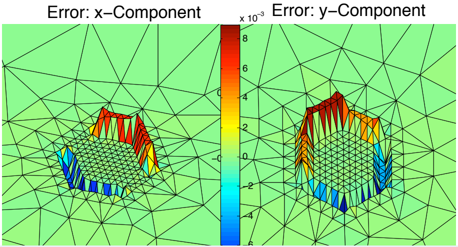
$$\delta\mathcal{E}^{\rm a}(y_{\sf F}) = 0$$

and

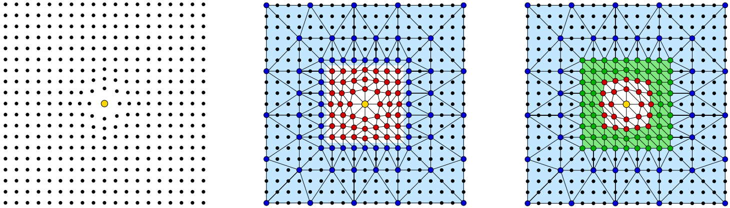
$$\delta\mathcal{E}^{\rm c}(y_{\sf F}) = 0,$$

but

$$\delta\mathcal{E}^{\rm qce}(y_{\sf F}) \neq 0 \text{ !}$$



A/C Coupling: Interface Correction



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

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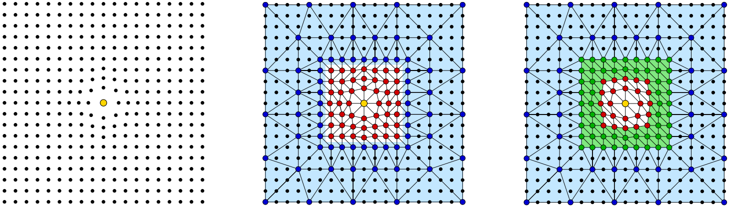


$$\mathcal{E}^{\rm ac}(y_h) = \sum_{x\in\mathscr{L}_{\rm a}} V_x + \sum_{x\in\mathscr{L}_{\rm i}} \tilde{V}_x + \int_{\Omega_{\rm c}} W(\nabla y_h)\,{\rm d}x$$

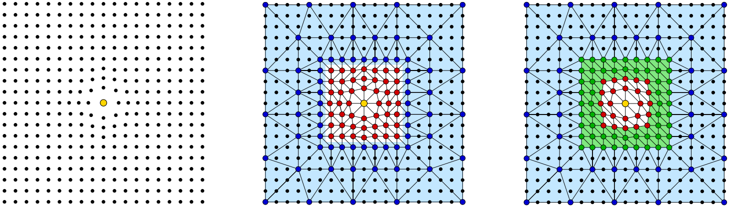
Construct $\tilde{V}$ s.t. $\delta\mathcal{E}^{\rm ac}(y_{\sf F}) = 0$ for all $\mathsf{F} \in \mathbb{R}^{d\times d}$.

Main Challenges:

- **Construction** of patch test consistent $\mathcal{E}^{\rm ac}$: still largely unsolved

  [Shimokawa et al; 2004], [E/Lu/Yang; 2006], [Shapeev; preprint], [Iyer/Gavini; preprint], [Ortner/Zhang; preprint], [Xiao/Belytschko, 2004], [Klein/Zimmermann, 2006], . . .

A/C Coupling: Interface Correction



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

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

Main Challenges:

- **Construction** of patch test consistent $\mathcal{E}^{\mathrm{ac}}$: still largely unsolved
  [Shimokawa et al; 2004], [E/Lu/Yang; 2006], [Shapeev; preprint], [Iyer/Gavini; preprint], [Ortner/Zhang; preprint], [Xiao/Belytschko, 2004], [Klein/Zimmermann, 2006], ...
- **Accuracy:** Does passing the patch test imply "good" accuracy?

Consisency of The Schemes

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

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

$$\tilde{V}_x = V\big(\tilde{g}_{x,r}; r \in \mathscr{R}\big)$$

$$\tilde{g}_{x,r} = \textstyle\sum_{s\in\mathscr{R}_x} C_{x,r,s} g_s$$

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

$\to$ geometric conditions only!

Theorem: [Ortner/Zhang, '11]

There exists a constant C that depends only on $M_2(V)$ and $M_3(V)$ such that

$$\|\delta\mathcal{E}^{\mathrm{ac}}(y) - \delta\mathcal{E}^{\mathrm{a}}(y)\|_{\mathscr{U}^{-1,p}} \le C\big(\|D^3y\|_{\ell^p(\Omega_{\mathrm{c}})} + \|D^2y\|^2_{\ell^{2p}(\Omega_{\mathrm{c}})} + \|D^2y\|_{\ell^p(\Omega_{\mathcal{I}})}\big)$$

Outlook on A/C Methods

Summary

- Ghost force removal ⇒ Patch test consistency ⇒ consistency
- Construction of practical energy-based a/c methods
- Sharp consistency error estimates through stress based formulation

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Open Problems

- Stability
- A/C coupling at surfaces
- Implementation, benchmarks, applications

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Major Open Problems

- A/C methods for multi-lattices
- A/C methods for Coulomb interaction
- A/C methods for electronic structure models (done only for insulators)
- A/C methods for molecular dynamics

Consequence of Patch Test Consistency

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

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

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

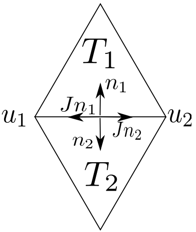
Lemma:
$\exists$ a function $\psi({\sf F}, T) \in {\rm N}_1(\mathscr{T})^2$, such that

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

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

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

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



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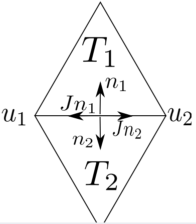
- For general deformation y, deformation gradient average for patch $\omega_f = (T_1 \cup T_2)$, ${\sf F}_f(y) = ⨍_{\omega_f} \nabla y \,{\rm d}x$,
  Corrector function: $\hat\psi(y; \cdot) = \sum_{f\in\mathscr{F}} \psi\big({\sf F}_f(y); m_f\big)\zeta_f$
- Define the 'modified' stress function,

$$\widehat{\Sigma}_{\rm ac}(y; T) := \Sigma_{\rm ac}(y; T) - {\sf J}\nabla\hat\psi(y; T), \qquad \text{for } T \in \mathscr{T}.$$

  - $\widehat{\Sigma}_{\rm ac}(y_{\sf F}; T) = \partial W({\sf F}) = \Sigma_{\rm a}(y_{\sf F}; T)$



Consisency of The Schemes

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

"Theorem:" [Ortner/Zhang]

There exists a constant C that depends only on $M_2(V)$ and $M_3(V)$ such that

$$\big\|\delta\mathcal{E}^{\mathrm{ac}}(y) - \delta\mathcal{E}^{\mathrm{a}}(y)\big\|_{\mathscr{U}^{-1,p}} \le C\big(\|\nabla^3 y\|_{\ell^p(\Omega_{\mathrm{c}})} + \|\nabla^2 y\|^2_{\ell^{2p}(\Omega_{\mathrm{c}})} + \|\nabla^2 y\|_{\ell^p(\Omega_{\mathcal{I}})}\big).$$

Proof of Consistency

$$\langle \delta\mathcal{E}^{\mathrm{ac}}(y) - \delta\mathcal{E}^{\mathrm{a}}(y), u\rangle = \sum_{T\in\mathscr{T}} (\Sigma_{\mathrm{ac}}(y;T) - \Sigma_{\mathrm{a}}(y;T)) : \nabla u$$
$$= \sum_{T\in\mathscr{T}} (\widehat{\Sigma}_{\mathrm{ac}}(y;T) - \Sigma_{\mathrm{a}}(y;T)) : \nabla u$$

1. $T \in \Omega_{\mathcal{A}}$, $\widehat{\Sigma}_{\mathrm{ac}}(y;T) = \Sigma_{\mathrm{a}}(y;T)$,
2. $T \in \Omega_{\mathcal{C}}$, $\widehat{\Sigma}_{\mathrm{ac}}(y;T) - \Sigma_{\mathrm{a}}(y;T) = \Sigma_{\mathrm{c}}(y;T) - \Sigma_{\mathrm{a}}(y;T)$, 2nd order consistency
3. $T \in \Omega_{\mathcal{I}}$, Let $y_T = y_{\nabla y(T)}$, we have,

$$\begin{aligned}|\widehat{\Sigma}_{\mathrm{ac}}(y;T) - \Sigma_{\mathrm{a}}(y;T)| &\le |\widehat{\Sigma}_{\mathrm{ac}}(y;T) - \partial W(\nabla y(T))| + |\partial W(\nabla y(T)) - \Sigma_{\mathrm{a}}(y;T)| \\ &= |\widehat{\Sigma}_{\mathrm{ac}}(y;T) - \widehat{\Sigma}_{\mathrm{ac}}(y_T;T)| + |\Sigma_{\mathrm{a}}(y_T;T) - \Sigma_{\mathrm{a}}(y;T)| \\ &\le C\|\nabla y(T) - \nabla y\|_{\ell^\infty} \le C|D^2 y|\end{aligned}$$

$\Rightarrow$

$$\left\|\delta\mathcal{E}^{\mathrm{ac}}(y) - \delta\mathcal{E}^{\mathrm{a}}(y)\right\|_{\mathscr{U}^{-1,p}} \le C\big(\|\nabla^3 y\|_{\ell^p(\Omega_{\mathrm{c}})} + \|\nabla^2 y\|^2_{\ell^{2p}(\Omega_{\mathrm{c}})} + \|\nabla^2 y\|_{\ell^p(\Omega_{\mathcal{I}})}\big).$$