Atomistic/continuum coupling schemes for solids
(a priori error analysis of a prototypical energy-based coupling scheme)

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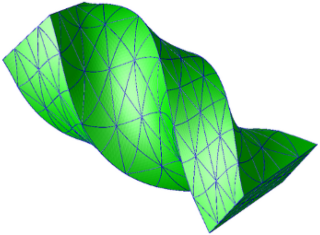
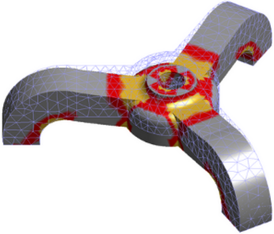
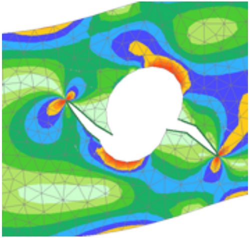
Continuum Solid Mechanics (Elasticity)

- Reference domain $\Omega \subset \mathbb{R}^d$, Deformation $y : \Omega \to \mathbb{R}^d$
- Minimize **stored energy**

$$\min \mathcal{E}^{\mathrm{c}}(y) := \int_\Omega \left[W(Dy) - g \cdot y \right] \mathrm{d}x, \qquad y \in \mathscr{Y}.$$

- Galerkin discretization: choose $\mathscr{Y}_h \subset \mathscr{Y}$, $\dim \mathscr{Y}_h < +\infty$,

$$\min \mathcal{E}^{\mathrm{c}}(y_h), \qquad y_h \in \mathscr{Y}_h.$$

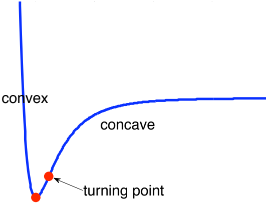
images taken from GETFEM++ website

Atomistic Mechanics

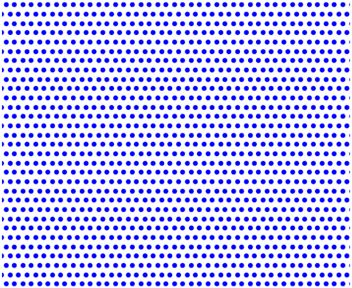
- **Atomistic body** with N atoms at positions $\mathbf{y} = (y_n)_{n=1}^{N} \in \mathbb{R}^{d \times N}$
- **Total energy** of configuration $\mathbf{y}$:

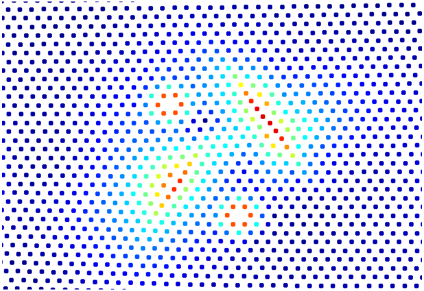
$$\mathcal{E}^{\mathrm{a}}(\mathbf{y}) = \sum_{n \neq k} \phi(|y_n - y_k|) - \langle \mathbf{g}, \mathbf{y} \rangle$$

  - ϕ : Lennard–Jones type potential
  - $\mathbf{g}$: external forces;
    for simplicity assume dead loads



- **Find local minimizer of** $\mathcal{E}^{\mathrm{a}}(\mathbf{y})$ over all admissible configurations $\mathbf{y}$!





Overview

1. **The simplest A/C hybrid energy:**
   - 1D model problem
   - energy-based QC method *(brutal energy mixing)*
   - the problem of ghost forces
   - ghost forces vs. consistency, part 1
2. Energy-based ghost-force removal; Consistency:
   - quasinonlocal QC *(bond-based coupling)*
   - ghost force vs. consistency, part 2 & 3
   - outlook to 2D/3D
3. Stability & Error estimates:
   - abstract framework
   - stability analysis via strain gradients
   - a rigorous error estimates

A 1D Model Problem

Periodic displacements:

$$\mathscr{U} = \{\mathbf{u} = (u_n)_{n\in\mathbb{Z}} : u_{n+N} = u_n, \textstyle\sum_{n=1}^{N} u_n = 0\},$$
$$\mathscr{Y} = \{\mathbf{y} = (y_n)_{n\in\mathbb{Z}} : y_n = x_n + u_n \text{ where } \mathbf{u} \in \mathscr{U}\}.$$

Atomistic energy: *(next-nearest neighbour pair interactions)*

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

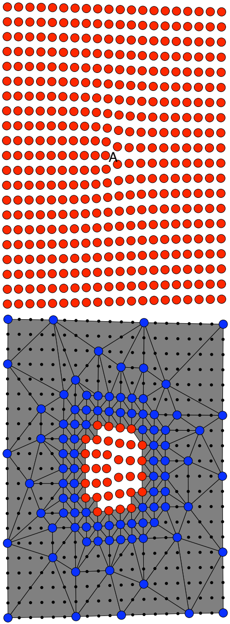
where $\quad \mathcal{E}_n^{\mathrm{a}}(\mathbf{y}) = \frac{1}{2}\{\phi(y_{n-1}' + y_n') + \phi(y_n') + \phi(y_{n+1}') + \phi(y_n' + y_{n+1}')\}.$

Continuum finite element model with $h = \varepsilon$:

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

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

The Energy-Based Quasicontinuum Method

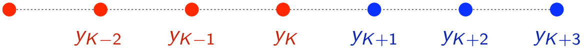


- Choose atomistic and continuum regions:

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

- Define a/c hybrid energy *("brutal energy mixing")*

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



[Tadmor, Miller, Ortiz; 1996]

The Ghost Forces = Patch Test (1)

- $\mathbf{g} = 0 \Rightarrow$ exact solution is the reference lattice: $\mathbf{y}^{\mathrm{a}} = \mathbf{x}$.
- Continuum model is exact here: $\nabla \mathcal{E}^{\mathrm{a}}(\mathbf{x}) = \nabla \mathcal{E}^{\mathrm{c}}(\mathbf{x}) = 0$
- Patch test for $\mathcal{E}^{\mathrm{qc}}(\mathbf{y}) = \varepsilon \sum_{\mathcal{N}^{\mathrm{a}}} \mathcal{E}^{\mathrm{a}}_{\boldsymbol{n}} + \varepsilon \sum_{\mathcal{N}^{\mathrm{c}}} \mathcal{E}^{\mathrm{c}}_{\boldsymbol{n}}$:

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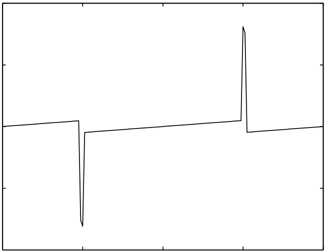
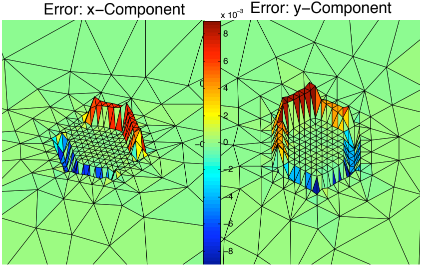
The ghost forces: $\nabla \mathcal{E}^{\mathrm{qc}}(\mathbf{x}) \neq 0$ at the interface

1D:



2D:



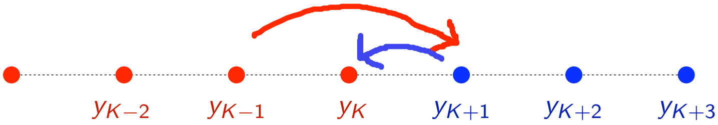
The Ghost Forces = Patch Test (2)

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

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

But if we insert $\mathbf{y}_{\mathrm{a}} = \mathbf{x}$ into $\nabla \mathcal{E}^{\mathrm{qc}}$: ("consistency error")

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



Ghost Force vs. Consistency, Part 1

Theorem

Ghost forces $\Rightarrow$ *high consistency error* $\Rightarrow$ *low accuracy.*

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Theorem

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Proof.

1. Observation: $\nabla_{L^2} = \varepsilon^{-1}\nabla_{\ell^2} = \varepsilon^{-1}\nabla =: \nabla_\varepsilon$
2. Consistency Error = a2c Model Error + Coupling Error
   + ~~Discretization Error~~
3. Insert calculation from previous page:

$$\begin{aligned} & \|\nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}(\mathbf{y}^{\mathrm{a}})\|_{\mathrm{L}^\infty} \sim \varepsilon^{-1} \\ \Rightarrow \quad & \|\nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}(\mathbf{y}^{\mathrm{a}})\|_{\mathrm{W}^{-1,\infty}} \gtrsim 1 \\ \Rightarrow \quad & \|\mathbf{y}^{\mathrm{a}} - \mathbf{y}^{\mathrm{qc}}\|_{\mathrm{W}^{1,\infty}} \gtrsim 1. \end{aligned}$$

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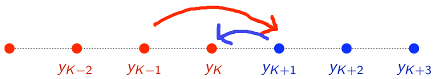
Ghost Force Removal



Observation: ghost forces can arise from asymmetry in the interaction

Idea: concentrate on bonds rather than atoms.

$$\mathcal{E}^{\mathrm{a}}(\mathbf{y}) = \varepsilon \sum_n \phi(y_n') + \varepsilon \sum_n \phi(y_n' + y_{n+1}')$$

$$\mathcal{E}^{\mathrm{c}}(\mathbf{y}) = \varepsilon \sum_n \phi(y_n') + \varepsilon \sum_n \phi(2y_n') = \int W(Dy)\,\mathrm{d}x$$

Here, going from atomistic to continuum can be understood as follows:

$$\phi(y_n' + y_{n+1}') \approx \tfrac{1}{2}\{\phi(2y_n') + \phi(2y_{n+1}')\}$$

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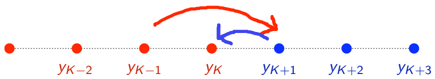

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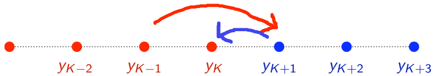
$\leadsto$ **new A/C hybrid energy**:

$$\mathcal{E}^{\mathrm{qc}}(\mathbf{y}) = \varepsilon \sum_n \phi(y_n') + \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{a}}} \phi(y_n' + y_{n+1}') + \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{c}}} \{\tfrac{1}{2}\phi(2y_n') + \tfrac{1}{2}\phi(2y_{n+1}')\}$$

Ghost Force Removal



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$\rightsquigarrow$ **new A/C hybrid energy**:

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$$= \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{a}}} \mathcal{E}_n^{\mathrm{a}} + \int_{\Omega^{\mathrm{c}}} W(Dy)\,\mathrm{d}x + \text{interface correction}$$

Ghost Forces vs. Consistency, Part 2

Easy to check that $\nabla\mathcal{E}^{\rm qc}(\mathbf{x}) = 0$; does this imply higher accuracy?

Theorem

$$\|\nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}) - \nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y})\|_{\mathsf{W}^{-1,p}} \lesssim \varepsilon \|\mathbf{y}''\|_{\mathsf{L}^p(\mathcal{N}^{\rm i})} + \varepsilon^2 \|\mathbf{y}'''\|_{\mathsf{L}^p(\mathcal{N}^{\rm c})} + \varepsilon^2 \|\mathbf{y}''\|^2_{\mathsf{L}^{2p}(\mathcal{N}^{\rm c})}$$

Ghost Forces vs. Consistency, Part 2

Easy to check that $\nabla \mathcal{E}^{\rm qc}(\mathbf{x}) = 0$; does this imply higher accuracy?

Theorem

$$\|\nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}) - \nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y})\|_{\mathsf{W}^{-1,p}} \lesssim \varepsilon \|\mathbf{y}''\|_{\mathsf{L}^p(\mathcal{N}^{\rm i})} + \varepsilon^2 \|\mathbf{y}'''\|_{\mathsf{L}^p(\mathcal{N}^{\rm c})} + \varepsilon^2 \|\mathbf{y}''\|^2_{\mathsf{L}^{2p}(\mathcal{N}^{\rm c})}$$

Proof. Fix $\mathbf{u} \in \mathscr{U}$, bound $\langle \nabla_\varepsilon \mathcal{E}^{\rm a} - \nabla_\varepsilon \mathcal{E}^{\rm qc}, \mathbf{u} \rangle_\varepsilon$ above.

1. Calculate Fréchet derivative

$$\begin{aligned}\langle \nabla_\varepsilon \mathcal{E}^{\rm a} - \nabla_\varepsilon \mathcal{E}^{\rm qc}, \mathbf{u} \rangle_\varepsilon &= \varepsilon \sum_{n \in \mathcal{N}^{\rm c}} \Big\{ \phi'(y_n' + y_{n+1}')[u_n' + u_{n+1}'] \\ &\qquad - \phi'(2y_n')[u_n'] - \phi'(2y_{n+1}')[u_{n+1}'] \Big\} \\ &= \varepsilon \sum_{n \in \mathcal{N}^{\rm c}} T_n u_n' \leq \|T_n\|_{\mathsf{L}^p} \|\mathbf{u}'\|_{\mathsf{L}^{p'}}\end{aligned}$$

2. Estimate T_n using Taylor expansion:

$$T_n = \begin{cases} \phi'(y_{n-1}' + y_n') + \phi'(y_n' + y_{n+1}') - 2\phi'(2y_n'), & n \in \text{interior}(\mathcal{N}^{\rm c}) \\ \phi'(y_n' + y_{n+1}') - \phi'(2y_n'), & n \in \text{a/c interface}. \end{cases}$$

Ghost Forces vs. Consistency, Part 3

Remarks:

1. In 1D these results are generic! In 2D/3D it is unclear whether absence of ghost forces gives improved accuracy.
2. $\varepsilon = h$ is not necessary; analysis can admit general meshes.

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- **Local QC / Cauchy–Born:**

$$\|\nabla_\varepsilon \mathcal{E}^{\mathrm{a}} - \nabla_\varepsilon \mathcal{E}^{\mathrm{c}}\|_{\mathsf{W}_h^{-1,p}} \lesssim \|h\mathbf{y}_{\mathrm{a}}''\|_{\mathsf{L}^p}^2 + \dots$$

- **QCE with ghost force:**

$$\|\nabla_\varepsilon \mathcal{E}^{\mathrm{a}} - \nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}\|_{\mathsf{W}_h^{-1,p}} \lesssim \|h\mathbf{y}_{\mathrm{a}}''\|_{\mathsf{L}^p(\mathcal{N}^{\mathrm{c}})}^2 + \varepsilon\|\mathbf{y}_{\mathrm{a}}''\|_{\mathsf{L}^p(\mathcal{N}^{\mathrm{i}})} + \boldsymbol{\varepsilon}^{\mathbf{1/p}} + \dots$$

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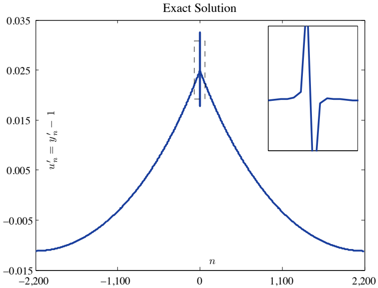
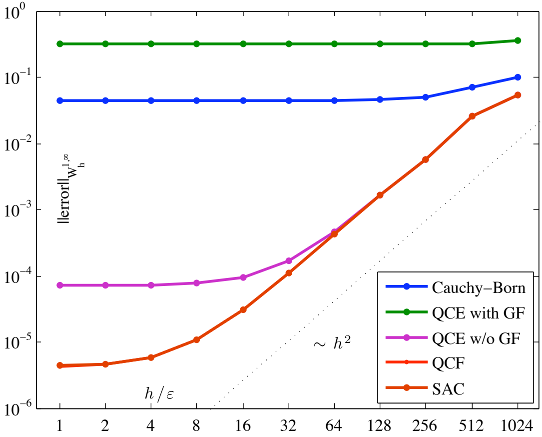
- **Force-based QC:** *(not discussed in this talk)*

$$\|\nabla_\varepsilon \mathcal{E}^{\mathrm{a}} - F^{\mathrm{qc}}\|_{\mathsf{W}_h^{-1,\infty}} \lesssim \|h\mathbf{y}_{\mathrm{a}}''\|_{\mathsf{L}^\infty(\mathcal{N}^{\mathrm{c}})}^2 + \dots$$

1D Numerical Experiment

$N = 1024$, $\phi(r) = \exp(-2\alpha(r-1)) - 2\exp(-\alpha(r-1))$





Extension to 2D

- **Crucial idea in 1D:**

$$\phi(y'_n + y'_{n+1}) \approx \tfrac{1}{2}\big\{\phi(2y'_n) + \phi(2y'_{n+1})\big\} = \frac{1}{2}\int_{x_{n-1}}^{x_{n+1}} \phi(y'(x))\,\mathrm{d}x$$

- **Natural generalization to dD:** identify $\mathbf{y}$ with P1-interpolant $\bar{y}(x)$ then

$$\phi(|y(\xi+\rho) - y(\xi)|) \approx \int_{t=0}^{1} \phi(|Dy(\xi + t\rho)\rho|)\,\mathrm{d}t$$

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- **Construction of QC method:** [Shapeev; preprint]

$$\begin{aligned}
&\sum_{(\xi,\xi+\rho)} \phi(|\bar{y}(\xi+\rho) - \bar{y}(\xi)|) \\
\approx\ &\sum_{(\xi,\xi+\rho)\in\mathcal{B}_{\mathrm{a}}} \phi(|\bar{y}(\xi+\rho) - \bar{y}(\xi)|) + \sum_{(\xi,\xi+\rho)\in\mathcal{B}_{\mathrm{c}}} \int_{t=0}^{1} \phi(|D\bar{y}(\xi+t\rho)\rho|)\,\mathrm{d}t \\
\overset{\mathbf{2D}}{=}\ &\sum_{(\xi,\xi+\rho)\in\mathcal{B}_{\mathrm{a}}} \phi(|\bar{y}(\xi+\rho) - \bar{y}(\xi)|) + \int_{\Omega_{\mathrm{c}}} W(D\bar{y})\,\mathrm{d}x + \text{interface correction}
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- **Consistency error estimate:** [O. & Shapeev; in prep.]

$$\langle \nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}) - \nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y}), \mathbf{u}\rangle \lesssim \Big\{ \inf_{\substack{\tilde{y}\in \mathrm{C}^2 \\ \tilde{y}(\xi)=y_\xi}} \|hD^2\tilde{y}\|_{\tilde{\mathrm{L}}^p(\Omega_{\rm c})} \Big\} \|D\bar{u}\|_{\mathrm{L}^{p'}(\Omega_{\rm c})}$$

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Abstract Framework

Assumptions on an exact solution:

- *Stability:* $\mathbf{y}_{\rm a}$ is a stable equlibrium of $\mathcal{E}^{\rm a}$:

$$\nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}_{\rm a}) = 0 \quad \text{and} \quad \nabla_\varepsilon^2 \mathcal{E}^{\rm a}(\mathbf{y}_{\rm a}) > 0$$

- *Smoothness:* $\mathbf{y}_{\rm a}$ is "smooth" in $\mathcal{N}^{\rm c}$.

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Outline of an Error Analysis:

1. *Consistency:* $\nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}(\mathbf{y}_{\mathrm{a}}) = \nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}(\mathbf{y}_{\mathrm{a}}) - \nabla_\varepsilon \mathcal{E}^{\mathrm{a}}(\mathbf{y}_{\mathrm{a}})$ is small
2. *Stability:* can we prove $\nabla_\varepsilon^2 \mathcal{E}^{\mathrm{qc}}(\mathbf{y}_{\mathrm{a}}) > 0$??
3. Inverse function theorem $\Rightarrow$

$$\exists\ \mathbf{y}_{\mathrm{qc}} \text{ s.t. } \nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}(\mathbf{y}_{\mathrm{qc}}) = 0, \quad \text{and}$$
$$\|\mathbf{y}'_{\mathrm{qc}} - \mathbf{y}'_{\mathrm{a}}\|_{\mathsf{L}^p} \lesssim \|\nabla_\varepsilon \mathcal{E}^{\mathrm{qc}}(\mathbf{y}_{\mathrm{a}}) - \nabla_\varepsilon \mathcal{E}^{\mathrm{a}}(\mathbf{y}_{\mathrm{a}})\|_{\mathsf{W}^{-1,p}}$$

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- *Stability:* $\mathbf{y}_{\rm a}$ is a stable equlibrium of $\mathcal{E}^{\rm a}$:

$$\nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}_{\rm a}) = 0 \quad \text{and} \quad \nabla_\varepsilon^2 \mathcal{E}^{\rm a}(\mathbf{y}_{\rm a}) > 0$$

- *Smoothness:* $\mathbf{y}_{\rm a}$ is "smooth" in $\mathcal{N}^{\rm c}$.

Outline of an Error Analysis:

1. *Consistency:* $\nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y}_{\rm a}) = \nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y}_{\rm a}) - \nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}_{\rm a})$ is small
2. *Stability:* can we prove $\nabla_\varepsilon^2 \mathcal{E}^{\rm qc}(\mathbf{y}_{\rm a}) > 0$?? $<<<$
3. Inverse function theorem $\Rightarrow$

$$\exists\ \mathbf{y}_{\rm qc} \text{ s.t. } \nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y}_{\rm qc}) = 0, \quad \text{and}$$
$$\|\mathbf{y}'_{\rm qc} - \mathbf{y}'_{\rm a}\|_{\mathsf{L}^p} \lesssim \|\nabla_\varepsilon \mathcal{E}^{\rm qc}(\mathbf{y}_{\rm a}) - \nabla_\varepsilon \mathcal{E}^{\rm a}(\mathbf{y}_{\rm a})\|_{\mathsf{W}^{-1,p}}$$

Task: Understand relationship between

$$\alpha^{\rm a}(\mathbf{y}) = \inf_{\|\mathbf{u}'\|_{\mathsf{L}^2}=1} \langle \nabla_\varepsilon^2 \mathcal{E}^{\rm a}(\mathbf{y})\mathbf{u}, \mathbf{u}\rangle \quad \text{and} \quad \alpha^{\rm qc}(\mathbf{y}) = \inf_{\|\mathbf{u}'\|_{\mathsf{L}^2}=1} \langle \nabla_\varepsilon^2 \mathcal{E}^{\rm qc}(\mathbf{y})\mathbf{u}, \mathbf{u}\rangle$$

Hessians & Strain Gradients (1)

Hessian of continuum energy:

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\mathrm{c}}(\mathbf{y})\mathbf{u}, \mathbf{u} \rangle = \varepsilon \sum_n \phi''(y_n')|u_n'|^2 + \varepsilon \sum_n 4\phi''(2y_n')|u_n'|^2$$

Hessian of atomistic energy:

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\mathrm{a}}(\mathbf{y})\mathbf{u}, \mathbf{u} \rangle = \varepsilon \sum_n \phi''(y_n')|u_n'|^2 + \varepsilon \sum_{n=1}^{N} \phi''(y_n' + y_{n+1}')|u_n' + u_{n+1}'|^2$$

Hessian of QC energy:

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\mathrm{qc}}(\mathbf{y})\mathbf{u}, \mathbf{u} \rangle = \varepsilon \sum_n \phi''(y_n')|u_n'|^2 + \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{a}}} \phi''(y_n' + y_{n+1}')|u_n' + u_{n+1}'|^2 + \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{c}}} \left\{ 2\phi''(2y_n')|u_n'|^2 + 2\phi''(2y_{n+1}')|u_{n+1}'|^2 \right\}$$

Hessians & Strain Gradients (1)

Hessian of continuum energy:

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\mathrm{c}}(\mathbf{y})\mathbf{u}, \mathbf{u} \rangle = \varepsilon \sum_n \phi''(y_n')|u_n'|^2 + \varepsilon \sum_n 4\phi''(2y_n')|u_n'|^2$$

Hessian of atomistic energy:

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\mathrm{a}}(\mathbf{y})\mathbf{u}, \mathbf{u} \rangle = \varepsilon \sum_n \phi''(y_n')|u_n'|^2 + \varepsilon \sum_{n=1}^{N} \phi''(y_n' + y_{n+1}')|u_n' + u_{n+1}'|^2$$

Hessian of QC energy:

$$\begin{aligned} \langle \nabla_\varepsilon^2 \mathcal{E}^{\mathrm{qc}}(\mathbf{y})\mathbf{u}, \mathbf{u} \rangle = \varepsilon \sum_n \phi''(y_n')|u_n'|^2 &+ \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{a}}} \phi''(y_n' + y_{n+1}')|u_n' + u_{n+1}'|^2 \\ &+ \varepsilon \sum_{n \in \mathcal{N}^{\mathrm{c}}} \{2\phi''(2y_n')|u_n'|^2 + 2\phi''(2y_{n+1}')|u_{n+1}'|^2\} \end{aligned}$$

Rewrite NNN terms using the *Polarisation Identity*:

$$|u_n' + u_{n+1}'|^2 = 2|u_n'|^2 + 2|u_{n+1}'|^2 - \varepsilon^2 |u_n''|^2$$

Hessians & Strain Gradients (2)

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\rm c}(\mathbf{y})\mathbf{u}, \mathbf{u}\rangle = \varepsilon \sum_n A_n^{\rm c} |u_n'|^2$$

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\rm a}(\mathbf{y})\mathbf{u}, \mathbf{u}\rangle = \varepsilon \sum_n A_n^{\rm a} |u_n'|^2 + \varepsilon^3 \sum_n B_n |u_n''|^2$$

$$\langle \nabla_\varepsilon^2 \mathcal{E}^{\rm qc}(\mathbf{y})\mathbf{u}, \mathbf{u}\rangle = \varepsilon \sum_n A_n^{\rm qc} |u_n'|^2 + \varepsilon^3 \sum_{n \in \mathcal{N}^{\rm a}} B_n |u_n''|^2$$

where $A_n^{\rm a} \approx A_n^{\rm qc}$ and $B_n \geq 0$

Theorem

1. $\alpha^{\rm a}(\mathbf{y}) \geq \alpha^{\rm qc}(\mathbf{y}) - C\varepsilon \|\mathbf{y}''\|_{L^\infty(\mathcal{N}^{\rm c})}$
2. $\alpha^{\rm qc}(\mathbf{y}) \geq \min_n A_n^{\rm qc}$
3. *If* $\mathbf{y}$ *is globally smooth then* $\alpha^{\rm qc} \geq \alpha^{\rm a} - O(\varepsilon)$

Error Estimate

Theorem (Existence and A Priori Error Estimate)

Let $\mathbf{y}_{\mathrm{a}}$ *be a stable equilibrium of* $\mathcal{E}^{\mathrm{a}}$ *s.t.* $\min_n A_n^{\mathrm{qc}} > 0$*. Then there exists a constant* $\delta > 0$ *such that, if*

$$\varepsilon \|\mathbf{y}''\|_{\mathrm{L}^\infty(\mathcal{N}^{\mathrm{c}})} + \varepsilon^{3/2} \|\mathbf{y}'''\|_{\mathrm{L}^2(\mathcal{N}^{\mathrm{c}})} + \varepsilon^{3/2} \|\mathbf{y}''\|^2_{\mathrm{L}^4(\mathcal{N}^{\mathrm{c}})} \le \delta,$$

then there exists a stable equlibrium $\mathbf{y}_{\mathrm{qc}}$ *of* $\mathcal{E}^{\mathrm{qc}}$ *s.t.*

$$\|\mathbf{y}'_{\mathrm{qc}} - \mathbf{y}'_{\mathrm{a}}\|_{\mathrm{L}^2} \lesssim \frac{1}{\alpha^{\mathrm{qc}}(\mathbf{y}_{\mathrm{a}})} \Big[\varepsilon \|\mathbf{y}''_{\mathrm{a}}\|_{\mathrm{L}^2(\mathcal{N}^{\mathrm{i}})} + \varepsilon^2 \big(\|\mathbf{y}'''_{\mathrm{a}}\|_{\mathrm{L}^2(\mathcal{N}^{\mathrm{c}})} + \|\mathbf{y}''_{\mathrm{a}}\|^2_{\mathrm{L}^4(\mathcal{N}^{\mathrm{c}})} \big) \Big]$$

Error Estimate

Theorem (Existence and A Priori Error Estimate)

Let $\mathbf{y}_{\rm a}$ *be a stable equilibrium of* $\mathcal{E}^{\rm a}$ *s.t.* $\min_n A_n^{\rm qc} > 0$. *Then there exists a constant* $\delta > 0$ *such that, if*

$$\varepsilon \|\mathbf{y}''\|_{\mathsf{L}^\infty(\mathcal{N}^{\rm c})} + \varepsilon^{3/2} \|\mathbf{y}'''\|_{\mathsf{L}^2(\mathcal{N}^{\rm c})} + \varepsilon^{3/2} \|\mathbf{y}''\|^2_{\mathsf{L}^4(\mathcal{N}^{\rm c})} \leq \delta,$$

then there exists a stable equlibrium $\mathbf{y}_{\rm qc}$ *of* $\mathcal{E}^{\rm qc}$ *s.t.*

$$\|\mathbf{y}'_{\rm qc} - \mathbf{y}'_{\rm a}\|_{\mathsf{L}^2} \lesssim \frac{1}{\alpha^{\rm qc}(\mathbf{y}_{\rm a})} \Big[\varepsilon \|\mathbf{y}''_{\rm a}\|_{\mathsf{L}^2(\mathcal{N}^{\rm i})} + \varepsilon^2 \big(\|\mathbf{y}'''_{\rm a}\|_{\mathsf{L}^2(\mathcal{N}^{\rm c})} + \|\mathbf{y}''_{\rm a}\|^2_{\mathsf{L}^4(\mathcal{N}^{\rm c})} \big) \Big]$$

Remarks:

- Can admit defects in the analysis, but need to modify the function space setting. [O. & Süli; 2008], [O.; 2010]
- Sharp stability in 2D/3D version is difficult (work in progress).

Atomistic/Continuum Hybrid Methods: POV

1. **Direct Coarse Graining without Coupling**
   - Force-based: [Knap & Ortiz; 2003], Energy-based: [Eidel & Stuchowsky; 2008]
   - Analysis: [Lin; 2003, 2008], [O. & Süli; 2008], [Luskin & O.; 2009]
   - Conclusion so far: not as simple as it sounds ...
2. **Energy Based Coupling**
   - Original QC (with GF): [Tadmor & Ortiz & Phillips; 1996]
   - Ghost force removal: [Shimokawa et al; 2004], [E & Lu & Yang; 2006], [Shapeev]
   - Analysis: 1D now fairly advanced; 2D in progress
   - Still some unresolved difficulties general interaction potentials ...
3. **Force Based Coupling**
   - Naturally free of ghost forces
   - Large number of different variants: Schmauder, Gumbsch; Shenoy, Rodney, Ortiz, Tadmor; Miller, Curtin; Luskin, Dobson; Parks, Bochev, Lehoucq; ...
   - Beautiful (and difficult) question open in their analysis.

Other Methods: Blending, Domain Decomposition, various methods for finite temperature, dynamics, DFT: Parks, Gunzburger, Seleson, Lehoucq, Karpov, Park, Rudd, Broughton, Ortiz, Gavini, Bhattacharya, E, Lu, Garcia–Cervera, Cances, Deleurence, Lewin, Legoll, ...