Analysis of Quasicontinuum Methods

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Part 1

Simple Atomistic Model
Derivation of the Local QC Method

Model Problem: Notation, Setup

- deformation of an infinite chain: $y = (y_\ell)_{\ell\in\mathbb{Z}}$;
  assume that displacement $u_\ell = y_\ell - \ell\varepsilon$ is N-periodic!
- $\varepsilon = 1/N$ =atomic spacing
- Displacement gradient: $u'_\ell = (u_\ell - u_{\ell-1})/\varepsilon$
- Stored energy (per period) of the deformed chain: $\mathcal{E}_{\mathrm{a}}(u)$
- Total energy: $E_{\mathrm{a}}(u) = \mathcal{E}_{\mathrm{a}}(u) - \sum_{\ell=1}^{N} \varepsilon f_\ell u_\ell$,
  where $f \in \mathbb{R}^{\mathbb{Z}}$ is a N-periodic dead load
- Admissible set: $\mathcal{X} = \{u \in \mathbb{R}^{\mathbb{Z}} : N\text{-periodic and } \sum_{\ell=1}^{N} u_\ell = 0\}$

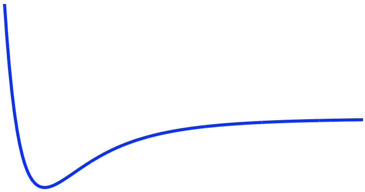
$$\text{Find} \qquad u_{\mathrm{a}} \in \operatorname*{argmin}_{\mathcal{X}} E_{\mathrm{a}}$$

Next-Nearest Neighbour Interaction

For this presentation: next-nearest neighbour pair interaction

$$\mathcal{E}_a(y) = \underbrace{\sum_{\ell=1}^{N} \varepsilon\phi\big(\varepsilon^{-1}(y_\ell - y_{\ell-1})\big)}_{\text{nearest-neighbour interaction}} + \underbrace{\sum_{\ell=1}^{N} \varepsilon\phi\big(\varepsilon^{-1}(y_{\ell+1} - y_{\ell-1})\big)}_{\text{next-nearest-neighbour interaction}}$$

ϕ is a smooth Lennard-Jones type potential.



Next-Nearest Neighbour Interaction

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$$\mathcal{E}_{\mathrm{a}}(u) = \sum_{\ell=1}^{N} \varepsilon\Big(\underbrace{\phi(1+u'_\ell)}_{\text{nearest-neighbour interaction}} + \underbrace{\phi(2+u'_\ell+u'_{\ell+1})}_{\text{next-nearest-neighbour interaction}} \Big)$$

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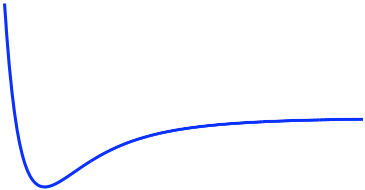

Next-Nearest Neighbour Interaction

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$$\mathcal{E}_{\mathrm{a}}(u) = \sum_{\ell=1}^{N} \varepsilon\Big(\underbrace{\phi_1(u'_\ell)}_{\text{nearest-neighbour interaction}} + \underbrace{\phi_2(u'_\ell + u'_{\ell+1})}_{\text{next-nearest-neighbour interaction}} \Big)$$

$$\phi_1(z) = \phi(1 + z)$$
$$\phi_2(z) = \phi(2 + z)$$

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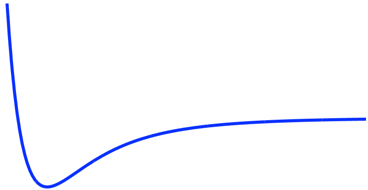

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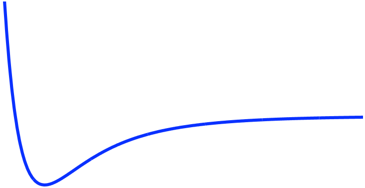

Captures some of the main characteristics of atomistic models:

- Non-convexity $\Rightarrow$ many local minimizers (non-uniqueness of solutions)
- Next-nearest neighbour interaction $\Rightarrow$ some amount of non-locality!

The Need (and Opportunity) for Approximations

$$\text{Find} \qquad u_a \in \operatorname*{argmin}_{\mathcal{X}} E_a$$

- $\mathcal{X}$ is finite dimensional $\Rightarrow$ in principle computable
- $N = \dim(\mathcal{X})$ is extremely large $\Rightarrow$ very expensive
- deformation/displacement is often 'smooth' except in localized regions (defects) $\Rightarrow$ can coarse-grain the atomistic model:
  - replace by simpler model ($\longleftarrow$ this talk)
  - remove degrees of freedom

('smooth' means u'_ℓ varies slowly!)

The Cauchy–Born Approximation

If u is 'smooth', then

$$\begin{aligned}
\mathcal{E}_{\mathsf{a}}(u) &= \sum_{\ell=1}^{N} \varepsilon\big(\phi_1(u'_\ell) + \phi_2(u'_\ell + u'_{\ell+1})\big) \\
&\approx \sum_{\ell=1}^{N} \varepsilon \underbrace{\big(\phi_1(u'_\ell) + \phi_2(2u'_\ell)\big)}_{=:\phi_{\mathsf{cb}}(u'_\ell)} \qquad = \int_0^1 \phi_{\mathsf{cb}}(u'(x))\,\mathrm{d}x =: \mathcal{E}_{\mathsf{cb}}(u)
\end{aligned}$$

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Cauchy–Born Model:

$$\mathcal{X}_{\mathrm{cb}} := \Big\{ u \in \mathrm{W}^{1,1}_{\#}[0,1] : \int_0^1 u\,\mathrm{d}x = 0 \Big\}$$

$$E_{\mathrm{cb}}(u) := \mathcal{E}_{\mathrm{cb}}(u) - \int_0^1 f u\,\mathrm{d}x$$

Does $\mathrm{argmin}_{\mathcal{X}_{\mathrm{cb}}} E_{\mathrm{cb}} \approx \mathrm{argmin}_{\mathcal{X}} E_{\mathrm{a}}$ *hold?*

The Local QC Method (QCL)

The Cauchy–Born Approximation: $E_{\mathsf{cb}}(u) = \int_0^1 \big(\phi_{\mathsf{cb}}(u') - fu\big)\,\mathrm{d}x$

$$\phi_{\mathsf{cb}}(z) = \phi(1+z) + \phi(2(1+z))$$

- The Local QC Method is a P1 Galerkin finite element discretization of the Cauchy–Born Approximation
- For simplicity: let the LQC mesh coincide with atomic lattice, i.e., $\mathcal{T} \sim \{\ell\varepsilon : \ell \in \mathbb{Z}\}$

  (we avoid having to analyze the discretization step, and concentrate on the approximation of the model)

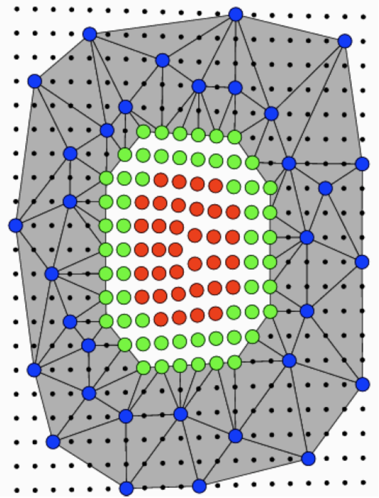
Find $\quad u_{\mathsf{lqc}} \in \operatorname*{argmin}_{\mathcal{X}} E_{\mathsf{lqc}},$

where $\quad E_{\mathsf{lqc}}(u) = \sum_{\ell=1}^{N} \varepsilon\big(\phi_{\mathsf{cb}}(u'_\ell) - f_\ell u_\ell\big)$

‘Proper’ QC Methods

In ‘proper’ QC methods:

- keep the atomistic model in the defect region
- use the Cauchy–Born approximation in the ‘smooth’ region
- couple the two models somehow



- Energy-Based Coupling (QCE) [Tadmor, Ortiz, Phillips; 1996]
- Quasi-nonlocal Coupling (QNL) [Shimoka et al; 2004]
- Geometrically-Consistent Scheme (QCGC) [E, Lu, Yang; 2006]
- Force-Based Coupling (QCF) [Dobson & Luskin; 2008]

- (Methods based on summation rules)

Other AtC Coupling Methods

- AtC Coupling by Blending (Fish, Parks, Gunzburger, Badia, . . .)
- Bridging-Scales Method (Karpov, Liu, Park, Hou, . . .)
- Coarse-Grained Molecular Dynamics (Rudd, Broughton, . . .)
- Methods based on Domain-Decomposition (Parks, Lehoucq, . . .)
- . . .

Part 2

A Very Basic Nonlinear Analysis

[E & Ming; 2005, 2006, preprint, preprint]
[O. & Süli; 2008]
[Dobson & Luskin; 2008]

Two fundamental questions

1. Given a local minimizer u_{a} of the atomistic model, does a local minimizer u_{lqc} of the Local QC Method exist such that $\|u_{\mathrm{a}} - u_{\mathrm{lqc}}\|_{?}$ is small?

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   - Finite Element Methods: [Dobrowolski & Rannacher; 1980], [Brezzi, Rappaz, Raviart; 1980, 1981, 1981]
   - QC Method: [E & Ming; 2005, 2006, . . .], [O. & Süli; 2008], [Luskin & O.; in preparation]

2. Given a local minimizer u_{lqc} of the Local QC Method does a local minimizer u_{a} of the atomistic model exist such that $\|u_{\mathrm{a}} - u_{\mathrm{lqc}}\|_{?}$ is small?
   - Finite Element Methods (*Computer assisted enclosure methods*): [Plum et al.; 1992, . . .], [Nakao et al.; 1993, . . .], [O.; 2008 preprint]
   - QC Methods: [O. & Süli; 2008], [Luskin & O.; in preparation]

Why this is important:

Consider quasistatic loading: $f = f(t)$, t varies in time, compute equilibria $u(t)$.

At which time t_* does an energy well become unstable?

- Onset of fracture
- Defect formation
- Onset and speed of dislocation motion
- ...

The Basic Strategy: Inverse Function Theorem

(for example, for question 1)

1. Setup two nonlinear systems:

$$E'_{\mathrm{a}} =: F_{\mathrm{a}} : \mathcal{X} \to \mathcal{Y} \qquad \text{and} \qquad E'_{\mathrm{lqc}} =: F_{\mathrm{lqc}} : \mathcal{X} \to \mathcal{Y}$$

2. If $F_{\mathrm{a}}(u_{\mathrm{a}}) = 0$, then

$$F_{\mathrm{lqc}}(u_{\mathrm{lqc}}) = 0 \qquad \Leftrightarrow \qquad F_{\mathrm{lqc}}(u_{\mathrm{lqc}}) - F_{\mathrm{lqc}}(u_{\mathrm{a}}) = F_{\mathrm{a}}(u_{\mathrm{a}}) - F_{\mathrm{lqc}}(u_{\mathrm{a}})$$

3. Apply Inverse Function Theorem: If $F'_{\mathrm{lqc}}(u_{\mathrm{a}})$ is an isomorphism and if $\|F_{\mathrm{a}}(u_{\mathrm{a}}) - F_{\mathrm{lqc}}(u_{\mathrm{a}})\|_{\mathcal{Y}}$ is small then there exists u_{lqc}, s.t. $F_{\mathrm{lqc}}(u_{\mathrm{lqc}}) = 0$ and $\|u_{\mathrm{a}} - u_{\mathrm{lqc}}\|_{\mathcal{X}}$ is small.

We will see that a sufficient condition for this to work is that u_a is smooth.

An Explicit Inverse Function Theorem

Lemma

Suppose $F : X \to Y$, $x_0 \in X$, $\|F(x_0)\|_Y \le \eta$, $\|F'(x_0)^{-1}\|_{[Y,X]} \le \sigma$, *and* $L := \mathrm{Lip}(F', B(x_0, 2\eta\sigma))$.
If $2L\eta\sigma^2 < 1$ *then there exists* $x \in X$ *such that* $F(x) = 0$ *and* $\|x - x_0\|_X \le 2\eta\sigma$.

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So we need:

- Residual Estimate: $\|E'_{\mathrm{a}}(u) - E'_{\mathrm{lqc}}(u)\| \le \eta(u)$
- Stability Estimate: $\|E''_{\mathrm{lqc}}(u)^{-1}\| \le \sigma(u)$
- Local Lipschitz Estimate: $\|E''_{\mathrm{lqc}}(v) - E''_{\mathrm{lqc}}(w)\| \le L\|v - w\|$

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So we need:

- Residual Estimate: $\|E_a'(u) - E_{lqc}'(u)\|_{-1} \le \eta(u)$
- Stability Estimate: $\|E_{lqc}''(u)^{-1}\|_{(-1,1)} \le \sigma(u)$
- Local Lipschitz Estimate: $\|E_{lqc}''(v) - E_{lqc}''(w)\|_{(1,-1)} \le L\|v - w\|_1$

Stability can be difficult unless we use an H^1-like topology:

$$\|v\|_{\mathcal{X}} := \|v\|_1 = \|v'\|_{\ell^2_\varepsilon} = \Big(\sum_{\ell=1}^{N} \varepsilon |v_\ell'|^2\Big)^{1/2}, \qquad v \in \mathcal{X}$$

$$\|g\|_{\mathcal{Y}} := \|g\|_{-1} = \sup_{\|v\|_{1,2}=1} |g[v]|, \qquad g \in \mathcal{X}^*$$

Residual Estimate

Best done in a weak formulation:

$$\mathcal{E}'_{\mathsf{lqc}}(u)[v] = \sum_{\ell=1}^{N} \varepsilon \phi'_{\mathsf{cb}}(u'_\ell) v'_\ell, \qquad \mathcal{E}'_{\mathsf{a}}(u)[v] = \sum_{\ell=1}^{N} \varepsilon R_\ell(u) v'_\ell$$

$$\text{where } \phi'_{\mathsf{cb}}(u'_\ell) = \phi'_1(u'_\ell) + 2\phi'_2(2u'_\ell),$$

$$\text{and } R_\ell(u) = \frac{1}{\varepsilon} \frac{\partial \mathcal{E}_{\mathsf{a}}(u)}{\partial u'_\ell} = \phi'_1(u'_\ell) + \phi'_2(u'_{\ell-1} + u'_\ell) + \phi'_2(u'_\ell + u'_{\ell+1})$$

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$$|R_\ell(u) - \phi'_{\mathrm{cb}}(u'_\ell)| \le M_2(|u'_\ell - u'_{\ell-1}| + |u'_{\ell+1} - u'_\ell|) = \varepsilon M_2(|u''_{\ell-1}| + |u''_\ell|).$$

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$$|R_\ell(u) - \phi'_{\mathrm{cb}}(u'_\ell)| \le M_2(|u'_\ell - u'_{\ell-1}| + |u'_{\ell+1} - u'_\ell|) = \varepsilon M_2(|u''_{\ell-1}| + |u''_\ell|).$$

$$|\mathcal{E}'_{\mathrm{lqc}}(u)[v] - \mathcal{E}'_{\mathrm{a}}(u)[v]| \le \sum_{\ell=1}^{N} \varepsilon |R_\ell(u) - \phi'_{\mathrm{cb}}(u'_\ell)||v'_\ell| \le 2\varepsilon M_2 \|u''\|_{\ell^p_\varepsilon} \|v'\|_{\ell^{p'}_\varepsilon}$$

$$\Rightarrow \quad \|E'_{\mathrm{a}}(u) - E'_{\mathrm{lqc}}(u)\|_{-1,2} \le 2\varepsilon M_2 \|u''\|_{\ell^2_\varepsilon}$$

Residual Estimates for Consistent QC Methods

First Order Consistent Methods:

- LQC: $\lesssim \varepsilon \|u''\|_{\ell^2_\varepsilon}$
- QNL: $\lesssim \varepsilon \|u''\|_{\ell^2_\varepsilon}$
- QCF: $\lesssim \varepsilon \|u''\|_{\ell^2_\varepsilon}$

Energy-Based Coupling:

- QCE: $\lesssim \sqrt{\varepsilon} \|u''\|_{\ell^2_\varepsilon}$

The Stability Estimate

H^1-stability = Coercivity:

$$F'_{\rm lqc}(u)[v,v] = \mathcal{E}''_{\rm lqc}(u)[v,v] = \sum_{\ell=1}^{N} \varepsilon \phi''_{\rm cb}(u'_\ell)|v'_\ell|^2 \geq c_{\rm lqc}(u)\|v'\|^2_{\ell^2_\varepsilon}.$$

(Note: $c_{\rm lqc}(u) \geq \min_\ell \phi''_{\rm cb}(u'_\ell)$)

If $c_{\rm lqc}(u) > 0$ then $F'_{\rm lqc}(u)$ is invertible and

$$\|F'_{\rm lqc}(u)^{-1}\|_{(-1,1)} = \frac{1}{c_{\rm lqc}(u)}$$

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Here everybody is cheating!

The Local Lipschitz Constant

We need:

$$|F'_{\mathsf{lqc}}(u)[v, w] - F'_{\mathsf{lqc}}(\tilde{u})[v, w]| \leq L\|u' - \tilde{u}'\|_{\ell^2_\varepsilon}\|v'\|_{\ell^2_\varepsilon}\|w'\|_{\ell^2_\varepsilon}$$

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$$\begin{aligned}
|F'_{\mathrm{lqc}}(u)[v,w] - F'_{\mathrm{lqc}}(\tilde{u})[v,w]| &= \Big|\sum_{\ell=1}^{N} \big(\phi''_{\mathrm{cb}}(u'_\ell) - \phi''_{\mathrm{cb}}(\tilde{u}'_\ell)\big) v'_\ell w'_\ell\Big| \\
&\le \max_{\ell=1,\dots,N} \big|\phi''_{\mathrm{cb}}(u'_\ell) - \phi''_{\mathrm{cb}}(\tilde{u}'_\ell)\big| \, \|v'\|_{\ell^2_\varepsilon}\|w'\|_{\ell^2_\varepsilon} \\
&\le M_3\|u' - \tilde{u}'\|_{\ell^\infty}\|v'\|_{\ell^2_\varepsilon}\|w'\|_{\ell^2_\varepsilon} \\
&\le M_3\varepsilon^{-1/2}\|u' - \tilde{u}'\|_{\ell^2}\|v'\|_{\ell^2_\varepsilon}\|w'\|_{\ell^2_\varepsilon}
\end{aligned}$$

So $L = M_3\varepsilon^{-1/2}$ because of an inverse inequality.

Existence + Error Estimate

Recall the Inverse Function Theorem:

$$2L\eta\sigma^2 < 1 \Rightarrow \exists\, x \in X \text{ s.t. } F(x) = 0 \text{ and } \|x - x_0\|_X \le 2\eta\sigma$$

If $E_{\mathrm{a}}'(u_{\mathrm{a}}) = 0$ then

- $2\eta\sigma = 4M_2\varepsilon\|u_{\mathrm{a}}''\|_{\ell^2_\varepsilon}/c_{\mathrm{lqc}}(u_{\mathrm{a}})$
- $2L\eta\sigma^2 = 4M_2M_3\varepsilon^{1/2}\|u_{\mathrm{a}}''\|_{\ell^2_\varepsilon}/c_{\mathrm{lqc}}(u_{\mathrm{a}})^2$

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- $2\eta\sigma = 4M_2\varepsilon\|u_{\rm a}''\|_{\ell^2_\varepsilon}/c_{\rm lqc}(u_{\rm a})$
- $2L\eta\sigma^2 = 4M_2M_3\varepsilon^{1/2}\|u_{\rm a}''\|_{\ell^2_\varepsilon}/c_{\rm lqc}(u_{\rm a})^2$

So, if $c_{\rm lqc}(u_{\rm a}) > 0$ and $u_{\rm a}$ is also sufficiently smooth, i.e.,

$$\|u_{\rm a}''\|_{\ell^2} < \frac{c_{\rm lqc}(u_{\rm a})^2\varepsilon^{-1/2}}{4M_2M_3},$$

then there exists $u_{\rm lqc} \in \mathcal{X}$ s.t. $E_{\rm lqc}'(u_{\rm lqc}) = 0$ and $E_{\rm lqc}$ such that

$$\|u_{\rm lqc}' - u_{\rm a}'\|_{\ell^2_\varepsilon} \le 4M_2\varepsilon\|u_{\rm a}''\|_{\ell^2_\varepsilon}/c_{\rm lqc}(u_{\rm a}).$$

Further Results

From previous slide:

- If $E'_{\rm a}(u_{\rm a}) = 0$, $c_{\rm lqc}(u_{\rm a}) > 0$, and $u_{\rm a}$ is *sufficiently smooth* then $\exists\, u_{\rm lqc}$ s.t. $E'_{\rm lqc}(u_{\rm lqc}) = 0$ and $\|u'_{\rm a} - u'_{\rm lqc}\|_{\ell^2_\varepsilon} \lesssim \varepsilon / c_{\rm lqc}(u_{\rm a})$.

Repeating the proof verbatim:

- If $E'_{\rm lqc}(u_{\rm lqc}) = 0$, $c_{\rm a}(u_{\rm lqc}) > 0$, and $u_{\rm lqc}$ is *sufficiently smooth* then $\exists\, u_{\rm a}$ s.t. $E'_{\rm a}(u_{\rm a}) = 0$ and $\|u'_{\rm a} - u'_{\rm lqc}\|_{\ell^2_\varepsilon} \lesssim \varepsilon / c_{\rm a}(u_{\rm lqc})$.

Further Results

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- If $E_a'(u_a) = 0$, $c_{lqc}(u_a) > 0$, and u_a is *sufficiently smooth* then $\exists\, u_{lqc}$ s.t. $E_{lqc}'(u_{lqc}) = 0$ and $\|u_a' - u_{lqc}'\|_{\ell^2_\varepsilon} \lesssim \varepsilon / c_{lqc}(u_a)$.

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Along very similar lines, corresponding results can be proven for all first-order consistent QC methods:

- Constrained Atomistic Approximation [O. & Süli; 2008]
- Force-based QC method [Dobson & Luskin; 2008]
- Quasi-nonlocal coupling (≈ geometrically-consistent QC method) [E & Ming; preprint]

BUT . . .

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BUT ... Nobody has adressed the stability issue (properly) so far!

Sharp Stability Estimates!

We need a result along the following lines:

If u is sufficiently smooth then $c_{\mathrm{a}}(u) \approx c_{\mathrm{lqc}}(u)$.

$\Rightarrow$ equivalence of stable equilibria
(up to a controlled approximation error)

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If u is sufficiently smooth then $c_{\mathrm{a}}(u) \approx c_{\mathrm{lqc}}(u)$.

$\Rightarrow$ equivalence of stable equilibria
(up to a controlled approximation error)

Why this is non-trivial: $\mathcal{E}_{\mathrm{a}}$ is non-local, while $\mathcal{E}_{\mathrm{lqc}}$ is local

$$\Rightarrow \qquad \|\mathcal{E}_{\mathrm{a}}''(u) - \mathcal{E}_{\mathrm{lqc}}''(u)\| \gtrsim 1 \qquad \text{for all } u.$$

So we really have to concentrate on the stability constants themselves . . .

A First Example

Compare $c_{\mathrm{a}}(0)$ and $c_{\mathrm{lqc}}(0)$:

- The QCL Hessian:

$$\mathcal{E}''_{\mathrm{lqc}}(0)[v,v] = \sum_{\ell=1}^{N} \varepsilon \underbrace{\phi''_{\mathrm{cb}}(0)}_{=\phi''(1)+4\phi''(2)} |v'_\ell|^2 = \phi''_{\mathrm{cb}}(0)\|v'\|^2_{\ell^2_\varepsilon}$$

- The Atomistic Hessian:

$$\mathcal{E}''_{\mathrm{a}}(0)[v,v] = \sum_{\ell=1}^{N} \varepsilon\big(\phi''(1)|v'_\ell|^2 + \phi''(2)|v'_\ell + v'_{\ell+1}|^2\big)$$

- Use the identity $|v'_\ell + v'_{\ell+1}|^2 = 2|v'_\ell|^2 + 2|v'_{\ell+1}|^2 - |v'_{\ell+1} - v'_\ell|^2$ to obtain

$$\begin{aligned}\mathcal{E}''_{\mathrm{a}}(0)[v,v] &= \sum_{\ell=1}^{N} \varepsilon\big(\phi''(1) + 4\phi''(2)\big)|v'_\ell|^2 - \phi''(2)\varepsilon^2 \sum_{\ell=1}^{N} |v''_\ell|^2 \\ &= \phi''_{\mathrm{cb}}(0)\|v'\|^2_{\ell^2_\varepsilon} - \phi''(2)\varepsilon^2\|v''\|^2_{\ell^2_\varepsilon}.\end{aligned}$$

A First Example (ctd.)

From previous slide:

$$\mathcal{E}''_{\mathrm{lqc}}(0)[v,v] = \phi''_{\mathrm{cb}}(0)\|v'\|_{\ell^2_\varepsilon}$$
$$E''_{\mathrm{a}}(0)[v,v] = \phi''_{\mathrm{cb}}(0)\|v'\|_{\ell^2_\varepsilon} - \phi''(2)\varepsilon^2\|v''\|^2_{\ell^2_\varepsilon}.$$

Typically: $\phi''(2) < 0$!

Proposition

If $\phi''(2) < 0$ *then* $c_{\mathrm{a}}(0) = c_{\mathrm{lqc}}(0) - \varepsilon^2\mu^2\phi''(2)$

(where $\mu = \min_v \|v''\|_{\ell^2_\varepsilon} / \|v'\|_{\ell^2_\varepsilon}$*)*

- QNL/QCGC: same result $c_{\mathrm{qnl}}(0) = c_{\mathrm{lqc}}(0) = c_{\mathrm{a}}(0) + O(\varepsilon^2)$
- QCF: **?** (non-conservative, needs inf-sup)
- QCE: $c_{\mathrm{a}}(0) \geq c_{\mathrm{qce}}(0) + O(1)$

The A Priori Result

Lemma (Stability of $\mathcal{E}''_{\mathrm{a}}$ implies stability of $\mathcal{E}''_{\mathrm{lqc}}$)

$$c_{\mathrm{lqc}}(u) \geq c_{\mathrm{a}}(u) - C\varepsilon^{2/3}\big(\|u''\|_{\ell^\infty} + \min_\ell |\phi''(2u'_\ell)|\big) =: \tilde{c}_{\mathrm{a}}(u).$$

Theorem (Existence of QC Solutions)

If $E'_{\mathrm{a}}(u_{\mathrm{a}}) = 0$, $\tilde{c}_{\mathrm{a}}(u_{\mathrm{a}}) > 0$, *and* $\|u''_{\mathrm{a}}\|_{\ell^2_\varepsilon} < C\varepsilon^{-1/2}\tilde{c}_{\mathrm{a}}(u_{\mathrm{a}})^2$ *then there exists a strict local minimizer* $u_{\mathrm{lqc}} \in \mathcal{X}$ *of* E_{lqc}, *and*

$$\|u'_{\mathrm{a}} - u'_{\mathrm{lqc}}\|_{\ell^2_\varepsilon} \lesssim \varepsilon\|u''_{\mathrm{lqc}}\|_{\ell^2_\varepsilon}/\tilde{c}_{\mathrm{a}}(u_{\mathrm{a}})$$

In words: *If u_{a} is a smooth and stable equilibrium of the atomistic model, then there exists a nearby LQC solution.*

The A Posteriori Result

Lemma (Stability of $\mathcal{E}''_{\mathrm{lqc}}$ implies stability of $\mathcal{E}''_{\mathrm{a}}$)

$$c_{\mathrm{a}}(u) \geq c_{\mathrm{lqc}}(u) - C\varepsilon \|u''\|_{\ell^\infty} =: \tilde{c}_{\mathrm{lqc}}(u).$$

Theorem (Reliability of the QC Method)

If $E'_{\mathrm{lqc}}(u_{\mathrm{lqc}}) = 0$, $\tilde{c}_{\mathrm{lqc}}(u_{\mathrm{lqc}}) > 0$, and $\|u''_{\mathrm{lqc}}\|_{\ell^2_\varepsilon} < C\varepsilon^{-1/2}\tilde{c}_{\mathrm{lqc}}(u_{\mathrm{lqc}})^2$, then there exists a strict local minimizer $u_{\mathrm{a}} \in \mathcal{X}$ of E_{a}, and

$$\|u_{\mathrm{a}} - u_{\mathrm{lqc}}\|_{\ell^2_\varepsilon} \lesssim \varepsilon \|u''_{\mathrm{lqc}}\|_{\ell^2_\varepsilon} / \tilde{c}_{\mathrm{lqc}}(u_{\mathrm{lqc}}).$$

In words: *If u_{lqc} is a stable equilibrium of LQC and sufficiently smooth then there exists a stable equilibrium u_{a} of the atomistic model.*

Extensions, Open Problems: 2D/3D

- CB/QCL: ok for small deformations [E & Ming; 2006]:
  - Prove that $c_{\mathrm{cb}}(0) \geq \hat{c}_{\mathrm{a}}(0)$
  - Deduce $c_{\mathrm{cb}}(u) \geq \frac{1}{2}\hat{c}_{\mathrm{a}}(u)$ for small deformations: $\|\nabla u\|_{\mathrm{L}^\infty} \leq \delta$
  - Given u_{lqc}, use asymptotic analysis to compute $\hat{u}_{\mathrm{lqc}}$ with $O(\varepsilon^2)$ residual in the atomistic model and $\|\nabla u_{\mathrm{lqc}}' - \nabla \hat{u}_{\mathrm{lqc}}\|_{\ell^\infty}$ under control.
- Stability: the sharp stability estimate of 1D is false! One needs to be much more careful.
- CB/QCL for large deformations: probably ok with arguments along the same lines (?)
- LQC, QNL, QCGC whould be doable, but will require a lot of work

Further Extension/Open Problems

Non-Uniform Meshes: On non-uniform meshes we really need to avoid the inverse inequality.

- 1D is ok, but needs slightly different techniques
  Basically define $F_{\mathrm{a/qc}} : \mathrm{W}^{1,\infty} \to \mathrm{W}^{-1,\infty}$ [O. & Süli; 2008]
- In 2D/3D: fully nonlinear analysis out of reach for the moment: essentially requires $\mathrm{W}^{1,\infty}$ estimates on non-uniform meshes
- But sharp residual and stability estimates should still be doable

Further Extension/Open Problems

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Other AtC Coupling Methods:

- AtC Coupling by Blending (Fish, Parks, Gunzburger, Badia, . . .)
- Bridging-Scales Method (Karpov, Liu, Park, Hou, . . .)
- Coarse-Grained Molecular Dynamics (Rudd, Broughton, . . .)
- Methods based on Domain-Decomposition (Parks, Lehoucq, . . .)
- . . .