A New Predictor-Corrector Method for Efficient Modeling of Surface Effects

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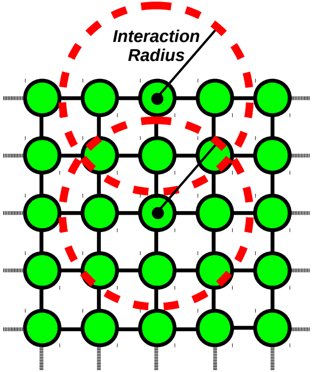
SIAM Conference on Computational Science and Engineering (CSE17)
February 28, 2017

Physical Motivation 1

- Well-known that surfaces exhibit different behavior than interior (bulk)



Physical Motivation 2

Example of Surface Influence

- Iron, platinum, and gold exhibit HCP lattice structure in the {100} surfaces as opposed to square lattice of interior due to tensile stress at surface

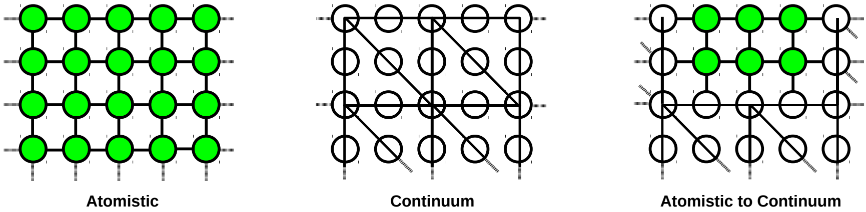
Length-Scale Dependence

- At the nanoscale, surface stresses can drive structural changes beyond the surface into interior
- Size-dependent material properties and phase transformations

Goal

- Solve a molecular statics problem to find ground states and predict surface-driven effects in nanostructures

Challenges with Common Approaches



- Purely atomistic approach is computationally expensive
- Bulk continuum models do not account for surface effects and are length-scale independent
- Atomistic-to-Continuum coupling methods may lose their efficiency with certain surface geometries

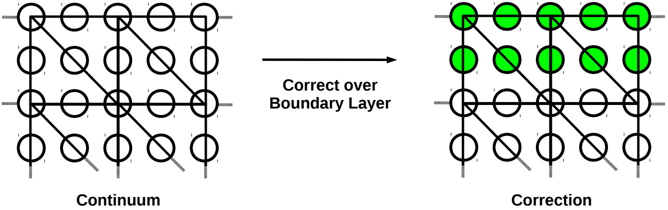
New Approach

Goal

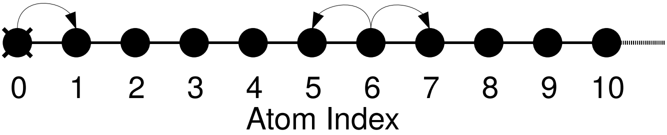
- Solve a molecular statics problem to find ground states and predict surface-driven effects in nanostructures
- Balance needs of accuracy and computational efficiency

Key Points

- Continuum methods already capture bulk behaviors efficiently and well
- Surface effects are extremely localized



Atomistic Model



- Atoms interact via nearest-neighbor, many-body forces
- 0-th atom held fixed

Site Energy Formulation in Terms of Strain

$$\mathcal{E}^{\mathrm{a}}(u) := V^{\mathrm{surf}}(u_0') + \sum_{\ell=1}^{\infty} V(u_{\ell-1}', u_\ell'),$$

- Strain represents change in reference bond length
- u is displacement, u' is displacement gradient (strain)

Site Energy Properties

Assumptions

(i) $V \in C^k(\mathbb{R}^2)$ and $V^{\mathrm{surf}} \in C^k(\mathbb{R})$ with $k \geq 3$;

(ii) V, V^{surf} and all permissible partial derivatives are bounded;

(iii) $V(0,0) = 0$;

(iv) $\partial^2 V(0,0) > 0$;

(v) $\inf_{\{|(r,s)|>\varepsilon\}} V(r,s) > 0$ for any $\varepsilon > 0$;

(vi) For any $s \in \mathbb{R}$, $\lim_{r\to\infty} V(r,s) = V^{\mathrm{surf}}(s)$.

Energy Cost of Surface

$$\inf_{s\in\mathbb{R}} V^{\mathrm{surf}}(s) > 0$$

Atomistic Problem

Space of Displacements

$$\mathcal{U} := \{u : \mathbb{Z}_{\geq 0} \to \mathbb{R} \mid u(0) = 0 \text{ and } u' \in \ell^2(\mathbb{Z}_{\geq 0})\}$$

- Finite-energy configurations
- Equip $\mathcal{U}$ with H^1-seminorm $|u|_{H^1} = \|u'\|_{\ell^2(\mathbb{Z}_{\geq 0})}$

Applied Forces

- $f : \mathbb{Z}_{\geq 0} \to \mathbb{R}$ with $f \in \mathcal{U}^*$
- Permanently applied, static forces

Atomistic Problem

Given a force $f \in \mathcal{U}^*$, we seek a minimizer

$$u^{\mathrm{a}} \in \arg\min\{\mathcal{E}^{\mathrm{a}}(u) - \langle f, u\rangle_{\mathbb{Z}_{\geq 0}} \mid u \in \mathcal{U}\}$$

Existence and Decay

Theorem (Existence)

There exists a minimizer of $\mathcal{E}^{\mathrm{a}} : \mathcal{U} \to \mathbb{R} \cup \{+\infty\}$.

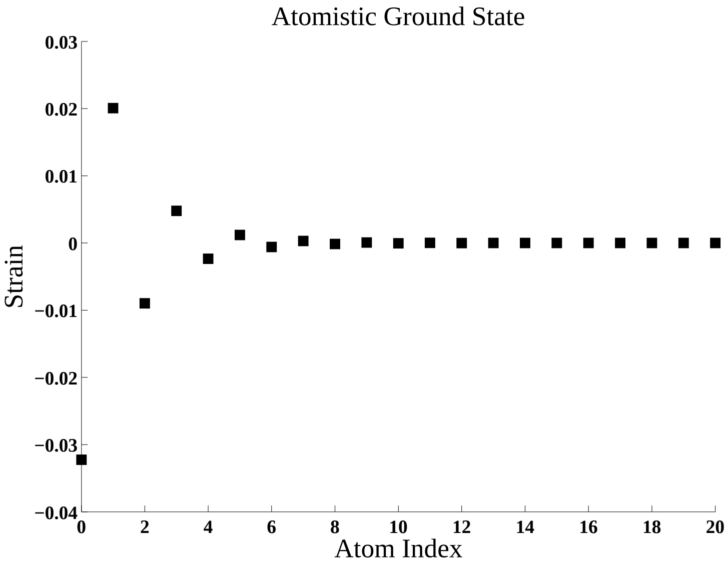
- No explicit solution in general
- Not necessarily unique

Theorem (Exponential Decay)

Let $u_{\mathrm{cr}}^{\mathrm{a}}$ *be a critical point of* $\mathcal{E}^{\mathrm{a}}$. *Then, there exists* $0 \leq \mu_{\mathrm{a}} < 1$ *such that*

$$|(u_{\mathrm{cr}}^{\mathrm{a}})'_{\ell}| \lesssim \mu_{\mathrm{a}}^{\ell} = e^{\log(\mu_a)\ell} \qquad \textit{for all} \quad \ell \in \mathbb{Z}_{\geq 0}.$$

Example of Surface Effects



Stability

- Assume that there exists an *atomistic stability constant* $c_a > 0$ such that

$$\langle \delta^2 \mathcal{E}^a(u^a_{gr}) v, v \rangle \geq c_a \| v' \|^2_{\ell^2(\mathbb{Z}_{\geq 0})} \quad \text{for all } v \in \mathcal{U}.$$

- An element $u^a \in \mathcal{U}$ is a strongly stable solution to the atomistic problem iff it satisfies the Euler-Lagrange equation

$$\langle \delta \mathcal{E}^a(u^a), v \rangle = \langle f, v \rangle \quad \text{for all } v \in \mathcal{U}$$

as well as the above stability condition.

Corollary

There exist $\varepsilon, C > 0$ such that, for all $f \in \mathcal{U}^*$ with $\|f\|_{\mathcal{U}^*} < \varepsilon$, the atomistic problem has a unique, strongly-stable solution with $\|(u^a - u^a_{gr})'\|_{\ell^2} \leq C \|f\|_{\mathcal{U}^*}$.

Cauchy-Born (Continuum) Model

- Derived from a limiting process involving the underlying lattice and potential

Energy

$$\mathcal{E}^{\mathrm{cb}}(u) := \int_0^\infty W(\nabla u(x))\,dx \quad \text{for } u \in \mathcal{U}^{\mathrm{cb}}, \quad \text{where } W(F) = V(F,F)$$

Space of Displacements

$$\mathcal{U}^{\mathrm{cb}} := \left\{ u \in H^1_{\mathrm{loc}}(0,\infty) \mid \nabla u \in L^2(0,\infty) \text{ and } u(0) = 0 \right\}$$

Cauchy-Born Problem

$$u^{\mathrm{cb}} \in \arg\min\{\mathcal{E}^{\mathrm{cb}}(u) - \langle f, u\rangle_{\mathbb{R}_+} \mid u \in \mathcal{U}^{\mathrm{cb}}\}$$

Error in Cauchy-Born Method

Proposition

The unique minimizer of $\mathcal{E}^{\mathrm{cb}}$ *in* $\mathcal{U}^{\mathrm{cb}}$ *is* $u^{\mathrm{cb}} = 0$. *Its atomistic residual is bounded by*

$$\sup_{v \in \mathcal{U}, \|v'\|_{\ell^2(\mathbb{Z}_{\geq 0})} = 1} |\langle \delta\mathcal{E}^{\mathrm{a}}(0), v \rangle| = \|\delta\mathcal{E}^{\mathrm{a}}(0)\|_{\mathcal{U}^*} = |\partial_F V^{\mathrm{surf}}(0)|.$$

In particular, $\|(u^{\mathrm{a}}_{\mathrm{gr}} - u^{\mathrm{cb}})'\|_{\ell^2} \geq M^{-1} |\partial_F V^{\mathrm{surf}}(0)|$, *where* M *is the global Lipschitz constant of* $\delta\mathcal{E}^{\mathrm{a}}$.

Corrector Model

Given *predictor* u^{cb}, let

$$\mathcal{E}^{\Gamma}(q; F_0) = V^{\mathrm{surf}}(F_0 + q_0') - W(F_0) - q_0' \partial_F W(F_0) + \sum_{j=1}^{\infty} \Big(V(F_0 + q_{j-1}', F_0 + q_j') - W(F_0) - q_j' \partial_F W(F_0) \Big) ,$$

where $F_0 := \nabla u^{\mathrm{cb}}(0)$.

Corrector Problem

For $L \in \mathbb{N} \cup \{\infty\}$, corrector strain on $[0, L]$ is found by solving

$$q_L \in \arg\min\{\mathcal{E}^{\Gamma}(q; F_0) \mid q \in \mathcal{Q}_L\},$$

where

$$\mathcal{Q}_L := \{q \in \mathcal{U} \mid q_\ell' = 0 \text{ for all } \ell \geq L\}. \quad \text{In particular,} \quad \mathcal{Q}_\infty = \mathcal{U}.$$

Predictor-Corrector Solution

- For $\|f\|_{\mathcal{U}^*}$ sufficiently small and L sufficiently large, solutions exist for the Cauchy-Born and corrector problems

Predictor-Corrector Solution

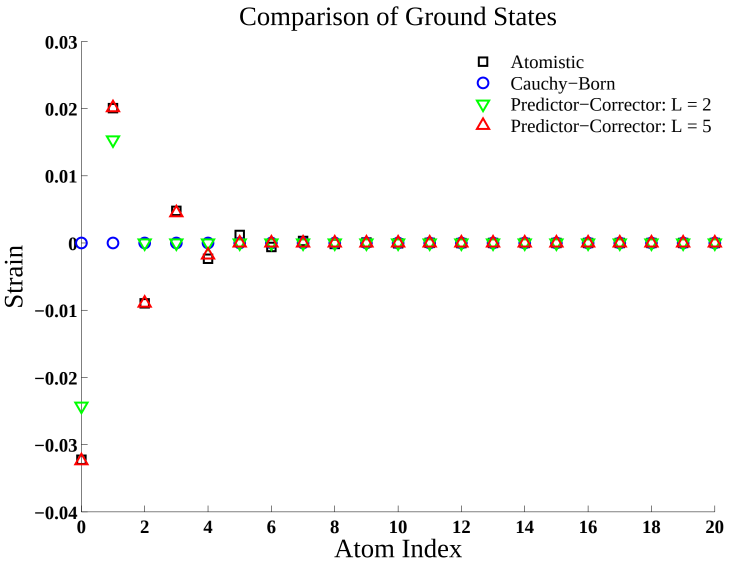
$$u_L^{\mathrm{pc}} := \Pi_{\mathrm{a}} u^{\mathrm{cb}} + q_L$$

Theorem

There exists an $\varepsilon > 0$ such that, for all $f \in \mathcal{U}^*$ with $\|f\|_{\mathcal{U}^*} < \varepsilon$, there exists an atomistic solution $u^{\mathrm{a}} \in \mathcal{U}$ to the atomistic problem satisfying

$$\left\|(u^{\mathrm{a}})' - (u_L^{\mathrm{pc}})'\right\|_{\ell^2} \lesssim \mu_q^L + |\nabla^2 u^{\mathrm{cb}}(0)| + \|\nabla^2 u^{\mathrm{cb}}\|_{L^4}^2 + \|\nabla^3 u^{\mathrm{cb}}\|_{L^2} + \|\nabla f\|_{L^2}.$$

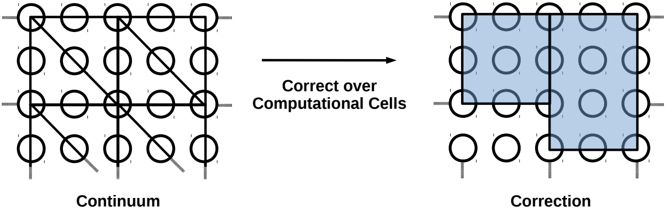
Ground States



Higher Dimensions

Computational Cells

- Tangential periodic boundary conditions
- Apply uniform strain from surface elements
- Additional approximations possible



Conclusion

- Surface effects are extremely localized
- Cauchy-Born method can be post-processed to capture surface effects
- Error analysis is sharp

Theorem

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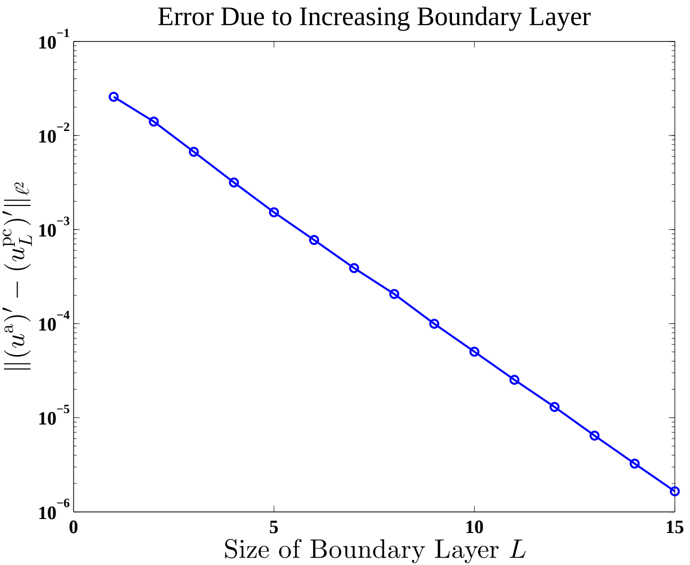
Exponential Convergence Due to Surface Error



Long Wavelength Limit

Error estimate in terms of force:

$$\left\|(u^{\mathrm{a}})' - (u_L^{\mathrm{pc}})'\right\|_{\ell^2} \lesssim \mu_q^L + |f(0)| + \|f\|_{L^4}^2 + \|\nabla f\|_{L^2}$$

Let λ^{-1} denote a length-scale over which we expect elastic strains to vary. Consider

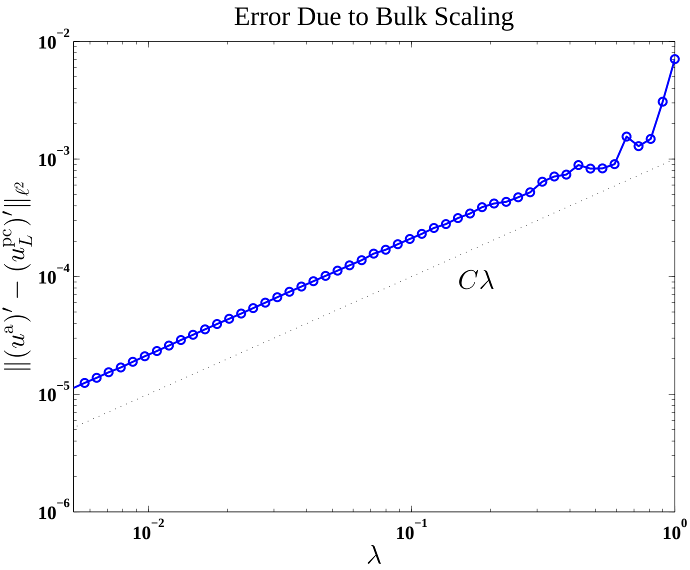
$$f_\ell^{(\lambda)} := \lambda \hat{f}(\lambda \ell).$$

Then,

$$\left\|(u^{\mathrm{a}})' - (u_L^{\mathrm{pc}})'\right\|_{\ell^2} \lesssim \mu_q^L + \lambda + \lambda^{3/2}.$$

Define $\hat{f}(x) = \cos(3\pi x/8)\chi_{[0,4)}(x)$, where $\chi_A(x)$ denotes the characteristic function, and $f_\ell = \lambda \hat{f}(\lambda \ell)$.

Long Wavelength Error



Residual Error in Presence of Forces