Optimising Multiscale Defect Computations

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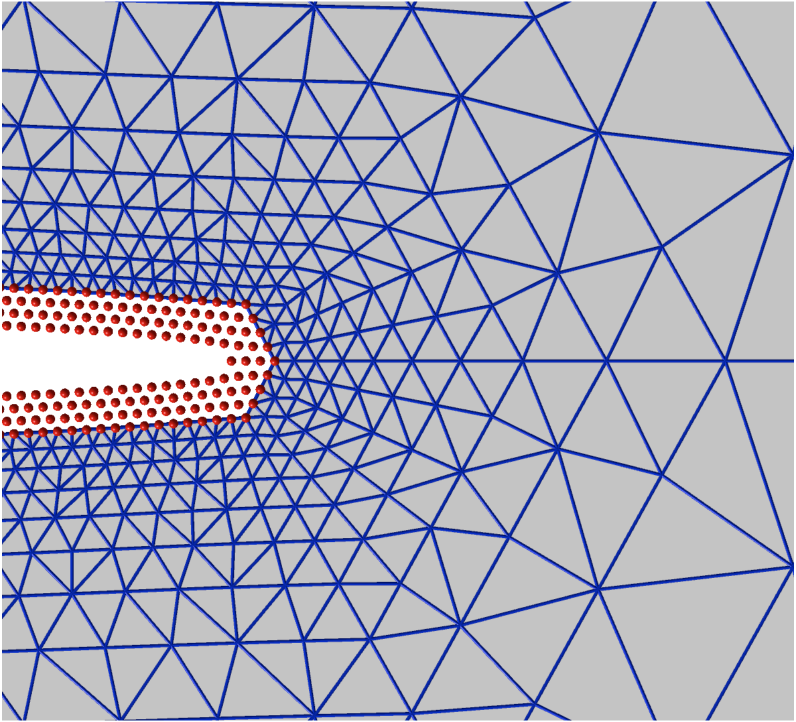

The A/C Team

- **Amhurst:** Matthew Dobson
- **Brown:** Xingjie (Helen) Li
- **Crete:** Charalambos Makridakis
- **Jiaotong:** Lei Zhang
- **Minneapolis:** **Mitch Luskin**, Alex Shapeev (previously Lausanne), Andrew Binder, Derek Olsen
- **UCLA:** Brian Van Koten
- **Oxford:** Endre Süli, Hao Wang, Tom Hudson
- **Warwick:** Florian Theil, CO, Dave Packwood

Continuum Mechanics and Molecular Mechanics

Continuum Elastostatics:

- Reference domain $\Omega \subset \mathbb{R}^d$
- Displacement $u : \Omega \to \mathbb{R}^d$

$$\min E^{c}(u) - (f, u)_{\Omega} := \int_{\Omega} W(\nabla u)\, \mathrm{d}x - \int_{\Omega} f \cdot u \, \mathrm{d}x$$

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Molecular Statics:

- Refence domain $\rightsquigarrow$ **index set**: $\Lambda \subset \mathbb{Z}^d$
- Displacement: $u : \Lambda \to \mathbb{R}^d$

$$\min E^{\mathrm{a}}(u) - (f, u)_\Lambda := \sum_{\xi \in \Lambda} V\big(Du(\xi)\big) - \sum_{\xi \in \Lambda} f(\xi) \cdot u(\xi)$$

Continuum Mechanics and Molecular Mechanics

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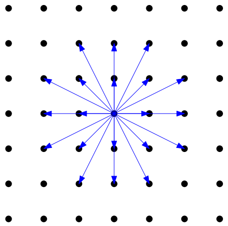


- $Du(\xi) := \{u(\xi + \rho) - u(\xi)\}_{\rho \in \mathbb{Z}^d}$
- $V(Du(\xi))$ = energy of atom ξ

Admissible Interaction Potentials

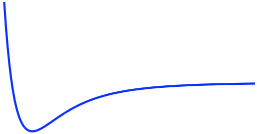
$$E^{\mathrm{a}}(u) = \sum_{\xi \in \Lambda} V\big(Du(\xi)\big)$$

$y := \Lambda + u$

- **Pair potentials:**

  $$E_{\mathrm{a}}(y) = \sum_{(i,j)} \phi(r_{ij}) = \sum_i \frac{1}{2} \sum_{j \neq i} \phi(r_{ij})$$

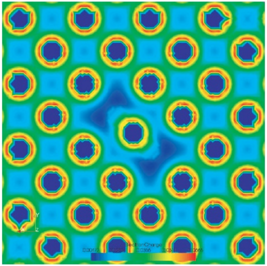
  $r_{ij} = |y_i - y_j|,$



$\phi(r) = r^{-12} - 2r^{-6}$

- **Embedded atom method:**

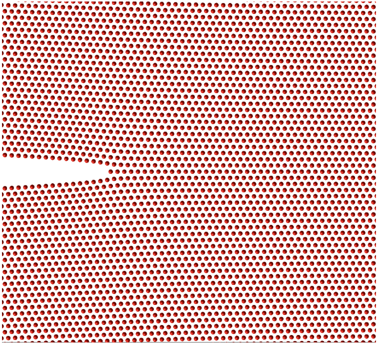
  $$E_{\mathrm{a}}(y) = \sum_i \left[\frac{1}{2} \sum_j \phi_2(r_{ij}) + F\Big(\textstyle\sum_j \rho(r_{ij}) \Big) \right]$$

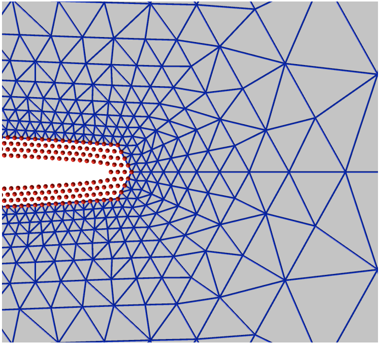


- $\angle$-Potentials, BOPs, GAPs, ...
- ~~Coulomb, DFT~~

Coarse-Graining

Applications: defect energies, defect interaction, void growth, crack growth, ...



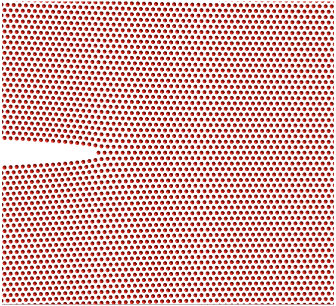


Treat coarse graining as a numerical analysis problem.

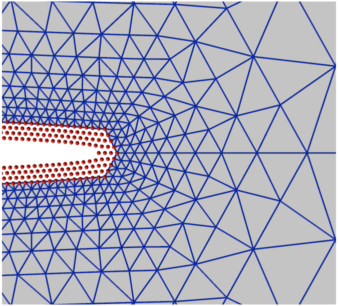
"Early" Results:

- Blanc, Le Bris, Lions (2002), Blanc, Le Bris, Legoll (2005)
- Lin (2003, 2007), CO, Süli (2008), Dobson, Luskin (2008)

Mathematical Question



$y^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}$



$y^{\mathrm{ac}} \in \arg\min E^{\mathrm{ac}}$

Can we talk about **error versus computational cost** in a meaningful way?

$$\|y^{\mathrm{a}} - y^{\mathrm{ac}}\|_{?} \lesssim (\mathrm{WORK})^{-R}$$

$$|E^{\mathrm{a}}(y^{\mathrm{a}}) - E^{\mathrm{ac}}(y^{\mathrm{ac}})| \lesssim (\mathrm{WORK})^{-S}$$

other quantities of interest? which norms?

Along the way learn how to **optimally** implement a/c coupling methods?

Strategy

1. Formulate well-posed model problem, precise mathematical question.
2. Estimate error of multiscale method in terms of approximation parameters.
3. Optimise choice of approximation parameter to reduce the error estimate to $\mathrm{ERROR} \lesssim \mathrm{WORK}^{-R}$
4. Implement the optimised scheme and check that the prediction is correct.

Model Problem

- Reference domain:

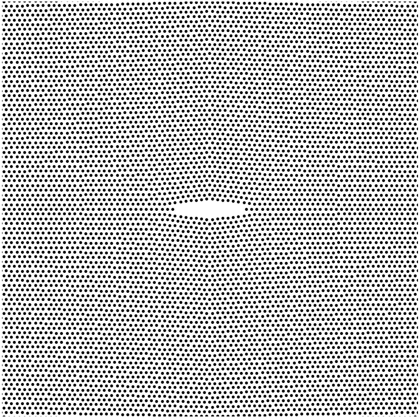
  $\Lambda := \mathsf{A} \cdot \mathbb{Z}^2 \setminus \text{crack}$

- Admissible displacements:

$$\mathscr{U} := \{ u : \Lambda \to \mathbb{R}^2, \|\nabla u\|_{L^2} < \infty, \; u(\xi) \sim 0 \text{ as } |\xi| \to \infty \},$$

  (space of finite energy displacements)

- Energy-difference functional:



$$E^{\mathrm{a}}(u) := \sum_{\xi \in \Lambda} \Big(V\big(D(\mathrm{id}+u)(\xi)\big) - V\big(D\mathrm{id}(\xi)\big) \Big)$$

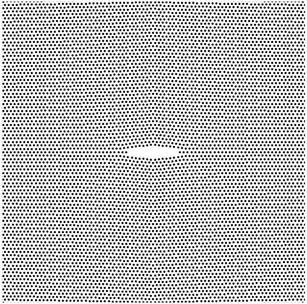
$$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$$

Since $\dim \mathscr{U} = \infty$, u^{a} is not directly computable!

(Notes: atomic spacing $= O(1)$; $\nabla u =$ gradient of a smooth interpolant; similar for ∇^2.)

Approximation Strategy

Approximations: rest of the talk, understand these approximations

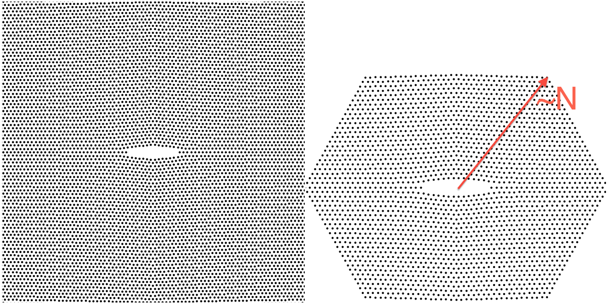


$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$

Approximation Strategy

Approximations: rest of the talk, understand these approximations

1. Reduction to finite domain (far-field boundary condition)

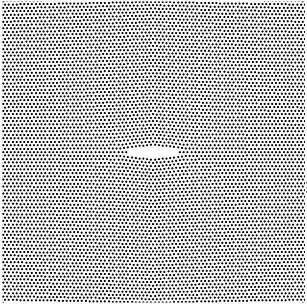


$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$ $\quad$ $u^{\mathrm{a}}_N \in \arg\min E^{\mathrm{a}}(\mathscr{U}_N)$

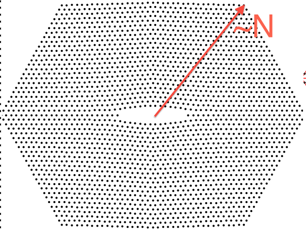
Approximation Strategy

Approximations: rest of the talk, understand these approximations

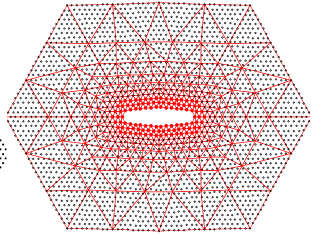
1. Reduction to finite domain (far-field boundary condition)
2. Remove degrees of freedom (coarsening error)



$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$



$u^{\mathrm{a}}_N \in \arg\min E^{\mathrm{a}}(\mathscr{U}_N)$

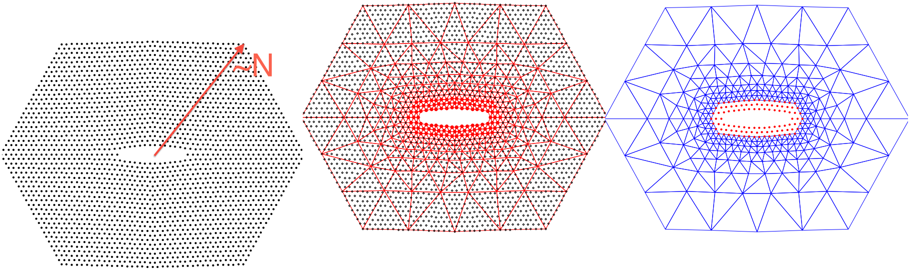


$u^{\mathrm{a}}_h \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$

Approximation Strategy

Approximations: rest of the talk, understand these approximations

1. Reduction to finite domain (far-field boundary condition)
2. Remove degrees of freedom (coarsening error)
3. Replace atomistic with continuum model (model error)

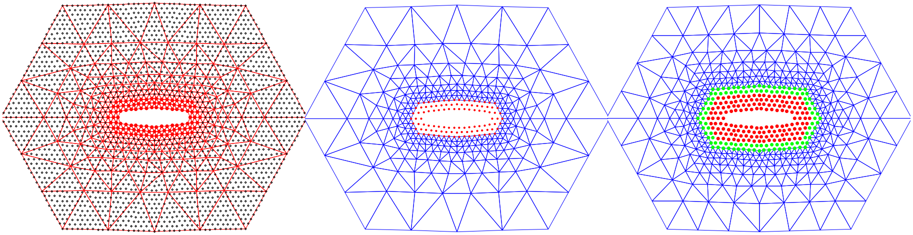


$u_N^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}_N)$ $u_h^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$ $u^{\mathrm{ac}} \in \arg\min E^{\mathrm{ac}}(\mathscr{U}_h)$

Approximation Strategy

Approximations: rest of the talk, understand these approximations

1. Reduction to finite domain (far-field boundary condition)
2. Remove degrees of freedom (coarsening error)
3. Replace atomistic with continuum model (model error)
4. **Interface correction**



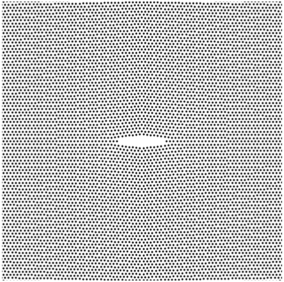
$u_h^{\rm a} \in \arg\min E^{\rm a}(\mathscr{U}_h)$ $u^{\rm ac} \in \arg\min E^{\rm ac}(\mathscr{U}_h)$ $u^{\rm ac+} \in \arg\min E^{\rm ac+}(\mathscr{U}_h)$

Approx. 1: Reduction to a Finite-Dimensional Space

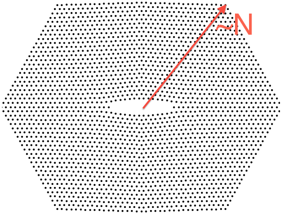
$$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$$

Since $\dim \mathscr{U} = \infty$, u^{a} is not directly computable!

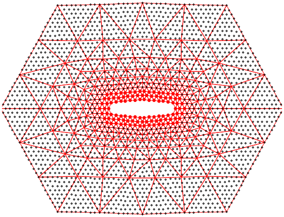
- Choose a finite-dimensional subspace $\mathscr{U}_h \subset \mathscr{U}$



$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$



$u^{\mathrm{a}}_N \in \arg\min E^{\mathrm{a}}(\mathscr{U}_N)$

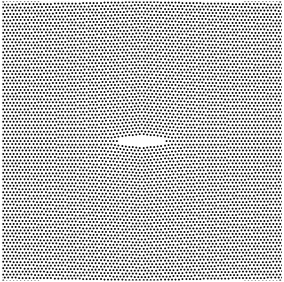


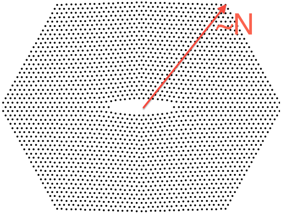
$u^{\mathrm{a}}_h \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$

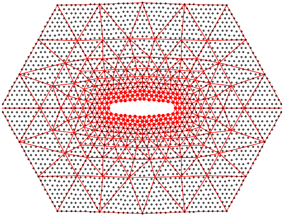
= **Galerkin Projection**

Theorem: Let u^{a} be stable and $\mathrm{dist}(u^{\mathrm{a}}, \mathscr{U}_h)$ sufficiently small, then there exists $u^{\mathrm{a}}_h \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$ such that the best approximation property holds: $\|\nabla u^{\mathrm{a}} - \nabla u^{\mathrm{a}}_h\|_{L^2} \lesssim \inf_{v_h \in \mathscr{U}_h} \|\nabla u^{\mathrm{a}} - v_h\|_{L^2}$

Analysis of the Best Approximation Error







1. **Decay of elastic field (Assumption):** (rigorous justification?)

$$|\nabla u^{\mathrm{a}}(x)| \lesssim |x|^{-2}, \qquad |\nabla^2 u^{\mathrm{a}}(x)| \lesssim |x|^{-3} \qquad \text{as } |x| \to \infty.$$

2. **Far-field error:**

$$\|\nabla u^{\mathrm{a}} - \nabla(\eta_N u^{\mathrm{a}})\|_{L^2} \lesssim \|\nabla u^{\mathrm{a}}\|_{L^2(\mathbb{R}^d \setminus B_{N/2})} \lesssim N^{-1}$$

3. **Finite element error:**

$$\|\nabla u^{\mathrm{a}} - \nabla I_h(\eta_N u^{\mathrm{a}})\|_{L^2} \lesssim \|h \nabla^2 u^{\mathrm{a}}\|_{L^2(\Omega^{\mathrm{c}})} + N^{-1}$$

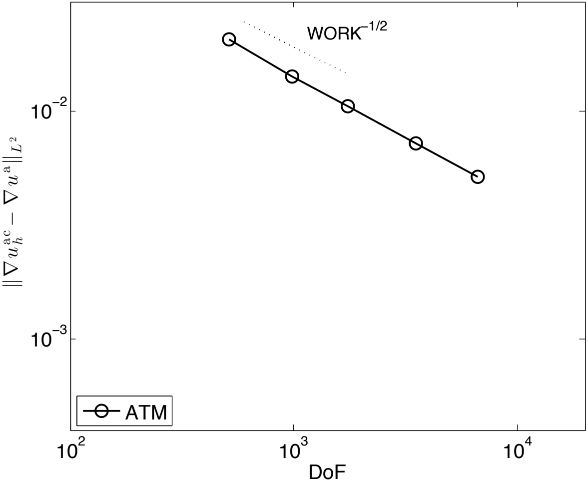
Reference: Direct Atomistic Simulation

$$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}), \qquad u^{\mathrm{a}}_N \in \arg\min E^{\mathrm{a}}(\mathscr{U}_N).$$

Theorem: If N is suff. large then $\exists\, u^{\mathrm{a}}_N \in \arg\min E^{\mathrm{a}}(\mathscr{U}_N)$ s.t.

$$\|\nabla u^{\mathrm{a}} - \nabla u^{\mathrm{a}}_N\|_{L^2} \lesssim N^{-1} \approx \mathrm{WORK}^{-1/2}$$

Di-Vacancy under shear and stretch

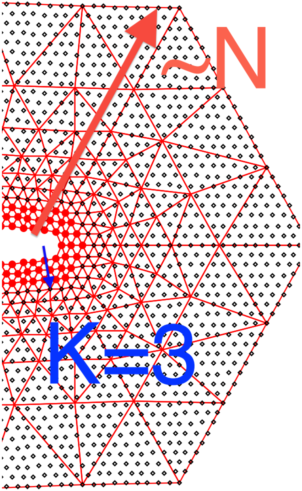


Optimising the Finite Element Mesh

$$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}), \qquad u_h^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h).$$

Then, we conjecture that

$$\|\nabla u^{\mathrm{a}} - \nabla u_h^{\mathrm{a}}\|_{L^2} \lesssim \|h\nabla^2 u^{\mathrm{a}}\|_{L^2(\mathbb{R}^d \setminus B_K)} + N^{-1}.$$



1. Fix K, N, assume $|\nabla^2 u^{\mathrm{a}}| \sim |x|^{-3}$, optimise h:

$$h(x) \approx \left(\frac{|x|}{K}\right)^{3/2}$$

$$\Rightarrow \quad \|h\nabla^2 u^{\mathrm{a}}\|_{L^2(\mathbb{R}^d \setminus B_K)} \approx \left(\int_K^N r r^{-6} \left(\tfrac{r}{K}\right)^3 \mathrm{d}r\right)^{1/2}$$

$$\approx K^{-2}.$$

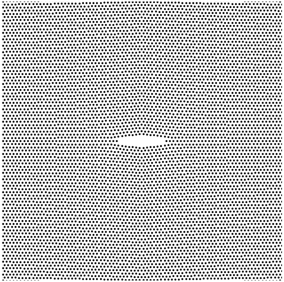
2. Can now bound best approx. error:

$$\mathrm{dist}(\nabla u^{\mathrm{a}}, \mathscr{U}_h) \lesssim K^{-2} + N^{-1}.$$

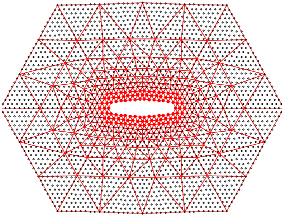
Now balance the finite element and far-field error: $N \sim K^2$.

$$\mathrm{dist}(\nabla u^{\mathrm{a}}, \mathscr{U}_h) \lesssim K^{-2} \approx N^{-1}.$$

The first multiscale scheme



$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U})$

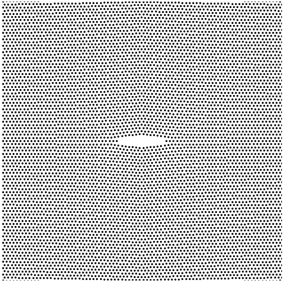


$u_h^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$

Theorem: Let K be given, $N \approx K^2$ and $h(x) \approx (|x|/K)^{3/2}$. Then, for K sufficiently large, there exists $u_h^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$, s.t.

$$\|\nabla u^{\mathrm{a}} - \nabla u_h^{\mathrm{a}}\|_{L^2} \lesssim K^{-2} \approx N^{-1} \approx \mathrm{DOF}^{-1}$$

The first multiscale scheme



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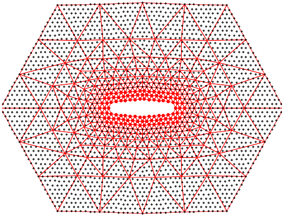

$u^{\mathrm{a}}_h \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h)$

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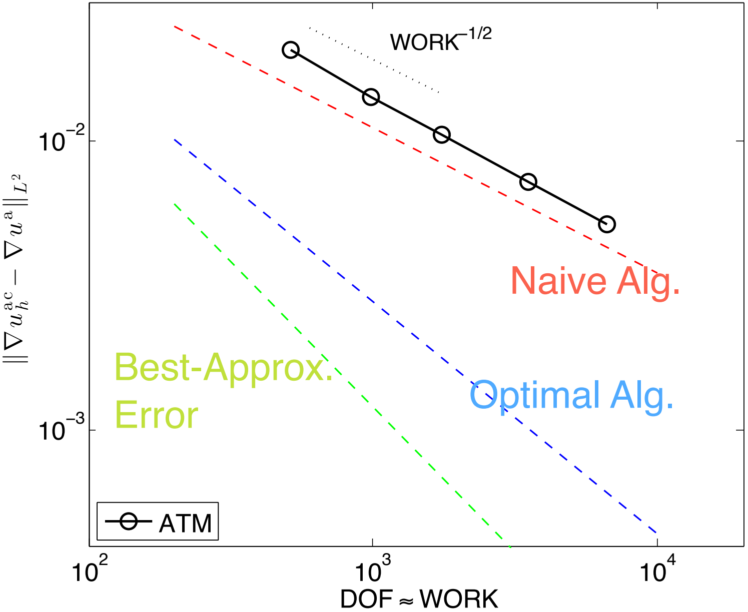
$$\|\nabla u^{\mathrm{a}} - \nabla u^{\mathrm{a}}_h\|_{L^2} \lesssim K^{-2} \approx N^{-1} \approx \mathrm{DOF}^{-1}$$

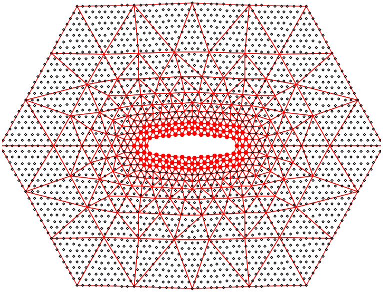
BUT: $\mathrm{DOF} \not\approx \mathrm{WORK}$! With a naive algorithm, $\mathrm{WORK} \approx N^2$

(with "optimal" algorithm $\mathrm{WORK} \approx N^{5/4}$, but near-impossible to implement)

Hypothetical $\mathrm{WORK} = \mathrm{DOF}$ algorithm



What about quadrature?



Luskin, CO (2009):

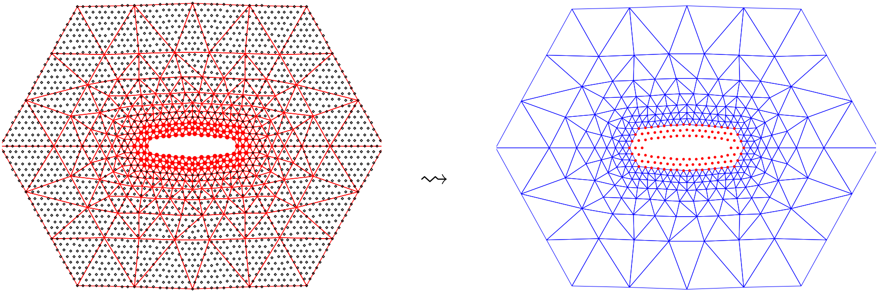
- element-based quadrature ⇝ effectively Cauchy–Born approximation ⇝ rest of the talk
- node-based quadrature is inconsistent (unless one applies expensive pre-processing techniques [Eidel/Stuchowsky, 2009])

A/C Coupling Methods (a selection)

1. **Ancestors**
   - Tewari (1973), Mullins (1982), Kohlhoff, Schmauder, Gumbsch (1989, 1991)
   - Quasicontinuum method: Tadmor, Phillips, Ortiz (1995)
2. **Force-based coupling**
   - Dead-load GF removal: Shenoy, Miller, Rodney, Tadmor, Phillips, Ortiz (1999)
   - AtC: Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2007, . . .)
   - CADD: Shilkrot & Curtin & Miller (2002, . . .)
   - Force-based A/C: Dobson/Luskin (2008), Dobson/Luskin/CO (2010)
   - Stress-based A/C: Makridakis/CO/Süli (2011); . . .
3. **Quadrature approaches**
   - Knap/Ortiz (2003), Eidel/Stuchowski (2009), Gunzburger/Zhang (2010,2011), Lin (2007)
   - Luskin/CO (2009): analysis
4. **Blending methods**
   - Overlapping domains: Belytschko & Xiao (2004), Klein & Zimmerman (2006), Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2008)
   - Conservative: Van Koten, Luskin (2011); Luskin, CO, Van Koten (2012)
   - Force-blending: Lu, Ming (preprint); Li, Luskin, CO (2012); . . .
5. **Ghost Force Removal**:
   - Geometry reconstruction: Shimokawa *et al* (2003), E, Lu, Yang (2006) CO (2012); CO, Zhang (preprint)
   - Other ideas: Shapeev (2012); CO, Shapeev (2012), Iyer, Gavini (2010)

Original Quasicontinuum Method

[Tadmor, Phillips, Ortiz, 1995]



- **QCE Method:** apply CB approximation in each blue triange

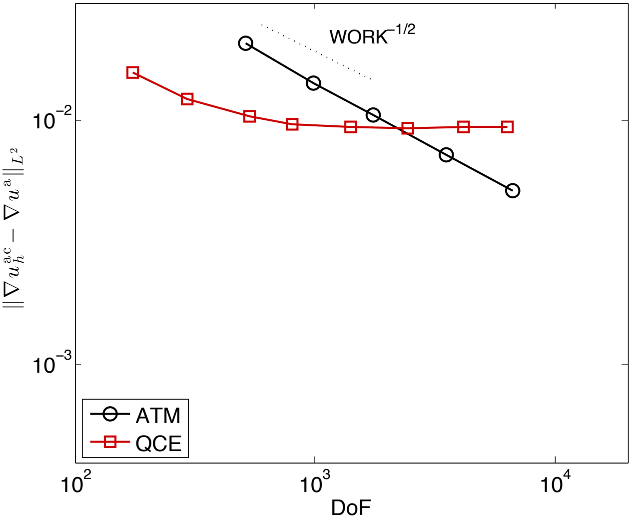
$$E^{\mathrm{a}}(u_h) \approx E^{\mathrm{qce}}(u_h) := \sum_{\xi \in \Lambda^{\mathrm{a}}} V\big(Du_h(\xi)\big) + \sum_{T \subset \Omega^{\mathrm{c}}} \mathrm{vol}[T]\, W(\nabla u_h|_T)$$

where $W(\mathsf{F}) = V(\mathsf{F} \cdot \mathbb{Z}^d)$ (Cauchy–Born stored energy density)

WORK: $\#\Lambda^{\mathrm{a}} + \#\{T\}$

Accuracy of QCE

For QCE $\text{WORK} \approx \text{DOF}$!



Failure of "Patch Test"

Test Problem: $\Lambda := \mathsf{A} \cdot \mathbb{Z}^d$ (no defect, no external forces)

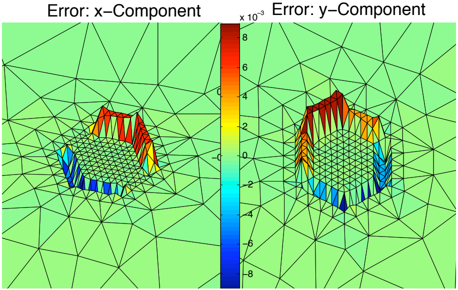
$$\min E^{\rm qce}(u_h) := \sum_{\xi \in \Lambda^{\rm a}} V(Du_h(\xi)) + \int_{\Omega^{\rm c}} W(\nabla u_h)\,{\rm d}x$$

QCE fails the **patch test**:

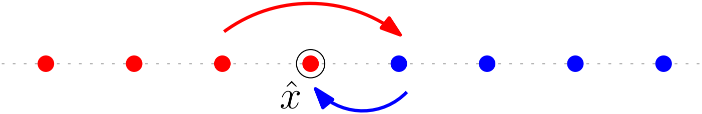
$$\delta E^{\rm a}(0) = 0$$

$$\delta E^{\rm c}(0) = 0,$$

$$\delta E^{\rm qce}(0) \neq 0 \text{ !}$$



Explanation: interaction asymmetry across interface



The Fundamental Theorem of Numerical Analysis (1)

Theorem (Lax/Richtmyer, 1956):
CONVERGENCE $\Leftrightarrow$ STABILITY + CONSISTENCY

$$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}) \;\rightsquigarrow\; u_h^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}_h) \;\rightsquigarrow\; u_h^{\mathrm{ac}} \in \arg\min E_h^{\mathrm{ac}}(\mathscr{U}_h)$$

ERROR EQUATION

Definition: The **consistency error** associated with u^{a} is defined by

$$\eta_h^{\mathrm{ac}}(u^{\mathrm{a}}) := \big\|\delta E^{\mathrm{a}}(u^{\mathrm{a}}) - \delta E_h^{\mathrm{ac}}(u^{\mathrm{a}})\big\|_{\mathscr{U}_h^*} := \sup_{\substack{v_h \in \mathscr{U}_h \\ \|\nabla v_h\|_{L^2}=1}} \big\langle \delta E^{\mathrm{a}}(u^{\mathrm{a}}) - \delta E_h^{\mathrm{ac}}(u^{\mathrm{a}}), v_h \big\rangle$$

Theorem ($\not\Leftarrow$): Suppose that $\|\delta^2 E_h^{\mathrm{ac}}\| \leq C$, then

$$\|\nabla u^{\mathrm{a}} - \nabla u_h^{\mathrm{ac}}\|_{L^2} \geq C^{-1}\big[\mathrm{dist}(u^{\mathrm{a}}, \mathscr{U}_h) + \eta_h^{\mathrm{ac}}(u^{\mathrm{a}})\big].$$

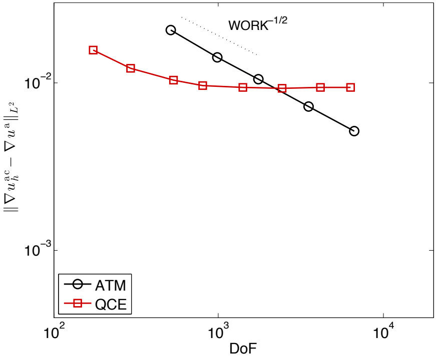
In-Consistency of QCE

Proposition: $\eta_h^{\mathrm{qce}}(u^{\mathrm{a}}) \gtrsim 1$

Proof: force error = O(1) at a/c interface

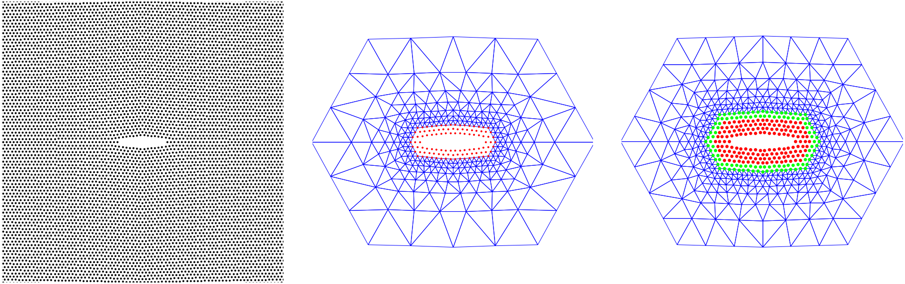
- 1D, linear, NNN: Dobson, Luskin (2009)
- any dimension, NNN: folklore

(Inconsistency: No approximation parameter drives this QCE error to zero.)



A General Class of A/C Coupling Methods

How can we remove the interface error? Shimokawa et al (2003)



$$E^{\rm ac}(u_h) = \sum_{\xi\in\Lambda^{\rm a}} V(Du_h(\xi)) + \sum_{\xi\in\Lambda^{\rm i}} \tilde{V}_\xi(Du_h(\xi)) + \int_{\Omega^{\rm c}} W(\nabla u_h)\,{\rm d}x$$

How should we choose $\tilde{V}_\xi$?

1. Cheap: $\mathrm{WORK} \approx \mathrm{DOF}$!; 2. Improve over QCE accuracy!

The Patch Tests:

$$E^{\mathrm{ac}}(u_h) = \sum_{\xi \in \Lambda^{\mathrm{a}}} V(Du_h(\xi)) + \sum_{\xi \in \Lambda^{\mathrm{i}}} \tilde{V}_\xi(Du_h(\xi)) + \int_{\Omega^{\mathrm{c}}} W(\nabla u_h) \,\mathrm{d}x$$

1. Energy Consistency: "$E^{\mathrm{ac}}(u) \approx E^{\mathrm{a}}(u)$"

$$E^{\mathrm{ac}}(\mathsf{F}x) = E^{\mathrm{a}}(\mathsf{F}x) \qquad \forall \mathsf{F} \in \mathbb{R}^{d \times d} \qquad \text{(E)}$$

Note $\tilde{V}_\xi = V$ gives QCE, so (E) is not sufficient!

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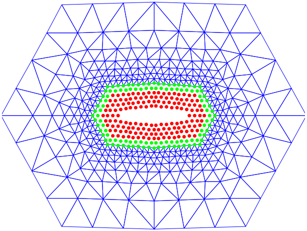

2. Force Consistency: "$\delta E^{\mathrm{ac}}(u) \approx \delta E^{\mathrm{a}}(u)$"

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

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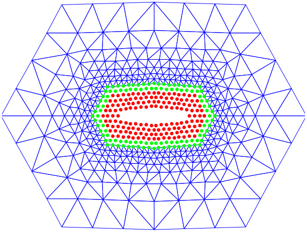

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Constructions of $\tilde{V}_\xi$ s.t. (E) and (F) are satisfied?

- Shimokawa et al (2003), E/Lu/Yang (2006), CO/Zhang (2012)
- Alternative approaches: Shapeev (2011, 2012), Iyer/Gavini (2011)

The Fundamental Theorem of Numerical Analysis (2)

Theorem (Lax/Richtmyer, 1956):
CONVERGENCE $\Leftrightarrow$ STABILITY + CONSISTENCY

$$u^{\mathrm{a}} \in \arg\min E^{\mathrm{a}}(\mathscr{U}) \qquad u_h^{\mathrm{ac}} \in \arg\min E_h^{\mathrm{ac}}(\mathscr{U}_h)$$

recall consistency error: $\eta_h^{\mathrm{ac}}(u^{\mathrm{a}}) := \big\|\delta E^{\mathrm{a}}(u^{\mathrm{a}}) - \delta E_h^{\mathrm{ac}}(u^{\mathrm{a}})\big\|_{\mathscr{U}_h^*}$

Theorem ($\Leftarrow$): Let u^{a} be stable in the a/c model, i.e., $\exists\gamma > 0$ s.t.

$$\langle \delta^2 E_h^{\mathrm{ac}}(u^{\mathrm{a}}) v_h, v_h\rangle \geq \gamma \|\nabla v_h\|_{L^2}^2.$$

and suppose that $\mathrm{dist}(u^{\mathrm{a}}, \mathscr{U}_h) + \eta_h^{\mathrm{ac}}(u^{\mathrm{a}})$ are sufficiently small; then there exists $u_h^{\mathrm{ac}} \in \arg\min E_h^{\mathrm{ac}}(\mathscr{U}_h)$ such that

$$\|\nabla u^{\mathrm{a}} - \nabla u_h^{\mathrm{ac}}\|_{L^2} \lesssim \gamma^{-1}\big[\mathrm{dist}(u^{\mathrm{a}}, \mathscr{U}_h) + \eta_h^{\mathrm{ac}}(u^{\mathrm{a}})\big]$$

Consistency of QNL-type Methods

From the Fundamental Theorem, and the best-approximation error analysis, we conjecture

$$\|\nabla u^{\mathrm{a}} - \nabla u_h^{\mathrm{ac}}\|_{L^2} \lesssim \|h\nabla^2 u^{\mathrm{a}}\|_{L^2(\Omega^{\mathrm{c}})} + \eta_h^{\mathrm{ac}}.$$

Theorem: [CO; 2012], [CO, Shapeev; preprint], [CO, Zhang; in prep.]

Suppose that E_h^{ac} satisfies **(F)** and **(E)** * * *, then

$$\eta_h^{\mathrm{ac}}(u^{\mathrm{a}}) \lesssim \|\nabla^2 u^{\mathrm{a}}\|_{L^2(\Omega^{\mathrm{c}})}.$$

$\rightsquigarrow$ ideal situation that the consistency error is dominated by the best-approximation error!

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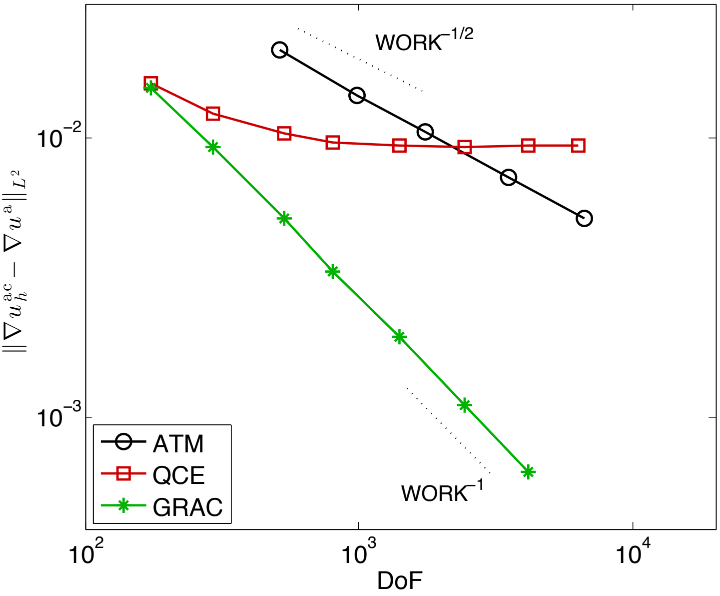
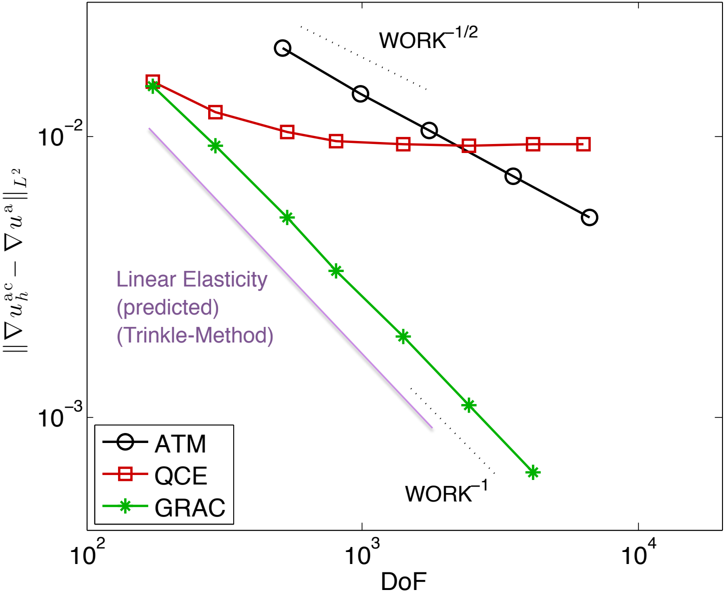
Corollary: Suppose that E_h^{ac} satisfies conditions of previous theorem, that it is **stable** (work in progress), and that $h = h(K), N = N(K)$ are chosen as before. Then, for K sufficiently large, there exists $u_h^{\mathrm{ac}} \in \arg\min E_h^{\mathrm{ac}}(\mathscr{U}_h)$ such that

$$\|\nabla u^{\mathrm{a}} - \nabla u_h^{\mathrm{ac}}\|_{L^2} \lesssim K^{-2} \approx \mathrm{DOF}^{-1} \approx \mathrm{WORK}^{-1}.$$

Numerical Experiment



Nonlinear versus Linear Elasticity



What is there left to do?

QNL-type methods are extremely difficult to construct in general. At the moment, they are practical methods for:

- 1D
- 2D, pair interactions (3D pair for the adventurous [Shapeev, 2012])
- 2D, first-neighbour many-body interactions
  (probably 2D, up to 3rd, 4th neighbours is ok [work in progress])
- 3D, interfaces without corners

A more practical alternative at present are **blending methods**:
[Xiao, Belytschko; 2003, 2004]
[Luskin, Vankoten; 2011], [Luskin, CO, Vankoten; 2012]

Fun Fact

If we can "spread" an error, then we control it in ℓ^2:

$$g(\xi) := \begin{cases} K^{-1}, & \xi = 1, \dots, K \\ 0, & \text{o.w.} \end{cases}$$

$$\Rightarrow \quad \|g\|_{\ell^2} = \left(\sum_{\xi=1}^{K} K^{-2} \right)^{1/2} = K^{-1/2}.$$

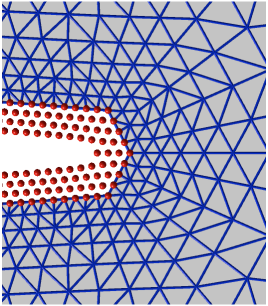
By constrast:

$$\|g\|_{\ell^1} = \sum_{\xi=1}^{K} K^{-1} = 1.$$

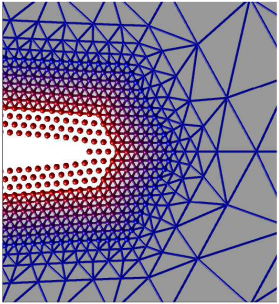
Blending

Belytschko & Xiao (2004)

Idea: Spread the interface ⇒ spread the error?



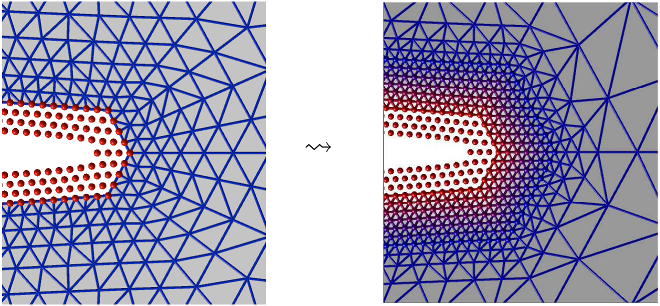
$\rightsquigarrow$



Blending

Belytschko & Xiao (2004)

Idea: Spread the interface $\Rightarrow$ spread the error?



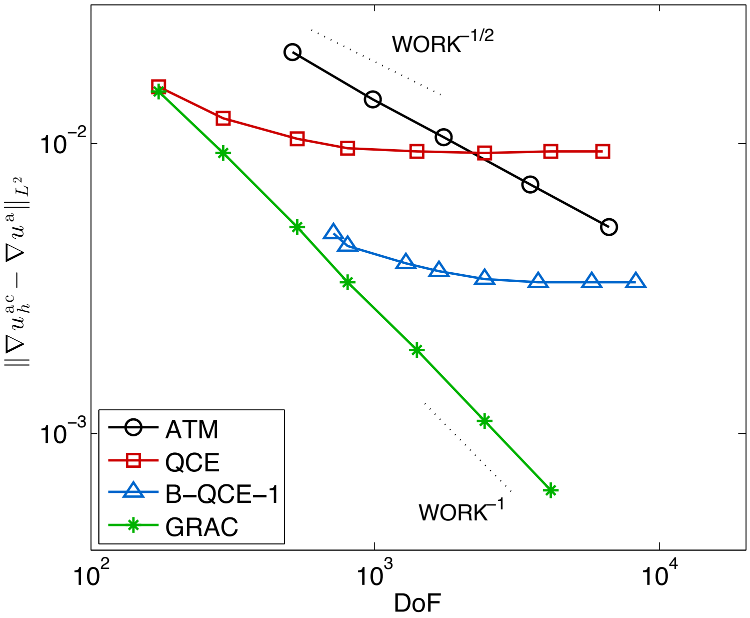
$$E^b(u_h) := \sum_{\xi \in \Lambda^{\mathrm{a}}} \beta(\xi) V(Du_h(\xi)) + \int_{\Omega^{\mathrm{c}}} (1-\beta) W(\nabla u_h)\,\mathrm{d}x$$

β = "smooth" blending function

[Luskin, Vankoten; 2011]
[Luskin, VanKoten, CO (2012)]

Approximation Parameters: $K, N, \mathscr{T}_h, \beta$

Numerical Experiment



Consistency of Blending

$$u_h^b \in \arg\min E^b(\mathscr{U}_h)$$

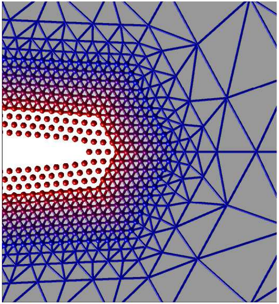
$$E^b(u_h) := \sum_{\xi \in \Lambda^{\mathrm{a}}} \beta(\xi) V(Du_h(\xi)) + \int_{\Omega^{\mathrm{c}}} (1-\beta) W(\nabla u_h) \,\mathrm{d}x$$

Theorem: 1D: Van Koten, Luskin (2012); dD: CO, Van Koten (in prep)

$$\eta_h^b(u^{\mathrm{a}}) \lesssim \|\nabla^2 \beta\|_{L^2} + \|\nabla^2 u^{\mathrm{a}}\|_{L^2(\Omega^c \cup \Omega^b)}$$

This tells us how to optimally choose β!

Optimal Blending



K atomistic layers
$L-K$ blending layers
rest is continuum

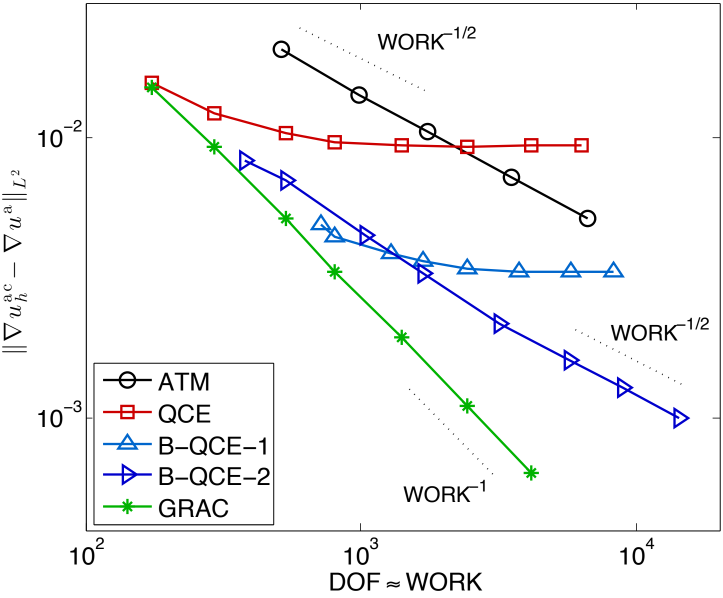
$$\mathrm{WORK} \approx \mathrm{DOF} \approx L^2.$$

$$\begin{aligned}\mathrm{ERR}^2 &\lesssim \|\nabla^2\beta\|_{L^2}^2 + \|h\nabla^2 u^{\mathrm{a}}\|_{L^2(\Omega^c\cup\Omega^b)}^2 \\ &\approx (L-K)^{-3}L + (L-K)^{-2}\log(L/K)\end{aligned}$$

If we choose $L \approx 2K$, then

$$\Rightarrow \quad \mathrm{ERR} \lesssim \mathrm{WORK}^{-1/2}$$

Numerical Result



Conclusion

Summary:

- Consistency estimates help to identify the key **approximation parameters**, even in fairly complex multiscale simulations.
- Optimising the choice of approximation parameters and **balancing errors** leads to formulations of multiscale methods with (quasi-)optimal work/accuracy and **without additional tuning of parameters**.

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- Consistency estimates help to identify the key **approximation parameters**, even in fairly complex multiscale simulations.
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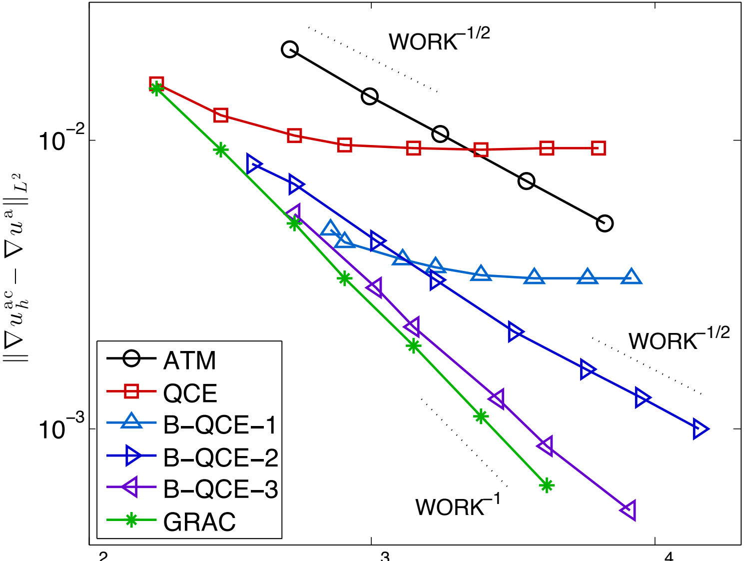
Towards a benchmark standard for multiscale methods?

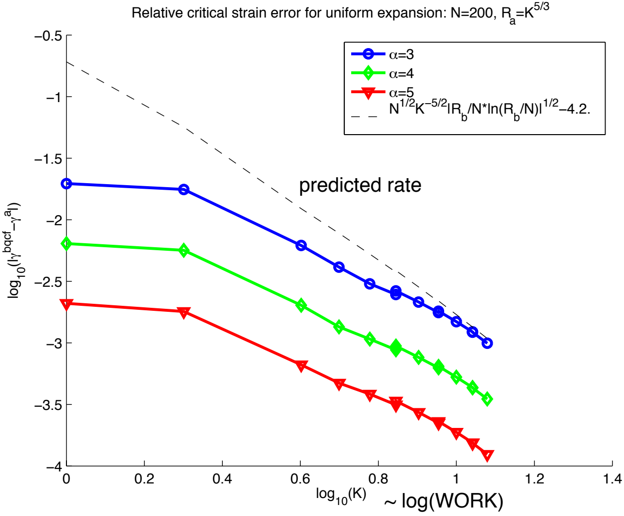
Further Observations: The Preasymptotic Regime?

Observation of Van Koten: in the preasymptotic regime, if $\mathrm{BW} \sim K^2$, then the "preasymptotic rate" is improved:



Further Directions: Error in the Critical Load

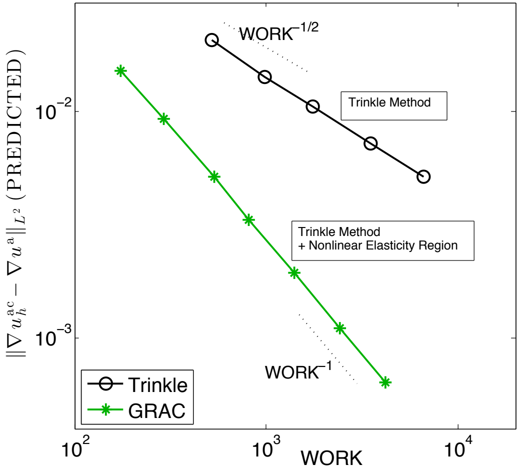
Error in the critical load under quasi-static loading [Li, Luskin, CO, Shappev; in prep.]



Further Directions: 2D Dislocations

Now the far-field error would be infinite, if we used a finite cut-off.

- **"Trinkle-Method":** atomistic core coupled to linear elasticity
- **Optimal A/C Coupling:** add region with nonlinear elasticity



(First observed by Shapeev.)