Atomistic/Continuum Multiscale Methods

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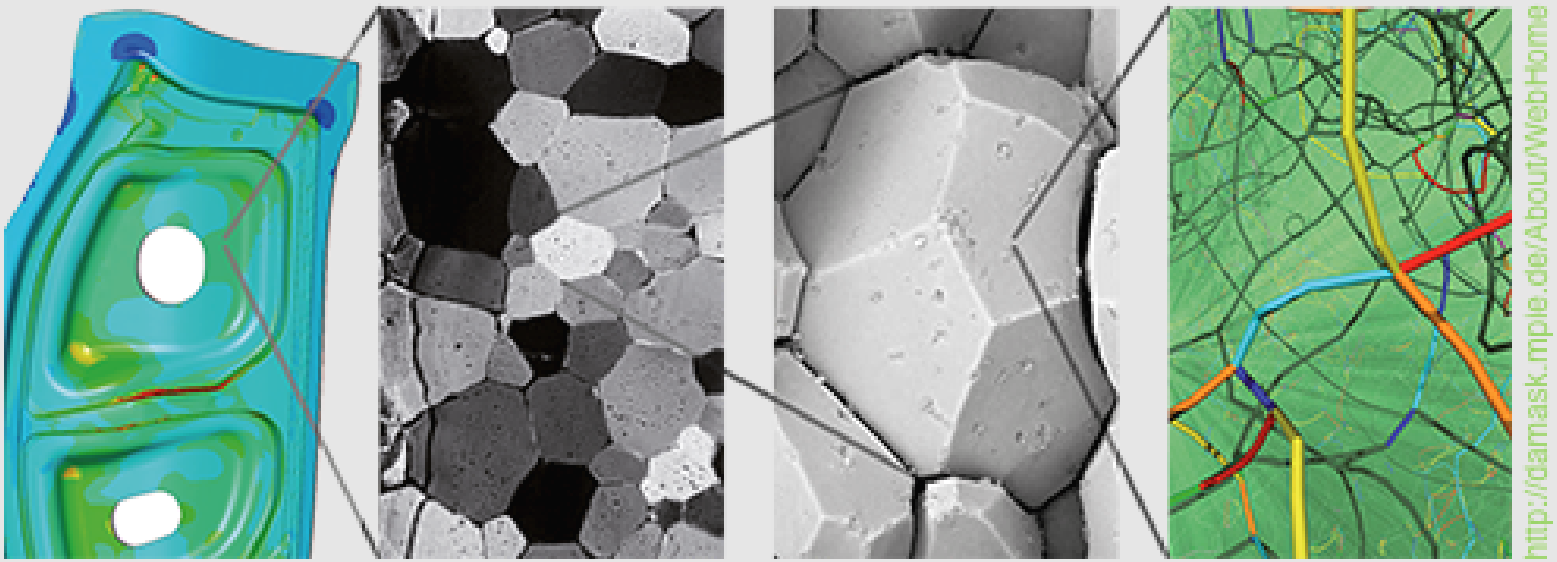
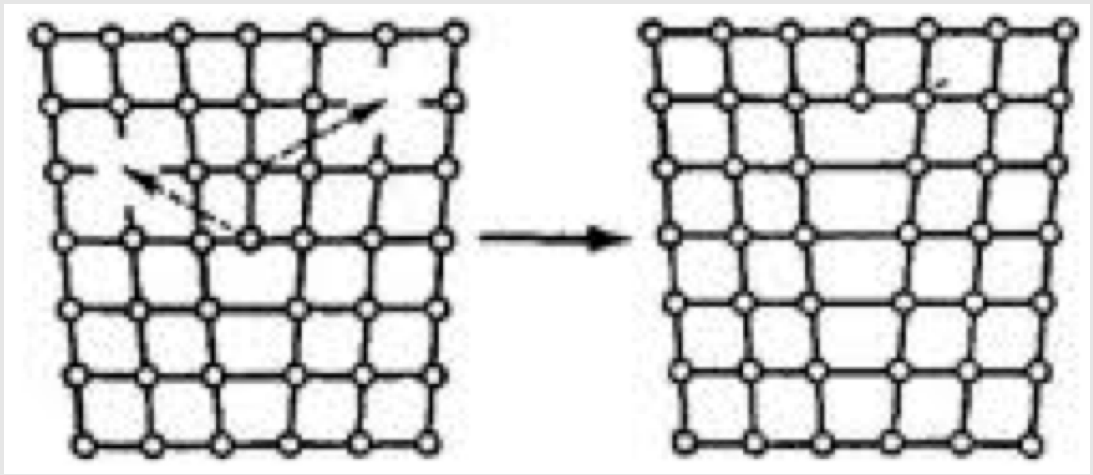
Motivation: Multi-scale Plasticity

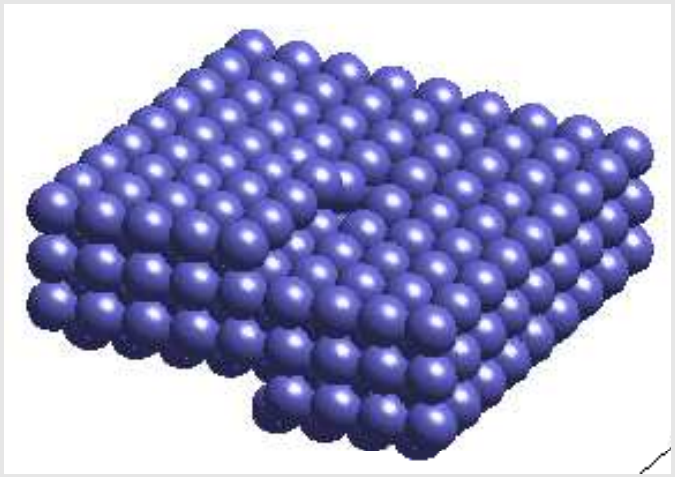


Continuum Mechanics

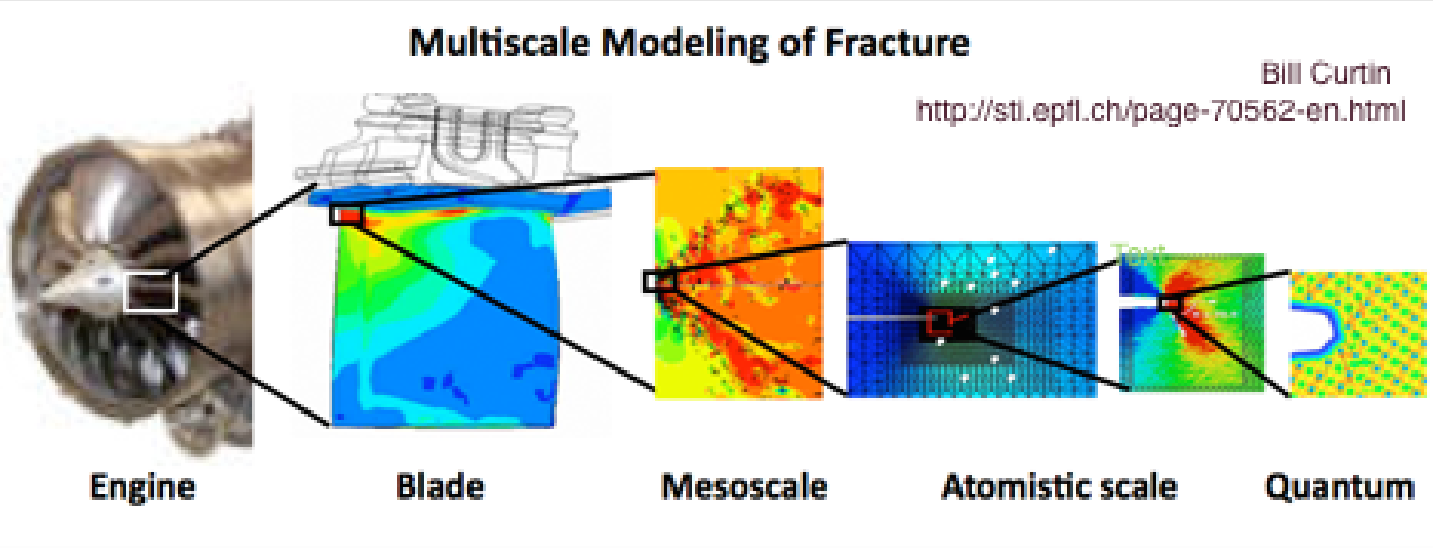
Dislocation Dynamics

Atomistic Mechanics

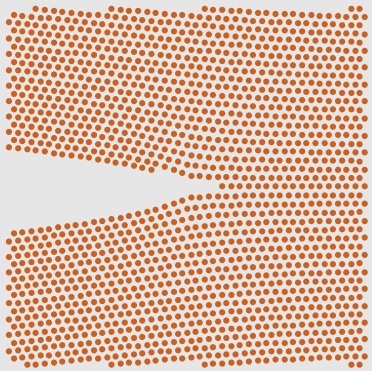


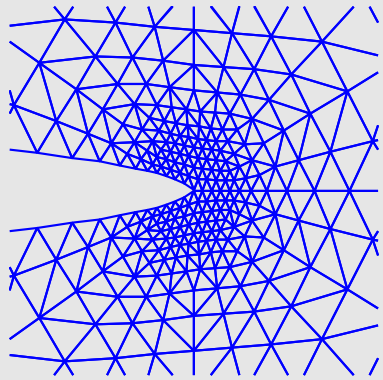


Motivation: Multiscale Fracture



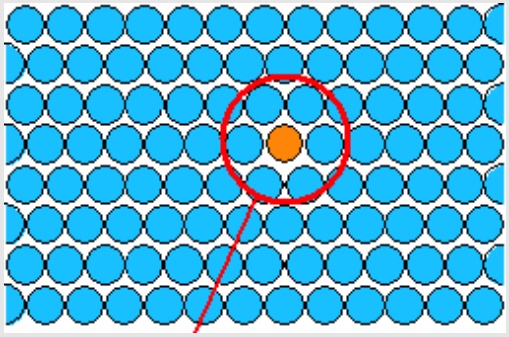
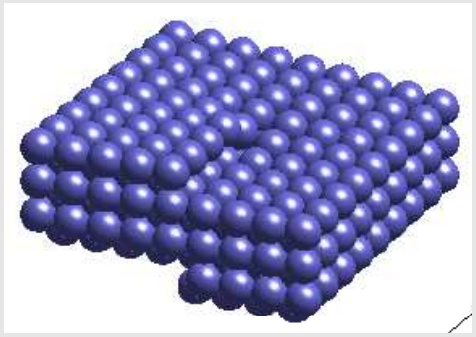
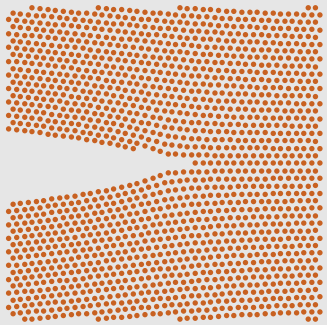
- **Fun Fact:** At least 5% of the world's energy resources are used to grind up rocks. This is essentially a fracture problem.
- Griffith fracture $\boxed{\dot{\ell}(G - G_{\text{crit}}) = 0}$ is rarely true at scales of interest.
- Again use molecular simulation to inform continuum models.



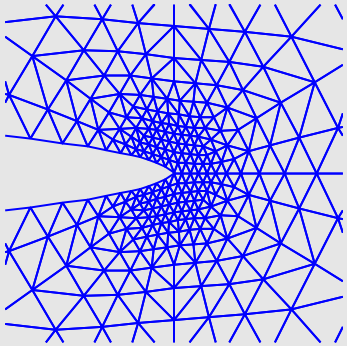
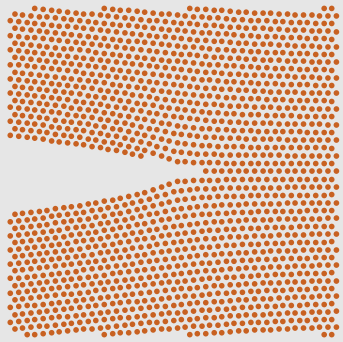


Motivation: This Lecture

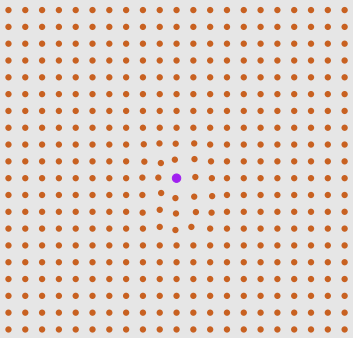
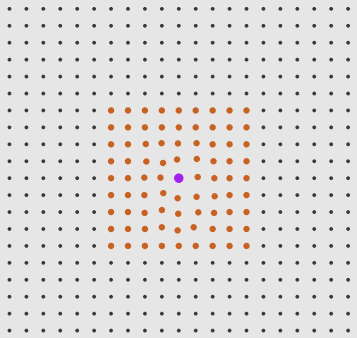
- Analysis and Numerics for Crystalline Defects

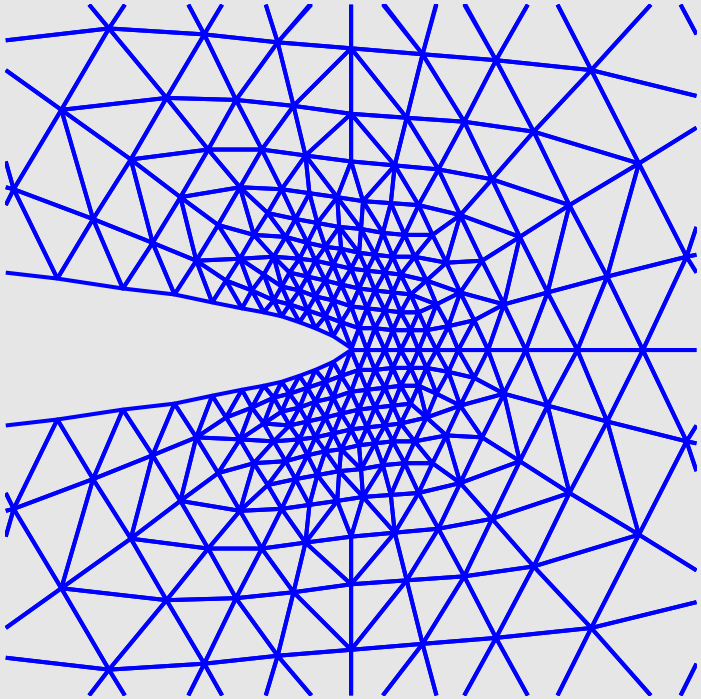
- Discrete (atomistic) problems vs PDEs

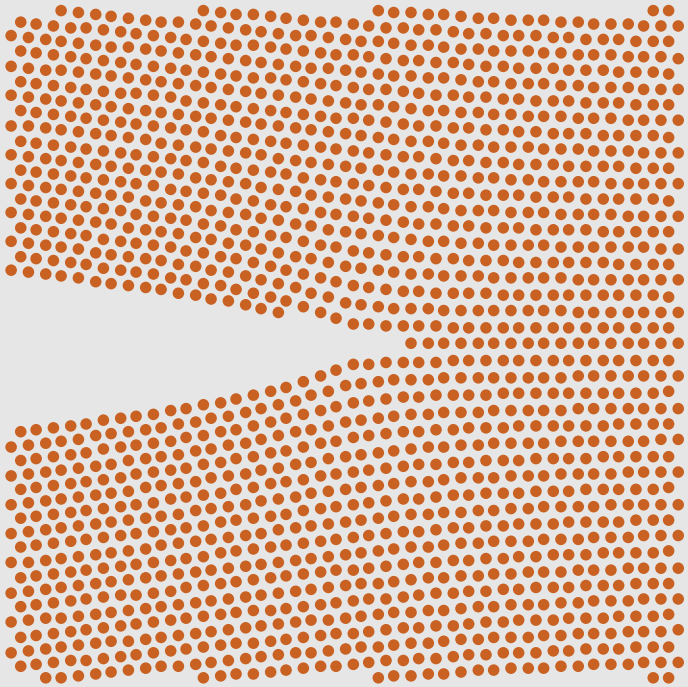



- Make Precise what is The Problem, Simulation, and the Error.

Motivation: Discrete-vs-PDE





$$\min_{b.c.} \mathcal{E}^{\mathrm{c}}(u) := \int_{\Omega} W(\nabla u)\,\mathrm{d}x$$

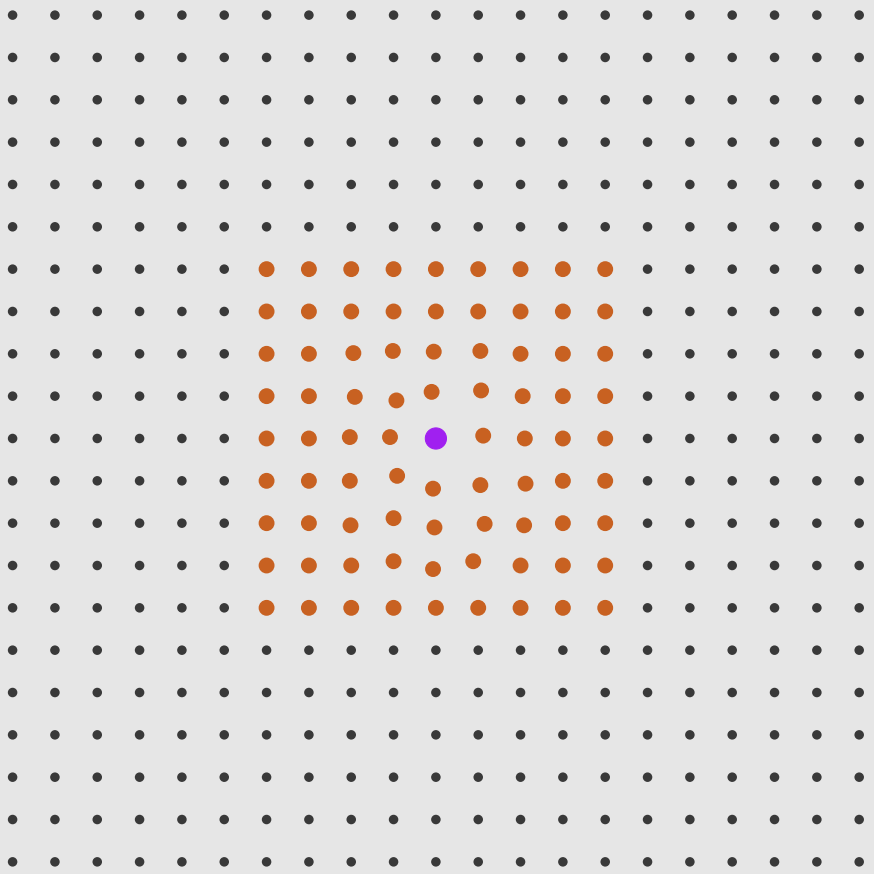
- Domain $\Omega \subset \mathbb{R}^d$
- Displacement $u : \Omega \to \mathbb{R}^d$
- ∇u : standard displacement gradient
- W : strain energy density

$$\min_{\text{b.c.}} \mathcal{E}^{\mathrm{a}}(u) := \sum_{\ell \in \Lambda} V\big(Du(\ell)\big)$$

- Domain $\Lambda \subset \mathbb{Z}^d$
- Displacement: $u : \Lambda \to \mathbb{R}^d$
- $Du(\ell) := \{u(\ell + \rho) - u(\ell)\}_{\rho \in \mathcal{R}}$
- $V(Dy(\ell)) =$ site energy of atom ℓ

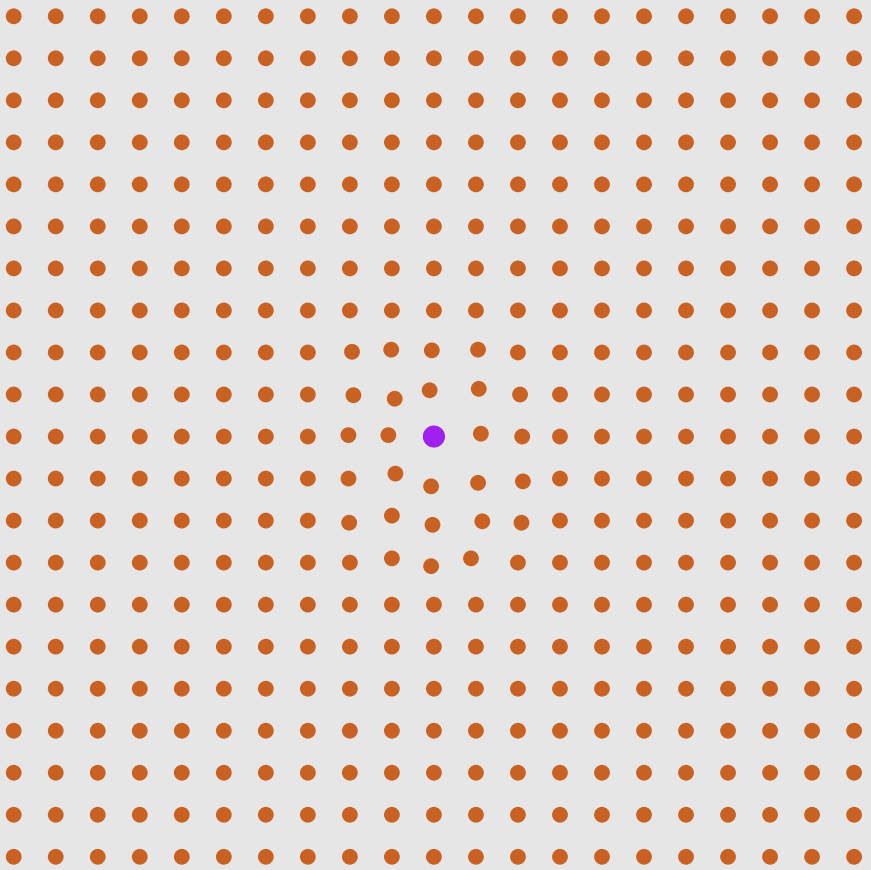
Motivation: The Simulation and The Problem

The Simulation:



$u_h \in \arg\min\{E_h(v) \mid v_h \in V_h\}$

What we mean by this simulation: configuration (and quantities of interest) of a defect in $\mathbb{Z}^d$.



$u \in \arg\min\{E(v) \mid v \in V\}$

Motivation: Aims of this Analysis

- understand, consolidate, improve existing models and computational methods
- feedback into method development
- huge area in computational science, but relatively new for applied mathematics, there is genuine interest in input from mathematics.
- **IMPORTANT CAVEAT:** these lectures only cover a very simple situation ("Dirichlet problem"). The ideas must be extended into many diverse directions to become widely useful ("Navier Stokes, Helmholtz, Fokker-Planck, . . .)" I will discuss this at the end of the lectures.

Outline of Lectures

0. Motivation ✓
1. Variational Problem in $\mathbb{Z}^d$
   - Discrete energy space
   - "Well-posedness" of energy-difference formulation
2. Boundary Conditions for Numerical Simulation
   - Dirichlet conditions
   - Regularity and Approximatio Error Estimates
   - REVISION CLASS: Linearised elasticity as a boundary condition
3. Atomistic/Continuum Multiscale Scheme
   - Cauchy–Born model
   - The ghost force problem
   - A/c coupling via blending
   - Proof of consistency estimate, sketch of error estimate
   - Fine-tuning for simulation
4. Outlook
   - Some open problems
   - Perspective of the field

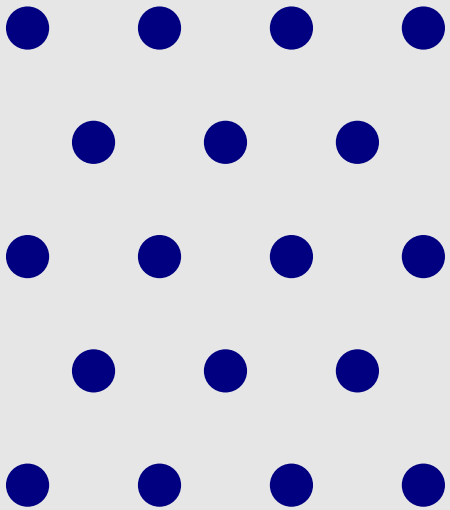
Part 1:
Variational Problem in $\mathbb{Z}^d$

The Lattice

The computational domain is a lattice $\Lambda = \mathrm{A}\mathbb{Z}^d$, $\mathrm{A} \in SO(d)$

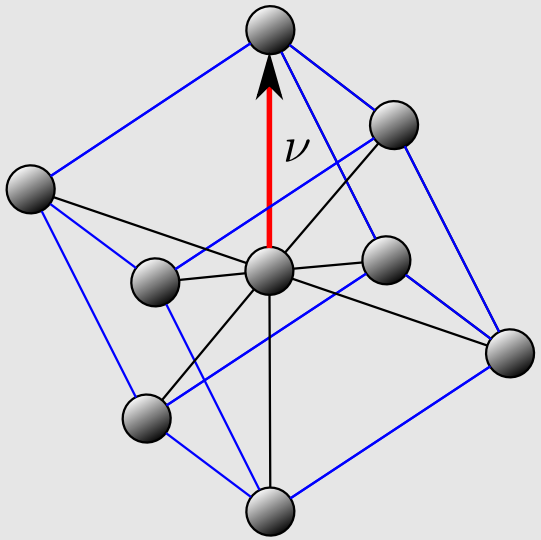
Example 1:
triangular lattice in 2D

$$\mathrm{A} = \begin{bmatrix} 1 & \cos(\pi/3) \\ 0 & \sin(\pi/3) \end{bmatrix}$$



Example 2:
body-centered cubic (bcc) in 3D

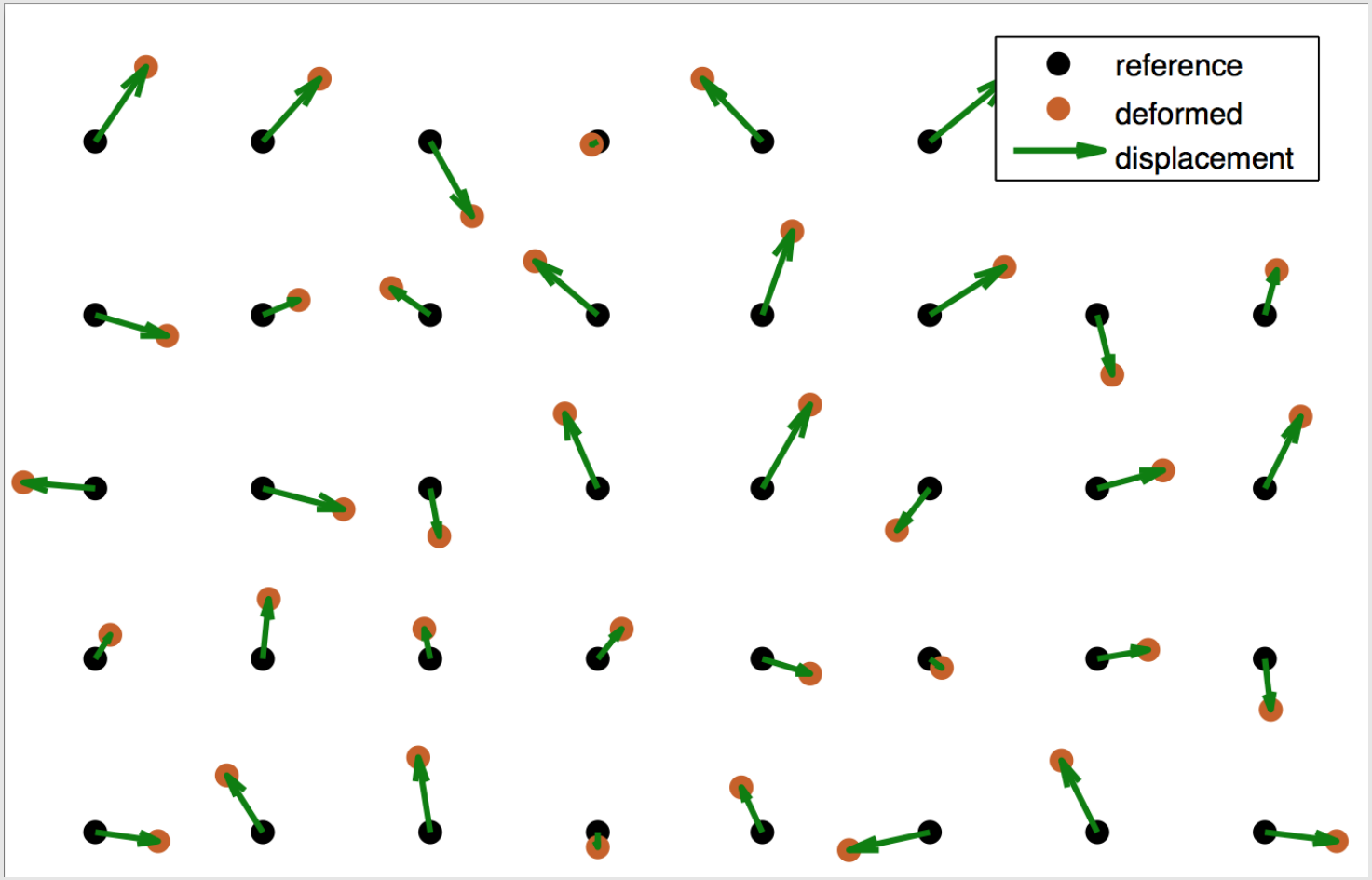
$$\mathrm{A} = \begin{bmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 1/2 \\ 0 & 0 & 1/2 \end{bmatrix}$$



But for simplicity we can just take $\Lambda = \mathbb{Z}^d$.

Kinematics

- Material points: $\ell \in \Lambda$
- Reference configuration: $x(\ell) = \ell$
- Displacement: $\boxed{u : \Lambda \to \mathbb{R}^d}$
- Deformation: $y = x + u$



Site Potential

For a displacement u, the energy associated with a site ℓ is

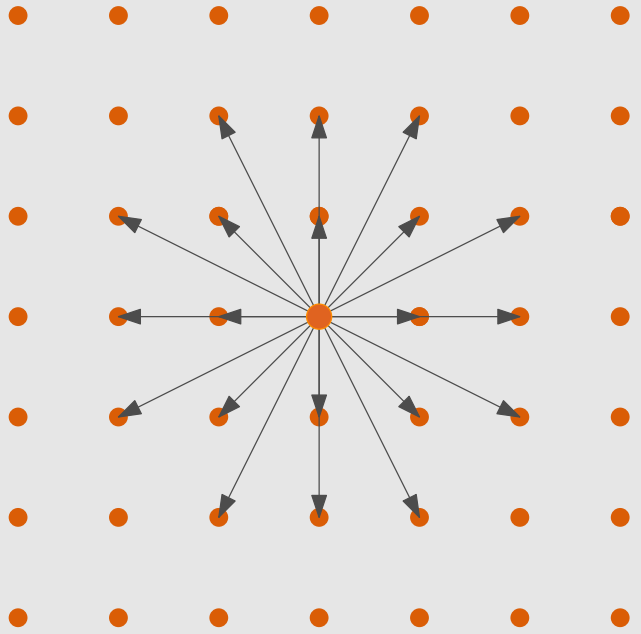
$$\boxed{V(Du(\ell))}$$

- Site energy should be translation invariant, i.e., depends only on $k \mapsto (u(k) - u(\ell))$.
- Interaction range: $\mathcal{R} \subset \Lambda \setminus \{0\}$ finite, point symmetry $-\mathcal{R} = \mathcal{R}$;
- Strain of bond $(\ell, \ell + \rho)$, $\rho \in \mathcal{R}$ is

$$D_\rho u(\ell) := u(\ell + \rho) - u(\ell)$$

Hence, the site energy is a function of

$$\boxed{Du(\ell) := (D_\rho u(\ell))_{\rho \in \mathcal{R}}} \quad .$$



Assumption 1 (V).

$V \in C^k((\mathbb{R}^d)^{\mathcal{R}})$, $\quad V(\mathbf{0}) = 0$, $\quad$ *point symmetric* $V((-g_{-\rho})_{\rho \in \mathcal{R}}) = V(\boldsymbol{g})$

Site Energy - Notes

Notes:

- $V(\mathbf{0}) = 0$ simply normalised the energy so that $u = 0$ has zero-site energy. Suppose, that we do not make this assumption, then we would, on the next slide define an "energy-difference functional" instead of an "energy functional": $E(u) = \sum_\ell V(Du(\ell)) - V(\mathbf{0})$, and then proceed as before. So in fact the "correct" way to think about V is that it is a site energy-*difference* and E is a total energy-*difference*.
- V has no ℓ-dependence, this means that all atoms are of the same species; generalisations to multi-lattices are possible: here each site is occupied by A species, the displacement is now $\mathbf{u} = (u_a)_{a \in A}$ and $V = \sum_{a \in A} V_a((u_b(\ell + \rho) - u_a(\ell)))$.
- Assumption C^k is unrealistic as $V \to \infty$ as atoms collide ($y(\ell + \rho) - y(\ell) \to 0$). To overcome this, we could restrict the definition to displacements such that the deformation $|y(\ell') - y(\ell)| \geq c|\ell - \ell'|$. See, e.g., [27]
- However, our later analysis will be purely local, in neighbourhood of a well-behaved deformation where V is in fact smooth. We can circumvent some boring technicalities by making the assumption $V \in C^k$ globally.

Energy

The energy of a displacement is simply the sum over site energies,

$$\mathcal{E}^{\mathrm{a}}(u) := \sum_{\ell \in \Lambda} V(Du(\ell))$$

This is well-defined for compact displacements, i.e., for

$$u \in \dot{\mathcal{U}}^{\mathrm{c}} := \left\{ v : \Lambda \to \mathbb{R}^d \,\middle|\, \mathrm{supp}(Dv) \text{ compact} \right\}$$

It is also well-defined if $Du \in \ell^1$. But intuitively, it must be possible to define the total energy in the **energy space**

$$\dot{\mathcal{U}}^{1,2} := \left\{ v : \Lambda \to \mathbb{R}^d \,\middle|\, Dv \in \ell^2 \right\}.$$

The associated (semi-)norm is $\| \cdot \|_{\dot{\mathcal{U}}^{1,2}} = \| D \cdot \|_{\ell^2}$.

Lemma 2 (Extension Lemma).

(a) *$\dot{\mathcal{U}}^{\mathrm{c}} \subset \dot{\mathcal{U}}^{1,2}$ is dense: $\forall u \in \dot{\mathcal{U}}^{1,2}\, \exists u_j \in \dot{\mathcal{U}}^{\mathrm{c}}$ s.t. $Du_j \to Du$ in ℓ^2.*
(b) *$\mathcal{E}^{\mathrm{a}} : (\dot{\mathcal{U}}^{\mathrm{c}}, \| D \cdot \|_{\ell^2}) \to \mathbb{R}$ is continuous, hence there exists a unique continuous extension to $\dot{\mathcal{U}}^{1,2}$, which we still denote by $\mathcal{E}^{\mathrm{a}}$.*
(c) *$\mathcal{E}^{\mathrm{a}} \in C^k(\dot{\mathcal{U}}^{1,2})$, in the sense of Frechet.*

This completes the definition of the energy functional. See also the following remarks.

Proof of Extension Lemma

- (a) is an EXERCISE
- (b) For $u \in \dot{\mathcal{U}}^{\rm c}$,

$$\mathcal{E}(u) = \sum_{\ell \in \Lambda} \Big(V(Du(\ell)) - V(\mathbf{0}) - \langle \delta V(\mathbf{0}), Du(\ell) \rangle \Big) + \sum_{\ell \in \Lambda} \langle \delta V(\mathbf{0}), Du(\ell) \rangle.$$

- Summation by parts: $\sum_{\ell \in \Lambda} \langle \delta V(\mathbf{0}), Du(\ell) \rangle = 0$,
- Taylor expansion: $\Big| V(Du(\ell)) - V(\mathbf{0}) - \langle \delta V(\mathbf{0}), Du(\ell) \rangle \Big| \lesssim |Du(\ell)|^2$, so

$$\mathcal{E}'(u) = \sum_{\ell \in \Lambda} \Big(V(Du(\ell)) - \langle \delta V(\mathbf{0}), Du(\ell) \Big)$$

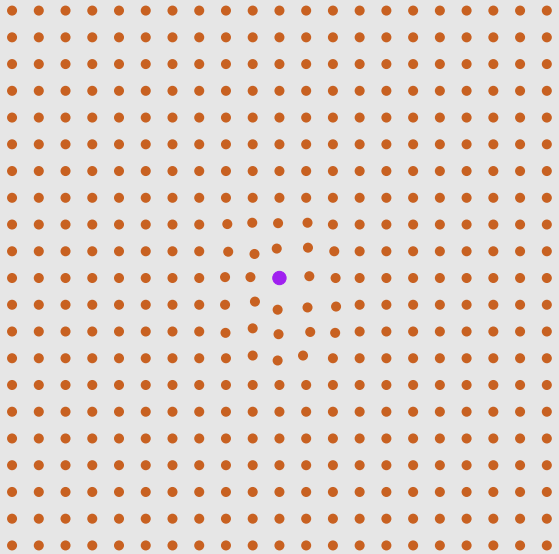
  is also well-defined for $u \in \dot{\mathcal{U}}^{1,2}$.
- TODO: prove $\mathcal{E}' \in C^k(\dot{\mathcal{U}}^{1,2})$ in the sense of Frechet. EXERCISE □

Notes:

- The proof indicates that, in fact, $\dot{\mathcal{U}}^{1,2}$ is the **largest space** to which $\mathcal{E}$ can be continuously extended. This is a strong indicator that we have a good function space setting. EXERCISE

Introducing the Defect

Introducing an **Impurity** into the host crystal (replace atom $\ell = 0$ with a different species)



This corresponds simply to replacing the site energies $V(Du(\ell))$ with $\tilde{V}_\ell(Du(\ell))$ for $\ell \in \{0\} \cup \mathcal{R}$. We write the perturbed (total) energy as

$$\mathcal{F}^{\rm a}(u) := \mathcal{E}^{\rm a}(u) + \mathcal{P}(u)$$

Assumption 3 (P).

$\mathcal{P} \in C^k(\dot{\mathcal{U}}^{1,2})$, translation invariant (i.e., $\mathcal{P}(u+c) = \mathcal{P}(u)$) and local, i.e., a function of only $Du(\ell)$, $|\ell| \le R_{\rm def}$, for some $R_{\rm def} > 0$.

Notes on the Defect

Notes:

- Other point defects can be introduced analogously, or with modified notation. All subsequent results can be extended to arbitrary point defects. See [9] for more detail.
- There are many other important classes of defects: dislocations, cracks, etc. We will discuss more on this at the end of the lectures. For now, we just mention that straight dislocation lines can still be incorporated into this framework, but this requires a little additional work. Cracks are essentially an open problem.
- For dislocations: Briefly, the idea is to decompose $u = u^{\rm pred} + u^{\rm corr}$, where $u^{\rm pred}$ is a predictor displacement that can, e.g., be obtained from continuum linearised elasticity and $u^{\rm corr}$ supplies the missing atomistic information. (E.g., for a pure screw dislocation in anti-plane deformation, $u^{\rm pred}(x) = \frac{b}{2\pi} \arg(x_1 + ix_2)$.)
  Since $\nabla u^{\rm pred} \sim |x|^{-1}$ it has infinite energy, however the corrector $u^{\rm corr} \in \dot{\mathcal{U}}^{1,2}$. Hence, we consider the energy-difference $\mathcal{E}(u) = \sum_{\ell \in \Lambda} V(Du^{\rm pred}(\ell) + Du(\ell)) - V(Du^{\rm pred}(\ell))$.
  One can again prove that this is well-defined, etc, and then continue similarly as in the point defect case.
  This procedure can also be thought of as supplying the far-field boundary condition $u(x) \sim u^{\rm pred}(x)$ as $|x| \to \infty$.
  Again, see [9] for more details.

The Variational Problem

With our results so far, we have shown that the following problem is well formulated:

$$\boxed{\bar{u}^{\mathrm{a}} \in \operatorname{arg\,min} \left\{ \mathcal{F}^{\mathrm{a}}(u) \,\middle|\, u \in \dot{\mathcal{U}}^{1,2} \right\}} \tag{1}$$

We will always understand this in the sense of local minimality.

Remarks:

- Uniqueness cannot be true, unless we "design" the interatomic potential to prevent lattice symmetries.
- Existence of minimisers is a property of $V, \mathcal{P}$, i.e., of the model. Except in rare circumstances it cannot be proven. (again: unless we "design" our potential so that we get an existence result via the direct method)
- In the following we shall assume existence of some minimiser (not necessarily unique) and study (i) properties of the minimiser, (ii) how to approximate it computationally.

Stability

(1) $\Rightarrow \delta\mathcal{F}^{\mathrm{a}}(\bar{u}^{\mathrm{a}}) = 0$ and $\delta^2\mathcal{F}^{\mathrm{a}}(\bar{u}^{\mathrm{a}}) \geq 0$, i.e. the hessian is positive semi-definite. This is almost never sufficient for analysis. We will therefore employ a stronger stability definition.

We say that a displacement u is **strongly stable** if

$$\exists \gamma > 0 \quad \text{s.t.} \quad \langle \delta^2\mathcal{F}^{\mathrm{a}}(u)v, v\rangle \geq \gamma \|Dv\|_{\ell^2}^2 \quad \forall v \in \dot{\mathcal{U}}^{\mathrm{c}}.$$

Assumption 4 (S).

There exists a strongly stable solution $\bar{u}^{\mathrm{a}}$ to (1).

Remarks

- If any $u \in \dot{\mathcal{U}}^{1,2}$ is strongly stable, then the reference crystal must be stable as well, i.e., EXERCISE

$$\langle \delta^2\mathcal{E}^{\mathrm{a}}(0)v, v\rangle \geq \gamma \|Dv\|_{\ell^2}^2 \tag{2}$$

- (2) is precisely the discrete analogue of the Legendre–Hadamard condition (ellipticity), $\mathbb{C}_{i\alpha}^{j\beta} v_i v_j k_\alpha k_\beta \geq \gamma |v|^2 |k|^2$, for elliptic systems $\mathrm{div}\mathbb{C} : \nabla u = 0$.

Notes:

- **Why the strong stability assumption:** all our subsequent analysis will rely on linearisation techniques. For example, we will linearise the equation at infinity to deduce rates of decay for the elastic fields. We will use the inverse function theorem to deduce existence of solutions of the approximation schemes. All these technques require that the linearisation of the problem contains "much" of the problems information. Without the strong stability assumption this is simply false.
  For example, we cannot use the inverse function theory for the function $f(x) = x^3$ to deduce the existene of a solution to $x^3 = \epsilon$ for ϵ small, due to the fact that all information about x^3 is lost upon linearisation.

Part 2:

Boundary Conditions for Numerical Simulation

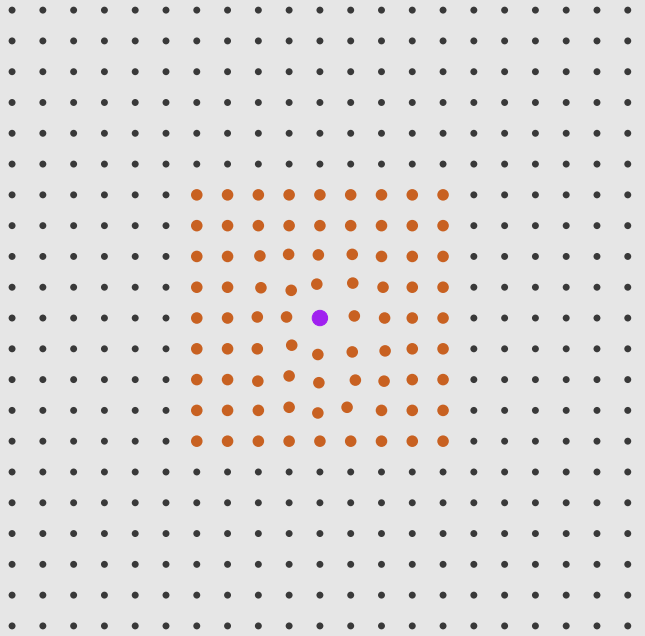
A Basic Galerkin Approximation

Remember, the reason we developed the discrete variational problem was to give a meaning to crystal defect simulations in finite domains, explaining these as approximations to the infinite-domain problem.

The Simplest Approximation Scheme:

- Computational Domain:
  $\Omega_R \subset \Lambda$ s.t. $(B_R \cap \Lambda) \subset \Omega_R$
- "Coarse" admissible space:
  $\dot{\mathcal{U}}_R := \left\{ u \in \dot{\mathcal{U}}^{\rm c} \,\middle|\, u = 0 \text{ in } \Lambda \setminus B_R \right\}$
- Approximate Variational Problem:

$$\bar{u}^{\rm a}_R \in \arg\min \left\{ \mathcal{F}^{\rm a}(u) \,\middle|\, u \in \dot{\mathcal{U}}_R \right\} \qquad (3)$$



With the tools we have so far we can prove the following:

Proposition 5.

Let $k \geq 3$, $\bar{u}^{\rm a}$ be a strongly stable solution of (1), then, for R sufficiently large, there exists $\bar{u}^{\rm a}_R$ solution to (3) such that $\|D\bar{u}^{\rm a}_R - D\bar{u}^{\rm a}\|_{\ell^2} \to 0$ as $R \to \infty$.

The Main Tools for the Analysis

Lemma 6 (Inverse Function Theorem – IFT).

X Hilbert, $x_0 \in X$; $m, \gamma, \eta > 0$, $r := 2\eta/\gamma$ such that (i) $\mathcal{G} \in C^1(B_R(x_0); X^*)$ with $\|\delta\mathcal{G}(x) - \delta\mathcal{G}(x')\|_{L(X,X^*)} \leq m\|x - x'\|_X$ for $x, x' \in B_r(x_0)$;

(ii) **Stability:** $\langle \delta\mathcal{G}(x_0)v, v\rangle \geq \gamma\|v\|_X^2 \quad \forall v \in X$;

(iii) **Consistency:** $\langle \mathcal{G}(x_0), v\rangle \leq \eta\|v\|_X \qquad (\text{i.e. } \|\mathcal{G}\|_{X^*} \leq \eta)$

and the "saturation assumption" $2\eta m\gamma^{-2} < 1$ holds, then $\exists\,!\,\bar{x} \in X$ such that

$$\mathcal{G}(\bar{x}) = 0, \qquad \|\bar{x} - x_0\|_X \leq 2\frac{\eta}{\gamma} \quad \text{and} \quad \langle \delta\mathcal{G}(\bar{x})v, v\rangle \geq \gamma\big(1 - 2\eta m\gamma^{-2}\big)\|v\|_X^2.$$

Notes:

- Normally in the inverse function theorem we start with a solution $\mathcal{G}(x_0) = 0$ and then perturb the right-hand side. The idea of the above result is to think of x_0 solving $\mathcal{G}(x_0) = \mathcal{G}(x_0)$ where the right-hand side is small, so changing the right-hand side to 0 is a small perturbation.
- Proof is an left as an exercise; hint: set $\bar{x} = x_0 + u$, rewrite as a fixed point problem $\mathcal{G}(\bar{x}) = 0 \quad \Leftrightarrow \quad \delta\mathcal{G}(x_0)u = -\mathcal{G}(x_0) + \big[\delta\mathcal{G}(x_0)u + \mathcal{G}(x_0) - \mathcal{G}(x_0 + u)\big]$, and apply Banach's fixed point theorem.

Proof of Proposition 5

1. $\dot{\mathcal{U}}^{\mathrm{c}} \subset \dot{\mathcal{U}}^{1,2}$ dense $\Rightarrow \exists\, u_R \in \dot{\mathcal{U}}_R$ s.t. $\|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \to 0$ as $R \to \infty$. Let $R_1 > 0$ such that $\|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \leq 1$ for $R \geq R_1$.
2. In the IFT we set $X = \dot{\mathcal{U}}_R$, $x_0 = u_R$, $\mathcal{G} = \delta\mathcal{F}^{\mathrm{a}}|_{\dot{\mathcal{U}}_R}$.
3. Since $k \geq 3$, $\delta\mathcal{F}^{\mathrm{a}}$ and $\delta^2\mathcal{F}^{\mathrm{a}}$ are Lipschitz in $B_1(\bar{u}^{\mathrm{a}})$ with Lip. const. $m_1, m > 0$. Therefore,

$$\begin{aligned}
\|\delta\mathcal{F}^{\mathrm{a}}(u_R)\|_{\dot{\mathcal{U}}^{-1,2}} &= \|\delta\mathcal{F}^{\mathrm{a}}(u_R) - \delta\mathcal{F}^{\mathrm{a}}(\bar{u}^{\mathrm{a}})\|_{\dot{\mathcal{U}}^{-1,2}} \leq m_1\|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2} =: \eta_R, \\
\langle\delta^2\mathcal{F}^{\mathrm{a}}(u_R)v, v\rangle &\geq \langle\delta^2\mathcal{F}^{\mathrm{a}}(\bar{u}^{\mathrm{a}})v, v\rangle - m\|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2}\|Dv\|_{\ell^2}^2 \\
&\geq \left(\gamma - \tfrac{m}{m_1}\eta_R\right)\|Dv\|_{\ell^2}^2 \geq \frac{\gamma}{2}\|Dv\|_{\ell^2}^2,
\end{aligned}$$

   the last inequality, provided that R is sufficiently large.
4. Since $\eta_R \to 0$, we obtain, for R sufficiently large all conditions of IFT are satisfies, so IFT implies existence of a solution to (3) with $\|D\bar{u}_R^{\mathrm{a}} - Du_R\|_{\ell^2} \leq 4m_1\gamma^{-1}\|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2}$.
   (note that 4 can be replaced with any number > 1.)
   and so, $\|D\bar{u}_R^{\mathrm{a}} - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \lesssim \|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \to 0$. Positivity of $\delta\mathcal{G}(\bar{x})$ (final statement of the lemma) implies that $\bar{u}_R^{\mathrm{a}}$ is a local minimiser. □

Quantifying the Approximation Error

Exact Problem:

$$\bar{u}^{\mathrm{a}} \in \arg\min\{\mathcal{F}^{\mathrm{a}}(v) \,|\, v \in \dot{\mathcal{U}}^{1,2}\}$$

Simulation:

$$\bar{u}_R^{\mathrm{a}} \in \arg\min\{\mathcal{F}^{\mathrm{a}}(v) \,|\, v \in \dot{\mathcal{U}}_R\}$$

From the convergence proof we get the stronger result

$$\|D\bar{u}_R^{\mathrm{a}} - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \leq C_R \|Du_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2},$$

where $C_R \to \gamma^{-1}$ as $R \to \infty$ and $u_R \in \dot{\mathcal{U}}_R$ is arbitrary. This is analogous to to Céa's Lemma / best-approximation error estimates in FEM.

Lemma 7 (Best Approximation Error Estimate).

There exists $C > 0$ such that, for all $u \in \dot{\mathcal{U}}^{1,2}$ there exists $u_R \in \dot{\mathcal{U}}_R$ satisfying

$$\|Du - Du_R\|_{\ell^2} \leq C \|Du\|_{\ell^2(\Lambda \setminus B_{R/2})}.$$

$\rightsquigarrow$ **We need a decay estimate for Du!**

Proof of Lemma 7

Instead of proving this result, we prove a continuous analogue. The proof of the discrete result is tedious unless one first introduced some machinery that makes it a corollary of its continuous version. (we will actually introduce this in the last part of the lecture)
So let $u \in \dot{H}^1(\mathbb{R}^d), d > 1$. We define a mollifier $\eta \in C^1(\mathbb{R}^d)$ with $\eta(x) = 1$ in $|x| < 1/2$, $\eta = 0$ in $|x| > 1$, $0 \leq \eta \leq 1$, and set

$$u_R(x) := \eta(x/R)\big(u(x) - \langle u \rangle_{A_R}\big), \qquad A_R := B_R \setminus B_{R/2},$$

then clearly $u_R \in \dot{H}^1, \nabla u_R$ has support B_R and further

$$\begin{aligned}
\nabla u_R(x) &= R^{-1}\nabla\eta(x/R)\big(u - \langle u \rangle_{A_R}\big) + \eta(x/R)\nabla u, \\
\nabla(u - u_R) &= (1 - \eta(x/R))\nabla u + R^{-1}\nabla\eta(x/R)\big(u - \langle u \rangle_{A_R}\big), \\
\|\nabla(u - u_R)\|_{L^2} &\leq \|\nabla u\|_{B'_{R/2}} + \|\nabla\eta\|_{L^\infty} R^{-1}\|u - \langle u \rangle_{A_R}\|_{L^2} \leq C\|\nabla u\|_{L^2(B'_{R/2})},
\end{aligned}$$

where in the last inequality we used the Poincaré inequality for A_R with scales linearly with R. □

Regularity: What should we expect?

We can think of $\delta\mathcal{F}^{\mathrm{a}} = 0$ as a discrete and nonlinear version of

$$-\Delta u = f, \quad x \in \mathbb{R}^d, \quad \operatorname{supp}(f) \subset B_1, \quad \int f = 0.$$

(these conditions corresponding to locality and translation invariance of $\mathcal{P}$).
Let G be the Green's function, then

$$\nabla u(x) = \int \nabla G(x') f(x - x') \, \mathrm{d}x' = \int \Big(\nabla G - (\nabla G)_{B_1(x)} \Big) f(x - x') \, \mathrm{d}x'$$

(Since $\int f = 0$, we can subtract the mean of G.) Hence, we obtain

$$|\nabla u(x)| \lesssim \|\nabla^2 G\|_{L^\infty(B_1(x))} \lesssim |x|^{-d}$$

More generally, once could prove (under suitable assumptions on f) that

$$|\nabla^j u(x)| \lesssim |x|^{1-d-j}.$$

We can think of this as a **regularity estimate** at $x = \infty$.

Notes on PDE in $\mathbb{R}^d$

Notes:

- The equation $-\Delta u = f, x \in \mathbb{R}^d$ can be solved in the homogeneous Sobolev space

$$\dot{H}^1 := \left\{ u \in H^1_{\mathrm{loc}}(\mathbb{R}^d) \,\middle|\, \nabla u \in L^2 \right\}.$$

  This can be made a Hilbert space by considering equivalence classes. $\{u + c | c \in \mathbb{R}\}$. If $f \in L^2(\mathbb{R}^d)$, $\mathrm{supp}(f)$ compact and $\int f = 0$, then it is easy to see (Lax Milgram) that there exists a unique solution in this space.
- In general, the equation can be solved for any right-hand side of the form $\mathrm{div} g, g \in L^2$.
- It can also be checked that, if $\int f \neq 0$, then no solution exists. In this case, the solution has a component that decays like the Green's function.

Regularity Theorem

Theorem 8 (Regularity).

Let $u \in \dot{\mathcal{U}}^{1,2}$ with $\delta\mathcal{F}^{\mathrm{a}}(u) = 0$, and assume the lattice is stable (2), then

$$|Du(\ell)| \leq C|\ell|^{-d}.$$

Consequence for the best-approximation error:

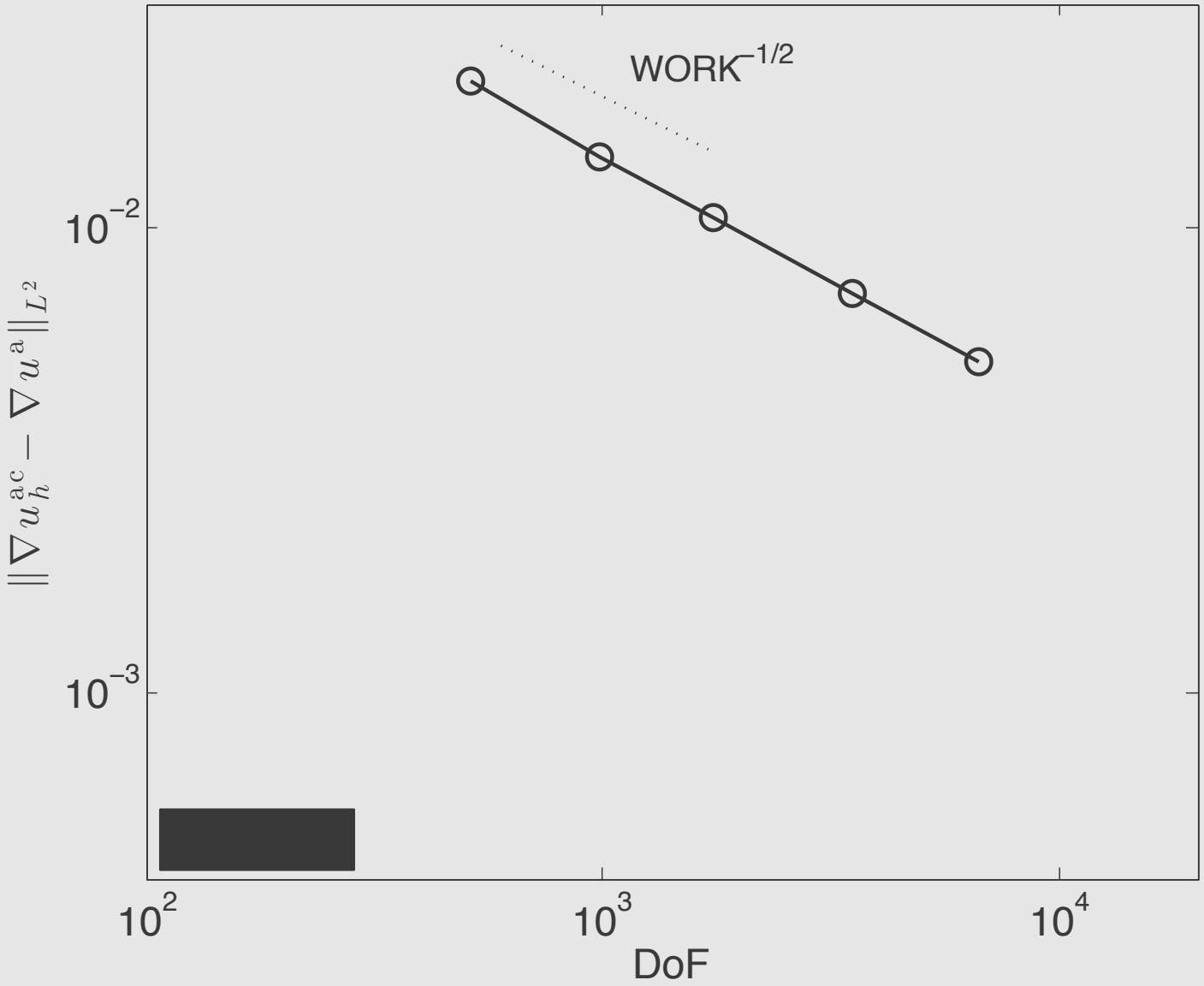
$$\|Du - Du_R\|_{\ell^2} \lesssim \|Du\|_{\ell^2(\Lambda \setminus B_{R/2})} \approx \left(\int_{R/2}^{\infty} r^{d-1} r^{-2d} \right)^{1/2} \approx R^{-d/2}.$$

Theorem 9 (Convergence Rate).

Let $k \geq 3$, $\bar{u}^{\mathrm{a}}$ be a strongly stable solution to (1), then for R suff. large $\exists!\, \bar{u}^{\mathrm{a}}_R$ solution to (3) such s.t. $\|D\bar{u}^{\mathrm{a}}_R - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \lesssim R^{-d/2} \approx (DOF)^{-1/2}.$

Numerical Confirmation

Numerical Test: divacancy in triangular lattice, NN EAM toy model



Proof of the Regularity Theorem – Sketch

1. **Linearisation:** Let $H := \delta^2 \mathcal{E}^{\rm a}(0)$, $u = \bar{u}^{\rm a}$, $v \in \dot{\mathcal{U}}^{\rm c}$. The intuition is that "near ∞", $\delta \mathcal{F}^{\rm a}(u) = 0$ reduces essentially to $Hu = 0$. In other words, far from the defect, linearised (lattice) elasticity is sufficient. This is in particular supported by the fact that $Du \in \ell^2$ implies $|Du(\ell)| \to 0$ uniformly as $|\ell| \to \infty$. This **key observation** one of the main things that distinguish discrete problems from continuous ones.

$$\begin{aligned} \langle Hu, v \rangle &= \langle Hu - \delta \mathcal{E}^{\rm a}(u) - \delta \mathcal{P}(u), v \rangle \\ &= \sum_{\ell \in \Lambda} \Big\{ \langle \delta^2 V(0) Du + \delta V(0) - \delta V(Du), Dv \rangle \Big\} - \langle \delta \mathcal{P}(u), v \rangle, \end{aligned}$$

Since $|\delta^2 V(0) Du + \delta V(0) - \delta V(Du)| \lesssim |Du|^2$ we obtain

$$\langle Hu, v \rangle = \langle g^{\rm def} + g, Dv \rangle \quad \text{where} \quad |g(\ell)| \lesssim |Du(\ell)|^2.$$

To continue it is sufficient to assume that

$$\langle Hu, v \rangle = \langle g, Dv \rangle, \qquad |g(\ell)| \lesssim |\ell|^{-p} + |Du(\ell)|^2,$$

for some $p > d$. ($p = d$ is also possible, then some log-factors come into the estimates; this is needed for the dislocation case)

2. **Lattice Green's Function:** It can be shown that there exists a lattice Green's function $G : \Lambda \to \mathbb{R}^d$, with the properties that $|D^j G(\ell)| \lesssim |\ell|^{2-d-j}$ and

$$u(\ell) = \langle Hu, G(\ell - \cdot)\rangle = \langle g, DG(\ell - \cdot)\rangle, \qquad Du(\ell) = \langle g, D^2 G(\ell - \cdot)\rangle.$$

(There is a corresponding continuum linear elasticity Green's function, which behaves asymptotically the same as G, and G inherits its far-field properties.)
If we did not have the $|Du|^2$ dependence on the right-hand-side (i.e. if the problem were linear) then we could now directly estimate $|Du(\ell)| \lesssim |\ell|^{-d}$.

3. **Dealing with the nonlinearity:** Let $w(r) := \|Du\|_{\ell^\infty(\Lambda \setminus B_r)}$, then the key idea is to estimate $w(2r)$ in terms of $w(r)$. From the recursion we will get, we will then be able to prove the result. This is similar to the Campanato approach to regularity for elliptic systems, but in our case applied at $x = \infty$.
Let $|\ell| \geq 2r$, then after a tedious but not difficult calculation, one obtains that

$$|Du(\ell)| \lesssim \sum_k \Big((1 + |k|)^{-p} + |Du(k)|^2 \Big) (1 + |\ell - k|)^{-d} \ldots$$

$$\ldots \leq C(1 + 2r)^{-d} + \eta(r) w(r),$$

where $\eta(r) \to 0$ as $r \to \infty$. Multiplying with $(1 + r)^{-d}$ we obtain, for a new constant C,

$$(1 + 2r)^d w(2r) \leq C + \eta(r)(1 + r)^d w(r).$$

Now set $v(r) := (1 + r)^d w(r)$, then we have $v(2r) \leq C + \eta(r) v(r)$. Since $\eta(r) \to 0$, for $r \geq r_0$, we have $\eta(r) \leq 1/2$, so in fact, $v(2r) \leq C + \frac{1}{2} v(r)$. Let $F := \sup_{r \leq r_0} v(r)$, then by induction

$$v(r) \leq C + \frac{1}{2}\left(C + \frac{1}{2}\left(\ldots \left(C + \frac{1}{2} F \right) \ldots \right) \right) \leq 2C + 2^{-N(r)} F,$$

where $N(r) \lesssim \log(r)$; in particular $v(r) \leq C_1$. This concludes the proof.

Part 3:
Revision Class

Exercises

1. (a) Let $\dot{\mathcal{U}}^{1,p} = \{u : \Lambda \to \mathbb{R}^d \,|\, Du \in \ell^p(\Lambda)\}$, $1 \le p \le \infty$. Which space is largest, which is smallest? Compare with Sobolev spaces $W^{1,p}(\Omega)$, where Ω is a bounded domain.
   (b) Analogously, prove that $\ell^2 \subset \dot{\mathcal{U}}^{1,2}$, but not vice-versa. Again contrast this with the embedding for the Sobolev spaces $L^2(\Omega)$, $W^{1,2}(\Omega)$, Ω bounded. Is the embedding $\ell^2 \subset \dot{\mathcal{U}}^{1,2}$ compact?
   (c) Prove that $\dot{\mathcal{U}}^{1,2}_{[]} := \{[u] \,|\, u \in \dot{\mathcal{U}}^{1,2}\}$, where $[u] = \{u + c \,|\, c \in \mathbb{R}\}$, with natural associated norm is a Hilbert space.
   (d) Prove that $\dot{\mathcal{U}}^{\rm c}$ is dense in $\dot{\mathcal{U}}^{1,2}$ (in the sense that $\dot{\mathcal{U}}^{\rm c}_{[]}$ is dense in $\dot{\mathcal{U}}^{1,2}_{[]}$). (You may use Lemma 7 for this. If you want to complete its proof, then read ahead to learn about the $\tilde{v}$ interpolant on slide 39)

2. (a) Complete the proof of the extension lemma.
   (b) Explain the remark after the proof of the extension lemma: Suppose that $\mathcal{E}^{\rm a}$ is stable in the reference state, i.e, $\langle \delta^2 \mathcal{E}^{\rm a}(0) v, v\rangle \ge \gamma \|Dv\|^2_{\ell^2}$ for all $v \in \dot{\mathcal{U}}^{\rm c}$. Under this assumption show that $\dot{\mathcal{U}}^{1,2}$ is indeed the largest space from the class $\dot{\mathcal{U}}^{1,p}$ to which $\mathcal{E}^{\rm a}$ can be continuously extended.

3. Prove (2).
   HINT: use the fact that, if $Du \in \ell^2(\Lambda)$, then $|Du(\ell)| \to 0$ uniformly as $|\ell| \to \infty$. Choose a test function $v \in \dot{\mathcal{U}}^{\rm c}$ and "shift" it to infinity.

Exercises

LIN-Method: Using a harmonic approximation of the interaction outside a core region $\Omega \supset (\Lambda \cap B_R)$ amounts to defining a modified energy functional

$$\mathcal{E}_R^{\rm lin}(u) = \sum_{\ell \in \Omega} V(Du(\ell)) + \sum_{\ell \in \Lambda \setminus \Omega} Q(Du(\ell)),$$

$$\text{where} \qquad Q(Du) = V(0) + \langle \delta V(\mathbf{0}), Du \rangle + \tfrac{1}{2} \langle \delta^2 V(\mathbf{0}) Du, Du \rangle.$$

Setting $\mathcal{F}_R^{\rm lin} := \mathcal{E}_R^{\rm lin} + \mathcal{P}$, in the LIN method we solve

$$\bar{u}_R^{\rm lin} \in \operatorname{arg\,min} \left\{ \mathcal{F}_R^{\rm lin}(u) \,\middle|\, u \in \dot{\mathcal{U}}^{1,2} \right\}. \tag{4}$$

This is still infinite-dimensional, but it can be reduced to a finite-dimensional problem using lattice Green's functions (similar to FEM-BEM coupling). We will not be concerned with this, but focus on the resulting error.

4. Prove the following result; the exponent α is something you should determine from your proof.

Theorem 10.

Let $k \geq 3$, $\bar{u}^{\rm a}$ be a strongly stable solution to (1), then there exist C, α, R_0 such that, for $R \geq R_0$, there exists a unique solution $\bar{u}_R^{\rm lin}$ to (4) such that $\|D\bar{u}_R^{\rm lin} - D\bar{u}^{\rm a}\|_{\ell^2} \leq R^{-\alpha}$.

Exercises

Outline for exercise 4:

- Prove that $\mathcal{E}_R^{\mathrm{lin}} \in C^k(\dot{\mathcal{U}}^{1,2})$.
- Prove that

$$\|\delta\mathcal{E}_R^{\mathrm{lin}}(u) - \delta\mathcal{E}^{\mathrm{a}}(u)\|_{\dot{\mathcal{U}}^{-1,2}} \lesssim \|Du\|^2_{\ell^4(\Lambda\setminus\Omega_R)}, \tag{5}$$

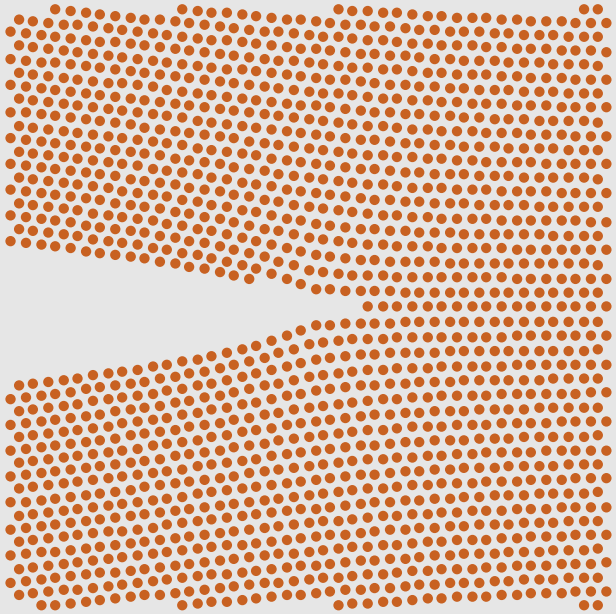
$$\|\delta^2\mathcal{E}_R^{\mathrm{lin}}(u) - \delta^2\mathcal{E}^{\mathrm{a}}(u)\|_{L(\dot{\mathcal{U}}^{1,2},\dot{\mathcal{U}}^{-1,2})} \lesssim \|Du\|_{\ell^\infty(\Lambda\setminus\Omega_R)} \tag{6}$$

- Consistency: conclude that $\|\delta\mathcal{E}_R^{\mathrm{lin}}(\bar{u}^{\mathrm{a}})\|_{\dot{\mathcal{U}}^{-1,2}} \lesssim R^{-\alpha}$, where $\bar{u}^{\mathrm{a}}$ is a stable solution of (1). (Here is the step where you find α)
- Apply the inverse function theorem to conclude the proof.

Part 4:
Coarse-Graining the Far-Field via Atomistic/Continuum Approach

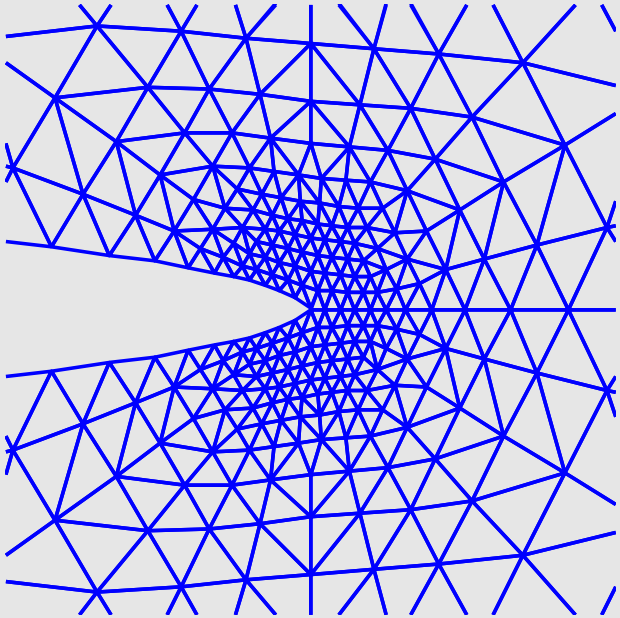
Physical Motivation

Atomistic Model



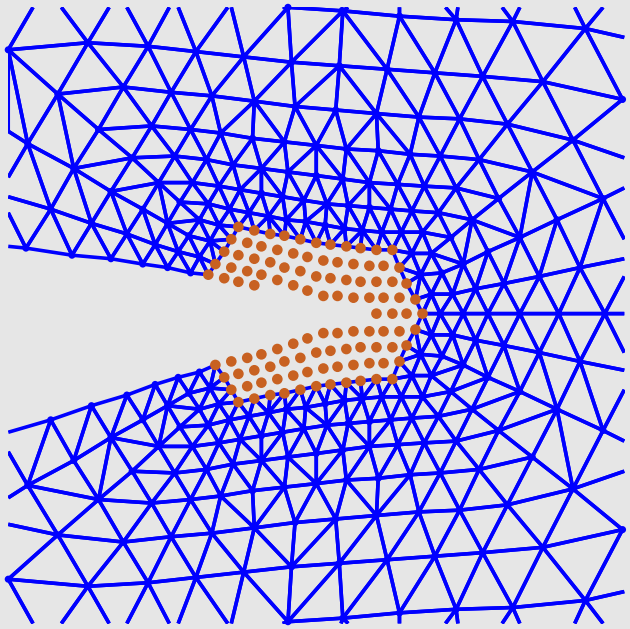
- Requires huge computational domain because of long-ranged elastic field
- intractable except for extremely high crack speeds

Continuum Model



- does not model bond-breaking (chemistry) accurately
- generic crack tip singularity does not capture the complexity of the crack tip
- but considered accurate for the elastic far-fields!

Hybrid Model



- accuracy of atomistic model at crack tip
- cheap computational cost and "sufficient accuracy" of continuum model for far-fields

Analytical Motivation: Higher Regularity

Theorem 11.

Let $\bar{u}^{\mathrm{a}}$ be a strongly stable solution of (1), then, for $j \leq k-2$,

$$|D^j \bar{u}^{\mathrm{a}}(\ell)| \lesssim |\ell|^{1-d-j}$$

(The proof is analogous to Theorem 8.)

Interlude: For the rest of this lecture it is convenient to identify all lattice functions $v : \Lambda \to \mathbb{R}^d$ with a $C^{2,1}$-smooth interpolant. The details of the construction are unimportant, so we do not show them, but only state the important facts: there exists a piecewise Q^5-interpolant (multi-quintic) which we denote by $\tilde{v} : \mathbb{R}^d \to \mathbb{R}^d$ such that

$$\tilde{v}(\ell) = v(\ell) \qquad \forall \ell \in \mathbb{Z},$$

$$\|\nabla^j \tilde{v}\|_{L^p(Q)} \leq C_1 \|D^j v\|_{\ell^p(Q \cap \Lambda)} \leq C_2 \|\nabla \tilde{v}\|_{L^p(\omega_Q)} \qquad \forall Q = \otimes[\ell_i, \ell_i + 1], \ell \in \Lambda, j \leq 3.$$

Theorem 11 can now be restated EXERCISE as

$$|\nabla^j \tilde{u}^{\mathrm{a}}(x)| \lesssim |x|^{1-d-j}, \qquad 1 \leq j \leq k-2. \tag{7}$$

In the following we drop the tilde, and unless stated otherwise we always identify a function with its $C^{2,1}$-interpolant, i.e., $v \equiv \tilde{v}$.

Notes:

- The $\tilde{v}$ interpolant is contructed as follows: for $\Lambda = \mathbb{Z}^d$, let $Q = \otimes(\ell_i, \ell_i + 1)$ be a "cell" in the lattice. To define a multi-quintic interpolant on that cell, we have 6^d degrees of freedom, which we can fill by prescribing $\nabla^\alpha \tilde{v}(k)$ at the 2^d corners k of the hypercube Q, where $\alpha \in \mathbb{N}^d$ is a multi-index with the restriction $|\alpha|_\infty \leq 2$. (note that the number of DOFs and the number of conditions, $2^d \times 3^d$, matches.)
  To that end, we denote

$$
\begin{aligned}
D_i^{\mathrm{nn},0} v(\ell) &:= v(\ell), \\
D_i^{\mathrm{nn},1} v(\ell) &:= (v(\ell + e_i) - v(\ell - e_i))/2, \\
D_i^{\mathrm{nn},2} v(\ell) &:= v(\ell + e_i) - 2v(\ell) + v(\ell - e_i),
\end{aligned}
$$

  and $D^{\mathrm{nn},\alpha} := D^{\mathrm{nn},\alpha_1} \cdots D^{\mathrm{nn},\alpha_\mathrm{d}}$ and then define

$$
\nabla^\alpha \tilde{v}(k) = D^{\mathrm{nn},\alpha} v(k),
$$

  for the corners k of the hypercube.
  A proof that this interpolant is well-defined, and that it leads to a $C^{2,1}$-interpolant of v is given in [17]. (quite possibly it can also be found in a textbook somewhere?)

Analytical Motivation: Exploiting the Regularity

Recall the **atomistic Energy:** $\mathcal{E}^{\mathrm{a}}(u) = \sum_{\ell \in \Lambda} V\big(\{D_\rho u(\ell)\}_\rho\big)$

Expansion of V:

$$\begin{aligned} V(Du) = V(\mathbf{0}) &+ \langle \delta V(\mathbf{0}), Du\rangle \\ &+ \tfrac{1}{2}\langle \delta^2 V(\mathbf{0}) Du, Du\rangle \\ &+ \tfrac{1}{6}\delta^3 V(\mathbf{0}) : (Du)^{\otimes 3} \\ &+ \tfrac{1}{24}\delta^4 V(\mathbf{0}) : (Du)^{\otimes 4} \\ &+ \dots \end{aligned}$$

Only the quadratic expansion is in general practical because this makes evaluating the far-field cheap through Green's function techniques.

Expansion of Du:

$$V(\{D_\rho u\}) = V(\{\nabla_\rho u + \tfrac{1}{2}\nabla_\rho^2 u + \dots\}).$$

We will truncate at ∇u,

$$V(Du) \approx V\big(\{\nabla_\rho u\}_\rho\big) =: W(\nabla u)$$

$\rightsquigarrow$ **Cauchy–Born Approximation**.
(Higher-order expansions lead into a strange variant of strain-gradient theories [1])

Thm 11 $\Rightarrow \nabla^3 u \ll \nabla^2 u \ll \nabla u$!

Remark: Expanding either (i) W from the Cauchy–Born model; or (ii) the Du in lattice linearised elasticity both leads to continuum linearised elasticity. In that respect, the diagram is commutative.

Short Summary of the CB Model

$$D_\rho u(\ell) = u(\ell+\rho) - u(\ell) = \nabla_\rho u(\ell) + \tfrac{1}{2}\nabla_\rho^2 + O(|\nabla^3 u|),$$

(here, and throughout we mean by $O(|\nabla^j f|)$, that the missing term is bounded above by $\|\nabla^j f\|_{L^\infty(\omega)}$ where ω is some "suitable" uniformly bounded neighbourhood)

Crucial consequence of Thm 11:

at the atomic scale, $\ldots \nabla^3 u \ll \nabla^2 u \ll \nabla u \ll u$!

This motivates the continuum model (as an approximation to $\mathcal{E}^{\rm a}$)

$$\mathcal{E}^{\rm c}(u) = \int_{\mathbb{R}^d} W(\nabla u)\,{\rm d}x, \qquad W(\mathsf{F}) = V\big((\mathsf{F}\rho)_{\rho\in\mathcal{R}}\big).$$

Theorem 12.

(some technical conditions [27]) Let Λ be stable (2), $F \in H^1(\mathbb{R}^d) \cap H^2_\infty(\mathbb{R}^2)$ (a dead-load force) and $f_\epsilon(\ell) := \epsilon f(\epsilon\ell)$, then for $\|F\|_{H^1\cap H^2_\infty}$ and ε suff. small, $\exists!$ $u^{\rm a}_\varepsilon, U^{\rm c}$ s.t.

$$u^{\rm a}_\varepsilon \in \arg\min\big\{\mathcal{E}^{\rm a}(u) - \langle f_\varepsilon, u\rangle \,|\, u \in \dot{\mathcal{U}}^{1,2}\big\}, \quad -{\rm div}\partial W(\nabla U^{\rm c}) = F,$$

$$\|Du^{\rm a}_\varepsilon - Du^{\rm c}_\varepsilon\|_{L^2} \lesssim \|F\|_{H^1} \approx \|D^3\bar{u}^{\rm a}\|_{\ell^2} + \|D^2\bar{u}^{\rm a}\|^2_{\ell^4},$$

$$\|\nabla U^{\rm a}_\varepsilon - \nabla U^{\rm c}\|_{L^2} \lesssim \varepsilon^2\|F\|_{H^1} \approx \varepsilon^2\big(\|\nabla^3 U^{\rm c}\|_{L^2} + \|\nabla^2 U^{\rm c}\|^2_{L^4}\big)$$

where $U^{\rm a}_\varepsilon(x) = \varepsilon u^{\rm a}_\varepsilon(\varepsilon^{-1}x)$, $u^{\rm c}_\varepsilon(x) = \varepsilon^{-1}U^{\rm c}(\varepsilon x)$. (the CB model is **second-order** *accurate)*

Additional Notes on the CB Model

Notes:

- The result on the previous slide is taken from [27], a similar result, with similar approach is also taken in [8]. Previous/recent results leading up to this result are [2, 23].
- A rough outline of the proof is the following:
  1. First, prove that (2) implies that $\partial^2 W(0)$ is elliptic (Legendre–Hadamard). This is classical, but for a recent discussion see [11]. Knowing this means we can apply all sorts of classical stability and regularity results for the CB Model.
  2. Solve the associated PDE with external force at macro-scale:

$$\operatorname{div}_X \partial W(\nabla U(X)) + F(X) = 0, \qquad U \in \dot{H}^1(\mathbb{R}^d) \cap \dot{H}^3(\mathbb{R}^d).$$

     For $\|F\|_{H^1}$ sufficiently small, existence and local uniqueness follows from IFT and some elliptic regularity.
  3. Rescale: discrete force $f_\varepsilon(\ell) := \varepsilon F(\varepsilon \ell)$, trial solution $\hat{u}_\varepsilon(x) := \varepsilon^{-1} U(\varepsilon x)$, and estimate its residual

$$\begin{aligned} \left| \langle \delta \mathcal{E}^{\mathrm{a}}(\hat{u}_\varepsilon) - f_\varepsilon, v \rangle \right| &\lesssim \|\nabla^3 \hat{u}_\varepsilon\|_{L^2(\mathbb{R}^d)} + \|\nabla^2 \hat{u}_\varepsilon\|^2_{L^4(\mathbb{R}^d)} \\ &\approx \varepsilon^2 \left(\|\nabla^3 U\|_{L^2(\mathbb{R}^d)} + \|\nabla^2 U\|^2_{L^4(\mathbb{R}^d)} \right) \lesssim \varepsilon^2 \|F\|_{H^1(\mathbb{R}^d)}. \end{aligned}$$

  4. Apply IFT to obtain a unique $u_\varepsilon \in \dot{\mathcal{U}}^{1,2}$ such that

$$\|Du_\varepsilon - D\hat{u}_\varepsilon\|_{\ell^2} \lesssim \varepsilon^2 \|F\|_{H^1}.$$

Notes:

- The key to getting second-order accuracy is the point symmetry of V. Here, I show this for the energy, but a similar argument applies also for the forces (we will see this later): let $\nabla_{\mathcal{R}} u := \{\nabla_\rho u\}_{\rho \in \mathcal{R}}$, then

$$\begin{aligned} V(\{D_\rho u(\ell)\}) &= V(\{\nabla_\rho u + \tfrac{1}{2}\nabla_\rho^2 u + O(|\nabla^3 u|)\}) \\ &= V(\nabla_{\mathcal{R}} u) + \sum_\varsigma V_{,\varsigma}(\nabla_\rho u) \cdot [\tfrac{1}{2}\nabla_\rho^2 u + O(|\nabla^3 u|)] + O(|\nabla^2 u|^2) \\ &= V(D_{\mathcal{R}} u) + \tfrac{1}{2}\sum_\varsigma V_{,\varsigma}(\nabla_\rho u) \cdot \nabla_\varsigma^2 u + O\Big(|\nabla^3 u| + |\nabla^2 u|^2\Big). \end{aligned}$$

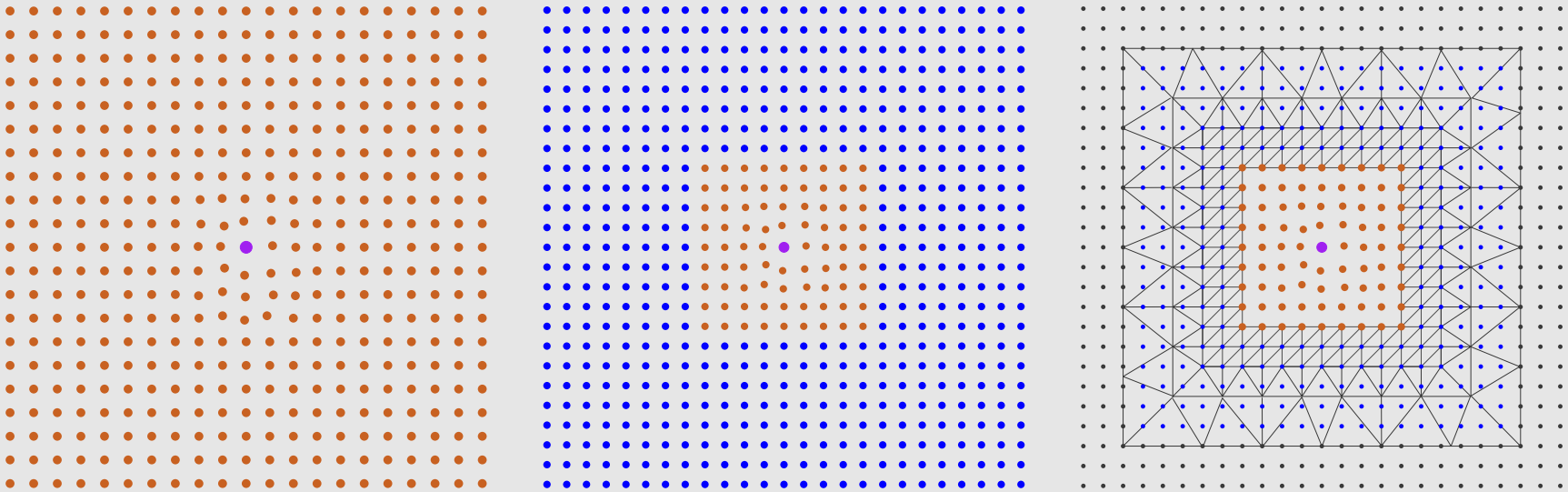
Now the point symmetry $V(\{-g_{-\rho}\}_\rho) = V(\{g_\rho\})$ implies

$$V_{,-\varsigma}(\{\mathrm{F}\rho\}_\rho) = -V_{,\varsigma}(\{\mathrm{F}\rho\}_\rho),$$

so we obtain that

$$\tfrac{1}{2}\sum_\varsigma V_{,\varsigma}(\nabla_{\mathcal{R}} u) \cdot \nabla_\varsigma^2 u = 0.$$

The Simplest A/C Coupling: "QCE"



- Atomistic Region: $\Lambda^{\mathrm{a}} \subset \Lambda$
- Continuum Region: $\Omega^{\mathrm{c}} := \mathbb{R}^d \setminus \bigcup_{\ell \in \Lambda^{\mathrm{a}}} \mathrm{vor}(\ell)$, $\quad (\mathrm{vor}(\ell) := \otimes_{i=1}^{d} (\ell_i - 1/2, ell_i + 1/2]$
- The Hybrid energy functional: $\boxed{\mathcal{E}^{\mathrm{ac}}(u) := \sum_{\ell \in \Lambda^{\mathrm{a}}} V(Du(\ell)) + \int_{\Omega^{\mathrm{c}}} W(\nabla u)\,\mathrm{d}x}$

  (remember we identified discrete functions with a $C^{2,1}$-interpolant)
  We can prove an extension lemma to show that $\mathcal{E}^{\mathrm{ac}} \in C^k(\dot{\mathcal{U}}^{1,2})$.

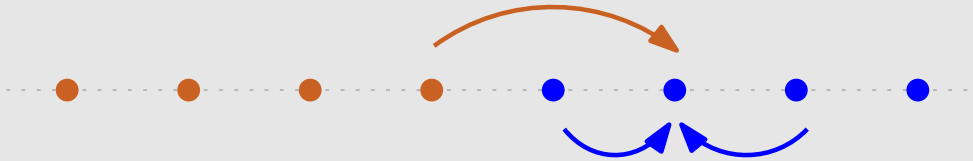
Assuming that the atomistic region surrounds the influence of the defect $\mathcal{P}$, we define $\mathcal{F}^{\mathrm{ac}}(u) := \mathcal{E}^{\mathrm{ac}}(u) + \mathcal{P}(u)$ and solve

$$\bar{u}^{\mathrm{ac}} \in \arg\min \left\{ \mathcal{F}^{\mathrm{ac}}(u) \,\middle|\, u \in \dot{\mathcal{U}}^{1,2} \right\}. \tag{8}$$

(In practise need domain truncation and finite element discretisation; we will return to this! But for simplicity, we first consider simplified schemes.)

The Ghost Force Problem

Suppose $\mathcal{P} \equiv 0$ and Λ is stable (2), then $\bar{u}^{\mathrm{a}} \equiv 0$ is a stable solution of the atomistic problem (1). It turns out that $\boxed{\delta\mathcal{E}^{\mathrm{ac}}(0) \neq 0}$, i.e., $u = 0$ is not a solution of the A/C method, i.e., the A/C method **fails the patch test**.



Proposition 13 (Failure of Patch Test).

Let $\mathcal{P} = 0$ and Λ stable (2), then there exists a constant $c > 0$ such that, whenever $\Lambda^{\mathrm{a}} \neq \emptyset$, $\|D\bar{u}^{\mathrm{ac}} - D\bar{u}^{\mathrm{a}}\|_{\ell^2} \geq c$.

Sketch of Proof:

1. Compute forces, $f(\ell) := \frac{\partial \mathcal{E}^{\mathrm{ac}}(0)}{\partial u(\ell)}$, show for certain ℓ in a neighbourhood of the interface that they are bounded below, $|f(\ell)| \geq c' > 0$.
2. $\|\delta\mathcal{E}^{\mathrm{ac}}(0)\|_{\dot{\mathcal{U}}^{-1,2}} \gtrsim \|\delta\mathcal{E}^{\mathrm{ac}}(0)\|_{\ell^2} > 0$. (recall that $\ell^2 \subset \dot{\mathcal{U}}^{1,2}$ so $\dot{\mathcal{U}}^{-1,2} \subset \ell^2$)
3. Inverse of the error estimate:

$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{ac}}\|_{\ell^2} \gtrsim \|\delta\mathcal{E}^{\mathrm{ac}}(\bar{u}^{\mathrm{a}}) - \delta\mathcal{E}^{\mathrm{ac}}(\bar{u}^{\mathrm{ac}})\|_{\dot{\mathcal{U}}^{-1,2}} = \|\delta\mathcal{E}^{\mathrm{ac}}(\bar{u}^{\mathrm{ac}})\|_{\dot{\mathcal{U}}^{-1,2}}\| \geq c > 0. \square$$

Notes on the Ghost Force Problem

Notes:

- The first rigorous results on the ghost force problem (1D, pair potential models) are given in[4, 5, 25]. It is shown by an elementary analysis of the finite difference equations that the effect of the ghost force decays exponentially away from the interface. Such results do not, however extend to 2D/3D. For a/c interfaces with corners, the ghost force effects can decay only algebraically. A precise and general analysis of this case is still open.
- A more severe problem though that the ghost forces imply is that they change the bifurcation diagram [6, 16].

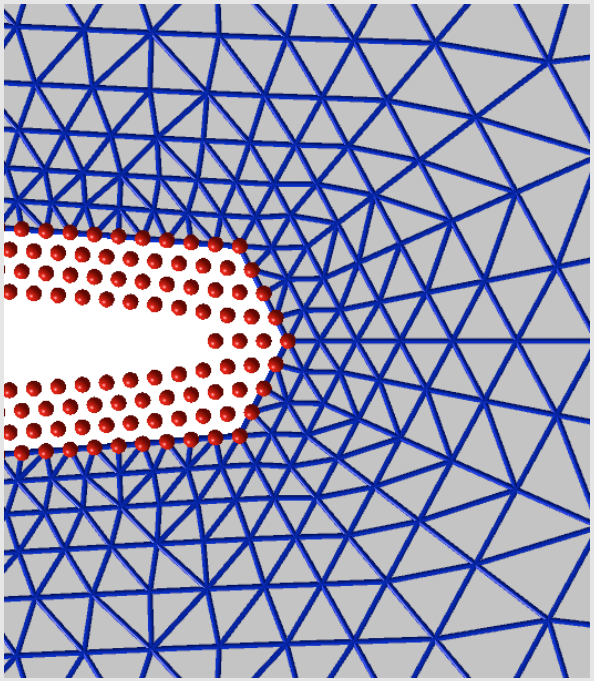
The Zoo of A/C Methods

see also Tadmor, Miller (2009) "benchmark of **fourteen** a/c methods" [24]

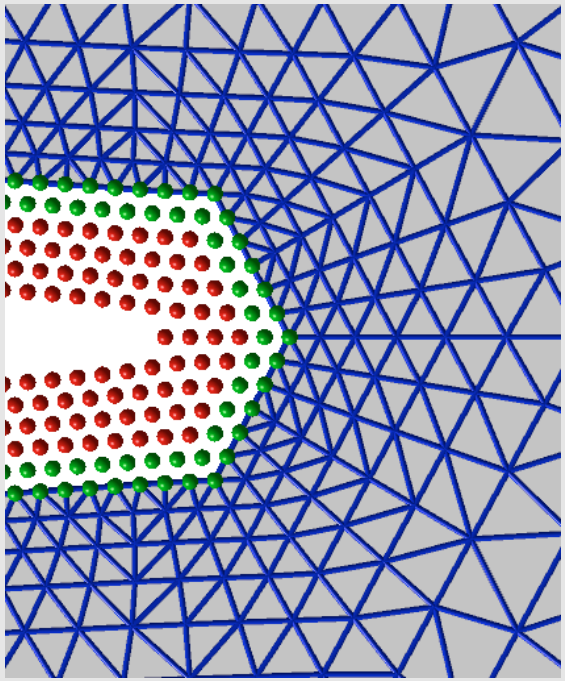
1. **Force-based coupling**
   - FeAt: Kohlhoff, Schmauder, Gumbsch (1989, 1991) [14]
   - Dead-load GF removal: Shenoy, Miller, Rodney, Tadmor, Phillips, Ortiz (1999) [31]
   - AtC: Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2007, . . .)
   - CADD: Shilkrot & Curtin & Miller (2002, . . .)
2. **Blending methods:** "diffusive interface"
   - Belytschko & Xiao (2004) [33]
   - Klein & Zimmerman (2006) [12]
   - Parks, Gunzburger, Fish, Badia, Bochev, Lehoucq, et al. (2008)
3. **Ghost Force Removal**:
   - Geometry reconstruction: Shimokawa *et al* (2003) [32], E, Lu, Yang (2006) [7] CO, Zhang (2012, 2014) [28]
   - Special cases: Shapeev (2012, 2013); Iyer, Gavini (2010); [30] Makridakis, Mitsoudis, Rosakis (2014) [22]
4. **Quadrature approaches**
   - Knap/Ortiz (2003) [13], Eidel/Stuchowski (2009) [10], Gunzburger/Zhang (2010,2011), Lin (2007)
     (Luskin/CO (2009) [19]: all of them are "inconsistent" in realistic situations)

Further variations: weak equality constraints (matching) vs. strong equality constraints (patching), optimal control approaches, domain decomposition framework, different classes of continuum models, . . .

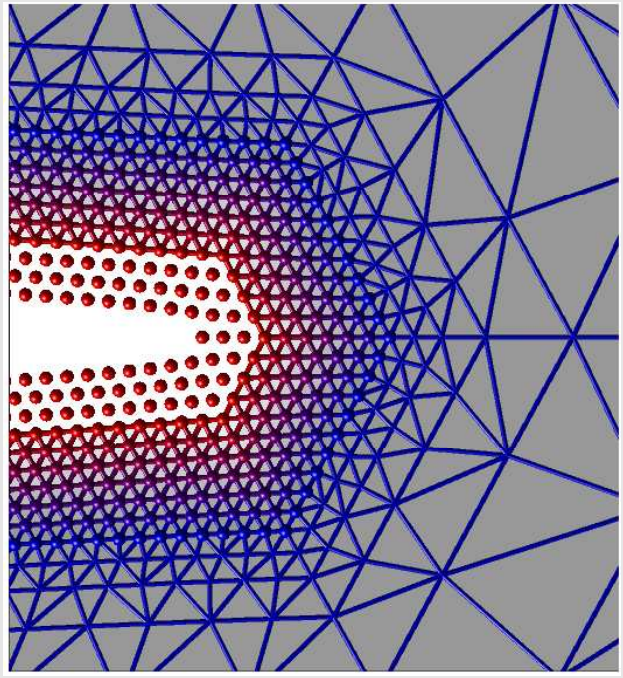
The Three Main Ideas in Pictures



force-based

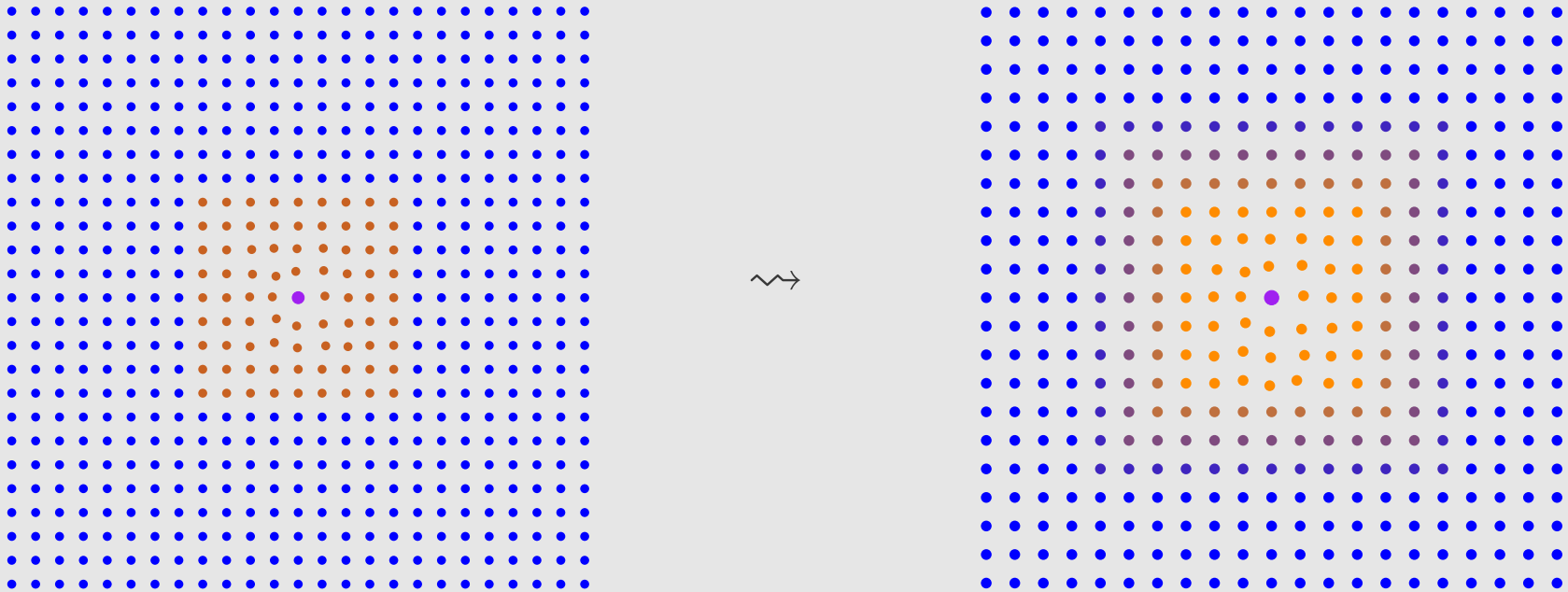


buffer atoms



blending

Blending / Diffuse Interface Method



$$\mathcal{E}^{\mathrm{b}}(u) = \sum_{\ell \in \Lambda} (1 - \beta(\ell)) V(Du(\ell)) + \int_{\mathbb{R}^d} \beta W(\nabla u) \, \mathrm{d}x$$

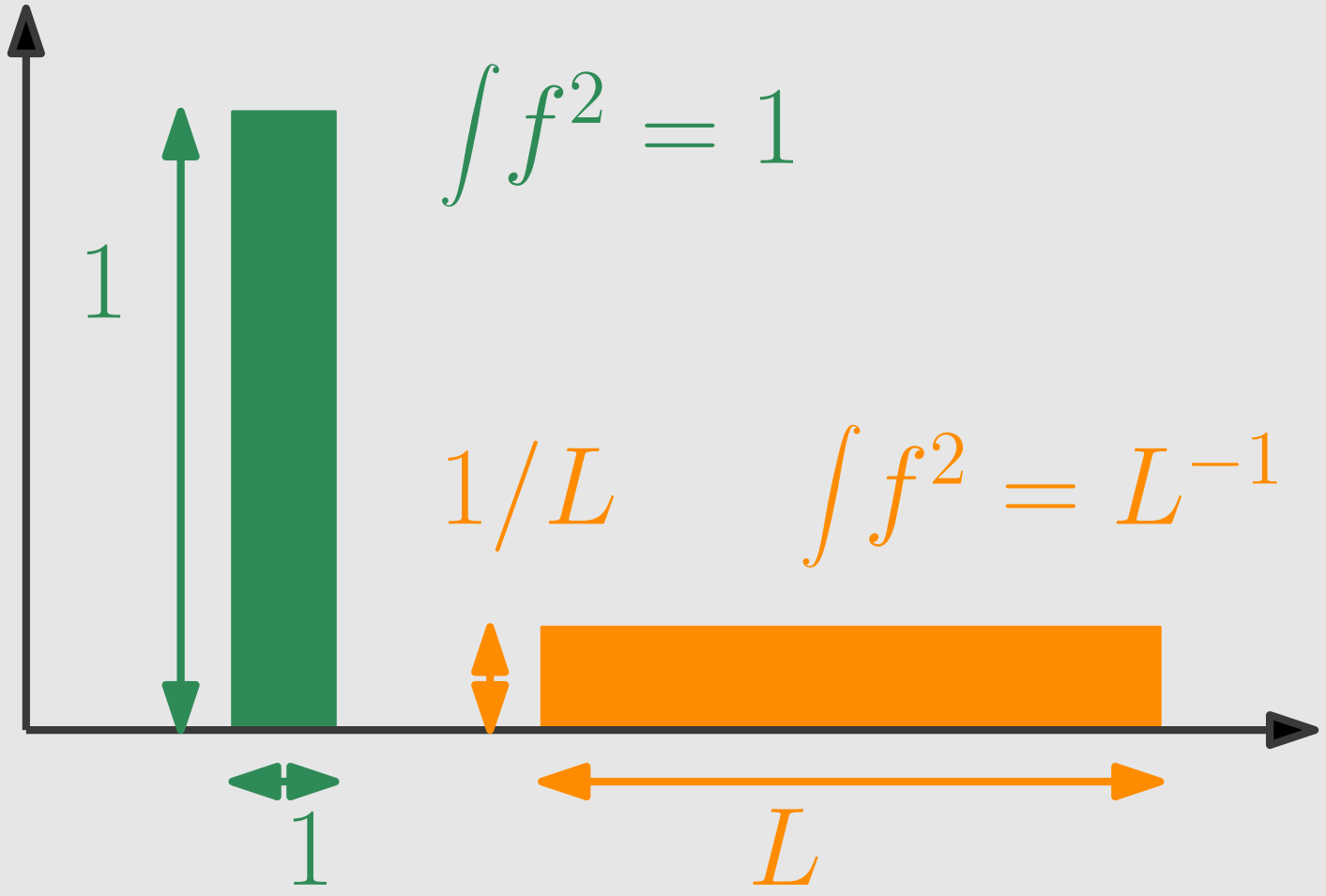
Belytschko/Xiao/2004 [33],
Badia/Parks/Bochev/Gunzburger/Lehoucq/2008,
Bauman/Dhia/Elkhodja/Oden/Prudhomme/2008

Luskin/Vankoten/2011 [15],
Luskin/CO/Vankoten/2012 [21]
Li/Ortner/Shapeev/Vankoten [17]

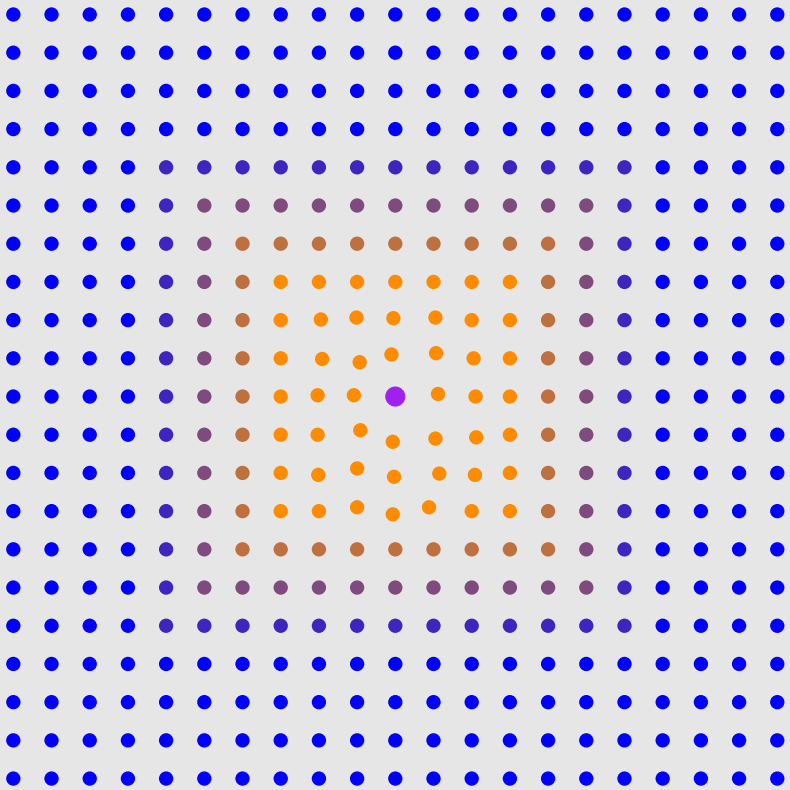
The B-QCE Scheme:

$$\bar{u}^{\mathrm{b}} \in \arg\min \{ \mathcal{F}^{\mathrm{b}}(u) \mid u \in \dot{\mathcal{U}}^{1,2} \} \tag{9}$$

Why Blending Should Work



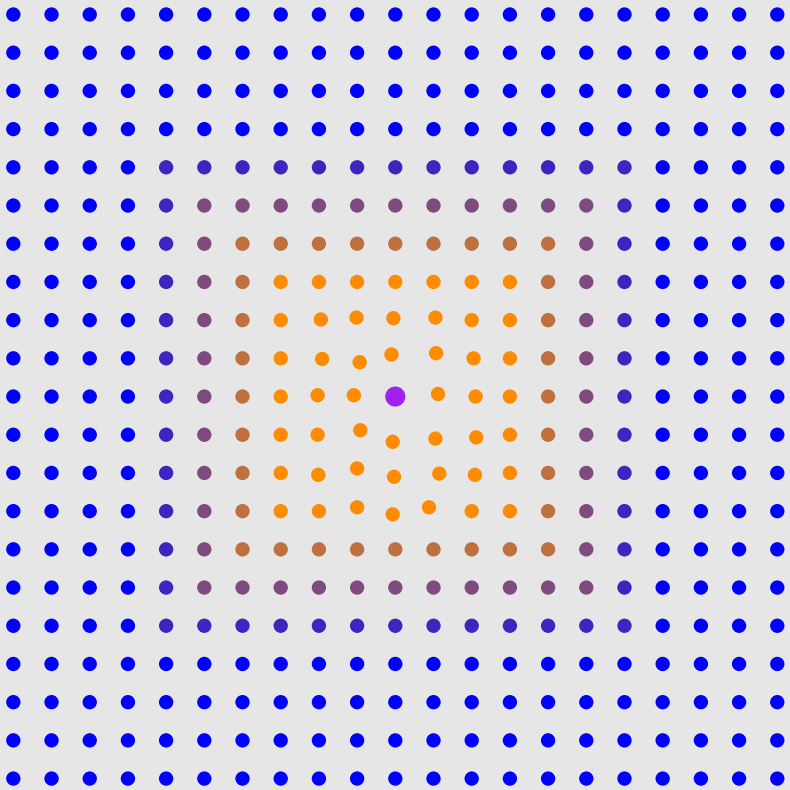
Why a Numerical Analysis



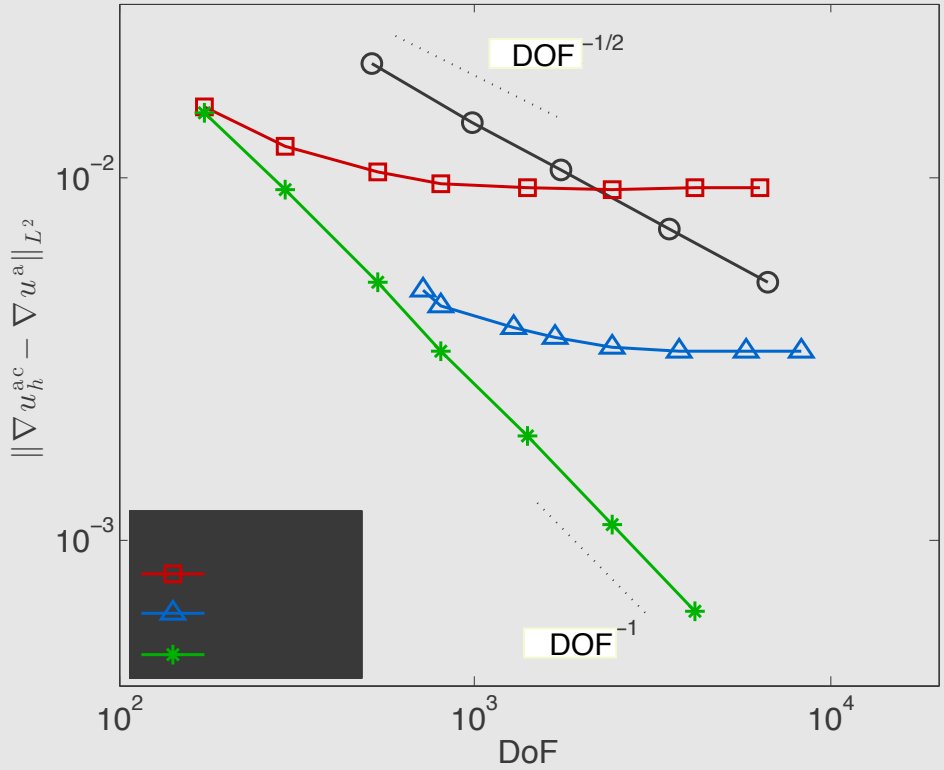
$$\mathcal{E}^{\mathrm{b}}(u) = \sum_{\ell \in \Lambda} (1 - \beta(\ell)) V(Du(\ell)) + \int_{\mathbb{R}^d} \beta W(\nabla u) \, \mathrm{d}x$$

Approximation Parameters: 1. atomistic region, 2. blending region, 3. blending function β, ~~4. mesh size h~~

Why a Numerical Analysis



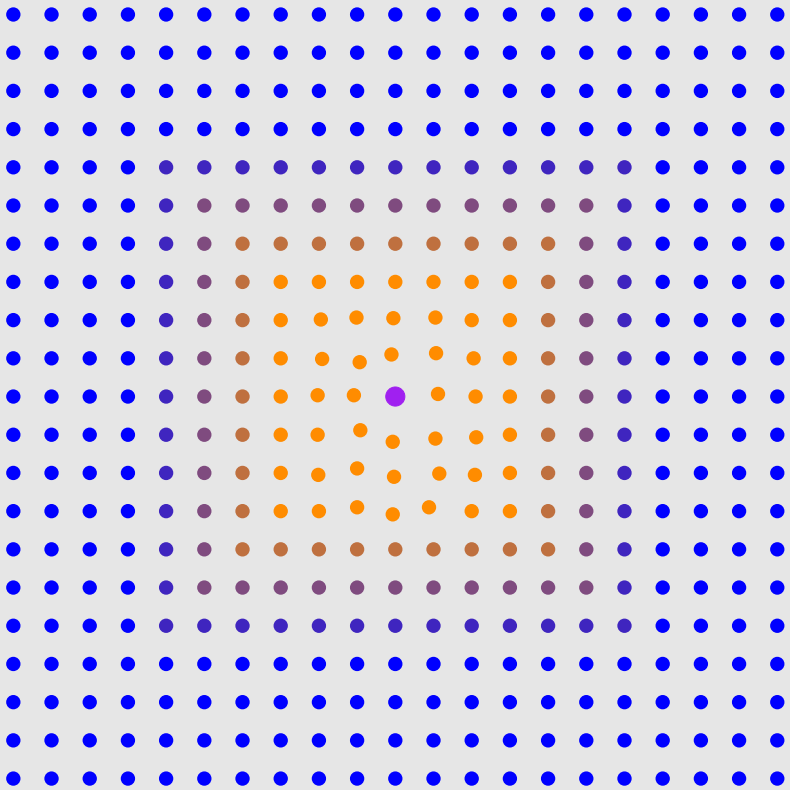
Di-vacancy, blending width 5.



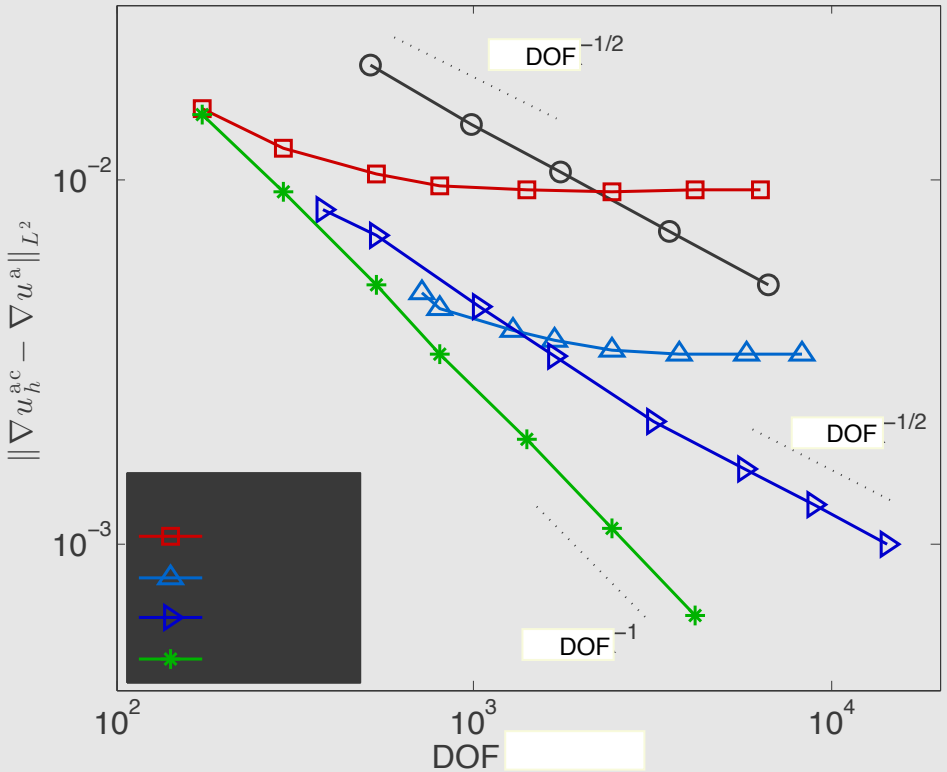
$$\mathcal{E}^{\mathrm{b}}(u) = \sum_{\ell \in \Lambda} (1 - \beta(\ell))\, V\big(Du(\ell)\big) + \int_{\mathbb{R}^d} \beta\, W(\nabla u)\, \mathrm{d}x$$

Approximation Parameters: 1. atomistic region, 2. blending region, 3. blending function β, ~~4. mesh size h~~

Why a Numerical Analysis



Di-vacancy, optimised blending



$$\mathcal{E}^{\mathrm{b}}(u) = \sum_{\ell \in \Lambda} (1 - \beta(\ell)) V(Du(\ell)) + \int_{\mathbb{R}^d} \beta W(\nabla u) \, \mathrm{d}x$$

Approximation Parameters: 1. atomistic region, 2. blending region, 3. blending function β, ~~4. mesh size h~~

Outline of The Error Estimate

Recall the general strategy to prove an error estimate via IFT:

- $X := \dot{\mathcal{U}}^{1,2}$, $x_0 := \bar{u}^{\mathrm{a}}$
- Stability estimate

$$\langle \delta^2 \mathcal{F}^{\mathrm{b}}(\bar{u}^{\mathrm{a}})v, v\rangle \geq \gamma_\beta \|Dv\|_{\ell^2}^2$$

- Consistency Estimate

$$\langle \delta \mathcal{F}^{\mathrm{b}}(\bar{u}^{\mathrm{a}}), v\rangle \leq \eta_\beta \|Dv\|_{\ell^2}$$

- If $L\eta_\beta(\gamma_\beta)^{-2} < 1$ then we obtain $\bar{u}^{\mathrm{b}}$ solution to (9) s.t.

$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim \eta_\beta$$

Proof of Consistency in 1D

The full estimate is fairly technical; see [17]. Instead we show a 1D proof from [20] (extends an earlier proof by Van Koten [15]), which shows most of the key ideas. Further, we assume that $\mathcal{T}_h$ has full atomistic resolution, i.e., $\mathcal{T}_h = \{(\ell, \ell+1) \,|\, \ell \in \mathbb{Z}\}$. In this case:

$$\mathcal{E}^{\rm b}(u) = \sum_{\ell\in\mathbb{Z}} (1-\beta(\ell)) V(Du(\ell)) + \int_{\mathbb{R}} \beta W(\nabla u)\,{\rm d}x$$

$$\langle \delta\mathcal{E}^{\rm b}(u), v\rangle = \sum (1-\beta)\langle \delta V(Du), Dv\rangle + \int \beta W'(\nabla u)\nabla v\,{\rm d}x,$$

$$\begin{aligned}\langle \delta\mathcal{E}^{\rm b}(u) - \delta\mathcal{E}^{\rm a}(u), v\rangle &= \int \beta W'(\nabla u)\nabla v\,{\rm d}x - \sum \langle \delta V(Du), Dv\rangle \\ &= \sum_{\rho\in\mathcal{R}} \left\{ \int \beta V_{,\rho}(\nabla_{\mathcal{R}} u)\nabla_\rho v\,{\rm d}x - \sum V_{,\rho}(Du) D_\rho v(\ell) \right\}\end{aligned}$$

$$\nabla_{\mathcal{R}} u = (\nabla_\rho u)_{\rho\in\mathcal{R}}, \quad \nabla_\rho u = \rho\nabla u$$

Taylor expansion easily implies that $V_{,\rho}(\nabla_{\mathcal{R}} u) = V_{,\rho}(Du) + O(|\nabla^2 u|)$, but v has no regularity so we cannot show $D_\rho v \approx \nabla_\rho v$. This is **nonlocality** vs. **locality** issue is the **core issue** in translating between atomistic and continuum models.

$$\langle \delta\mathcal{E}^{\mathrm{b}}(u) - \delta\mathcal{E}^{\mathrm{a}}(u), v\rangle = \sum_{\rho\in\mathcal{R}} \left\{ \int \beta V_{,\rho}(\nabla_{\mathcal{R}} u)\nabla_\rho v \,\mathrm{d}x - \sum \beta V_{,\rho}(Du) D_\rho v(\ell) \right\}.$$

In 1D (and in 1D only!) we can write

$$\boxed{D_\rho v(\ell) = \int \chi_{\ell,\rho} \nabla_\rho v \,\mathrm{d}x}$$

where $\chi_{\ell,\rho}(x) = |\rho|^{-1}, x \in \mathrm{conv}\{\ell, \ell+\rho\}$ and 0 otherwise.
We can now continue:

$$\begin{aligned}\langle \delta\mathcal{E}^{\mathrm{b}}(u) - \delta\mathcal{E}^{\mathrm{a}}(u), v\rangle &= \sum_{\rho\in\mathcal{R}} \left\{ \int \beta V_{,\rho}(\nabla_{\mathcal{R}} u)\nabla_\rho v \,\mathrm{d}x - \int \left[\sum_\ell \beta(\ell) V_{,\rho}(Du)\chi_{\ell,\rho} \right] \nabla_\rho v \,\mathrm{d}x \right\} \\ &= \int \sum_{\rho\in\mathcal{R}} \left\{ \beta\rho V_{,\rho}(\nabla_{\mathcal{R}} u(x)) - \sum_\ell \beta(\ell) V_{,\rho}(Du(\ell))\rho\chi_{\ell,\rho} \right\} \nabla v(x) \,\mathrm{d}x\end{aligned}$$

We have now removed the "bad non-locality" by shifting it into a "good non-locality" which we can remove via Taylor expansions:

- $\beta(\ell) = \beta(x) + \nabla\beta(x)(\ell - x) + O(\nabla^2\beta)$
- $V_{,\rho}(Du) = V_{,\rho}(\nabla_{\mathcal{R}} u) + \sum_\varsigma V_{,\rho\varsigma}(D_\varsigma u(\ell) - \nabla_\varsigma u(x)) + O(|\nabla^2 u|^2)$
- $D_\rho u(\ell) = \nabla_\rho u(x) + \frac{1}{2}\nabla_\rho^2 u(x) + \nabla_\rho \nabla_{\ell - x} u(x) + O(\nabla^3 u)$

This is a tedious calculation, the details of which can be found in [20]. In addition to the Taylor expansions we also need, that at element-midpoints $x = k + 1/2, k \in \mathbb{Z}$,

$$\sum_\ell \chi_{\ell,\rho}(x) = 1, \qquad \sum_\ell (\ell - x)\chi_{\ell,\rho}(x) = -\tfrac{\rho}{2}.$$

Here is roughly what happens: (we write $\beta = \beta(x), \nabla\beta = \nabla\beta(x)$ and so forth)

$$\begin{aligned}
\sum_\ell \beta(\ell) V_{,\rho}(Du(\ell))\rho\chi_{\ell,\rho} &= \sum_\ell \rho\chi_{\ell,\rho}\Big(\beta + \nabla\beta(\ell - x)\Big)\Big(V_{,\rho} + \sum_\varsigma V_{,\rho\varsigma}(D_\varsigma u - \nabla_\varsigma u)\Big) + O(|\nabla^2\beta| + |\nabla^2 u|^2) \\
&= \sum_\ell \rho\chi_{\ell,\rho}\beta V_{,\rho} + \sum_\ell \rho\chi_{\ell,\rho}\beta \sum_\varsigma V_{,\rho\varsigma}\Big(\tfrac{1}{2}\nabla_\varsigma^2 u + \nabla_\varsigma \nabla_{\ell - x} u\Big) \\
&\quad + \sum_\ell \rho\chi_{\ell,\rho}\nabla_{\ell-x}\beta V_{,\rho} + O\Big(|\nabla^2\beta| + |\nabla^2 u|^2 + |\nabla^3 u| + |\nabla\beta\nabla^2 u|\Big) \\
&= \beta\rho V_{,\rho} + \beta\nabla^2 u \sum_\varsigma V_{,\rho\varsigma}\Big(\tfrac{1}{2}\rho\varsigma^2 - \tfrac{1}{2}\rho^2\varsigma\Big) - \tfrac{1}{2}V_{,\rho}\rho^2\nabla\beta + O\Big(\dots\Big).
\end{aligned}$$

Now we go back into the sum over ρ:

$$\begin{aligned}
\sum_{\rho\in\mathcal{R}}\Big\{\beta\rho V_{,\rho}(\nabla_{\mathcal{R}} u(x)) - \sum_\ell \beta(\ell) V_{,\rho}(Du(\ell))\rho\chi_{\ell,\rho}\Big\} &= \sum_\rho \Big\{\beta\nabla^2 u \sum_\varsigma V_{,\rho\varsigma}\Big(\tfrac{1}{2}\rho\varsigma^2 - \tfrac{1}{2}\rho^2\varsigma\Big) - \tfrac{1}{2}V_{,\rho}\rho^2\nabla\beta\Big\} \\
&\quad + O\Big(\dots\Big)
\end{aligned}$$

The final step is exploiting point symmetry of V: Assumption (V) implies $V_\rho = -V_{,-\rho}$ and $V_{,\rho\varsigma} = V_{,(-\rho)(-\varsigma)}$, so we obtain

$$\cdots = \underbrace{\tfrac{1}{2}\nabla^2 u \sum_{\rho,\varsigma} V_{,\rho\varsigma}\left(\rho\varsigma^2 - \rho^2\varsigma\right)}_{=0} + O\Big(|\nabla^2\beta| + |\nabla^2 u|^2 + |\nabla^3 u| + |\nabla\beta\nabla^2 u|\Big)$$

Remark on Generalisation to 2D/3D: [17]
The only step that does not generalise to 2D/3D is $D_\rho u(\ell) = \int \chi_{\ell,\rho}\nabla_\rho u \,\mathrm{d}x$. In fact it is also true if we allow line integrals, but this does not help since we need to convert it to a volume integral. In 2D there is a small miracle in that bond integrals can be summed to become volume integrals [30]. In 3D no such miracle exists (to the best of my knowledge), instead we resort to very careful mollification argument. We identify lattice fuctions $v : \mathbb{Z}^d \to \mathbb{R}^d$ with their Q1 intepolants. Let ζ be the Q1 hat-function centered at 0 and define $v^* := \zeta * v$. Then we obtain

$$\begin{aligned} D_\rho v^*(\ell) &= \int_0^1 \nabla_\rho v^*(\ell + t\rho)\,\mathrm{d}t = \int_0^1 \int \zeta(\ell + t\rho - x)\nabla_\rho v(x)\,\mathrm{d}x\,\mathrm{d}t \\ &= \int_{\mathbb{R}^d} \chi_{\ell,\rho}(x)\nabla_\rho v(x)\,\mathrm{d}x, \qquad \chi_{\ell,\rho}(x) := \int_0^1 \zeta(\ell + t\rho - x)\,\mathrm{d}t. \end{aligned}$$

The key in the analysis is then to exploit the invertibility of the operation $v \mapsto v^*$ (true due to discreteness!) and to transfer back and forth between v and v^* as needed.
An alternative route might be to employ the ideas in [23]?

Full Statement of the Consistency Error Estimate

Generalising to 2D/3D we finally arrive at the following result.

Theorem 14.

Let $u \in \dot{\mathcal{U}}^{1,2}$, then for each $v_h \in \dot{\mathcal{U}}(\mathcal{T}_h)$ there exists $u \in \dot{\mathcal{U}}^{\mathrm{c}}$ such that

$$\left|\langle \delta\mathcal{E}^{\mathrm{b}}(\Pi_{R,h}u), v_h\rangle - \langle \delta\mathcal{E}^{\mathrm{a}}(u), v\rangle\right|'' \lesssim '' \|\nabla^2\beta\|_{L^2} + \|\nabla\beta\nabla^2 u\|_{L^2} + \|\beta\nabla^3 u\|_{L^2} + \|\beta\nabla^2 u\|_{L^4}^2 .$$

(legend: blending error, continuum modelling error)

Notes:

- The " $\lesssim$ " indicates that I've sligthly simplified the statement of the result. The "true estimate" is what I stated + higher-order terms, or alternatively one can state an estimate that looks more complicated but is qualitatively equivalent.

Very Rough Sketch of Stability

The proof of stability is even more involved than the proof of consistency. In 1D it is still somewhat elementary [20], but in 2D/3D it is fairly involved: [17]
The idea is to take a sequence of approximation parameters $(\beta_j, \mathcal{T}_j)$ with $R_j^{\mathrm{a}} \uparrow \infty$ and of minimising test functions $v_j \in \dot{\mathcal{U}}_j$ (the space is now indexed by j) such that $\|\nabla v_j\|_{L^2} = 1$ and $\left\langle \left(\delta^2\mathcal{E}^{\mathrm{b}}(\Pi_{h,j}y) + \delta^2\mathcal{P}(\Pi_{h,j}y)\right) v_j, v_j \right\rangle = \gamma_j^{\beta}$. Due to the bound $\|\nabla v_j\|_{L^2} = 1$, we can extract a weakly convergent subsequence (still denoted by v_j). This sequence is then decomposed into three components (scales): $v_j = v_j^{\mathrm{a}} + v_j^{\mathrm{b}} + v_j^{\mathrm{c}}$, for each of which we use a different stability argument:

- ∇v_j^{a} converges strongly at the atomic scale. It is concentrated near the defect core, hence for a sufficiently large atomistic region stability of the defect implies stability for this test function.
- ∇v_j^{b} converges weakly to zero at the atomic scale but strongly at the "interfacial scale"; i.e., after a rescaling $w_j^{\mathrm{b}}(x) = \delta v_j^{\mathrm{b}}(x/\epsilon)$, where $\epsilon \approx (R^{\mathrm{a}})^{-1}$ and δ so that $\|\nabla w_j^{\mathrm{b}}\|_{L^2} = \|\nabla v_j^{\mathrm{b}}\|_{L^2}$. This scaling keeps the interface (i.e., $\mathrm{supp}(\nabla\beta)$) near $|x| = 1$ as $\varepsilon \to 0$. Consistency of B-QCE implies that the action of the B-QCE hessian on this test function is approximately the same as that of the Cauchy–Born hessian, hence stability of the continuum model implies stability for this component of the test function.
- ∇v_j^{c} converges weakly to zero both at the atomic and "interfacial scale" (which means that it is not concentrated near a defect or interface). We can then exploit that, for a subsequence, $v_j^{\mathrm{c}} \to 0$ strongly in $L^2(B_{R^{\mathrm{b}}})$ to reduce the action of the B-QCE hessian on this test function to the independent actions of the linearized atomistic and continuum operators which are both stable.
- All cross-terms can be neglected in the limit as $j \to \infty$ due to an approximate orthogonality between the three components.

Incorporating Regularity

Having proven a consistency and a stability estimate (we skip the Lipschitz estimate), we check that the consistency error $\to 0$ (this happens as $R^{\mathrm{a}} \to \infty$; it is easy to see) and the IFT therefore yields an error estimate

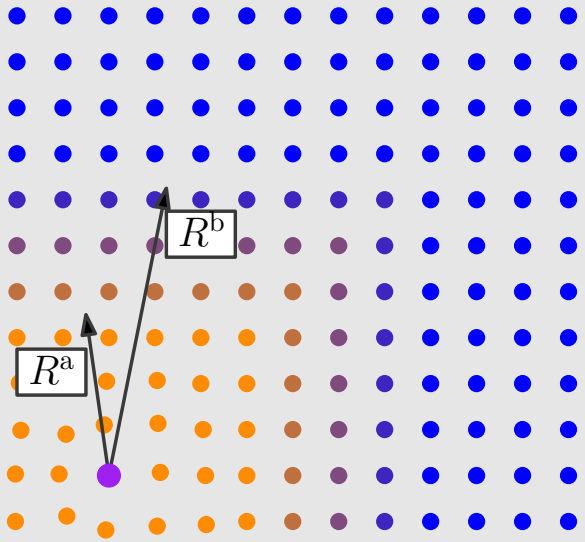
$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim \|\nabla^2\beta\|_{L^2} + \|\nabla\beta\nabla^2 u\|_{L^2} + \left\|\beta\nabla^3 u\right\|_{L^2} + \left\|\beta\nabla^2 u\right\|_{L^4}^2$$

Assuming that $u = \bar{u}^{\mathrm{a}}$ and employing the regularity estimate $|\nabla^j u| \lesssim |x|^{1-d-j}$ to obtain

$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim \|\nabla^2\beta\|_{L^2} + \|\nabla\beta\,|x|^{-d-1}\|_{L^2} + \left\|\beta|x|^{-d-2}\right\|_{L^2} + \left\|\beta|x|^{-d-1}\right\|_{L^4}^2$$

Introduce the radii $R^{\mathrm{a}}, R^{\mathrm{b}}$ as in the figure: to be precise, we need that

$$B_{R^{\mathrm{a}}} \subset \{\beta = 0\}, \quad B'_{R^{\mathrm{b}}} \subset \{\beta = 1\}$$



Some elementary estimates

$$\left\|\beta|x|^{-d-2}\right\|_{L^2} \lesssim \left(\int_{R^{\mathrm{a}}}^{\infty} r^{d-1} r^{-2d-4}\,\mathrm{d}r\right)^{1/2} \lesssim (R^{\mathrm{a}})^{-2-d/2},$$

$$\left\|\beta|x|^{-d-1}\right\|_{L^4}^2 \lesssim \left(\int_{R^{\mathrm{a}}}^{\infty} r^{d-1} r^{-4d-4}\right)^{1/2} \lesssim (R^{\mathrm{a}})^{-2-3d/2}.$$

We arrive at: $\boxed{\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim \|\nabla^2\beta\|_{L^2} + \|\nabla\beta\,|x|^{-d-1}\|_{L^2} + (R^{\mathrm{a}})^{-2-d/2}}$.

Optimising B-QCE: β

We have arrived at

$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim \|\nabla^2\beta\|_{L^2} + \|\nabla\beta\,|x|^{-d-1}\|_{L^2} + (R^{\mathrm{a}})^{-2-d/2}$$

To continue analysing the rate of convergence, we must now choose β. Since we have the precise dependence of the error on β we know exactly how to choose it: $\Delta^2\beta = 0$ subject to b.c. $\beta = 0$ in $B_{R^{\mathrm{a}}}$ and $\beta = 1$ in $B_{R^{\mathrm{c}}}$. In 1D this means that β is a cubic spline [15]. In practise, this is very useful for implementatin (solve this problem in a preprocessing step [21].)

It turns out for the error estimate we the following:

$$\beta \in C^{1,1}, \qquad |\nabla\beta| \le C_\beta (R^{\mathrm{b}} - R^{\mathrm{a}})^{-1}, \qquad C_\beta (R^{\mathrm{b}} - R^{\mathrm{a}})^{-2}. \tag{10}$$

(this is easy to achieve by choosing a radial β) This yields

$$\|\nabla\beta|x|^{-d-1}\|_{L^2} \lesssim (R^{\mathrm{b}} - R^{\mathrm{a}})^{-1} \left(\int_{R^{\mathrm{a}}}^{R^{\mathrm{b}}} r^{d-1} r^{-2d-2} \right)^{1/2} \lesssim (R^{\mathrm{b}} - R^{\mathrm{a}})^{-1} (R^{\mathrm{a}})^{-1-d/2},$$

$$\|\nabla^2\beta\|_{L^2} \lesssim (R^{\mathrm{b}} - R^{\mathrm{a}})^{-2} \left[(R^{\mathrm{b}})^d - (R^{\mathrm{a}})^d \right]^{1/2}$$

We see that the the term $\|\nabla^2\beta$ is by far the worst. Its rate becomes quasi-optimal if

$$c_\beta R^{\mathrm{a}} \le R^{\mathrm{b}} - R^{\mathrm{a}} \le C_\beta R^{\mathrm{a}}, \tag{11}$$

and in this case we obtain the **convergence rate**

$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim (R^{\mathrm{a}})^{-2+d/2} + (R^{\mathrm{a}})^{-2-d/2}$$

Convergence Rates

Summarising what we have so far obtained:

Theorem 15 (BQCE Convergence).

Let $\bar{u}^{\mathrm{a}}$ be a strongly stable solution of (1), β satisfy (10, 11) where C_β, c_β are independent of R^{a}. Then, for sufficiently large R^{a}, there exists $\bar{u}^{\mathrm{b}}$ solution to (9) such that $\boxed{\|D\bar{u}^{\mathrm{a}} - D\bar{u}^{\mathrm{b}}\|_{\ell^2} \lesssim (R^{\mathrm{a}})^{-2+d/2}}$

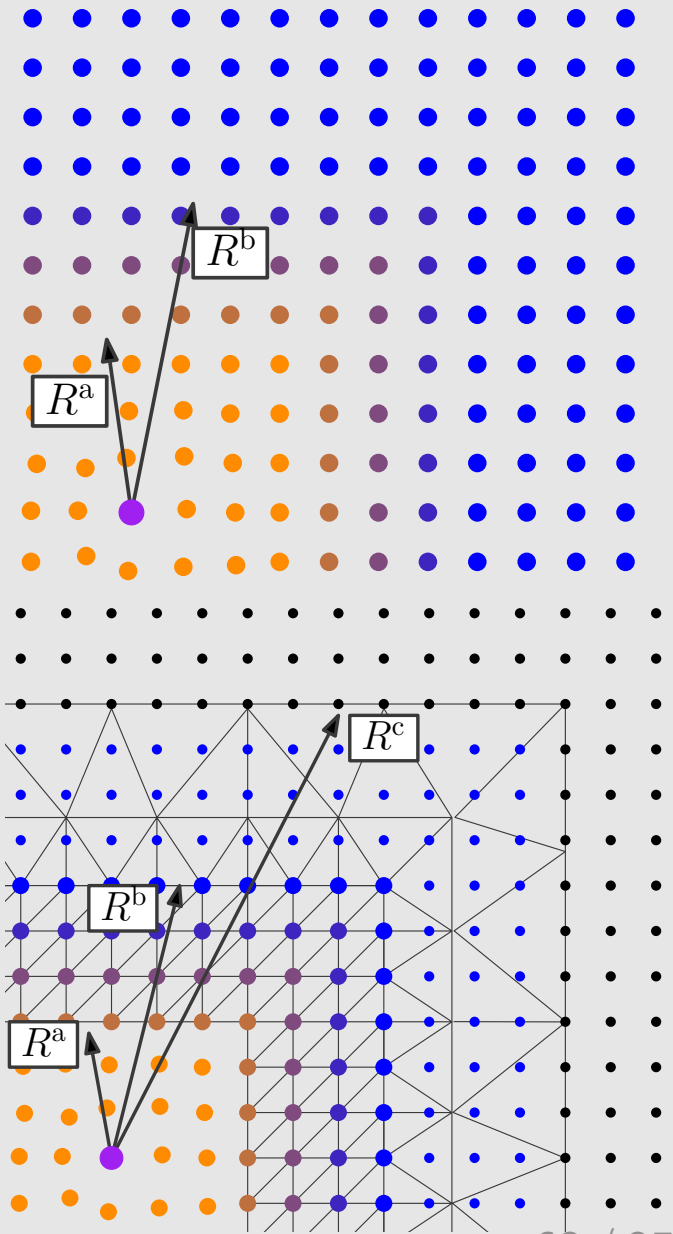
Remarks:

- In 2D, the BQCE rate is the same as that of the trivial atomstic truncation scheme. The complex multi-scale idea has gained us nothing! In 3D, the BQCE scheme is worse than the truncation scheme!
- Is the rate really optimal? We will see after some remarks on implementation.

Convergence Rate with P1-FEM

- Keep blending width $R^{\mathrm{b}} - R^{\mathrm{a}} \approx R^{\mathrm{a}}$
- Create finite element mesh $\mathcal{T}_h$
  - full atomistic resolution in atomistic and blending region
  - coarseing with rate $h(x) \approx (|x|/R^{\mathrm{a}})^{3/2}$
  - Total computational domain $\Omega_h = \cup \mathcal{T}_h$ has radius $R^{\mathrm{c}} \approx (R^{\mathrm{a}})^2$
- $\dot{\mathcal{U}}(\mathcal{T}_h) = \Big\{ v_h : \mathbb{R}^d \to \mathbb{R}^d \,|\, \text{p.w. aff.}, \; v_h = 0 \text{ in } \Omega_h' \Big\}.$
- FEM-BQCE functional ($Q_h \equiv$ midpt quadrature)

$$\mathcal{E}_h^{\mathrm{b}}(u_h) = \sum (1-\beta) V(Du_h) + \int_{\Omega_h} Q_h \big[\beta W(\nabla u_h)\big].$$



Theorem 16.

$\bar{u}^{\mathrm{a}}$ strongly stable soln of (1), R^{a} suff. lge., then $\exists\, ! \bar{u}_h^{\mathrm{b}} \in \arg\min\{(\mathcal{E}_h^{\mathrm{b}} + \mathcal{P})(u_h) \,|\, u_h \in \dot{\mathcal{U}}(\mathcal{T}_h)\}$ *s.t.*

$$\|D\bar{u}^{\mathrm{a}} - D\bar{u}_h^{\mathrm{b}}\|_{\ell^2} \lesssim (R^{\mathrm{a}})^{-2+d/2} + (R^{\mathrm{a}})^{-1-d/2}.$$

Numerical Implementation

1. Choose R^{a}, then $R^{\mathrm{b}} = 2R^{\mathrm{a}}$, $Rc = (R^{\mathrm{a}})^2$
2. Construct a finite element mesh and corresponding domain Ω_h according to these radii, with the optimal coarsening rate.
3. Compute a blending function β. In practise, this is best done by solving a discrete bi-Laplace problem. [21]

$$\min \|\Delta_h \beta_h\|_{L^2} \quad \text{subj. to } \beta_h = \begin{cases} 0, \text{atomistic region. e.g., } |x| \leq R^{\mathrm{a}}, \\ 1, \text{continuum region, e.g., } |x| \geq R^{\mathrm{b}} \end{cases}$$

   where Δ_h is some arbitrary discrete Laplacian.

4. Supply energy and forces for

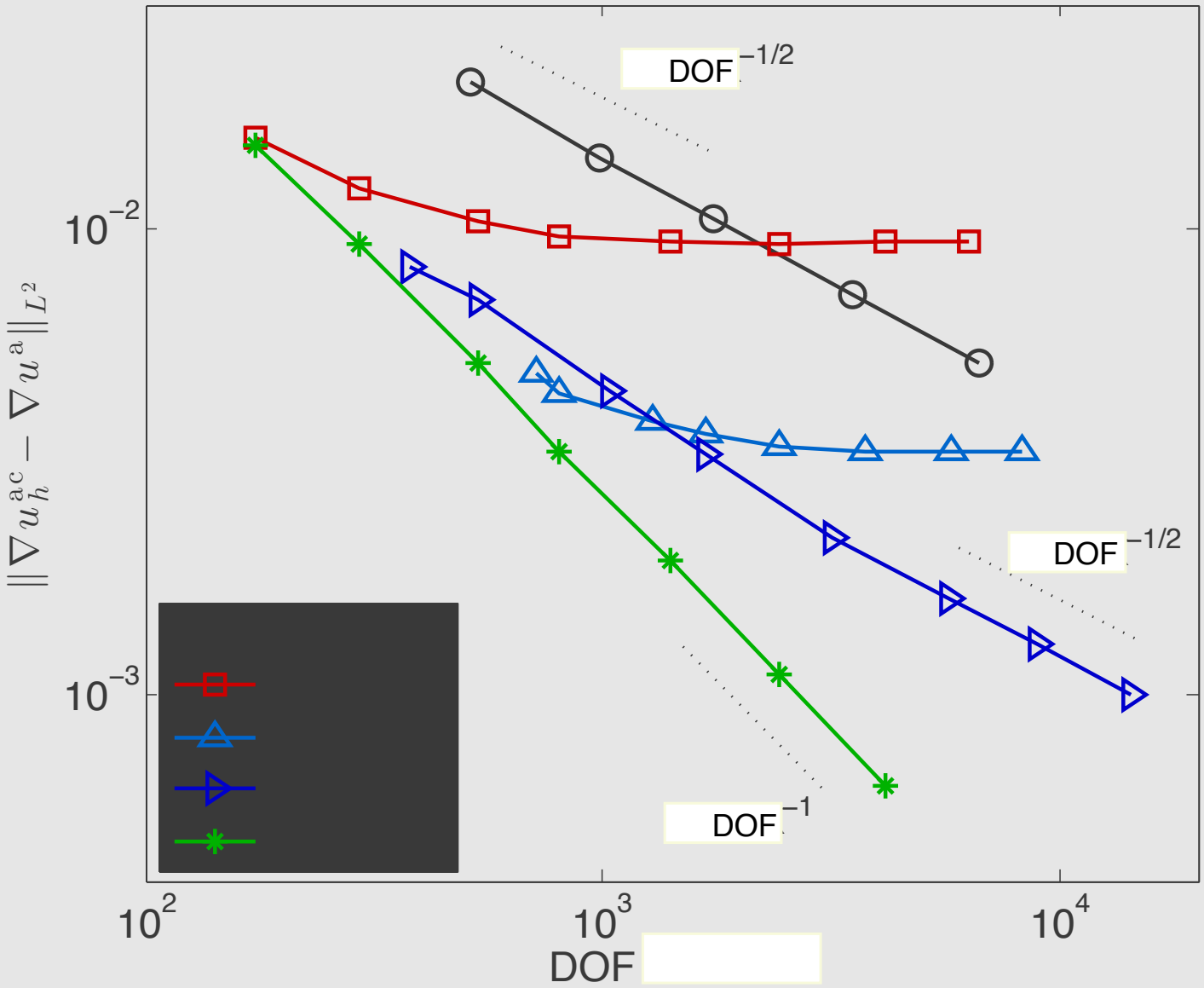
$$\mathcal{E}_h^{\mathrm{b}}(u_h) = \sum_{\ell \in \Lambda} (1 - \beta(\ell)) V(Du_h(\ell)) + \int Q_h \left[\beta W(\nabla u_h)\right] \mathrm{d}x,$$

   where Q_h is the mid-point quadrature operator.

5. Minimise $\mathcal{E}_h^{\mathrm{b}} + \mathcal{P}$ using a gradient scheme (ideally preconditioned.)

Numerical Confirmation of the Rate

Numerical Test: divacancy in triangular lattice, NN EAM toy model



Ghost-Force Removal

Motivation:

- Recall that the "ghost forces" $\delta\mathcal{E}^{\mathrm{ac}}(0) \neq 0$ are not removed, but only smeared out i.e. we still have $\delta\mathcal{E}^{\mathrm{b}}(0) \neq 0$. We can also see this if we dig deeper into the consistency error estimate: the $\|\nabla^2\beta\|_{L^2}$ term can be made more precise:

$$\|\nabla^2\beta\|_{L^2} \quad \rightsquigarrow \quad \big\| \, |\nabla^2\beta| \, |\delta V(\nabla_{\mathcal{R}} u)| \, \big\|$$

  Can we remove them altogether?

- But, motivated by the proof of the extension lemma, we can easily remove these by "renormalising" the atomistic energy

$$\mathcal{E}^{\mathrm{a}}(u) = \sum V(Du) = \sum \Big(V(Du) - \langle \delta V(\mathbf{0}), Du \rangle \Big) =: \sum V'(Du)$$

  Let the corresponding strain energy function be $W'(\mathsf{F}) := V(\mathsf{F} \cdot \mathcal{R})$.

- While the new site potential V' does not change $\mathcal{E}^{\mathrm{a}}$, it does change $\mathcal{E}^{\mathrm{b}}$:

$$\mathcal{E}^{\mathrm{gb}}(u) := \sum_{\ell \in \Lambda} (1 - \beta(\ell)) V'(Du(\ell)) + \int \beta W(\nabla u) \, \mathrm{d}x$$

  With the total energy $\mathcal{F}^{\mathrm{gb}} = \mathcal{E}^{\mathrm{gb}} + \mathcal{P}$ we solve

  The GFC-B-QCE Scheme: $\boxed{\bar{u}^{\mathrm{gb}} \in \operatorname{arg\,min} \left\{ \mathcal{F}^{\mathrm{gb}}(u) \,|\, u \in \dot{\mathcal{U}}^{1,2} \right\}}$ (12)

Notes on the GFC-B-QCE Scheme

Notes:

- An alternative interpretation of the GFC-B-QCE scheme (which gives it its name) is to remove the "ghost forces" as follows:

$$\mathcal{E}^{\mathrm{gb}}(u) := \mathcal{E}^{\mathrm{b}}(u) + \langle \delta\mathcal{E}^{\mathrm{a}}(0) - \delta\mathcal{E}^{\mathrm{b}}(0), u \rangle.$$

  It is easy to see that these are equivalent formulations, however the new formulation is much easier to extend to more complex situations (dislocations, cracks, problems with boundaries, etc).
  The dead load correction obviously achieves that $\langle \delta\mathcal{E}^{\mathrm{gb}}(0), u \rangle = 0$.
  More generally, one could remove the ghost force in some predictor $\hat{u}$; see [29].
- The idea of static ghost-forces correction originates (to my knowledge) from [31]. It is somewhat under debate whether the scheme schould be considered energy-based or force-based [3]; it depends heavily on the context. In our context it is clearly energy-based.
- There is so far no rigorous analysis of the pure GFC scheme in 2D/3D, due to the fact that as for all sharp-interface schemes, proving stability is very difficult.

Error Estimate for GFC-B-QCE

We only look at the leading term, assuming all our previous optimisations on β:

$$\begin{aligned}\| \, |\nabla^2 \beta| \, |\delta V'(\nabla_{\mathcal{R}} u)| \, \|_{L^2} &\lesssim (R^{\rm b} - R^{\rm a})^{-2} \|\delta V'(\nabla_{\mathcal{R}} u) - \delta V'(\mathbf{0})\|_{L^2(B_{R^{\rm b}} \setminus B_{R^{\rm a}})} \\ &\lesssim (R^{\rm b} - R^{\rm a})^{-2} (R^{\rm a})^{-d/2} \approx (R^{\rm a})^{-2-d/2}.\end{aligned}$$

Remark: This matches the error contribution from the continuum model! That is, the GFC-B-QCE scheme is **optimal** among all a/c coupling schemes where the continuum model is of first-order.

Theorem 17 (GFC-BQCE Convergence).

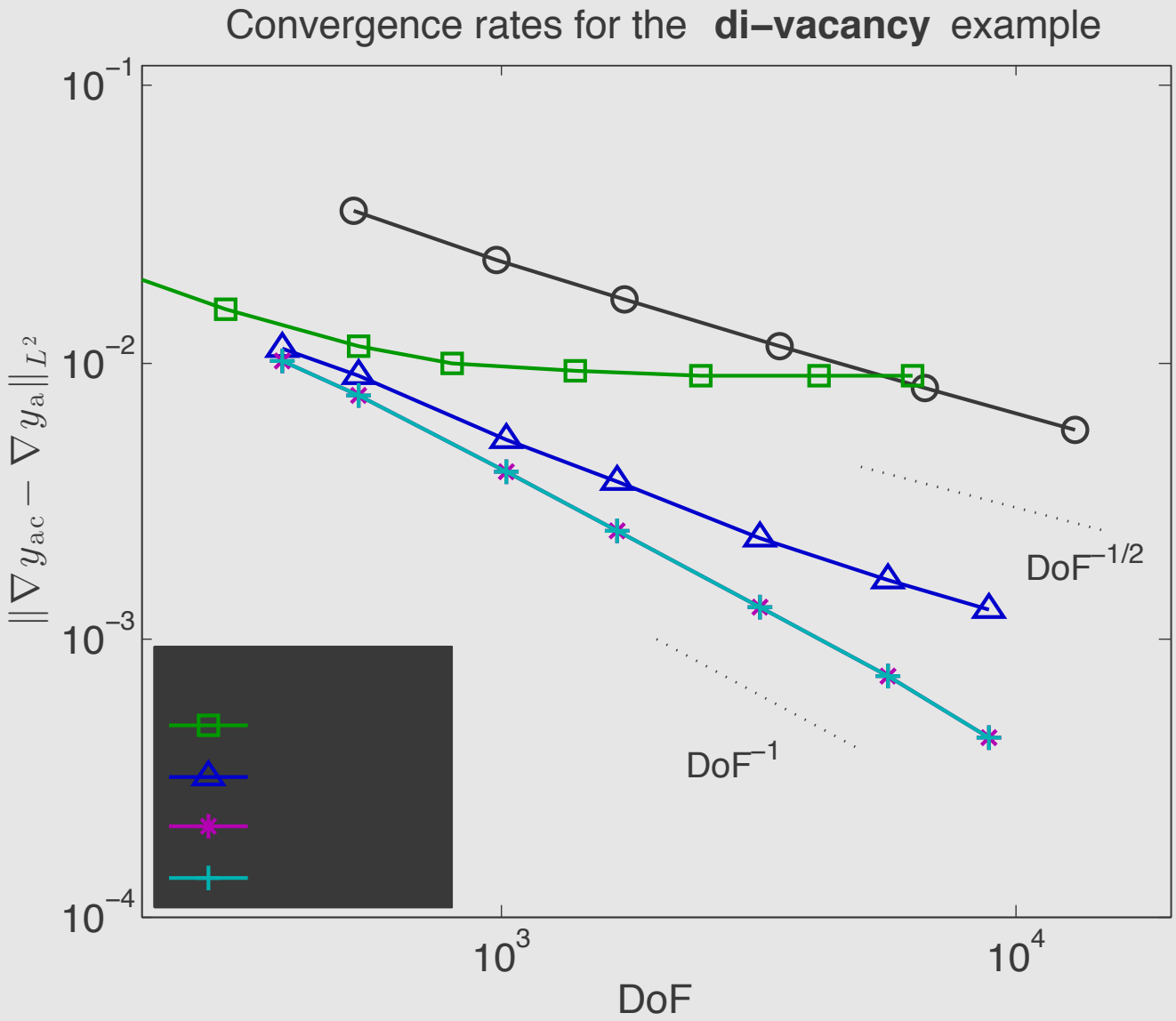
Let $\bar{u}^{\rm a}$ be a strongly stable solution of (1), β satisfy (10, 11) where C_β, c_β are independent of $R^{\rm a}$. Then, for sufficiently large $R^{\rm a}$, there exists $\bar{u}^{\rm gb}$ solution to (9) such that $\|D\bar{u}^{\rm a} - D\bar{u}^{\rm gb}\|_{\ell^2} \lesssim (R^{\rm a})^{-2-d/2}$

Remarks:

- Adding P1-FEM and truncation to the method yields the rate $(R^{\rm a})^{-1-d/2}$
- For optimal rate, use P2-FEM discretisation. (This extension is possible.)

Numerical Confirmation of the Rate

Numerical Test: divacancy in triangular lattice, NN EAM toy model



Appendix A: Outlook

Some Obvious Directions (that Require Attention)

- **A Posteriori Model Adaptivity:**
  1. A posteriori error control of course;
  2. Optimise approximation parameters on the fly to also optimise the prefactor, not just the rate;
  3. Evolve the atomistic region with the defect;
  4. Place atomistic region where defect nucleates.
- **Stability of sharp-interface** coupling (as opposed to our blending method) E.g., it can be shown that within the QNL class (the only known general class of energy-based sharp-interface couplings) no "universally stable" variant exists [26].
  1. How large is the stability error, i.e., is this ever a problem?
  2. Are force-based sharp-interface methods stable? For a first step, see [18].
- **Complex Crystals:** if more than one specis of atom occurs in the crystal, they still arrange into a periodic environment (but not a Bravais lattice anymore). Point symmetry of the crystal and of the interaction is now lost. What is the consequence of this? (see publications by [Abdulle/Shapeev/Lin], [Dobson/Elliot/Luskin/Tadmor], [Vankoten/Ortner], ...)
- **Charged Defects:** depending on who you talk to even the model seems to be unclear? (e.g., Mott/Littleton vs. PBCs?) This seems particularly difficult for charged defects on surfaces. Because of Coulomb interaction, both the interaction and the elastic fields are long-ranged. Both are more difficult to treat analytically. Important applications, e.g., in semiconductor design, energy storage, etc.

Perspective

- Multi-scale modelling has become a huge subdiscipline of applied mathematics. What I have discussed in these notes is a still small niche: numerical analysis of coarse-graining schemes for atomistic models. I have discussed one particular example which we understand well (though not completely!) But there are **many** other coarse-graining schemes that are still waiting to receive similar attention.
- **2013 Nobel Prize in Chemistry:** "for the development of multiscale models for complex chemical systems".

  This is often confused to mean "for the introduction of the QM/MM scheme", but in reality it was given for the development of "coarse-grained" molecular simulation as a whole, including the development of interatomic potentials (as coarse-graining of Born-Oppoenheimer MD).
- The state of multi-scale modelling is roughly where finite-difference methods were before the CFL condition. There are few precise "regulations" to follow in constructing good coarse-graining schemes. As a result a considerable proportion of human resources goes into generating, fine-tuning and **calibrating** atomistic models and coarse-graining schemes. A continued effort to develop a mathematical foundation for molecular simulation in general and coarse-graining in particular will lead to automated procedures, and simulation by "press of a button" (cf. FENICS).
- (this is all aside from the obvious improvements in accuracy, performance and reliability that a rigorous mathematical foundation can bring.)

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Appendix C: Solutions

Solution Exercise 1

(a) $\ell^1 \subset \ell^p \subset \ell^\infty$, hence $\dot{\mathcal{U}}^{1,\infty}$ is the largest and $\dot{\mathcal{U}}^{1,1}$ the smallest. By contrast, $L^\infty \subset L^p \subset L^1$ provided the domain is bounded (or, measure finite) so in this case $W^{1,1}$ is the largest, $W^{1,\infty}$ the smallest.
The important point here is that on lattices $\ell^2 \subset \ell^\infty$, which is the main reason that linearisation arguments (Inverse function theorem) can be applied in the energy space. By contrast one cannot normally apply IFT arguments to quasilinear PDE $\mathrm{div} S(\nabla u)$, when taking $u \in W^{1,2}$, because the linearisation error is not controlled. Instead one then resorts monotonicity or convexity arguments.

(b) immediate corollary of triangle inequality. The embedding is not compact; take $u_n(\ell) = \delta(k_n - \ell)$ where $|k_n| \to \infty$.

(c) This just follows from the fact that $\|Du - Dv\|_{\ell^2} = 0$ implies $u = v + c$.

(d) For this, we just employ Lemma 7. If we believe it (we didn't actually prove it), then we can now just use the fact that $\|Du\|_{\ell^2(\Lambda \setminus B_{R/2})} \to 0$ as $R \to \infty$, due to the fact that $|Du(\ell)|^2 \in \ell^1$.
If we do want to prove Lemma 7 properly, then all we need is a discrete Poincaré inequality, but this requires considerable machinery. An easier technique is to triangulate the lattice, then get an interpolant $\bar{u}$ of u, so that we get $\|\bar{u} - \langle \bar{u} \rangle_{A_R}\| \lesssim R\|\nabla \bar{u}\|$ and then show some norm-equivalences. This is done in [9].

Solution Exercise 2

(a) We need to prove that $\mathcal{E}' \in C^k$; $k \geq 2$. We show that $\mathcal{E}' \in C$. We first write

$$\Phi(Du) := V(Du) - \langle \delta V(\mathbf{0}), Du \rangle = \int_0^1 (1-t) \langle \delta^2 V(tDu) Du, Du \rangle \, \mathrm{d}t.$$

Fix $u \in \dot{\mathcal{U}}^{1,2}$ and take $v \to u$ in $\dot{\mathcal{U}}^{1,2}$; wlog $\|Du - Dv\|_{\ell^\infty} \leq 1$. There is a modulus of continuity ω for $\delta^2 V$ in the domain $\{\boldsymbol{g} \in (\mathbb{R}^d)^{\mathcal{R}} \,|\, |\boldsymbol{g}| \leq \|Du\|_{\ell^\infty} + 1\}$, hence we obtain

$$\begin{aligned}
|\Phi(Du) - \Phi(Dv)| &\leq \left| \int_0^1 (1-t) \langle [\delta^2 V(tDu) - \delta^2 V(tDv)] Du, Du \rangle \, \mathrm{d}t \right| + \text{quadratic ter} \\
&\leq \int_0^1 \omega\big(t |Du(\ell) - Dv(\ell)|\big) |Du(\ell)|^2 \, \mathrm{d}t + \text{quad. terms} \\
&\leq \omega\big(\|Du - Dv\|_{\ell^\infty}\big) \|Du\|_{\ell^2} + \text{quad. terms.}
\end{aligned}$$

The quadratic terms are of course continuous and further, $\|Du - Dv\|_{\ell^\infty} \to 0$ as $\|Du - Dv\|_{\ell^2} \to 0$. Hence, $\mathcal{E}' \in C(\dot{\mathcal{U}}^{1,2})$.

To show that $\mathcal{E}' \in C^2$ (with $k = 2$) we just expand,

$$\begin{aligned}\mathcal{E}'(u+v) &= \sum_\ell \Phi(Du + Dv) \\ &= \sum_\ell \Big(\Phi(Du) + \langle \delta\Phi(Du), Dv\rangle + \tfrac{1}{2}\langle \delta^2\Phi(Du)Dv, Dv\rangle \\ &\qquad + \int_0^1 \langle [\delta^2 V(Du + tDv) - \delta^2 V(Du)]Dv, Dv\rangle \Big),\end{aligned}$$

and arguing as before we obtain that the remainder tends to zero as $Dv \to 0$ in ℓ^2.

(b) Let $u \in \dot{\mathcal{U}}^{\mathrm{c}}$. If $Du \to 0$ in ℓ^p for some $p < 2$, then in particular $Du \to 0$ in ℓ^2 and hence $\mathcal{E}^{\mathrm{a}}(u) \to 0$.
Now suppose we take $Du \to 0$ in ℓ^p for $p > 2$, but $\|Du\|_{\ell^2} \to \infty$. In this case, $\mathcal{E}^{\mathrm{a}}(u) \to \infty$, i.e., $\mathcal{E}^{\mathrm{a}}$ is not continuous. A simple way to see this is to write

$$\mathcal{E}^{\mathrm{a}}(u) = \int_0^1 (1-t)\langle \delta^2\mathcal{E}(tu)u, u\rangle \,\mathrm{d}t \geq \tfrac{1}{2}\langle \delta^2\mathcal{E}(0)u, u\rangle - C\|Du\|_{\ell^\infty}\|Du\|_{\ell^2}^2.$$

Upon rescaling, we can in fact obtain $\mathcal{E}^{\mathrm{a}}(u) \to c$ for any $c \in [0, \infty]$. It remains to show that such a sequence exists. To that end we just consider a mollifier μ and define $u_R(\ell) := R^\alpha \mu(\ell/R)$. One can then quickly see that $\|Du_R\|_{\ell^p} \approx R^{\alpha + d/p - 1}$, and by adjusting α we can obtain $Du_R \to 0$ in any ℓ^p space.

Solution Exercise 3

Pick an arbitrary $v \in \dot{\mathcal{U}}^{\mathrm{c}}$ with support contained in B_R, say, and define $v_m(\ell) := v(\ell - m)$. Then,

$$\begin{aligned}
\|Dv\|_{\ell^2}^2 \gamma = \gamma \|Dv_m\|_{\ell^2}^2 &\leq \langle \delta^2 \mathcal{E}^{\mathrm{a}}(u) v_m, v_m \rangle \\
&= \sum_{\ell \in \Lambda \cap B_R(m)} \langle \delta^2 V(Du) Dv, Dv \rangle \\
&= \langle \delta^2 \mathcal{E}^{\mathrm{a}}(0) v_m, v_m \rangle + \sum_{\ell \in \Lambda \cap B_R(m)} \langle [\delta^2 V(Du) - \delta^2 V(\mathbf{0})] Dv, Dv \rangle \\
&\leq \langle \delta^2 \mathcal{E}^{\mathrm{a}}(0) v, v \rangle + \sup_{|\ell| > |m| - R} \omega(|Du(\ell)|) \|Dv\|_{\ell^2},
\end{aligned}$$

But $\sup_{|\ell|>|m|-R} \omega(|Du(\ell)|) \to 0$ as $|m| \to \infty$, so in the limit we obtain the stated result.

Solution Exercise 4

We follow the outline given after the statement of the problem. The first step, $\mathcal{E}_R^{\mathrm{lin}} \in C^k$ is analogous to proving the $\mathcal{E}^{\mathrm{a}} \in C^k$. Note in particular that $\delta Q(\mathbf{0}) = \delta V(\mathbf{0})$ so the "renormalisation" does not change.

Proof of (5) (estimate for $\delta\mathcal{E}_R^{\mathrm{lin}} - \delta\mathcal{E}^{\mathrm{a}}$):

$$\begin{aligned}\langle \delta\mathcal{E}_R^{\mathrm{lin}}(u) - \delta\mathcal{E}^{\mathrm{a}}(u), v\rangle &= \sum_{\Omega'} \langle \delta V(Du) - \delta Q(Du), Dv\rangle \\ &= \sum_{\Omega'} \langle \delta V(Du) - \delta V(\mathbf{0}) - \delta^2 V(\mathbf{0})Du, Dv\rangle.\end{aligned}$$

Since $V \in C^3$, we have $|\delta V(Du) - \delta V(\mathbf{0}) - \delta^2 V(\mathbf{0})Du| \le C|Du|^2$, where C depends only on $\|Du\|_{\ell^\infty}$. So we obtain

$$\langle \delta\mathcal{E}_R^{\mathrm{lin}}(u) - \delta\mathcal{E}^{\mathrm{a}}(u), v\rangle \lesssim \sum_{\Omega'} |Du|^2|Dv| \le \|Du\|^2_{\ell^4(Om')}\|Dv\|_{\ell^2}.$$

Proof of (6) (estimate for $\delta^2\mathcal{E}_R^{\mathrm{lin}} - \delta^2\mathcal{E}^{\mathrm{a}}$): analogously to the last step,

$$\begin{aligned}\langle\langle \delta^2\mathcal{E}^{\mathrm{a}}(u) - \delta^2\mathcal{E}_R^{\mathrm{lin}}(u)]v, v\rangle &= \sum_{\ell\in\Omega'} \langle [\delta^2 V(Du) - \delta^2(\mathbf{0})]Dv, Dv\rangle \\ &\lesssim \sum_{\Omega'} |Du||Dv|^2 \le \|Du\|_{\ell^\infty(\Omega')}\|Dv\|^2_{\ell^2}.\end{aligned}$$

This works because $k \ge 3$.

To employ the IFT we set $X = \dot{\mathcal{U}}^{1,2}, x_0 = \bar{u}^{\rm a}$ (note there is no approximation necessary here since the computational space is the same as the problem space!), $\mathcal{G} = \delta\mathcal{E}_R^{\rm lin}$. Then we obtain from Theorem 8 that

$$\begin{aligned}\|\mathcal{G}(x_0)\| &= \|\delta\mathcal{E}_R^{\rm lin}(\bar{u}^{\rm a})\|_{\dot{\mathcal{U}}^{-1,2}} = \|\delta\mathcal{E}_R^{\rm lin}(\bar{u}^{\rm a}) - \delta\mathcal{E}^{\rm a}(\bar{u}^{\rm a})\|_{\dot{\mathcal{U}}^{-1,2}} \\ &\le C\|D\bar{u}^{\rm a}\|_{\ell^4}^2 \le C\left(\int_R^\infty r^{d-1} r^{-4d}\right)^{1/2} \le CR^{-3d/2} =: \eta.\end{aligned}$$

Further, from (6) we obtain that

$$\langle \delta^2\mathcal{E}_R^{\rm lin}(\bar{u}^{\rm a})v, v\rangle \ge \gamma_R \|Dv\|_{\ell^2}^2,$$

where $\gamma_R \to \gamma$ as $R \to \infty$. Lipschitz continuity of $\delta^2\mathcal{E}_R^{\rm lin}$ is easy to show along similar lines. Hence, the IFT gives us existence of a uniquye $\bar{u}_R^{\rm lin}$ satisfying (4) and $\|D\bar{u}_R^{\rm lin} - D\bar{u}^{\rm a}\|_{\ell^2} \le CR^{-3d/2}$.

Rate of Convergence of LIN

Interstitial in 2D triangular lattice, EAM-type NN interaction