Exercises

There are far too many exercises to cover during the summer school. The idea of providing these was to give interested readers the opportunity for a self-study introduction to a/c coupling. In the tutorials we will cover primarily the exercises on the B-QCE method.

Atomistic Model, General Background

Exercise 1 Prove Lemma 2.1.

Hint: Let \( u \in U \) be defined by \( u'_m = 1 \) and \( u'_\ell = 0 \) for \( m \neq \ell \). Then construct an approximating sequence from \( U_0 \).

Exercise 2 Prove Lemma 2.2.

Hint: This is a slightly involved proof. Show first that you can replace \( \phi_i(r) \) with \( \psi_i(r) := \phi_i(r) - \phi'_i(0)r \), i.e., redefine \( E_a(u) = \sum_\ell \{ \psi_1(u'_\ell) + \psi_2(u'_\ell + u'_{\ell+1}) \} \). Note that \( |\psi_i(r)| \lesssim r^2 \) and use this to show that the new form of \( E_a \) is well-defined on \( U \) and \( C^3 \).

Exercise 3 Recall that \( U \) is the closure of \( U_0 \), and according to Exercise 2, \( E_a(u) \sim \|u\|_U^2 \) hence the closure is taken in the correct “energy norm”.

Prove that, if \( u \in U \) then \( |u_\ell| \leq C \ell^{1/2} \). Show that this estimate is essentially sharp. Why does this not contradict the far-field boundary condition \( u_\ell \sim 0 \) as \( \ell \to \infty \)?

Exercise 4 Show that \( \langle f, u \rangle \lesssim C\|u'\|_{\ell^2} \) if and only if there exists \( g \in \ell^2 \) such that \( f_\ell = g'_\ell \). Show that \( C = \|g\|_{\ell^2} \) is the optimal constant.

Exercise 5 Prove Lemma 2.3.

Exercise 6 1. Let \( K \in \mathbb{N} \) be arbitrary. Prove that \( \|\delta E^{\text{qce}}(0)\|_{U_K} \geq \frac{1}{\sqrt{2}}|\phi'_2(0)| \).

2. Moreover (after introducing the FE spaces) prove that, if \( K - 1, K \) are finite element nodes (repatoms) then we still have \( \|\delta E^{\text{qce}}(0)\|_{U_K} \geq \frac{1}{\sqrt{8}}|\phi'_2(0)| \).

The Cauchy–Born Model

Exercise 7 Review the derivation of the Cauchy–Born approximation. Make this more precise by showing that, if

\[
E^c(u) := \int_0^\infty W(\nabla u) \, dx = \sum_{\ell=1}^\infty W(u'_\ell),
\]
then
\[ |\mathcal{E}^a(u) - \mathcal{E}^c(u)| \lesssim \|u''\|_{\ell^1} + \|u''\|_{\ell^2}^2. \]

Explain why this is a second-order estimate. This is a bit surprising, since the construction would indicate only a first-order approximation. Can you think of the reason why it is second-order?

**Exercise 8** Prove a sharp consistency estimate for the Cauchy–Born model:
\[ \langle \delta \mathcal{E}^a(u) - \delta \mathcal{E}^c(u), v \rangle \lesssim \left( \|u''\|_{\ell^2} + \|u''\|_{\ell^2}^2 \right). \]

Explain again, why this is a second-order estimate.

**Exercise 9** Stability for a homogeneous deformation: Show that, if
\[ \langle \delta^2 \mathcal{E}^a(0)v, v \rangle \geq c_0 \|v'\|_{\ell^2}^2 \quad \forall v \in U_0, \]
then also
\[ \langle \delta^2 \mathcal{E}^c(0)v, v \rangle \geq c_0 \|v'\|_{\ell^2}^2 \quad \forall v \in U_0, \]
but not vice-versa.

Hint: show that \( \inf \delta^2 \mathcal{E}^a(0) > 0 \) always implies \( \inf \delta^2 \mathcal{E}^c(0) > 0 \). But show that if \( \phi''_2(0) > 0 \) and \( \phi''_1(0) < 0 \), then it is possible that \( \delta^2 \mathcal{E}^c(0) \) is unstable while \( \delta^2 \mathcal{E}^a(0) \) is stable.

**Exercise 10** Prove a stability estimate for the Cauchy–Born model: Suppose that \( u \in U \) is atomistically stable:
\[ \langle \delta^2 \mathcal{E}^a(u)v, v \rangle \geq c_0 \|v'\|_{\ell^2}^2 \quad \forall v \in U_0. \]
Show that there exists \( \epsilon > 0 \) such that, if \( \|u''\|_{\ell^\infty} \lesssim \epsilon \), then
\[ \langle \delta^2 \mathcal{E}^a(u)v, v \rangle \geq c_0 \|v'\|_{\ell^2}^2. \]

Hint: Write \( \langle \delta^2 \mathcal{E}^a(u)v, v \rangle = \sum_{\ell} A_\ell \|v'\|_{\ell^2}^2 + B_\ell \|v''\|_{\ell^2}^2. \) Now use a localisation argument to show that \( A_\ell \geq c_0/2 \) provided that \( \|u''\|_{\ell^\infty} \) is sufficiently small.

**Exercise 11** Combine the foregoing exercises to prove a rigorous second-order error estimate for the Cauchy–Born model.

**Exercise 12** 1. Sharper consistency error analysis for the QNL method: In the same setting as Lemma 8, prove that
\[ \|\delta \mathcal{E}^a(u) - \delta \mathcal{E}^{\text{qnl}}(u)\|_{U^*} \lesssim |u''_K| + \|u''\|_{\ell^2(\Lambda_{\kappa})} + \|u''\|_{\ell^2(\Lambda_{\kappa})}^2. \]
Assuming that \( u \) satisfies (DH), deduce that \( \|\delta \mathcal{E}^a(u) - \delta \mathcal{E}^{\text{qnl}}(u)\|_{U^*} \lesssim K^{-\alpha - 1}. \)

2. Does the same (or a similar) estimate hold for nearest-neighbour many-body interactions as in Example 22?
Results on the FE coarsening error

**Exercise 13** Let $J_h : \mathcal{U} \to \text{P1}(\mathcal{T}_h)$ be the nodal interpolant ($J_h \neq I_h$)! Prove the interpolation error estimate

$$\|\nabla u - \nabla J_h u\|_{L^2} \lesssim h \|\nabla^2 \tilde{u}\|_{L^2(K,N)}$$

for any choice of $\tilde{u} \in C^{1,1}$ s.t. $\tilde{u}(\ell) = u_\ell$ for all $\ell \in \mathbb{Z}$. Deduce that

$$\|\nabla u - \nabla I_h u\|_{L^2} \lesssim h \|\nabla^2 \tilde{u}\|_{L^2(K,N)} + N^{1/2-\alpha}.$$  

Hint: if you don’t know the standard 1D interpolation error estimates, try to derive this result using Friedrich’s / Poincaré’s inequalities.

**Exercise 14** Prove Lemma 6.2.

(Hint: Suppose that $|\nabla^2 \tilde{u}(x)| \lesssim x^{-\alpha-1}$ for $x \geq r_0$ (as suggested by (DH)). Write the error as a functional $\text{Err}(h)$ of the mesh size $h \in L^\infty(K,N)$ and the number of degrees of freedom as another functional $\text{DoF}(h)$. Now minimize $\text{Err}$ subject to $\text{DoF}$ held fixed.)

**Exercise 15** Prove Lemma 6.3. (DIFFICULT)

(Hint: first try the standard interpolation error analysis. This will fail because we need a Poincaré inequality. But the Poincaré constant on $[0,N]$ is $O(N)$. Instead, try to employ the weighted Poincaré inequality

$$\|w^{-1}u\|_{L^2(K,\infty)} \leq \frac{1}{\log K} \|\nabla u\|_{L^2(K,\infty)} \quad \forall u \in \mathcal{U},$$

where $w(x) = x \log^2(x)$.)

The **B-QCE Method**

The B-QCE method is defined by

$$\mathcal{E}^\text{bqce}(u) := \sum_{\ell=0}^{\infty} \left\{ (1 - \beta_\ell) \Phi^a_\ell(u) + \beta_\ell \Phi^c_\ell(u) \right\};$$

see slides for further detail.

**Exercise 16** 1. Prove a basic consistency estimate for the B-QCE method:

$$\|\delta E^a(u) - \delta \mathcal{E}^\text{bqce}(u)\|_{\mathcal{U}^*} \lesssim \|\beta''\|_\varepsilon + \|u''\|_{\mathcal{E}^2(\Delta K_{\ell-1})}.$$  

2. Improved consistency estimate for the B-QCE method: Prove that

$$\|\delta E^a(u) - \delta \mathcal{E}^\text{bqce}(u)\|_{\mathcal{U}^*} \lesssim \|\beta''\|_\varepsilon + \|\beta' u''\|_\varepsilon + \|u'''\|_{\mathcal{E}^2(\Delta K_{\ell-1})} + \|u''\|_{\mathcal{E}^2(\Delta K_{\ell-1})}^2,$$

where $\beta' u''$ is understood as pointwise multiplication.
Exercise 17  Linear blending function: Suppose that we use the blending function 
\[ \beta_\ell = \begin{cases} 
0, & \ell = 0, \ldots, K, \\
(\ell - K)/(L - K), & \ell = K + 1, \ldots, L - 1, \\
1, & \ell = L, L + 1, \ldots.
\end{cases} \]
Suppose, in addition, that \(L - K \leq K\) (why should we always require this anyhow?) and that \(u\) satisfies (DH). Prove that, for \(K\) sufficiently large,
\[ \|\delta E^a(0) - \delta E^{\text{bqce}}(0)\| U^* \gtrsim (L - K)^{-1}. \]

Exercise 18  Prove that, if
\[ \langle \delta^2 E^a(0)v, v \rangle \geq c_0 \|v\|^2_{L^2} \quad \forall v \in U_0, \]
then, there exists a constant such that
\[ \langle \delta^2 E^{\text{qnl}}(0)v, v \rangle \geq (c_0 - C(L - K)^{-1/2})\|v\|^2_{L^2} \quad \forall v \in U_0. \]
In particular, if \(L - K\) is sufficiently large, the \(\delta^2 E^{\text{qnl}}(0)\) is stable.

Exercise 19  Apply the foregoing estimates and extend the stability analysis for the QNL method, to prove an existence and convergence result for the B-QCE method.

Error Estimates for the Energy
In these exercises, we show that in all three “consistent” approximation ATM, QNL, B-QCE, the convergence rate is typically doubled. To simplify notation, we define the total energies
\[ E^a(u) := \mathcal{E}^a(u) - \langle f, u \rangle \quad \text{and} \quad E^*(u_h) := \mathcal{E}^*(u_h) - \langle f, u_h \rangle \]
for \(* \in \{\text{qnl, bqce}\}\).

Exercise 20  In the setting of Theorem 4.2, prove that
\[ \big| E^a(u^a) - E^a(u^a_N) \big| \lesssim N^{1-2\alpha}. \]

Exercise 21  In the setting of Theorem 6.4, prove that
\[ \big| E^a(u^a) - E^{\text{qnl}}(u^{\text{qnl}}) \big| \lesssim J^{-1-2\alpha} + \log(J)J^{-\alpha-3/2} \]
Hint: Split the energy error as follows:
\[ \big| E^a(u^a) - E^{\text{qnl}}(u^{\text{qnl}}) \big| \leq \big| E^a(u^a) - E^a(I_h u^a) \big| + \big| E^a(I_h u^a) - E^{\text{qnl}}(I_h u^a) \big| + \big| E^{\text{qnl}}(I_h u^a) - E^{\text{qnl}}(u^{\text{qnl}}) \big|. \]

Exercise 22  In the setting of Theorem 7.3, what is the convergence rate for the energy,
\[ \big| \{ E^a(u^a) - \langle f, u^a \rangle \} - \{ E^{\text{bqce}}(u^{\text{bqce}}) - \langle f, u^{\text{bqce}} \rangle_h \} \big| \lesssim ??? \]
Hint: see the hint in Exercise 20.
Many-Body Interactions

The following exercises are intended to show how some of the ideas developed in these lectures can be extended to many-body interactions.

**Exercise 23** Suppose that the atomistic energy is given by a general nearest-neighbour model of the form

\[ \mathcal{E}^a(u) = \sum_{\ell=0}^{\infty} \Phi^a_{\ell}(u), \quad \text{where} \quad \Phi^a_{\ell}(u) = V(u_{\ell-1}, u_{\ell+1}) \quad \text{for} \quad \ell \geq 2. \]

1. Derive the Cauchy–Born model. (Hint: \( W(F) = V(F, F) \).)
2. Construct the QCE energy and show that it has no ghost forces, i.e., prove that \( \delta \mathcal{E}^{\text{qce}}(u_F) = 0 \) for all \( F \), provided that \( V(r, s) = V(s, r) \).
   (Note that \( \delta \mathcal{E}^{\text{qce}}(u_F) \) must be defined with care since \( u_F \notin \mathcal{U} \); however, it is ok if we test with displacements from \( \mathcal{U}_N \).)
3. Show how the QNL method for 2nd-neighbour pair interactions can be derived in this way.

**Exercise 24** Construction of a ghost-force free scheme from second-neighbour many-body interactions: Let the atomistic energy be given by

\[ \mathcal{E}^a(u) := \sum_{\ell=0}^{\infty} \Phi^a_{\ell}(u), \quad \text{where} \quad \Phi^a_{\ell}(u) := V(u_{\ell-2} - u_{\ell}, u_{\ell-1} - u_{\ell}, u_{\ell+1} - u_{\ell}, u_{\ell+2} - u_{\ell}), \]

and \( V \) possesses the symmetry \( V(-g_{-2}, -g_{-1}, -g_1, -g_2) = V(g_2, g_1, g_{-1}, g_{-2}) \). Define the QNL-type interface potentials

\[ \Phi^i_{\ell}(u) := V(u_{\ell-2} - u_{\ell}, u_{\ell-1} - u_{\ell}, u_{\ell+1} - u_{\ell}, 2(u_{\ell+1} - u_{\ell})), \quad \text{for} \quad \ell = K, K + 1, \]

and the QNL-type energy

\[ \mathcal{E}^{\text{qnl}}(u) := \sum_{\ell=0}^{K-1} \Phi^a_{\ell}(u) + \sum_{\ell=K}^{K+1} \Phi^i_{\ell}(u) + \sum_{\ell=K+2}^{\infty} \Phi^c_{\ell}(u). \]

1. Prove that \( \delta \mathcal{E}^{\text{qnl}}(F x) = 0 \) for all \( F \in \mathbb{R} \).
2. (DIFFICULT) Can you generalize the method to third neighbours?

**Exercise 25** (DIFFICULT) For the method(s) derived in Exercise 23, prove an optimal consistency error estimate. Can you come up with an argument that would apply to any a/c coupling energy that has no ghost forces?

Hint: Show that the first variation of any a/c coupling can be written in the form

\[ \langle \delta \mathcal{E}^{\text{ac}}(u), v \rangle = \sum_{\ell=1}^{\infty} \sigma^*_\ell(u) \cdot v_{\ell}, \]

Show that \( \sigma_\ell(F x) = W'(F) \) for all \( F \), i.e., if \( u \) is locally homogeneous, then \( \sigma_\ell \) equals the Cauchy–Born stress. Conclude that \( |\sigma^*_\ell(u) - \sigma^a_\ell(u)| \lesssim \|u''\|_{\ell=\infty}(\mathcal{N}_\ell) \) where \( \mathcal{N}_\ell \) is a suitable neighbourhood of \( \ell \).

**Exercise 26** (DIFFICULT) Formulate the B-QCE method for second-neighbour many-body interactions and prove an analogous consistency estimate.