Quasi-continuum Approximation Through A 1D Periodic Example

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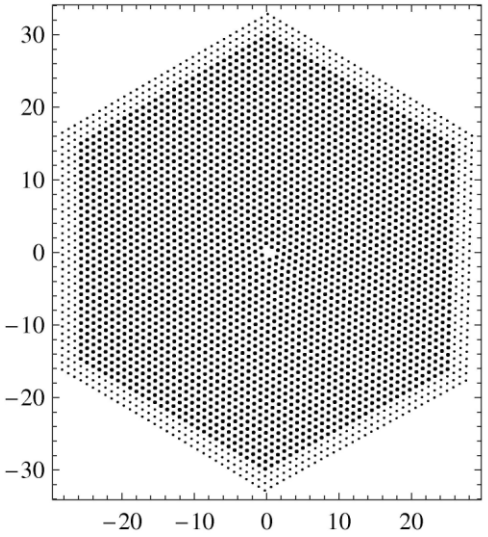
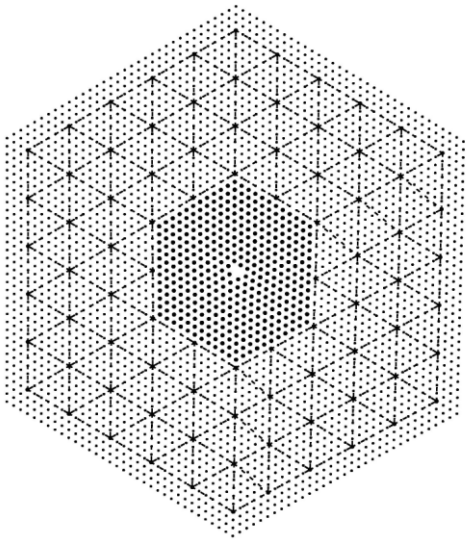
Atomistic model

Atomistic-to-Continuum (multi-scale modeling)



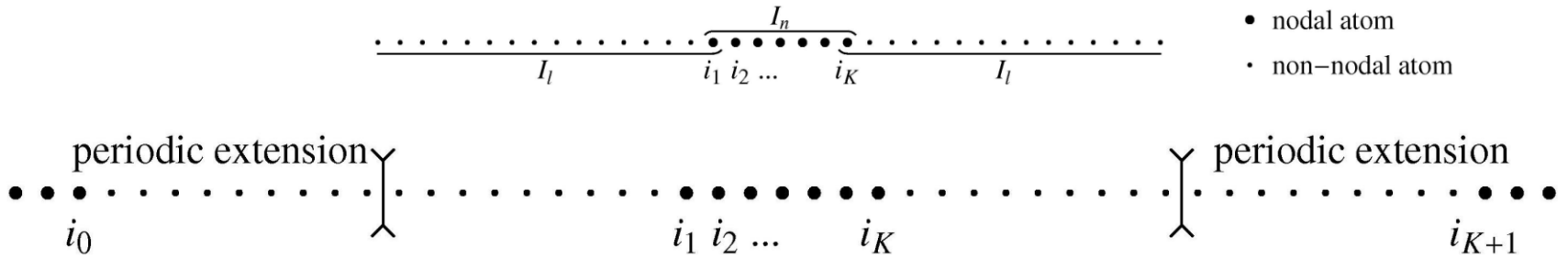


Outline

- **Ghost force at atomistic/continuum interfaces (with A Shapeev)**
  - Explaining ghost force using a periodic 1D example
  - Quasi-nonlocal method and geometrically consistent reconstruction
  - Finite element projection and comparison
- **Quasicontinuum for complex lattice atomistic systems (with A Abdulle and A Shapeev)**
  - Atomistic model with different species of atoms
  - QC method for simple lattice system doesn't work
  - Error analysis based on a discrete homogenization theory

Ghost force

One-dimentional periodic atomistic model, providing that deformed configuration x_i: $x_N = x_0 + 1$ and fixed configuration $X_i = i\epsilon$ in $[0, 1]$, $N\epsilon = 1$.

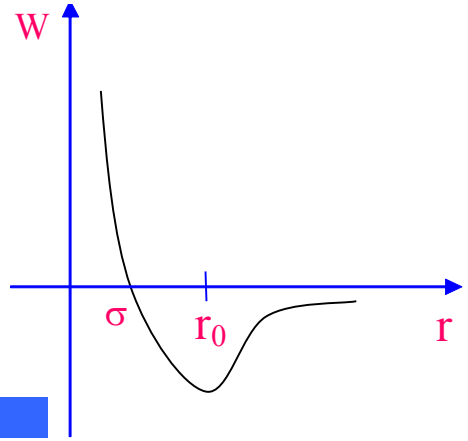


Consider external force acting on each atom. Associated energies:

$$E_{int} = \frac{\epsilon}{2} \sum_{i=1}^{N} \sum_{j=i-n}^{i+n} W(\frac{|x_i - x_j|}{\epsilon}), \quad E_{ext} = -\epsilon \sum_{i=1}^{N} f_i(x_i - X_i)$$

An equilibrium solution with no external force

$x_i = \epsilon i$ (choosing $\epsilon = r_0$)



QC approximation

$$E_{tot}^{QC} = E_{local}^{QC} + E_{nonlocal}^{QC}$$

where

$$E_{local}^{QC} = (i_1 - i_0)\frac{\epsilon}{2}\sum_{m=-n}^{n} W\left(|m|\frac{x_{i_1} - x_{i_0}}{(i_1 - i_0)\epsilon}\right)$$

and

$$E_{nonlocal}^{QC} = \frac{\epsilon}{2}\sum_{i=i_1}^{i_K}\sum_{j=i-n}^{i+n} W\left(\frac{|x_i - x_j|}{\epsilon}\right)$$

To explain the ghost force let us compute the force on the atom i_2 assuming first and second nearest neighbor interaction, i.e. $n = 2$

Cauchy-Born rule: Computing the energy contribution of a representative atom (better to be near the center of the element) and extending it over the whole element

$$E_{tot}^{QC} = \frac{\epsilon}{2}\left(\cdots + W\left(\frac{|x_{i_1} - x_{i_2}|}{\epsilon}\right)\right.$$
$$+W\left(\frac{|x_{i_2} - x_{i_2-2}|}{\epsilon}\right) + W\left(\frac{|x_{i_2} - x_{i_1}|}{\epsilon}\right) + W\left(\frac{|x_{i_2} - x_{i_3}|}{\epsilon}\right) + W\left(\frac{|x_{i_2} - x_{i_4}|}{\epsilon}\right)$$
$$\left.+W\left(\frac{|x_{i_3} - x_{i_2}|}{\epsilon}\right) + W\left(\frac{|x_{i_4} - x_{i_2}|}{\epsilon}\right) + \cdots\right)$$

At the equilibrium position, the force acting on i_2

$$\frac{\partial E_{tot}^{QC}}{\partial x_{i_2}} = \frac{1}{2}\left(W'\left(\frac{x_{i_2} - x_{i_1}}{\epsilon}\right)\right.$$
$$+W'\left(\frac{x_{i_2} - x_{i_2-2}}{\epsilon}\right) + W'\left(\frac{x_{i_2} - x_{i_1}}{\epsilon}\right) - W'\left(\frac{x_{i_3} - x_{i_2}}{\epsilon}\right) - W'\left(\frac{x_{i_4} - x_{i_2}}{\epsilon}\right)$$
$$\left.-W'\left(\frac{x_{i_3} - x_{i_2}}{\epsilon}\right) - W'\left(\frac{x_{i_4} - x_{i_2}}{\epsilon}\right)\right) = -\frac{1}{2}W'(2) \neq 0$$

-- ghost force due to the QC approximation

Quasi-nonlocal method (QNL) Shimokawa et al'04

Replacing $W\left(\frac{x_{i_2}-x_{i_2-2}}{\epsilon}\right)$ by $W\left(\frac{2(x_{i_2}-x_{i_1})}{\epsilon}\right)$

That is, one side treated as local, the other side treated as nonlocal

Now at equilibrium

$$\frac{\partial E_{tot}^{QC}}{\partial x_{i_2}} = \frac{1}{2}\left(W'\left(\frac{x_{i_2}-x_{i_1}}{\epsilon}\right)\right.$$

$$+2W'\left(\frac{2(x_{i_2}-x_{i_1})}{\epsilon}\right)+W'\left(\frac{x_{i_2}-x_{i_1}}{\epsilon}\right)-W'\left(\frac{x_{i_3}-x_{i_2}}{\epsilon}\right)-W'\left(\frac{x_{i_4}-x_{i_2}}{\epsilon}\right)$$

$$\left.-W'\left(\frac{x_{i_3}-x_{i_2}}{\epsilon}\right)-W'\left(\frac{x_{i_4}-x_{i_2}}{\epsilon}\right)\right)=0$$

Only work for $n=2$

E, Lu and Yang 06, C Ortner Math Comp to appear

Geometrically consistent reconstruction (GCR)

E, Lu and Yang'06

Reconstruct positions of certain atoms before interaction

For instance, in the interaction of atoms i2 and i2-2 of QNL, the position of atom i2-2 is reconstructed as xi2 + 2(xi1-xi2)

Reconstruction is sought in the form of a linear combination of the nonlocal reconstruction and local reconstruction:

$$x_j^{reconstructed} = C_{ij}x_j + (1-C_{ij})(x_i + (j-i)(x_{i+sgn(j-i)} - x_i))$$

C_{ij} is determined in advance to eliminate the ghost force

The reconstruction is not unique. For n=2 there is one construction such that GCR=QNL. But unlike QNL, it works for n>2 as well

Divide all atom pairs $\langle i, j \rangle$ into groups: The vectors connecting the pairs within each group will have the same distance R_n and are parallel to the same direction τ_m in equilibrium.

Geometrical consistency:

$$\sum_{|r_i(j)|=R_n, r_i(j) \| \tau_m} \mathrm{sgn}(r_i(j) \cdot \tau_m) \frac{\partial R_i(j)}{\partial x_k} = 0$$

$R_i(j) = x_j^{reconstructed}$ and $r_i(j) = X_j - X_i$ denotes the relative position of atom j w.r.t. atom i in the equilibrium state.

Reason: the force acting on atom k is (writing $E_{int} = \sum_i E_i$)

$$f_k = \frac{\partial E_{int}}{\partial x_k} = \sum_i \frac{\partial E_i}{\partial x_k} = \sum_{i,j} \frac{\partial E_i}{\partial x_j} \frac{\partial R_i(j)}{\partial x_k}$$

$$= \sum_{n,m} \sum_{|r_i(j)|=R_n, r_i(j)\|\tau_m} \left[\mathrm{sgn}(r_i(j)\cdot\tau_m) \frac{\partial E_i}{\partial x_j} \right] \cdot \left[\mathrm{sgn}(r_i(j)\cdot\tau_m) \frac{\partial R_i(j)}{\partial x_k} \right].$$

The first term is independent of i and j due to invariance of the energy under translation and point inversion w.r.t. the equilibrium lattice points.

Analysis: Ming and Yang SIAM MMS 2009

One example for n<4:

$$C_{ij}^{GCR} = \begin{cases} 1 & (i,j) = (i_1 - 1, i_1) \text{ or } (i_K + 1, i_K), \\ 1 & (i,j) = (i_1 - 1, i_1 + 1) \text{ or } (i_K + 1, i_K - 1), \\ 1 & (i,j) = (i_1 - 1, i_1 + 2) \text{ or } (i_K + 1, i_K - 2), \\ 2/3 & (i,j) = (i_1 - 2, i_1 + 1) \text{ or } (i_K + 2, i_K - 1), \\ 1/3 & (i,j) = (i_1 + 1, i_1 - 2) \text{ or } (i_K - 1, i_K + 2), \\ C_{ij}^{QC} & \text{otherwise} \end{cases}$$

$$C_{ij}^{QC} = \begin{cases} 0 & i < i_1 \text{ or } i > i_K \\ 1 & i_1 < i < i_K \\ 1 & i \in \{i_1, i_K\} \text{ and } i_i < j < i_K \\ 0 & i \in \{i_1, i_K\} \text{ and } (j < i_1 \text{ or } j > i_K) \end{cases}$$

Finite Element Projection (QCP)

-- Simply a finite element method to the atomistic model, having been used as a coarsening method in e.g. Rudd & Broughton'98,05, Ortner & Suli'08

We emphasize it as a ghost force removing method and a starting point to develop ghost force free summation rule.

$$E_{int}^{QCP} = \frac{\epsilon}{2} \sum_{i=1}^{N} \sum_{j=i-n}^{i+n} W\left(\frac{|x_i - x_j|}{\epsilon}\right)$$

The same as the exact energy formulation but in local region

$$x_i = \frac{i_1 - i}{i_1 - i_0} x_{i_0} + \frac{i - i_0}{i_1 - i_0} x_{i_1}$$

We can show that the method has no ghost force under a general setting of any dimension

Analytical comparison of QCP, QNL and GCR

$$\frac{\partial E_{int}^{QNL}}{\partial x_{i_2}} - \frac{\partial E_{int}^{QCP}}{\partial x_{i_2}} \approx \frac{\epsilon}{2}(D^2 x_{i_1}) W'' \left(\frac{2(x_{i_1} - x_{i_1 - 1})}{\epsilon} \right)$$ when n=2

$$\frac{\partial E_{int}^{QCP}}{\partial x_{i_2}} - \frac{\partial E_{int}^{GCR}}{\partial x_{i_2}} \approx \frac{2}{9} W'' \left(\frac{3(x_{i_1} - x_{i_1 - 1})}{\epsilon} \right) O(\epsilon D^2 x_{i_1})$$ when n=3

where $\frac{2}{9} W'' \left(\frac{3(x_{i_1} - x_{i_1 - 1})}{\epsilon} \right)$ is rather small (≈ 0.003 if the interatomic distance is approximately equal to $\epsilon = r_0$).

Lin and Shapeev Preprint 2009

It's always possible to find a set of GCR coefficients s.t. GCR=QCP

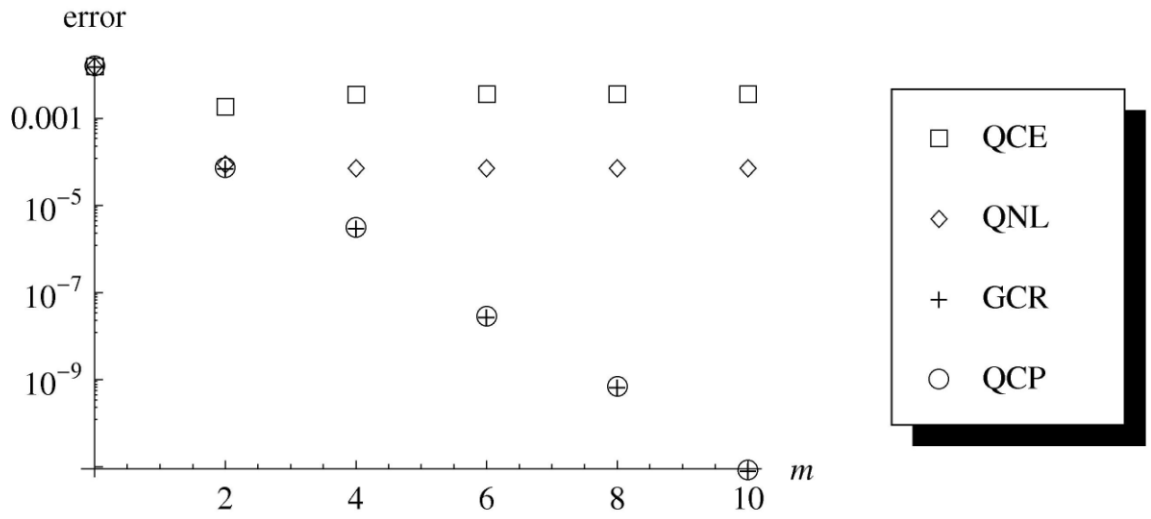
e.g. when n=3 the following will do

$$\tilde{C}_{ij}^{GCR} = \begin{cases} 1 & (i,j) = (i_1 - 1, i_1) \text{ or } (i_K + 1, i_K), \\ 1 & (i,j) = (i_1 - 1, i_1 + 1) \text{ or } (i_K + 1, i_K - 1), \\ 1 & (i,j) = (i_1 - 2, i_1 + 1) \text{ or } (i_K + 2, i_K - 1), \\ 1 & (i,j) = (i_1 - 1, i_1 + 2) \text{ or } (i_K + 1, i_K - 2), \\ 2/3 & (i,j) = (i_1 - 3, i_1 + 1) \text{ or } (i_K + 3, i_K), \\ 1/3 & (i,j) = (i_1, i_1 - 3) \text{ or } (i_K, i_K + 3), \\ C_{ij}^{QC} & \text{otherwise} \end{cases}$$

Numerical comparison of QCP, QNL and GCR

1D Test with localized external force

$$f_i = \begin{cases} -1 & i = N/2 \\ 1 & i = N/2+1 \\ 0 & \text{otherwise} \end{cases}$$

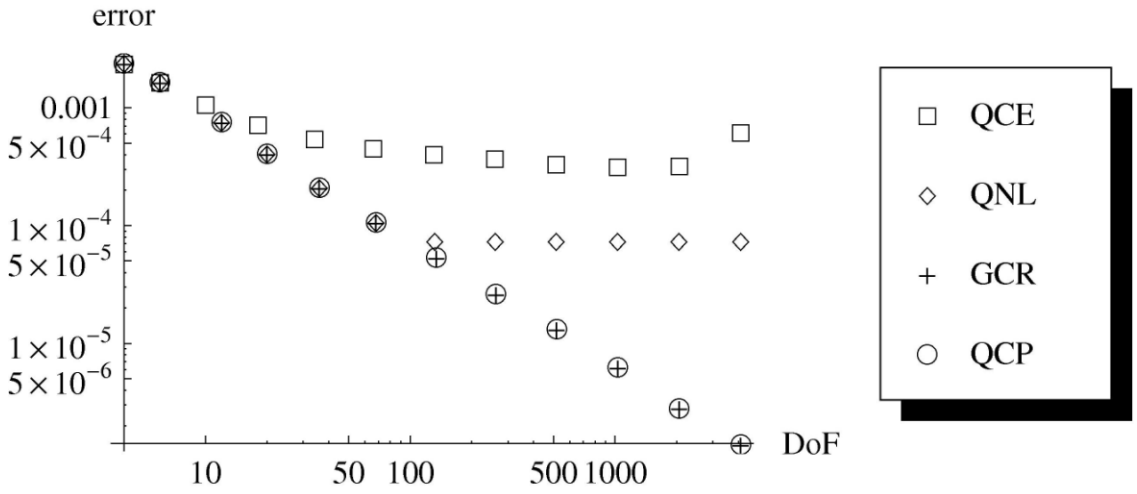


$N = 10000$ and error in $W^{1,\infty}$

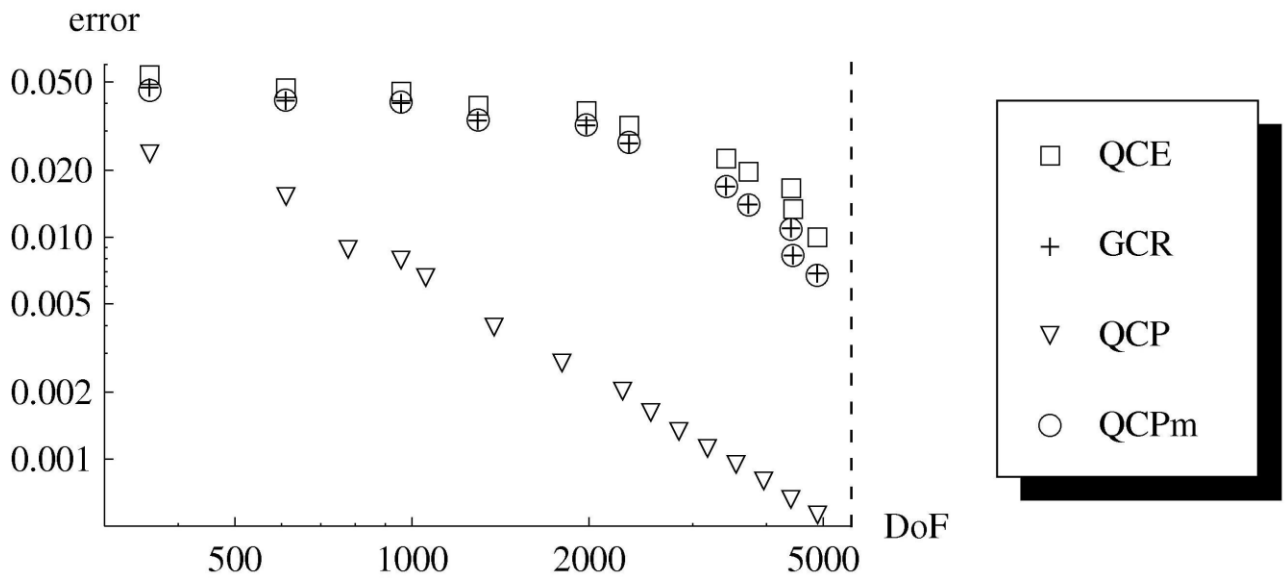
1D Test with localized external force $\mathbf{f} = \mathbf{f}^{irr} + \mathbf{f}^{reg}$

where

$$f_i^{irr} = \begin{cases} 10 & i = N/2 \\ -10 & i = N/2+1 \\ 0 & \text{otherwise} \end{cases} \qquad f_i^{reg} = \frac{1}{N} \sin\left(1 + \frac{2\pi i}{N}\right)$$



2D Test with a point defect (Screw dislocation)



Inconsistency error at edges of finite elements: (Lin SINUM07)

$$\sup_k \left(\frac{b_i}{m_i} \right) = O\left(\frac{\epsilon}{h} \right)$$

if elements are large in comparison with the atomistic scale.

Remark:

Further reduction of the summation cost (atom-based summation and element-based summation):
1D: relatively easy
2D or higher dimension: difficult and may cause unphysical force inside the local region (examples in E, Lu and Yang 2006). How to reduce the summation cost without introducing unphysical force? Shapeev Preprint 2010 (2D)

Analysis: open

Complex Crystalline Materials

Consider 1D periodic problem: reference configuration: $X_i = \epsilon i$

Deformed atom position: $x_i = X_i + u_i$ where u_i is the displacement

Periodicity: $u_{i+N} = u_i \quad \forall i$

$$E_{int}(u) = \epsilon \sum_{i=1}^{N} \sum_{j=i+1}^{i+n} W_{i,j}\left(\frac{x_j - x_i}{\epsilon}\right) = \epsilon \sum_{i=1}^{N} \sum_{j=i+1}^{i+n} W_{i,j}\left(j - i + \frac{u_j - u_i}{\epsilon}\right)$$

$$= \epsilon \sum_{i=1}^{N} \sum_{r=1}^{n} W_{i,i+r}(r + rD_r u_i) = \sum_{r=1}^{n} \langle \Phi_r(D_r u) \rangle$$

Notations: $(\Phi_r(z))_i = W_{i,i+r}(r + rz_i)$, $D_r u_i = \frac{u_{i+r} - u_i}{r\epsilon}$ and $D_1 u_i = Du_i = \frac{u_{i+1} - u_i}{\epsilon}$.

$$E_{ext}(u) = -\epsilon \sum_{i=1}^{N} f_i u_i = -\langle f, u \rangle$$

"Variational" formulation:

$$\frac{dE_{int}}{dt}(u+tv) + \frac{dE_{ext}}{dt}(u+tv)|_{t=0} = 0$$

Equilibrium equation:

$$E'_{int}(u;v) + E'_{ext}(v) = 0 \quad \forall v \in \mathbb{R}^N_{per}$$

where

$$\begin{aligned} E'_{ext}(v) &= -\langle f, v\rangle \\ E'_{int}(u;v) &= \sum_{r=1}^{n} \langle \Phi'_r(D_r u), D_r v\rangle \\ (\Phi'_r(z))_i &= rW'_{i,i+r}(r + rz_i) \end{aligned}$$

Solvability requires $\langle f\rangle = 0$; Uniqueness condition: $\langle u\rangle = 0$

Nearest neighbor interaction:

$$\langle \Phi'_1(Du), Dv\rangle = \langle f, v\rangle \quad \forall\, v \in R^N_{per}$$

Linearize at a given $\bar{u}_i$:

$$(\Phi_r'(D_r u))_i \approx rW'_{i,i+r}(r+rD_r\bar{u}_i)+r^2W''_{i,i+r}(r+rD_r\bar{u}_i)D_r(u_i-\bar{u}_i)$$

Upon defining $\psi_r = [r^2W''_{i,i+r}(r + rD_r\bar{u}_i)]_{i=1}^N$ we have a linearized model

$$\sum_{r=1}^{n} \langle \psi_r D_r u, D_r v\rangle = \langle \bar{f}, v\rangle$$

Nearest neighbor interaction:

$$\langle \psi_1 Du, Dv\rangle = \epsilon \sum_{i=1}^{N} \psi_{1i} Du_i, Dv_i = \langle \bar{f}, v\rangle$$

Next we will look at an example with linear nearest neighbor interaction. For convenience we will denote $\psi = \psi_1$, $\psi_i = \psi_{1i}$and $f = \bar{f}$. The model becomes

$$\langle \psi Du, Dv\rangle = \langle f, v\rangle$$

Recap of QC

$$u^H: \quad u_i^H = \frac{i_{k+1}-i}{i_{k+1}-i_k} u_{i_k}^H + \frac{i-i_k}{i_{k+1}-i_k} u_{i_{k+1}}^H \ (i_k < i < i_{k+1})$$

Taking a representative atom $i_k < i_k^{rep} < i_{k+1}$ and denoting $H_k = \epsilon(i_{k+1} - i_k)$ we have

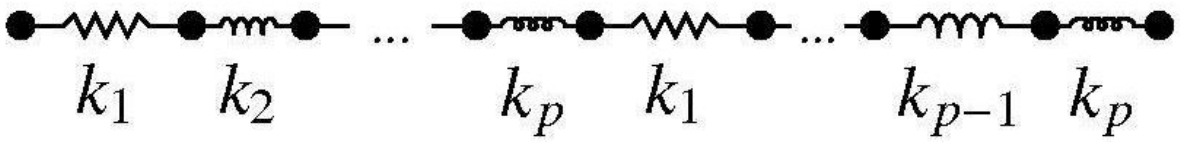
$$\langle \psi Du^H, Dv^H \rangle = \sum_{k=1}^{K} \epsilon \sum_{i=i_k}^{i_{k+1}-1} \psi_i Du_i^H Dv_i^H \approx \sum_{k=1}^{K} H_k \psi_{i_k^{rep}} Du_{i_k^{rep}}^H Dv_{i_k^{rep}}^H$$

where

$$Du_{i_k^{rep}}^H = \frac{u_{i_k^{rep}+1}^H - u_{i_k^{rep}}^H}{\epsilon} = \frac{u_{i_{k+1}}^H - u_{i_k}^H}{(i_{k+1}-i_k)\epsilon} = \frac{u_{i_{k+1}}^H - u_{i_k}^H}{H_k}$$

Cauchy-Born rule: Computing the energy contribution of a representative atom (better to be near the center of the element) and extending it over the whole element

A 1D complex lattice model



Complex lattices are defined as a union of a number of simple lattices. A straightforward application of QC would fail. For example, bonds oscillate 2-periodically, i.e. $p = 2$ in above figure or $\psi = (\psi_1, \psi_2, \psi_1, \psi_2, \ldots, \psi_1, \psi_2)$

Under nearest neighbor interaction, it is a spring-mass system where masses are located at $x_i = X_i + u_i$ connected with ideal springs with spring constants $k_i = \psi_i/\epsilon,\ i = 1, 2.$

If we apply the QC straightforwardly the numerical tensor of this two spring system is (for simplicity assuming the nodal number i_k is even)

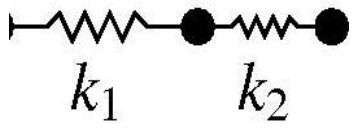
$$\psi_{i_k^{rep}} = \begin{cases} \psi_1 & i_k^{rep} \text{ is odd} \\ \psi_2 & i_k^{rep} \text{ is even} \end{cases}$$

Even if we calculate energy of each element accurately (not only at the repatom):

$$\langle \psi Du^H, Dv^H \rangle = \sum_{k=1}^{K} \epsilon \sum_{i=i_k}^{i_{k+1}-1} \psi_i Du_i^H Dv_i^H$$

$$= \sum_{k=1}^{K} \epsilon \left(\sum_{i_k}^{i_{k+1}-1} \psi_i \right) Du_{i_k}^{H}{}_{rep} Dv_{i_k}^{H}{}_{rep} = \sum_{k=1}^{K} H_k \frac{\psi_1 + \psi_2}{2} Du_{i_k}^{H}{}_{rep} Dv_{i_k}^{H}{}_{rep}$$

This time, numerical tensor is $\frac{\psi_1+\psi_2}{2}$.



Consider a two-spring system (spring constants k_1, k_2 corresponding displacements d_1, d_2) exerted with a force f. Let the unified spring constant be k each.

Then the total displacement $d = d_1 + d_2$. Hooke's law gives:

$$f/(2k) = f/k_1 + f/k_2$$

i.e. the unified spring constant: $k = \left((k_1^{-1} + k_2^{-1})/2 \right)^{-1}$ (harmonic average), indicating that a naive application of the QC fails.

QC for complex lattices

Tadmor, Smith, Bernstein and Kaxiras 1999

(Also see E and Ming 2007, Dobson, Elliott, Luskin and Tadmor 2007)

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An improved Caughy-Born rule (Stakgold 1950): introducing shifts between the simple comprising lattice sites.

$$u_i^H = \frac{i_{k+1} - i}{i_{k+1} - i_k} u_{i_k}^H + \frac{i - i_k}{i_{k+1} - i_k} u_{i_{k+1}}^H + \frac{1 + (-1)^i}{2} q_k, \qquad i_k < i < i_{k+1}$$

(in the two-spring example $d_2 = \frac{k_1}{k_2} d_1$ since $k_1 d_1 = k_2 d_2$. So we can write $d_2 = d_1 + q$, where $q = (\frac{k_1}{k_2} - 1) d_1$ is the shift)

$$E(\cdot) = \min_q E(\cdot, q)$$

Just like introducing an extra basis function $v_k^q = \frac{1+(-1)^i}{2}$ (bubble) in the element $i_k < i < i_{k+1}$. So we have an extra equation for q_k:

$$\langle \psi Du^H, Dv_k^q \rangle + \sum_{m=1}^{K} q_m \langle \psi Dv_m^q, Dv_k^q \rangle = 0 \quad \text{(internal eqn)}$$

(the summation is actually done only in element k and $m = k$)

So $q_k = q_k(Du^H_{i_k^{rep}}) = \epsilon \frac{\psi_2 - \psi_1}{\psi_2 + \psi_1} Du^H_{i_k^{rep}}$ $\qquad Du_i^H = Du^H_{i_k^{rep}} \; \forall i \in (i_k, i_{k+1})$

Now we can obtain

$$\langle \psi Du^H, Dv^H \rangle = \sum_{k=1}^{K} H_k \frac{2\psi_1\psi_2}{\psi_1 + \psi_2} Du^H_{i_k^{rep}} Dv^H_{i_k^{rep}}$$

So the numerical tensor $\psi = \frac{2\psi_1\psi_2}{\psi_1+\psi_2} = \left(\frac{\psi_1^{-1} + \psi_2^{-1}}{2} \right)^{-1}$ is accurate by using the improved Cauchy-Born rule.

Discrete homogenization

Assume that micro atomistic interaction is periodic with period $p\epsilon$

Displacement $u = u(X_i, X_i/\epsilon)$, where $X_i \in \epsilon\mathbb{Z}$ (macro or slow variable) and $Y_i = X_i/\epsilon \in \mathbb{Z}$ (micro or fast variable)

Periodicity: $u(X_i, Y_{j+p}) = u(X_i, Y_j)$and $u(X_{i+N}, Y_j) = u(X_i, Y_j)$

Asymptotic (two-scale) expansion:

$$u = u^0(X_i, Y_j) + \epsilon u^1(X_i, Y_j) + \epsilon^2 u^2(X_i, Y_j) + \dots$$

Note $D = D_X T_Y + \epsilon^{-1} D_Y = D_X + \epsilon^{-1} D_Y T_X$and $T^{-1} = T_X^{-1} T_Y^{-1}$

Consider linearised model with nearest neighbor interaction:

$$\langle \psi^\epsilon Du, Dv\rangle_X = \langle f, v\rangle_X \text{ or strong form: } -D^*\psi^\epsilon(Du) = f$$

where $\psi^\epsilon(X_i) = \psi(X_i, X_i/\epsilon) = \psi(X_i, Y_i)$ (p-periodic in Y)

Discrete integration by parts: $\langle u, Dv\rangle = -\langle T^{-1}Du, v\rangle$ gives $D^* = -T^{-1}D = -T_Y^{-1}(T_X^{-1}D_X + \epsilon^{-1}D_Y)$

We have (assuming f is independent of Y and $\psi \geq c > 0$)

$$-(T_X^{-1} D_X + \epsilon^{-1} D_Y)(\psi D_X T_Y u^0 + \epsilon^{-1} \psi D_Y u^0 + \epsilon \psi D_X T_Y u^1 + \psi D_Y u^1$$
$$+\epsilon^2 \psi D_X T_Y u^2 + \epsilon \psi D_Y u^2 + \ldots) = T_Y f = f$$

Collecting $O(\epsilon^{-2})$ terms:

$$-D_Y(\psi D_Y u^0) = 0 \qquad u^0 : \ p - \text{periodic in } Y$$

$\Rightarrow$ u^0 is a function of X: i.e. $u^0(X_i, Y_j) = u^0(X_i)$

Collecting $O(\epsilon^{-1})$ terms:

$$u^1(X_i, Y_j) = \chi(X_i; Y_j) D_X u^0(X_i),$$

where χ satisfies

$$-D_Y(\psi D_Y \chi) = D_Y \psi \qquad \chi : p - \text{periodic in } Y$$

Collecting $O(\epsilon^0)$ terms leads to the homogenized equation:

$$-D_X(\psi^0 D_X u^0) = T_X f, \quad \psi^0 = \langle \psi \ (1 + D_Y \chi) \rangle_Y$$

In the case of linear nearest neighbor interaction, we can calculate $\psi^0 = \langle \psi(1 + D_Y \chi) \rangle_Y$ explicitly.

The discrete homogenization gives the same correct tensor

$$\psi^0 = \langle C(X_i) \rangle_Y = (\psi_1^{-1} + \psi_2^{-1})^{-1}/2$$

We can actually show that under this periodic setting the QC for complex lattice and an appropriately processed discrete homogenization are equivalent even for general nonlinear finite range interactions.

Abdulle, Lin and Shapeev, A review of multiscale computational methods for complex crystals, Manuscript 2010

Error analysis of discrete homogenization

Abdulle, Lin and Shapeev Preprint arXiv.1006.0378 2010

Assume $0 < c_\psi \leq \psi(X_i, Y_j), \psi^0 \leq C_\psi$ and $\|D_X \psi\|_{L^\infty(N,p)} \leq C'_\psi$.

Write the asymptotic solution

$$u^c(X_i) = u^0(X_i) + \epsilon \chi(X_i, X_i/\epsilon) D_X u^0(X_i)$$

Then

$$|u^c - u|_{H^1} \leq C\epsilon \|f\|_{L^2}, \quad |\langle u^c \rangle_X| \leq C\epsilon^2 \|f\|_{L^2}$$

and

$$\|u^0 - u\|_{L^2} \leq C\epsilon \|f\|_{L^2}$$

in the case of linear nearest neighbor interaction.

Homogenized quasicontinuum (HQC)

Numerical methods to deal with continuum homogenization elliptic problems: (i) Multiscale finite element method (See Babuska, Hou, Wu, Efendiev, etc.); (ii) Heterogeneous multiscale method (See E, Engquist, etc.).

Sampling domain (taken near the center of the element):

$$S_k^{\text{rep}} = \left\{ X_i : X_{i_k}^{\text{rep}} \leq X_i < X_{i_k}^{\text{rep}} + p\epsilon \right\}.$$

Define the atomistic interaction energy of the HQC method

$$E^{\text{HQC}}(u^H) = \sum_{S_k \in \mathcal{T}} H_k \sum_{r=1}^{n} \left\langle \Phi_r^{\epsilon}(D_r R_k(u^H)) \right\rangle_{X_i \in S_k^{\text{rep}}},$$

where $R_k\left(u^H\right)$, defined below, is the microfunction constrained by u^H in the sampling domain S_k^{rep}, and $\Phi_r^{\epsilon}(z)(X_i) = W_r(r + rz(X_i))$.

The functional derivative of the above energy reads

$$(E^{\mathsf{HQC}})'(u^H; v^H)$$
$$= \sum_{S_k \in \mathcal{T}} H_k \sum_{r=1}^{n} \left\langle (\Phi_r^\epsilon)'(D_r \mathcal{R}_k(u^H)), D_r \mathcal{R}_k'(u^H; v^H) \right\rangle_{X_i \in S_k^{\mathsf{rep}}}$$

Microproblem: Given a function $u^H \in U^H_{per}$, $\mathcal{R}_k\left(u^H\right)$ is a function defined on S_k^{rep} such that $\mathcal{R}_k\left(u^H\right) - u^H \in U^p_{\#}(\epsilon\mathbb{Z})$ and

$$\sum_{r=1}^{n} \left\langle (\Phi_r^\epsilon)' \left(D_r \mathcal{R}_k \left(u^H \right) \right), \ D_r s \right\rangle_{X_i \in S_k^{\mathsf{rep}}} = 0 \quad \forall s \in U^p_{\#}(\epsilon\mathbb{Z})$$

Motivation: $\mathcal{R}_k(u^H) = u^H + \omega$ is something like u^c. For example, linear nearest neighbor case: $\langle \psi D\omega, Ds \rangle_{X_i \in S_k^{rep}} = -\langle \psi D u^H, Ds \rangle_{X_i \in S_k^{rep}}$
Changing variable to $Y_i = X_i/\epsilon$, i.e. write $\omega = \tilde{\omega}(X_i/\epsilon) = \tilde{\omega}(Y_i)$ we have

$$\epsilon^{-1} \langle \psi D_Y \tilde{\omega}, D_Y s \rangle_Y = -D_X u^H \langle \psi, D_Y s \rangle_Y$$

So ω is something like $\epsilon D_X u^H \chi(\cdot, X_i/\epsilon)$. Denote

$$u^{H,c} = \text{ periodically extended } \mathcal{R}_k(u^H) \text{ in each element}$$

Error analysis

Abdulle, Lin and Shapeev Preprint arXiv.1006.0378 2010

Consider the linear nearest neighbor case:

$$(E^{\mathsf{HQC}})'(u^H; v^H)$$
$$= \sum_{S_k \in \mathcal{T}} H_k \sum_{r=1}^{n} \left\langle \psi_c^\epsilon D\mathcal{R}_k(u^H), D\mathcal{R}_k(v^H) \right\rangle_{X_i \in S_k^{\mathsf{rep}}} = \langle f, v^H \rangle$$

where $\psi_c^\epsilon(X_i) := \psi(X_{i_k^c}, X_i/\epsilon),\ \forall X_i \in S_k^{rep}$, choosing $X_{i_k^c}$ in a distance of $O(\epsilon)$ from the center of the element, and

$$\langle \psi_c^\epsilon D\mathcal{R}_k(u^H), Ds \rangle_{X_i \in S_k^{rep}} = 0$$

Assume conditions for ψ as before. Then

$$|u^H - u^0|_{H^1} \leq CH\|f\|_{L^2}, \quad \|u^H - u^0\|_{L^2} \leq C(H^2\|f\|_{L^2} + \epsilon\|f\|_{H^{-1}})$$

$$\|u^H - u\|_{L^2} \leq C(H^2 + \epsilon)\|f\|_{L^2}$$

$$|u^{H,c} - u|_{H^1} \leq CH\|f\|_{L^2}, \quad \|u^{H,c} - u\|_{L^2} \leq C(H^2\|f\|_{L^2} + \epsilon\|f\|_{H^{-1}})$$

If ψ only depends on Y, then no $\epsilon\|f\|_{H^{-1}}$ in above estimates.

Numerical examples

1D linear: $p = 2$ and number of interacting neighbors $n = 3$. The potential is defined as

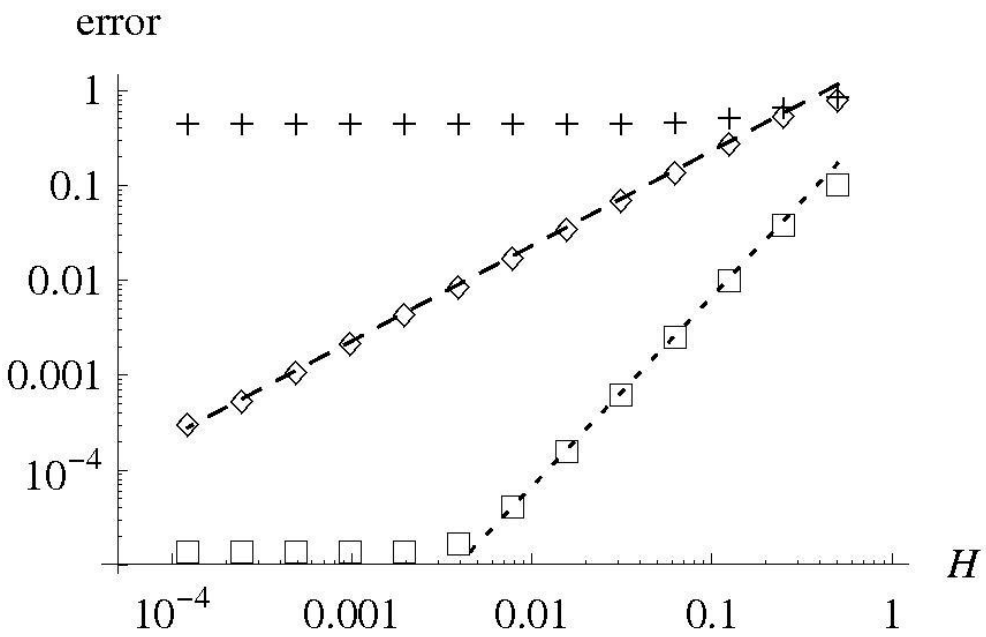
$$W_{i,i+r}(z) = \frac{1}{2} k_{i,i+r} 3^{1-r} (z - r)^2 \quad (1 \leq r \leq n),$$

where

$$k_{i,i+r} = \begin{cases} 1 & i \text{ is even} \\ 2 & i \text{ is odd} \end{cases}$$

$N = 2^{14} = 16384$, and the external force was taken as

$$f_i = \sin(1 + 2\pi X_i).$$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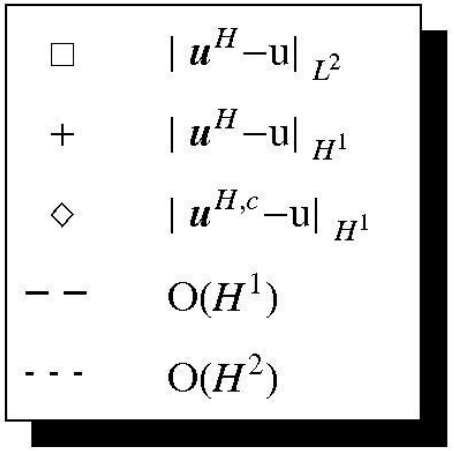
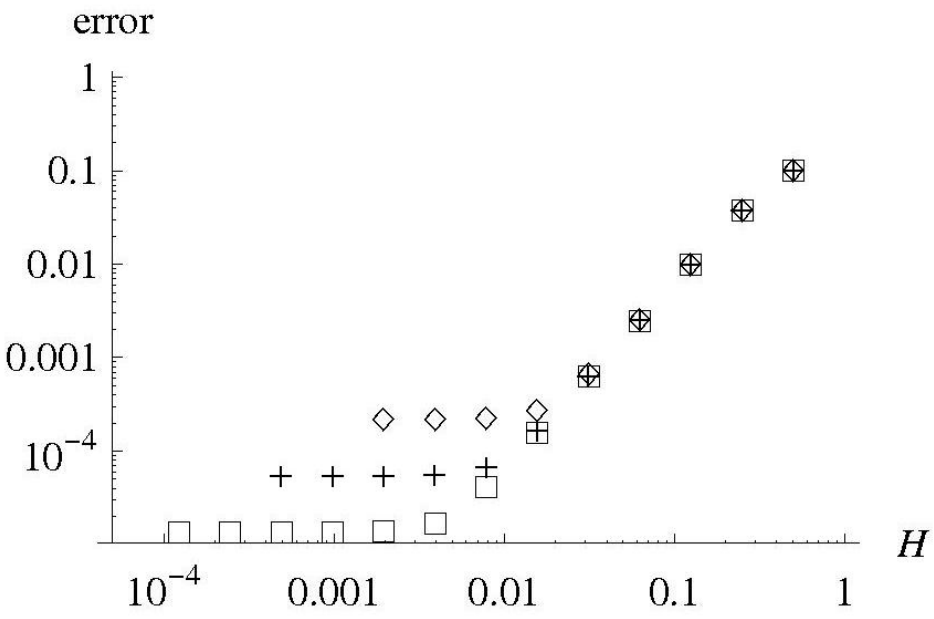

$|u^H - u|_{L^2}$
$|u^H - u|_{H^1}$
$|u^{H,c} - u|_{H^1}$
$O(H^1)$
$O(H^2)$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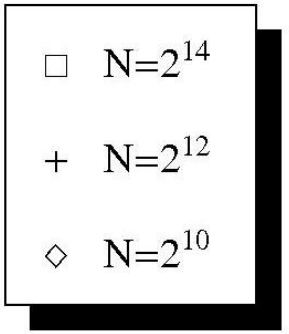

N=2^{14}
N=2^{12}
N=2^{10}

$\|u^H - u\|_{L^2}$

1D nonlinear: Lennard-Jones potential

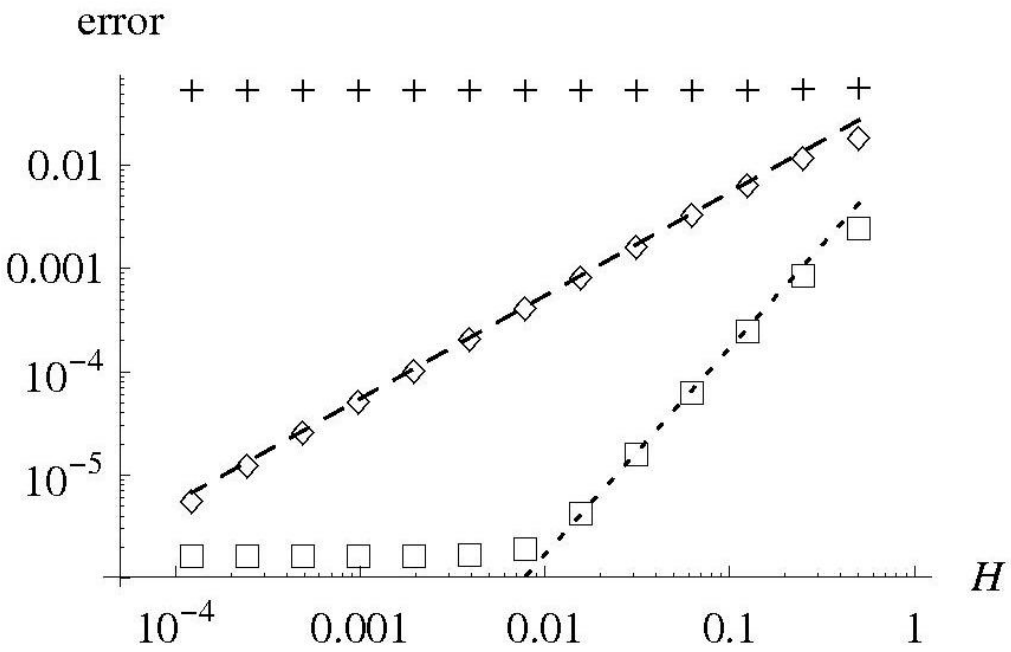
$$\varphi_{i,i+r}(z) = -2\left(\frac{z}{l_{i,i+r}}\right)^{-6} + \left(\frac{z}{l_{i,i+r}}\right)^{-12} \qquad (1 \le r \le R)$$

with the varying equilibrium distance

$$l_{i,i+r} = \begin{cases} 1 & i \text{ is even} \\ 9/8 & i \text{ is odd.} \end{cases}$$

The external force was taken as

$$f_i = 50 \sin\left(1 + 2\pi X_i\right).$$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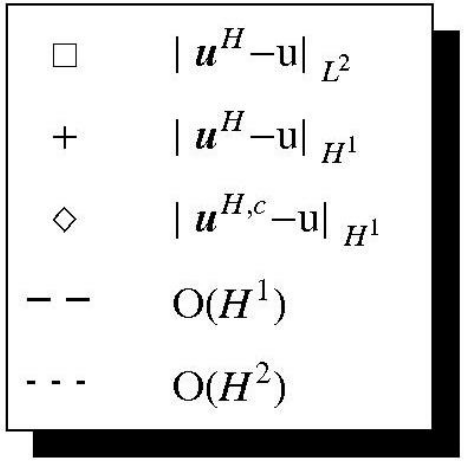
$|u^H - u|_{L^2}$
$|u^H - u|_{H^1}$
$|u^{H,c} - u|_{H^1}$
$O(H^1)$
$O(H^2)$

Summary

- Ghost force is shown in the local/nonlocal interface in a simple lattice case. No ghost force in the case of nearest neighbor interaction.
- Under a 1D periodic setting QNL, GCR and QCP are introduced and compared. QNL can remove ghost force for n=2. GCR and QCP can do for all interacting range n. GCR is general but requires a priori tabulated coefs of reconstruction and is problem-dependent. QCP is specific, easy to implement, works as good as GCR in all cases. Challenging of element summation in 2D and 3D.
- Complex lattice – equivalence to an appropriately processed discrete homogenization, analysis may be done through the discrete homogenization framework
- Ghost force removing strategies can be used to deal with atomistic/continuum interface with complex lattice structures.