Understanding Quasicontinuum Method

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The world is multiscale

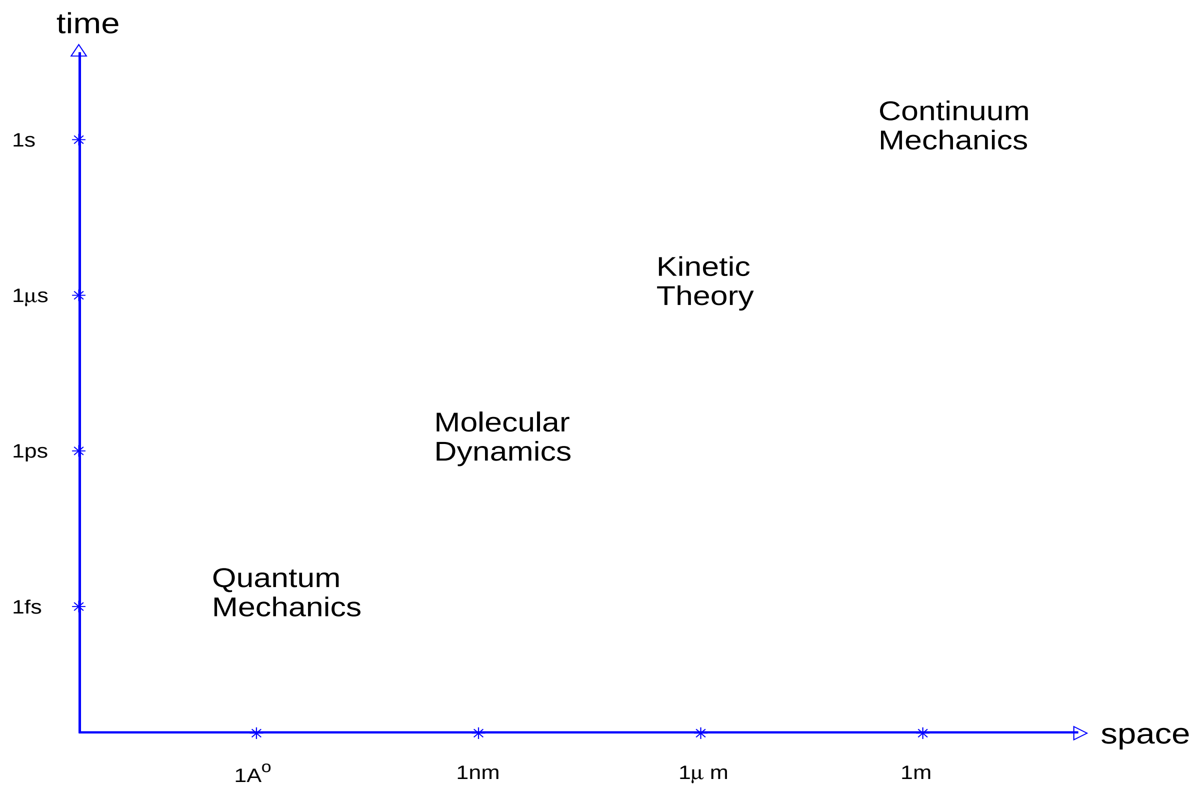


Fig. 1: Commonly used laws of physics at different scales

- Resolving the macroscopic model; but usually lacks of solid foundation and too coarse; validation?
- Turn to microscopic model; too complex to resolve and too huge data to retrieve useful info. predicative?

Examples of multiscale models/methods

- Chemistry: Quantum Mechanics and Molecular Mechanics Method (QM-MM) (WARSHEL & LEVITT, 1976)
- Car-Parrinello Molecular Dynamics (CPMD, 1985, avoid empirical potentials, compute force fields directly from electronic structure information)
- Kinetic schemes in gas dynamics
- Material Science: CPMD (1985); QuasiContinuum method (TADMOR, ORTIZ & PHILLIPS, 1996)
- ...
- General feature: concurrent coupling (on-the-fly) domain decomposition

Q: stability? accuracy?

Al (1 1 1) Nanoindentation: MD analysis

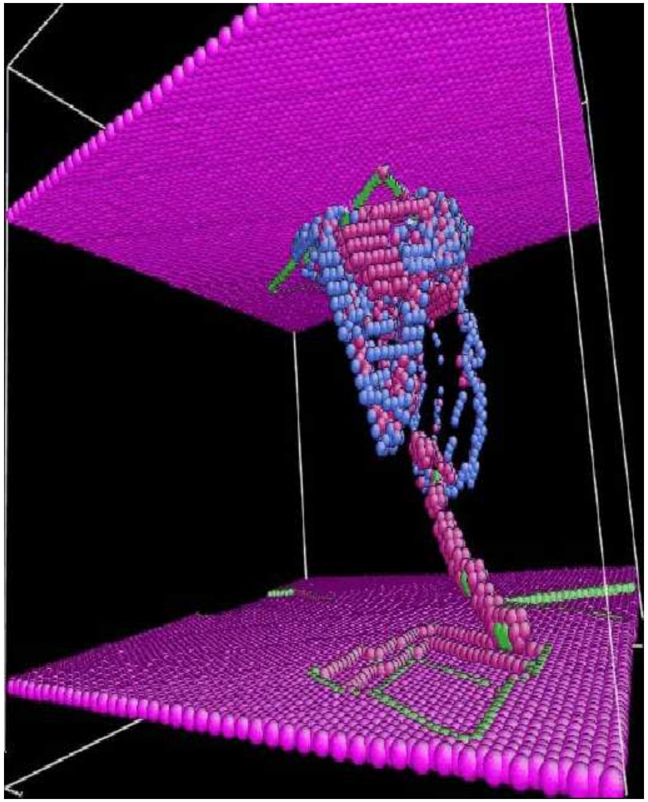
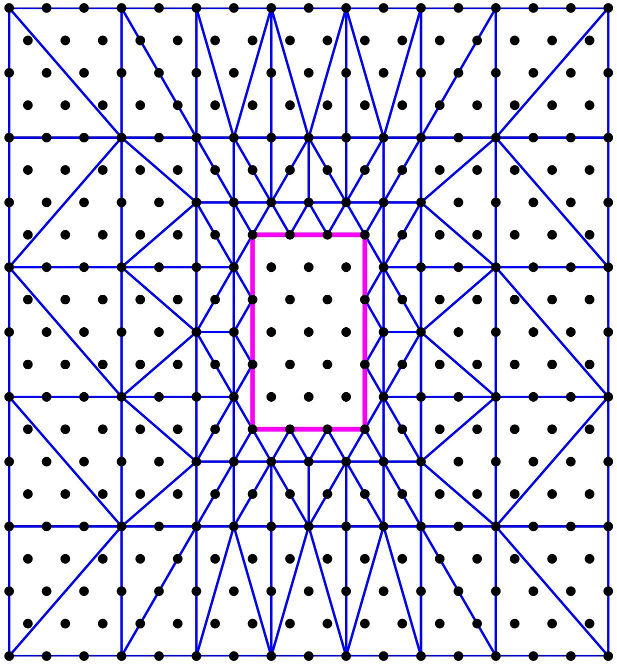


Fig. 2: J. Li et al, Nature, **418**(2002), 307

- Atomistic model is a must-be
- Long range elastic field is equally important (large cells)
- The vast majority of atoms in MD moves according to the smooth elastic field $\Longrightarrow$MD wasteful!
- Coupled atomistic continuum model description
- MD Molecular Dynamics without all the atoms

Quasicontinuum method: methodology



- Adaptive modeling and mesh refinement procedure
  - local region (nonlinear elasticity modeling); nonlocal region (atomistic modeling)
  - Representative atoms define the triangulation, near defects, the mesh becomes fully atomistic
- Use continuum model to reduce the Degree Of Freedom without losing the atomistic detail

http://www.qcmethod.com

- Original papers:
  - TADMOR, ORTIZ AND PHILLIPS, Phil. Mag. **96**(1996), 1529–1563
  - KANP AND ORTIZ, J. Mech. Phys. Solids, **49**(2001), 1899–1923
- Review papers:
  - MILLER AND TADMOR, J. Comput. Aided Mat. Des., **9**(2002), 203–239
  - MRS Bulletin **32**(2007), Nov., 920–926
  - Modeling Simul. Mater. Sci. Eng. **17**(2009), (053001)
- Similar ideas may be found in A. BRANDT, Multigrid methods in lattice field computations, Nuclear Phys. B, Proc. Suppl. **26**(1992), 137–180

Continuum & atomistic models of crystalline solids

Nonlinear elasticity model $\quad \boldsymbol{u} : \Omega \to \mathbb{R}^3$ displacement field

$$I(\boldsymbol{u}) = \int_\Omega \Big(W(\nabla \boldsymbol{u}(\boldsymbol{x})) - \boldsymbol{f}(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}) \Big) \mathrm{d}\,\boldsymbol{x}$$

$W =$ stored energy function density $\quad \boldsymbol{f} =$ external force

minimizing $I(\boldsymbol{u})$ in suitable space subject to certain boundary condition

$\boldsymbol{x}_j =$ position of j-th atom at undeformed state

$\boldsymbol{y}_j =$ position of j-th atom at deformed state

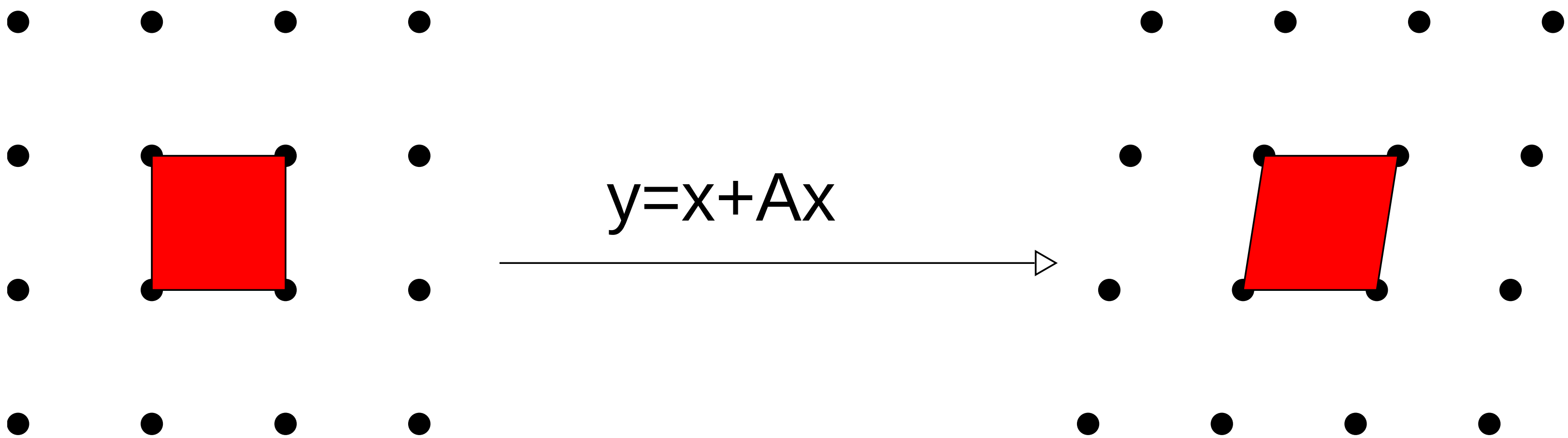
$$E^{\text{tot}}\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\} = \sum_{i,j} V_2(\boldsymbol{y}_i, \boldsymbol{y}_j) + \sum_{i,j,k} V_3(\boldsymbol{y}_i, \boldsymbol{y}_j, \boldsymbol{y}_k) + \cdots$$

$$\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\} = \operatorname{argmin} \left\{ E^{\text{tot}}\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\} - \sum_{i=1}^{N} f(\boldsymbol{x}_i)\boldsymbol{y}_i \right\}$$

Question: can we relate W to the atomistic model?

Q: Given a matrix $\boldsymbol{A} \in \mathbb{R}^{3\times 3}$ $W_{\text{CB}}(\boldsymbol{A}) = ?$

A: Deform the crystal uniformly by $\boldsymbol{y} = \boldsymbol{x} + \boldsymbol{A}\boldsymbol{x}$



$W_{\text{CB}}(\boldsymbol{A}) =$ energy of unit cell at the deformed configuration

Example: $V =$ Lennard-Jones potential $\zeta =$ Riemann-zeta function

$$W_{\text{CB}}(A) = \frac{\zeta^2(6)}{\zeta(12)}\varepsilon_0\left(|1+A|^{-12} - 2|1+A|^{-6}\right)$$

- Choose representative atom $N_{\text{rep}} \ll N \quad \boldsymbol{u}_i = \sum_{\alpha=1}^{N_{\text{rep}}} S_\alpha(\boldsymbol{x}_i)\boldsymbol{u}_\alpha$
- Calculate local energy

$$E^{\text{local}} = \sum_K \int_K W_{\text{CB}}(\nabla \boldsymbol{u}(\boldsymbol{x}))\,\text{d}\,\boldsymbol{x}$$

- Calculate nonlocal energy: choose each atom as rep-atom and using the atomistic model to compute the nonlocal energy
- Calculate total energy

$$E_{\text{QC}}^{\text{tot}} = E^{\text{local}} + E^{\text{nonlocal}}$$

- Minimizing the total energy

$$\boldsymbol{u}_{\text{QC}} = \operatorname{argmin}\left\{E_{\text{QC}}^{\text{tot}} - \sum f(\boldsymbol{x})(\boldsymbol{x} + \boldsymbol{u}(\boldsymbol{x}))\right\}$$

- X_H =linear finite element

$$W_{\mathsf{LQC}}(\nabla \boldsymbol{V}) := \sum_{K \in \mathcal{T}_H} |K| W_{\mathsf{CB}}(\nabla \boldsymbol{V}), \qquad \boldsymbol{V} \in X_H$$

- $W_{\mathsf{CB}}(\nabla \boldsymbol{V}) =$ stored-energy function obtained from CB rule
- Minimization problem:

$$\begin{aligned} \boldsymbol{u}_{\mathsf{QC}} &= \operatorname*{argmin}_{V \in X_H} \left\{ W_{\mathsf{LQC}}(\nabla V) - \int_\Omega fV \right\} \\ &= \operatorname*{argmin}_{\boldsymbol{V} \in X_H} \left\{ \int_\Omega W_{\mathsf{CB}}(\nabla V) - \int_\Omega fV \right\} \end{aligned}$$

- Conclusion: local QC is a finite element approximation of Cauchy-Born elasticity problem!

Why we need to understand QC?

- Motivation
  - Successful method for modeling static properties of crystalline solids at zero temperature
  - The simplest example for understanding the algorithmic issues in coupled atomistic/continuum methods:
    - Temperature $= 0$
    - No dynamics
- Objective
  - Whether the matching between the continuum and atomistic models causes large error? consistency
  - Whether new numerical instabilities can arise as a result of atomistic/continuum coupling? stability

State of the art of QC analysis

- Many groups: Lin; E et al; Le Bris & Lions; Luskin et al; Süli et al; Oden; Prudhomme $\cdots$
- This is a very good problem: the simplest one to understand the atomistic/continuum coupled multiscale/multiphysics method: no temperature; no dynamics so far
- This is a new type of problem for numerical analysis community

$\cdots$ `rigorous understanding of QC and related multiscale algorithms remain open` $\cdots$ [J.M. Ball, Some open problems in elasticity, 2002]

Understanding QC: our framework

- Consistency problem
  - Consistency in the bulk: understanding the passage

    $$\text{atomistic model} \xrightarrow{\text{Cauchy-Born rule}} \text{continuum model}$$

  - Consistency at the interface: understanding ghost force
    - Ghost force $\Longrightarrow$ large error
    - Ghost force free schemes converge? what is the convergence rate?
    - Core: quantify ghost force
- Stability problem:
  - stability is crucial for CB rule
  - ghost-force induces instability?
- Approach: classical NA; Lax Thm. $+$ Strang's approach for nonlinear finite difference schemes

Validity of Cauchy-Born rule: consistency

- Consider a one-dimensional chain: $x_i = i\epsilon$ with $\epsilon =$equilibrium bond length
- Assume $y_i = x_i + u(x_i)$ with u a smooth function

$$V = \frac{1}{2}\sum_{i\neq j} V_0(y_i - y_j)$$

$$\simeq \frac{1}{2}\sum_{i}\Big(\sum_{j\neq i} V_0\Big(1 + \frac{\mathrm{d}u}{\mathrm{d}x}(x_i)\Big)j\epsilon\Big)$$

$$= \sum_i W\Big(\frac{\mathrm{d}u}{\mathrm{d}x}(x_i)\Big) \simeq \int W\Big(\frac{\mathrm{d}u}{\mathrm{d}x}(x)\Big)\mathrm{d}\,x$$

$$W(A) = \frac{1}{2\epsilon}\sum_i V_0\Big((1+A)i\epsilon\Big)$$

- The simplest CB rule
- X. Blanc, C. Le Bris & P.-L. Lions (2002) for pair-wise emperical potentials + some QM models

Validity of Cauchy-Born rule: stability

- Continuum level (Born criteria)≡ *Elastic stiffness tensor* is positive definite
- Atomic level (Lindemann criteria) ≡*Phonon spectra* (dispersion relation for the lattice waves) is non-degenerate("positive definite")

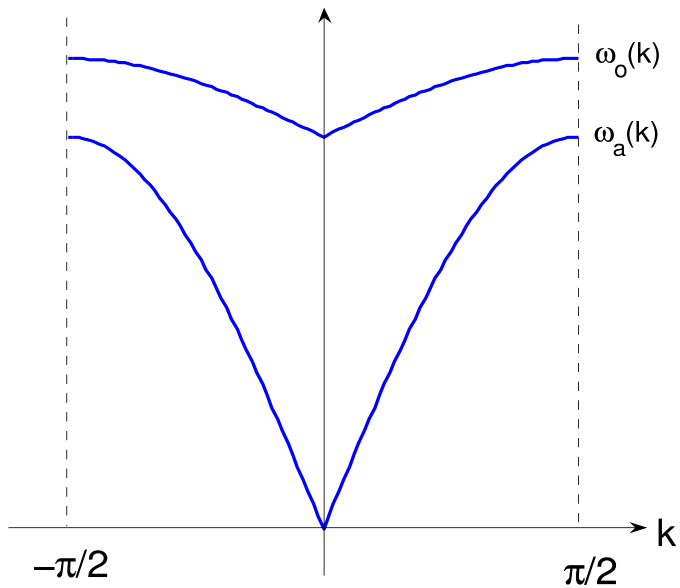
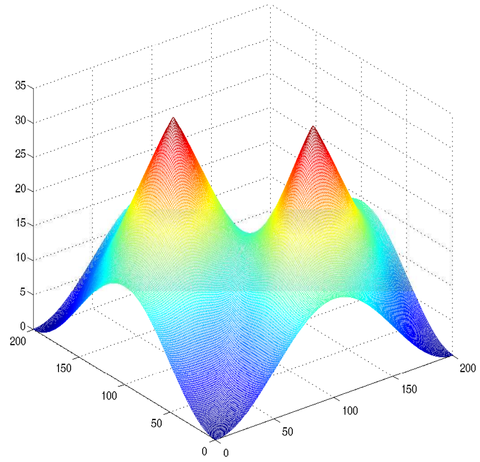


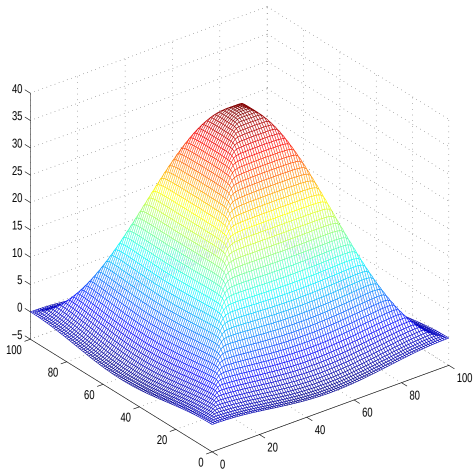
Fig. 3: phonon spectrum of the complex lattice

Validity of Cauchy-Born rule: counterexample

- Set-up
  - Lennard-Jones potential
  - next nearest neighborhood interaction
- △ lattice: Cauchy-Born rule is valid
- □ lattice: Cauchy-Born rule is invalid
  - Cauchy-Born rule gives negative shear modulus
  - phonon spectra is degenerate



(a) triangular lattice



(b) square lattice

Theorem for CB rule [E & M, ARMA, 07]

If Born criterion is true, and for $p > d$, there $\exists K, R$ s.t. for any $\|\boldsymbol{f}\|_{L^p} \leq K$, $\exists | \boldsymbol{u}_{\text{CB}}$ of the continuum problem s.t. $\|\boldsymbol{u}_{\text{CB}}\|_{W^{2,p}} \leq R$, and $\boldsymbol{u}_{\text{CB}}$ is a $W^{1,\infty}-$local minimizer

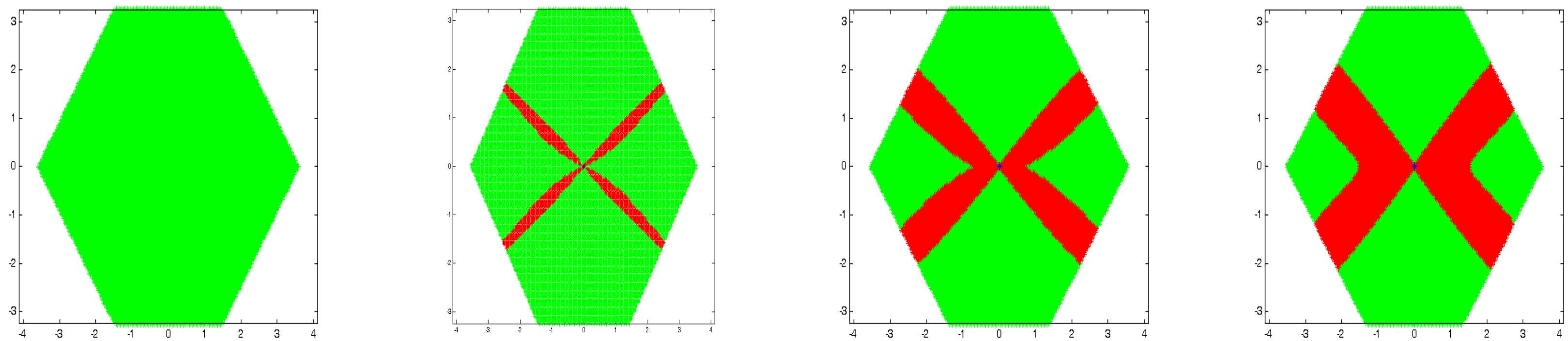
If Lindemann criterion is true, and for $p > d, \exists K$ s.t. for any $\boldsymbol{f} \in W^{6,p}(\Omega; \mathbb{R}^d)$ and $\|\boldsymbol{f}\|_{L^p} \leq K$, then the atomistic model has a local minimizer $\{\boldsymbol{y}_{\text{atom}}\}$ nearby, i.e.,

$$\|D_+(\boldsymbol{y}_{\text{atom}} - \boldsymbol{y}_{\text{CB}})\|_{\ell_2} \leq C\epsilon$$

where $\boldsymbol{y}_{\text{CB}} = \{\boldsymbol{y}_{\text{CB}}\}_j = \boldsymbol{x}_j + \boldsymbol{u}_{\text{CB}}(\boldsymbol{x}_j)$, $\epsilon =$ lattice constant

Examples of triangular lattice instability

Triangular lattice with LJ potentials: $x-$direction tension

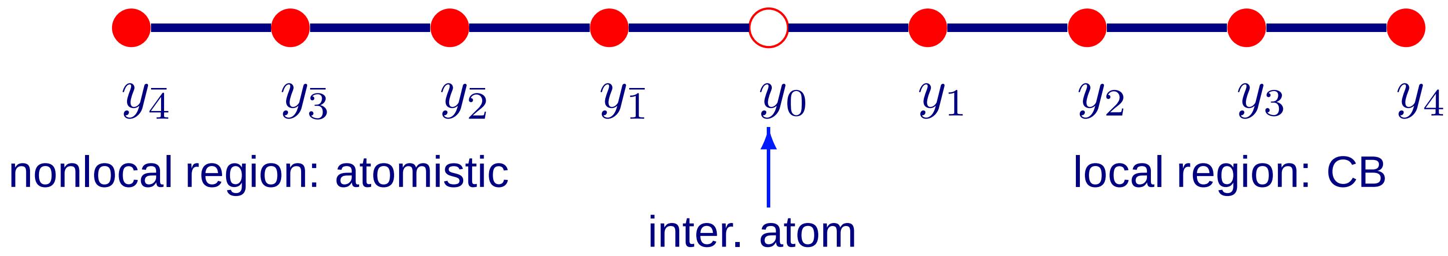


(c) $\epsilon_{xx} = 0.12$ (d) $\epsilon_{xx} = 0.13$ (e) $\epsilon_{xx} = 0.15$ (f) $\epsilon_{xx} = 0.17$

- 1st Brillouin zone of deformed triangular lattice under uniaxial strain. Green $\omega(\boldsymbol{k}) > 0$; Red $\omega(\boldsymbol{k})$ has imaginary part
- The stability condition is sharp! Violation of these conditions signals of the plasticity deformation or structural phase transformation (J. Li & S. Yip et al.)

- Consistency in the bulk (for simple system, the two models should produce consistent results) Under Born and Lindmann stability criteria
  - The atomistic model is a consistent approximation of Cauchy-Born elasticity model
  - Cauchy-Born elasticity model is a consistent coarse-graining of the atomistic model
  - This result is valid for $d = 1, 2, 3$
- Refer to `J.L. Ericksen, On the Cauchy-Born rule, Mathematics and Mechanics of Solids 13: 199-220, 2008`
- Quantitative estimate in CB is key to QC analysis

Definition: at the equilibrium state, the forces on the atom is $\neq 0$; i.e. the equilibrium state is no longer at equilibrium



$$f_{\bar{1}} = -V'(r_{\bar{3}\bar{1}}) - V'(r_{\bar{2}\bar{1}}) + V'(r_{\bar{1}0}) + \frac{1}{2}V'(r_{\bar{1}1})$$

$$f_0 = -V'(r_{\bar{2}0}) - V'(r_{\bar{1}0}) + V'(r_{01}) + 2V'(2r_{01})$$

$$f_1 = -\frac{1}{2}V'(r_{\bar{1}1}) - 2V'(2r_{01}) - V'(r_{01}) + V'(r_{12}) + 2V'(2r_{12})$$

At equilibrium state: ϵ=bond length

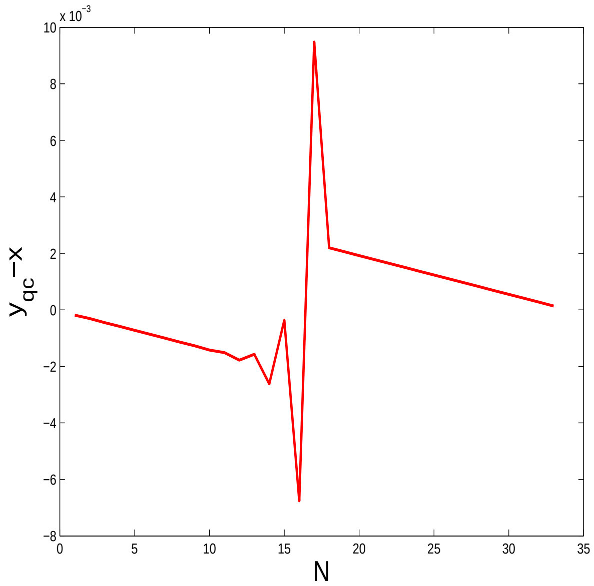
$$f_{\bar{1}} = -\frac{1}{2}V'(2\epsilon) \qquad f_0 = V'(2\epsilon) \qquad f_1 = -\frac{1}{2}V'(2\epsilon)$$

Violation of patch test in finite element language

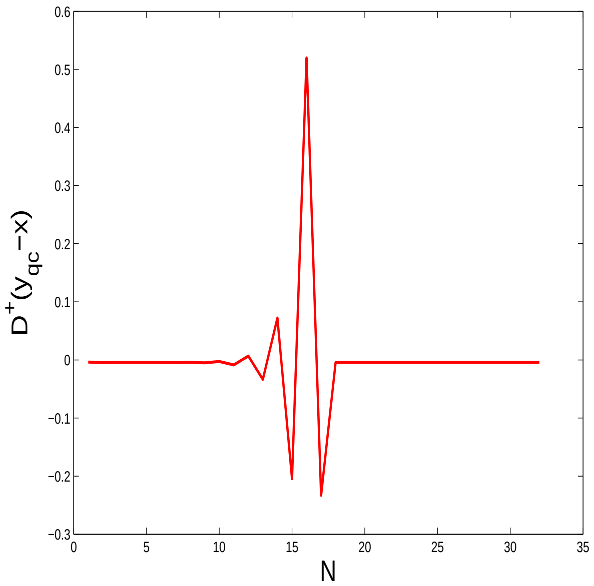
- harmonic potential (re-scale): $V = (1/2)|r/\epsilon|^2$
- 2nd neighbor interaction (NNN)

$$\mathcal{D}\boldsymbol{y}_{\text{QC}} = \boldsymbol{f}.$$

$$\mathcal{D} = \frac{1}{\epsilon^2}\left(\begin{array}{cccccccccc}
4 & -1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & 4 & -1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & -1 & 4 & -1 & -1 & \cdots & \cdots & \cdots & \cdots & 0 \\
 & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\
\hline
0 & \ldots & -1 & -1 & 7/2 & -1 & -1/2 & \ldots & \ldots & 0 \\
0 & \ldots & \ldots & -1 & -1 & 7 & -5 & \ldots & \ldots & 0 \\
0 & \ldots & \ldots & \ldots & -1/2 & -5 & 21/2 & -5 & \ldots & 0 \\
\hline
0 & \ldots & \ldots & \ldots & \ldots & -5 & 10 & -5 & \ldots & 0 \\
 & & & & & & \ddots & \ddots & \ddots & \\
0 & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & -5 & 10 & -5 \\
0 & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & 0 & -5 & 10
\end{array}\right)$$



(g) Profile for $\boldsymbol{y}_{\mathrm{QC}} - \boldsymbol{x}$



(h) Profile for $D_+(\boldsymbol{y}_{\mathrm{QC}} - \boldsymbol{x})$

Fig. 4: Error profile for the original QC solu.

Explicit solution without forcing

$$\widehat{\boldsymbol{y}} \equiv \boldsymbol{y}_{\mathsf{QC}} - \boldsymbol{x}, \qquad D_+ y_i \equiv (y_{i+1} - y_i)/\epsilon.$$

$$f(z) = 14 + 5z, \quad g(z) = 11 + 4z,$$

$$\omega_1 = \frac{1}{2}(-3 + \sqrt{5}), \omega_2 = -\frac{1}{2}(3 + \sqrt{5}), \gamma = \alpha g(\omega_1) + \beta g(\omega_2)$$

$$\widehat{y}_i = \begin{cases} (i+N)\gamma + \alpha f(\omega_1) + \beta f(\omega_2) + \alpha \omega_1^{i+N} + \beta \omega_2^{i+N}, & \text{if} \quad i = -N, \dots, 0, \\ (i - N - 1)\gamma & \text{if} \quad i = 1, \dots, N. \end{cases}$$

$$D_+ \widehat{y}_i = \begin{cases} \frac{\gamma}{\epsilon} + \frac{\alpha}{\epsilon}\omega_1^{i+N}(\omega_1 - 1) + \frac{\beta}{\epsilon}\omega_2^{i+N}(\omega_2 - 1), & \text{if} \quad i = -N, \dots, \bar{1}, \\ -\frac{2\gamma}{\epsilon}N - \frac{\alpha f(\omega_1) + \beta f(\omega_2)}{\epsilon} - \frac{\alpha\omega_1^N + \beta\omega_2^N}{\epsilon}, & \text{if} \quad i = 0, \\ \gamma/\epsilon, & \text{if} \quad i = 1, \dots, N - 1 \end{cases}$$

Rigorous estimate for 1-d: toy model

y_{QC} = solution of the original QC with harmonic potential

- error estimate

$$|D_+(y_i - x_i)| \leq C\left(\epsilon + \exp\left[-|i| \ln \frac{3+\sqrt{5}}{2}\right]\right), \qquad i = -N, \ldots, 0,$$
$$|D_+(y_i - x_i)| \leq C\epsilon, \qquad i = 1, \ldots, N.$$

- lower bound:

$$D_+(y_{-1} - x_{-1}) \geq \frac{1}{5}, \qquad N \geq 4.$$

- Interface width $= \mathcal{O}(\epsilon|\ln \epsilon|)$; outside interface, error $= \mathcal{O}(\epsilon)$
- Similar results have been obtained by Dobson & Luskin

Ghost force induced plasticity behavior (I)

$$V_{\text{Morse}}(r) = D_e[(1 - e^{-a(r-r_e)})^2 - 1]$$

$r =$ separation between atoms; $r_e =$ lattice parameter, $D_e =$ well depth; $a \simeq$ width

Modified Morse potential

$$V_{\text{Modify}}(r) = \begin{cases} V_{\text{Morse}}(r) + \delta\Big[\cos\big(100\pi(r - 0.72)\big) + 1\Big] & .71 < r < .73 \\ V_{\text{Morse}}(r) & r \leq .71 \text{ or } r \geq .73 \end{cases}$$

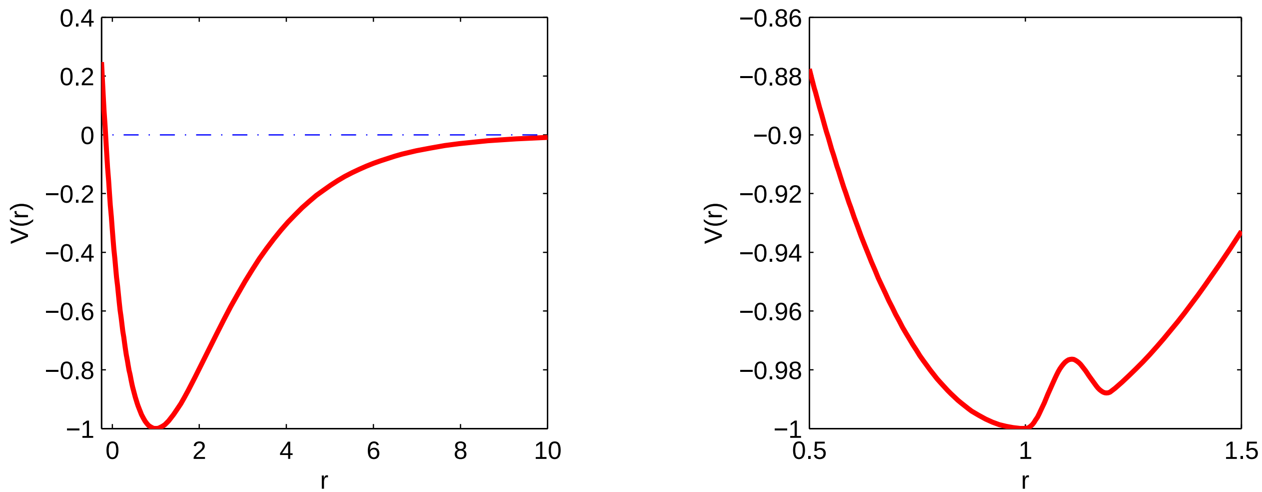


Fig. 5: Conventional and modified Morse potential.

Ghost force induced plasticity behavior (II)

- parameters $N = 21, r_e = 1.0, D_e = 1.0, a_e = 0.6$ 2nd interaction
- Other examples demonstrated the influence of the ghost force may be found in J. Mech. Phys. Solids, 47(1999), 611–642; Phy. Rew. B **69**(2004), 214104

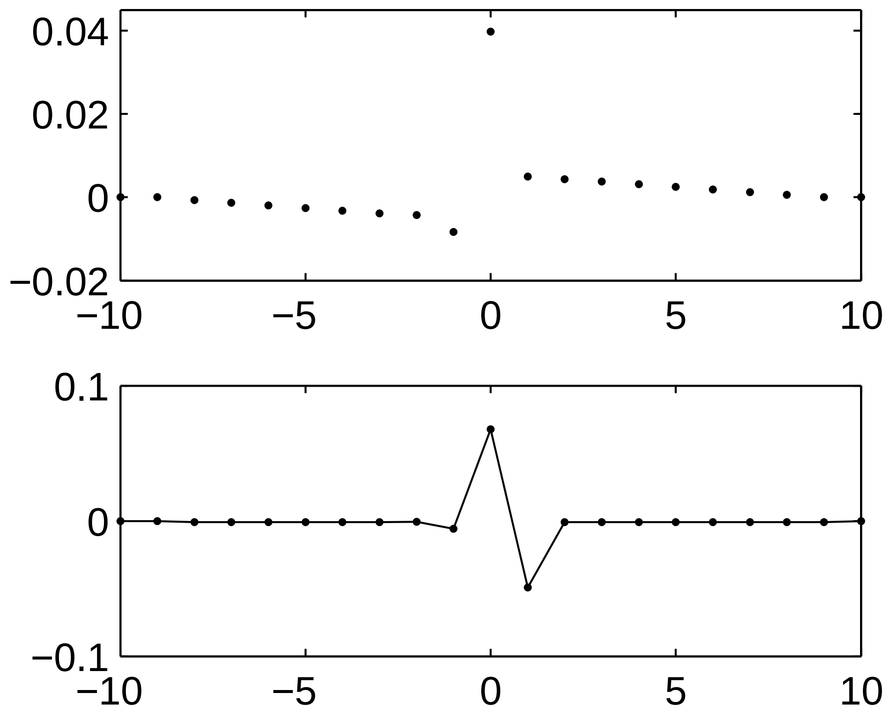
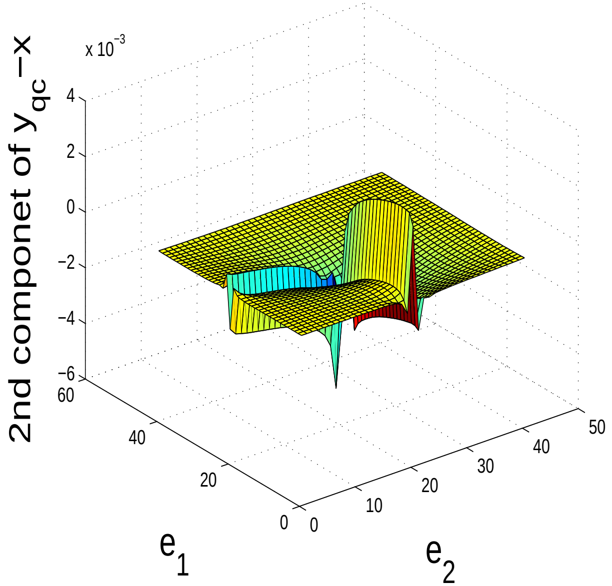
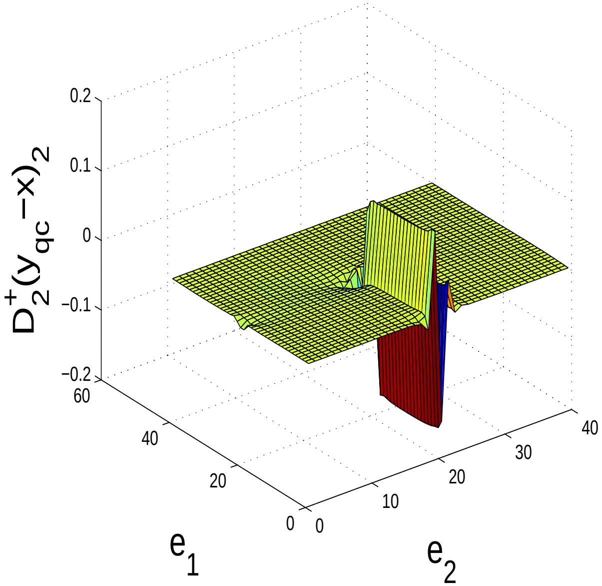


Fig. 6: Displacement & disp. grad. of atoms for original QC

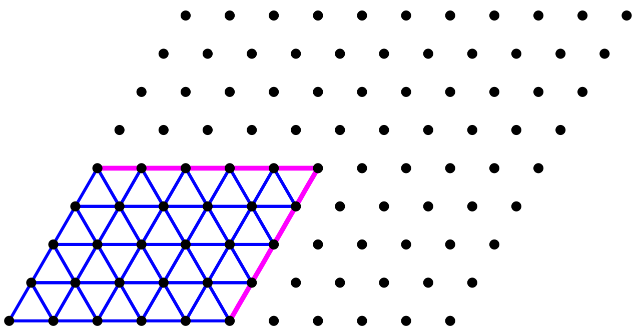
Ghost force in 2d



(a) Profile for $\boldsymbol{y}_{\text{QC}} - \boldsymbol{x}$

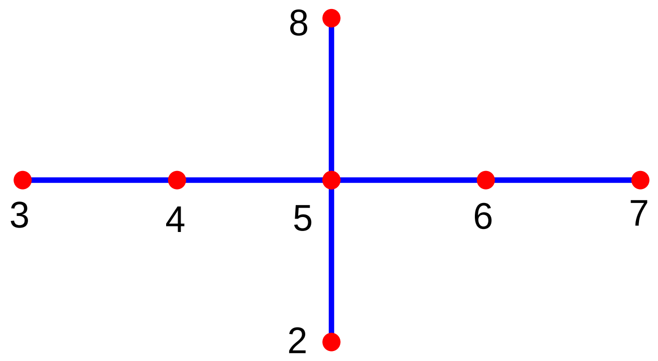


(b) Profile for $D_+(\boldsymbol{y}_{\text{QC}} - \boldsymbol{x})$

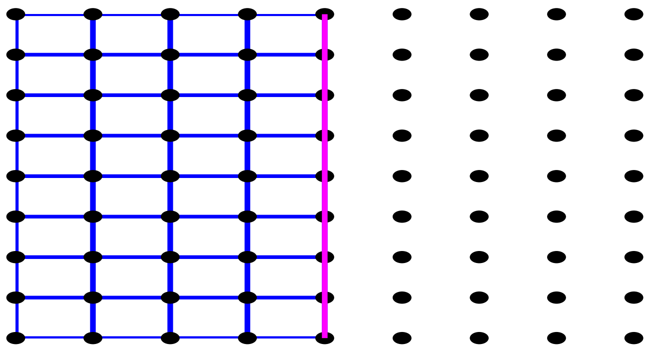


- Ghost force leads to $\mathcal{O}(1)$ error (discrete gradient) around the interface
- interface width $= \mathcal{O}(\epsilon|\ln \epsilon|)$; outside interface, error $= \mathcal{O}(\epsilon)$

Ghost force in 2d: explicit example (I)



(c) interaction range



(d) planar interface for square lattice;

Left=Continuum; Right=Atomic

- harmonic potential
- Dirichlet boundary condition imposed on boundaries
- special case: $x-$direction$=$Dirichlet BC; $y-$direction$=$periodic BC, reduces to $1-$d case

Ghost force in 2d: explicit example (II)

$$(\boldsymbol{y}_{\mathrm{QC}} - \boldsymbol{x})(m,n) = \begin{cases} \displaystyle\sum_{k=1}^{2N-1} a_k \sinh[(M+m)\alpha_k] \sin\frac{k\pi}{2N}(N+n), & \text{continuum} \\ \displaystyle\sum_{k=1}^{2N-1} \Big(b_k F_m(\gamma_k,\delta_k) + c_k f_m(\gamma_k,\delta_k)\Big) \sin\frac{k\pi}{2N}(n+N), & \text{atomistic} \end{cases}$$

$$\cosh\alpha_k = 1 + \frac{\lambda_k}{5}, \quad \lambda_k = 2\sin^2\frac{k\pi}{4N}$$

$$\cosh\gamma_k = \frac{1}{4}\Big(1 + \sqrt{25+8\lambda_k}\Big), \cosh\delta_k = \frac{1}{4}\Big(-1 + \sqrt{25+8\lambda_k}\Big)$$

$$F_m(\gamma,\delta) = \sinh[(M-m)\gamma] + 2\sinh\gamma\Big(\cosh[(M-m)\gamma] - \cosh[(M-m)\delta]\Big)$$

$$f_m(\gamma,\delta) = F_m(\delta,\gamma)$$

$a_k, b_k, c_k =$ certain parameters

Ghost force in 2d: explicit example (II)

- Error estimate $m = -M, \ldots, M, n = -N, \ldots, N$

$$|(\boldsymbol{y}_{\text{QC}} - \boldsymbol{y}_{\text{atom}})(m,n)| \le C\epsilon \exp\left[-\frac{|m|\pi}{5N}\right]$$

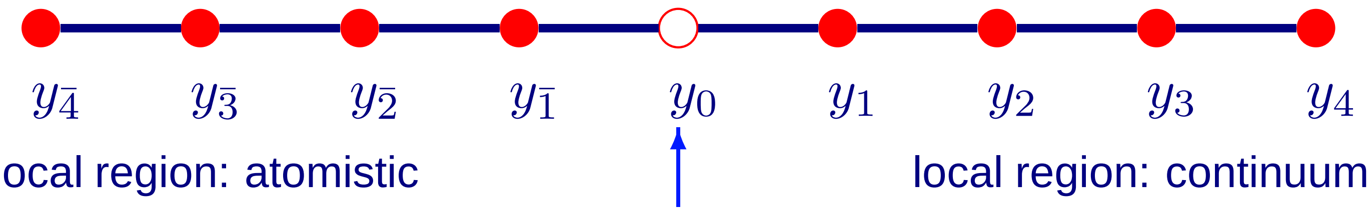
$$|D(\boldsymbol{y}_{\text{QC}} - \boldsymbol{y}_{\text{atom}})(m,n)| \le C \exp\left[-\frac{|m|\pi}{5N}\right]$$

- Lower bound: there exists c such that

$$|D(\boldsymbol{y}_{\text{QC}} - \boldsymbol{y}_{\text{atom}})(0,n)| \ge c.$$

- Interface width $= \mathcal{O}(\epsilon|\ln\epsilon|)$; outside interface, error for discrete gradient $= \mathcal{O}(\epsilon)$
- Conjecture: the above conclusion remains true for nonplanar interface; also for more general lattice structure

- Nonlocal region: solve the equilibrium equations from atomistic model
- Local region: solve the equilibrium equations from CB elasticity



$$f_i = -\frac{1}{\epsilon}\Big\{V'\Big(\frac{y_i - y_{i-2}}{\epsilon}\Big) + V'\Big(\frac{y_i - y_{i+2}}{\epsilon}\Big) + V'\Big(\frac{y_i - y_{i-1}}{\epsilon}\Big) + V'\Big(\frac{y_i - y_{i+1}}{\epsilon}\Big)\Big\}, \quad \text{nonlocal Reg.}$$

$$f_i = -\frac{1}{\epsilon}\Big\{V'\Big(\frac{y_i - y_{i-1}}{\epsilon}\Big) + V'\Big(\frac{y_i - y_{i+1}}{\epsilon}\Big) + 2V'\Big(\frac{2(y_i - y_{i-1})}{\epsilon}\Big) + 2V'\Big(\frac{2(y_i - y_{i+1})}{\epsilon}\Big)\Big\} \quad \text{Local Reg}$$

No ghost force!

Other ghost-force free methods

- Quasi-nonlocal QC (Shimokawa, Mortensen, Schiøtz and Jacobsen, 04)
- Geometrically consistent schemes (E, Lu, Yang, 06)
- In contrast to force-based QC, these two methods are based on energy

Theorem for Local QC method [E & M, 05]

If Born criteria is true, there exists constant κ, such that if $\|\boldsymbol{f}\|_{L^p(\Omega)} \leq \kappa$ with $p > d$, then

$$\|\boldsymbol{u}_{\text{CB}} - \boldsymbol{u}_{\text{QC}}\|_{H^1} \leq CH$$

$\boldsymbol{u}_{\text{CB}} =$ continuum solution obtained using $W = W_{\text{CB}}$

If Lindemann criteria is true, let $\boldsymbol{y}_{\text{QC}} = \boldsymbol{x} + \boldsymbol{u}_{\text{QC}}(\boldsymbol{x})$, there exists a local minimizer $\boldsymbol{y}$ of the atomistic model nearby, i.e.,

$$\|D_+(\boldsymbol{y} - \boldsymbol{y}_{\text{QC}})\|_\infty \leq C\big(\epsilon + H\big)$$

Corollary: Local QC method is stable whenever the atomistic model is stable

Quantify local truncation error

$\boldsymbol{y}_{\text{atom}}$ = the solution of the atomistic model

$$\text{Local Truncation Error} = (\mathcal{L}^{\epsilon}_{\text{atom}} - \mathcal{L}^{\epsilon}_{\text{qc}})(\boldsymbol{y}_{\text{atom}})$$

- Original QC

$$\text{LTE} = (\mathcal{L}^{\epsilon}_{\text{atom}} - \mathcal{L}^{\epsilon}_{\text{qc}})(\boldsymbol{y}_{\text{atom}}) = \begin{cases} \mathcal{O}(1/\epsilon) & \text{near interface} \\ \mathcal{O}(\epsilon^2) & \text{away from interface} \end{cases}$$

- $\text{LTE} = \mathcal{O}(\epsilon^2)$ forced-based QC
- Quasi-nonlocal QC & geometrically consistent scheme

$$\text{LTE} = \begin{cases} \mathcal{O}(1) & \text{near interface} \\ \mathcal{O}(\epsilon^2) & \text{away from interface} \end{cases}$$

Refined structure of the local truncation error

Observation: symmetry of lattice and the translation invariance of the potential function makes LTE $\simeq$ discrete divergence form

$$\text{LTE}_i = -\frac{1}{\epsilon}\Big\{V'\Big(\frac{y_i - y_{i-2}}{\epsilon}\Big) + V'\Big(\frac{y_i - y_{i+2}}{\epsilon}\Big) - 2V'\Big(\frac{2(y_i - y_{i-1})}{\epsilon}\Big) - 2V'\Big(\frac{2(y_i - y_{i+1})}{\epsilon}\Big)\Big\} = D_+ Q_i,$$

$$Q_i = V'\Big(\frac{y_i - y_{i-2}}{\epsilon}\Big) + V'\Big(\frac{y_{i+1} - y_{i-1}}{\epsilon}\Big) - 2V'\Big(\frac{y_i - y_{i-1}}{\epsilon}\Big)$$

$Q_i = \mathcal{O}(\epsilon^2)$ $\quad$ $\text{LTE}_i = D_+ Q_i = \mathcal{O}(\epsilon^2)$ $\quad$ Taylor expansion

Estimate the consistency error

- forced based QC;

$$|\,\text{LTE}\,| \simeq \mathcal{O}(\epsilon^2)$$

- Q-QC; geometrically consistent scheme

$$|\,\langle\,\text{LTE}, \boldsymbol{w}\rangle\,| \leq C\epsilon \|\,\boldsymbol{w}\,\|_d$$

- In short $\quad \|\text{LTE}\|_{-d} \leq C\epsilon$

$$\|\boldsymbol{F}\|_{-d} = \sup_{\boldsymbol{w}\in\mathbb{R}^{2N+1}} \frac{\langle\,\boldsymbol{F}, \boldsymbol{w}\rangle}{\|\,\boldsymbol{w}\,\|_d}$$

Spijker, 1968; Tikhonov & Samarskiĭ, 1962

$$\|\,\boldsymbol{w}\,\|_d := \Big(\Big|\,\frac{w_1}{\epsilon}\,\Big|^2 + \Big|\,\frac{w_{2N+1}}{\epsilon}\,\Big|^2 + \sum_{i=1}^{2N}\Big|\,\frac{w_{i+1}-w_i}{\epsilon}\,\Big|^2\Big)^{1/2}.$$

Under certain stability condition on phonon spectra

$$\langle \mathcal{H}\boldsymbol{w}, \boldsymbol{w} \rangle \geq \Lambda \| \boldsymbol{w} \|_d^2$$

$$\mathcal{H}_{ij} = \frac{\partial^2 E}{\partial y_i \partial y_j}|_{\boldsymbol{x}} \qquad \text{Q-QC, GCS}$$

$$\mathcal{H}_{ij} = -\frac{\partial f_i}{\partial y_j}|_{\boldsymbol{x}} \qquad \text{force-based QC}$$

1. Translation invariance of $E \Longrightarrow \sum_j H_{ij} = 0 = \sum_i H_{ij}$
2. For any $\boldsymbol{w} \in \mathbb{R}^N$

$$\langle \mathcal{H}\boldsymbol{w}, \boldsymbol{w} \rangle = \sum_{ij} H_{ij} w_i w_j = -\frac{1}{2} \sum_{ij} (w_i - w_j) H_{ij} (w_i - w_j)$$

discrete Fourier transform; stab. cond. $\Downarrow$

$$\geq \lambda_1 \sum_i \sum_{|j-i| \leq M} \left| \frac{w_i - w_j}{\epsilon} \right|^2$$

Error estimate of ghost-force free QC [M & Yang, 09]

Suppose $V=$ LJ, there exists a threshold δ such that if f is smaller than δ in a suitable norm, then there exists a solution $\boldsymbol{y}$ near the atomistic solution:

$$\| D_+(\boldsymbol{y}_{\text{fqc}} - \boldsymbol{y}_{\text{atom}}) \|_\infty \le C\epsilon^2$$

$$\| D_+(\boldsymbol{y} - \boldsymbol{y}_{\text{atom}}) \|_\infty \le C\epsilon \qquad \boldsymbol{y} = \boldsymbol{y}_{\text{qqc}}, \boldsymbol{y}_{\text{gcs}}$$

$$\| D_+\boldsymbol{z} \|_\infty = \max_{1\le i\le N-1} |D_+ z_i| = \max_{1\le i\le N-1} |z_i - z_{i-1}|/\epsilon$$

- The convergence rate is sharp
- A reminiscent of Supra-convergence (Kreiss, Manteuffel, Swartz, Wendroff & White, Math. Comput. 1986)
- stability+consistency $\Longrightarrow$ convergence (Lax theorem)

Convergence of the original QC

- Consistency error

$$|\,\text{LTE}\,| = \mathcal{O}(1/\epsilon) \qquad \|\text{LTE}\|_{-d} = \mathcal{O}(1)$$

- The original QC is stable

$$\langle\,\mathcal{H}\boldsymbol{w},\boldsymbol{w}\rangle \geq \Lambda\|\,\boldsymbol{w}\,\|_d^2$$

- Convergence rate

$$\|D_+(\boldsymbol{y}_{\text{QC}} - \boldsymbol{y}_{\text{atom}})\|_{\ell_2} + \|\,\boldsymbol{y}_{\text{QC}} - \boldsymbol{y}_{\text{atom}}\,\|_\infty \leq C\epsilon^{1/2}$$

- The original QC converges with half-order rate

Error estimate for 2d problem

Set-up: 2d triangular lattice+harmonic potential; planar interface

- Consistency error for QQC

$$\|\text{LTE}\|_{-d} = \mathcal{O}(\epsilon) \qquad \text{very subtle}$$

- QQC is stable
- Convergence

$$\|D_+(\boldsymbol{y}_{\text{qqc}} - \boldsymbol{y}_{\text{atom}})\|_\infty \leq C\epsilon$$

- main issues for extension to more general cases:
  - consistency analysis: how to employ symmetry: lattice and potential
  - stability analysis: discrete Fourier analysis (phonon analysis): take into account into boundary condition

- Non-planar interface: new ghost-force free schemes are required, particularly for energy-based method; no serious tests so far (ongoing work)
- Planar interface: understanding nonlocal QC in high dimension with more general case (ongoing work)
- understanding other atomistic/continuum coupled method (many quasi-QC), e.g.,Coupled Atomistic and Discrete Dislocation mechanics (Shilkrot, Miller & Curtin); More ambitious project: QM/MM; CPMD; more efforts are needed to better understand microscopic models, such as `electronic structure models, molecular dynamics, Monte Carlo method`...

- Examples shows (1d + 2d) ghost-force is dangerous, e.g.,
  1. leads to unphysical plasticity deformation: trigger the solu. jump into unphysical local minimizer basin
  2. spoils the solution, e.g. deteriorate the accuracy or there is no accuracy at all in certain norm
  3. This seems quite generic for atomistic-continuum coupled methods, or even more general multiscale method or multilevel coupled method
- Ghost force free schemes converge with order in $W^{1,\infty}-$norm
  - 1d: FQC converges with $2-$order; QQC & GCS converge with $1-$order
  - 2d: QQC converges with $1-$order
- Key issue
  - consistent in the bulk: stability condition is key
  - consistent at interface: quantify the Local Truncation Error is quite subtle, in particularly for $d \geq 2$

Feedback for classical NA

- Numerical Analysis tools do help out in understanding QC
  - taking into account features of the problem: lattice symmetry, invariance of potential
  - limitation: zero temperature &no dynamics
- NA must be used carefully: choose a right norm to measure the error
  - Pointwise $W^{1,\infty}$norm is appropriate in this set-up
  - The original QC converges with $1/2$-order in discrete H^1 norm and pointwise L^∞ norm while still leads to WRONG physical picture
- Force-based QC is good (analysis aspect of view); but `This can lead to slower convergence and even spurious solutions, but the methods are reasonably robust if used carefully; Miller & Tadmor, MRS Bulletin, 07`