Some Mathematical and Numerical Issues in Multiscale Modeling

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Multiscale modeling has had a lot of successes

- Quantum mechanics-Molecular mechanics (QM-MM) methods (1975, Warshel and Levitt)
- Car-Parrinello molecular dynamics (1985, avoid empirical potentials, compute force fields directly from electronic structure information)
- Kinetic schemes in gas dynamics
- Quasicontinuum method (1996, Tadmor, Ortiz and Phillips)
- ......

There are still many fundamental issues

Focus on:
Difficulties with coupled atomistic (electronic structure) -continuum methods,
from the viewpoint of numerical analysis:

- Boundary conditions
- Consistency
- Stability

Illustrated using simple examples.

Major difficulty: Microsopic models, such as molecular dynamics and electronic structure models, are very poorly understood.

Boundary conditions

Consistency

Stability

Linear and sublinear scaling algorithms

Molecular dynamics

$$m_j \frac{d^2 \mathbf{x}_j}{dt^2} = \mathbf{F}_j = -\frac{\partial V}{\partial \mathbf{x}_j}$$

Electronic structure models

- Wave functions for the electrons (Kohn-Sham density functional theory, tight-binding models, etc)
- Electron density (Orbital-free density functional theory)

Boundary conditions for MD and QM models

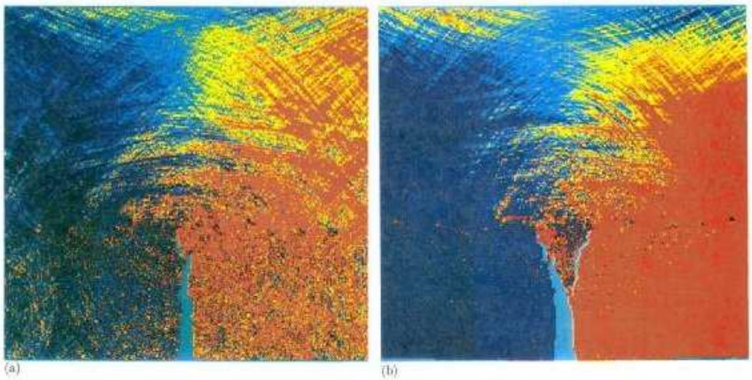
Super-cell: making things periodic.

Effect of boundary condition more pronounced due to the fact that we can only simulate rather small systems.

What would it be like if all finite element calculations are restricted to periodic boundary conditions?

Boundary conditions: Phonon reflection from MD simulation of solids

Dirichlet type of boundary condition is used.



(Holian et al., Phys. Rev. B, 1998).

Boundary condition for MD simulation of solids

Main objective: Use a small system to mimic the behavior of much larger system.

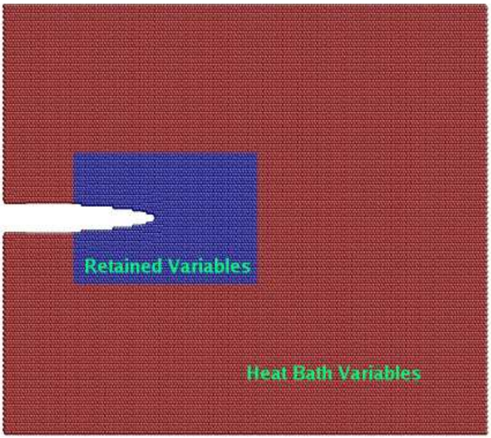
Obvious analogy with ABC (absorbing boundary condition for wave equation)

Key differences:

- Small k expansion not enough, phonons exist at all k.
- Finite temperature: Also need to take phonons from the environment.

Problem formulation

Eliminate heat bath variables



The right perspective: Mori-Zwanzig formalism

A simple linear example

$$\frac{\mathrm{d}p}{\mathrm{d}t} = A_{11}p + A_{12}q,$$
$$\frac{\mathrm{d}q}{\mathrm{d}t} = A_{21}p + A_{22}q.$$

Objective: Obtain a closed model for p.

$$q(t) = e^{A_{22}t}q(0) + \int_0^t e^{A_{22}(t-\tau)}A_{21}p(\tau)\,\mathrm{d}\tau.$$

$$\begin{aligned}\frac{\mathrm{d}p}{\mathrm{d}t} &= A_{11}p + A_{12}\int_0^t e^{A_{22}(t-\tau)}A_{21}p(\tau)\,\mathrm{d}\tau + A_{12}e^{A_{22}t}q(0)\\ &= A_{11}p + \int_0^t K(t-\tau)p(\tau)\,\mathrm{d}\tau + f(t),\end{aligned}$$

- $K(t) = A_{12}e^{A_{22}t}A_{21}$ is the *memory kernel*
- $f(t) = A_{12}e^{A_{22}t}q(0)$ is the *noise term*, if we think of $q(0)$ as a random variable.

General Mori-Zwanzig formalism

1. Projection operator (conditional expectation),

$$\mathcal{P}g = E(g|\text{retained variables}), \mathcal{Q} = I - \mathcal{P}.$$

2. For any function of the retained variables: φ,

$$\frac{d}{dt}\varphi(t) = e^{t\mathcal{L}}\mathcal{L}\varphi(0) = e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\varphi(0) + e^{t\mathcal{L}}\mathcal{Q}\mathcal{L}\varphi(0),$$

3. Dyson's formula,

$$e^{t\mathcal{L}} = e^{t\mathcal{Q}\mathcal{L}} + \int_0^t e^{(t-s)\mathcal{L}}\mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}ds.$$

4. Generalized Langevin equation:

$$\begin{aligned} \frac{d}{dt}\varphi(t) &= e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\varphi(0) + \int_0^t e^{(t-s)\mathcal{L}}K(s)ds + R(t). \\ R(t) &= e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\varphi(0), \quad K(t) = \mathcal{P}\mathcal{L}R(t). \end{aligned}$$

Recent literature: Chorin et al. on "Optimal prediction".

- Universal strategy for eliminating degrees of freedom.
- By itself, it is almost useless. The key is to make approximations.

Mori-Zwanzig formalism for MD (Xiantao Li and E)

Partition of the system: $\mathbf{u} = (\mathbf{u}_I, \mathbf{u}_j), \quad \mathbf{v} = (\mathbf{v}_I, \mathbf{v}_j)$
The thermodynamic force: $e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\mathbf{v}_I(0) = -\frac{\partial W}{\partial \mathbf{u}_I}$.
The effective free energy:

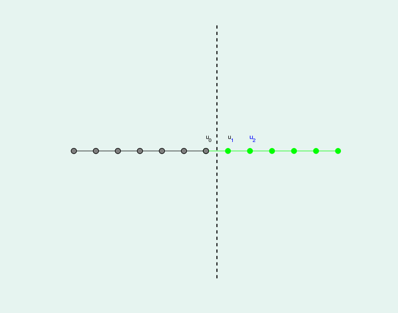
$$W(\mathbf{u}_I, T) = -k_B T \ln Z, \quad Z = \int e^{-\frac{V(\mathbf{u}_I, \mathbf{u}_j)}{k_B T}} d\mathbf{u}_j,$$

The memory term: $-\int_0^t \Theta(\tau)\dot{\mathbf{u}}_I(t-\tau)d\tau$.
The generalized Langevin equation:

$$m\ddot{\mathbf{u}}_I = -\nabla_{\mathbf{u}_I} W - \int_0^t \Theta(\tau)\dot{\mathbf{u}}_I(t-\tau)d\tau + R(t) + \mathbf{f}^{ex}(t).$$

Example:

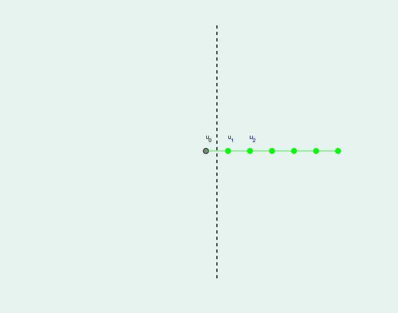
$$\begin{cases} \ddot{u}_j & = & \phi'(u_{j+1} - u_j) - \phi'(u_j - u_{j-1}) \\ \ddot{u}_j & = & u_{j+1} - 2u_j + u_{j-1}, \quad j \leq 0. \end{cases}$$



Example:

$$\ddot{u}_0 = \phi'(u_1 - u_0) - \int_0^t \theta(\tau)\dot{u}_0(t-\tau)d\tau + R.$$

$$\theta(t) = \frac{J_2(2t)}{t}.$$



Local memory kernels

(E and Huang, 2001; Li and E, 2006–2007)

- the memory kernel is independent of the temperature
- at zero temperature, similar to absorbing BC for wave equations

Basic principles:

1. Efficiency: local kernels
2. Stability: positive-definite kernels
3. Consistency: fluctuation-dissipation theorem

Variational approach at $T = 0$

Given the stencil (cost), find the best approximate kernels.

Note the lack of a small parameter.

1. Express $\Theta(t)$ in the form of,

$$\Theta(t) = \int_{-\infty}^{+\infty} \Gamma(s)\Gamma(t+s)^T ds.$$

   $\Gamma(t)$ is local:

$$\Gamma_{ij}(t) = 0, \text{ if } |\mathbf{r}_i - \mathbf{r}_j| > r_c, \text{ or } |t| > t_c.$$

2. Objective functions

$$\min_{\Gamma(t)} \int e(\omega; \Gamma) W(\omega) d\omega.$$

3. Choose the functional: e.g. Total energy of reflected phonons.

Sample the random noise

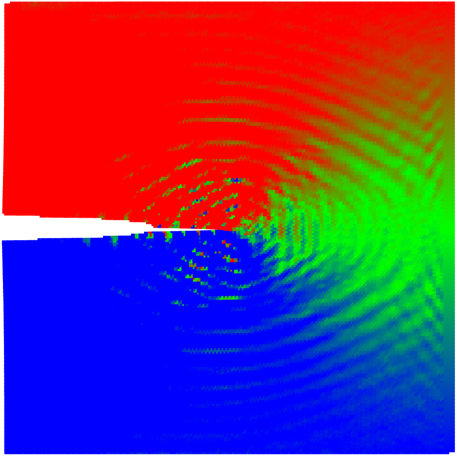
The random noise $R(t)$ is a stationary Gaussian process. The fluctuation-dissipation theorem is satisfied:

$$\left\langle R(t)R(0)^T \right\rangle = k_B T\Theta(t).$$

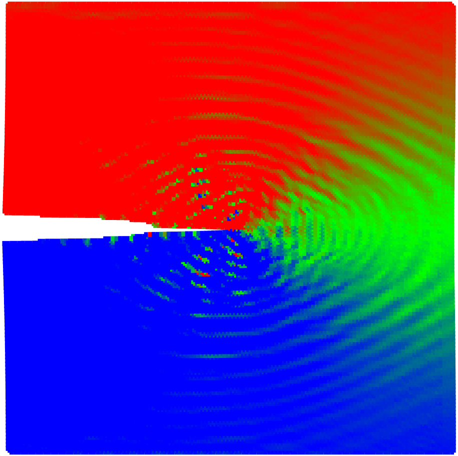
Let $W(t)$ be white noise with variance $k_B TI$, then,

$$R(t) = \sum_k \int \Gamma(s)W(t-s)ds.$$

Case studied 1: fracture simulation

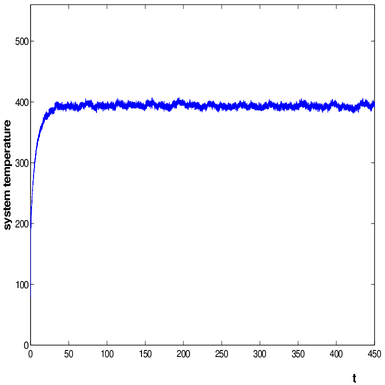


Fixed boundary condition.

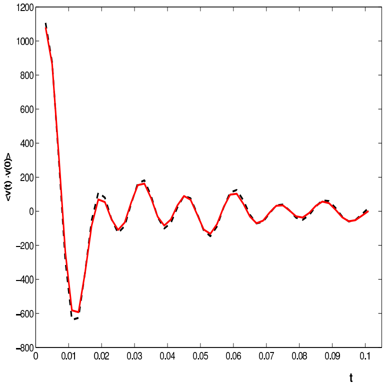


Variational boundary condition.

Case studied 2: finite temperature in 3D BCC Iron



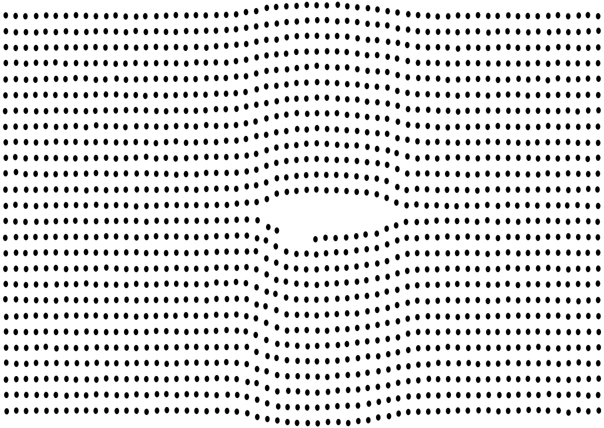
System temperature.



Velocity autocorrelation.

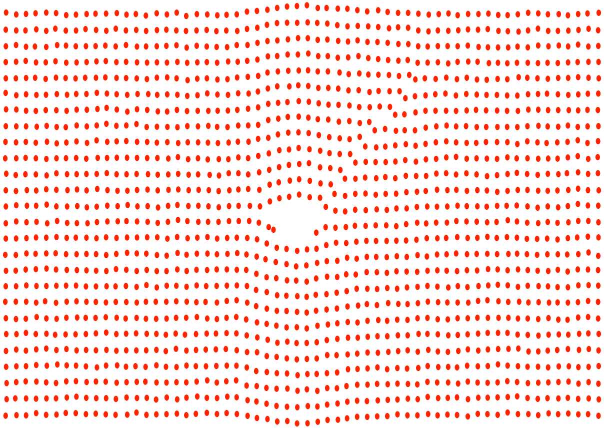
Can be used as a “first-principle-based” thermostat.

Case studied 3: finite temperature crack simulation



At zero temperature

Case studied 3: finite temperature crack simulation



At finite temperature 500K

Consistency between the MD and the continuum model

Outside region (eliminated region) is not just a heat bath, but a piece of material modeled by continuum equations (with a temperature field).

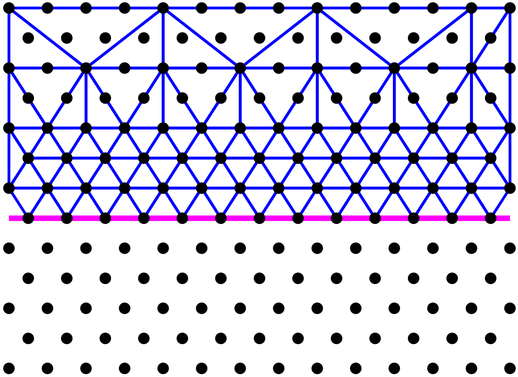
Work in progress by Xiantao Li and E

Will look at a special case:

Quasicontinuum method (Tadmor et al. 1996)

- Temperature $= 0$
- No dynamics

Quasicontinuum method



- An adaptive mesh and model refinement procedure
- Based on linear finite elements
- Representative atoms define the triangulation
- Near defects, the mesh becomes fully atomistic
- Local (continuum) and nonlocal (atomistic) regions

Consistency

- Consistency in the bulk: For simple systems, the two models should produce consistent results.
- Consistency at the local-nonlocal interface.

Consistency between atomistic and continuum models

Nonlinear elasticity theory:

$$E(\mathbf{u}) = \int_\Omega W(\nabla \mathbf{u}) d\mathbf{x}$$

$W(\cdot)$ = stored energy density.
In linear elasticity, W = a quadratic function of $\nabla \mathbf{u}$.

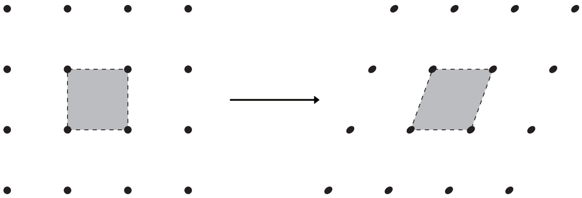
$$E(\{\mathbf{y}_1, \cdots, \mathbf{y}_N\}) = \sum_{i,j} V_2(\mathbf{y}_i, \mathbf{y}_j) + \sum_{i,j,k} V_3(\mathbf{y}_i, \mathbf{y}_j, \mathbf{y}_k) + \cdots$$

Question: Can we relate W to the atomistic model?

The Cauchy-Born rule

Given A, a 3×3 matrix, $W(A) = ?$

Deform the crystal uniformly: $\mathbf{y}_j = \mathbf{x}_j + A\mathbf{x}_j = (I + A)\mathbf{x}_j$



$W(A)$ = energy density of deformed unit cell, computed according to the given atomistic or electronic structure model.

Validity of Cauchy-Born rule: Consistency

One dimension model: $x_k = k\varepsilon$.

Assume: $y_k = x_k + u(x_k)$ and u is a **smooth** function.

$$
\begin{aligned}
V &= \frac{1}{2}\sum_{i\neq k} V_0(y_i - y_k) \qquad (1)\\
&\approx \frac{1}{2}\sum_{i}\left(\sum_{k\neq i} V_0(1+\frac{du}{dx}(x_i))k\varepsilon\right)\\
&= \sum_{i} W\left(\frac{du}{dx}(x_i)\right)\varepsilon \approx \int W\left(\frac{du}{dx}(x)\right)dx,
\end{aligned}
$$

where

$$
W(A) = \frac{1}{2\varepsilon}\sum_{k} V_0((1+A)k\varepsilon)
$$

X. Blanc, C. Le Bris and P. L. Lions (2002) considered general case, including some QM models.

Validity of Cauchy-Born rule: Counterexample

Example: Lennard-Jones potential, next nearest neighbor interaction

- *Triangular* lattice, Cauchy-Born rule is valid
- *Square* lattice, Cauchy-Born gives **negative shear modulus (unstable)**, can't speak of elasticity theory.

Validity of Cauchy-Born rule: Stability

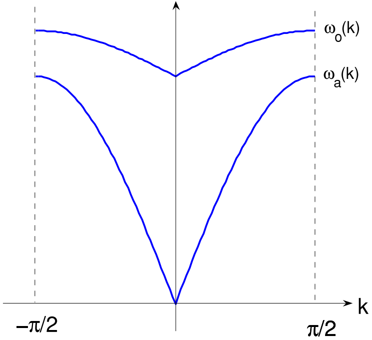
- Continuum level (Born criteria) – *Elastic stiffness tensor* is positive definite
- Atomic level (Lindemann criteria) – *Phonon spectra* (dispersion relation for the lattice waves) remain "positive definite"
- Electronic level – Disperson relation for the *charge-density waves and spin waves*

Phonon stability condition

Acoustic branch: dynamics of the Bravais lattice

Optical branch: relative motion of the internal degrees of freedom

1st Brillouin zone: Voronoi cell of the origin of the dual lattice



Consistency in the bulk

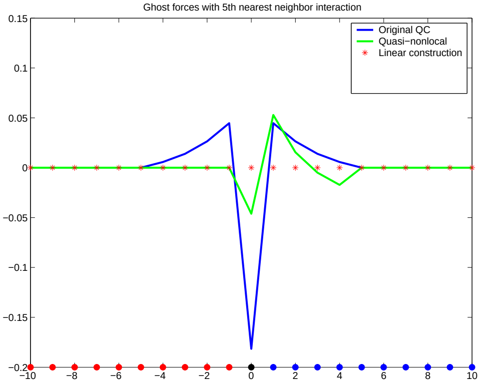
Under these conditions, the solutions to the Cauchy-Born continuum model and the atomistic model are close.

- E and Ming (2007), molecular mechanics models.
- E and Lu (2008), several classes of quantum mechanics models.

These conditions are sharp!!
Violation of the stability conditions signals onset of plastic deformation or structural (or electronic) phase transformation.
Related work of Ju Li, S. Yip et al. (Λ-criterion),
R. Elliott et al.

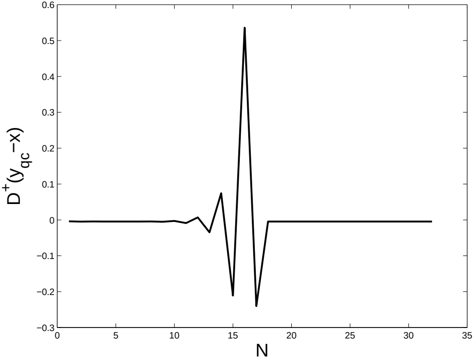
Consistency at the loca-nonlocal interface

The issue of "ghost force" (e.g. in quasicontinuum methods)



- Left side: using continuum model based on the Cauchy-Born rule (effectively a nearest neighbor model).
- Right side: Using full atomistic model, next nearest neighbor interaction.

Explicit solution for quadratic potential (E, Ming and Yang, 08)



1. The deformation gradient has $\mathcal{O}(1)$ error at the interface.
2. The influence of the ghost force decays exponential fast away from the interface.
3. Away from an interfacial region of width $\mathcal{O}(\varepsilon|\log(\varepsilon)|)$, the error in the deformation gradient is of $\mathcal{O}(\varepsilon)$ (see also recent work of Dobson and Luskin).

Removing the ghost force

Ghost force may induce numerical artifacts (e.g. plastic deformation) at the interface.

- Force-based approach (Tadmor et al., Miller, Dobson and Luskin)
- Quasi-nonlocal atoms (Jacobson et al.)
- Geometrically consistent scheme (E, Lu and Yang)

Classical numerical analysis viewpoint:

- Truncation error $= O(\varepsilon)$ in a weak sense
- Stability conditions (similar to the ones discussed above)

Uniform $O(\varepsilon)$ accuracy for smooth solutions.

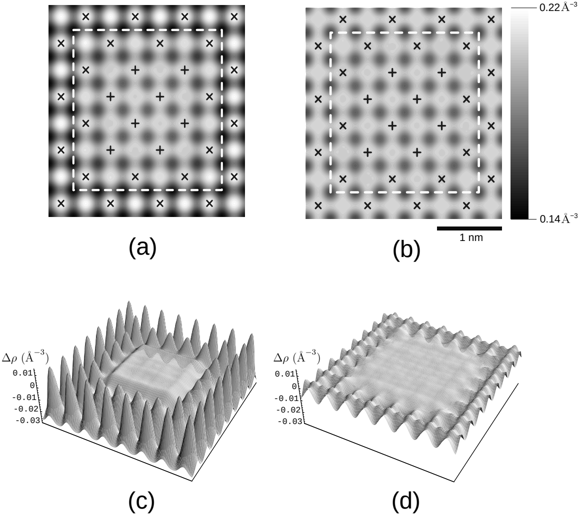
Related work in the math literature:

- Dobson and Luskin
- Ortner and Süli
- Blanc, Legoll and Le Bris

Improving atomistic/continuum coupling for solids:

- MAAD: Abraham, Bernstein, Broughton and Kaxiras
- Bridge domain: Xiao and Belytschko
- Bridge scales: W. K. Liu et al.
- AtC approach: Gunzburger et al., Lehoucq et al.
- M. Robbins
- ......

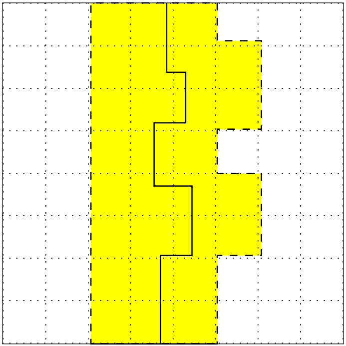
Ghost force for the coupled OF-DFT/EAM method (Choly, Lu, E, Kaxiras)



Loss of fluctuations

Example: Coupled KMC-continuum models of epitaxial crystal growth (Schulze, Smereka and E):

- Around the step-edges, use KMC, since fluctuations are important
- On the terraces, use continuum (e.g. diffusion) models



Mean position and variance of step edge

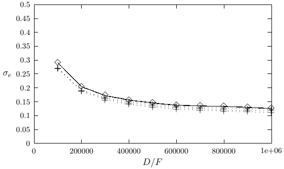


Figure 6: The time and space averaged surface adatom density for the KMC simulations (diamonds) and the hybrid scheme (crosses) using cell-widths $M = \{20, 25, 40\}$.

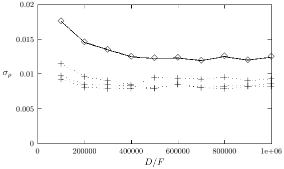


Figure 7: The standard deviation (in time) of the surface averaged adatom density as a function of the ratio D/F. The solid curve (diamonds) are from the KMC simulations and the remaining curves are for the hybrid scheme with cell-widths $M = \{20, 25, 40\}$ sites per cell.

Other examples: See work of Garcia, Bell and Donev, et al.

Boundary conditions

Consistency

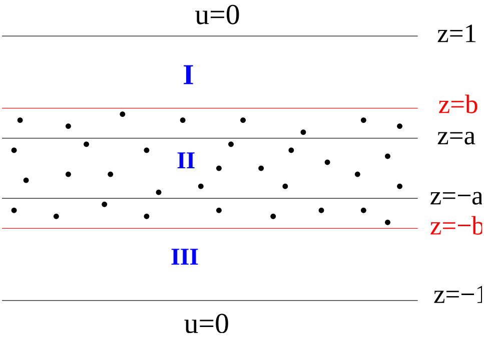
Stability

Linear and sublinear scaling algorithms

Stability of coupled continuum/MD methods

Work of Weiqing Ren (NYU)

- Example of fluids
- General strategy: Domain decomposition (with overlap)
- Coupling:



In continuum region (I, III): $\rho u_t - \mu u_{zz} = 0$

In particle region (II): $m \frac{d^2 \mathbf{x}_j}{dt^2} = \mathbf{f}_j$

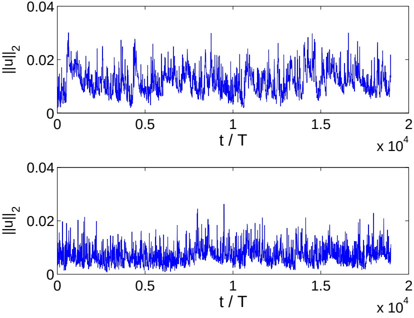
Four coupling schemes:

1. velocity(MD)-velocity(C),
2. velocity(MD)-flux(C),
3. flux(MD)-velocity(C),
4. flux(MD)-flux(C)

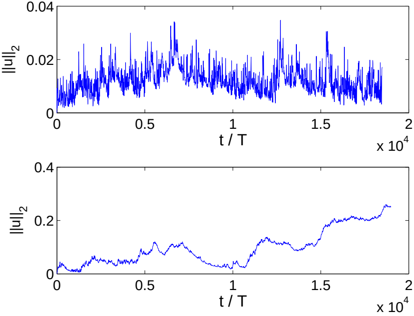
Particular features as a domain decomposition method

- The MD (molecular dynamics) domain is very small.
- Statistical error cannot be avoided

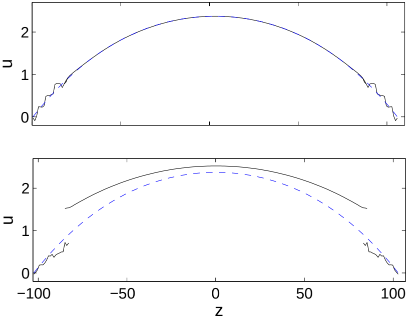
Numerical solutions for equilibrium states



Upper panel: velocity-velocity
Lower panel: flux-velocity



Upper panel: velocity-flux
Lower panel: flux-flux


u
2
1
0
u
2
1
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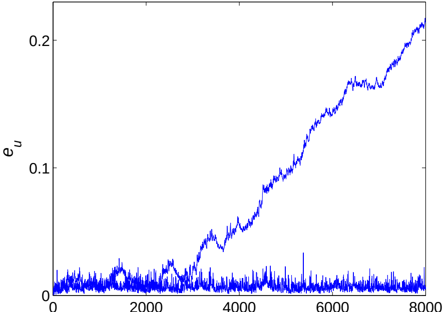
−50
0
50
100
z


e_u
0.2
0.1
0
0
2000
4000
6000
8000

Steady-state calculation: $T_c = \infty$

Amplification factors g for the four schemes:

- velocity-velocity, flux-velocity

$$u_n(z) = \sum_{i=1}^{n} g^{n-i} \xi_i \frac{1-z}{1-a}, \qquad \langle \|u_n\|_2 \rangle \leq \left(\frac{1}{3(1-g^2)} \right)^{1/2} \sigma_v$$

ξ_i: Statistical errors in velocity BC; $\quad \sigma_v = \langle \xi_i^2 \rangle$
$g = \frac{a(1-b)}{b(1-a)}$ for velocity-velocity; $\quad g = \frac{a}{a-1}$ for flux-velocity

- velocity-flux, flux-flux

$$u_n(z) = \sum_{i=1}^{n} g^{n-i} \xi (z-1)$$

$g = \frac{b-1}{b}$ for velocity-flux; ($g > 1 \rightarrow$ Diverge)
$g = 1$ for flux-flux $\rightarrow \langle \|u_n\|_2 \rangle \leq 3^{-1/2}(1-a) n^{1/2} \sigma_\tau$

Stability: Finite T_c

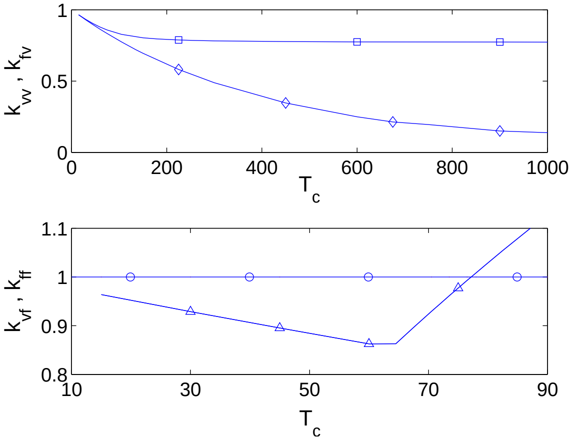


Figure: The amplification factor g versus $T_c/\Delta t$ for the four schemes: VV (squares), FV (diamonds), VF (triangles) and FF (circles).

Remarks:

- There are many different variants of atomistic/continuum coupling schemes.
- Errors and artifacts are difficult to understand.
- What I have described are examples of efforts to try to put things on a solid foundation.

Boundary conditions

Consistency

Stability

Linear and sublinear scaling algorithms

Linear scaling algorithms

Cost $\sim$ number of degrees of freedom

Examples:

- Multi-grid method
- Fast multipole method
- Linear scaling algorithms in electronic structure analysis
- ......

Sublinear scaling algorithms

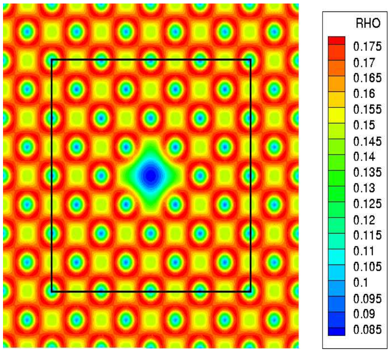
Cost $\ll$ number of degrees of freedom (in the microscopic) model

- Quasicontinuum method
- AtC methods

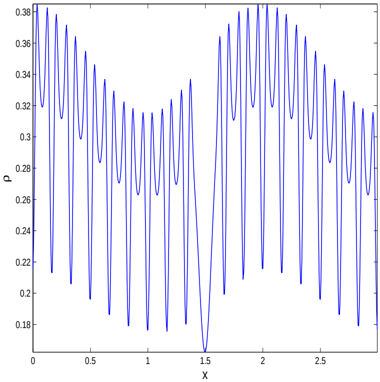
Most multiscale methods are sublinear scaling algorithms.

Sub-linear scaling algorithm for electronic structure analysis

García-Cervera, Lu and E (2007)

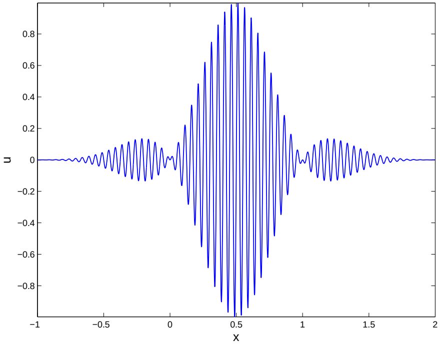


Electron density distribution of Al in the presence of vacancies



A slice of the electron density (modulated problem).

An analogy: Wave propagation and geometric optics



$$\partial_t^2 u = C(x)^2 \Delta u;$$

$$u(x,0) = A_0(x) e^{i\frac{\phi_0(x)}{\epsilon}}.$$

Solving the wave equation directly: $O(\varepsilon^{-1})$ operations (linear scaling algorithm).

Geometric optics approximation:

Ansatz: $u(x,t) = A(x,t)\exp\left(i\frac{\varphi(x,t)}{\epsilon}\right) + \cdots\cdots$

$$\partial_t\varphi + C(x)|\nabla\varphi| = 0;$$

$$\partial_t A + C(x)\frac{\nabla\varphi\cdot\nabla A}{|\nabla\varphi|} + \frac{C(x)^2\Delta\varphi - \partial_t^2\varphi}{2C(x)|\nabla\varphi|}A = 0.$$

Solving these equation require $O(1)$ (independent of ε) operations.

In the general case, solve these limit equations away from caustics, and solve the original problem near caustics.
This requires $o(\varepsilon^{-1})$ operations, hence **sub-linear scaling algorithm**.

Combine asymptotic analysis and numerical methods

Asymptotics for density functional theory

$\{\psi_k = \psi_k(\mathbf{y}), k = 1, \cdots, N\} =$ A set of N orthonormal orbitals:

$$I_\varepsilon(\{\psi_k\}) = \varepsilon^2 \sum_{k=1}^{N} \int_{\mathbb{R}^3} |\nabla \psi_k(\mathbf{y})|^2 \, \mathrm{d}\mathbf{y} + \int_{\mathbb{R}^3} \epsilon_{\mathrm{xc}}(\rho)\rho(\mathbf{y}) \, \mathrm{d}\mathbf{y}$$
$$+ \frac{\varepsilon}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{(\rho - m)(\mathbf{y})(\rho - m)(\mathbf{y}')}{|\mathbf{y} - \mathbf{y}'|} \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{y}'.$$

$\varepsilon =$ atomic length scale, e.g. the lattice constant.

$\rho(\mathbf{y}) = \sum_k |\psi_k|^2(\mathbf{y})$ is the electron density.

Input to the model: The atoms. $m(\mathbf{y}) = \sum_{\mathbf{y}_i \in \varepsilon L \cap \Omega} m_i^a(\mathbf{y} - \mathbf{y}_i) =$ (pseudo)-ionic potential (describing the atoms in the system).

- $\{\mathbf{y}_j\} =$ positions of the nuclei (ions).
- $\{m_j^a\} =$ describe the types of atoms

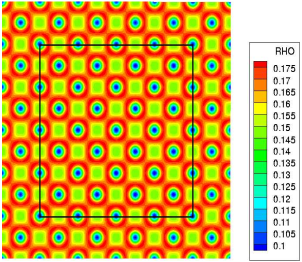
Ansatz (first variable is Eulerian, second is Lagrangian):

$$\psi_\alpha(y, \frac{x}{\varepsilon}) = \frac{1}{\varepsilon^{3/2}}\psi_{\alpha,0}(y, \frac{x}{\varepsilon}) + \frac{1}{\varepsilon^{1/2}}\psi_{\alpha,1}(y, \frac{x}{\varepsilon}) + \varepsilon^{1/2}\psi_{\alpha,2}(y, \frac{x}{\varepsilon}) + \cdots$$

$$\rho(y, \frac{x}{\varepsilon}) = \frac{1}{\varepsilon^{3}}\rho_0(y, \frac{x}{\varepsilon}) + \frac{1}{\varepsilon^{2}}\rho_1(y, \frac{x}{\varepsilon}) + \frac{1}{\varepsilon^{1}}\rho_2(y, \frac{x}{\varepsilon}) + \cdots$$

$$\phi(y, \frac{x}{\varepsilon}) = \phi_0(y, \frac{x}{\varepsilon}) + \varepsilon\phi_1(y, \frac{x}{\varepsilon}) + \varepsilon^2\phi_2(y, \frac{x}{\varepsilon}) + \cdots .$$

$\psi_\alpha(y,z)$ **decays for large** z
$\rho(y,z)$ and $\phi(y,z)$ are periodic in z.



Electron density distribution of Al

Leading order: Electronic structure of a uniformly deformed infinite lattice

$\{\psi_\alpha\}$, where α numbers the valence electrons in a unit cell.
$\nabla_1 = \nabla_y, \nabla_2 = \nabla_z$.

$$
\begin{aligned}
&-\Delta_2^x \psi_{\alpha,0}(y,z) + V_{xc,0}(\rho_0)\psi_{\alpha,0}(y,z) - \phi_0(y,z)\psi_{\alpha,0}(y,z) \\
&\qquad + \sum_{\alpha', z_j \in L} \lambda_{\alpha\alpha' j,0}(y)\psi_{\alpha',0}(y, z - z_j) = 0; \\
&-\Delta_2^x \phi_0(y,z) = 4\pi(m_0 - \rho_0)(y,z); \\
&\int_{\mathbb{R}^3} \psi_{\alpha,0}(y,z)\psi_{\alpha',0}(y, z - z_j)\,\mathrm{d}z = \delta_{\alpha\alpha'}\delta_{0j}/\det(I + \nabla u(x)).
\end{aligned}
$$

$\Delta_2^x = ((I + \nabla u(x))^{-\mathrm{T}}\nabla_2)^2$, the coefficients come from the coordinate change, $y = x + u(x)$.

- This is a system of equations in z – the fast variables. y enters only as parameters.
- It is a periodic system, but the equation is formulated over the whole space.

The continuum limit and the Cauchy-Born rule

$$E(u) = \int_\Omega W_{\rm CB}(\nabla u(x))\ {\rm d}x$$

Variational formulation

$$W_{\rm CB}(A) = \inf_{\{\psi\}} W(A, \{\psi_\alpha(\cdot; A)\}) = \inf_{\{\psi\}} \frac{\det(I + A)}{|\Gamma|} I_A(\{\psi\})$$

$$\begin{aligned} I_A = \sum_\alpha \int_{\mathbb{R}^3} |(I + A)^{-\rm T} \nabla \psi_\alpha(z; A)|^2\ {\rm d}z + \int_\Gamma \varepsilon_{{\rm xc},0}(\rho(z; A))\rho(z; A)\ {\rm d}z \\ + \frac{1}{2} \iint_{\Gamma\times\Gamma} (\rho - m_{\rm CB})(z; A) G(z - z'; A)(\rho - m_{\rm CB})(z'; A)\ {\rm d}z\, {\rm d}z'. \end{aligned}$$

Γ= unit cell, G is the periodic Green's function.

Next order equations:

$$
\begin{aligned}
&-\Delta_2^x \psi_{\alpha,1}(y,z) + V_{xc,0}(\rho_0)\psi_{\alpha,1}(y,z) \\
&\quad + V_{xc,1}(\rho_0,\rho_1)\psi_{\alpha,0}(y,z) - \phi_0\psi_{\alpha,1}(y,z) - \phi_1\psi_{\alpha,0}(y,z) \\
&\quad + \sum_{\alpha',z_j\in L}\Big(\lambda^{(y)}_{\alpha\alpha' j,0}\nabla_1\psi_{\alpha',0}(y,z-z_j)(I+\nabla u)\cdot z_j \\
&\quad + \lambda^{(y)}_{\alpha\alpha' j,0}\psi_{\alpha',1}(y,z-z_j) + \lambda^{(y)}_{\alpha\alpha' j,1}\psi_{\alpha',0}(y,z-z_j)\Big) = 0; \\
&-\Delta_2^x \phi_1(y,z) = 4\pi(m_1(y,z) - \rho_1(y,z)); \\
&\int_{R^3} \psi_{\alpha,0}(y,z)\psi_{\alpha',1}(y,z-z_j) \\
&\quad + \psi_{\alpha,0}(y,z)\nabla_1\psi_{\alpha',0}(y,z-z_j)(I+\nabla u)\cdot z_j \,\mathrm{d}z = 0.
\end{aligned}
$$

- Again, this is a set of equations in the fast variable. Differentiation in y only enters through the forcing term in the constraint equation.

How do we make use of the asymptotics results to design sublinear scaling algorithms?

See talk by Carlos Garcia-Cervera

Summary: 1. Model error and solution error

$E_{tot} = E_I + E_{II} + E_{int}$

Example: Coupled QM-continuum methods (E and Lu)

1. The whole domain is decomposed to the union of a continuum region (Ω_c) and QM (orbital-free DFT models) region (Ω_{qm}) .
2. In the continuum region Ω_c, use Cauchy-Born rule.

Two levels of Cauchy-Born rule:

- Cauchy-Born energy density
- Cauchy-Born electron density

$$I_A(\rho_{ns}, \Omega) = I(\rho_{\mathrm{CB}}, \Omega_s) + I(\rho_{ns}, \Omega_{ns}) + E_{int}(\rho).$$

$$I_B(\rho_{ns}, \Omega) = \int_{\Omega_s} W_{\mathrm{CB}}(\nabla u)\, \mathrm{d}x + I(\rho_{ns}, \Omega_{ns}) + E_{int}(\rho).$$

$$E_{int}(\rho) = \varepsilon \iint_{y(\Omega_s)\times y(\Omega_{ns})} \frac{(\rho_{\mathrm{CB}} - m)(y)(\rho_{ns} - m)(y')}{|y - y'|}\, \mathrm{d}y\, \mathrm{d}y'.$$

Lemma: (E and Lu, 2007) Assume that the displacement of the atoms is smooth, then

- For model A, the error for the force on atoms is $o(1)$.
- For model B, the error for the force on atoms is $O(1)$.

2. Linear scaling vs. sublinear scaling algorithms

Sublinear scaling algorithms usually rely on some results from asymptotic analysis.

Concluding remarks

- Understanding the fundamental numerical issues in multiscale methods is a rather challenging task. More efforts are needed to better understand microscopic models, such as electronic structure models, molecular dynamics and Monte Carlo methods.

- The basic purpose of multiscale modeling is to get rid of bad models. However, it is not a step forward to replace bad models by bad numerics.
- In the early days of numerical weather forcasting, Richardson made a lot of progress using an unstable numerical scheme, the Richardson scheme. But further progress was only possible after we understood basic issues about stability and accuracy of numerical methods.