User-GFMD: Greens Function Molecular Dynamics

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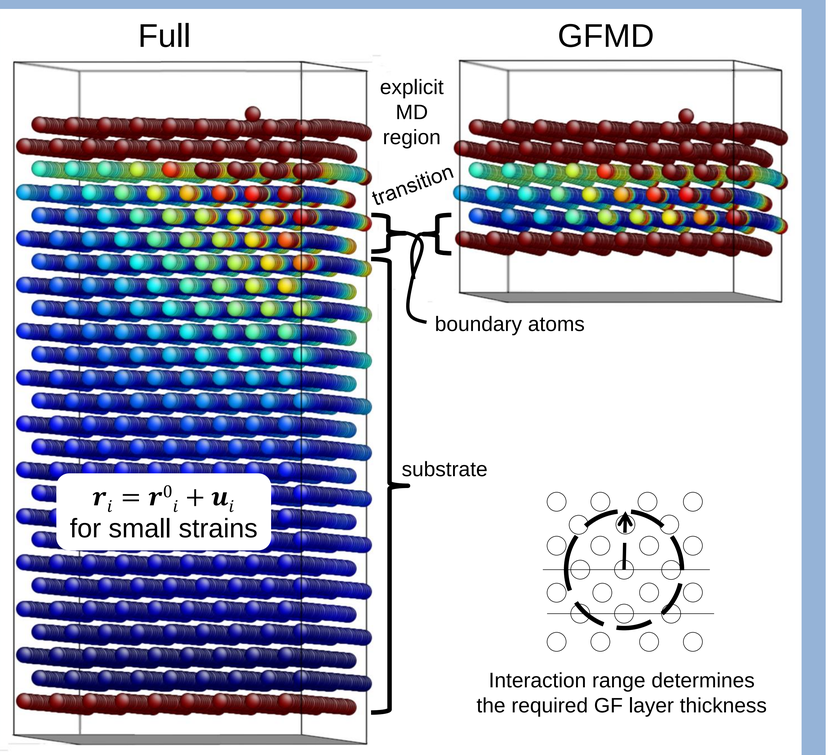
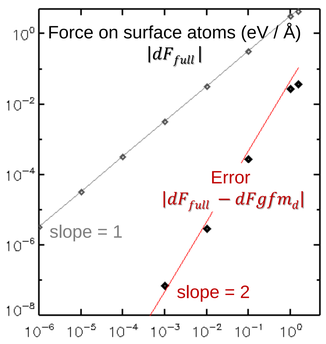
Accelerate MD by replacing part of crystalline substrate with its linear response



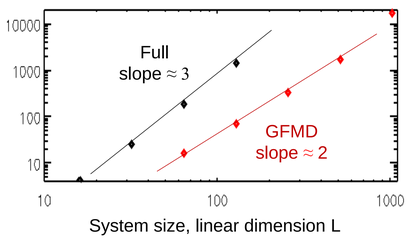
Interaction range determines the required GF layer thickness

$O(u^2)$ convergence



~O($N_{boundary}$) runtime

Processor-seconds *per MD step*



Also, smaller MD system → Convergence time decreased

Can be implemented on GPU

Method derivation

Break up Hamiltonian, Taylor expand in the lattice region

"Lattice region" will refer to the region of boundary + substrate atoms.
The Hamiltonian is

$$U = \underbrace{\frac{1}{2}\sum_{i=1}^{N_{explicit}}\sum_{j,k,\ldots=1}^{N} V(\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{r}_k\ldots)}_{U_{explicit}} + \underbrace{\frac{1}{2}\sum_{i=1}^{N_{lattice}}\sum_{j,k,\ldots=1}^{N} V(\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{r}_k\ldots)}_{U_{lattice}}$$

For small strains, expand about ideal lattice to approximate

$$U_{lattice} \approx U_0 - \sum_{i=1}^{N}\boldsymbol{f}_i\boldsymbol{u}_i + \frac{1}{2}\sum_{i,j=1}^{N}\boldsymbol{u}_i\boldsymbol{D}_{ij}\boldsymbol{u}_j$$

where $\boldsymbol{D}_{ij} = \boldsymbol{\nabla}_i\boldsymbol{\nabla}_j U_{lattice}$ and $\boldsymbol{f}_i = -\boldsymbol{\nabla}_i U_{lattice}$

Surface Greens function provides the forces on boundary atoms due to $U_{lattice}$

The total force on a boundary atom *i* has terms from both $U_{explicit}$ and $U_{lattice}$

$$f_i^{boundary} = fi^{exp} + fi^{lattice} = fi^{exp} + fi - \sum_j D_{ij}u_j$$

f_i is independent of displacements and can be precomputed. The last term can be written in Fourier space as $\tilde{f}_i(q) \equiv \widetilde{\boldsymbol{D}}_{\beta-\alpha}(\vec{q})\tilde{u}_{(q)}$

if atom *i* is in lattice layer α and *j* in layer β. The intra-plane Fourier transform is defined for atom *j* in layer α as

$$\widetilde{\boldsymbol{D}}_{\beta-\alpha}(\vec{q}) = \sum_{k \text{ in layer } \beta}\boldsymbol{D}_{jk}e^{-i\vec{q}\cdot(\overrightarrow{\boldsymbol{R}_{j0}}-\overrightarrow{\boldsymbol{R}_{k0}})}$$

Since the equation of motion is linear in lattice atom displacements, this force can be found from the problem's Greens function $\widetilde{\Phi}_{ij}$

$$\tilde{f}_i(q) = \widetilde{\Phi}_{ij}(q)\tilde{u}(q)$$

The transform of *u*, the 3x3 multiplication for each q, and the inverse transform of $\tilde{f}$ occur in each time step, running in O($N_{boundary}$ ln $N_{boundary}$)

Pre-computing the surface Greens function; procedure integrates out quadratic degrees of freedom

$\widetilde{\Phi}_{ij}$ can be rapidly computed in time O(L^2 lnL). It is given for example by this continued fraction relation, iterated for each lattice layer.

$$\widetilde{\Phi}_{ij} = U_0 - V\cfrac{1}{U - V\cfrac{1}{U - V\cfrac{1}{\ddots + V} + V} + V}V +$$

where U and V are given by $\widetilde{D}_{\alpha-\beta} = \begin{cases} U_0 \text{ if } \alpha=\beta=0 \\ U \text{ if } \alpha=\beta\neq 0 \\ V \text{ if } \alpha-\beta=1 \end{cases}$

Implementation

atom_style gfmd
: stores boundary atoms' equilibrium lattice positions
Geometry file: id type x y z i j k x0 y0 z0

fix_gfmd
: applies restoring force towards equilibrium configuration
fix myfix gfmdgroup FCC100 static ${spring1} ${spring2}

patch pair_eam.cpp
: prevents application of forces from original $U_{lattice}$ term

Interaction range implemented (nn = "nearest neighbors"):

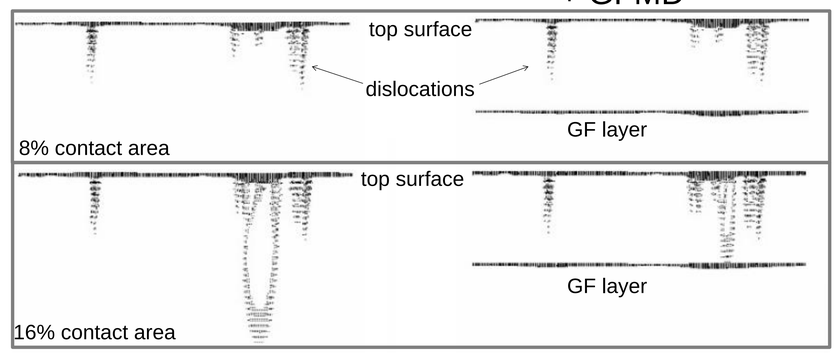
	Pair potentials	EAM	Stillinger-Weber
FCC 100	Up to 3rd nn	Up to 3rd nn	
Diamond 100			1st nn

Bottom boundary rigid or free
Also isotropic linear elasticity, laterally periodic or free
Statics and zero temperature
Single underlying Hamiltonian → No ghost forces

Example application

Lattice dislocations, nucleated by pressure at the top surface, are captured nicely above the GF layer

Full — 16 lattice planes (MD) + GFMD



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