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An improved version of the Green's function molecular dynamics method ☆,☆☆

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ABSTRACT

This work presents an improved version of the Green's function molecular dynamics method (Kong et al., 2009; Campañá and Müser, 2004 [1,2]), which enables one to study the elastic response of a three-dimensional solid to an external stress field by taking into consideration only atoms near the surface. In the previous implementation, the effective elastic coefficients measured at the Γ-point were altered to reduce finite size effects: their eigenvalues corresponding to the acoustic modes were set to zero. This scheme was found to work well for simple Bravais lattices as long as only atoms within the last layer were treated as Green's function atoms. However, it failed to function as expected in all other cases. It turns out that a violation of the acoustic sum rule for the effective elastic coefficients at Γ (Kong, 2010 [3]) was responsible for this behavior. In the new version, the acoustic sum rule is enforced by adopting an iterative procedure, which is found to be physically more meaningful than the previous one. In addition, the new algorithm allows one to treat lattices with bases and the Green's function slab is no longer confined to one layer.

New version program summary

Program title: FixGFC/FixGFMD v1.12
Catalogue identifier: AECW_v1_1
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AECW_v1_1.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 206 436
No. of bytes in distributed program, including test data, etc.: 4 314 850
Distribution format: tar.gz
Programming language: C++
Computer: All
Operating system: Linux
Has the code been vectorized or parallelized?: Yes. Code has been parallelized using MPI directives.
RAM: Depends on the problem
Classification: 7.7
External routines: LAMMPS (http://lammps.sandia.gov/), MPI (http://www.mcs.anl.gov/research/projects/mpi/), FFT (http://www.fftw.org/)
Catalogue identifier of previous version: AECW_v1_0
Journal reference of previous version: Comput. Phys. Comm. 180 (2009) 1004
Does the new version supersede the previous version?: Yes
Nature of problem: Green's function molecular dynamics (GFMD) is a coarse-graining method that enables one to investigate the full elastic response of an interface between a semi-infinite solid and a contact while taking only the surface atoms in the solid into consideration. The effect of long-range elastic deformations on the surface atoms from the semi-infinite solid is replaced by effective elastic interactions, thus reducing the problem from three dimensions to two dimensions without compromising the physical essence of the problem.

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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Solution method: See "Nature of problem".

Reasons for new version: The basic theory underlying the new version is essentially the same as the previous one, while the special treatment to reduce the finite size effect on effective elastic coefficients at the Γ-point is now realized in a physically meaningful manner. Finite size effects are an important issue in molecular dynamics simulations, particularly for GFMD, they result in a violation of the acoustic sum rule (ASR) for the effective elastic coefficients measured at the Γ-point (Φ^{Γ}). In the previous implementation, the effective elastic coefficients measured at the Γ-point were altered by setting their eigenvalues corresponding to the acoustic modes to zero. This scheme was found to work well for simple Bravais lattices as long as only atoms within the last layer were treated as Green's function atoms. However, it failed to function as expected in all other cases. We therefore adopt a new algorithm to enforce the ASR for Φ^{Γ} (Kong, 2010 [3]) which is implemented in this revision.

Summary of revisions: Assuming the lattice under study consists of surface unit cells with n basis atoms labeled by $k = 1, 2, \ldots, n$. When all atoms in the lattice are moved by the same amount, i.e., the crystal is rigidly translated, the force on any atom must be zero. This is known as the translational invariance, leading to the so-called acoustic sum rule: $\sum_{k'} \Phi_{k\alpha,k'\beta}(\Gamma) = 0$ where $\Phi_{k\alpha,k'\beta}(\Gamma)$ is the $k\alpha, k'\beta$ component of the effective elastic coefficients at the Γ-point; we will denote it as Φ^{Γ} hereafter. α and β enumerate the Cartesian directions. In addition, Φ^{Γ} should be Hermitian (or symmetric, since at the Γ-point, the imaginary part of Φ^{Γ} is zero.) because of the commutative nature of the force constants: $\Phi^{\Gamma}_{k\alpha,k'\beta} = \Phi^{\Gamma}_{k'\beta,k\alpha}$. These two properties are expected for Φ^{Γ}, yet the ASR is not satisfied during the measurement (done by FixGFC) because of the finite size effect. A scheme is therefore needed to enforce ASR on Φ^{Γ} afterwards, while the symmetric nature of Φ^{Γ} should be retained.

We list below the detailed scheme adopted to enforce ASR implemented in the improved version of GFMD together with some other revisions to the code after the previous release.

1. In FixGFMD, the previously employed method to rescale the effective elastic coefficients at Γ is obsoleted. Instead, an iterative procedure is adopted to enforce the acoustic sum rule on Φ^{Γ} (Kong, 2010 [3]).
   (i) $\sum_{k'} \Phi_{k\alpha,k'\beta} = 0$ is enforced by subtracting each element involved by a constant term; this procedure removes the violation of the acoustic sum rule, while in turn, usually destroys the symmetry of the force constant matrix.
   (ii) Symmetry is restored by replacing $\Phi_{k\alpha,k'\beta}$ and $\Phi_{k'\beta,k\alpha}$ with their average value; this will ensure the symmetry of the matrix, however, it will break the acoustic sum rule slightly.
   (iii) The above steps are repeated for several iterations, followed by a "symmetric ASR": similar to step (i), $\sum_{k'} \Phi_{k\alpha,k'\beta} = 0$ is enforced but only elements with $k' \geqslant k$ are subtracted by a constant value, while setting $\Phi_{k'\beta,k\alpha} = \Phi_{k\alpha,k'\beta}$.
2. In FixGFC, the surface lattice vectors and the relative positions of each atom in the surface unit cell are also computed and written to the binary file, which can be used in FixGFMD to set the equilibrium positions in the Green's function slab based on their lattice indices.
3. In FixGFMD, it is now possible to output the total forces applied on atoms in the Green's function slab before applying the elastic forces as a thermal quantity for LAMMPS (http://lammps.sandia.gov [6]). It is also possible to reset these forces to zero before applying the elastic forces.
4. In both FixGFC and FixGFMD, the dependence on MPI-enabled FFTW 2.1.5 was lifted. The Fourier transformations are now accomplished by calling the FFT3d wrapper from standard package "kspace" of LAMMPS (Plimpton, 1995; Plimpton et al., 1997; http://lammps.sandia.gov [4,5,6]).

Restrictions: By adopting the new method to enforce the acoustic sum rule, the restriction that atoms in the Green's function slab must be in the same layer is lifted, while it is still necessary to ensure that the mean equilibrium positions of atoms in the Green's function slab satisfy the Born–von Karman boundary condition. In addition, only deformations within the harmonic regime are expected in the slab during Green's function molecular dynamics simulations.

Additional comments: The new version is not compatible with the previous one: the contents in the binary file are different and therefore the effective elastic coefficients measured by the previous version of FixGFC cannot be used by the current version of FixGFMD.

Running time: FixGFC varies from minutes to days, like a typical molecular dynamics simulation, depending on the system size, the number of processors used, and the complexity of the force field. FixGFMD varies from seconds to hours, depending on the system size and the number of processors used.

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