Implementation of THB1 potential library with core-shell approximation - Srinivasan Mahendran

Aim

To model dislocations in forsterite with computational efficiency, THB1 is an empirical potential developed to model forsterite and its high-pressure polymorphs (Price and Parker 1987) is chosen. As a part of my PhD thesis I have implemented this THB1 potential library to Large-scale Atomic/Molecular Massively Parallel simulator (LAMMPS) open source code. The analytical expressions of force field implemented to the code and algorithm are as follows.

Analytical forces

THB1 potential contains an electrostatic term (Wolf Summation – Wolf et al. 1999), a short range Buckingham term, a harmonic spring term and a three body term. Analytical expressions from first derivative of aforementioned energy terms are as follows

Coulombic – Wolf summation term

$$f_{Coulomb\,\alpha} = \sum_{\substack{j\neq i \\ (r_{ij}<R_c)}} q_i q_j \left\{ \begin{array}{c} \left(\frac{erfc(\alpha R_c)}{r_{ij}^2} + \frac{2\alpha}{\pi^{1/2}}\frac{exp\left(-\alpha^2 r_{ij}^2\right)}{r_{ij}}\right)\times\frac{r_{ij\alpha}}{r_{ij}} \\ -\left(\frac{erfc(\alpha R_c)}{R_c^2} + \frac{2\alpha}{\pi^{1/2}}\frac{exp(-\alpha^2 R_c^2)}{R_c}\right)\times\frac{r_{ij\alpha}}{R_c}\Big|_{r_{ij}=R_c} \end{array} \right\} \quad (1)$$

Short range Buckingham term

$$f_{Short\,\alpha} = \left(-6C_{ij}r_{ij}^{-6} + \frac{A_{ij}}{B_{ij}}exp\left(-\frac{r_{ij}}{B_{ij}}\right)\times r_{ij}\right)\times\frac{r_{ij\alpha}}{r_{ij}^2}\,, r_{ij} < R_B \quad (2)$$

Harmonic spring term

$$f_{spring\,\alpha} = -\left(K_1 + \frac{K_2 r_i^2}{6}\right)r_{i\alpha}\,, r_i < R_{spring} \quad (3)$$

Three body term

$$f_{THB\,i\alpha} = -f_{THB\,j\alpha} - f_{THB\,k\alpha} \quad (4)$$

$$f_{THB\,j\alpha} = A_{11}r_{ij\alpha} + A_{12}r_{ik\alpha} \quad (5)$$

$$f_{THB\,k\alpha} = A_{22}r_{ik\alpha} + A_{12}r_{ij\alpha} \quad (6)$$

Where,

$$\Delta\theta = \left(\theta_{ijk} - \theta_0\right) \quad (7)$$

$$A = -2\,\Delta\theta\sin\theta_{ijk} \quad (8)$$

$$A_{11} = \frac{A\cos\theta_{ijk}}{r_{ij}^2} \quad (9)$$

$$A_{12} = \frac{A}{\left(r_{ij}\times r_{ik}\right)} \quad (10)$$

$$A_{22} = \frac{A\cos\theta_{ijk}}{r_{ik}^2} \quad (11)$$

References

- Price G D and Parker S C 1987 The Lattice Dynamics of Forsterite *Mineralogical Magazine* **51** 157–170
- Wolf D, Keblinski P, Phillpot S R and Eggebrecht J 1999 Exact method for the simulation of Coulombic systems by spherically truncated, pairwise r^{-1} summation *The Journal of Chemical Physics* **110** 8254

Algorithm

Step:

1. Start

2. Collect data about atomic positions from main program

3. Read data about parameters and cut-off for potential library

4. Start energy and force computation nested loop

4.1. Set i < Number of atoms

4.1.1. Calculate self-energy of ion

4.2. Set j < Number of atoms where j != i (For loop)

4.2.1. Calculate distance R_ij between i and j

4.2.2. If R_ij < Cut off for spring term

4.2.2.1. Compute Energy and force from spring term

4.2.3. Else,

4.2.3.1. If Rij < Coulombic term cut-off distance

4.2.3.2. Compute Coulombic Wolf summation energy and force, End If

4.2.3.3. If Rij < Short range Buckingham tem cut-off distance

4.2.3.4. Compute Buckingham term energy and force, End If

4.2.4. End If

4.3. End the j loop of two-body term

4.4. Commence the three-body term calculation

4.4.1. Set jj < Number of atoms where jj != i

4.4.1.1. Calculate distance R_THB_ij between i and jj

4.4.1.2. If R_THB_ij > three body cut-off, skip particle

4.4.1.3. Else, set kk < Number of atoms where k != i && k != j

4.4.1.3.1. Compute distance R_THB_ik between i and kk

4.4.1.3.2. If R_THB_ik < three body cut-off, compute three body term energy and force

4.5. Update force and energy

5. Stop module.

Solution:

LAMMPS has different modules to do specific tasks, in which *Pair Style* represents a set of potential libraries. THB1 potential library has been implemented to this module. The implemented files lie in *src* folder with name *pair_core_shell.cpp* and *pair_core_shell.h*.

To compile the code

```
$ cd lammps-core_shell/src/STUBS        # Clean object files
$ make clean
$ cd lammps-core_shell/src/
$ make clean-all

$ cd STUBS/
$ make
$ cd ../src/
$ make serial                           # To compile the code in serial
```

To run the code, an example to perform minimization of a unit cell using conjugate gradient minimizer is given in *sample* folder in *lammps-core_shell* directory. To run the example,

```
$ cd lammps-core_shell/sample/minimize/

$ ../.. /src/lmp_serial < initial.in
```