ReadMe

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About this project

This project is dedicated for Undergraduate Computational Physics Course at Tsinghua, University, lectured by Prof. Wu Jian and assisted by Ph.D student Li Yang.

Based on MATLAB, we developed a Molecular Dynamics program for basic simulations.

The algorithm we adopted included Verlet algorithm and two multistep algorithm including Predictor-Corrector-4 and Predictor-Corrector-6 algorithm. Compared to Verlet, the multistep methods approximately takes double time and memory. Usage of particular algorithm may be specified first several lines in MDmain.m.

In MDmain.m, we incorporated two-body potentials including Lennard-Jones potential and Morse potential, whose parameters may be read from external files. Other two-body potentials can be easily added to the progamme. Three-body potentials, however, need a modification in general stucture to be incorporated.

MDmain.m also includes a visual output module visualising motion of particles. For efficiency concern, it's recommended to shut this module in most cases.

Our program performs simulations for a system of 1000 atoms for approximately 10 time steps per second on a personal computer, or 100 atoms for 200 time steps per second. Efficiency may be increased with furthur optimization.

Since this program is dedicated for a course in a Chinese University, most code comments as well as a former course report are in Chinese. The

course report also include a variable table for the convenience of further development.

Other programs

Apart from MDmain.m, we also posted a MATLAB and a Python program for specific applications. Detailed information may be found in our course report in Chinese. In brief, the MATLAB project simulated a graphene being deformed by external force. The Python project incorporated a many-body effect which added penalty to twisted bond angle of graphene.