Programming of a simple molecular dynamic simulation using open source software

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Molecular Dynamics (MD) simulation is a technique for computing equilibrium and dynamic properties of a classical many-body system. The key ingredients in carrying out a MD simulation are the potentials used to model intermolecular interactions, the integration algorithms and the periodic boundary conditions (PBC) to conserve the total energy of the system.

Researchers generally use expensive software packages to run model simulations and therefore, face many limitations when further improvements and expansions are required. Open source software provides much more freedom and more expansion capabilities in programming. Thus, in this research project a simple MD simulation model was developed using java 6.0 programming language and equilibrium of a real gas under Lennard-Jones(LJ) potential with periodic boundary conditions was studied using the simulation programme.

Only small systems and relatively short run times for MD simulation were considered here as a first step and some qualitative properties of simple macroscopic systems are studied. Finding optimum time step (Δt) for the simulation is very important in order to reach equilibrium conditions and thus, Δt was found to be 0.015 for the model studied in here. The total energy of the system was conserved with a remarkable accuracy, up to about 1%.Verlet algorithm was tested and ΔE_{max} showed a variation of approximately $(\Delta t)^2$. as

expected. The total energy E was found to be a monotonically increasing function of T. Energy was computed for LJ solids having square and triangular lattice structures. Triangular lattice exhibited lower energy.

Further modifications, improvements and expansions of the MD simulation programme to handle more complex systems are feasible without much difficulty.

Key words: *Lennard-Jones(LJ) potential. Molecular Dynamics, Periodic boundary conditions*