Abstract

Molecular Dynamics (MD) is a numerical simulation of the time evolution of interacting particles. In the process of defining particles position/movement, this simulation uses the information of the velocity and the acceleration from the previous time step. These is the problem of 1st order ordinary differential equation (ODE 1), therefore this method will require the numerical integration technique to define current position from the information of velocity and acceleration from the past. In recent works, most of the MD simulation is performed by employing Velocity Verlet method in serial fashion. The problem occurs when we simulate large number of particles, the simulation require very long computation time. To address this problem we tried to implement 4th order Runge Kutta method in the simulation, furthermore in addition to that we perform the calculation of acceleration in parallel by employing *Compute Unified Device Architecture* (CUDA) programming scheme. This scenario prove significant improvement in respect to the simulation time. We able to obtain 3 times speedup in the implementation of Velocity Verlet method, and 2.9 times speedup in the Runge-Kutta method implementation, all of this benchmark is performed with employing the parallel acceleration calculation with respect to serial ones.