The code implements the parallel algorithm of molecular dynamics using mpi, and the efficiency of which has been compared with the sequential program. The simulation has been done using 8 atoms and 4 processors. Since the problem size is small, the computation:communication ratio is also small in magnitude. Therefore, the parallel version of the program spent most of the time on communication which makes the paralleled implementation much slower than sequential version.

To compile the code:
type make in linux terminal, make sure the mpicc compiler has been properly installed

To run the code:
type mpirun -np 4 ./molecule.x

Output example:

pass: 0 process ID: 1 Eproc: 2.23607 guest atoms: 2 3
pass: 0 process ID: 3 Eproc: 3.60555 guest atoms: 6 7
pass: 1 process ID: 3 Eproc: 16.8652 guest atoms: 4 5
pass: 0 process ID: 0 Eproc: 1 guest atoms: 0 1
pass: 1 process ID: 0 Eproc: 11.5694 guest atoms: 6 7
pass: 0 process ID: 2 Eproc: 3 guest atoms: 4 5
pass: 1 process ID: 2 Eproc: 13.5694 guest atoms: 2 3
pass: 2 process ID: 2 Eproc: 13.5694 guest atoms: 0 1
pass: 1 process ID: 1 Eproc: 9.11438 guest atoms: 0 1
pass: 2 process ID: 1 Eproc: 21.1051 guest atoms: 6 7
pass: 2 process ID: 3 Eproc: 16.8652 guest atoms: 2 3
pass: 2 process ID: 0 Eproc: 20.491 guest atoms: 4 5
Energy calculated by parallel programming is: 72.0307
time elapsed: 0.000239
Energy calculated by sequential program is: 72.0307
time elapsed: 1.00001e-06