

PROJECT PROPOSAL FOR COMPUTATIONAL PHYSICS COURSE

RAJDEEP.MOHAN.CHATTERJEE

February 21, 2010

I propose to do a project on classical molecular dynamics the details of which are as follows:

Consider N particles confined in an insulated cubical box, interacting with the well known Lennard-Jones potential and study the evolution of this system. One expects the Energy of the system to be conserved. This would serve as a test on the stability of the algorithm used to solve the resulting equations of motion.

I have divided the project into the following sub-parts that I would like to implement/study:

- Use different algorithms to implement the time evolution of the system and compare them for stability of the result, and the complexity in terms of the number of basic operations per iteration. I would like to study the effects of two different boundary conditions. First the periodic boundaries, and then impermeable boundaries that scatter the particles elastically. Also study the effect of changing the power law dependence of the interacting potential.
- Try and maximize N (provided all the particles fit in the box) and check whether the result seems reasonable for the given computer hardware. Check to what extent the algorithms respect the time reversal symmetry of the equations of motion.
- Check for a given initial condition how long the system takes to equilibrate. Then at equilibrium whether the various thermodynamic parameters reach their expected theoretical values. Also see whether there exists a relation between the initial average kinetic energy per particle(due to initial conditions) and the final equilibrated value.
- Carry out the same procedure for the system now in contact with a heat bath.
- If time permits I would also study the effect of the earth's gravitational potential on such a system changing the box dimension and boundary condition in the vertical direction suitably to see if the result corresponds to that given by the barometric equations.