PROJECT PROPOSAL FOR COMPUTATIONAL PHYSICS COURSE

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I propose to study the implementation of the time evolution of a system of N particles in contact with a heat bath.

1 DESCRIPTION OF THE PROBLEM:

- particles are contained in a cubical box of some length L which is kept in contact with a heat bath at some temperature T.
- The box has periodic boundary conditions.
- The particles interact pairwise with the Lennard-Jones potential(and also with the heat bath).
- Initially the particles will be allotted random positions inside the box and random velocities.

2 ALGORITHMS TO BE STUDIED AND IMPLEMENTED:

There are two parts to this:

2.0.1 :- Implement the time evolution of the system:

- Study how to implement the time evolution of the above system by solving the Newton's equations of motion for each of the particles subject to the above boundary condition.
- This will be done using the velocity verlet algorithm.
- The specific study would be to determine the equilibration time as a function of T.
- The interaction with the heat bath will be done using the Andersen Thermostat method.

2.0.2 :- Implement random number generators relevant to the problem:

- Implement a uniform deviates random number generator. This will be used to assign the initial conditions to the system and also to pick the particles that we consider to be interacting with the heat bath at a given time step. I will use an algorithm that implements the Minimal Standard Random Number Generator for this purpose.
- The particles that interact with the heat bath are assigned velocities drawn from the Maxwell-Boltzmann distribution at T. Thus I will convert the uniform deviates random number into one that follows the above distribution using the Box-Muller method.