# "Molecular Dynamic simulations of the atoms of a Noble gas using the Lennard-Jones potential"

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## Abstract

We use molecular simulations to reduce the cost of experiment and search space. Through it, we can select the best result from simulations and do experiment with the selected parameters. In Molecular Dynamic (MD), you start with a given number of atoms and you want to be able to simulate to predict how these atoms will be moving according to time. The result is a trajectory of all particles in the system as a function of time. Time averages and other properties can be calculated. Parallelizing MD code is important, because MD simulation is very time-consuming and expensive. The main reason for that is you should calculate all forces between all atoms of the system. For large number of atoms it might be impractical. The goal of this project is to run MD simulations with large number of atoms using parallel version of force field function. We first make sure that the parallel code generates the same force values, and then we compare its performance to the serial code. At the end we will make the trajectory of the simulation.

To implement the MD method, what we need is the initial positions and initial velocity of the atoms. So, this depends potentially on the temperature. The second key ingredient we need is the interatomic energy function. Eq. (1) is an expression for the total energy of the system.

$$E_{total} = E_{bond} + E_{angle} + E_{dihedral} + E_{electrostatic} + E_{van\ der\ Waals} \quad \textbf{Eq. (1)}$$

The first three terms of Eq. (1) are assigned to covalent bonds and the rest are related to noncovalent bonds. In this simulation, because we suppose that the atoms are for a Noble gas, there is no bond between atoms. So, all the covalent bonds terms will be zero. Another assumption of our system is that the atoms are electronically neutral. Therefore, the electrostatic energy will be zero too. Our simplified energy equation is shown in Eq. (2), which is also called Lennard-Jones potential. where $r_{ij}$ is the distance between two interacting particles, $\varepsilon_{ij}$ is the depth of the potential well, and $r_m$ is the distance at which the particle-particle potential energy is zero.

$$E_{(R)} = \sum_{i<j}^{atoms} \varepsilon_{ij} \left[\left(\frac{r_m}{r_{ij}}\right)^{12} - 2\left(\frac{r_m}{r_{ij}}\right)^{6}\right] \quad \textbf{Eq. (2)}$$

The question is that if we know the energies between atoms, how can we determine the motions, or trajectories of the atoms. The forces on each atom are given by the gradient of the energy function with respect to the atomic positions. For instance, the force on particle 0 in x direction can be calculated using Eq.(3):

$$F_{x0} = -\frac{\partial E}{\partial x_0} = -\frac{\partial}{\partial x_0}\left[\sum_{i=i}^{n-1}\sum_{j=i+1}^{n}\left[\left(\frac{r_m}{r_{ij}}\right)^{12} - 2\left(\frac{r_m}{r_{ij}}\right)^{6}\right]\right] = -\sum_{j=0}^{atoms}\frac{\partial}{\partial r_{0j}}\left[\left[\left(\frac{r_m}{r_{ij}}\right)^{12} - 2\left(\frac{r_m}{r_{ij}}\right)^{6}\right]\right]\frac{\partial r_{0j}}{\partial x_0} \quad \textbf{Eq. (3)}$$

A brief procedure of updating atom positions is shown in Fig. (1).

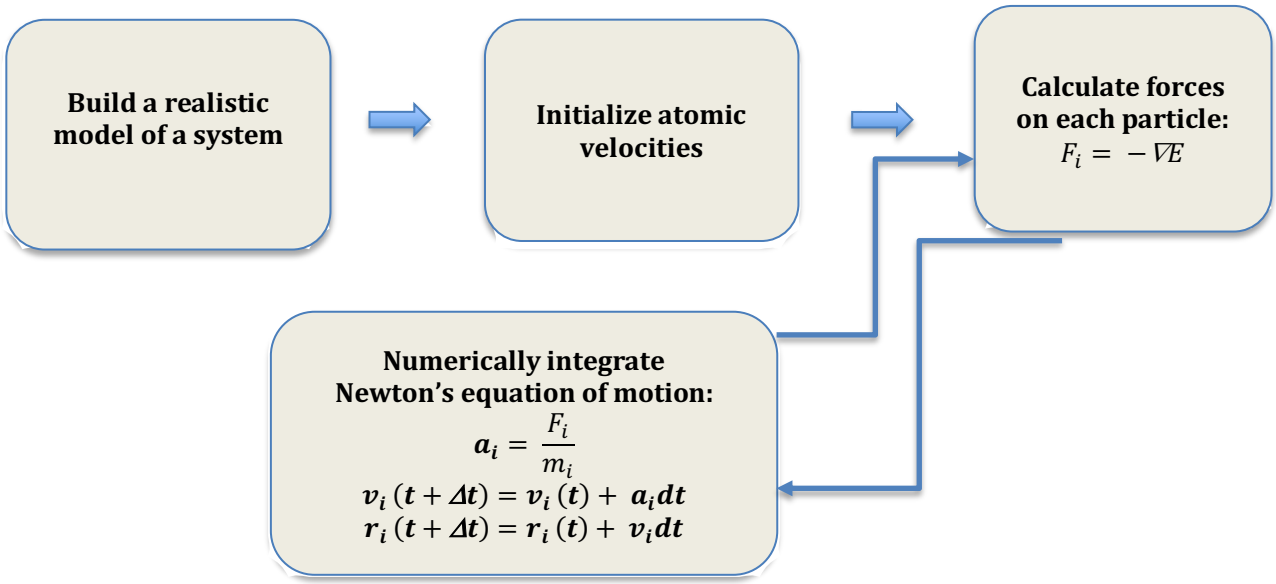


**Fig. (1)** Procedures of a Molecular Dynamic simulation

## Tools

The critical part of the code that parallelization can help the speed of running the simulation, is calculating forces on each particle. The point is that we probably cannot have parallel computing for each individual atom. Because for each atom the calculation of each iteration is dependent on the previous iteration result. In fact, to obtain the current position and velocity of each atom, the previous values are needed. However, we can do the calculation of force for the whole systems in parallel. One important point that we should take it into consideration is that for moving to the next time step, the calculations for all atoms at the previous steps should be done. So, two probable ways to do that are using "mutex" and "lock_gurad" or using "OpenMP" tools.

## Data Set

In this project we do not use real experimental data. Our data is generated using random generator function (mt19937 gen(rd())).

## Success

The goal of paralleling this MD simulation is reducing the run time of serialized version. Another goal may be optimizing the number of threads.

## References

- Eijkhout, Victor. "*Introduction to high performance scientific computing*", (2010).

-Andrew, R. Leach. "Molecular modeling principles and applications." *Prentice Hall, London* (2001).

- https://www.openmp.org/resources/refguides/

- https://en.wikipedia.org/wiki/Lennard-Jones_potential