



JOINT INSTITUTE FOR NUCLEAR RESEARCH

FINAL REPORT ON

MOLECULAR DYNAMICS SIMULATION RESEARCH (FROM ATOMIC FRAGMENTS TO MOLECULAR COMPOUND)

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ABSTRACT

MD (Molecular dynamics) simulation is very useful method to held physics experiments. It is inexpensive, also you may see a lot combinations of the experiments. As well as it can measure many parameters of the experiments and it is time-saving method. Nowadays MD simulation is method which be between theory and experiment. In this report, MD simulation is discussed. There are discussion of equations , force fields , numerical calculation in the report. Nowadays, there are a lot of MD simulation force fields such as GROMACS, CHARMM , DL_POLY , AMBER and others. In this Interest program, we studied DL_POLY and AMBER force fields.

Introduction

Molecular Dynamics (MD) simulation is a computational technique used to study the dynamic behavior of molecules and materials at the atomic and molecular levels. By numerically solving Newton's equations of motion, MD simulations provide insights into the motion, interactions, and thermodynamics of systems over time. This powerful tool has applications in various fields, including chemistry, biochemistry, physics, and materials science, enabling researchers to explore complex phenomena and gain a deeper understanding of molecular behavior.

In MD simulations, atoms and molecules are represented as particles with defined masses and forces. The system's evolution is tracked over time, allowing researchers to observe how the positions and velocities of these particles change. This approach provides a dynamic perspective on phenomena such as protein folding, chemical reactions, and material properties.

Key components of an MD simulation include the force field, which describes the potential energy surface governing interactions between particles, and the integration algorithm, used to numerically solve equations of motion. Simulations can range from nanoseconds to microseconds, offering a glimpse into processes occurring at different timescales. (Fig1)

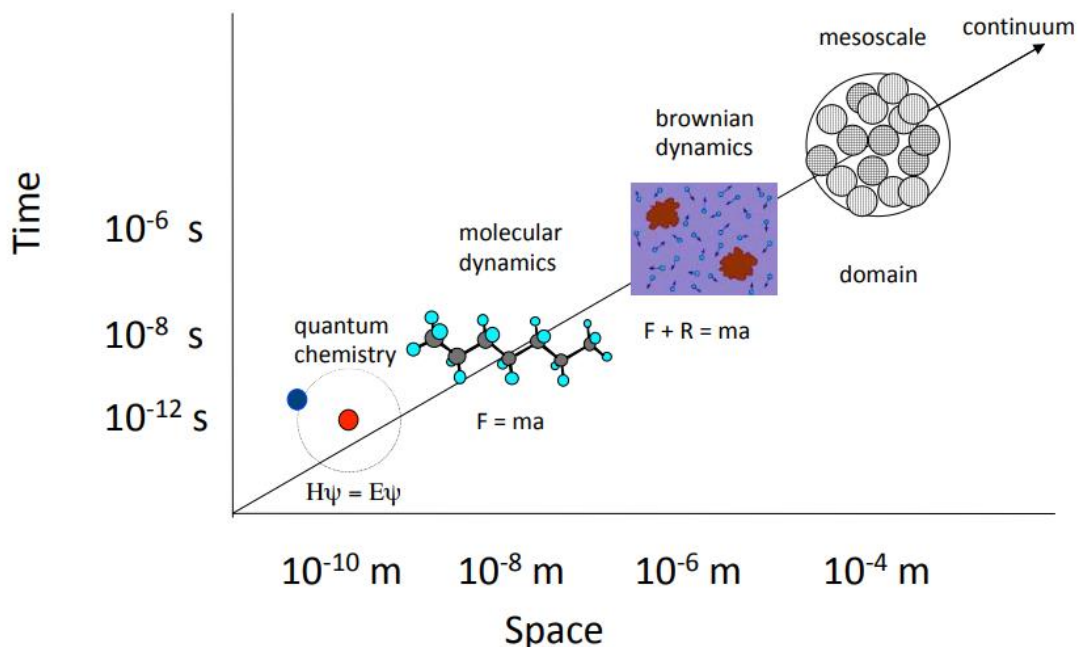


Figure 1. The figure shows the size of the system and the time of occurrence of the processes in it.

MD simulations contribute valuable data for validating experimental results, predicting molecular behavior under various conditions, and designing new drugs

or materials. As computational power continues to advance, MD simulations become increasingly sophisticated, playing a pivotal role in advancing our understanding of molecular dynamics and contributing to scientific discoveries. Additionally, MD simulations provide a way to explore molecular systems that may be challenging or impractical to study experimentally. The method allows researchers to investigate the effects of temperature, pressure, and other environmental factors on molecular structures and behaviors.

One notable aspect of MD simulations is their ability to capture the stochastic nature of molecular motion, revealing intricate details about fluctuations, conformational changes, and transitional states. This level of detail is often difficult to achieve solely through experimental methods. MD simulations have become integral in fields like drug discovery, where understanding the dynamics of biomolecular interactions is crucial.

The Basic equations

MD simulations are based on Newton's laws as mentioned earlier.

$$m_1 \frac{dv_1}{dt} = F_1(r_1, r_2, \dots), \quad \frac{dr_1}{dt} = v_1$$

$$m_2 \frac{dv_2}{dt} = F_2(r_1, r_2, \dots), \quad \frac{dr_2}{dt} = v_2$$

.....

$$m_i \frac{dv_i}{dt} = F_i(r_1, r_2, \dots), \quad \frac{dr_i}{dt} = v_i$$

.....

Here, i is the sequence number of the molecule. r is the coordinate of the molecule. But you can see these equations are very a lot. And, we need to use numerical calculations for solving these. Firstly, we need to know field potential:

$$\vec{F}_i = -\vec{\nabla}U(\vec{R})$$

In the matter environment have many potentials. This field potential consists of the following components:

$$U(\mathbf{r}) = U_b + U_\theta + U_\varphi + U_\omega + U_{LJ} + U_{el} + U_{HB} + \dots$$

Here

Valence length potential:

$$U_b = \frac{1}{2} \sum_b K_b (r - b_0)^2$$

Valence angle potential:

$$U_{\theta} = \frac{1}{2} \sum_{\theta} K_{\theta} (\theta - \theta_0)^2$$

Torsion dihedral potential:

$$U_{\varphi} = \frac{1}{2} \sum_{\varphi} K_{\varphi} [\cos(n\varphi - \delta) + 1]$$

Lennar-Jones potential:

$$U_{LJ} = \sum_{i,j} \left[\frac{A}{r_{ij}^{12}} - \frac{B}{r_{ij}^6} \right]$$

Electrostatics potential:

$$U_{el} = \sum_{i,j} \frac{q_i q_j}{\epsilon r_{ij}}$$

Hydrogen bonding potential:

$$U_{HB} = \sum_{i,j} \left[\frac{A'}{r_{ij}^{12}} - \frac{B'}{r_{ij}^{10}} \right]$$

You can learn more about these potentials in the pictures below.

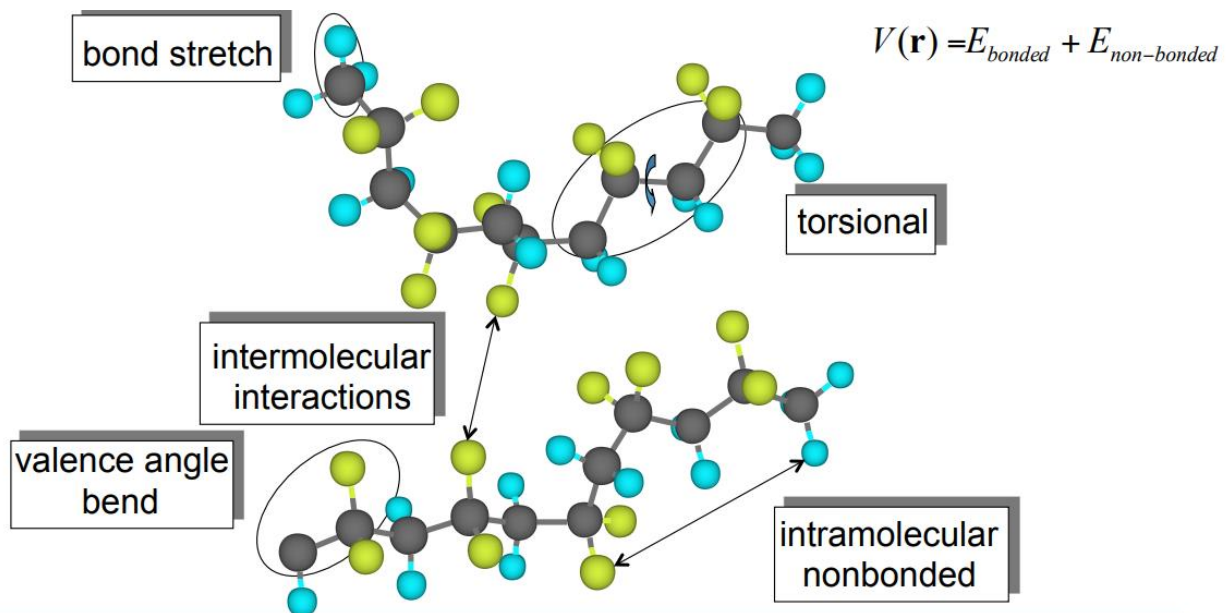
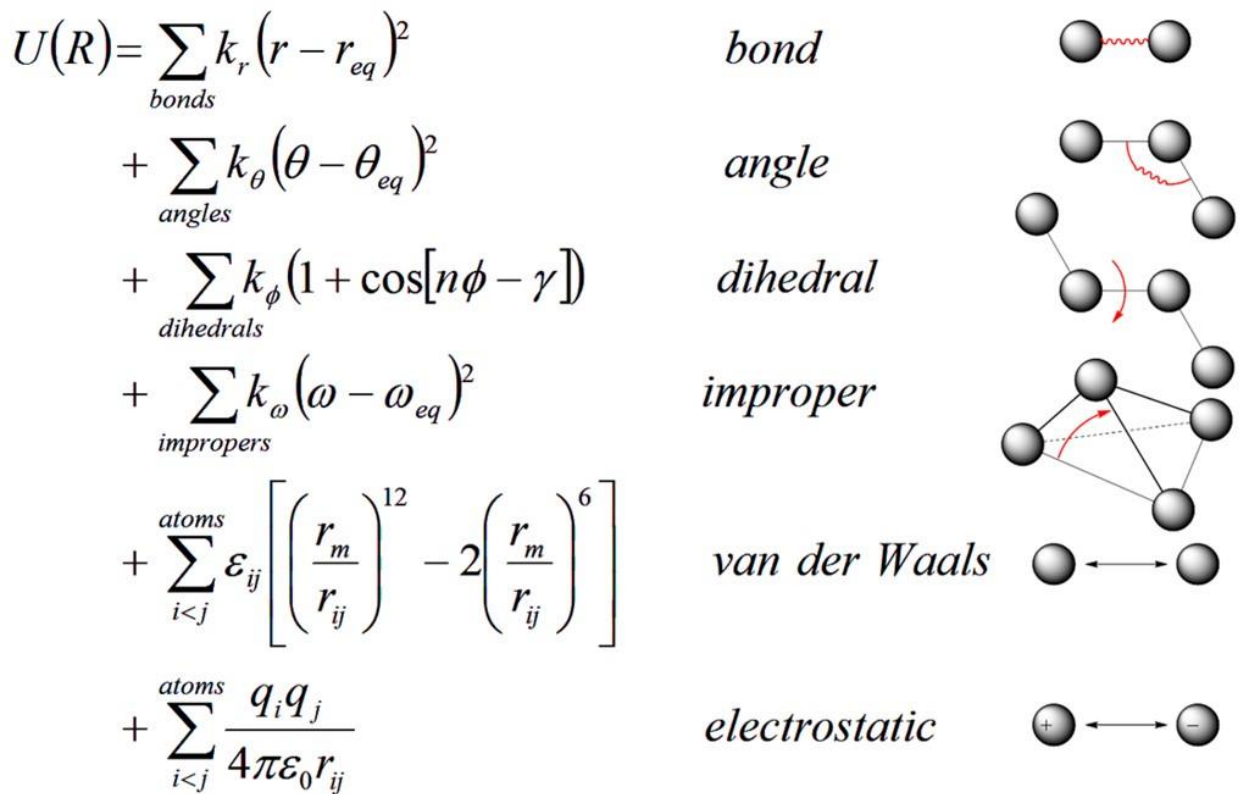


Figure 2. The pictures show that potentials and their location on the molecule.

Lennar Jones potential

The solid and liquid states of rare-gas elements Ne, Ar, Kr, Xe have closed-shell electron configurations. Thus, that molecules do not interact each other with covalent or metallic bonding. Nevertheless, they have a interaction via very weak van der Waals bonds which are perturbational in nature in these elements. Van der Waals forces arise from the fact that the centers of positive (nuclear) and negative (cloud of electrons) charges of an atom do not overlap. Under the influence of this force, the potential energy of the interaction between molecules or atoms is called the Lennar-Jones potential.

$$u_{LJ}(r) = \frac{A}{r^{12}} - \frac{B}{r^6} = 4\epsilon_{LJ} \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

The r^{-12} is used to approximate the strong Pauli repulsion that results from electron orbitals overlapping, while the r^{-6} term describes weaker attractive forces acting between local dynamically induced dipoles in the valence orbitals. While the attractive term is physically realistic (London dispersive forces have r^{-6} distance dependence), the repulsive term is a crude approximation of exponentially decaying repulsive interaction. The too steep repulsive part often leads to an overestimation of the pressure in the system.

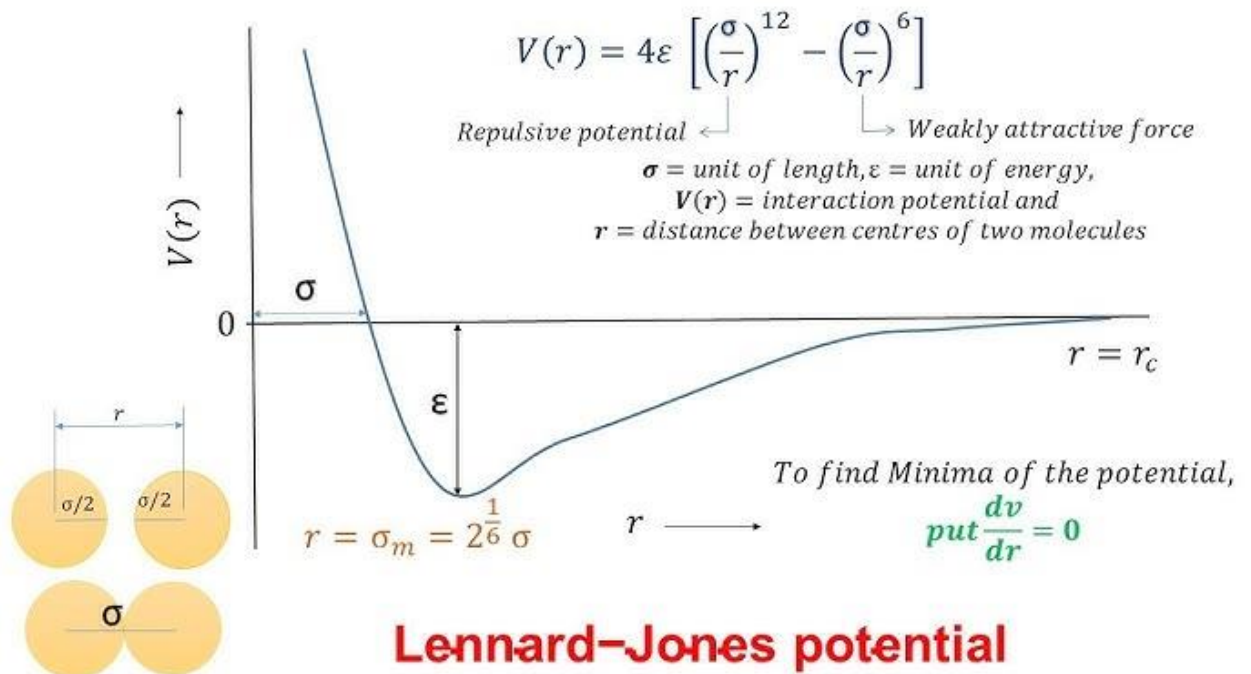


Figure 3. Lennar-Jones potential.

Species	ϵ/k_B (K)	σ (Å)
He	10.22	2.56
Ne	35.6	2.75
Ar	120	3.40
Kr	171	3.60
Xe	220	4.10
N ₂	95.5	3.74
CH ₄	148.4	3.81
CF ₄	151.4	4.75
H ₂	39.4	2.81
O ₂	118	3.58
CO	100	3.76
CO ₂	309	3.36
C ₂ H ₄	470	2.5
C ₂ H ₆	243	3.95
C ₃ H ₈	242	5.64
C(CH ₃) ₄	232	7.44
C ₆ H ₆	830	3.4
C ₆ H ₆ -CH ₄ O	1018.2	2.896
C ₆ H ₆ -C ₂ H ₆ O	553.5	4.651
C ₆ H ₆ -C ₃ H ₆ O	632.1	4.620
C ₆ H ₆ -C ₄ H ₁₀ O	1122.3	3.425

Figure 4. The table parameters of Lennar-Jones potential.

Numerical calculation

Molecular dynamics (MD) simulations involve the numerical calculation of the motion of atoms and molecules over time by solving Newton's equations of motion. This involves:

1. Calculating the forces acting on each atom or molecule based on their positions and interactions with other particles (e.g., using force fields or quantum mechanics methods).

2. Integrating the equations of motion to determine the new positions and velocities of the particles at each time step.

3. Updating the system energy, temperature, pressure, and other relevant properties based on the computed positions and velocities.

These numerical calculations are typically performed using specialized software packages that implement various algorithms, such as Verlet or Leapfrog integration, for efficient and accurate MD simulations. Let us consider Velet and Leapfrog algorithms.

Verlet algorithm:

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + \frac{1}{2} \mathbf{a}(t)\Delta t^2 + \dots$$

$$\mathbf{r}(t - \Delta t) = \mathbf{r}(t) - \mathbf{v}(t)\Delta t + \frac{1}{2} \mathbf{a}(t)\Delta t^2 + \dots$$

$$\mathbf{r}(t + \Delta t) + \mathbf{r}(t - \Delta t) = 2\mathbf{r}(t) + \mathbf{a}(t)\Delta t^2 + \dots$$

$$\mathbf{r}(t + \Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t - \Delta t) + \mathbf{a}(t)\Delta t^2 + \dots$$

$$\mathbf{v}(t) = \frac{\mathbf{r}(t + \Delta t) - \mathbf{r}(t - \Delta t)}{2\Delta t} + \dots$$

$$e(t) = \mathcal{O}(\Delta t^4)$$

$$E(t) = \mathcal{O}(\Delta t^3)$$

Leapfrog algorithm:

$$\begin{aligned}
 v_{i+1/2} &= v_i + a_i \frac{\Delta t}{2}, \\
 x_{i+1} &= x_i + v_{i+1/2} \Delta t, \\
 v_{i+1} &= v_{i+1/2} + a_{i+1} \frac{\Delta t}{2},
 \end{aligned}$$

This picture shows that both algorithms.

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Leapfrog Algorithm

- Eliminates addition of small numbers $O(\delta t^2)$ to differences in large ones $O(\delta t^0)$
- Algorithm

$$\begin{aligned}
 \mathbf{r}(t + \delta t) &= \mathbf{r}(t) + \mathbf{v}(t + \frac{1}{2} \delta t) \delta t \\
 \mathbf{v}(t + \frac{1}{2} \delta t) &= \mathbf{v}(t - \frac{1}{2} \delta t) + \frac{1}{m} \mathbf{F}(t) \delta t
 \end{aligned}$$
- Mathematically equivalent to Verlet algorithm

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) + \left[\mathbf{v}(t - \frac{1}{2} \delta t) + \frac{1}{m} \mathbf{F}(t) \delta t \right] \delta t$$

r(t) as evaluated from previous time step

$$\mathbf{r}(t) = \mathbf{r}(t - \delta t) + \mathbf{v}(t - \frac{1}{2} \delta t) \delta t$$

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) + \left[(\mathbf{r}(t) - \mathbf{r}(t - \delta t)) + \frac{1}{m} \mathbf{F}(t) \delta t^2 \right]$$

$$\mathbf{r}(t + \delta t) = 2\mathbf{r}(t) - \mathbf{r}(t - \delta t) + \frac{1}{m} \mathbf{F}(t) \delta t^2 \quad \text{original algorithm}$$

Figure 5. Verlet and Leapfrog algorithms.

Future Goals

I am senior student National university of Uzbekistan. I have several goals in the future. My study field include quantum physics and nuclear physics . I am going to learn thermonuclear reaction and controlled fusion. It is my field in the future. I am certain that it will be major future energy source.

Acknowledgement

First of all, I would like to thank my project supervisor Kholmurzo Kholmurodov who gave us his time and shared his knowledge. Through him , I learned a lot about molecular dynamics simulations. I would also like to thank the organizers of this project. I believe that such projects will help many students to find their academic career.

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