

JOINT INSTITUTE FOR NUCLEAR RESEARCH  
Frank Laboratory of Neutron Physics

## **FINAL REPORT**

### **MD-SIMULATION RESEARCH**

**(FROM ATOMIC FRAGMENTS TO MOLECULAR COMPOUND)**

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## 1 ABSTRACT

Molecular dynamics (MD) is another approach for the investigation of the atom location in space. In this approach, a single-point model is replaced by a dynamic model in which the nuclear system is forced into motion. The simulation of the motion is realized by the numerical solution of the classical Newtonian dynamic equations. The set of possible atom locations gives, for example, conformational ensemble profile for a given molecule. MD can also provide information on thermodynamic and dynamic properties of the molecules.

Molecular dynamics (MD) simulation is becoming an invaluable tool for studying biomolecular structure and dynamics, the relationship between which is central to understanding important cellular processes.

During the course, we covered the following areas:

- 1: The basic equations, potentials and simulation techniques;
- 2: The computer code description for simulation of liquid model (Lenard-Jones potential);
- 3: The use of selected general-purpose code for the simulation of ionic, polymeric and biochemical molecular systems;
- 4: The theory of the basics of hybrid MD approach
- 5: MD test modeling.

## 2 INTRODUCTION

### 2.1 The basic equations and the force field potentials

$$m_i \frac{d^2 r_i(t)}{dt^2} = F_i(r)$$

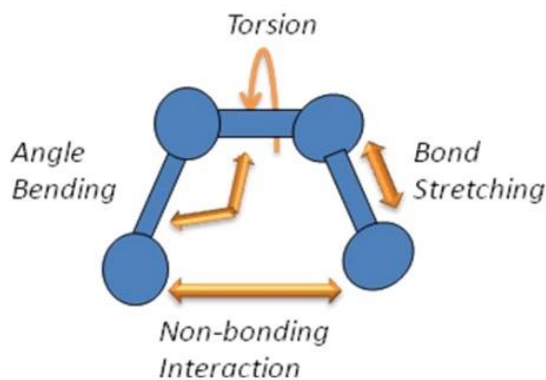
Equation above is the most important equation on which molecular dynamics are based, and as everyone knows, it represents Newton's second law.

A molecular dynamics simulation requires the definition of a potential function, or a description of the terms by which the particles in the simulation will interact.

Empirical potentials used in chemistry are frequently called force fields, while those used in materials physics are called just empirical or analytical potentials.

Most force fields in chemistry are empirical and consist of a summation of bonded forces associated with chemical bonds, bond angles, and bond dihedrals, and non-bonded forces associated with van der Waals forces and electrostatic charge.

illustration of the specified forces is shown in the picture below.



Corresponding potentials are shown below.

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

Van der Waals Interaction Potential:

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

Valence length potential,

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

Electrostatics potential,

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

Valence angle potential,

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

Hydrogen bonding potential,

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

Torsion dihedral potential,

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

Valence length potential describes bond stretching.

Valence angle potential describes angle bending of three atoms.

Torsion dihedral potential describes torsion of four atoms.

The hydrogen bond potential is often implicitly parameterized as a combination of Lennard-Jones (L-J) and electrostatic terms. In force fields that use an explicit hydrogen bonding term, the hydrogen bond potential is typically a distance-dependent function without any directional component.

## MD simulation research

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When studying proteins in solution it is apparent that electrostatic interactions play a role in folding, conformational stability, and other chemical-physical properties, so there is Electrostatics potential too.

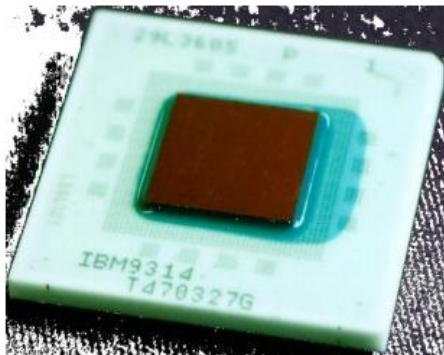
The Ewald summation for Coulomb interaction is a correct approach taking into account periodicity

In the Ewald summation the electrostatics coulomb potential,

$$\frac{1}{4\pi\epsilon_0} \sum_{n < j}^N \frac{q_j q_n}{r_{nj}}$$

To calculate Ewald's sums, chips with very good performances vary in millions of dollars.

The Ewald sums are realized under special-purposes architectures, like as *MDGRAPE-2* & 3 (Fig. 8).

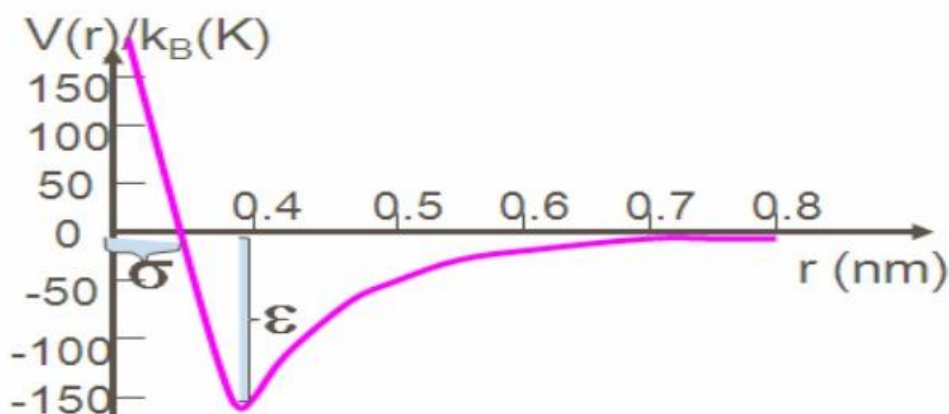


The Van der Waals force is a weak, short-range force that arises from temporal fluctuations of the charge distribution. This force can attract ideal gas atoms together. Ideal gas atoms are electrically neutral so there is no Coulomb attraction between them. The average dipole moment of an ideal gas atom is zero but the charge fluctuates around its average position and can temporarily create a dipole moment. This dipole moment induces a response in the neighboring atom such that there is a net attractive force between the atoms. The average over the attractive forces caused by the charge fluctuations is the Van der Waals force.

The bonds between atoms held together by Van der Waals forces are weak with a bond energy of a few meV. The Van der Waals bond potential is often approximated by a Lennard Jones potential of the form.

$$U(R) = 4\epsilon \left[ \left( \frac{\sigma}{R} \right)^{12} - \left( \frac{\sigma}{R} \right)^6 \right].$$

where the two terms represent repulsive and attractive interactions, respectively, and the parameters, and  $\sigma$  are expressed as a combination of parameters of atoms  $i$  and  $j$ , and  $\epsilon$  corresponds to the depth of the potential, which is typically a small number.



The radial distribution function (RDF) describes how the density of surrounding matter varies as a function of the distance from a point.

$$\rho g(r) = \frac{1}{N} \left\langle \sum_i^N \sum_{j \neq i}^N \delta[r - r_{ij}] \right\rangle$$

Order parameter is widely used for distinguishing of the equilibrium states

$$\begin{aligned} \gamma_x &= \frac{1}{N} \sum \cos(4\pi x_i/a) \\ \gamma_y &= \frac{1}{N} \sum \cos(4\pi y_i/a) \\ \gamma_z &= \frac{1}{N} \sum \cos(4\pi z_i/a) \\ \gamma &= \frac{1}{3} [\gamma_x + \gamma_y + \gamma_z] \end{aligned}$$

Boltzmann distribution (also called Gibbs distribution) is a probability distribution or probability measure that gives the probability that a system will be in a certain state as a function of that state's energy and the temperature of the system.

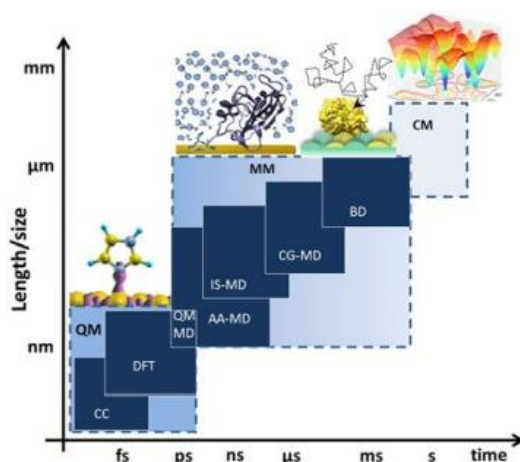
$$H_x(t) = \int_{-\infty}^{+\infty} f(v_x) \ln f(v_x) dv_x$$



## 3 MD SIMULATION

When it comes to MD simulation, one of the main problems is the length of the simulation. The time it takes to perform a simulation can be great due to the lack of performance of the computer systems we use. If the Moore's law (number of transistors in a dense integrated circuit (IC) doubles about every two years) maintained its accuracy in the future, these simulations could be executed significantly more quickly. But as The Moore's law is known, a solution is sought in the transition from silicon to graphene technology.

The picture under shows time and length scales of different simulation technique.



**Fig. 2.** Typical time and length scales of different simulation techniques: quantum mechanics (QM), including coupled cluster (CC) and DFT methods (inset adapted with permission from Iori *et al.* 2008). Copyright (2008) American Chemical Society); molecular mechanics (MM) including all-atom molecular dynamics (AA-MD) simulations, implicit solvent and coarse grained MD (IS-MD and CG-MD), and the Brownian dynamics (BD) technique; and continuum mechanics (CM). The ranges of time and length scales are approximate.

# MD simulation research

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There is a wide selection of software that can be used for MD simulation.

## 1.AMBER

The term "Amber" refers to two things. First, it is a set of molecular mechanical force fields for the simulation of biomolecules (these force fields are in the public domain, and are used in a variety of simulation programs). Second, it is a package of molecular simulation programs .

## 2.CHARMM

Chemistry at Harvard Macromolecular Mechanics (CHARMM) is the name of a widely used set of force fields for molecular dynamics, and the name for the molecular dynamics simulation and analysis computer software package associated with them

## 3.DL\_POLY

DL\_POLY is a general purpose classical molecular dynamics (MD) simulation software.DL\_POLY general design provides scalable performance from a single processor workstation to a high performance parallel computer.

In addition to the above, there is more software such as NAMD and GROMACS

A flowchart scheme → *input: CONFIG, CONTROL, FIELD; output: OUTPUT, REVCON, HISTORY*

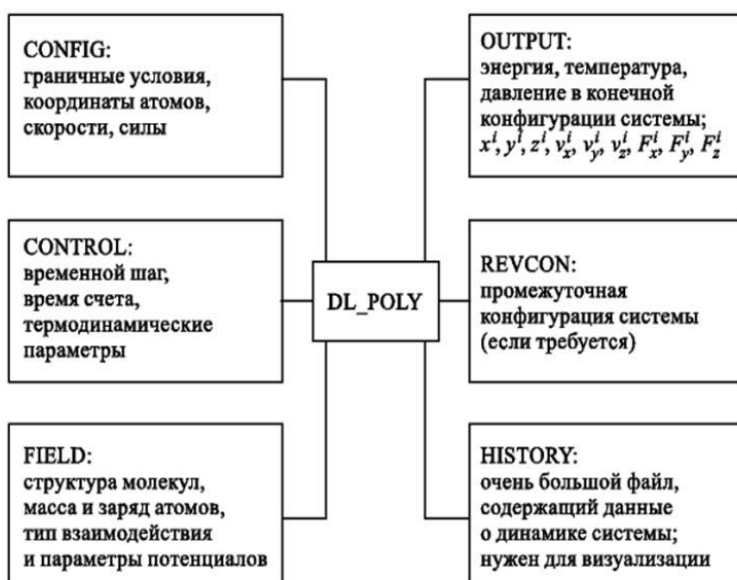


Fig. 26. A flowchart scheme of the input and output files of DL\_POLY.

### **4 CONCLUSION**

During the course, I gained knowledge of the simulation of physical and biochemical nanostructures, as well as the design of new structures, as well as the necessary theoretical knowledge

Given the long time the MD simulation has been performed, perhaps the biggest improvement would be reducing the timing of the simulation. As mentioned so far, the size of the chips has decreased twice every two years, which is why the speed and performance of those chips have improved, that's what the law of the man is talking about. But as we've reached the limits where this law is already scheduling, it's important to find a solution and make this tradition of cip reduction continue. Solution sought by replacing silicon technology with graphene, but this issue remains open.

## **5 FUTURE WORK**

After finishing my bachelor studies, I plan to enroll in master's studies, where I would like to apply and expand the knowledge of molecular dynamics acquired in this course.

### **6 Acknowledgement**

I primarily thank Professor Kholmurzo Kholmurodov, who was my professor and mentor during this course, and who managed to pass on knowledge to me in the most efficient and best way, I also thank the Joint Institute for Nuclear Research, Dubna, Russia on the opportunity to gain broad knowledge.

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