JOINT INSTITUTE FOR NUCLEAR RESEARCH
Frank laboratory of Neutron Physics

FINAL REPORT ON THE INTEREST PROGRAMME
Wave 13

INTRODUCTORY COURSE "MD-SIMULATION RESEARCH (FROM ATOMIC FRAGMENTS TO MOLECULAR COMPOUND)"

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Abstract

The goal of this project is to provide an introduction course to the modeling and design of physical and biochemical nanostructures, systems, and compounds in the field of molecular biology.

Contents:

I. Introduction

Molecular modeling is a set of methods for studying the structure and properties of molecules using computational techniques with visualization of the results, providing a three-dimensional representation of what is happening in a molecular system.

The MD method is based on an approximate numerical solution of Newton's equations. By solving the equations iteratively, one obtains the trajectory of a particle's motion r(t). The time step is usually measured in femtoseconds (10^{-15} s), and the total duration of observing the trajectory reaches nanosecond intervals (10^{-9} s) and, in rare cases, reaches a microsecond. Since the computational formulas only approximate the exact formulas, an error accumulates with each step. As a result, the discrepancy between the analytical and numerical solutions can be very large. However, there is a clearly defined event horizon within which computational errors can be neglected.

Modeling Stages

When modeling molecular structures, the following stages are performed:

1. Selection of the interaction model
2. Selection of boundary conditions
3. Selection of the computer code (software package – DL_POLY, AMBER, CHARMM, NAMD, etc.)
4. Selection of initial conditions
5. Performing the modeling
6. Analysis of the results

The basic equations and the force field potentials

Molecular dynamics of conventional use is based on II Newton' law:

$$m_i \frac{d^2 \boldsymbol{r}_i(t)}{dt^2} = \boldsymbol{F}_i(\boldsymbol{r}), \quad i = 1,2,\dots,n$$

$$\{\boldsymbol{r}_i, m_i, \boldsymbol{F}_i\}$$

$$\boldsymbol{r} = \{r_1, r_2, \ldots, r_n\};\ U(\boldsymbol{r})$$

$$\boldsymbol{F}_i(\boldsymbol{r}) = -\frac{\partial U(\boldsymbol{r})}{\partial \boldsymbol{r}_i}$$

$$m_i \frac{d^2 \boldsymbol{r}_i(t)}{dt^2} = \boldsymbol{F}_i\big(\boldsymbol{r}_i(t)\big) - \gamma_i m_i \frac{d\boldsymbol{r}_i(t)}{dt} + R_i(t)$$

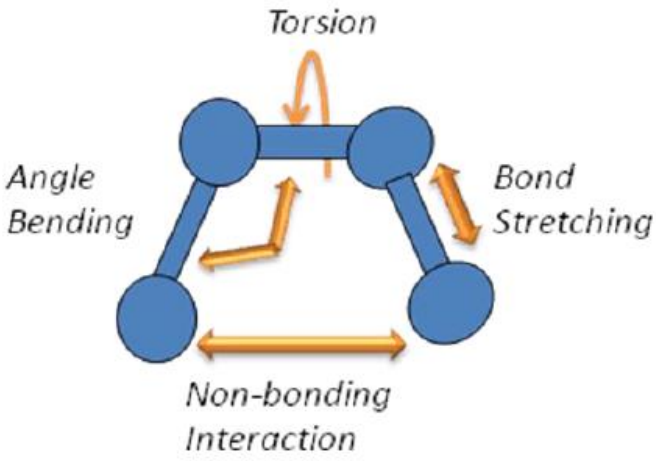


Fig. 1. *Chemical bonds (bond stretching, angle bending, torsion) and non-bonding interaction)*

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

where U_b is the bond potential, U_θ is the valence angle potential, U_φ is the torsion angle potential, U_ω is the planar group potential, U_{LJ} is the van der Waals interaction potential, U_{el} is the electrostatic interaction potential, and U_{HB} is the hydrogen bond potential (Fig. 1)

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

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

Van-der-Waals interaction potential (12-6 or Lennard-Jones (l_j))

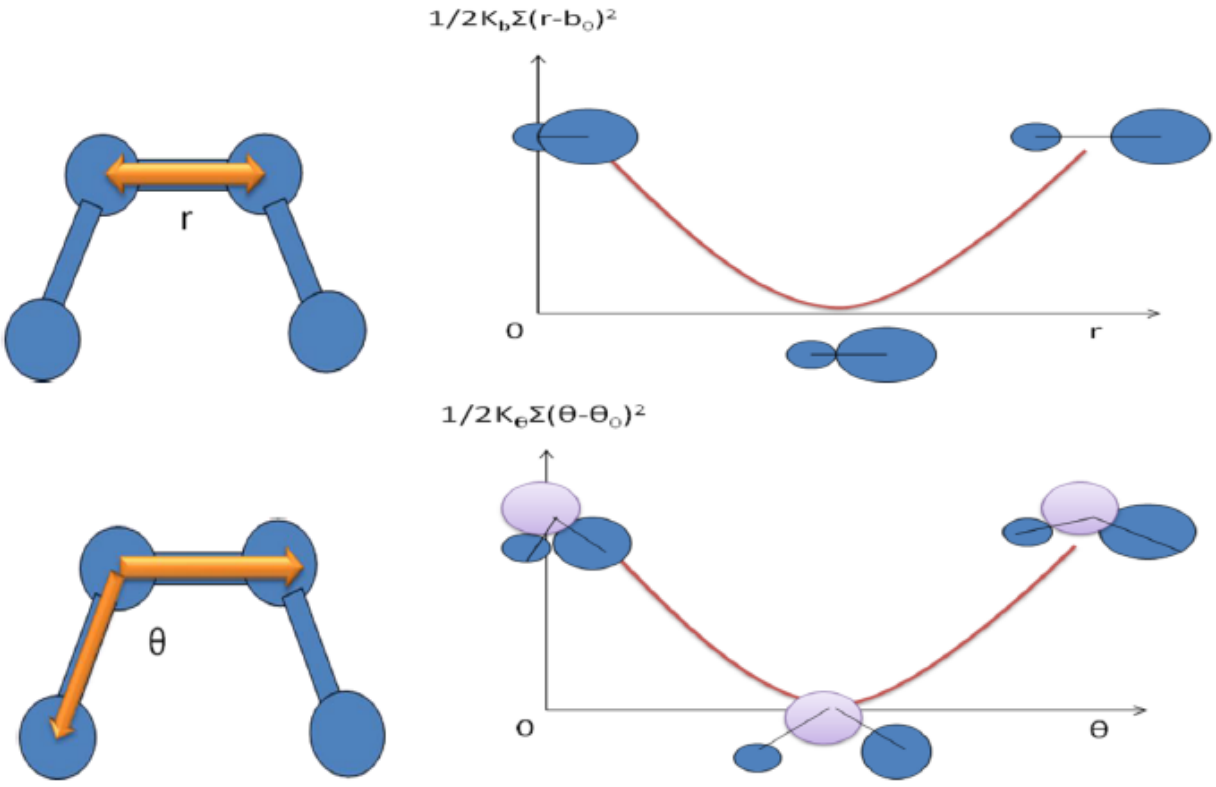
$$U_{LJ} = \sum_{i,j}[\frac{A}{r_{i,j}^{12}} - \frac{B}{r_{i,j}^{6}}]$$

Electrostatics potential

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

Hydrogen bonding potential

$$U_{HB} = \sum_{i,j}[\frac{A'}{r_{i,j}^{12}} - \frac{B'}{r_{i,j}^{6}}]$$



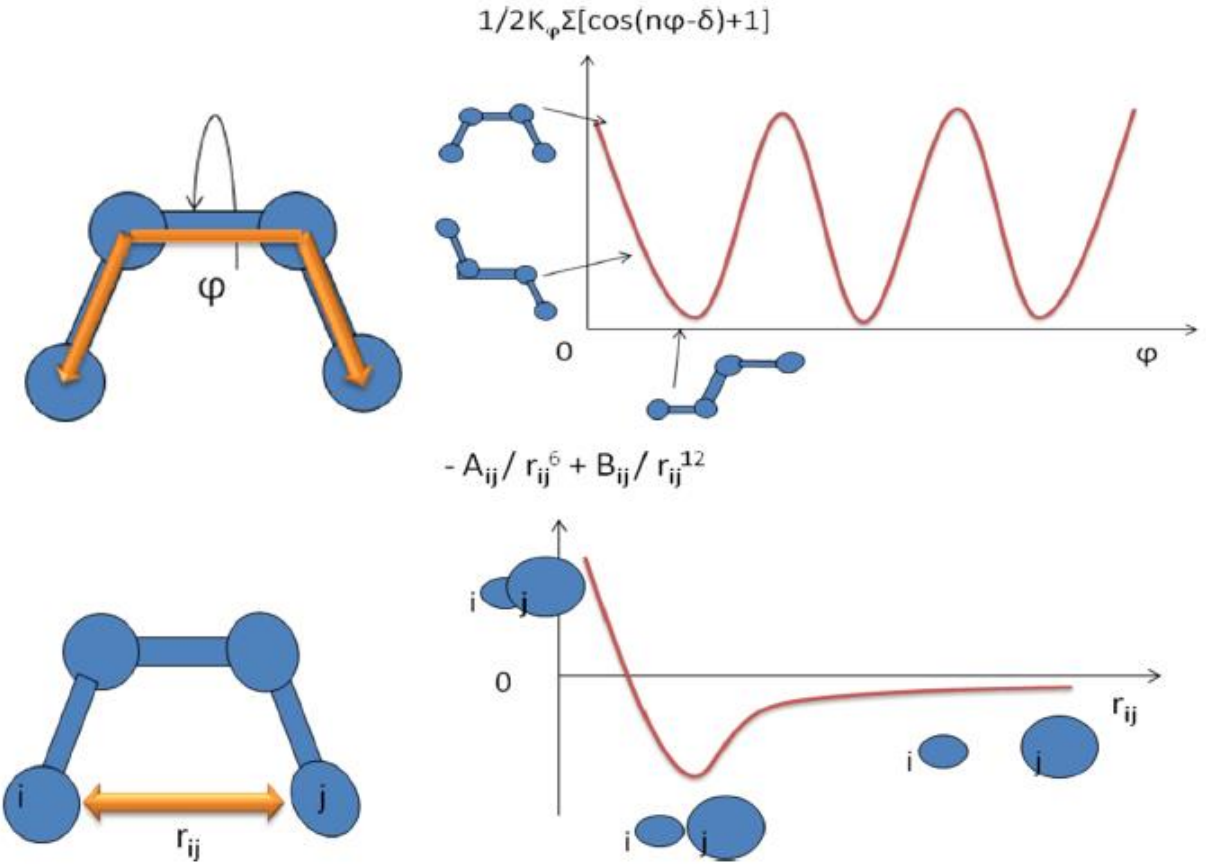


Fig. 2. *Graphs of chemical potentials*

Lennard-Jones (l_j) potential

The Lennard–Jones potential can be used to describe gases, liquids, and solids. The Lennard–Jones potential has the form

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

where ε is the depth of the potential well, σ is the van der Waals atomic diameter (the "effective atomic diameter") — the distance at which the repulsive and attractive forces between atoms balance each other (Fig. 3)

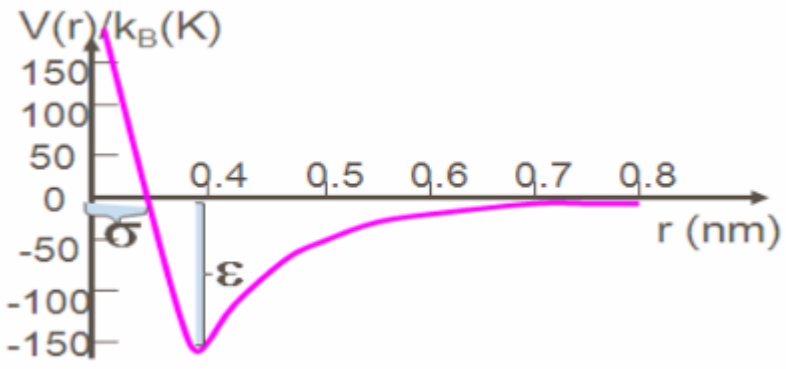


Fig. 3. *The Lennard-Jones potential energy dependence on the atom-atomic distance*

At large distances, atoms attract each other, which corresponds to the term $\{\frac{\sigma}{r}\}^6$, and the interaction potential is negative.At small distances, atoms repel each other, which corresponds to the term $\{\frac{\sigma}{r}\}^{12}$, and the interaction potential is positive. The form of the repulsive potential has no theoretical justification, but it is used in practice because it is convenient to compute. An exponential dependence is considered more physically justified.

атом	ε/k_B (K)	σ (nm)
H	8.6	0.281
He	10.2	0.228
C	51.2	0.335
N	37.3	0.331
O	61.6	0.295
F	52.8	0.283
Ne	47.0	0.272
S	183.0	0.352
Cl	173.5	0.335
Ar	119.8	0.341
Br	257.5	0.354
Kr	164.0	0.383

Table 1. *The LJ (Lennard-Jones)-parameters of* ε *and* σ *for different atoms*

The values of the potential well depth and effective diameters are tabulated quantities (Table 1). If the system consists of different types of atoms, the parameters are averaged according to the following mixing rules.The Lorentz-Berthelot mixing rule:

$$\sigma_{CS} = \frac{\sigma_{cc} + \sigma_{ss}}{2}$$

$$\sigma_{CS} = (\sigma_{cc} * \sigma_{ss})^{1/2}$$

MD Simulation Software

Several common software can be used in MD simulations such as:

- **AMBER** (Assisted Model Building with Energy Refinement): A suite of biomolecular simulation programs that began in the late 1970s. 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

- **DL_POLY:** is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov, W. Smith, A.M. Elena, and so on

- **NAMD** (Nano-scale Molecular Dynamics): A parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems

- **GROMACS** (Groningen Machine for Chemical Simulation): A versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles

- **LAMMPS** (Large-scale Atomic/Molecular Massively Parallel Simulator): A classical molecular dynamics code with a focus on materials modeling

- **CHARMM** (Chemistry at Harvard Macromolecular Mechanics): A program widely used for macromolecular simulations, including energy minimization and molecular dynamics

Applications and Future Work

As a 2nd year master student in photonics department, faculty of physics at the National University of Uzbekistan I am working on my master's thesis work titled "Coherent properties of the field in optical channels under conditions of ray chaos". I study the dynamics of speckle patterns passing through a diffuser. An approach to detecting the localization and statistical analysis of wavefront dislocations based on experimental interferograms is proposed. By changing the polarization angle of the light incident on the ground glass surface, the observed speckle structure can be controlled.

In my work, optical speckles arise from multiple scattering events inside a complex medium (optical fiber) or from uneven surface (frosted glass, tracing paper). MD simulations similarly track the motion and interaction of many particles in a complex environment. This analogy makes MD a useful tool in fields where wave propagation, disorder, and statistical behavior play key roles.

1. Modeling Disordered Media. MD simulation techniques can be used to generate realistic models of disordered materials such as ground glass surfaces or diffusers.

These atomistic models help predict:

- local surface roughness
- scattering centers
- correlation lengths of the medium, which directly influence speckle structure formation and wavefront dislocations

2. MD for Optical and Photonic Systems. Although MD is primarily used for atomic-scale interactions, advanced models can support the study of light–matter interactions in nanostructures, helping bridge optical experiments and microscopic structure. This opens possibilities for comparing dynamic behavior of complex media, including systems exhibiting speckle formation, scattering, and wavefront distortions.

3. Statistical Mechanics Approaches

Applying MD-inspired statistical mechanics to speckle data could strengthen analysis of:

- localization of dislocations
- distributions of phase singularities
- coherence fluctuations in chaotic regimes

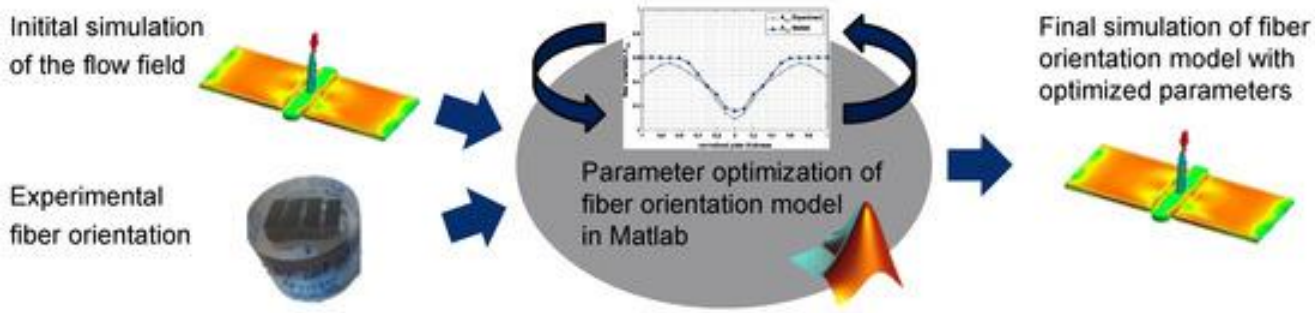


Fig.4. *Process scheme of the fiber orientation optimization tool.*

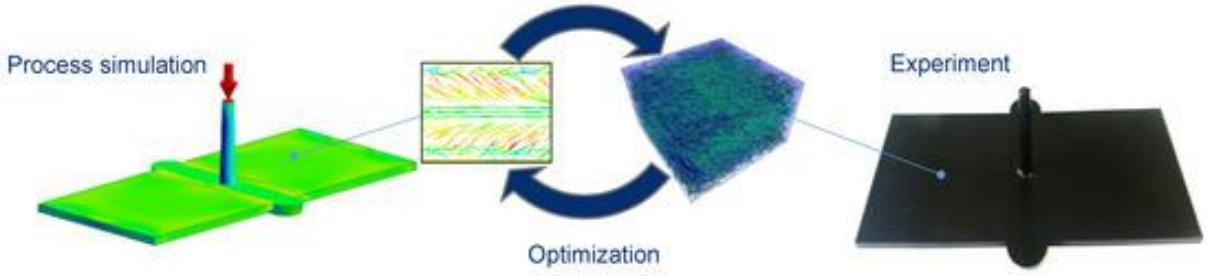


Fig.5. *Reverse engineering of fiber microstructure properties at a specific position.*

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