1 Installation

To get the code you can download archive or execute the following commands in the terminal:

```
git clone https://github.com/zhmurov/MD
```

To compile, run 'make' from the code directory:

```
cd MD/
make
```

This will produce 'mrg-cg2' executable which is the program. To run simulations, first make sure that you have had topology, coordinate, parameter and configure file. You should pass the configuration file as the first parameter to the program (the description of this file follows):

```
<instalation-path>/mrg-cg2 <config_file>.conf
```

2 Configuration file

2.1 Input

device — ID of NVidia card to run simulations on. Use "nvidia-smi" or "deviceQuery" from NVidia SDK to check devices ids.

topology_file — path to the structure topology file. Format "*.top".

parameter_file — path to the interaction parameters file (DNA-Ions, DNA-Protein, Protein-Ions). Includes potential parameters: BONDSCLASS2ATOM, ANGLECLASS2, GAUSSEXCLUDED.

coordinates_file — path to the structure initial coordinates file. Format "*.xyz".

structure_file — path to the file with parameters of fixed atoms. Format "*.pdb".

2.2 Calculation

timestep — time-scale of one simulation step. Units: ps.

run — number of simulation steps, natural number.

temperature — temperature. Units: K.

seed — random seed, determines a random spread of the initial velocities of the system.

pbc_xlo — the minimum x coordinate of the box of periodically specified conditions. Units: nm.

pbc_ylo — the minimum y coordinate of the box of periodically specified conditions. Units: nm.

pbc_zlo — the minimum z coordinate of the box of periodically specified conditions. Units: nm.

pbc_xhi — the maximum x coordinate of the box of periodically specified conditions. Units: nm.

pbc_yhi — the maximum y coordinate of the box of periodically specified conditions. Units: nm.

pbc_zhi — the maximum z coordinate of the box of periodically specified conditions. Units: nm.

fix_momentum — conserve rotational momentum of the system

- fix_momentum_freq — frequency with which the rotational momentum will be zeroed

integrator — switch on one of the following integrators: "leap-frog", "velocity-verlet", "leap-frog-nose-hoover", "leap-frog-new", "leap-frog-overdumped", "steepest-descent".

- nose-hoover-tau — nose-hoover thermostat parameter.
- nose-hoover-T0 — nose-hoover thermostat parameter.
- max_force — steepest-descent parameter.

langevin — switch on the Langevin dynamics.

- langevin_seed — parameter of the random velocity distribution in the Langevin dynamics.
- damping — Langevin parameter.

2.3 Potentials

fene — switch on FENE potential (amino acid bond in one thread). Switches: "on/off". NECESSARY for protein calculations.

lennardjones — switch on Lennard-Jones potential. Switches: "on/off". NECESSARY for protein calculations.

repulsive — switch on repulsive potential. Switches: "on/off". NECESSARY for protein calculations, But is not needed in the calculations of the general DNA-protein model.

- rep_eps — the depth of the potential well.
- rep_sigm — zero interaction energy distance.

bondclass2atom — switch on bond interaction along the DNA chain. Switches: "on/off". NECESSARY for protein calculations. Potential parameters are in parameter file.

angleclass2 — switch on angle interaction along the DNA chain. Switches: "on/off". NECESSARY for protein calculations. Potential parameters are in parameter file.

gaussexcluded — switch on interactions between DNA, ions and protein. Switches: "on/off". NECESSARY for protein calculations. Potential parameters are in parameter file.

- pairs_cutoff — radius of a small pairs list (nm).
- pairs_freq — frequency of the small pairs list update.
- possible_pairs_cutoff — radius of a big pairs list (nm).
- possible_pairs_freq — frequency of the big pairs list update.

pppm — switch on P^3M (Particle–Particle-Particle–Mesh) method. Switches: "on/off". NECESSARY for protein calculations.

- pppm_order — P^3M order. Default value: 5.
- pppm_accuracy — P^3M accuracy.

coulomb — switch on the electrostatic potential. Switches: "on/off". NECESSARY for protein calculations. Potential parameters are in parameter file.

- dielectric — permittivity, real. Default value: 1.0.

- nb_cutoff — nonbonded interaction distance (nm).
- coul_cutoff — Coulomb potential interaction distance (nm).

push_sphere — switch on pushing sphere potential. Switches: "on/off".

- ps_center_of_sphere — pushing sphere center coordinates.
- ps_radius0 — pushing sphere initial radius.
- ps_radius — pushing sphere final radius.
- ps_update_freq — frequency of sphere coordinates update.
- ps_harmonic — set compression potential as harmonic. Switches: "on/off". If disabled, Lennard-Jones potential is used by default.
- ps_sigma — the depth of the potential well for repulsive Lennard-Jones potential.
- ps_epsilon — coefficient of restitution (in case of harmonic potential) / zero interaction energy distance (in case of repulsive Lennard-Jones potential)
- ps_mask — switch on particles compression. Switches: "on/off". By default, only DNA particles are compressed.
- ps_mask_pdb_filename — containing compressible atoms parameters file. Format "*.pdb".

fixation — switch on particle fixation. Switches: "on/off".

- fix_atomtype — type of fixed particles (1 – DNA, 2 – Na^+, 3 – Cl^-, 4 – protein)

indentation — switch on indentation potential. Switches: "on/off".

- ind_tip_radius — radius of the virtual sphere representing cantilever tip (nm).
- ind_base_coord — current cantilever base coordinates (nm)
- ind_tip_coord — current cantilever tip coordinate (nm)
- ind_base_freq — the frequency of cantilever base displacement by ind_vel.
- ind_n — substrate cantilever tip normal vector (vector).
- ind_vel — the value define the displacement of the virtual particle, representing cantilever base, every ind_base_freq steps. Actual cantilever base velocity can be calculated as $ind\_vel/(ind\_base\_freq-timestep)$
- ind_ks — spring constant of the cantilever (kJ/mol nm^2).
- ind_eps — repulsive energy factor for Lennard-Jones potential (kJ/mol).
- ind_sigm — repulsive distance for the Lennard-Jones potential. Note that potential is shifted to the surface of the cantilever tip sphere (nm).

- sf_coord — current surface coordinate (nm).
- sf_n — substrate surface normal vector (vector).
- sf_eps — repulsive energy factor for the surface Lennard-Jones potential (kJ/mol).
- sf_sigm — repulsive distance for the surface Lennard-Jones potential (nm).

2.4 Output

psf_filename — the path to save the topology. Format: "*.psf".
dcd_filename — filename to write coordinates output. Format: "*.dcd".
dcd_freq — frequency of writing out structure coordinates in .dcd output file in course of simulation. Natural number.
energy_filename — name of the output file to save resulted energy. Format: "*.dat".
energy_freq — frequency of writing out energy in output file in course of simulation. Natural number.
output_xyz — switch on final coordinates saving. Switches: "on/off".
output_xyz_file — filename to write final coordinates output. Format "*.xyz".
ps_presure_filename — filename to write pushing sphere pressure output. Fromat: "*.dat".
pdb_cant_filename — name of the output file with the position of cantilever tip. Format: "*.pdb".
dcd_cant_filename — name of the output file with the coordinates of cantilever tip. Format: "*.dcd".

2.5 Example

Consider an example of configuration file (see Tab. **??**). There is equilibration simulation of dna system for 1 ns trajectory.

```
device                  2           # NVidia GPU device index
```

Input files, including topology file in Gromacs format (.top), LAMMPS-style .dat file with parameters for Bond Class 2, Angle Class 2 and Gauss-excluded potentials and coordinate file in .xyz format.

```
name                    dna
topology_file           <name>.top
parameter_file          par.dat
coordinates_file        <name>.xyz
```

Parameters for integrator:

```
timestep                0.005       # 5 fs time step
run                     200000      # 1 ns trajectory
temperature             300
seed                    5464754
integrator              leap-frog-nose-hoover
nose-hoover-tau         100
nose-hoover-T0          300
```

Box with boundary conditions:

```
pbc_xlo                  -20          # Low coordinate x of the box
pbc_ylo                  -20          # Low coordinate y of the box
pbc_zlo                  -20          # Low coordinate z of the box
pbc_xhi                   20          # High coordinate x of the box
pbc_yhi                   20          # High coordinate y of the box
pbc_zhi                   20          # High coordinate z of the box
```

Potentials:

```
bondclass2atom           on
angleclass2              on
gaussexcluded            on
pairs_cutoff             4
pairs_freq               10
possible_pairs_cutoff    7
possible_pairs_freq      100
pppm                     on
pppm_order               5
pppm_accuracy            0.00001
coulomb                  on
dielectric               80.0
nb_cutoff                1.5
coul_cutoff              3
```

Output:

```
psf_filename             <name>_equil.psf
dcd_filename             <name>_equil.dcd
dcd_freq                 20
energy_filename          <name>_out_equil.dat
energy_freq              20
output_xyz on
output_xyz_file          <name>_equil.final.coord.xyz
```