User Manual of `DPDWetting` (Ver 3.1) Simulation Software

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1 Modules

`DPDWetting` includes the main simulation module and analysis modules. The usage of the program is:

```
mpirun -np [number of cores] dpdwetting [module name] [options],
```

or

```
dpd [module name] [options]
```

Here is an example of the main module of the software.

```
mpirun -np 8 dpd run -c conf.gro -p control.in -t topol.top -o impact
```

The names of modules are listed as follows:

- Main module

  `run`*: Main dpd simulation module

- Modules for general purposes

  `trjtogro`: Converting a binary trajectory to a gro file (ASCII)

  `rdf`: Radial distribution functions

  `surfrdf`: 2D particle distribution function on a given surface

  `avgstress`: Average stress

  `velacf`: Velocity auto-correlation function

- Modules for droplet analysis

  `dropsize`: Droplet diameter, base diameter, diameter of the second layer from the surface, contact angle, and height of the droplet as a function of time

  `velocity`: Droplet velocity in each direction as a function of time

  `rdensity`: Averaged radial density

  `sphstress`*: Spherical stress from the trajectory

  `polads`: Polymer adsorption on the surface as a function of time

  `polstretch`: Stretching amount of polymer as a function of time

  `surfcov`: Surface coverage by polymer

  `jumpfreq`: Jumping frequency defined in the molecular kinetic theory

  `surfrdf`: 2D radial distribution function of particles adsorbed on a solid surface

  `depori`: Second Legendre Polynomial of backbone vectors of adsorbed polymers

  `dropzd`: Particle density profile along z-coordinate

- Modules for capillary bridge analysis

  `brdgsize`: Contact angles of a capillary bridge

  `brdgvel`: Average velocities of particles in a capillary bridge

  `brdgpc`: Polymer concentration adsorbed on the contact line region

  `brdgac`: Polymer concentration in the adsorption layer

  `brdgclvel`: Contact line velocity of each component

  `brdgezd`: Density profile along z-coordinate

  `brdgjpf`: Jumping frequencies defined in the molecular kinetic theory

  `brdgslvel`: Slip velocity

  `brdgvelx`: Average x-velocity at different z position

  `brdgvelxz`: Average x-, and z- velocities

  `brdgald`: Density profile at the first adsorption layer

  `brdgzd`: Density profile of liquid particles along z

  `brdgxzd`: Density map of liquid particles on a xz-plane

  `brdgcline`: Contact line position as a function of time

  `brdginterf`: 3D interface points at a given time

  `brdggpd`: Particle density in grooves for rough surfaces

- Modules for polymer analysis

  `polsize`: Module for polymer size(end-to-end distance, radius of gyration...) as a function of time and its distribution averaged over all simulation time

  `polevrlx`: Module for polymer end-to-end vector relaxation time

  `bondlen`: Module for average bond length as a function of time

  `polsmsf`: Module for single molecule structure factor

  `msd`: Module for mean square displacements

  `polsubsize`: Module for subchain sizes of polymer

  `polorient`: Module for orientational order parameter

*: Only these modules support multi-core.

The main simulation module requires basically three input files, initial configuration (`.gro`), topology (`.top`), and control (`.in`) files. The first line is the comment.

The analysis modules additionally require an output from the main module, trajectory (`.trj` or `.gro`)), force (`.frc`) or stress(`.str`) file depending on the module. One can use following options to specify input and output file names.

`-c`: (default: conf.gro) Input initial configuration file

`-t`: (topol.top) Input topology file

`-p`: (control.in) Input control file

`-o`: Prefix for output files

`-l`: (log.out) Output log file

`-x`: (traj.trj or traj.gro) Output trajectory file

`-f`: (force.frc) Output force file

`-s`: (stress.str) Output stress file

`-r`: (check.ckp) Checkpoint file to generate

`-restart`: Checkpoint file to restart simulation

`-ss`: (sslog.out) Output log file for slip-springs

2 Initial Configuration

Initial conformation is given by GROMACS ASCII format, "gro". Brief format of the file is as below.

```
Example initial configuration
124000
    1POL      P    1  54.782  17.861   5.524  -1.386  -0.247  -0.345
    1POL      P    2  54.309  18.355   5.630   0.632   0.259   0.892
    1POL      P    3  53.732  18.079   5.567   0.643   0.123  -0.146
    1POL      P    4  53.293  17.623   5.558   1.223   0.031  -0.964
    1POL      P    5  52.647  17.785   5.454  -0.832   0.433   0.789
    1POL      P    6  53.209  18.130   5.626   0.525  -0.754   0.326
    1POL      P    7  53.713  18.668   5.598   0.096   0.089   0.773
    1POL      P    8  53.061  18.631   5.528  -1.215  -0.124   0.316
    1POL      P    9  52.544  18.425   5.716   2.707   1.564  -0.235
    1POL      P   10  52.483  19.096   5.588   0.284  -0.381   0.525
    1POL      P   11  53.003  19.519   5.594  -0.567  -0.931   0.482
    1POL      P   12  53.426  20.026   5.559  -1.096  -0.832  -1.142
    1POL      P   13  53.056  20.574   5.611  -0.220   1.366  -1.603
    1POL      P   14  53.752  20.604   5.745   0.684  -0.803   0.081
```

The first line is a comment, and the second line is the number of particles in a system. Configuration is given as the order of [molecule number], [molecule name] , [particle name], [particle number], [position x], [position y], [position z], [velocity x], [velocity y], [velocity z]. Spacing between values has to be exact and the following format should be used ("%5d%-5s%5s%5d%8.3f%8.3f%8.3f%8.4f%8.4f%8.4f"). One can fine more information from GROMACS official manual.(https://manual.gromacs.org/)

3 Control variables

Control variables for simulation has to be specified in a separate file, which looks as below.

```
temperature     1.0     ;temperature
totalsteps      1000    ;total integration steps
timestep        0.02    ;integration time step
integrator      vv      ;integration method
nonbonded       mdpd    ;nonbonded interaction type
bondlength      harmonic ;bondlength interaction type
;randseed        123123 ;random seed
gamma           4.5     ;gamma
cellcutoff      1.0     ;cutoff distance of a cell
rmcomvfreq      100     ;frequency of removing center of mass motion
rmcomvdir       x y z   ;axis of removing center of mass motion
xtrjfreq        100     ;frequency of writing trajectory
xlogfreq        50      ;frequency of writing log
xstrfreq        100     ;frequency of writing stress
xfrcfreq        100     ;frequency of writing force
wall            solid z     ;boundary condition for walls
wallposz        5.0 26.0    ;positions of walls
wallshear       xz 0.002    ;direction and rate of the steady shear
wallshrgrp      WAL RAL     ;molecule name of the sheared walls
```

Argument and the value has to be separated by space or tab, and any values or strings behind the character ";" is taken as a comment and is ignored. Here, one can find a list of the supported control variables. Default values are given in the parenthesis.

- `temperature` (default: 1.0) The temperature of the simulation given to the DPD random force.
- `timestep` (0.02) The integration time step.
- `gamma` (4.5) The coupling parameter of the drag force in DPD simulation.
- `saferatio` (10.0) The multiplication factor to the number of beads in a domain for memory allocation.
- `maxforce` (100.0) The maximum force to stop energy minimization.
- `lambda` (0.5) The division factor for the estimation of the velocity at $t + \Delta t/2$ by DPD velocity-Verlet algorithm.
- `cellcutoff` (1.0) The cut-off distance for the cell-list. This has to be larger than the longest cutoff distance of the non-bonded interaction.
- `totalsteps` The number of integration steps for whole simulation.
- `dumpbinary` (yes) `yes`: Outputs are written binary if yes. `no`: Written in text format.
- `xtrjfreq` (100) A frequency to write a trajectory
- `xlogfreq` (1) A frequency to write a log
- `xstrfreq` A frequency to write stress of each particle
- `xfrcfreq` A frequency to write force of each particle
- `rmcomvreq` A frequency to remove center-of-mass motion
- `rmcomvdir` (x y z) A direction of the removal of the center-of-mass motion
- `randseed` A seed of a random number generator
- `dumpfrozen` (no)

  `no`: Data of frozen particles is not written in trajectory, stress, and force files.

  `yes`: It's written.

- `integrator`

  `vv`: Velocity-Verlet algorithm

  `emin`: Energy minimization

  `vv-sllod`: SLLOD Velocity-Verlet algorithm (under deformation)

- `pullspringk` A constant of springs pulling all particles toward a fixed point in a simulation box. Followed by the direction of pulling in case it is not isotropic (x/y/z/xy/yz/xz)
- `pullcenter` (Center of the box) A position of the fixed point to which the springs are attached
- `gravity` External gravitational field. Followed by direction (x/y/z)

- `nonbonded` Potential function for non-bonded interactions

    dpd: Dissipative particle dynamics

    mdpd: Multi-body dissipative particle dynamics

- `bondlength` (harmonic) Potential function for bond length

- `wall` Wall boundary condition followed by direction (x/y/z)

    solid: Reflective boundary condition

- `wallposx/wallposy/wallposz` Position of two walls along z-direction

- `slipspring` (0) The total number of slip-springs

- `sscutoff` (1.5) The cutoff distance of slip-springs

- `seqnmcsteps` (0) The number of MC steps per each sequence

- `seqndpdsteps` (0) The number of DPD steps per each sequence

- `ssparam` (0.0 0.0) The spring constant and the average bond length of the slip-spring

- `sspoltype` (linear)

    – `linear`: Slip-spring algorithm for linear / branched polymer (with ends)

    – `ring`: Silp-spring algorithm for ring polymer (without ends)

- `intrassbias` Bias for intramolecular slipspring for ring-type slip-spring algorithm

- `wallshear` Direction of the wall-induced shear (xy/xz/yx/yz/zx/zy)

- `wallshrgrp` Two groups which move in opposite direction to induce shear

- `liquidgrps` The molecule name of liquid groups for analysis

4 Topology

Force field has to be given in a topology file. An example force field looks like this.

```
;System information
[ System ]
; Mol_nameNum_of_mols
       POL        25
       SOL     99500
       WAL     12000    frozen
       RAL     12000    frozen

;Molecule Atom Information
[ SOL Atoms ]
;   Aindex     Atype      mass
         0         S       1.0

[ POL Atoms ]
;   Aindex     Atype      mass
         0         P       1.0
         1         P       1.0
         2         P       1.0
         3         P       1.0
         4         P       1.0
         5         P       1.0
         6         P       1.0
         7         P       1.0
         8         P       1.0
         9         P       1.0
        10         P       1.0

;Molecule Bond Information
[ POL Bonds ]
;   index1    index2     btype
         0         1        PP
         1         2        PP
         2         3        PP
         3         4        PP
         4         5        PP
         5         6        PP
         6         7        PP
         7         8        PP
         8         9        PP
         9        10        PP

[ WAL Atoms ]
;   Aindex     Atype      mass
         0         W       1.0

[ RAL Atoms ]
;   Aindex     Atype      mass
         0         W       1.0

;Nonbonded Parameters
[ Nonbonded ]
;   Atype1    Atype2         B       r_B         A       r_A
         S         S     25.00      0.75    -40.00      1.00
         S         W     25.00      0.75    -10.00      1.00
         W         W     25.00      0.75    -40.00      1.00
         S         P     25.00      0.75    -40.00      1.00
         P         P     25.00      0.75    -40.00      1.00
         P         W     25.00      0.75    -30.00      1.00

;Bond length Parameters
[ Bondlength ]
;    btype         k        l0
        PP    300.00     0.650
```

The topology file always starts with "[System]" argument which includes molecule names and the number of molecules. If the molecules are frozen in space, for example, wall particles in an impact

simulation, it has to be specified with "frozen" after the number of particles.

The particle information in each molecule is given in the argument "[{Molecule name} Atoms]". Here, the molecule name used in "[System]" has to be given in {Molecule name} and this should be the same with the one used in the configuration file. For each molecule, index, type, and mass of particles are given. The information for chemical bonds in a molecule is given in "[{Molecule name} Bonds]". It should contain the indices of two particles of each bond and the name of the bond type.

Non-bonded parameter of MDPD (or DPD) force field is given in "[Nonbonded]". It contains the names of particles of each interaction pair, and its the repulsive amplitude, the cutoff distance of the repulsion, the attractive amplitude, and the cutoff of the attraction in order. For DPD simulation specified by the control variable "nonbonded dpd", only repulsive ampltude and cutoff are given.

Bond length parameter is given by "[Bondlenth]" argument, which contains the type of bond, spring constant, and the equilibrium bond length. Harmonic potential is used for the bond length force.