MPMDP Tutorial

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1 Introduction

This tutorial introduces the molecular dynamics code MPMDP (Multi-purpose molecular dynamics package), which simulates a single particle type with Lennard-Jones pair interactions, DPD, or hybrid particle-field MD. The Berendsen, Andersen, and the Lowe-Andersen thermostats and the Berendsen barostat are implemented. This code also supports shear flow non-eq. simulations and multi-particle collision dynamics (MPCD) for cell-based hydrodynamics. The code also supports slip-springs for entangled simulations of polymer melts.

2 Requirements

To use MPMDP, you need to have Julia installed and the following packages:

- Formatting
- Distributions
- ProgressMeter
- Debugger
- Statistics
- LinearAlgebra
- Random
- FFTW

You can install these packages using the following command in the Julia REPL:

```
import Pkg; Pkg.add("Formatting"); Pkg.add("Distributions");
    Pkg.add("ProgressMeter"); Pkg.add("Debugger"); Pkg.add("
    Statistics"); Pkg.add("LinearAlgebra"); Pkg.add("Random");
    Pkg.add("FFTW")
```

3 Input Files

To run MPMDP, you need two input files: control.txt and a coordinate file (e.g. input.data). The control.txt file configures the simulation, while the coordinate file contains the initial configuration of the particles.

3.1 Example control.txt

Here is an example of a control.txt file with descriptions for every single point:

```
timestep 0.007
temperature 0.7
n_steps 1000000
traj_freq 1000
log_freq 1000
data_file input.data
traj_file trj.xyz
log_file logger_MD.txt
init_velocity Z
# Non-bonded interactions:
# LJ_12_6 epsilon sigma
# non_bonded_interactions LJ_12_6 1 1
non_bonded_interactions original_hPF_Interactions 0.1 10 10 10
thermostat Berendsen_Thermostat 1
# thermostat Andersen_Thermostat 1
# thermostat Lowe-Andersen_Thermostat 1
# Special features:
# collisions MPCD 2 1 130
# slip_springs 10 500 500 20 2 n
# shear highest only 1 20 15
# shear_sample_freq 100
```

3.2 Control Parameters in control.txt

Here is an explanation of each control parameter in the control.txt file:

- **timestep**: The time duration of each simulation step. Example: `timestep 0.007`.
- **temperature**: The target temperature of the simulation. Example: `temperature 0.7`.
- **n_steps**: The total number of simulation steps to be executed. Example: `n_steps 1000000`.
- **traj_freq**: How often to write the trajectory data. Example: `traj_freq 1000`.
- **log_freq**: How often to write the log data. Example: `log_freq 1000`.

- **data_file**: The file containing the initial particle coordinates. Example: `data_file input.data`.
- **traj_file**: The file to store the trajectory data. Example: `traj_file trj.xyz`.
- **log_file**: The file to store the log data. Example: `log_file logger_MD.txt`.
- **init_velocity**: Set the initial velocity distribution. Use Z for zero, G for Gaussian, or R for reading from a restart file. Example: `init_velocity Z`.
- **non_bonded_interactions**: Define the non-bonded interaction potential. Example: `non_bonded_interactions LJ_12_6 1 1` for Lennard-Jones 12-6 potential with epsilon 1 and sigma 1. For using hybrid particle-field MD, the parameters are κ (the compressibility parameter) and the number of cells in x, y and z dimension. The particle density should be higher than the number of cells. Example: `non_bonded_interactions original_hPF_interactions 0.1 10 10 10` for hPF with κ 0.1 and 10 cells each, in the x, y, and z dimension.
- **thermostat**: Choose the thermostat type. Options are Berendsen_Thermostat, Andersen_Thermostat, and Lowe-Andersen_Thermostat. Example: `thermostat Berendsen_Thermostat 1`.
- **collisions**: Enable Multi-particle Collision Dynamics (MPCD) by specifying cell size, collision frequency, and collision angle. Example: `collisions MPCD 2 1 130`.
- **slip_springs**: Define the slip-springs parameters, including the number of slip-springs, number of MD steps, number of MC steps, k, r_0, and restart option. Example: `slip_springs 10 500 500 20 2 n`.
- **shear**: Enable shear flow by specifying shear mode, number of exchanged particles, number of slabs, and frequency. Example: `shear highest only 1 20 15`.
- **shear_sample_freq**: Set the frequency of saving information about the shear flow. Example: `shear_sample_freq 100`.

3.3 Minimal example control.txt

Most parameters take default values, e.g. you will not have to specify file names, but you can.

```
timestep 0.007
temperature 0.7
n_steps 1000000
traj_freq 1000
log_freq 1000
init_velocity Z
non_bonded_interactions LJ_12_6 1 1
thermostat Berendsen_Thermostat 1
```

4 Running the Simulation

With the input files (control.txt and input.data) prepared, you can execute the following command to run the simulation from the same folder as your input files:

```
julia /your_path/MPMDP/source/start.jl
```

5 Analysis

The MPMDP package comes with several MD analysis tools, such as the MSD, VACF, and polymer analysis tools. Find them in MPMDP/tools.