molsim tutorial

J.S. Hansen

Februaray 2022, v. 0.9

1 Introduction

molsim is a GNU Octave/Matlab package for molecular dynamics simulation library. molsim supports simulations of

- Standard Lennard-Jones systems (solid, liquids, gasses, etc)
- Molecular systems with bond, angle, and torsion potentials
- Confined flow systems, eg., Couette and Poiseuille flows
- Charged systems using shifted force and Wolf methods
- Dissipative particle dynamics systems
- and more

The package also supports a series of run-time sampling functionalities.

molsim is basically a wrapper for the seplib library, which is a light-weight flexible molecular dynamics simulation library written in ISO-C99. The library is CPU-based and offers shared memory parallisation; this parallisaton is supported by the molsim package. The algorithms used in seplib is based on the books by Allen & Tildesley, Rapaport, Frenkel & Smith, and R. Sadus, see Ref. [**?**].

In this text

```
>>
```

indicates GNU Octave or Matlab command prompt. This

```
$
```

indicates the shell prompt.

2 Installation

2.1 GNU Octave

GNU Octave's package manager offers a very easy installation. From

`https://github.com/jesperschmidthansen/molsim/`

download and save the current release `molsim-<version>.tar.gz` in a directory of your choice. Start GNU Octave and if needed change directory to the directory where the file is saved.

```
>> pkg install molsim-<version>.tar.gz
```

Check contact by

```
>> molsim('hello')
Hello
```

In case this fails, check the path where molsim is install by

```
>> pkg list molsim
```

If the path is not in your GNU Octave search path add this using the `addpath` command.

2.2 Matlab

From

`https://github.com/jesperschmidthansen/seplib/`

download and save the current release `seplib-<version>.tar.gz` in a directory of your choice. Unpack, configure and build the library

```
$ tar zxvf seplib-<version>.tar.gz
$ cd seplib
$ ./configure
$ make
$ cd octave
```

To build the mex-file enter Matlab

```
$ matlab -nodesktop
```

Then build the

```
>> buildmex
```

Depending on the system this will build a molsim.mex¡archtype¿ file. You can copy this file to a directory in your Matlab searce path.

3 First quick example: The Lennard-Jones liquid

Listing 1 shows the simplest script simulating a standard Lennard-Jones system.

Listing 1

```
1: cutoff = 2.5; epsilon = 1.0; sigma = 1.0; aw=1.0;

2: molsim('set', 'lattice', [10 10 10], [12 12 12]);
3: molsim('load', 'xyz', 'start.xyz');

4: for n=1:10000

5:   molsim('reset');
6:   molsim('calcforce', 'lj', 'AA', cutoff, sigma, epsilon, aw);
7:   molsim('integrate', 'leapfrog');

8: end

9: molsim('clear');
```

Line 1: Specification of the Lennard-Jones interaction potential.
Line 2: Writes initial particle positions and velocities to default file start.xyz. System dimension is set to $10 \times 10 \times 10$, and box lengths to $12 \times 12 \times 12$.
Line 3: The initial configuration is loaded
Line 4 & 8: Molecular dynamics main loop. 10^4 iterations are performed
Line 5: Everything reset
Line 6: Calculate force between particles of type A using the interaction parameter specifications
Line 7: Integrate forward in time
Line 9: Free all memory allocated.