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Contents

1 Requirements

1.1 Cuda

```
$ sudo rm /etc/apt/sources.list.d/cuda*
$ sudo apt remove --autoremove nvidia-cuda-toolkit
$ sudo apt remove --autoremove nvidia-*
$ sudo apt-get purge nvidia*
$ sudo apt-get autoremove
$ sudo apt-get autoclean
$ sudo rm -rf /usr/local/cuda*
```

```
$ sudo apt update
$ sudo add-apt-repository ppa:graphics-drivers
$ sudo apt-key adv --fetch-keys
http://developer.download.nvidia.com/compute/cuda/repos/ubuntu1804/x86_64/7fa2af80.pub
$ sudo bash -c 'echo "deb
http://developer.download.nvidia.com/compute/cuda/repos/ubuntu1804/x86_64 /" >
/etc/apt/sources.list.d/cuda.list'
$ sudo bash -c 'echo "deb
http://developer.download.nvidia.com/compute/machine-learning/repos/ubuntu1804/x86_64 /" >
/etc/apt/sources.list.d/cuda_learn.list'
```

```
$ sudo apt update
$ sudo apt install cuda-10-0
$ sudo apt install libcudnn7
```

```
$ echo 'export PATH=/usr/local/cuda/bin${PATH:+:${PATH}}' >> ~/.bashrc
```

1.2 Cmake 2.8+

```
$ sudo apt-get install cmake
```

1.3 VMD

Visual Molecular Dynamics (VMD) is a powerful toolkit that can be used in order to visualize, design structures, animate and analyse trajectories. The link for VMD dowmload: https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD.

```
$ tar zxvf vmd-1.9.3.***.tar.gz
$ cd vmd-1.9.3
$ sudo nano configure
```

Change installation directory if necessary.

```
$ ./configure
$ cd src
$ make install
```

2 Compiling a code

Go to the **mt_assembly_hydrolysis** directory.
First of all, open **Makefile** with a text editor. Find the flags:

- CMAKE_SOURCE_DIR
- CMAKE_BINARY_DIR

and change the value to the directory where your **mt_assembly_hydrolysis** is located. Also search in the file for "# The main all target" and change the paths where it necessary. In the same folder run:

```
$ cmake .
```

Press ***c*** to configure and then press ***t***. Scroll down until the option ***CUDA_SEPARABLE_COMPILATION*** and make sure that it is turned ON by pressing [enter]. Press ***c*** and then press ***g*** to generate and exit. After that run

```
$ make
```

This will create the binary file **mt** in the same folder that you could use to run the code.

3 Initial structure preparation

3.1 Coordinate- and angle-files creation

Go to the **mt_assembly_hydrolysis/scripts** folder and run

```
$ python2 concentration.py C
```

where ***C*** is the concentration in μM. If you want to change the size of the cylinder box, open the file with a text editor and change the values of the radius and the height of the cylinder: ***rep_r*** (the radius of the cylinder box, 80 nm by default) and ***rep_h*** (the height of the cylinder box, 400 nm by default). The value of the height will define the maximum length of the MT.
After script is run, the further instructions will be displayed:

```
Free particles # (dimers) = 120

Recommended extra# of dimers = 109

1) Launch python make_mt_cncntr.py length extra#

2) Compile with LJ and REPULSIVE, no MORSE, no ASSEMBLY, no MT_LENGTH, no CONCentration.
3) Simulate *.pdb files for 10 million steps and fix = 1, runnum = 1;
4) Take result.pdb as initial structure
5) Compile with LJ, CONC, MORSE, ASSEMBLY, MT_LENGTH
6) Simulate trajectory with any runnum, fix = 1 and so on.
```

Here, the number of free dimers is the number of dimers present in the solution at any given time. Recommended extra number is the number of 'inactive' dimers that are stored outside the box and released into the box if some dimers are attached to the MT lattice to maintain a constant concentration. Length is the initial length of the MT (in monomers, should be even).
The next step is to create the very first initial pdb-file. Before we start the assemble from the seed, we need to create a long MT, so launch

```
$ python make_mt_cncntr.py 2 109
```

and change the values of the length and the number of free dimers to the values you need. The coordinate- and angle-files are located in the

mt_assembly_hydrolysis/scripts/structs and named as **xyz_2_109.pdb** and **ang_2_109.pdb**

3.2 Free dimers concentration and start of the MD run

Create a folder **name1**. Copy **mt** binary file form **mt_assembly_hydrolysis** to this folder. Copy all configuration files from the folder **config_for_dis** into **name1**. In **config.conf** change the names of coordinate- and angle-files in the field "#file to read coordinates from". Also create folder **dcd** and put **xyz_2_109.pdb** and **ang_2_109.pdb** inside of it. Run:

```
$ ./mt config.conf
```

The first part of the simulation will be just a diffusion of free dimers from the top of the cylinder. After the distibution of the dimers will be uniform the actual run will start. It is recommended to restart the simulation from this point by saving one of the intermediate frames as a new pdb-file (for both, angles and coordinates) and start new simulation with these pdb-files as initial..

3.3 Configuration files

Here, some parameters that could be changed will be described

3.3.1 cond.conf

- is_const_conc - condition if concentration of free dimers is constant (yes/no)
- conc - the concentration of free dimers (value in μM)
- hydrolysis - condition if there is a hydrolysis in the simulation (yes/no)
- khydro - the hydrolysis rate constant (value in 1/s)

3.3.2 morf.conf

The only parameter that could be changed in this configuration file is ***rep_h*** if you changed it previously.

3.3.3 config.conf

- device - the ID of the GPU you want to use for the calculations
- rseed - the seed for the random number generator. Change it every time you work with the new system
- dt - time step in ps. Decrease it if you have any problems with steric clashes
- stride - the frequency of updating and saving of output files
- steps - the total number of steps
- coordinates_xyz - the path to the initial coordinate file
- coordinates_ang - the path to the initial angle file
- fix - the number of layers (in monomers, so should be even) that will be fixed.
- runnum - the number of runs that will be processed in parallel. Not recommended to set the value higher than 5
- tubule_length - condition if the output file with MT length will be saved (yes/no)
- output_energy - condition if the output file with energies will be saved (yes/no)
- output_force - condition if the output file with forces will be saved (yes/no)

The rest of the parameters were parameterized and tuned but could be changed at your own risk.
