AWSEM tutorial

Requirements

Linux
VMD 1.9.3 [http://www.ks.uiuc.edu/]
Grace [http://plasma-gate.weizmann.] or GNUplot (sudo apt-get gnuplot grace)
Python (sudo apt-get python python-pip – sudo pip install biopython – sudo pip install numpy)
LAMMPS and AWSEM (attached file – read README.md file for installation)

1) Untar the programs file we sent you.

```
tar -xvf 'lammps-awsem.tar.bz2'
```

Or download a zip from https://github.com/Tatotavella/Workshop-3_PBATEOTW_Chile

Go to lammps-awsem/src and write:

```
make clean
make all
```

Check if a lmp_serial file appears in lammps-awsem/bin

2) Go to Tools folder and run

```
dir = lammps-awsem
cd $dir/tools
cd lammps-awsem/tools
./install_tools.sh
```

3) Make a folder to run the examples **inside lammps-awsem** folder.

```
mkdir monomer    (you have to be in lammps-awsem folder!!)
cp ../bin/lmp_serial ./monomer/  (copy executable to folder)
```

4) **Monomer structure prediction**

a) Go to PDB and download the protein with the code 1R69 (https://www.rcsb.org/structure/1r69)
b) Copy 1r69.pdb inside monomer directory
c) Run the script to generate initial LAMMPS files **(from within monomer folder)**:

```
../tools/PdbCoords2Lammps.sh 1r69 1r69
```

d) File copying:

```
cp $dir/parameters/* .
cp $dir/monomer_backup_files/unfold.restart .
```

```
cp $dir/monomer_backup_files/1r69.mem .

python $dir/src/awsemmd-CGpH/create_project_tools/GetCACADistancesFile.py 1r69
rnative.da t

python $dir/src/awsemmd-CGpH/create_project_tools/GetCACoordinatesFromPDB.py 1r69
nativecoords.dat
```

Go to JPRED homepage: http://www.compbio.dundee.ac.uk/www-jpred/

Feed the sequence from fasta file into JPRED. Choose to continue carrying out a Jpred prediction. When the prediction is complete, look at the prediction in “ViewSimple”

Copy the JPRED prediction into a new text file, called IDjpred
Call command to generate ssweight file

```
python $dir/create_project_tools/GenSswight.py IDjpred ssweight
```

Edit 1r69.in file:

Go to the read_data line and write:

```
read_restart unfolded.restart.1r69
```

Go to the velocity attribute and write:

```
velocity 800.0 XXXXXXX
```

where in the “XXXXXX” you have to write any number of 7 digits (This is the random seed!)
Go to the fix 1 line and replace by:

```
fix             1 all nvt temp 800.0 200.0 100.0
```

Under the fix 2 add the calculation of extra variables:

```
compute     qw alpha_carbons qwolynes rnative.dat 2 0.15
variable    qw equal c_qw
compute     rg alpha_carbons gyration
variable    rg equal c_rg
compute qo alpha_carbons qonuchic cutoff 12.0 (continues next line)
        nativecoords.dat 1.2
variable    qo equal c_qo
compute     tc beta_atoms totalcontacts 6.5 2
variable    tc equal c_tc
variable    S_T equal step
variable    E_P equal pe
```

```
variable     T_E equal temp
```

And under this add the file writing **(in one line)**:

```
fix    4 all print 1000 "${S_T} ${T_E} ${qw} ${rg} ${qo} ${tc}
${E_P}" file extra_variables.dat screen no
   title "# Tstep Temp Qw Rg Qo Tc Energy"
```

Got to the thermo line and write:

```
thermo       1000
```

Go to the dump line and write:

```
dump         1 all atom 1000 dump.lammpstrj
```

Go to the run line and write:

```
run          1000000
```

e) Run your simulation!

```
./lmp_serial < 1r69.in
```

5) Follow https://github.com/adavtyan/awsemmd/wiki for dimer prediction or monomer prediction steps.

7) You can try with a protein of your own interests.

8) You can follow AMH-Go calculations.

9) Try to repeat calculations with the fragment memory style.