

```

1 #####EQUILIBRATION RUN#####
2 structure                step3_input.psf
3 coordinates              step3_input.pdb
4
5 set temp                  310.15;
6
7 set outputname            step4_equilibration;
8
9 # read system values written by CHARMM (need to convert uppercases to lowercases)
10 exec tr "\[:upper:\]" "\[:lower:\]" < ../step3_pbcsetup.str | sed -e "s/ =//g" >
   step3_input.str
11 source                   step3_input.str
12
13 temperature              $temp;
14
15 outputName                $outputname;      # base name for output from this run
16                                     # NAMD writes two files at the end, final
17                                     # in the format of first-dyn.coor and
18                                     # first-dyn.vel
19 firsttimestep             0;                # last step of previous run
20 restartfreq               50000;            # 500 steps = every 1ps
21 dcdfreq                   50000;
22 dcdUnitCell               yes;              # the file will contain unit cell info in
   the style of
23                                     # charmm dcd files. if yes, the dcd files
24                                     # will contain
25                                     # unit cell information in the style of
26                                     # charmm DCD files.
27 xstFreq                   50000;            # XSTFreq: control how often the extended
   system configuration
28                                     # will be appended to the XST file
29 outputEnergies            50000;            # 125 steps = every 0.25ps
30                                     # The number of timesteps between each
31                                     # energy output of NAMD
32 outputTiming              50000;            # The number of timesteps between each
   timing output shows
33                                     # time per step and time to completion
34
35 # Force-Field Parameters
36 paraTypeCharmm            on;               # We're using charmm type parameter file(s)
37                                     # multiple definitions may be used but only
38                                     # one file per definition
39
40 parameters                toppar/par_all36m_prot.prm
41 parameters                toppar/par_all36_na.prm
42 parameters                toppar/par_all36_carb.prm
43 parameters                toppar/par_all36_lipid.prm
44 parameters                toppar/par_all36_cgenff.prm
45 parameters                toppar/par_interface.prm
46 parameters                toppar/toppar_all36_moreions.str
47 parameters                toppar/toppar_all36_nano_lig.str
48 parameters                toppar/toppar_all36_nano_lig_patch.str
49 parameters                toppar/toppar_all36_synthetic_polymer.str
50 parameters                toppar/toppar_all36_synthetic_polymer_patch.str
51 parameters                toppar/toppar_all36_polymer_solvent.str
52 parameters                toppar/toppar_water_ions.str
53 parameters                toppar/toppar_dum_noble_gases.str
54 parameters                toppar/toppar_ions_won.str
55 parameters                toppar/toppar_all36_prot_arg0.str
56 parameters                toppar/toppar_all36_prot_c36m_d_aminoacids.str
57 parameters                toppar/toppar_all36_prot_fluoro_alkanes.str
58 parameters                toppar/toppar_all36_prot_heme.str
59 parameters                toppar/toppar_all36_prot_na_combined.str
60 parameters                toppar/toppar_all36_prot_retinol.str
61 parameters                toppar/toppar_all36_prot_model.str
62 parameters                toppar/toppar_all36_prot_modify_res.str
63 parameters                toppar/toppar_all36_na_nad_ppi.str
64 parameters                toppar/toppar_all36_na_rna_modified.str

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60 parameters toppar/toppar_all136_lipid_sphingo.str
61 parameters toppar/toppar_all136_lipid_archaeal.str
62 parameters toppar/toppar_all136_lipid_bacterial.str
63 parameters toppar/toppar_all136_lipid_cardiolipin.str
64 parameters toppar/toppar_all136_lipid_cholesterol.str
65 parameters toppar/toppar_all136_lipid_dag.str
66 parameters toppar/toppar_all136_lipid_inositol.str
67 parameters toppar/toppar_all136_lipid_lnp.str
68 parameters toppar/toppar_all136_lipid_lps.str
69 parameters toppar/toppar_all136_lipid_mycobacterial.str
70 parameters toppar/toppar_all136_lipid_miscellaneous.str
71 parameters toppar/toppar_all136_lipid_model.str
72 parameters toppar/toppar_all136_lipid_prot.str
73 parameters toppar/toppar_all136_lipid_tag.str
74 parameters toppar/toppar_all136_lipid_yeast.str
75 parameters toppar/toppar_all136_lipid_hmmm.str
76 parameters toppar/toppar_all136_lipid_detergent.str
77 parameters toppar/toppar_all136_lipid_ether.str
78 parameters toppar/toppar_all136_carb_glycolipid.str
79 parameters toppar/toppar_all136_carb_glycopeptide.str
80 parameters toppar/toppar_all136_carb_imlab.str
81 parameters toppar/toppar_all136_label_spin.str
82 parameters toppar/toppar_all136_label_fluorophore.str
83 parameters ../lig/lig.prm # Custom topology and parameter files for LIG
84
85 # Nonbonded Parameters
86 exclude scaled1-4 # non-bonded exclusion policy to use
87 "none,1-2,1-3,1-4,or scaled1-4"
88 # 1-2: all atoms pairs that are bonded are
89 # going to be ignored
90 # 1-3: 3 consecutively bonded are excluded
91 # scaled1-4: include all the 1-3, and
92 # modified 1-4 interactions
93 # electrostatic scaled by 1-4scaling factor
94 1.0
95 # vdW special 1-4 parameters in charmm
96 # parameter file.
97
98 1-4scaling 1.0
99 switching on
100 vdwForceSwitching on; # New option for force-based switching of vdW
101 # if both switching and vdwForceSwitching
102 # are on CHARMM force
103 # switching is used for vdW forces.
104
105 # You have some freedom choosing the cutoff
106 cutoff 12.0; # may use smaller, maybe 10., with PME
107 switchdist 10.0; # cutoff - 2.
108 # switchdist - where you start to switch
109 # cutoff - where you stop accounting for
110 # nonbond interactions.
111 # correspondence in charmm:
112 # (cutnb,ctofnb,ctonnb =
113 # pairlistdist,cutoff,switchdist)
114 # stores the all the pairs with in the
115 # than cutoff( + 2.)
116 pairlistdist 16.0;
117 distance it should be larger
118 # 20 redo pairlists every ten steps
119 stepspercycle 20;
120 pairlistsPerCycle 2; # 2 is the default
121 # cycle represents the number of steps
122 # between atom reassignments
123 # this means every 20/2=10 steps the
124 # pairlist will be updated
125
126 # Integrator Parameters
127 timestep 2.0; # fs/step
128 rigidBonds all; # Bound constraint all bonds involving H are
129 fixed in length
130 nonbondedFreq 1; # nonbonded forces every step
131 fullElectFrequency 1; # PME every step

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117
118 # Constant Temperature Control ONLY DURING EQUILB
119 reassignFreq      10000;          # reassignFreq: use this to reassign
velocity every 500 steps
120 reassignTemp      $temp;
121
122 # Periodic Boundary conditions. Need this since for a start...
123 cellBasisVector1  $a    0.0    0.0;      # vector to the next image
124 cellBasisVector2  0.0    $b    0.0;
125 cellBasisVector3  0.0    0.0    $c;
126 cellOrigin        0.0    0.0    $zcen;    # the *center* of the cell
127
128 wrapWater          on;              # wrap water to central cell
129 wrapAll            on;              # wrap other molecules too
130 wrapNearest        off;            # use for non-rectangular cells (wrap to the
nearest image)
131
132 # PME (for full-system periodic electrostatics)
133 PME                yes;
134 PMEInterpOrder     6;              # interpolation order (spline order 6 in
charmm)
135 PMEGridSpacing     1.0;            # maximum PME grid space / used to calculate
grid size
136
137 # Constant Temperature Control
138 langevin            on
139 langevinDamping     1.0
140 langevinTemp        $temp
141 langevinHydrogen    off
142
143 constraints         on
144 consexp             2
145 consref             restraints/prot_posres.ref
146 conskfile           restraints/prot_posres.ref
147 conskcol            B
148 constraintScaling   1.0
149
150 minimize            50000
151 run                 5000000;        # 10ns
152 #####PRODUCTION RUN#####
153 structure           step3_input.psf
154 coordinates         step3_input.pdb
155
156 set temp             310.15;
157 outputName          step5_production; # base name for output from this run
158                                     # NAMD writes two files at the end, final
                                     # coord and vel
159                                     # in the format of first-dyn.coor and
                                     # first-dyn.vel
160
161 set inputname        step4_equilibration;
162 binCoordinates       $inputname.coor; # coordinates from last run (binary)
163 binVelocities        $inputname.vel;  # velocities from last run (binary)
164 extendedSystem       $inputname.xsc;  # cell dimensions from last run (binary)
165
166 dcdfreq              5000;
167 dcdUnitCell          yes;            # the file will contain unit cell info in
the style of
168                                     # charmm dcd files. if yes, the dcd files
                                     # will contain
169                                     # unit cell information in the style of
                                     # charmm DCD files.
170 xstFreq              5000;          # XSTFreq: control how often the extended
system configuration
171                                     # will be appended to the XST file
172 outputEnergies       5000;          # 5000 steps = every 10ps
173                                     # The number of timesteps between each
                                     # energy output of NAMD
174 outputTiming         5000;          # The number of timesteps between each

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timing output shows
175                                     # time per step and time to completion
176 restartfreq           5000;         # 5000 steps = every 10ps
177
178 # Force-Field Parameters
179 paraTypeCharmm         on;           # We're using charmm type parameter file(s)
180                                     # multiple definitions may be used but only
                                      # one file per definition
181 parameters             toppar/par_all36m_prot.prm
182 parameters             toppar/par_all36_na.prm
183 parameters             toppar/par_all36_carb.prm
184 parameters             toppar/par_all36_lipid.prm
185 parameters             toppar/par_all36_cgenff.prm
186 parameters             toppar/par_interface.prm
187 parameters             toppar/toppar_all36_moreions.str
188 parameters             toppar/toppar_all36_nano_lig.str
189 parameters             toppar/toppar_all36_nano_lig_patch.str
190 parameters             toppar/toppar_all36_synthetic_polymer.str
191 parameters             toppar/toppar_all36_synthetic_polymer_patch.str
192 parameters             toppar/toppar_all36_polymer_solvent.str
193 parameters             toppar/toppar_water_ions.str
194 parameters             toppar/toppar_dum_noble_gases.str
195 parameters             toppar/toppar_ions_won.str
196 parameters             toppar/toppar_all36_prot_arg0.str
197 parameters             toppar/toppar_all36_prot_c36m_d_aminoacids.str
198 parameters             toppar/toppar_all36_prot_fluoro_alkanes.str
199 parameters             toppar/toppar_all36_prot_heme.str
200 parameters             toppar/toppar_all36_prot_na_combined.str
201 parameters             toppar/toppar_all36_prot_retinol.str
202 parameters             toppar/toppar_all36_prot_model.str
203 parameters             toppar/toppar_all36_prot_modify_res.str
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205 parameters             toppar/toppar_all36_na_rna_modified.str
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207 parameters             toppar/toppar_all36_lipid_archaeal.str
208 parameters             toppar/toppar_all36_lipid_bacterial.str
209 parameters             toppar/toppar_all36_lipid_cardiolipin.str
210 parameters             toppar/toppar_all36_lipid_cholesterol.str
211 parameters             toppar/toppar_all36_lipid_dag.str
212 parameters             toppar/toppar_all36_lipid_inositol.str
213 parameters             toppar/toppar_all36_lipid_lnp.str
214 parameters             toppar/toppar_all36_lipid_lps.str
215 parameters             toppar/toppar_all36_lipid_mycobacterial.str
216 parameters             toppar/toppar_all36_lipid_miscellaneous.str
217 parameters             toppar/toppar_all36_lipid_model.str
218 parameters             toppar/toppar_all36_lipid_prot.str
219 parameters             toppar/toppar_all36_lipid_tag.str
220 parameters             toppar/toppar_all36_lipid_yeast.str
221 parameters             toppar/toppar_all36_lipid_hmmm.str
222 parameters             toppar/toppar_all36_lipid_detergent.str
223 parameters             toppar/toppar_all36_lipid_ether.str
224 parameters             toppar/toppar_all36_carb_glycolipid.str
225 parameters             toppar/toppar_all36_carb_glycopeptide.str
226 parameters             toppar/toppar_all36_carb_imlab.str
227 parameters             toppar/toppar_all36_label_spin.str
228 parameters             toppar/toppar_all36_label_fluorophore.str
229 parameters             ../lig/lig.prm # Custom topology and parameter files for LIG
230
231 # Nonbonded Parameters
232 exclude                 scaled1-4    # non-bonded exclusion policy to use
    "none,1-2,1-3,1-4,or scaled1-4"
233                                     # 1-2: all atoms pairs that are bonded are
                                      # going to be ignored
234                                     # 1-3: 3 consecutively bonded are excluded
235                                     # scaled1-4: include all the 1-3, and
                                      # modified 1-4 interactions
236                                     # electrostatic scaled by 1-4scaling factor
                                      # 1.0
237                                     # vdW special 1-4 parameters in charmm

```

```

238 1-4scaling 1.0
239 switching on
240 vdWForceSwitching on; # New option for force-based switching of vdW
241 # if both switching and vdWForceSwitching
# are on CHARMM force
242 # switching is used for vdW forces.
243
244 # You have some freedom choosing the cutoff
245 cutoff 12.0; # may use smaller, maybe 10., with PME
246 switchdist 10.0; # cutoff - 2.
247 # switchdist - where you start to switch
248 # cutoff - where you stop accounting for
nonbond interactions.
249 # correspondence in charmm:
250 # (cutnb,ctofnb,ctonnb =
pairlistdist,cutoff,switchdist)
251 pairlistdist 16.0; # stores the all the pairs with in the
distance it should be larger
252 # than cutoff( + 2.)
253 stepspercycle 20; # 20 redo pairlists every ten steps
254 pairlistsPerCycle 2; # 2 is the default
255 # cycle represents the number of steps
between atom reassignments
256 # this means every 20/2=10 steps the
pairlist will be updated
257
258 # Integrator Parameters
259 timestep 2.0; # fs/step
260 rigidBonds all; # Bound constraint all bonds involving H are
fixed in length
261 nonbondedFreq 1; # nonbonded forces every step
262 fullElectFrequency 1; # PME every step
263
264 wrapWater on; # wrap water to central cell
265 wrapAll on; # wrap other molecules too
266 wrapNearest off; # use for non-rectangular cells (wrap to the
nearest image)
267
268 # PME (for full-system periodic electrostatics)
269 PME yes;
270 PMEInterpOrder 6; # interpolation order (spline order 6 in
charmm)
271 PMEGridSpacing 1.0; # maximum PME grid space / used to calculate
grid size
272
273 # Constant Pressure Control (variable volume)
274 useGroupPressure yes; # use a hydrogen-group based
pseudo-molecular viral to calcualte pressure and
275 # has less fluctuation, is needed for rigid
bonds (rigidBonds/SHAKE)
276 useFlexibleCell no; # yes for anisotropic system like membrane
277 useConstantRatio no; # keeps the ratio of the unit cell in the
x-y plane constant A=B
278
279 # Constant Temperature Control
280 langevin on; # langevin dynamics
281 langevinDamping 1.0; # damping coefficient of 1/ps (keep low)
282 langevinTemp $temp; # random noise at this level
283 langevinHydrogen off; # don't couple bath to hydrogens
284
285 # Constant pressure
286 langevinPiston on; # Nose-Hoover Langevin piston pressure
control
287 langevinPistonTarget 1.01325; # target pressure in bar 1atm = 1.01325bar
288 langevinPistonPeriod 50.0; # oscillation period in fs. correspond to
pgamma T=50fs=0.05ps
289 # f=1/T=20.0(pgamma)
290 langevinPistonDecay 25.0; # oscillation decay time. smaller value
parameter file.

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corresponds to larger random
291
292                                     # forces and increased coupling to the
                                     Langevin temp bath.
293 langevinPistonTemp      $temp;    # Equal or smaller than piston period
294                                     # coupled to heat bath
295 # run
296 run                      20000000;    # 80ns
297
```