

Sample Input for Frenkel & Smit Case Study 4

The file below is the input script run distributed with the original distribution of Frenkel and Smit's case study 4. Relevant variables for the run are highlighted in blue. In each case, the value of these variables is set in the line underneath the list of variable names. The highlighted variable names are defined below after the script listing.

```
#!/bin/csh -f

foreach temp (0.728)
  echo " --- temp ${temp} "
  echo " --- temp ${temp} " >> out
  cat > fort.15 <<endofdata
  ibeg , delt tmax tequil nsamp
  0 0.001 .5 0.00 1
  npart temp rho rcp iseed
  108 ${temp} 0.8442 2.5 123456
  scale temp
  .true. 0.728
  iout igr iout2 ivacf t0vacf t0stress iout3 iout4
  33 10 34 10000000 100 100000 35 36
  samp1 samp2 tdifmax
  .true. .false. 100
endofdata
cp lj.res fort.11
time ../Source/MD >> out
cp fort.21 lj.res
mv fort.66 lj.prt
mv fort.33 lj.gr
#perform block analysis
cp lj.prth fort.31
mv lj.prt fort.32
../Appendix/block >> out
rm fort.*
end
exit
```

Variable Definitions: Note that all dimensional quantities are in reduced units.

delt = time step in reduced units

tmax = total length of run

tequil = interval at beginning of run not used for data averaging*

nsamp = # of steps between two samples for static averages

npart = # of particles in system

temp (first time) = temperature assigned for initial velocity distribution

rho = density

rcp = cutoff radius for Lennard-Jones potential

iseed = seed for random number generator

scale = logical variable to indicate whether velocity rescaling is used in initialization

temp (second time) = assigned temperature after velocity scaling**

igr = # of time steps between averaging of data for radial distribution function, $g(r)$

*For example, if $tmax = 2.0$ and $tequil = 1.5$, data is only averaged over the last 0.5 units of time.

**Note that velocity rescaling is applied at the end of the equilibration run.