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 , \textcolor{blue}{delt} t\textcolor{blue}{max} tequil nsamp
    0 0.001 .5 0.00 1
    npart \textcolor{blue}{temp} rho rcp iseed
    108 \$\{temp\} 0.8442  2.5  123456
    scale \textcolor{blue}{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.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textit{delt}</td>
<td>time step in reduced units</td>
</tr>
<tr>
<td>\textit{tmax}</td>
<td>total length of run</td>
</tr>
<tr>
<td>\textit{tequil}</td>
<td>interval at beginning of run not used for data averaging*</td>
</tr>
<tr>
<td>\textit{nsamp}</td>
<td># of steps between two samples for static averages</td>
</tr>
<tr>
<td>\textit{npart}</td>
<td># of particles in system</td>
</tr>
<tr>
<td>\textit{temp} (first time)</td>
<td>temperature assigned for initial velocity distribution</td>
</tr>
<tr>
<td>\textit{rho}</td>
<td>density</td>
</tr>
<tr>
<td>\textit{rcp}</td>
<td>cutoff radius for Lennard-Jones potential</td>
</tr>
<tr>
<td>\textit{iseed}</td>
<td>seed for random number generator</td>
</tr>
<tr>
<td>\textit{scale}</td>
<td>logical variable to indicate whether velocity rescaling is used in initialization</td>
</tr>
<tr>
<td>\textit{temp} (second time)</td>
<td>assigned temperature after velocity scaling**</td>
</tr>
<tr>
<td>\textit{igr}</td>
<td># of time steps between averaging of data for radial distribution function, g(r)</td>
</tr>
</tbody>
</table>

*For example, if \textit{tmax} = 2.0 and \textit{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.