Molecular Dynamics

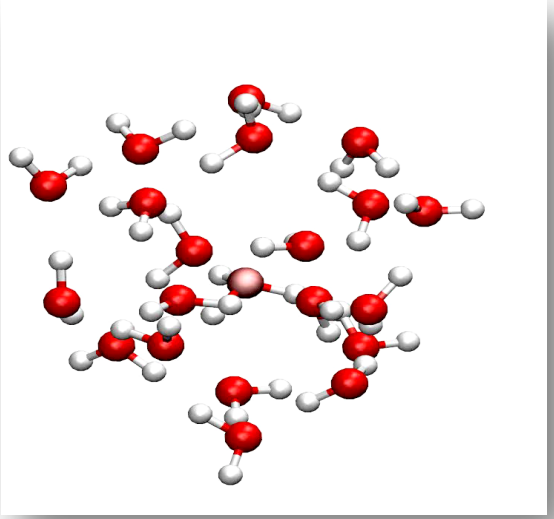
Tutorial

Starting Structure and Visualization

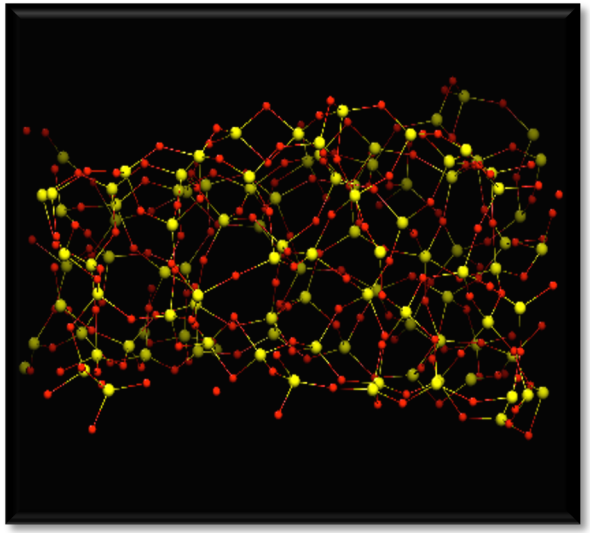
Coordinates of starting configuration:

1) From Crystal Structure

2) Built based on chemical intuition



Water Clusters



Amorphous Silica

Using DLPOLY for MD Simulations

Now we will compile the code. To do this move to the **srcmod** directory which is a sub-directory of MDTutorial.

Type: **make clean** (to delete any files from old compilations)

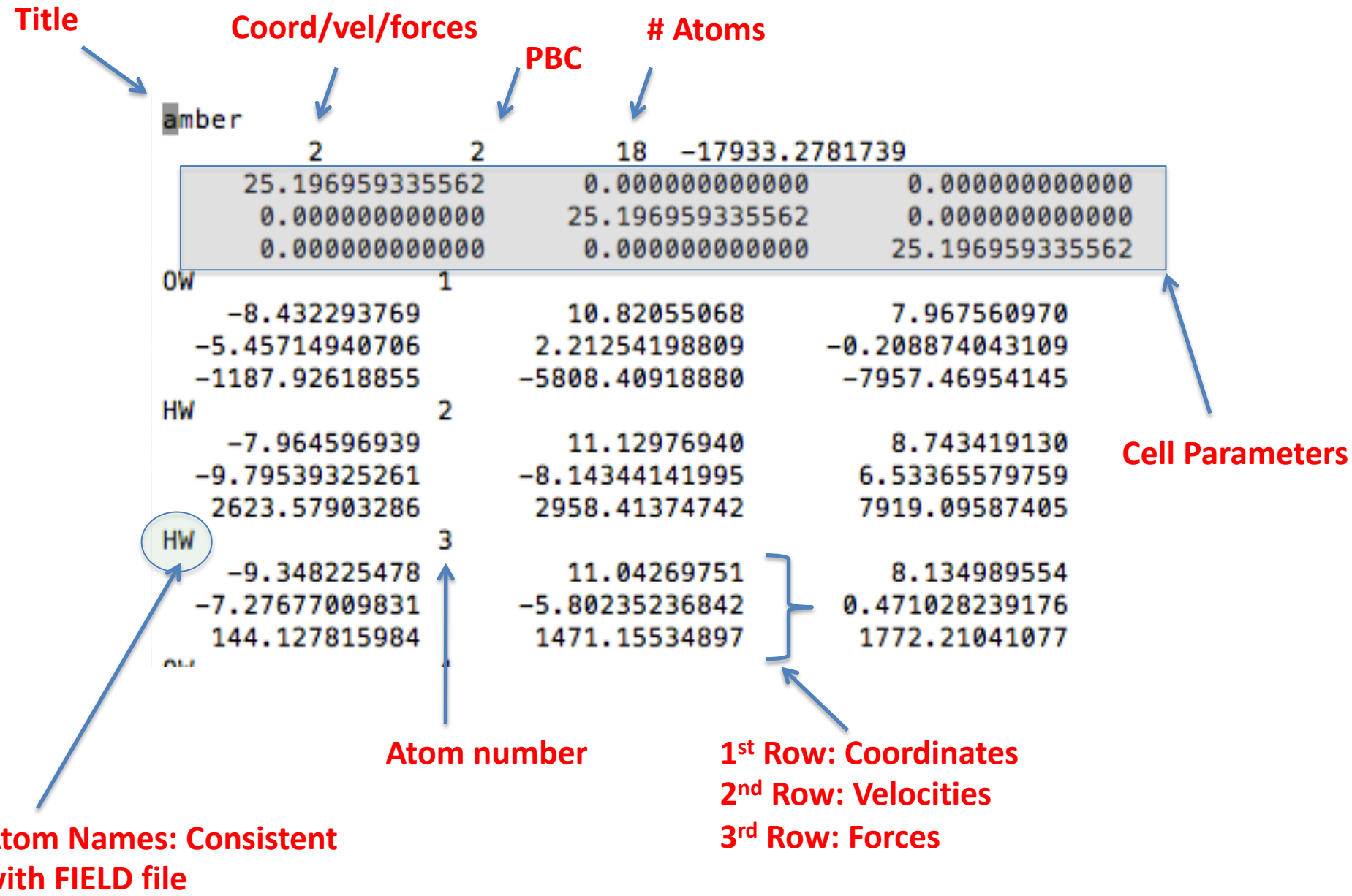
Type: **make gfortran** (you should see that the different files in that directory are getting compiled

Once this is successfully completed you should see a DLPOLY.X executable in the execute directory which is one directory above the current one you are working in. Simply do: **ls –al ../execute/**

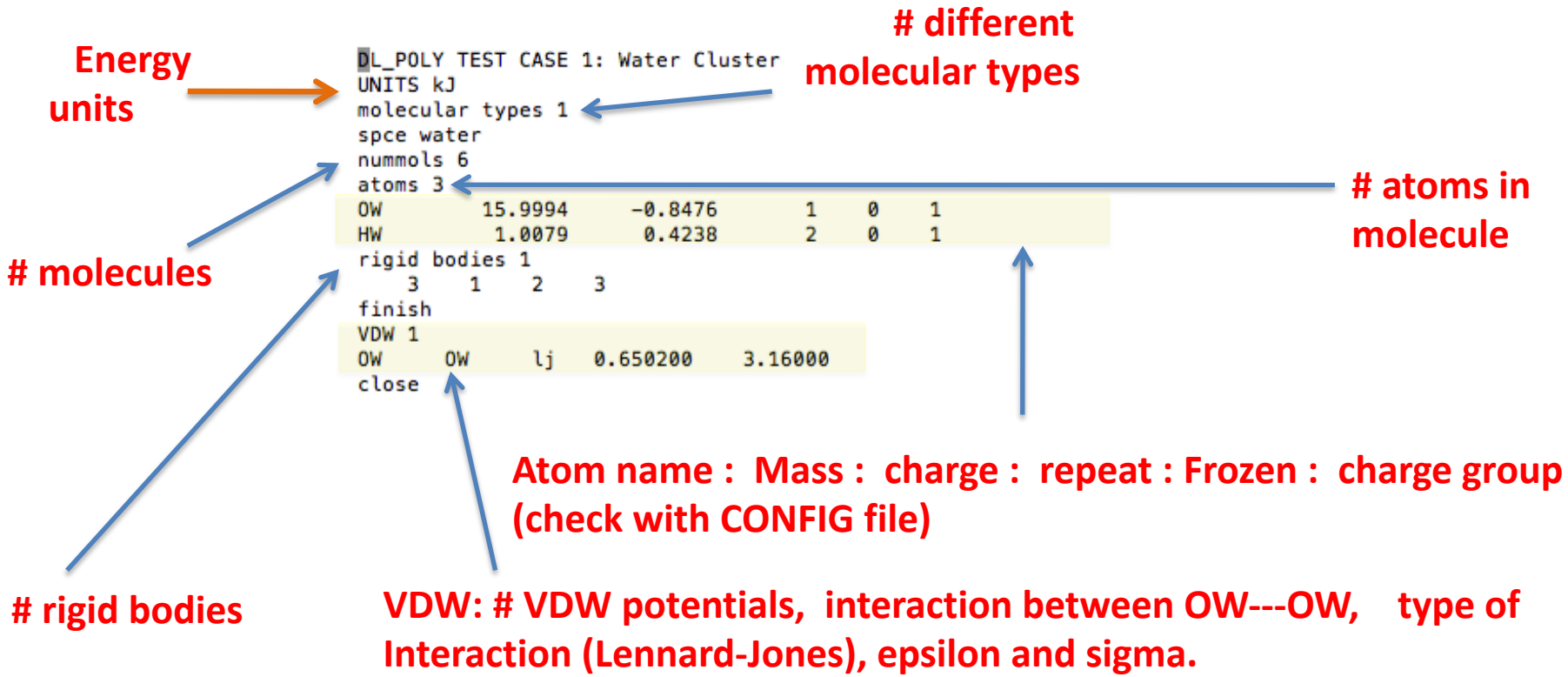
To run DLPOLY do: ../execute/DLPOLY.X

NOTE: TO RUN DLPOLY.X YOU NEED THE CONFIG, CONTROL AND FIELD FILES IN THE DIRECTORY YOU ARE WORKING IN. IF YOU TRY IT AS ABOVE, YOU SHOULD GET AN ERROR IN THE OUTPUT FILE. THIS IS A GOOD SIGN. AFTER YOU GET TO THIS STEP, GET ON SLACK AND SAY "YES I GOT THE ERROR"!

DLPOLY input files: CONFIG



DLPOLY input files: FIELD



DLPOLY input files: CONTROL

```
DL_POLY TEST CASE 3: Polymer in Water

integrator leap frog

temperature          100
pressure           0.001

ensemble nvt hoover 0.2

steps               5000

equilibration          0
scale                  0
print                100
stack                100
stats                 10

timestep           0.005
delr width        1.2000
cutoff             9.000
rvdw cutoff        9.000

shake tolerance    1.0E-6
ewald precision    1.0E-6

#ewald sum 0.36 2 2 2

cap forces 100.

rdf                10 0.05
print rdf
zden

#plumed on
#plumedfile plumed.dat

traj nstraj 0 istraj 100 keytrj 0

job time          50000000.00
close time           1000.00

finish
```

Numerical Integrator for F=ma (variant of Verlet)

Ensemble (NVE, NVT), thermostat type

Printing options

MD steps

equilibration steps : use with cap-forces

Temperature scaling

MD timestep: 5 fs (units in ps)

Cutoff: coulomb cutoff, rvdw: short range

Bond constraints

Ewald parameters

Equilibration

Printing options for g(r), Z-Density

PLUMED: Free energies etc

Printing options for HISTORY file

Job time (useful for supercomputer jobs)

Files Generated in DLPOLY

OUTPUT: Human readable, Simulation Parameters, Simulation Progress

HISTORY: Trajectory of atomic coordinates, velocities and forces

STATIS: Data file with MD statistics

REVCON: Restart configuration file same format as CONFIG

REVIVE: Accumulated statistical data should be renamed REVOLD for restarts.

RDFDAT: Radial distribution function data.

ZDNDAT: Z-Density data.

Useful Script/Commands to Use

After each DLPOLY MD simulation there will be a file called STATIS that contains A LOT of information on the conserved quantity, temperature, potential energy etc etc

We will use a small function pickstatis to extract some information from the STATIS file so that we can plot it in xmgrace or another plotting tool.

Then we run it as: **pickstatis 1 < STATIS > output.dat**

```
amber
 ENERGY UNITS=kjoule/mol
        10  1.000000E-02        38
-1.649997E+02  1.046468E+02 -1.793576E+02  3.273406E+01 -2.120917E+02
 0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00 -2.078088E+02
 1.438820E+02  1.356022E+02 -6.121436E+02  2.120134E+02  0.000000E+00
 0.000000E+00  0.000000E+00  0.000000E+00  1.599722E+04  0.000000E+00
 0.000000E+00  0.000000E+00  9.000000E+01  9.000000E+01  9.000000E+01
 0.000000E+00 -4.385401E-02  7.635280E-04  1.281173E-02 -8.090824E-02
-5.659242E-03 -2.724850E-02 -5.659242E-03 -2.734355E-02  1.176846E-02
-2.724850E-02  1.176846E-02 -2.331026E-02
        20  2.000000E-02        38
-1.650015E+02  1.189566E+02 -1.813283E+02  3.707538E+01 -2.184037E+02
 0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00 -1.985262E+02
 1.646710E+02  1.085466E+02 -6.728105E+02  2.183279E+02  0.000000E+00
 0.000000E+00  0.000000E+00  0.000000E+00  1.599722E+04  0.000000E+00
 0.000000E+00  0.000000E+00  9.000000E+01  9.000000E+01  9.000000E+01
 0.000000E+00 -3.433674E-02  3.229768E-03  5.126958E-02 -7.000306E-02
-1.858430E-02 -1.758878E-02 -1.858430E-02 -2.165889E-02  4.486834E-03
-1.758878E-02  4.486834E-03 -1.134827E-02
        30  3.000000E-02        38
-1.650030E+02  1.200132E+02 -1.814975E+02  4.219710E+01 -2.236946E+02
 0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00 -1.834095E+02
 1.545521E+02  6.492823E+01 -7.443439E+02  2.236215E+02  0.000000E+00
 0.000000E+00  0.000000E+00  0.000000E+00  1.599722E+04  0.000000E+00
 0.000000E+00  0.000000E+00  9.000000E+01  9.000000E+01  9.000000E+01
 0.000000E+00 -1.882574E-02  7.217556E-03  1.115517E-01 -2.933750E-02
-2.497997E-02 -1.005571E-02 -2.497997E-02 -1.858436E-02  2.296176E-04
-1.005571E-02  2.296176E-04 -8.555354E-03
```

After each run within the various Exercises please save your data using:

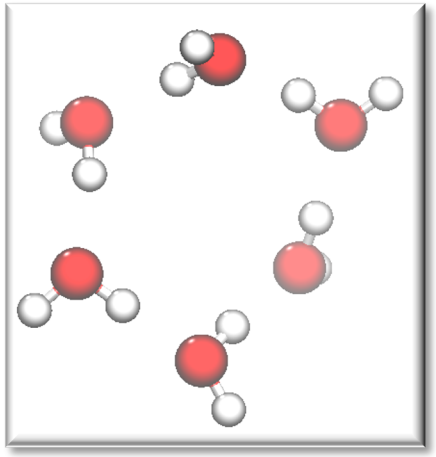
mv DEBUG.dat HISTORY OUTPUT RDFDAT REVCON REVIVE STATIS ZDNDAT Run1

Run1 is just the name of a directory you create

MD Exercises I: Choosing Timestep

Exercise 1

Water Hexamer



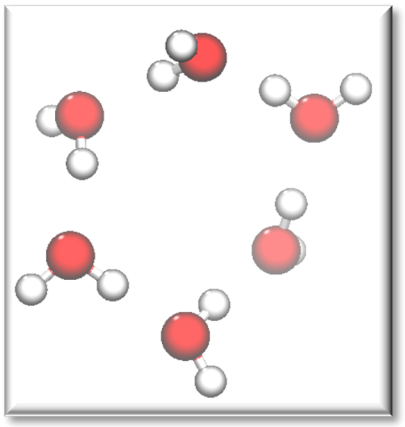
$$\mathbf{r}^N(t+\Delta t) = 2\mathbf{r}^N(t) - \mathbf{r}^N(t-\Delta t) + \Delta t^2\,\mathbf{a}^N(t) + \cdots$$

How do you choose the timestep?

Q1: What could you do to get away with larger timesteps?

Q2: What physically controls the magnitude of the timestep you can take in a simulation?

Exercise II & III: Thermostats



Water Cluster

Simulating systems in the NVT ensemble:

- Choosing the time-constant ?
- Temperature to simulate ?

Q1: How do we know that the system is equilibrated?

Q2: Why does the temperature fluctuate?

Q3: How would the fluctuations in temperature change as we made the system larger?

Q4: Compare and discuss differences between O-O g(r) for simulations thermostatted at 100K and 200K simulations. (Exercise 3 in Tutorial.html)

Visualizing a Trajectory

Type: **vmd** in the terminal

Load the HISTORY file in to VMD

In the terminal type the following:

package require pbctools
pbc set {25.19 25.19 25.19} –all
pbc box