# Problem Set 5

For Problem1 1 see the tar file rdf.tar which contains the code and results. (To open a "tar" archive in unix, type: tar –xvf rdf.tar)

For 2 and 3 see the tar file diatomic.tar. For both the soft and hard bond cases, there is a modified subroutine lattice, which puts the atoms into dimers separated by length 1 (=sigma).

The soft bond case in addition has small changes inparams.inc and subroutine readdat (and fort.10) to input the spring constant. Subroutines mcmove and toterg now call a new subroutine enerb, which adds the bond contributions to the Lennard-Jones ones - new terms erb and virb toadded to energy & virial, respectively. mc_soft.f is the complete code.

In the hard case, instead of calls to enerb, subroutine mcmove has been modified to alternate between rotation and translation moves. The LJ energy between the two atoms in a molecule is irrelevant because it's constant, but subroutine eneri was be modified to omit this term, to avoid counting it twice. Also, subroutine readdat (and fort.10) are modified to read the rotational move parameter gamma (the counterpart of the maximum translation dr). Subroutine adjust should be modified to separately vary gamma and dr so that each has a 50% success rate relative to the total number of attempts, but this is not included in the modified code.