Problem Set 3

For Problems 1 and 4, see the tar files rdf.tar and block_variance.tar, which contain the code and results. (To open a "tar" archive in unix, type: tar –xvf rdf.tar)

For 2 and 3, there is a revised subroutine lattice which places the molecules oriented in the x-direction in two planes of 25 each, parallel to the y-z plane, and numbers them so that the molecules contain atoms 1&2, 3&4, etc.

For Problem 2 there is a revised subroutine mcmove, which allows for separate translations and rotations. To complete a new program, one would also have separate adjust routines to vary the maximum displacements for the two moves.

For Problem 3 there is a complete revised program set in soft_mol.tar.