Class 2: Molecular Dynamics

1. Use `rdesktop` to login to the Windows Terminal Server at `minsc.oerc.ox.ac.uk` (use your supercomputer login credentials). *Note:* please do not hammer the terminal server with large calculations.

2. Draw a glucose molecule in GaussView, and save it as a .mol file. Start HyperChem and load the .mol file.

3. Set the calculation method (Menu/Setup) to Molecular Mechanics/AMBER and run the geometry optimization.

4. Run a 1-picosecond MD trajectory (Menu/Compute/Molecular Dynamics) at 10K, then another 1-picosecond MD trajectory at 400K, then another trajectory at 1000K. Observe the dynamics and the fact that the chemical bonds do not break.

5. Add water and a periodic box (12 x 12x 12 Å) to the system (Menu/Setup/Periodic Box) and switch the display to ball-and-cylinder (Display/Rendering). Display the hydrogen bonds (Display/Recompute H Bonds).

6. Optimize the geometry and watch the water arrange itself into a hexagonal lattice. Observe water jumps across the periodic box and hydrogen bonds between water molecules across the opposite boundaries.

7. Run a 1-picosecond MD trajectory with an option to store the snapshots in a file. Observe the size of the resulting .snp file.

8. Run a 1-picosecond MD trajectory with an option to display the time dependence of system parameters. Observe the conservation of energy and the noisy time dependence of the system temperature.

9. Create a 15x15x15 Å box of water, optimize the geometry and run a 5-picosecond MD trajectory with the temperature set to decrease from 400K to 200K over the course of the trajectory. Observe the freezing of water.