

The images in this solutions file were made with VMD/NAMD/BioCoRE/JMV/other software support. VMD/NAMD/BioCoRE/JMV/ is developed with NIH support by the Theoretical and Computational Biophysics group at the Beckman Institute, University of Illinois at Urbana-Champaign. Courtesy of the Theoretical and Computational Biophysics group at the Beckman Institute, University of Illinois at Urbana-Champaign. Used with permission.

## 10.675 Assignment #5

due 11/23/04

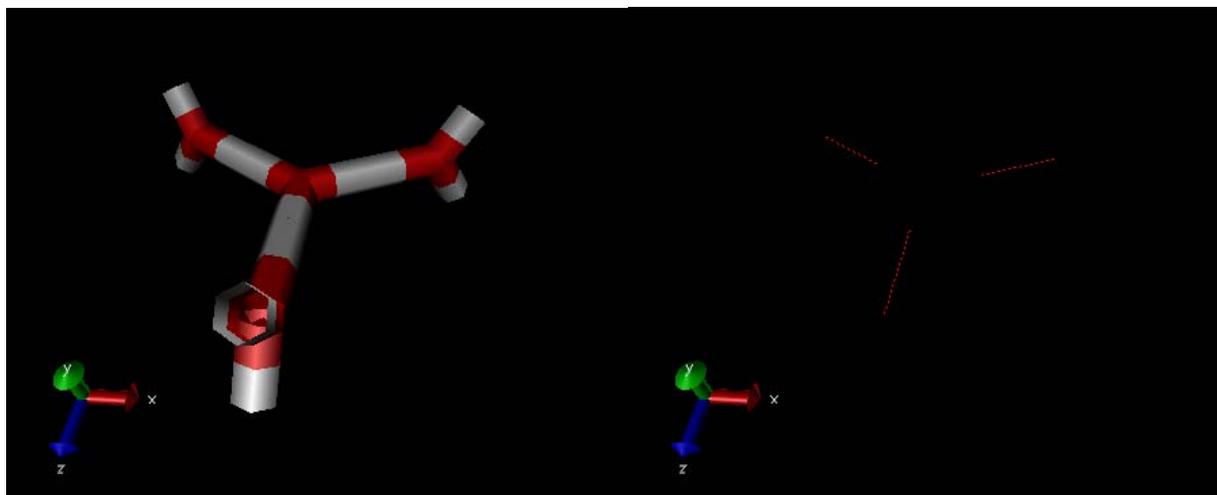
In this problem set, you will use CPMD to study the dynamics of a proton transferring among water molecules ( $\text{H}_2\text{O}$ ). And you can compare what you observe with the literature report (Ref: *Nature*, vol. **397**, 1999, 601).

Solution:

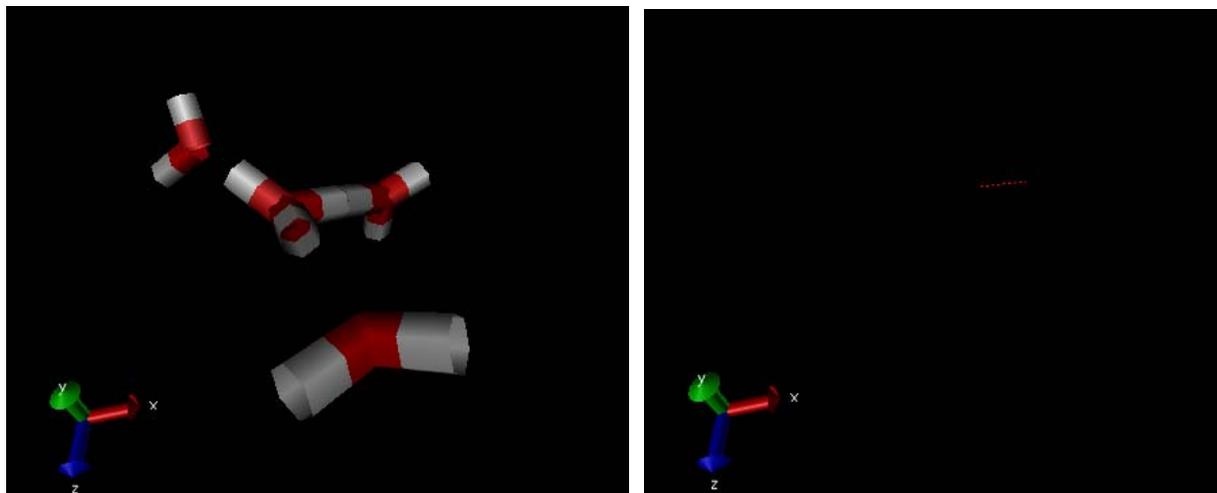
The detailed procedure has been described in the problem statement. Here in the solution, we will only present the snapshots from the simulations (5000 steps).

**[Left: DynamicBond; Right: Hydrogen Bond]**

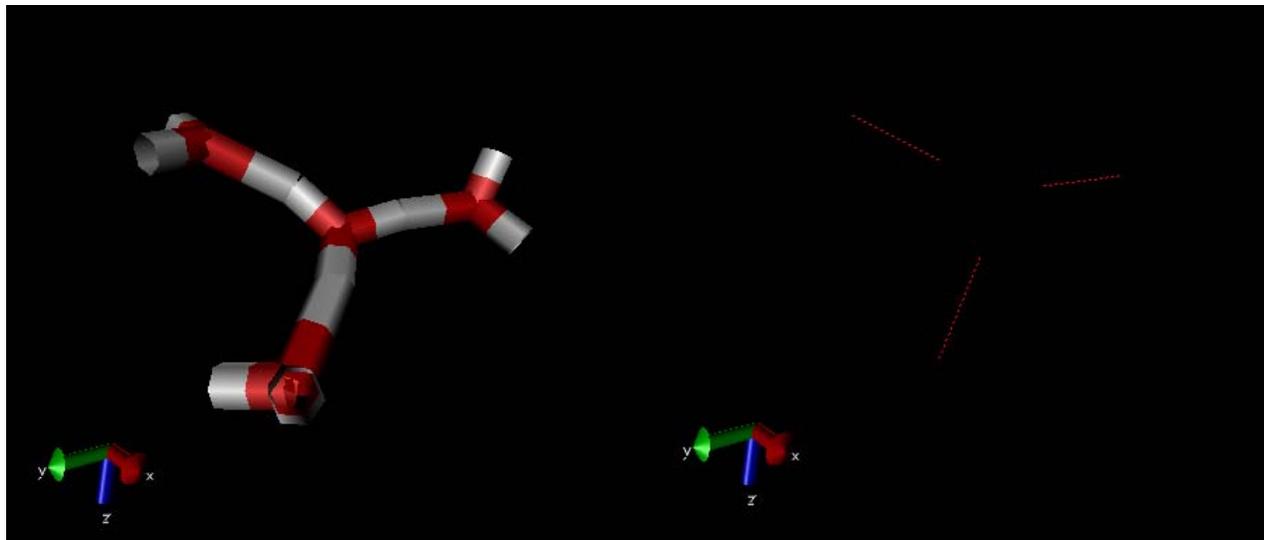
Snapshot 1 (Frame 1):  $\text{H}_9\text{O}_4^+$  has an  $\text{H}_3\text{O}^+$  core that donates three hydrogen bonds to its neighboring  $\text{H}_2\text{O}$  molecules. (Similar to Fig. 1a in Ref.)



Snapshot 2 (Frame 141): One of the three protons of the  $\text{H}_3\text{O}^+$  core migrates along its hydrogen bond and forms an  $\text{H}_5\text{O}_2^+$ , in which this proton is equally shared between two water molecules. (Similar to Fig. 1b in Ref.)



Snapshot 3 (Frame 335):  $\text{H}_9\text{O}_4^+$  formed again. And there are three hydrogen bonds in the system again.



Snapshot 4 (Frame 434): Further migration of a different proton in  $\text{H}_3\text{O}^+$  forms another  $\text{H}_5\text{O}_2^+$  with one hydrogen bond. (Similar to Fig. 1d in Ref.)

