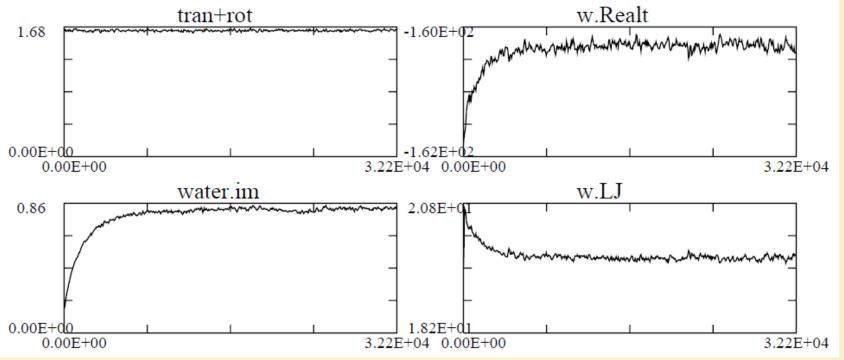
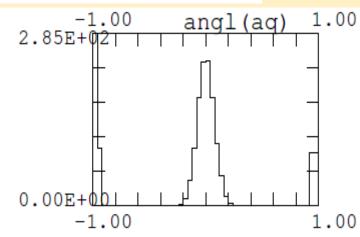
Molecular Dynamics Simulation of Water and Ice by TIP5P Code

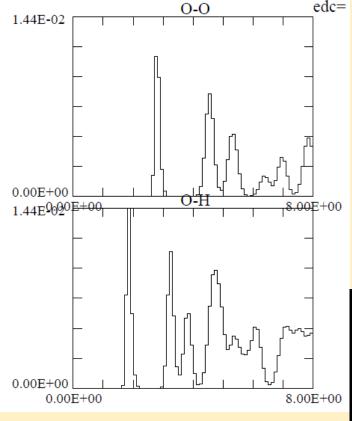
Motohiko Tanaka, Ph.D., Prof. Graduate School of Chubu University Kasugai 487-8501, Japan

Simulation starting from ice at 230 K



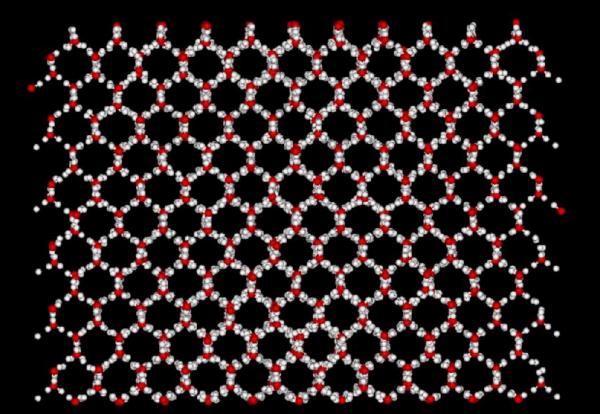
At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity E_0= 10x10^6 V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at time of t=32,200. Right: cosine distribution of water in the x-direction. No oscillations are really found at imposed large electric field.



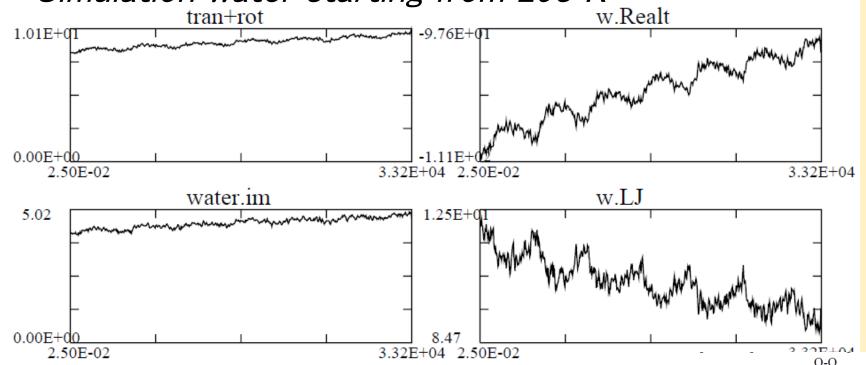


Time t=32,000 of temperature 230 K. Left: a) pair distribution functions of O-O atoms b) O-H atoms for R=0-8 Angstrom. Peaks are well separated at this temperature. Right: scatter plot of water molecules where

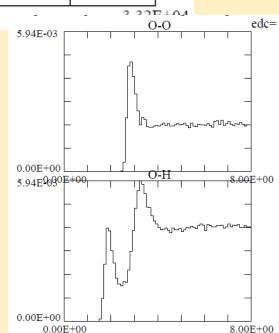
6-membered rings are formed for frozen ice.

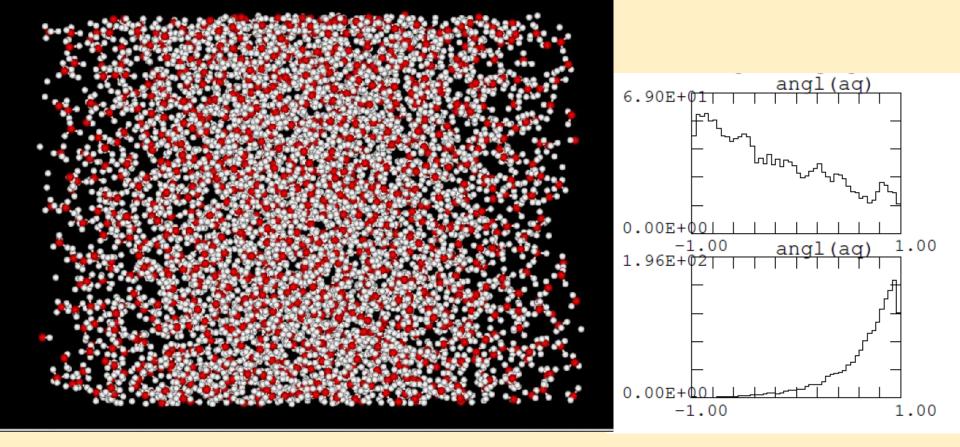


Simulation water starting from 298 K



Time t=33,200 starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with E_0= 5x10^6 V/cm (about 3.2 periods). Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy. Right: pair distribution functions of a) O-O atoms, b) O-H atoms in R=0-8 Angstrom. O and H atoms are thus mixed showing heavy water interactions. Compare with the frozen ice of 230 K.





At t=33,000 of water molecules at 298 K. Left: scatter plot of water, b) x-directional cosine distribution for the cross bins in (-1.0,1.0). Due to phase lag of molecules compared to imposed electric field, water is largely heated,