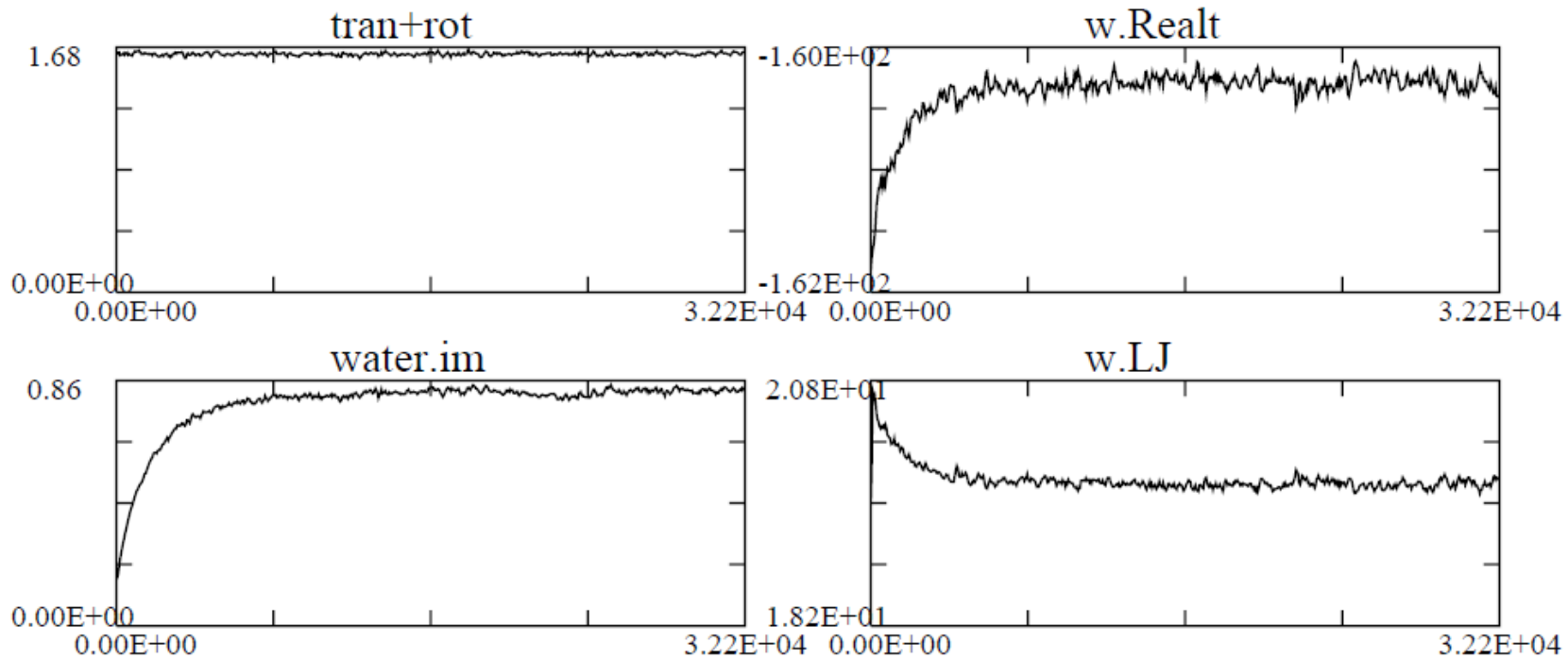


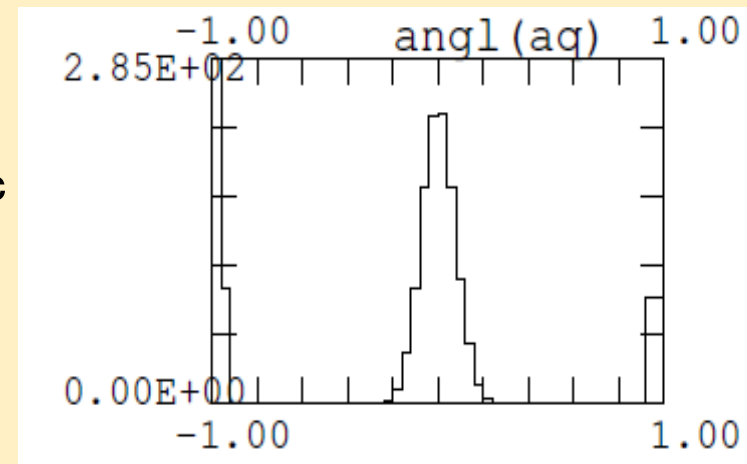
Figures - Molecular dynamics simulation of water and ice by TIP5P code

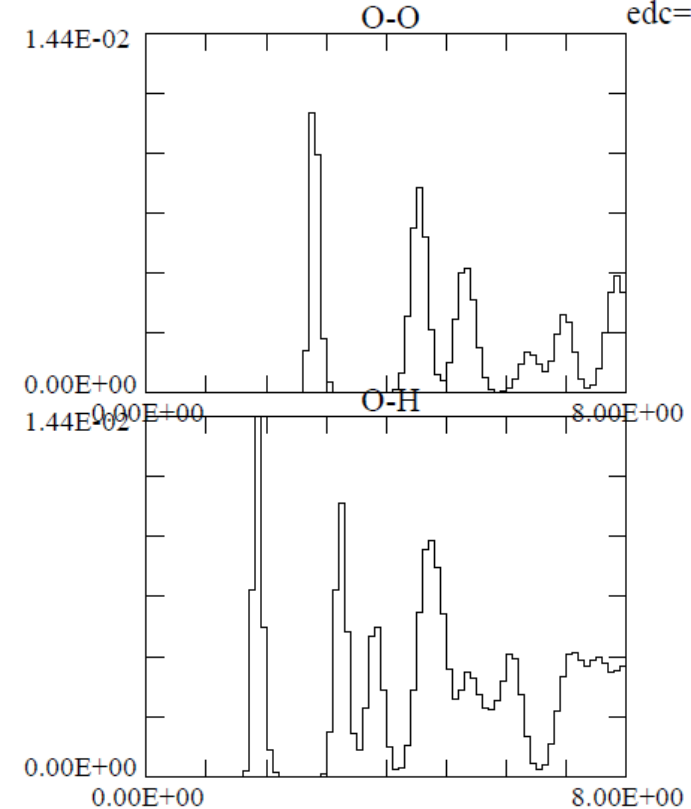
Motohiko Tanaka, Ph.D., Prof.
Graduate School of Chubu University
Kasugai 487-8501, Japan

Simulation starting from ice state at 230 K



At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity $E_0 = 10 \times 10^6$ 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.

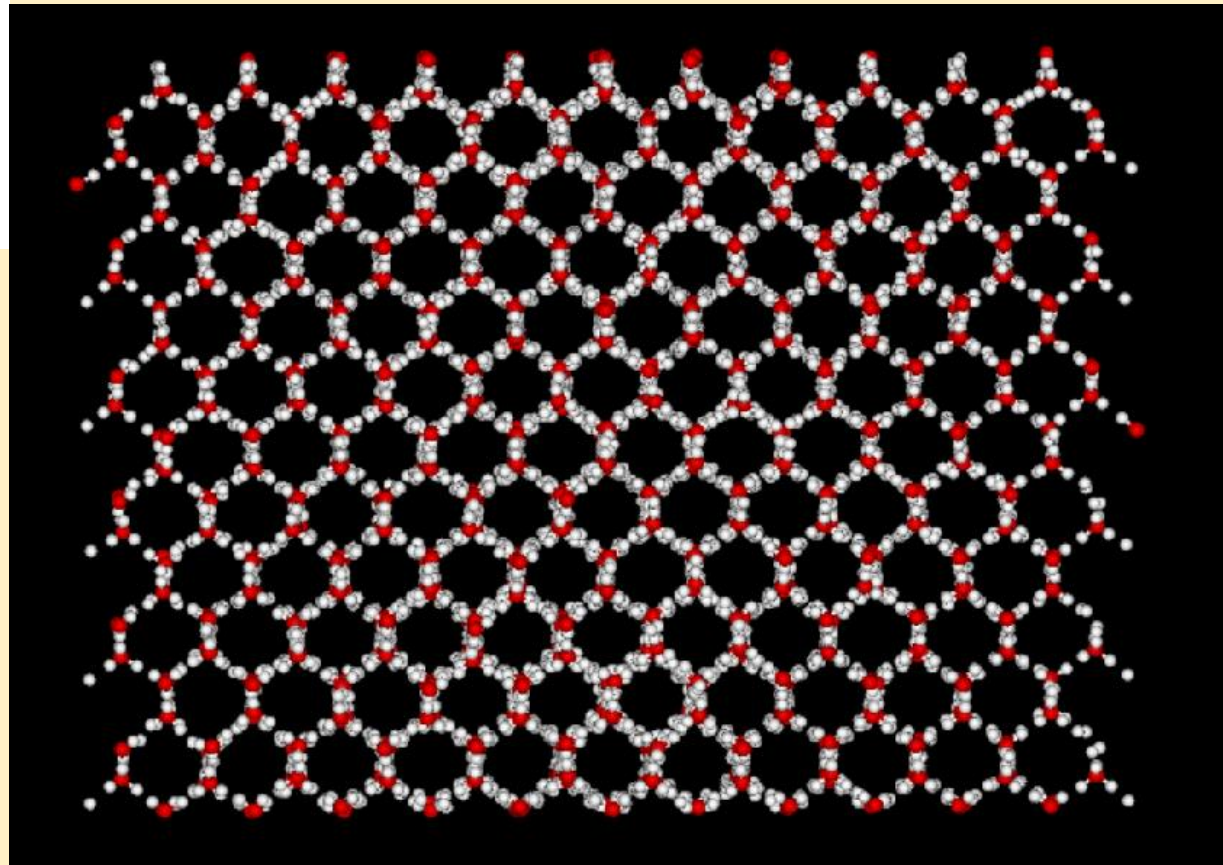




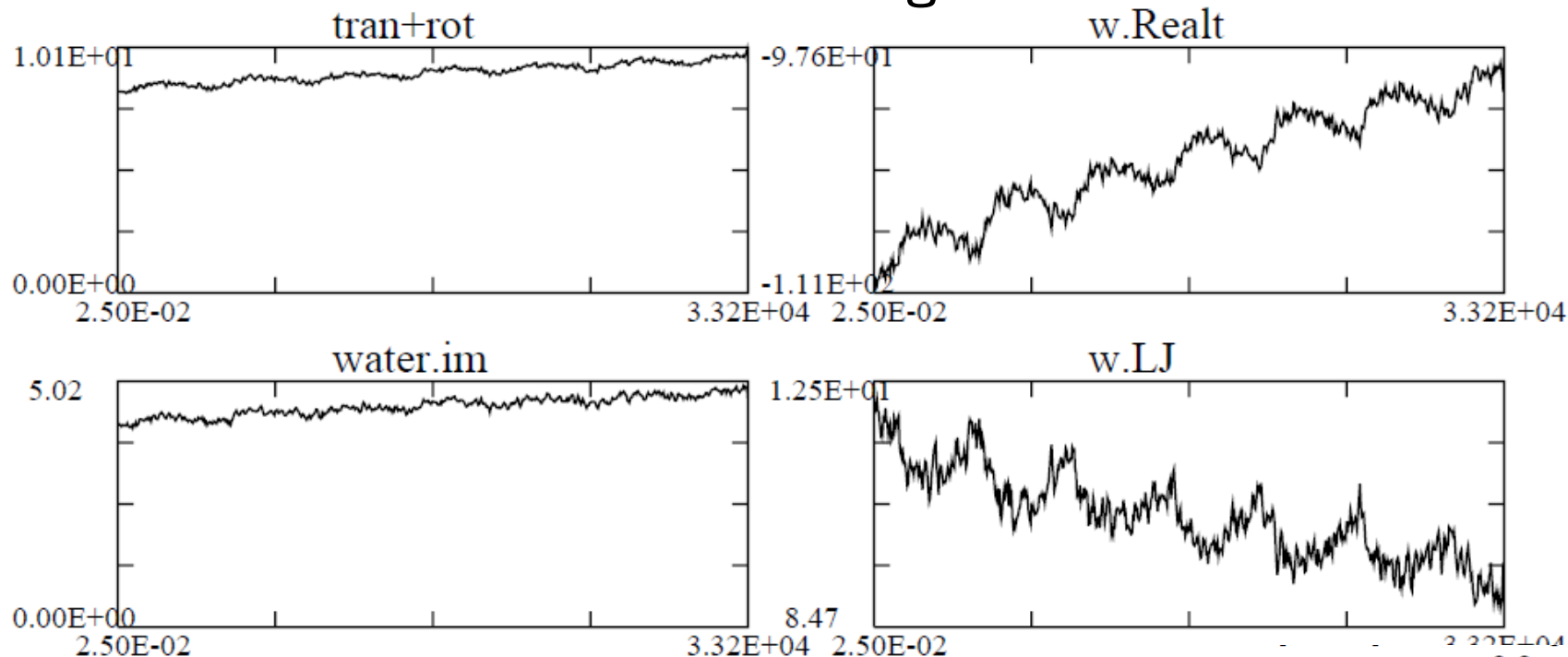
Time $t=32,000$ of temperature 230 K.

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.



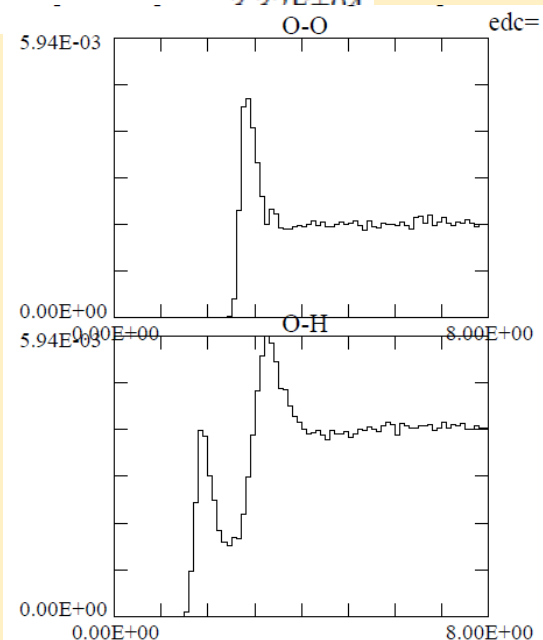
Simulation water state starting from 298 K

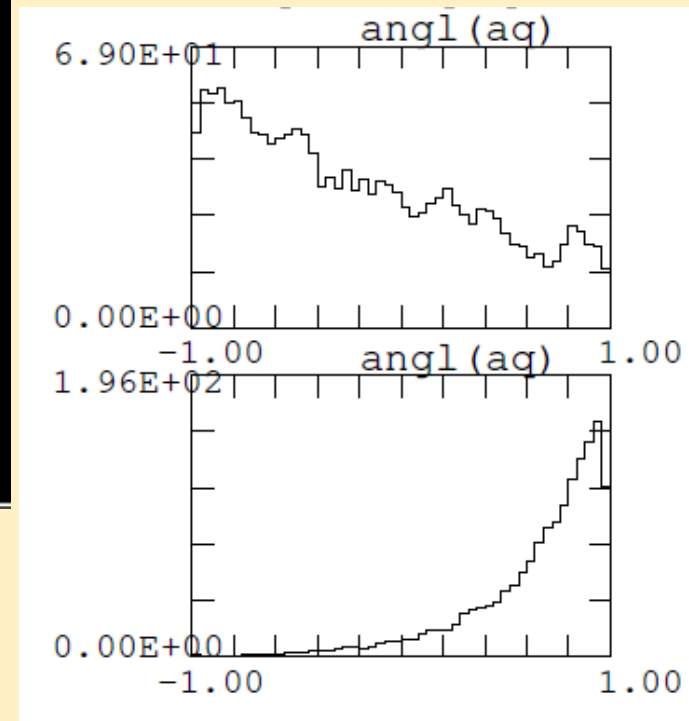
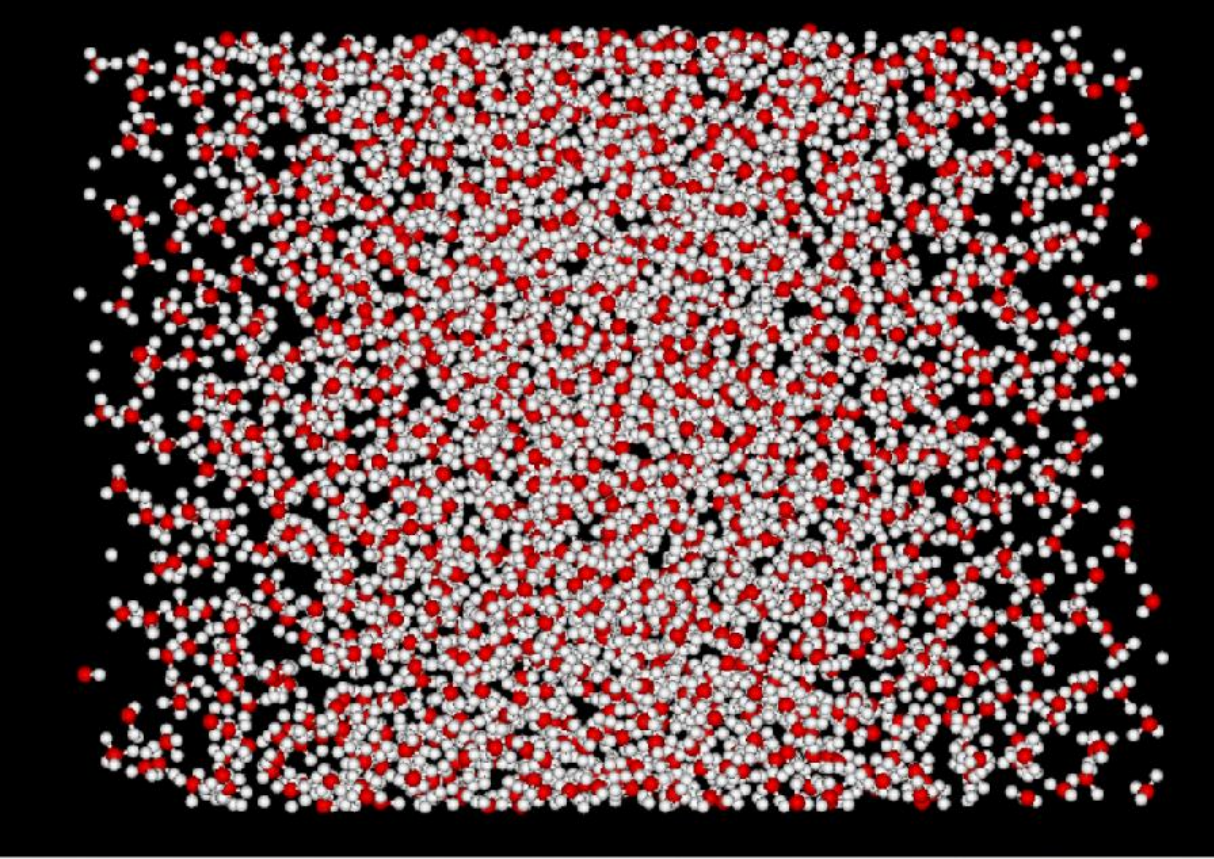


Time $t=33,200$ starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with $E_0 = 5 \times 10^6$ V/cm (about 3.2 periods).

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.

Left: scatter plot of water, b) x-directional cosine distribution for the cross section $x = (-1, 1)$. Due to phase lag of molecules compared to imposed electric field, water is largely heated,