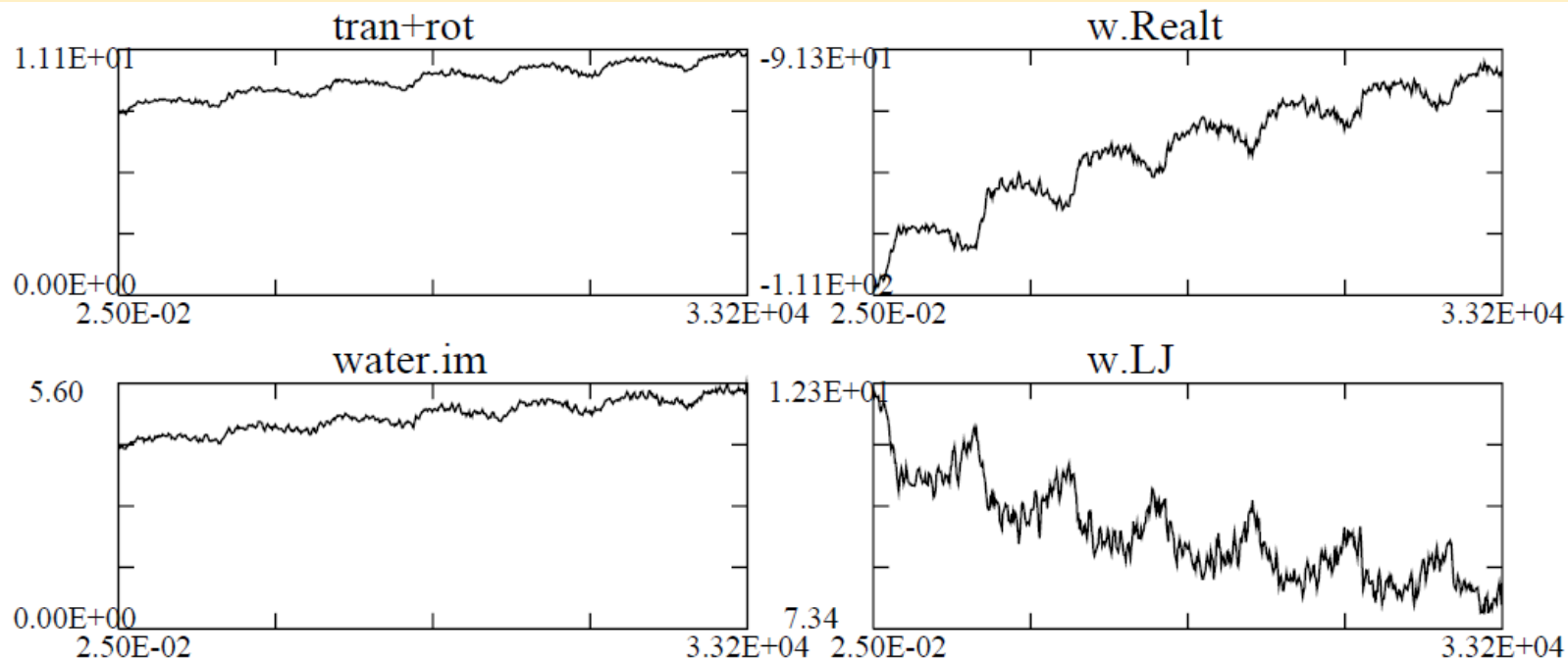


Molecular Dynamics Simulation of Water and Ice by TIP5P Code

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

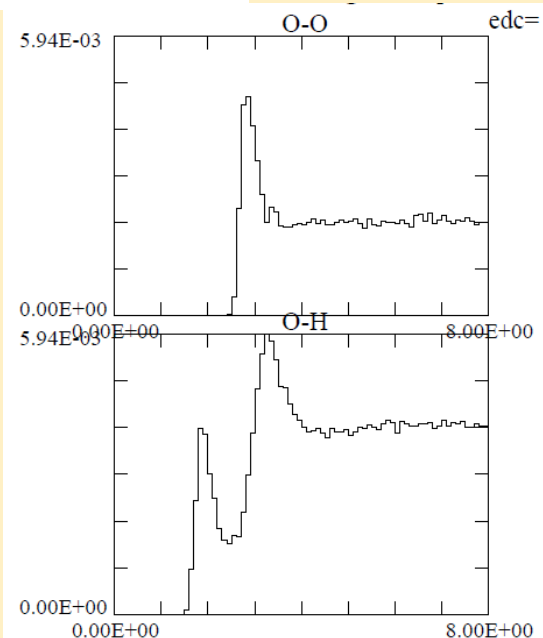
* Simulation water starting from 298 K *

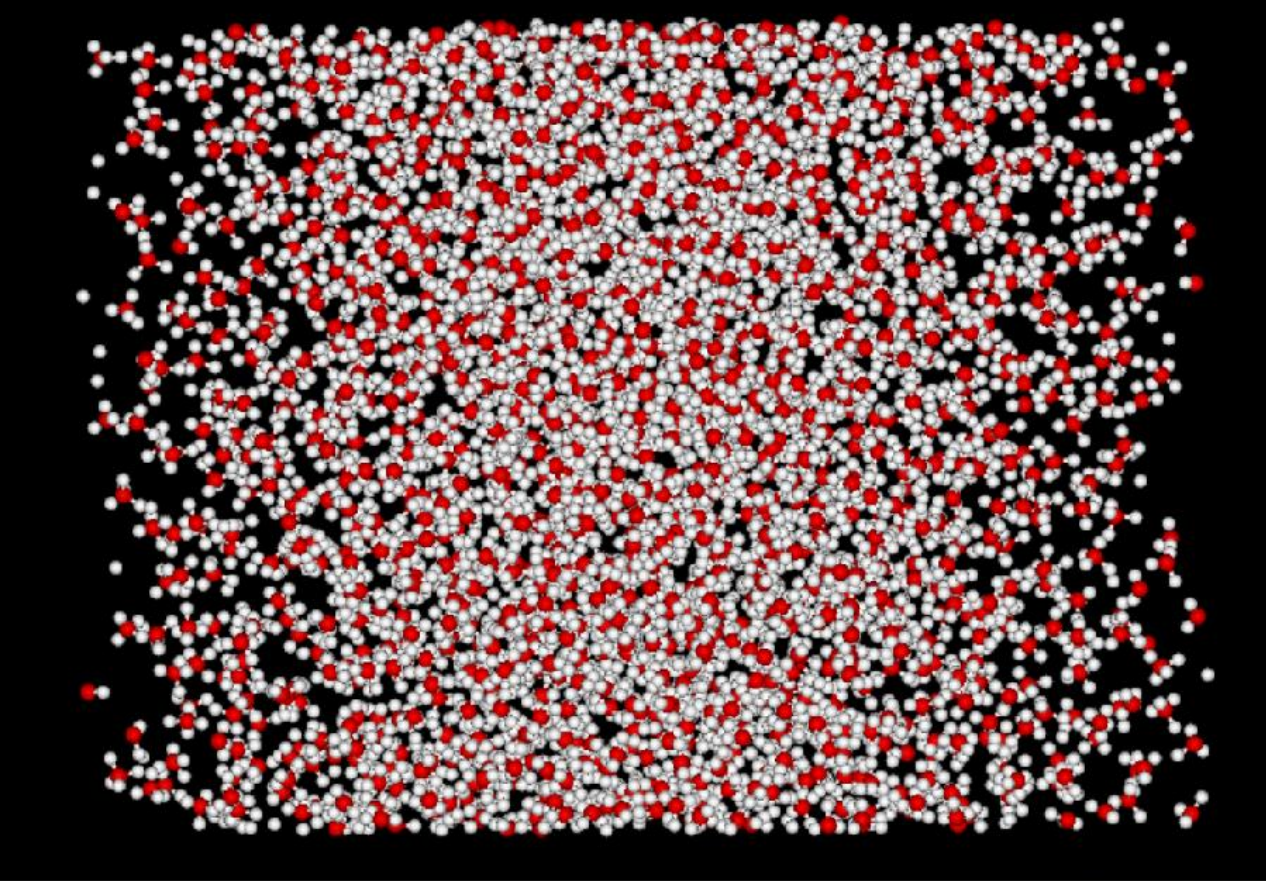


Time $t=33,200$ starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with $E_0 = 5 \times 10^6$ V/cm (about 3.2 periods).

Left: a) Total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy.

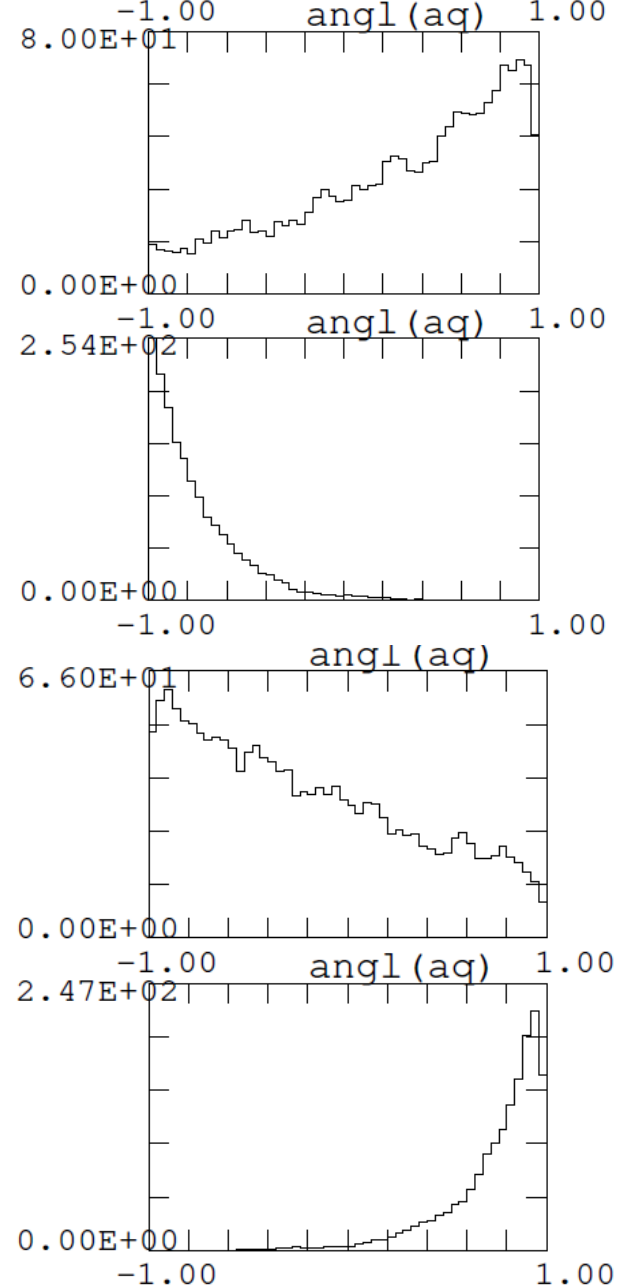
Right: Pair distribution functions of a) O-O atoms, b) O-H atoms in $R=0-8$ Angstrom. O and H atoms are thus mixed showing heavy water interactions. Compare with the frozen ice of 230 K.



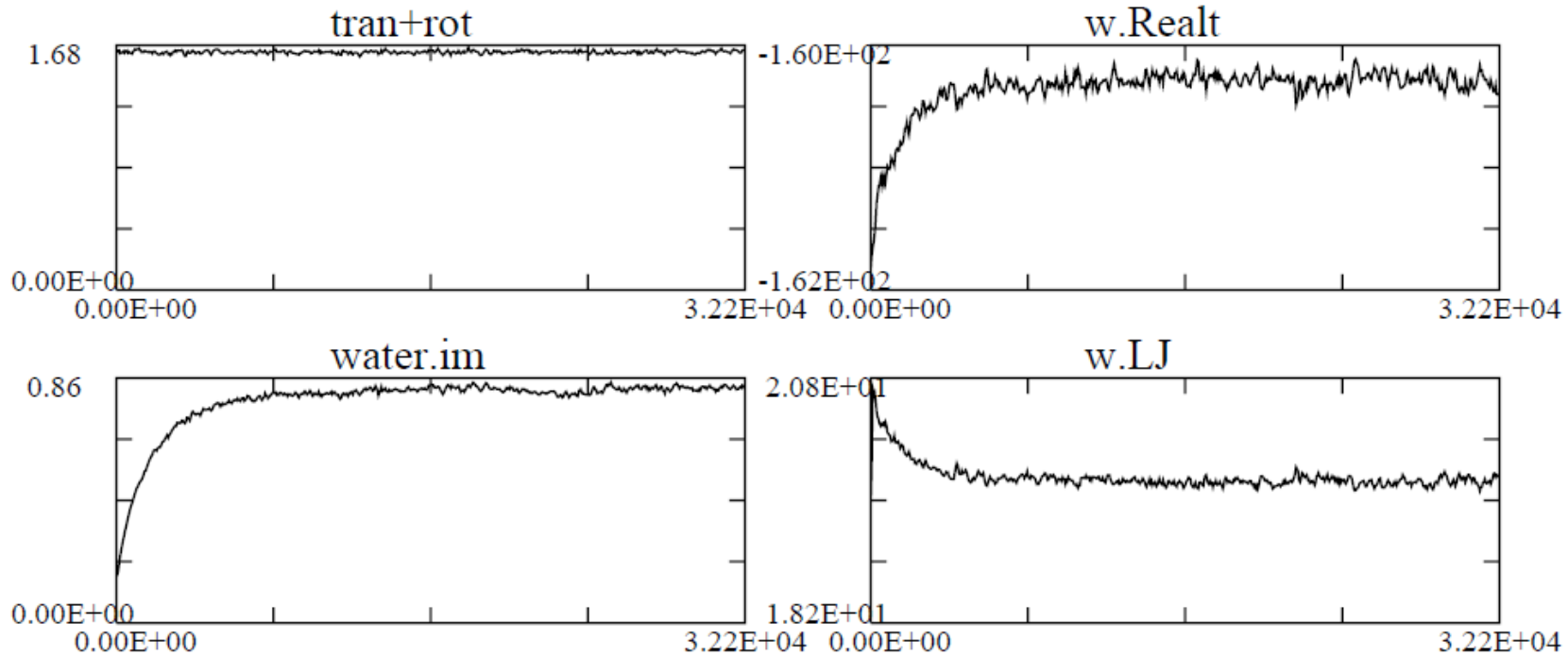


Water molecules at 298 K.

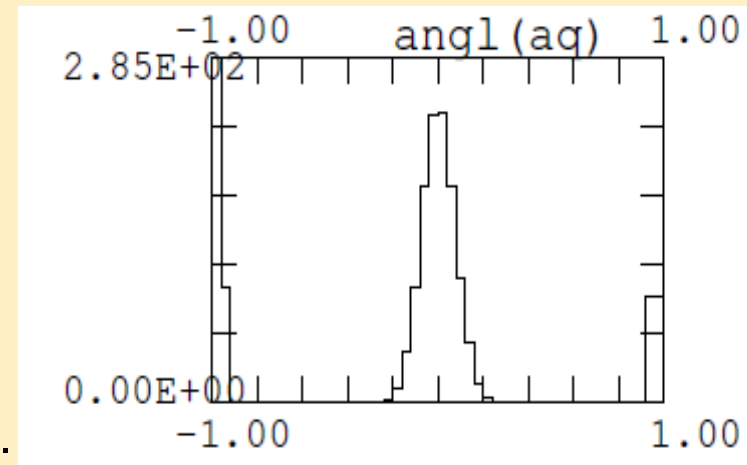
Left: Scatter plot of water at $t=32,500$, b) x-directional cosine distribution for the cross bins of $(-1.0, 1.0)$ at $t=27,500$ to $32,500$. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

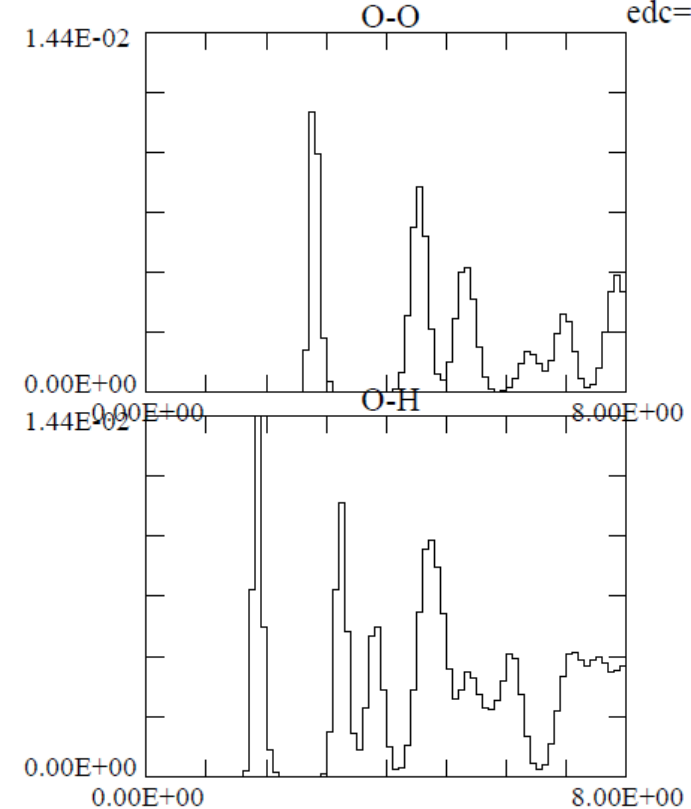


** Simulation starting from ice at 230 K **



At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity $E_0 = 5 \times 10^6$ 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 Bins $(-1,1)$ of the x-direction. No oscillations are really found at the 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.

