

Molecular Dynamics Simulations of Water and Ice by TIP5P Code

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

Dielectric constant of water and ice

Water dielectric constant in temperature. It changes slowly for less than 273 K, and after phase transition it becomes rapidly for > 273 K. (Eyring et al., PNAS, 1966).

Water T (K), Dielectric constant of liquid

273 K 88 $\leftarrow 298$ K, $\epsilon = 80$

373 K 56

473 K 35

Ice I, T (K), Dielectric constant

273 K 91.5

262.3 K 95.0

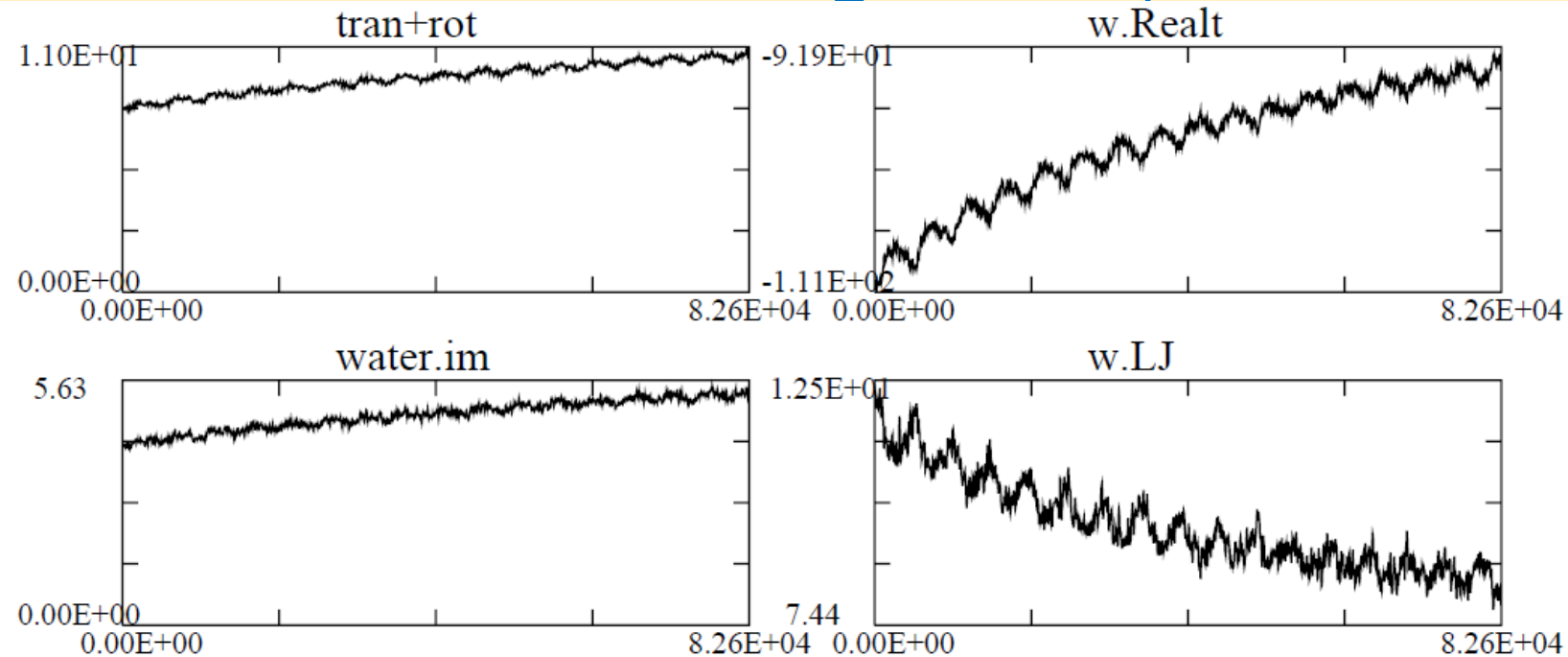
252.2 K 97.4

241 K 100

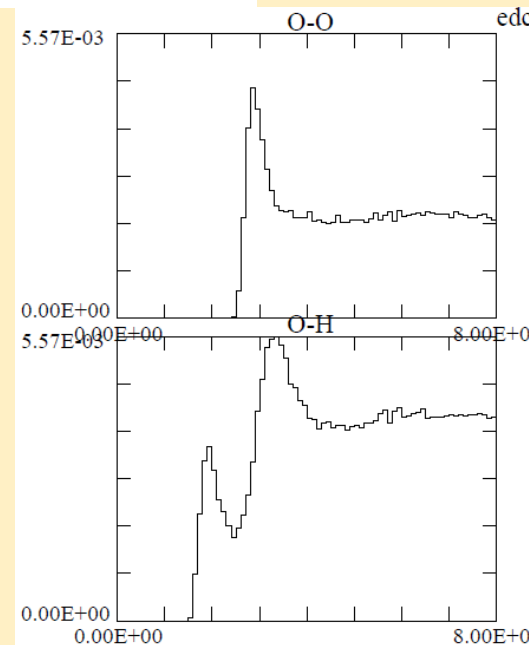
228.4 K 104 $\leftarrow 230$ K, $\epsilon = 104$

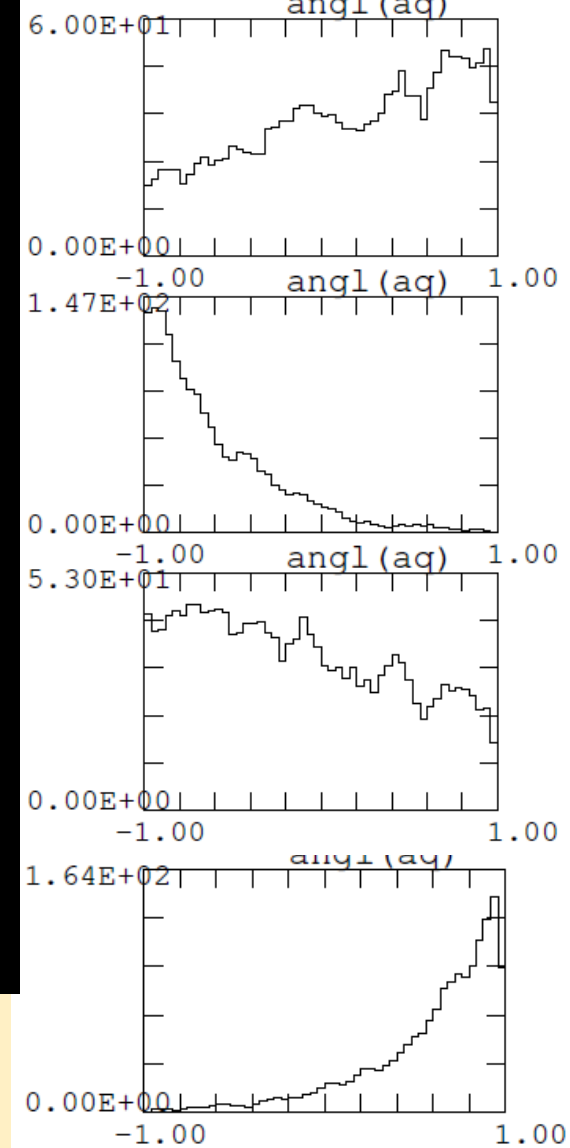
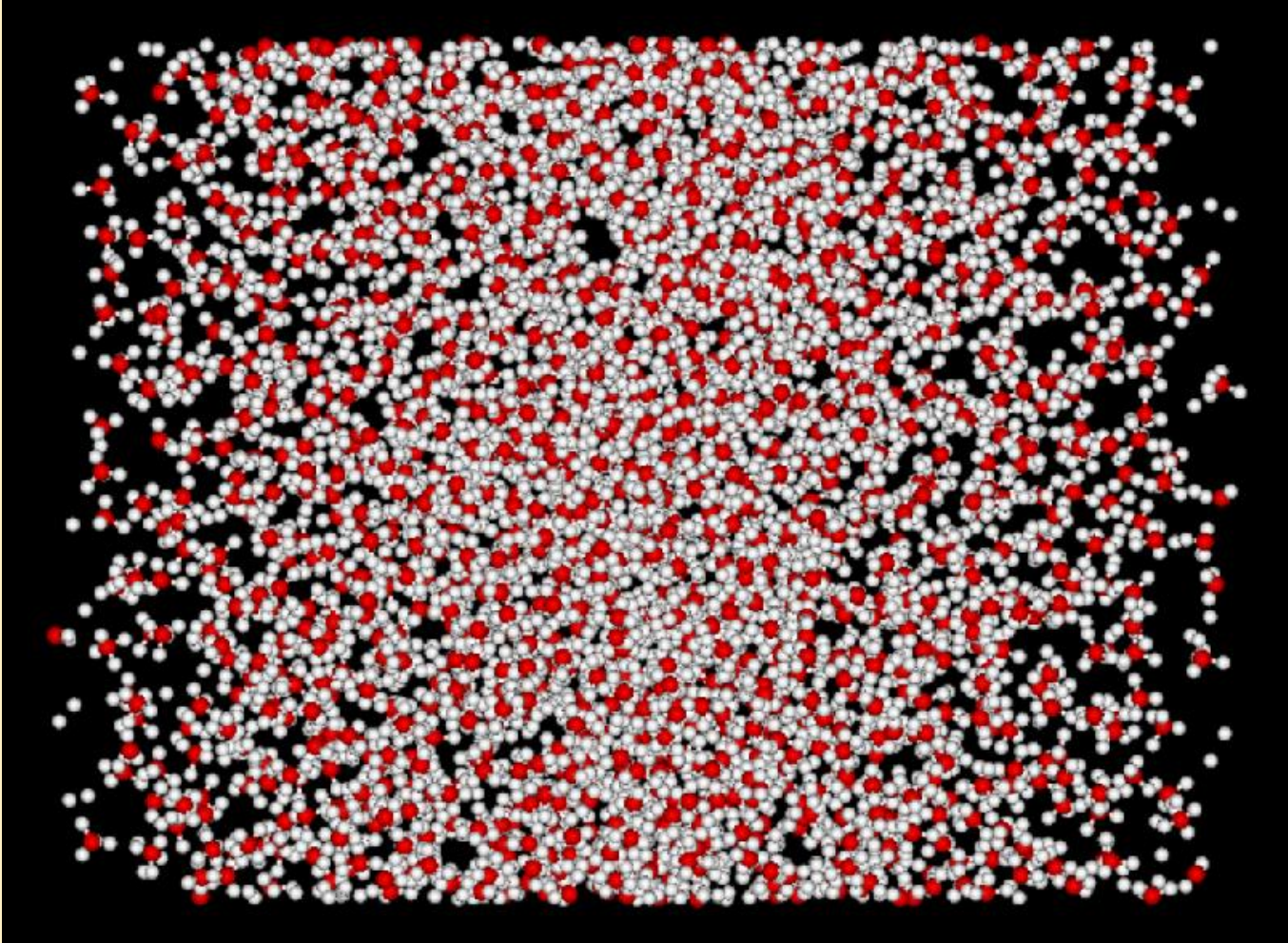
216.3 K 114

Simulation water starting at 298 K, NVE



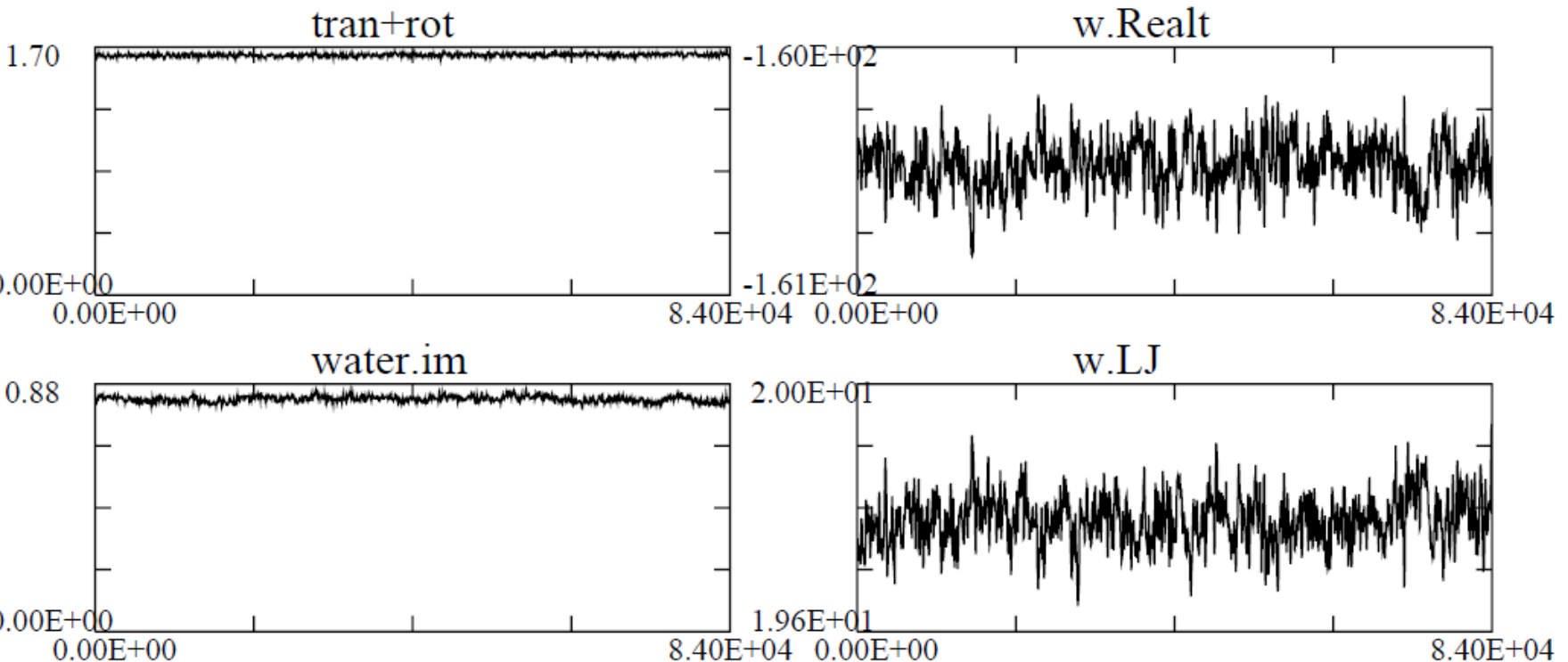
The time $t=82,600$ starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with $E_0 = 5 \times 10^6$ V/cm and NV run (by 8.3 periods). Left: a) Total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy. The final temperature is about 405 K. 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.



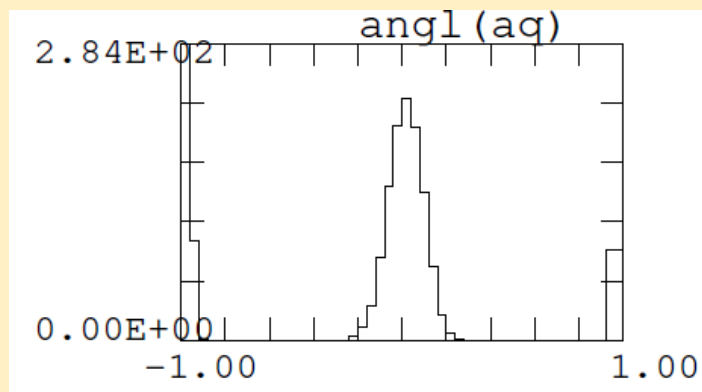


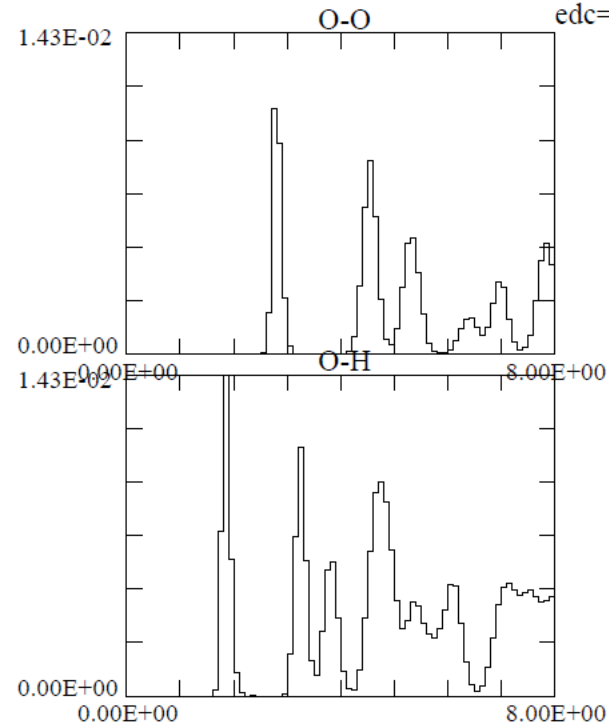
Water molecules starting 298 K.
 Left: Scatter plot of water at $t=80,000$, b) x-directional cosine distribution for the cross bins of $(-1.0, 1.0)$ at $t=72,500$ to $80,000$. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

Simulation starting at ice 230 K, NVE

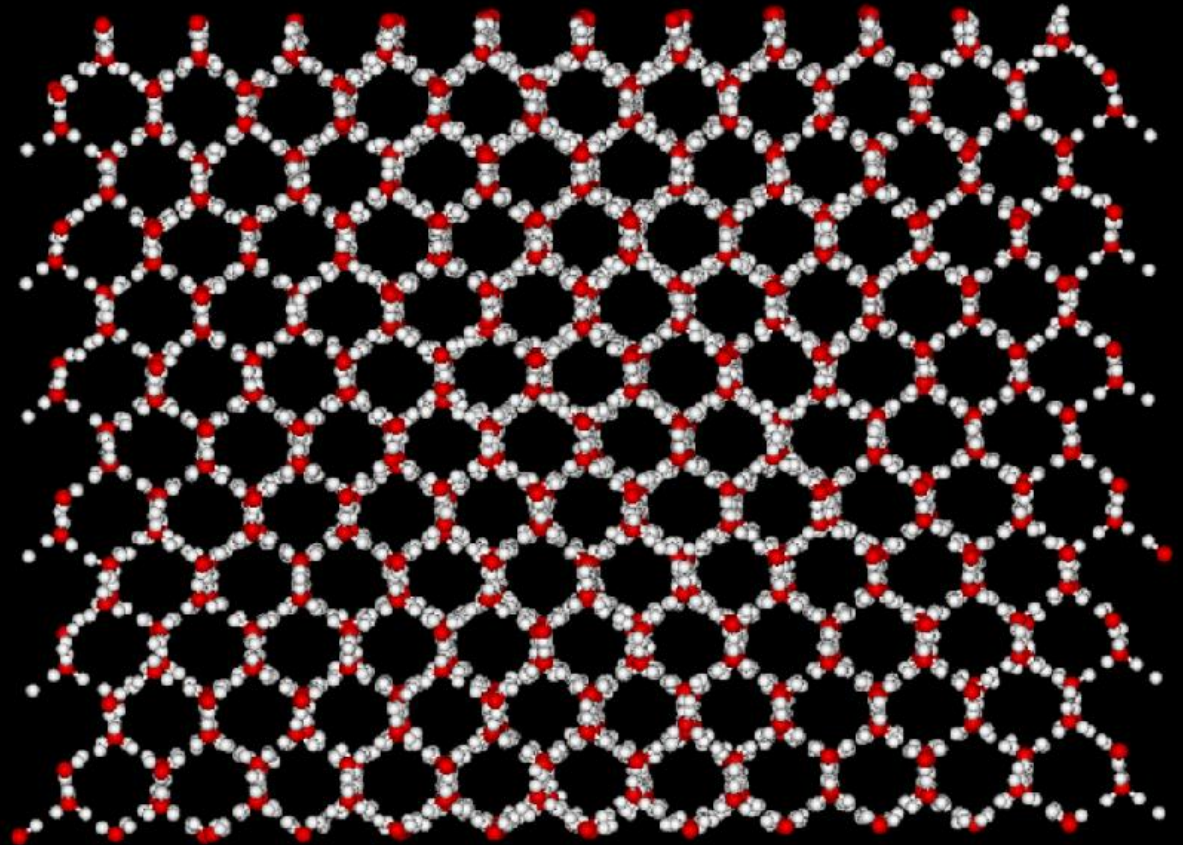


At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity $E_0 = 5 \times 10^6$ V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at the time of $t=84,000$. Right: cosine distribution of water in Bins $(-1,1)$ of the x-direction. No oscillations are really found at the imposed electric field.





Time $t=80,000$ of the 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 ice is frozen by 6-membered water clusters.



References

1. M. Hobbs, M. Jhon, and H. Eyring, PNAS, 1966.
2. “Classical Mechanics”, H. Goldstein, C. Poole, J. Safko, 3rd Edition, Pearson Education Inc., England, 2003.
3. ”Microwave heating of water, ice and saline solution: Molecular dynamics study”, M.Tanaka and M.Sato, J.Chem.Phys., 126, 034509 1-9 (2007).
4. “Microwave heating of water and ice by TIP5P code”, M. Tanaka, <https://github.com/Mtanaka77/> (May 2023).
5. “Microwave heating and collapse of methane hydrate by molecular dynamics simulations, M. Tanaka, M. Sato, and S. Nakatani, arXiv.1909.01024, Cornell University, 2019, USA