Molecular Dynamics Simulations of Water and Ice by TIP5P Code

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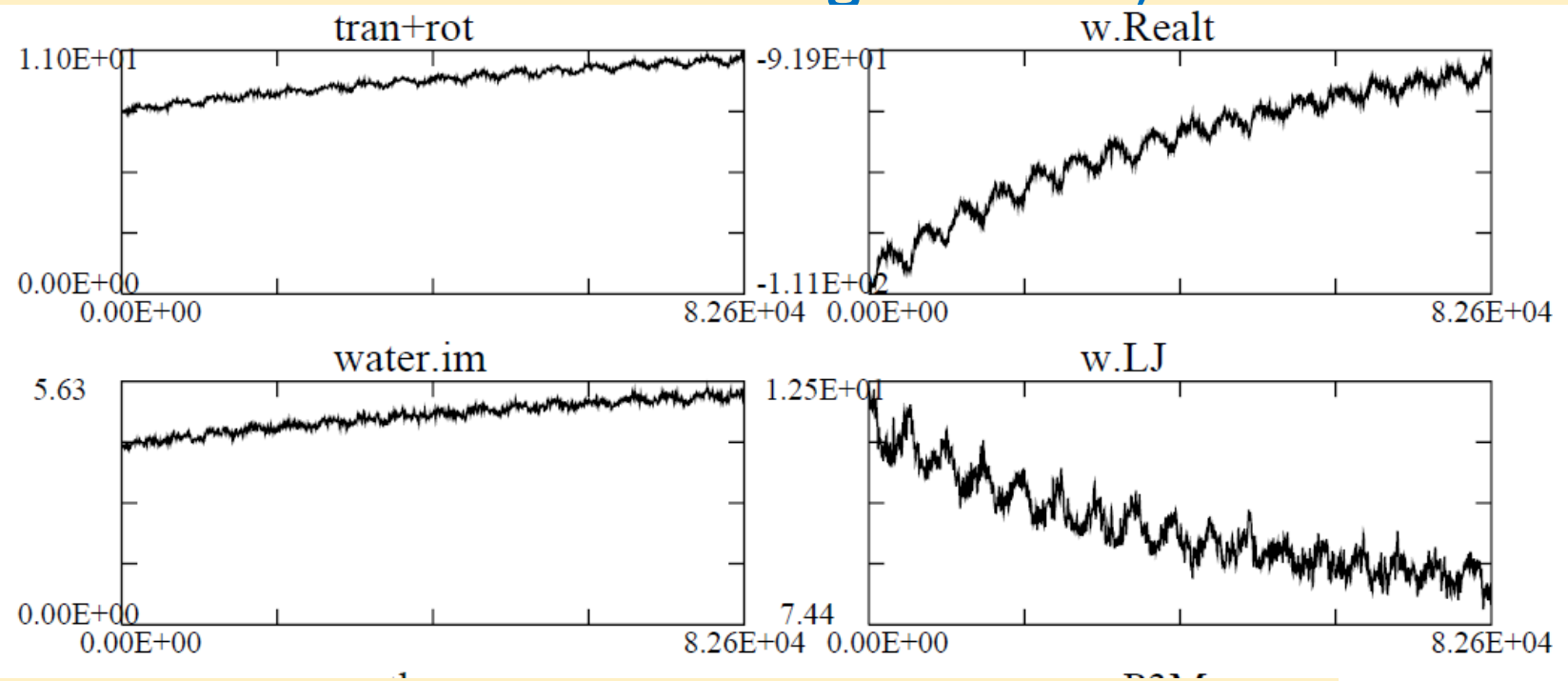
Dielectric constant of water and ice

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

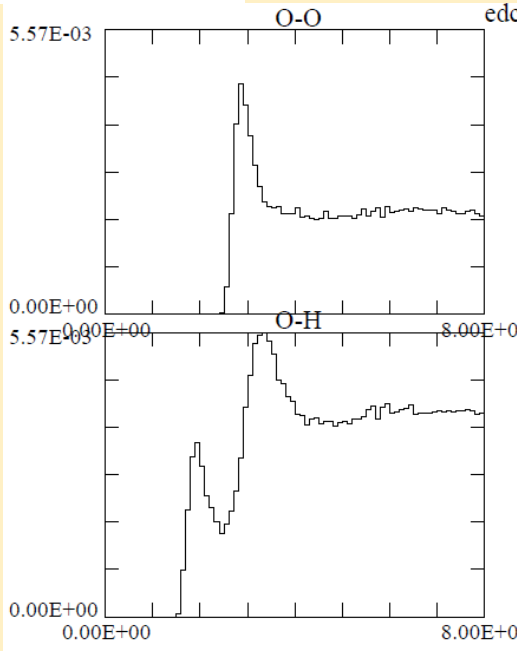
Water T (K)	Dielectric constant of liquid
273 K	88 <- 298 K, $\varepsilon = 80$
373 K	56
473 K	35

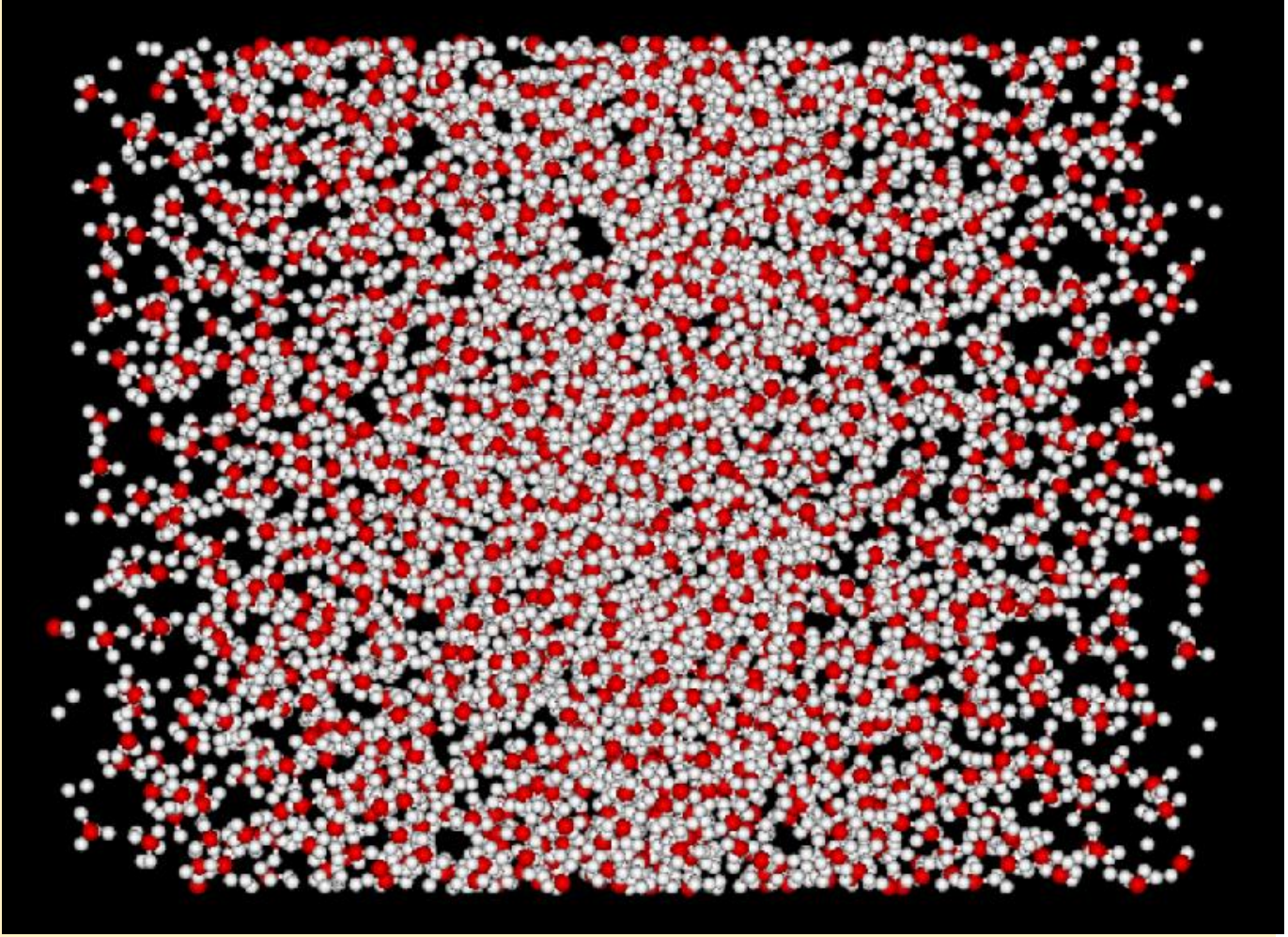
Ice I, T (K)	Dielectric constant
273 K	91.5
262.3 K	95.0
252.2 K	97.4
241 K	100
228.4 K	104 <- 230 K, $\varepsilon = 104$
216.3 K	114

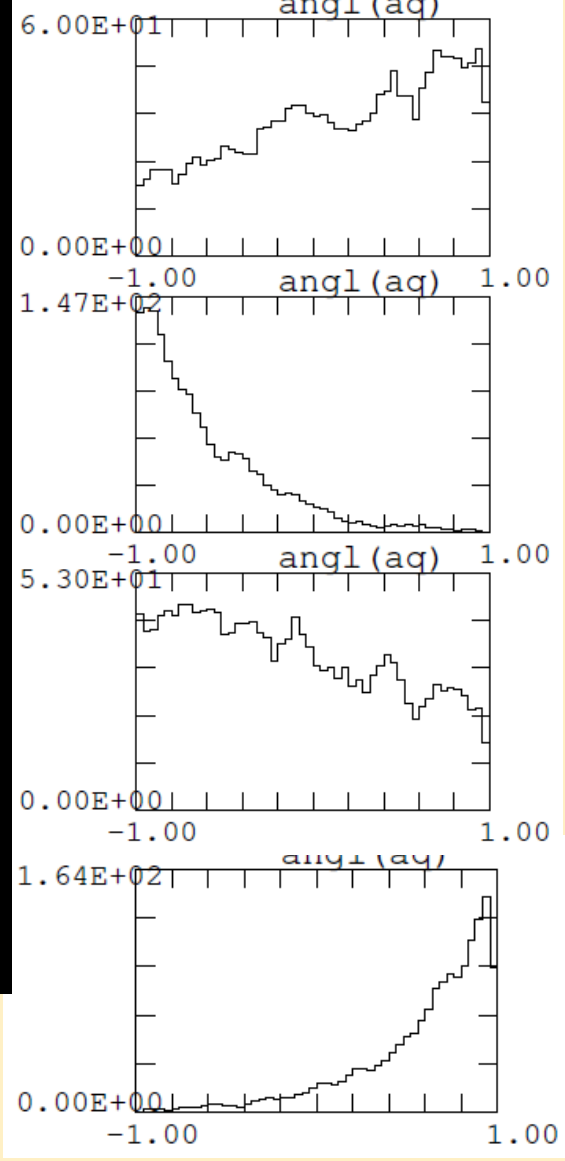
Simulation water starting at 298 K, NVE



The time t=82,600 starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with E_0= 5x10^6 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.

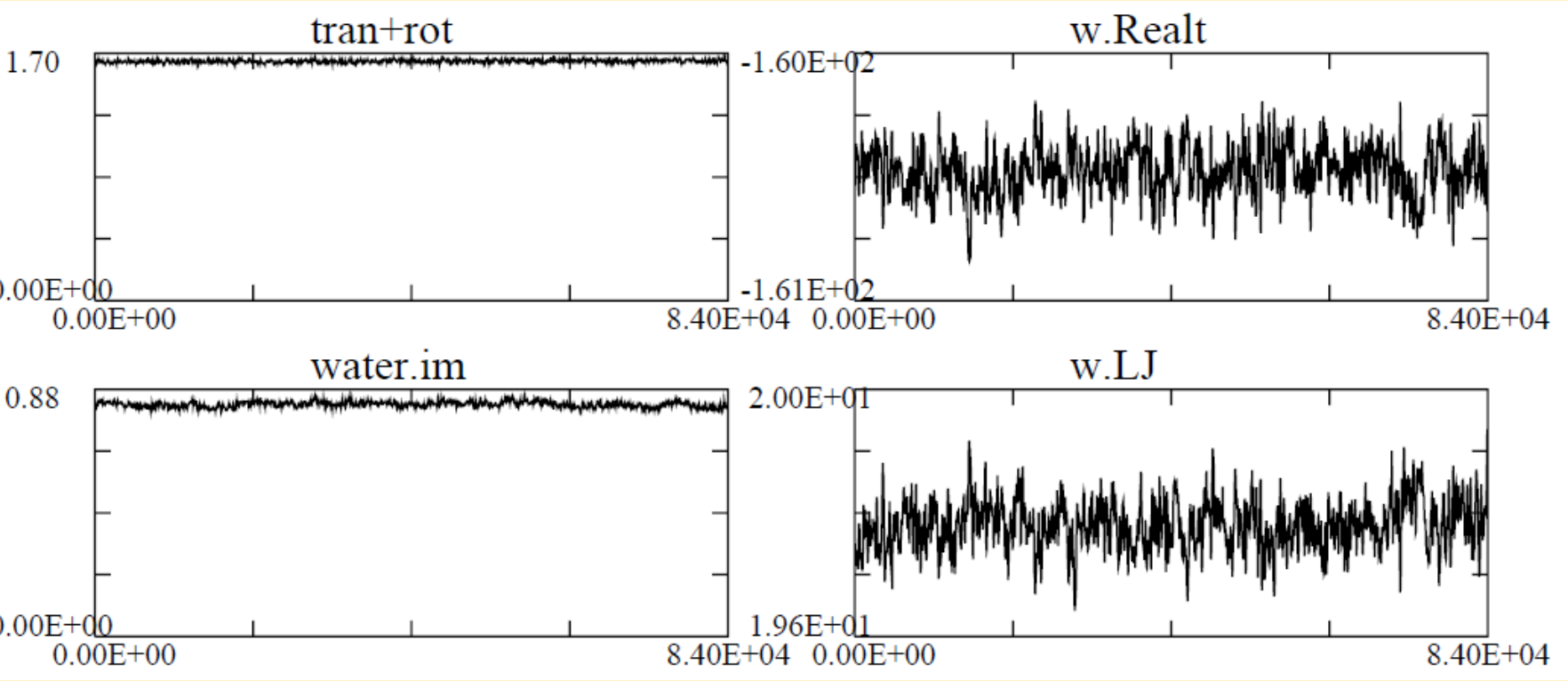




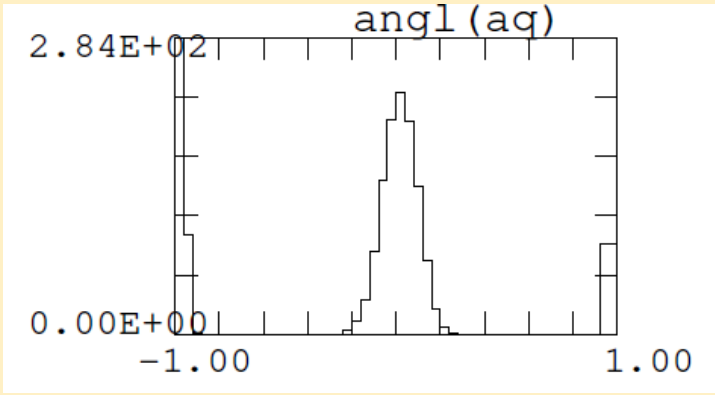


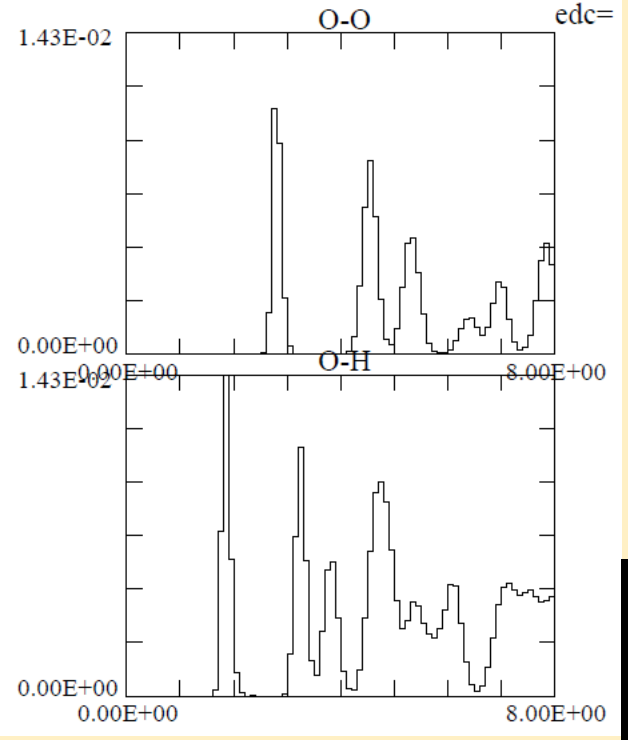
Water molecules starting 298 K.
Left: Scatter plot of water at t=80,000, b) x−directional cosine distribution for the cross bins of (−1.0,1.0) at t=72,500 to 80,000. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

Simulation starting at ice 230 K, NVE

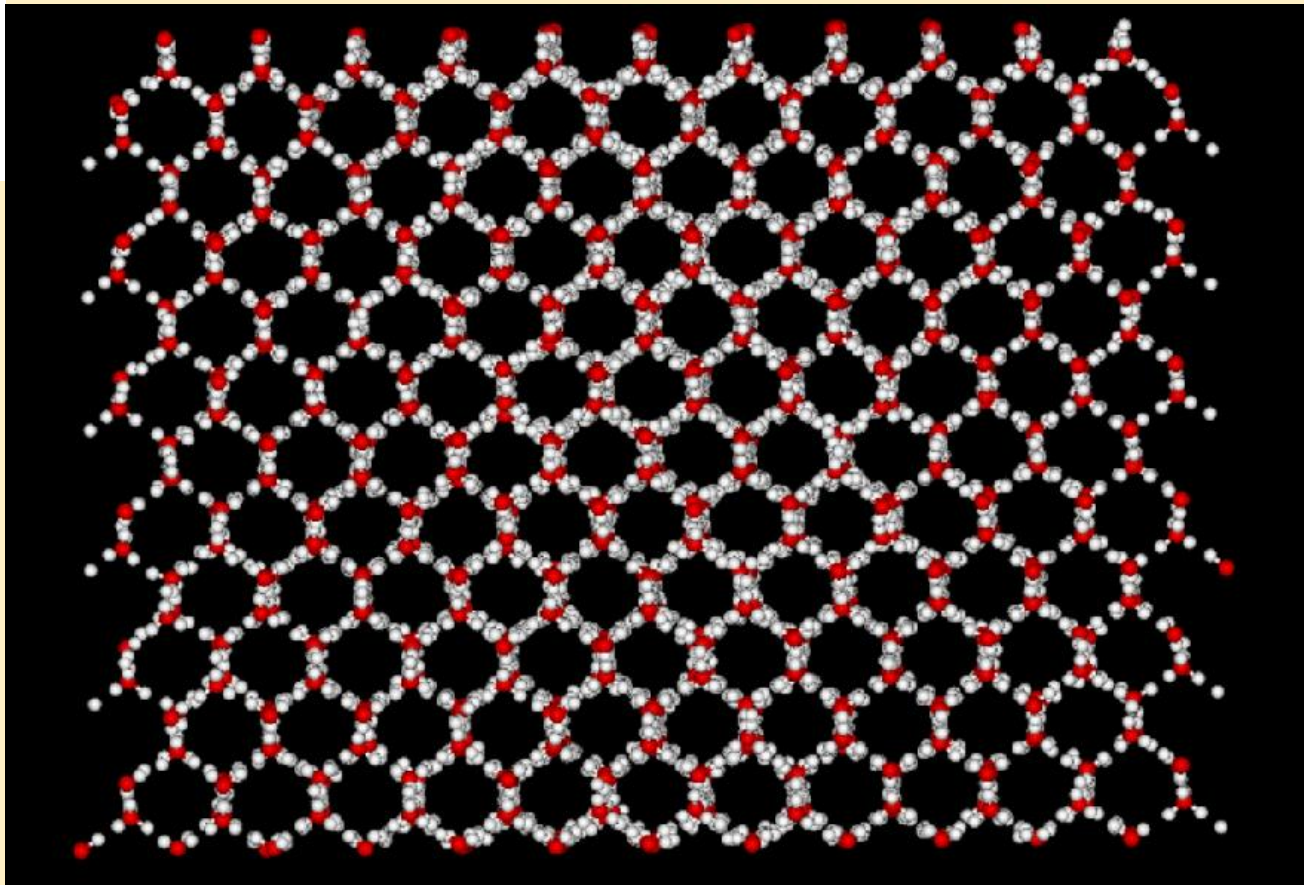


At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity E_0= 5x10^6 V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at the time of t=84,000. Right: cosine distribution of water in Bins (-1,1) 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. Poolee, 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