

Molecular Dynamics Simulations of Water and Ice by TIP5P Code

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Dielectric constant of water and ice [Ref. 3]

Water dielectric constant changes in temperature.
It decreases slowly and for 273 K it changes rapidly
(Hobbs, Jhon, Eyring, PNAS, 1966).

Water T (K), Dielectric constant of liquid

273 K 88 <− 298 K,

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

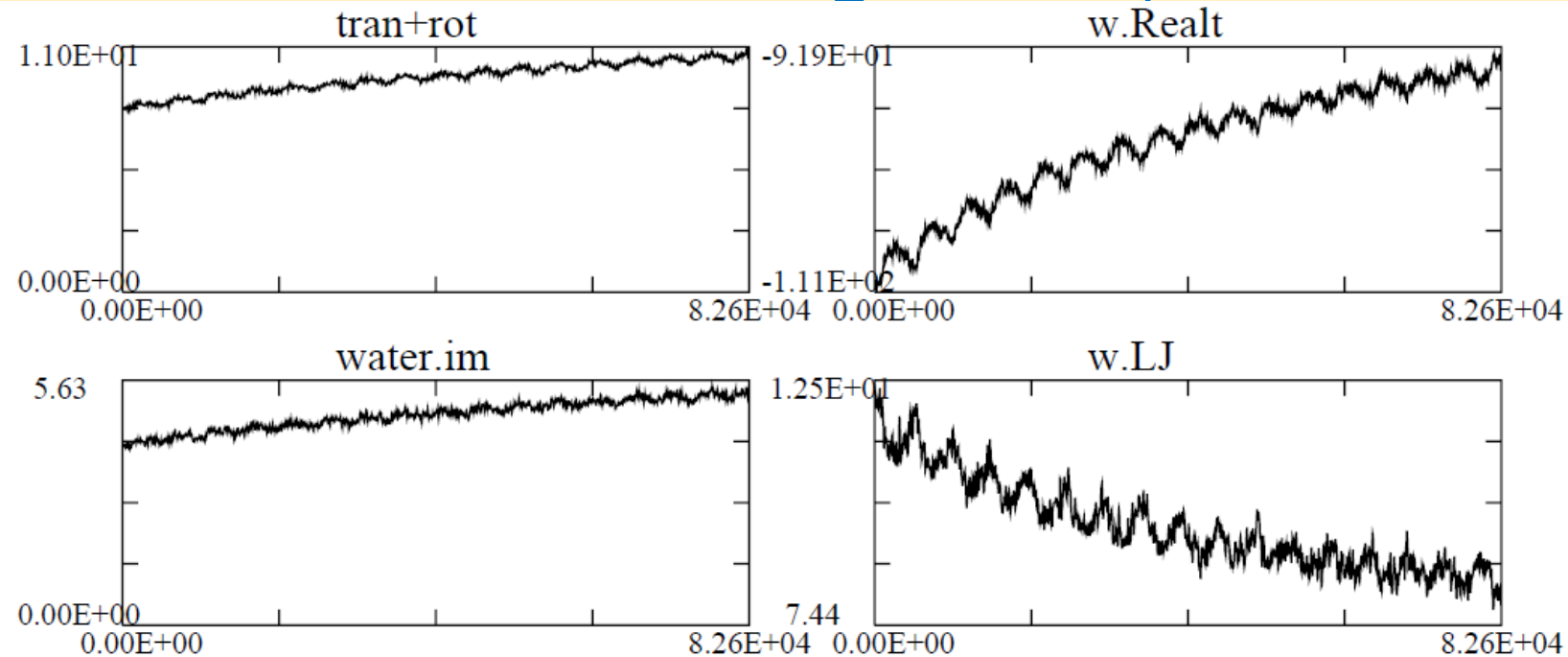
241 K 100

228.4 K 104 <− 230 K,

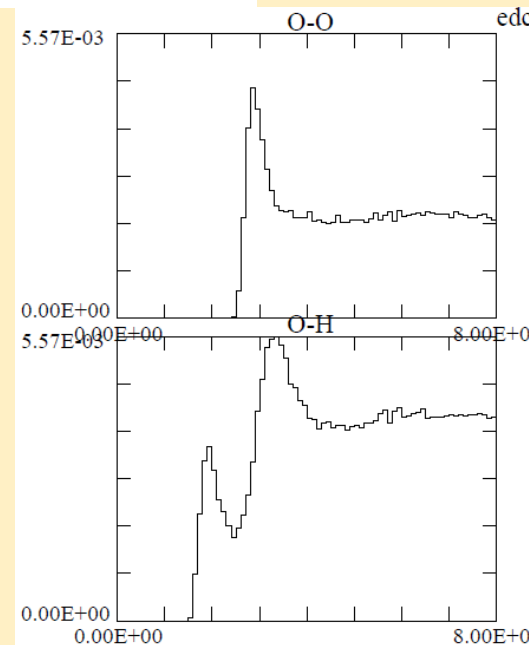
216.3 K 114

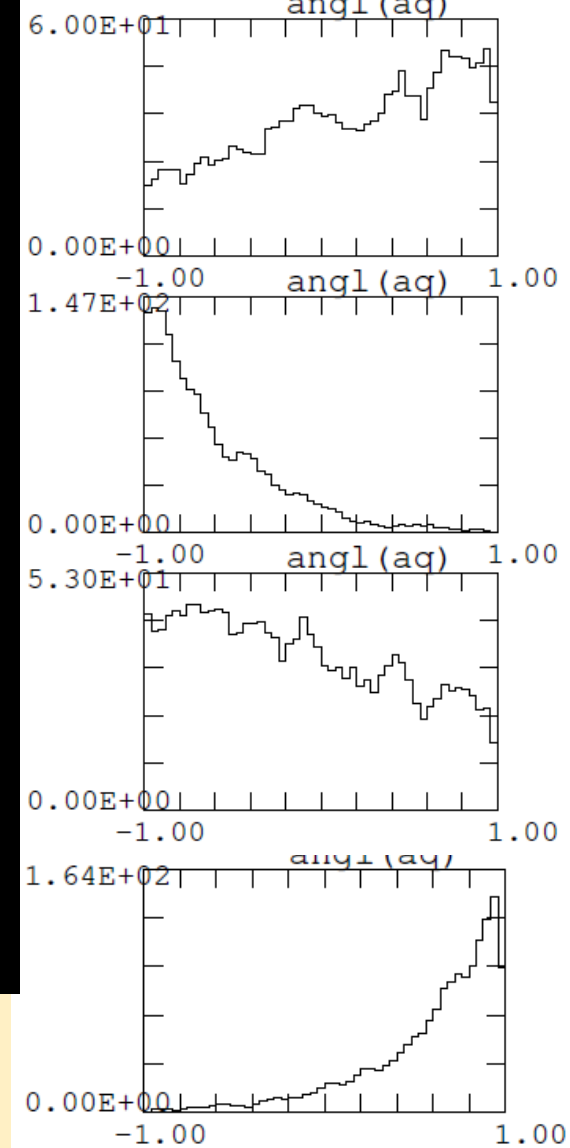
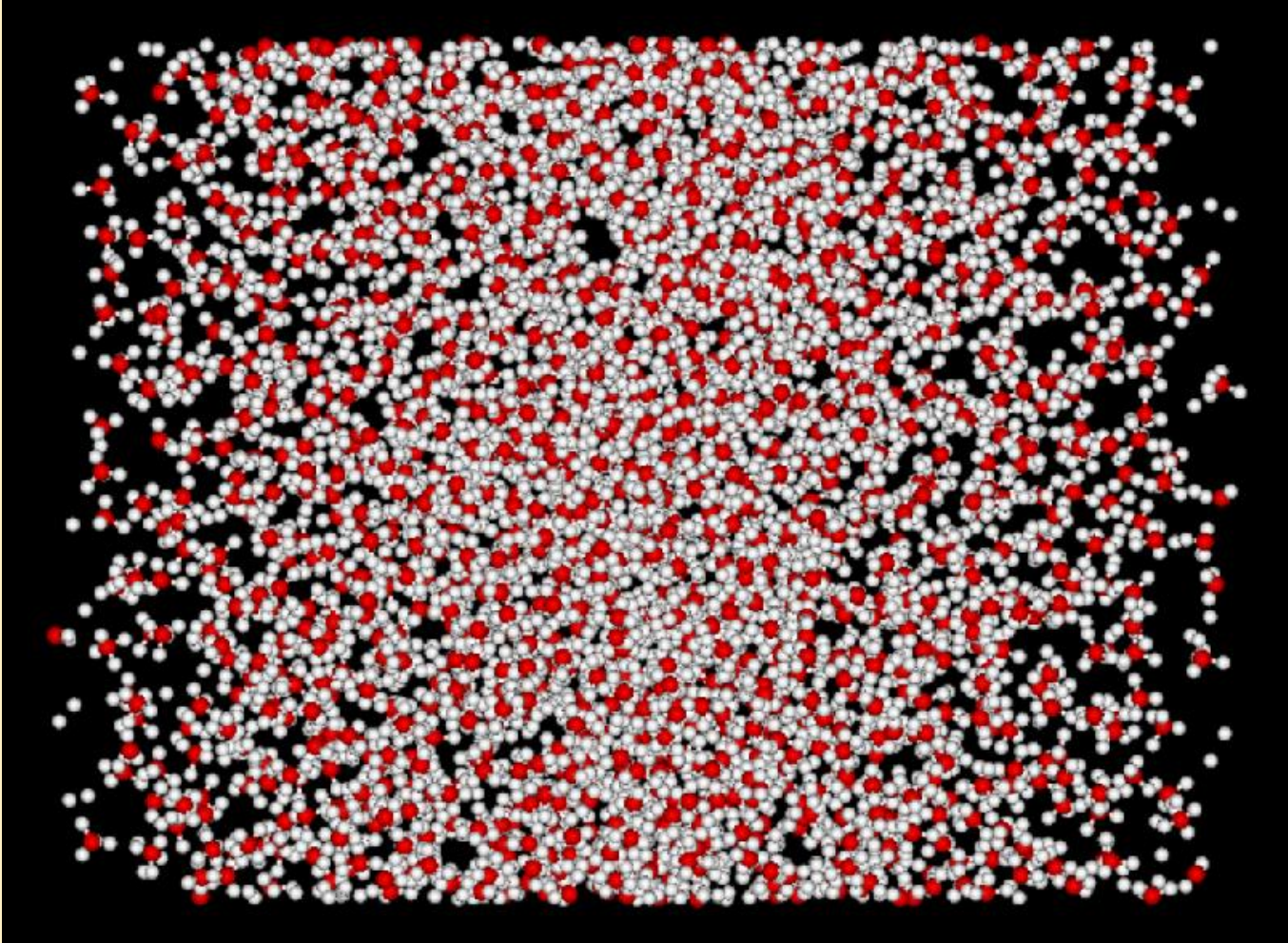
$\epsilon = 104$

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.

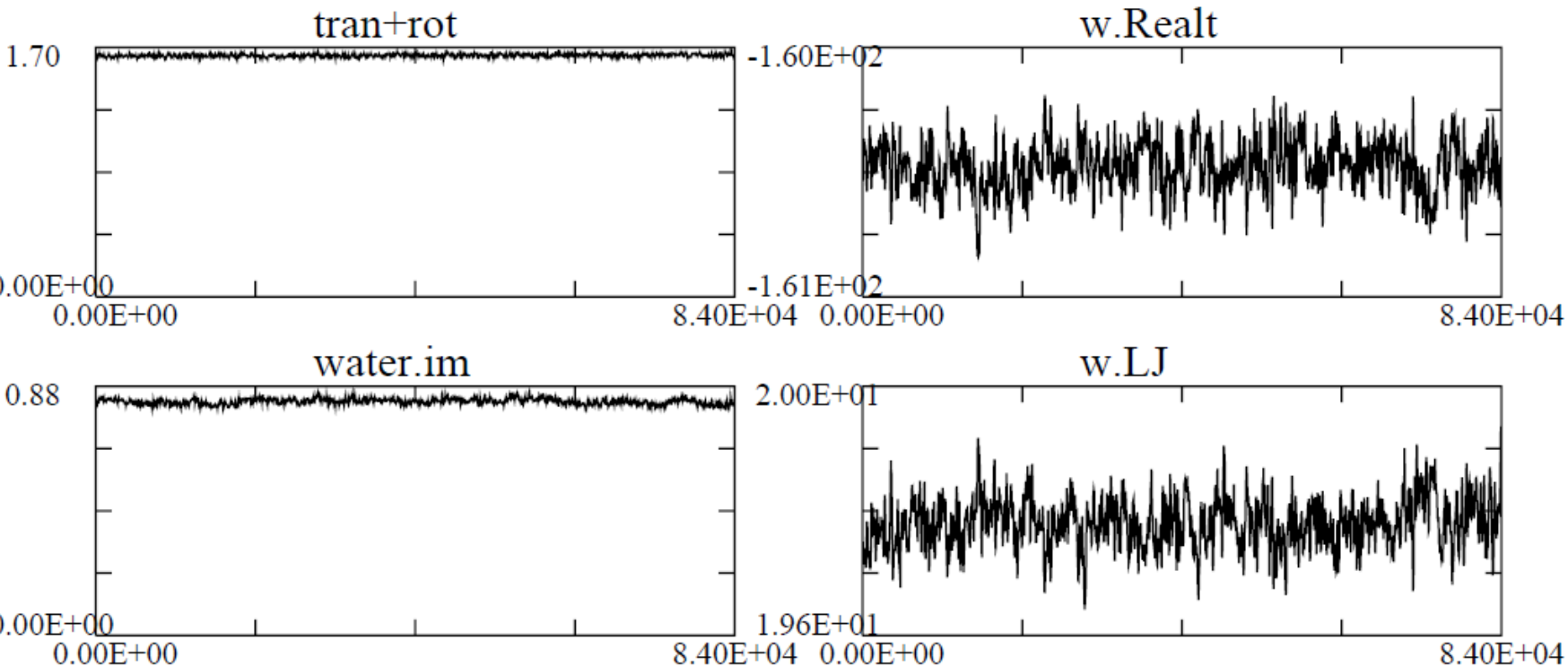




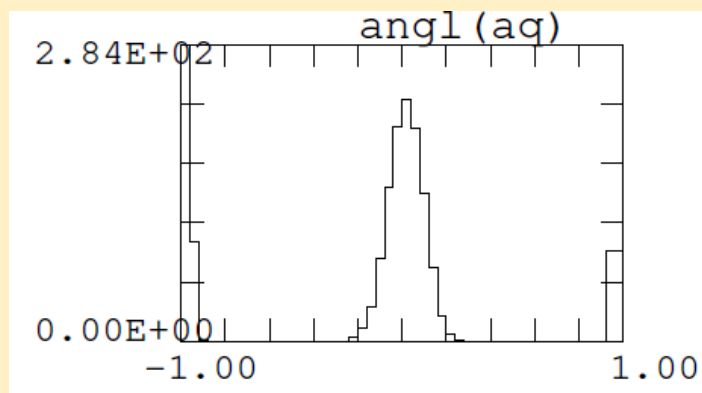
Water molecules starting 298 K.

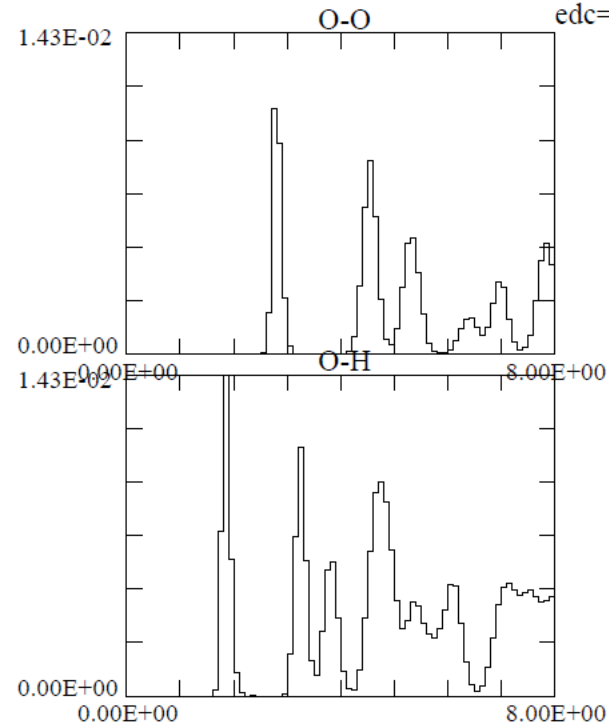
Left: Scatter plot of water at $t=80,000$, b) x-directional cosine distribution for the cross bins of $(-1.0, 1.0)$ at $t=72,500$ to $80,000$. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

Simulation starting at ice 230 K, NVE

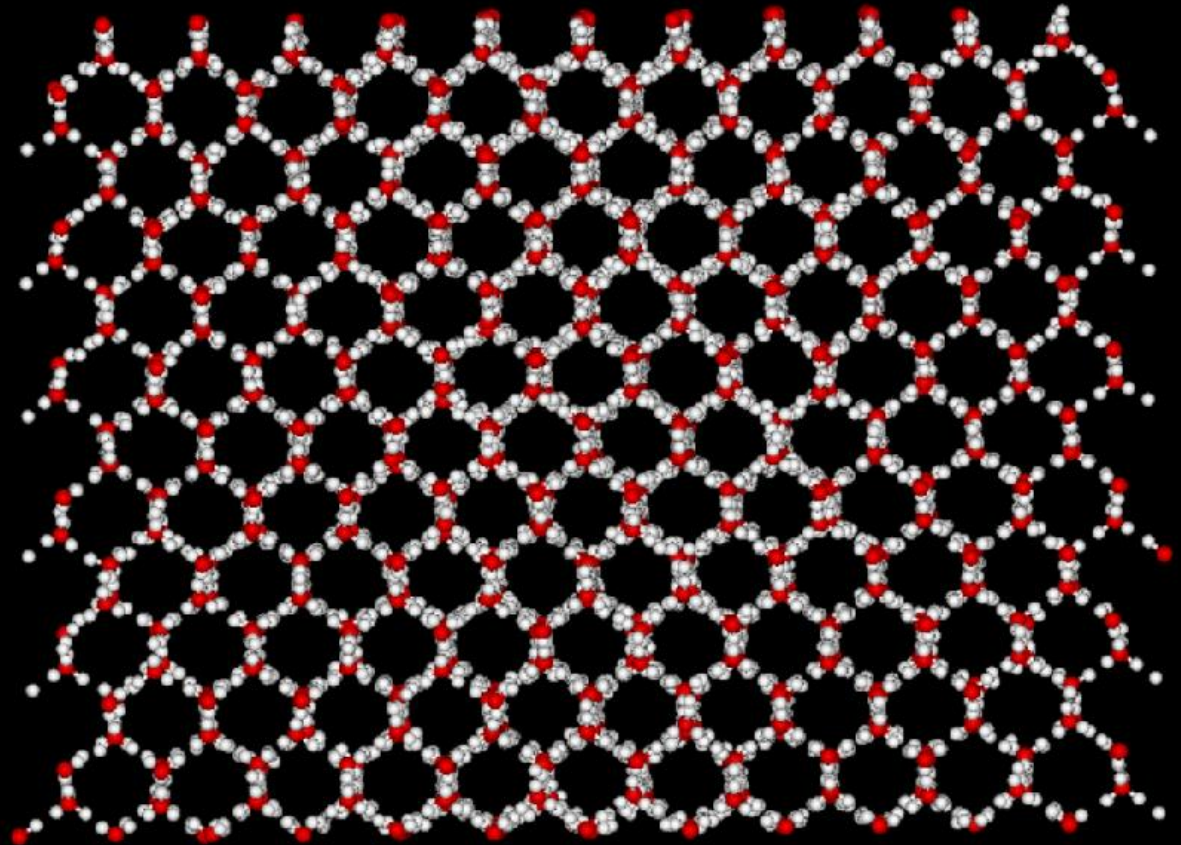


At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity $E_0 = 5 \times 10^6$ V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at the time of $t=84,000$. Right: cosine distribution of water in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

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3. “Microwave heating of water and ice by TIP5P code”, M. Tanaka, <https://github.com/Mtanaka77/> (May 2023).
4. “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