Molecular Dynamics Simulation of Water and Ice by TIP5P Code

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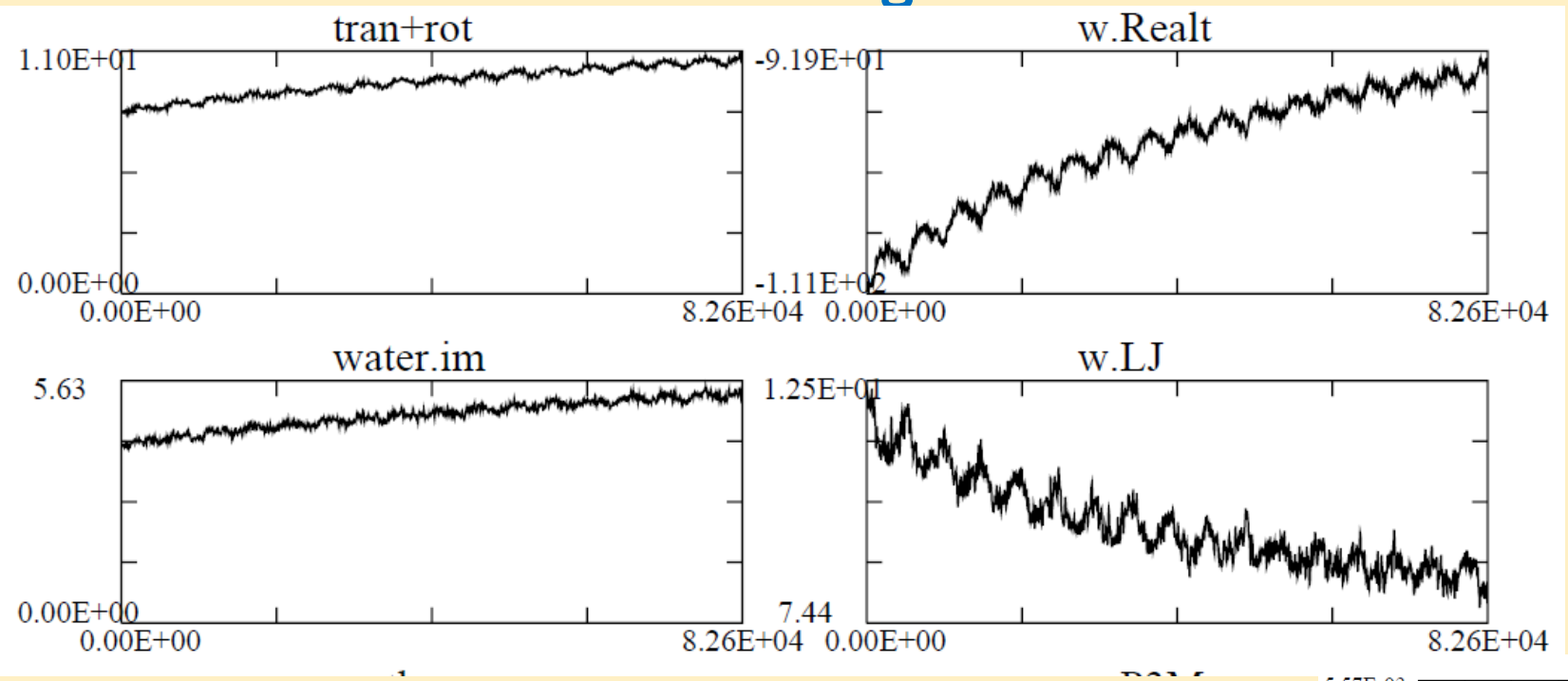
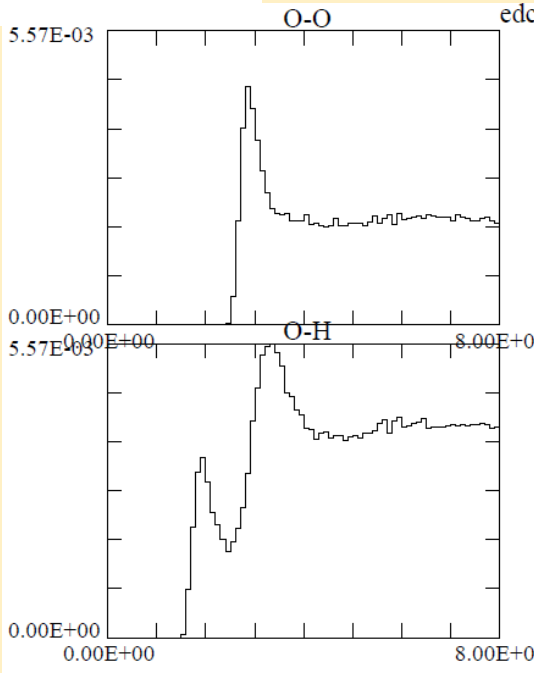
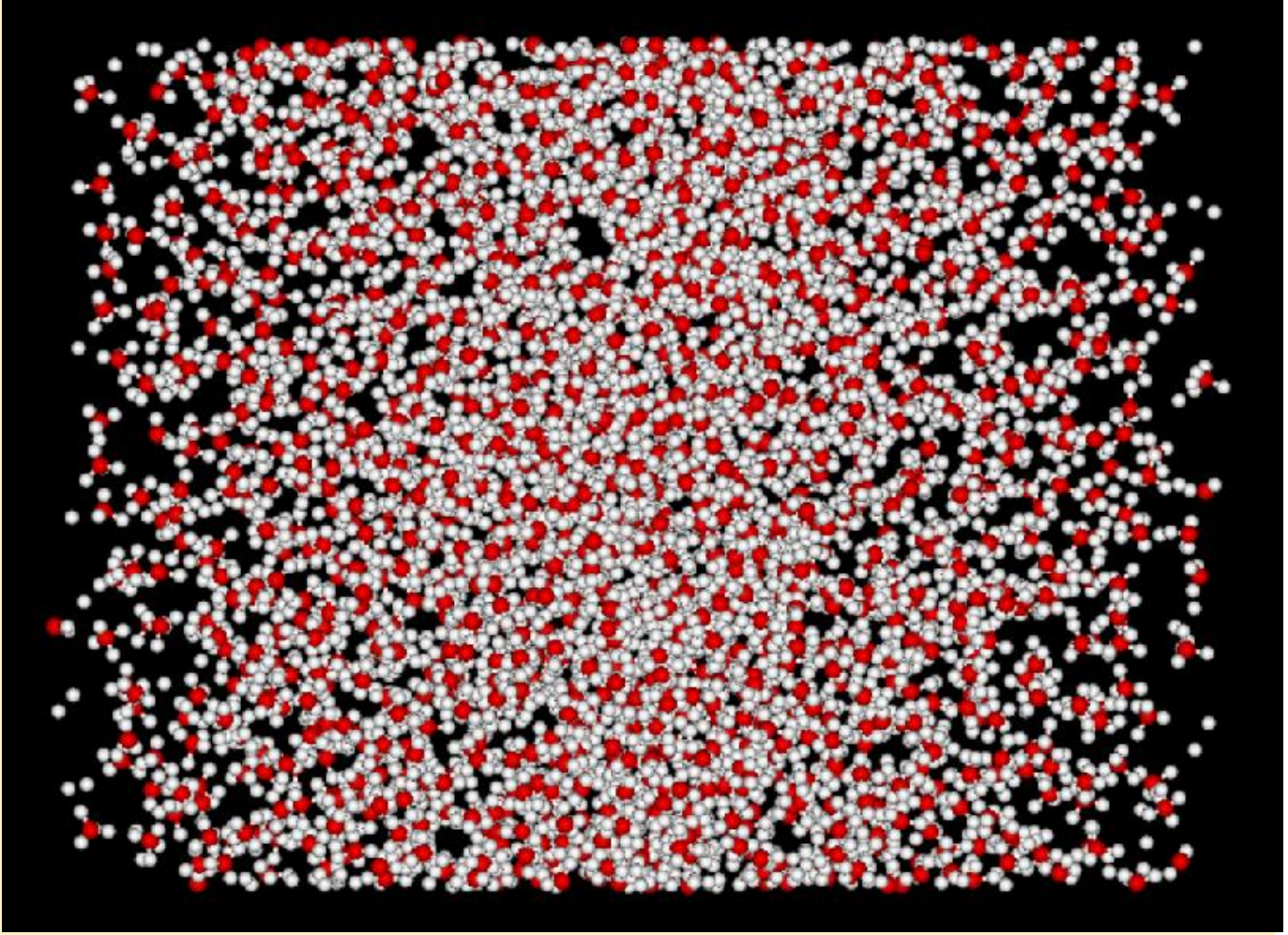
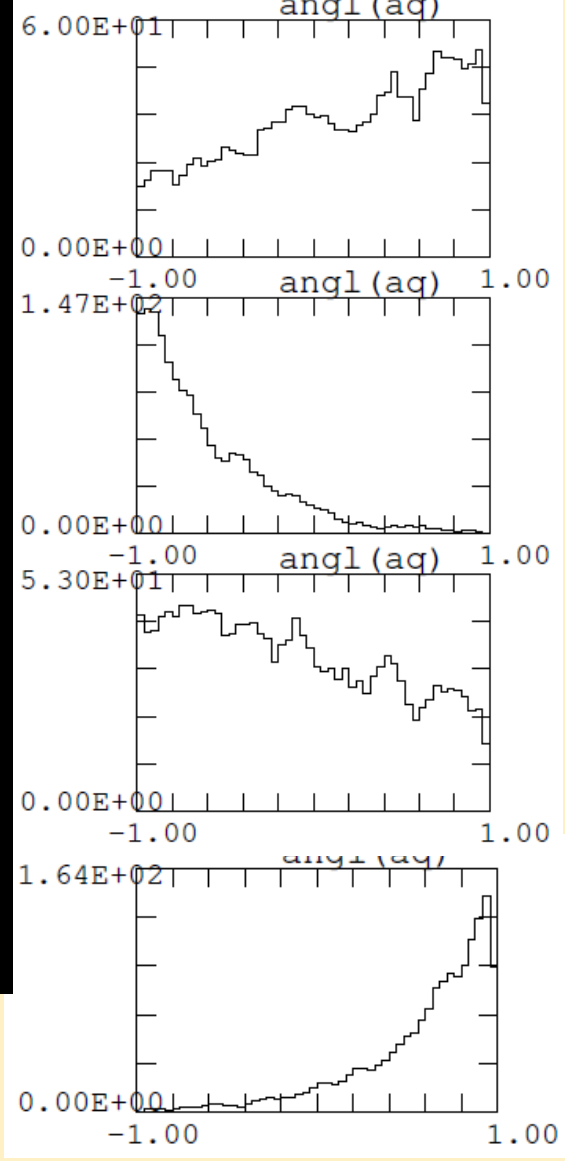
* Simulation water starting from 298 K



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.

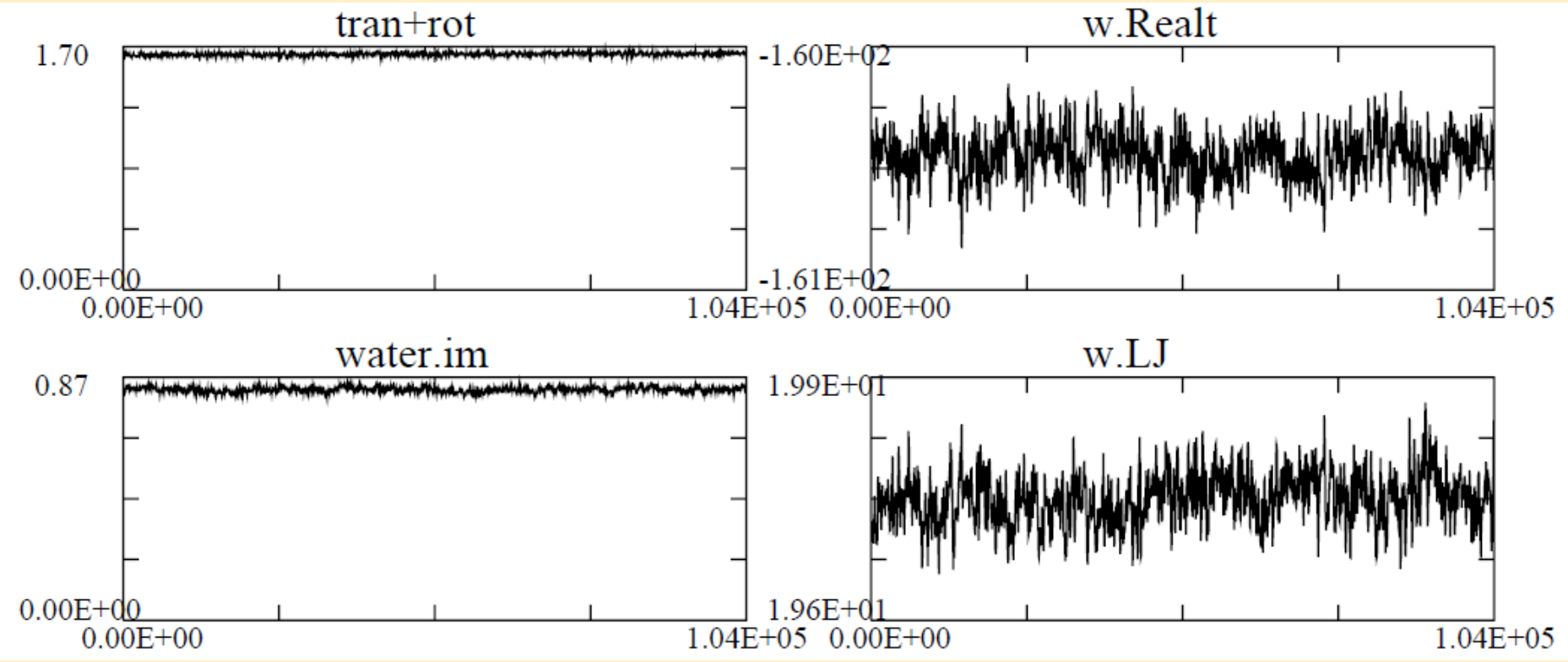




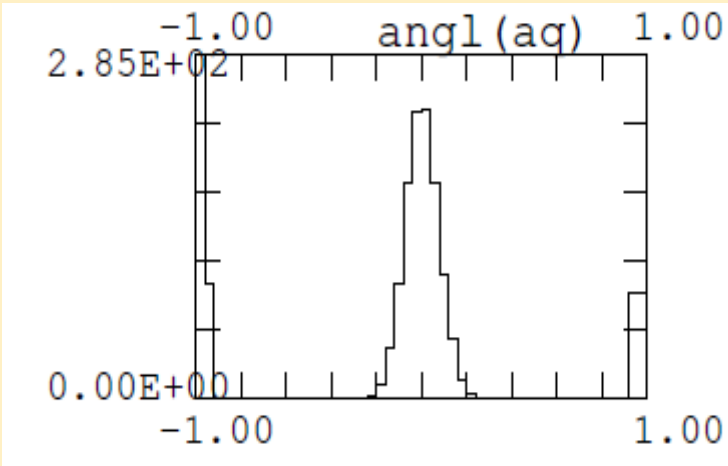


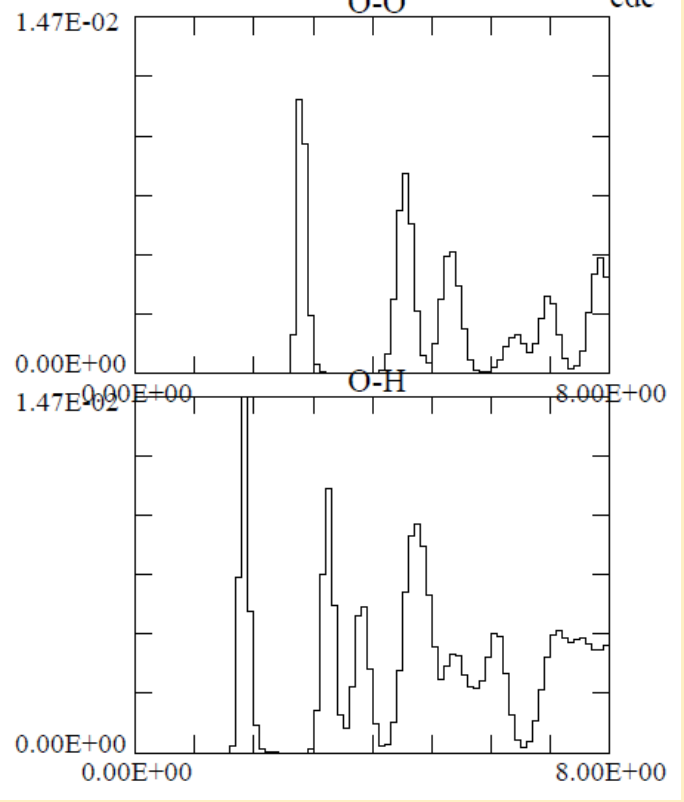
Water molecules starting 298 K.
Left: Scatter plot of water at t=80,000, b) x−directional cosine distribution for the cross bins of (−1.0,1.0) at t=72,500 to 80,000. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

* Simulation starting 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= 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=104,000. 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=104,000 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 6–membered rings are formed for frozen ice.