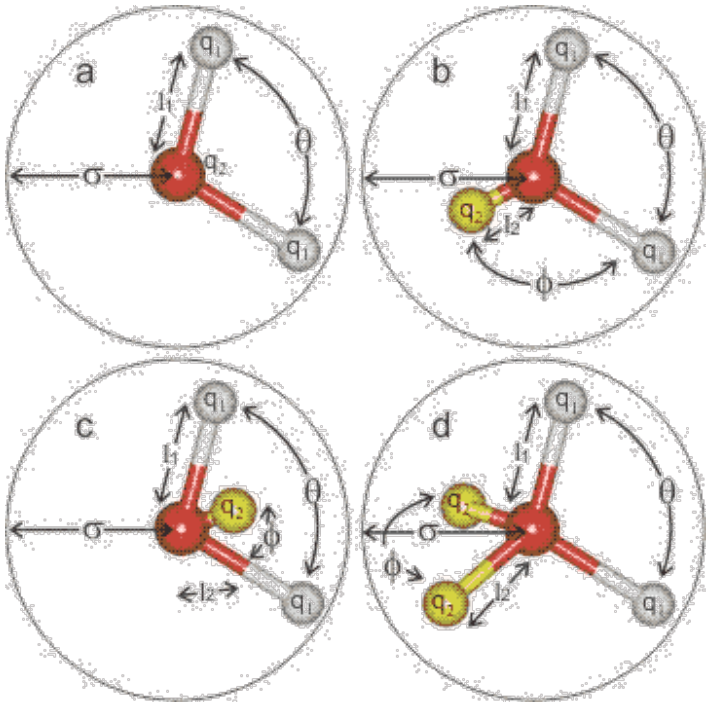
Liquid water MD simulation

A lot of stories on water:

Please refer to the excellent web-site
Martin Chaplin's "**Water Structure and Science**"

http://www.lsbu.ac.uk/water/index2.html

Model	Type	σ / Å	ϵ / kJ mol^{-1}	l_1 Å	l_2 Å	q_1 (e)	q_2 (e)	θ°	φ°
SPC/E	a	3.166	0.650	1.0000	-	+0.4238	-0.8476	109.47	-
TIP3P	a	3.15061	0.6364	0.9572	-	+0.4170	-0.8340	104.52	-
TIP4P	c	3.15365	0.6480	0.9572	0.15	+0.5200	-1.0400	104.52	52.26
TIP4P-Ew	c	3.16435	0.680946	0.9572	0.125	+0.52422	-1.04844	104.52	52.26
TIP5P-Ew	d	3.097	0.7448	0.9572	0.70	+0.2410	-0.2410	104.52	109.47



Water model potential

SPC/E: H. J. C. Berendsen, J. R. Grigera and T. P. Straatsma, The missing term in effective pair potentials, *J. Phys. Chem.* **91** (1987) 6269-6271.

TIP3P: W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey, and M. L. Klein, Comparison of simple potential functions for simulating liquid water, *J. Chem. Phys.* **79** (1983) 926-935

TIP4P: W. L. Jorgensen and J. D. Madura, Temperature and size dependence for monte carlo simulations of TIP4P water, *Mol. Phys.* **56** (1985) 1381-1392.

TIP4P-Ew: H. W. Horn, W. C. Swope, J. W. Pitera, J. D. Madura, T. J. Dick, G. L. Hura and T. Head-Gordon, Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew, *J. Chem. Phys.* **120** (2004) 9665-9678.

TIP5P-Ew: S. W. Rick, A reoptimization of the five-site water potential (TIP5P) for use with Ewald sums, *J. Chem. Phys.* **120** (2004) 6085-6093.

TIP5P: M. W. Mahoney and W. L. Jorgensen, A five-site model for liquid water and the reproduction of the density anomaly by rigid, nonpolarizable potential functions, *J. Chem. Phys.* **112** (2000) 8910-8922.

Calculated results：classical MD

Model	Dipole moment	Dielectric constant	Self diffusion, 10^{-5} cm^2/s	Average configurational energy, kJ mol^{-1}	Density maximum, °C	Expansion coefficient, 10^{-4} $°C^{-1}$
Exp.	2.95	78.4	2.30	-41.5	+3.984	2.53
SPC/E	2.35	71	2.49	-41.5	-38	5.14
TIP3P	2.35	82	5.19	-41.1	-91	9.2
TIP4P	2.18	53	3.29	-41.8	-25	4.4
TIP4P-Ew	2.32	62.9	2.4	-46.5	+1	3.1
TIP5P-Ew	2.29	92	2.8	-	+8	4.9

All the data is at 25°C and 1 atm

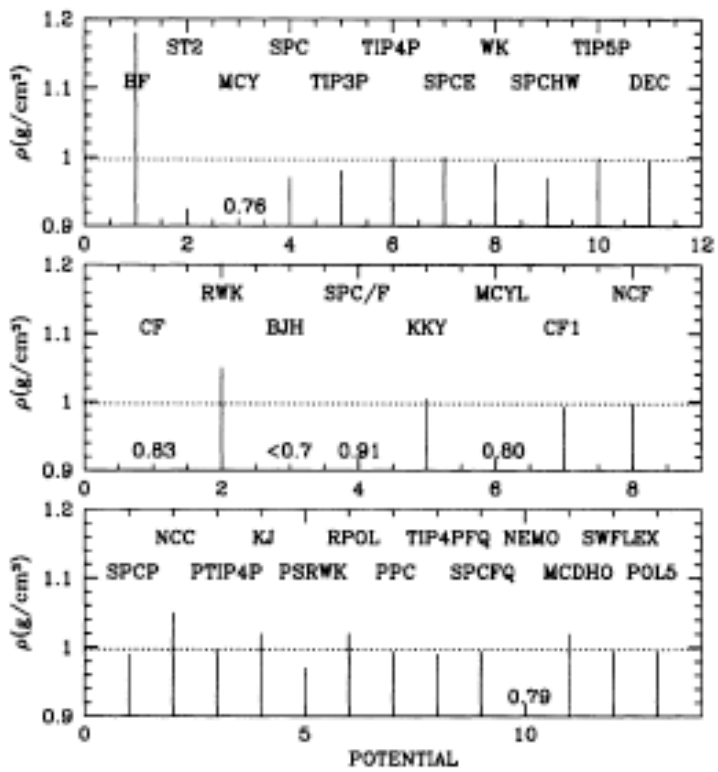
==>The popular models SPC, SPC/E, TIP3P and TIP4P produce poor agreement with water's melting point (giving melting points of 190 K, 215 K, 146 K and 232 K respectively)

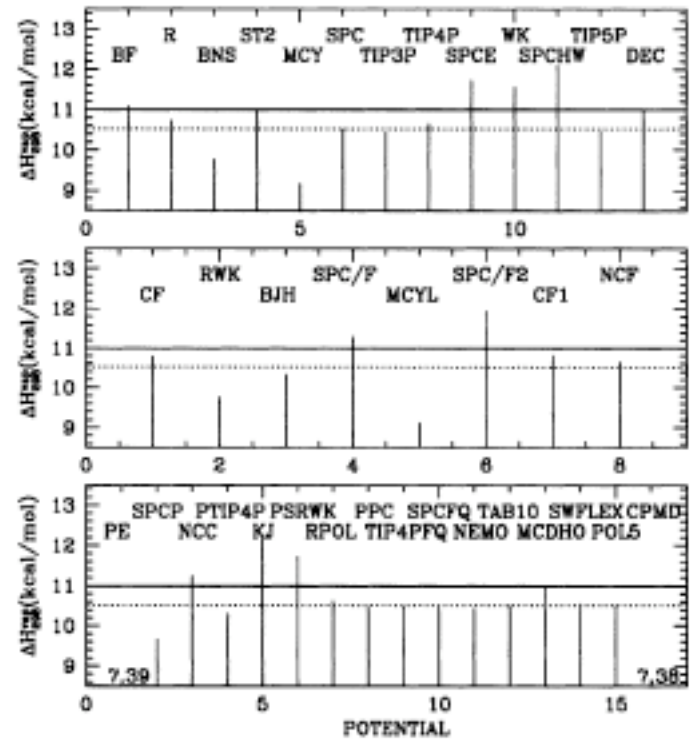
==>The popular TIP4P model underestimates the tetrahedrality of the water molecule's environment, which explains its poor estimate of the dielectric constant. It is, however, remarkably good at qualitatively describing water's phase diagram. The SPC/E and TIP4P models are reported as failing to properly describe the experimental O···O radial distribution function. The TIP3P and SPC show particularly poor agreement, the TIP4P, SPC/E and PPC show improved agreement.

Journal of Molecular Liquids 101/1–3 (2002) 219–260

A REAPPRAISAL OF WHAT WE HAVE LEARNT DURING THREE DECADES OF COMPUTER SIMULATIONS ON WATER

Bertrand Guillot





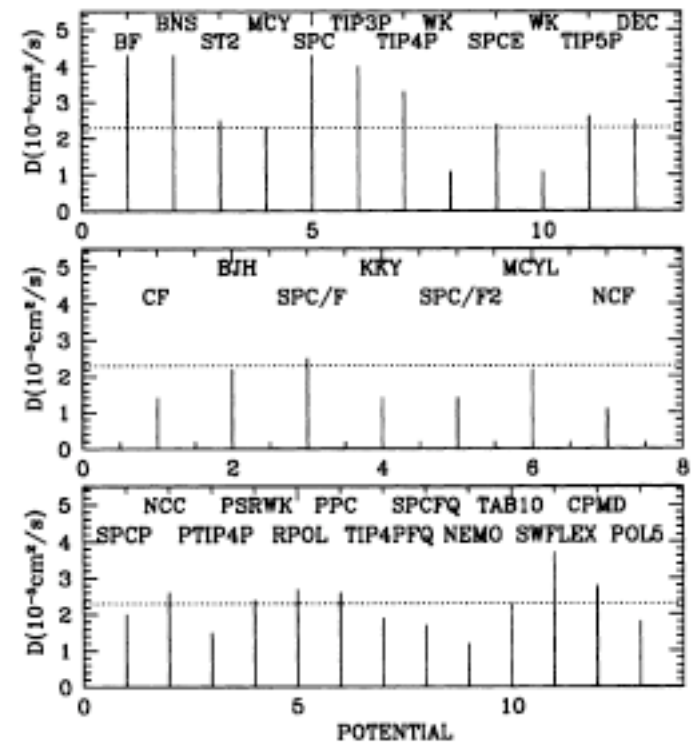
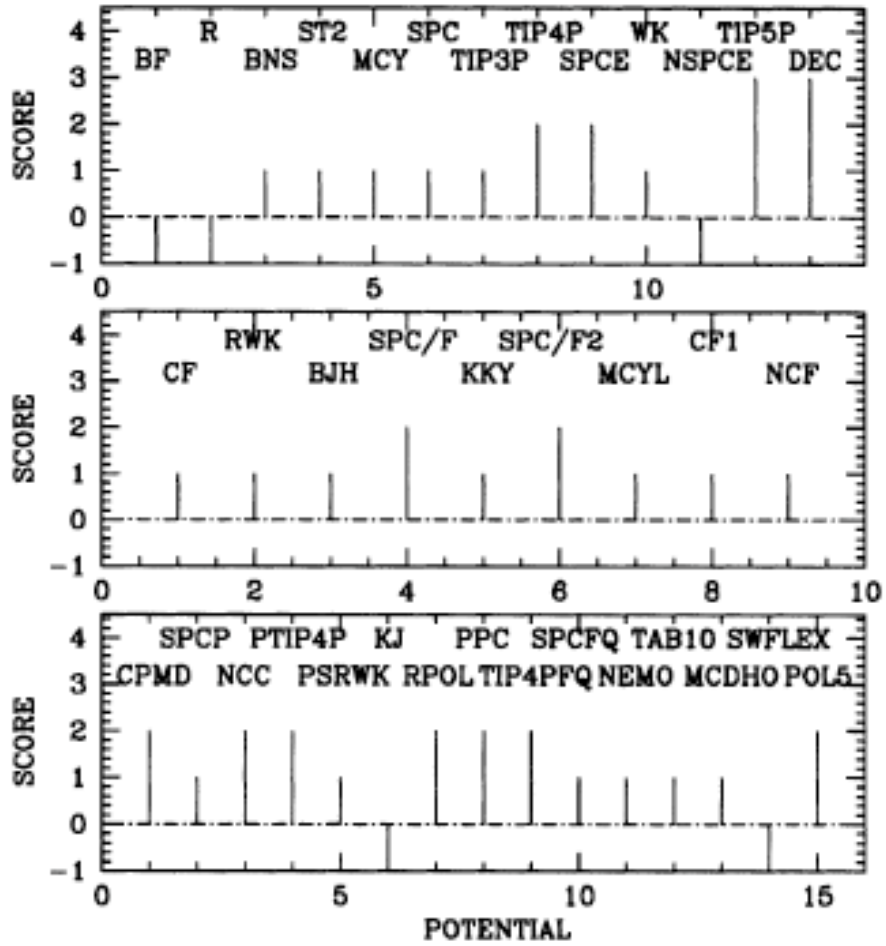


Figure 1. Density of simulated water at 298K and 1bar for different model potentials (see Table):top panel (rigid models), middle panel (flexible models) and bottom panel (polarizable models). The dotted line indicates the experimental value for H_2O (0.997g/cm3).

model potential SCORE

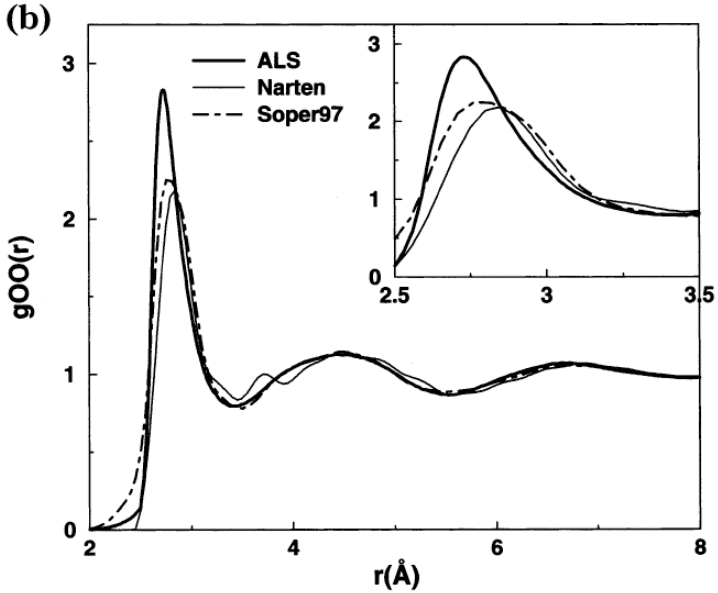


==> We will use SPC/E and TIP4P/Ew models.

Figure 5. Ability of the model potentials to reproduce structure data of liquid water at ambient conditions (see text): -1 suggests a bad description, +1 when it is acceptable, +2 when the description is good and +3 when the agreement is excellent (see Fig.4 for an illustration).

flexible model: time consuming and not improved from rigid model

Polarizable model: so far not significantly improved, but maybe important for ion solvation, for interface, and for ILs



line). (b) Comparison of experimentally derived $g_{OO}(r)$ data. ALS, X-ray[40] (thick solid line); Narten,[70] X-ray (thin solid line); Soper, Bruni, and Ricci,[103] neutron 1997 (dot–dash line).

ALS2000 and Soper 2000

ALS:X-ray 2000
Narten: X-ray 1972
Soper: Neutron 97
Soper 2000:reanalysis of 1997 data

Chem. Rev. **2002**, *102*, 2651–2670

Water Structure from Scattering Experiments and Simulation

Teresa Head-Gordon*

Department of Bioengineering, University of California at Berkeley, and Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720

Greg Hura

Graduate Group in Biophysics, University of California at Berkeley, and Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720

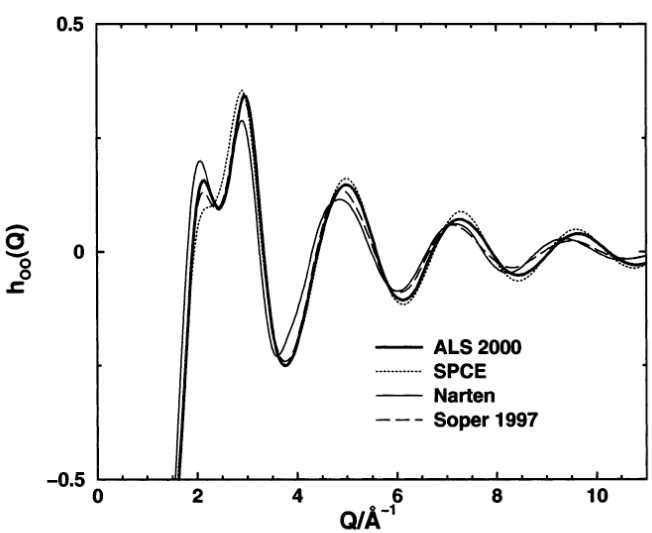


Figure 3. $h_{OO}(Q)$ from experiment and simulation. Legend: Narten and Levy[63] (thin solid line); Soper, Bruni, and Ricci[103] (dot–dash line); Hura et al.[40] (thick solid line); SPC/E[24] (dotted line). The curve for Narten and Levy is $H_M(Q)$ taken from their paper;[62] the curve for Soper et al. is taken from applying a Fourier transform to the $g_{OO}(r)$ given in ref 103.

good agreement !!
SPC/E and ALS2000

Radial distribution function(**RDF**) from **exp. and MD.**

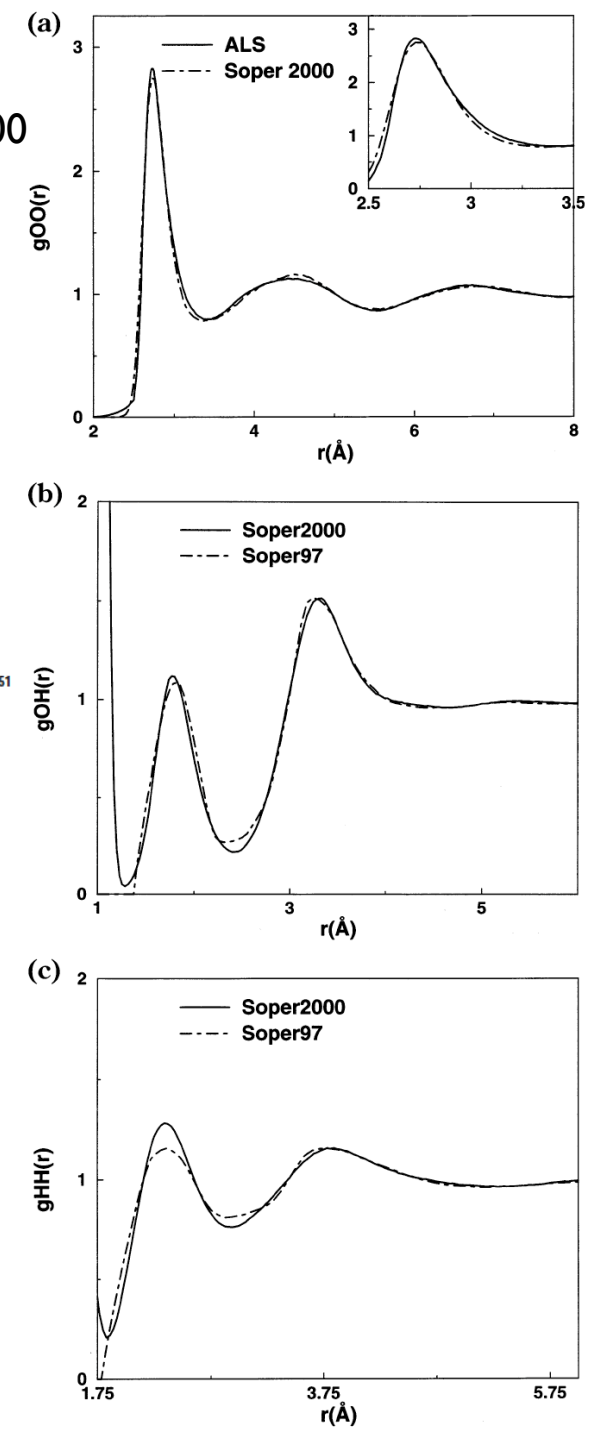


Figure 4. Comparison of neutron data on pure water at 25 °C and 1 atm. **(a)** Comparison of ALS X-ray experimental $g_{OO}(r)$[40,41] (solid line) with reanalysis of Soper neutron data, 2000[5] (dashed line). Comparison of neutron data on pure water at 25 °C and 1 atm in 1997[103] (dot–dash line) and 2000[116] (solid line) for **(b)** $g_{OH}(r)$ and **(c)** $g_{HH}(r)$.

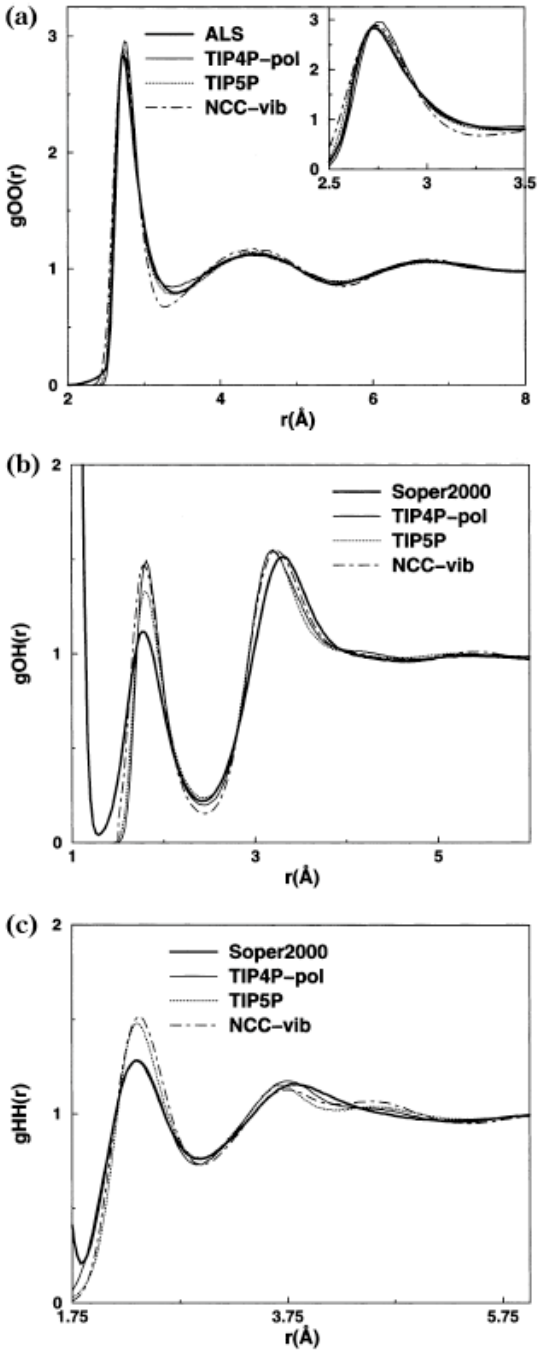


Figure 5. Comparison of experimental radial distribution functions (thick solid line) with simulations using empirical force fields for the TIP4P-pol-1[31] (thin solid line), TIP5P[27] (dotted line), and NCC-vib[29] (dot–dash line) models: (a) $g_{OO}(r)$, (b) $g_{OH}(r)$, and (c) $g_{HH}(r)$.

Classical model potentials can explain the Exp. results very well.

Exp. results are also improving.

Radial distribution function from exp. and MD.

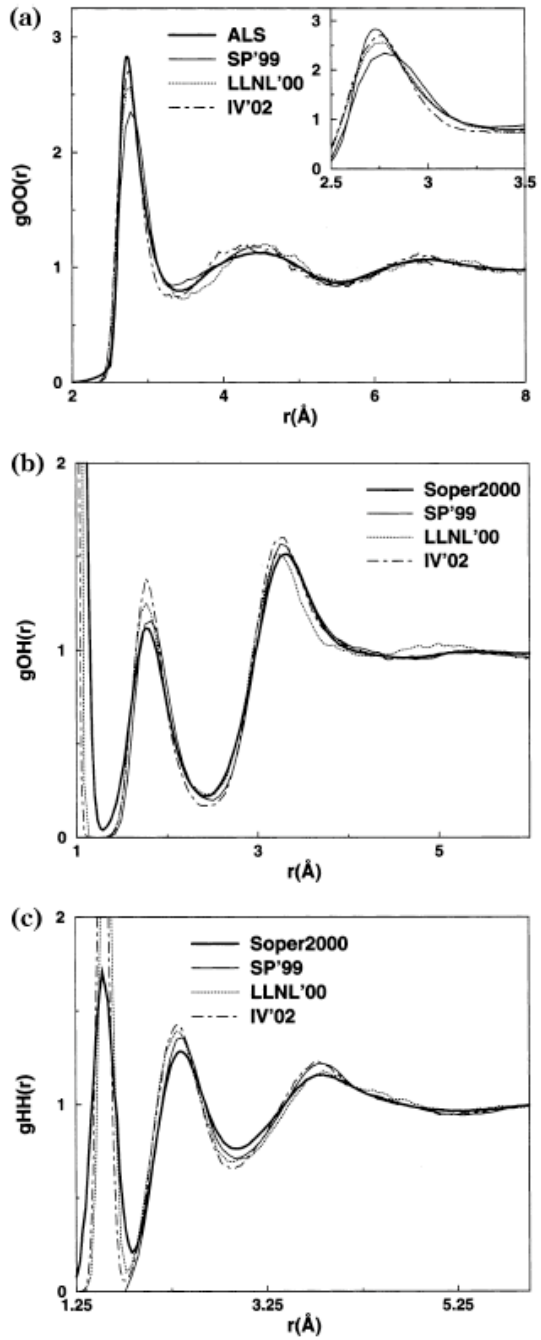


Figure 6. Comparison of experimental scattering data with ab initio molecular dynamics simulations. ALS X-ray experimental $g_{OO}(r)$ (thick solid line), ab initio simulation of 10 ps for 64 water molecules, average ionic temperature of 318 K from Silvestrelli and Parrinello[36] (thin solid line), recent ab initio simulation by Schwegler et al.,[187] 3 ps for 54 water molecule average ionic temperature of ~294 K (dotted line), ab initio simulation of 12 ps for 64 water molecules, average ionic temperature of 307 K from Izvekov and Voth[38] (dot–dash line): (a) $g_{OO}(r)$, (b) $g_{OH}(r)$, (c) $g_{HH}(r)$.

first-pinciples MD is getting better.

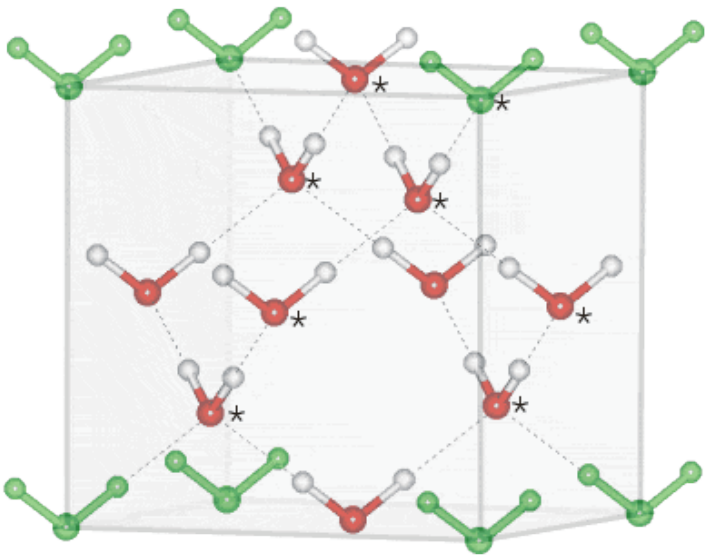
Here we use one of the water model SPC/E or TIP4P-Ew

1) L-J interaction is oxygen-oxygen only.
2) rigid molecule is assumed. ==> Cal. become faster
   O-H distance is const.
   angle H-O-H is const.
==> Cal. become faster
==> but neglect the vibrational degree of freedom.
==> we should select how we impose the constraints on bond length and bond angle.

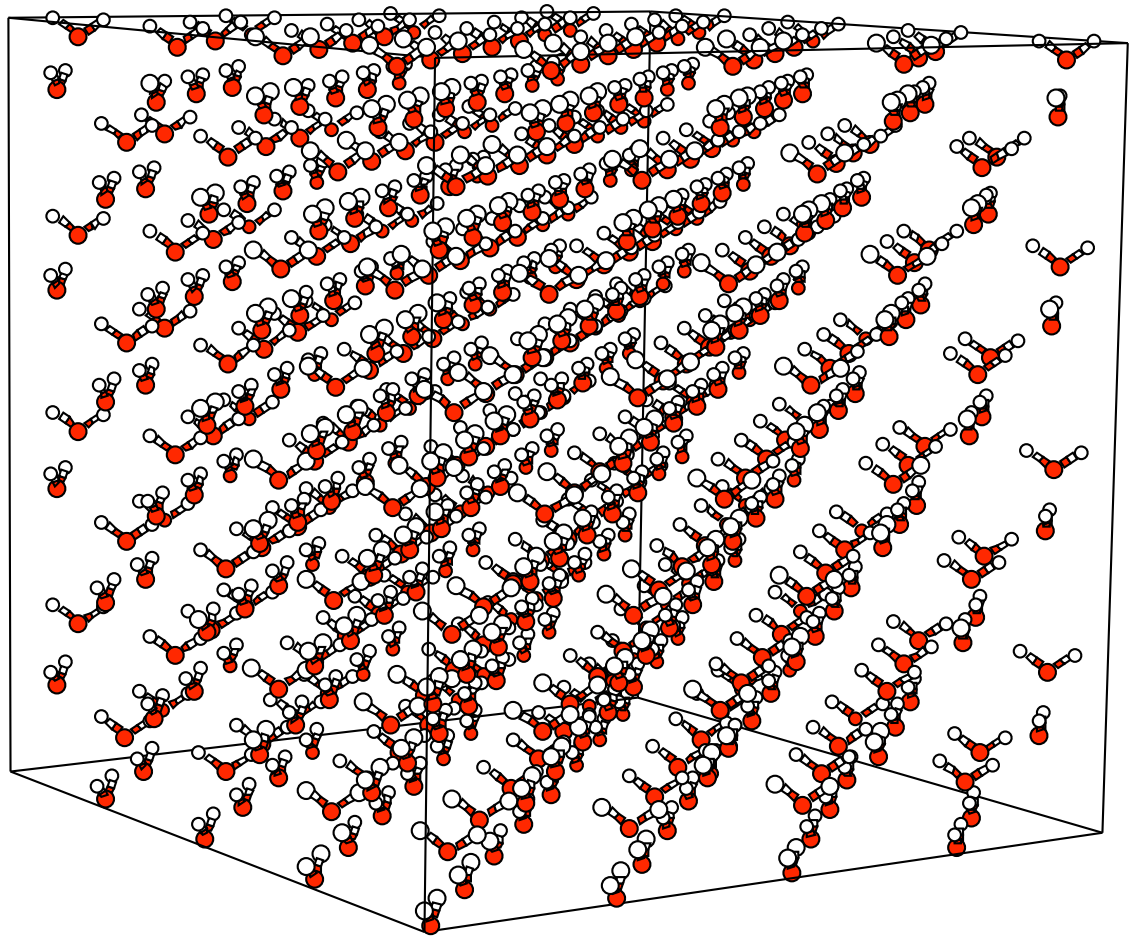
3) no electrostatic interaction between the intramolecular atoms.

initial configuration: ice?

Cubic Ice



fcc + half the tetrahedral sites are filled.



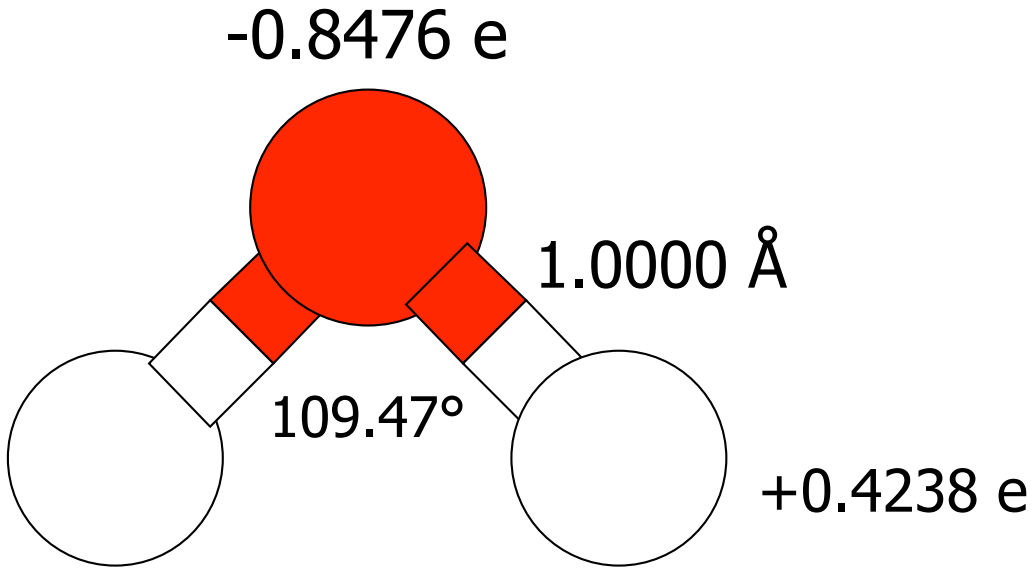
ρ / g cm-3 = 0.996516

H2O all site(fcc+t-site)= 512

liquid water all atom number= 1536

ax,ay,az,volume= 24.86, 24.86, 24.86 Å 15370.0

SPC/E model



r(OH)=1.0000 Å
θ(HOH)=109.47
are fixed.

intermolecular interaction

z(O)=-0.8476 *e*
z(H)=0.4238 *e*
ε(O) = 0.650 kJ mol^{-1}
σ(O) = 3.166 Å

CONFIG

```
H2O liquid SPCE water at  300 K
         2          1
   24.8632886676       .0000000000       .0000000000
    .0000000000     24.8632886676       .0000000000
    .0000000000       .0000000000     24.8632886676
  OW    1
 -12.4316443338    -12.4316443338    -12.4316443338
   -.1157118156      -.1006883860       .0252069353
    .0000000000       .0000000000       .0000000000
  HW    2
 -11.8542984133    -11.8542984133    -11.8542853673
   -.1157118156      -.1006883860       .0252069353
    .0000000000       .0000000000       .0000000000
  HW    3
 -13.0089902543    -13.0089902543    -11.8542853673
   -.1157118156      -.1006883860       .0252069353
    .0000000000       .0000000000       .0000000000
  OW    4
 -10.8776887921    -10.8776887921    -10.8776887921
   -.0944489040       .0834090526      -.0070384049
    .0000000000       .0000000000       .0000000000
  HW    5
 -10.3003428716    -11.4550347126    -10.3003298256
   -.0944489040       .0834090526      -.0070384049
    .0000000000       .0000000000       .0000000000
  HW    6
 -11.4550347126    -10.3003428716    -10.3003298256
   -.0944489040       .0834090526      -.0070384049
    .0000000000       .0000000000       .0000000000
...
  OW 1534
    7.7697777086      10.8776887921      10.8776887921
    .0179460404       .0359122702       .0141856681
    .0000000000       .0000000000       .0000000000
  HW 1535
    8.3471236291      10.3003428716      11.4550477586
    .0179460404       .0359122702       .0141856681
    .0000000000       .0000000000       .0000000000
  HW 1536
    7.1924317881      11.4550347126      11.4550477586
    .0179460404       .0359122702       .0141856681
    .0000000000       .0000000000       .0000000000
```

FIELD

```
H2O SPC/E
units  kJ
molecules 1
SPCE water
nummols 512
atoms 3
   OW        15.9996    -0.8476
   HW        1.0008      0.4238
   HW        1.0008      0.4238
constraints  3
    1    2    1.0000
    1    3    1.0000
    2    3    1.63298
finish
vdW 3
    OW      OW    lj  0.6507346    3.165492
    OW      HW    lj  0.0          3.165492
    HW      HW    lj  0.0          0.0
close
```

SPC/E model

CONTROL NVE

```
SPC/E model of water

integrator velocity verlet
temperature      300.00
ensemble nve

steps          150000
equilibration   100000
multiple step        1
scale               10
print               50
stack              100
stats               10
rdf                  1
traj     1   100  0

timestep        0.001
cutoff          9.50
delr width      0.5000
ewald precision 1d-6
shake tolerance  1.0E-5
quaternion tolerance  1.0E-5
print rdf

job time           150000.00
close time            500.00

finish
```

CONTROL NPT 300 K 1 atom

```
SPC/E model of water

integrator velocity verlet
temperature      300.00
ensemble npt hoover 0.1 0.2

steps          150000
equilibration   100000
multiple step        1
scale               10
print               50
stack              100
stats               10
rdf                  1
traj     1   100  0

timestep        0.001
cutoff          9.50
delr width      0.5000
ewald precision 1d-6
shake tolerance  1.0E-5
quaternion tolerance  1.0E-5
print rdf
pres  0.001

job time           150000.00
close time            500.00

finish
```

SPC/E model

NVE : microcanonical ensemble

==> total energy conserved

==> directly linked to mechanics

==> $k_B T$ = kinetic energy

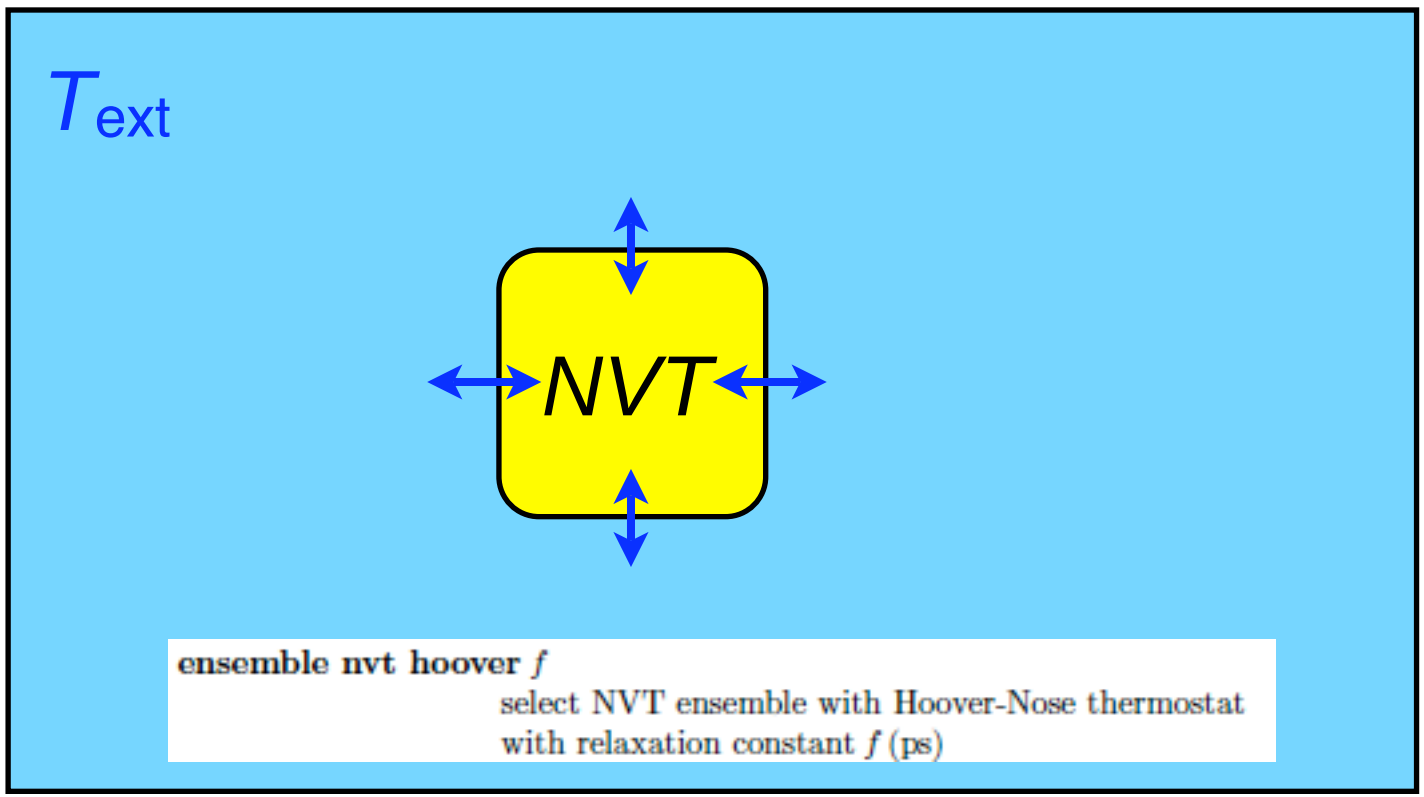
Temperature fluctuates

but the termal average should be the same

NVT : canonical ensemble

==> *T* keeps constant and
the heat exchange (or momentum exchange)
with the virtual reservoir (thermostat)

===> some tricks are needed.
Nose-Hoover algorithm is only well defined!!



ensemble nvt hoover *f*

select NVT ensemble with Hoover-Nose thermostat
with relaxation constant *f* (ps)

2.5.4.1 Nosé - Hoover Thermostat

In the Nosé-Hoover algorithm [20] Newton's equations of motion are modified to read:

$$\frac{d\underline{r}(t)}{dt} = \underline{v}(t)$$

$$\frac{d\underline{v}(t)}{dt} = \frac{\underline{f}(t)}{m} - \chi(t)\underline{v}(t) \qquad (2.231)$$

$$(2.232)$$

The friction coefficient, χ, is controlled by the first order differential equation

$$\frac{d\chi(t)}{dt} = \frac{N_f k_B}{Q}(\mathcal{T}(t) - T_{\rm ext}) \qquad (2.233)$$

where $Q = N_f k_B T_{\rm ext} \tau_T^2$ is the effective 'mass' of the thermoststat, τ_T is a specified time constant (normally in the range [0.5, 2] ps) and N_f is the number of degrees of freedom in the system. $\mathcal{T}(t)$ is the instantaneous temperature of the system at time t.

In the VV version of DL_POLY_2

$$\begin{aligned}
\chi(t+\tfrac{1}{2}\Delta t) &\leftarrow \chi(t) + \frac{\Delta t N_f k_B}{2Q}(\mathcal{T}(t) - T_{\rm ext}) \\
\underline{v}'(t) &\leftarrow \underline{v}(t) - \frac{\Delta t}{2}\chi(t+\tfrac{1}{2}\Delta t)\underline{v}(t) \\
\underline{v}(t+\tfrac{1}{2}\Delta t) &\leftarrow \underline{v}'(t) + \frac{\Delta t}{2}\frac{\underline{f}(t)}{m} \\
\underline{r}(t+\Delta t) &\leftarrow \underline{r}(t) + \Delta t\, \underline{v}(t+\tfrac{1}{2}\Delta t) \\
& \quad call \quad rattle(R) \\
\underline{v}'(t+\Delta t) &\leftarrow \underline{v}(t+\tfrac{1}{2}\Delta t) + \frac{\Delta t}{2}\frac{\underline{f}(t+\Delta t)}{m} \\
& \quad call \quad rattle(V) \\
\chi(t+\Delta t) &\leftarrow \chi(t+\tfrac{1}{2}\Delta t) + \frac{\Delta t N_f k_B}{2Q}(\mathcal{T}(t+\Delta t) - T_{\rm ext}) \\
\underline{v}(t+\Delta t) &\leftarrow \underline{v}'(t+\Delta t) - \frac{\Delta t}{2}\chi(t+\Delta t)\underline{v}'(t+\Delta t)
\end{aligned}$$

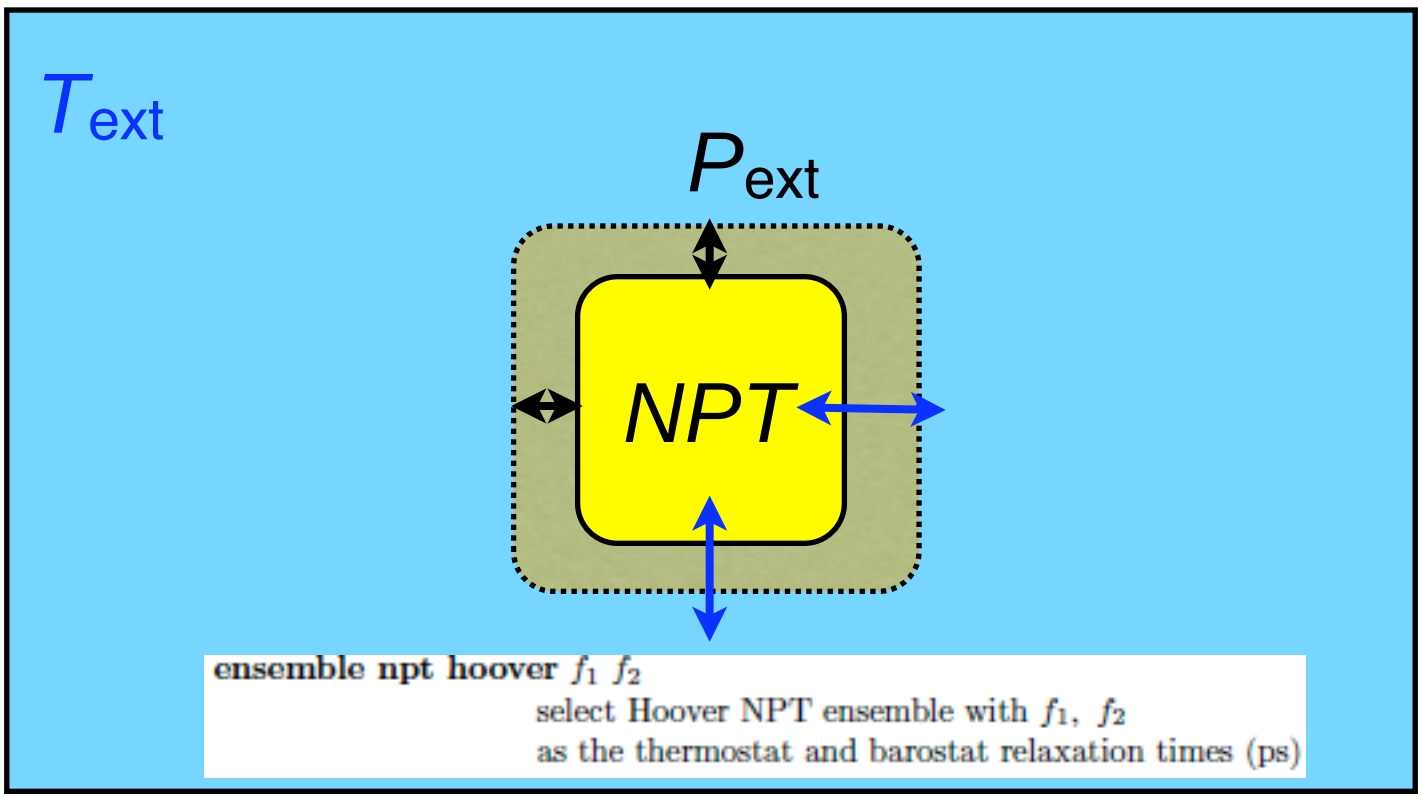
The conserved quantity is derived from the extended Hamiltonian for the system which, to within a constant, is the Helmholtz free energy:

$$\mathcal{H}_{\rm NVT} = U + KE + \frac{1}{2}Q\chi(t)^2 + \frac{Q}{\tau_T^2}\int_o^t \chi(s)ds$$

NPT ensemble

==> *T* and *P* keeps constant and
the heat exchange and cell size change
dynamically.

===> Hoover barostat method is only well defined!!



ensemble npt hoover f_1 f_2

select Hoover NPT ensemble with f_1, f_2
as the thermostat and barostat relaxation times (ps)

Cell size variation

For isotropic fluctuations the equations of motion are:

$$\begin{aligned}
\frac{d\underline{r}(t)}{dt} &= \underline{v}(t) + \eta(\underline{r}(t) - \underline{R}_0) \\
\frac{d\underline{v}(t)}{dt} &= \frac{\underline{f}(t)}{m} - [\chi(t) + \eta(t)]\,\underline{v}(t) \\
\frac{d\chi(t)}{dt} &= \frac{N_f k_B}{Q}(\mathcal{T}(t) - T_{\text{ext}}) + \frac{1}{Q}(W\eta(t)^2 - k_B T_{\text{ext}}) \\
\frac{d\eta(t)}{dt} &= \frac{3}{W}V(t)(\mathcal{P}(t) - P_{\text{ext}}) - \chi(t)\eta(t) \\
\frac{dV(t)}{dt} &= [3\eta(t)]V(t)
\end{aligned} \tag{2.246}$$

where $Q = N_f k_B T_{\text{ext}} \tau_T^2$ is the effective 'mass' of the thermostat and $W = N_f k_B T_{\text{ext}} \tau_P^2$ is the effective 'mass' of the barostat. N_f is the number of degrees of freedom, η is the barostat friction coefficient, R_0 the system centre of mass, τ_T and τ_P are specified time constants for temperature and pressure fluctuations respectively, $\mathcal{P}(t)$ is the instantaneous pressure and V the system volume.

The conserved quantity is, to within a constant, the Gibbs free energy of the system:

$$\mathcal{H}_{NPT} = U + KE + \mathcal{P}_{\text{ext}}V(t) + \frac{1}{2}Q\chi(t)^2 + \frac{1}{2}W\eta(t)^2 + \int_o^t (\frac{Q}{\tau_T^2}\chi(s) + k_B\mathcal{T}_{\text{ext}})ds \tag{2.247}$$

The implementation in the VV algorithm follows the scheme:

$$
\begin{aligned}
\chi(t+\tfrac{1}{2}\Delta t) &\leftarrow \chi(t) + \frac{\Delta t N_f k_B}{2Q}(\mathcal{T}(t) - T_{\text{ext}}) + \frac{\Delta t}{2Q}(W\eta(t)^2 - k_B T_{\text{ext}}) \\
\underline{v}'(t) &\leftarrow \underline{v}(t) - \frac{\Delta t}{2}\chi(t+\tfrac{1}{2}\Delta t)\underline{v}(t) \\
\eta(t+\tfrac{1}{2}\Delta t) &\leftarrow \eta(t) + \frac{\Delta t}{2}\left\{\frac{3V(t)}{W}(\mathcal{P}(t) - P_{\text{ext}}) - \chi(t)\eta(t)\right\} \\
\underline{v}''(t) &\leftarrow \underline{v}'(t) - \frac{\Delta t}{2}\eta(t+\tfrac{1}{2}\Delta t)\underline{v}'(t) \\
\underline{v}(t+\tfrac{1}{2}\Delta t) &\leftarrow \underline{v}''(t) + \frac{\Delta t}{2}\frac{\underline{f}(t)}{m} \\
\underline{r}(t+\Delta t) &\leftarrow \underline{r}(t) + \Delta t\, \underline{v}(t+\tfrac{1}{2}\Delta t) \\
&\quad call \quad rattle(R) \\
V(t+\Delta t) &\leftarrow V(t)\exp\left[3\Delta t\, \eta(t+\tfrac{1}{2}\Delta t)\right] \\
\underline{\underline{\mathbf{H}}}(t+\Delta t) &\leftarrow \exp\left[\Delta t\, \eta(t+\tfrac{1}{2}\Delta t)\right]\underline{\underline{\mathbf{H}}}(t) \\
\underline{v}'(t+\Delta t) &\leftarrow \underline{v}(t+\tfrac{1}{2}\Delta t) + \frac{\Delta t}{2}\frac{\underline{f}(t+\Delta t)}{m} \\
&\quad call \quad rattle(V) \\
\eta(t+\Delta t) &\leftarrow \eta(t+\tfrac{1}{2}\Delta t) + \frac{\Delta t}{2}\left\{\frac{V(t+\Delta t)}{W}(\mathcal{P}(t+\Delta t) - P_{\text{ext}}) - \chi(t+\Delta t)\eta(t+\Delta t)\right\} \\
\underline{v}''(t+\Delta t) &\leftarrow \underline{v}'(t+\Delta t) - \frac{\Delta t}{2}\eta(t+\Delta t)\underline{v}'(t+\Delta t) \\
\chi(t+\Delta t) &\leftarrow \chi(t+\tfrac{1}{2}\Delta t) + \frac{\Delta t N_f k_B}{2Q}(\mathcal{T}(t+\Delta t) - T_{\text{ext}}) + \frac{\Delta t}{2Q}(W\eta(t+\Delta t)^2 - k_B T_{\text{ext}}) \\
\underline{v}(t+\Delta t) &\leftarrow \underline{v}''(t+\Delta t) + \frac{\Delta t}{2}\chi(t+\Delta t)\underline{v}''(t+\Delta t)
\end{aligned}
\tag{2.250}
$$

SPC/E model: *NVE* ensemble results

time elapsed since job start = 27144.723 seconds

temp 2.9618E+02 K r.m.s. fluctuation 6.3217E+00 K

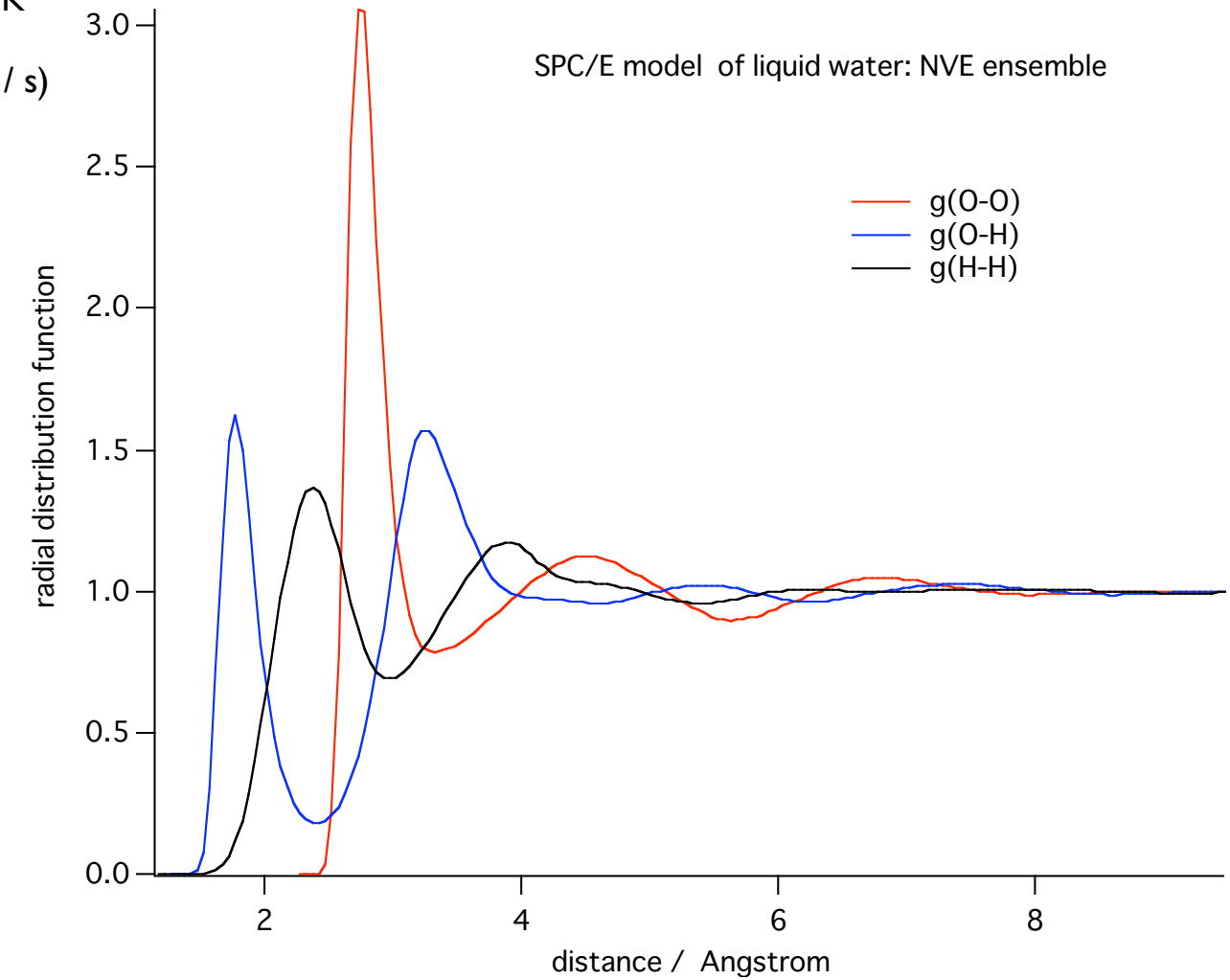
Approximate 3D Diffusion coefficients (10^-9 m^2 / s)

atom	D
OW	2.6341E+00
HW	2.6341E+00

Average pressure tensor

-8.2421E-02	2.9661E-02	5.1028E-03
2.9661E-02	-3.2231E-02	2.5959E-02
5.1028E-03	2.5959E-02	-8.3213E-02

trace/3. -6.5955E-02 katom

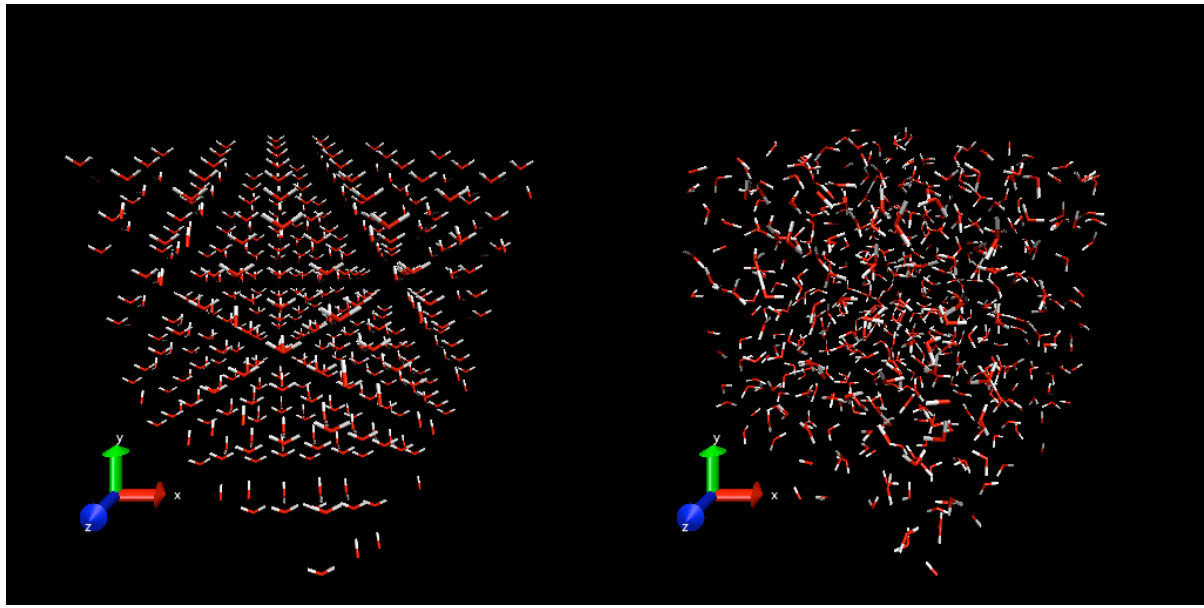


SPC/E model: *NPT* ensemble results

T = 3.0011E+02 K r.m.s. fluc. 7.1254E+00 K

Approximate 3D Diffusion coefficients (10^-9 m^2 / s)

atom	D
OW	2.4579E+00
HW	2.4818E+00



movie

Average pressure 1.2925E-03 katom

Average pressure tensor			r.m.s. fluctuations		
-3.3618E-02	1.3665E-02	3.6790E-02	6.2210E-01	5.0643E-01	5.1488E-01
1.3665E-02	-1.0684E-02	5.6640E-03	5.0643E-01	6.1777E-01	5.0854E-01
3.6790E-02	5.6640E-03	4.8179E-02	5.1488E-01	5.0854E-01	6.2829E-01

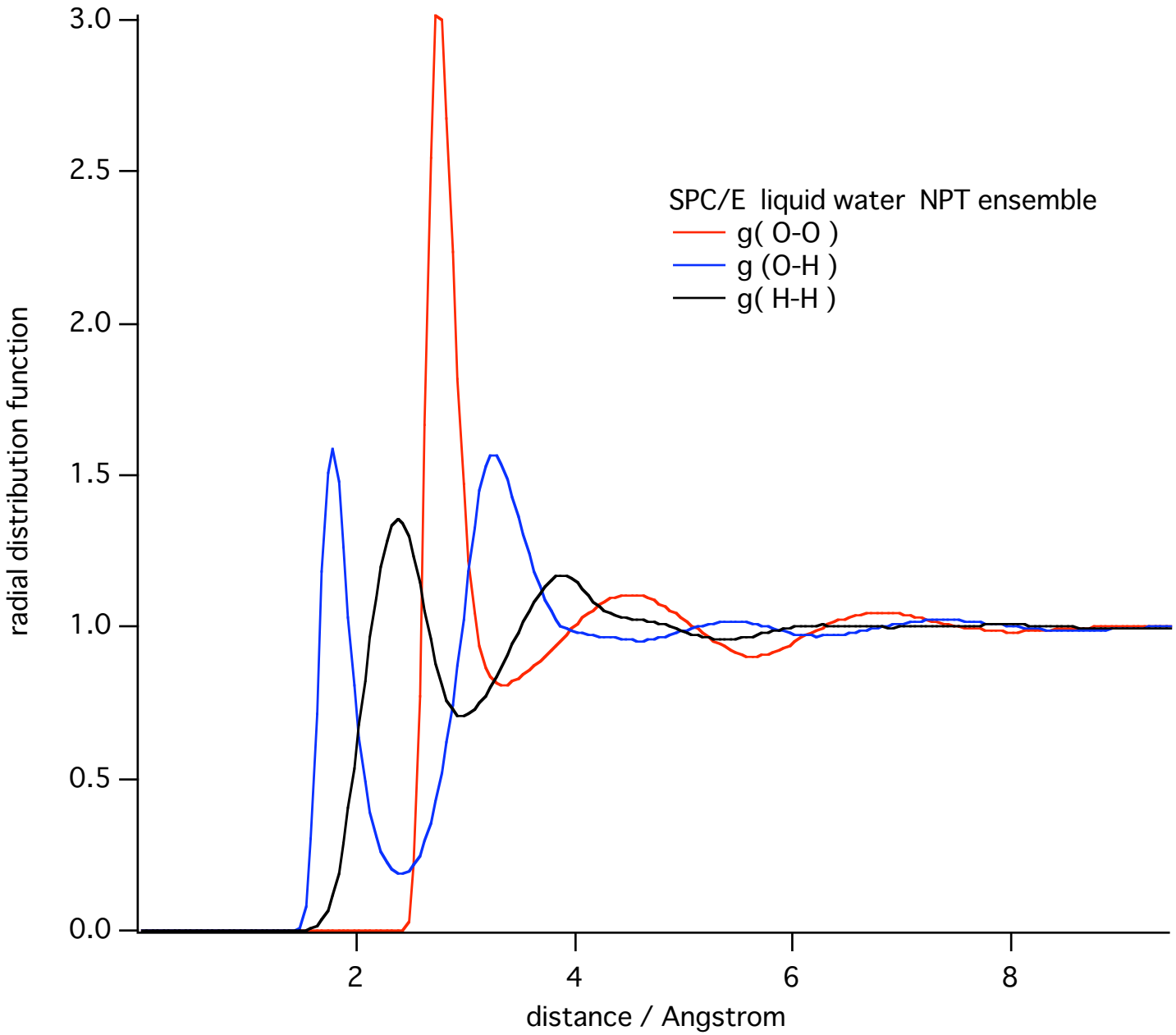
trace/3. 1.2925E-03

Average cell vectors			r.m.s. fluctuations		
24.8372539181	.0000000000	.0000000000	7.1583E-02	0.0000E+00	0.0000E+00
.0000000000	24.8372539181	.0000000000	0.0000E+00	7.1583E-02	0.0000E+00
.0000000000	.0000000000	24.8372539181	0.0000E+00	0.0000E+00	7.1583E-02

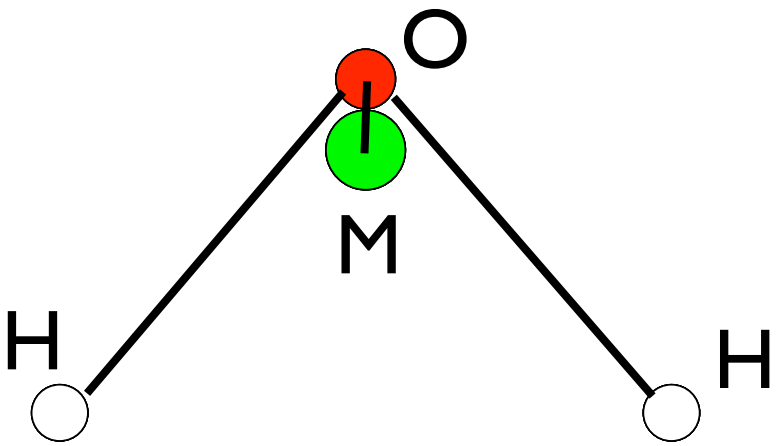
time elapsed since job start = 24121.500 seconds

SPC/E model: *NPT* ensemble results

cf. exp. results



TIP4P/Ew model

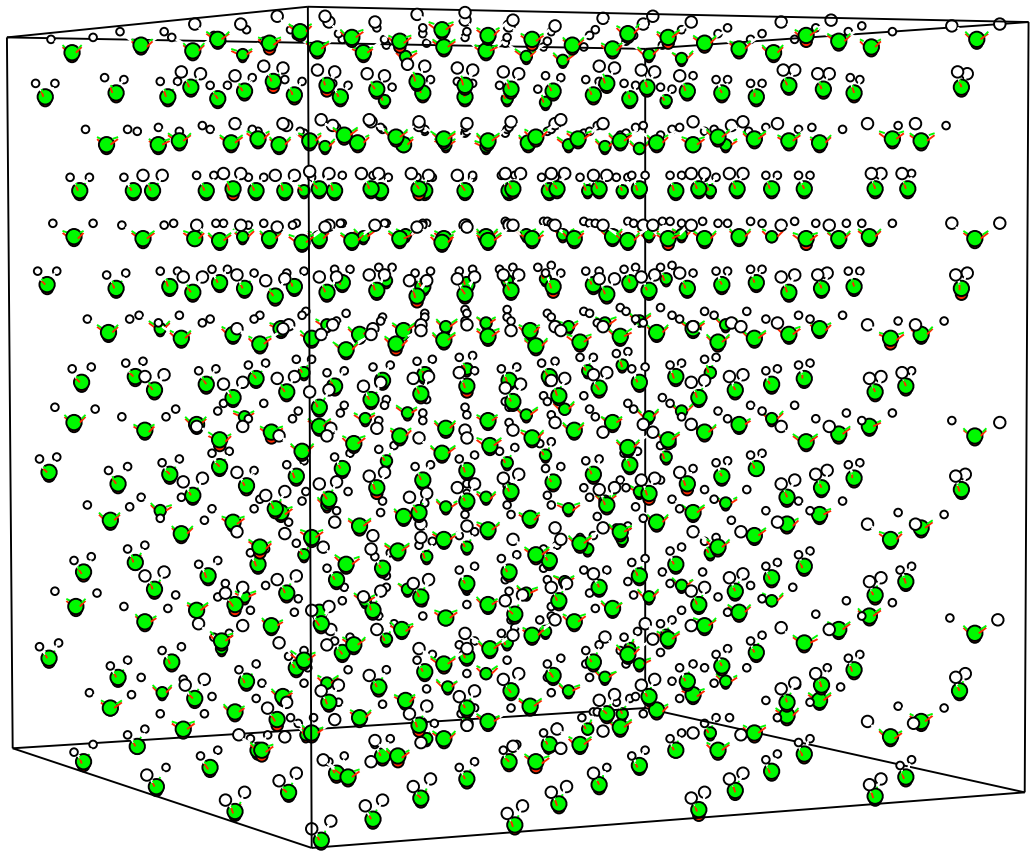


M: dummy charge site

r(OH)=0.9572 Å
r(OM)=0.125 Å
θ(HOH)=104.52
θ(MOH)=52.26
are fixed.

z(M)=-1.04844 *e*
z(H)=0.52422 *e*
ε(O) = 0.680946 kJ mol^{-1}
σ(O) = 3.16435 Å

mass of M is zero.



CONFIG

```
TIP4P H2O liquid water 300 K
         2          1
    24.8632889271        .0000000000        .0000000000
      .0000000000      24.8632889271        .0000000000
      .0000000000        .0000000000      24.8632889271
   OW    1
  -12.4316444636     -12.4316444636     -12.4316444636
    -.1157118180       -.1006883881        .0252069358
      .0000000000        .0000000000        .0000000000
   HW    2
  -11.8963997541     -11.8963997541     -11.8457621869
    -.1157118180       -.1006883881        .0252069358
      .0000000000        .0000000000        .0000000000
   HW    3
  -12.9668891730     -12.9668891730     -11.8457621869
    -.1157118180       -.1006883881        .0252069358
      .0000000000        .0000000000        .0000000000
   MW    4
  -12.4316444636     -12.4316444636     -12.3066444636
    -.1157118180       -.1006883881        .0252069358
      .0000000000        .0000000000        .0000000000
   OW    5
  -10.8776889056     -10.8776889056     -10.8776889056
    -.0944489059        .0834090543       -.0070384050
      .0000000000        .0000000000        .0000000000
   HW    6
  -10.3424441962     -11.4129336150     -10.2918066290
    -.0944489059        .0834090543       -.0070384050
      .0000000000        .0000000000        .0000000000
   HW    7
  -11.4129336150     -10.3424441962     -10.2918066290
    -.0944489059        .0834090543       -.0070384050
      .0000000000        .0000000000        .0000000000
   MW    8
  -10.8776889056     -10.8776889056     -10.7526889056
    -.0944489059        .0834090543       -.0070384050
      .0000000000        .0000000000        .0000000000
```

FIELD

```
H2O TIP4P
units  kJ
molecules 1
TIP4P  water
nummols 512
atoms 4
   OW        15.9996     0.0
   HW        1.0008      0.52422
   HW        1.0008      0.52422
   MW        0.0        -1.04844
constraints  3
    1    2    0.95720000
    1    3    0.95720000
    2    3    1.51390065
rigid 1
    2    1    4
finish
vdW 6
    OW      OW    lj  0.680946     3.16435
    OW      HW    lj  0.0          0.0
    HW      HW    lj  0.0          0.0
    OW      MW    lj  0.0          0.0
    HW      MW    lj  0.0          0.0
    MW      MW    lj  0.0          0.0
close
```

CONTROL NVE

```
TIP4P  model of water

integrator velocity verlet
temperature      300.00
ensemble nve

steps          150000
equilibration   100000
multiple step        1
scale               10
print               50
stack              100
stats               10
rdf                  1
traj     1   100  0

timestep        0.001
cutoff          9.50
delr width      0.5000
ewald precision 1d-6
shake tolerance  1.0E-5
quaternion tolerance  1.0E-5
print rdf

job time           300000.00
close time            500.00

finish
```

CONTROL NPT 300 K 1 atom

```
TIP4P  model of water

integrator velocity verlet
temperature      300.00
ensemble npt hoover 0.1 0.2

steps          150000
equilibration   100000
multiple step        1
scale               10
print               50
stack              100
stats               10
rdf                  1
traj     1   100  0

timestep        0.001
cutoff          9.50
delr width      0.5000
ewald precision 1d-6
shake tolerance  1.0E-5
quaternion tolerance  1.0E-5
print rdf
pres  0.001

job time           300000.00
close time            500.00

finish
```

TIP4P/Ew model: *NVE* ensemble results

movie

temp_tot 3.0270E+02 K r.m.s. fluctn. 6.4702E+00 K

Approximate 3D Diffusion coefficients (10^-9 m^2 / s)

atom	D
OW	2.6537E+00
HW	2.6627E+00
MW	2.6538E+00

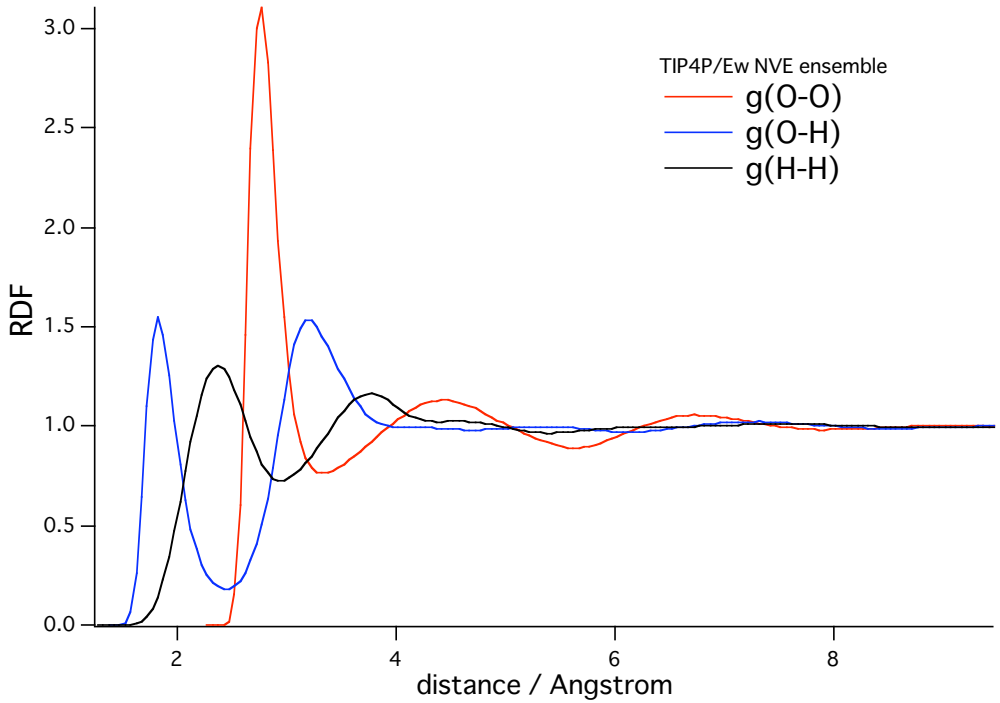
Average pressure tensor

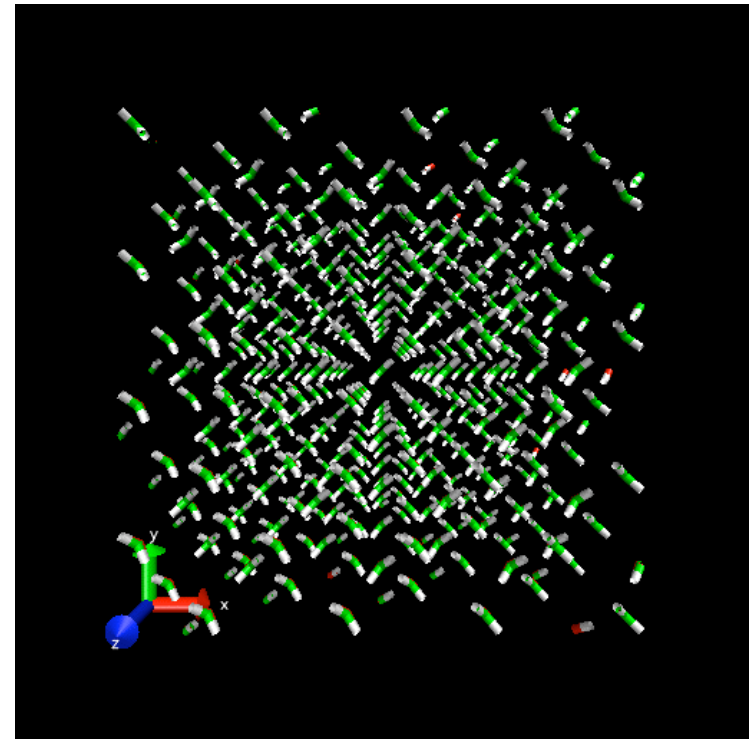
4.8443E-02	6.8694E-03	1.4413E-02
6.8694E-03	3.8647E-02	2.9359E-02
1.4413E-02	2.9359E-02	4.2101E-02

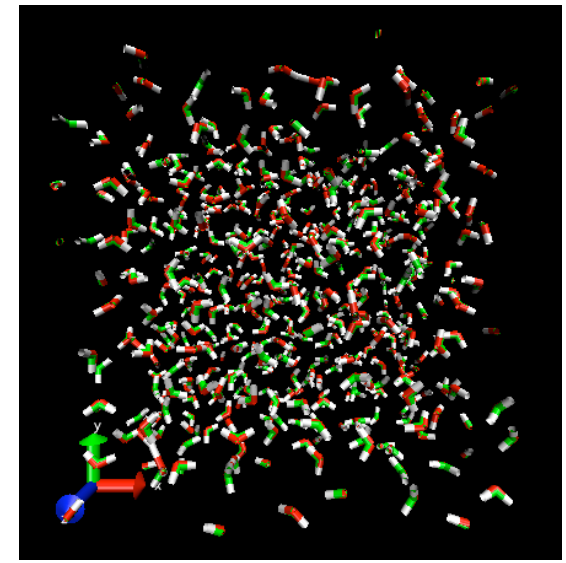
r.m.s. fluctuations

7.6492E-01	5.0866E-01	5.1297E-01
5.0866E-01	7.9529E-01	5.0658E-01
5.1297E-01	5.0658E-01	8.0716E-01

trace/3. 4.3064E-02







time elapsed since job start = 34789.530 seconds

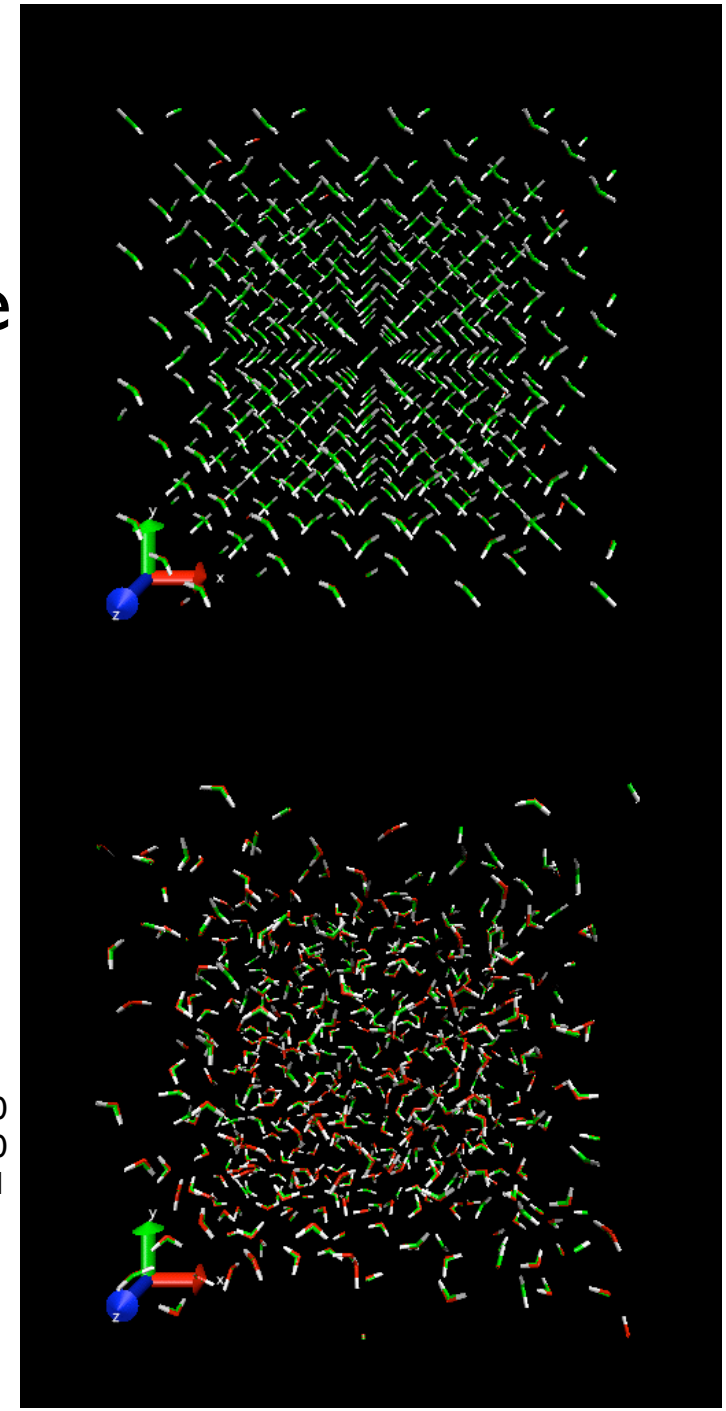
TIP4P/Ew model: *NPT* ensemble results

Temp. 2.9996E+02 K +- 7.7193E+00

Approximate 3D Diffusion coefficients
(10^-9 m^2 / s)

atom	D
OW	2.5677E+00
HW	2.5421E+00
MW	2.5601E+00

movie



Average pressure tensor

2.3043E-02	-3.2620E-02	1.5465E-02
-3.2620E-02	4.4084E-03	-1.0378E-02
1.5465E-02	-1.0378E-02	-1.3775E-02

r.m.s. fluctuations

8.9626E-01	5.0277E-01	4.8920E-01
5.0277E-01	8.5233E-01	4.9858E-01
4.8920E-01	4.9858E-01	8.6417E-01

trace/3. 4.5587E-03

Average pressure
4.5587E-03 katom

Average cell vectors

24.8869811588	.0000000000	.0000000000
.0000000000	24.8869811588	.0000000000
.0000000000	.0000000000	24.8869811588

r.m.s. fluctuations

1.0249E-01	0.0000E+00	0.0000E+00
0.0000E+00	1.0249E-01	0.0000E+00
0.0000E+00	0.0000E+00	1.0249E-01

time elapsed since job start = 34773.057 seconds

TIP4P/Ew model: *NPT* ensemble results

cf. exp. results