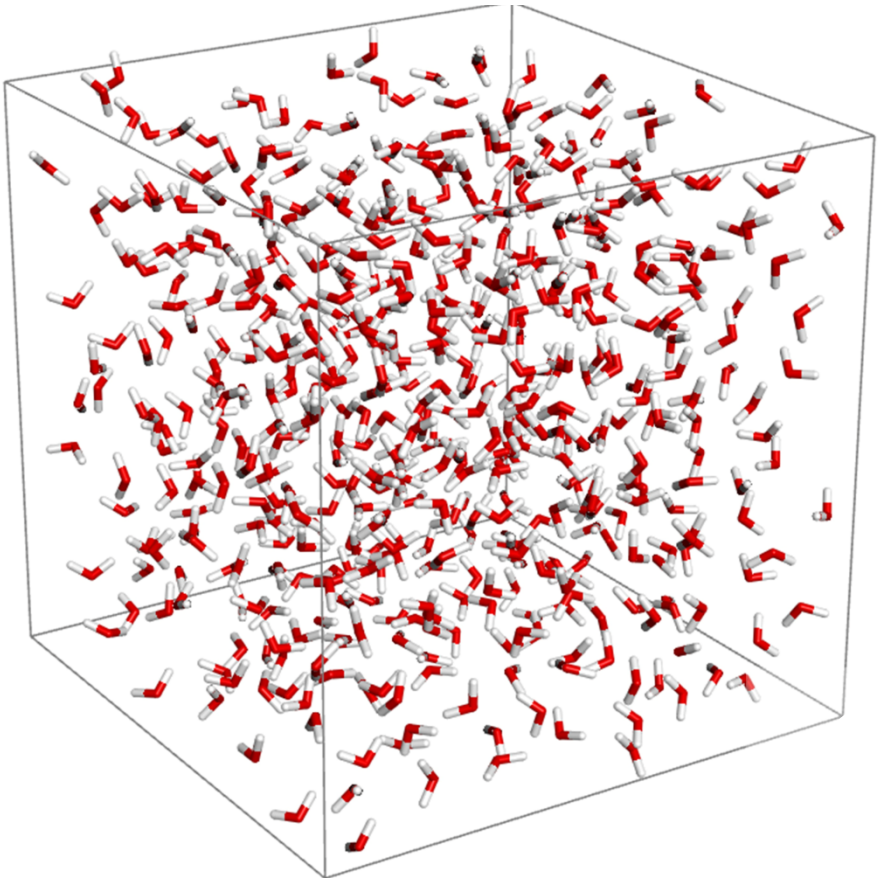
Molecular dynamics (MD, PIMD)

1. Calculation setup

The following setup is used.

- Method : PIMD
- Ensemble : NVT (canonical ensemble)
- Potential : MM (classical potential)
- System : H_2O (64 molecules)
- Number of beads : 1, 16
- Boundary : periodic boundary condition

A snapshot of the system is shown below.



2. Results

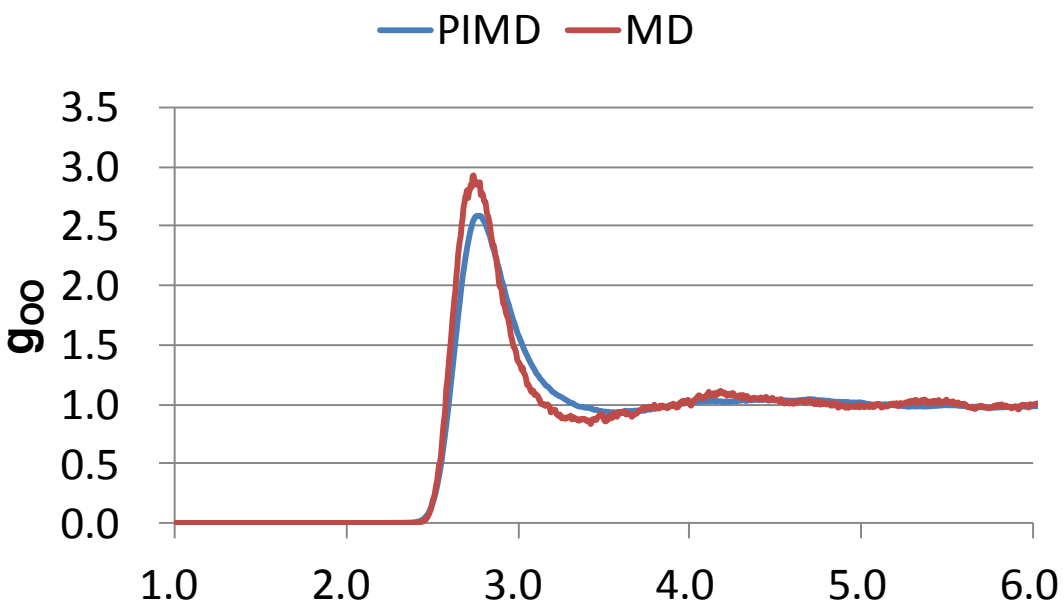
As shown below, the total energy, the potential energy, the instantaneous temperature and the wall clock time of each step are printed in “standard.out”.

```
================================================================================
   step     energy [au]  potential [au]  temp [K]  wall clock time
--------------------------------------------------------------------------------
      0    26.72593499     2.46109108   300.00  2016-03-04 金 10:56:18.58
     10    26.72154291     1.54702217   324.08  2016-03-04 金 10:56:26.55
     20    26.72283571     1.36784139   275.43  2016-03-04 金 10:56:34.20
     30    26.72304579     1.25660900   266.65  2016-03-04 金 10:56:42.04
     40    26.72294052     1.06831460   272.57  2016-03-04 金 10:56:49.69
     50    26.72336575     1.06198721   282.97  2016-03-04 金 10:56:57.34
     60    26.72311093     0.90714165   315.20  2016-03-04 金 10:57:05.05
     70    26.72327800     0.83548383   329.52  2016-03-04 金 10:57:17.62
     80    26.72332197     0.77974987   324.63  2016-03-04 金 10:57:25.24
     90    26.72314060     0.68389906   314.84  2016-03-04 金 10:57:38.35
    100    26.72323059     0.65248203   298.57  2016-03-04 金 10:57:45.97
...omitted...
```

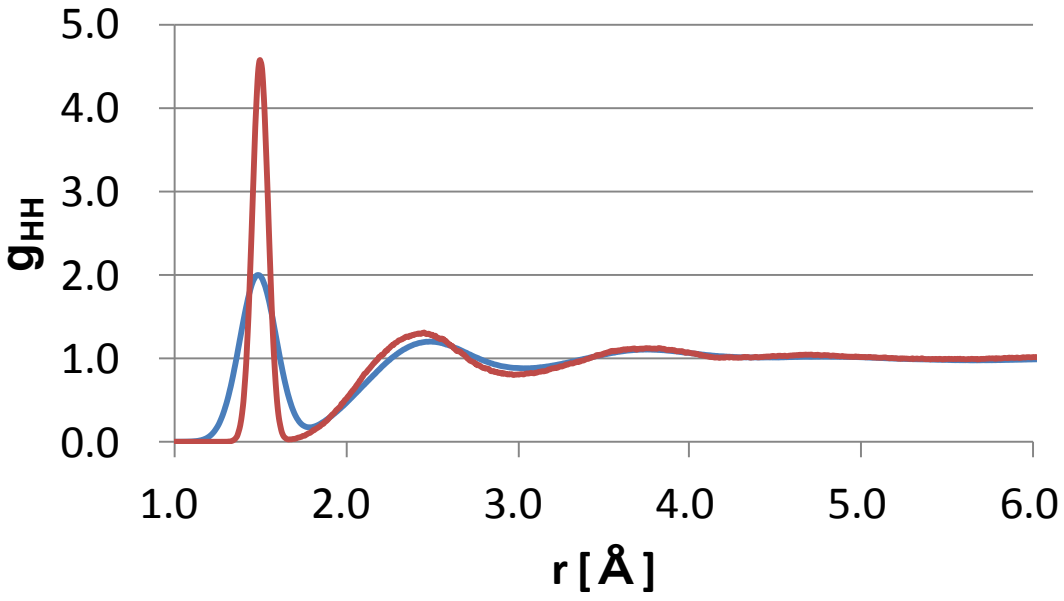
The radial distribution functions are printed in “rdf.out”.

```
          ============================================================
            1   2          r [au]      rdf: n(r)      rdf: g(r)
          ------------------------------------------------------------
            0   0      1.00000000     0.00000000     0.00000000
            0   0      1.01000000     0.00000000     0.00000000
            0   0      1.02000000     0.00000000     0.00000000
            0   0      1.03000000     0.00000000     0.00000000
            0   0      1.04000000     0.00000000     0.00000000
            0   0      1.05000000     0.00000000     0.00000000
            0   0      1.06000000     0.00000000     0.00000000
            0   0      1.07000000     0.00000000     0.00000000
            0   0      1.08000000     0.00000000     0.00000000
            0   0      1.09000000     0.00000000     0.00000000
            0   0      1.10000000     0.00000000     0.00000000
            0   0      1.11000000     0.00000000     0.00000000
            0   0      1.12000000     0.00000000     0.00000000
            0   0      1.13000000     0.00000000     0.00000000
            0   0      1.14000000     0.00000000     0.00000000
            0   0      1.15000000     0.00000000     0.00000000
                                ...omitted...
```

The hydrogen-hydrogen and oxygen-oxygen radial distributions are shown below. For comparison, the results of classical molecular dynamics (for the case of number of beads = 1) are also shown. One can see the importance of nuclear quantum effects.



(oxygen-oxygen radial distributions)



(hydrogen-hydrogen radial distributions)