AICTE QIP Short Term Training Program

on

Applications of Molecular Simulations and Machine Learning in Research

LAMMPS
Large-scale Atomic/Molecular Massively Parallel Simulator

WORKSHOP

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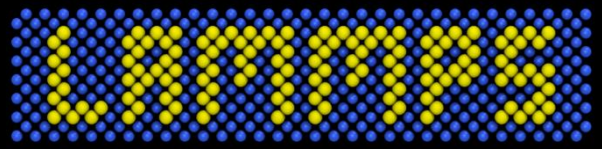
Overview

- Introduction To LAMMPS
- Examples From LAMMPS Website
- Input Script – Lennard Jones
- Input Files Generation Tools – A Brief Introduction
- SPCE Water
- Hexane – Water mixture

Introduction to 

- LAMMPS – Large-Scale Atomic/Molecular Massively Oarallel Simulator.
- Development began in the mid 1990s at the Sandia National Laboratories. Released as open source code in 2004.
- LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.
- Can be run on single processor or in parallel with GPU acceleration support.
- Modular code with most functionality in optional packages.
- Open Source Repository on GitHub.

- Features of LAMMPS:
  - 221 different pair styles
  - 17 bond styles
  - 22 angle styles
  - 17 dihedral style
  - 13 improper style
  - 264 fixes
  - 138 computes

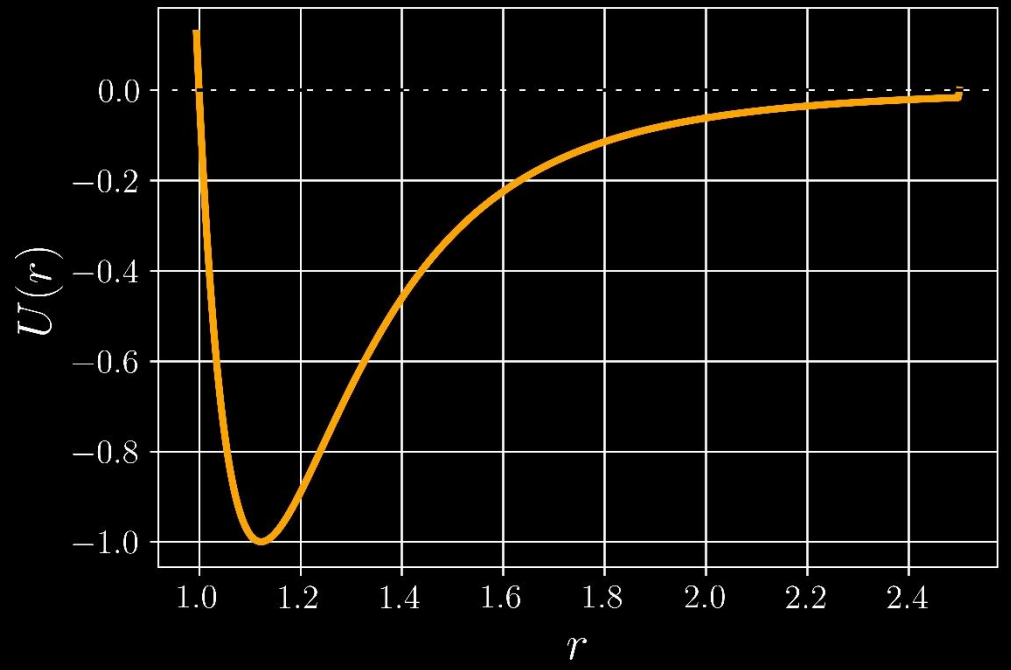
- Post processing tools
  - Pizza.py
  - MDAnalysis
  - VMD etc..

Some examples from LAMMPS website

- Blood Flow in Capilaries : https://www.lammps.org/movies/mp4/blood.mp4
- Rhodopsin in solvated lipid bilayer: https://www.lammps.org/movies/mp4/rhodo.mp4
- Flow of water and ions thru a silica pore : https://www.lammps.org/movies/mp4/pore.mp4
- Au nanowire formation and extension: https://www.lammps.org/movies/mp4/nanowire2.mp4

Example Input Script – Lennard Jones

```
########################## System Setup ##############################
variable        eq_step             equal  1e5
variable        pro_step            equal  1e5
variable        dt                  equal  0.001
variable        thermo_step         equal  1000
variable        epsilon             equal  1
variable        sigma               equal  1.0
variable        part_num            equal  1000
variable        lj_cut              equal  3.5*${sigma}
variable        eq_dump             equal  1e3
variable        pro_dump            equal  1e3
variable        box_length          equal   ceil((${part_num}/${rho})^(1/3))
```



Example Input Script – Lennard Jones

```
######################## Initialization ##########################
units                   lj
dimension               3
boundary                p p p
atom_style              atomic
lattice                 sc ${rho}
region                  box block 0.0 ${box_length} 0.0 ${box_length} 0.0 ${box_length}
create_box              1 box
create_atoms            1 box
mass                    1 1.0
```

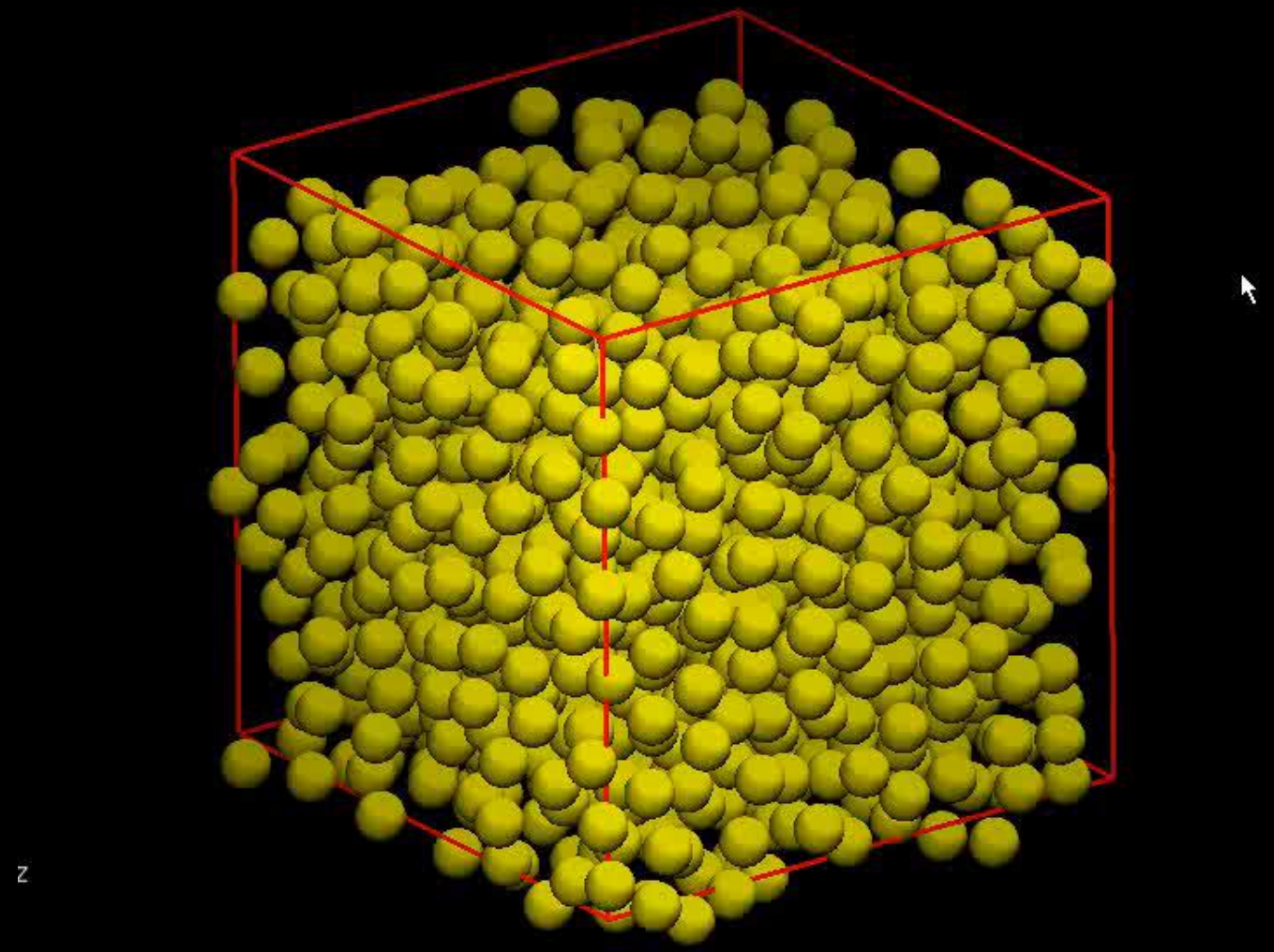
Example Input Script – Lennard Jones

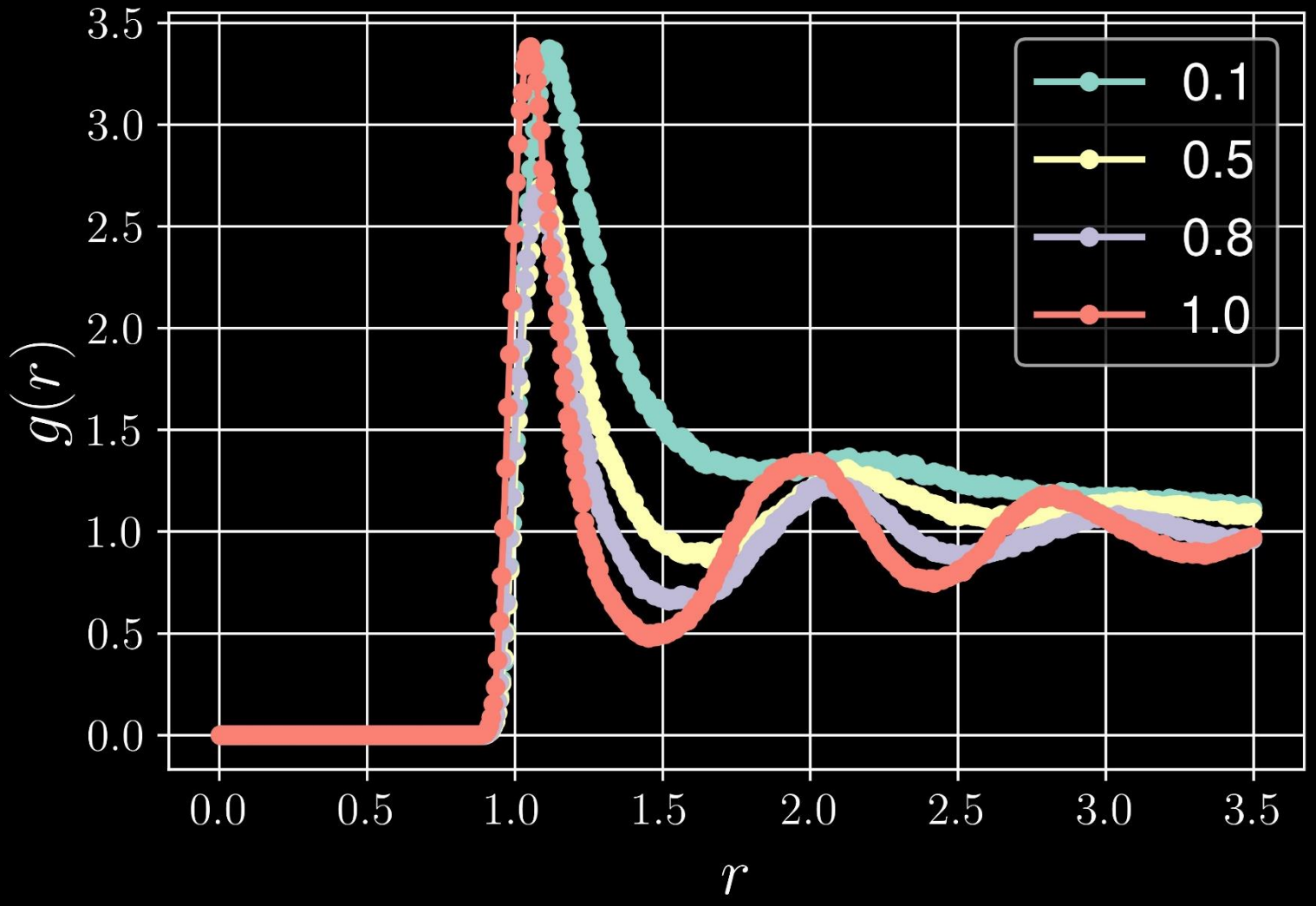
```
###################### Force Parameters ########################
pair_style          lj/cut ${lj_cut}
pair_modify         shift yes
pair_coeff          1 1 ${epsilon} ${sigma} ${lj_cut}
min_style           sd
minimize            1.0e-6 1.0e-8 1000 10000
velocity            all create 1.0 89387 dist gaussian
```

Example Input Script – Lennard Jones

```
############################ RUN ################################
fix                 1 all nvt temp 1.0 1.0 10 #NoseHoover
thermo_style    custom step temp press pe ke etotal density
thermo              ${thermo_step}

timestep            ${dt}
fix                 3 all print ${thermo_step} "$S $T $P ${Pe} ${Ke} $E ${EP}" file equilibration.dat
compute             RDF all rdf 500 1 1 cutoff 3.5
fix                  5 all ave/time 10 100 ${pro_step} c_RDF[*] file rdf_${rho}.dat mode vector
dump                1 all custom ${eq_dump} dump.equilibration id x y z

run                 ${eq_step}

write_restart       equilibrium.restart
```

Results



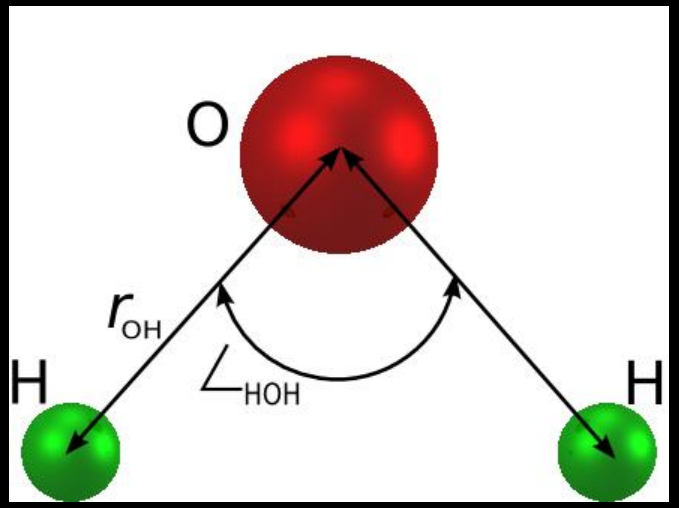

0.1
0.5
0.8
1.0
$g(r)$
r
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5

Input Data Generation Tools

- VMD Topotools : TopoTools by Axel Kohlmeyer
- Moltemplate : https://www.moltemplate.org/
- ATB : Automated Topology Builder and Repository
- Avogadro : https://avogadro.cc/

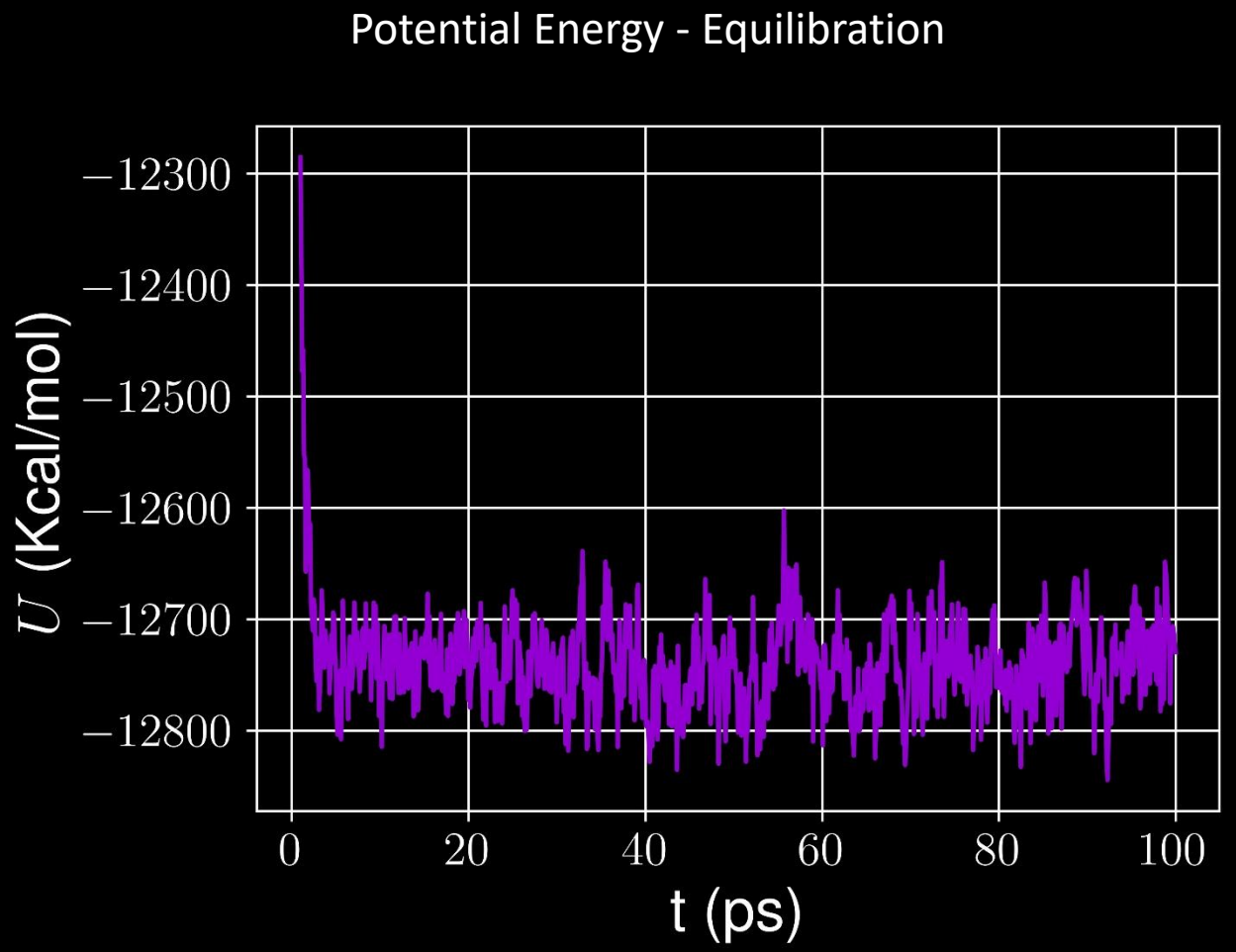
SPCE - Water

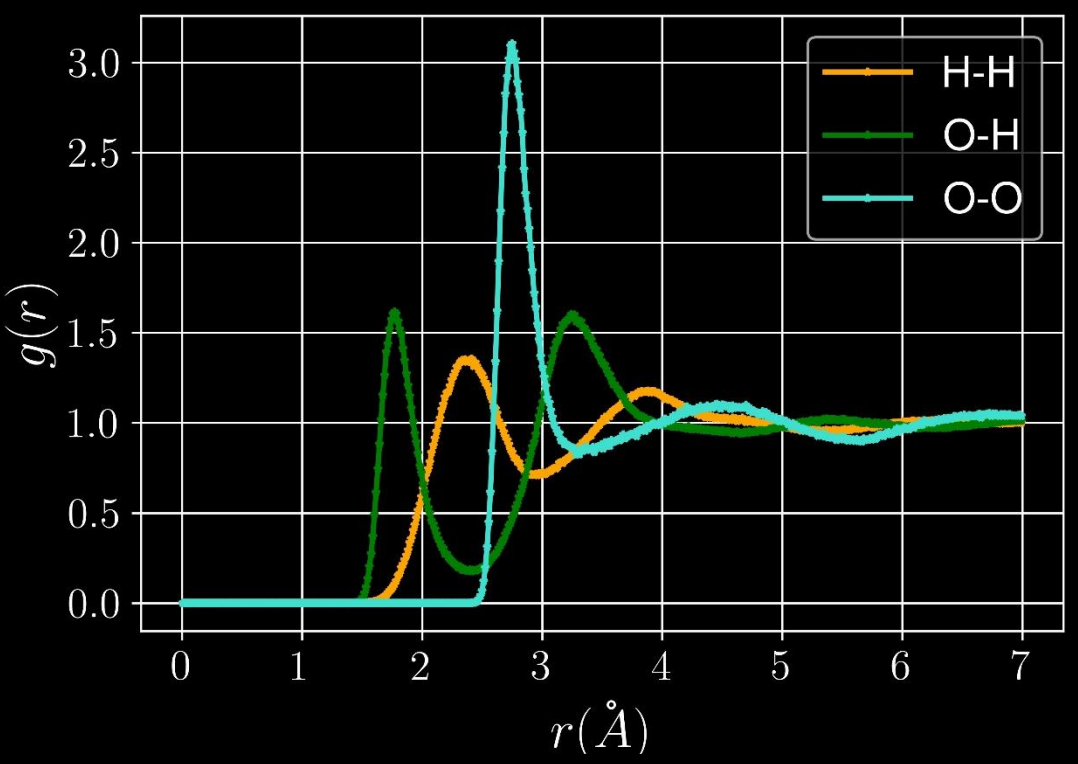
- Input Files : GitHub
- 100 ps equilibration
- 4 ns of non equilibrium run with simple shear
  Using SSLOD algorithm.

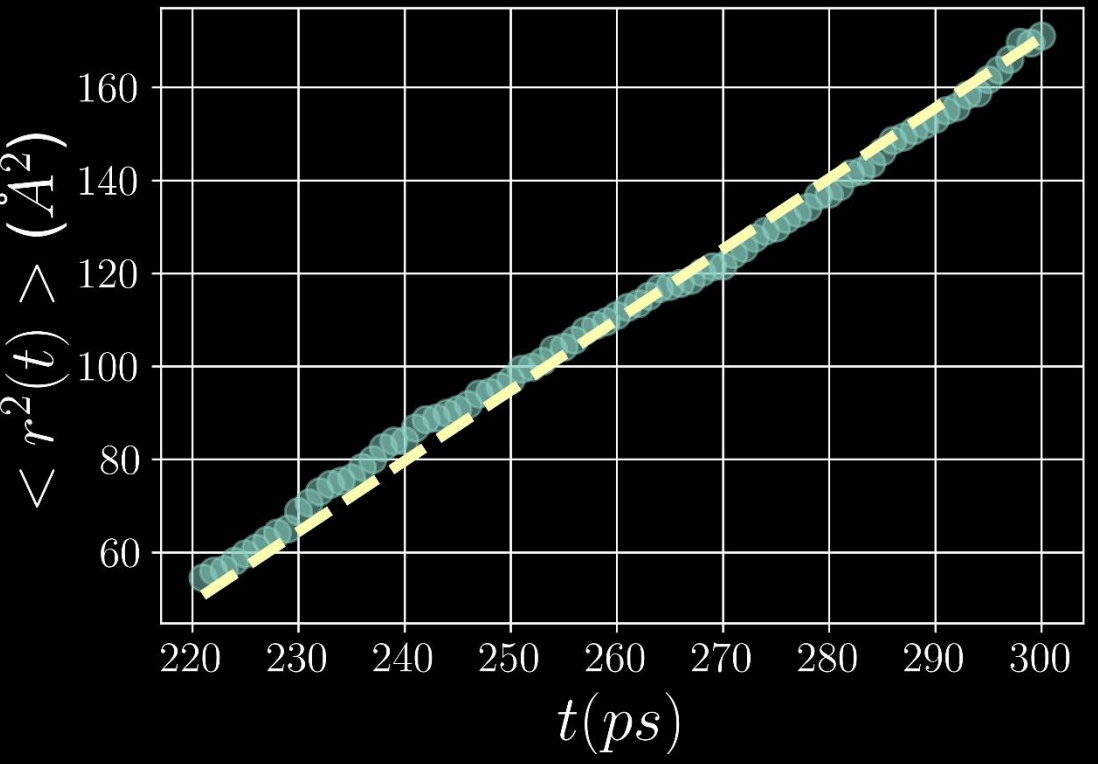


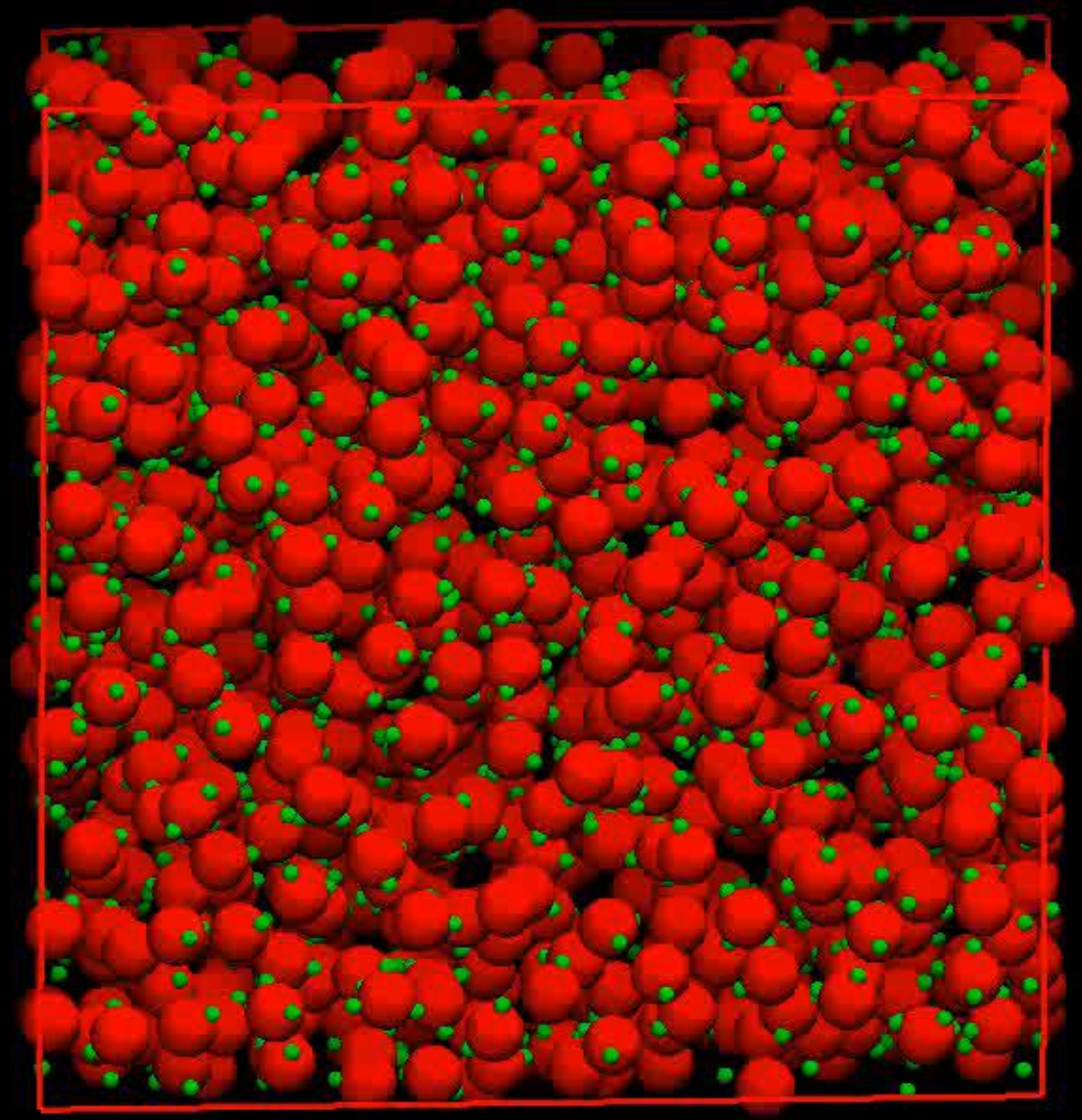
Parameter	Value
σ_O	3.166 Å
ϵ	0.650 KJ/mol
r_{OH}	1.00Å
θ_{HOH}	109.47°
q_0	-0.8476e
q_H	$\lvert q_o \rvert/2$

Results

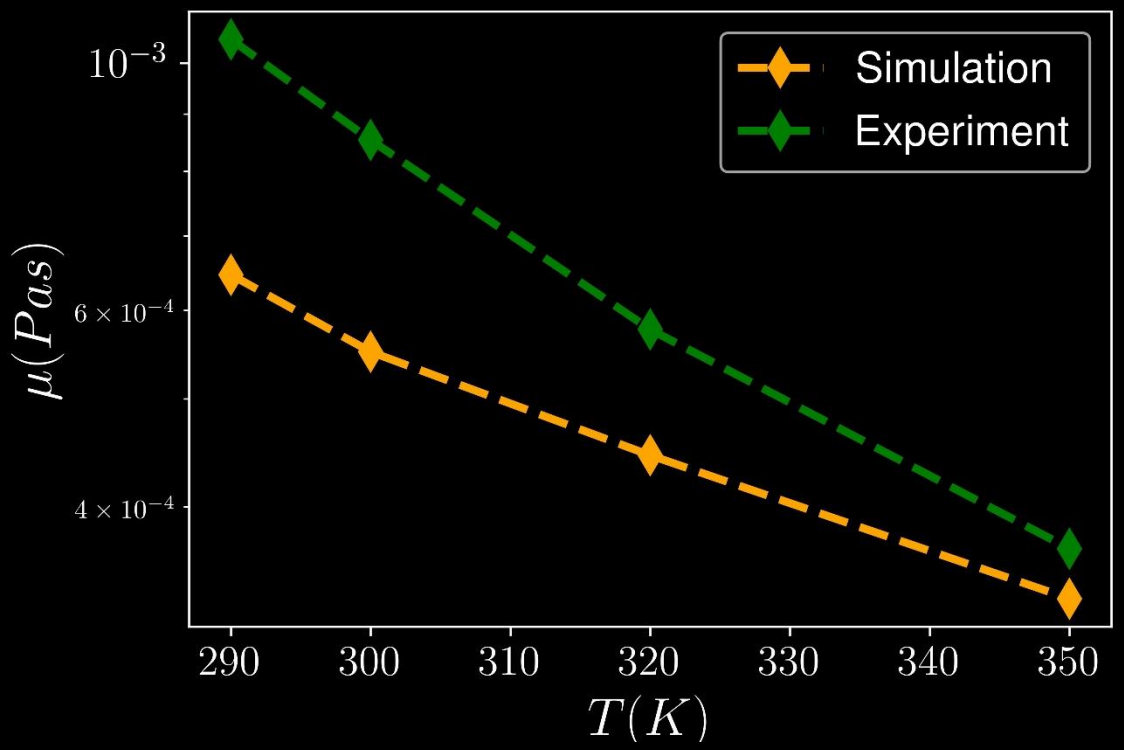

Potential Energy - Equilibration
−12300
−12400
−12500
−12600
−12700
−12800
U (Kcal/mol)
0
20
40
60
80
100
t (ps)


H-H
O-H
O-O
$g(r)$
$r(\AA)$
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
1
2
3
4
5
6
7

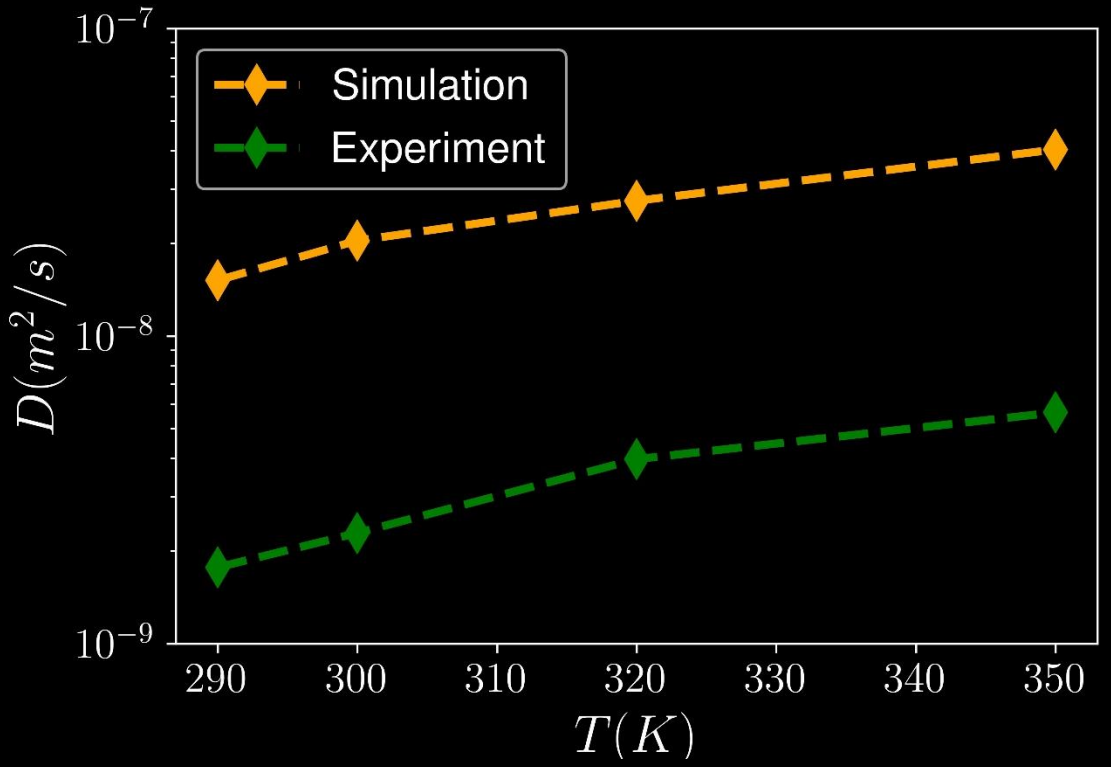

$< r^2(t) > (\AA^2)$
$t(ps)$
60
80
100
120
140
160
220
230
240
250
260
270
280
290
300



Viscosity calculated using $-\frac{\sigma_{xy}}{\dot{\gamma}}$



Diffusivity calculated from MSD

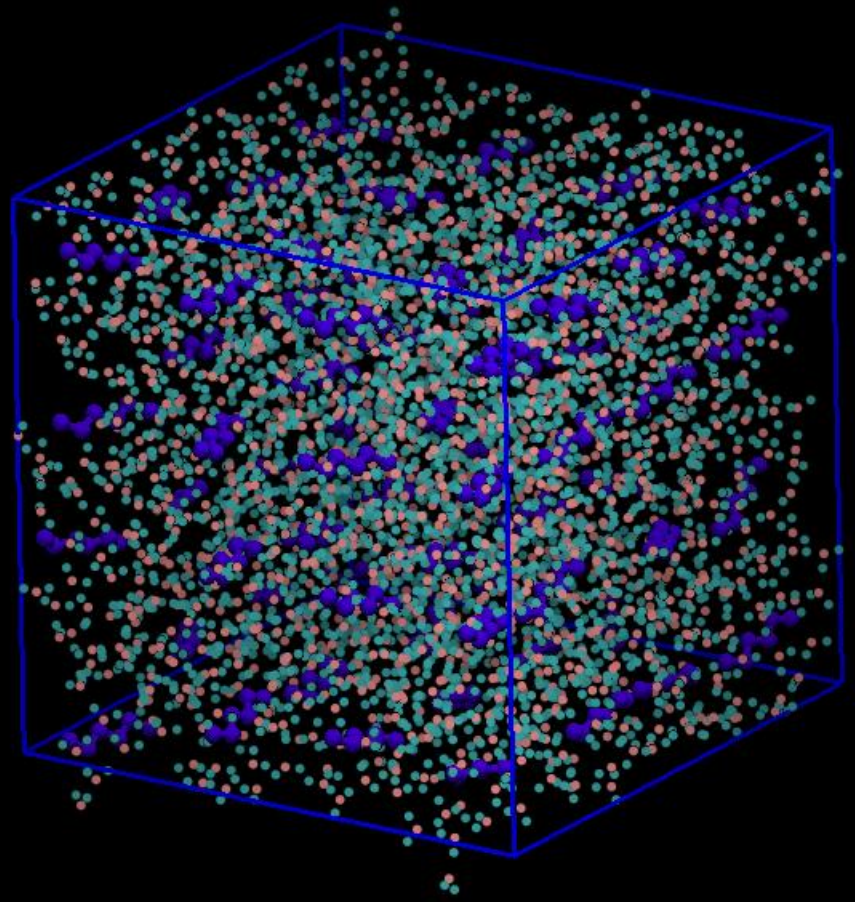


https://www.engineeringtoolbox.com/water-dynamic-kinematic-viscosity-d_596.html

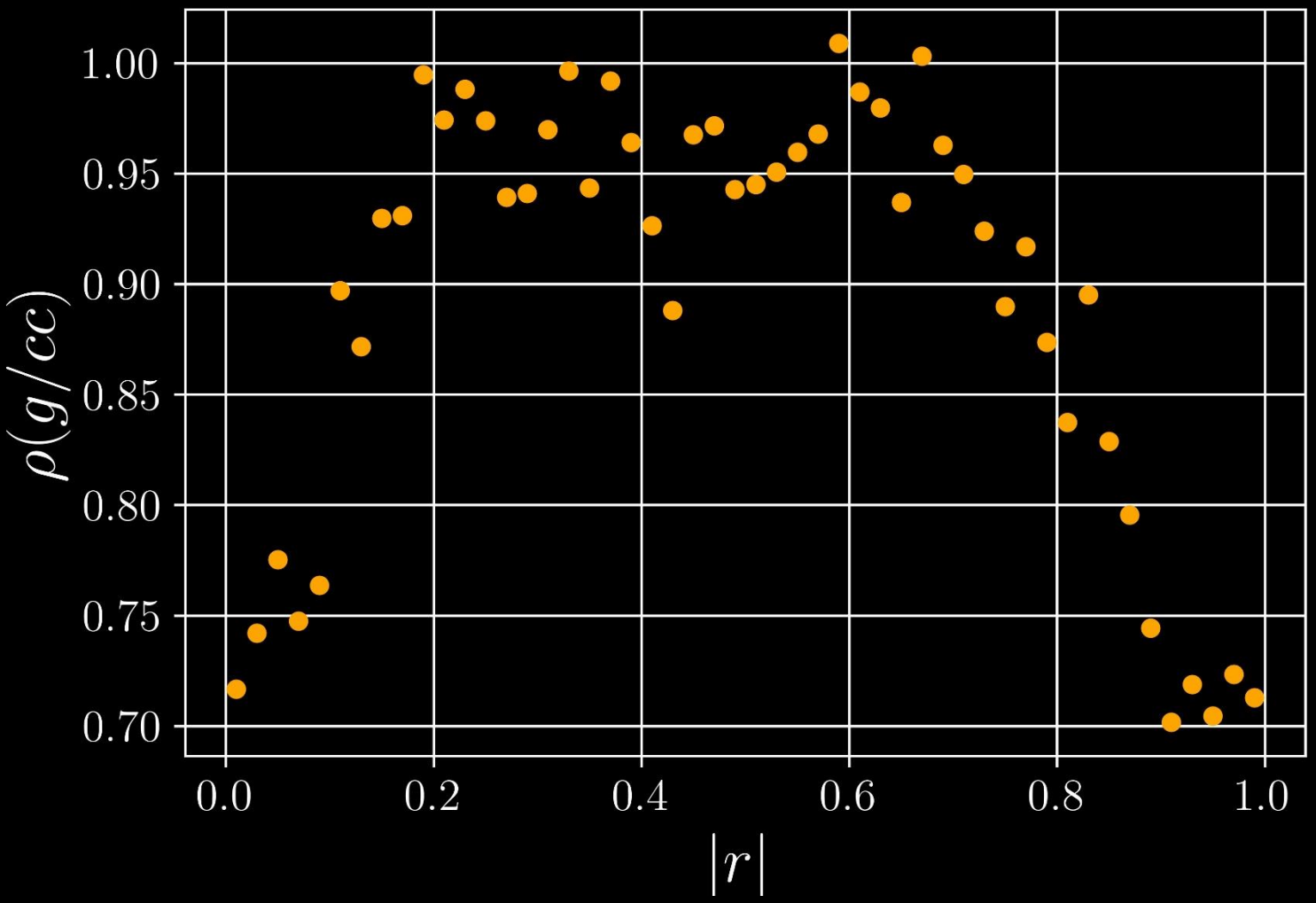
Physical Chemistry Chemical Physics, Vol. 2, 4740–4742 (2000). DOI: 10.1039/B005319H

Hexane – Water mixture

- OPLSAA forcefield
- System generated using Moltemplate
- 4ns equilibration run
- Input Files : GitHub



Show trajectory


1.00
0.95
0.90
0.85
0.80
0.75
0.70
$\rho(g/cc)$
0.0
0.2
0.4
0.6
0.8
1.0
$|r|$