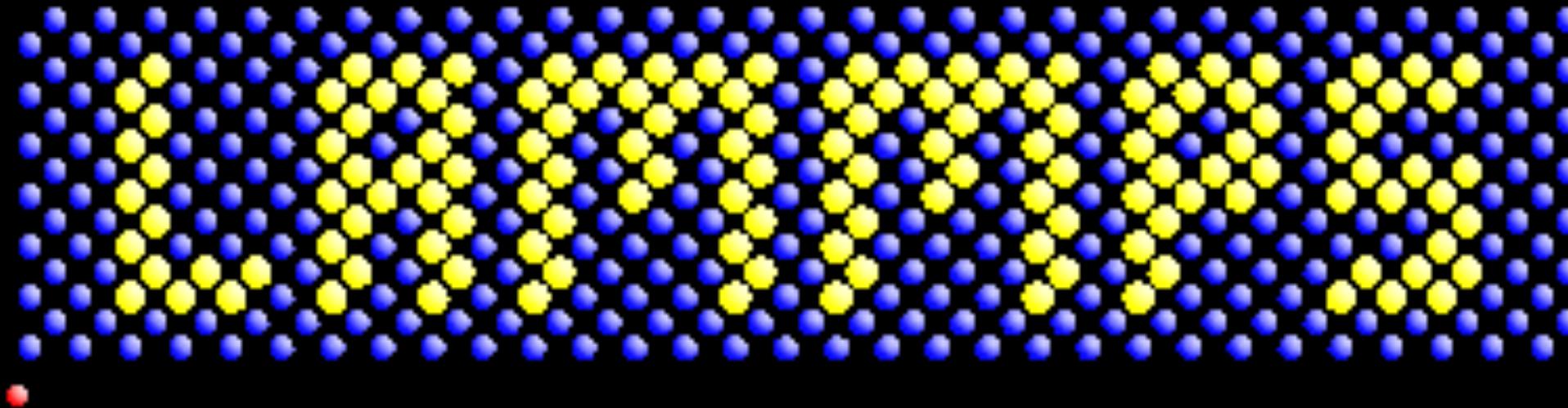


LAMMPS: A Powerful Tool for Large-scale Molecular Dynamics Simulations- Part I

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LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)

*Developed in mid 90's in collaboration between **two national labs** (**Sandia** and **LNNL**) and **three companies** (**Cray**, **Bristol Myers Squibb** and **DuPont**)*

Original LAMMPS in **FORTRAN**.

Rewritten in **C++** in 2004.

Three Main Advantages

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Versatility and generalizability

A large number of methods and force-fields already implemented in LAMMPS, more so than other open-source MD packages.

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Coding is far less complicated than other packages.

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Surrogacy

Possible to use LAMMPS library to call it from within your own code, using it as an MD **engine** from within external packages.

What is Needed for a LAMMPS Simulation?

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Input Script File:

A text file specifying different aspects of the simulation (integrator, ensemble, force-fields, live analyses, output, etc).

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Usually necessary

Configuration File:

A text or binary file containing **particle positions** (and possibly **velocities**), plus some information about force-fields, masses & ensembles.

Uncommon

Force-field File:

A text file including further information about the force-field. (Only needed for specialized force-fields).

Run a Simple LAMMPS Simulation

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Goal:

Simulate a Lennard-Jone liquid at $T^*=2$ and $\rho^*=1$.

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Step 2: Prepare an initial configuration.

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units lj                      # Units for quantities. (lj = reduced units)
atom_style atomic              # What features does each atom have?
boundary p p p                 # Boundary conditions in each dimension.
```

Step 2: Prepare an initial configuration.

```
lattice fcc 1.0
region myBox block -0.5 5.5 -0.5 5.5 -0.5 5.5
create_box 1 myBox
create_atoms 1 region myBox
```

Run a Simple LAMMPS Simulation

Goal:

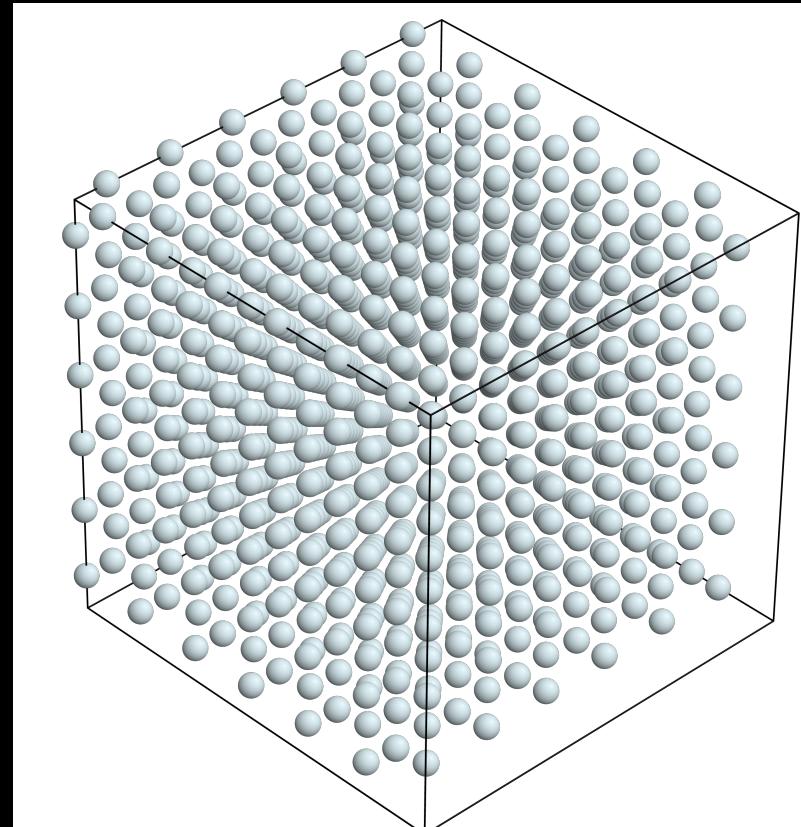
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Step 2: Prepare an initial configuration.

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```
pair_style lj/cut 2.5
pair_modify shift yes
pair_coeff 1 1 1.0 1.0 2.5
```

Run a Simple LAMMPS Simulation

Goal:

Simulate a Lennard-Jone liquid at $T^*=2$ and $\rho^*=1$.

Step 3: Specify the interatomic potential (FF).

```
pair_style lj/cut 2.5  
pair_modify shift yes  
pair_coeff 1 1 1.0 1.0 2.5
```

Step 4: Specify the ensemble & other implementation details.

Run a Simple LAMMPS Simulation

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Simulate a Lennard-Jone liquid at $T^*=2$ and $\rho^*=1$.

Step 3: Specify the interatomic potential (FF).

```
pair_style lj/cut 2.5
pair_modify shift yes
pair_coeff 1 1 1.0 1.0 2.5
```

Step 4: Specify the ensemble & other implementation details.

```
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
```

Run a Simple LAMMPS Simulation

Goal:

Simulate a Lennard-Jone liquid at $T^*=2$ and $\rho^*=1$.

Step 3: Specify the interatomic potential (FF).

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pair_style lj/cut 2.5
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mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
```

Step 5: Run the simulation.

Run a Simple LAMMPS Simulation

Goal:

Simulate a Lennard-Jone liquid at $T^*=2$ and $\rho^*=1$.

Step 3: Specify the interatomic potential (FF).

```
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pair_modify shift yes
pair_coeff 1 1 1.0 1.0 2.5
```

Step 4: Specify the ensemble & other implementation details.

```
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
```

Step 5: Run the simulation.

```
thermo 100
run 100000
```

Run a Simple LAMMPS Simulation

Goal:

Simulate a Lennard-Jone liquid at $T^*=2$ and $\rho^*=1$.

```
LAMMPS (2 Aug 2023 - Update 3)
# Specify basic aspects of the simulation.
units lj      # Units for quantities. (lj = reduced units)
atom_style atomic # What features does each atom have?
boundary p p p      # Boundary conditions in each dimension.

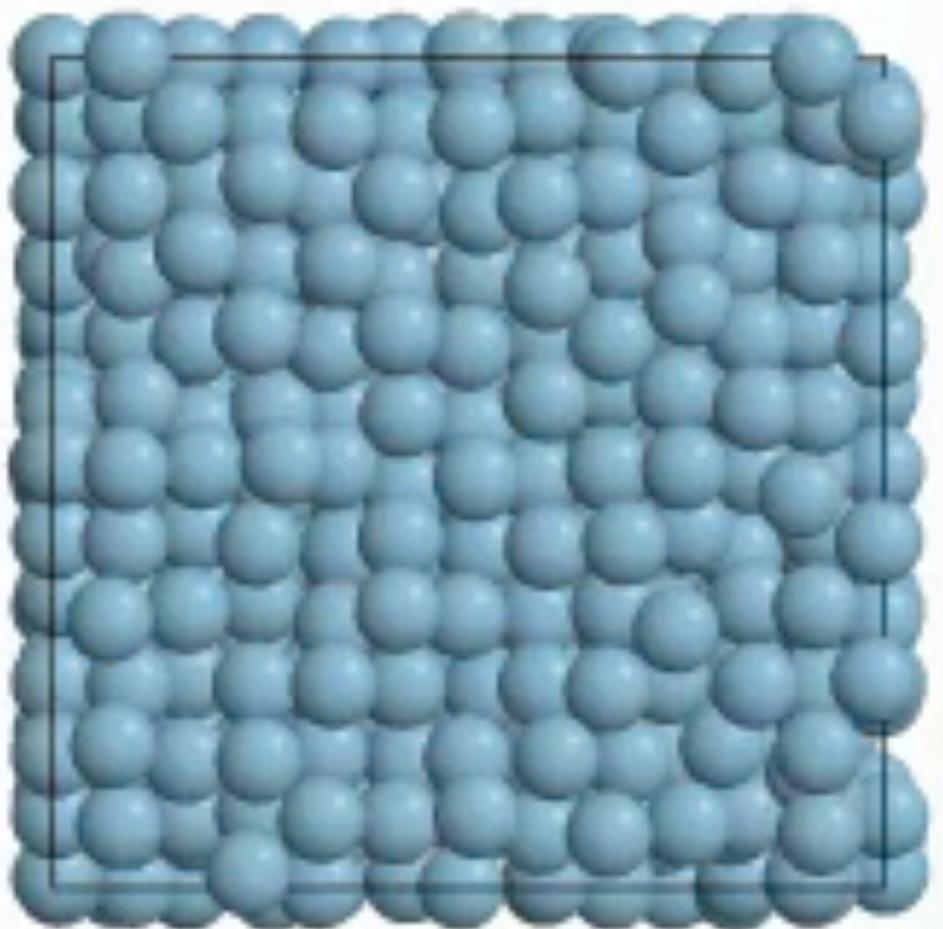
# Prepare initial structure.
lattice fcc 1.0
Lattice spacing in x,y,z = 1.5874011 1.5874011 1.5874011
region myBox block -0.5 5.5 -0.5 5.5 -0.5 5.5
create_box 1 myBox
Created orthogonal box = (-0.79370053 -0.79370053 -0.79370053) to (8.7307058 8.7307058 8.7307058)
1 by 1 by 1 MPI processor grid
create_atoms 1 region myBox
Created 864 atoms
using lattice units in orthogonal box = (-0.79370053 -0.79370053 -0.79370053) to (8.7307058 8.7307058 8.7307058)
create_atoms CPU = 0.000 seconds

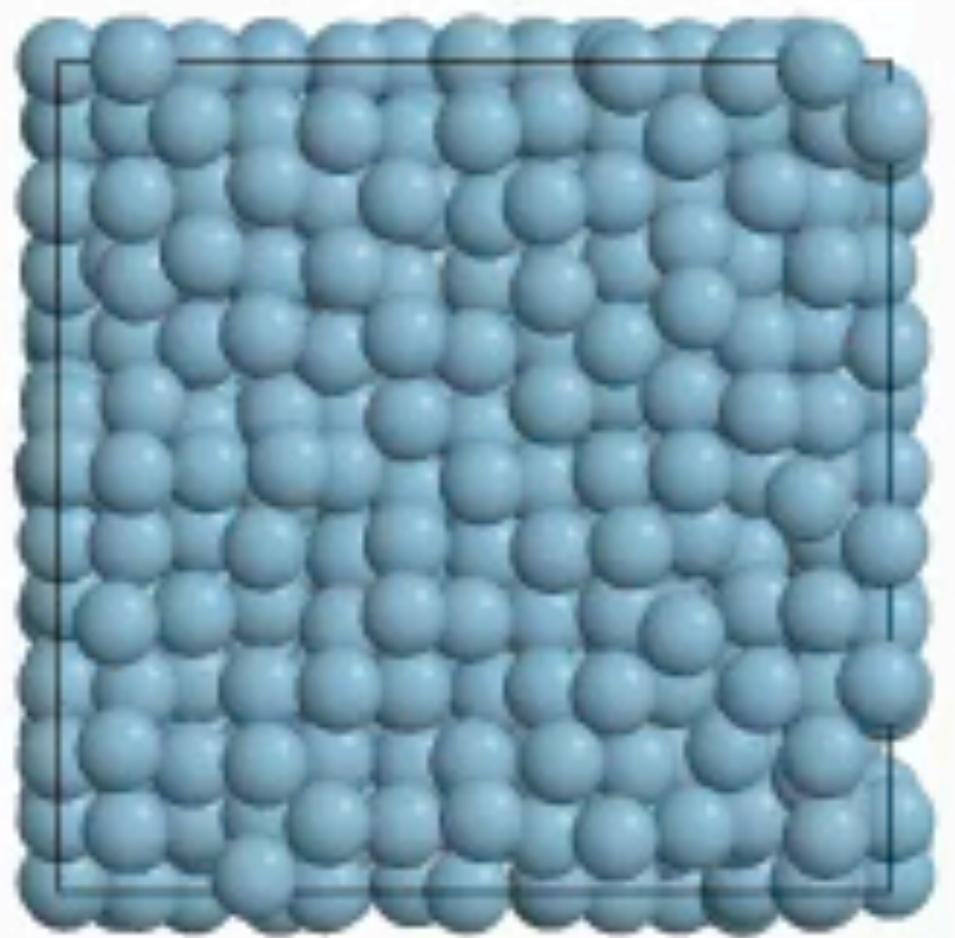
# Specify the interatomic potential.
pair_style lj/cut 2.5
pair_modify shift yes
pair_coeff 1 1 1.0 1.0 2.5

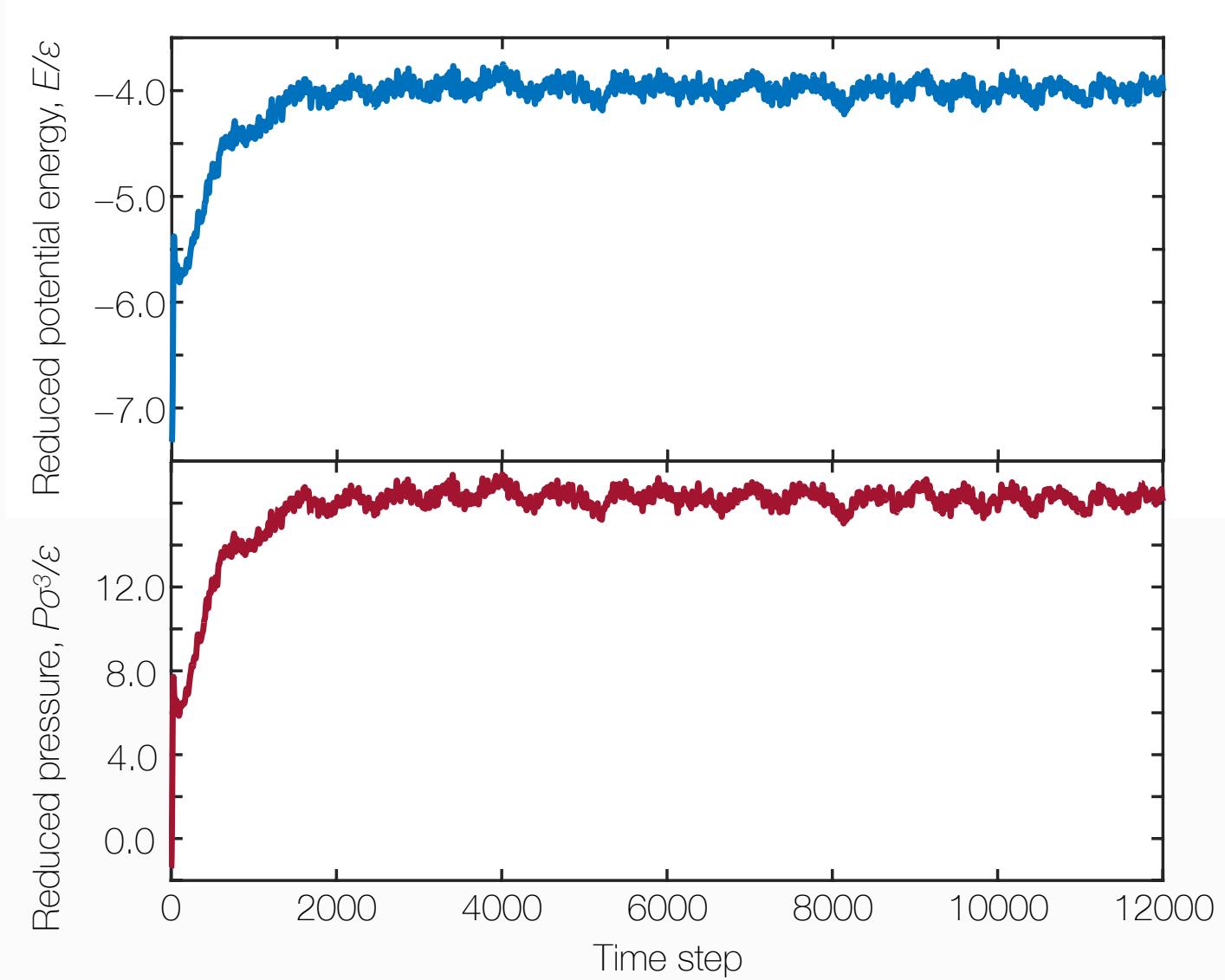
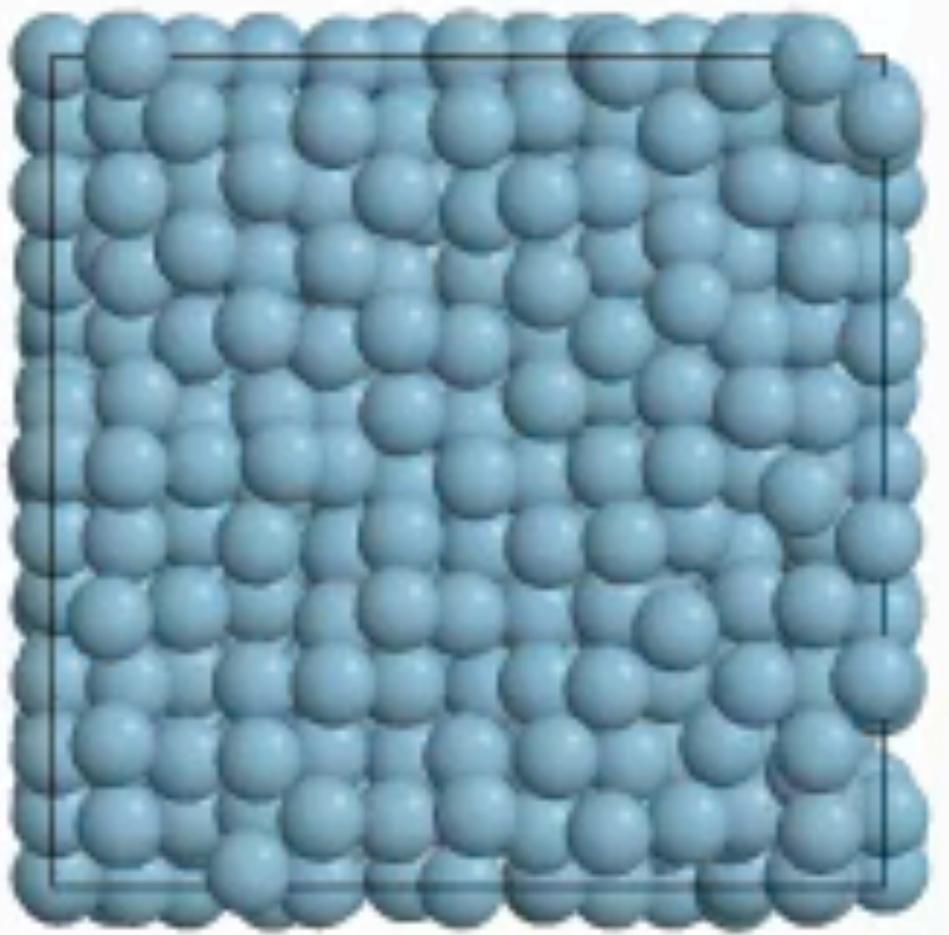
# Integration details,
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
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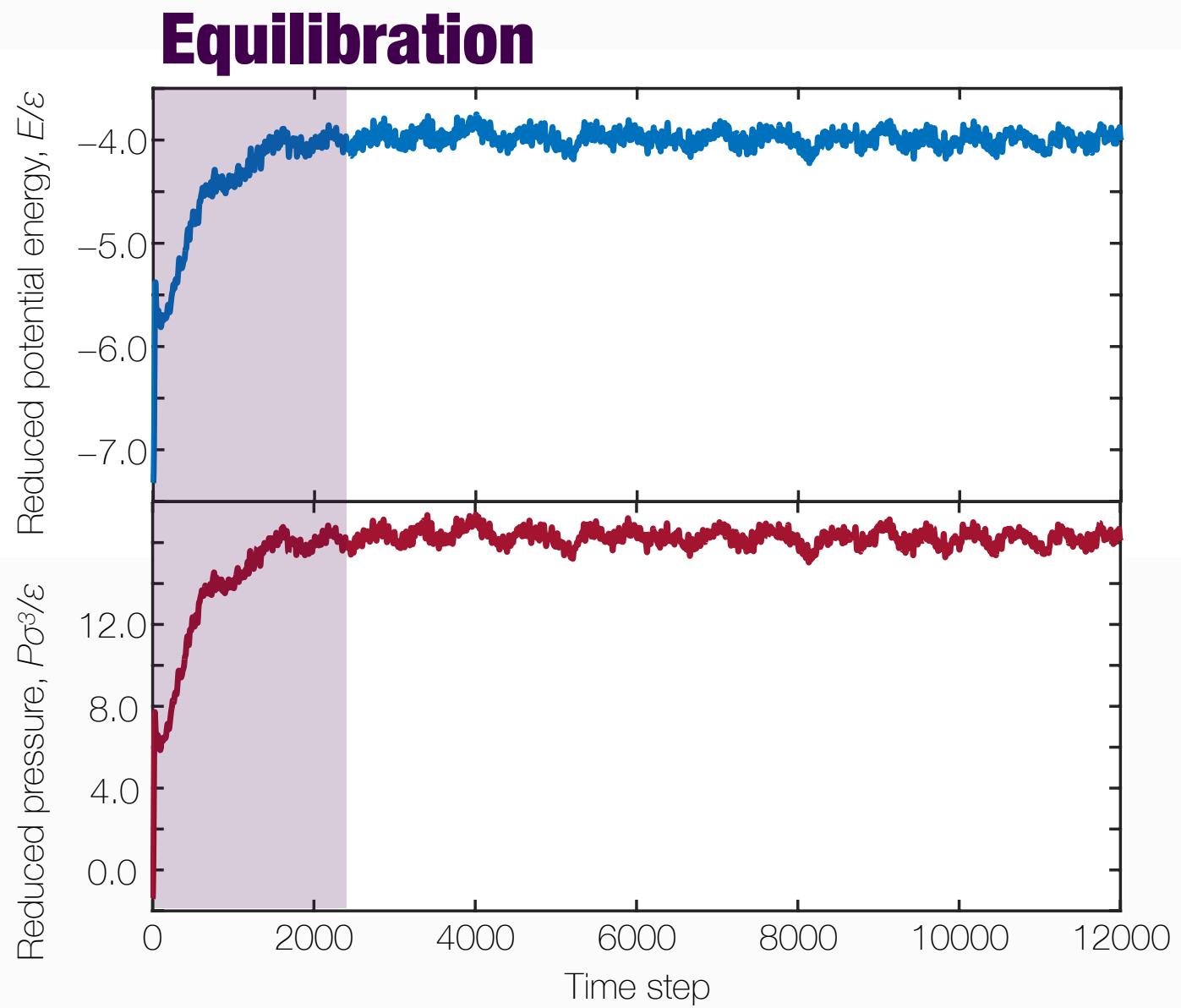
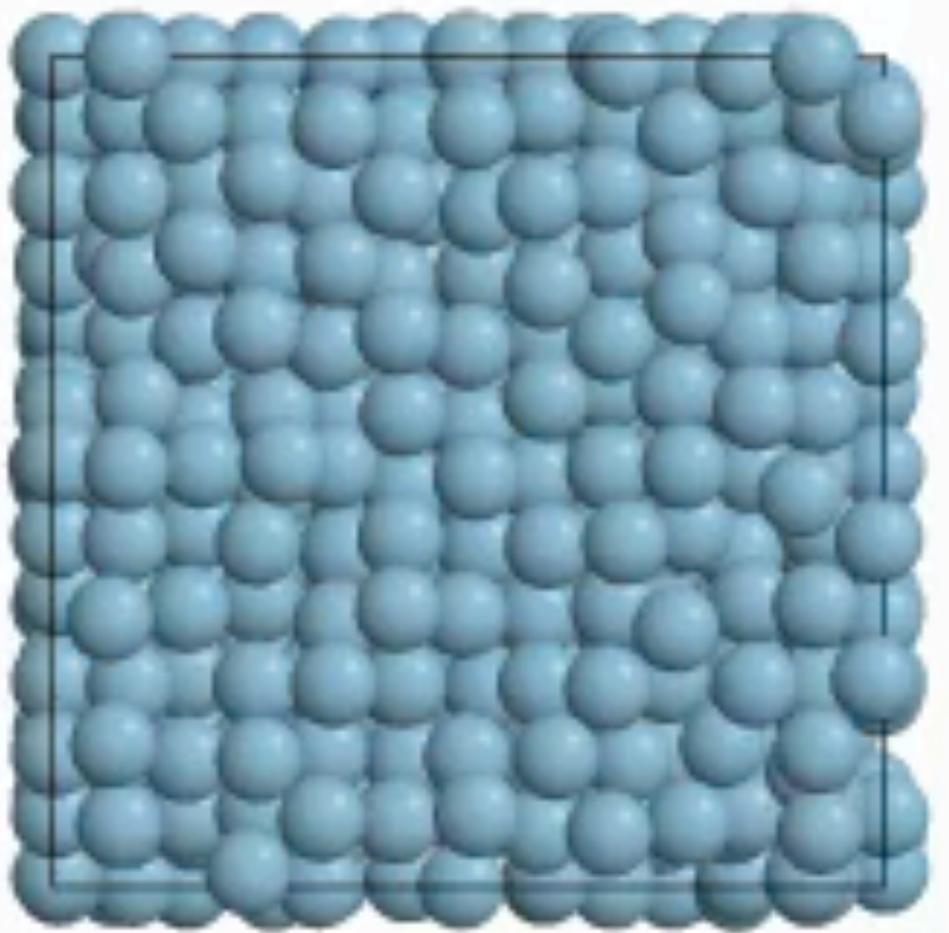
```
# Save the starting configuration.
write_data starting.dat.out
System init for write_data ...
Generated 0 of 0 mixed pair_coeff terms from geometric mixing rule
Neighbor list info ...
update: every = 1 steps, delay = 0 steps, check = yes
max neighbors/atom: 2000, page size: 100000
master list distance cutoff = 2.8
ghost atom cutoff = 2.8
binsize = 1.4, bins = 7 7 7
1 neighbor lists, perpetual/occasional/extral = 1 0 0
(1) pair lj/cut, perpetual
    attributes: half, newton on
    pair build: half/bin/atomonly/newton
    stencil: half/bin/3d
    bin: standard

# Run the simulation.
thermo 100
run 100000
Generated 0 of 0 mixed pair_coeff terms from geometric mixing rule
Per MPI rank memory allocation (min/avg/max) = 3.173 | 3.173 | 3.173 Mbytes
Step      Temp       E_pair      E_mol      TotEng      Press
        0     2      -7.3210321      0      -4.3245043   -1.3958896
    100    1.142423     -5.7775119      0      -4.0658608    6.095448
    200    1.3285217     -5.5636209      0      -3.5731448   7.3600912
    300    1.5299072     -5.2881155      0      -2.9959109   9.011835
    400    1.7141339     -4.9674496      0      -2.3992246  10.803728
    500    1.9308627     -4.7418912      0      -1.8489493  12.248392
    600    2.1560817     -4.6675128      0      -1.4371334  12.791065
    700    2.1231454     -4.5885377      0      -1.4075056  13.171636
    800    2.0013568     -4.6342072      0      -1.6356466  12.849316
```











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# Specify basic aspects of the simulation.
units lj    # Units for quantities. (lj = reduced units)
atom_style atomic # What features does each atom have?
boundary p p p    # Boundary conditions in each dimension.
# Prepare initial structure.
lattice fcc 1.0
region myBox block -0.5 5.5 -0.5 5.5 -0.5 5.5
create_box 1 myBox
create_atoms 1 region myBox
# Specify the interatomic potential.
pair_style lj/cut 2.5
pair_modify shift yes
pair_coeff 1 1 1.0 1.0 2.5
# Integration details,
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
# Save the starting configuration.
write_data starting.dat.out
# Equilibrate the system.
thermo 100
run 10000
# Compute the RDF
comm_modify mode single cutoff 5
compute myRDF all rdf 160 cutoff 4.0
fix rdfAvgFix all ave/time 20 1 20 c_myRDF[*] ave running file nvt-T2.rdf overwrite mode vector
# Compute the potential energy and pressure
variable myPE equal pe
variable myPress equal press
fix thAvgFix all ave/time 10 100 1000 v_myPE v_myPress file nvt-T2-thermo.txt
# Production run
run 90000
# Save the final configuration.
write_data melted.dat.out
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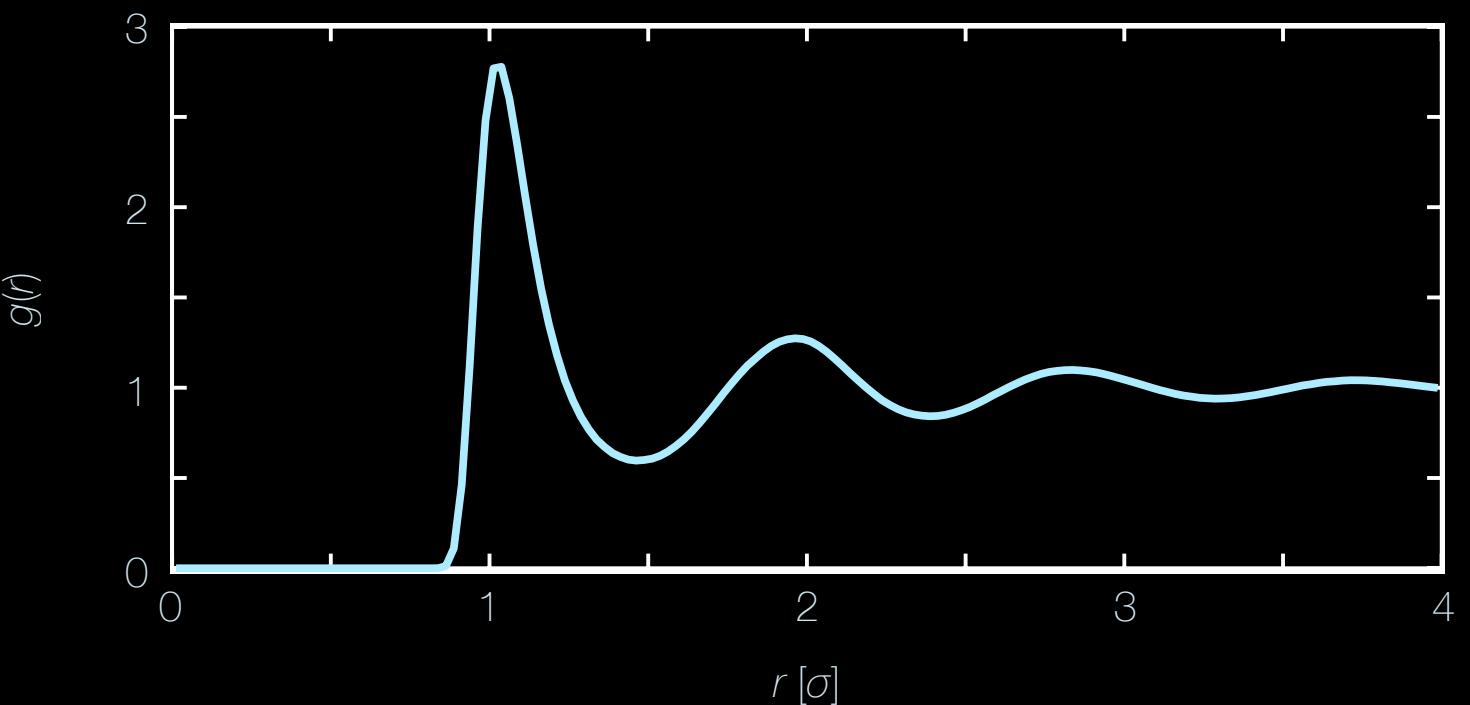


```
# Time-averaged data for fix rdfAvgFix
# TimeStep Number-of-rows
# Row c_myRDF[1] c_myRDF[2] c_myRDF[3]
100000 160
1 0.0125 0 0
2 0.0375 0 0
3 0.0625 0 0
4 0.0875 0 0
5 0.1125 0 0
6 0.1375 0 0
7 0.1625 0 0
8 0.1875 0 0
9 0.2125 0 0
10 0.2375 0 0
11 0.2625 0 0
12 0.2875 0 0
13 0.3125 0 0
14 0.3375 0 0
15 0.3625 0 0
16 0.3875 0 0
17 0.4125 0 0
18 0.4375 0 0
19 0.4625 0 0
20 0.4875 0 0
21 0.5125 0 0
22 0.5375 0 0
23 0.5625 0 0
24 0.5875 0 0
25 0.6125 0 0
26 0.6375 0 0
27 0.6625 0 0
28 0.6875 0 0
29 0.7125 0 0
30 0.7375 0 0
31 0.7625 0 0
32 0.7875 0 0
33 0.8125 7.44733e-06 1.54287e-06
34 0.8375 0.000418226 9.36006e-05
35 0.8625 0.011841 0.0028579
36 0.8875 0.110419 0.030151
```

```

# Time-averaged data for fix rdfAvgFix
# TimeStep Number-of-rows
# Row c_myRDF[1] c_myRDF[2] c_myRDF[3]
100000 160
1 0.0125 0 0
2 0.0375 0 0
3 0.0625 0 0
4 0.0875 0 0
5 0.1125 0 0
6 0.1375 0 0
7 0.1625 0 0
8 0.1875 0 0
9 0.2125 0 0
10 0.2375 0 0
11 0.2625 0 0
12 0.2875 0 0
13 0.3125 0 0
14 0.3375 0 0
15 0.3625 0 0
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30 0.7375 0 0
31 0.7625 0 0
32 0.7875 0 0
33 0.8125 7.44733e-06 1.54287e-06
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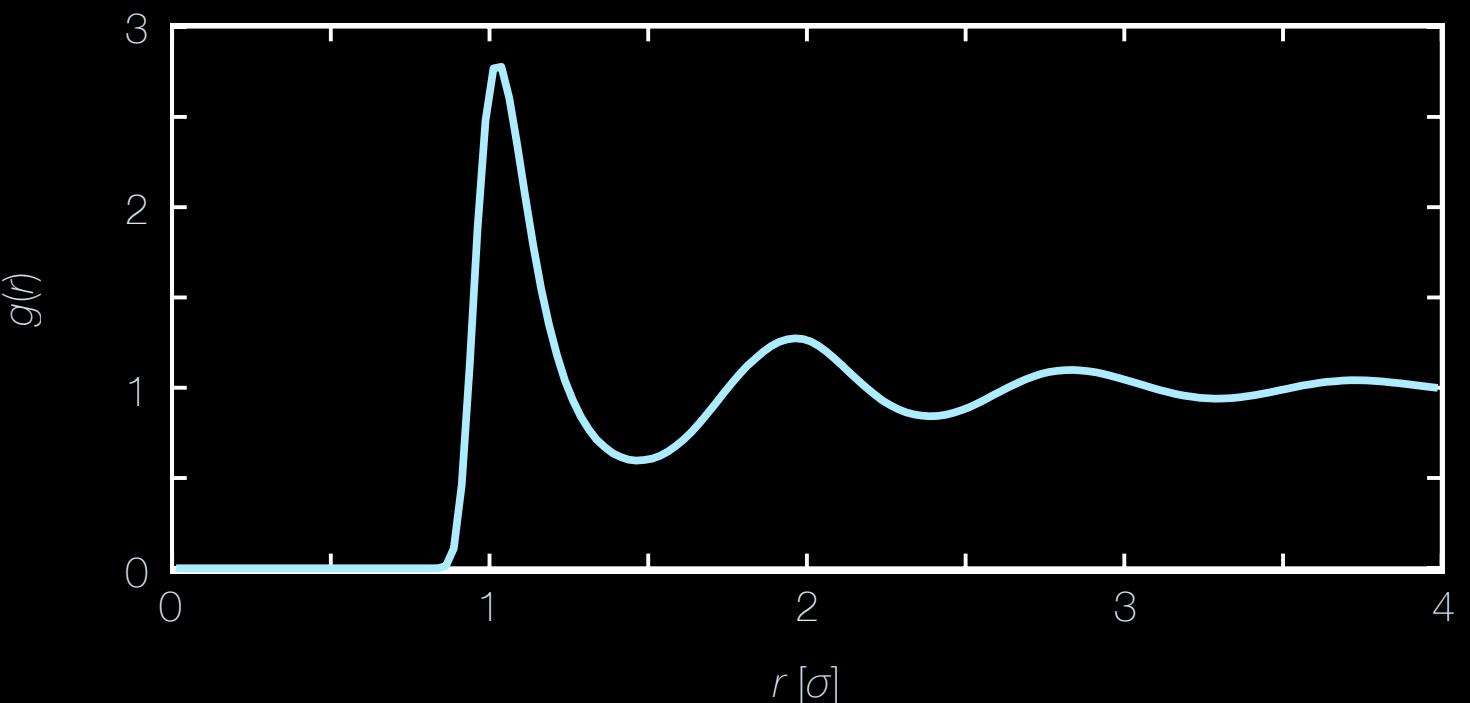
```



```

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# TimeStep Number-of-rows
# Row c_myRDF[1] c_myRDF[2] c_myRDF[3]
100000 160
1 0.0125 0 0
2 0.0375 0 0
3 0.0625 0 0
4 0.0875 0 0
5 0.1125 0 0
6 0.1375 0 0
7 0.1625 0 0
8 0.1875 0 0
9 0.2125 0 0
10 0.2375 0 0
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12 0.2875 0 0
13 0.3125 0 0
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```



```

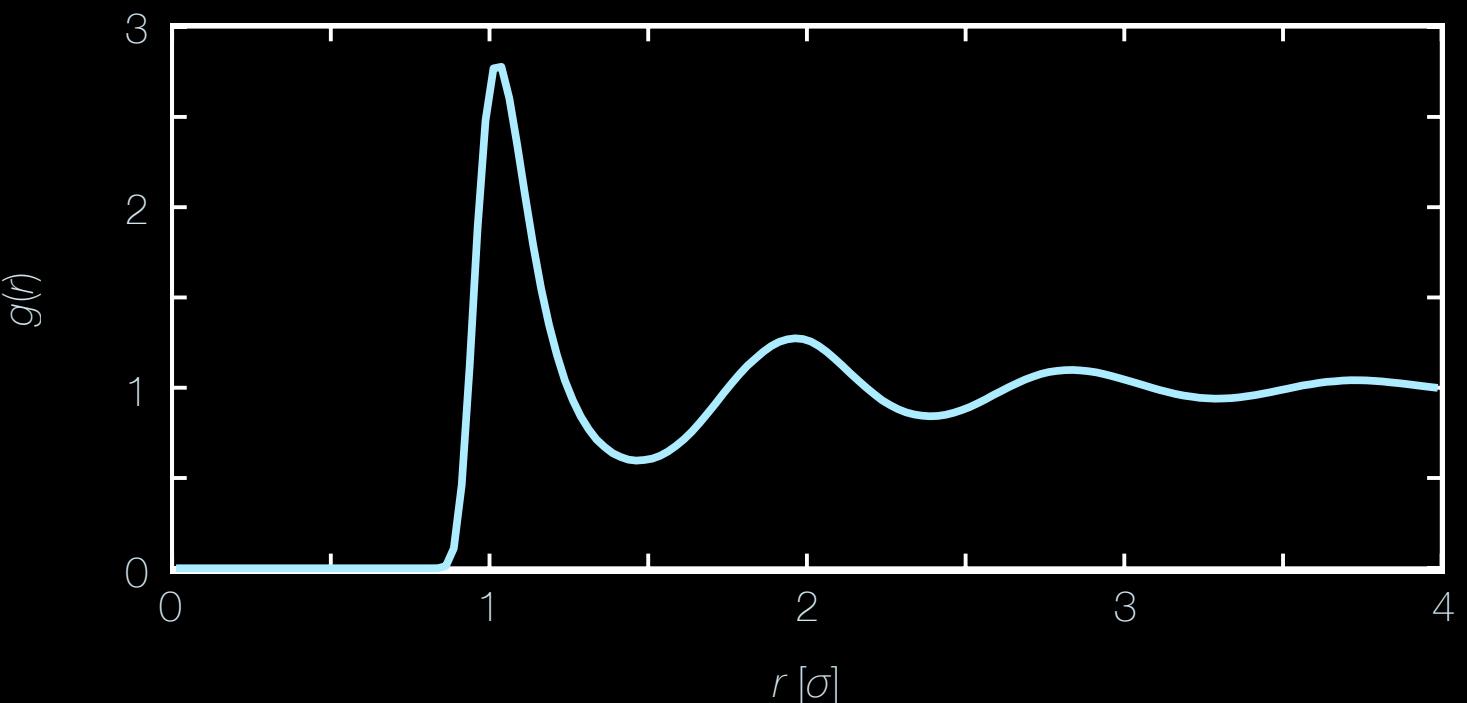
# Time-averaged data for fix thAvgFix
# TimeStep v_myPE v_myPress
11000 -3.96102 16.3791
12000 -3.95183 16.4508
13000 -3.94512 16.46
14000 -4.00331 16.1505
15000 -3.96473 16.373
16000 -4.0134 16.1062
17000 -4.00544 16.1246
18000 -3.99571 16.2072
19000 -3.95334 16.4358
20000 -3.99483 16.1924
21000 -3.98551 16.2581
22000 -4.02115 16.0528
23000 -3.99541 16.2037

```

```

# Time-averaged data for fix rdfAvgFix
# TimeStep Number-of-rows
# Row c_myRDF[1] c_myRDF[2] c_myRDF[3]
100000 160
1 0.0125 0 0
2 0.0375 0 0
3 0.0625 0 0
4 0.0875 0 0
5 0.1125 0 0
6 0.1375 0 0
7 0.1625 0 0
8 0.1875 0 0
9 0.2125 0 0
10 0.2375 0 0
11 0.2625 0 0
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13 0.3125 0 0
14 0.3375 0 0
15 0.3625 0 0
16 0.3875 0 0
17 0.4125 0 0
18 0.4375 0 0
19 0.4625 0 0
20 0.4875 0 0
21 0.5125 0 0
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24 0.5875 0 0
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```



```

# Time-averaged data for fix thAvgFix
# TimeStep v_myPE v_myPress
11000 -3.96102 16.3791
12000 -3.95183 16.4508
13000 -3.94512 16.46
14000 -4.00331 16.1505
15000 -3.96473 16.373
16000 -4.0134 16.1062
17000 -4.00544 16.1246
18000 -3.99571 16.2072
19000 -3.95334 16.4358
20000 -3.99483 16.1924
21000 -3.98551 16.2581
22000 -4.02115 16.0528
23000 -3.99541 16.2037

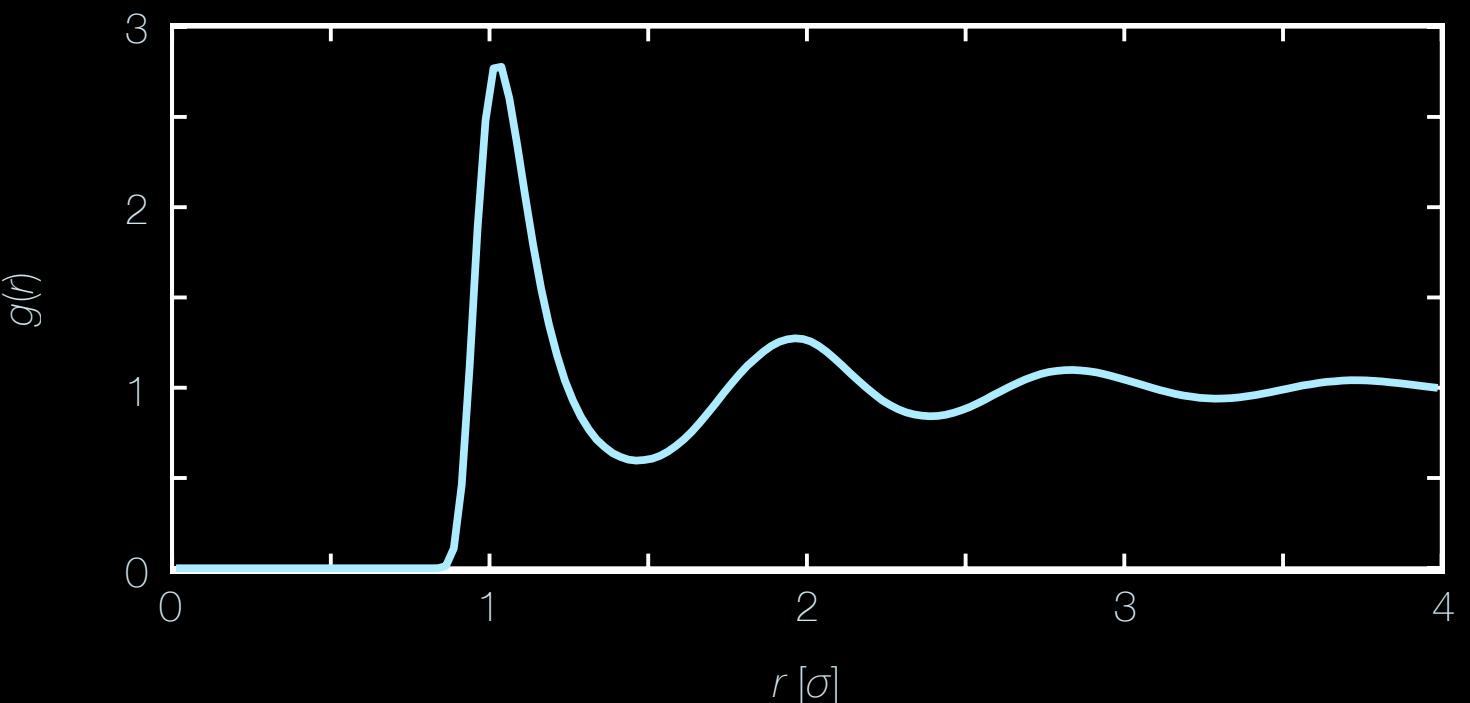
```

$$E_{\text{mean}} / N \varepsilon = -3.97$$

```

# Time-averaged data for fix rdfAvgFix
# TimeStep Number-of-rows
# Row c_myRDF[1] c_myRDF[2] c_myRDF[3]
100000 160
1 0.0125 0 0
2 0.0375 0 0
3 0.0625 0 0
4 0.0875 0 0
5 0.1125 0 0
6 0.1375 0 0
7 0.1625 0 0
8 0.1875 0 0
9 0.2125 0 0
10 0.2375 0 0
11 0.2625 0 0
12 0.2875 0 0
13 0.3125 0 0
14 0.3375 0 0
15 0.3625 0 0
16 0.3875 0 0
17 0.4125 0 0
18 0.4375 0 0
19 0.4625 0 0
20 0.4875 0 0
21 0.5125 0 0
22 0.5375 0 0
23 0.5625 0 0
24 0.5875 0 0
25 0.6125 0 0
26 0.6375 0 0
27 0.6625 0 0
28 0.6875 0 0
29 0.7125 0 0
30 0.7375 0 0
31 0.7625 0 0
32 0.7875 0 0
33 0.8125 7.44733e-06 1.54287e-06
34 0.8375 0.000418226 9.36006e-05
35 0.8625 0.011841 0.0028579
36 0.8875 0.110419 0.030151

```



```

# Time-averaged data for fix thAvgFix
# TimeStep v_myPE v_myPress
11000 -3.96102 16.3791
12000 -3.95183 16.4508
13000 -3.94512 16.46
14000 -4.00331 16.1505
15000 -3.96473 16.373
16000 -4.0134 16.1062
17000 -4.00544 16.1246
18000 -3.99571 16.2072
19000 -3.95334 16.4358
20000 -3.99483 16.1924
21000 -3.98551 16.2581
22000 -4.02115 16.0528
23000 -3.99541 16.2037

```

$$E_{\text{mean}} / N \varepsilon = -3.97$$

$$P_{\text{mean}} \sigma^3 / \varepsilon = 16.29$$

Starting from a pre-saved configuration

```
# Specify basic aspects of the simulation.
units lj    # Units for quantities. (lj = reduced units)
atom_style atomic # What features does each atom have?
boundary p p p    # Boundary conditions in each dimension.
# Specify the interatomic potential.
pair_style lj/cut 2.5
pair_modify shift yes
# Read a data file containing starting configuration
read_data melted.dat.out
# Optional, but better to include (in case info missing from data file)
pair_coeff 1 1 1.0 1.0 2.5
# Integration details,
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
# Save checkpoints along the trajectory
restart 20000 LJ-T2-rho1-rst
# Create a trajectory for further analysis/post-processing.
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz
dump_modify myDump sort id
# Run the simulation.
thermo 100
run 100000
```

Starting from a pre-saved configuration

```
# Specify basic aspects of the simulation.  
units lj    # Units for quantities. (lj = reduced units)  
atom_style atomic # What features does each atom have?  
boundary p p p    # Boundary conditions in each dimension.  
# Specify the interatomic potential.  
pair_style lj/cut 2.5  
pair_modify shift yes  
# Read a data file containing starting configuration  
read_data melted.dat.out  
# Optional, but better to include (in case info missing from data file)  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp 2.0 2.0 0.25  
velocity all create 2.0 4928459 dist gaussian  
# Save checkpoints along the trajectory  
restart 20000 LJ-T2-rho1-rst  
# Create a trajectory for further analysis/post-processing.  
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz  
dump_modify myDump sort id  
# Run the simulation.  
thermo 100  
run 100000
```

A Typical Data File

A Typical Data File

```
LAMMPS data file via write_data, version 2 Aug 2023, timestep = 100000, units = lj
```

```
864 atoms
```

```
1 atom types
```

```
-0.7937005259840997 8.730705785825096 xlo xhi
```

```
-0.7937005259840997 8.730705785825096 ylo yhi
```

```
-0.7937005259840997 8.730705785825096 zlo zhi
```

```
Masses
```

```
1 1
```

```
Pair Coeffs # lj/cut
```

```
1 1 1
```

```
Atoms # atomic
```

```
813 1 -0.7689461301142977 0.7800062157809646 -0.38429757614666415 0 1 1
```

```
80 1 -0.17404446254176928 -0.1696516471907801 8.340409425564513 1 0 -1
```

```
639 1 8.094998976206686 8.526353678882293 8.558990011292014 -1 0 0
```

```
473 1 0.8704026531389637 -0.25460256503726586 -0.5276023495628914 0 0 1
```

```
670 1 1.4443100240531723 8.265577319775666 -0.1893750225727789 -1 0 1
```

```
.....
```

```
Velocities
```

```
813 3.023141009895317 1.2903672987595027 -0.7566085625088316
```

A Typical Data File

```
LAMMPS data file via write_data, version 2 Aug 2023, timestep = 100000, units = lj
```

```
864 atoms
```

```
1 atom types
```

```
-0.7937005259840997 8.730705785825096 xlo xhi  
-0.7937005259840997 8.730705785825096 ylo yhi  
-0.7937005259840997 8.730705785825096 zlo zhi
```

```
Masses
```

```
1 1
```

```
Pair Coeffs # lj/cut
```

```
1 1 1
```

```
Atoms # atomic
```

```
813 1 -0.7689461301142977 0.7800062157809646 -0.38429757614666415 0 1 1  
80 1 -0.17404446254176928 -0.1696516471907801 8.340409425564513 1 0 -1  
639 1 8.094998976206686 8.526353678882293 8.558990011292014 -1 0 0  
473 1 0.8704026531389637 -0.25460256503726586 -0.5276023495628914 0 0 1  
670 1 1.4443100240531723 8.265577319775666 -0.1893750225727789 -1 0 1
```

```
.....
```

```
Velocities
```

```
813 3.023141009895317 1.2903672987595027 -0.7566085625088316
```

***Can prepare your own data file
using a third-party package or
your own code!***

A Few More Additions!

```
# Specify basic aspects of the simulation.
units lj    # Units for quantities. (lj = reduced units)
atom_style atomic # What features does each atom have?
boundary p p p    # Boundary conditions in each dimension.
# Specify the interatomic potential.
pair_style lj/cut 2.5
pair_modify shift yes
# Read a data file containing starting configuration
read_data melted.dat.out
# Optional, but better to include (in case info missing from data file)
pair_coeff 1 1 1.0 1.0 2.5
# Integration details,
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
# Save checkpoints along the trajectory
restart 20000 LJ-T2-rho1-rst
# Create a trajectory for further analysis/post-processing.
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz
dump_modify myDump sort id
# Run the simulation.
thermo 100
run 100000
```

A Few More Additions!

```
# Specify basic aspects of the simulation.  
units lj    # Units for quantities. (lj = reduced units)  
atom_style atomic # What features does each atom have?  
boundary p p p    # Boundary conditions in each dimension.  
# Specify the interatomic potential.  
pair_style lj/cut 2.5  
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# Read a data file containing starting configuration  
read_data melted.dat.out  
# Optional, but better to include (in case info missing from data file)  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp 2.0 2.0 0.25  
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run 100000
```

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units lj    # Units for quantities. (lj = reduced units)  
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# Specify the interatomic potential.  
pair_style lj/cut 2.5  
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read_data melted.dat.out  
# Optional, but better to include (in case info missing from data file)  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp 2.0 2.0 0.25  
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restart 20000 LJ-T2-rho1-rst  
# Create a trajectory for further analysis/post-processing.  
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz  
dump_modify myDump sort id  
# Run the simulation.  
thermo 100  
run 100000
```

Write periodic binary outputs to start fresh simulations!

A Few More Additions!

```
# Specify basic aspects of the simulation.
units lj    # Units for quantities. (lj = reduced units)
atom_style atomic # What features does each atom have?
boundary p p p    # Boundary conditions in each dimension.
# Specify the interatomic potential.
pair_style lj/cut 2.5
pair_modify shift yes
# Read a data file containing starting configuration
read_data melted.dat.out
# Optional, but better to include (in case info missing from data file)
pair_coeff 1 1 1.0 1.0 2.5
# Integration details,
mass 1 1.0
timestep 0.0025
fix ensFix all nvt temp 2.0 2.0 0.25
velocity all create 2.0 4928459 dist gaussian
# Save checkpoints along the trajectory
restart 20000 LJ-T2-rho1-rst
# Create a trajectory for further analysis/post-processing.
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz
dump_modify myDump sort id
# Run the simulation.
thermo 100
run 100000
```

A Few More Additions!

```
# Specify basic aspects of the simulation.  
units lj    # Units for quantities. (lj = reduced units)  
atom_style atomic # What features does each atom have?  
boundary p p p    # Boundary conditions in each dimension.  
# Specify the interatomic potential.  
pair_style lj/cut 2.5  
pair_modify shift yes  
# Read a data file containing starting configuration  
read_data melted.dat.out  
# Optional, but better to include (in case info missing from data file)  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp 2.0 2.0 0.25  
velocity all create 2.0 4928459 dist gaussian  
# Save checkpoints along the trajectory  
restart 20000 LJ-T2-rho1-rst  
# Create a trajectory for further analysis/post-processing.  
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz  
dump_modify myDump sort id  
# Run the simulation.  
thermo 100  
run 100000
```

A Few More Additions!

```
# Specify basic aspects of the simulation.  
units lj    # Units for quantities. (lj = reduced units)  
atom_style atomic # What features does each atom have?  
boundary p p p    # Boundary conditions in each dimension.  
# Specify the interatomic potential.  
pair_style lj/cut 2.5  
pair_modify shift yes  
# Read a data file containing starting configuration  
read_data melted.dat.out  
# Optional, but better to include (in case info missing from data file)  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp 2.0 2.0 0.25  
velocity all create 2.0 4928459 dist gaussian  
# Save checkpoints along the trajectory  
restart 20000 LJ-T2-rho1-rst  
# Create a trajectory for further analysis/post-processing.  
dump myDump all custom 250 nvt-T2-rho1-dump.xyz id type x y z vx vy vz  
dump_modify myDump sort id  
# Run the simulation.  
thermo 100  
run 100000
```

Create a long “bare” trajectory for post-processing, visualization or transfer to other packages.

A Typical Dump File

A Typical Dump File

```
ITEM: Timestep
0
ITEM: Number of Atoms
864
ITEM: Box Bounds pp pp pp
-7.9370052598409968e-01 8.7307057858250960e+00
-7.9370052598409968e-01 8.7307057858250960e+00
-7.9370052598409968e-01 8.7307057858250960e+00
ITEM: Atoms id type x y z vx vy vz
1 1 -0.460001 6.71873 0.1299 2.75499 2.04401 -0.499415
2 1 5.06938 4.93808 2.84887 1.46912 -3.3227 -0.325835
3 1 8.37534 0.114851 1.93991 1.16774 -0.109902 3.45937
4 1 2.4004 1.96077 6.54152 -0.422939 -1.30187 -1.43718
5 1 1.28181 6.71877 3.44022 -1.77102 0.911424 2.84987
6 1 0.762845 1.11275 4.22049 -0.336543 -0.935257 -0.810099
7 1 5.34442 5.4529 2.07625 -1.50284 -1.04324 -1.70678
8 1 8.19373 5.0113 -0.104749 0.0638107 -0.637271 -0.398029
9 1 1.66126 7.51044 5.47042 0.14022 0.0947027 0.831843
10 1 5.70331 3.96422 7.58096 -0.805547 -0.370405 0.280985
11 1 7.79485 5.17263 3.18285 0.318948 0.393109 1.02244
12 1 8.62021 5.93558 -0.19867 -0.235391 0.487304 -1.13593
13 1 0.713081 3.73732 0.688987 -0.601049 -1.39198 -2.53684
14 1 4.75175 8.05159 2.47969 2.04589 0.718168 0.762836
15 1 4.34178 8.19972 -0.129279 0.488617 0.819358 -0.197692
16 1 7.09782 7.30505 5.2013 -1.13335 -1.26086 0.180832
17 1 0.412103 -0.789558 3.85691 0.690659 0.351547 0.536481
18 1 0.668403 2.71232 0.700827 0.600151 -1.35037 2.41296
19 1 -0.157543 4.19247 0.45575 1.045 1.03258 0.690863
20 1 6.87458 2.04552 7.24267 -0.564621 -1.3646 -1.87772
21 1 5.00925 3.67059 2.03951 -1.16097 -1.45397 1.67865
```

Run LAMMPS Yourself!

```
# Specify basic aspects of the simulation.  
units lj      # Units for quantities. (lj = reduced units)  
atom_style atomic# What features does each atom have?  
boundary p p p    # Boundary conditions in each dimension.  
# Prepare initial structure.  
lattice sc ${numDen}  
region myBox block 0 10 0 10 0 10  
create_box 1 myBox  
create_atoms 1 region myBox  
# Specify the interatomic potential.  
pair_style lj/cut 2.5  
pair_modify shift yes  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp ${T_target} ${T_target} 0.25  
velocity all create ${T_target} 4928459 dist gaussian  
# Save the starting configuration.  
write_data starting.dat.out  
# Run the simulation.  
thermo 100  
run ${eqSteps}  
# Save the final configuration.  
write_data equil-rho${numDen}-T${T_target}.dat.out
```

```
# Specify basic aspects of the simulation.  
units lj      # Units for quantities. (lj = reduced units)  
atom_style atomic# What features does each atom have?  
boundary p p p    # Boundary conditions in each dimension.  
pair_style lj/cut 2.5  
read_data ${confFileName}  
pair_modify shift yes  
pair_coeff 1 1 1.0 1.0 2.5  
# Integration details,  
mass 1 1.0  
timestep 0.0025  
fix ensFix all nvt temp ${T_target} ${T_target} 0.25  
velocity all create ${T_target} ${mySeed} dist gaussian  
thermo 100  
# Compute the RDF  
comm_modify mode single cutoff 5  
compute myRDF all rdf ${nRdfBins} cutoff ${rdfCutoff}  
fix rdfAvgFix all ave/time 20 1 20 c_myRDF[*] ave running  
file ${tag}-T${T_target}.rdf overwrite mode vector  
# Compute the potential energy and pressure  
variable myPE equal pe  
variable myPress equal press  
fix thAvgFix all ave/time 10 100 1000 v_myPE v_myPress file  
${tag}-T${T_target}-thermo.txt  
# Production run  
run ${prodSteps}
```

Run LAMMPS Yourself!

Run LAMMPS Yourself!

Step 1: Start an interactive job on Bridges-2.

```
srun -p RM-shared -n 1 --pty bash -I
```

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```
srun -p RM-shared -n 1 --pty bash -I
```

Step 2: Load modules & copy LAMMPS binary & run scripts to appropriate folders.

```
module load intel-compiler
module load intel-mpi
module load intel-mkl
cp /ocean/projects/see22002p/shared/LAMMPS/bin/lmp_mpi .
cp /ocean/projects/see22002p/shared/LAMMPS/LJ-Bulk/in.nvt-
generate-general .
cp /ocean/projects/see22002p/shared/LAMMPS/LJ-Bulk/in.nvt-
general-rdf .
```

Run LAMMPS Yourself!

Step 1: Start an interactive job on Bridges-2.

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```

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cp /ocean/projects/see22002p/shared/LAMMPS/LJ-Bulk/in.nvt-
generate-general .
cp /ocean/projects/see22002p/shared/LAMMPS/LJ-Bulk/in.nvt-
general-rdf .
```

Step 3: Generate a starting configuration at the specified density and temperature.

```
./lmp_mpi -in in.nvt-generate-general -v numDen ${rho} -v
T_target ${T} -v eqSteps ${mySteps}
```

Group ID	Temperature	Number Density	Equilibrium Steps
1	2.0	1.05	20000
2	1.8	0.95	20000
3	1.5	1.00	20000
4	1.0	0.90	20000

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```
srun -p RM-shared -n 1 --pty bash -I
```

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```
module load intel-compiler
module load intel-mpi
module load intel-mkl
cp /ocean/projects/see22002p/shared/LAMMPS/bin/lmp_mpi .
cp /ocean/projects/see22002p/shared/LAMMPS/LJ-Bulk/in.nvt-
generate-general .
cp /ocean/projects/see22002p/shared/LAMMPS/LJ-Bulk/in.nvt-
general-rdf .
```

Step 3: Generate a starting configuration at the specified density and temperature.

```
./lmp_mpi -in in.nvt-generate-general -v numDen ${rho} -v
T_target ${T} -v eqSteps ${mySteps}
```

Step 4: Use the generated configuration to start a production run using the following script.

```
./lmp_mpi -in in.nvt-general-rdf -v confFileName
equil-rho${rho}-T${T}.dat.out -v T_target ${T} -v
mySeed 2024${grpId} -v nRdfBins ${n} -v rdfCutoff ${rMax} -v tag prod-rho${rho} -v prodSteps 80000
```

Choose \${rMax} as the largest value possible for your box size, and \${N} so that each RDF bin is 0.025 thick.

Group ID	Temperature	Number Density	Equilibrium Steps
1	2.0	1.05	20000
2	1.8	0.95	20000
3	1.5	1.00	20000
4	1.0	0.90	20000

Typical Outputs

Typical Outputs

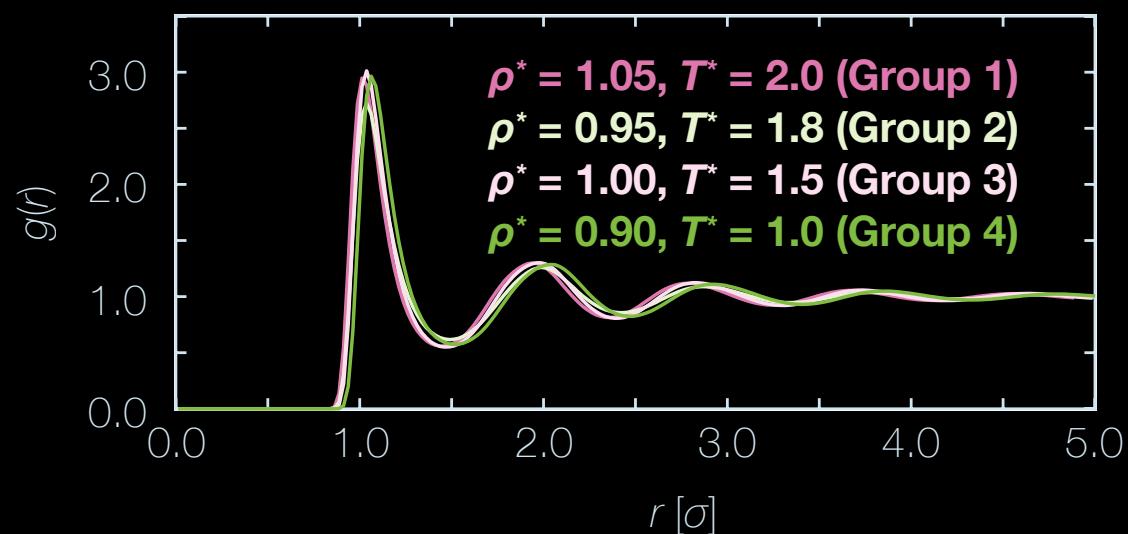
Group ID	Temperature	Number Density	Equilibration Steps
1	2.0	1.05	20000
2	1.8	0.95	20000
3	1.5	1.00	20000
4	1.0	0.90	20000

Typical Outputs

Group ID	Temperature	Number Density	Equilibration Steps	Maximum distance	Bin Count
1	2.0	1.05	20000	4.900	196
2	1.8	0.95	20000	5.075	203
3	1.5	1.00	20000	5.000	200
4	1.0	0.90	20000	5.175	207

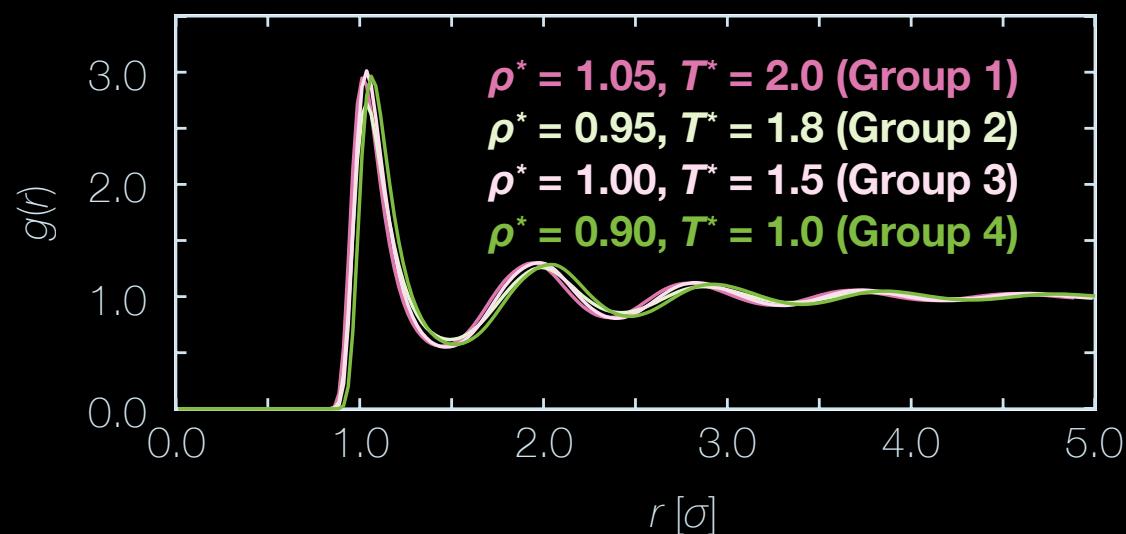
Typical Outputs

Group ID	Temperature	Number Density	Equilibration Steps	Maximum distance	Bin Count
1	2.0	1.05	20000	4.900	196
2	1.8	0.95	20000	5.075	203
3	1.5	1.00	20000	5.000	200
4	1.0	0.90	20000	5.175	207



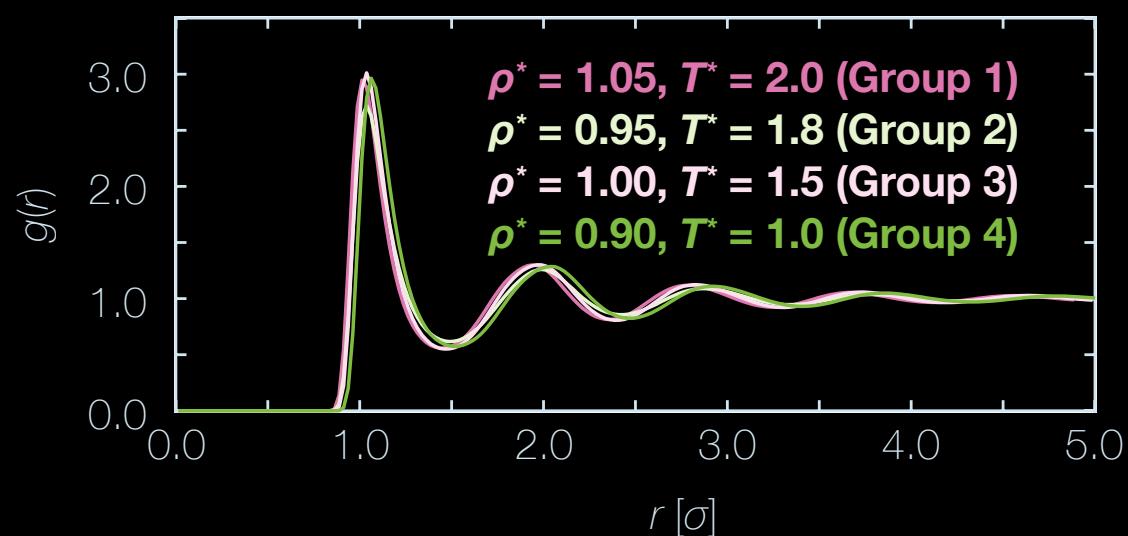
Typical Outputs

Group ID	Temperature	Number Density	Equilibration Steps	Maximum distance	Bin Count	Potential Energy
1	2.0	1.05	20000	4.900	196	-3.82
2	1.8	0.95	20000	5.075	203	-4.30
3	1.5	1.00	20000	5.000	200	-4.61
4	1.0	0.90	20000	5.175	207	-5.09



Typical Outputs

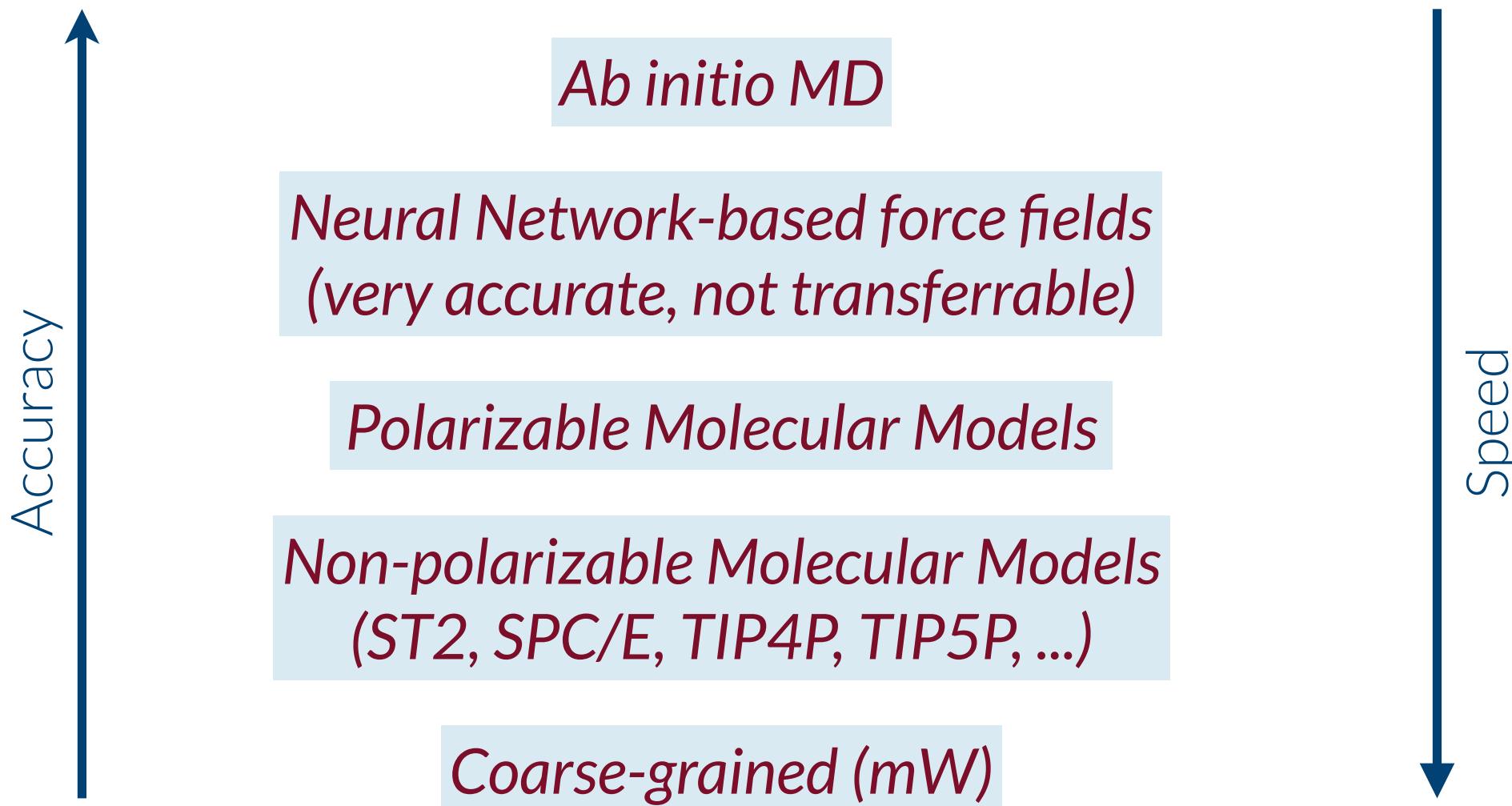
Group ID	Temperature	Number Density	Equilibration Steps	Maximum distance	Bin Count	Potential Energy	Pressure
1	2.0	1.05	20000	4.900	196	-3.82	20.48
2	1.8	0.95	20000	5.075	203	-4.30	11.44
3	1.5	1.00	20000	5.000	200	-4.61	12.59
4	1.0	0.90	20000	5.175	207	-5.09	4.19



Water

A More Complex System

Water Models: Timescales & Nucleation



Modeling Water

Atomistic Representations

Modeling Water

Atomistic Representations

Comprised of a handful of charged LJ sites connected via bonds & angles.

Modeling Water

Atomistic Representations

Comprised of a handful of charged LJ sites connected via bonds & angles.

Bonds & angles usually frozen to avoid high-frequency O-H vibrations allowing the use of larger time steps (typically 2 fs).

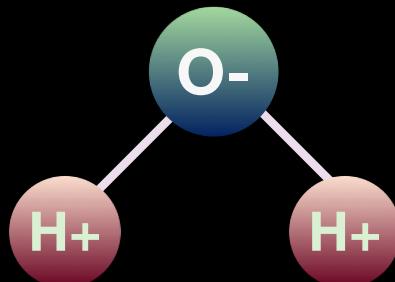
Modeling Water

Atomistic Representations

Comprised of a handful of charged LJ sites connected via bonds & angles.

Bonds & angles usually frozen to avoid high-frequency O-H vibrations allowing the use of larger time steps (typically 2 fs).

Three-site models



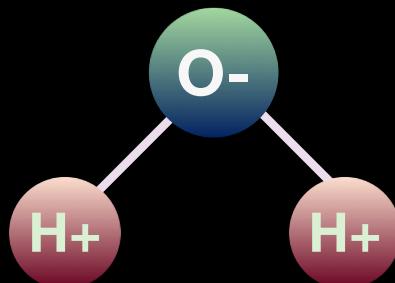
Modeling Water

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Three-site models



TIP3P, SPC, SPC/E

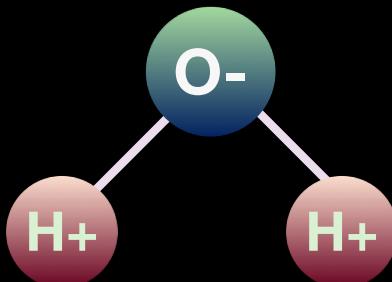
Modeling Water

Atomistic Representations

Comprised of a handful of charged LJ sites connected via bonds & angles.

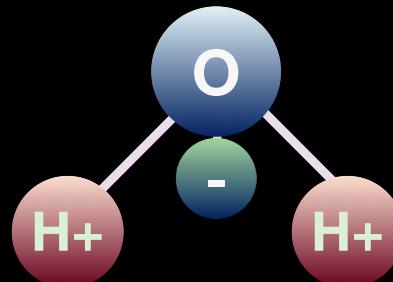
Bonds & angles usually frozen to avoid high-frequency O-H vibrations allowing the use of larger time steps (typically 2 fs).

Three-site models



TIP3P, SPC, SPC/E

Four-site models



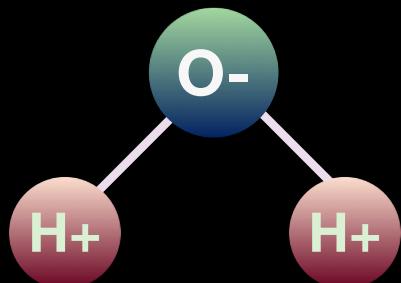
Modeling Water

Atomistic Representations

Comprised of a handful of charged LJ sites connected via bonds & angles.

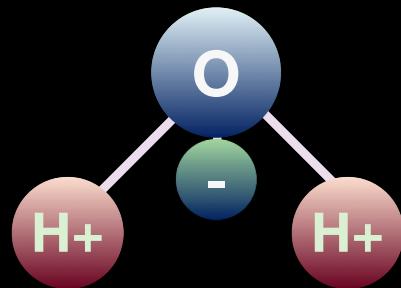
Bonds & angles usually frozen to avoid high-frequency O-H vibrations allowing the use of larger time steps (typically 2 fs).

Three-site models

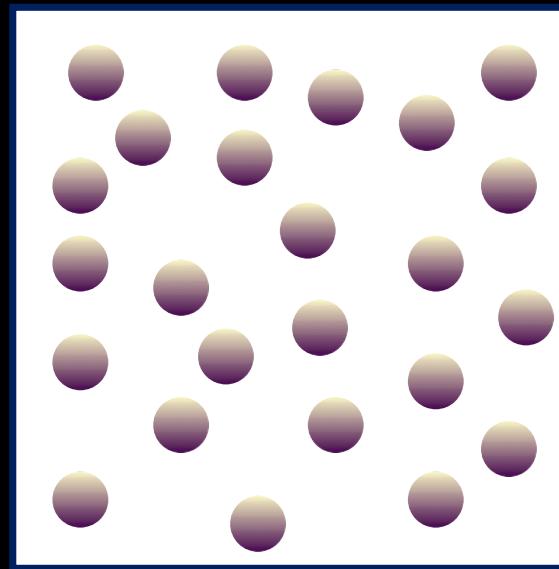


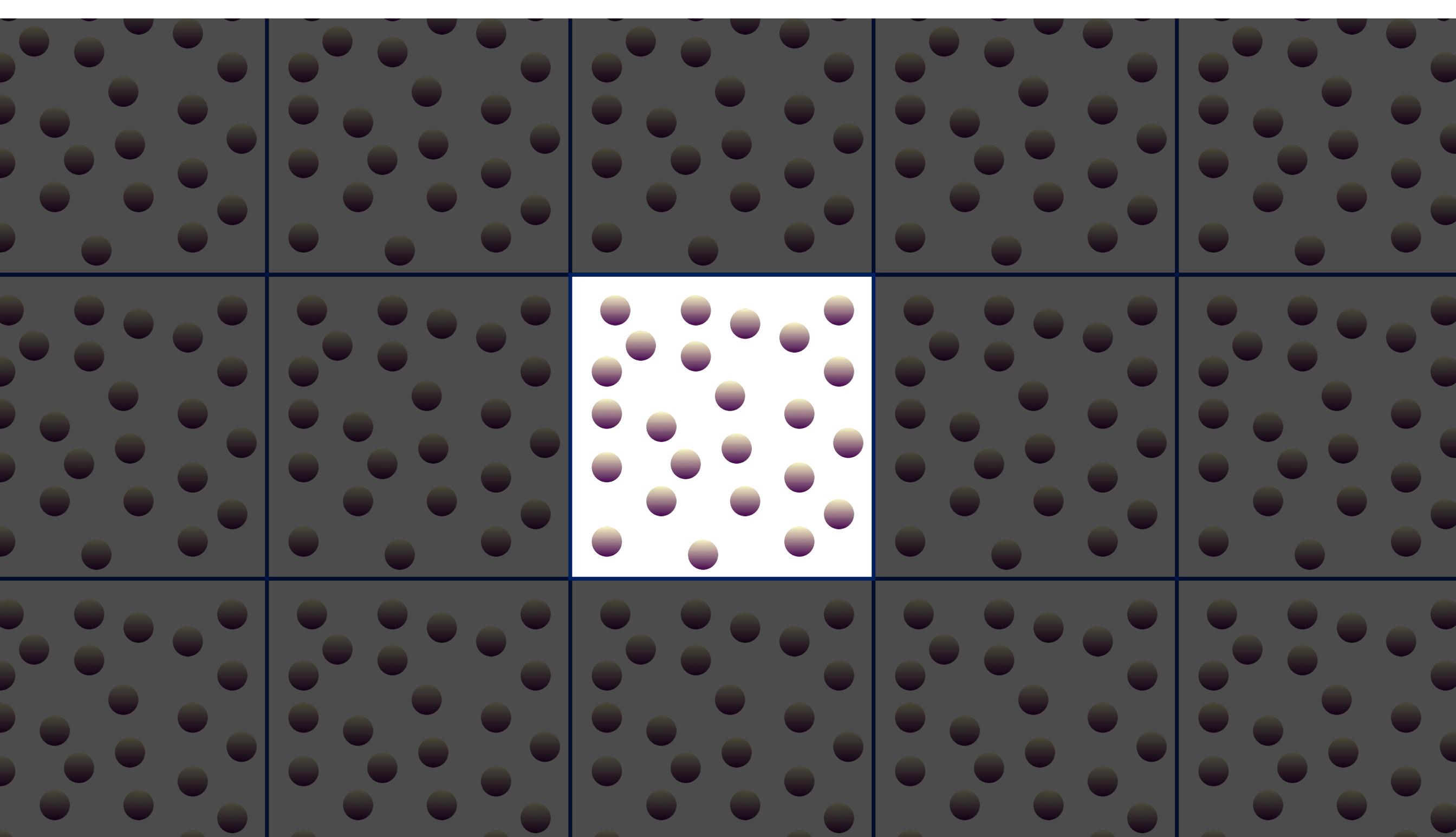
TIP3P, SPC, SPC/E

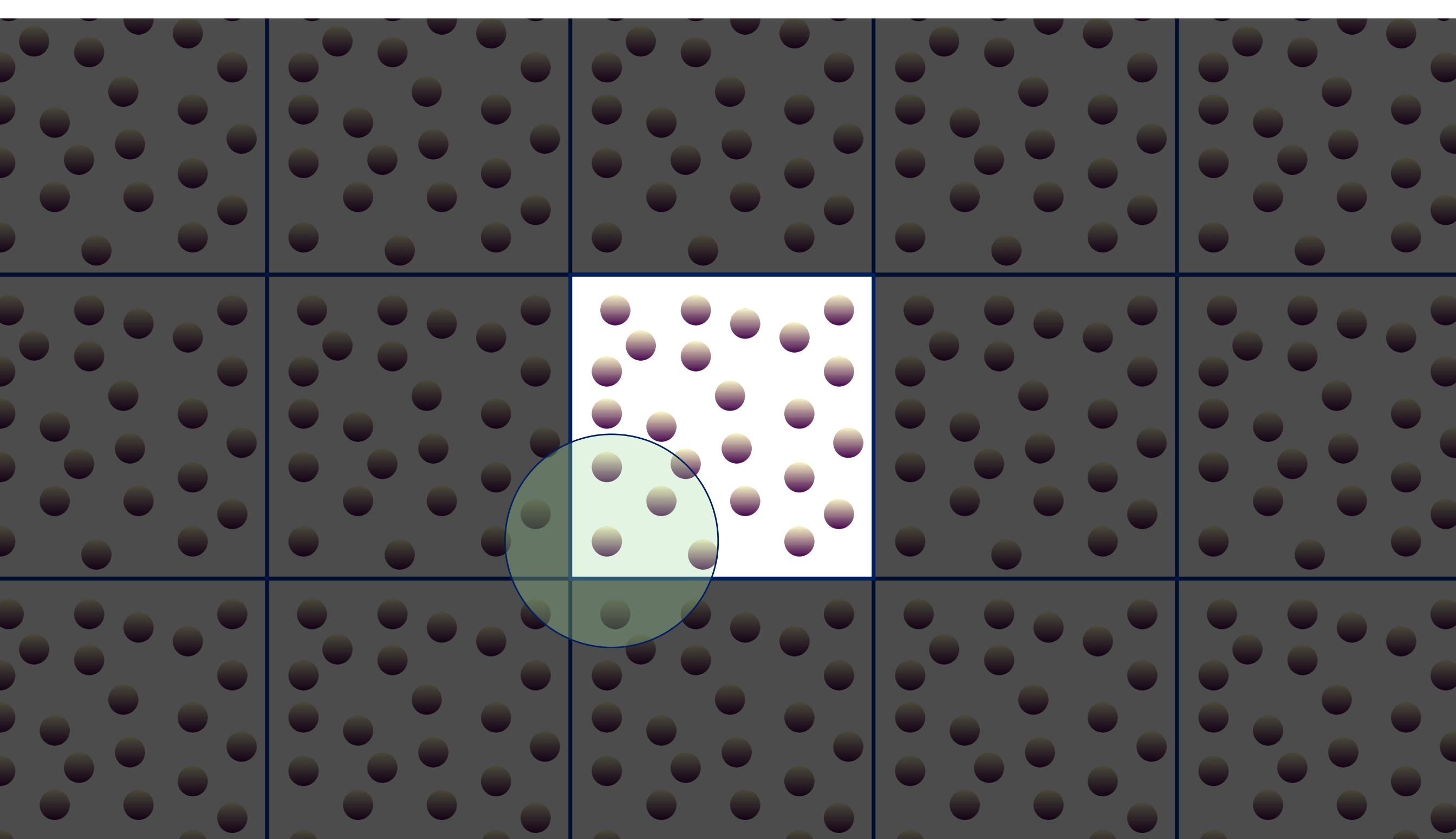
Four-site models



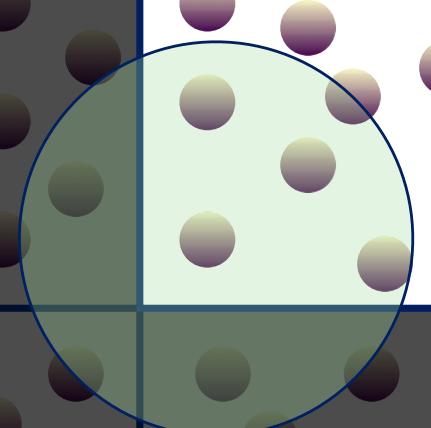
TIP4P, TIP4P/2005, TIP4P/Ice





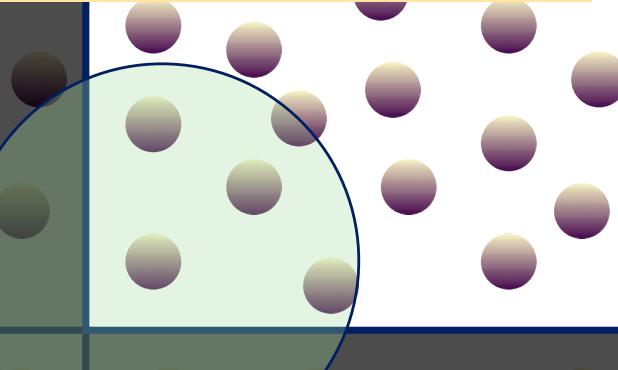


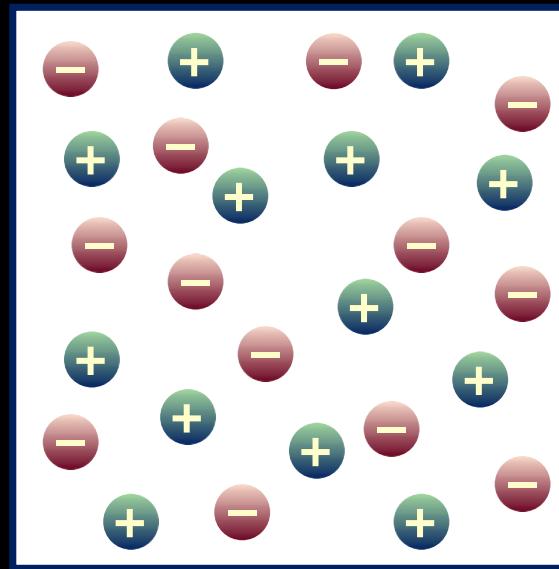
$$u_{\text{tail}} = \frac{\rho}{2} \int_{r_c}^{\infty} 4\pi r^2 u(r) dr$$

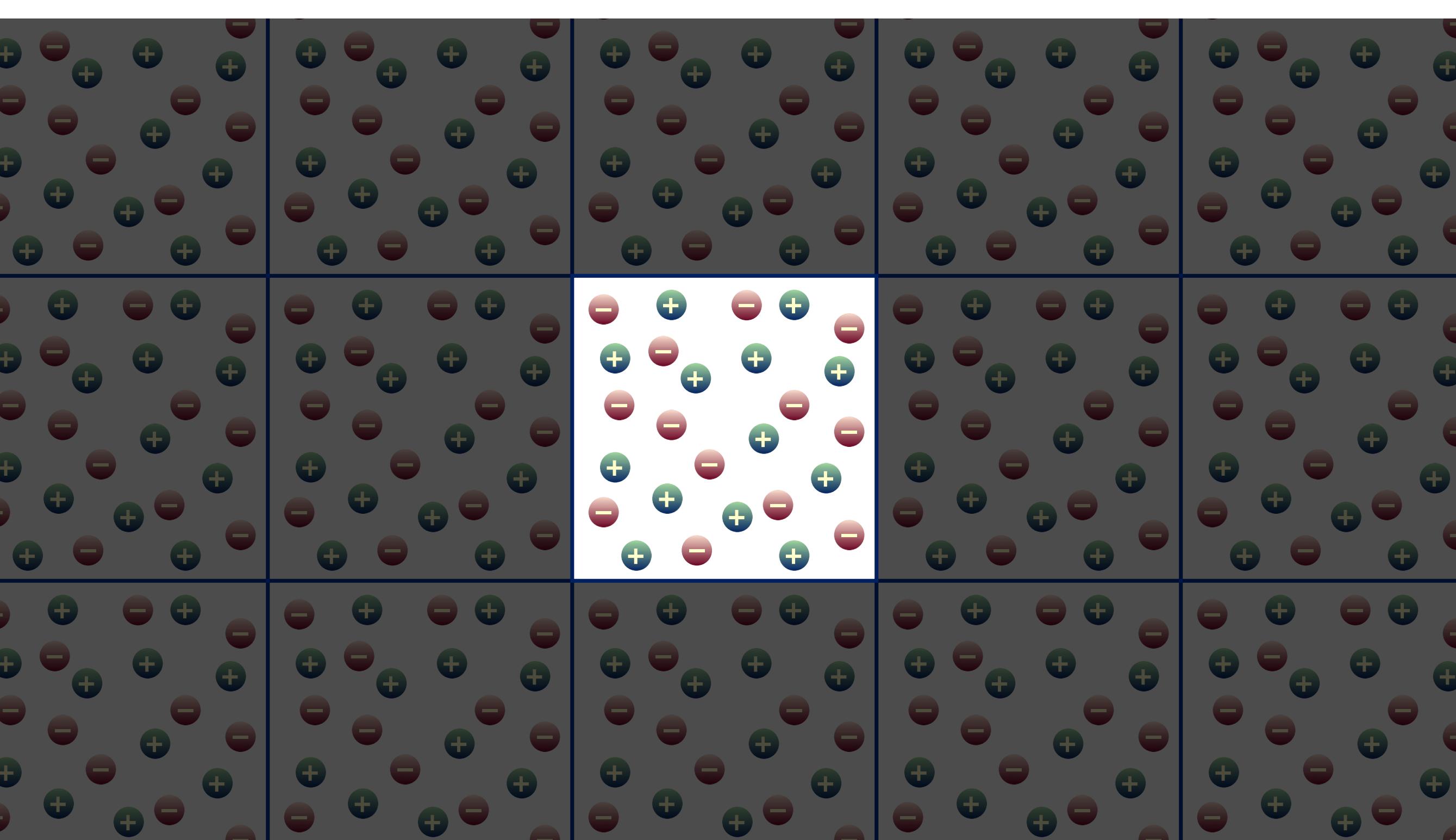


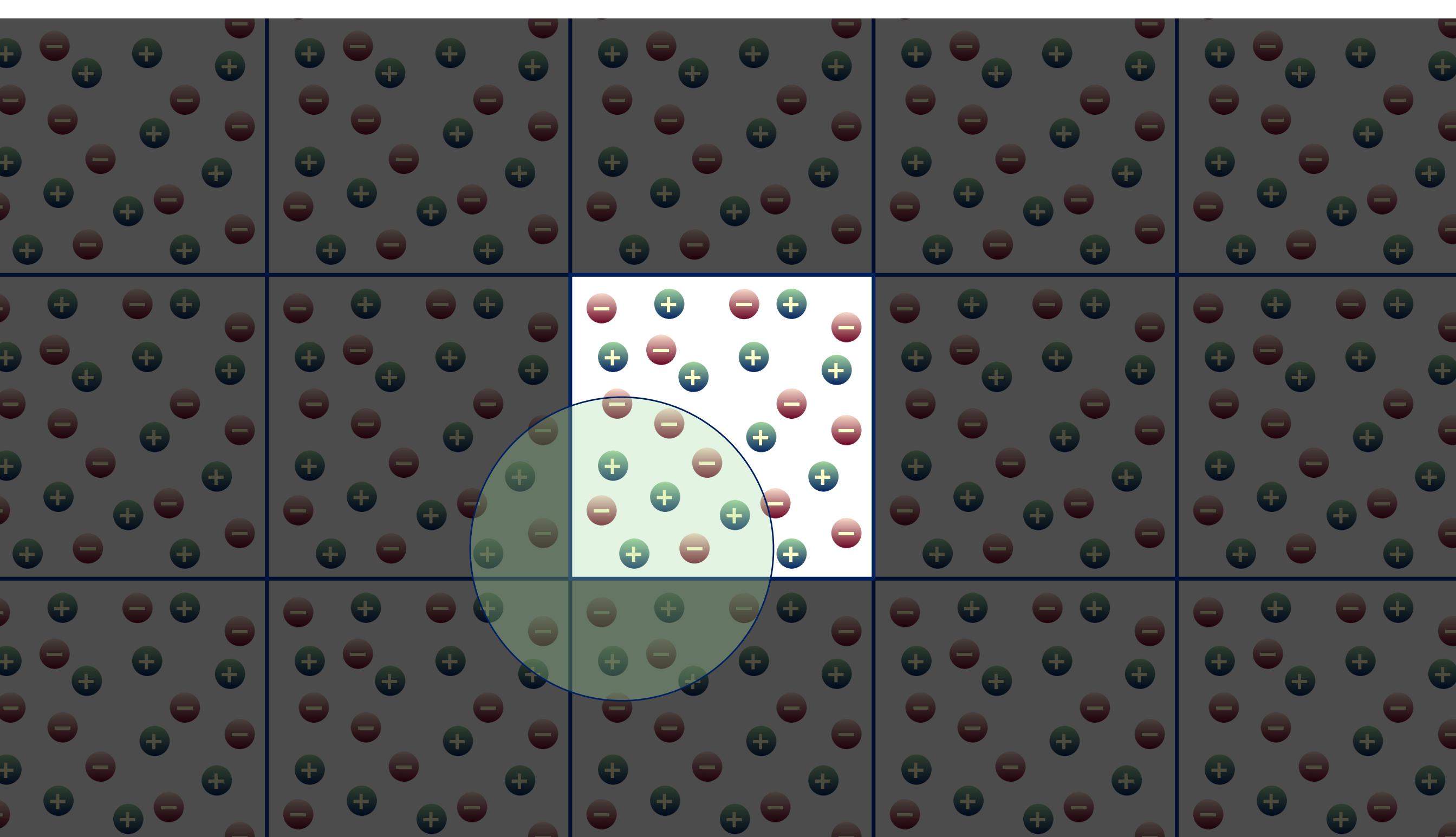
$$u_{\text{tail}}^{\text{LJ}} = \frac{8}{3} \pi \rho \epsilon \sigma^3 \left[\frac{1}{3} \left(\frac{\sigma}{r_c} \right)^9 - \left(\frac{\sigma}{r_c} \right)^3 \right]$$

$$u_{\text{tail}} = \frac{\rho}{2} \int_{r_c}^{\infty} 4\pi r^2 u(r) dr$$

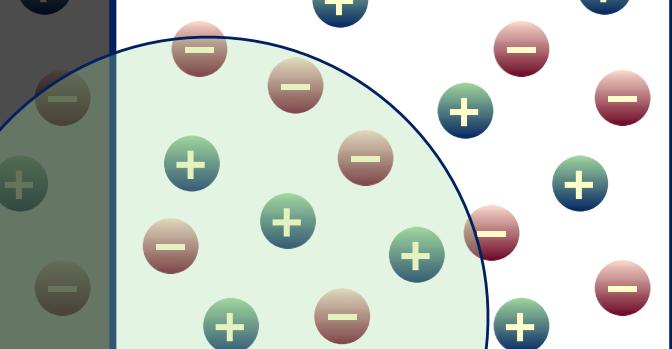








$$u_{\text{tail}} = \frac{\rho}{2} \int_{r_c}^{+\infty} 4\pi r^2 \frac{qq'}{4\pi\epsilon r} dr = \frac{\rho qq'}{2\epsilon} \int_{r_c}^{+\infty} r dr = \infty$$



$$u_{\text{tail}} = \frac{\rho}{2} \int_{r_c}^{+\infty} 4\pi r^2 \frac{qq'}{4\pi\epsilon r} dr = \frac{\rho qq'}{2\epsilon} \int_{r_c}^{+\infty} r dr = \infty$$

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

No cutoff allowed for long-range electrostatic potentials!

Ewald Summation

Ewald Summation

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

Ewald Summation

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

$$\rho(r) = \sum_i q_i \delta(\mathbf{r} - \mathbf{r}_i) = \underbrace{\sum_i q_i \left(\frac{\alpha}{\pi} \right)^{\frac{3}{2}} e^{-\alpha |\mathbf{r} - \mathbf{r}_i|^2}}_{\rho_{\text{short-range}}(\mathbf{r})} + \underbrace{\sum_i q_i \left[\delta(\mathbf{r} - \mathbf{r}_i) - \left(\frac{\alpha}{\pi} \right)^{\frac{3}{2}} e^{-\alpha |\mathbf{r} - \mathbf{r}_i|^2} \right]}_{\rho_{\text{long-range}}(\mathbf{r})}$$

Ewald Summation

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

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$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \left[\frac{1}{2} \sum_{i \neq j} \frac{q_i q_j \text{erfc}(|\mathbf{r}_{ij} \sqrt{\alpha}|)}{|\mathbf{r}_{ij}|} + \frac{1}{2V} \sum_{\mathbf{k} \neq \mathbf{0}} \frac{4\pi |\rho(\mathbf{k})|^2}{|\mathbf{k}|^2} e^{-|\mathbf{k}|^2/4\alpha} - \sqrt{\frac{\alpha}{\pi}} \sum_i q_i^2 \right]$$

Ewald Summation

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

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Gaussian cloud
(Short-range)

Ewald Summation

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

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Gaussian cloud
(Short-range)

Fourier Space
(Long-range)

$$\rho(\mathbf{k}) = \sum_i q_i e^{-i\mathbf{k} \cdot \mathbf{r}_i}$$

$$\mathbf{k} = \left(\frac{2\pi n_x}{L_x}, \frac{2\pi n_y}{L_y}, \frac{2\pi n_z}{L_z} \right)$$

Ewald Summation

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum'_{i,j} \sum_{\mathbf{k} \in \mathbb{Z}^3} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j + k_x L_x \mathbf{e}_x + k_y L_y \mathbf{e}_y + k_z L_z \mathbf{e}_z|}$$

$$\rho(r) = \sum_i q_i \delta(\mathbf{r} - \mathbf{r}_i) = \underbrace{\sum_i q_i \left(\frac{\alpha}{\pi} \right)^{\frac{3}{2}} e^{-\alpha|\mathbf{r} - \mathbf{r}_i|^2}}_{\rho_{\text{short-range}}(\mathbf{r})} + \underbrace{\sum_i q_i \left[\delta(\mathbf{r} - \mathbf{r}_i) - \left(\frac{\alpha}{\pi} \right)^{\frac{3}{2}} e^{-\alpha|\mathbf{r} - \mathbf{r}_i|^2} \right]}_{\rho_{\text{long-range}}(\mathbf{r})}$$

$$U_{\text{elect}} = \frac{1}{4\pi\epsilon_0\epsilon_r} \left[\frac{1}{2} \sum_{i \neq j} \frac{q_i q_j \operatorname{erfc}(|\mathbf{r}_{ij} \sqrt{\alpha}|)}{|\mathbf{r}_{ij}|} + \frac{1}{2V} \sum_{\mathbf{k} \neq 0} \frac{4\pi |\rho(\mathbf{k})|^2}{|\mathbf{k}|^2} e^{-|\mathbf{k}|^2/4\alpha} - \sqrt{\frac{\alpha}{\pi}} \sum_i q_i^2 \right]$$

Gaussian cloud
(Short-range)

Fourier Space
(Long-range)

**Self Interaction
Correction**

$$\rho(\mathbf{k}) = \sum_i q_i e^{-i\mathbf{k} \cdot \mathbf{r}_i}$$

$$\mathbf{k} = \left(\frac{2\pi n_x}{L_x}, \frac{2\pi n_y}{L_y}, \frac{2\pi n_z}{L_z} \right)$$

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary  p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
mass 1 15.9994
mass 2 1.008
pair_style lj/cut/coul/long 10.0
pair_coeff 1 1 0.1553 3.166 #0-0 interaction - epsilon (kcal/mol), sigma (Angstroms), ljcutoff (optional)
pair_coeff 2 2 0.0 1.0
pair_coeff 1 2 0.0 1.0
bond_style harmonic #Only needed for energy minimization, otherwise zero.
bond_coeff 1 500 1.00
angle_style harmonic #Only needed for energy minimization, otherwise zero.
angle_coeff 1 100 109.47
molecule water spce.mol
create_atoms 0 random 400 34564 NULL mol water 25367 overlap 2.0 # Randomly insert 400 molecules into the box.
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.
thermo 100 # Output frequency.
thermo_style custom step temp pe ke etotal press
log spc_minimization.log
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
neighbor 3.0 bin # Thickness of the neighbor shell
neigh_modify delay 0 every 1 check yes
fix     fixwater all shake 0.0001 100 0 b 1 a 1 # Freeze bonds & angles
timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

A Simple LAMMPS Script to Simulate Water SPC/E Model

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timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary   p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
mass 1 15.9994
mass 2 1.008
pair_style lj/cut/coul/long 10.0
pair_coeff 1 1 0.1553 3.166 #0-0 interaction - epsilon (kcal/mol), sigma (Angstroms), ljcutoff (optional)
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bond_style harmonic #Only needed for energy minimization, otherwise zero.
bond_coeff 1 500 1.00
angle_style harmonic #Only needed for energy minimization, otherwise zero.
angle_coeff 1 100 109.47
molecule water spce.mol
create_atoms 0 random 400 34564 NULL mol water 25367 overlap 2.0 # Randomly insert 400 molecules into the box.
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.
thermo 100 # Output frequency.
thermo_style custom step temp pe ke etotal press
log spc_minimization.log
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
neighbor 3.0 bin # Thickness of the neighbor shell
neigh_modify delay 0 every 1 check yes
fix     fixwater all shake 0.0001 100 0 b 1 a 1 # Freeze bonds & angles
timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

Randomly insert a given number of molecules into the box

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension   3
boundary   p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
mass 1 15.9994
mass 2 1.008
pair_style lj/cut/coul/long 10.0
pair_coeff 1 1 0.1553 3.166 #0-0 interaction - epsilon (kcal/mol), sigma (Angstroms), ljcutoff (optional)
pair_coeff 2 2 0.0 1.0
pair_coeff 1 2 0.0 1.0
bond_style harmonic #Only needed for energy minimization, otherwise zero.
bond_coeff 1 500 1.00
angle_style harmonic #Only needed for energy minimization, otherwise zero.
angle_coeff 1 100 109.47
molecule water spce.mol
create_atoms 0 random 400 34564 NULL mol water 25367 overlap 2.0 # Randomly insert 400 molecules into the box.
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.
thermo 100 # Output frequency.
thermo_style custom step temp pe ke etotal press
log spc_minimization.log
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
neighbor 3.0 bin # Thickness of the neighbor shell
neigh_modify delay 0 every 1 check yes
fix     fixwater all shake 0.0001 100 0 b 1 a 1 # Freeze bonds & angles
timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

Water molecule. SPC/E geometry

3 atoms
2 bonds
1 angles

Coords

1	0.00000	-0.06461	0.00000
2	0.81649	0.51275	0.00000
3	-0.81649	0.51275	0.00000

Types

1	1	# O
2	2	# H
3	2	# H

Molecules into the box

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary  p p p # Periodic box.
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mass 1 15.9994
mass 2 1.008
pair_style lj/cut/coul/long 10.0
pair_coeff 1 1 0.1553 3.166 #0-0 interaction - epsilon (kcal/mol), sigma (Angstroms), ljcutoff (optional)
pair_coeff 2 2 0.0 1.0
pair_coeff 1 2 0.0 1.0
bond_style harmonic #Only needed for energy minimization, otherwise zero.
bond_coeff 1 500 1.00
angle_style harmonic #Only needed for energy minimization, otherwise zero.
angle_coeff 1 100 109.47
molecule water spce.mol
create_atoms 0 random 400 34564 NULL mol water 25367 overlap 2.0 # Randomly insert 400 molecules into the box.
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.
thermo 100 # Output frequency.
thermo_style custom step temp pe ke etotal press
log spc_minimization.log
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
neighbor 3.0 bin # Thickness of the neighbor shell
neigh_modify delay 0 every 1 check yes
fix     fixwater all shake 0.0001 100 0 b 1 a 1 # Freeze bonds & angles
timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary  p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
mass 1 15.9994
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angle_coeff 1 100 109.47
molecule water spce.mol
create_atoms 0 random 400 34564 NULL mol water 25367 overlap 2.0 # Randomly insert 400 molecules into the box.
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.
thermo 100 # Output frequency.
thermo_style custom step temp pe ke etotal press
log spc_minimization.log
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
neighbor 3.0 bin # Thickness of the neighbor shell
neigh_modify delay 0 every 1 check yes
fix     fixwater all shake 0.0001 100 0 b 1 a 1 # Freeze bonds & angles
timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

Kspace solver

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary  p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
mass 1 15.9994
mass 2 1.008
pair_style lj/cut/coul/long 10.0
pair_coeff 1 1 0.1553 3.166 #0-0 interaction - epsilon (kcal/mol), sigma (Angstroms), ljcutoff (optional)
pair_coeff 2 2 0.0 1.0
pair_coeff 1 2 0.0 1.0
bond_style harmonic #Only needed for energy minimization, otherwise zero.
bond_coeff 1 500 1.00
angle_style harmonic #Only needed for energy minimization, otherwise zero.
angle_coeff 1 100 109.47
molecule water spce.mol
create_atoms 0 random 400 34564 NULL mol water 25367 overlap 2.0 # Randomly insert 400 molecules into the box.
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.
thermo 100 # Output frequency.
thermo_style custom step temp pe ke etotal press
log spc_minimization.log
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
neighbor 3.0 bin # Thickness of the neighbor shell
neigh_modify delay 0 every 1 check yes
fix     fixwater all shake 0.0001 100 0 b 1 a 1 # Freeze bonds & angles
timestep 1.0 # dt needs to be small for equilibration.
thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary   p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
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unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

Generally applied in complex systems to remove overlaps

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
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create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
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log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
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fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

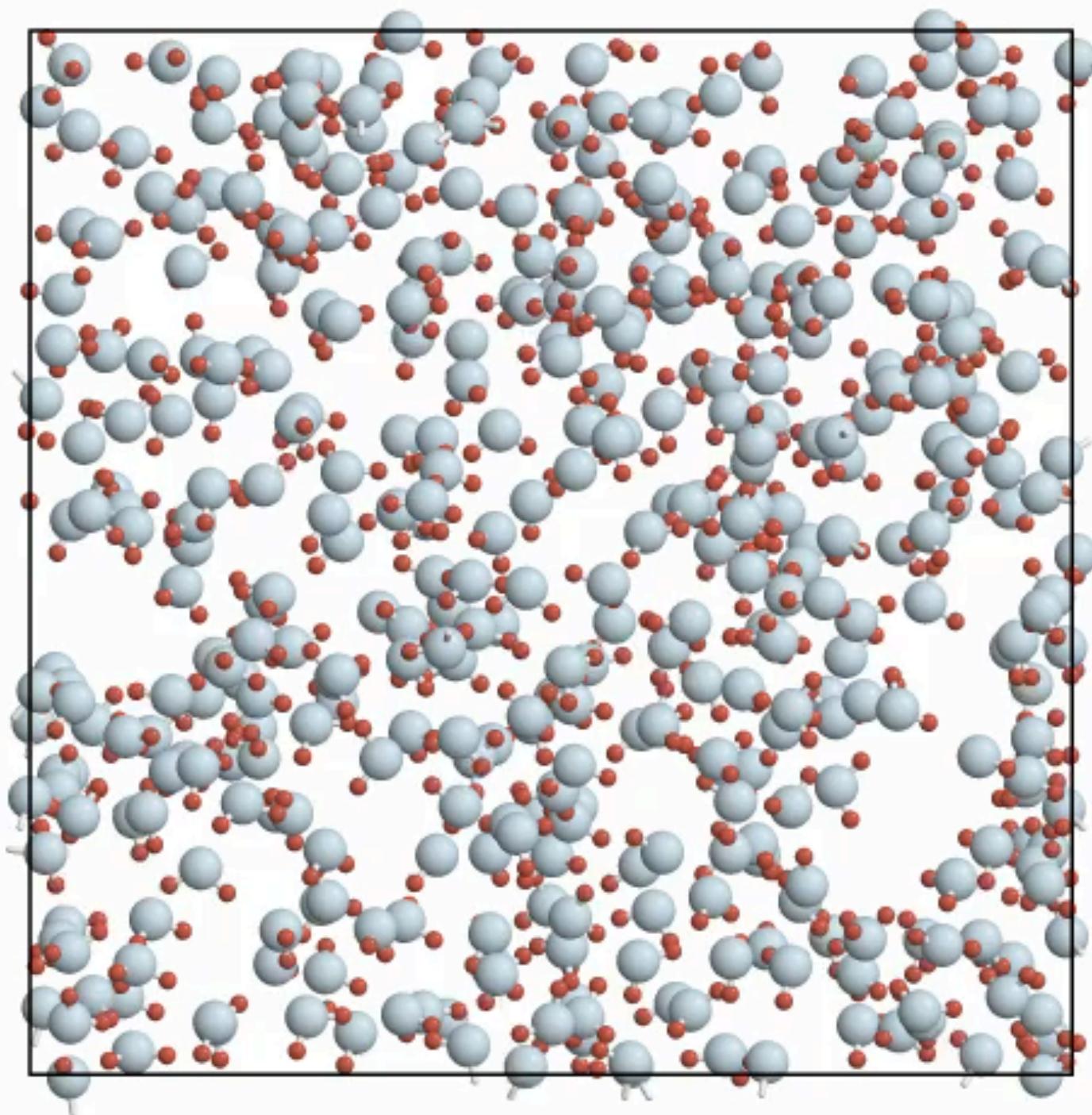
A Simple LAMMPS Script to Simulate Water SPC/E Model

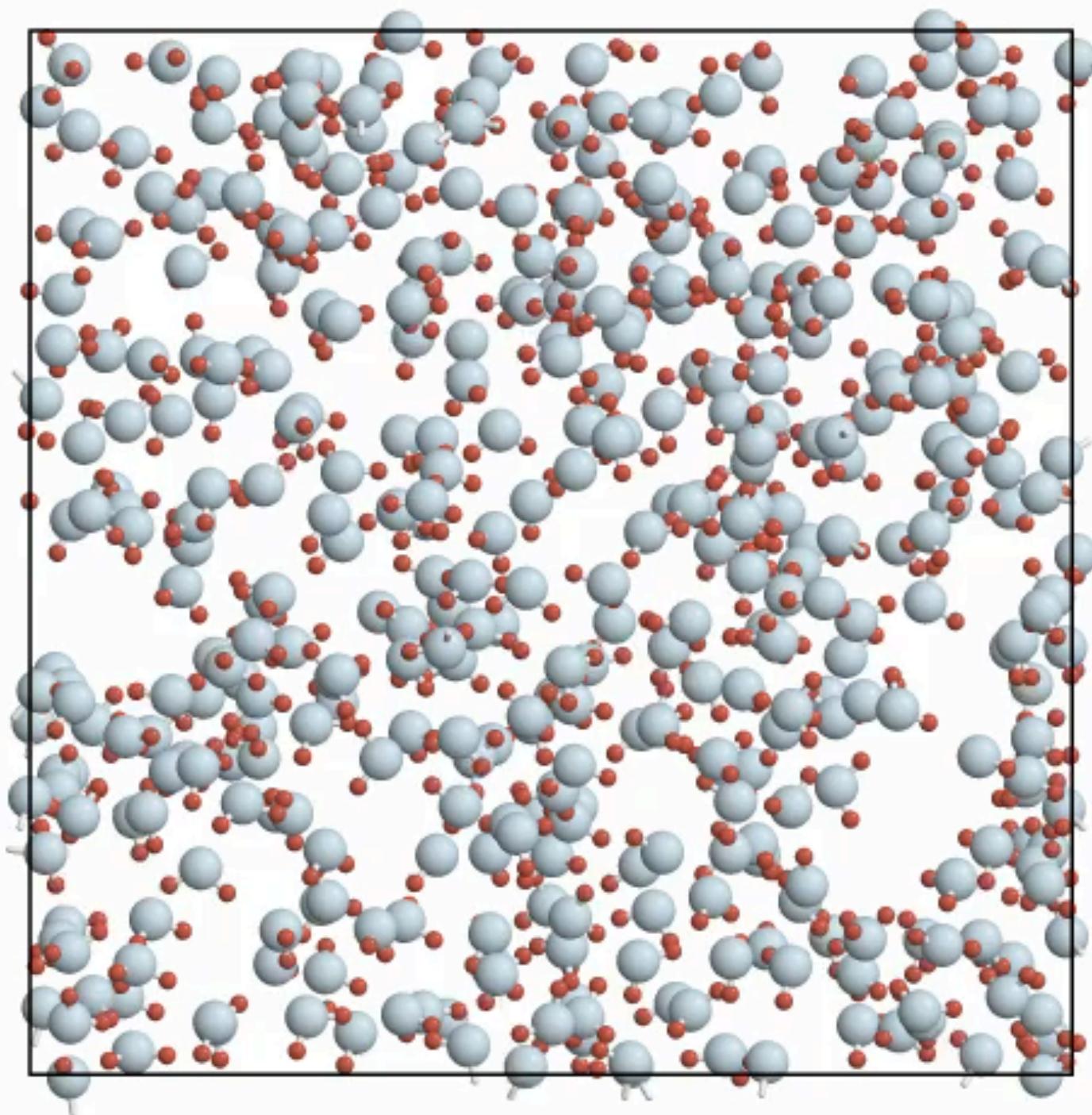
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units      real    # Real units
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boundary   p p p # Periodic box.
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thermo_style custom step temp press density etotal
log     spc_equilibration.log
fix     ensFix all nvt temp 298.0 298.0 100.0 # NVT equilibration
run     50000 #run simulation
unfix   ensFix
fix     ensFix all npt temp 298.0 298.0 100.0 iso 1.0 1.0 1000.0 # NPT equilibration
run     100000
write_data spce-equil.dat
```

Shake freezes bonds & angles

A Simple LAMMPS Script to Simulate Water SPC/E Model

```
units      real    # Real units
atom_style full    # Full atomic features (type,parent,charge,position)
dimension 3
boundary  p p p # Periodic box.
region box block 0 30 0 30 0 30 # Region to introduce molecules
create_box 2 box bond/types 1 angle/types 1 extra/bond/per/atom 2 extra/angle/per/atom 1 extra/special/per/atom 2
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run     100000
write_data spce-equil.dat
```





A Few Adventures with Water

Q1: Why is energy minimization necessary?

A Few Adventures with Water

Q1: Why is energy minimization necessary?

Step 1: Start an interactive job with one core, and copy the script `in.spce-faulty` from the following folder to your folder of interest:

```
/ocean/projects/see220002p/shared/LAMMPS/Water-Bulk/in.spce-faulty
```

A Few Adventures with Water

Q1: Why is energy minimization necessary?

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```
/ocean/projects/see220002p/shared/LAMMPS/Water-Bulk/in.spce-faulty
```

Step 2: Open the script **in.spce-faulty** and comment out the following line:

```
create_atoms 0 random 800 34564 NULL mol water 25367 overlap 1.0 # Randomly insert 400 molecules into the box.  
kspace_style pppm 1.0e-4 # PPPM solver for long-range interactions.  
thermo 100 # Output frequency.  
thermo_style custom step temp pe ke etotal press  
log spc_minimization.log  
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
```

A Few Adventures with Water

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log spc_minimization.log  
minimize 1.0e-4 1.0e-6 1000 10000 # Minimize energy (to remove overlaps).
```

Step 3: Run the script with LAMMPS.

```
/ocean/projects/see220002p/shared/LAMMPS/bin/lmp_mpi -in in.spce-faulty
```

A Few Adventures with Water

Q1: Why is energy minimization necessary?

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```
/ocean/projects/see220002p/shared/LAMMPS/bin/lmp_mpi -in in.spce-faulty
```

What happens? Why?

A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?

A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?

Group ID	Water Model
1	SPC/E
2	TIP3P
3	TIP4P
4	TIP4P/2005

A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?

Step 1: Copy your groups input, analysis script and batch file to the appropriate folder?

Group ID	Water Model
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4	TIP4P/2005

A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?

Step 1: Copy your groups input, analysis script and batch file to the appropriate folder?

```
cp /ocean/projects/see22002p/shared/LAMMPS/Water-Bulk/in.${FF}-prod .
cp /ocean/projects/see22002p/shared/LAMMPS/Water-Bulk/${FF}-equil-T298-P1.dat .
cp /ocean/projects/see22002p/shared/LAMMPS/Water-Bulk/analysis.cmd .
```

Group ID	Water Model
1	SPC/E
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A Few Adventures with Bulk Water

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```

Step 2: Launch the submission script.

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A Few Adventures with Bulk Water

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```
cp /ocean/projects/see22002p/shared/LAMMPS/Water-Bulk/in.${FF}-prod .
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cp /ocean/projects/see22002p/shared/LAMMPS/Water-Bulk/analysis.cmd .
```

Step 2: Launch the submission script.

```
sbatch analysis.cmd ${FF} 298 1 50000
```

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1	SPC/E
2	TIP3P
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A Few Adventures with Bulk Water

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cp /ocean/projects/see22002p/shared/LAMMPS/Water-Bulk/analysis.cmd .
```

Step 2: Launch the submission script.

```
sbatch analysis.cmd ${FF} 298 1 50000
```

Step 3: Plot the OO RDF in the \${FF}.rdf file. Identify the height of the first peak and the loci of the first two valleys.

Group ID	Water Model
1	SPC/E
2	TIP3P
3	TIP4P
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A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?

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sbatch analysis.cmd ${FF} 298 1 50000
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Step 3: Plot the OO RDF in the \${FF}.rdf file. Identify the height of the first peak and the loci of the first two valleys.

Step 4: Estimate average density from the last line of the \${FF}.thermo.txt file.

Group ID	Water Model
1	SPC/E
2	TIP3P
3	TIP4P
4	TIP4P/2005

A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?

Step 1: Copy your groups input, analysis script and batch file to the appropriate folder?

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```
sbatch analysis.cmd ${FF} 298 1 50000
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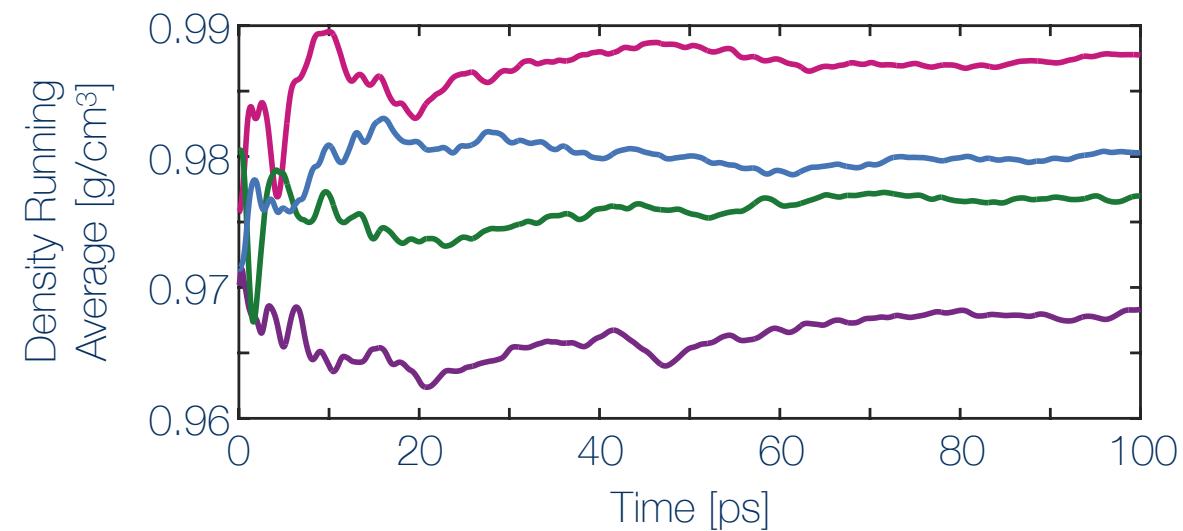
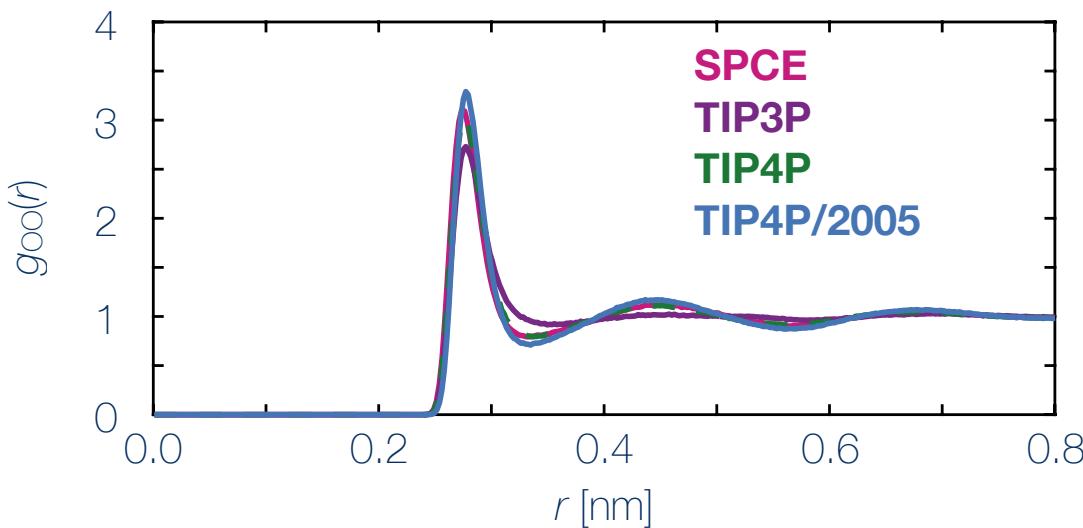
Step 4: Estimate average density from the last line of the \${FF}.thermo.txt file.

Step 5: Plot the running averages to assess how reliable your estimates are.

Group ID	Water Model
1	SPC/E
2	TIP3P
3	TIP4P
4	TIP4P/2005

A Few Adventures with Bulk Water

Q2: How to compute properties of bulk water for different models?



Group ID	Water Model	Mean Density (g/cm ³)	1st RDF Valley (nm)	2nd RDF Valley (nm)	Height of the First Peak
1	SPC/E	0.9877	3.30	5.6	3.1
2	TIP3P	0.9683	3.55	5.8	2.7
3	TIP4P	0.9769	3.35	5.7	3.0
4	TIP4P/2005	0.9802	3.35	5.7	3.3

A Few Adventures with Bulk Water

Q4: Analyze angular distribution of water dipoles

A Few Adventures with Bulk Water

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Step 1: Use the `.dipole.out` file to extract molecular dipoles into X.

A Few Adventures with Bulk Water

Q4: Analyze angular distribution of water dipoles

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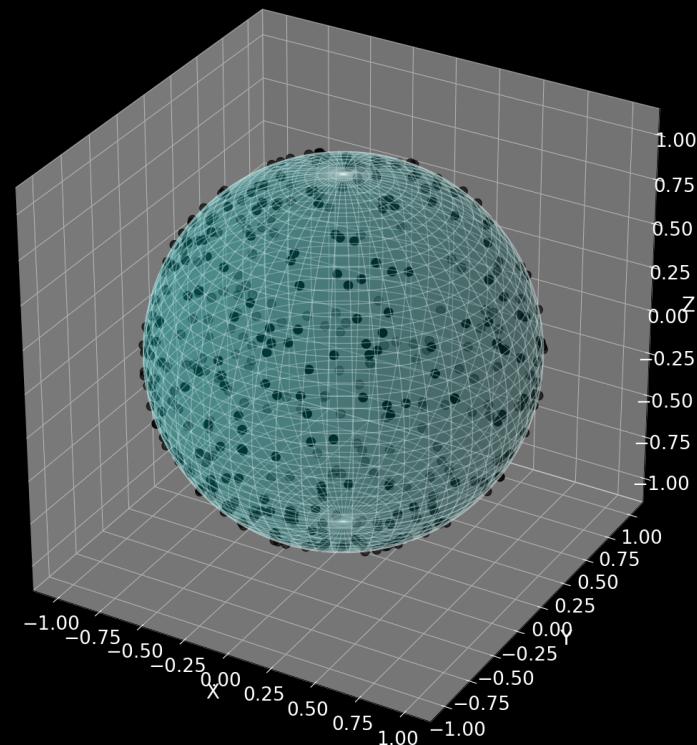
Step 2: Create an angular distribution of those dipoles and plot them.

A Few Adventures with Bulk Water

Q4: Analyze angular distribution of water dipoles

Step 1: Use the `.dipole.out` file to extract molecular dipoles into X.

Step 2: Create an angular distribution of those dipoles and plot them.

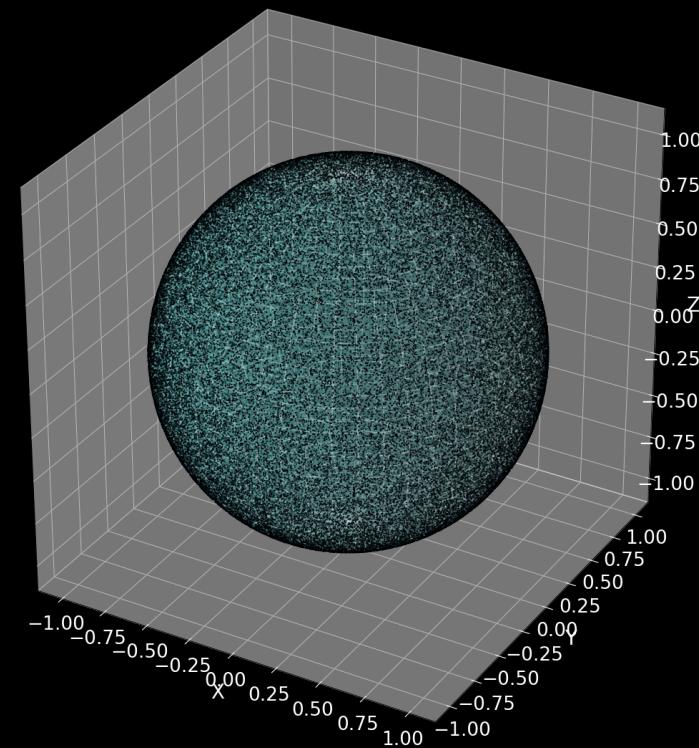
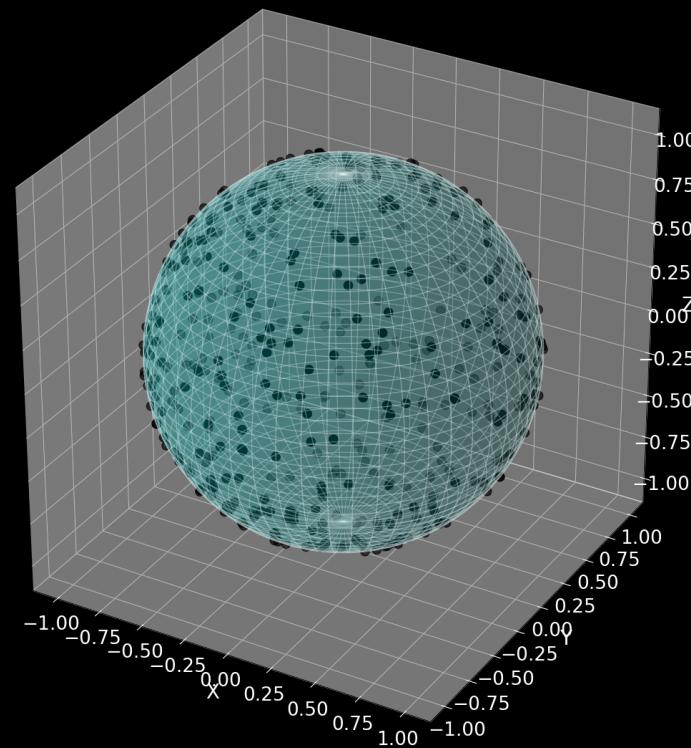


A Few Adventures with Bulk Water

Q4: Analyze angular distribution of water dipoles

Step 1: Use the `.dipole.out` file to extract molecular dipoles into X.

Step 2: Create an angular distribution of those dipoles and plot them.



Your Nighttime Adventure

Use the LAMMPS scripts and input configurations in the Water-Bulk folder to launch simulations aimed at computing your group's model's C_p (heat capacity) at 298 K and 1 bar.