

MateriApps LIVE! Hands-on LAMMPS tutorial

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Outline

- About LAMMPS
 - Force Fields
- LAMMPS examples
 - Execution of melt, micelle, colloid
 - Visualization by VMD
 - Change from 2D to 3D for micelle
 - Increasing the number of atoms

About LAMMPS

Large-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator

<https://lammps.sandia.gov/>

- Download
<https://lammps.sandia.gov/download.html>
- Manual
<https://lammps.sandia.gov/doc/Manual.html>
- Error messages
<https://lammps.sandia.gov/doc/Errors.html>

Please read the documents carefully.

Force Fields



- LAMMPS Force Fields
https://lammps.sandia.gov/doc/99/force_fields.html
- Database
Interatomic Potentials Repository Project
<https://www.ctcms.nist.gov/potentials/>
ex) Al-Ni: <https://www.ctcms.nist.gov/potentials/Al-Ni.html>

LAMMPS examples

- LAMMPS examples

MateriApps LIVE!: `/usr/share/lammps/examples`

- About examples

<https://lammps.sandia.gov/doc/Examples.html>

- 2D

- **colloid**, crack, flow, friction,
micelle, nemd, obstacle, shear

For polymer

- 3D

- **melt**, peptide

- Force Fields

- dreiding, kim, reax

- Speeding up

- cuda, gpu, intel

例	説明
melt	rapid melt of 3d LJ system
micelle	self-assembly of small lipid-like molecules into 2d bilayers
colloid	big colloid particles in a small particle solvent, 2d system
peptide	dynamics of a small solvated peptide chain (5-mer)

examples/melt(1)

Commands

https://lammps.sandia.gov/doc/commands_list.html

Content of in.melt

```
# 3d Lennard-Jones melt

units          lj
atom_style     atomic

lattice        fcc 0.8442
region         box block 0 10 0 10 0 10
create_box     1 box
create_atoms   1 box
mass           1 1.0

velocity       all create 3.0 87287

pair_style     lj/cut 2.5
pair_coeff    1 1 1.0 1.0 2.5

neighbor       0.3 bin
neigh_modify   every 20 delay 0 check no

fix            1 all nve
```

examples/melt(2)

```
#dump           id all atom 50 dump.melt  
  
#dump      2 all image 25 image.*.jpg type type &  
#       axes yes 0.8 0.02 view 60 -30  
#dump_modify 2 pad 3  
  
#dump      3 all movie 25 movie.mpg type type &  
#       axes yes 0.8 0.02 view 60 -30  
#dump_modify 3 pad 3  
  
thermo      50  
run        250
```

Ready to run

- Make directory (ex: \$HOME/lammps)

```
$ cd $HOME
```

```
$ mkdir lammps
```

- Change the directory (\$HOME/lammps)

```
$ cd lammps
```

- Copy the example files(melt, micelle, colloid)

```
$ cp -r /usr/share/lammps/examples/melt ./
```

```
$ cp -r /usr/share/lammps/examples/micelle ./
```

```
$ cp -r /usr/share/lammps/examples/colloid/ ./
```

Running of melt(1)

- Change the directory

```
$ cd melt
```

- See the directory contents

```
$ ls
```

```
in.melt  log.27Nov18.melt.g++.1  log.27Nov18.melt.g++.4
```

- Run in.melt

```
$ lammmps < in.melt
```

```
LAMMPS (4 Feb 2020)
```

```
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread.
```

```
(../comm.cpp:90)
```

```
using 1 OpenMP thread(s) per MPI task
```

```
...
```

```
Total # of neighbors = 151513
```

```
Ave neights/atom = 37.8783
```

```
Neighbor list builds = 12
```

```
Dangerous builds not checked
```

```
Total wall time: 0:00:00
```

If "Total wall time" is displayed without error message, normal execution

- A log file log.lammps is generated

Running of melt(2)

- Job running 4 processes

```
$ mpirun -oversubscribe -n 4 lammps < in.melt
```

LAMMPS (4 Feb 2020)

...

1 by 2 by 2 MPI processor grid

...

Performance: 90089.282 tau/day, 208.540 timesteps/s

22.1% CPU use with 4 MPI tasks x 1 OpenMP threads

...

If you have more than 3 cores in your machine

Running of melt(3)



- Job running 4 threads

\$ OMP_NUM_THREADS=4 lammps < in.melt

LAMMPS (4 Feb 2020)

using **4** OpenMP thread(s) per MPI task

...

Performance: 115561.777 tau/day, 267.504 timesteps/s

97.6% CPU use with 1 MPI tasks x **4** OpenMP threads

...

If you have more than 3 cores in your machine

Running of micelle and colloid



- micelle : self-assembly of small lipid-like molecules into 2d bilayers
Change the directory
\$ cd \$HOME/lammps/micelle
\$ lammps < in.micelle

(注) Running by ver. 4 Feb 2020

WARNING: Communication cutoff 1.42246 is shorter than a bond length based estimate of 1.425. This may lead to errors. (./comm.cpp:686)

You should ignore this warning for this tutorial.

(This warning does not appear for the execution by ver. 29 Mar 2020.)

- colloid : big colloid particles in a small particle solvent, 2d system
Change the directory
\$ cd \$HOME/lammps/colloid
\$ lammps < in.colloid

Visualization by VMD(1)

- Change the directory (\$HOME/lammpas/melt)
\$ cd \$HOME/lammps/melt
- Rewrite in.melt by emacs
\$ emacs in.melt &

Visualization by VMD(2)

- Open emacs

emacs@malive.local

File Edit Options Buffers Tools Help ?

3d Lennard-Jones melt

```

units      lj
atom_style atomic

lattice    fcc 0.8442
region     box block 0 10 0 10 0 10
create_box 1 box
create_atoms 1 box
mass       1 1.0

velocity   all create 3.0 87287

pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5

neighbor   0.3 bin

```

in.melt Top L1 (Fundamental)-----

Welcome to GNU Emacs, one component of the GNU/Linux operating system.

[Emacs Tutorial](#) Learn basic keystroke commands
[Emacs Guided Tour](#) Overview of Emacs features at gnu.org
[View Emacs Manual](#) View the Emacs manual using Info
[Absence of Warranty](#) GNU Emacs comes with ABSOLUTELY NO WARRANTY
[Copying Conditions](#) Conditions for redistributing and changing Emacs
[Ordering Manuals](#) Purchasing printed copies of manuals
To quit a partially entered command, type Control-g.

This is GNU Emacs 23.4.1 (i486-pc-linux-gnu, GTK+ Version 2.24.10) of 2012-09-10 on murphy, modified by Debian Copyright (C) 2012 Free Software Foundation, Inc.

Dismiss this startup screen Never show it again.

-U:%%- *GNU Emacs* All L3 (Fundamental)-----

For information about GNU Emacs and the GNU system, type C-h C-a.

Welcome to GNU Emacs, one component of the GNU/Linux operating system.

Emacs Tutorial Learn basic keystroke commands
Emacs Guided Tour Overview of Emacs features at gnu.org
View Emacs Manual View the Emacs manual using Info
Absence of Warranty GNU Emacs comes with ABSOLUTELY NO WARRANTY
Copying Conditions Conditions for redistributing and changing Emacs
Ordering Manuals Purchasing printed copies of manuals
To quit a partially entered command, type Control-g.

This is GNU Emacs 23.4.1 (i486-pc-linux-gnu, GTK+ Version 2.24.10) of 2012-09-10 on murphy, modified by Debian Copyright (C) 2012 Free Software Foundation, Inc.

Dismiss this startup screen Never show it again.

② Click this (blue letters) ① Check the box

emacs@malive.local

File Edit Options Buffers Tools Help ?

3d Lennard-Jones melt

```

units      lj
atom_style atomic

lattice    fcc 0.8442
region     box block 0 10 0 10 0 10
create_box 1 box
create_atoms 1 box
mass       1 1.0

velocity   all create 3.0 87287

pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5

neighbor   0.3 bin
neigh_modify every 20 delay 0 check no

fix        1 all nve

#dump      id all atom 50 dump.melt

#dump      2 all image 25 image.*.jpg type type &
#           axes yes 0.8 0.02 view 60 -30
#           pad 3

#dump      3 all movie 25 movie.mpg type type &
#           axes yes 0.8 0.02 view 60 -30
#           pad 3

thermo    50
run       250

```

in.melt All L1 (Fundamental)-----

Wrote /home/user/.emacs

Visualization by VMD(3)

Rewrite in.melt

```
# 3d Lennard-Jones melt

units          lj
atom_style     atomic

lattice        fcc 0.8442
region         box block 0 10 0 10 0 10
create_box     1 box
create_atoms   1 box
mass           1 1.0

velocity       all create 3.0 87287

pair_style     lj/cut 2.5
pair_coeff    1 1 1.0 1.0 2.5

neighbor       0.3 bin
neigh_modify   every 5 delay 0 check no
fix            1 all nve

dump          id all atom 5 dump.melt
...

```

Change from 20 to 5

Remove #, and change from
50 to 5

Visualization by VMD(4)

- Run modified in.melt

```
$ lammps < in.melt
```

If "Total wall time" is displayed without
error message,
normal execution

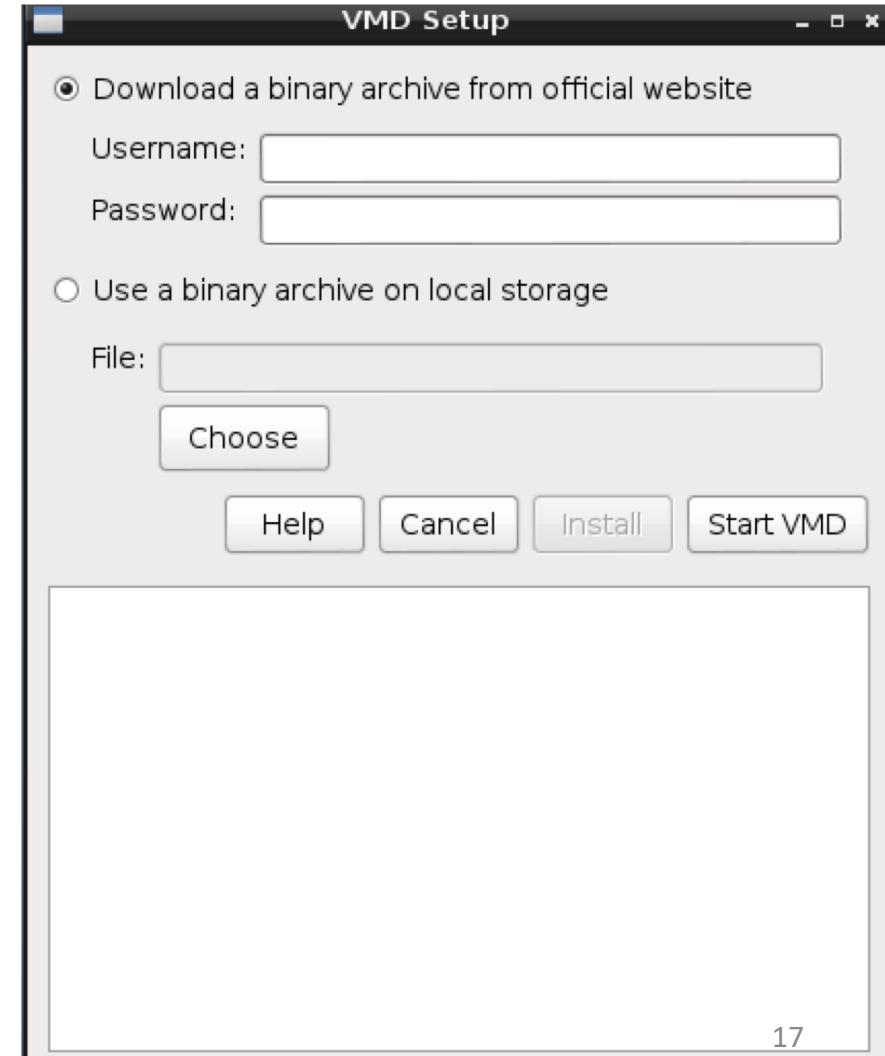
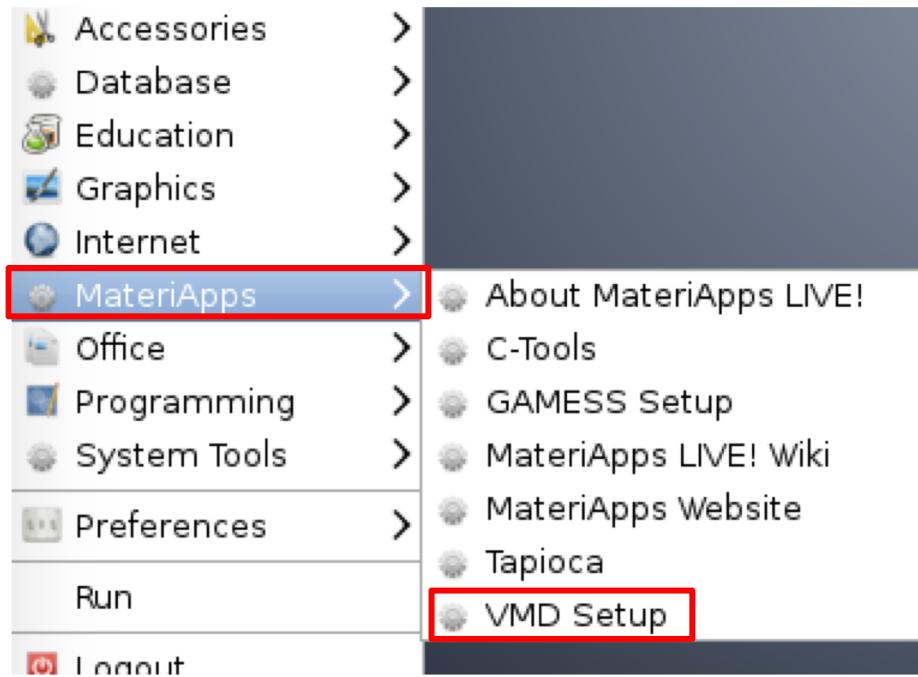
- Check creating dump.melt

```
$ ls
```

dump.melt in.melt.org in.melt log.lammps

Visualization by VMD(5)

- Open VMD
Select “VMD Setup” of “MateriApps”



Visualization by VMD (6)

- Create your account
(If you have your account, you don't need to create it.)

- Visit VMD web site

Download VMD - Theoretical and Computational Biophysics Group

<https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD>

NIH CENTER FOR MACROMOLECULAR MODELING & BIOINFORMATICS | UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Type Keywords

SEARCH

THEORETICAL *and* COMPUTATIONAL BIOPHYSICS GROUP



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Software Downloads

Download VMD:

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. Visit the [VMD website](#) for complete information and documentation.

Selecting an archive below will lead to a user registration and login page. Your download will continue after you have registered or logged in.

Version 1.9.4 LATEST ALPHA (2017-12-21) Platforms:

Click

Latest pre-release ALPHA test version

- [LINUX_64 OpenGL, CUDA, OptiX, OSPRay](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86_64 SSE, with CUDA 9.x, OptiX, OSPRay)
- [MacOS X OpenGL \(32-bit Intel x86\)](#) (Apple Mac OS-X (10.10.x or later) with hardware OpenGL (native bundle))

Visualization by VMD(7)

- Input username and password
(You create new username and password)

If you have a username and password, you don't need to create new ones.

Registration/Login

You will need a username and password to download software.

If this is your first download, please choose a username and password to register.
Current NAMD or VMD users, please enter your existing username and password.

Username:

Password:

① Input Username and Password

Note: You can't use rist2018 because it already exists.

② Click the button

Your download will continue after you have registered or logged in.

Visualization by VMD(8)

- Registration

New User Registration

New User Registration for 'rist2018':

First and Last Name:

Kanako Yoshizawa

Email Address:

yoshizawa@rist.or.jp

Affiliation:

Academic Government Industrial Other (specify)

The number of people using TCBG software at my site is:

1 2-4 5-10 11-20 21 or more

I use TCBG software primarily for:

Research Teaching Commerce Personal

The work I do with TCBG software is funded (at least partially) by NIH:

Yes No

Re-enter password for confirmation:

Register

If you have a username and password, you don't need to create new ones.

① Input your information

② Click the button

Visualization by VMD (9)

- Agree

Software Downloads

Welcome! Account created for 'rist2018'.

Please remember your password for future downloads.

You may avoid logins for 6 months by saving a cookie on your browser:

If you have a username and password, you don't need to create new ones.

VMD 1.9.4 for Linux (RHEL 6.x) 64-bit x86_64 w/ SSE, CUD

To download this software you must agree to abide by the terms of the following license:

UNIVERSITY OF ILLINOIS
VISUAL MOLECULAR DYNAMICS SOFTWARE LICENSE AGREEMENT

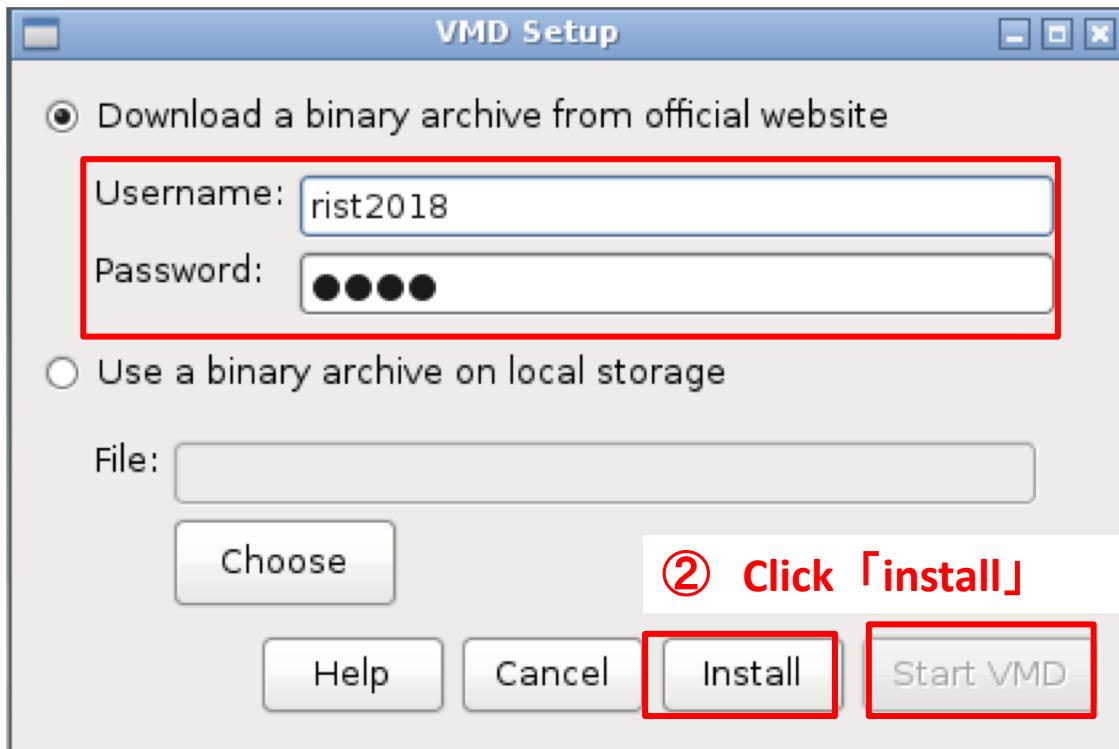
Upon execution of this Agreement by the party identified below ("Licensee"), The Board of Trustees of the University of Illinois ("Illinois"), on behalf of The Theoretical and Computational Biophysics Group ("TCBG") in the Beckman Institute, will provide the Visual Molecular Dynamics ("VMD") software in Executable Code and/or Source Code form ("Software") to Licensee, subject to the following

terms and conditions. For purposes of this Agreement, Executable Code is the compiled code, which is ready to run on Licensee's computer. Source code consists of a set of files which contain the actual program commands that are compiled to form the Executable Cod

Click the button

Visualization by VMD(10)

- Input username and password for 「VMD Setup」



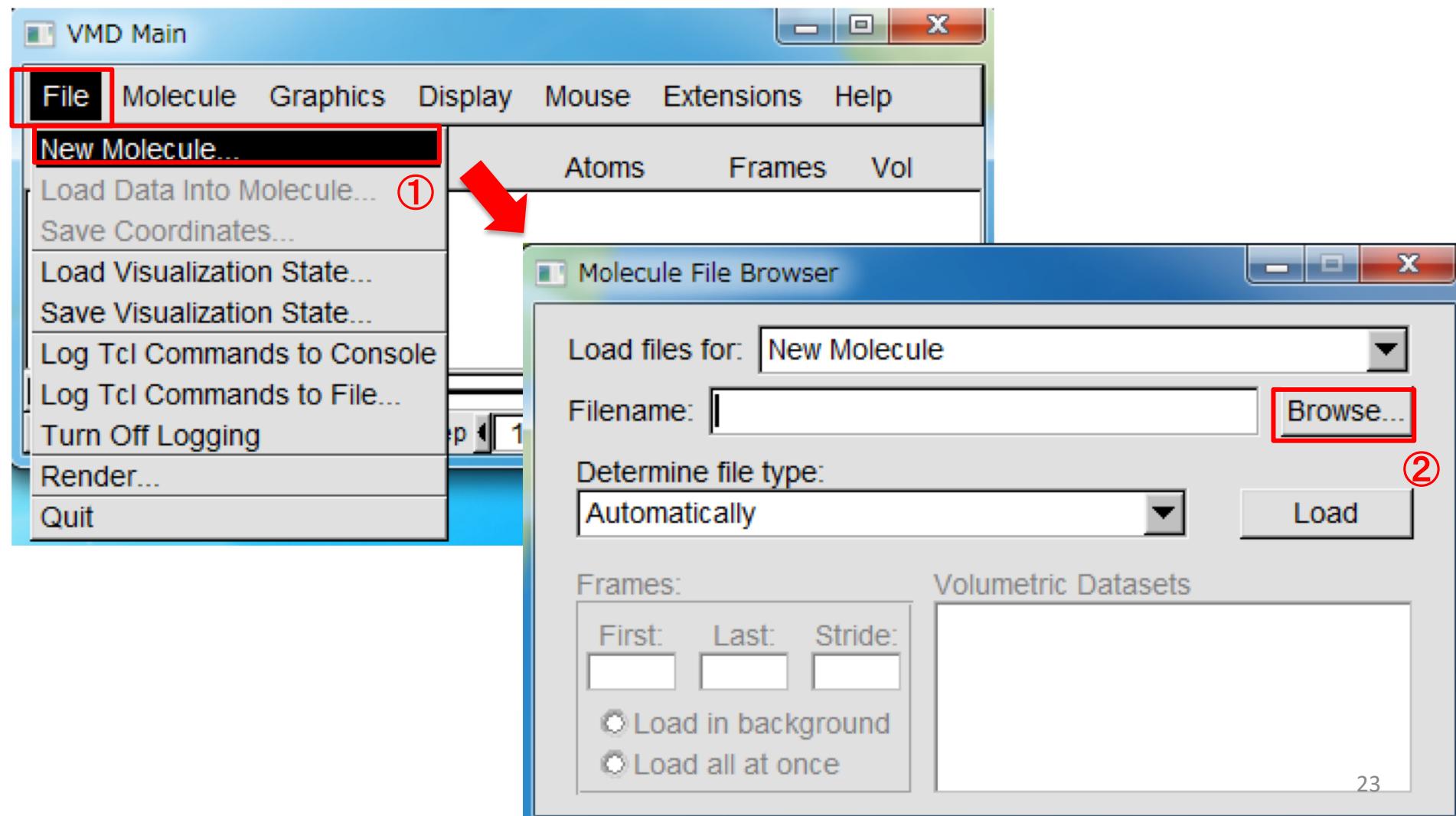
① Input username and password

② Click 「install」

③ If the setup is complete, you click "Start VMD"

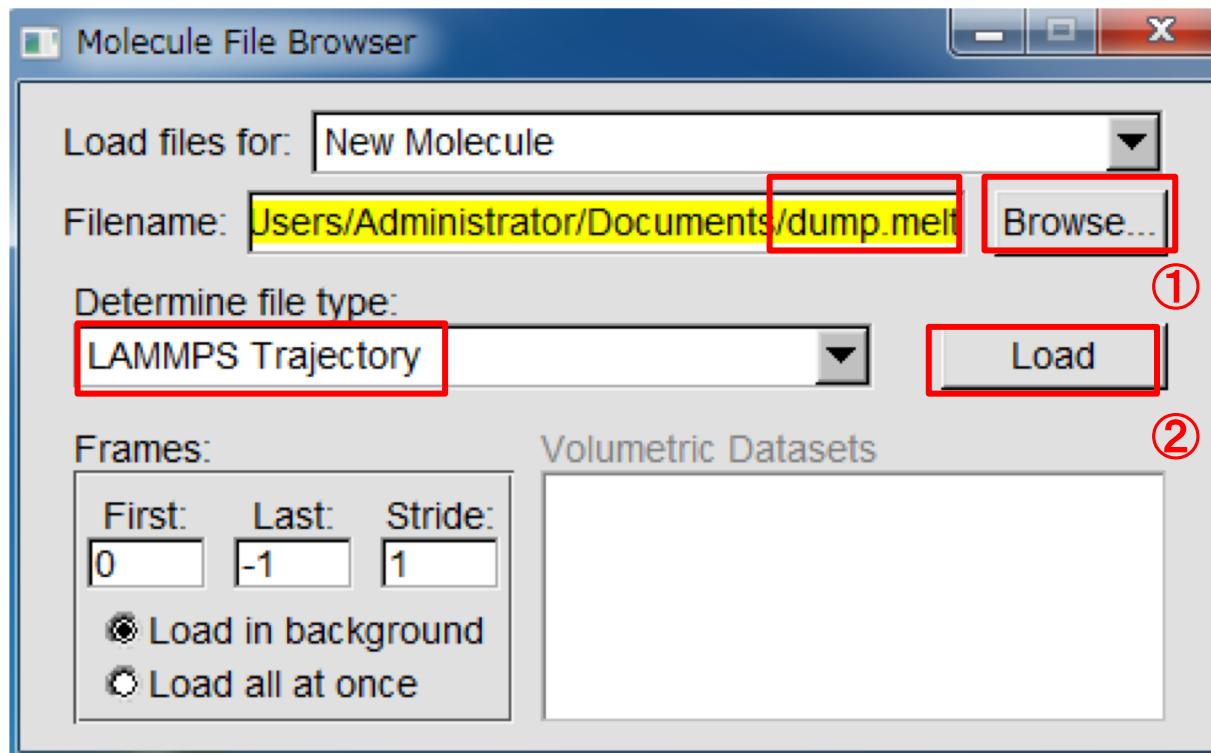
Visualization by VMD(11)

- Open dump.melt



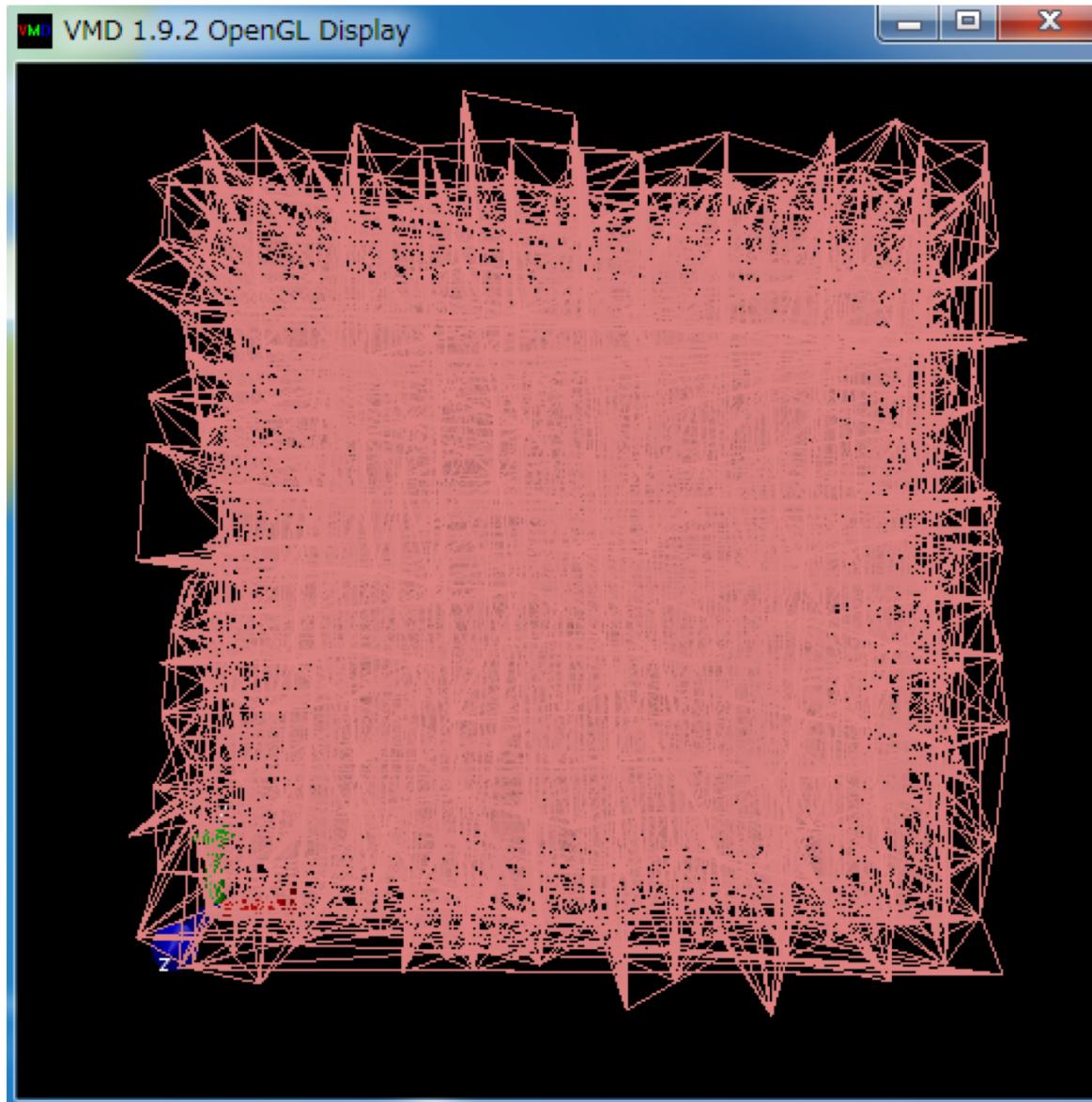
Visualization by VMD(12)

- Select "LAMMPS Trajectory"



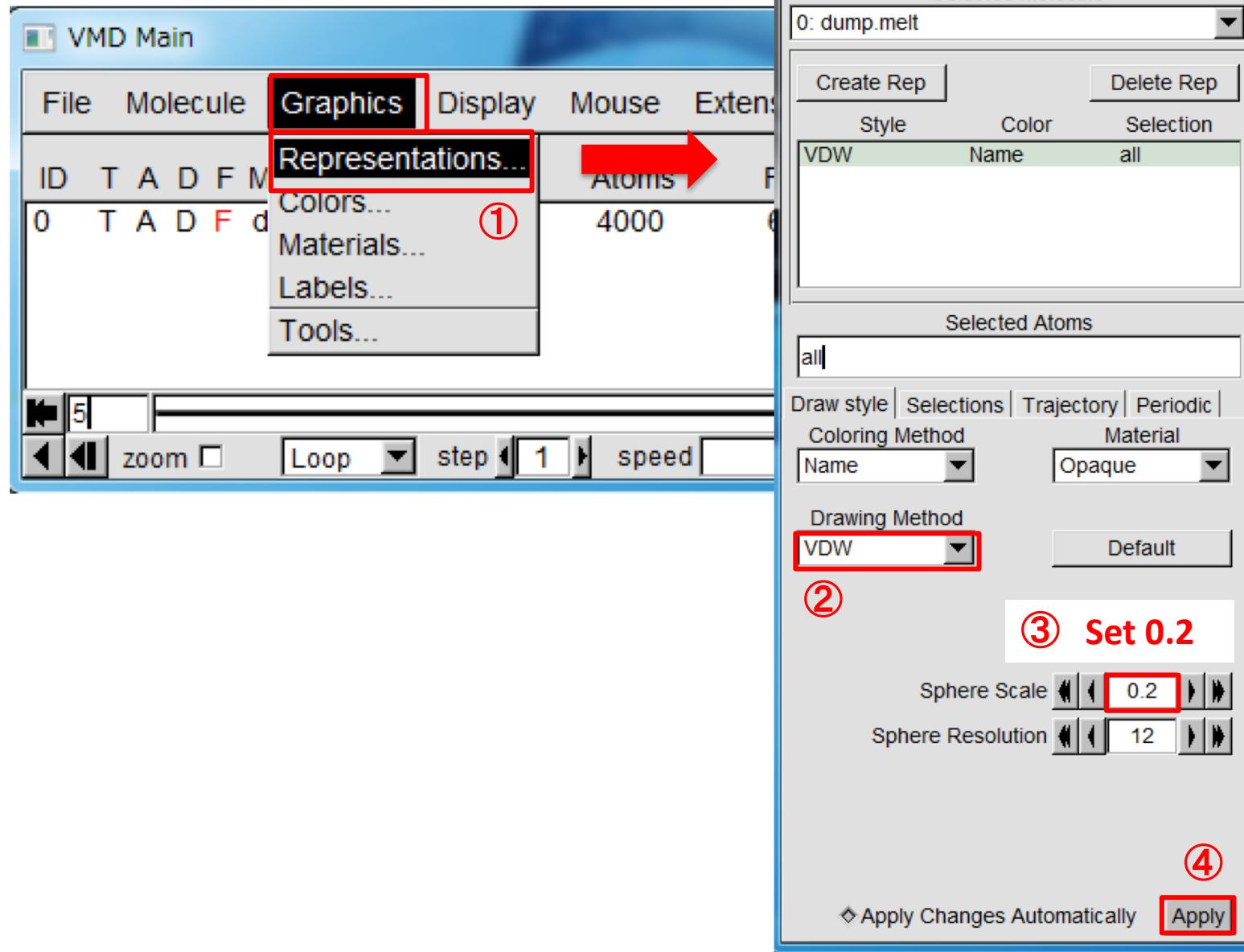
Visualization by VMD(13)

- Open the Display



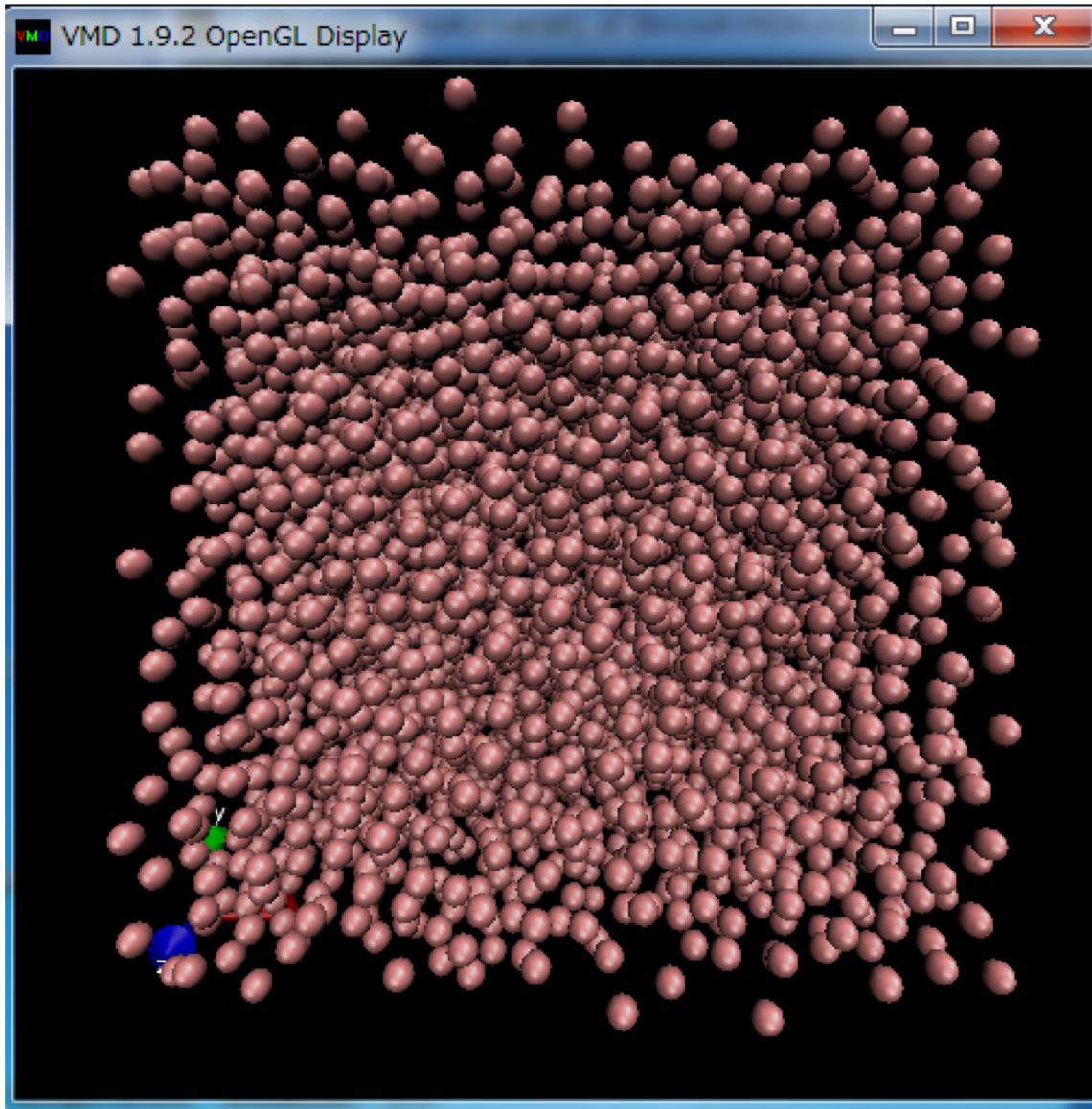
Visualization by VMD(14)

- Set "Representations"



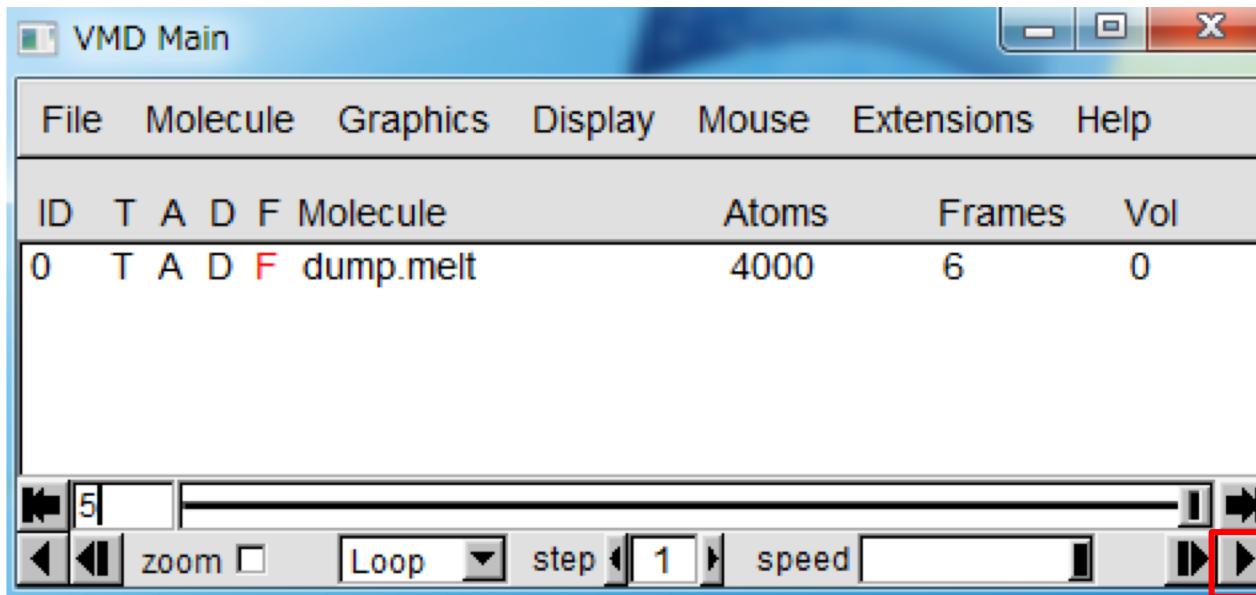
Visualization by VMD(15)

- Open the Display again



Visualization by VMD(16)

- Start MD



Click the button

Visualization of micelle and colloid

1. Create dump files of micelle and colloid
2. Open the dump files by VMD

Visualization of micelle(1)

Rewrite in.micelle

```
# 2d micelle simulation

dimension 2

neighbor 0.3 bin
neigh_modify delay 5

atom_style bond

# Soft potential push-off

read_data data.micelle
special_bonds fene

...
fix 1 all nve
...
thermo 1000

dump 1 all atom 2000 dump.micelle
```

← Remove #

Visualization of micelle(2)

```
#dump      2 all image 2000 image.*.jpg type type zoom 1.6
#dump_modify 2 pad 5 adiam 1 0.5 adiam 2 1.5 adiam 3 1.0
adiam 4 0.75

#dump      3 all movie 2000 movie.mpg type type zoom 1.6
#dump_modify 3 pad 5 adiam 1 0.5 adiam 2 1.5 adiam 3 1.0
adiam 4 0.75

reset timestep 0
run    500000
```

Increase the number of steps

Visualization of micelle (2)

- Run modified in.micelle

```
$ lammmps < in.micelle
```

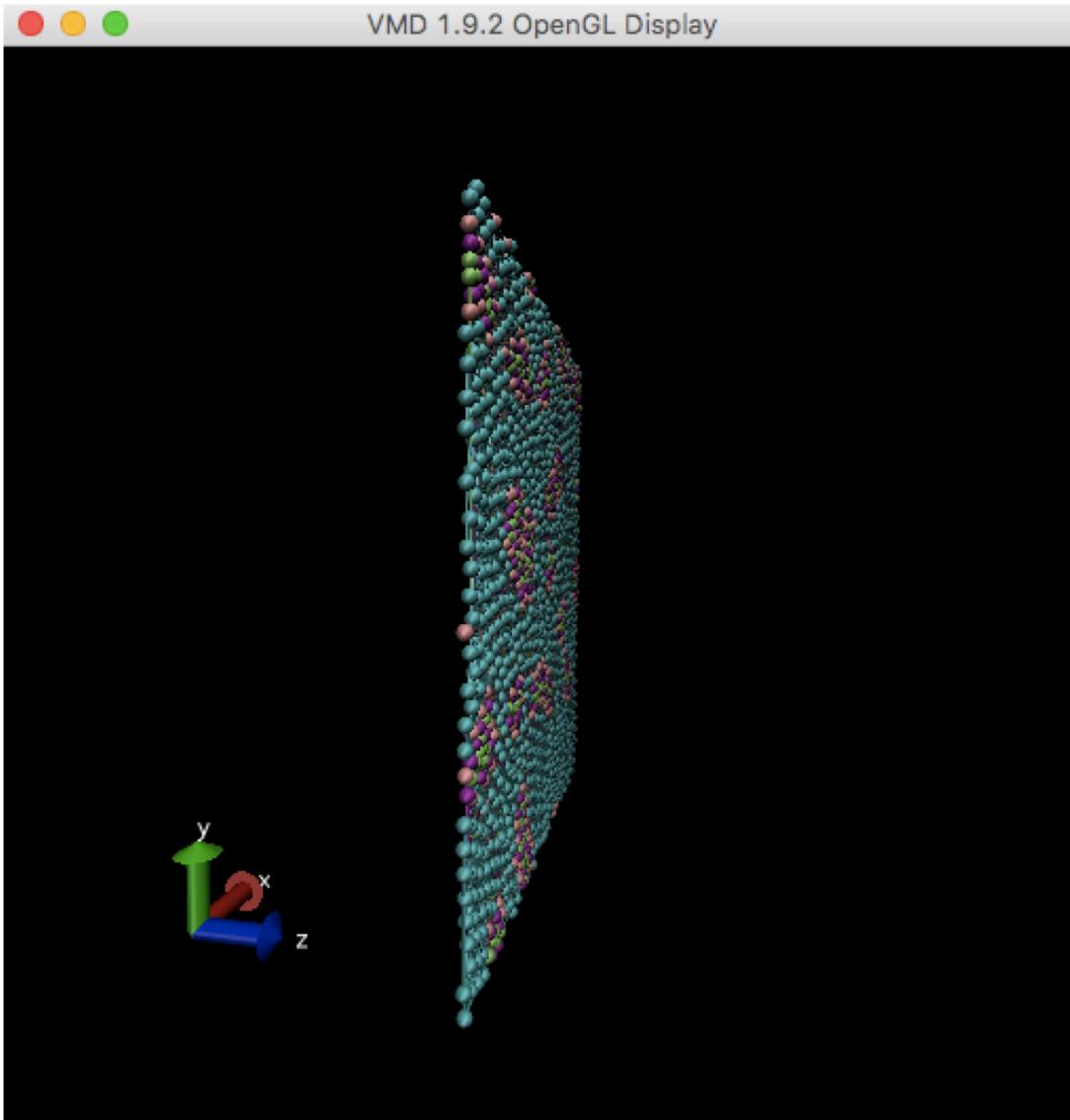
If "Total wall time" is displayed without
error message,
normal execution

- Check creating dump.micelle

```
$ ls  
data.micelle  dump.micelle  log.lammps  
def.micelle  in.micelle
```

Visualization of micelle (3)

- Open dump.micelle



Change from 2D to 3D for micelle

1. Rewrite in.micelle and data.micelle from 2D to 3D
 2. Visualization of 3D micelle
-
- Make directory (ex: \$HOME/lammps/micelle3d)
\$ cd \$HOME/lammps
\$ mkdir micelle3d
 - Copy in.micelle and data.micelle
\$ cp ./micelle/in.micelle ./micelle3d
\$ cp ./micelle/data.micelle ./micelle3d
 - Rewrite in.micelle and data.micelle
\$ cd ./micelle3d
\$ emacs in.micelle &
\$ emacs data.micelle &

Running of 3D micelle(1)

Rewrite in.micelle (input file)

```
# 3d micelle simulation                                bond_coeff    1 50.0 0.75
# dimension   2                                     velocity      all create 0.45 2349852
neighbor      0.3 bin                               variable      prefactor equal ramp(1.0,20.0)
neigh_modify  delay 5
atom_style    bond
# Soft potential push-off
# fix          1 all npt temp 1.0 1.0 1.0 iso 3.0 3.0 10.0
fix           2 all temp/rescale 100 0.45 0.45 0.02 1.0
fix           3 all adapt 1 pair soft a * * v_prefactor
# fix          4 all enforce2d
read_data     data.micelle                         thermo       50
replicate     1 1 36                                run          1000
special_bonds tene
pair_style    soft 1.12246                          unfix        3
pair_coeff    * * 0.0 1.12246                      → continuation
bond_style    harmonic
```

Running of 3D micelle (3)

Rewrite in.micelle (input file)

→ continuation

Main run

pair_style lj/cut 2.5

solvent/head - full-size and long-range

pair_coeff 1 1 1.0 1.0 2.5

pair_coeff 2 2 1.0 1.0 2.5

pair_coeff 1 2 1.0 1.0 2.5

tail/tail - size-averaged and long-range

pair_coeff 3 3 1.0 0.75 2.5

pair_coeff 4 4 1.0 0.50 2.5

pair_coeff 3 4 1.0 0.67 2.5

solvent/tail - full-size and repulsive

pair_coeff 1 3 1.0 1.0 1.12246

pair_coeff 1 4 1.0 1.0 1.12246

thermo 1000

dump 1 all atom 2000 dump.micelle

#dump 2 all image 2000 image.*.jpg type type
zoom 1.6

#dump_modify 2 pad 5 adiam 1 0.5 adiam 2 1.5
adiam 3 1.0 adiam 4 0.75

#dump 3 all movie 2000 movie.mpg type type
zoom 1.6

#dump_modify 3 pad 5 adiam 1 0.5 adiam 2 1.5
adiam 3 1.0 adiam 4 0.75

reset_timestep 0

run 60000

If this execution time is large,
you should reduce the
number of steps.

Running of 3D micelle (4)

Rewirte data.micelle (data file)

LAMMPS 3d micelle data file

1200 atoms

1 1.000000

2 1.000000

3 1.000000

4 1.000000

0 angles

0 dihedrals

0 impropers

Atoms

4 atom types

1 139 2 0.000 0.000 0.000

1 bond types

2 0 1 1.195 0.000 0.000

0 angle types

3 0 1 2.390 0.000 0.000

0 dihedral types

4 0 1 3.586 0.000 0.000

0 improper types

5 0 1 4.781 0.000 0.000

...

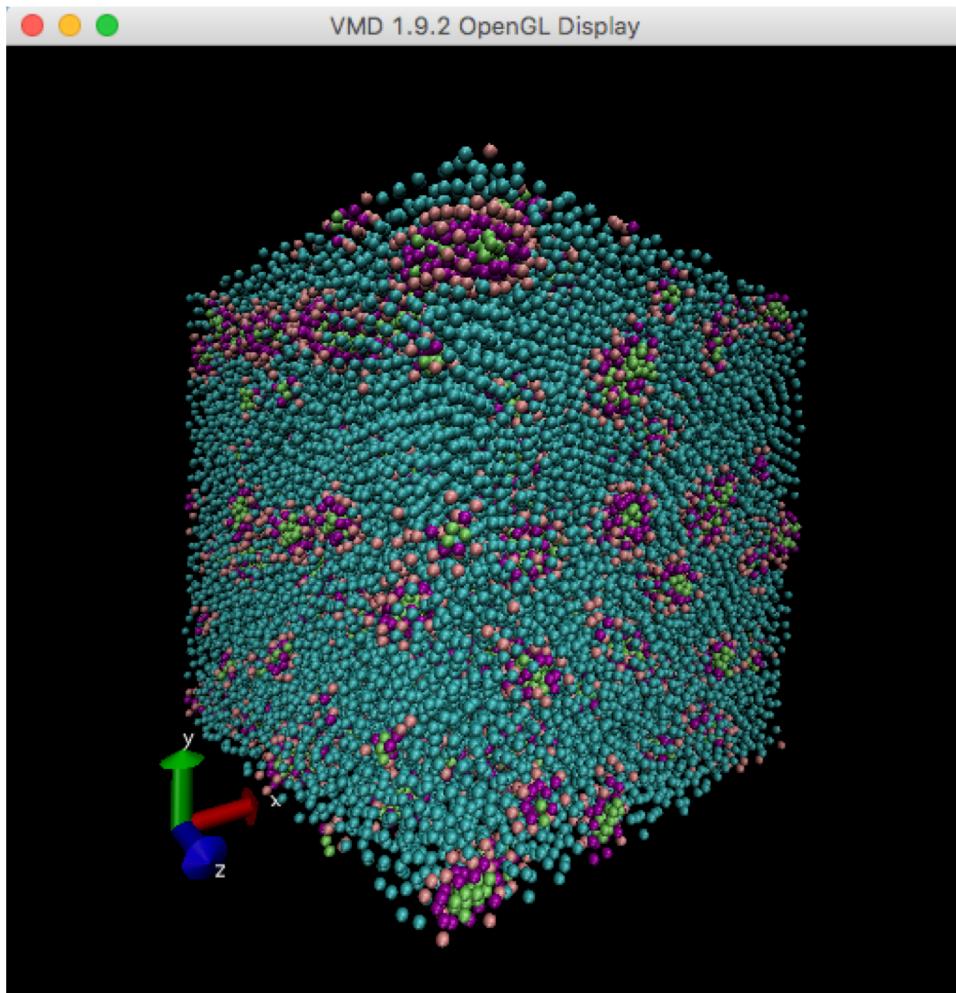
0.0000000E+00 35.85686 xlo xhi

0.0000000E+00 35.85686 ylo yhi

0.0000000E+00 0.996023889 zlo zhi

Running of 3D micelle (4)

- Run modified in.micelle and data.micelle
\$ lammmps < in.micelle
- Open dump.micelle



Increasing the number of atoms (1)

- Make directory (ex: \$HOME/lammps/melt2)
\$ cd \$HOME/lammps
\$ mkdir melt2
- Change the directory (\$HOME/lammps/melt2)
\$ cd melt2
- Copy in.melt
\$ cp/melt/in.melt ./
- Rewrite in.melt
\$ emacs in.melt

Increasing the number of atoms (2)

Rewrite in.melt

```
# 3d Lennard-Jones melt

units          lj
atom_style     atomic

lattice        fcc 0.8442
region         box block 0 40 0 40 0 40
create_box     1 box
create_atoms   1 box
mass           1 1.0

velocity       all create 3.0 87287

pair_style     lj/cut 2.5
pair_coeff     1 1 1.0 1.0 2.5

neighbor       0.3 bin
neigh_modify   every 20 delay 0 check no

fix            1 all nve
```

Change from 4,000 atoms
to 256, 000 atoms

Increasing the number of atoms (3)



- Run modified in.melt
\$ lammps < in.melt
- Show the log file
\$ cat log.lammps

...

Created 256000 atoms

...