计算物质科学
教育部重点实验室(复旦大学)
Key Laboratory of Computational Physical Sciences
(Fudan University), Ministry of Education

复旦大学
FUDAN UNIVERSITY

Thermal Conductivity Calculation of Argon by Molecular Dynamics

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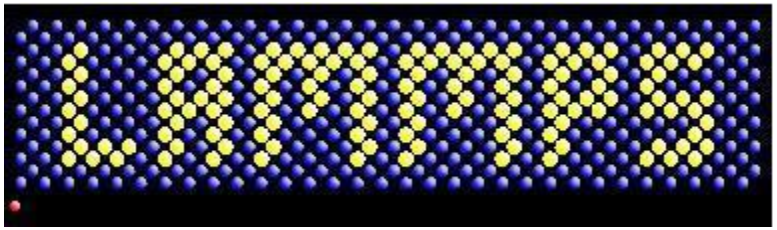
Basic Understanding of LAMMPS

LAMMPS

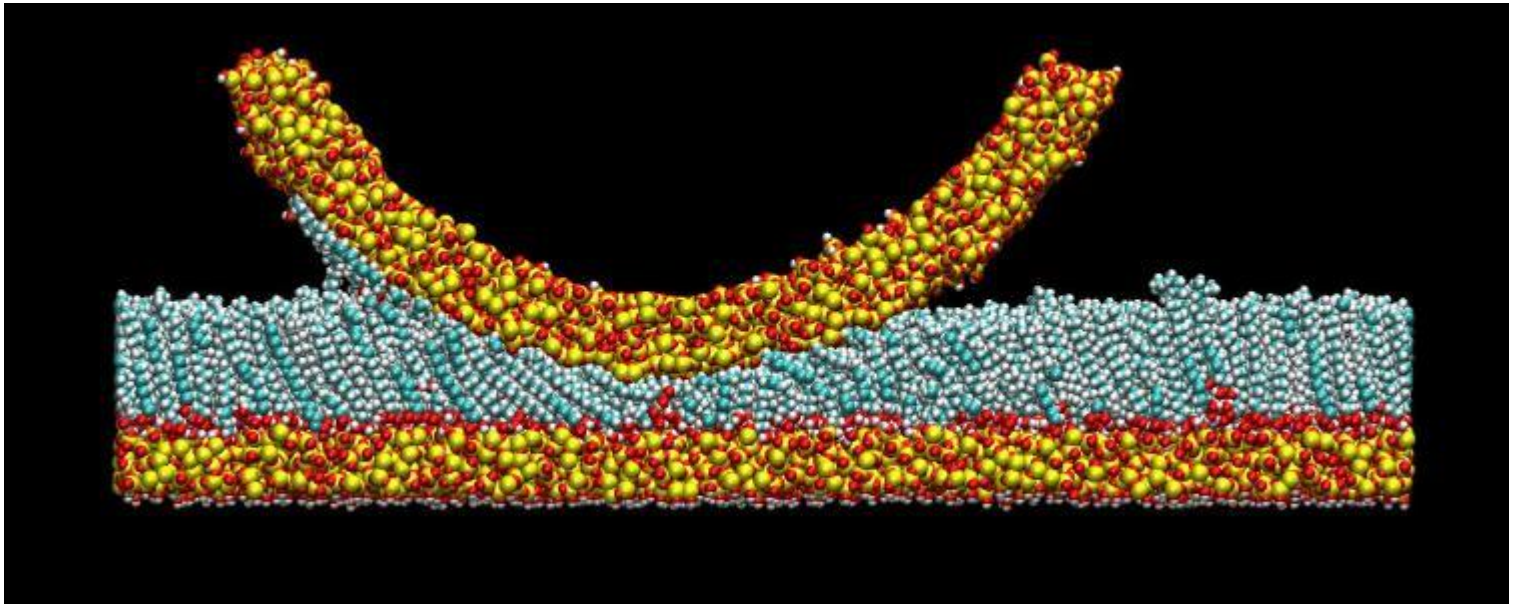


Large-scale Atomic/Molecular Massively Parallel Simulator

大规模原子分子并行模拟器

Based on C++ , which is efficiency is easy to extend

Implements of many kinds of applications



Environment

Linux

- basic

cd -- go into a directory
cd .. -- go into parent directory
cd - -- go into the last directory
tab -- auto complete

ls – view the file list
mkdir – make directory
rm – remove file
rm –r – remove directory

- ssh

ssh xggong@10.92.2.163
password: gjzzw224
./ZHANGJIANG.sh

remote console

- Winscp

host:10.92.2.163
username : xggong
password : gjzzw224
cd zhangjiang

remote filesystem

- Vim & Sublime Text

text editor

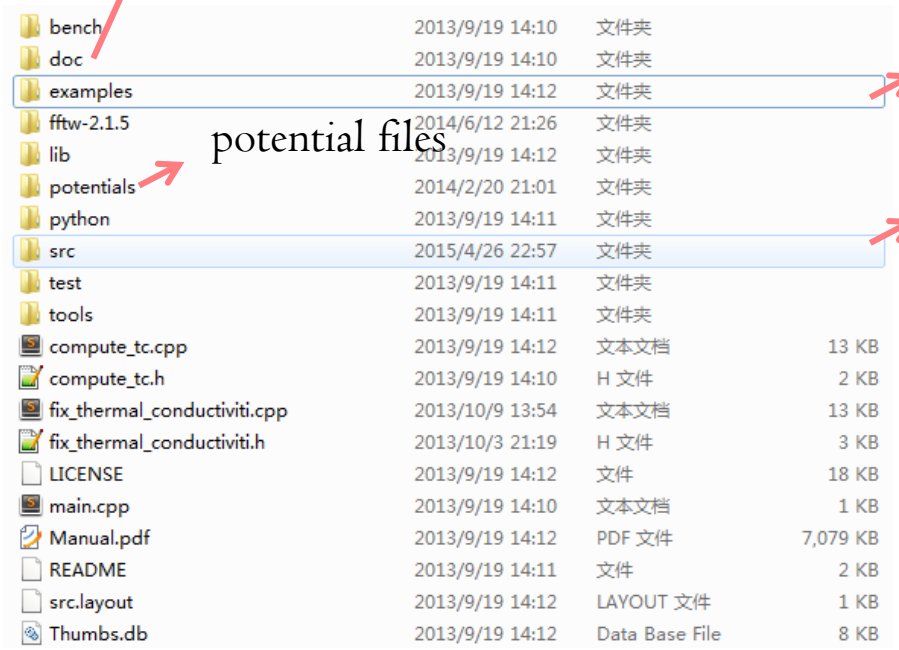
- Tar

download lammps.tar.gz at http://lammps.sandia.gov/download.html
tar xvf lammps.tar.gz

extract files

Source structure of LAMMPS

manual



scripts

potential files

cpp source

src

- packages like "manybody" → make yes-manybody
- user-packages like "user-phonon" copy the code in MANYBODY into current folder
- MAKE
- cpp & h

Compiling

cd stubs
make
make serial

you get lmp_serial

- g++ & Makefile

```
g++ -c hello.cpp –o hello.o
g++ -c world.cpp –o world.o
g++  hello.o world.o –o helloworld
```

compile
link

Makefile : dependency translation

```
all : hello.o world.o
        g++ hello.o world.o -o helloworld
hello.o: hello.c
        g++ -c hello.c -o hello.o
world.o: world.c
        g++ -c world.c -o world.o
```

⇔

```
objects = hello.o world.o
all : $(objects)
        g++ $(objects) -o helloworld
$(objects):%.o : %.c
        g++ -c $< -o $@
```

make

Excution

./lmp_serial <in.lmp

mpirun –n 2 lmp_parallel <in.lmp >log.out

pbs

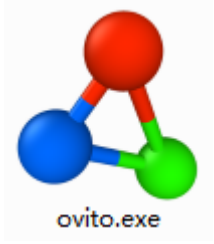
qsub
qstat
qdel

§ Excute in Windows

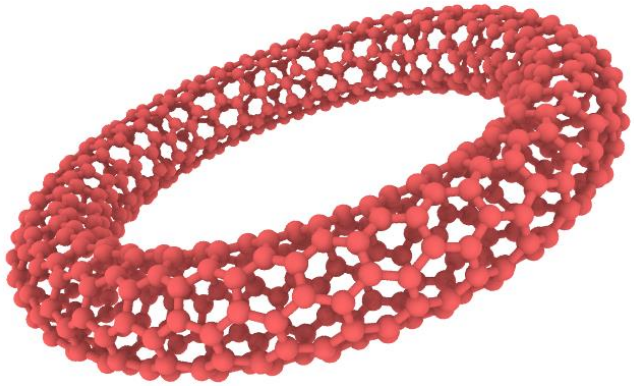
download lammps at http://rpm.lammps.org/windows.html
ctrl+r
cmd
lammps.exe<in.lmp

Visualization

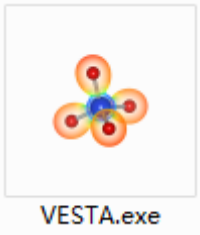
§ VMD,ovito,qutemol



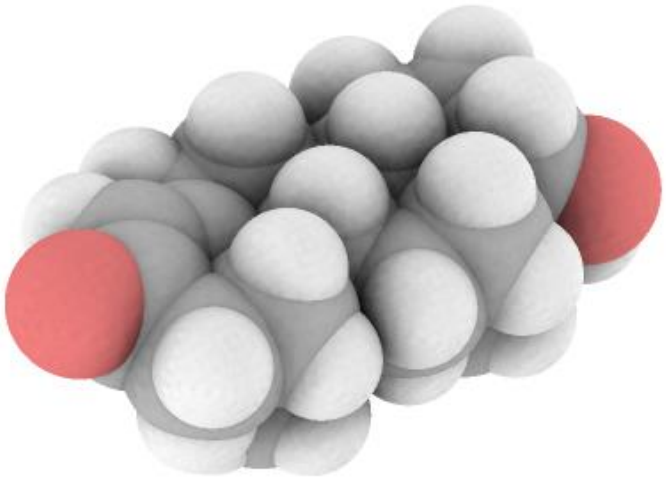
rendering, coloring
animation



animation, biomolecule
render, interactive MD

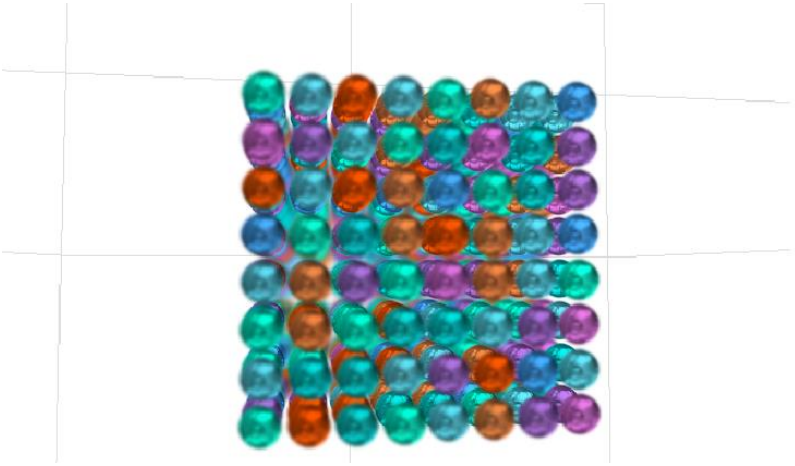


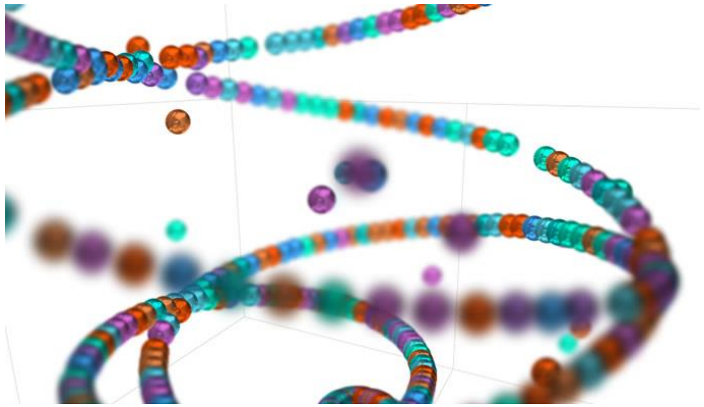
electronic structure

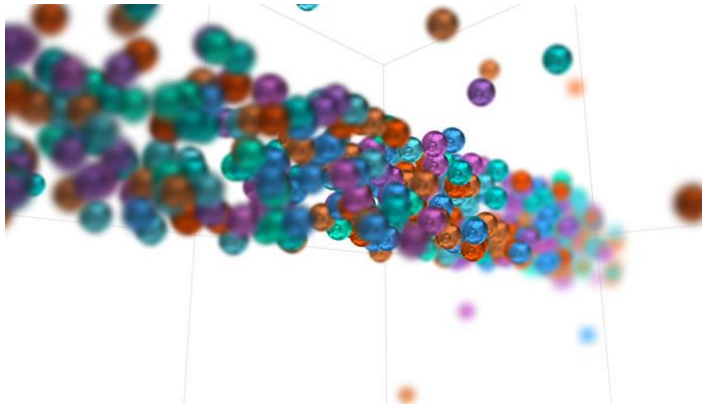


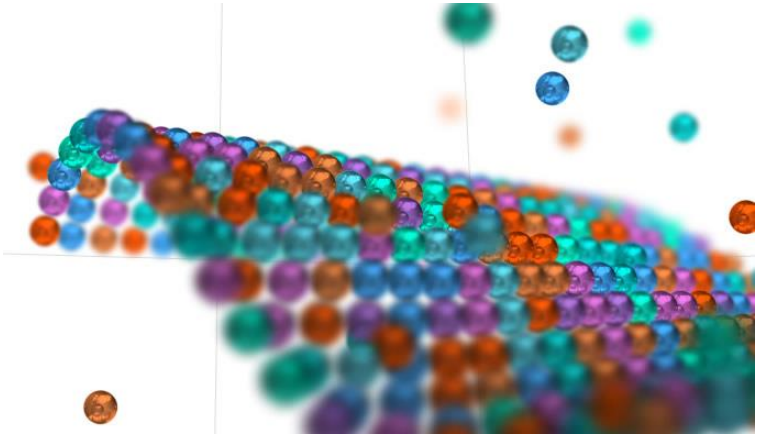
realistic rendering

Visualization









LAMMPS script

§ Manual

http://lammps.sandia.gov/doc/Manual.html

§ Setup

§ Material

```
# 3d Lennard-Jones nvt ensemble
units           metal      #unit system : metal ,lj, si ...
atom_style      atomic
boundary p p p             #boundary type
lattice         fcc 5.41229                #lattice type and constant
region          box1 block 0 5 0 5 0 5 units lattice   #geometrical objects,  named as box1
create_box      1 box1     #use box1 to define the space where atoms are in . there’ s 1
                           type of atoms
create_atoms    1 box      #create the type 1 atom at all the lattice sites within the box
mass            1 39.948                                  #mass of atom type 1

pair_style      lj/cut 8.5125                  #define potential and set cut radius
pair_coeff      * * 0.0103235761 3.405 8.5125  #for all types of atoms set parameter

neighbor        2.0 bin                        #neighbor list type and size
neigh_modify    every 2 delay 10 check yes     #update rate
```

LAMMPS script

```
timestep        0.001                                   #1(fs)
dump d1 all atom 20 dump.lammpstrj                      # output structure to file , labeled as d1
dump_modify   d1 sort id                                # sort according to id

thermo          20                                      #output to screen every 20 steps
thermo_style    custom step  temp pe etotal lx ly lz    #which value to be output
velocity        all create 40 1234567 mom yes  rot yes dist gaussian
        #initial velocity to 40K with Gaussian distribution of seed 1234567
        ,moveout drift and remained rotation
fix             a1 all nvt temp 40.0  40.0  0.1       #NVT with start T=40, end T=40,
                                                        relaxation time=0.1 (ps)
region          box2 block 0 3 0 5 0 5 units lattice
group           g1 region box2                          # define group using box2
compute T1 g1 temp # define a compute name as T1,calculating the temperature of g1

fix sqo1 all ave/time 1 5000 10000 c_T1 c_thermo_temp c_thermo_pe file log.Ave
                        # average and output, compute T1 is excuted, so as 2 default computes
run             10000
                                                        #run for 10000 times  (10ps)
```

- Device
- Measure

Ensemble

```
boundary p p p
```

```
p – periodic
s – free: scale as needed
m – free with lower limit
f – lost if leave out
```

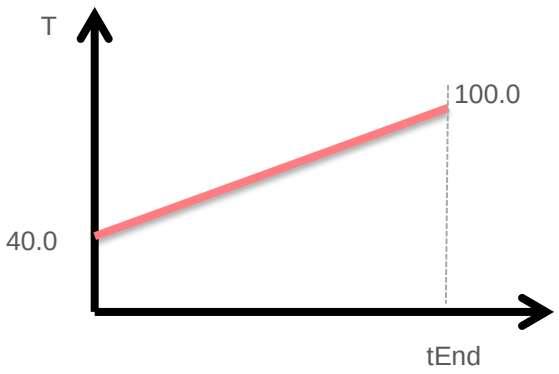
```
fix ID group-ID ave/time Nevery Nrepeat Nfreq
```

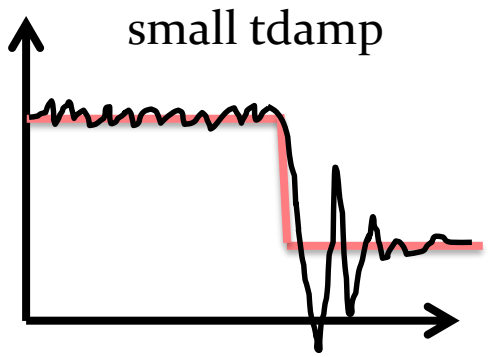
```
Nevery Nrepeat Nfreq=2 3 10
```

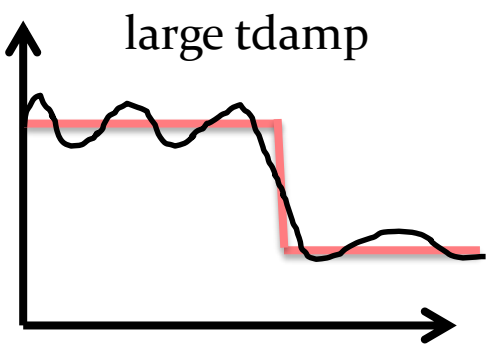
```
                10          20          30
6 8 10    16 18 20    26 28 30
          ↓           ↓           ↓
          ave         ave         ave
```

```
fix a1 all nvt temp 40.0  100.0
```
Tdamp

Tdamp is usually 0.01*timestep



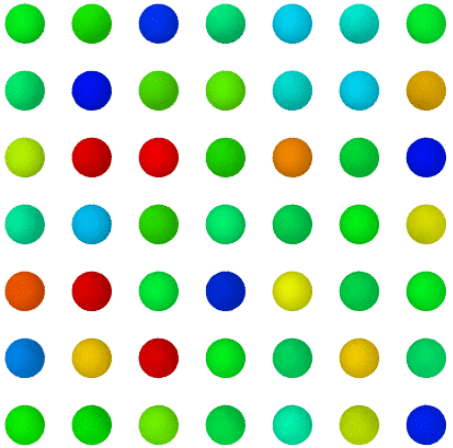




Example

§ Melt

```
units                   lj
atom_style              atomic
boundary s s s  #nano-particle

lattice                 fcc 0.8442
region box block 0 3 0 3 0 1  #a small region
create_box              1 box
create_atoms            1 box
mass                    1 1.0

velocity     all create .1 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     #verlet algorithm
compute ke all ke/atom     #kinetic energy of every atom
dump a all custom 10 dump.melt id type xs ys zs c_ke  #besides dump/atom we want c_ke
dump_modify             a sort id
thermo 50
run 1000
```

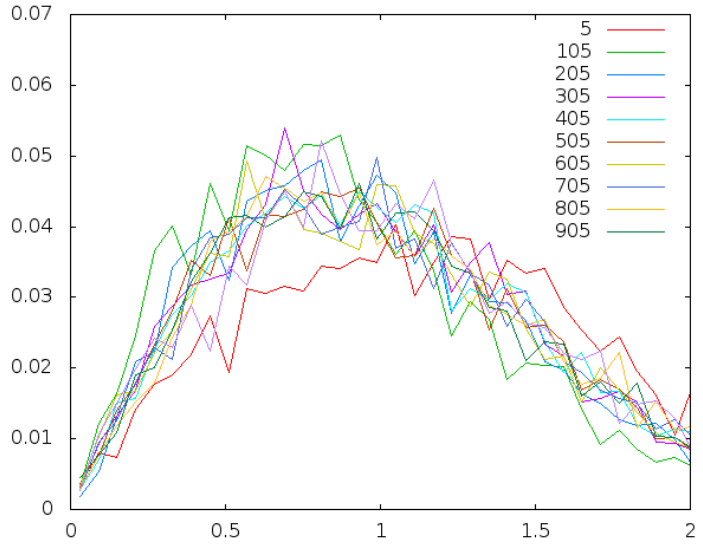


coloring according to ke
using Ovito (top view)

Example

§ histogram

#the velocity distribution of sum atoms

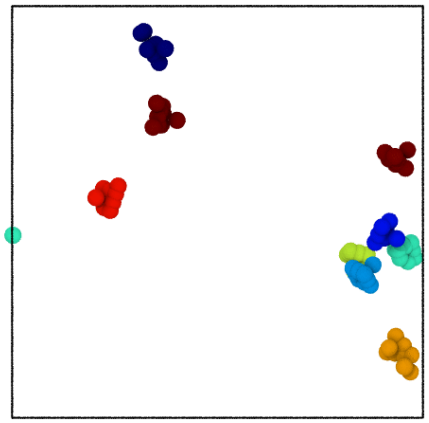



```
units           lj
atom_style atomic
boundary p p p

region 1 block 0 10 0 10 0 10
create_box 1 1
create_atoms 1 box
mass 1 1

timestep .001
pair_style       lj/cut 3
pair_coeff      * * 1 1
velocity all create 1 17 rot yes dist  gaussian
fix 1 all nve
variable velo atom sqrt(vx*vx+vy*vy+vz*vz)      #the scalar velocity
fix 2 all ave/histo 1 4 5 0 3 50 v_velo mode vector file histo.txt
                                        #the velocity distribution of every atom

thermo 100
dump 1 all atom 10 dump.lammpstrj
run 1000
```

Example

Lammps

Examples § Rigid body



```
# Simple rigid body system
units                   lj
atom_style              atomic
pair_style  lj/cut 2.5
read_data  data.rigid
velocity     all create 100.0 4928459
# unconnected bodies
group                   clump1 id <> 1 9  #define groups according to ids ranges
group                   clump2 id <> 10 18
group                   clump3 id <> 19 27
group                   clump4 id <> 28 36
group                   clump5 id <> 37 45
group                   clump6 id <> 46 54
group                   clump7 id <> 55 63
group                   clump8 id <> 64 72
group                   clump9 id <> 73 81
fix 1 all rigid group 9 clump1 clump2 clump3
clump4 clump5 clump6 clump7 clump8 clump9 #define 9 rigid bodies
```

Homework

- 用lammps重复上次课的作业
- 用lammps计算Ar理想气体的融化曲线，求出融化温度

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THANK FOR YOUR ATTENTION!

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