Install Parallel Lammps on Ubuntu

tags: Research records Molecular dynamics

Install required packages

```
sudo su                                    #Open the administrator mode, enter the password and co
```

```
                    apt-get install gcc                    #Install gcc
```

```
                    apt-get install g++                    #Install g++
```

```
                     apt-get install gfortran              #Install gfortran
```

```
                      apt-get install make                 #Install make
```

Download the required documents

Open the terminal in the home directory:

```
#New lammps folder
mkdir lammps
```

```
#Enter lammps
cd lammps
```

```
#Download fftw-3.3.8.tar.gz
wget http://www.fftw.org/fftw-3.3.8.tar.gz
```

```
#Download mpich-3.3.2.tar.gz
wget http://www.mpich.org/static/downloads/3.3.2/mpich-3.3.2.tar.gz
```

```
#Download lammps-stable.tar.gz
wget https://lammps.sandia.gov/tars/lammps-stable.tar.gz
```

Unzip

```
#After decompression, fftw-3.3.8
tar -xvf fftw-3.3.8.tar.gz
```

```
#After decompression, it is mpich-3.3.2
tar -xvf mpich-3.3.2.tar.gz
```

```
#After decompression is lammps-3Mar20
tar -xvf lammps-stable.tar.gz
```

Install fftw

Enter the /lammps-3Mar20/src/MAKE/OPTIONS path. From the Makefile.fftw file, you can see that the default fftw calling path of lammps is /usr/local. For the convenience of subsequent compilation of lammps, install fftw to this path.

```
cd lammps/src/MAKE/OPTIONS
vim Makefile.fftw
```

```
FFT_INC =       -DFFT_FFTW3 -I/usr/local/include
FFT_PATH =      -L/usr/local/lib
FFT_LIB =       -lfftw3
```

```
cd fftw-3.3.8
```

```
sudo ./configure --prefix=/usr/local --enable-float
```

./configure --prefix=/usr explanation

Linux ./configure --prefix command

```
sudo make -j          #-j means that there is no core limit for calling and compiling
```

```
sudo make install  # sudo is over, I haven't had a problem with sudo before
```

```
cd                                  #Return to the root directory
```

Install MPICH

Enter the \lammps-3Mar20\src\MAKE\OPTIONS path, open the Makefile.g++_mpich_link file, and check the following content to know that the default mpich calling path of lammps is /usr/local.

```
MPI_INC =       -DMPICH_SKIP_MPICXX -DOMPI_SKIP_MPICXX=1 -I/usr/local/include
MPI_PATH =      -L/usr/local/lib
MPI_LIB =       -lmpich -lmpl -lpthread
```

```
cd lammps/mpich-3.3.2
```

```
sudo ./configure --prefix=/usr/local
```

```
sudo make -j
```

```
sudo make install
```

```
cd ..                #Return to the parent directory
```

Install lammps

```
cd lammps/lammps-3Mar20/src
```

```
sudo make mpi -j
```

If successful, a file of lmp_mpi will be generated

Note: lammps installs 3 dependency packages by default, MANYBODY, KSPACE, and MOLECULE. If there are other dependent packages needed, just enter the commands separately in the /lammps-3Mar20/src folder:

```
1.      make  package-status (View dependent package status)
2.      make  yes-*** (install *** dependent package)
3.      make  no-*** (delete *** dependent packages)
4.      make mpi -j
```

Just regenerate the executable file lmp_mpi
Note: Do not make yes-all, it will get stuck. . . You can install the package according to your needs. For the first installation, I added three packages: MANYBODY, KSPACE, and MOLECULE:

```
make yes-MANYBODY
make yes-KSPACE
```

```
make yes-MOLECULE
sudo make mpi -j
```

test

```
#Return to the root directory
cd
```

```
#Enter the shear folder
cd lammps/lammps-3Mar20/examples/shear
#
vi in.shear
```

Uncomment: #dump 1 all atom 100 dump.shear, run the test after saving and exiting

```
/usr/local/bin/mpirun -np 6 /home/yuabaoqiang/lammps/lammps-3Mar20/src/lmp_mpi < in.shear
```

- mpirun is under /usr/local/bin
- 6 is my audit
- lmp_mpi is under /home/yuabaoqiang/lammps/lammps-3Mar20/src
- in.shear is my in file

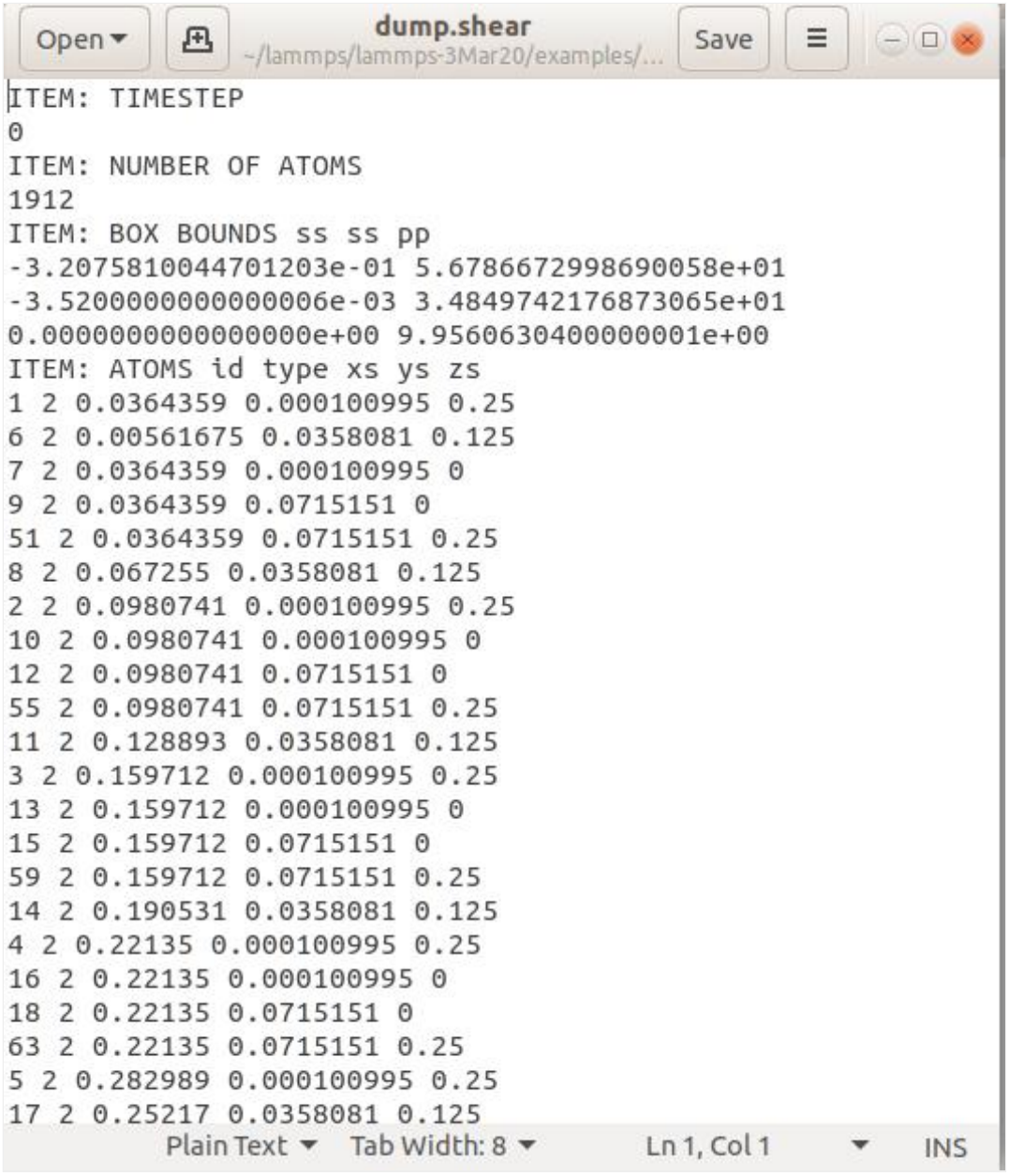
Run interface:

```
  Time step     : 0.001
Per MPI rank memory allocation (min/avg/max) = 3.352 | 3.355 | 3.362 Mbytes
Step Temp E_pair E_mol TotEng Press Volume
       0          300   -8317.4367            0   -8263.8067   -7100.7667     19
547.02
      25    218.45854   -8271.4152            0   -8232.3621    5664.5251     19
547.02
      50          300   -8237.5513            0   -8183.9213    14095.181    196
90.916
      75    295.96592   -8230.5173            0   -8177.6084    14553.581    197
57.713
     100          300   -8248.8926            0   -8195.2626    8400.5188    198
05.732
Loop time of 0.0460751 on 6 procs for 100 steps with 1912 atoms

Performance: 187.520 ns/day, 0.128 hours/ns, 2170.371 timesteps/s
99.2% CPU use with 6 MPI tasks x no OpenMP threads

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 0.035214   | 0.038055   | 0.041519   |   1.2 | 82.59
Neigh   | 0.0010753  | 0.0012574  | 0.0015705  |   0.6 |  2.73
Comm    | 0.0018911  | 0.0055716  | 0.0087402  |   3.6 | 12.09
```

dump file:



In order to simplify the running command, you can write the folder where the running file is located into the PATH path
Open the terminal on the desktop:

```
vi .bashrc
```

Add text directly at the bottom:
Note that the file path is written according to your actual situation.

```
export PATH=/usr/local/bin:/usr/local/lib:/usr/local/include:/home/yuanbaoqiang/lammps/lammps-3Mar20/src:$PATH
```

```
#Make the environment effective
source .bashrc
```

Test again

```
cd lammps/lammps-3Mar20/examples/shear
```

```
mpirun -np 6 lmp_mpi < in.shear
```

Then it works perfectly~

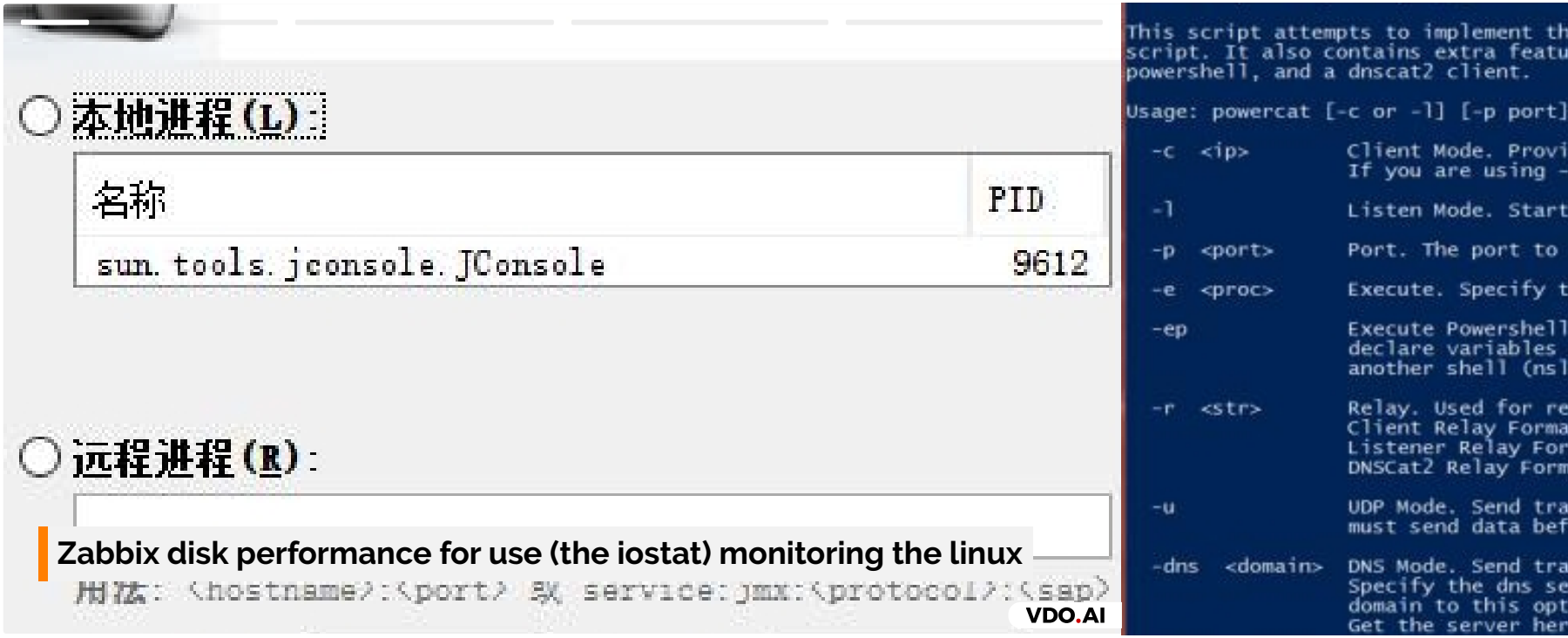
reference:

There are many online posts, but they are all similar. You can refer to multiple versions and choose the one that suits you.

Installation of lammps under ubuntu

lammps-mpi parallel installation

2018 version of lammps installation tutorial (for Xiaobai)



Zabbix disk performance for use (the iostat) monitoring the linux

Intelligent Recommendation

Lammps molecular dynamics software + Intel MPI parallel compiler efficient version of Linux complete installation tutorial

Brief introduction LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on a parallel computer. It is by Sandia National Laboratories (Sandia National Laboratories) US ...

Mac Install Ubuntu 18.04 based on Parallel Desktop Modify the IP address (connected to wifi mode)

Ubuntu 18.04 Use modify ip to modify using netplan Note: The following format needs to be written in accordance with the yaml format, otherwise the configuration will not be recognized, and a space wi...

Install linux virtual machine (ubuntu) and Intel parallel XE 2013 (ifort2013) under VM

Install ubuntu and ifort2013 under VM to run your own mode Due to the new crown epidemic, I can only work at home. Many important files and programs are left on the Linux machine in the office, and th...

Record-lammps

Input script： Error message %%%%%%%%%%%%%%% To be continued...

Parallel Ubuntu and MacOS exchange data

Configuration process on Linux After that, you can get the ip address of Linux, remember this ip, you will use it later. (The tutorial I saw before said that the ip address can also be obtained with t...

More Recommendation

Install ubuntu

I have itchy for a long time, I haven't played ubuntu for a long time, I will record it myself. Mirror manufacturing Domestic mirror station Download imagehttps://mirrors.tuna.tsinghua.edu.cn/ub...

Install Ubuntu

Further information may be found in /var/log/syslog. Do you want to try running this step again before continuing? if you do not, your installation may fail entirely or may be broken. at...

Ubuntu install

1.install qq 1>.download 2>.install 2.confit network 3.install jdk...

ubuntu install

Install ubuntu on VMware Workstation The official website of ubuntu: https://ubuntu.com/download You can download the latest version of Ubuntu image on the official website. It is recommended that eve...

Install ubuntu

table of Contents First, the purpose: 1. Want to know: install ubuntu 2. Reference 1. Windows10 installation ubuntu dual system tutorial (the most detailed in absolute history) 2. Ubuntu mirror downlo...

Related Posts

- Centos install GPU parallel lammps
- Install lammps on Ubuntu
- lammps use diary 1 win 10 to download and install the parallel version of lammps and related software
- Installation of lammps under ubuntu
- Lammps parallel installation tutorial under win
- Install MPI + VTK on Ubuntu 16.04 for parallel rendering
- lammps how to install the package on a supercomputing platform
- How to install and run lammps (serial) in win
- Macbook Ubuntu install and run the first program by parallel desktops c
- Linux/Ubuntu download and install Intel Parallel Studio XE

Popular Posts

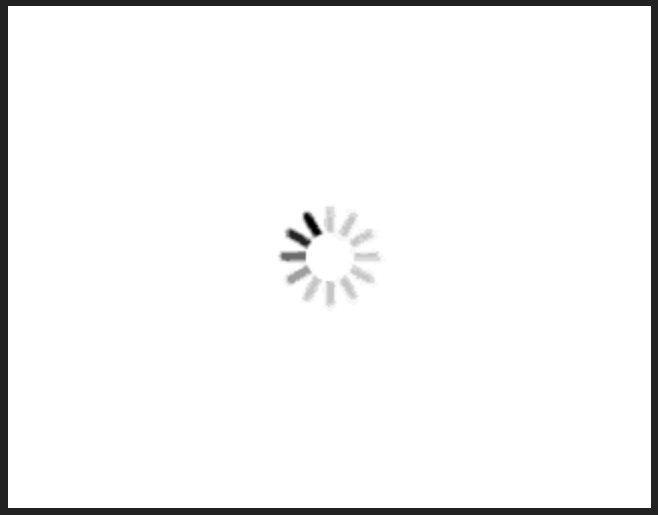
- Humor
- What is the meaning of changing the video md5?
- Spark：【error】System memory 259522560 must be at least 471859200
- (C++) Sword refers to offer-40: a number that appears only once in the array (knowledge transfer ability)
- Java OOM problem
- vue-create component
- Simple example of C# calling Python script, IronPython (reproduced)
- A large number of examples of java regular expressions and common constructors
- Third C language program debugging
- How does Shopify build a website? Learn to use Shopify in 9 steps to quickly build your own website!

TOP

Recommended Posts

- hdu 1121 Complete the Sequence (DP polynomial differential)
- Thinking in Java, Fourth Edition Chapter individual exercises
- The big difference between file data calculation file with the Java computing [emphasis! ! !]
- DeforGAN: Use GAN to realize StarCraft and open the full map plugin!
- Transfer statement in loop control
- python study notes
- network programming

- An array of related content
- Li Wei: OJ: 1156: singular variable plural
- org.apache.ibatis.binding.BindingException: Invalid bound statement (not found)



Related Tags

Centos

GPU

lammps

ubuntu

other

----------Linux----------

VTK

Parallel Computing

Spike camp

ifort

TOP