

search

Install Parallel Lammps on Ubuntu

tags: [Research records](#) [Molecular dynamics](#)

Install required packages

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

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

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

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

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

[TOP](#)

Download the required documents

Open the terminal in the home directory:

```
1 | #New lammps folder  
2 | mkdir lammps
```

```
1 | #Enter lammps  
2 | cd lammps
```

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

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

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

Unzip

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

TOP

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

```
1 | #After decompression is lammgs-3Mar20  
2 | tar -xvf lammgs-stable.tar.gz
```

Install fftw

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

```
1 | cd lammgs/src/MAKE/OPTIONS  
2 | vim Makefile.fftw
```

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

```
1 | cd fftw-3.3.8
```

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

`./configure --prefix=/usr` explanation

Linux `./configure --prefix` command

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

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

```
1 | 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 -lmpi -lpthread
```

```
1 | cd lammps/mpich-3.3.2
```

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

```
1 | sudo make -j
```

TOP

```
1 | sudo make install
```

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

Install lammmps

```
1 | cd lammmps/lammmps-3Mar20/src
```

```
1 | sudo make mpi -j
```

If successful, a file of `Imp_mpi` will be generated

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

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

Just regenerate the executable file `Imp_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:

```
1 | make yes-MANYBODY
2 | make yes-KSPACE
```

TOP

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

test

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

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

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

```
1 /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

TOP


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:

TOP




Open ▾



dump.shear

Save

≡



~/lammps/lammps-3Mar20/examples/...

```
ITEM: TIMESTEP
0
ITEM: NUMBER OF ATOMS
1912
ITEM: BOX BOUNDS ss ss pp
-3.2075810044701203e-01 5.6786672998690058e+01
-3.52000000000000006e-03 3.4849742176873065e+01
0.0000000000000000e+00 9.9560630400000001e+00
ITEM: ATOMS id type xs ys zs
1 2 0.0364359 0.000100995 0.25
6 2 0.00561675 0.0358081 0.125
7 2 0.0364359 0.000100995 0
9 2 0.0364359 0.0715151 0
51 2 0.0364359 0.0715151 0.25
8 2 0.067255 0.0358081 0.125
2 2 0.0980741 0.000100995 0.25
10 2 0.0980741 0.000100995 0
12 2 0.0980741 0.0715151 0
55 2 0.0980741 0.0715151 0.25
11 2 0.128893 0.0358081 0.125
3 2 0.159712 0.000100995 0.25
13 2 0.159712 0.000100995 0
15 2 0.159712 0.0715151 0
59 2 0.159712 0.0715151 0.25
14 2 0.190531 0.0358081 0.125
4 2 0.22135 0.000100995 0.25
16 2 0.22135 0.000100995 0
18 2 0.22135 0.0715151 0
63 2 0.22135 0.0715151 0.25
5 2 0.282989 0.000100995 0.25
17 2 0.25217 0.0358081 0.125
```

Plain Text ▾ Tab Width: 8 ▾ Ln 1, Col 1 ▾ INS

TOP

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:

```
1 | vi .bashrc
```

Add text directly at the bottom:

Note that the file path is written according to your actual situation.

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

```
1 | #Make the environment effective
2 | source .bashrc
```

Test again

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

```
1 | 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.

TOP

[Installation of lammeps under ubuntu](#)

[lammeps-mpi parallel installation](#)

[2018 version of lammeps installation tutorial \(for Xiaobai\)](#)

☐ 本地进程 (L):

名称	PID
sun.tools.jconsole.JConsole	9612

☐ 远程进程 (R):

用法: <hostname>:<port> 或 service:jmx:<protocol>:<sap>

VDO.AI

This script attempts to implement the script. It also contains extra features like powershell, and a dnscat2 client.

Usage: powercat [-c or -l] [-p port]

-c <ip> Client Mode. Provide IP address. If you are using -c, you must specify -p.

-l Listen Mode. Start listening on the port.

-p <port> Port. The port to listen on.

-e <proc> Execute. Specify the process to execute.

-ep Execute Powershell. Execute Powershell commands. You can declare variables and use them in the script.

-r <str> Relay. Used for relay mode. Client Relay Format: <ip>:<port> Listener Relay Format: <ip>:<port> DNSCat2 Relay Format: <ip>:<port>

-u UDP Mode. Send traffic over UDP. You must send data before you can receive data.

-dns <domain> DNS Mode. Send traffic over DNS. Specify the dns server domain to this option. Get the server here: <url>

Intelligent Recommendation

TOP

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 ...

```
rtos-master:/etc/netplan# cat 50-cloud-init.yaml
# This file is generated from information provided by
# cloud-init. Changes to it will not persist across an instance.
# cloud-init's network configuration capabilities, write a
# /cloud.cfg.8/99-disable-network-config.cfg with the follow
# config: disabled)

1:
  eth1:
    dhcp4: no
    dhcp6: no
    addresses: [10.0.0.1]
    optional: true
    gateway4: 10.0.0.254
    nameservers:
      addresses: [8.8.8.8]
2
rtos-master:/etc/netplan#
```

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...

TOP

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 image<https://mirrors.tuna.tsinghua.edu.cn/ubuntu...>



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...

TOP

Ubuntu install

1.install qq 1>.download 2>.install 2.confir 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...



TOP

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](#)

TOP



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

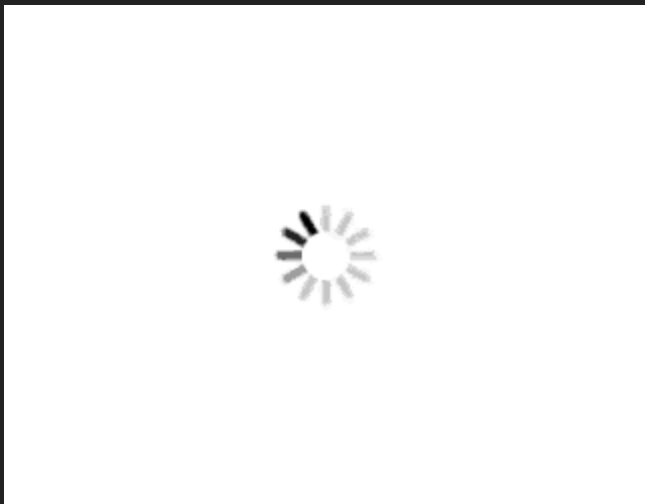


Recommended Posts

- [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](#)

TOP

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



Related Tags

Centos

GPU

lamps

ubuntu

other

-----Linux-----

VTK

Parallel Computing

Spike camp

ifort

TOP



TOP

