Lab1 Report

软件安装

- [x] 下载OpenMPI、BLAS和HPL的源代码并编译安装

集群搭建

- [x] 克隆虚拟机
- [x] 配置虚拟机互联
- [x] 测试节点间通信

性能测试

- [x] 在虚拟机集群上使用openMPI运行HPL性能测试，记录测试结果

Bonus（选做）

- [ ] 配置NFS并复现实验
- [ ] 使用Docker复现实验
- [ ] 使用Spack复现实验

---

1. 虚拟机的搭建

我搭建的虚拟机环境配置如下：

```
Hypervisor : VMware Workstation Pro 17.5.2
OS : ubuntu-18.04.6-64bit
Hard Disk : 20GB
Memory : 4096MB
Network Adapter : NAT
Other Devices : 2CPU cores
```

装机完成后为虚拟机下载必要的build-seeential软件包，其中包含了全面的编译器和构建工具

```
sudo apt update
sudo apt install build-essential
```

2. 任务一：从源码构建OpenMPI和HPL

接下来的构建和安装分为三个部分

2.1 BLAS & CBLAS

BLAS

```
wget "http://www.netlib.org/blas/blas-3.12.0.tgz"
tar xvf blas-3.12.0.tgz
cd BLAS-3.12.0
make
```

前三句话没有问题，`make`的时候会报错

```
make : gfortran :No such file or directory
```

提示缺少了gfortran，需要下载:`sudo apt install gfortran`
再次`make`后将刚下载到的库文件复制到系统库文件

```
sudo cp blas_LINUX.a /usr/local/lib/libblas.a
```

```
lee@ubuntu:~/BLAS-3.12.0$ cp blas_LINUX.a /usr/local/lib/libblas.a
cp: cannot create regular file '/usr/local/lib/libblas.a': Permission denied
lee@ubuntu:~/BLAS-3.12.0$ sudo cp blas_LINUX.a /usr/local/lib/libblas.a
```

```
lee@ubuntu:~/openmpi-5.0.3$ cd /usr/local/lib
lee@ubuntu:/usr/local/lib$ ls
libblas.a  python3.6
```

CBLAS

```
wget http://www.netlib.org/blas/blast-forum/cblas.tgz
tar -xvf cblas.tgz
```

接下来我们的目标是接下来我们要编译CBLAS文件，得到cblas_LINUX.a

`make`之前需要修改Makefile。打开Makefile.in，可以看到

```
lee@ubuntu: ~/CBLAS
File  Edit  View  Search  Terminal  Help

#-----------------------------------------------------------------------
# Platform
#-----------------------------------------------------------------------

PLAT = LINUX

#-----------------------------------------------------------------------
# Libraries and includes
#-----------------------------------------------------------------------

BLLIB = /Users/julie/Documents/Boulot/lapack-dev/lapack/trunk/blas_LINUX.a
CBLIB = ../lib/cblas_$(PLAT).a

#-----------------------------------------------------------------------
# Compilers
#-----------------------------------------------------------------------

CC = gcc
FC = gfortran
LOADER = $(FC)

#-----------------------------------------------------------------------
                                                          29,1          50%
```

我们需要指定BLAS库的路径，刚刚我们已经把blas_LINUX.a复制到了系统库文件，修改路径如下

```
lee@ubuntu: ~/CBLAS
File  Edit  View  Search  Terminal  Help

#-----------------------------------------------------------------------------
# Platform
#-----------------------------------------------------------------------------

PLAT = LINUX

#-----------------------------------------------------------------------------
# Libraries and includes
#-----------------------------------------------------------------------------

BLLIB = /usr/local/lib/libblas.a
CBLIB = ../lib/cblas_$(PLAT).a

#-----------------------------------------------------------------------------
# Compilers
#-----------------------------------------------------------------------------

CC = gcc
FC = gfortran
LOADER = $(FC)

#-----------------------------------------------------------------------------
-- INSERT --                                                    26,31         50%
```

这样就可以make

```
lee@ubuntu: ~/CBLAS
File  Edit  View  Search  Terminal  Help

                CALL STEST1(SASUMTEST(N,SX,INCX),STEMP,STEMP,SFAC)
                                                      1
Warning: Rank mismatch in argument ‘strue1’ at (1) (scalar and rank-1) [-Wargume
nt-mismatch]
gfortran  -o xscblat1 c_sblat1.o c_sblas1.o ../lib/cblas_LINUX.a /usr/local/lib/
libblas.a
gcc -I../include -O3 -DADD_ -c c_dblas1.c
gfortran -O3   -c c_dblat1.f
c_dblat1.f:214:48:

                CALL STEST1(DNRM2TEST(N,SX,INCX),STEMP,STEMP,SFAC)
                                                      1
Warning: Rank mismatch in argument ‘strue1’ at (1) (scalar and rank-1) [-Wargume
nt-mismatch]
c_dblat1.f:218:48:

                CALL STEST1(DASUMTEST(N,SX,INCX),STEMP,STEMP,SFAC)
                                                      1
Warning: Rank mismatch in argument ‘strue1’ at (1) (scalar and rank-1) [-Wargume
nt-mismatch]
gfortran  -o xdcblat1 c_dblat1.o c_dblas1.o ../lib/cblas_LINUX.a /usr/local/lib/
libblas.a
gcc -I../include -O3 -DADD_ -c c_cblas1.c
```

P.S. 中间有几条warning，但没有error

```
lee@ubuntu:~/CBLAS$ cd lib
lee@ubuntu:~/CBLAS/lib$ ls
cblas_LINUX.a
lee@ubuntu:~/CBLAS/lib$
```

成功在 /CBLAS/lib中生成了cblas_LINUX.a 把它也复制到`/usr/local/lib/libcblas.a`

```
sudo cp cblas_LINUX.a /usr/local/lib/libcblas.a
```

2.2 OpenMPI

```
wget "https://download.open-mpi.org/release/open-mpi/v5.0/openmpi-5.0.3.tar.gz"
tar xvf openmpi-5.0.3.tar.gz
cd openmpi-5.0.3
```

下载好后安装在特定的路径`/usr/local/openMPI`

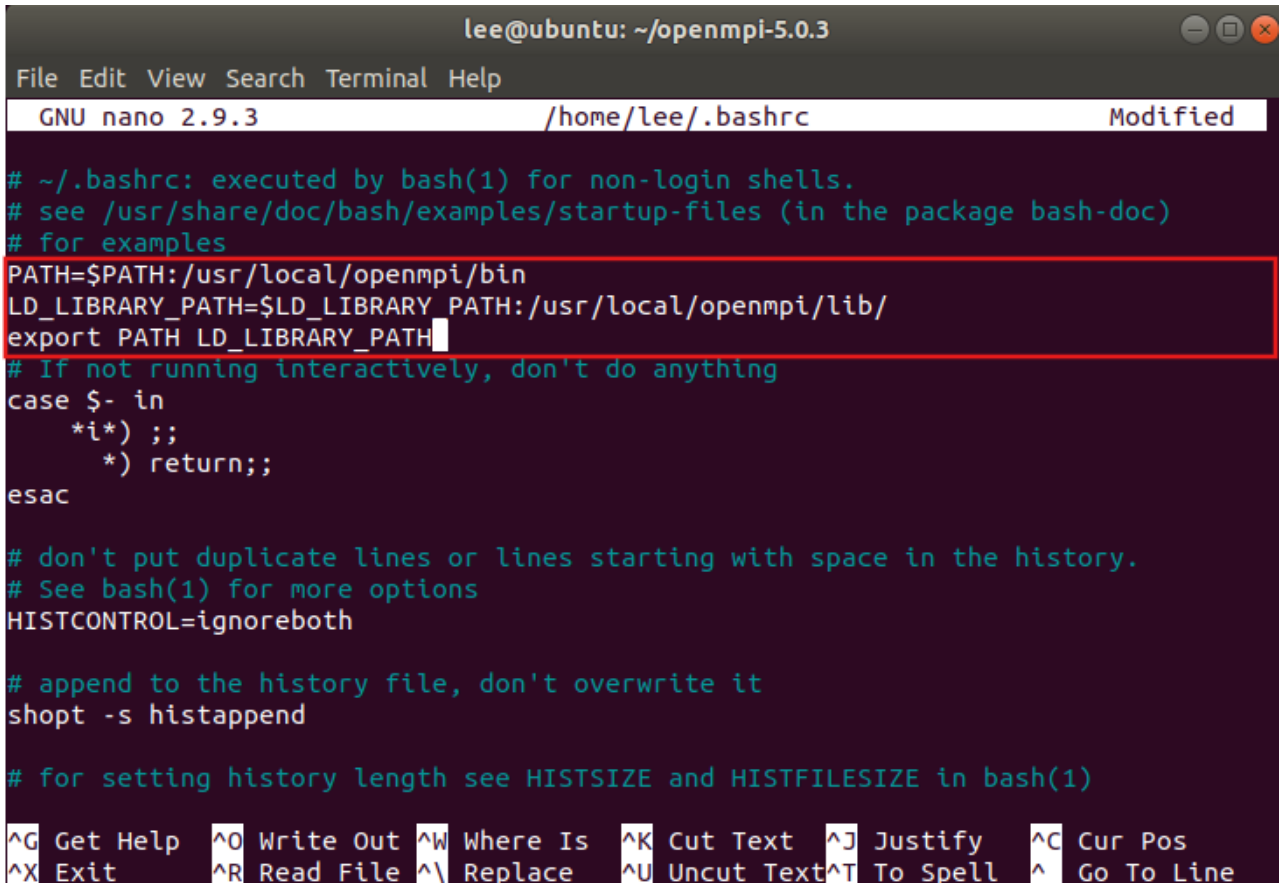
```
./configure --prefix=/usr/local/openMPI
make
sudo make install
```

漫长的等待后安装完成

接下来需要修改`PATH`和`LD_LIBRARY_PATH`(之后讲MPI的时候会提到)，我是使用nano打开修改的

```
nano ~/.bashrc
```

在`.bashrc`的最上面配置环境变量



最后运行一下使修改生效

```
source ~/.bashrc
```

2.3 HPL

```
wget https://netlib.org/benchmark/hpl/hpl-2.3.tar.gz
tar -xvf hpl-2.3.tar.gz
cd hpl-2.3
```

为HPL构建提供一个合适的Makefile文件

```
cp setup/Make.Linux_PII_CBLAS ./Make.Linux_PII
```

对这个Make.Linuc_PII文件进行修改

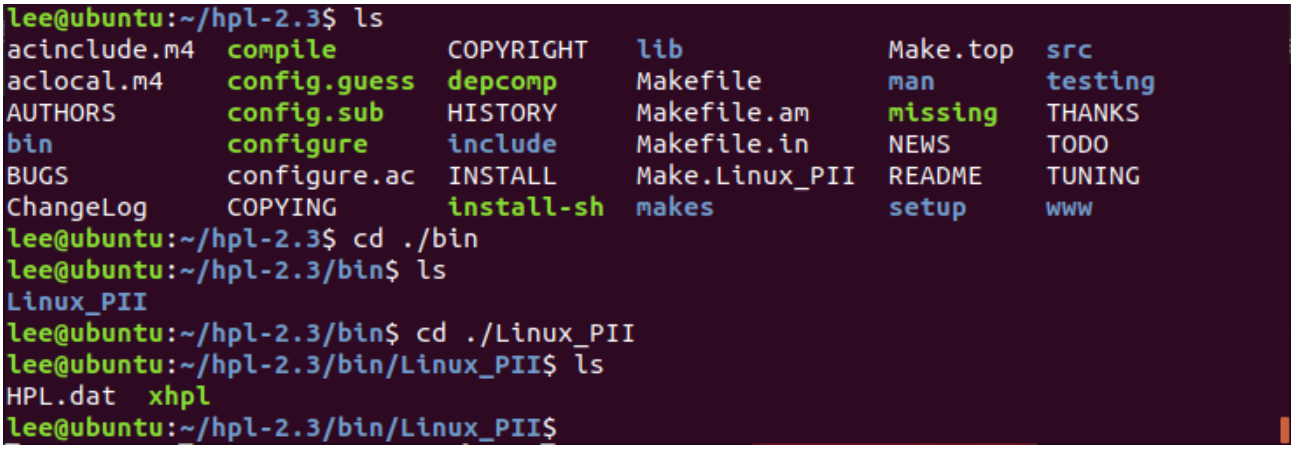
```
ARCH         = Linux_PII_CBLAS -> Linux_PII
TOPdir       = $(HOME)/hpl-2.3 -> /home/lee/hpl-2.3
MPdir        = /usr/local/mpi ->/usr/local/openmpi
MPinc        = -I$(MPdir)/include
MPlib        = $(MPdir)/lib/libmpich.a -> $(MPdir)/lib/libmpi.so
LAdir        = $(HOME)/netlib/ARCHIVES/Linux_PII -> /home/lee/CBLAS
```

```
LAinc        =
LAlib        = $(LAdir)/libcblas.a $(LAdir)/libatlas.a -> /usr/local/lib/libcblas.a
/usr/local/lib/libblas.a -lgfortran
CC           = /usr/bin/gcc -> /usr/local/openMPI/bin/mpicc
```

修改完成后，根据刚才修改的Makefile去make

```
make arch=Linux_PII
```

可以在`/hpl-2.3/bin/Linux_PII`目录下找到的可执行文件xhpl



P.S 任务一源码构建的内容虽然看起来不甚复杂，但对于新手属实不友好。前置实验对Angband的构建中，对安装路径强调的不多，在实验文档中说 ./configure # 不带参数，将默认安装到 /usr/local/ 下，此时不需要修改 PATH 和 LD_LIBRARY_PATH 等；如果你使用 --prefix 参数指定了安装路径，则可能需要修改 PATH 和 LD_LIBRARY_PATH。
但在第一次使用尝试（ubuntu）的时候内存不足，第二次改用Debian发现并没有下载到local里，而是在/home/lee/下，BLAS也完全没有配好，既没有把库放在正确的位置，也没有在Makefile.Linux_PII中修改成正确的路径，导致一直error，花了很长时间一度很崩溃。第三次尝试又换回ubuntu，configure的时候用了--prefix指定/usr/local，添加了PATH和LD_LIBRTARY_PATH环境变量，按照Makefile去放置库

```
/usr/bin/ld: cannot find /home/dqy/BLAS-3.12.0/blas_LINUX.a: No such file or dir
ectory
/usr/bin/ld: cannot find /usr/local/lib/libmpich.so: No such file or directory
collect2: error: ld returned 1 exit status
```

3. 任务二：使用HPL测试虚拟机集群的性能

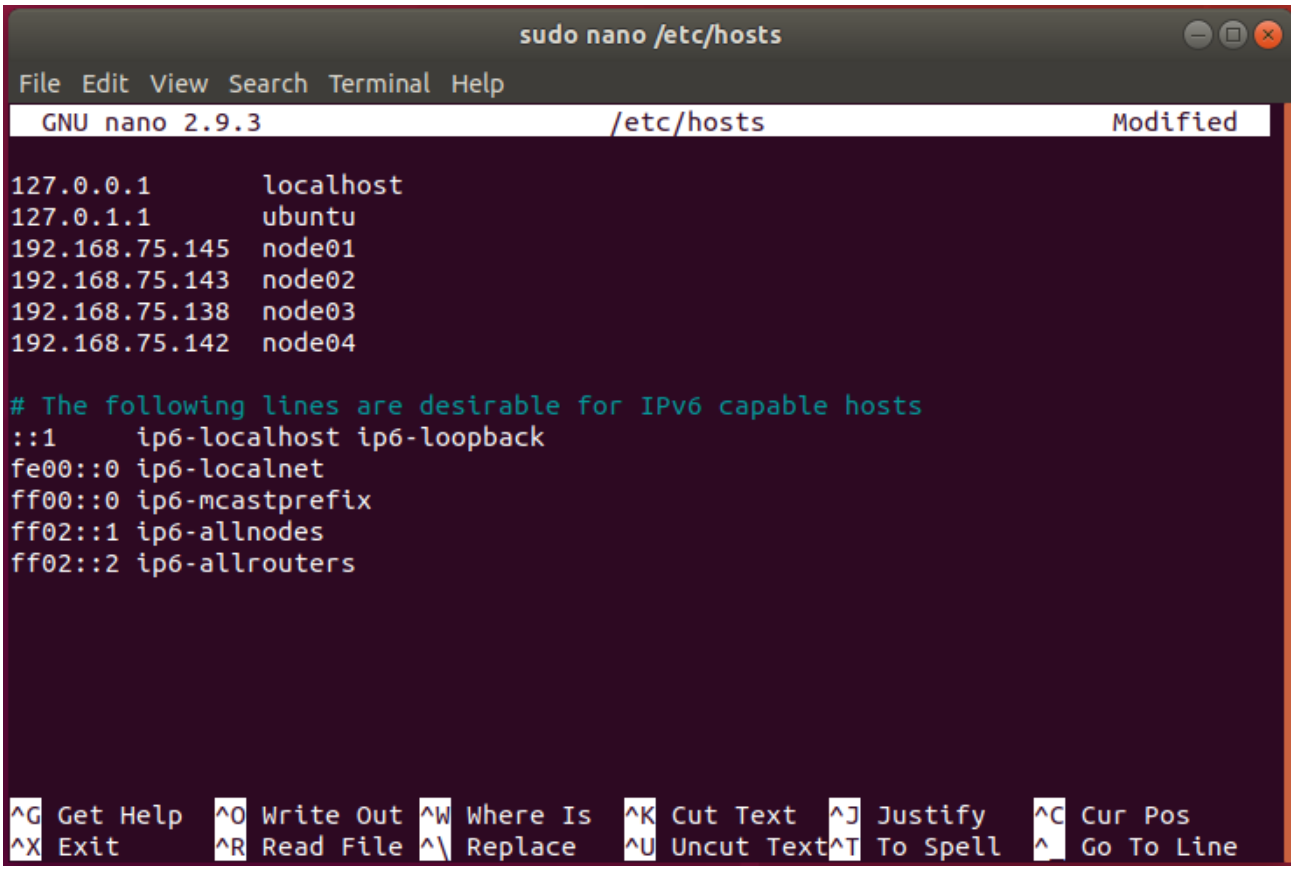
3.1 集群节点间的连接与互访

用VMware Workstation自带的功能克隆虚拟机，命名为node01，node02，node03，node04。
在克隆时选择*完整克隆*

注意，不只是在 Hypervisor 中修改名字，还需要在虚拟机中修改 /etc/hostname 我们可以用 `sudo nano /etc/hostname`来修改名称,之后`reboot`重启

```
# 查看各台虚拟机的ip地址:
ip addr
node01: 192.168.75.145
node02: 192.168.75.143
node03: 192.168.75.138
node04: 192.168.75.142
```

获取后在node01中修改`/etc/hosts`文件，添加其他节点的地址



根据ssh原理，我们需要在主节点(node01)上生成公钥，把公钥放到node02/03/04上，建立链接。(这一过程类似于第一次登录ZJU集群时的操作)

```
ssh-keygen # 注意不需要为密钥设置密码，全程回车即可
ssh-copy-id user@hostname  #e.g.ssh-copy-id lee@node02
```

```
lee@node01:~
File  Edit  View  Search  Terminal  Help
Generating public/private rsa key pair.
Enter file in which to save the key (/home/lee/.ssh/id_rsa):
Created directory '/home/lee/.ssh'.
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /home/lee/.ssh/id_rsa.
Your public key has been saved in /home/lee/.ssh/id_rsa.pub.
The key fingerprint is:
SHA256:jgFOgD0GWUMhZMTFrghEyB58jjpUi06mS4Qutf1WLws lee@node01
The key's randomart image is:
+---[RSA 2048]----+
|@%Oo             |
|=B+*             |
|+.O.+            |
|oO.* .           |
|%..o. . S        |
|*=. .  +.        |
|oo   .E...       |
|.     o.. .      |
|      .  .o      |
+----[SHA256]-----+

~ ..................................................... took 9s | at 23:17:05
>
```

P.S 这里有个小失误，由于是重装了一台ubuntu来做的，所以之前没有装openssh-server和openssh-client，应该先装好再克隆的

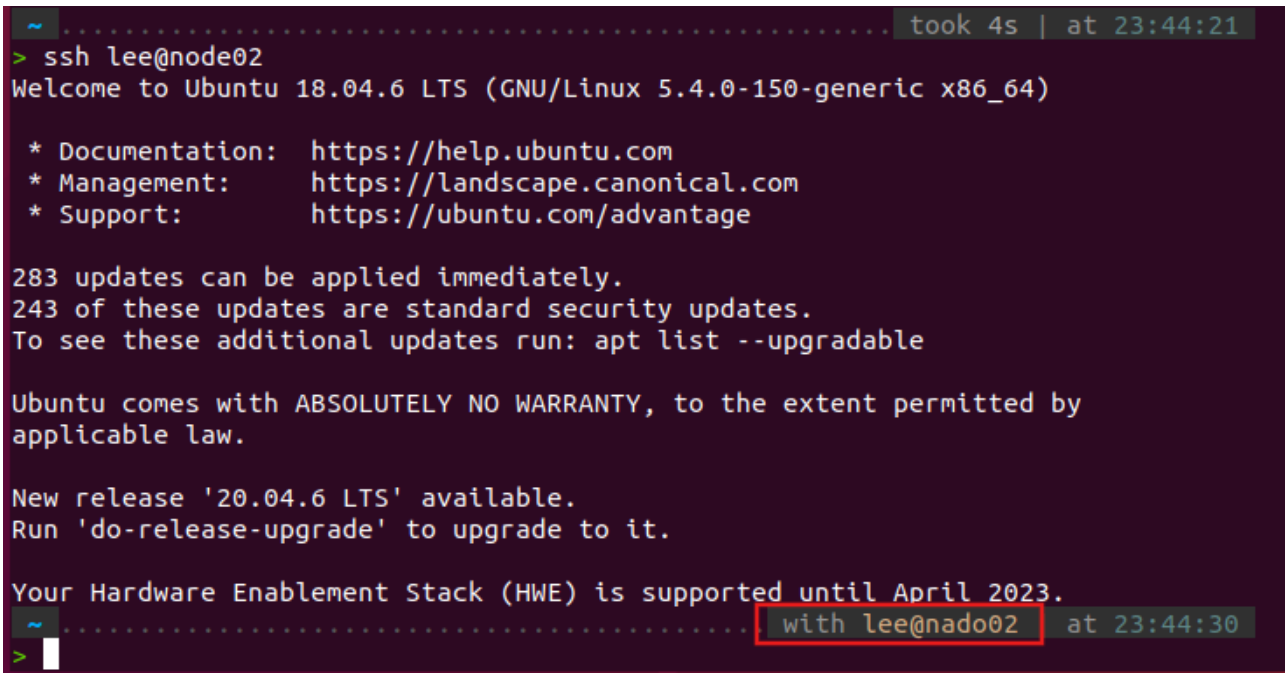
```
~ ..................................................... took 6s | at 23:27:28
> ssh-copy-id lee@node02
/usr/bin/ssh-copy-id: INFO: attempting to log in with the new key(s), to filter
out any that are already installed

/usr/bin/ssh-copy-id: ERROR: ssh: connect to host node02 port 22: Connection ref
used
```

之后再操作就不会error了

```
~ ..................................................................... at 23:28:08
> ssh-copy-id lee@node02
The authenticity of host 'node02 (192.168.75.137)' can't be established.
ECDSA key fingerprint is SHA256:hsHvhBETaJcW15beekGTyM7368Q1Hmpg0VayLG+CTB0.
Are you sure you want to continue connecting (yes/no)? yes
/usr/bin/ssh-copy-id: INFO: attempting to log in with the new key(s), to filter
out any that are already installed
/usr/bin/ssh-copy-id: INFO: 1 key(s) remain to be installed -- if you are prompt
ed now it is to install the new keys
lee@node02's password:

Number of key(s) added: 1

Now try logging into the machine, with:   "ssh 'lee@node02'"
and check to make sure that only the key(s) you wanted were added.
```

根据提示尝试登录node02

```
ssh lee@node02
```

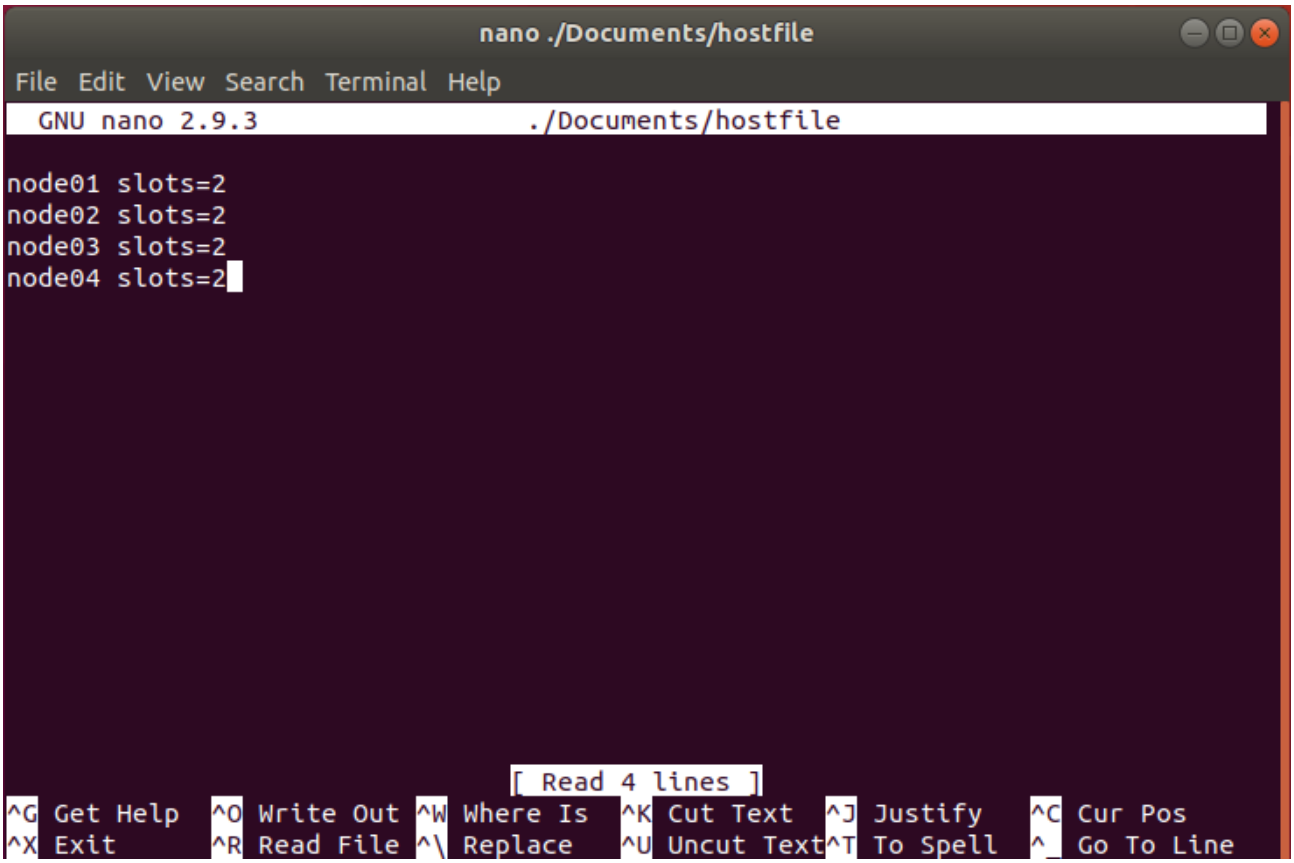


红框处表面我们已经可以从node01登录node02的shell了

对node03/node04做同样的操作

3.2 测试MPI运行

在node01上写一个hostfile，指定节点和进程数(直接新建就好，这里我建在了`/home/Documents`)



P.S 这个slots似乎是与当时设置的cores有关的，在前面测试MPI能否正常运行的时候，执行`mpirun -n 2 hello_c`是可以的，如果超过2个MPI processes就会error。似乎是MPI会计算CPU的算力上限，给出限制。

SOLVED:设置环境变量声明`export OMP_NUM_THREADS=8`就可以设定线程数量

```
There are not enough slots available in the system to satisfy the 6
slots that were requested by the application:
```

```
Hello, world, I am 0 of 2, (Open MPI v5.0.3, package: Open MPI lee@ubuntu Distri
bution, ident: 5.0.3, repo rev: v5.0.3, Apr 08, 2024, 105)
Hello, world, I am 1 of 2, (Open MPI v5.0.3, package: Open MPI lee@ubuntu Distri
bution, ident: 5.0.3, repo rev: v5.0.3, Apr 08, 2024, 105)
lee@ubuntu:~/openmpi-5.0.3/examples$
```

简单测试MPI可以正常运行

```
mpirun --hostfile hostfile cat /etc/hostname
```

```
lee@node01:~/Documents
File  Edit  View  Search  Terminal  Help
 the list of known hosts.
--------------------------------------------------------------------------
PMIx was unable to find a usable compression library
on the system. We will therefore be unable to compress
large data streams. This may result in longer-than-normal
startup times and larger memory footprints. We will
continue, but strongly recommend installing zlib or
a comparable compression library for better user experience.

You can suppress this warning by adding "pcompress_base_silence_warning=1"
to your PMIx MCA default parameter file, or by adding
"PMIX_MCA_pcompress_base_silence_warning=1" to your environment.
--------------------------------------------------------------------------
node01
node01
nado02
nado02
nado03
nado03
node04
node04

 ~/Documents ..................................................... at 06:07:20
>
```

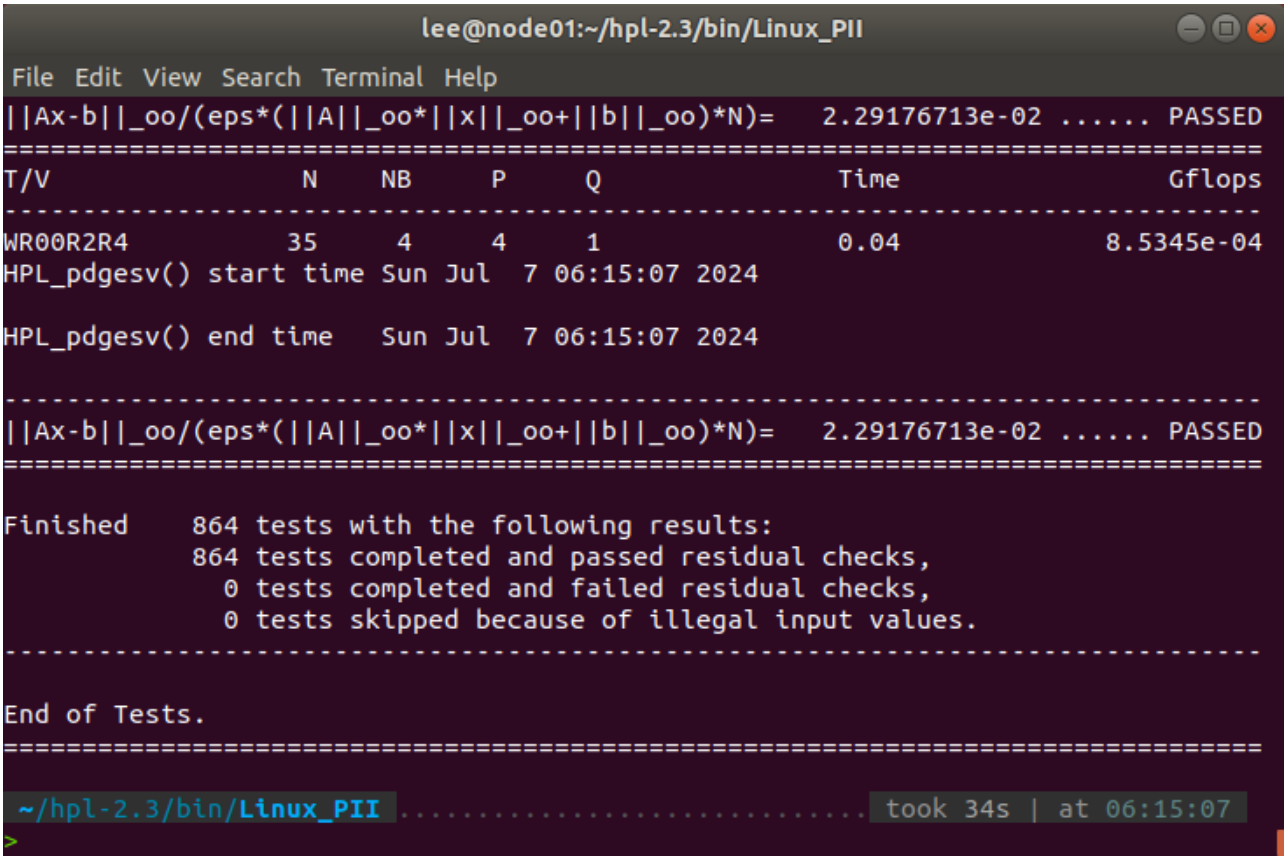
3.3 运行HPL

切换工作目录到`HPL`所在目录，`xhpl`需要在工作目录下找到`HPL.dat`

```
cd /hpc-2.3/bin/Linux_PII
```

找到xphl可执行文件，运行

```
mpirun --hostfile /home/lee/Documents/hostfile ./xhpl
```



运行成功！

P.S 在写实验报告的时候第二次过了一下流程，发现ssh居然连不上了，后来发现虚拟机重启后IP地址也变了(?)，需要修改`hosts`文件。

4.Bonus尝试（未成功）

其实我完全还不清楚要怎么用Docker来复现集群的搭建，但我觉得Docker容器和虚拟机应该是十分类似的，我的基本想法是：在一个ubuntu容器中搭建一个类似之前The One一样的主节点，把它创建成镜像。用这个镜像再创建三个容器（类似于克隆虚拟机），让他们互相ping通，形成集群。概括来说是一台主机、四个容器的结构。

但由于时间和能力有限，只在一个Docker容器中复现了The One的环境配置，并手动构建了镜像，这里只记录了遇到的问题，其他步骤与The One的配置一样

新的ubuntu-container进去后只有root用户，需要自己创建一个用户、下载sudo，并把该用户添加到sudoers file中

使用root用户权限，打开 /etc/sudoers ，添加

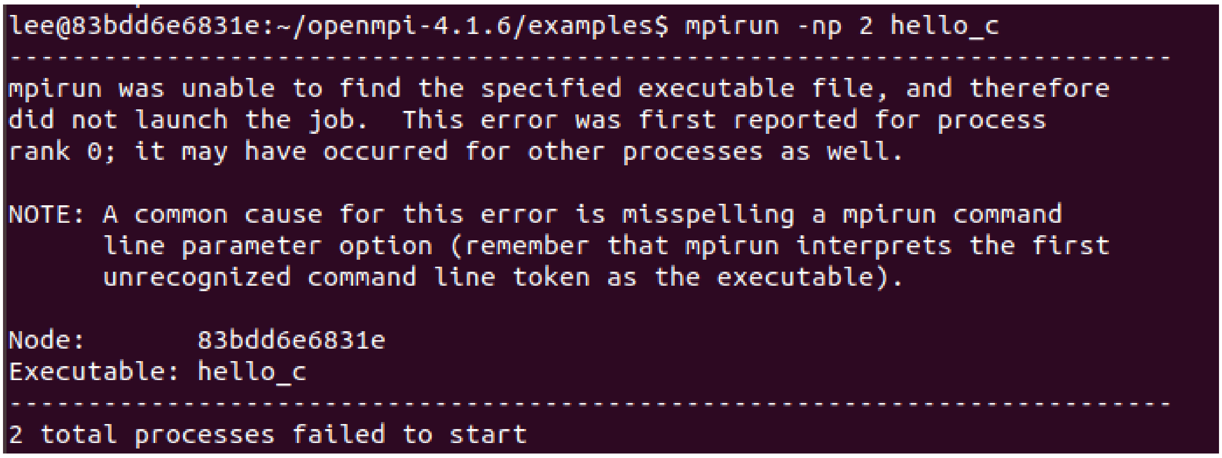
```
lee ALL=(ALL) ALL
```

在配置CBLAS进行make的时候，本来的warning变成了error，需要在Makefile.in中对编译选项进行修改

```
FC=gfortran --> FC=gfortran -fallow-argument-mismatch
```

忽略这个报错，之后就可以正常make

之后的构建与之前完全一致，但在测试OpenMPI的时候出现了问题

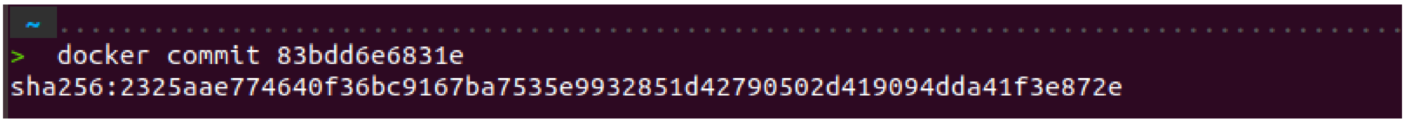


```
lee@83bdd6e6831e:~/openmpi-4.1.6/examples$ mpirun -np 2 hello_c
--------------------------------------------------------------------------
mpirun was unable to find the specified executable file, and therefore
did not launch the job.  This error was first reported for process
rank 0; it may have occurred for other processes as well.

NOTE: A common cause for this error is misspelling a mpirun command
      line parameter option (remember that mpirun interprets the first
      unrecognized command line token as the executable).

Node:       83bdd6e6831e
Executable: hello_c
--------------------------------------------------------------------------
2 total processes failed to start
```

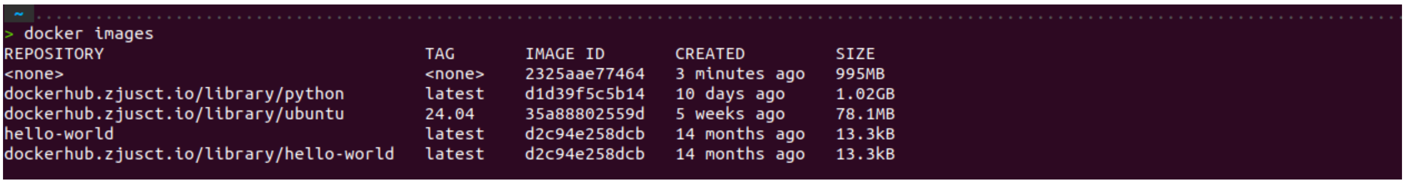
由于时间问题，该报错仍然没有解决

手动构建镜像后可以再 `images` 中查看到该镜像

```
docker commit 83bdd6e6831e
```



```
~
>  docker commit 83bdd6e6831e
sha256:2325aae774640f36bc9167ba7535e9932851d42790502d419094dda41f3e872e
```

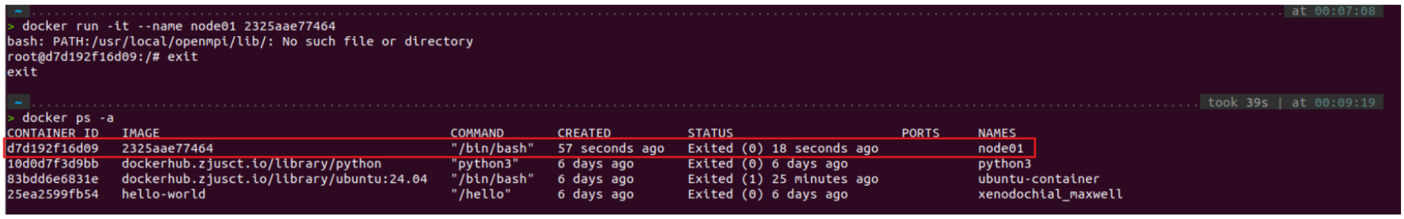


```
~
> docker images
REPOSITORY                               TAG       IMAGE ID       CREATED          SIZE
<none>                                   <none>    2325aae77464   3 minutes ago    995MB
dockerhub.zjusct.io/library/python       latest    d1d39f5c5b14   10 days ago      1.02GB
dockerhub.zjusct.io/library/ubuntu       24.04     35a88802559d   5 weeks ago      78.1MB
hello-world                              latest    d2c94e258dcb   14 months ago    13.3kB
dockerhub.zjusct.io/library/hello-world  latest    d2c94e258dcb   14 months ago    13.3kB
```

我们可以用

```
docker run -it --name node01 2325aae77464
```

来生成一个使用该镜像的容器



```
~                                                                                    at 00:07:08
> docker run -it --name node01 2325aae77464
bash: PATH:/usr/local/openmpi/lib/: No such file or directory
root@d7d192f16d09:/# exit
exit

~                                                                        took 39s | at 00:09:19
> docker ps -a
CONTAINER ID   IMAGE                                   COMMAND       CREATED          STATUS                       PORTS     NAMES
d7d192f16d09   2325aae77464                            "/bin/bash"   57 seconds ago   Exited (0) 18 seconds ago              node01
10d0d7f3d9bb   dockerhub.zjusct.io/library/python      "python3"     6 days ago       Exited (0) 6 days ago                  python3
83bdd6e6831e   dockerhub.zjusct.io/library/ubuntu:24.04   "/bin/bash"   6 days ago       Exited (1) 25 minutes ago              ubuntu-container
25ea2599fb54   hello-world                             "/hello"      6 days ago       Exited (0) 6 days ago                  xenodochial_maxwell
```

后续应该需要设置容器的网络来实现相互的链接

5. 总结

至此，Lab1的大部分工作告一段落。说实话，这对大佬来说当然是轻而易举的事情，作为一个之前连linux和虚拟机都从来没碰过的纯纯小白，当意识到有一个小集群运行在自己电脑上时，还是相当激动的。
我不确定会在HPC这条路上走多远，但很高兴，已经开始了

```
hello new world
```