







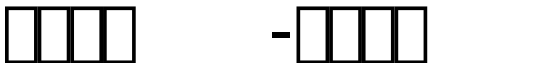




-  _____
-  _____
-  _____
-  _____
-  _____
-  _____
-  _____
-  _____
-  _____



1. 
2. 

Web

5. Web x fwd ssh sftp

SSH

2. Username: /10.1.0.101/self yaoge yaoge/10.1.0.101/self

SFTP

2. Username: /10.1.0.101/self yaoge yaoge/10.1.0.101/self



4. passwd 8

5.

VPN



VPN

1. VPN
2. VPN

eScience VPN

1. VPN Client
2. njucm.yaoge123.com
3. 4433
4.
5. VPN eScience



1. SFTP SFTP
2. ZMODEM rz sz
3.
4.



USB 3.0

ext4/XFS/exFAT

- ext4/XFS Linux Linux)
- exFAT Windows Linux

Windows WSL(Windows Subsystem for

目录

- 1. 目录 fsa
 - 2. 目录 myquota
 - 3. 目录 7
 - 4. 目录
- <10% >10%

access

目录

1. 目录 Web
 2. 目录 Web <https://access.nju.edu.cn>
 3. 目录
 4. 目录 RFC 6238 TOTP APP
 5. 目录 APP
 6. 目录
- “ ”

Web

1. 目录 Web <https://access.nju.edu.cn>
2. 目录
3. 目录 APP
4. 目录 Java
5. Web xfce4/vnc ssh Web SFTP
6. 目录 Applications - Settings - Display - Resolution

SSH

1. 目录 access.nju.edu.cn 22 目录 njucm.yaoge123.com 5022
2. Username: 目录
3. Password: 目录 + 目录 YaoGe123 APP 123456
4. SSH X11-Forwarding
5. SSH Putty Xshell Bitvise SSH Client iTerm2 Termius.....

SFTP

1. 192.168.1.101 access.nju.edu.cn 22 njucm.yaoge123.com 5022
2. Username: yaoge123
3. Password: YaoGe123 + APP 123456
4. SFTP /hpc_login1 sftp (10.1.0.101)/self /fsa/home/yaoge123
5. SFTP Xftp(Windows) WinSCP Bitvise SSH Client Termius(macOS) FileZilla LFTP
- Xftp (Sessions) (Properties) (Options) (Use main connection only)

• WinSCP (Background Transfers)

• FileZilla (Site) (Transfer Settings) (Limit number of simultaneous connections) (Maximum number of connections) 1
6. SFTP SFTP Drive SSHFS
- SFTP Drive "Authentication Type" "Keyboard Interactive"

1. 5
2. access.nju.edu.cn
3. Shell PS1 \$ +
4. passwd 8
5.

--	--	--	--

--	--	--	--

The diagram illustrates the structure of an email address using a sequence of boxes representing characters. It shows the full address, the domain part, and the local part separately, along with a combined representation.

Full address: yaoge@hpc.nju.edu.cn

Domain part: @hpc.nju.edu.cn

Local part: yaoge

Combined representation: yaoge@hpc.nju.edu.cn

--	--	--	--

- 
- 

--	--	--

- [] seaf-cli [] Linux []
- [] seaf-file-applet
- [] seadrive [] Linux []
- [] seadrive-gui

--	--	--	--	--	--	--	--	--

1. Token

```
curl -d 'username=<username>@hpc.nju.edu.cn' -d 'password=<password>'
https://box.nju.edu.cn/api2/auth-token/
```

- [illegible]

```
[account]
server = https://box.nju.edu.cn
username = <username>@hpc.nju.edu.cn
token = <token>
is_pro = true
[general]
client_name = hpc-login
[cache]
size_limit = 10GB
clean_cache_interval = 10
```

3.

```
seadrive -c ~/seadrive.conf -f -d ~/.seadrive/data -l ~/.seadrive/data/logs/seadrive.log ~/SeaDrive
```

4. Transport endpoint is not connected fusermount -u ~/SeaDrive

5.

1.

```
mkdir ~/Seafile
```

2.

```
seaf-cli init -d ~/Seafile
```

3.

```
seaf-cli start
```

4. ID

```
seaf-cli list-remote -s https://box.nju.edu.cn -u <username>@hpc.nju.edu.cn
```

5. ID

```
seaf-cli sync -s https://box.nju.edu.cn -u <username>@hpc.nju.edu.cn -l <library-id> -d <folder>
```

```
seaf-cli download -s https://box.nju.edu.cn -u <username>@hpc.nju.edu.cn -l <library-id> -d <folder>
```

6.

seaf-cli status

7.

seaf-cli desync -d <folder>

8.

seaf-cli stop

☐ rclone ☐

rclone

rclone

1.

rclone

module load rclone

2.

rclone

~/.config/rclone/

rclone.conf

<username>

```
; hpc_box  
[hpc_box]  
type = seafile  
url = https://box.nju.edu.cn  
user = <username>@hpc.nju.edu.cn  
; true  
2fa = false
```

3.

<password>

rclone config update hpc_box pass <password>

4.

rclone ls hpc_box:

5.

<library>

rclone mkdir hpc_box:<library> --seafile-create-library

rclone mkdir hpc_box:test --seafile-create-library `test`

6.

```
rclone copy <destination_path> hpc_box:<source_path>
```

```
# myfile.txt   
#rclone copy myfile.txt hpc_box:test  myfile.txt  test   
# myfolder   
#rclone copy myfolder hpc_box:test  myfolder   
myfolder  test 
```

7.

```
rclone copy hpc_box:<source_path> <destination_path>
```

```
# `test` myfile.txt   
#rclone copy hpc_box:test/myfile.txt .  `test` myfile.txt   
# `test` myfolder   
#rclone copy hpc_box:test/myfolder .  `test` myfolder  
 myfolder 
```

8.

```
rclone copy hpc_box:<source_path> <destination_path> -P --no-traverse
```

```
# `test` myfile.txt   
#rclone copy hpc_box:test/myfolder . -P --no-traverse  `test` myfolder  
 myfolder 
```

9. rclone - commands
 rclone - seafiler rclone - storage systems



```

$ module Environment Modules
$ module Environment Module
(load) (unload) (switch)
$ module
/etc/profile ~/.bashrc ~/.bash_profile Environment Module
$ source Environment Module
$ module
Environment Modules
```



- module module help
- module avail
- module list
- module load MODULEFILE
- module unload MODULEFILE
- module switch OLD_MODULEFILE NEW_MODULEFILE module unload OLD_MODULEFILE; module load NEW_MODULEFILE
- module purge
- module whatis MODULEFILE
- module display MODULEFILE
- module use
- module unuse

Bash

```

$ Bash Login Shell
$ Login Shell Bash
$ Login Shell tcsh
```

```

#!/bin/tcsh # Shell
#BSUB ...
...
```

```
...  
#BSUB -L /bin/bash #[] [] [] [] Login Shell[] Bash  
...
```



```
$ module avail #[] [] [] [] [] [] [] []
```

```
----- /fs00/software/modulefiles -----  
gcc/5.2.0             impi/5.0.3.048  
iccifort/15.0.3       ips/2011sp1u3  
ics/2013              ips/2015u3  
ics/2013sp1u1         openmpi/1.10.0-gcc-5.2.0  
imkl/11.2.3           openmpi/1.10.0-iccifort-15.0.3
```

```
$ module list #[] [] [] [] [] []
```

```
No Modulefiles Currently Loaded. #[] [] [] [] [] []
```

```
$ icc --version #[] icc[] [] []
```

```
-bash: icc: command not found
```

```
$ module whatis ips/2015u3 #[] [] [] [] [] []
```

```
ips/2015u3           : Intel Parallel Studio XE 2015 Update 3 Cluster Edition
```

```
$ module load ips/2015u3 #[] [] [] []
```

```
$ icc --version
```

```
icc (ICC) 15.0.3 20150407
```

```
Copyright (C) 1985-2015 Intel Corporation. All rights reserved.
```

```
$ module list #[] [] [] [] [] []
```

```
Currently Loaded Modulefiles:
```

```
1) ips/2015u3
```

```
$ module unload ips/2015u3 #[] [] [] []
```



```
$ module use
```

```
Search path for module files (in search order):
```

```
/fs00/software/modulefiles
```

```
$ module avail
```

```
--- /fs00/software/modulefiles ---
```

```
gcc/12.1.0
```

```
.....
```

```
$ module use /fs00/software/modulefiles/oneapi/2024.0 #[] MODULEPATH[][]
```

```
$ module use
```

```
Search path for module files (in search order):
```

```
/fs00/software/modulefiles/oneapi/2024.0
```

```
/fs00/software/modulefiles
```

```
$ module avail
```

```
--- /fs00/software/modulefiles/oneapi/2024.0 ---
```

```
mkl32/2024.0
```

```
compiler/2024.0.2
```

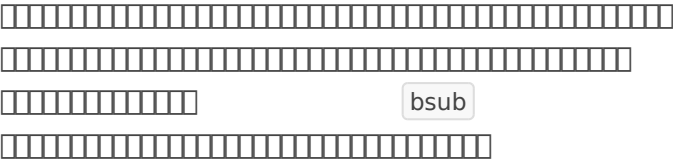
```
mkl/2024.0
```

```
.....
```

```
--- /fs00/software/modulefiles ---
```

```
gcc/12.1.0
```

```
.....
```



bsub

bsub



bsub [options] command [arguments]

- [options] bsub CPU
- command MPI mpirun
- [arguments]

“ e5v3ib 24 MPI

```
$ bsub -q e5v3ib -n 24 "module load oneapi/2024.0/mpi && mpirun ./app"
Job <3206000> is submitted to queue <e5v3ib>
```

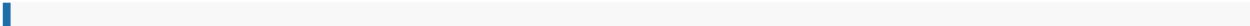


bsub < jobfile

jobfile shell

#BSUB [options]
command [arguments]

#BSUB bsub



e5v3ib

48

MgSiO3

out

err

Intel MPI

0

```

$ cat job.lsf
#BSUB -q e5v3ib
#BSUB -n 48
#BSUB -J MgSiO3
#BSUB -o out
#BSUB -e err
module load ips/2018u4
mpirun ./app

$ bsub < job.lsf
Job <3207099> is submitted to queue <e5v3ib>.

```

```

$ bsub -q e5v3ib -n 48 -J MgSiO3 -o out -e err "module load ips/2018u4;mpirun ./app"
Job <3207099> is submitted to queue <e5v3ib>.

```

bsub

- -J job_name

- -n min_tasks[,max_tasks] CPU -n 4 4~8 -n 4,8
- -m bmggroup hostname/hostgroup !
 +[num] c04n01 c04n02 -m "c04n01
 c04n02" f01n01~n03 f01n01 f01n02 -m "f01n01+2
 f01n02+1 f01n03"
- -R "res_req" -R largemem
- -R "select[hname!=host_name]" host_name && -R
 "select[hname!=x001 && hname!=x002]" x001 x002
- -x
- -W [hour:]minute kill

CPU

- R affinity[core:cpubind=core:membind=localprefer:distribute=pack] MPI CPU

- r all
- Q "exit_code [exit_code ...]" ~

- l %j JOBID -o -oo output_%j -o /dev/null
- K
- i input_file
- o output_file
- e error_file

GPU

-gpu GPU GPU CPU GPU CPU

-gpu : num=1:mode=shared:mps=no:j_exclusive=yes

- num=number GPU
- mode=shared | exclusive_process GPU shared Nvidia/AMD DEFAULT compute mode exclusive_process Nvidia EXCLUSIVE_PROCESS
- mps=yes | no Nvidia Multi-Process Service (MPS) MPS GPU MPS CUDA Context GPU
- aff=yes | no GPU-CPU -R affinity[core:cpubind=core:membind=localprefer:distribute=pack] GPU-CPU



```

#####
# bsub ##### -w 'dependency_expression'
#####

```

- `-w 'done(job_ID | "job_name")'` ##### `job_ID` `job_name` ##### `DONE`##### `0`
- `-w 'ended(job_ID | "job_name")'` ##### `job_ID` `job_name` ##### `EXIT` `DONE`
- ##### `&&` (AND) `||` (OR) `!` (NOT)
- ##### `1`#####

`###`_____

MPI/OpenMP

OpenMP (Open Multi-Processing) ##### MPI (Message
Passing Interface) ##### OpenMP
MPI
#####

OpenMP `#####` MPI ##### NUMA##### OpenMP
NUMA##### MPI
MPI##### NUMA
#####

`mpirun`##### `LSB_MCPU_HOSTS`##### MPI
CPU##### MPI/OpenMP##### MPI
#####

1. `#BSUB -n` ##### CPU##
2. #####

source /fs00/software/lsf/misc/ompthreads.sh [N]
3. `#####` MPI ##### OpenMP ##### `OMP_NUM_THREADS`
CPU
#####





- LSB_JOBID[] ID
- LSB_QUEUE[]
- LSB_JOBNAME[]
- LSB_DJOB_NUMPROC[] CPU[]
- LSB_DJOB_HOSTFILE[]
- LSB_HOSTS[] CPU[]
- LSB_MCPU_HOSTS[] CPU[]

```
LSB_DJOB_NUMPROC=6
LSB_HOSTS="node1 node1 node1 node2 node2 node2"
LSB_MCPU_HOSTS="node1 3 node2 3"
```

```
$ cat $LSB_DJOB_HOSTFILE
node1
node1
node1
node2
node2
node2
```

```
## LSB_HOSTS [ ] LSB_MCPU_HOSTS [ ] LSB_MCPU_HOSTS
[ ] LSB_HOSTS [ ] LSB_HOSTS [ ] 4096 [ ]
LSB_MCPU_HOSTS[ ]
```



[] e52660 []

```
$ bsub -q e52660 ./app
Job <3279929> is submitted to queue <e52660>.
$ cat job.lsf
#BSUB -q e52660
```

```
./app
```

```
$ bsub < job.lsf
```

```
Job <3279930> is submitted to queue <e52660>.
```

MPI

MPI 

mpirun 



48 

Intel MPI 

e5v3ib 

```
$ bsub -q e5v3ib -n 48 "module load ips/2018u4;mpirun ./app"
```

```
Job <3280120> is submitted to queue <e5v3ib>.
```



48 

Open MPI 

e5v3ib 

```
$ cat job.lsf
```

```
#BSUB -q e5v3ib
```

```
#BSUB -n 48
```

```
module load iccifort/15.0.3 imkl/11.2.3 openmpi/1.10.0-iccifort-15.0.3
```

```
mpirun ./app
```

```
$ bsub < job.lsf
```

```
Job <3280122> is submitted to queue <e5v3ib>.
```

OpenMP

OpenMP 

-n 

CPU 



64 

OpenMP 

e7v4ib 

-nt 

```
$ bsub -q e7v4ib -n 64 "./app-nt ${LSB_DJOB_NUMPROC}"
```

```
Job <3348175> is submitted to queue <e7v4ib>.
```



64 

OpenMP 

e7v4ib 

OMP_NUM_THREADS



```
$ cat job.lsf
```

```
#BSUB -q e7v4ib
```

```
#BSUB -n 64

OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"

./app

$ bsub < job.lsf
Job <3348182> is submitted to queue <e7v4ib>.
```

MPI/OpenMP

 MPI  6  OpenMP 

          OMP_NUM_THREADS  

```
#BSUB -q 6140ib
#BSUB -n 72
export OMP_NUM_THREADS=6
source /fs00/software/lsf/misc/ompthreads.sh
module load ips/2018u4
mpirun ./run
```

```
#BSUB -q 6140ib
#BSUB -n 72
source /fs00/software/lsf/misc/ompthreads.sh 6
module load ips/2018u4
mpirun ./openmx -nt 6
```

GPU

    1  GPU   e5v4p100ib 

```
bsub -q e5v4p100ib -gpu num=1 ./gpu_app
```

    4  GPU   62v100ib    GPU-CPU 

```
bsub -q 62v100ib -gpu "num=4:aff=yes" ./gpu_app
```



命令	説明
<code>bjobs</code>	実行中のジョブの一覧を出力する
<code>bjobs -l JOBID</code>	指定したジョブの詳細情報を出力する
<code>bhist</code>	実行履歴の一覧を出力する
<code>bhist -l JOBID</code>	指定したジョブの実行履歴の詳細情報を出力する
<code>bpeek JOBID</code>	指定したジョブの標準出力/標準エラー出力をリアルタイムで表示する
<code>bkill JOBID</code>	指定したジョブを強制終了させる
<code>btopy JOBID</code>	指定したジョブのトップレベルのディレクトリを出力する
<code>bbot JOBID</code>	指定したジョブのボトムレベルのディレクトリを出力する



`bjobs` 実行中のジョブの一覧を出力する

ステータス	説明
PEND	実行待ちのジョブ
PROV	実行中のジョブ sbatchd 実行中 PROV 実行中
PSUSP	実行待ちのジョブ LSF 実行待ち
RUN	実行中のジョブ
USUSP	実行待ちのジョブ LSF 実行待ち
SSUSP	実行待ちのジョブ LSF 実行待ち
DONE	完了したジョブ 0 完了
EXIT	終了したジョブ

UNKN	UNKN
UNKN	<div> <div>UNKN</div> <div> <div>①</div> <div>②</div> </div> </div>
WAIT	
ZOMBI	<div> <div>①</div> <div> <div>kill</div> <div>UNKN</div> <div>②</div> <div>LSF</div> <div>ID</div> <div>③</div> <div>LSF</div> <div>ZOMBI</div> <div>ZOMBI</div> <div>EXIT</div> <div>MultiCluster</div> <div>ZOMBI</div> <div>ZOMBI</div> <div>ZOMBI</div> </div> </div>



```
bwait -w "wait_condition" [-t timeout]
```

bjobs bwait

- w wait_condition bsub -w
- t timeout 1-525600

--	--	--	--

--	--	--

[illegible]Linux

```
/test  /test/1  /test/2  /test
```

[illegible][illegible][illegible]

--	--	--	--	--

```
bgadd /test#
```

```
bsub -g /test# bsub
```

--	--	--	--	--

```
bjgroup /test#
```

--	--	--	--	--

```
bgdel /test#####
```

```
bjobs -g /test
```

```
bkill -g /test 0#
```

--	--	--	--

[illegible]

ID

```
bsub -j "arrayName[indexList, ...]"
```

[illegible]

indexList = start[-end[:step]]

%I %J %I %J ID
LSB_JOBINDEX

```
bsub -J "myArray[1-10]" myJob# 10
bsub -J "myArray[1-10]" -i "input.%I" -o "output.%I" myJob#
bkill 123[1]# jobid 123
bkill 123# jobid 123
```

1 CPU

4x5650

```
$ cat job.lsf
#BSUB -q x5650
./a.out >& 1.out
./a.out >& 2.out
./a.out >& 3.out
./a.out >& 4.out

$ bsub < job.lsf
Job <3366369> is submitted to queue <x5650>.
```

N CPU N CPU
wait

□

12□□□□□□□□□□□□□□□□

x5650□□□□□□□□□□

```
$ cat job.lsf
#BSUB -q x5650
#BSUB -n 12
( ./a.out >& 1.out )&
( ./a.out >& 2.out )&
( ./a.out >& 3.out )&
( ./a.out >& 4.out )&
( ./a.out >& 5.out )&
( ./a.out >& 6.out )&
( ./a.out >& 7.out )&
( ./a.out >& 8.out )&
( ./a.out >& 9.out )&
( ./a.out >& 10.out )&
( ./a.out >& 11.out )&
( ./a.out >& 12.out )
wait
```

```
$ bsub < job.lsf
Job <3366370> is submitted to queue <x5650>.
```




bqueues

```
$ bqueues
QUEUE_NAME    PRIO STATUS      MAX JL/U JL/P JL/H NJOBS  PEND  RUN  SUSP
x7542!        50 Open:Active    - - - - 24  0 24  0
e5645!        50 Open:Active    - - - -  0  0  0  0
e52643tgb!    50 Open:Active    - - - -  8  0  8  0
.....
6226rib       30 Open:Active    - - - -  0  0  0  0
5218          30 Open:Active    - - - -  0  0  0  0
6230r         30 Open:Active    - - - - 32  0 32  0
```

- QUEUE_NAME
- PRIO
- STATUS Open/Closed
Active/Inact Open:Active
- Open:Inact
- NJOBS CPU
- PEND CPU
- RUN CPU
- SUSP CPU



bqueues -l

```
$ bqueues -l e5v3ib

QUEUE: e5v3ib
-- CPU: 2*E5-2680v3, RAM: 256GB/128GB, NET: 56Gb FDR InfiniBand
.....

SCHEDULING POLICIES: FAIRSHARE EXCLUSIVE
```

```
USER_SHARES: [root=, 999999] .....
```

SHARE_INFO_FOR: e5v3ib/

USER/GROUP	SHARES	PRIORITY	STARTED	RESERVED	CPU_TIME	RUN_TIME	ADJUST	GPU_RUN_TIME
------------	--------	----------	---------	----------	----------	----------	--------	--------------

```
root= 999999 202255.328 0 0 8456.5 1542 0.000 0
```

• • • • •

USERS: all ~test/

HOSTS: f01+10 f02+10 f03+10 f04+10 f05s+10 f05l/

RES_REQ: span[ptile=24]

Maximum slot reservation time: 43200 seconds



lshosts[][][#][][][][]

```
lshosts -gpu# GPU
```

Isload

			#						
--	--	--	---	--	--	--	--	--	--

Isload -gpu GPU

```
Isload -gpuload# GPU
```

bhosts[][][][#][][][][]



□□□□ /fs00/reports/bjobs/ □□□□□□□□□□□□□□□□

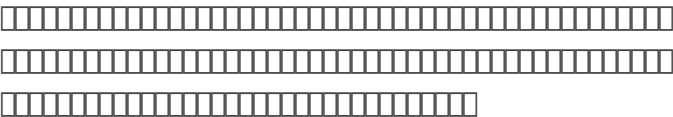
```
/fs00/reports/bjobs/bjobs.20130728070457  2013  07  28  07  04  57
```

bjobs -uall -w



/fs00/reports/process

- CPU
- CPU
- 2 CPU



Apptainer

2021 11 Singularity Linux Apptainer Apptainer
Docker HPC Apptainer Singularity Image File (SIF) Singularity
Singularity Singularity Singularity



Singularity Image File (SIF)



/fs00/software/singularity-images/ SIF



Docker Hub SIF

- Docker Hub `apptainer build ubuntu.sif docker://ubuntu`
- NVIDIA NGC `apptainer build ngc_cuda.sif docker://ngc.nju.edu.cn/nvidia/cuda`
- docker save `apptainer build abc.sif docker-archive://abc.tar`



- `apptainer build --fix-perms --sandbox build docker://ubuntu`
- `apptainer shell build/`
- `apt` `make`
- `exit`
- SIF `apptainer build abc.sif build`

root

CI

git.nju.edu.cn CI/CD kaniko Docker build ocr.sif docker://reg.nju.edu.cn/yaoge123/ocr apptainer

CI/CD Docker



```
#BSUB -q 62v100ib
#BSUB -gpu num=4

apptainer exec --nv cuda.sif app
```



- nv NVIDIA GPUs & CUDA
- bind/-B src[:dest[:opts]]



- Apptainer
- Apptainer User Guide
- Docker Hub
- NVIDIA NGC



p.nju.edu.cn



p.nju.edu.cn



```
curl -X POST https://p.nju.edu.cn/api/portal/v1/login -H "Content-type: application/json" -d
```

```
'{"username":"<username>","password":"<password>"}
```

```
curl -X POST https://p.nju.edu.cn/api/portal/v1/logout -H "Content-type: application/json" -d '{}'
```

```
curl -s "http://p2.nju.edu.cn/portal_io/login?username=<username>&password=<password>"
```

```
curl -s http://p2.nju.edu.cn/portal_io/logout
```

**

**

conda

pip



- mirror.nju.edu.cn conda pip
- git
-



<https://table.nju.edu.cn/dtable/view-external-links/custom/hpc-internet/>

SSH/SFTP no matching host key type found

```
SSH/SFTP no matching host key type found. Their offer: ssh-rsa,ssh-dss -o
HostKeyAlgorithms=+ssh-rsa ~/.ssh/config HostKeyAlgorithms +ssh-rsa
```



pip

```
Python root pip install -t
```

```
cd scikit-opt-master
pip install -t $HOME .
```

```
 ~/.bashrc
```

```
export PYTHONPATH=$HOME:$PYTHONPATH
```



CPU

- 1. CPU

```
Python Python OMP_NUM_THREADS
NUMEXPR_NUM_THREADS OPENBLAS_NUM_THREADS MKL_NUM_THREADS
```

```
export OMP_NUM_THREADS=$LSB_DJOB_NUMPROC
export NUMEXPR_NUM_THREADS=$LSB_DJOB_NUMPROC
export OPENBLAS_NUM_THREADS=$LSB_DJOB_NUMPROC
export MKL_NUM_THREADS=$LSB_DJOB_NUMPROC
```

2. CPU

#BSUB -R affinity[core:cpubind=core:membind=localprefer:distribute=pack]

3. #BSUB -x

MAX(1000,MIN(((30000-)/10,(20000-)/6))

UNKWN

UNKWN

1.

2.