Reedbush Quick Start Guide

Information Technology Center The University of Tokyo

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Index

- 1. Index
- 2. Cygwin installation (1)
- 3. Cygwin installation (2)
- 4. Building SSH key
- 5. Access to Web Portal
- 6. Change Password
- 7. Change password successfully
- 8. Re-login to Web portal
- 9. Upload public key (1)10. Upload public key(2)11. Upload public key(3)

- 12. Upload public key(4)
- 13.Login
- **14. Your Directory**
- 15. Building program
- 16.Compile and Run
- 17. Batch script
- 18.Batch script sample(1)
- **19.Batch script sample(2)**
- 20. Running Batch job
- 21. Deleting batch job
- 22. Application software

Cygwin installation (1)

- Install Cygwin
 - Download setup-x86_64.exe(64bit) or setupx86.exe(32bit) from http://cygwin.com/index.html, run it.
 - Click X11's Default at Package selection window, it change to "Install"

Click X11's Default

1

| Cygwin Setup - Select Package | | VVI | п | 00 | WSJ |
|-------------------------------|--------|------|------|-------------|--------------------------------------|
| Select packages to install | / | | | | |
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| ✓ Hide obsolete packages | | | | | , |
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It change to "Install", they are ready to be installed.

| E | Cygwin Set | up - Select | Packages | | | | | | | | | x |
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Cygwin installation (2)

– Search OpenSSH and click it. It will change install target from "Skip".

| | | Search OpenSSH |
|---|---|---|
| Cygwin Setup - Select Packages Select Packages Select Packages Select packages to initial errich logenplath Category Current Debug Operault Debug Operault Debug Operault | Exeep @ Durr Esp View Datecry Bin? Src? Stee Package | Box is changed to checked if you click. |
| 22p2-1 072p1-1 | ⊠ 731k. openssh: The OpenSSH server ar | |
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Building SSH key

- Open Cygwin64 Terminal or UNIX/Mac Terminal.
- Run ssh-keygen.
 - Public key "id_rsa.pub" and private key "id_rsa" is build on your home directory/.ssh.

| \$ ssh-keygen -t rsa Generating public/private rsa key pair. Enter file in which to save the key (/home/username/.ssh/id_rsa): Created directory '/home/username/.ssh'. | Run ssh-keygen |
|--|--|
| Enter passphrase (empty for no passphrase): Enter same passphrase again: Your identification has been saved in /home/username/.ssh/id_rsa. Your public key has been saved in /home/username/.ssh/id_rsa.pub. The key fingerprint is: SHA256:NedyH2JayWknq87pQlvaLVs3omJK2ZijB8iR9Qnwf4 username@host The key's randomart image is: +[RSA 2048]+ S.% o S.% o =o++ oo . =BP0=+to 0. | Enter your passphrase Re-Enter your passphrase |
| =++++.o.+=. +[SHA256]+ \$ | 4 |

Access to Web Portal

- Access to following site with your browser.
 https://reedbush-www.cc.u-tokyo.ac.jp
- Login to Web Portal.



Change Password

- Change your password on "Change Password" for the first time.
- Password policy
 - more than 8 characters.
 - the use of both upper-case and lower-case letters
 - inclusion of one or more numerical digits
 - inclusion of special characters, such as @, #, \$
 - not be a dictionary word



Change password successfully

• Click "Return to Login"



• Return to Login and retry if you failed to change password.

Re-login to Web portal

• Login with new password.



Upload public key (1)

• Click "SSH Configuration"

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| Login: z: | Module Index Au | uthorized Keys | ^ | |
| Change Language | No authorized keys have been registe | ered. | | |
| System Documentation System Information | Add a new SSH 2 authorized key. | | | |
| SSH Configuration | | | | |
| Ogout | | | | |
| | | | — 1. Click | "SSH Configuration" |
| | | | | |
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- At first time, "No authorized keys have been registered" appears.
- Click "Add a new SSH 2 authorized key."

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| Change Language | No authorized keys have been registe | ered. | | | |
| System Documentation System Information | Add a new SSH 2 authorized key. | | | | |
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| | | | 1. Click | "Add a new | SSH 2 authorized key. |
| | | | | | |
| | | | ~ | | |

Upload public key(2)

• "Add Authorized Key" window



 Copy your public key "HOMEDIR/.ssh/id_rsa.pub" on your terminal.



Upload public key(3)

- Paste this public key on "Key digits"
 - Confirm key doesn't include carriage return before you paste it.
- Confirm your public key format is "ssh-rsa key-digits key's name (user@host)".



Confirm that ssh-rsa or ssh-dss is in header, new line character is not included. RSA key should be more than 2048bits, DSA key should be more than 1024bits.

Upload public key(4)

- Confirm your key is registered at "Authorized Keys".
- "No authorized keys have been registered" appears if your key is invalid.



Login

- Login to Reedbush-u frontend server with ssh.
- Hostname: reedbush.cc.u-tokyo.ac.jp

| % ssh -l username reedbush.cc.u-tokyo.ac.jp Authenticating with public key ″rsa-key-20160612″ The authenticity of host 'localhost (∵1)' can't be established | It appears for the first time only |
|--|------------------------------------|
| RSA key fingerprint is XX:XX:XX:XX:XX:XX:XX:XX:XX:XX:XX:XX:XX: | Answer "yes". |
| Are you sure you want to continue connecting (yes/no)? yes | |
| Warning: Permanently added 'localhost' (RSA) to the list of known hosts. | |
| Passphrase for key rsa-key-20160612 : | |
| | - Enter passphrase. |
| | |
| | |
| | |
| | |

Your Directory

- /home/group_name/account_name
 - Default directory when you login.
 - Setting environment variables
 - Maximum 2GB
 - Home directory is unavailable to run batch job because compute node doesn't mount it.
- /lustre/group_name/account_name
 - Working directory
 - [number of subscription nodes]TB: Group Course
 4TB: when your group subscribes 4 nodes.
 8TB: when your group subscribes 8 nodes.
 - 1TB: Personal Course
 - Build and run your program at this directory.

Building program

- Default development environment
 - Intel C,C++,Fortran Compiler
 - Intel MPI
 - You are able to change your development environment with module command.
- module
 - You can switch compiler and mpi environment with module command.
 - When you run batch job, you have to load same modules as when you compile.

```
List your module environment

$ module list

Currently Loaded Modulefiles:

1) intel/16.0.3.210 2) intel-mpi/5.1.3.210

Load module

$ module load intel/16.0.3.210 intel-mpi/5.1.3.210
```

Compile and Run

- Compile and Run
 - Serial job (Intel Compiler)
 - icc、ifort
 - Parallel job (Intel MPI)
 - mpiicc、mpiifort

Example \$ mpiicc -o a.out -O2 mpiprogram.c \$ mpirun -np 2 ./a.out Hello World from Process 0 of 2 running on reedbush-u1 Hello World from Process 1 of 2 running on reedbush-u1

Batch script

- Move to your /lustre directory, make batch script.
- The following lines is necessary.
 - #!/bin/sh
 - #PBS -q [Queue name]
 - #PBS -l select=[number of nodes]:mpiprocs=[number of MPI processes/per node]:ompthreads=[number of OpenMP threads/per proccess]
 - #PBS -W group_list=[group name]
 - #PBS -I walltime=[wall time]
 - cd \$PBS_O_WORKDIR
 - [Initializing module]
 - [Load programing environment]
 - [Running program]
- Option
 - #PBS -N [Job name]

Batch script sample(1)

- Be sure to make and run on your /lustre directory.
- See run.sh(red character)
- Select appropriate queue for walltime and number of nodes which you'd like to use.

Ex) Serial job

\$ cd /lustre/group/username \$ cat ./run.sh #!/bin/sh #PBS -q u-short #PBS -l select=1:mpiprocs=1:ompthreads=1 #PBS -W group_list=mygroup #PBS -l walltime=02:00:00 cd \$PBS_O_WORKDIR . /etc/profile.d/modules.sh module load intel/16.0.3.210 ./a.out > ./output.log 2>&1

Your job will fail if it uses over 244GB per node.

| Queue name | Number of nodes | Walltime | |
|-----------------|-----------------|----------|--|
| u-debug | 1-16 | 30min | |
| (u-interactive) | - | - | |
| u-interactive_1 | 1 | 30min | |
| u-interactive_4 | 2-4 | 10min | |
| u-short | 8 | 4H | |
| (u-regular) | - | - | |
| u-small | 4-16 | 48H | |
| u-medium | 17-32 | 48H | |
| u-large | 33-64 | 48H | |
| u-x-large | 65-128 | 24H | |

Batch script sample(2)

- See run.sh(red character)
- Select appropriate queue for walltime and number of nodes which you'd like to use.

| 256MPI job | Hybrid parallel job |
|--|--|
| (8nodes x 32 MPI processes) | (8nodes x 2 MPI processes x 18 OpenMP threads) |
| <pre>\$ cd /lustre/group/username</pre> | <pre>\$ cd /lustre/group/username</pre> |
| \$ cat ./run.sh | \$ cat ./run.sh |
| #!/bin/sh | #!/bin/sh |
| #PBS -q u-short | #PBS -q u-short |
| <pre>#PBS -l select=8:mpiprocs=32:ompthreads=1 #PBS -W group_list=mygroup #PBS -l walltime=02:00:00 cd \$PBS_O_WORKDIR . /etc/profile.d/modules.sh module load intel/16.0.3.210 intel-mpi/5.1.3.210 mpirun ./a.out > ./output.log 2>&1</pre> | <pre>#PBS -I select=8:mpiprocs=2:ompthreads=18 #PBS -W group_list=mygroup #PBS -I walltime=02:00:00 cd \$PBS_O_WORKDIR . /etc/profile.d/modules.sh module load intel/16.0.3.210 intel-mpi/5.1.3.210 mpirun ./a.out > ./output.log 2>&1</pre> |

Your job will fail if it uses over 244GB per node.

Running Batch job

qsub to submitting batch script



- rbstat to show job status
 - Example

| \$ rbsta | t | | | | | | | |
|----------|----------|---------|---------|---------|----------------|----------|-------|------|
| JOB_ID | JOB_NAME | STATUS | PROJECT | QUEUE | START_DATE | ELAPSE | TOKEN | NODE |
| 123 | STDIN | RUNNING | XXXX | u-short | 06/27 19:56:41 | 00:00:00 | 0.0 | 1 |
| 124 | STDIN | QUEUED | XXXX | u-short | 06/27 19:56:48 | 00:00:00 | 0.0 | 1 |
| | | | | | | | | |

Deleting batch job

• qdel to delete batch job.

\$ qdel [Job ID]

• Example

| \$ rbstat | Ē | | | | | | | |
|-----------|----------|---------|---------|---------|----------------|---------------|-------|------|
| JOB_ID | JOB_NAME | STATUS | PROJECT | QUEUE | START_DATE | ELAPSE | TOKEN | NODE |
| 123 | STDIN | RUNNING | XXXX | u-short | 06/27 19:56:41 | 00:00:00 | 0.0 | 1 |
| 124 | STDIN | QUEUED | XXXX | u-short | 06/27 19:56:48 | 00:00:00 | 0.0 | 1 |
| | 24 | | | | | | | |
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| S rbstat | | | | | | | | |
| JOB ID | JOB NAME | STATUS | PROJECT | QUEUE | START DATE | FLAPSE | TOKEN | NODE |
| 123 | STDIN | RUNNING | XXXX | u-short | 06/27 19:56:41 | 00:00:00 | 0.0 | 1 |
| | | | | | | | | |
| | | | | | | | | |

Application software

- A list of software installed on Reedbush-u system is shown by using "module avail"
- Load application module which you use.

| \$ module avail |
|--|
| /lustre/app/modulefiles/compiler /intel/16.0.3.210(default) pgi/16.5 |
| |
| |
| /lustre/app/modulefiles/application abinit-mp/7.0 bwa/0.7.13 gatk/3.5 openfoam/3.0.1 samtools/1.3.1 akaikkr/cpa2002v009c feram/0.24.02 gromacs/5.1.2 openfoam/3.0.1-mpt spark/1.6.1 alps/2.1.1-r6176 frontflow_blue/8.1 kmr/1.8.1 openmx/3.8 xtapp/150401 bioperl/1.6.924 frontflow_blue/8.1_gnu modylas/1.0.4 phase0/2015.01 bioruby/1.5.0 frontistr/4.4 ncbi-blast/2.3.0 r/3.2.5 \$ module load openfoam/3.0.1 |