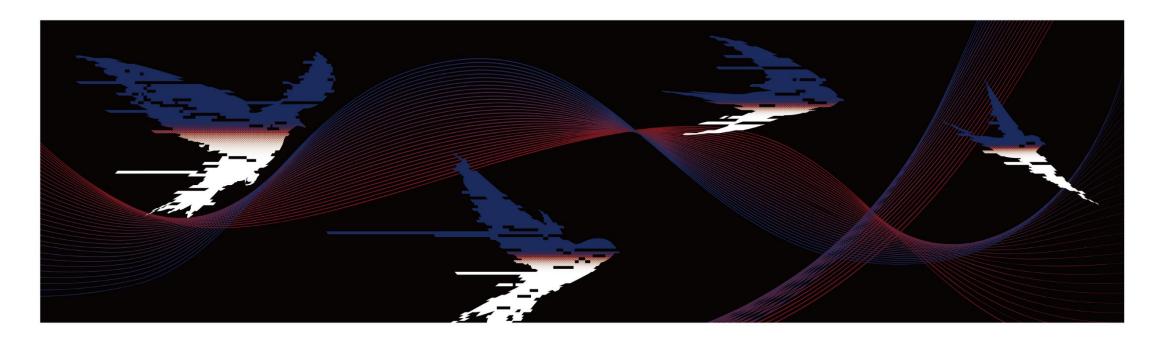


Introduction to TSUBAME (Linux basics)





Contents

- Overview of TSUBAME4
- Introduction of Linux
- File operation
- Various commands
- Run programs on compute node (Job Submission)
- User environment



Overview of TSUBAME4

- System details
- Commercial applications
- Provided services
- Getting Started
- Usage of compute node
- T4 web page introduction



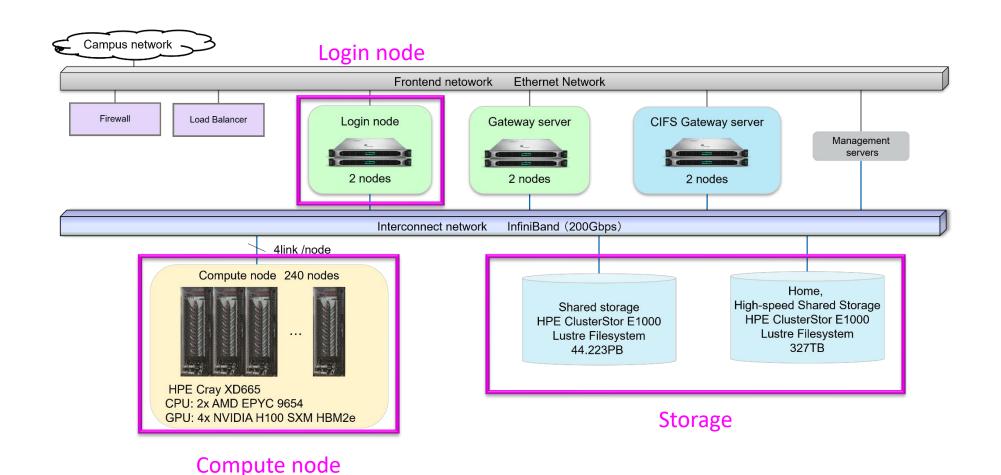
TSUBAME4

- TSUBAME4 is the supercomputer introduced on April 1st, 2024.
- Total 960 GPUs (NVIDIA H100)
- Theoretical computing performance
 - double precision performance (FP64): 66.8 PFLOPS
 - half precision performance (FP32): 952 PFLOPS
- Total memory capacity: 180 TiB
- Total SSD Capacity: 327TB
- Total HDD Capacity: 44.2PB
- 200 Gbps High speed network (inside T4 system)
- As a new utility, users can use computing resources through Web browser (Open OnDemand).
 - Various resource selection from 4 cores to high parallel computing / multiple GPUs for per job.
 - Obviously, the standard method (SSH) is provided.
- Programs developed at TSUBAME3 can be used without any changes.
 - Combination of x86_64 CPU x NVIDIA GPU x Linux OS

```
*1 TiB = 2^{40} B = 1,099,511,627,776 B
```



T4 System architecture





System details - Compute node

HPE Cray XD665 240 nodes

Item	Specification
CPU	AMD EPYC 9654 (2.4GHz) × 2CPU
# of cores/threads	96 cores / 192 threads × 2CPU
Memory size	768GiB
GPU	NVIDIA H100 SXM5 94GB HBM2e × 4
SSD	1.92TB NVMe U.2 SSD
Interconnect	InfiniBand NDR200 200Gbps × 4





System details - Storage and SW

Storage

Areas	Mount point	Capacity	Filesystem
High-speed storage area Home directory (SSD)	/gs/fs /home	372TB	Lustre
Large-scale storage area Common application deployment (HDD)	/gs/bs /apps	44.2PB	Lustre
Local scratch area	/local	1.92TB/node	xfs (SSD)

Software

- OS:Red Hat Enterprise Linux Server 9.4
- Commercial applications (see the following page)



Commercial applications

Software	description
ANSYS	Analysis Software
ANSYS/Fluent	Analysis Software
ANSYS/LS-DYNA	Analysis Software
ABAQUS/ABAQUS CAE	Analysis Software
Gaussian	Quantum chemistry calculation program
GaussView	Quantum chemistry calculation program Pre-Post tool
AMBER	Molecular dynamics calculation program
Materials Studio	Chemical Simulation Software
Discovery Studio	Chemical Simulation Software
Mathematica	Mathematical Processing Software
COMSOL	Analysis Software
Schrodinger	Chemical Simulation Software
MATLAB	Numerical calculation software
Arm Forge	Debugger
Intel oneAPI Compiler	Compiler, Development tool
NVIDIA HPC SDK Compiler	Compiler, Development tool

Activation is required for each application before use.

Activation can be done on T4 portal with TSUBAME point.

In a job session, environment for each application will be configured by module command.

Commercial applications except for Gaussian, debugger and compiler are for users on-campus.

Center for information infrastructure (CII), institute of Science Tokyo



Provided services

- Compute node
 - TSUBAME4 provids 240 nodes. (HPE Cray XD665)
- Storage
 - home directory (up to 25GiB for each user): for free
 - home directory for each user is located in /home/[0-9]/username.
 - Accessible from all nodes on the system.
 - High-speed/Largh-scale storage area: paid service (TSUBAME point required)
 - Group disk area composed of Lustre file system
 - High-speed storage -> SSD, Large-scale storage -> HDD
 - Scratch area (SSD): for free (available in running job)
 - Local scratch area
 - Shared scratch area



Paid Services in TSUBAME4

- Run jobs on compute node (pay-as-you-go)
- Compute node reservation
- 1-month node reservation (flat-rate system) <-- New
- Commercial applications used in T4 system (monthly payment) <-- New
- Parts of Commercial applications used in campus (annual payment) <-- New
- Group Disk

- When you activate paid services, "TSUBAME point" is required.
- You will get amount of "TSUBAME point" with your budget of research project.
- TSUBAME point will be expired until the end of faculty year. Cannot carry over to the next year.



Getting Started

[note] Participants in this course need to configure 1 and 2. TSUBAME point is necessary to submit jobs, use group disks and use commercial application.

- 1. Get a TSUBAME account (See https://www.t4.cii.isct.ac.jp/en/getting-account)
- 2. Create SSH key pair in local PC and upload the public key
- 3. Create group [by group administrator]
- 4. Configure group
 - Register budget code [by group admin.]
 - Purchase points [by group admin. or sub admin.]
 - Add users to the group [by group admin. and users]
 - Grant permission to users [by group admin. or sub admin.]
 - Configure group disks [by group admin. or auth. users]
 - Apply for using Apps. (activation) [by group admin. or auth. users]
 - <Another configuration if you need>
- 5. Submit jobs

Setup at TSUBAME4 potal



Usage of compute node

There are mainly 2 types of using compute node.

1. CLI use: SSH

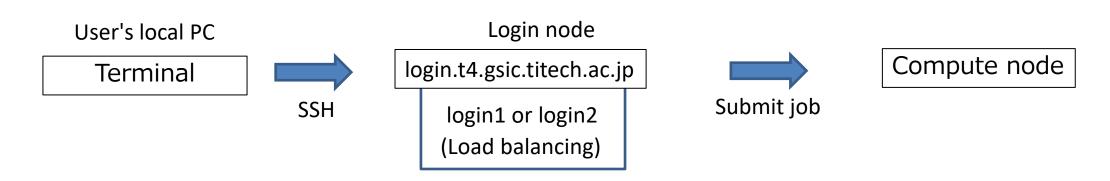
2. Web based use: Open OnDemand <-- New

• In this course, CLI use with SSH will be introduced.



Usage of compute node (SSH)

- Login to login node (SSH key authentication)
 - Perform the ssh command to access to login.t4.gsic.titech.ac.jp in a terminal, on your PC, then automatically login to one of the login node by load balancing.
- **On login node, running heavy processes are prohibited. When monitoring system finds such a process, it will kill them automatically.
- Integrated Development Environment (IDE) such as VS Code also uses large number of resources.
- **Upload SSH public key to server (via T4 portal) in advance. After upload SSH key, users finally can access login node. See TSUBAME Portal User's Guide.





TSUBAME information

- TSUBAME4 Computing Services (Homepage)
 - https://www.t4.cii.isct.ac.jp/en
- TSUBAME4 portal
 - https://portal.t4.gsic.titech.ac.jp/ptl/
 For user/group setting (e.g. SSH pubkey registration, point purchase, node reservation)
- X (formerly known as Twitter)
 - @TSUBAME_sc
 The latest news will be announced on X and T4 Homepage.
- If there is some inquiry about TSUBAME, post at "Contact Us" on T4 Homepage
 - https://www.t4.cii.isct.ac.jp/en/contact-t4



Introduction of Linux

- Overview of Linux
- Terminal
- Use terminal on Windows/Mac
- Remote login
- SSH key authentication
- Login to TSUBAME4
- Logout



Overview of Linux

- Linux is a family of open-source Unix-like operating systems based on the Linux kernel.
- Linux is a multitasking/multiuser Operating System.
- Linux distributions
 - Debian
 - Slackware Linux
 - SUSE Linux Enterprise Server (SLES)
 - Red Hat Enterprise Linux (RHEL)
 - CentOS

. .

- Authentication
 - Local login
 - username / password
 - Remote login
 - username / password
 - Key authentication <-- TSUBAME4 supports this authentication.



Terminal

- Using a standard terminal on Linux.
- The line which has a symbol such as "%", "\$" and ">" is called prompt. (In the example below, \$ is displayed.)
- Type a command on this line.

```
● GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$
```



Terminal emulators for Windows

- There are various terminal emulators for Windows.
 - Cygwin, PuTTY, Tera Term, Rlogin, MobaXterm, WSL
- MobaXterm seems to be convenient because they contains several services including X window system, VNC, port forwarding, ...
- Anyway, please try several terminal emulators and select the one you like.

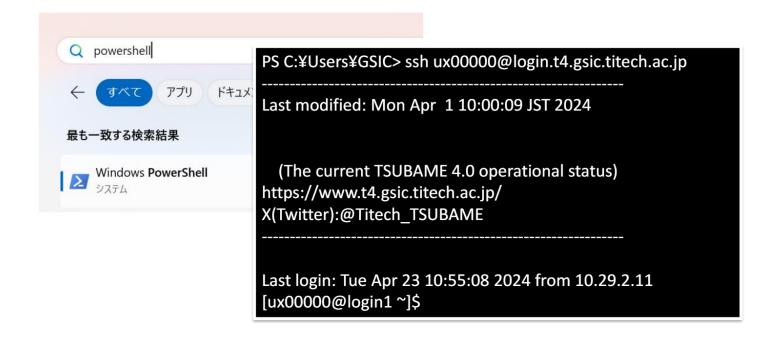
See also Available SSH client on Windows



Use PowerShell

- Start -> Type "powershell" in the search box and Enter.
- Execute SSH command.

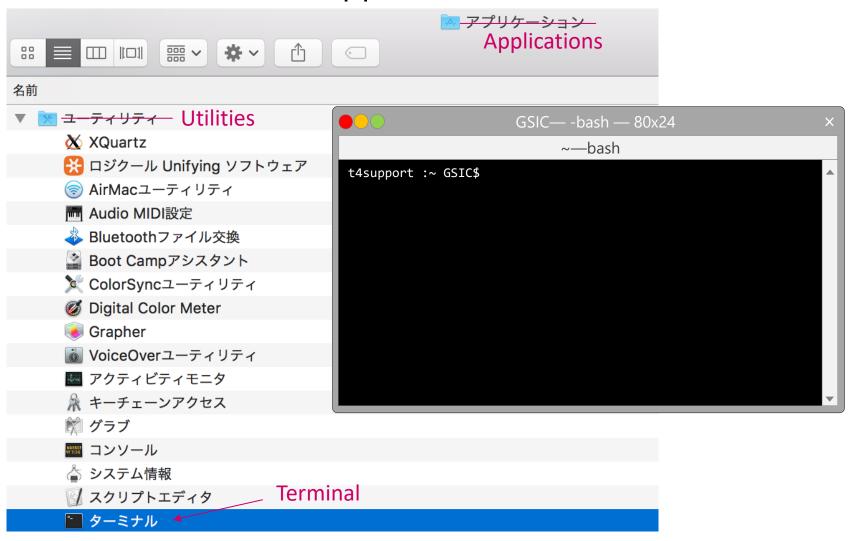
(Make sure to configure SSH key pair in advance)





Use terminal on Mac

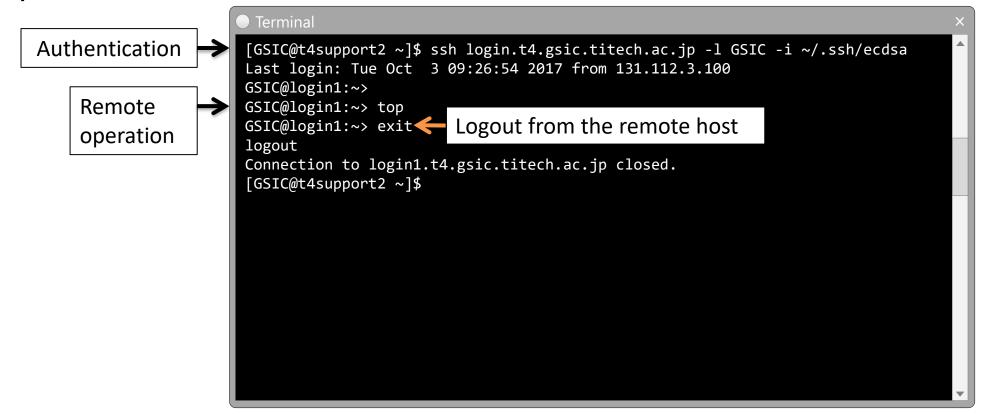
Applications > Utilities > Terminal.app





Remote login

- Remote host operation on a local host
- Commands are telnet, rlogin, ssh and so on.
- In TSUBAME, SSH public key authentication is supported from perspective of security.



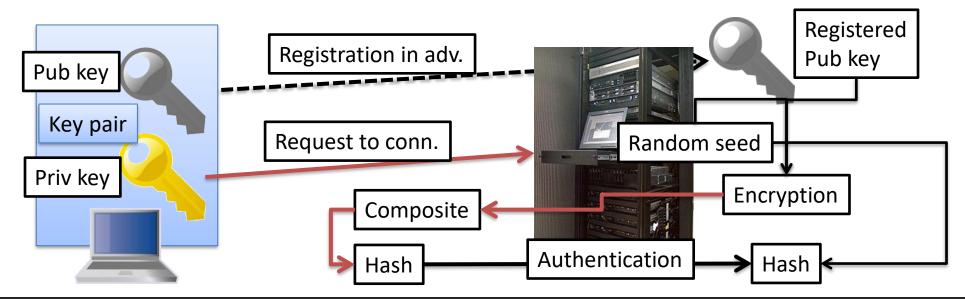


SSH key authentication

The authentication system consisits of a pair of keys, called public key and private key.

- Advantage
 - Only accessible from the machine which have the key = High security
- Disadvantage
 - It's a little hard for configure and management.

[NOTE] Recommend to set passphrase





Creating SSH key pair

Use ssh-keygen command

See https://www.t4.cii.isct.ac.jp/docs/faq.en/general/#keypair

```
GSIC— -bash — 80x24
                               ~—bash
t4support :~ GSIC$ ssh-keygen -t ecdsa
```



Upload public key

Upload public key to TSUBAME via T4 poral.

- https://portal.t4.gsic.titech.ac.jp/ptl/user/sshPublicKey?lang=en
- Check the text of public key (.pub), copy and paste it to the T4 potal page.





Exercise (Login to TSUBAME4)

- Input ssh command on a prompt to log in to TSUBAME4 with specifying a ssh key as shown below.
- Successfully logged in, a prompt username@loginX appears.

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ ssh login.t4.gsic.titech.ac.jp -l GSIC -i ~/.ssh/ecdsa
Last login: Tue Oct 3 09:26:54 2017 from 131.112.3.100

GSIC@login1:~>

# The following command is also the same meaning.
$ ssh GSIC@login.t4.gsic.titech.ac.jp -i ~/.ssh/ecdsa
```

You don't have to use your private key if you want to use TSUBAME from a Computer room's PC in campus. (password authentication)

Therefore, please execute ssh command without -i option while this seminar.

```
$ ssh login.t4.gsic.titech.ac.jp -l username
```



Logout

- Perform log out operation to finish your work.
- Check the followings before log out.
 - Data arrangement
 - Process (Check no program is running on the terminal)
- Log out operation
 - Type Ctrl and d keys at the same time (Ctrl-d)
 - Type logout -> Enter
 - Type exit -> Enter



Tips

- It is better to configure the terminal preference when you log in to TSUBAME to avoid the disconnect.
- Discribe the following parameteres in ~/.ssh/config if you use Mac, Cygwin, Linux and so on.

```
GSIC@t4support:~

File Edit View Help

[GSIC@t4support ~]$ cat ~/.ssh/config
ServerAliveInterval 120
ServerAliveCountMax 30
```



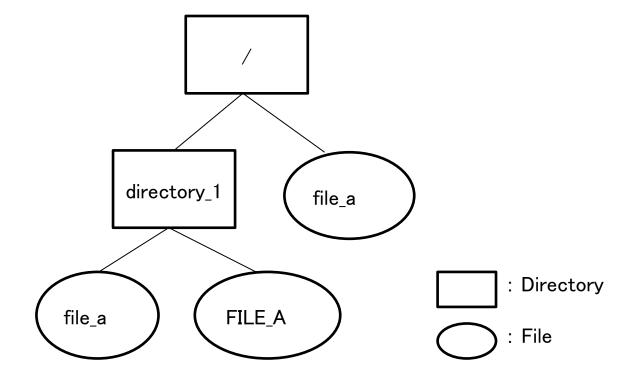
File Operation

- Filesystem
- File specification
- Information display commands
- Symbols
- Special characters
- File permission and attribute
- Newline difference amang OS
- Compression and extraction



Filesystem

- Represented in hierarchical structure
- File management with directory
- Ordinary file and special file





File specification

- The top of a hierarchical structure of a file system is called "root", represented as "/".
- How to access files
 - Absolute specification: Full specification from the root (/)
 - Relative specification: Specifies the location from current location

```
GSIC@t4support:~

File Edit View Help

[GSIC@t4support ~]$ ls /home/GSIC

Desktop

[GSIC@t4support ~]$ ls ../GSIC

Desktop
```



Symbols

- Command to confirm directory: pwd
- Home directory: ~
- One directory up: ...
- Current directory: .

```
GSIC@t4support:~

File Edit View Help

[GSIC@t4support2 ~]$ pwd
/home/GSIC

[GSIC@t4support2 ~]$ cd ..

[GSIC@t4support2 home]$ cd ~

[GSIC@t4support2 ~]$
```

*Use . (dot) to represent the current directory (current position)



Information display commands

pwd (to confirm where you are)

```
GSIC@t4support:~

File Edit View Help

[GSIC@t4support ~]$ pwd
/home/GSIC
```

Is (to display files in current or specified directory)

```
GSIC@t4support:~

File Edit View Help

[GSIC@t4support ~]$ 1s

Desktop
```



Special characters

Special characters representation can be used to specify file names.

*Metacharacter	Function	Usage
*	all character strings	ls *
?	one of any character	ls?
[character string]	one of character strings	ls [bc]
	one of the characters between character 1 and character 2	ls b[a-c]d

Special characters are also known as metacharacters. Metacharacters are symbols which do not have any meaning itself, however these become meaningful as a whole when combined with other characters.

^{*}Metacharacter



File permission and attribute

• |s -|

```
File Edit View Help

[GSIC@t4support2 hogehoge]$ 1s -1
合計 0
drwxrwxr-x. 2 GSIC users 6 10月 3 15:35 hoge
-rw-rw-r--. 1 GSIC users 0 10月 3 15:35 hogedoc

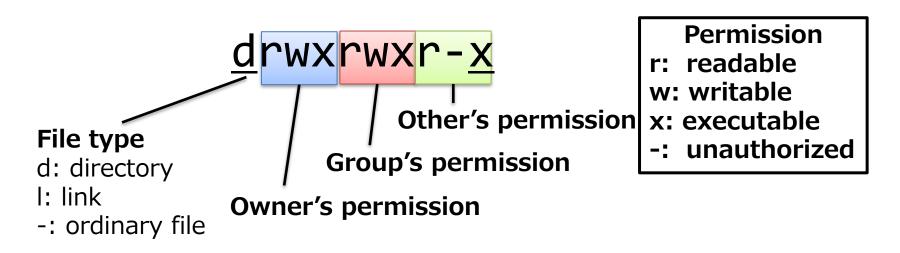
Attribute

Owner, Group

Timestamp

File name
```

Mode





Commands for file management

- Create directory % mkdir aaa
- Remove directory % rmdir aaa
- Change file attribute % chmod 755 aaa

```
*755 is called as bit representation, and it represents access rights for owner, group and others.
```

- 0 --- unauthorized
- 1 --x execute only
- 2 -w- write only
- 3 -wx
- 4 r-- read only
- 5 r-x
- 6 rw-
- 7 rwx full access

(Operation of administrator is as follows)

- Change owner # chown necapps aaa
- Change group # chgrp procon aaa



Different codes depending on OS

- Newline difference in text file
 - Unix/linux ¥n LF(line feed)
 - Macintosh ¥r CR(carriage return)
 - Win/Dos ¥r¥n CRLF
- [note] A text file contains Win/Dos-type newline cannot be read on Unix/linux system.
- Display code for 2-bite characters (e.g. Japanese)
 - Unix/Linux UTF-8/EUC
 - Macintosh/Windows UTF-8/S-JIS
- Conversion through nkf command
 - nkf -Lu abc_crlf.sh > abc_fl.sh



Compression and extraction

Compression

```
gzip atom45.tar
                                    \rightarrow atom45.tar.gz
    zip atom45.zip atom45
                                    \rightarrow atom45.zip
    lha a text.lzh *.txt
                                    \rightarrow text.lzh
    tar czvf atom45.tgz atom45 \rightarrow atom45.tgz
    tar cjf smpl.tar.bz2 smpldir
                                    \rightarrow smpl.tar.bz2
    bzip2 sample.txt
                                     \rightarrow sample.txt.bz2

    Extraction

    zcat atom45.tar.Z | tar -xvf -
    tar jxf sample.tar.bz2
    gzip -d atom45.tar.gz
                                   \rightarrow atom45.tar
    unzip book2nd.zip
    lha e text.lzh
    tar xzvf atom45.tgz
    bzip2 -d sample.txt.bz2
                                     \rightarrow sample.txt
```



Various commands

- Frequently used commands
- Commands for file operation
- Alias function
- Text editor (vi)
- Usage of commands
- Online manual
- Command concatenation



Frequently used commands

- ssh
- exit
- mkdir
- rmdir
- chmod
- chown
- chgrp
- nkf
- cd
- cp
- mv
- rm
- pwd

- Is
- vi
- emacs
- view
- tail
- cat ,more ,less
- find
- file
- grep
- diff ,sdiff
- man



Command operation

Usage

- Execute a command without any option
- Execute a command with options or arguments
- It is possible to combine multiple commands.

```
GSIC@t4support2:~
      Edit View
                     Help
[GSIC@t4support2 ~]$ ls
Desktop
[GSIC@t4support2 ~]$
[GSIC@t4support2 ~]$ 1s -1
drwxr-xr-x 2 GSIC users
                           512 Sep 13 10:15 Desktop
[GSIC@t4support2 ~]$
[GSIC@t4support2 ~]$ cal 10 2017
    October 2017
Su Mo Tu We Th Fr Sa
   2 3 4 5 6 7
 8 9 10 11 12 13 14
15 16 17 18 19 20 21
22 23 24 25 26 27 28
29 30 31
```



Commands for file operation

- cd change directory
- cp copy copy a file or a directory
- mv
 move
 move a file or a directory
- rm
 remove
 remove a file or a directory

```
GSIC@t4support2:~
     Edit View
                    Help
[GSIC@t4support2 hogehoge]$ ls
hoge hogedoc
[GSIC@t4support2 hogehoge]$ cd hoge
[GSIC@t4support2 hoge]$ ls
cast dust host
[GSIC@t4support2 hoge]$ cp cast fast
[GSIC@t4support2 hoge]$ ls
cast dust fast host
[GSIC@t4support2 hoge]$ mv host test
[GSIC@t4support2 hoge]$ ls
cast dust fast test
[GSIC@t4support2 hoge]$ rm dust
[GSIC@t4support2 hoge]$ ls
cast fast test
```

^{*}In cp, mv, rm commands, users are prompted for confirmation by –i option.

^{*}There is no command to restore the files that were removed once.



Alias function

- Adding alias to frequently used command or command line.
- alias can also be used as command.
- To unset alias, use unalias command.

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ cat .bashrc

# rm option
alias rm='rm -i'
```

By writing this way in .bashrc, loss of file by mistake can be prevented.

By mistake, if space is given such as rm * .txt , then all files in current directry will be deleted.

By setting the alias, users are prompted for confirmation before removing by -i option.



Text editor (vi)

An editor necessarily installed in Linux machine

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ vi hogedoc

~
~
~
~
~
~
~
~
"hogedoc" OL,

OC 0,0-1

All
```

Insert mode by i or a

Standby mode by Esc key

Delete one character by x, delete one line by dd

Save and exit editor by :wq

Wipe out all edits and quit (exit vi editor) by :q!

Undo the last change to the file by u

At the time standby mode, move using h, j, k, l, which is the function of \leftarrow , \downarrow , \uparrow , \rightarrow , respectively.

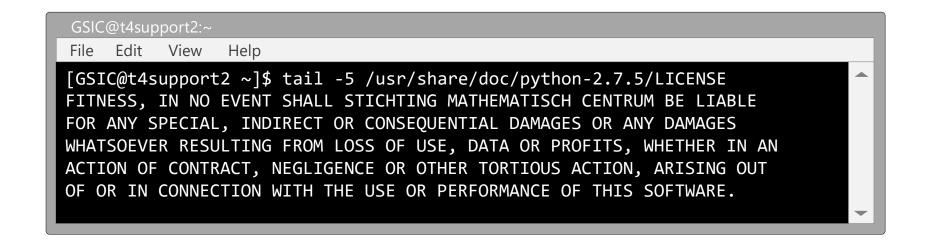


view

- An editor command similar to vi editor can be used.
- Open editor in read-only mode.
- Use to check the contents of file.



Displays last part of output to standard output



It is useful to output the calculation result to a file and periodically check the progress with the tail command.

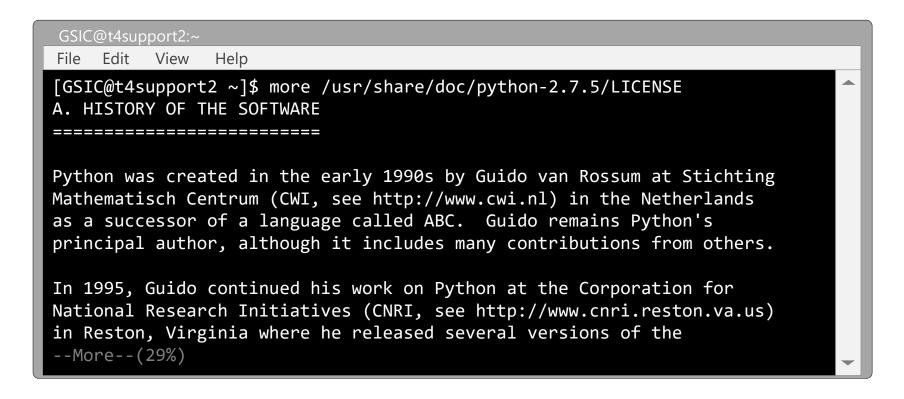
Please avoid running text output and tail commands successively through a program. (in order to avoid the heavy load on the machine)



cat, more and less

- Using cat to view the content of a file
- Using more/less to output the large size files in page

The contents of a file are displayed in page units. page feed is done with the space key.





- find is the command for get a file location.
 - \rightarrow It is convenient to use when you know part of file name or whole file name.
 - \rightarrow It is impossible to search within a directory without execution rights.
- There are which and whereis as similar commands

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ find . -name hoge -print ./hoge

[GSIC@t4support2 ~]$ which python
/usr/bin/python

[GSIC@t4support2 ~]$ whereis python
python: /usr/bin/python /usr/bin/python3.4 /usr/bin/python3.4m
/usr/bin/python2.7 /usr/bin/python2.7-config /usr/bin/python3.4-config /usr/bin/python3.4m-config /usr/lib/python3.4 /usr/lib/python2.7
/usr/lib64/python3.4 /usr/lib64/python /usr/lib64/python2.7
/usr/include/python3.4m /usr/lib64/python2.7 /usr/include/python3.4m /usr/lib64/python2.7
```



To check file type from character string.

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ file hoge
hoge: directory

[GSIC@t4support2 ~]$cd hoge
[GSIC@t4support2 hoge]$ file hogedoc
hogedoc: empty

[GSIC@t4support2 hoge]$ file hogedoc2
hogedoc: ASCII text
```



- Searches the character string in file
- Convenient to search strings in standard output (with pipe)

It is useful if this command is executed before performing character string search such as viewtier and more command.

```
GSIC@t4support2:~
File Edit View Help

[GSIC@t4support2 examples]$ grep mpi *.c
connectivity_c.c:#include <mpi.h>
hello_c.c:#include <mpi.h>
connectivity_c.c:#include <mpi.h>
connectivity_c.c: MPI_Status status;
(snip)
hello_c.c:#include "mpi.h"
hello_c.c: char version[MPI_MAX_LIBRARY_VERSION_STRING];
(snip)
[GSIC@t4support2 hoge]$ grep -i mpi *.c | more
(snip)
```



Displays the differences between two files.

- diff

sdiff

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ sdiff hello_c.c hello_cxx.cc

MPI_Init(&argc, &argv); | MPI::Init();

MPI_Comm_rank(MPI_COMM_WORLD, &rank); | rank = MPI::COMM_WORLD.Get_rank();

MPI_Comm_size(MPI_COMM_WORLD, &size); | size = MPI::COMM_WORLD.Get_size();

MPI_Get_library_version(version, &len); | MPI_Get_library_version(version, &len);
```



Online manual

- man command name/file name
- man -k keyword

```
GSIC@t4support2:~
     Edit View
                  Help
[GSIC@t4support2 examples]$ man ls
Man: find all matching manual pages (set MAN_POSIXLY_CORRECT to avoid this)
* ls (1)
  ls (1p)
Man: What manual page do you want?
Man:
NAME
      ls - list directory contents
SYNOPSIS
      ls [OPTION]... [FILE]...
DESCRIPTION
       List information about the FILEs (the current directory by default). Sort
entries alphabetically if none of -cftuvSUX nor --sort is specified.
       Mandatory arguments to long options are mandatory for short options too.
```

POSIX [Portable Operating System Interface for UNIX]

A set of standard operating system interfaces based on the UNIX, specified by IEEE. (extracted from e-word)



Command concatenation

Process can be executed collectively as program by combining commands.

- Connect command by semicolon (;)
- Connect command by pipe (|)
- Write the output of the command to file
- Input file in command
- Shell Programming (Shell script)



Semicolon

- Connects multiple commands by semicolon (grouping)
- After execution of command 1, command 2 and command 3 are executed in sequence.

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ uname; arch; hostname
Linux
x86_64
t4support2
```



Pipe

| (vertical bar)

Example:

Transfer the standard output obtained with cat to grep

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ cat /usr/mpi/gcc/openmpi-1.10.4/include/mpi.h | grep INDEX

#define MPI_T_ERR_INVALID_INDEX 57

MPI_COMBINER_INDEXED,

MPI_COMBINER_HINDEXED,

MPI_COMBINER_INDEXED_BLOCK,

MPI_COMBINER_INDEXED_BLOCK

MPI_COMBINER_HINDEXED_BLOCK
```



Redirection

- Create the stdout obtained with Is to Is.txt.
- >> Append the stdout obtained with Is to Is.txt.

```
GSIC@t4support2:~
     Edit View
                 Help
[GSIC@t4support2 ~]$ ls
Desktop hoge
[GSIC@t4support2 ~]$ ls > ls.txt
[GSIC@t4support2 ~]$ cat ls.txt
Desktop
hoge
[GSIC@t4support2 ~]$ ls >> ls.txt
[GSIC@t4support2 ~]$ cat ls.txt
Desktop
hoge
Desktop
hoge
ls.txt
```



Here document

- Transfer data from standard output to command (program)
 - Input from file

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ a.out < input.dat
```

Input from standard input

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ a.out << EndOfFile
100
EndOfFile
$
```



Background execution

- Command (program) which takes longer time in execution
- To do another task on the same terminal after starting a program.
 - → Execute the program as a background job
- To execute command, add "&" at the end of command.

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ find . -name xinit -print &

[1] 53254
```



View running process

- Process is execution unit of processing on OS
 - The following example shows three processes running.

```
GSICUSER00@r6i3n2:~> top
PID USER PR NI VIRT RES SHR S %CPU %MEM TIME+ COMMAND
354797 hpe_use+ 20 0 49.897g 456836 408116 R 14.286 0.173 0:02.09 pmemd.cuda.MPI
354798 hpe_use+ 20 0 49.897g 453680 407172 R 14.286 0.172 0:02.08 pmemd.cuda.MPI
3207 hpe_use+ 20 0 425428 60592 1356 S 2.640 0.092 30:26.49 a.out
```



- A job is a shell execution unit that combines commands / programs
 - Even when a command is connected by a pipe or the like, it is called a job.
 - jobs command to check running jobs with jobs command

```
GSIC@t4support2:~

File Edit View Help

[GSIC@t4support2 ~]$ sleep 30 &

[1] 3423

[GSIC@t4support2 ~]$ jobs

[1]+ Running sleep 30 &

[GSIC@t4support2 ~]$
```



Exercise

- Let's use the commands that have learned so far.
- Please execute the commands shown here in order.
 - (1) cd
 - (2) mkdir lesson
 - (3) cd lesson
 - 4 cp -r /gs/bs/soudan/UNIX/* ./
 - (5) cp sample.sh sample.txt
 - 6 file sample.txt
 - 7 vi sample.txt
 - Please edit somewhere appropriately in a file with vi
 - after editing, type Esc
 - :wq (save and quit)
 - (8) diff sample.sh sample.txt
 - (9) sdiff sample.sh sample.txt



Run programs on compute node (Job Submission)

- module command to set environment
- Batch job scheduler
- How to submit job



module command to set environment

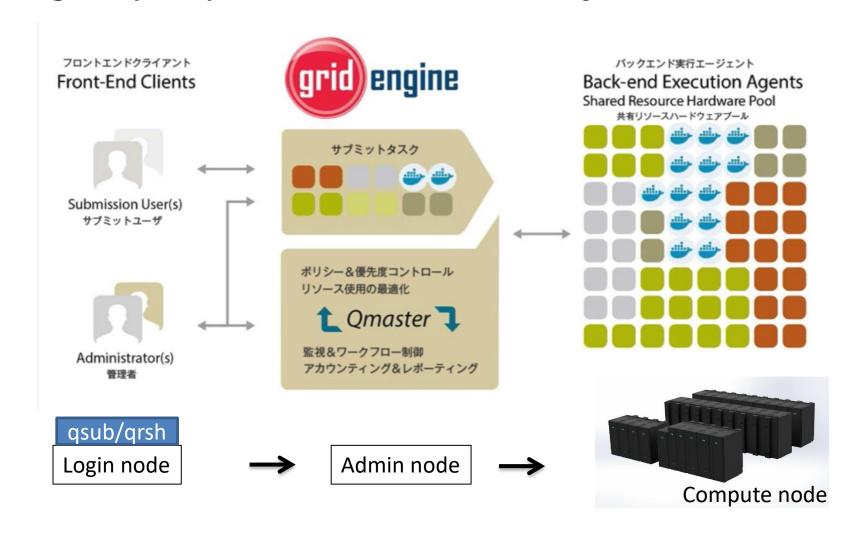
- When using TSUBAME4, load execution environment of the application you want with the module command. It needs to be done before executing the application.
- Example (Intel Compiler):
 - \$ module load intel
- To browse available modules
 - \$ module avail

Command	Operation	
module avail	List available modules	
module load	Load specific module's environment	
module list	List loaded modules	
module purge	Purge loaded modules	



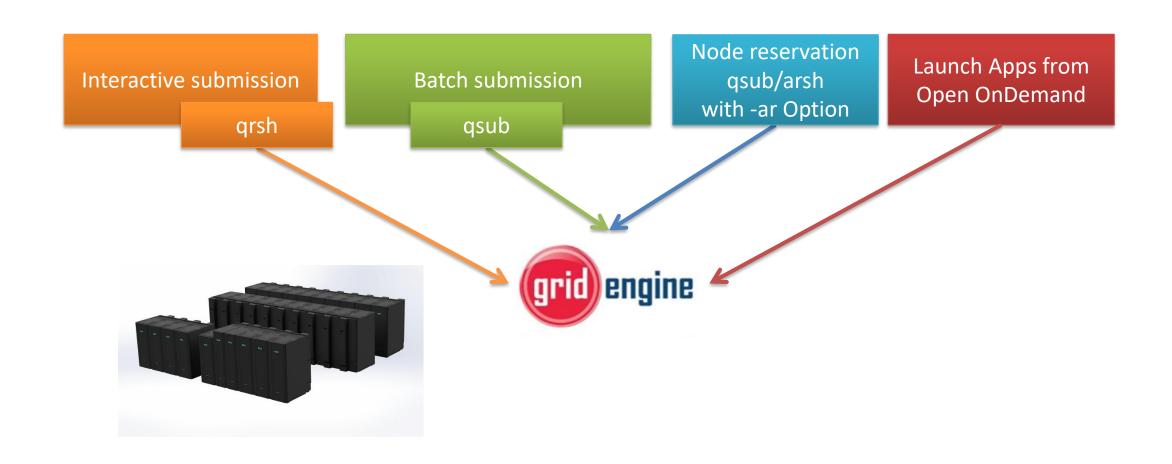
Batch job scheduler

Altair Grid Engine (AGE) is introduced as batch job scheduler.





Use Compute node (qsub/qrsh)





Flow from file creation to submit

- Prepare program you would like to use.
- Consider resouces need to use the job. (num. nodes, run time length)
- Select one of resource types.
 - node_f, node_q, cpu_4, or …
- Create a batch job script for job scheduler.
- Submit the job by qsub.
- Check job status.
- Check the result of the program after the job finished.



Resource Types

- Only node_f is permitted to login by SSH from another terminal.
- Effective use of TSUBAME point, appropriate

Туре	CPU cores	Memory (GB)	GPUs	Local scratch area (GB)
node_f	192	768	4	1920
node_h	96	384	2	960
node_q	48	192	1	480
node_o	24	96	1/2	240
gpu_1	8	96	1	240
gpu_h	4	48	1/2	120
cpu_160	160	368	0	96
cpu_80	80	184	0	48
cpu_40	40	92	0	24
cpu_16	16	36.8	0	9.6
cpu_8	8	18.4	0	4.8
cpu_4	4	9.2	0	2.4



Limits of job submission

- Limits
 - Run time
 - Maximum running time is 24 hours per job. (Reservation execution might be able to run for 1 week in some cases)
 - Number of available resources at the same time
 - 6144 slots (12288 slots on weekend)
 - Maximum degree of parallelism per job
 - 64 (Note: maximum effective capacity of node_f will be 32, because of the 6144-slot limitation)
 - Number of running jobs at the same time
 - 30 jobs per user (100 jobs on weekend)

If you submit jobs exceeding the limitations, the exceeded jobs' status become wait and does not run until the preceding running job ends.

*slots = physical cpu cores

See Resource Limit Values for more info.



Run programs on compute node

When a Job is submitted, The job scheduler will randomly allocate One/multiple node(s) of 240 compute node to a Job. Users can not select a specific compute node.

The followings are the commands to submit jobs.

- Interactive job submission (for small to medium scale)
 - Perform qrsh command. It is for directory log in to an interactive node.
 \$ qrsh -g TSUBAME_group -l resource_type -l max_run_time
 - Then you can run programs on the node.\$./a.out
- Batch job submission (for medium to large scale)
 - Perform qsub command. It is for submitting a job, on a login node.
 \$ qsub -g TSUBAME_group -I resource_type -I max_run_time batch_script.sh
 For using node reservation, add -ar reservation_number to qsub argument.



Submit job (Create job script)

Example of a job script

Refer to TSUBAME4.0 User's Guide.

https://www.t4.cii.isct.ac.jp/docs/handbook.en/jobs/#jobscript

```
#!/bin/bash
                  <-shebang
#$ -cwd
                 <-set to run on current directory
              <- job name
#$ -N test job
echo "this host is" `hostname` "."
```



Submit job (batch job)

qsub -l resource_type -l max_run_time -g TSUBAME_group jobscript.sh

See also https://www.t4.cii.isct.ac.jp/docs/handbook.en/jobs/#execute_qsub

```
GSIC@t4support:~

File Edit View Help

[ux00000@login1 ~]$ qsub -g TSUBAME_group sample.sh

#For trial, submit a job without -g option. Note that the limitation to a job execution is within 10min and 2 nodes.

[ux00000@login1 ~]$ qsub sample.sh
```



Submit Job (interactive job)

qrsh -l resource_type -l reserve_time -g TSUBAME_group

Refer to TSUBAME4.0 User's Guide.

https://www.t4.cii.isct.ac.jp/docs/handbook.en/jobs/#interactive

```
File Edit View Help

#General usage
#Interactive execution using node_f as resource type
[ux00000@login1 ~]$ qrsh -g GSIC -l node_f=1 -l h_rt=8:0:0

#For trial, submit a job without -g option. Note that the limitation to a job execution is within 10min and 2 nodes.

[GSIC@login1 ~]$ qrsh -l node_f=2 -l h_rt=0:10:0

[GSIC@r5i6n5 ~]$ (Run command here.)
```



batch queue control

Confirm that the job(s) has been submitted with qstat.

```
GSIC@t4support2:~
      Edit
            View
                   Help
GSIC@login1:~> qstat
                                                                      jclass slots ja-task-ID
iob-ID
          prior name
                                      state submit/start at
                                                              queue
                           user
         0.55500 PDF
                           GSICUSER00 r 10/04/2017 07:39:58 all.g@r2i4n6
93501
93578
         0.55500 QRLOGIN GSICUSER00 r
                                           10/04/2017 11:39:58 all.q@r6i3n2
                                                                             28
```

Delete the running job with qdel

```
GSIC@t4support2:~

File Edit View Help

GSIC@login1:~> qdel 93578

GSIC@login1:~> qstat

GSIC@login1:~>
```



The size of a running program

- Command to measure the memory size of running programs ps aux, top
- *Press q key to stop top command.

```
GSIC@t4support:~
      Edit
            View
                    Help
ux00000@r6n2:~> ps aux
                 PID %CPU %MEM
USER
                                    VSZ
                                               TTY STAT START
                                                                   TIME COMMAND
ux00000
              354797 13.2 0.1 52321684 490304 pts/1 Rl
                                                         13:19
                                                                   0:02 pmemd.cuda.MPI
              354798 13.2 0.1 52321348 487148 pts/1 Rl 13:19
                                                                  0:02 pmemd.cuda.MPI
ux00000
ux00000@r6n2:~> top
                                       SHR S
                                                              TIME+ COMMAND
PID USER
              PR NI
                        VIRT
                                RES
354797 hpe_use+ 20 0 49.897g 456836 408116 R 14.28<mark>6</mark> 0.173
                                                              0:02.09 pmemd.cuda.MPI
354798 hpe use+ 20 0 49.897g 453680 407172 R 14.286 0.172
                                                              0:02.08 pmemd.cuda.MPI
```



Forcely stop a program

Confirm the process ID of a running program.

Use either ps or top command. (the example is shown below.)

```
GSIC@t4support:~

File Edit View Help

ux00000@r6n2:~> ps aux | grep ux00000

354797 | 13.2 | 0.1 52321684 | 490304 | pts/1 | Rl | 13:19 | 0:02 | pmemd.cuda.MPI -0 -i | input -p | top -o | test | 354798 | 13.2 | 0.1 52321348 | 487148 | pts/1 | Rl | 13:19 | 0:02 | pmemd.cuda.MPI -0 -i | input -p | top -o | test | ux00000@r6n2:~> top

354797 | hpe_use+ 20 | 0 | 49.897g | 456836 | 408116 | R | 14.286 | 0.173 | 0:02.09 | pmemd.cuda.MPI | 354798 | hpe_use+ 20 | 0 | 49.897g | 453680 | 407172 | R | 14.286 | 0.172 | 0:02.08 | pmemd.cuda.MPI | Process ID
```

Execute kill command to stop the process.

```
GSIC@t4support:~

File Edit View Help

ux00000@r6n2:~> kill 354797 354798

# Forcely
ux00000@r6n2:~> kill -9 354797 354798
```



Process information gathering commands (1)

- Display the users logging in -> who command
- Display status of the users logging in -> w command

```
GSIC@t4support:~
     Edit View
                Help
[ux00000@t4support ~]$ who
GSIC
      pts/5
                2017-09-06 10:52 (:1)
GSIC
      pts/6
                2017-09-06 11:22 (:1)
TEST
      pts/2
                2017-09-07 10:05 (192.168.111.63)
GSICUSE pts/7
                2017-10-03 12:30 (:2)
GSICUSE pts/3
                2017-10-04 12:37 (192.168.111.63)
[ux00000@t4support ~]$ w
12:39:20 up 51 days, 3:29, 12 users, load average: 1.00, 1.01, 1.00
USER
              FROM
                           LOGIN@ IDLE JCPU PCPU WHAT
                            0611月10 ?xdm? 22days 22.80s gdm-session-worker
      pts/5
GSIC
              :1
                           0611月10 41days 0.25s 10:00 /usr/libexec/
GSIC
      pts/6
TEST
      pts/2
              GSICUSE pts/7
                            火12 24:09m 0.05s 0.05s bash
GSICUSE pts/3
```



Process information gathering commands (2)

Display the status of a node -> top command

```
GSIC@t4support:~
     Edit View
                   Help
[GSIC@t4support ~]$ top
Tasks: 784 total, 1 running, 781 sleeping, 2 stopped,
%Cpu(s): 0.1 us, 0.1 sy, 0.0 ni, 99.9 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
KiB Mem: 26377451+total, 14203016 used, 24957150+free,
                                                       3352 buffers
               0 total,
KiB Swap:
                              0 used,
                                            0 free. 10473748 cached Mem
                                      SHR S %CPU %MEM
               PR NI
                        VIRT RES
  PID USER
                                                           TIME+ COMMAND
225488 root
               20 0 371260 20796
                                     4816 S 2.990 0.008 118:58.30 nv-hostengine
               20 0 110076 66204 61604 S 0.332 0.025 0:19.26 systemd-journal
 1111 root
```

Display running processes -> ps command



Example (qsub)

Submit a batch job to TSUBAME (trial run)

```
$ qsub sample.sh
```

Check job status \$ qstat

If \${JOB_NAME}.o\${JOB_ID} and \${JOB_NAME}.e\${JOB_ID} are created in working directory, the job has already finished.



User environment

- Shell
- Environment variables
- HISTSIZE shell variable
- PATH variable
- File transfer
- SSH
- X-window system



Shell

- Shell is a computer program that exposes an operating system's services to a human user or other programs.
- The major compatible shells which TSUBAME4 supports, which available with chsh command, are as follows:
 - /bin/bash
 - /bin/tcsh
 - /bin/zsh
- chsh command to change a current shell
 - \$ chsh /bin/tcsh

It takes 5 minutes to reflect the change.



Load shell environment

In case of bash

 The order of profiles (configuration files) read when log in /etc/profile /etc/bashrc

```
~/.bash_profile
~/.bash_login (if ~/.bash_profile is not exist)
```

- ~/.bashrc is loaded whenever bash is executed.
- Editing the personal configuration file ~/.bashrc
 - PATH="/usr/local/bin:\$PATH"
 - export PATH
- After editing, re-login or execute "source .bashrc" to reflect.
- It is preferable to write alias here.
- In case of editing files, check properly before updating.
- Check it in another terminal.



Variables

- Shell variable
 - Variable valid in a current shell.
- Environment variable
 - Variable valid in every shell.



HISTSIZE shell variable

History

- Stores a predetermined number of commands most recently.
- It can be useful when executing the same (or similar) command.
- The number of history to be stored can be set arbitrarily.

Examples

- + export HISTSIZE=600 ⇒ History size will be set 600
- \$ history 3 \Rightarrow Shows 3 items in history list

534 cd

535 ls

536 history 3



PATH variable

- Set the location of command.
- The setting sometimes needs to be modified. For example, when a command or a program are installed or created by an individual.

```
File Edit View Help

[GSIC@t4support2 Program]$ 1s
a.out

[GSIC@t4support2 Program]$ a.out

If 'a.out' is not a typo you can use command-not-found to lookup the package that contains it, like this:
    cnf a.out

[GSIC@t4support2 Program]$ PATH=$PATH:.

[GSIC@t4support2 Program]$ a.out

14digit@M_PI=3.14159265358979

[GSIC@t4support2 Program]$
```

※ If it is described in .bashrc, it will be always enabled.



File transfer

- A system connected via a network is called a host.
- It is easy to transfer files among hosts via TCP/IP.
- Commands for the function
 - ftp, rcp, rsync, sftp, scp
- rsync, sftp, scp are available in TSUBAME.



Examples of rsync/sftp/scp

```
GSIC@t4support:~
File
    Edit View
                  Help
#rsync
[GSIC@t4support ~]$ rsync -av --progress -e "ssh -i .ssh/id_ecdsa -l ux00000"
login.t4.gsic.titech.ac.jp:/gs/bs/soudan/UNIX/testfile ./
receiving incremental file list
testfile
         990 100% 966.80kB/s
                                 0:00:00 (xfer#1, to-check=0/1)
sent 42 bytes received 1078 bytes 2240.00 bytes/sec
total size is 990 speedup is 0.88
[GSIC@t4support ~]$
#sftp
[GSIC@t4support ~]$ sftp -i ~/.ssh/id ecdsa ux00000@login.t4.gsic.titech.ac.jp
Connected to login.t4.gsic.titech.ac.jp.
sftp> get /gs/bs/soudan/UNIX/testfile
Fetching /gs/bs/soudan/UNIX/testfile to testfile
/gs/hbs/soudan/UNIX/testfile
sftp> exit
#scp
[GSIC@t4support ~]$ scp -i ~/.ssh/id ecdsa
ux00000@login.t4.gsic.titech.ac.jp:/gs/bs/soudan/UNIX/testfile .
testfile
```



SSH connection Examples

login to TSUBAME4 with login name (GSIC→GSCIUSER00)

```
GSIC@t4support:~

File Edit View Help

[GSIC@t4support ~]$ ssh login.t4.gsic.titech.ac.jp -l ux000000 -i ~/.ssh/id_ecdsa
Last login: Tue Oct 3 09:26:54 2017 from 131.112.3.100
ux00000@login1:~>
ux00000@login1:~> top
ux00000@login1:~> exit
```

login to TSUBAME4 as the same login name (GSCIUSER→GSCIUSER)

```
GSIC@t4support:~

File Edit View Help

[ux00000@t4support ~]$ ssh login.t4.gsic.titech.ac.jp -i ~/.ssh/id_ecdsa
Last login: Tue Oct 4 09:26:54 2017 from 131.112.3.100
ux00000@login1:~>
ux00000@login1:~> top
ux00000@login1:~> exit
```



X-Window system

- Used in various operating systems including Linux.
- Used for GUI applications
- Hardware independent
 - The system is pre-installed in Linux/Mac
 - Lots of software for Windows
 - Cygwin
 - MobaXterm
 - PuTTY/Tera Term/RLogin+VcXsrv/Xming



X-Window system

- Running X-Window applications
 - → Client program, server program
- X protocol, unique communication procedure
 - → Data exchange between client/server
 - Server side (Displayed side)
 Definition to allow display request from system
 % xhost +client_host_name
 - Client side (Displaying side)
 Specifies DISPLAY environment variables.
 % export DISPLAY=server_host_name

Please use Open OnDemand to run GUI application.

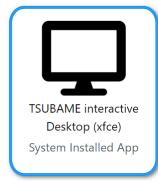


Usage of compute node (Open OnDemand)

- https://ood.t4.gsic.titech.ac.jp/
- Applications described as "interactive" are for free within campus.
- To use this service, check the followings:
 - Already configured password for your TSUBAME account
 - The e-mail sent from this service will be received.

Pinned Apps A featured subset of all available apps









for details, https://www.t4.cii.isct.ac.jp/docs/ood/ (In Japanese)

TSUBAME Desktop (xfce)

This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.

Select resource type

gpu_1	~
If you use resevation, only node_f, node_h, node_q, and node_o are available.	
Number of Request resources.	
1	
TSUBAME group	
tgz-jochu	~
Maximum run time(hh:mm:ss)	
24:00:00	
Specify the job execution time in the format hh:mm:ss. If Trial run is selected for	
TSUBAME group, the run time should be less than 10 minutes.	
Priority Option	
-5 Standard execution priority.	~
Reservation Number (AR ID)	
Launch	



Conclusion

That's all!
Thank you!



Get more information about T4

- Manuals
 - https://www.t4.cii.isct.ac.jp/en/manuals
 - TSUBAME4.0 User's Guide
 - https://www.t4.cii.isct.ac.jp/docs/handbook.en/
 - TSUBAME Portal User's Guide
 - https://www.t4.cii.isct.ac.jp/docs/portal.en/
 - Migration from TSUBAME3.0 to TSUBAME4.0
 - https://www.t4.cii.isct.ac.jp/docs/migration.en/
- This document is available at https://www.t4.cii.isct.ac.jp/en/lectures