

Linux-how-to

- In Linux, you should work with *terminal*, which is CUI (character user interface), a different interface from GUI (graphical user interface).
- The Gaussian is usually done in remote environment, because running Gaussian on your desktop/laptop is not a good idea as it demands large CPU power, memory, and hardware in/out.
- Thus it is recommended to run the Gaussian on supercomputers. Here, we mainly use TSUBAME, a Tokyo-Tech supercomputer.
- The usage of TSUBAME is introduced later. First, we will look into the basic linux commands.

Linux environment setup

Mac

- No need to do, just open "terminal.app".

Windows

- Install WSL2 (Windows service for linux ver.2); following is an example in Windows 10
 - i. Open "Windows Power Shell" or "Terminal" as Administrator.
 - ii. Type `wsl --set-default-version 2` (for safe)
 - iii. Type `wsl --install -d Ubuntu`.
 - iv. After installation is done, open `Ubuntu` in Application.
- When above doesn't work, check "Windows の機能の有効化、または無効化", then "Linux 用 Windows サブシステム", "仮想マシンプラットフォーム" is ON.

- You can access Windows system from Ubuntu like: `cd` to Desktop by `cd /mnt/c/Users/your_name/Desktop/`.

- It is useful to make symbolic link between Ubuntu and Windows like

```
cd  
ln -s /mnt/c/Users/your_user_name/Desktop/ desktop
```

- If some commands are unavailable (e.g. vi), install them by `sudo apt-get install vim`.

ssh

- To login the supercomputer from your environment, you need to use *ssh* so you have to set up it.

ssh key generation

- To make a ssh connection to remote environment, you need a *ssh-key*.
- There are two keys, a *public key* and *private key*.
- To generate these keys, execute `ssh-keygen` on your linux terminal.
- You can set your passphrase if you like.
- This makes following keys.
 - `~/.ssh/id_rsa` (private key)
 - `~/.ssh/id_rsa.pub` (public key)
- After generating this, you should upload the public key to the remote environment.
Keep a private key to your local environment.

Public key upload

1. Login a portal site with your internet browser.
2. Click "ssh public key registration" (or similar contents).
3. Copy the public key file (id_rsa_XXX.pub) generated by ssh-keygen.
4. Paste the above contents to some appropriate space.
5. Go back to terminal and login via: `ssh [account_name]@[login_node].ac.jp -i [private_key-file]`
 - In TSUBAME, `ssh [account_name]@login.t3.gsic.titech.ac.jp -i [private_key-file]`

ssh-config

- To make next login easier, it is better to set up the ssh configure file to make login easier.
- An example of TSUBAME is (minimal configuration),

```
Host tsubame
  HostName login.t3.gsic.titech.ac.jp
  User your_name
  IdentityFile /Users/your_name/.ssh/id_rsa_tsubame
```

- After that, you can login TSUBAME by `ssh tsubame`.

Basic linux commands

- `cd` : To change the current directory, `cd target_dir` . Note that `target_dir` should be a directory, not a file.
- `ls` : To list the files and directories in the current directory, you should `ls` .
- `cp` : To copy a file, you should `cp from_file to_file` .
- `pwd` : To display the current directory, type `pwd` .
- `less` : To see the contents of file. For files more than one page, place *space* key to see further. Type `q` to quit. If you type `shift + f` , it waits the reloading the file. This mode can be quitted by `ctrl + c` .
- `grep` : To extract a line with some keyword, type `grep "keyword" filename` .
- `mkdir` : To make a new directory, type `mkdir new_dir` .

Editor

- There are several editors in linux. Two editors are popular, *vi* and *emacs*.
- Here in this course we will use `vi`.
- You can use these editors in the remote environment.
- If you don't want to use vi/emacs, copy your target file to local PC and then use your favorite editor, then send it back to remote environment.

- However, your editor should output the text file with Linux-compatible newline code.
 - Newline code depends on the OS (operating system).
 - Linux and Mac (after Mac OS X) uses LF(Line Feed) and Windows uses CR (Carriage Return) + LF.
- So use VS Code, sakura editor, K2E, etc.

vi

- Minimal instruction of vi.
 - open file: `vi file.txt`
 - vi has two modes: command mode and insert mode
 - command mode to insert mode: `i`
 - insert mode to command mode: `esc`
 - you can put character only in the insert mode
 - move: `j` (down), `k` (up), `l` (right), `h` (left)
 - deleting character: `x` (no need to be insert mode)
 - save and exit: `:wq`
 - exit without saving: `:q!`

scp

- After making a ssh-login environment, you can use `scp` (means secure copy) to send/take file from/to remote environment.
 - send: `scp your_file login_node:directory`
 - take: `scp login_node:directory your_local_directory`

submitting jobs

- See "tsubame.md" for details.