Introduction

- 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, memotry, and hardware in/out.
- Thus it is recommented to run the Gaussian on supercomputes. 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.

Login

1. Login a portal site with your internet browser (Edge, Chrome, Safari etc.)
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 [your_account_name]@[login_node].ac.jp -i [your_private_keyfile]

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 quited 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, *vim* and *emacs*.
- To use vi, just type `vi target_file`.
- You can use these editors in the remote environment.
- If you do not want to use vi/emacs, *copy your target file to local PC and then use your favorite editor (like notepad), then send it back to remote environment*.

vi usage

- asdf

ssh

Key-generation

- `To make a ssh connection to remote environment, you need a *ssh-key*. There are two kyes, a *public key* and *private key*.
- To generate these keys, execute `ssh-keygen`.

```
ssh-keygen
```

- 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 remove environment. Keep a private key to your local environment.

scp

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

Submitting jobs

- pjsub?