

Practical Parallel Computing (実践的並列コンピューティング)

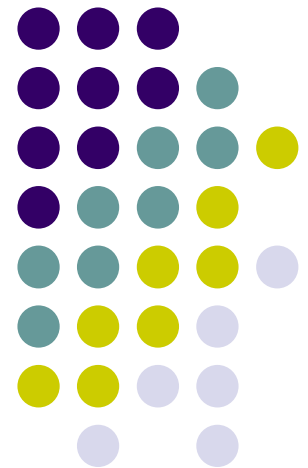
Introduction (1)

Apr 12, 2021

Toshio Endo

School of Computing & GSIC

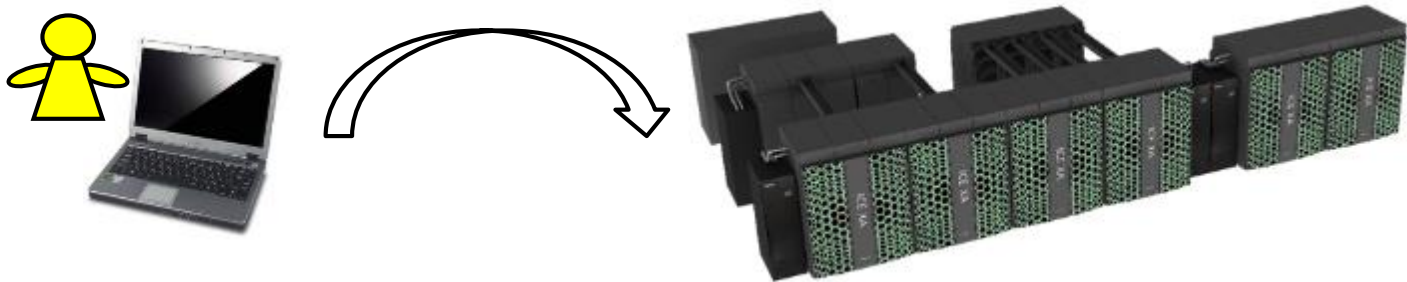
endo@is.titech.ac.jp



Purpose of This Course



- To learn parallel computing practically
 - Lecture + Practice
 - We will use the TSUBAME supercomputer from your PC





Overview of This Course

- Part 0: Introduction
 - 2 classes including today
- Part 1: **OpenMP** for shared memory programming
 - 4 classes
- Part 2: **GPU** programming
 - 4 classes, OpenACC and CUDA
- Part 3: **MPI** for distributed memory programming
 - 3 classes

In 2021, talk and presentations are done in English

奇数年度は英語です



Credits / 単位認定

Your score will be determined by the followings

- Each part (OpenMP, GPU, MPI) has homework.

Reports submission for 2 parts is required

- The due date will be about 1.5 weeks after each part finished
- (You can submit more than 2)

下記により採点・単位認定

- OpenMP, GPU, MPIの各パートで課題を出す。**2つのパートのレポート提出**を必須とする
 - 〆切は、各パート終了の約1.5週間後
 - (それ以上のレポート提出してもよい)



What We Do

We do

- Parallel programming by yourself
 - C language + something
 - CPU parallel programming and GPU parallel programming
- To evaluate speed-up of programs on TSUBAME supercomputer



What We Don't

We don't

- To use Python
- To learn usage of machine learning framework
- To learn usage of parallel computation libraries
- To learn variety of parallel algorithms
 - Consider to attend “CSC.T526 High Performance Scientific Computing”
- To program network or client-server applications



Requirements (1)

- Knowledge of basic C language
 - Pointers, malloc/free
 - Relation between pointers and arrays
- Knowledge of Pthread, Java threads is useful, but not required



Requirements (2)

- Knowledge of basic Linux commands
 - TSUBAME uses Linux OS
 - ls, cp, mkdir, gcc...
 - “make” command will help you
 - SSH public key authorization (SSH公開鍵認証)
- A PC to log-in to TSUBAME3 and Internet connection
 - For the remote course, you will need to open both Zoom window and a terminal window on your PC ☹



Supercomputers



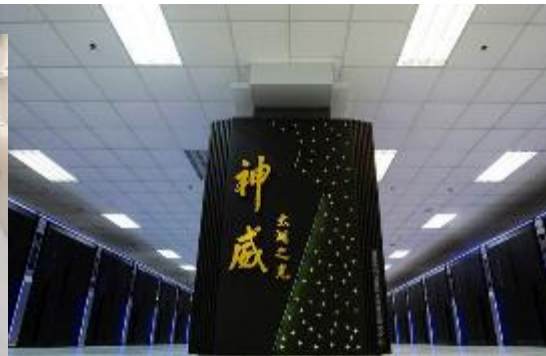
Fugaku
World No. 1



Tokyo Tech
TSUBAME3.0



Summit
World No.2

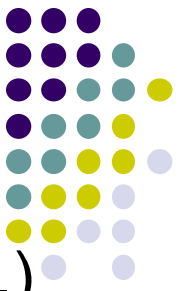


Taifulight

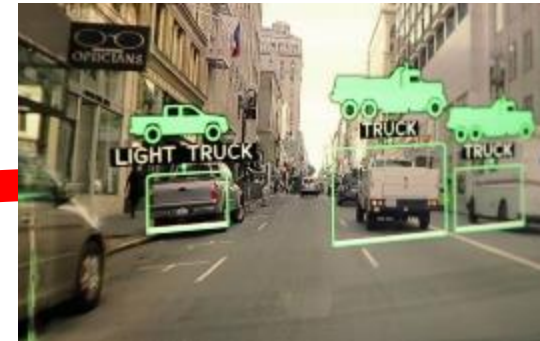
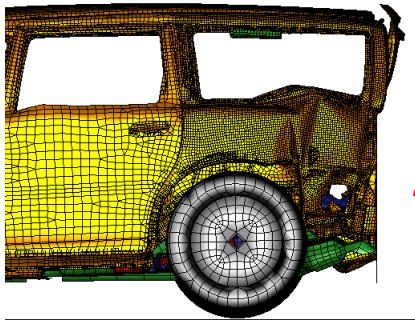
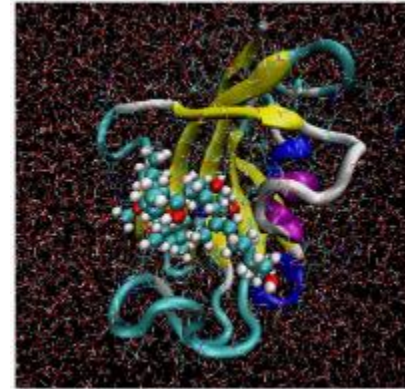
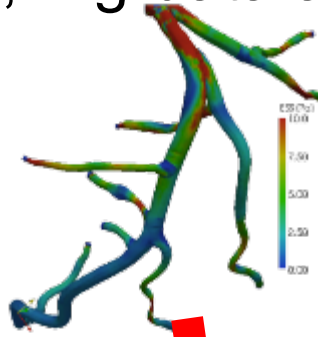


ABCI
AIST, Japan

What are Supercomputers (SCs) used for?



- Simulations (Fluid dynamics, molecular dynamics, etc.)
- Machine learning, Big-data analysis



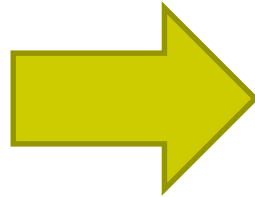
Difference with “Normal” Computers



- SCs are computers that support **much faster and much larger computation** than normal computers
 - Speeds are often compared in “Flops” = The number of possible add/subtract/multiplication operations per second



~60,000x!

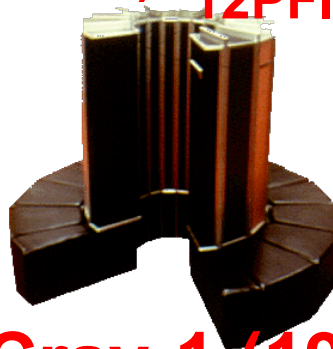


~200GFlops (2×10^{11} times per sec)

12PFlops (1.2×10^{16} times per sec)



PC in 1980



Cray-1 (1976)

160MFlops



Modern
Cell Phone

Why are Speed & Size Important?

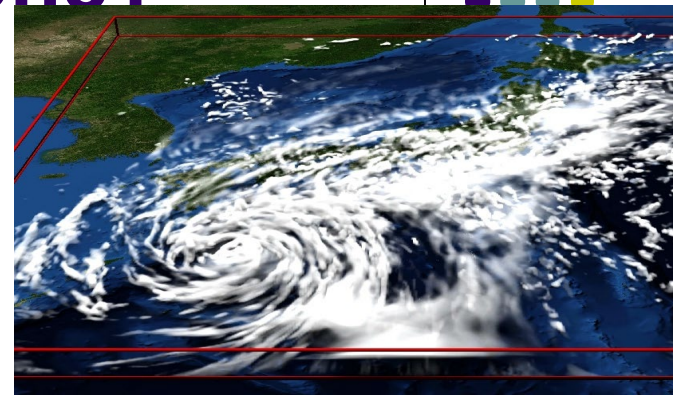


- For simulation & big-data analysis, **large number of computations** should be done speedily
 - ⇒ Want to obtain forecast of tomorrow weather by tomorrow (of course!)
 - ⇒ Want to develop and sell new medicine (than competitors)
- For simulation & big-data analysis, storing **large scale data** is needed
 - ⇒ Want to make discovery by comparing mass genome data
 - ⇒ Want to visualize motion of molecules for every time step

How is Weather Forecast done?

Motions of air, clouds, water are expressed by differential equations

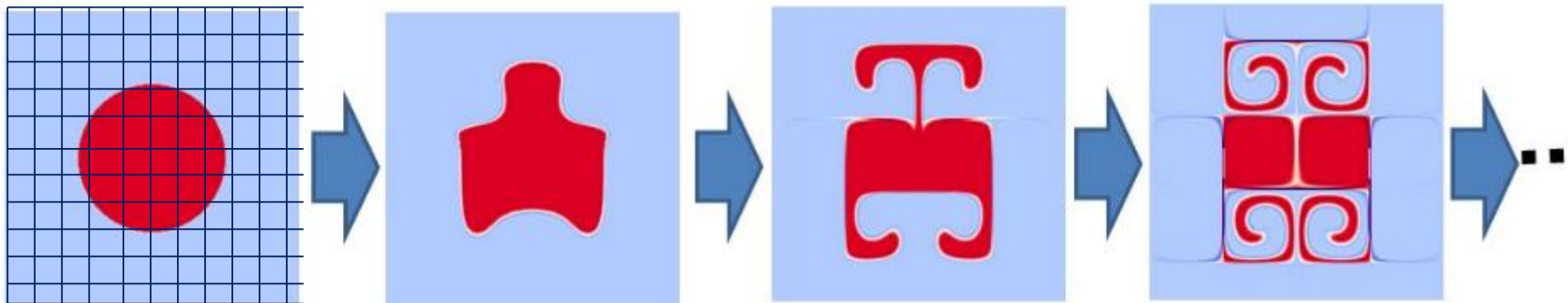
$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{v} - g \hat{\mathbf{z}}$$



But no analytical solution for them, generally

⇒ Instead, space and time are **discretized**

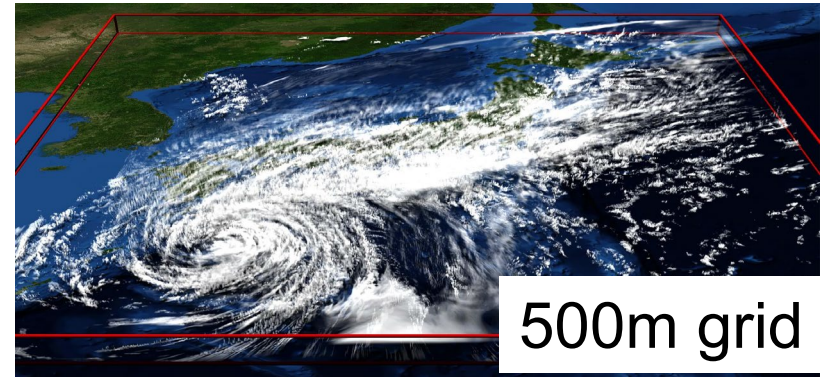
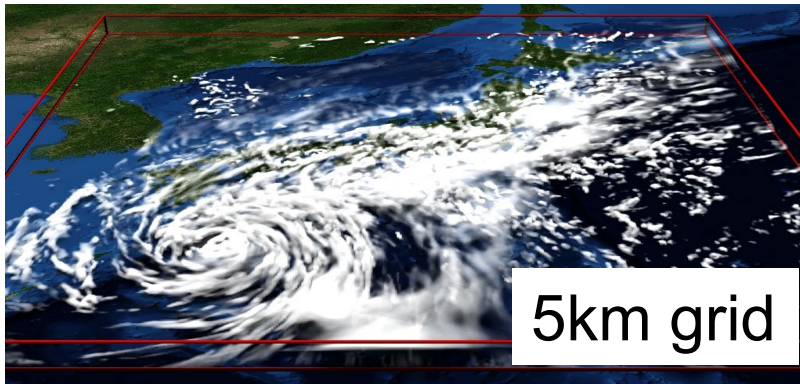
- The space is divided into small grids, expressed as an array
⇒ Each array element should be computed
- The time is divided into time steps
⇒ After a time step is computed, we go to next step, and so on



Why is Speed Important?



- Since we have to compute all points for every time step, computational complexity is
 - $O(\text{x-size} \times \text{y-size} \times \text{z-size} \times \text{time-steps})$



For better prediction, we need to make grid finer (arrays larger)

If resolution is 10x higher, we need **10000x** computations!
(10x10x10x10)

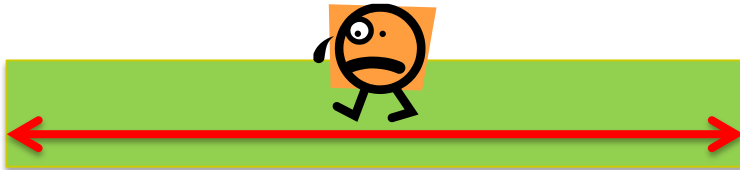
→ In future, we are going to 50m or smaller grids



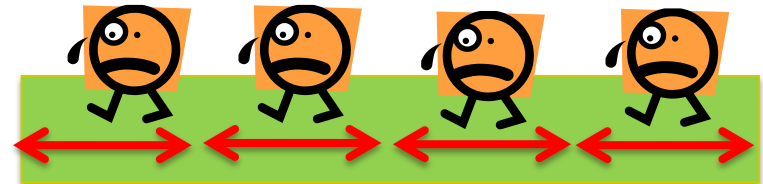
Why are SCs Fast?

- Do SCs have 10THz CPUs? → **No!!**
- Basic idea: **If multiple workers work cooperatively and simultaneously, they can do great tasks than a single worker** ⇒ **Parallel execution**

A worker is cultivating a large field



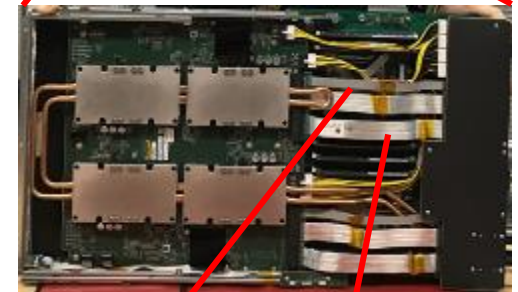
Multiple workers are working together → **fast!**



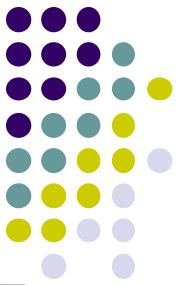
SC Structure is Hierarchical



- System = Many **nodes** (=computers) + **External storage**
 - They are connected by **Network**
- Node = Several **processors** (CPU etc.) + **Memory** + **Local storage**
 - They are connected by **PCI-e, QPI, etc.**
- Processor = Several **cores** + **Cache**



Structure of TSUBAME3 and Fugaku



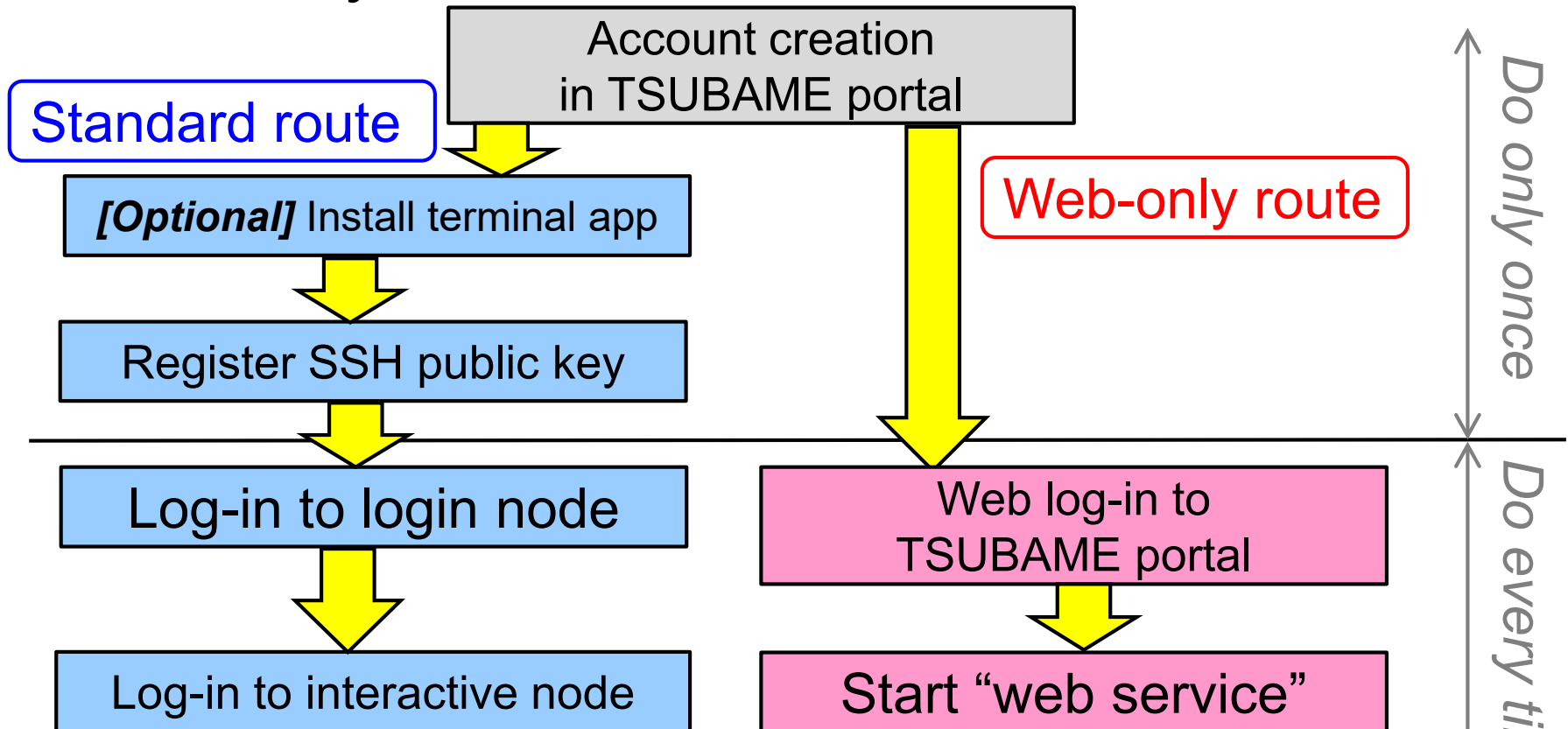
System	540 nodes	12.15PFlops	160,000 nodes	540PFlops
Node	2 CPUs + 4 GPUs	2 x 425GFlops + 4 x 5300GFlops = 22.05TFlops	1 CPU	3.38TFlops
Processor	CPU: 14 cores GPU: 56 SMXs	CPU: 425GFlops GPU: 5300GFlops	48 cores	3.38TFlops
Core	CPU core: 1.9GHz x 16 = 30.4GFlops GPU SMX: 1.48GHz x 64 = 94.6GFlops		2.2GHz x 32 = 70.4GFlops	

Here “Flops” shows speed in “double precision (FP64)”



Start to Use TSUBAME

- Two ways to use TSUBAME in this class



Also, please register to "[tga-ppcomp](#)" TSUBAME group
(see Today's homework)

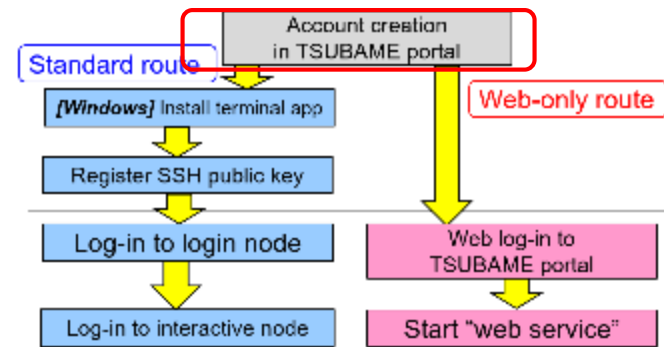
- ➔ Log-in and then click
“TSUBAME portal”



Standard route

Web-only route

Account Creation in TSUBAME Portal



- Visit **TokyoTech Portal / 東工大ポータル** and log-in



Click **“TSUBAME portal”**

➔ If you are new to TSUBAME, you will be taken to account creation pages

➔ You will get an account.

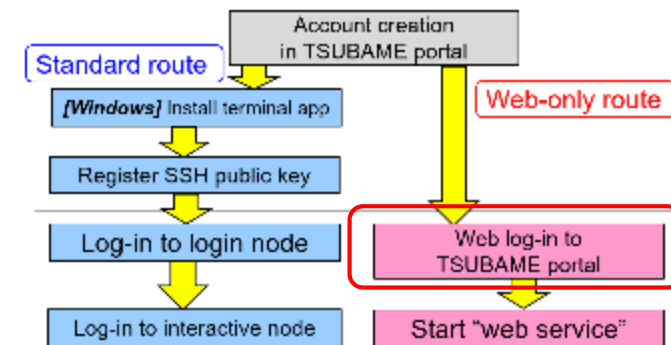
- Account name is same as the **student ID (like 20M12345)** for Tokyo Tech students

- For details, visit <https://www.t3.gsic.titech.ac.jp/> and click **“Getting Accounts” / “アカウント取得方法”**

Web-only route

Log-in to TSUBAME Portal

- Visit “Tokyo Tech portal”
- Log-in
- Click “TSUBAME portal”



Your account name

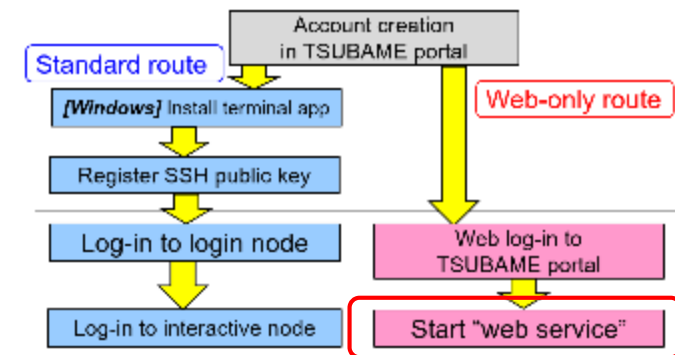
Will be used in “standard route”

Used in the next page

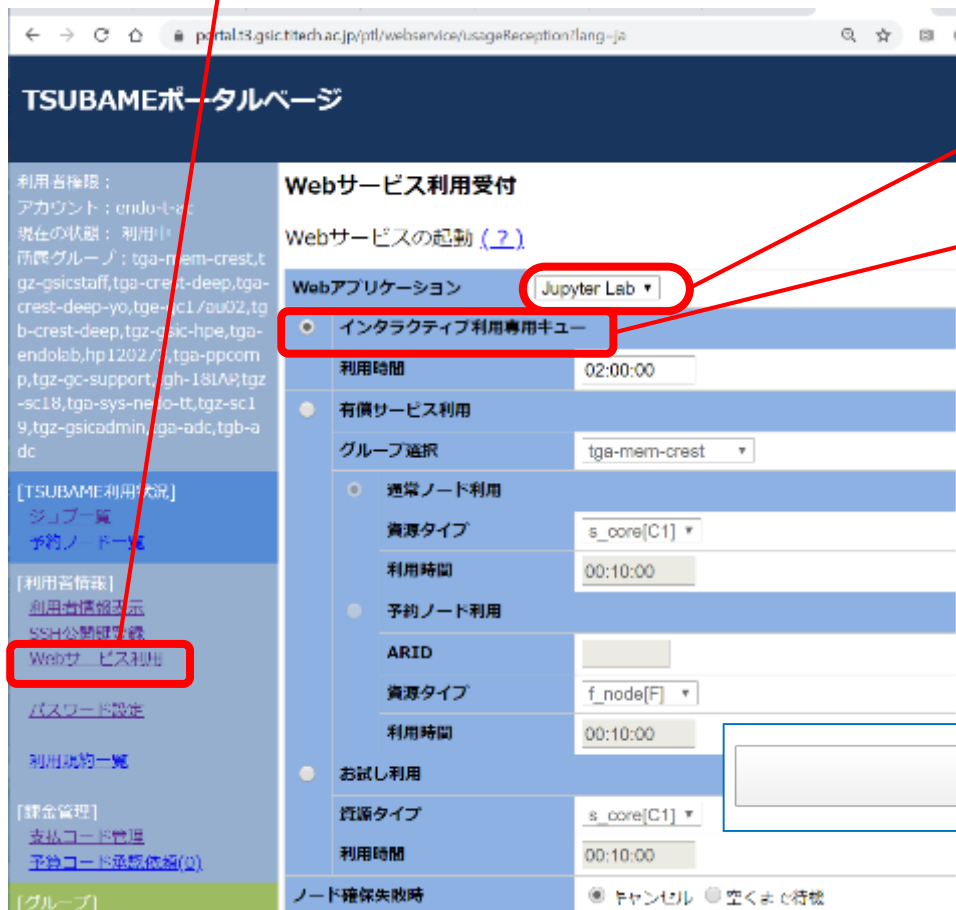


Web-only route

Start “Web Service” (1)



- In TSUBAME portal, click **Use Web service / Webサービス利用**

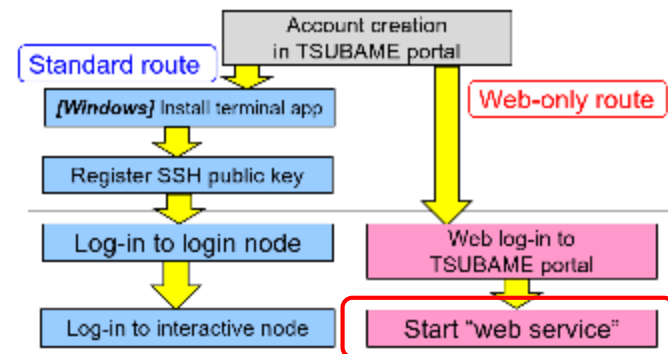


Choose
Jupyter Lab

Choose
Queue for interactive use only/
インタラクティブ専用キュー

And click
Start-up / 起動 button

Start “Web Service” (2)



- When you see a green row, please wait and push **update / 表示更新** button

状態	操作	グループ名	AR ID	JOB ID	CPU(core)	GPU	TIME(h)	登録	開始
準備中	キャンセル	--	--	7007687	7	1	02:00:00		
終了		--	--	7000686	7	1	12:00:00	2020/05/01 13:22:24	2020/05/01 13:22:30
終了		--	--	7000685	7	1	12:00:00	2020/05/01 13:19:00	2020/05/01 13:19:14

Wait for 1-2 minutes and “update”

状態	操作	グループ名	AR ID	JOB ID	CPU(core)	GPU	TIME(h)	登録	開始
実行中	表示	--	--	7007687	7	1	02:00:00	2020/05/06 12:54:18	2020/05/06 12:54:18
終了		--	--	7000686	7	1	12:00:00	2020/05/01 13:22:24	2020/05/01 13:22:30
終了		--	--	7000685	7	1	12:00:00	2020/05/01 13:19:00	2020/05/01 13:19:14

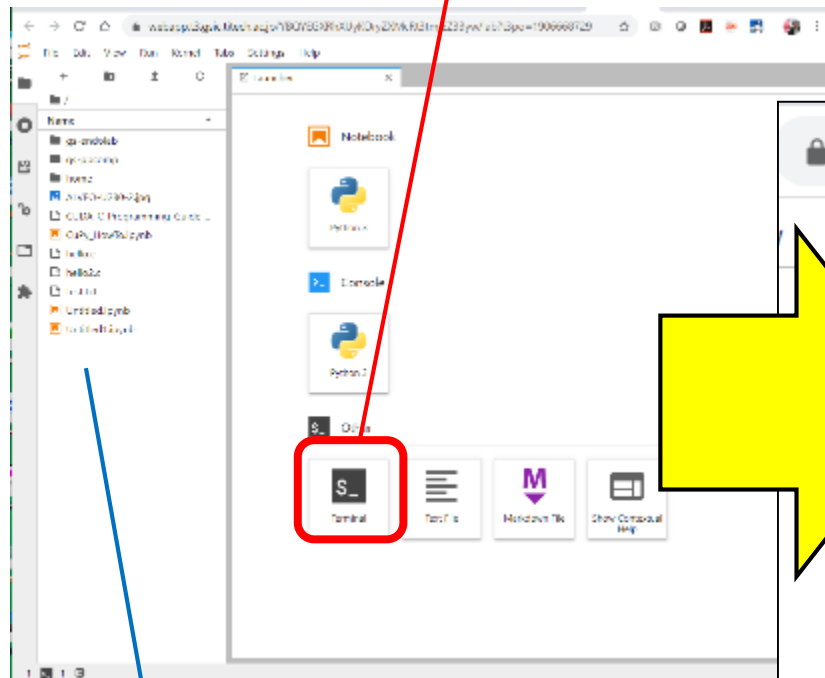
Please be patient...

- If you see a blue row, push **Display / 表示** button

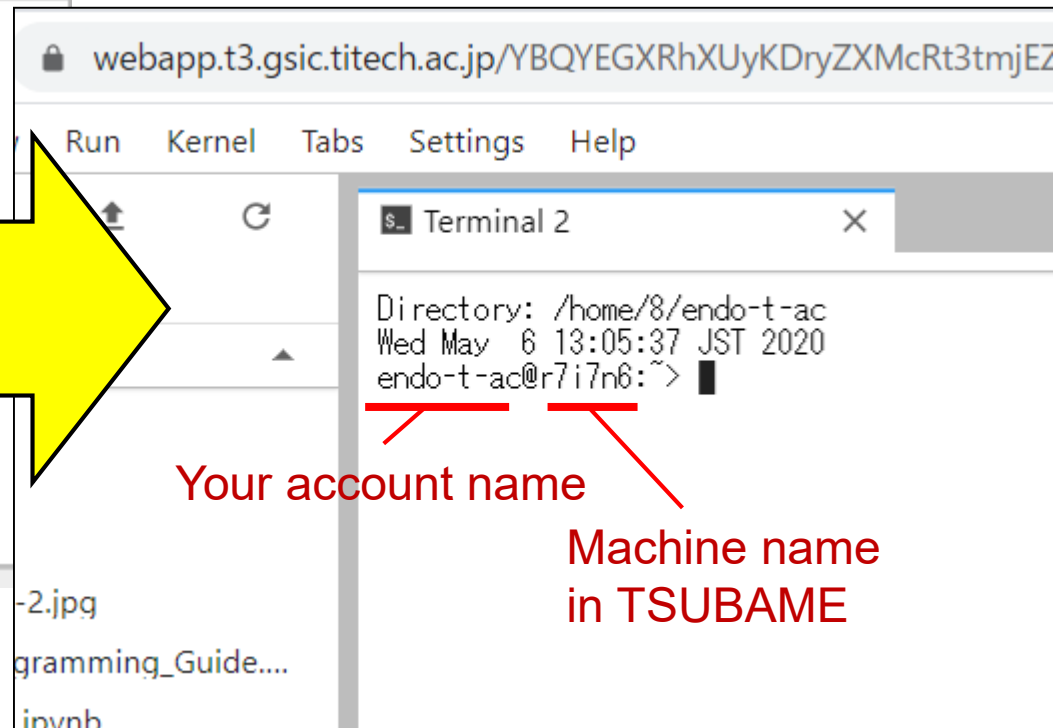
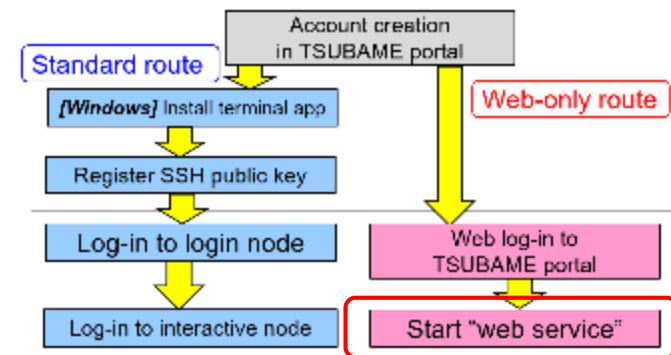
Web-only route

Start “Web Service” (3)

- You will see a “Jupyter” screen
- Click the **Terminal** icon



~/t3workspace/ directory
in TSUBAME



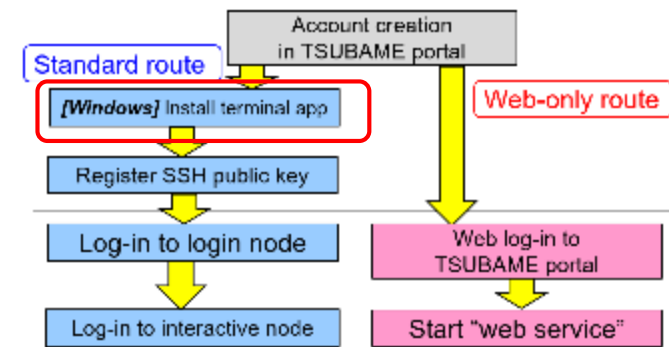
Your account name

Machine name
in TSUBAME

Standard route

[Optional] Install a Terminal Application

(In standard route) Your PC must have a terminal application that supports SSH protocol



On Mac

- Start **terminal** / ターミナル app → use **ssh** command



On Windows...

- Recently, **command prompt** / コマンドプロンプト is ok
 - On Windows10 after 2018, **ssh** command has been installed

Also you can install other applications

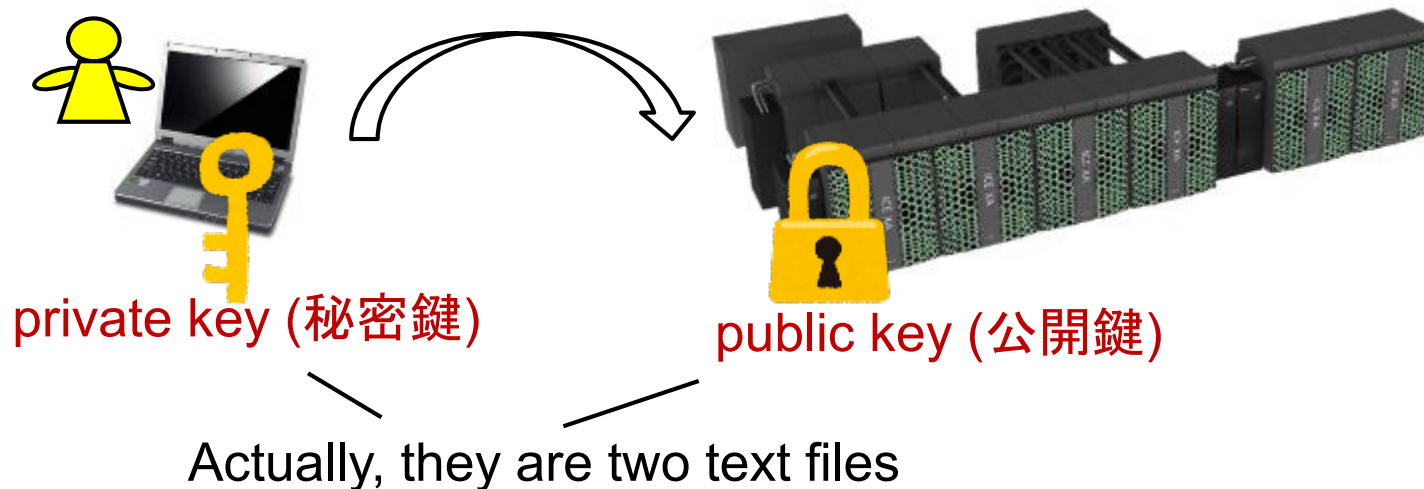
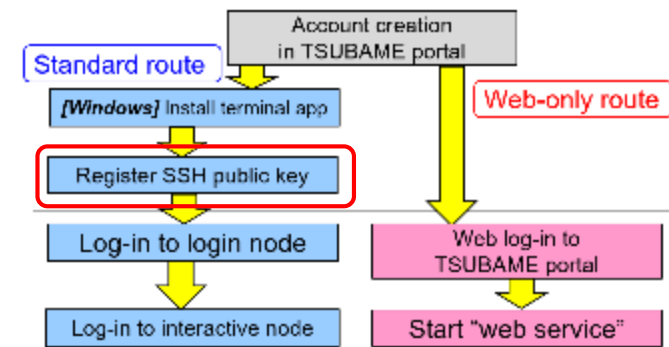
- MobaXterm on Windows**
- Putty on Windows/Mac**
- iTerm on Mac ...**

Or try google
“windows ssh client”
“mac ssh client”

Standard route

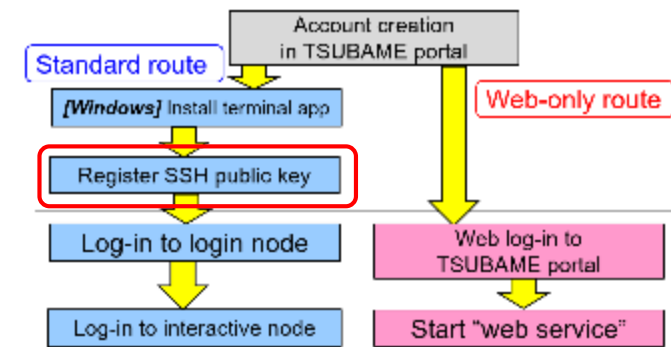
Register an SSH Public Key (1)

- To log-in to TSUBAME,
 - A password is NOT used
 - instead, **public key (公開鍵)** method is used



Standard route

Register an SSH Public Key (2)



Please create key-pair on your PC by yourself

- On Mac terminal or Windows command prompt

- Use **ssh-keygen** command
- Setting “**passphrase**” is strongly recommend
- ➔ Two files are created

In default,

private key → `.ssh/id_rsa` (Mac) `.ssh¥id_rsa` (Win)
public key → `.ssh/id_rsa.pub` (Mac) `.ssh¥id_rsa.pub` (Win)



- If you are using another terminal application, try Google

- Such as “mobaXterm public key”
- If you are asked the key format, choose “**OpenSSH**” format, NOT “ssh.com format”

Standard route

Register an SSH Public Key (3)

Register your public key on TSUBAME portal

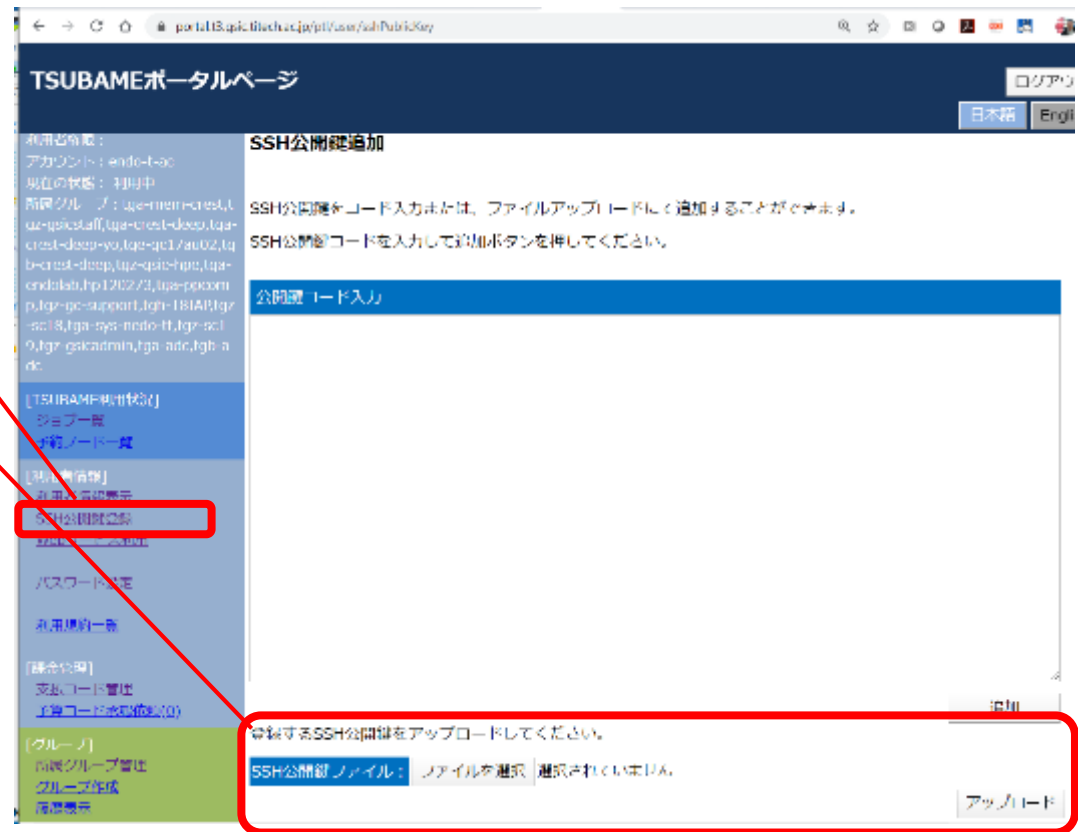
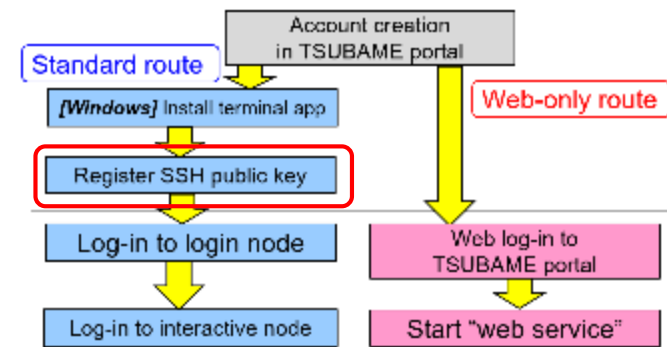
1. Click **Register SSH public key / SSH公開鍵登録**
2. Upload your **public key**
 - Don't upload the private key!!



id_rsa



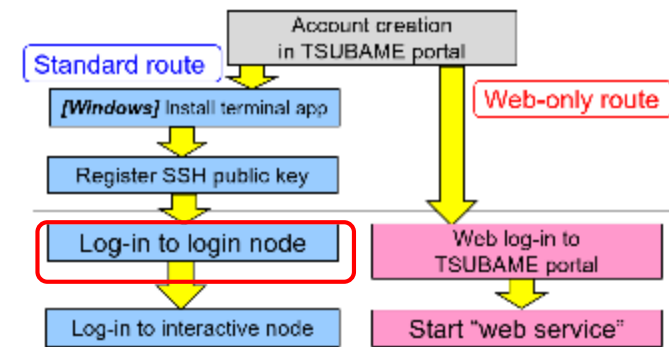
id_rsa.pub



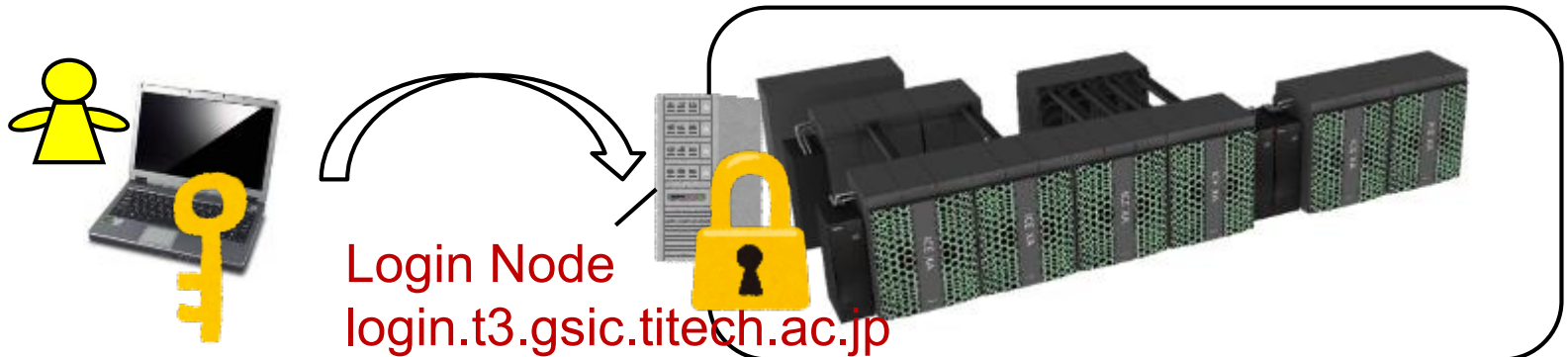
NOTE: The key is automatically added to
~/.ssh/authorized_keys on TSUBAME

Standard route

Log-in to TSUBAME Login Node



- On Mac terminal or Windows command prompt
`ssh -i [private key] [account]@login.t3.gsic.titech.ac.jp`
ex) `ssh -i .ssh/id_rsa 20M12345@login.t3.gsic.titech.ac.jp`



```
Last login: Wed May 6 13:30:17 2020 from 160.13.82.172
-----
Last modified: Apr 6 17:00:00 JST 2020

*** Do not run programs with high load average such as ISV ***
*** on login0 and 1. ***

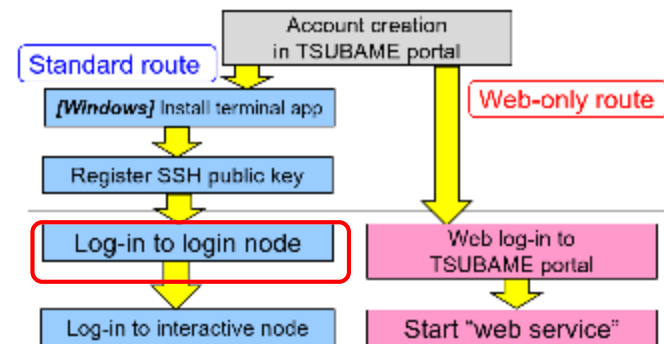
(The current TSUBAME 3.0 operational status)
http://www.t3.gsic.titech.ac.jp/
-----
endo-t-ac@login1:~>
```

← If successful,
you will see

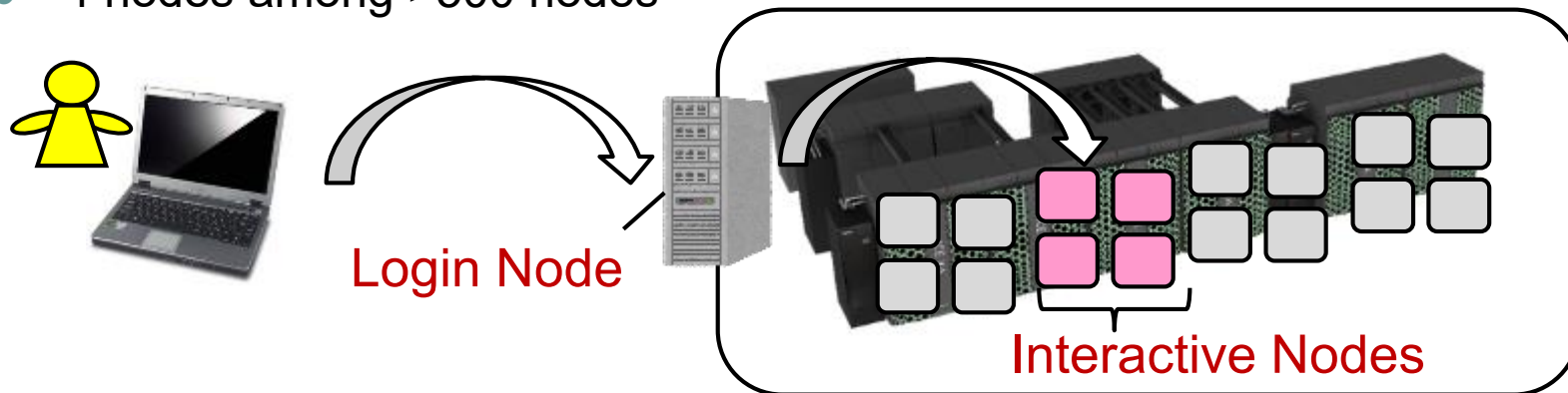
On other terminal
applications, try Google

Standard route

Log-in to Interactive Node



- Log-in nodes are only entrance of TSUBAME and not powerful, no GPU on them
- In this lecture, we mainly use “interactive nodes”
 - 4 nodes among >500 nodes



- On login node,
iqersh -l h_rt=2:00:00

NOTE: The command is changed in Apr 2021

If successful, you will see →

```
endo-t-ac@login1:~> qersh -q interactive -l h_rt=2:00:00
endo-t-ac@r7i7n6:~>
```



Notes in Using TSUBAME

- Use your account only by yourself

Standard route

- Don't share private or public keys with other people
- Login nodes are shared by many TSUBAME users.
Avoid running CPU/GPU heavy jobs there

[Interactive nodes]

Web-only route

Standard route

- Only users in Tokyo-Tech can use
- Each user can use only one session
- 7 CPU cores + 1 GPU (= $\frac{1}{4}$ node) are assigned
- CPU cores, GPU may be shared by several users → you may suffer from slow down



Today's Homework (1)

1. (If you are new to TSUBAME) please make your account on TSUBAME by 13:00, Apr 13

(まだ作ったことがなければ) TSUBAMEアカウントを、4月13日13:00までに作成してください

2. You will receive an invitation e-mail to [tga-ppcomp](#) TSUBAME group (no later than around 14:00, Apr 13). Please read it and accept the invitation.

[tga-ppcomp](#) TSUBAMEグループへの招待e-mailが届くはずですが(4月13日14時ごろまでに)。指示に従って招待を受けてください。



Today's Homework (2)

- If you cannot make an account by due time, please send an e-mail after account creation
- もし期限までにアカウントを作成できなければ、作成してから下記のようなe-mailを送ってください

To: ppcomp@el.gsic.titech.ac.jp

Subject: [TSUBAME3 ppcomp account](#)

Department name:

School year:

Name:

TSUBAME account name:

Then we will invite you to the TSUBAME group
その後、TSUBAMEグループへの招待を送ります

Contact/ Information on the Course



- About this course
 - e-mail ppcomp@el.gsic.titech.ac.jp
 - T2SCHOLA
 - <https://t2schola.titech.ac.jp/>
 - TSUBAME official site
 - <https://www.t3.gsic.titech.ac.jp>
 - Manuals are here
 - Tokyo Tech portal
 - <https://portal.titech.ac.jp/>
- ➔ Log-in and then click “TSUBAME portal”