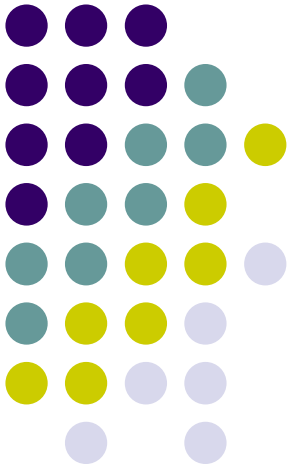
Practical Parallel Computing (実践的並列コンピューティング)

2025 Class No.1
Introduction Part
About Supercomputer



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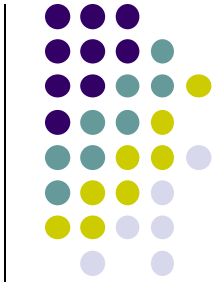
Purpose of This Course

- To learn parallel computing practically
  - Lecture + Practice
  - We will use the TSUBAME4.0 supercomputer from your PC

Your PC

TSUBAME4.0 Supercomputer

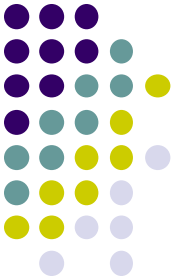
Overview of This Course



- Introduction Part
  - 2 classes including today
- OpenMP (OMP) Part
  - 4 classes
  - Report (required)
- OpenACC (ACC) Part
  - 2 classes
  - Report (required)
- CUDA Part
  - 3 classes
  - Report (elective)
- MPI Part
  - 3 classes
  - Report (elective)

In 2025, 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 has homework.

  3 Reports submission is required. Please see next page.

  - (You can submit more)

下記により採点・単位認定

- 各パートで課題を出す。3回のレポート提出を必須とする。詳細は次ページ
  - ∠切は、各パート終了の約1.5週間後
  - (それ以上のレポートを提出してもよい)

About Reports

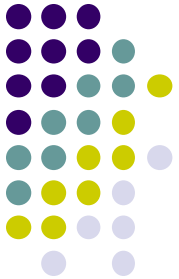
Different from past years

- Introduction Part
- OpenMP (OMP) Part
  - Problems [O1], [O2], [O3] or [O4] ➔ Select one and write a report
- OpenACC (ACC) Part
  - Problems [A1], [A2], [A3] or [A4] ➔ Select one and write a report
- CUDA Part
  - Problems [C1], [C2], [C3] or [C4]
- MPI Part
  - Problems [M1], [M2], [M3] or [M4]

} Select one and write a report

Each part has the due date, which will be about 1~1.5 weeks after each part finishes
各パート毎に〆切あり。パート終了後1~1.5週後の予定

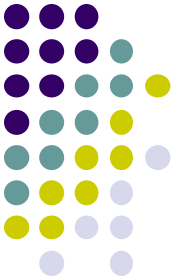
What We Do



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

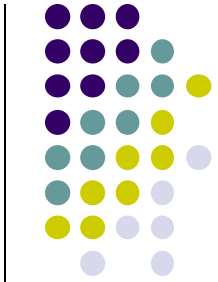
What We Don’t



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
  - Optional: SSH public key authorization (SSH公開鍵認証)

- A PC to log-in to TSUBAME4 and Internet connection
  - Such as “ScienceTokyo” wifi

Supercomputers

Fugaku (RIKEN)
World No. 6

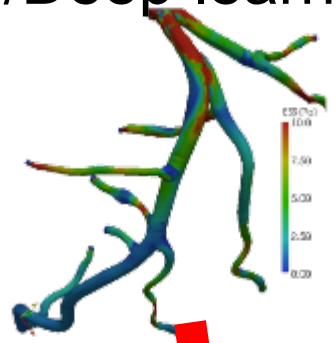
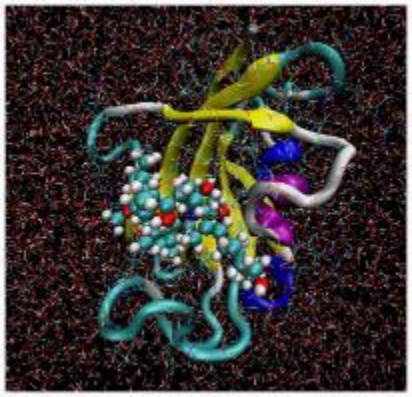
TSUBAME4.0
(Science Tokyo)

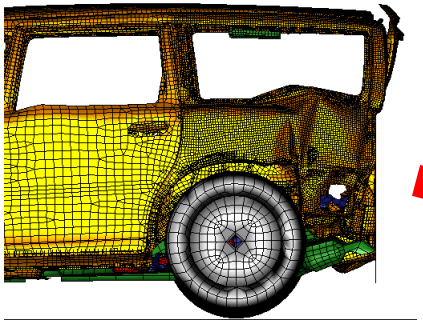
Frontier (LLNL, US)
World No.1

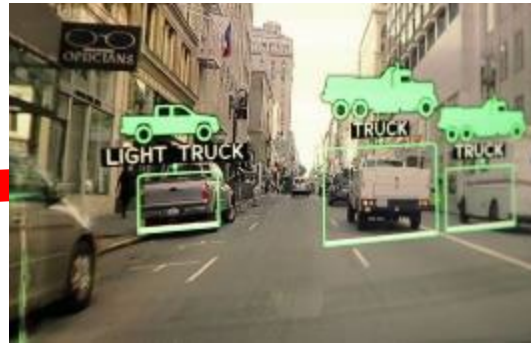
ABCI (AIST)

What are Supercomputers (SCs) used for?

- Simulations (Fluid dynamics, molecular dynamics, etc.)
- Machine learning/Deep 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

~130,000x!

TSUBAME4

~500GFlops (5×10^{11} times per sec)

67PFlops (6.7×10^{16} times per sec)

PC in 1980

<<

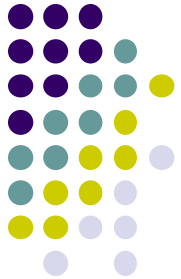
Cray-1 (1976)

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

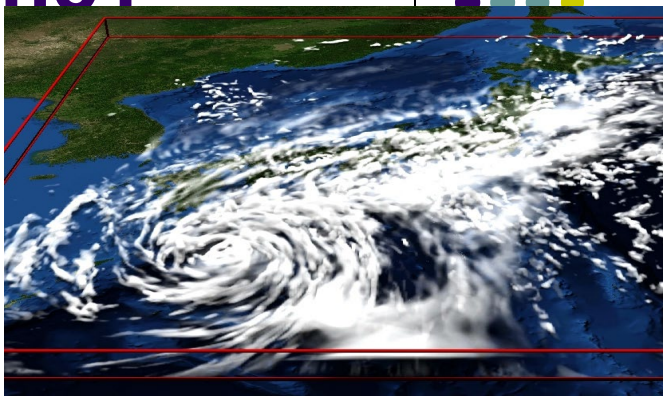
⇒Want to make discovery by comparing mass genome data

⇒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

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

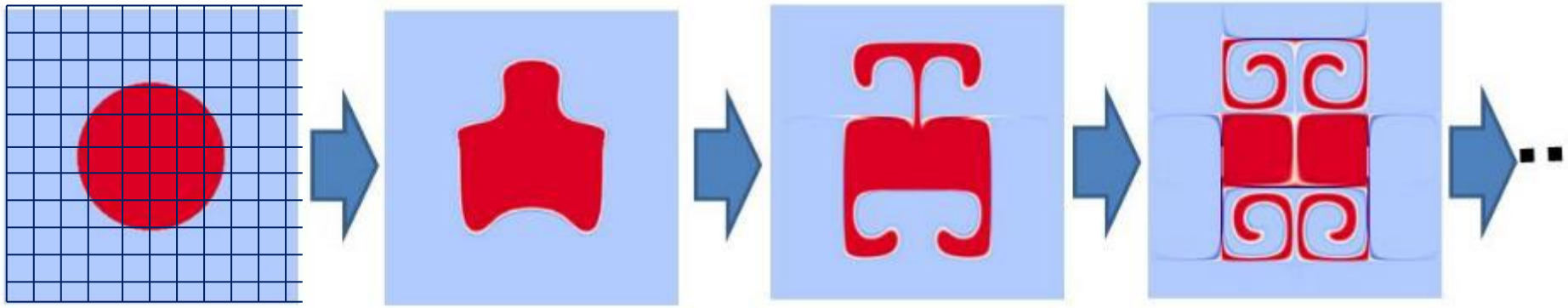


By Takayuki Aoki

But no analytical solution for them, generally

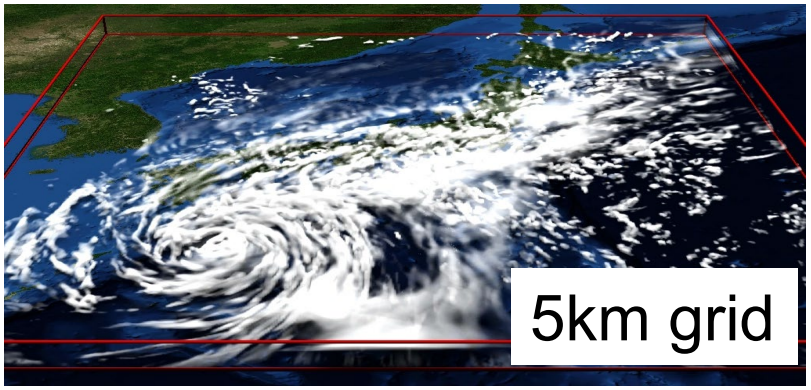
⇒ Instead, space and time are discretized

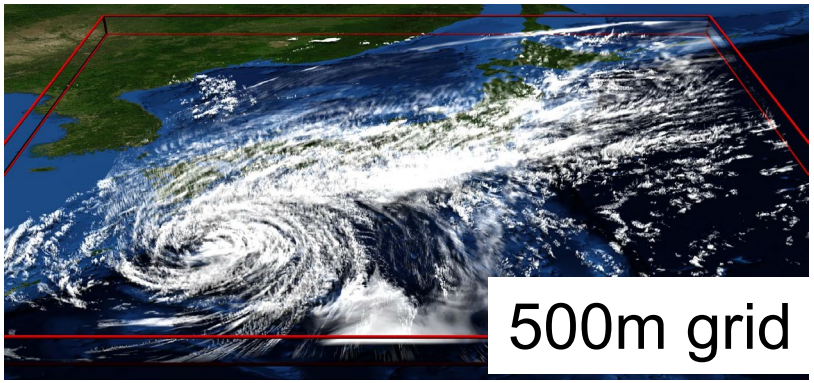
- The space is divided into small grids, expressed as an array
  ⇒ Each array element should be computed
- The time is divided into time steps
  ⇒ After a time step is computed, we go to next step, and so on



Why is Speed Important?

- Since we have to compute all points for every time step, computational complexity is
  - O(x-size × y-size × z-size × 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

Deep Learning (DL) needs SC

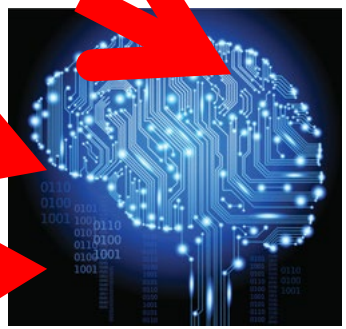
- Deep learning consists of "training phase" and "inference phase"
- Training requires supercomputers

In case of image recognition

Training

Done on supercomputers/cloud

Inputs are lots of images with correct answers

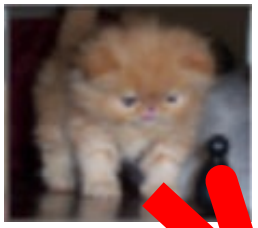


AI, actually numeric data

Copy data of AI

Inference

Done on cars/phones

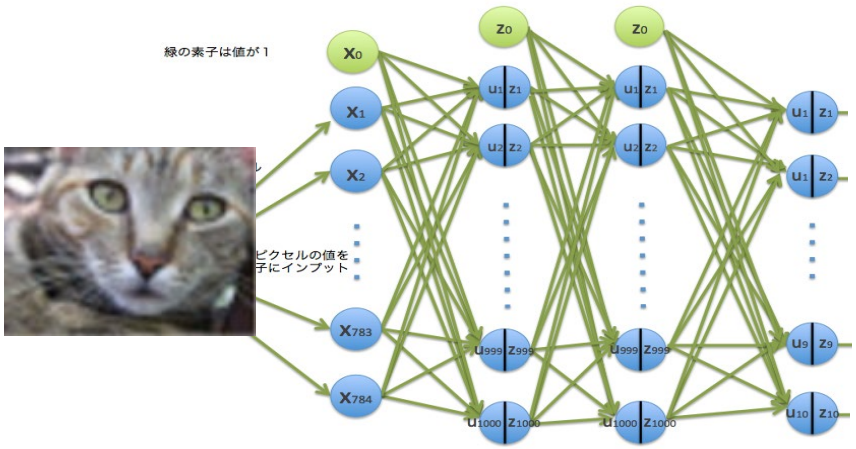


What's this?

A cat (75%)
A dog (24%?)

Training in DL Has Large Compute Complexity

- DL uses “network of neurons”
- (Roughly) “knowledge” is represented as connectivity of neurons
  - Sets of large parameter vectors, whose total sizes are $>10^4$, $>10^8$…
- Basic training method:
  - For an input image, it computes the current answer (≠ correct answer)
  - By using difference of current answer and correct answer, it updates its parameter vectors



Vertices are neurons
Arrows are connections,
which have numeric data

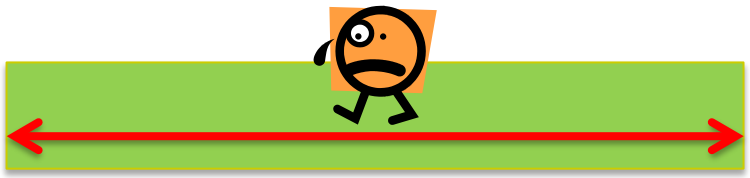
Compares current answer and correct answer, *“cat”*
→ It updates the knowledge (vectors) using the difference

Complexity of (Number of images × Sizes of parameter vectors × Number of repetitions) !!

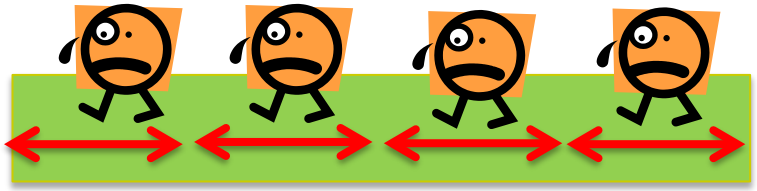
Why are SCs Fast?

- 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

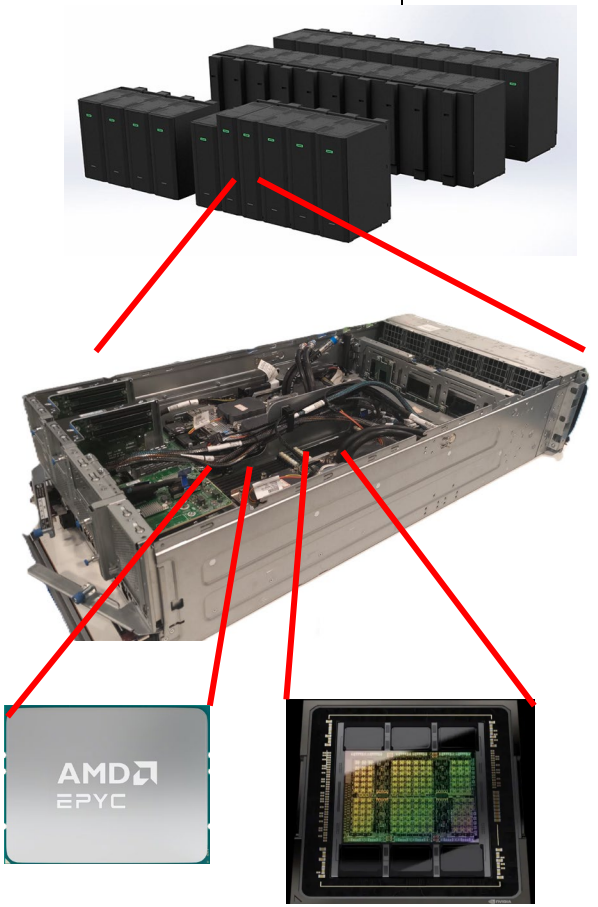


Multiple workers are working together → fast!



SC Structure is Hierarchical

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



Structure of TSUBAME4 and Fugaku


TSUBAME4

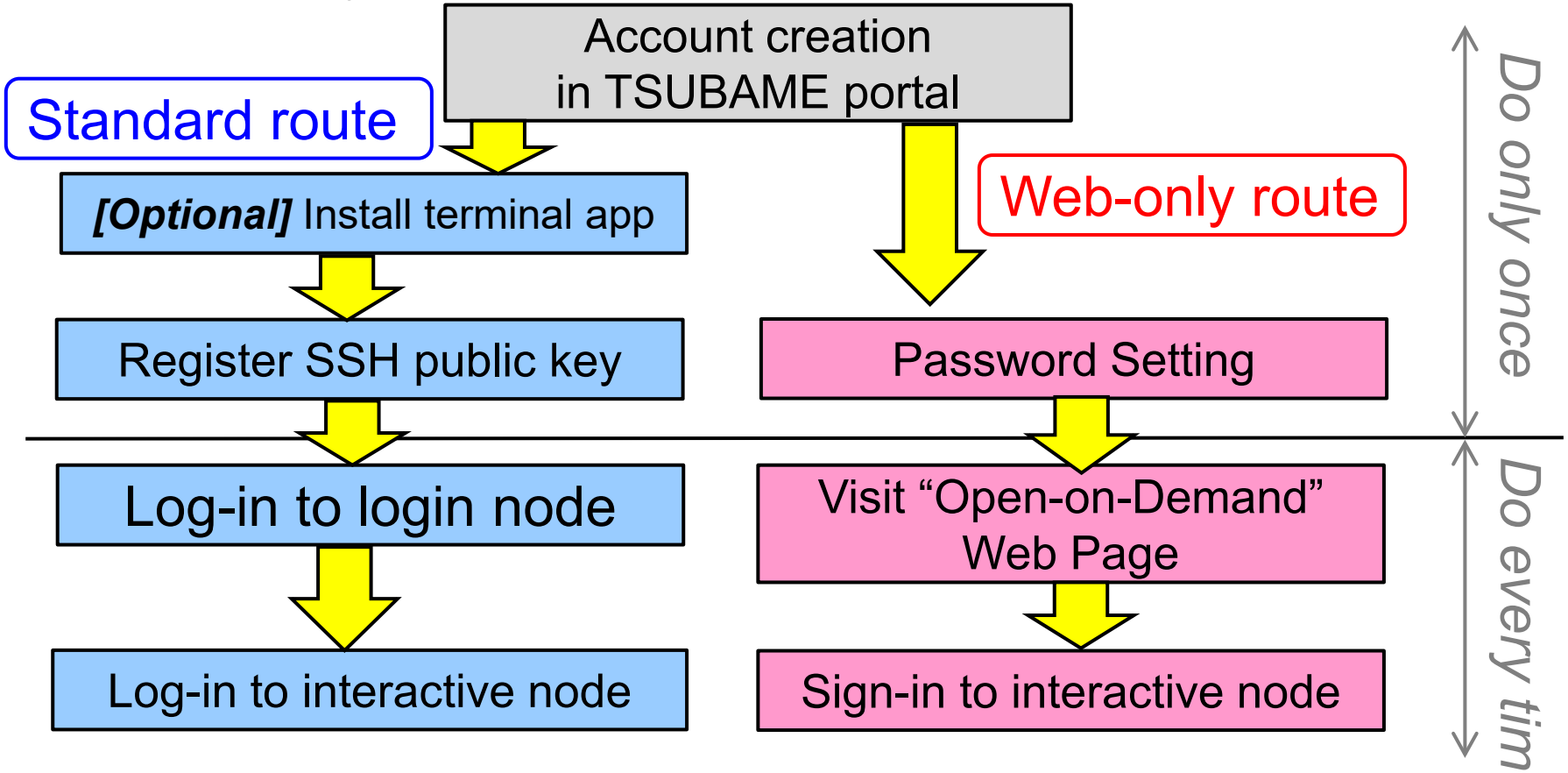

Fugaku

System	240 nodes	66.8PFlops	160,000 nodes	540PFlops
Node	2 CPUs + 4 GPUs	2 x 5.45TFlops + 4 x 66.9TFlops = 278.5TFlops	1 CPU	3.38TFlops
Processor	CPU: 96 cores GPU: 132 SMXs	CPU: 5.45TFlops GPU: 66.9TFlops	48 cores	3.38TFlops
Core	CPU core: 3.55GHz x 16 = 56.8GFlops GPU SMX: 507 Gflops (Tensor core)		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)

Important URLs about TSUBAME

- TSUBAME official site
  - https://www.t4.cii.isct.ac.jp
  - Manuals are here

For Science&Engineering students:

- (old) Tokyo Tech portal
  - https://portal.titech.ac.jp/

➔ Log-in and then click “TSUBAME portal”

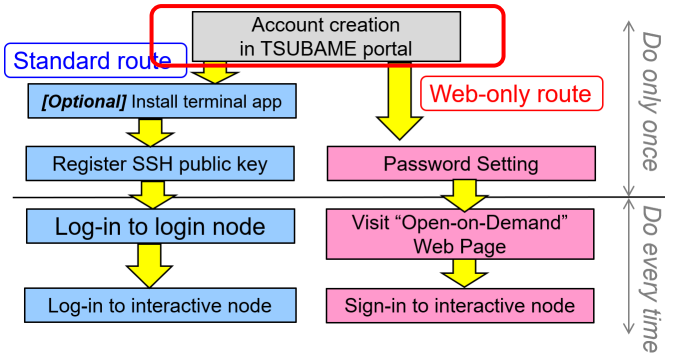
➔ Not “Science Tokyo” portal

For Medical students and others,

please see TSUBAME official site

Standard route | Web-only route

Account Creation in TSUBAME Portal



- Visit (old) TokyoTech Portal / (旧) 東工大ポータル and log-in
  - https://portal.titech.ac.jp/

Click "TSUBAME4 portal"

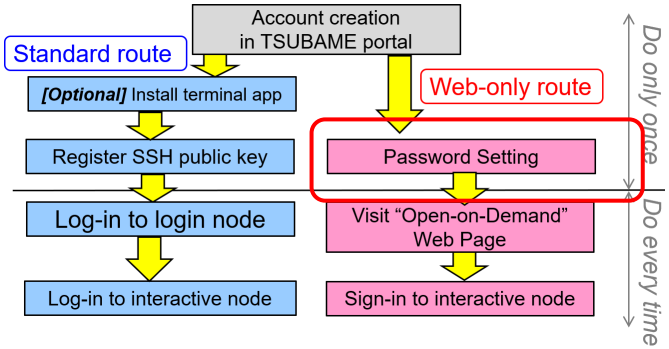
➔ If you are new to TSUBAME, you will be taken to account creation pages

➔ You will get an account.

- An account name looks like: *ux02345* (not the student ID)

- For details, visit https://www.t4.cii.isct.ac.jp/ and click "Getting Accounts" / "アカウント取得方法"

Web-only route



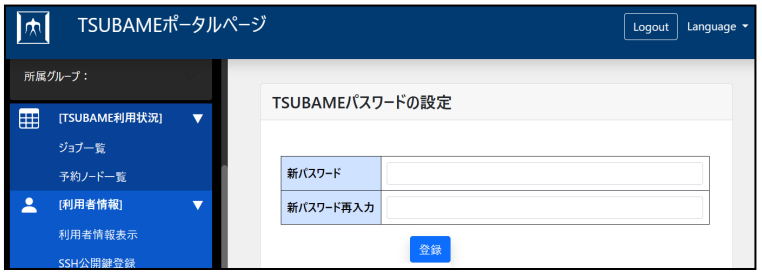
Password Setting

Go to "TSUBAME4 portal" again

- Visit "Tokyo Tech portal"
- Log-in
- Click "TSUBAME4 portal"

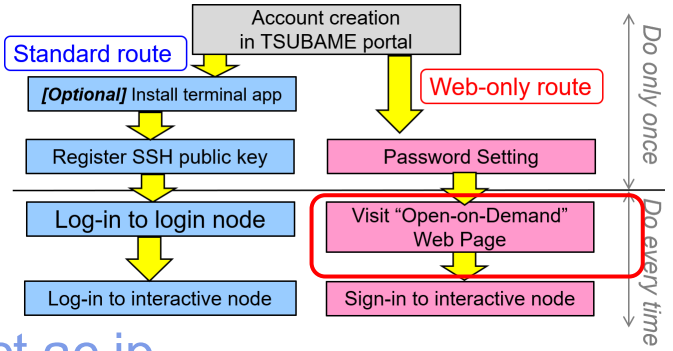
Your account name

Set a new password
→ used in next page



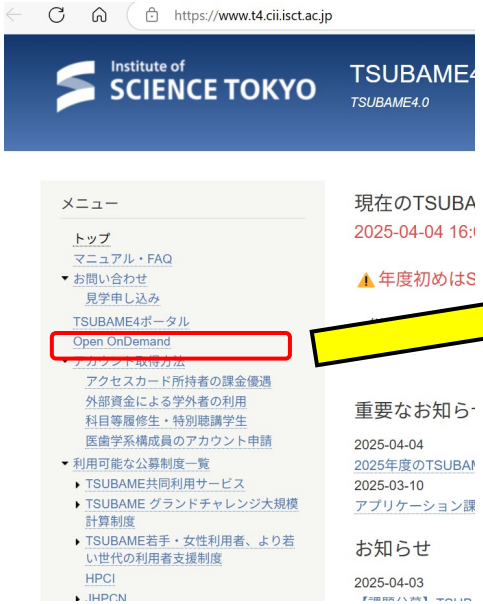
Web-only route

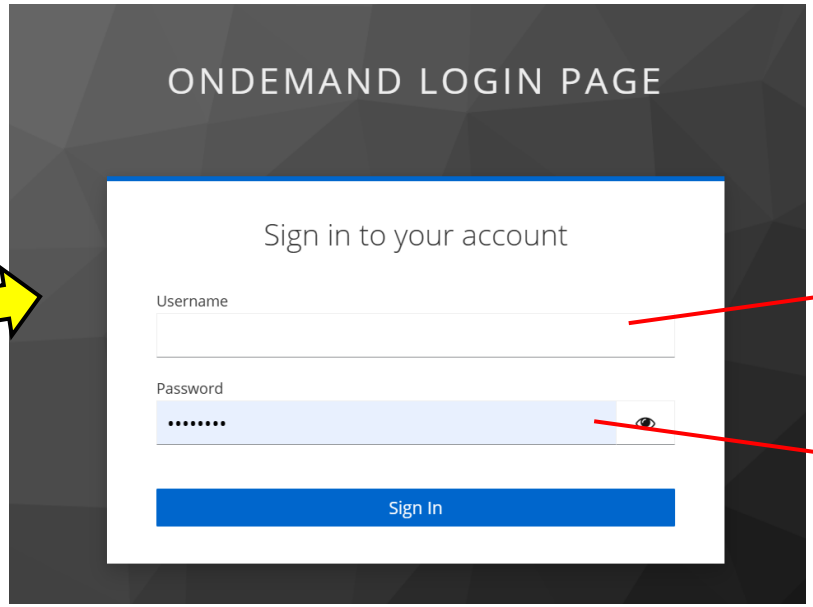
Visit “Open-on-Demand” Web Page



- Visit TSUBAME offial site https://www.t4.cii.isct.ac.jp

  ➔ Click “Open-on-Demand”





Type your TSUBAME account name

Type your password

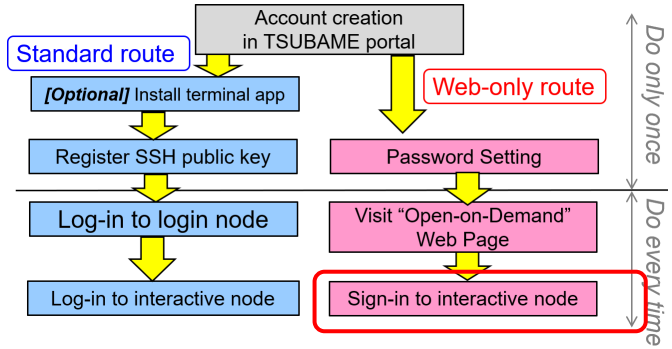
Two-factor authentication is used:

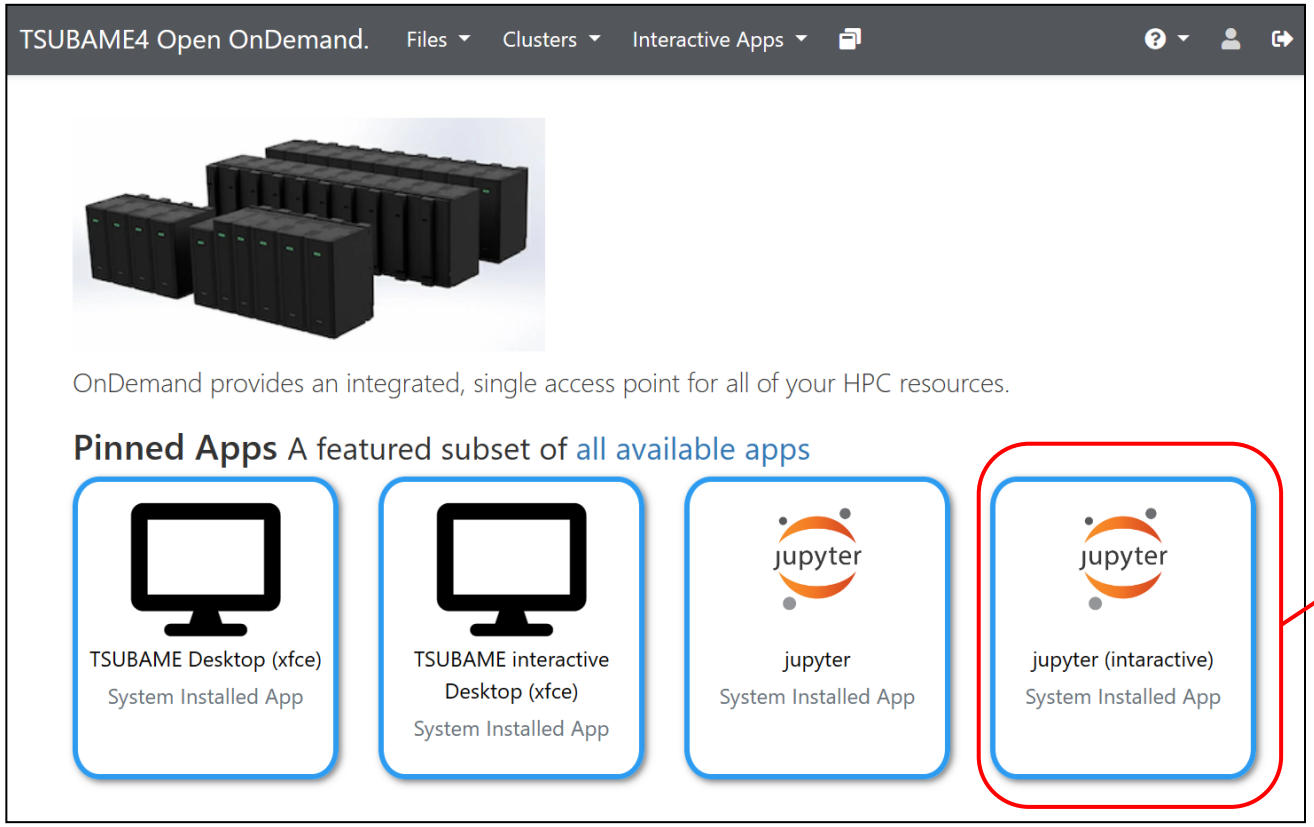
- You will receive an e-mail with “Access code”

  ➔ Type it

Web-only route

Start “Web Service” (1)

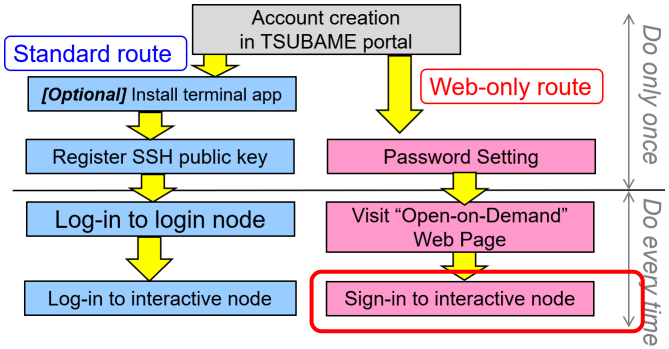


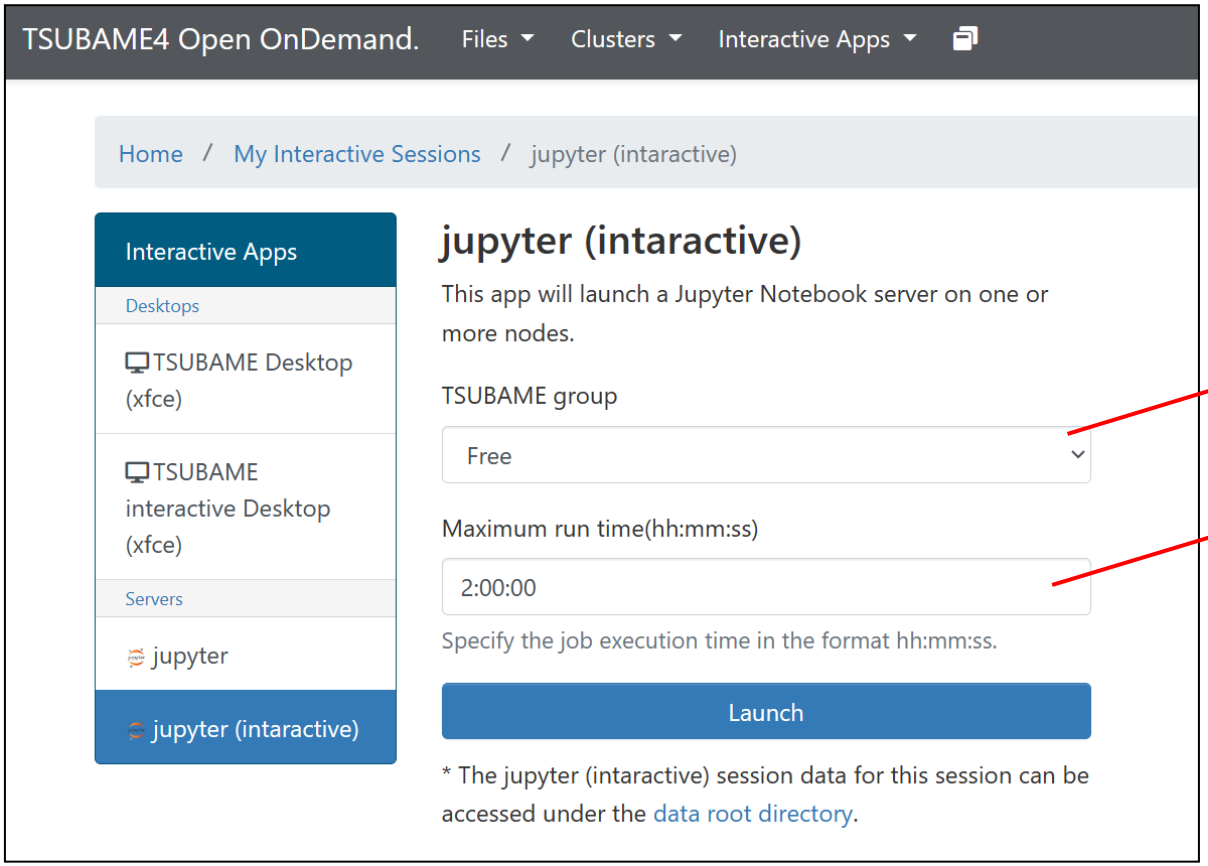


Select
jupyter (interactive)

Web-only route

Start “Web Service” (2)

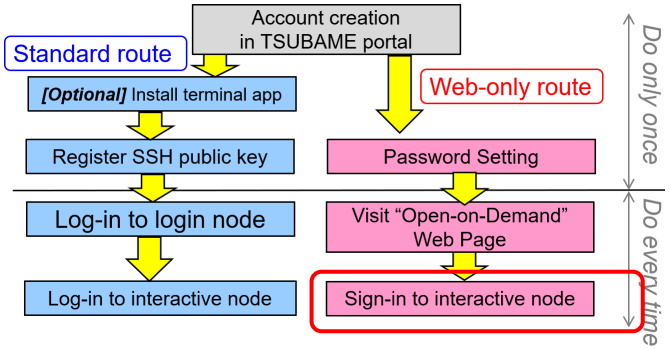




Select “free”

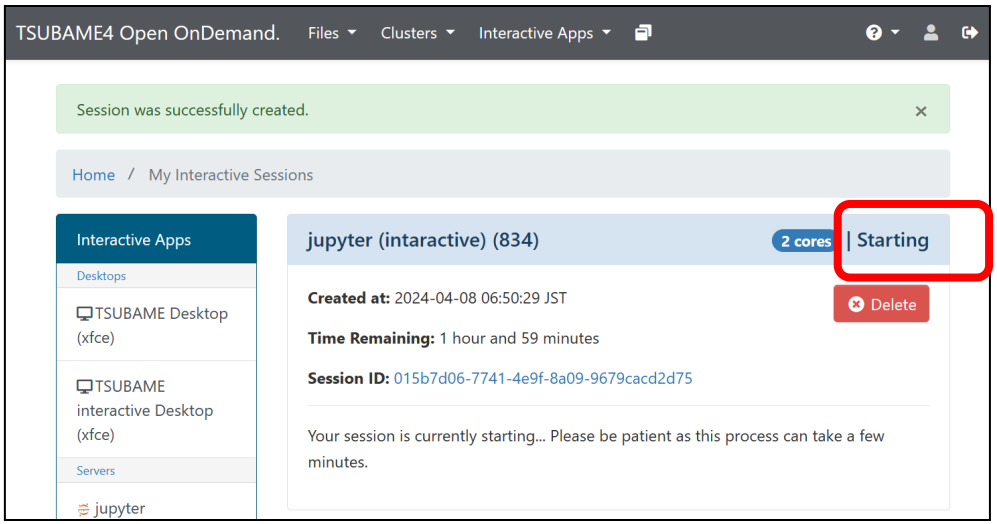
Type maximum time, such as “2:00:00”

Web-only route

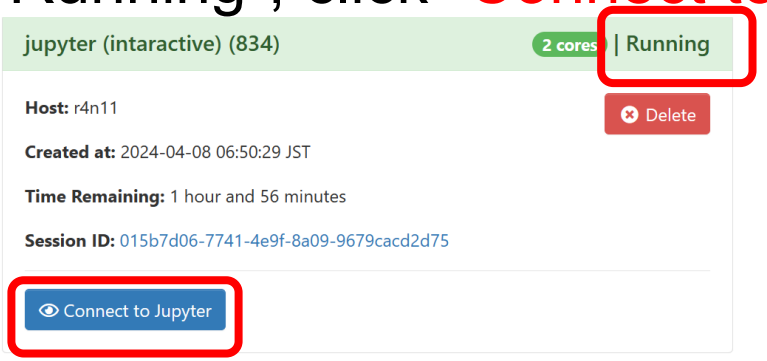


Start "Web Service" (3)

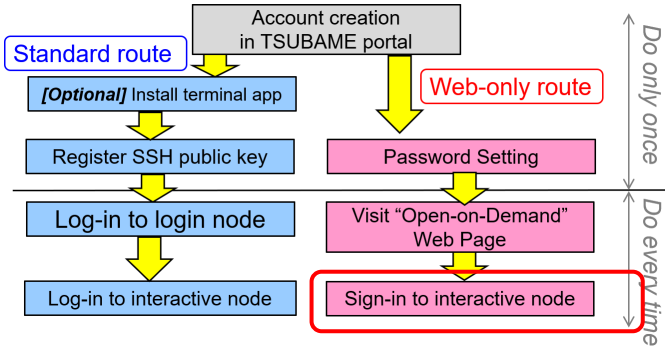
- Please wait until your session becomes "Running"



- If you see "Running", click "Connect to Jupyter"

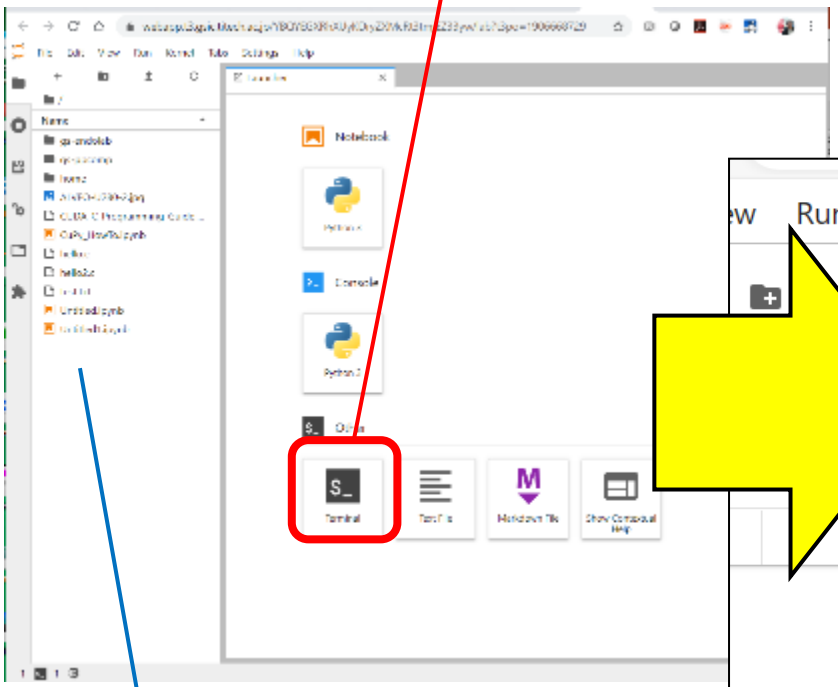


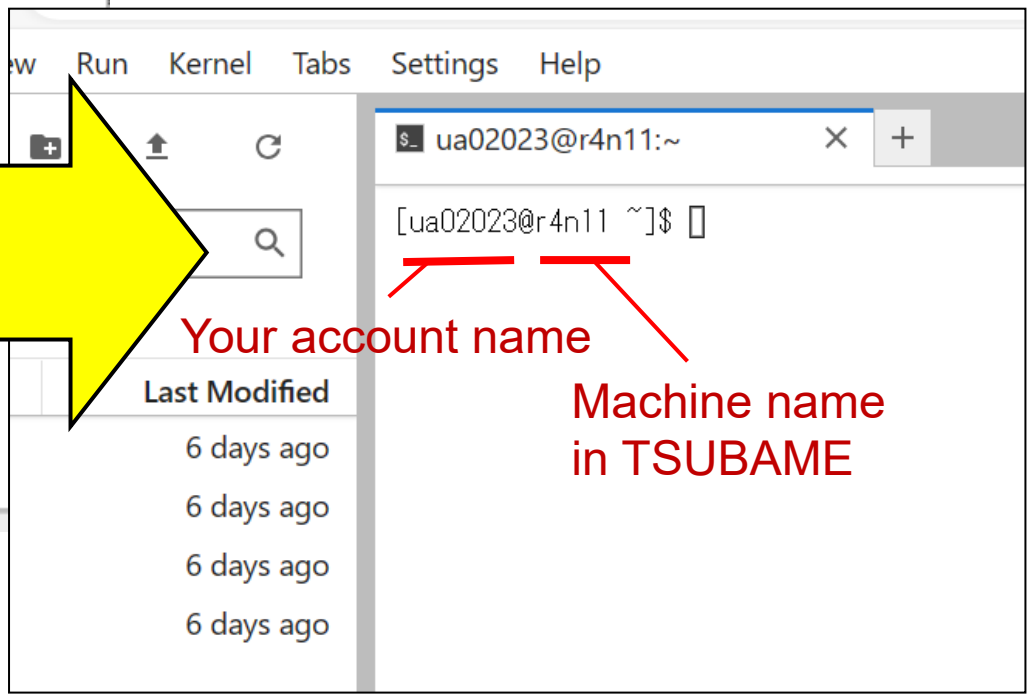
Web-only route



Start "Web Service" (4)

- You will see a "Jupyter" screen
- Click the Terminal icon



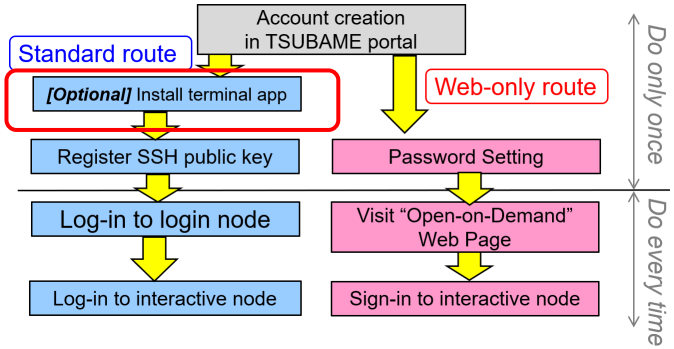


Your account name

Machine name
in TSUBAME

~/ (your home) directory
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

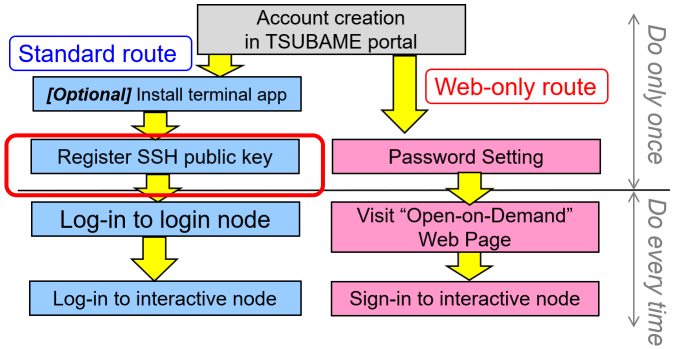
Also you can install other applications

- MobaXterm on Windows
- Putty on Windows/Mac
- iTerm on Mac …

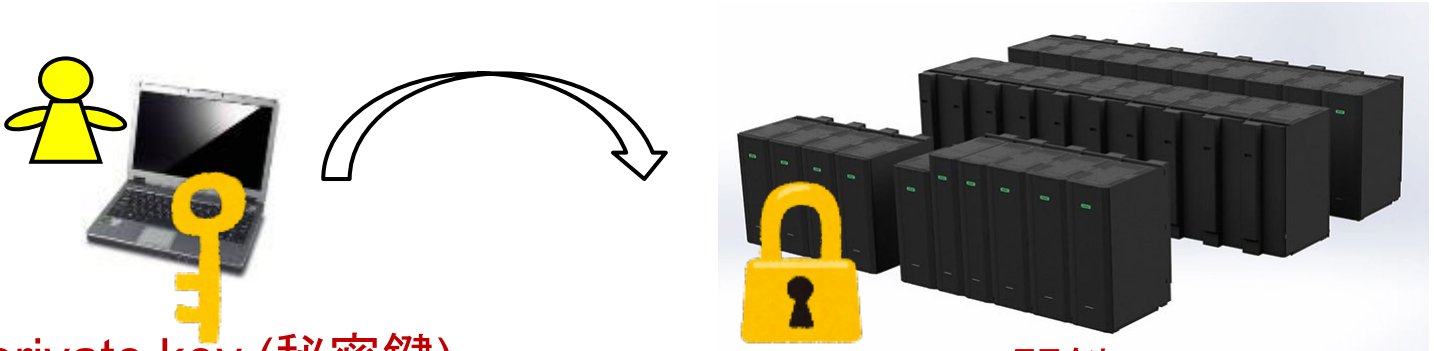
Or try google
"windows ssh client"
"mac ssh client"

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



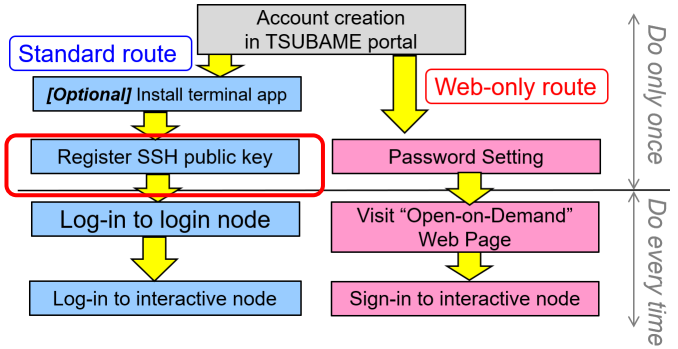
private key (秘密鍵)

public key (公開鍵)

Actually, they are two text files

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

  For example,

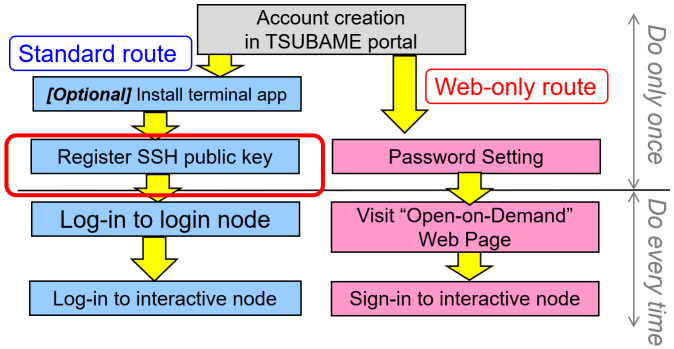
  private key → .ssh/id_ecdsa (Mac) .ssh¥id_ecdsa(Win)

  public key → .ssh/id_ecdsa.pub (Mac) .ssh¥id_ecdsa.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

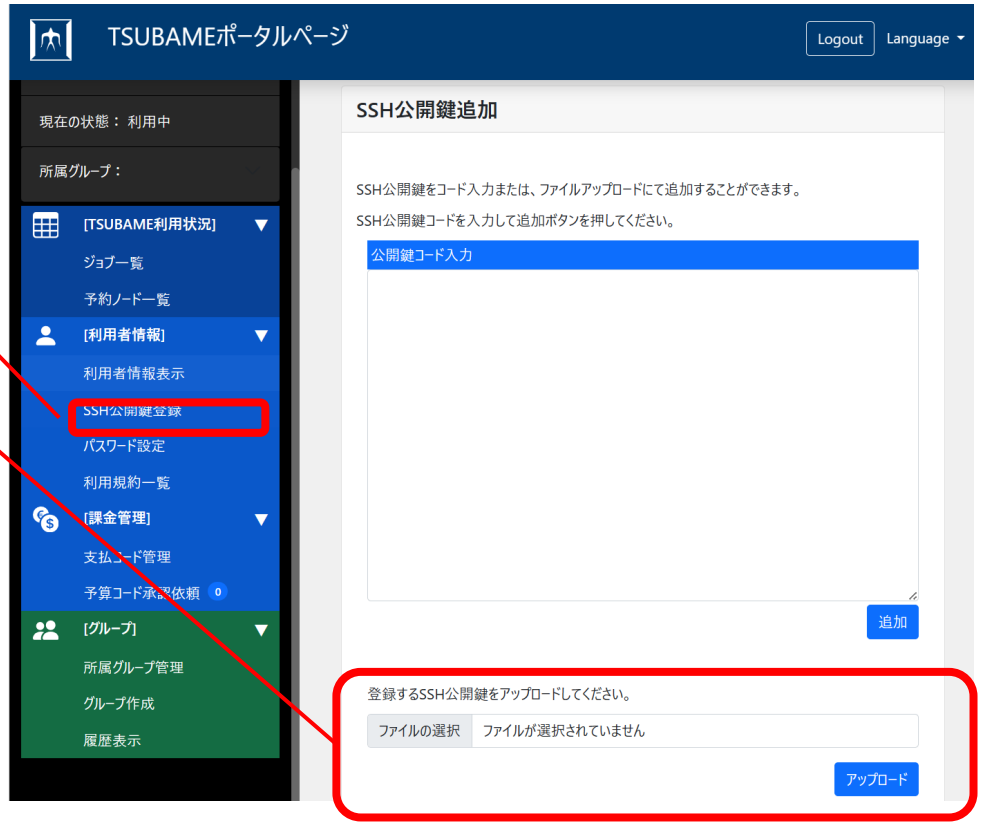
1. Click Register SSH public key / SSH公開鍵登録

2. Upload your public key

- Don't upload the private key!!

id_ecdsa

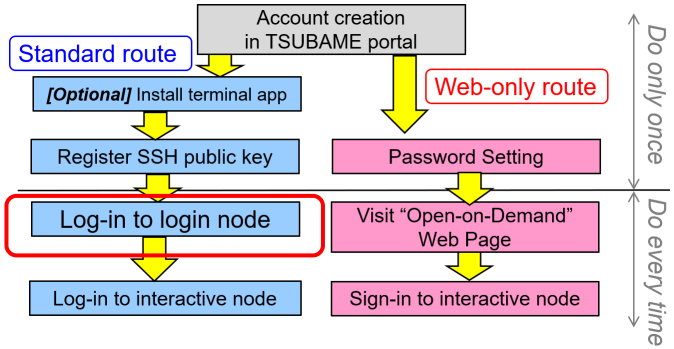
id_ecdsa.pub



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

Standard route

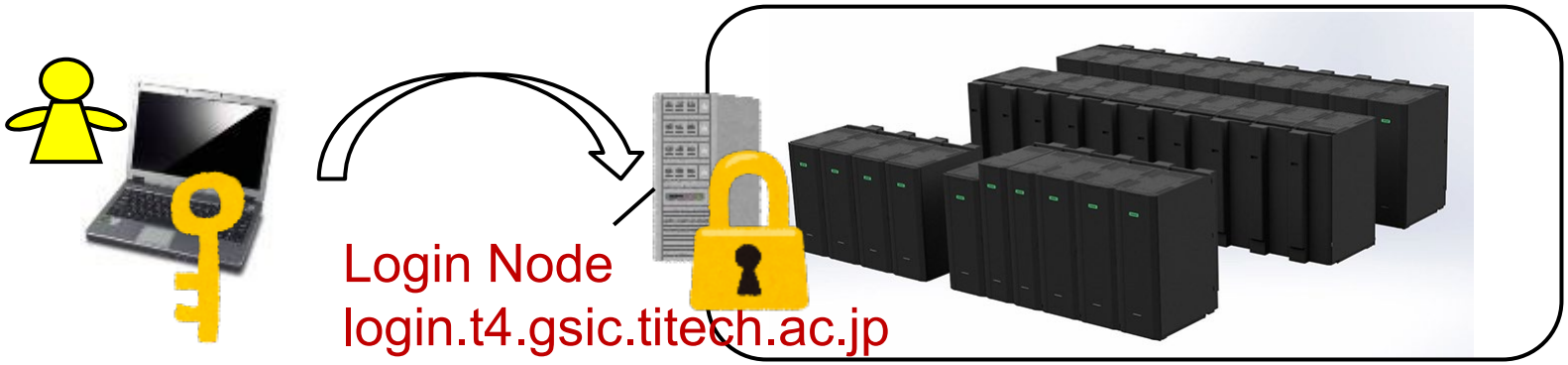
Log-in to TSUBAME Login Node



- On Mac terminal or Windows command prompt

  ssh -i *[private key] [account]*@login.t4.gsic.titech.ac.jp

  ex) ssh -i .ssh/id_rsa ux02345@login.t4.gsic.titech.ac.jp



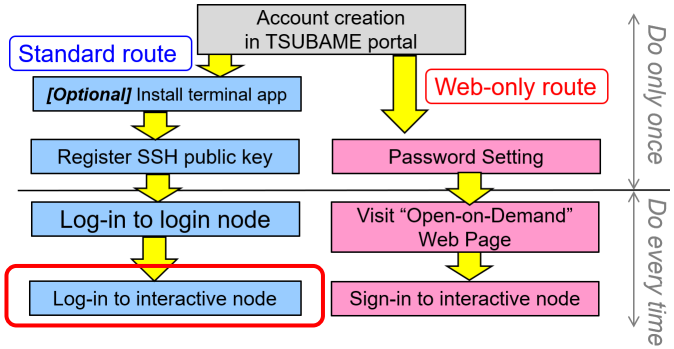

```
--------------------------------------------------------------------
Last modified: Mon Apr  1 10:00:09 JST 2024


    (The current TSUBAME 4.0 operational status)
https://www.t4.gsic.titech.ac.jp/      X(Twitter):@Titech_TSUBAME
--------------------------------------------------------------------

Last login: Wed Apr  3 18:41:29 2024 from 131.112.132.225
[ua02023@login1 ~]$
```

← If successful, you will see

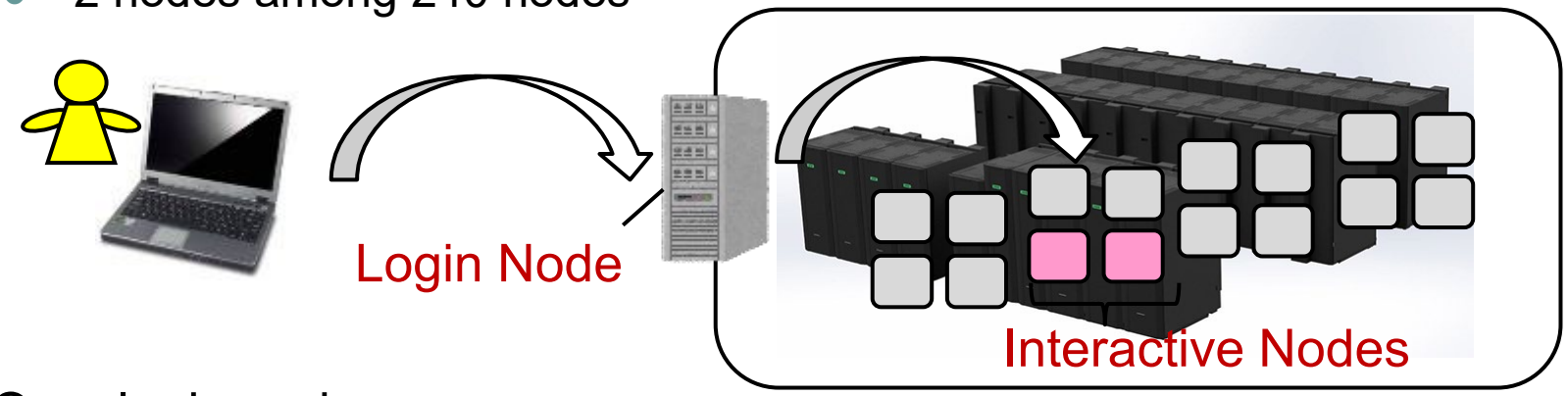
On other terminal applications, try Google

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"
  - 2 nodes among 240 nodes



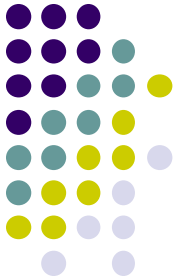
- On a login node,

  iqrsh -l h_rt=2:00:00

If successful, you will see ➔

```
[ua02023@login1 ~]$ iqrsh -l h_rt=2:00:00
[ua02023@r4n11 ~]$
```

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

- Each user can use only one session
- (24 CPU cores + 0.5 GPU) (= 1/8 node) are assigned
- CPU cores, GPU may be shared by several users → you may suffer from slow down

Today's Homework (1)

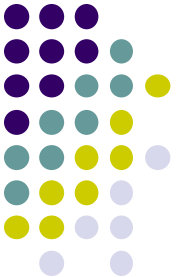
Please do 1&2 by 17:00, Aug 9. We accept it after this due time.
1と2を4/9 17:00までに行ってください。それより後でも受け付けます

1. (If you are new to TSUBAME) please make your account on TSUBAME
   (まだ作ったことがなければ) TSUBAMEアカウントを作成してください
2. Please inform the account name Science Tokyo LMS
   - Class #1: Today's homework

   Science Tokyo LMSからアカウント名を知らせてください
   - Class #1: Today's homework

   If submission from LMS does not work, please send it by e-mail to
   もしLMSからの提出がうまくいかなければ、e-mailで知らせてください
   endo@scrc.iir.isct.ac.jp

Today's Homework (2)

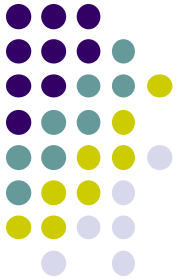


3. You will receive an invitation e-mail to tga-ppcomp TSUBAME group. Please read it and accept the invitation.

tga-ppcomp TSUBAMEグループへの招待e-mailが届くはずです。指示に従って招待を受けてください。

Also (if you are Science Tokyo students)
Please join Science Tokyo Slack Channel:
#dp-ppcomp-mcs-t418-2025

Contact/ Information on the Course



[About this course]

- e-mail endo@scrc.iir.isct.ac.jp
- Slides
  - https://github.com/toshioendo/ppcomp
  - ➔ 25slides
- Science Tokyo Slack Channel
  - #dp-ppcomp-mcs-t418-2025 Please join!

[About TSUBAME]

- https://www.t4.cii.isct.ac.jp TSUBAME's manuals are here
- (old) Tokyo Tech portal
  - https://portal.titech.ac.jp/

➔ Log-in and then click "TSUBAME4 portal"