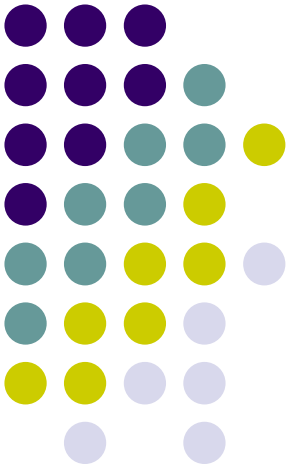
2019 Practical Parallel Computing (実践的並列コンピューティング) No. 1

Overview of the course & Basic usage of TSUBAME



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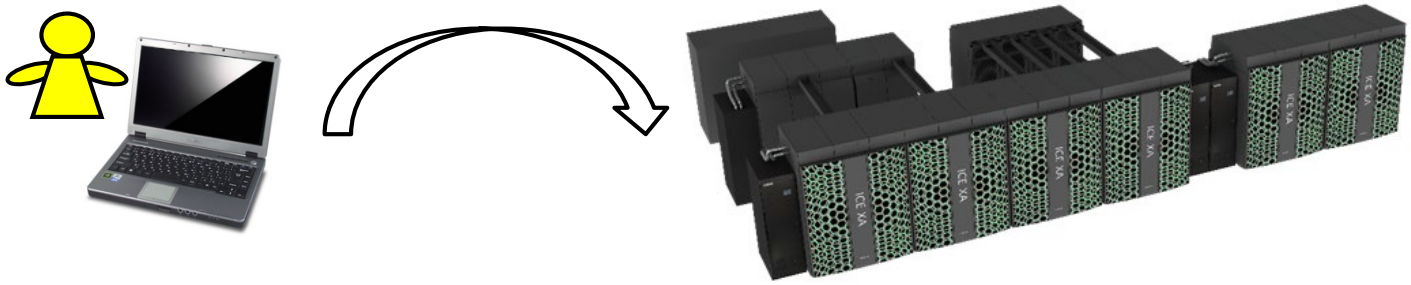
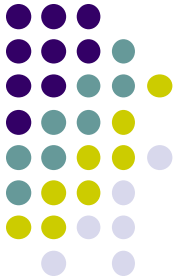
Purpose of This Course

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



- Plan
  - Introduction (2 classes including today)
  - Lecture about libraries/languages for parallel computing
    - OpenMP (4 classes)
    - MPI (4 classes)
    - GPU programming (4 classes)

Overview and Credits

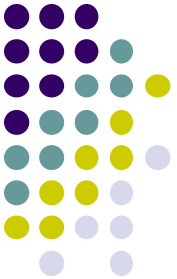


- Part 1: OpenMP for shared memory parallel programming
- Part 2: MPI for distributed memory parallel programming
- Part 3: GPU programming

Your score will be determined by the followings

- Each part has homework. Reports submission for 2 parts is required
  - The due date will be about two weeks after each part finished
  - (You can submit more)
- Also attendances will be considered

講義の流れと単位認定

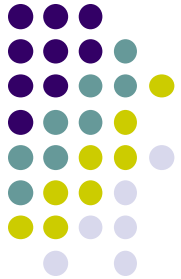


- Part 1: OpenMPによる共有メモリ並列プログラミング
- Part 2: MPIによる分散メモリ並列プログラミング
- Part 3: GPUプログラミング

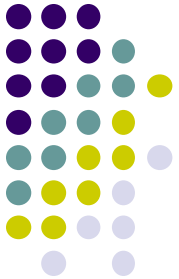
下記により採点・単位認定

- 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
  - ∠切は、各パート終了の約2週間後
  - (それ以上のレポート提出してもよい)
- 出席点

Required Knowledge



- This course uses C language as basis
  - Pointers, malloc/free
  - Relation between pointers and arrays
  - Knowledge of Pthread, Java threads is useful, but not required
- Basic Linux commands
  - TSUBAME uses Linux OS
  - ls, cp, mkdir, gcc…
  - SSH public key authorization (SSH公開鍵認証)
  - “make” would be helpful



What are supercomputers?

Variety of Supercomputers

K computer
World No.1 → No. 18
Will be replaced in 2021

TSUBAME3.0
No. 22

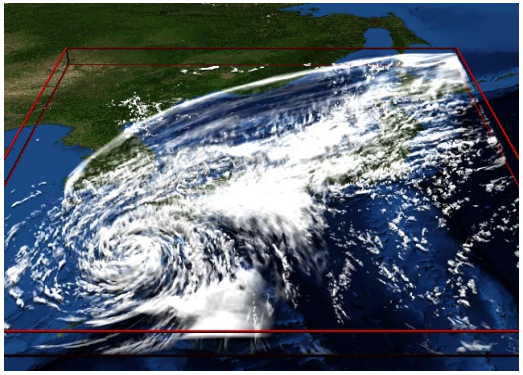
ABCI

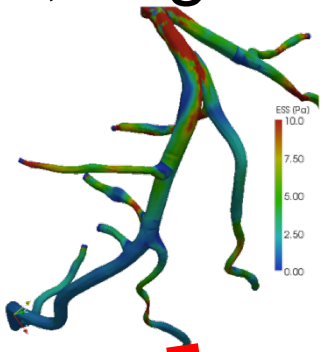
Summit
World No.1

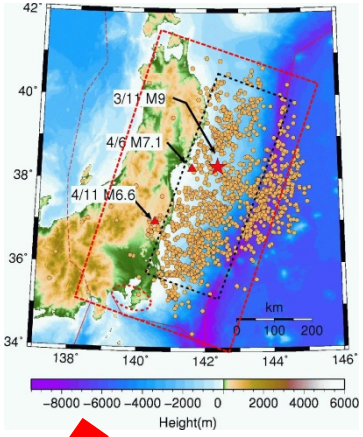
Taifulight

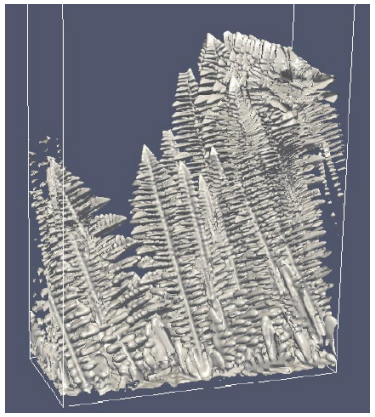
What are Supercomputers used for?

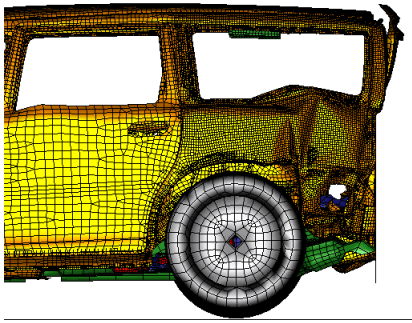
Simulations and Big-data analysis are important for area of science, engineering, security…

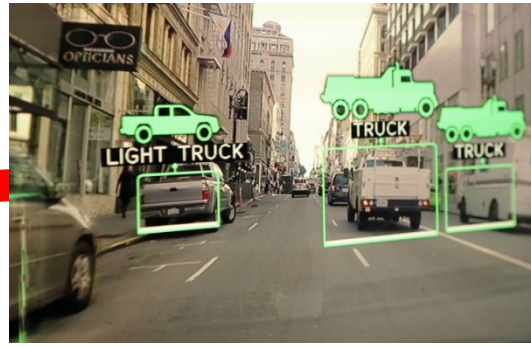












Difference with "Normal" Computers

- 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

~200GFlops (2×10^{11} times per sec)

~60,000x!

12PFlops (1.2×10^{16} times per sec)

PC in 1980

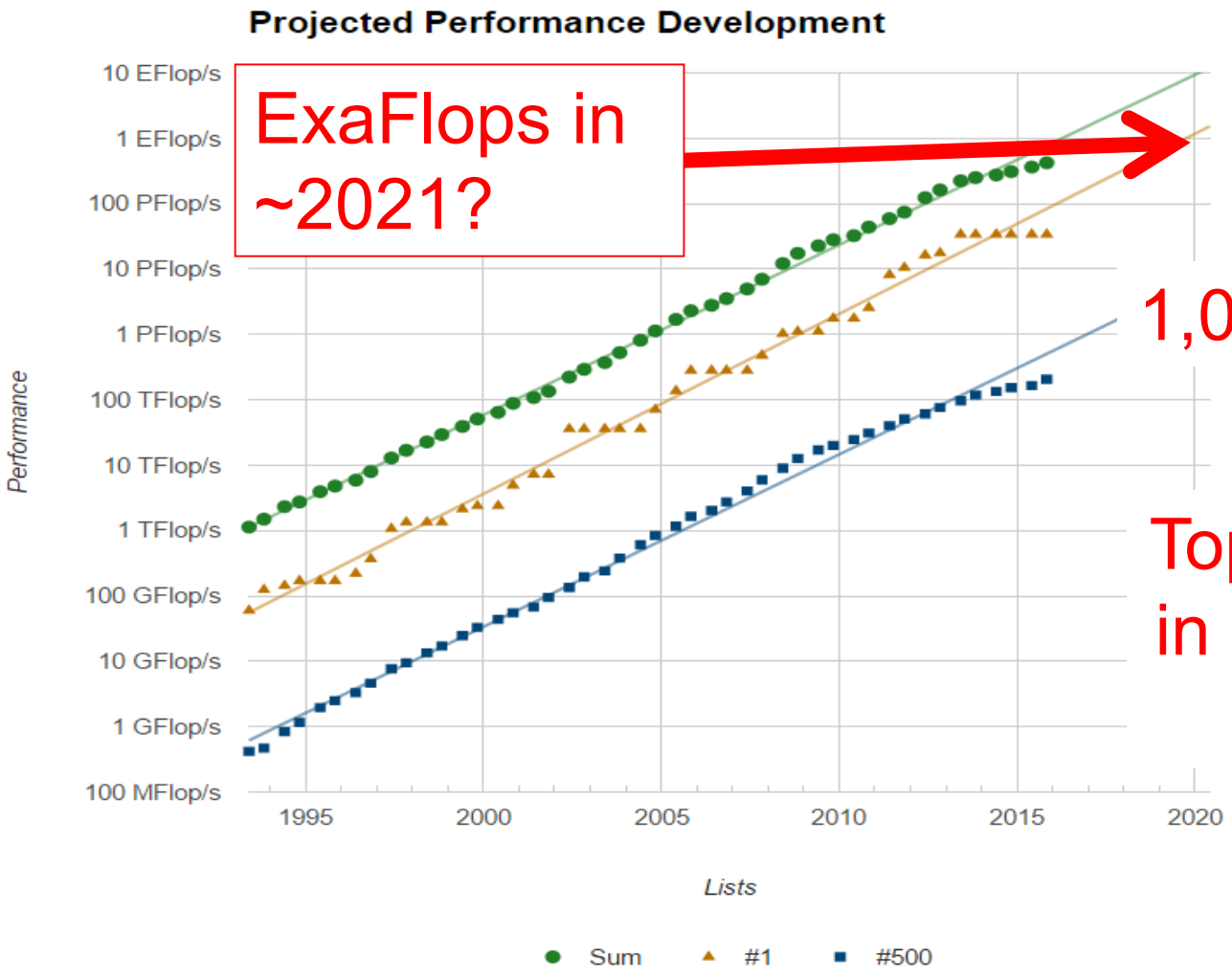
<<

Cray-1 (1976)
160MFlops

<<

Modern Cell Phone

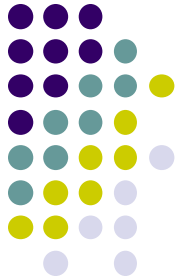
Development of Supercomputers (from www.top500.org)



1,000x in 10 years

Top Supercomputer in 1993 (60GFlops) < PC in 2019

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

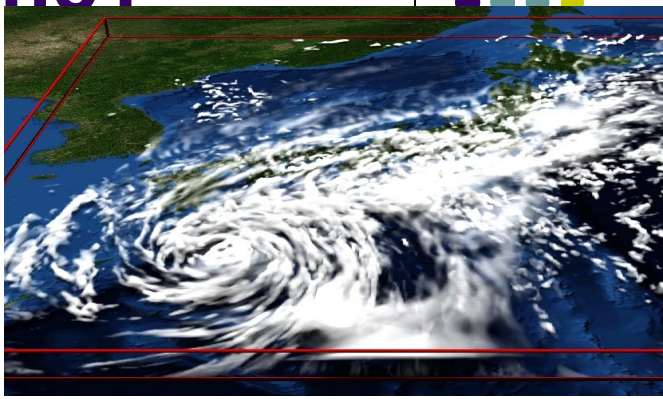
⇒Want to make discovery by comparing mass genome data

⇒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

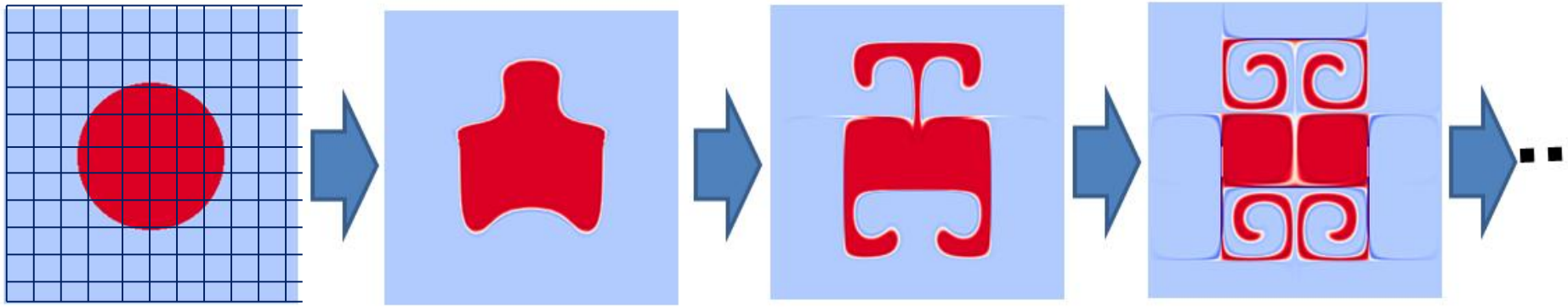
$$\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\frac{1}{\rho}\nabla p + \nu \Delta \boldsymbol{v} - g\hat{\boldsymbol{z}}$$



But no analytical solution for them, generally

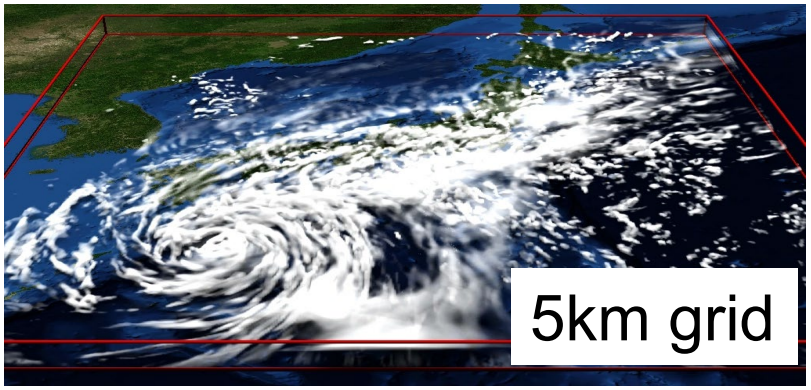
⇒ Instead, space and time are discretized

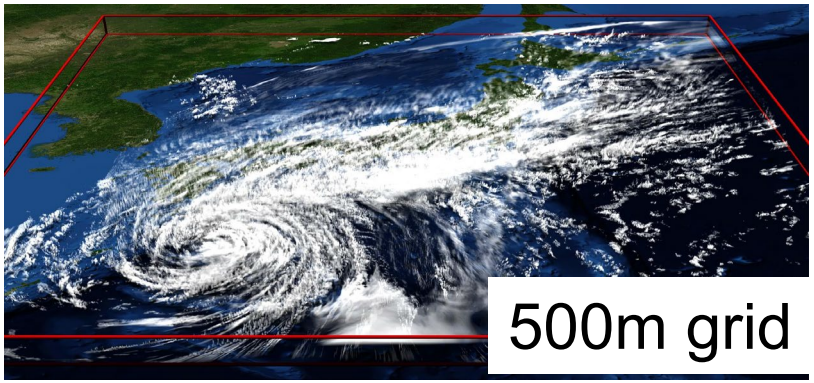
- The space is divided into small grids, expressed as an array
  ⇒ Each array element should be computed
- The time is divided into time steps
  ⇒ After a time step is computed, we go to next step, and so on



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)



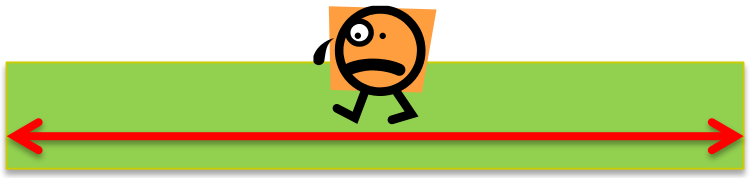


For better prediction, we need to make grid finer (arrays larger)
If resolution is 10x higher, we need 10000x computations! (10x10x10x10)
→ In future, we are going to 50m grid…

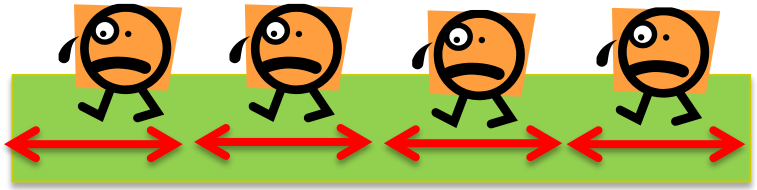
Why are SCs Fast?

- 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 work is cultivating a large field



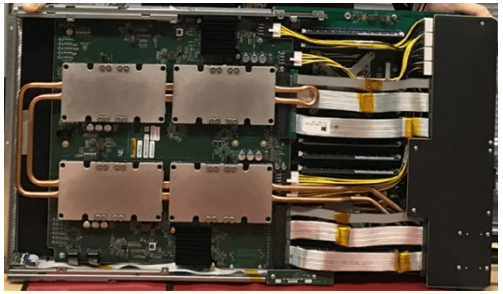
Multiple workers are working together → fast!



Hierarchical SC Structure

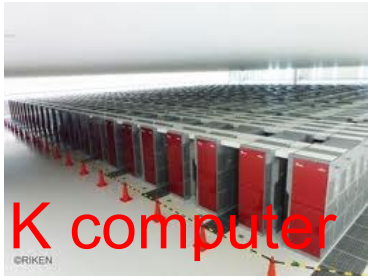
- System = Many nodes (=computers) + External storage
  - Parts are connected by Network

- Node = Several processors (CPU etc.) + Memory + Local storage
  - Parts are connected by PCI-e, QPI, etc.



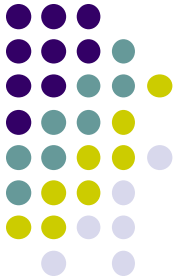
- Processor = Several cores + Cache

Structure of TSUBAME3 and K



System	540 nodes	12.15PFlops	88000 nodes	11.26PFlops
Node	2 CPUs + 4 GPUs	2 x 425GFlops + 4 x 5300GFlops = 22050GFlops	1 CPU	128GFlops
Processor	CPU: 14 cores GPU: 56 SMXs	CPU: 425GFlops GPU: 5300GFlops	8 cores	128GFlops
Core	CPU core: 1.9GHz x 16 = 30.4GFlops GPU SMX: 1.48GHz x 64 = 94.6GFlops		2GHz x 8 = 16GFlops	

"Flops" shows speed in "double precision"



TSUBAME Account

TSUBAME Account Creation

- Please visit https://www.t3.gsic.titech.ac.jp/
  - Click “Getting Accounts” / “アカウント取得方法”
  - Tokyo Tech members can create an account in TokyoTech Portal / 東工大ポータル
  - Basically the account name is same as student ID (like 19M12345…)

Notes after Account Creation

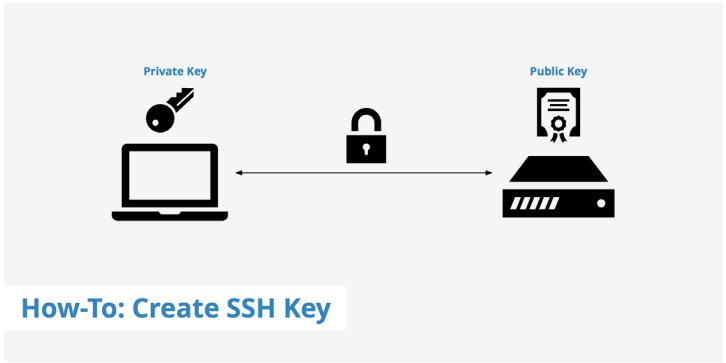
After account creation, do not forget

(1) To create SSH private key (秘密鍵) and public key (公開鍵) on your PC

- The method depends on Windows or Mac

(2) To “register SSH public key” / “SSH公開鍵登録” in the TSUBAME portal

- If you are not familiar with SSH, Please use web search
- “SSH public key Windows 10” or “SSH public key Mac”…



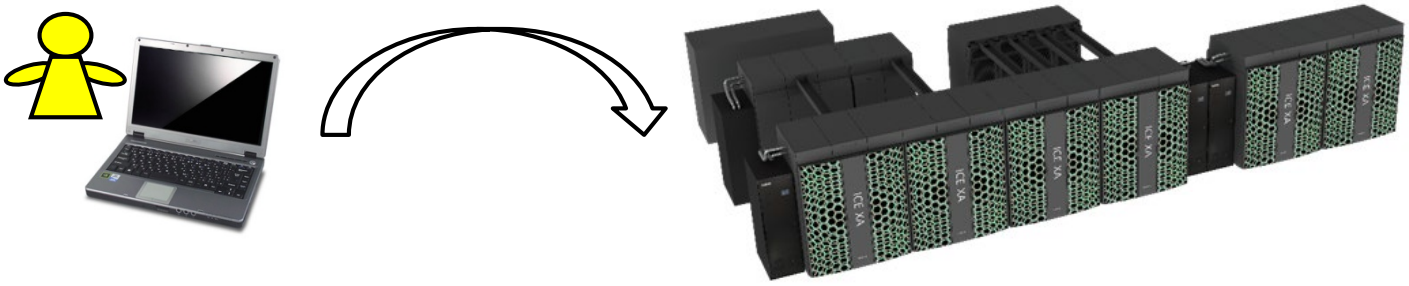
Do not mistake a private key for a public key

Login to TSUBAME

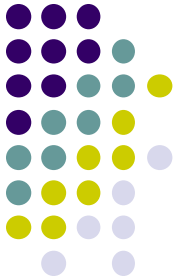
After Apr 5 10:00

- Use SSH to login TSUBAME
  - Putty, Teraterm+SSH in Windows
  - Terminal in Mac → ssh command
- Hostname: login.t3.gsic.titech.ac.jp

ssh –l [account] login.t3.gsic.titech.ac.jp



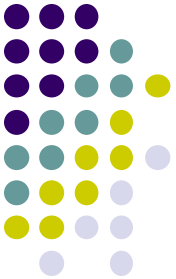
Note in This Course



Since each student logins to TSUBAME from this room,

- We recommend you to bring your laptop PC
  - If it is difficult, please practice in home
- Please install SSH terminal software
  - For Windows PC, “Putty” or “Teraterm+SSH” will work
  - For Mac, “Terminal” is already installed
    - Applications -> Utilities -> Terminal
- Make sure use can connect to Wifi network
  - We recommend “TokyoTech” Wifi network

Today's Homework



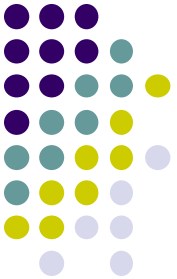
Please do the followings by Apr 15 (earlier is better)

- Please make your account on TSUBAME3
- Please send an e-mail to ppcomp@el.gsic.titech.ac.jp

Subject: TSUBAME3 ppcomp account
To: ppcomp@el.gsic.titech.ac.jp

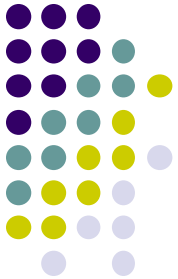
Lab name:
Department name:
School year:
Name:
Your TSUBAME account name:

TSUBAME Group in This Course



- Students of this course will become members of “tga-ppcomp” TSUBAME group
  - Use qsub/qrsh command with “-g tga-ppcomp”

Contact/ Information on the Course



- About this course
  - ppcomp@el.gsic.titech.ac.jp
- Tokyo Tech OCW
  - http://ocw.titech.ac.jp

→ Search with “Practical Parallel Computing”
「実践的並列コンピューティング」で検索