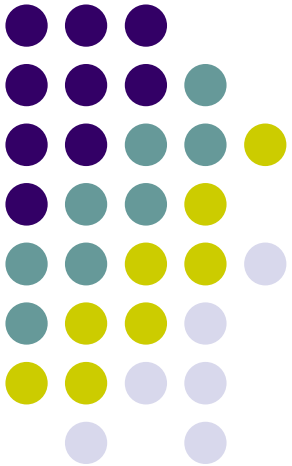
2018 Practical Parallel Computing (実践的並列コンピューティング) No. 1

Overview of the course &
Basic usage of TSUBAME

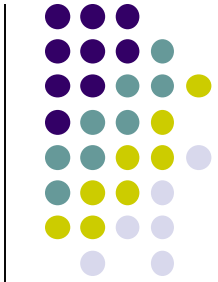


Toshio Endo

School of Computing & GSIC

endo@is.titech.ac.jp

Purpose of This Course



- To learn parallel computing practically
  - Lecture + Practice
  - We 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)

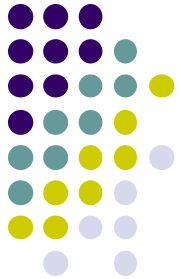
Materials, announcements will be found at OCW web page

- http://ocw.titech.ac.jp

→ Search “practical parallel computing”

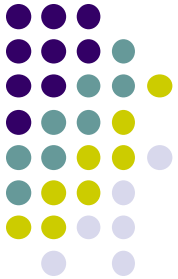
or「実践的並列コンピューティング」

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
  - ls, cp, mkdir, gcc…
  - “make” would be helpful

Overview and Credits

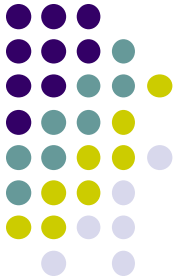


- Part 1: OpenMP for shared memory parallel programming
- Part 2: MPI for distributed memory parallel programming
- Part 3: GPU programming

Your score will be determined by the followings

- There is homework for each part. Submission of reports for 2 parts is required
  - The due date will be about two weeks after each part finished
  - (You can submit reports more)
- Also attendances will be considered

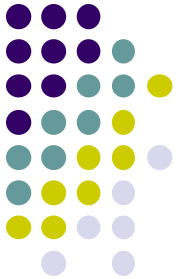
講義の流れと単位認定



- 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

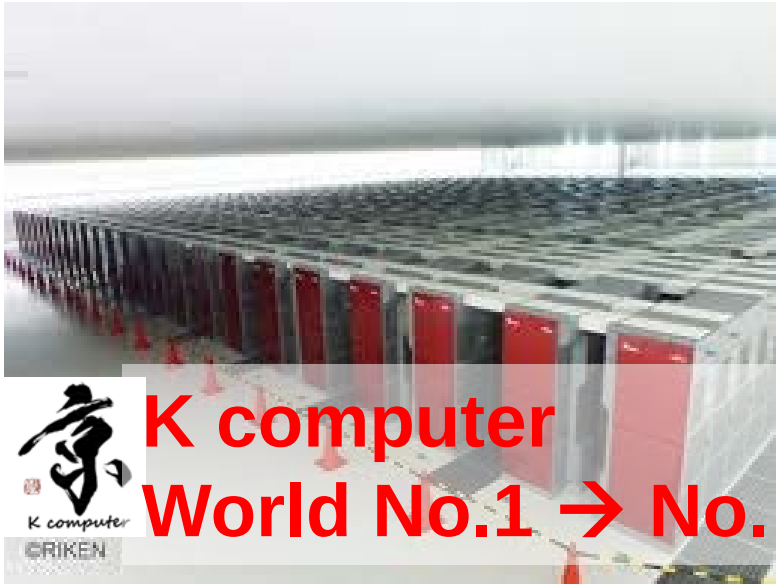
下記により採点・単位認定

- 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



What are supercomputers?

Variety of Supercomputers



K computer
World No.1 → No. 10

TSUBAME3.0
No. 13

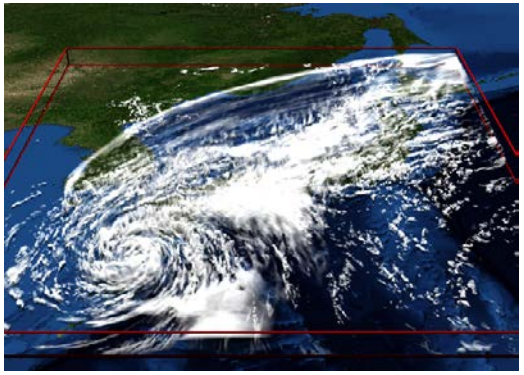
Oakforest-PACS

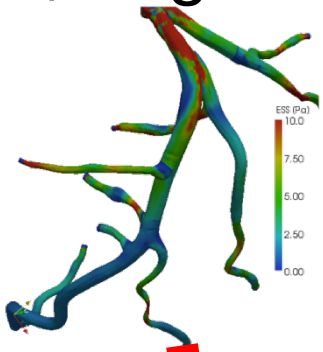
Jaguar

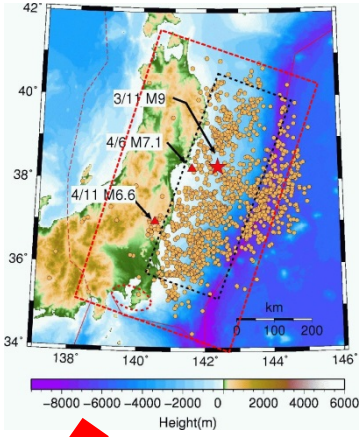
Taifulight
World No.1

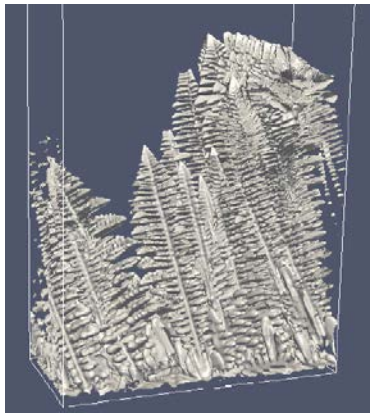
What are Supercomputers used for?

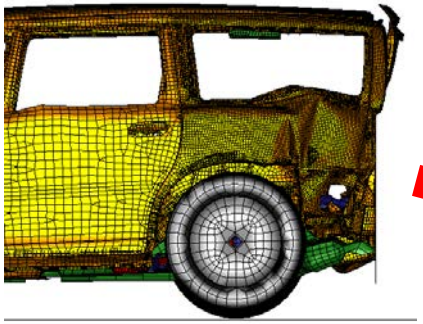
Simulations and Big-data analysis are important for area of science, engineering, security…

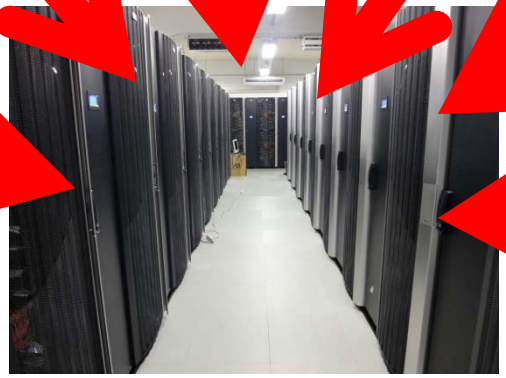


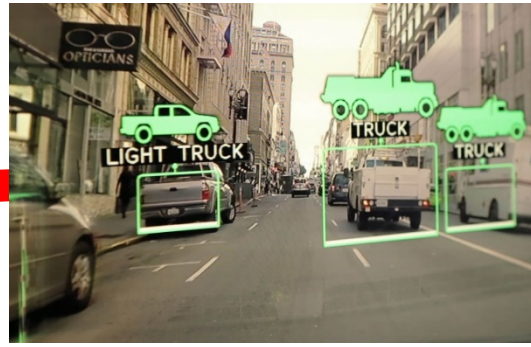












Difference with "Normal" Computers

- 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

~60,000x!

~200GFlops (3×10^{11} times per sec)

12PFlops (1.2×10^{16} times per sec)

<<

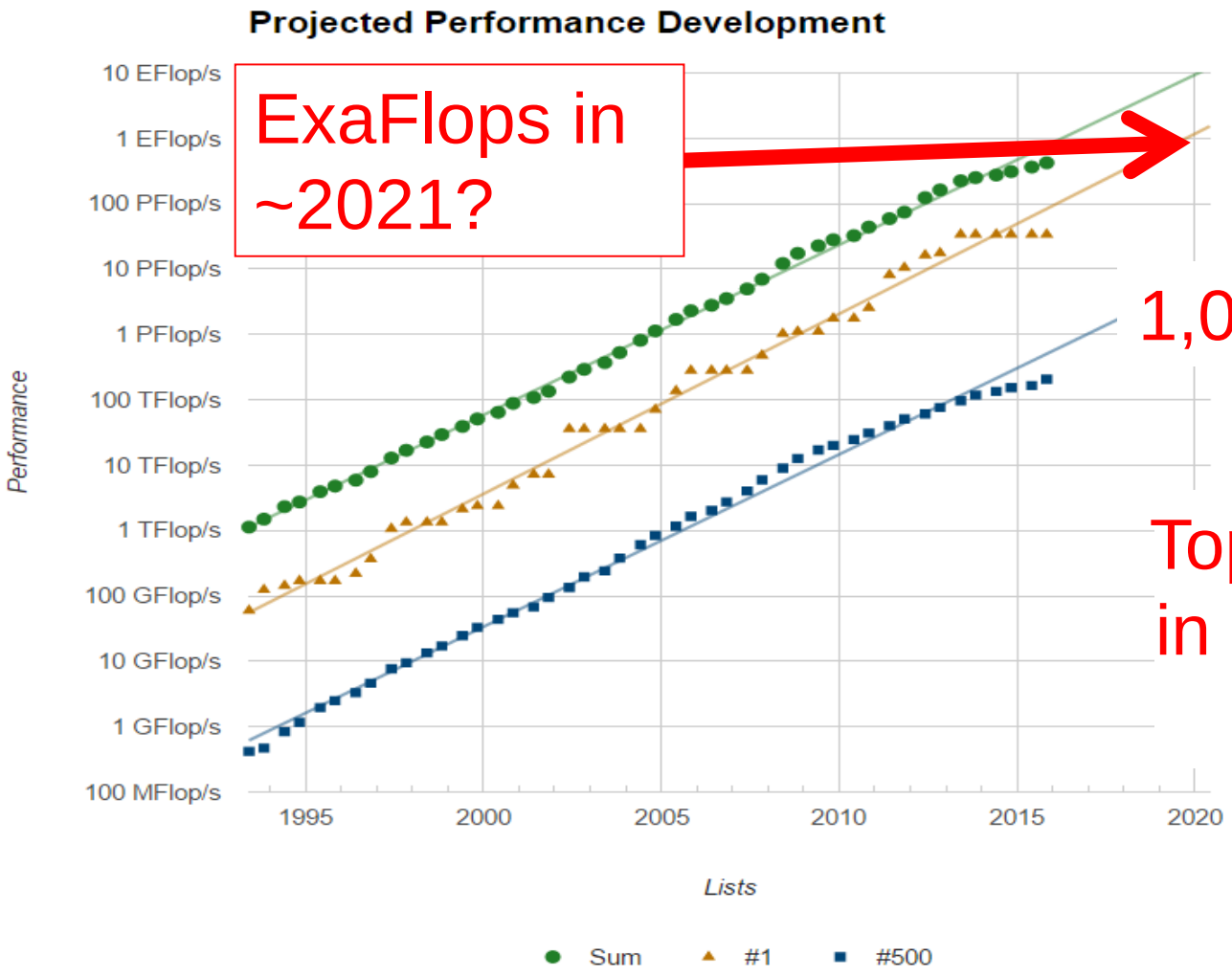
<<

PC in 1980

Cray-1 (1976)
160MFlops

Modern Cell Phone

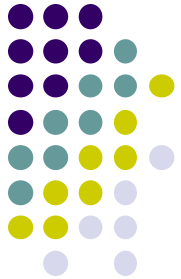
Development of Supercomputers
(from www.top500.org)



1,000x in 10 years

Top Supercomputer in 1993 (60GFlops) ≒ PC in 2011

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

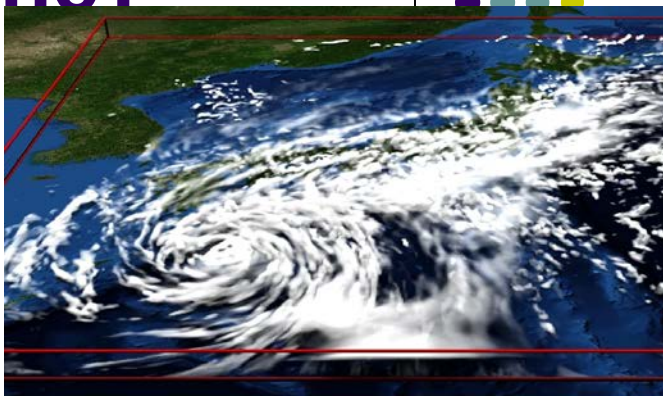
⇒Want to make discovery by comparing mass genome data

⇒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

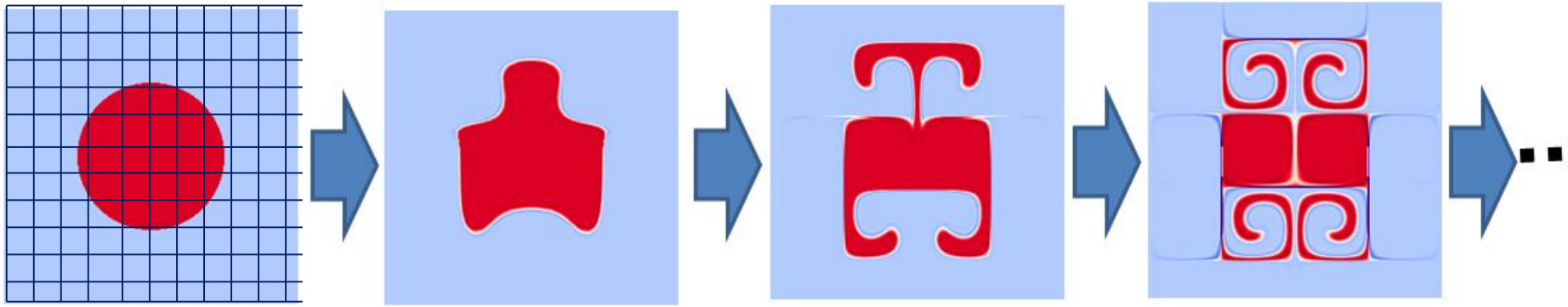
$$\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\frac{1}{\rho}\nabla p + \nu \Delta \boldsymbol{v} - g\hat{\boldsymbol{z}}$$



But no analytical solution for them, generally

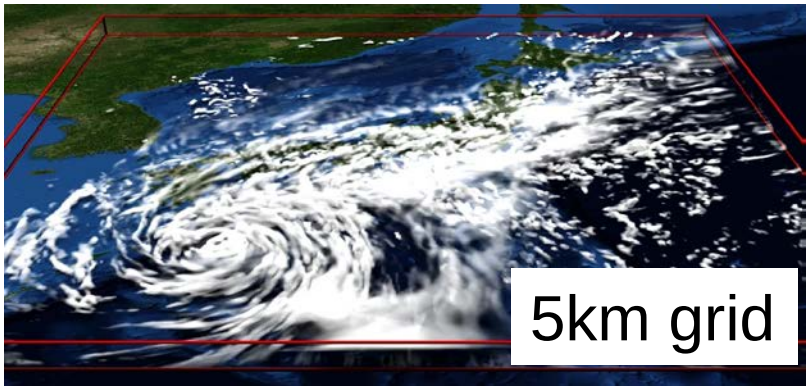
⇒ Instead, space and time are discretized

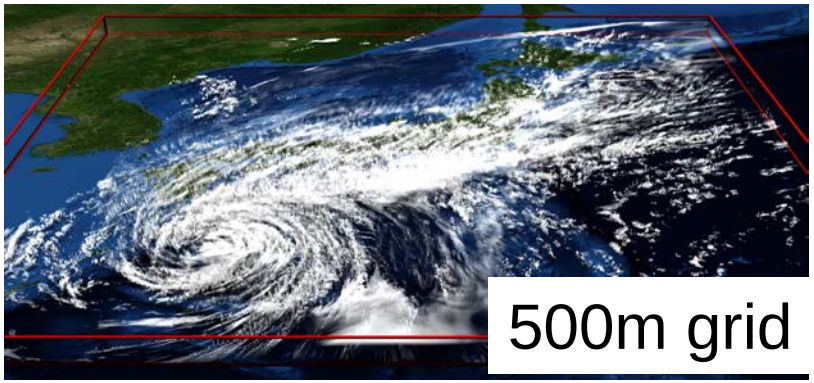
- The space is divided into small grids, expressed as an array
  ⇒ Each array element should be computed
- The time is divided into time steps
  ⇒ After a time step is computed, we go to next step, and so on



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)





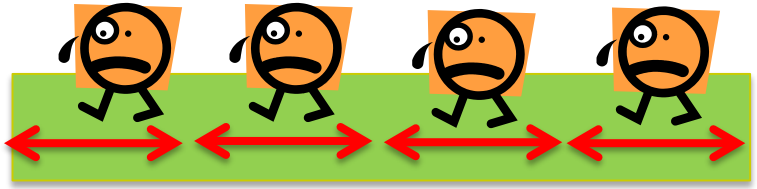
For better prediction, we need to make grid finer (arrays larger)
If resolution is 10x higher, we need 10000x computations! (10x10x10x10)
→ In future, we are going to 50m grid…

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

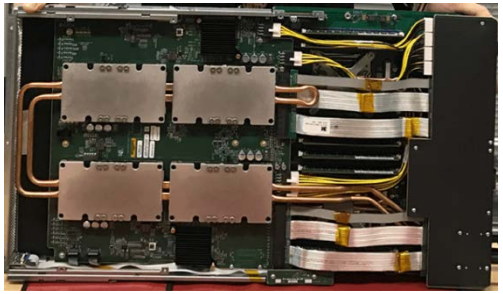
Multiple workers are working together → fast!



Hierarchical SC Structure

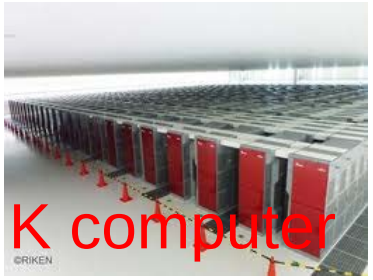
- System = Many nodes (=computers) + External storage
  - Parts are connected by Network

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



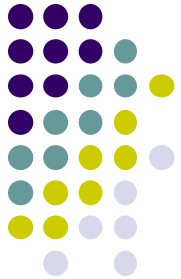
- Processor = Several cores + Cache

Structure of TSUBAME3 and K



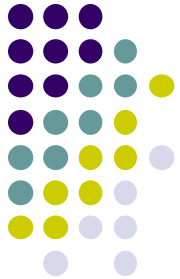
System	540 nodes	5.73PFlops	88000 nodes	11.26PFlops
Node	2 CPUs + 4 GPUs	2 x 425GFlops + 4 x 5300GFlops = 22050GFlops	1 CPU	128GFlops
Processor	CPU: 14 cores GPU: 56 SMXs	CPU: 425GFlops GPU: 5300GFlops	8 cores	128GFlops
Core	CPU core: 1.9GHz x 16 = 30.4GFlops GPU SMX: 1.48GHz x 64 = 94.6GFlops		2GHz x 8 = 16GFlops	

“Flops” shows speed in “double precision”



- “TSUBAME3 Guidance” is explained here

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”

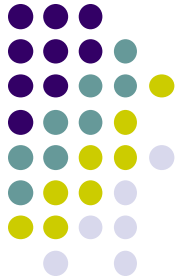
Please do the following by Apr 19 (earlier is better)

- Please make your account on TSUBAME3
  - Tokyo Tech Portal (portal.titech.ac.jp) → TSUBAME Portal
- 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:

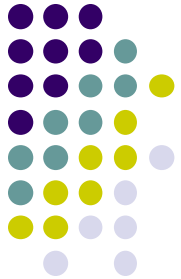
Note in This Course



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
- Make sure use can connect to Wifi network
  - We recommend “TokyoTech” Wifi network

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”School of 「実践的並列コンピューティング」で検索