

2017

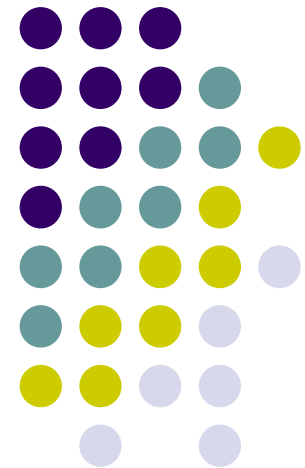
# Practical Parallel Computing (実践的並列コンピューティング)

No. 1

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Overview of the course &  
Basic usage of TSUBAME

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# Purpose of This Course



- To learn parallel computing practically
  - Lecture + Practice
  - We use the TSUBAME supercomputer from this room
- Plan
  - Lecture about libraries/languages for parallel computing
    - OpenMP
    - MPI
    - CUDA (a programming environment for GPUs)

Materials, announcements will be found at OCW web page

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

→ Search “practical parallel computing”



# 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...
  - Compilation, 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

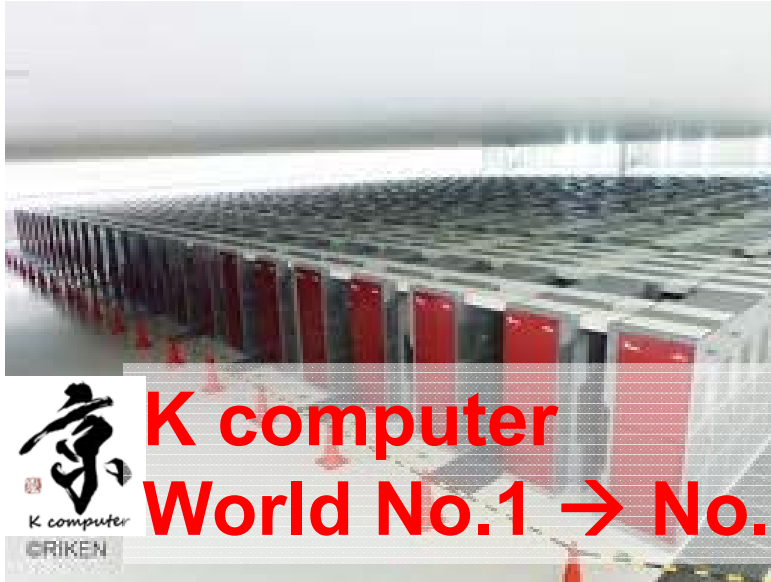
## 下記により採点・単位認定

- 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
  - 〆切は、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?

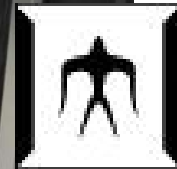
# Variety of Supercomputers (SC)



**K computer**  
**World No.1 → No. 7**



**TSUBAME2**  
**No. 4 → No. 40**



**Oakforest-PACS**



**Jaguar**

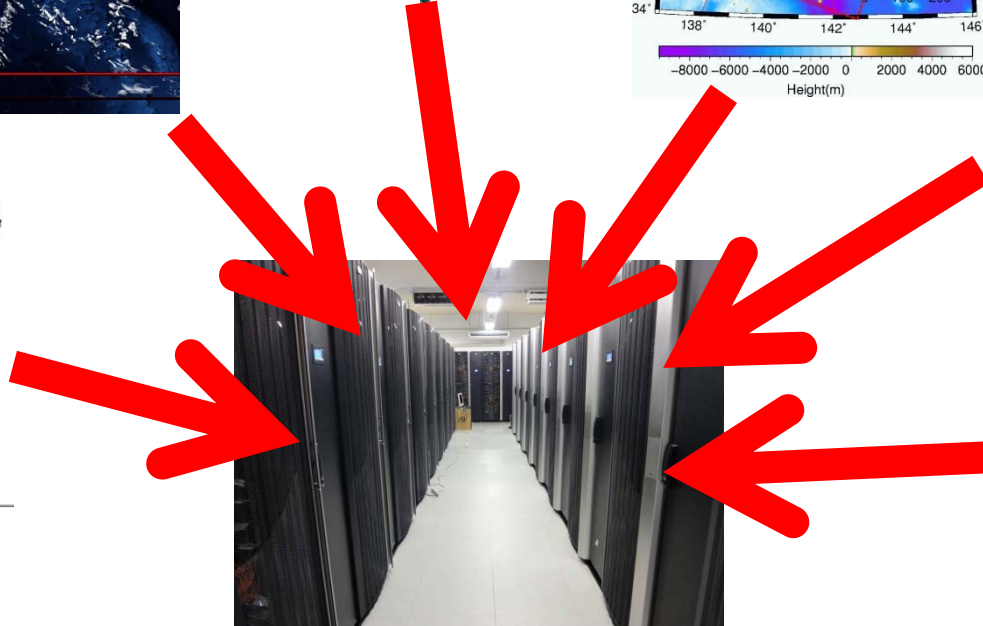
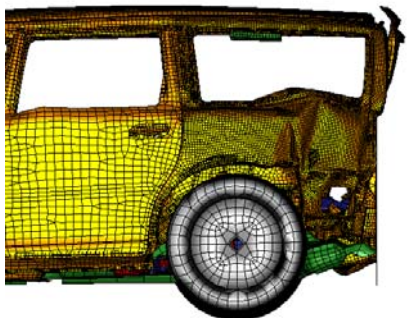
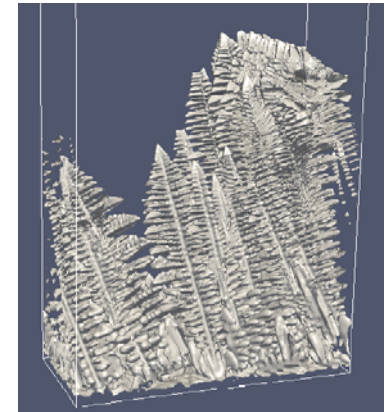
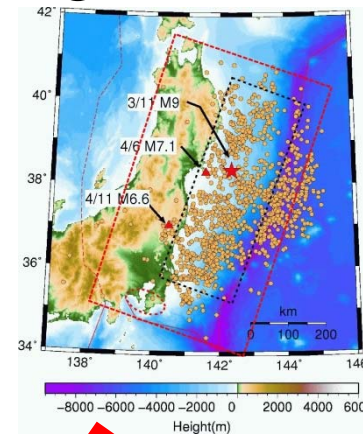
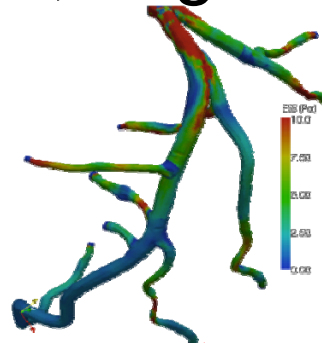
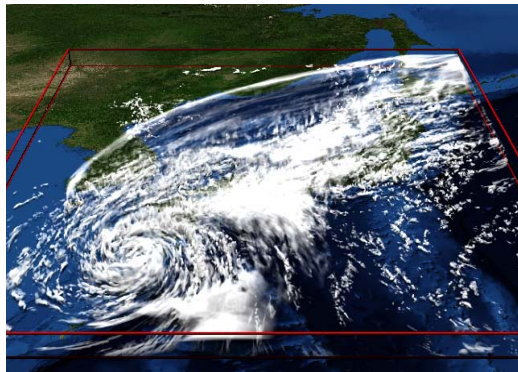


**Taifulight**  
**World No.1**



# What are Supercomputers used for?

Simulations and Big-data analysis are important for area of science, engineering, social...

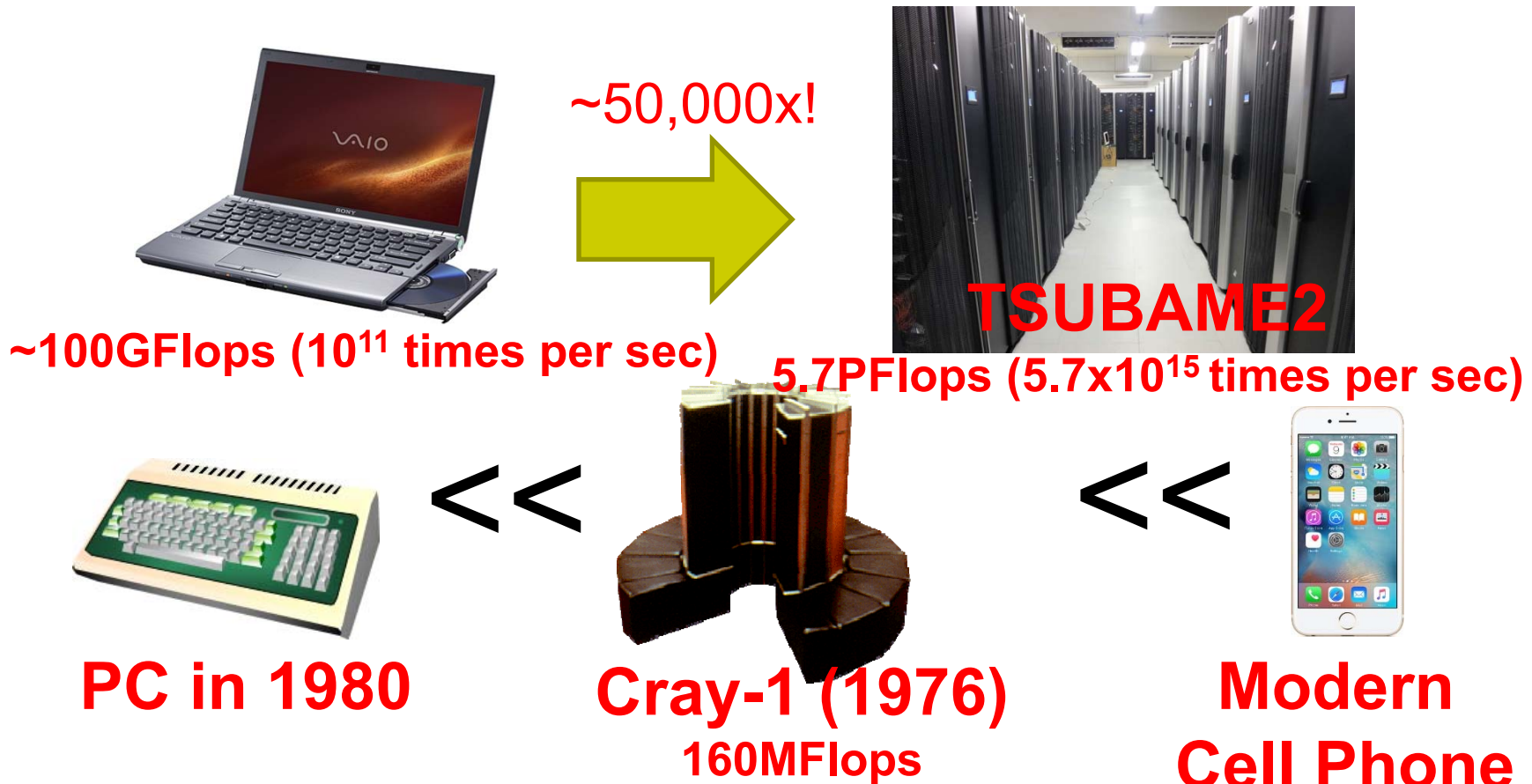




# Difference with “Normal” Computers



- 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



# Development of Supercomputers (1)

(from [www.top500.org](http://www.top500.org))

Linpack benchmark speed (Gflops)



Jun-93	CM-5/1024	60	LANL	US
Nov-93	Numerical Wind	60	LANL	Japan
Jun-94	XP/S140	60	LANL	US
Nov-94	Numerical Wind Tunnel	170	LANL	Japan
Jun-95	↓	170	↓	Japan
Nov-95	↓	170	↓	Japan
Jun-96	SR2201	170	↓	US
Nov-96	CP-PACS	1338	↓	US
Jun-97	ASCI I	1338	↓	US
Nov-97	↓	1338	↓	US
Jun-98	↓	1338	↓	US
Nov-98	↓	1338	↓	US
Jun-99	↓	2121	↓	US
Nov-99	↓	2379	↓	US
Jun-00	↓	2379	↓	US
Nov-00	ASCI White	4938	LLNL	US
Jun-01	↓	7226	↓	US
Nov-01	↓	7226	↓	US
Jun-02	Earth-Simulator	35860	ES Center	Japan
Nov-02	↓	35860	↓	Japan
Jun-03	↓	35860	↓	Japan

60GFlops

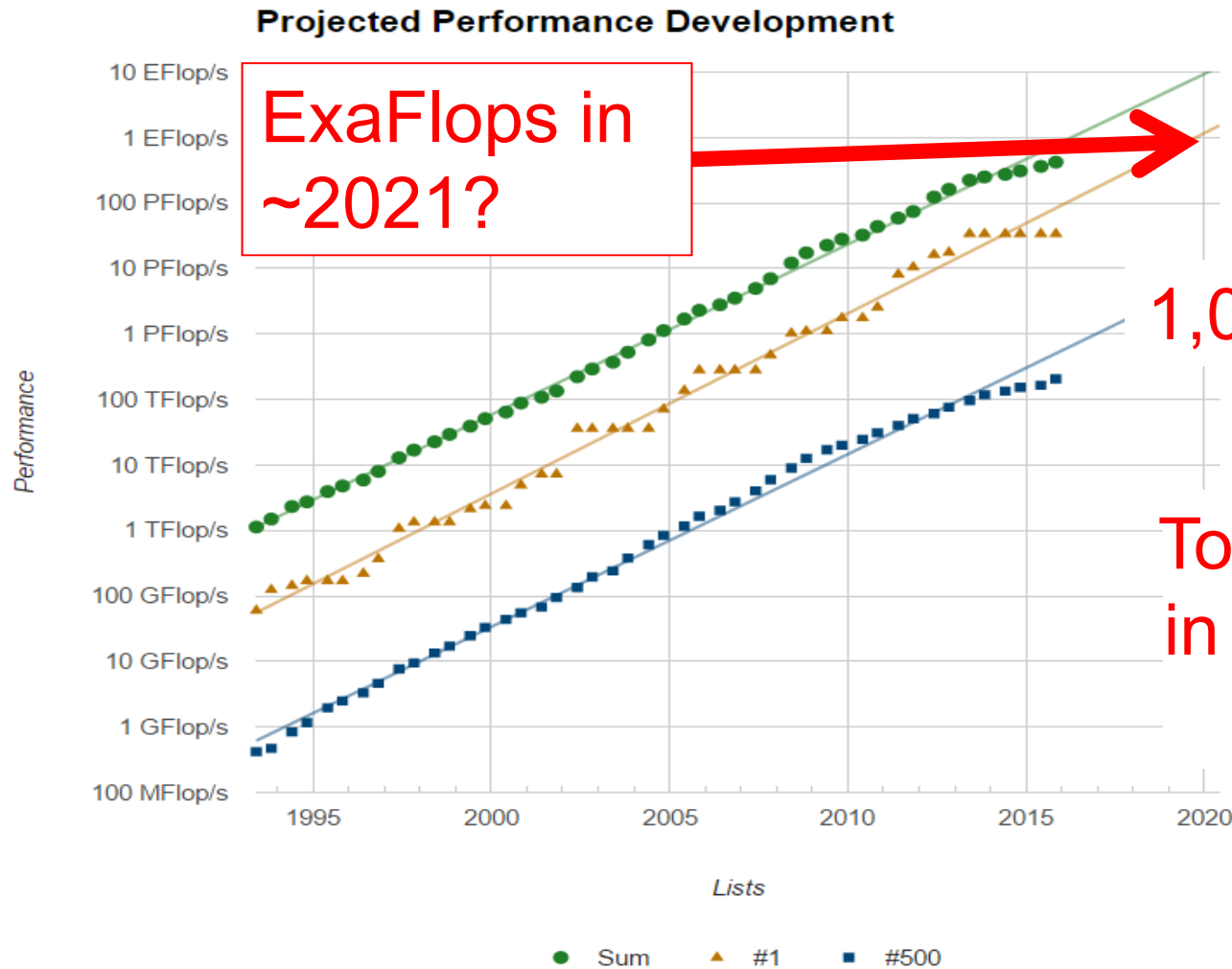
500,000x Faster in 20 years

33.9PFlops

Nov-03	↓	35860	↓	Japan
Jun-04	↓	35860	↓	Japan
Nov-04	BlueGene/L beta	70720	IBM/DOE	US
Jun-05	BlueGene/L	136800	DOE/NNSA/LLNL	US
Nov-05	↓	280600	↓	US
Jun-06	↓	280600	↓	US
Nov-06	↓	280600	↓	US
Jun-07	↓	280600	↓	US
Nov-07	↓	280600	↓	US
Jun-08	RoadRunner	1026000	↓	US
Nov-08	↓	1105000	↓	US
Jun-09	↓	1105000	↓	US
Nov-09	Jaguar	1759000	ORNL	US
Jun-10	↓	1759000	↓	US
Nov-10	Tianhe-1A	2566000	NSC	China
Jun-11	K computer	8162000	RIKEN AICS	Japan
Nov-11	↓	10510000	↓	Japan
Jun-12	Jaguar2	16324000	DOE/NNSA/LLNL	US
Nov-12	↓	16324000	DOE/SC/ORNL	US
Jun-13	Tianhe-2	33863000	NSC	China
Nov-13	↓	33863000	↓	China

# Development of Supercomputers (2)

(from [www.top500.org](http://www.top500.org))



1,000x in 10 years

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



# Why are Speed & Size Important?

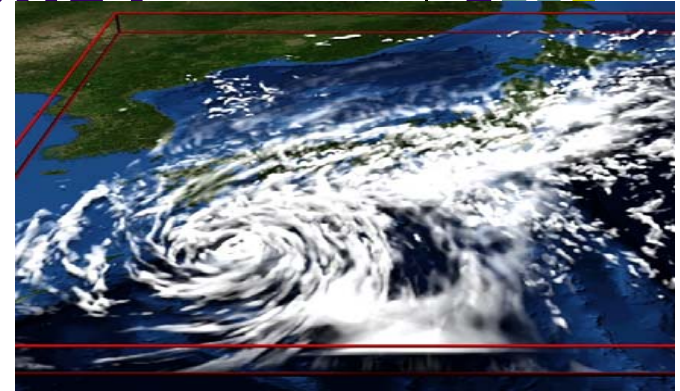


- For simulation & big-data analysis, **large number of computations** should be done speedily
  - ⇒ Want to obtain forecast of tomorrow weather by tomorrow (of course!)
  - ⇒ Want to develop and sell new medicine (than competitors)
- For simulation & big-data analysis, storing **large scale data** is 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

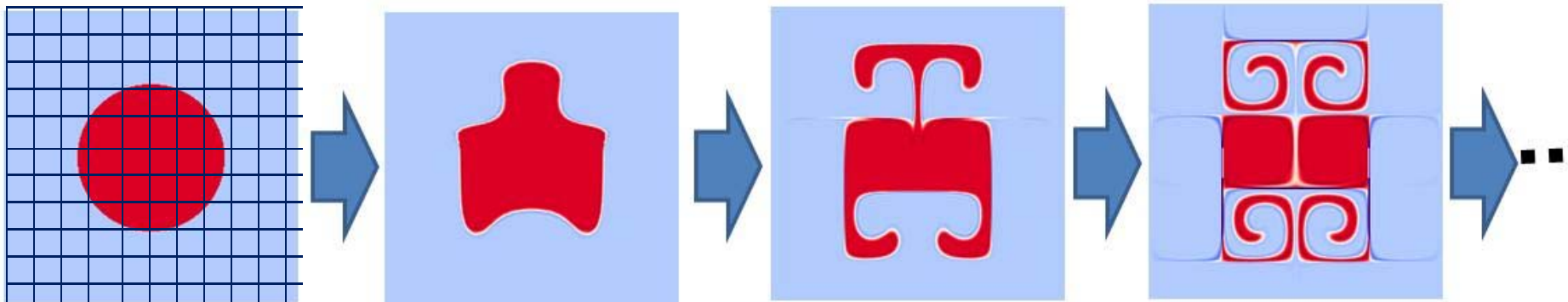
$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{v} - g \hat{\mathbf{z}}$$



But no analytical solution for them, generally

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

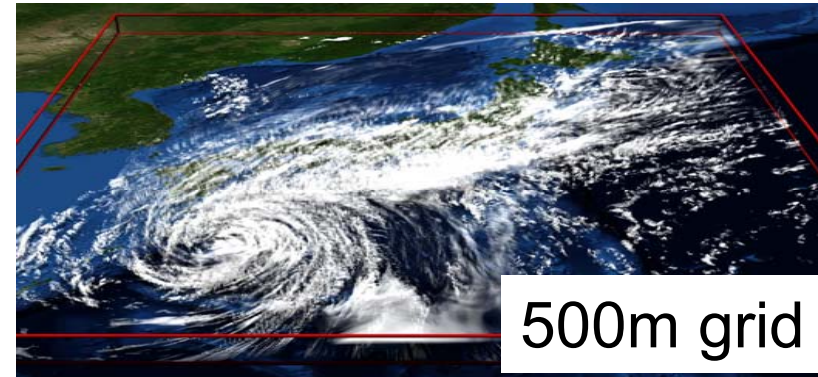
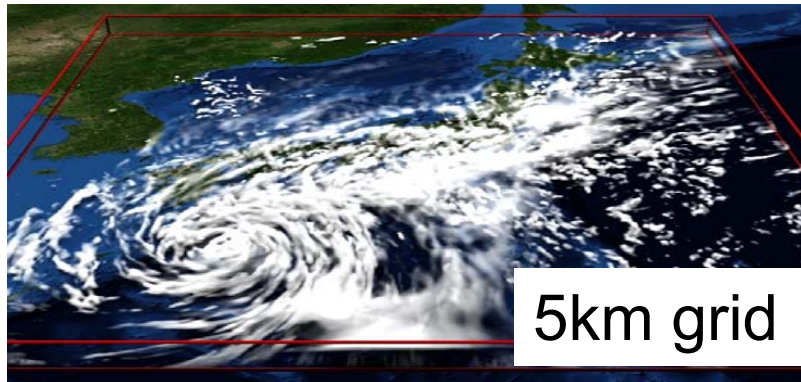
- The space is divided into small grids, expressed as an array  
⇒ Each array element should be computed
- The time is divided into time steps  
⇒ After a time step is computed, we go to next step, and so on



# 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 grid...





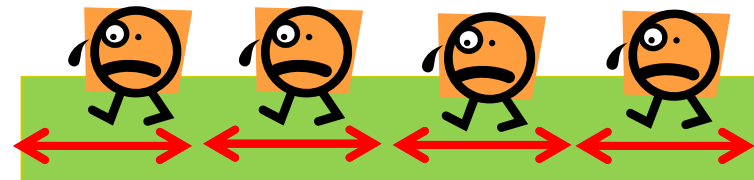
# Why are SCs Fast?

- 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!**



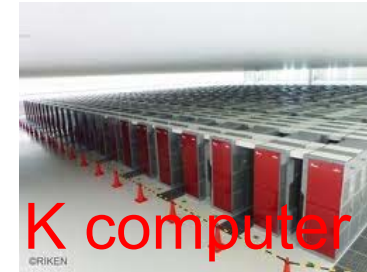


# Hierarchical SC Structure

- 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 TSUBAME2 and K



System	1408 nodes	5.73PFlops	88000 nodes	11.26PFlops
Node	2 CPUs + 3 GPUs	140GFlops + 3930GFlops = 4070GFlops	1 CPU	128GFlops
Processor	CPU: 6 cores GPU: 14 SMXs	CPU: 70GFlops GPU: 1310GFlops	8 cores	128GFlops
Core	CPU core: 2.93GHz x 4 = 11.7GFlops GPU SMX: 0.73GHz x 128 = 93.4GFlops		2GHz x 8 = 16GFlops	

*GPUs are focused in Part 3  
In this course*



- “TSUBAME2.5 Guidance” is explained here

# TSUBAME Group in This Course



- Students of this course will become members of “t2g-ppcomp” TSUBAME group
  - Use t2sub command with “-W grouplist=t2g-ppcomp”

Please do the following by Apr 20 (earlier is better)

- Please make your account on TSUBAME2
  - Tokyo Tech Portal (portal.titech.ac.jp) → TSUBAME2 Portal
- Please send an e-mail to [ppcomp@el.gsic.titech.ac.jp](mailto:ppcomp@el.gsic.titech.ac.jp)

Subject: TSUBAME2 ppcomp account

To: [ppcomp@el.gsic.titech.ac.jp](mailto:ppcomp@el.gsic.titech.ac.jp)

Lab name/Department name

School year

Name

Your TSUBAME account name

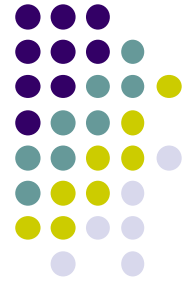


# Note in This Course

Since each student logs in 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](mailto:ppcomp@el.gsic.titech.ac.jp) (Endo)
- 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