Introduction to large-scale computing
大規模計算序論

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Contents

- Necessity of large-scale computing
- Methods of the large-scale computing(Mainly parallelization)
- Today's supercomputers
- Future direction of large-scale computing

Necessity of large-scale computing

- Systems we want to study have many atoms.
- The computational cost increases N^3, N^6, or exponentially.(N is the number of atoms, electrons,…)
- Some physical quantities needs a huge computational cost in spite of a small system(high accuracy).
- There is scientific and/or industrial significance obtained by large-scale computing.

Problems raised by large-scale computing

- Because of huge date must be handled, huge HDD and fast IO is needed. (~30PB in K computer, ~150PB in Fugaku)
- In shared PC clusters level, several troubles can also occur when you increase the number of atoms, the number of k-point sampling, cut-off energy, or the values of some parameters.
  - The data of wavefunctions in first-principles calculations (~ a few GB or more/job)
  - The data of atomic positions in MD (~300GB or more if you consider one million atoms and 10 million MD steps.)
  - You have to know the remaining capacity of the home directory and/or workspace.→It bothers other users if the HDD overflows.
  - You have to know the capacity of the memory of nodes. If your job uses the swap space, the calculation speed becomes very slow(10 times or more).
- The problem of data analysis including visualization.
  - It takes about 30 seconds to make one snap shot. If you need 1,000 pictures, it takes more than 8 hours.
- In some cases, data analysis costs more time than computational time.
- …

When we perform large-scale computing,…

- It costs huge computational time.
- In some cases, huge physical memory of CPU is needed.

- In order to solve these problems, we have to improve software codes to reduce the computational time and memory.

- Parallel computing is definitely necessary.

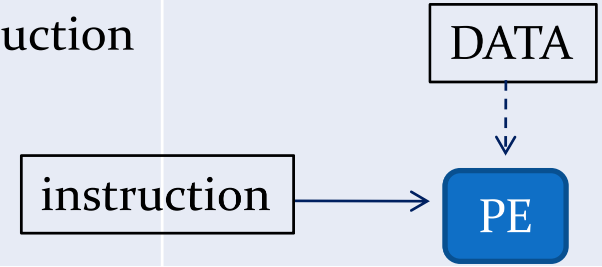
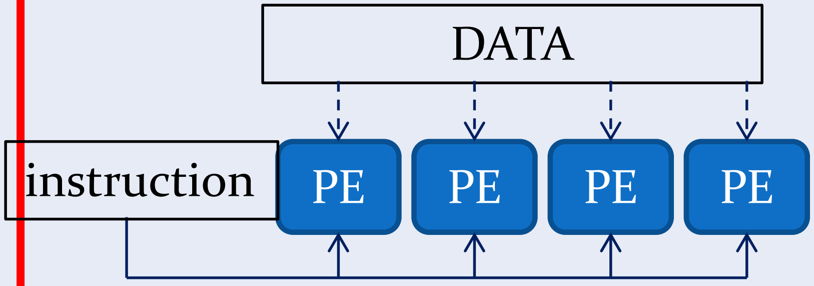
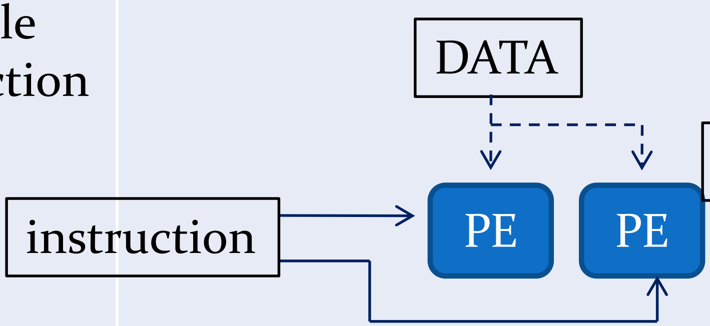
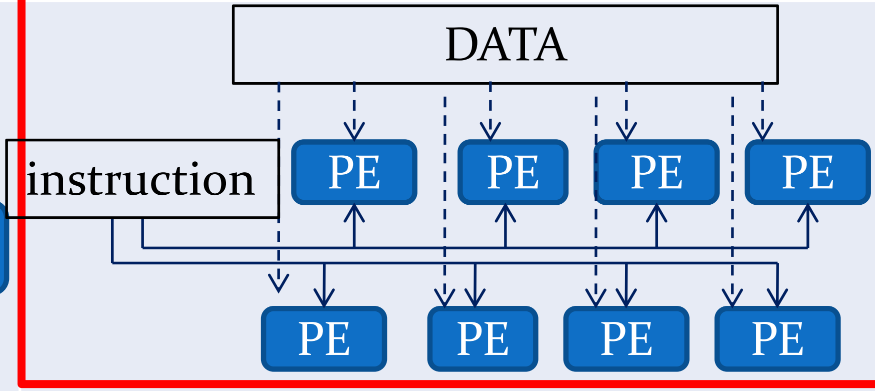
Methods for large-scale computing

- Speed-up techniques
  - Vectorization→SIMD
  - Parallelization
  - Order-*N* method(reduce the cost $o(N^p)\rightarrow o(N)(p=1)$)
  - Use of specialized machine or accelerator(GPU).
- These are used in a code depending on one's necessity.

The easiest way to speed up is to be able to realize it by choosing proper compile options(vectorization, Automatic parallelization, optimization,…).

Since it is not possible to speed up the code automatically, we have to tune the code significantly.

Concept of Flynn’s taxonomy

	Single data	Multiple data
	SISD	SIMD
Single instruction		
	MISD	MIMD
Multiple instruction		 DATA instruction PE PE PE PE PE PE PE PE

Vectorization

- A vector processor, or array processor, is a CPU that implements an instruction set containing instructions that operate on one-dimensional arrays of data called *vectors*(row, column, or diagonal elements, etc…).
- Vectorization is the method that we program a code to construct regularly-arrayed data, and process the data at a time by the vector CPU.
- Vectorization realizes the reduction of a CPU time.
- Today, this concept is included in SIMD.

Vector processing

```
do i=1,imax
   a(i) = c(i) ＋d(i)
   b(i) = c(i) ×d(i)
enddo
```

We tune to increase the part being processed at the deepest do-loop in multi do-loop.

Scalar processing

```
a(1) = c(1) ＋d(1)
b(1) = c(1) ×d(1)
a(2) = c(2) ＋d(2)
b(2) = c(2) ×d(2)
:
:
a(imax) = c(imax) ＋d(imax)
b(imax) = c(imax) ×d(imax)
```

Vector processing

```
a(1) = c(1) ＋d(1)
a(2) = c(2) ＋d(2)
:
:
a(imax) = c(imax) ＋d(imax)
b(1) = c(1) ×d(1)
b(2) = c(2) ×d(2)
:
:
b(imax) = c(imax) ×d(imax)
```

"a" array

"b" array

Order-*N*

- Realized by algorithm

→No approximation Ex.: Screened-KKR

- Realized by approximation of Hamiltonian

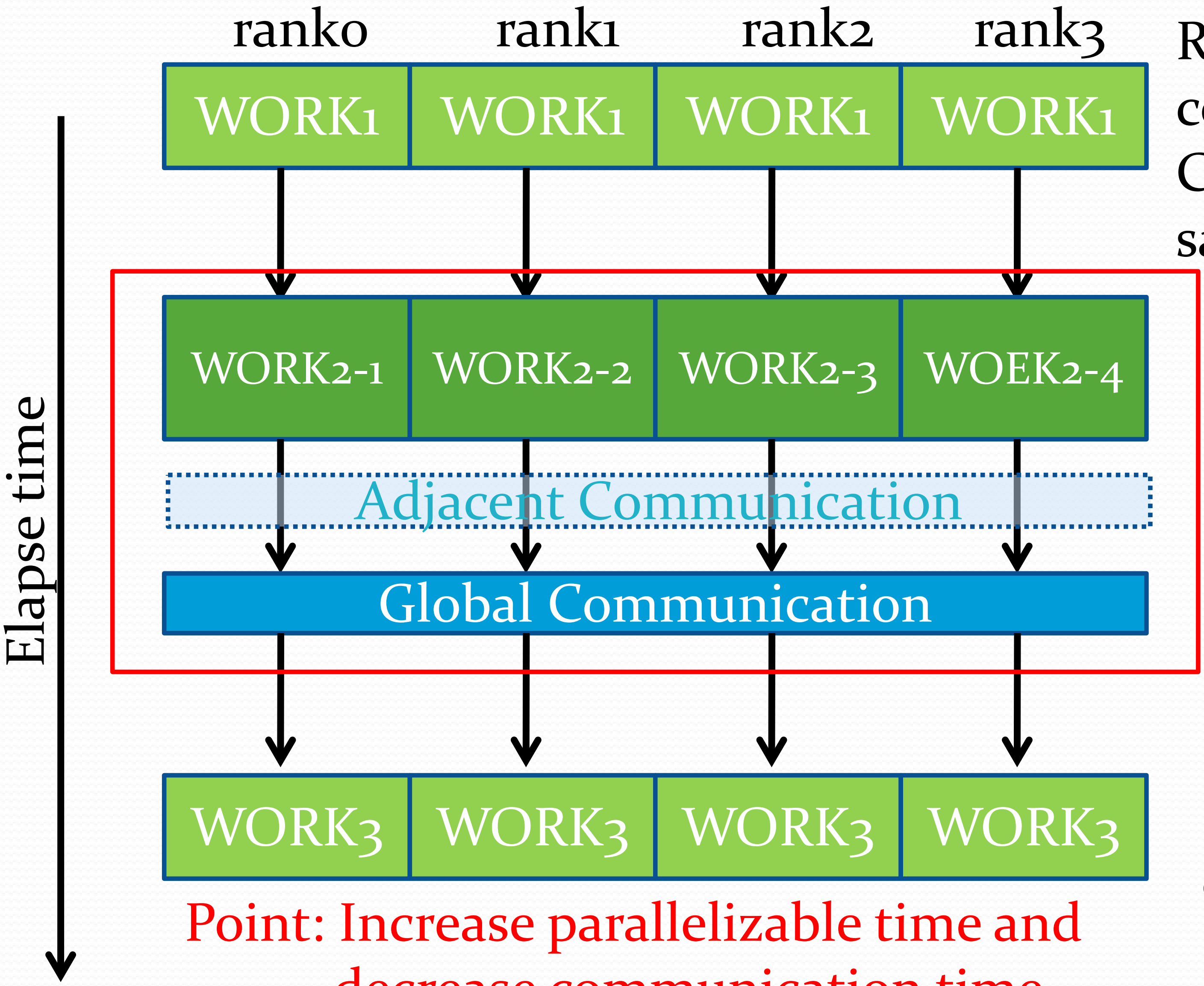
→Approximation by localization of interaction. This type of methods were actively studied in 90's.

  - Roughly speaking, matrices are block-diagonalized or including similar method.
  - $N \times N \rightarrow N \times N_{\mathrm{local}}$(fixed). If N increases, N_{local} not increase. (like a tight-binding approximation)
  - The accuracy of the approximation can be adjustable depending on a required accuracy.
  - One of the famous method is a Divide and conquer method（分割統治法）. This is used in "OpenMX(Ozaki)", "DC(Kobayashi and Nakai)",CONQUEST(Bowler, Miyazaki, Gillan)…

Parallelization

- This is the method to shorten the elapse time by sharing task with more than one CPU without changing the processing time of the task.
- This is used to share big memory(array).

Concept of parallelization



rank0 rank1 rank2 rank3

WORK1 WORK1 WORK1 WORK1

WORK2-1 WORK2-2 WORK2-3 WOEK2-4

Adjacent Communication

Global Communication

WORK3 WORK3 WORK3 WORK3

Elapse time

Redundant computation (all CPUs compute the same calculation)

Parallel computation (different CPU computes different calculation)

Redundant computation

Point: Increase parallelizable time and decrease communication time.

Problems in parallelization

- The ratio of parallelizable part in an elapse time on 1CPU sequential job is conclusive (Amdahl' law) .
- When we parallelize a software code, the data communication between nodes must occur. If the number of nodes increases, the communication time between nodes costs more than the computational time.(In the case of classical MD simulation, this is a crucial problem.)

Amdahl’s Law

Speed up ratio $\alpha_P \equiv \dfrac{t_1}{t_{N_{\text{core}}}}$

Elapse time of one job on 1 core

Elapse time of one job on *N* core

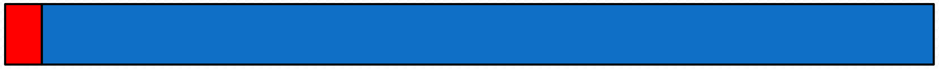
$$(\alpha_P)_{\max} = t_1 \times \left(\frac{1}{t_{N_{\text{core}}}} \right)_{\max} = \frac{1}{(1-P) + \dfrac{P}{N_{\text{core}}}}$$

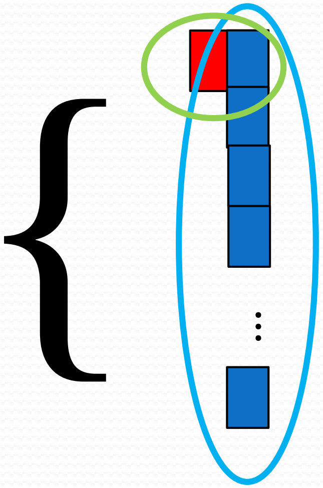
P: parallelizable time in a sequential job

Upper bound of parallelizable ratio

For examples,

Not parallelizable (1 sec.)   parallelizable (99 sec.)



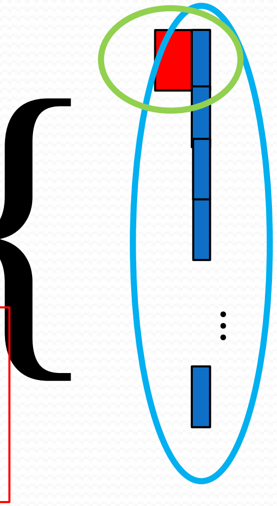


1+0.99=1.99 sec.(almost 50 times faster)

Even w
obtain

We have to increase the parallelizable part as possible.

We have to decrease the non parallelizable part as possible.



1+0.099=1.099 sec. (almost 91 times faster)

Although we uses 1000 processors, the efficiency does not become 100 times even!!!

We feel that the merit of parallelization does not increase even if the number of processors increases more and more.

Gustafson-Barsis' law

Speed-up ratio $\leq n + (1 - n)s$

n: the number of cores

s: the ratio of sequential computation(this part cannot parallelize.)

In this law, the communication time among nodes does not considered.

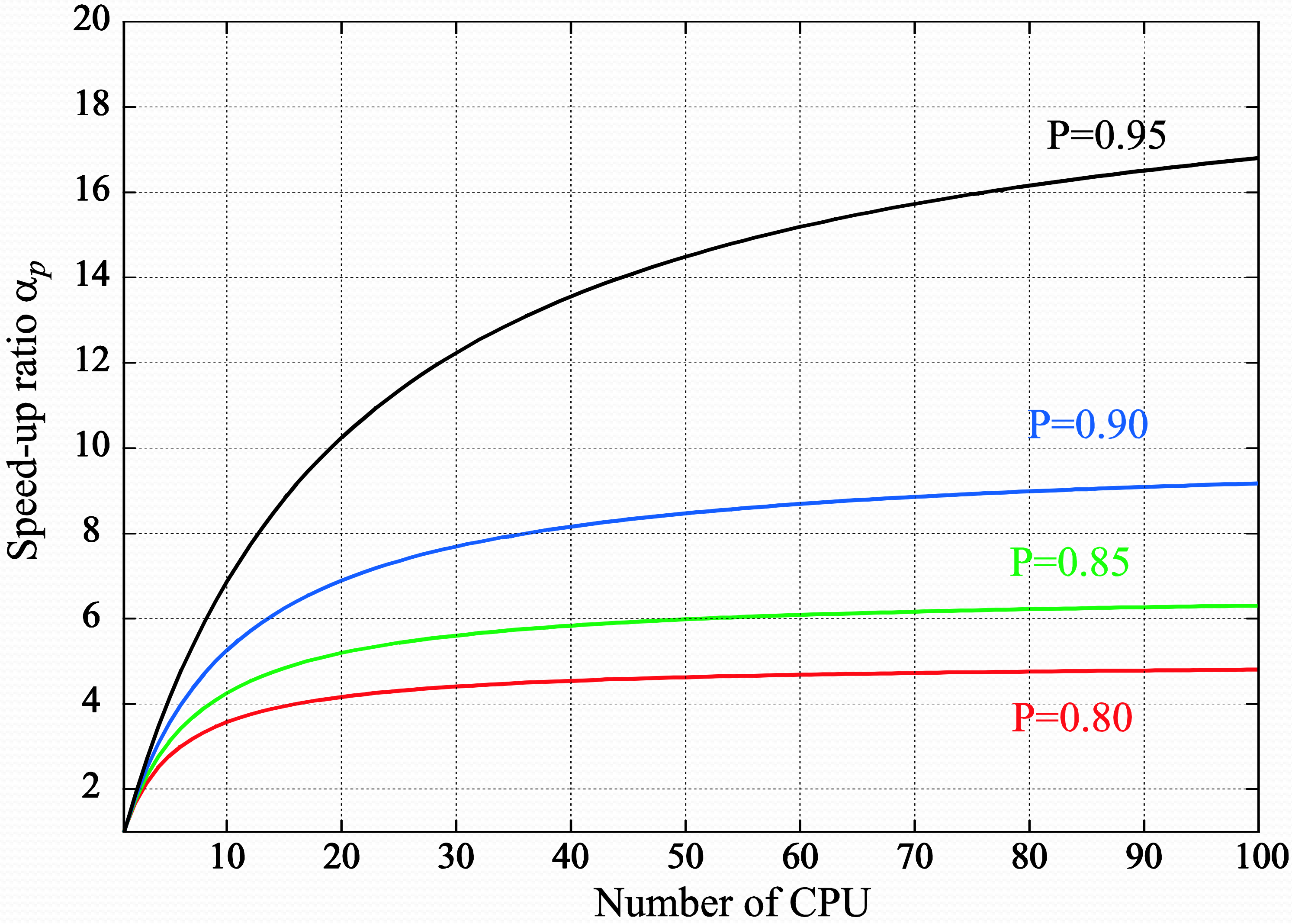
Indices of parallelization efficiency

- Strong scaling－The overall problem size (number of atoms or electrons etc…) is fixed and the number of processors is increased(based on Amdahl's law).
- Weak scaling－The problem size per processor is fixed and the overall problem size is increased with increasing processors(based on Gustafson's law). The processing of one processor is not changed. The ideal situation is the computation time should be constant even if the increase of the number of processors. If the computation time increases, we can see the non parallel part remains, and if the adjacent communication time increases, the method of the communication has a problem.

Reference: https://www.r-ccs.riken.jp/library/event/tokuronB_2020.html
https://www.slideshare.net/RCCSRENKEI/ss-232004088/1

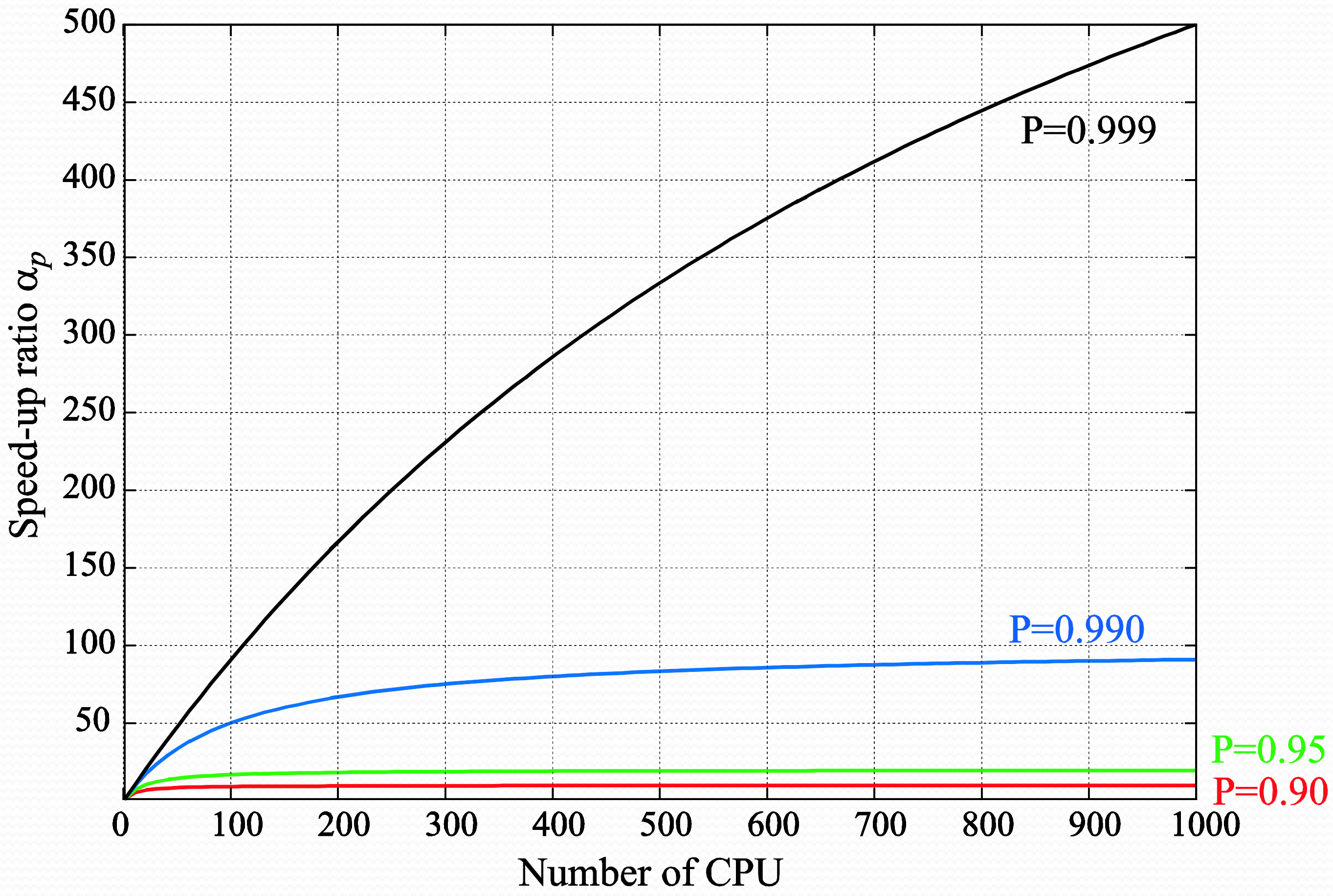
Example of Amdahl's law(1)

Caution! The communication time is not included.



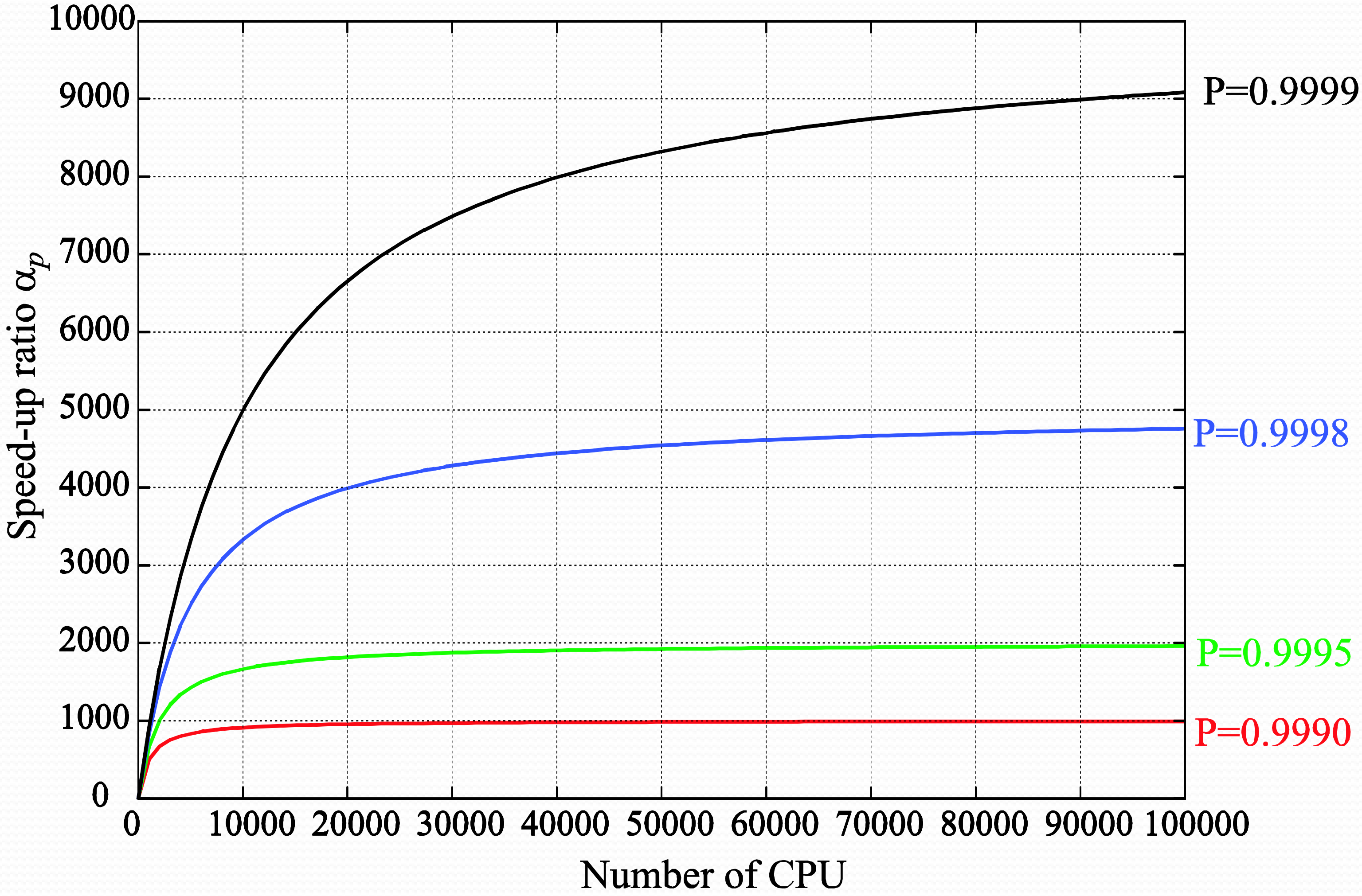
Ordinary calculations using PC cluster

Example of Amdahl's law(2)



Calculations using high-end PC cluster or supercomputers

Example of Amdahl’s law(3)

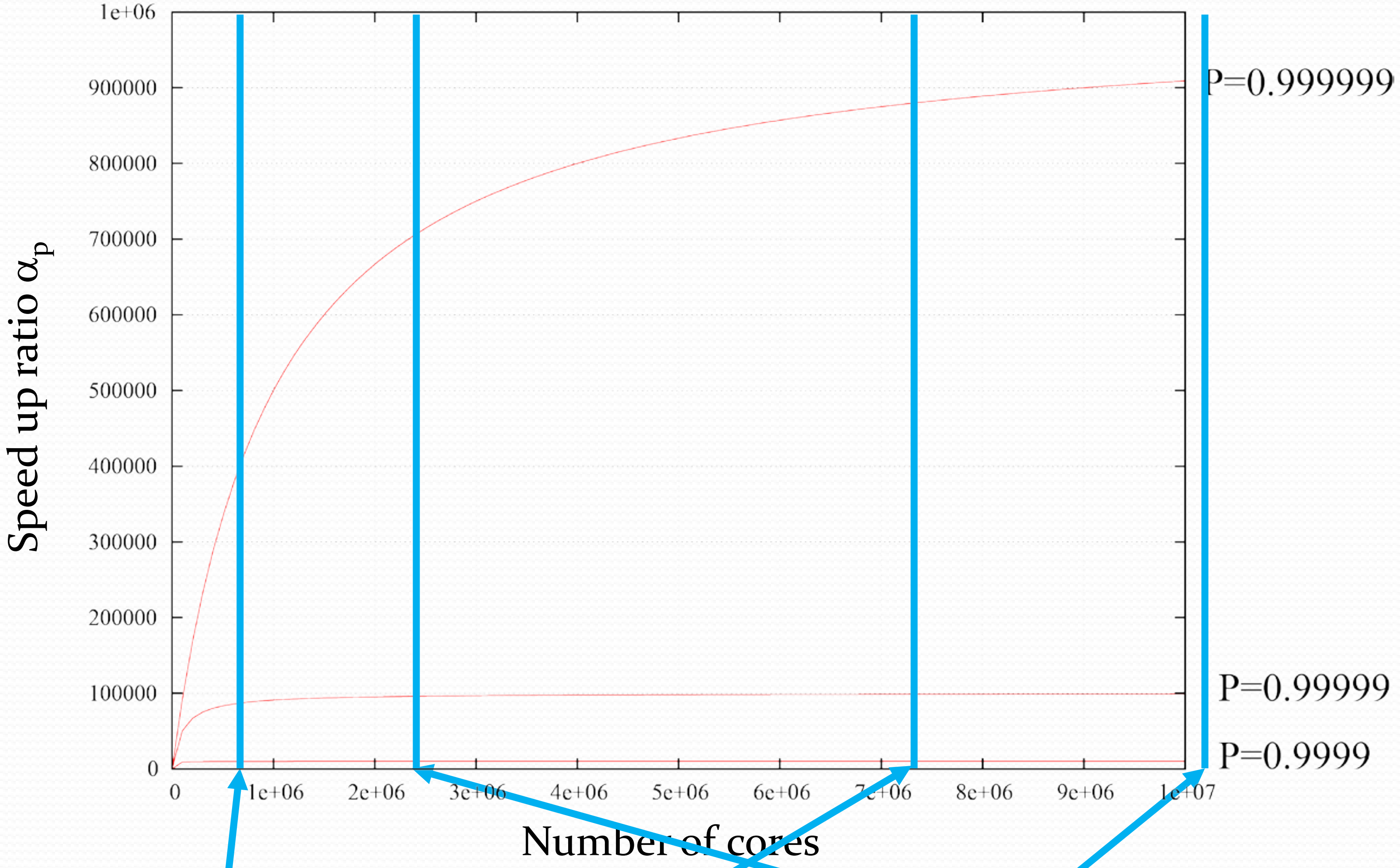


Fugaku: 7,299,072 cores

Calculations using high-end supercomputers

Example of Amdahl’s law(4)

Calculations using top class supercomputers in the world



K computer: 705,024 cores

Fugaku: 7,299,072 cores

Summit: 2,414,592 cores

Sunway TaihuLight: 10,649,600 cores

Even if you are just a user,

- you need to be aware of the parallelization efficiency of the software you use because you must effectively use machine time(machine point, or cost(usage fee)) you can use.
- you need to understand the characteristics of the computer and make efforts to increase the calculation efficiency.
- you need to choose the best compile options to make executable files.

For Intel compiler, -xHost, -axCORE-AVX2,…

- you need to choose the best parameters for the best performance of the software to obtain the best scientific results.

In DFT calculations, E_{cut}, k-point sampling,…
Fundamentally a model size,…

Parallel programming languages

- MPI(message passing interface)
  - The most versatile method.
  - Both core-to-core and node-to-node communication can be handled.
  - The programming may not be easy.
- OpenMP
  - Only core-to-core communication.
  - The programming may be easier than that of MPI.

(within non-complex case)

- PVM
- HPF(High Performance Fortran)

} Now, these are seldom used.

Example of parallelization with MPI

```
program main
include (mpif.h)
        …
call MPI_INIT(IERR)
call MPI_COMM_SIZE(MPI_COMM_WORLD,NPROCS,IERR)
call MPI_COMM_RANK(MPI_COMM_WORLD,MYRANK,IERR)
        …
call para_range(1, n, nprocs, myrank, ista, iend)
do i=ista, iend
        …
   a(i)=a(i)+value
enddo
 call MPI_ALLREDUCE(a,a1,n_element,
     & MPI_DOUBLE_PRECISION,
     & MPI_SUM, MPI_COMM_WORLD, IERR)
    …
call MPI_FINALIZE(IERR)
    …
end
```

ista, iend are the first array numbers allocated to each processor.

Each processor has only allocated elements of the array a() .

Sum up all elements of the array a() for all processors and distributed it for all processors (all processors have the same value of a()).

It is necessary to rewrite so as to calculate only the part allocated to each node and to communicate the data.

Execution: mpirun (or mpiexec) –np 4(# of parallel) ./a.out

Example of parallelization with OpenMP

```
program main
implicit none
integer omp_get_thread_num,I
double precision z(100), a, x(100), y
 do i= 1, 100
    z(i) = 0.0
    x(i) = 2.0
  end do
 a = 4.0
 y = 1.0
print *, “Welcome to the parallel world”
!$omp parallel
print *, “Excuted on”, omp_get_thread_num()
 call daxpy(z, a, x, y)
!$omp end parallel
end program main

subroutine daxpy(z, a, x, y)
integer I
double precision z(100), a, x(100), y
!$omp parallel do
 do i = 1, 100
    z(i) = a * x (i) + y
 enddo
 return
end
```

For simple parallelization, we only need to insert directives, so if we compile without parallelization options the directives are commented out, so basically we do not need to change the original code.

← Directive of the start of parallel processing

← Directive of the end of parallel processing

← Do parallel of just below do loop

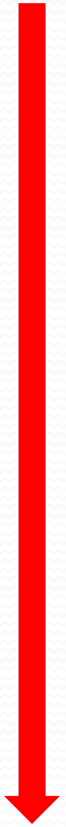
Execution: We do not use a special command.
Set environmental value
“OMP_NUM_THREADS=4” (# of parallel)

The difference between MPI and OpenMP

- OpenMP can be parallelizable only for cores which share the memory. We cannot make a large-scale parallelization code by using OpenMP only.
- The typical software codes which correspond to the large-scale parallelization are tuned by using MPI for its main part.
- The role of OpenMP is to assist the speed up of the code which is parallelized by using MPI.
- Even if you do not develop the software code, you have to know the details of the code in order to get maximum performance.

The other environments to develop parallel computing codes using GPU

easy



hard

- CUFFT, CUBLAS,…
  - Only call libraries to accelerate specific parts. The other parts do not be accelerated.
- OpenACC
  - a programming standard for parallel computing developed by Cray, CAPS, NVIDIA and PGI, designed to simplify parallel programming of heterogenious CPU/GPU system.
  - Very similar with OpenMP. In near future, OpenMP and OpenACC may be merged.
  - Fortran and C are supported.
- CUDA
  - a parallel computing platform and programming model created by NVIDIA and implemented by the graphics processing units (GPUs) that they produce. (only PGI Fortran can used.))

OpenACC(Open Accelerator)

```
program picalc
    implicit none
    integer, parameter :: n=1000000
    integer :: i
    real(kind=8) :: t, pi
    pi = 0.0
  !$acc parallel loop
    do i=0, n-1
      t = (i+0.5)/n
      pi = pi + 4.0/(1.0 + t*t)
    end do
  !$acc end parallel loop
    print *, 'pi=', pi/n
  end program picalc
```

As the development environment, the best results can be obtained by improving according to the message issued by the compiler.

http://www.nvidia.co.jp/object/openacc-gpu-directives-jp.html

http://www.cms-initiative.jp/ja/events/2014-haishin

http://www.r-ccs.riken.jp/library/event/tokuronB_180406.html

(The 14th lecture given by Dr. A. Naruse is useful.)

https://www.r-ccs.riken.jp/library/event/tokuronB_2020.html

(The 11th lecture given by Dr. A. Naruse is useful.)

The cutting-edge techniques

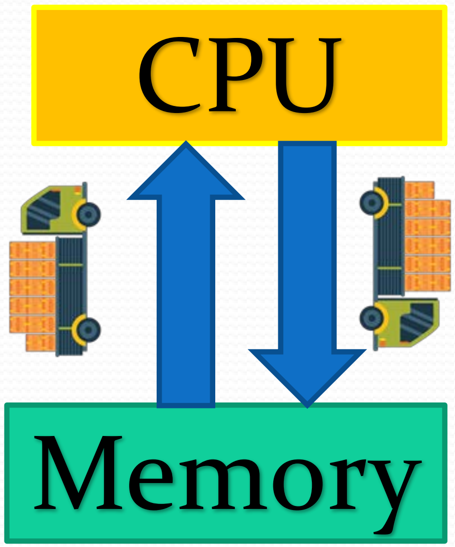
- Avoid memory wall problem(cache control)
  - Computing power>data transfer from memory to computing unit(CPU)→reuse the data on caches
- Pipeline processing
- Continuous access in do loop
- loop unrolling
- Divide data into blocks
- Use the highly-optimized libraries
- …

We have to know details of hardware to make highly optimized software codes.

Please see these sites;
(only Japanese) https://www.r-ccs.riken.jp/library/event/tokuronA_2019.html
https://www.r-ccs.riken.jp/library/event/tokuronB_2020.html

Memory wall problem

Old computer

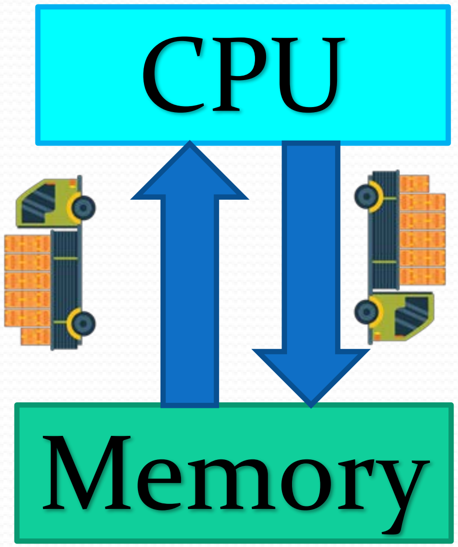


Computation performance (number of clocks) was slow (~10MHz)

The memory can not be accessed until a certain time passes

Sending data from memory to the CPU was slow, and the computation speed was also slow, so it was not the problem at “data transfer speed ≈ calculated speed”.

Today’s computer



The computation performance becomes extremely fast（~a few GHz)

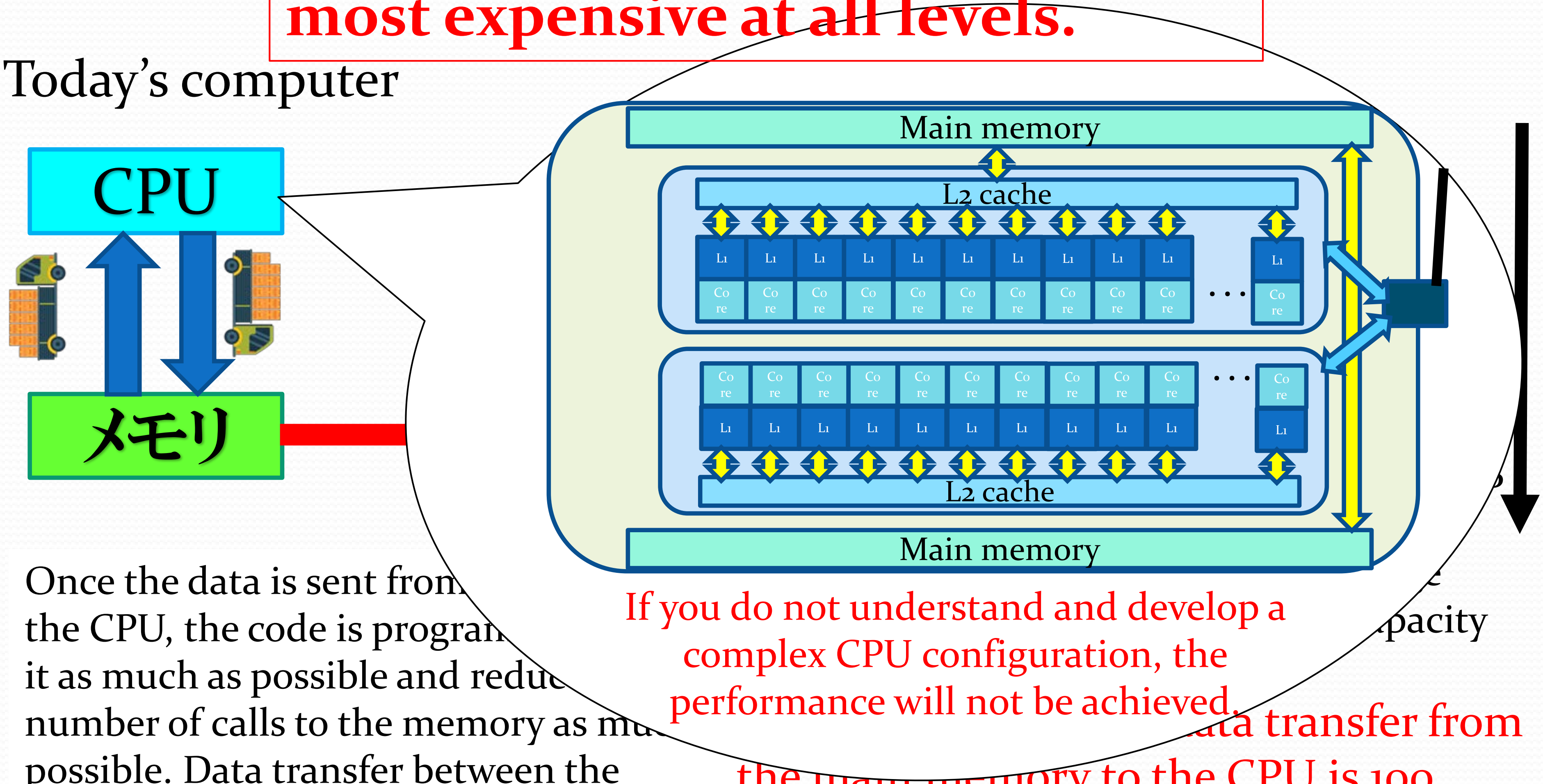
The fact that memory cannot be accessed only for a fixed time does not change much.

Sending data from the memory to the CPU is slow, but since the computing speed has become extremely fast, the CPU is waiting for a long time because of “the transfer speed << compute speed” (supplement with cache etc…).

Memory wall problem

Important!: Data transfer is the most expensive at all levels.

Today's computer



If you do not understand and develop a complex CPU configuration, the performance will not be achieved.

Once the data is sent from
the CPU, the code is progra
it as much as possible and reduc
number of calls to the memory as mu
possible. Data transfer between the
memory and the register or cache is fast,
but the capacity is small.

e
pacity

ta transfer from
the main memory to the CPU is 100
times longer than access to the data on
the register.

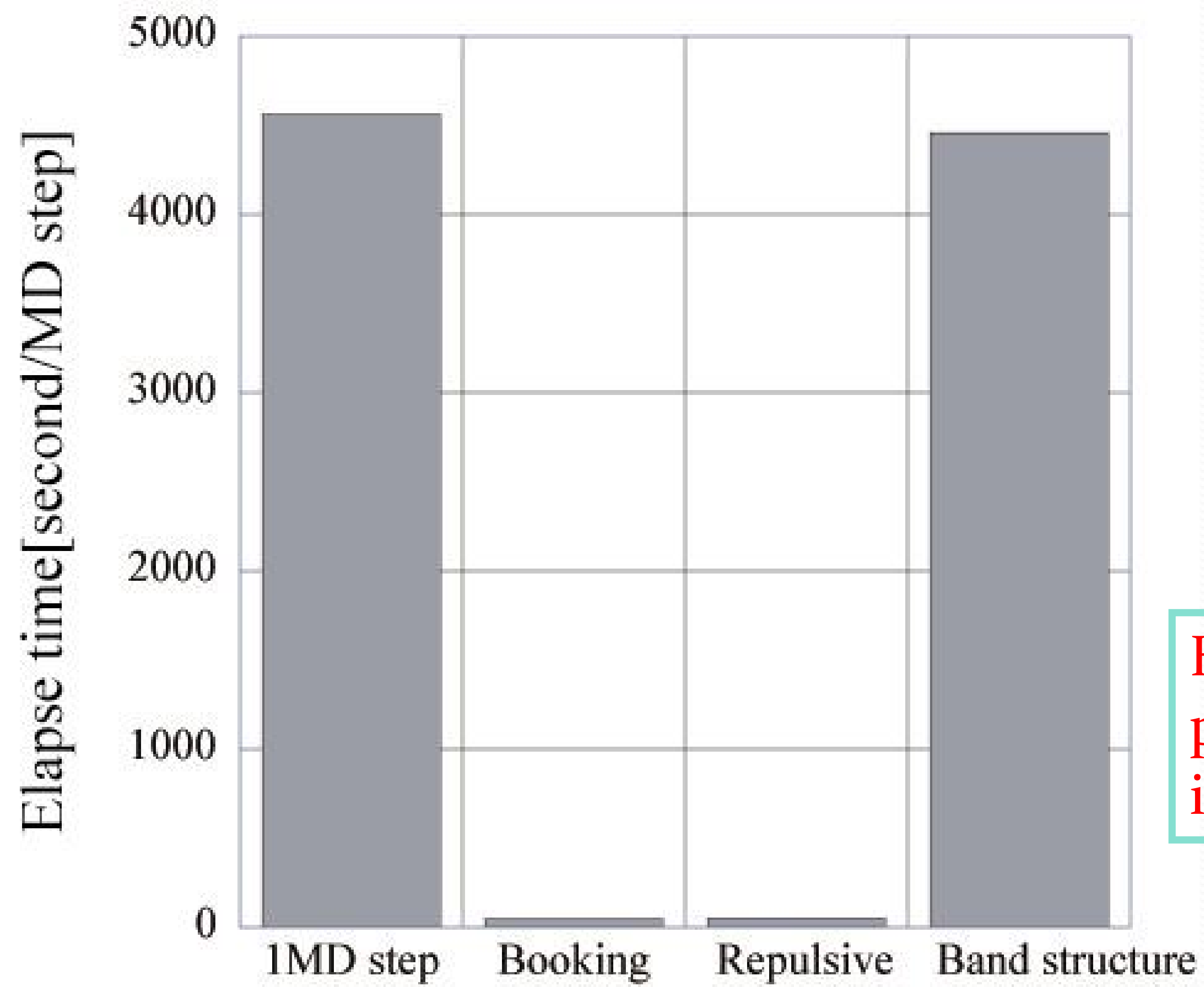
High performance Python

- In place of Fortran and C / C ++, which have been used in scientific computing in the past, HPC software development has been advanced in the USA by using Python.
- Python has overwhelming code readability compared to Fortran and C / C ++.

→It is more likely that the maintenance of the code will be continued without reading by experts.

- We do not need to write everything in Python. If we know that another language is faster than Python for a certain part, we should use the part in the original. We combine Python and the other language and improve the ease of maintenance. (It is said that Python is a "glue language" because it is a language that "sticks" programs in multiple languages.)

Analysis of the computational time in order-*N* tight-binding method



A electronic structure part occupies 97.6% of total elapse time in a sequential job.

↓

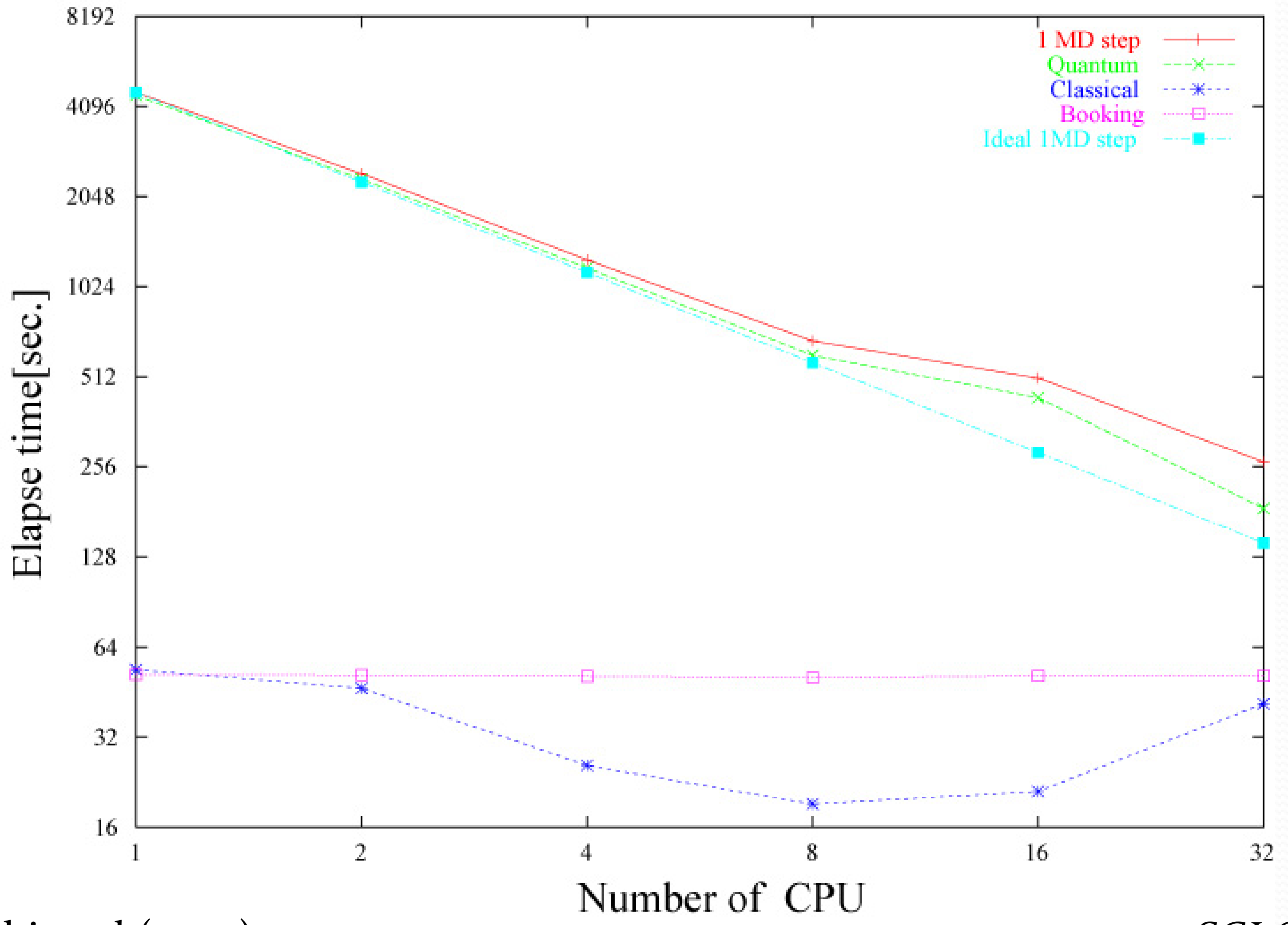
High parallelizability is expected.

Geshi et al.(2003)

Parallelization by means of MPI

- We used MPI_ALLREDUCE and MPI_BCAST to communicate data. (Although this is quite simple and includes useless data communication, the speed-up ratio was good.)
- We divided do-loop as outer as possible.
- In this method, we can make all matrix elements as long as we determine the atomic positions. These data determined from 1 MD step are stored in CPU memory of all node. Although almost all data are useless, we do not need to communicate the data among nodes and there is no loss of data communication.

Elapse time of each part as a function of the number of CPU

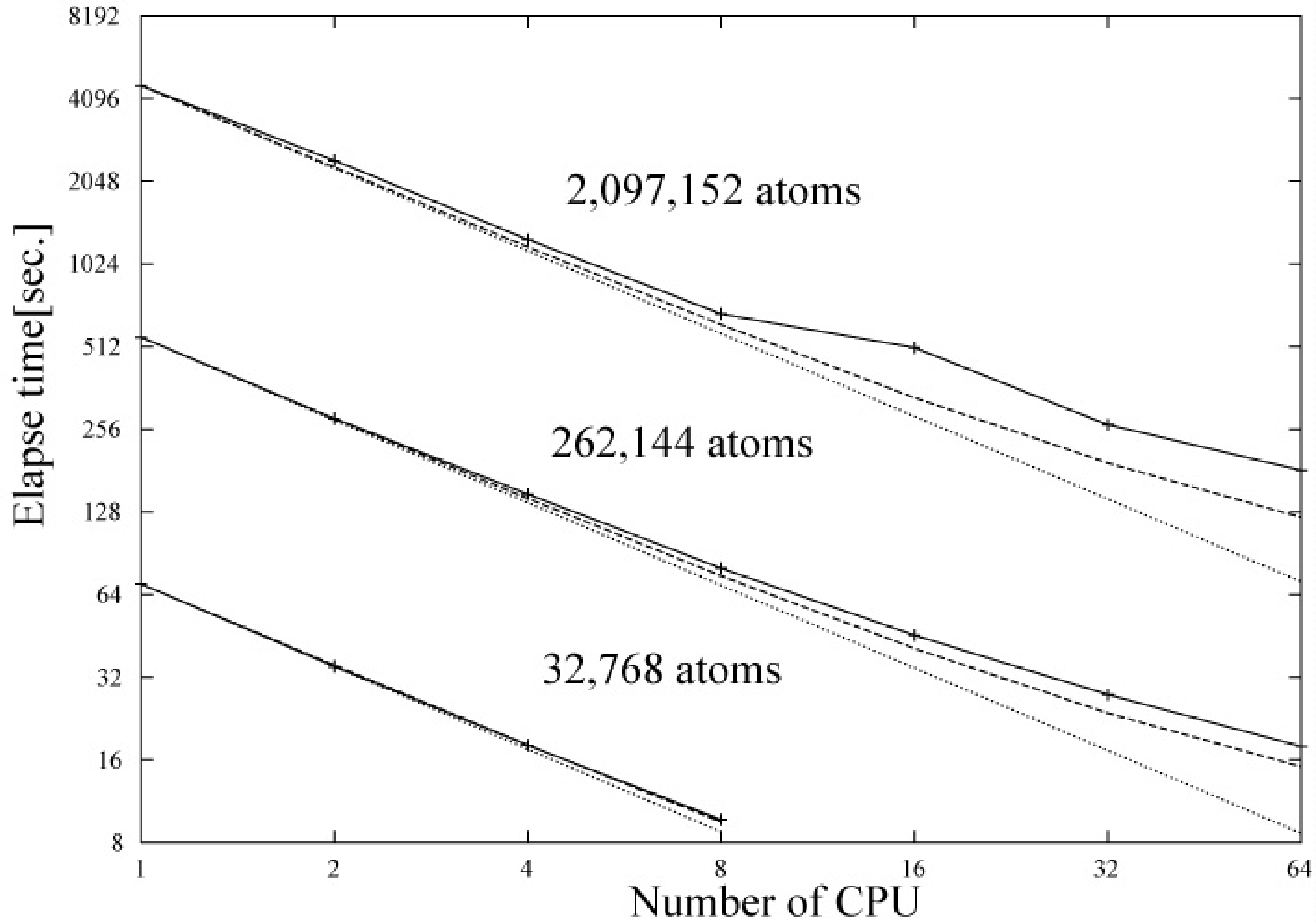


Geshi et al.(2003)

SGI Origin 3800

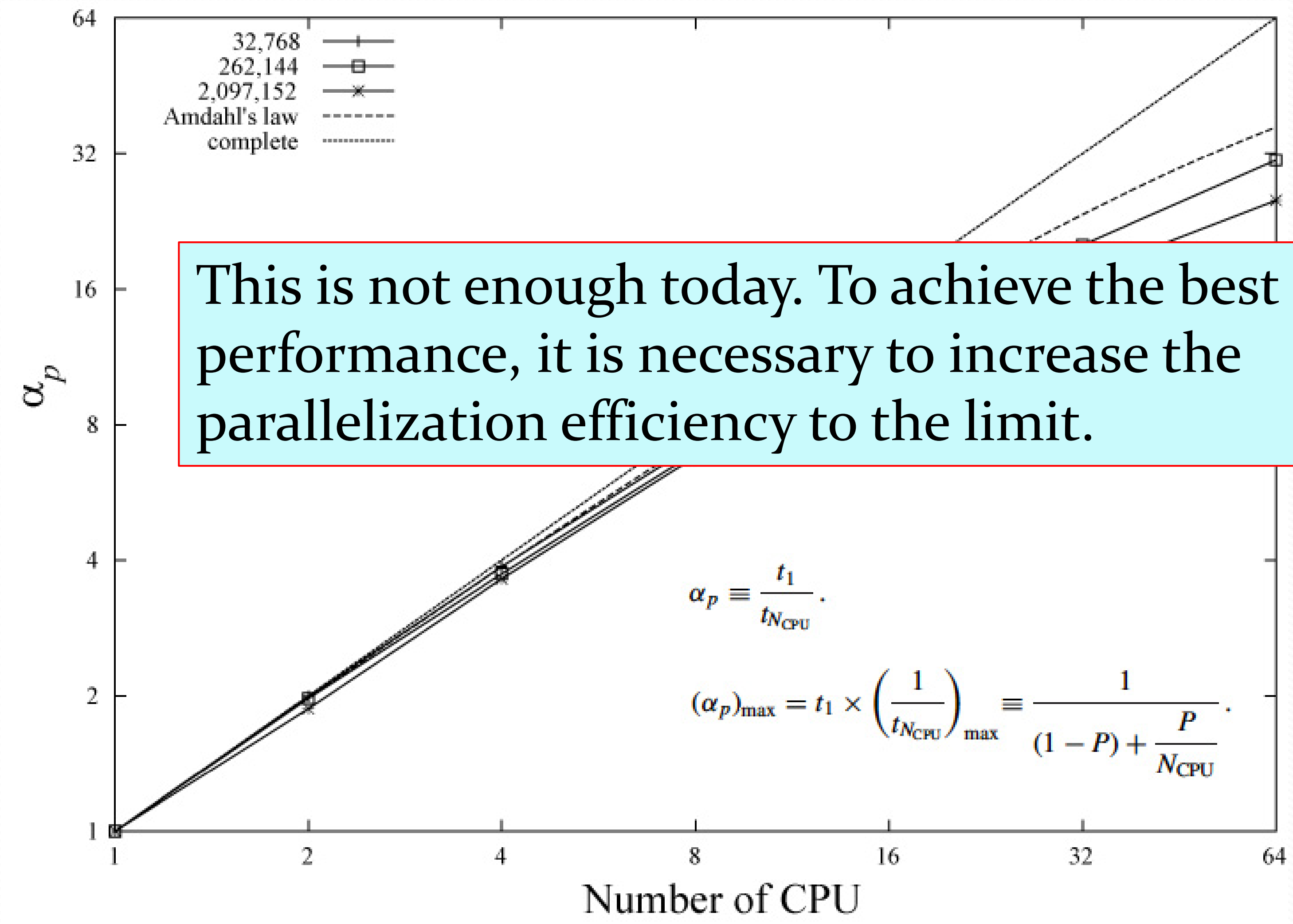
Elapse time as a function of the number of CPU

M. Geshi et al, J. Phys. Soc. Jpn. **72** ,2880 (2003).



Parallelization ratio

M. Geshi et al, J. Phys. Soc. Jpn. **72** ,2880 (2003).



$$\alpha_p \equiv \frac{t_1}{t_{N_{\mathrm{CPU}}}}.$$

$$(\alpha_p)_{\max} = t_1 \times \left(\frac{1}{t_{N_{\mathrm{CPU}}}}\right)_{\max} \equiv \frac{1}{(1-P)+\dfrac{P}{N_{\mathrm{CPU}}}}.$$

P=0.988

This is not enough today. To achieve the best performance, it is necessary to increase the parallelization efficiency to the limit.

Today’s supercomputers

Classes of parallel computers

- Multicore computing
  - a processor that includes multiple execution units ("cores") on the same chip.
- Symmetric multiprocessing
  - a computer system with multiple identical processors that **share memory** and connect via a bus.
- Distributed computing
  - a distributed memory computer system in which the processing elements are connected by a network.(**Cluster computing, Massive parallel processing, Grid computing**)
- Specialized parallel computers
  - Within parallel computing, there are specialized parallel devices that remain niche areas of interest. (**GPGPU,Application-specific integrated circuits, Vector processors**)

From http://en.wikipedia.org/wiki/Parallel_computing

The latest top 500 supercomputer list (2019.11)

https://www.top500.org/lists/top500/2019/11/

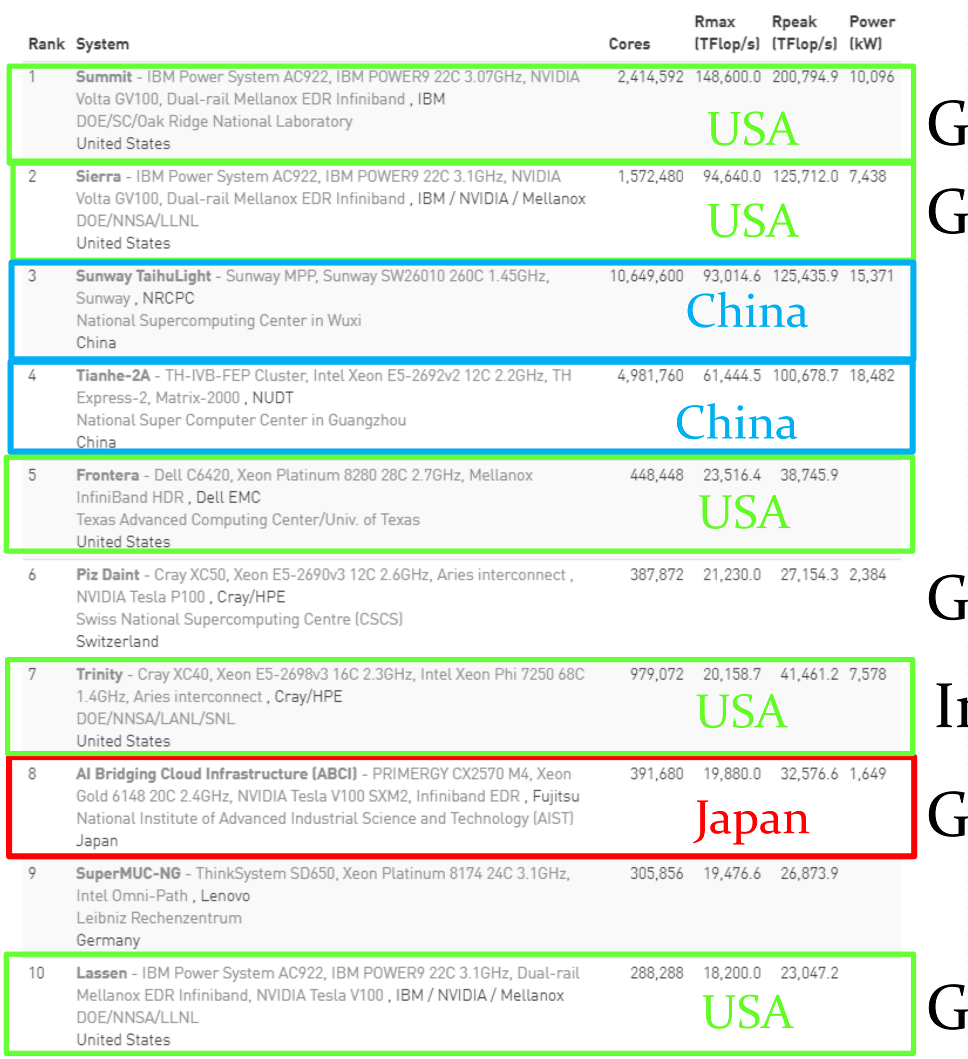
IBM製

● ●

Cray製

● ●

●



Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
2	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
3	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
4	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 , NUDT National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482
5	**Frontera** - Dell C6420, Xeon Platinum 8280 28C 2.7GHz, Mellanox InfiniBand HDR , Dell EMC Texas Advanced Computing Center/Univ. of Texas United States	448,448	23,516.4	38,745.9	
6	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray/HPE Swiss National Supercomputing Centre (CSCS) Switzerland	387,872	21,230.0	27,154.3	2,384
7	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray/HPE DOE/NNSA/LANL/SNL United States	979,072	20,158.7	41,461.2	7,578
8	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR , Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) Japan	391,680	19,880.0	32,576.6	1,649
9	**SuperMUC-NG** - ThinkSystem SD650, Xeon Platinum 8174 24C 3.1GHz, Intel Omni-Path , Lenovo Leibniz Rechenzentrum Germany	305,856	19,476.6	26,873.9	
10	**Lassen** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, Dual-rail Mellanox EDR Infiniband, NVIDIA Tesla V100 , IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	288,288	18,200.0	23,047.2	

GPU

GPU

GPU

Intel XeonPhi

GPU

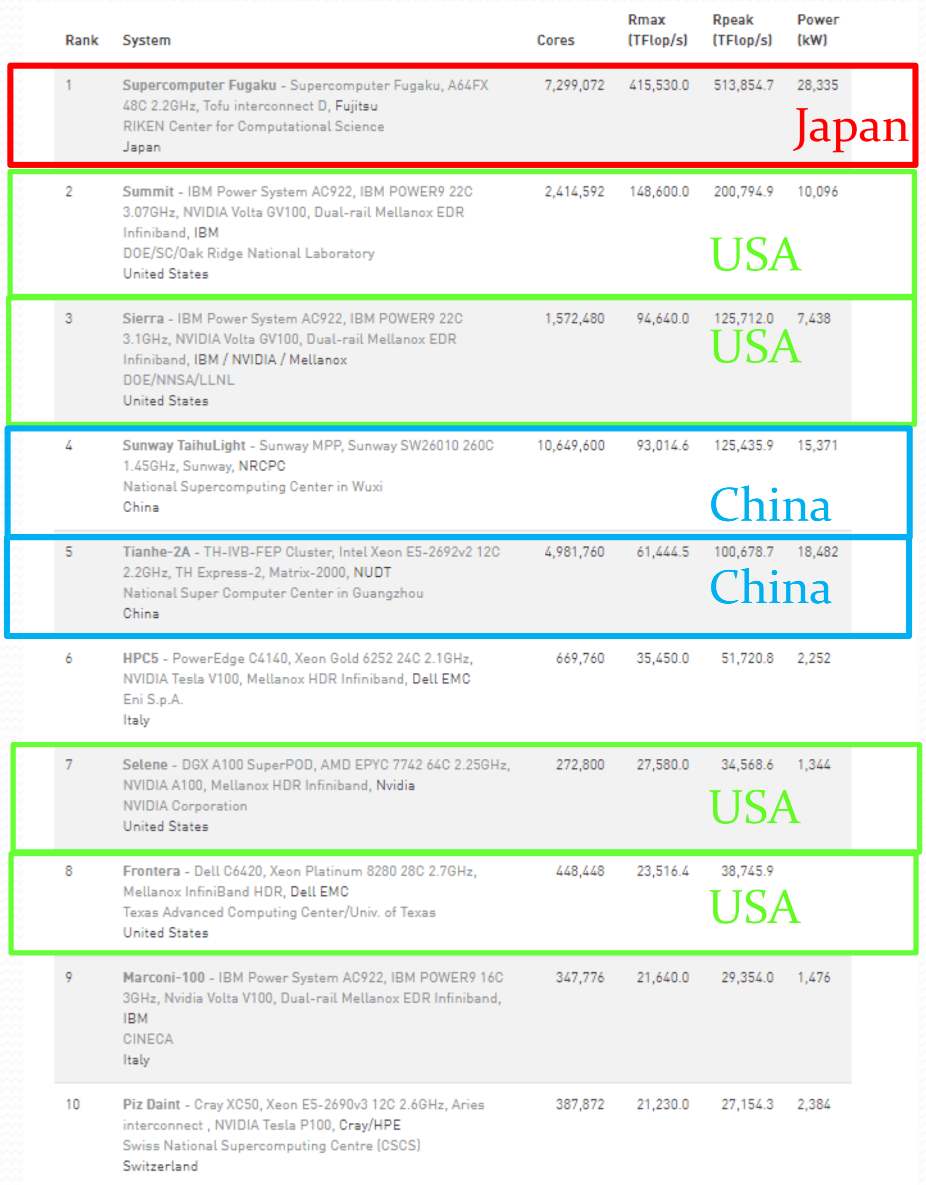
GPU

By the way, Oakforest-PACS is 15, and TSUBAME3.0 is 23. In total, 14 Japanese supercomputers are in the top 100.

Intel XeonPhi
(This architecture was gone.)

The latest top 500 supercomputer list (2020.6)(Latest)

https://www.top500.org/lists/top500/2020/06/



	Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)		
	1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,299,072	415,530.0	513,854.7	28,335	Japan	
●	2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096	USA	GPU
●	3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438	USA	GPU
	4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371	China	
	5	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, NUDT National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482	China	
●	6	**HPC5** - PowerEdge C4140, Xeon Gold 6252 24C 2.1GHz, NVIDIA Tesla V100, Mellanox HDR Infiniband, Dell EMC Eni S.p.A. Italy	669,760	35,450.0	51,720.8	2,252		GPU
	7	**Selene** - DGX A100 SuperPOD, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	272,800	27,580.0	34,568.6	1,344	USA	GPU
●	8	**Frontera** - Dell C6420, Xeon Platinum 8280 28C 2.7GHz, Mellanox InfiniBand HDR, Dell EMC Texas Advanced Computing Center/Univ. of Texas United States	448,448	23,516.4	38,745.9		USA	GPU
●	9	**Marconi-100** - IBM Power System AC922, IBM POWER9 16C 3GHz, Nvidia Volta V100, Dual-rail Mellanox EDR Infiniband, IBM CINECA Italy	347,776	21,640.0	29,354.0	1,476		GPU
	10	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100, Cray/HPE Swiss National Supercomputing Centre (CSCS) Switzerland	387,872	21,230.0	27,154.3	2,384		GPU

IBM製

Dell製

By the way, AI Bridging Cloud Infrastructure (AIBC)is 12, Oakforest-PACS is 18, and TSUBAME3.0 is 27. In total, 14 Japanese supercomputers are in the top 100.

LINPACK

- A software library for performing numerical linear algebra on digital computers.
- It is used for the performance assessment of supercomputers. In practice, High-Performance Linpack(HPL) is used.
- It makes use of the BLAS libraries for performing basic vector and matrix operations.
- The benchmark used in the LINPACK Benchmark is to solve a dense system of linear equations.

This benchmark shows nothing more than one side of performance of supercomputers.

HPC Challenge

The HPC Challenge benchmark consists of basically 7 tests:

- HPL - the Linpack TPP benchmark which measures the floating point rate of execution for solving a linear system of equations.
- DGEMM - measures the floating point rate of execution of double precision real matrix-matrix multiplication.
- STREAM - a simple synthetic benchmark program that measures sustainable memory bandwidth (in GB/s) and the corresponding computation rate for simple vector kernel.
- PTRANS (parallel matrix transpose) - exercises the communications where pairs of processors communicate with each other simultaneously. It is a useful test of the total communications capacity of the network.
- RandomAccess - measures the rate of integer random updates of memory (GUPS)
- FFT - measures the floating point rate of execution of double precision complex one-dimensional Discrete Fourier Transform (DFT).
- Communication bandwidth and latency - a set of tests to measure latency and bandwidth of a number of simultaneous communication patterns; based on b_eff (effective bandwidth benchmark).

http://www.hpcchallenge.org/

HPCG Benchmark(From 2014)

The High Performance Conjugate Gradients (HPCG) Benchmark project is an effort to create a new metric for ranking HPC systems. HPCG is intended as a complement to the High Performance LINPACK (HPL) benchmark, currently used to rank the TOP500 computing systems. The computational and data access patterns of HPL are still representative of some important scalable applications, but not all. HPCG is designed to exercise computational and data access patterns that more closely match a different and broad set of important applications, and to give incentive to computer system designers to invest in capabilities that will have impact on the collective performance of these applications.

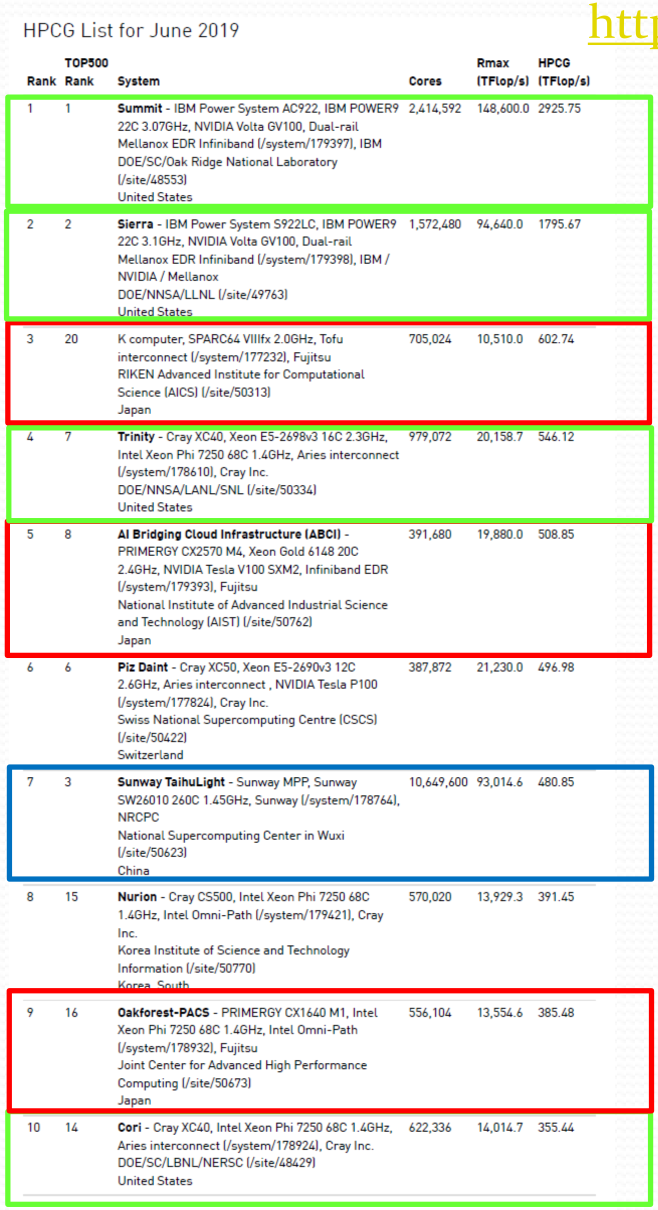
HPCG is a complete, stand-alone code that measures the performance of basic operations in a unified code:

- Sparse matrix-vector multiplication.
- Vector updates.
- Global dot products.
- Local symmetric Gauss-Seidel smoother.
- Sparse triangular solve (as part of the Gauss-Seidel smoother).
- Driven by multigrid preconditioned conjugate gradient algorithm that exercises the key kernels on a nested set of coarse grids.
- Reference implementation is written in C++ with MPI and OpenMP support.

https://www.top500.org/lists/hpcg/2017/11/

HPCG ranking(2019.6)

https://www.top500.org/lists/hpcg/2019/06/



HPCG List for June 2019

Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	HPCG (TFlop/s)
1	1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband (/system/179397), IBM DOE/SC/Oak Ridge National Laboratory (/site/48553) United States	2,414,592	148,600.0	2925.75
2	2	**Sierra** - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband (/system/179398), IBM / NVIDIA / Mellanox DOE/NNSA/LLNL (/site/49763) United States	1,572,480	94,640.0	1795.67
3	20	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect (/system/177232), Fujitsu RIKEN Advanced Institute for Computational Science (AICS) (/site/50313) Japan	705,024	10,510.0	602.74
4	7	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect (/system/178610), Cray Inc. DOE/NNSA/LANL/SNL (/site/50334) United States	979,072	20,158.7	546.12
5	8	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR (/system/179393), Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) (/site/50762) Japan	391,680	19,880.0	508.85
6	6	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 (/system/177824), Cray Inc. Swiss National Supercomputing Centre (CSCS) (/site/50422) Switzerland	387,872	21,230.0	496.98
7	3	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway (/system/178764), NRCPC National Supercomputing Center in Wuxi (/site/50623) China	10,649,600	93,014.6	480.85
8	15	**Nurion** - Cray CS500, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path (/system/179421), Cray Inc. Korea Institute of Science and Technology Information (/site/50770) Korea, South	570,020	13,929.3	391.45
9	16	**Oakforest-PACS** - PRIMERGY CX1640 M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path (/system/178932), Fujitsu Joint Center for Advanced High Performance Computing (/site/50673) Japan	556,104	13,554.6	385.48
10	14	**Cori** - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect (/system/178924), Cray Inc. DOE/SC/LBNL/NERSC (/site/48429) United States	622,336	14,014.7	355.44

USA GPU

USA GPU

Japan

USA Intel XeonPhi

Japan GPU

GPU

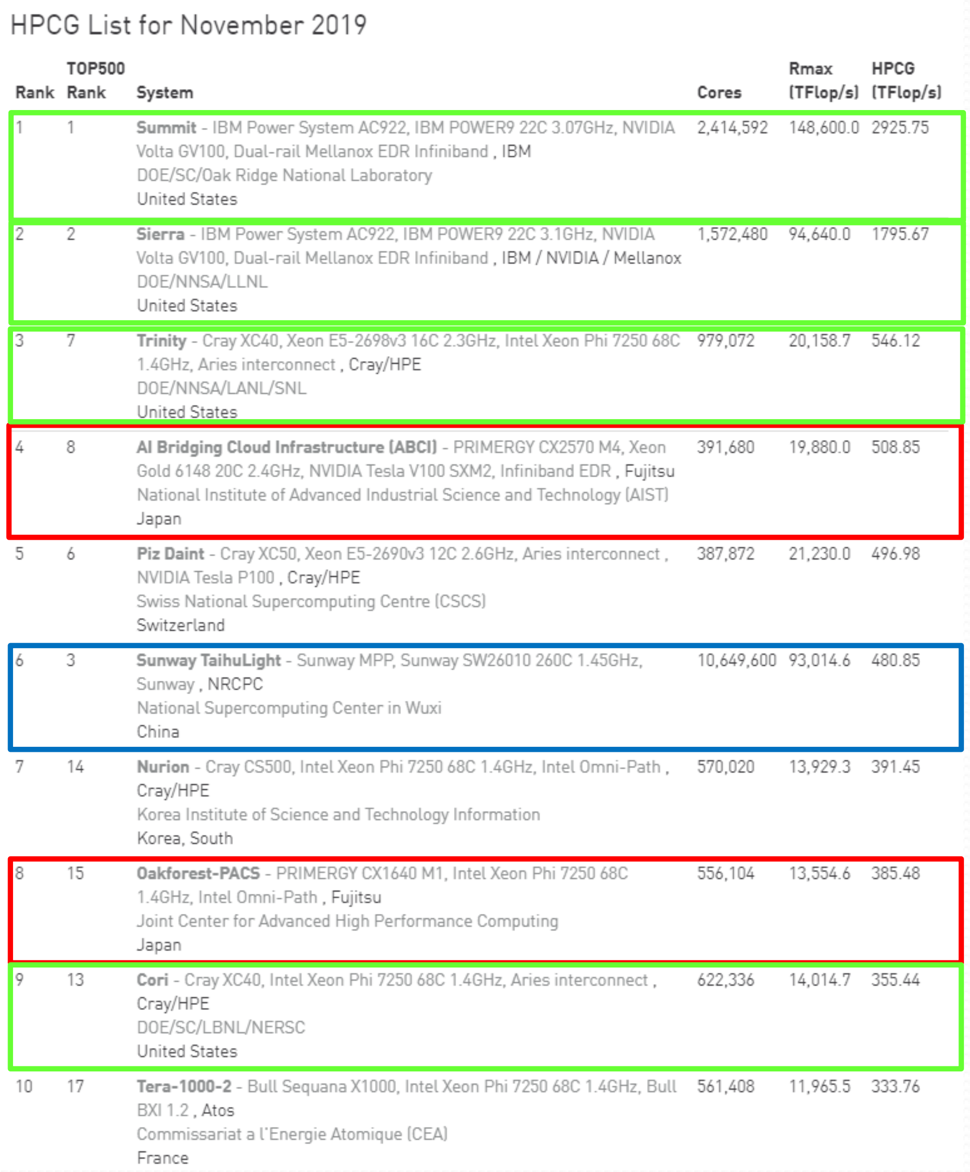
China GPU

Intel XeonPhi

Japan Intel XeonPhi

USA Intel XeonPhi

HPCG ranking(2019.11)



HPCG List for November 2019

Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	HPCG (TFlop/s)
1	1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	2925.75
2	2	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	1795.67
3	7	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray/HPE DOE/NNSA/LANL/SNL United States	979,072	20,158.7	546.12
4	8	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR , Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) Japan	391,680	19,880.0	508.85
5	6	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray/HPE Swiss National Supercomputing Centre (CSCS) Switzerland	387,872	21,230.0	496.98
6	3	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	480.85
7	14	**Nurion** - Cray CS500, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path , Cray/HPE Korea Institute of Science and Technology Information Korea, South	570,020	13,929.3	391.45
8	15	**Oakforest-PACS** - PRIMERGY CX1640 M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path , Fujitsu Joint Center for Advanced High Performance Computing Japan	556,104	13,554.6	385.48
9	13	**Cori** - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray/HPE DOE/SC/LBNL/NERSC United States	622,336	14,014.7	355.44
10	17	**Tera-1000-2** - Bull Sequana X1000, Intel Xeon Phi 7250 68C 1.4GHz, Bull BXI 1.2 , Atos Commissariat a l'Energie Atomique (CEA) France	561,408	11,965.5	333.76

USA GPU

USA GPU

USA Intel XeonPhi

Japan GPU

GPU

China

Intel XeonPhi

Japan Intel XeonPhi

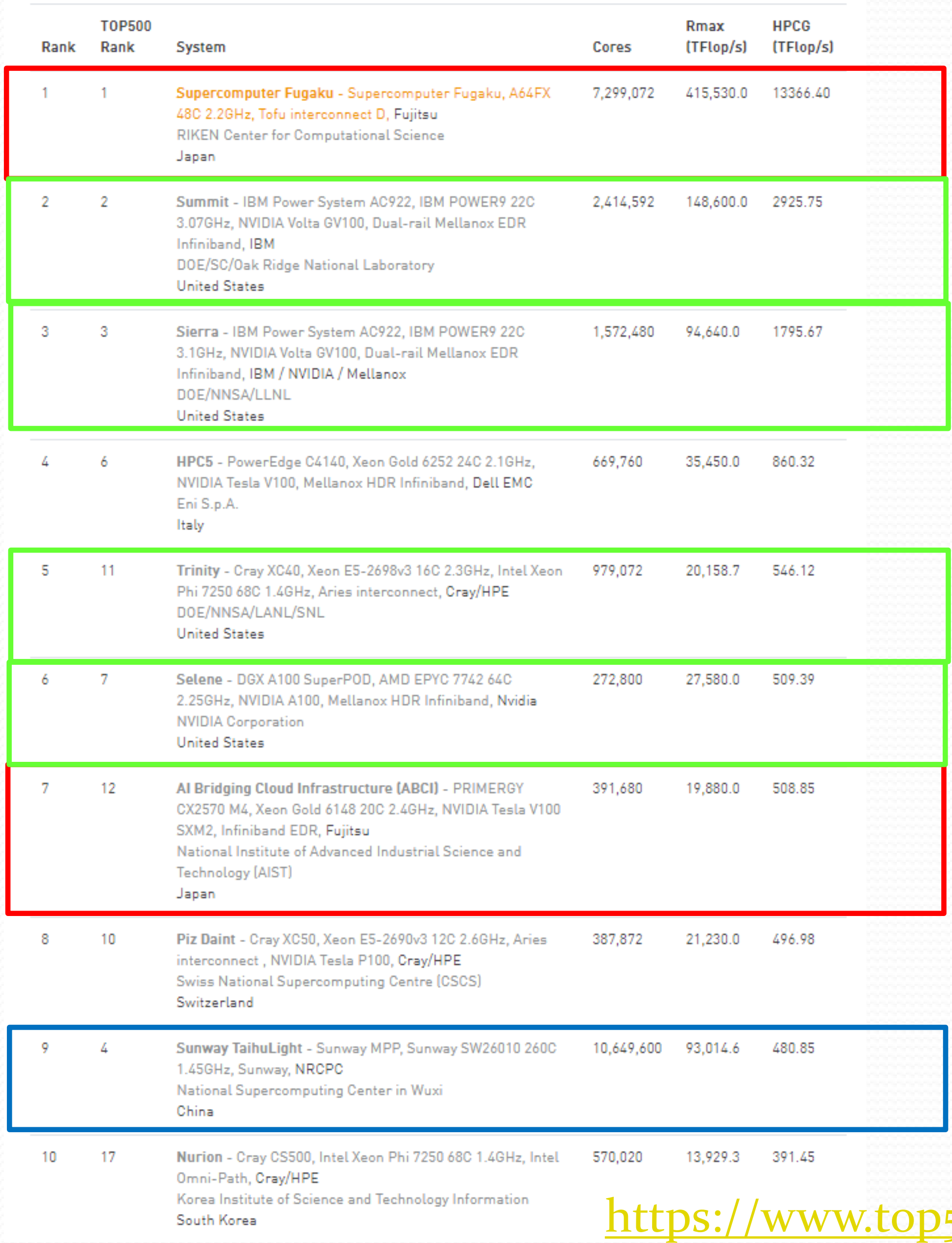
Intel XeonPhi

USA

Intel XeonPhi

https://www.top500.org/lists/hpcg/2019/11/

HPCG ranking(2020.6)(Latest)



Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	HPCG (TFlop/s)
1	1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,299,072	415,530.0	13366.40
2	2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	2925.75
3	3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	1795.67
4	6	**HPC5** - PowerEdge C4140, Xeon Gold 6252 24C 2.1GHz, NVIDIA Tesla V100, Mellanox HDR Infiniband, Dell EMC Eni S.p.A. Italy	669,760	35,450.0	860.32
5	11	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect, Cray/HPE DOE/NNSA/LANL/SNL United States	979,072	20,158.7	546.12
6	7	**Selene** - DGX A100 SuperPOD, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	272,800	27,580.0	509.39
7	12	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR, Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) Japan	391,680	19,880.0	508.85
8	10	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100, Cray/HPE Swiss National Supercomputing Centre (CSCS) Switzerland	387,872	21,230.0	496.98
9	4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	480.85
10	17	**Nurion** - Cray CS500, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path, Cray/HPE Korea Institute of Science and Technology Information South Korea	570,020	13,929.3	391.45

Japan

USA

GPU

USA

GPU

USA

GPU

Intel XeonPhi

USA

USA

GPU

Japan

GPU

GPU

China

Intel XeonPhi

https://www.top500.org/lists/hpcg/06/

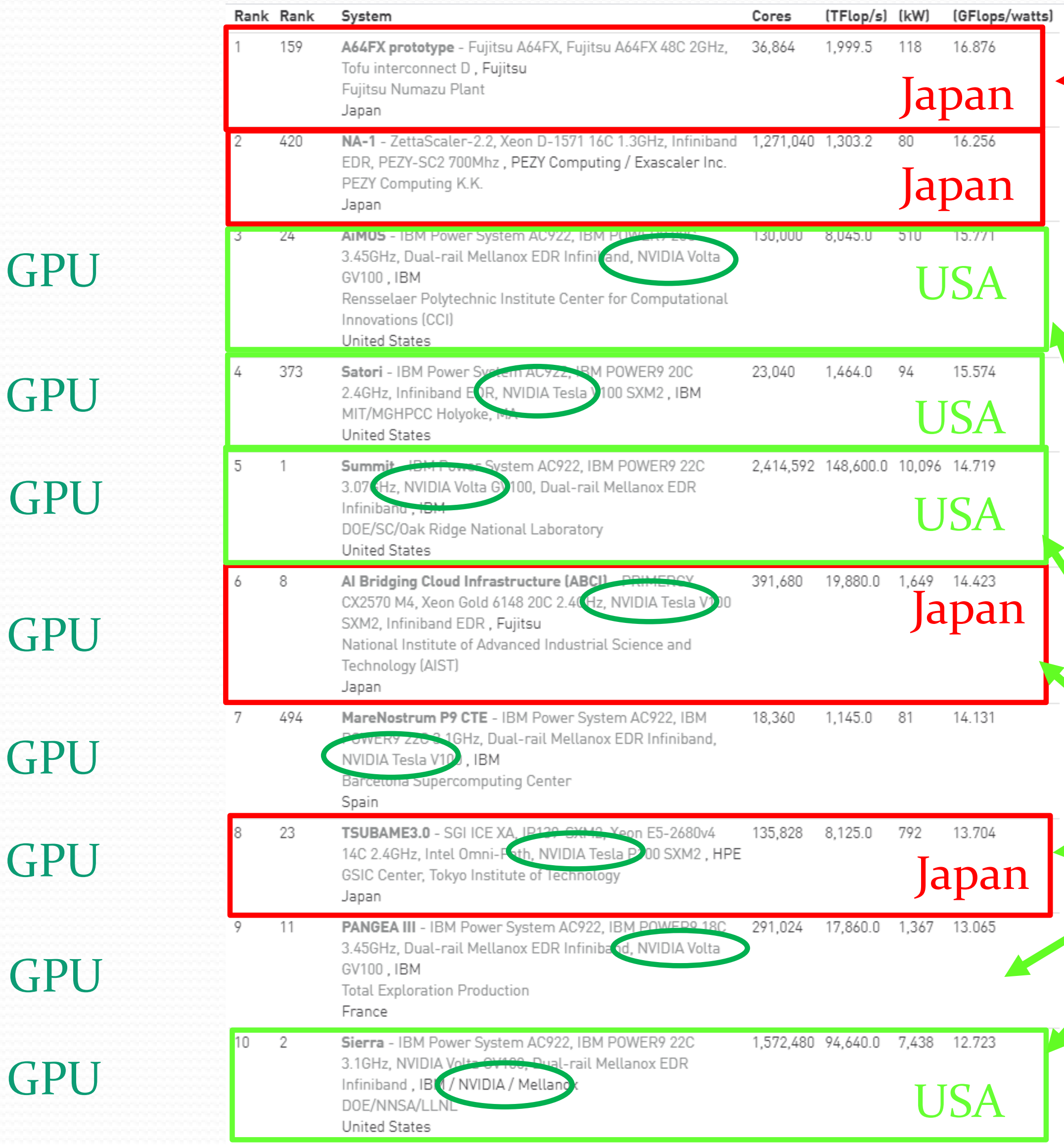
Green500(省エネスパコンリスト)

- The purpose of the Green500 is to provide a ranking of the most energy-efficient supercomputers in the world. For decades, the notion of "performance" has been synonymous with "speed" (as measured in FLOPS). This particular focus has led to the emergence of supercomputers that consume egregious amounts of electrical power and produce so much heat that extravagant cooling facilities must be constructed to ensure proper operation. In addition, the emphasis on speed as the ultimate metric has caused other metrics such as reliability, availability, and usability to be largely ignored. As a result, there has been an extraordinary increase in the total cost of ownership (TCO) of a supercomputer.

https://www.top500.org/lists/green500/2013/06/

Green 500(2019.11)

https://www.top500.org/lists/green500/2019/11/



Rank	Rank	System	Cores	(TFlop/s)	(kW)	(GFlops/watts)
1	159	**A64FX prototype** - Fujitsu A64FX, Fujitsu A64FX 48C 2GHz, Tofu interconnect D , Fujitsu Fujitsu Numazu Plant Japan	36,864	1,999.5	118	16.876
2	420	**NA-1** - ZettaScaler-2.2, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz , PEZY Computing / Exascaler Inc. PEZY Computing K.K. Japan	1,271,040	1,303.2	80	16.256
3	24	**AiMOS** - IBM Power System AC922, IBM POWER9 20C 3.45GHz, Dual-rail Mellanox EDR Infiniband, NVIDIA Volta GV100 , IBM Rensselaer Polytechnic Institute Center for Computational Innovations (CCI) United States	130,000	8,045.0	510	15.771
4	373	**Satori** - IBM Power System AC922, IBM POWER9 20C 2.4GHz, Infiniband EDR, NVIDIA Tesla V100 SXM2 , IBM MIT/MGHPCC Holyoke, MA United States	23,040	1,464.0	94	15.574
5	1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	10,096	14.719
6	8	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR , Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) Japan	391,680	19,880.0	1,649	14.423
7	494	**MareNostrum P9 CTE** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, Dual-rail Mellanox EDR Infiniband, NVIDIA Tesla V100 , IBM Barcelona Supercomputing Center Spain	18,360	1,145.0	81	14.131
8	23	**TSUBAME3.0** - SGI ICE XA, IP139-SXM2, Xeon E5-2680v4 14C 2.4GHz, Intel Omni-Path, NVIDIA Tesla P100 SXM2 , HPE GSIC Center, Tokyo Institute of Technology Japan	135,828	8,125.0	792	13.704
9	11	**PANGEA III** - IBM Power System AC922, IBM POWER9 18C 3.45GHz, Dual-rail Mellanox EDR Infiniband, NVIDIA Volta GV100 , IBM Total Exploration Production France	291,024	17,860.0	1,367	13.065
10	2	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	7,438	12.723

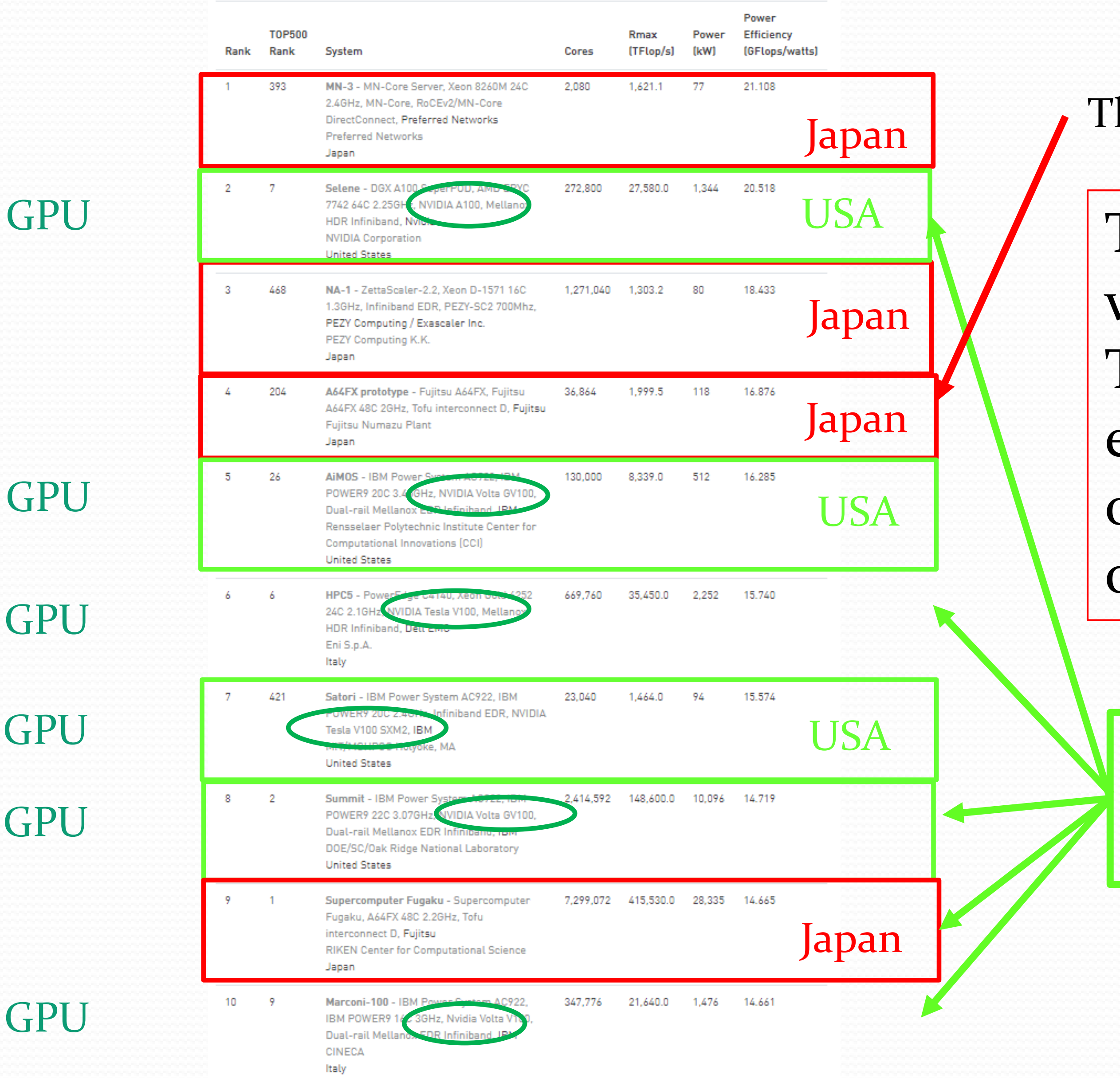
The prototype of Fugaku.

This list fluctuates violently every time. That is why emphasis is placed on the development of this technology.

These machines balance energy saving and computing performance.

Green 500(2020.6)(Latest)

https://www.top500.org/lists/green500/2020/06/



Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	Power (kW)	Power Efficiency (GFlops/watts)
1	393	**MN-3** - MN-Core Server, Xeon 8260M 24C 2.4GHz, MN-Core, RoCEv2/MN-Core DirectConnect, Preferred Networks Preferred Networks Japan	2,080	1,621.1	77	21.108
2	7	**Selene** - DGX A100 SuperPOD, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	272,800	27,580.0	1,344	20.518
3	468	**NA-1** - ZettaScaler-2.2, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz, PEZY Computing / Exascaler Inc. PEZY Computing K.K. Japan	1,271,040	1,303.2	80	18.433
4	204	**A64FX prototype** - Fujitsu A64FX, Fujitsu A64FX 48C 2GHz, Tofu interconnect D, Fujitsu Fujitsu Numazu Plant Japan	36,864	1,999.5	118	16.876
5	26	**AiMOS** - IBM Power System AC922, IBM POWER9 20C 3.45GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM Rensselaer Polytechnic Institute Center for Computational Innovations (CCI) United States	130,000	8,339.0	512	16.285
6	6	**HPC5** - PowerEdge C4140, Xeon Gold 6252 24C 2.1GHz, NVIDIA Tesla V100, Mellanox HDR Infiniband, Dell EMC Eni S.p.A. Italy	669,760	35,450.0	2,252	15.740
7	421	**Satori** - IBM Power System AC922, IBM POWER9 20C 2.4GHz, Infiniband EDR, NVIDIA Tesla V100 SXM2, IBM MIT/MGHPCC Holyoke, MA United States	23,040	1,464.0	94	15.574
8	2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	10,096	14.719
9	1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,299,072	415,530.0	28,335	14.665
10	9	**Marconi-100** - IBM Power System AC922, IBM POWER9 16C 3GHz, Nvidia Volta V100, Dual-rail Mellanox EDR Infiniband, IBM CINECA Italy	347,776	21,640.0	1,476	14.661

The prototype of Fugaku.

This list fluctuates violently every time. That is why emphasis is placed on the development of this technology.

These machines balance energy saving and computing performance.

K computer was working on 24h/365days

- K computer was active for public use on 24hours/365 days for general users.
  - Different from K-computer, almost all the top class machines of the top500 ranking are for closed users and are used for limited purposes.
- The several rankings showed that K computer was almighty.
- Users could optimize their code for K computer easier than for the other ones(in the sense that it did not use a special architecture like GPU).
- Fugaku will be operated in the same way as K-computer and the latest ranking shows that Fugaku is almighty.

Future direction of large-scale computing

From the above rankings

- From now on, both performance and energy-saving are important (half of the top 10 machine in the top500 make energy saving and computing performance highly compatible).
- The trend of many-core system with not so high frequency CPU is still going on. →Fugaku has 48 cores.
- Or many supercomputers have GPU and realize energy saving.
- As GPU is prominent in the field of AI and machine learning, this architecture will continue to be adopted in the future.
- However, I do not know whether supercomputers made up of GPU are effective in all fields or not.
- Probably, many supercomputers designed for data analysis and AI will appear after now.

However,…

- Effective performances measured by LINPACK or HPCG benchmarks are not necessarily accordance with the performance of our software codes. Usually, we spend so much effort to get better performance on supercomputers than typical PC clusters.
  →Fugaku, will be constructed for getting better performance for scientific application than benchmark programs (Co-design). (However, it may be the national mission to get the first prize of top 500 for taxpayers.→Achieved)
- The effort goes beyond knowledge and techniques of physicists, chemist, biologists,… We need those of computer scientists and numerical mathematicians and need to collaborate them.
- Fugaku will be also a computer for general purpose. It may be inferior to a dedicated machine.(cf. Anton (supercomputer for performing classical MD) is 100~1000 faster than normal supercomputers.)

Future direction1

- The tendency of architecture is multi cores or many cores (including SIMD,GPU, …).
- It is not easy to use all cores effectively.

(As personal opinion, I think that I do not have to worry about using all the cores and it is enough to get the best efficiency to obtain the calculation result.)

- Is it reasonable and proper to devote many researchers' effort to develop parallel efficiency? (very serious problem!!!)→ It should be better than before due to the accumulation of K computer.
- For DFT calculations, it may be difficult to speed-up the software by using GPU without breakthrough.
- We have to perform feasibility studies continuously to follow a leading-edge architecture.

Future direction2

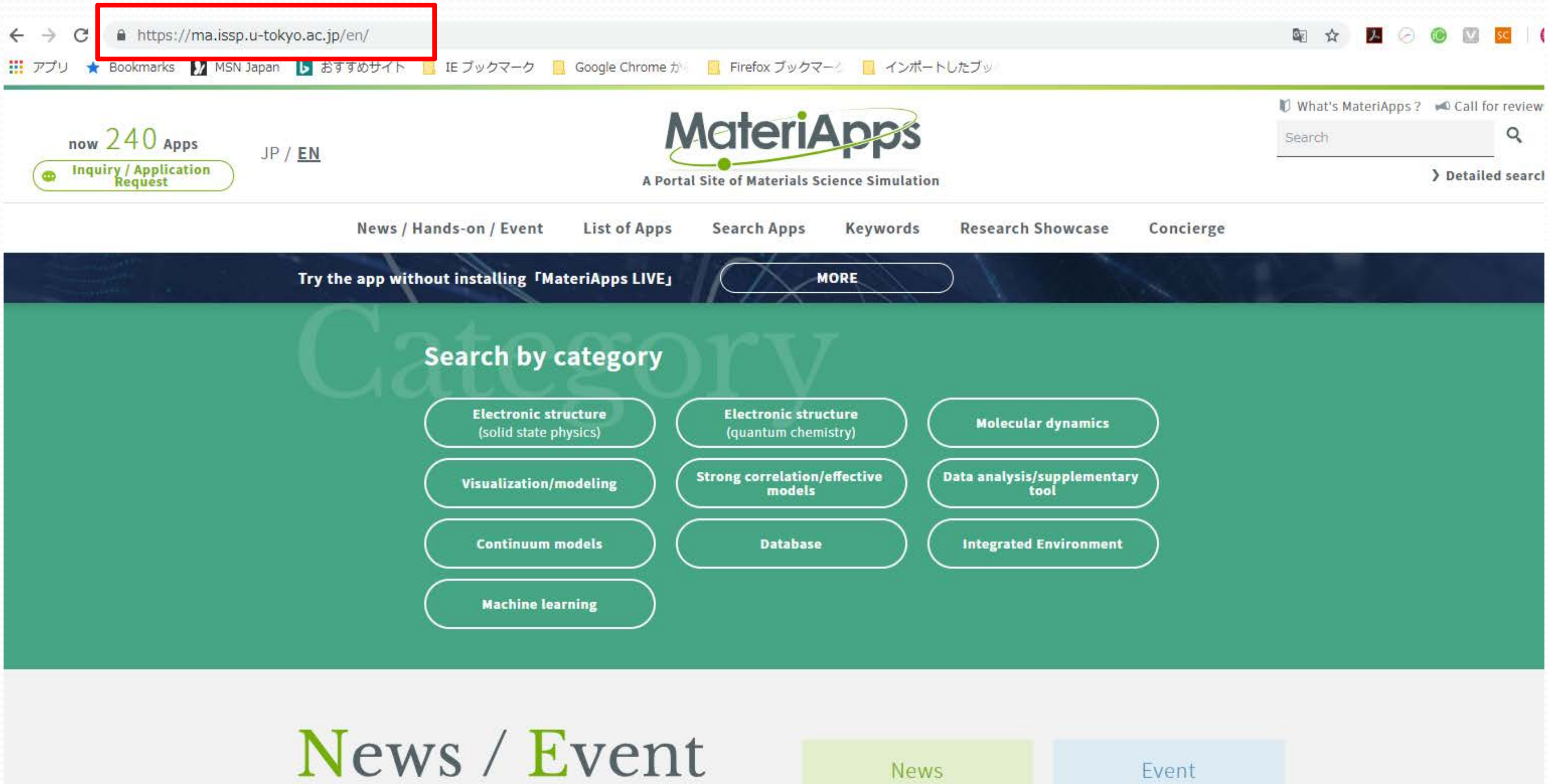
- The United States develops both architectures and programming language frameworks. We should contribute those.
- It is too much hard-pressed for physicists and chemists to cover computer science or numerical analysis.

  →it is needed to establish a system to promote to work together with computational scientists and computer scientists or experts of numerical analysis.
  →This is currently under development.
  (Computational Materials Science Forum is established.
  https://cms-forum.jp/)
- Still now, the guarantee of accuracy of calculation is inadequacy. There is no standard for summation of data from cores (threads) on MPI or OpenMP,… We must treat it carefully, otherwise our calculation may become meaningless.

Future direction3

- Today's amassed skills through K computer can be used during the next 10 years. (In Japan, Fugaku project, and the next project)
- However, the development of supercomputer must be stop in near future.(Prof. Hiraki said it was 2029. The reason is the necessity of huge electric power, failure of Moors' law, etc…)
- We should consider a new idea to get high performance of our own calculations for both software and hardware as soon as possible. We may undergo a paradigm shift before 2029.
- **For the time being, data transfer will continue to be the most costly at all levels.**
- The research on quantum computers is also advancing, and that will be a focus in the future.

MateriApps



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A Portal Site of Materials Science Simulation

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- Visualization/modeling
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- Data analysis/supplementary tool
- Continuum models
- Database
- Integrated Environment
- Machine learning

News / Event

News | Event

This portal site provides the information of applications that are used in materials science. You can find your desired application. “MateriApps LIVE” gives you an environment to perform open-source software codes without any installation process.

Finally,

- We should advance the development of human resources to be able to use supercomputers and/or HPC machines effectively.
- The relation between the ranking of top500 and the software code we use is not necessarily clear. We need to have the knowledge of the architecture of the supercomputers and/or the HPC machines if we'd like to maximize the performance of our software codes.
- We should cultivate people who can develop the software code.
- We should cultivate people who can effectively use scientific software codes to progress the researches. (CMD-WS, distance learning etc…)

Related texts

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Techniques of Speedup and Parallelization for General Purposes

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The Art of High Performance Computing for Computational Science, Vol. 2

Advanced techniques and examples for materials science

Springer

- These books are for developers.
- Integrates techniques for development on massively parallel computers such as supercomputers.
- Lecture videos and texts are available on the following site(Japanese only).

https://www.r-ccs.riken.jp/library/event/tokuronA_2019.html

https://www.r-ccs.riken.jp/library/event/tokuronB_2020.html