RIKEN International Summer School 2021

– Toward Society 5.0 –

Basics of Parallel Programming and Execution

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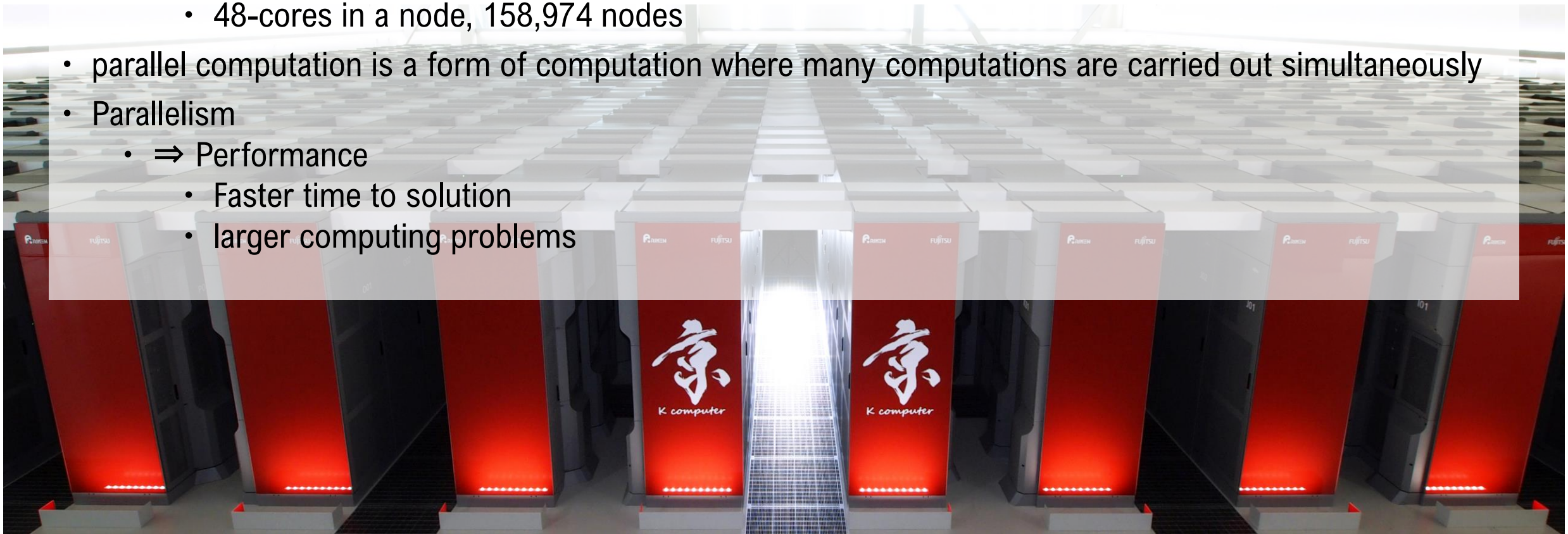
Agenda

1. Parallel computing and background
2. Parallel architectures
3. Some of important concepts to learn parallel programming
4. Setup your environment and login supercomputer Fugaku
5. Hands-on
   - OpenMP
   - MPI

Parallel Computing

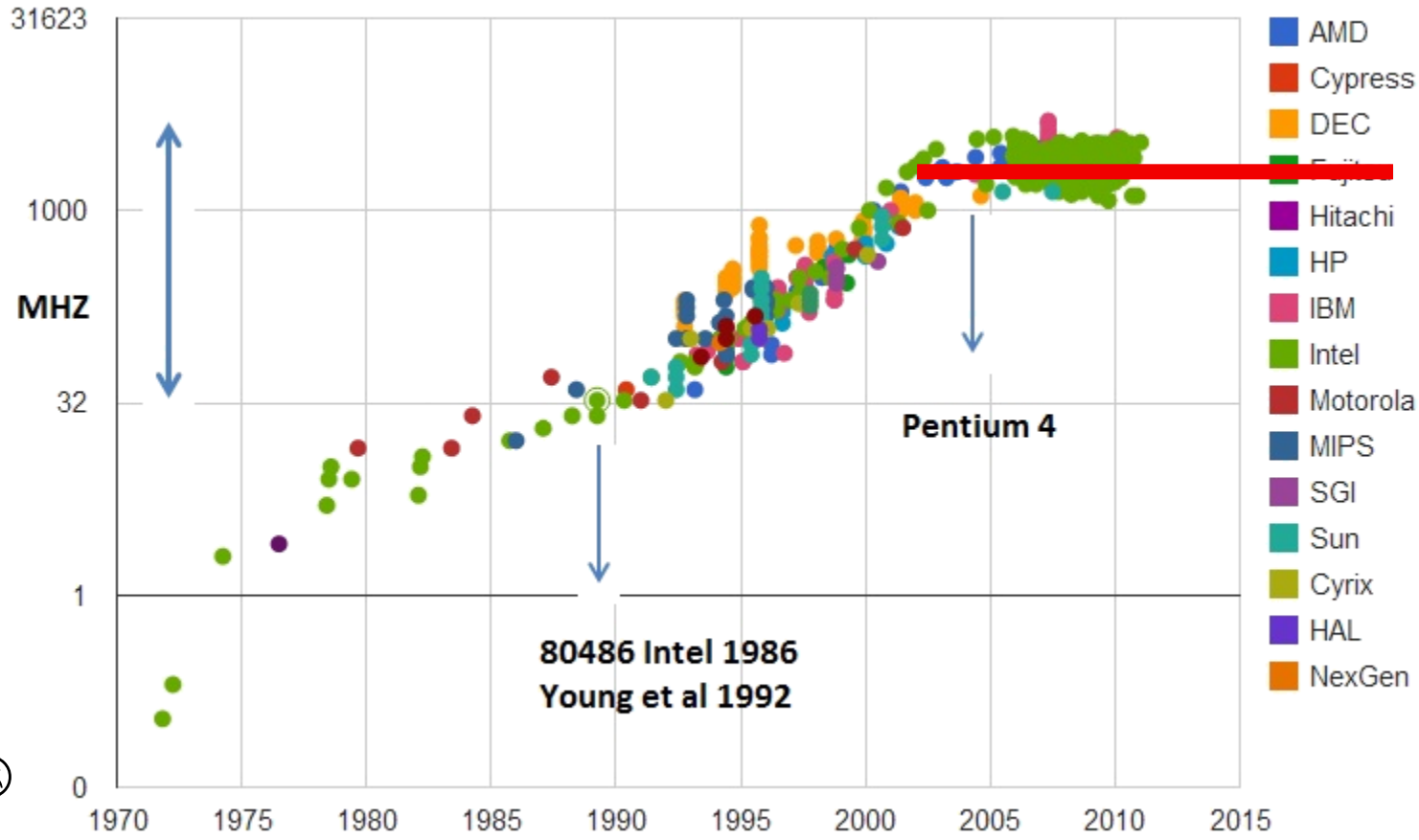
- parallel computer is a computer system that uses multiple processing elements (PEs) simultaneously
  - Apple A13 on IPhone 11 Pro/11 Pro Max
    - 2 Lighting cores, 4 Thunder cores
  - K-computer
    - 8-cores in a node, 88128 nodes
  - Supercomputer Fugaku
    - 48-cores in a node, 158,974 nodes
- parallel computation is a form of computation where many computations are carried out simultaneously
- Parallelism
  - ⇒ Performance
    - Faster time to solution
    - larger computing problems



Motivation of parallel computing

- Motivation: accelerate computation
  - Speedup based on frequency scaling ⇒ Limited due to the physical limits to transistor scaling
  - Energy consumption
    - approximately proportional to the CPU frequency, and to the square of the CPU voltage
  - ⇒ **Parallel computing**
    - consumption is proposal to the concurrency
- increase frequency
  - surely increase performance ☺
- increase concurrency
  - not always increase performance ☹
  - energy efficient

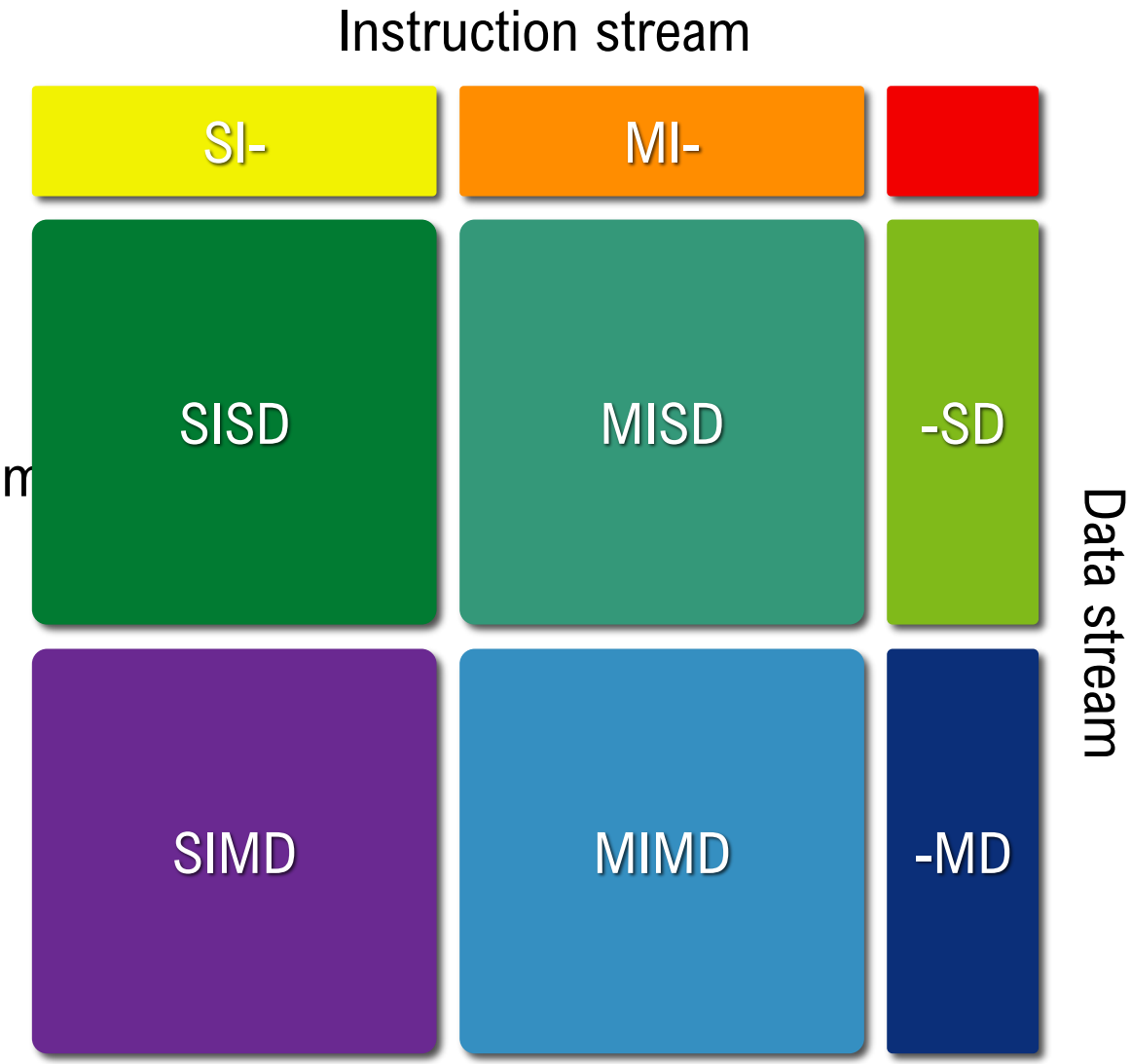
  ⇒ need to understand parallel computing



https://en.wikipedia.org/wiki/File:Clock_CPU_Scaling.jpg

Flynn's Taxonomy

- SISD Single Instruction stream, Single Data stream
  - No parallelism, entirely serial program
- SIMD Single Instruction stream, Multiple Data stream
  - the same operation over different data
- MISD Multiple Instruction stream, Single Data stream
  - (rarely used)
  - Multiple instructions operate on one data stream
- MIMD Multiple Instruction stream, Multiple Data stream
  - Multiple independent processors simultaneously executing different instructions on different data
- Modern HPC systems : hybrids of these categories

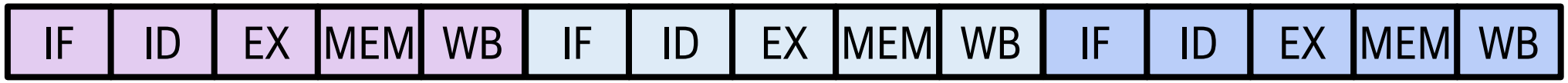


Parallel architectures supporting parallelism

- instruction-level parallelism
- SIMD
- distributed parallel system
- shared memory parallel system

Types of parallelism: instruction-level parallelism

- performing a number of instructions during a single clock cycle
- a program is a stream of instructions



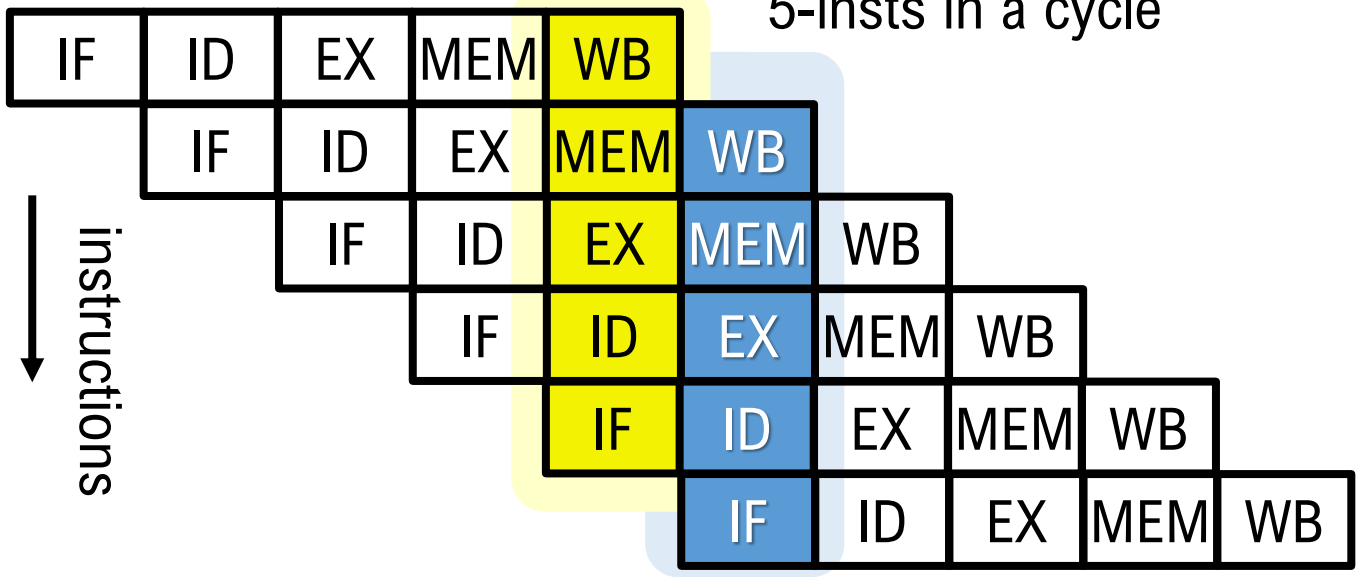
time

parallelization based on "**pipelining**"

time

5-insts in a cycle

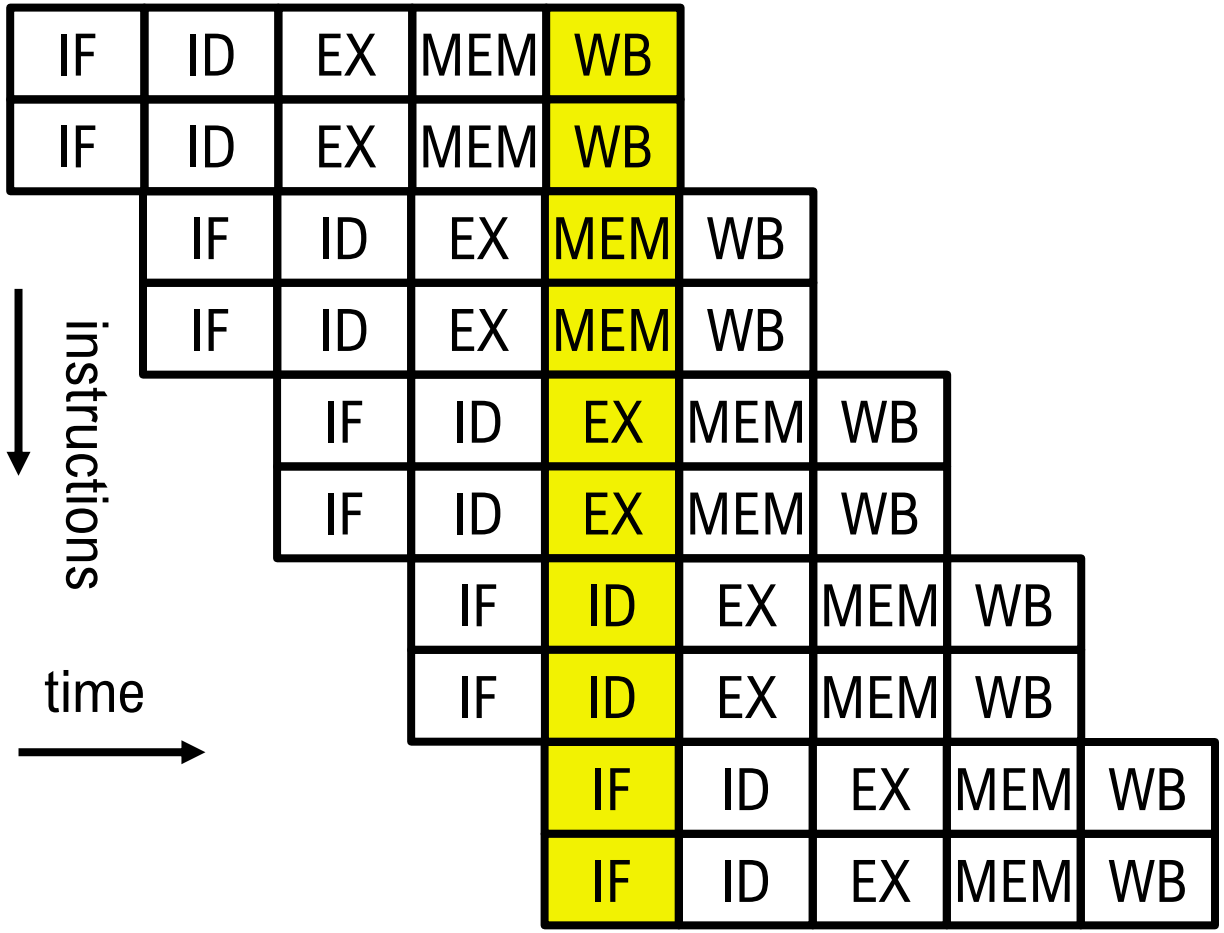
5-insts in a cycle



IF: Instruction Fetch
ID: Instruction Decode
EX: Execute
MEM: Memory access
WB: Register Write Back

Types of parallelism: instruction-level parallelism

- performing a number of instructions during a single clock cycle
- a program is a stream of instructions
- modern processors can issue more than one instruction at a cycle
  - ex: K computer
    - 4 instructions per cycle / core
- out-of-order execution
- instruction level parallelism



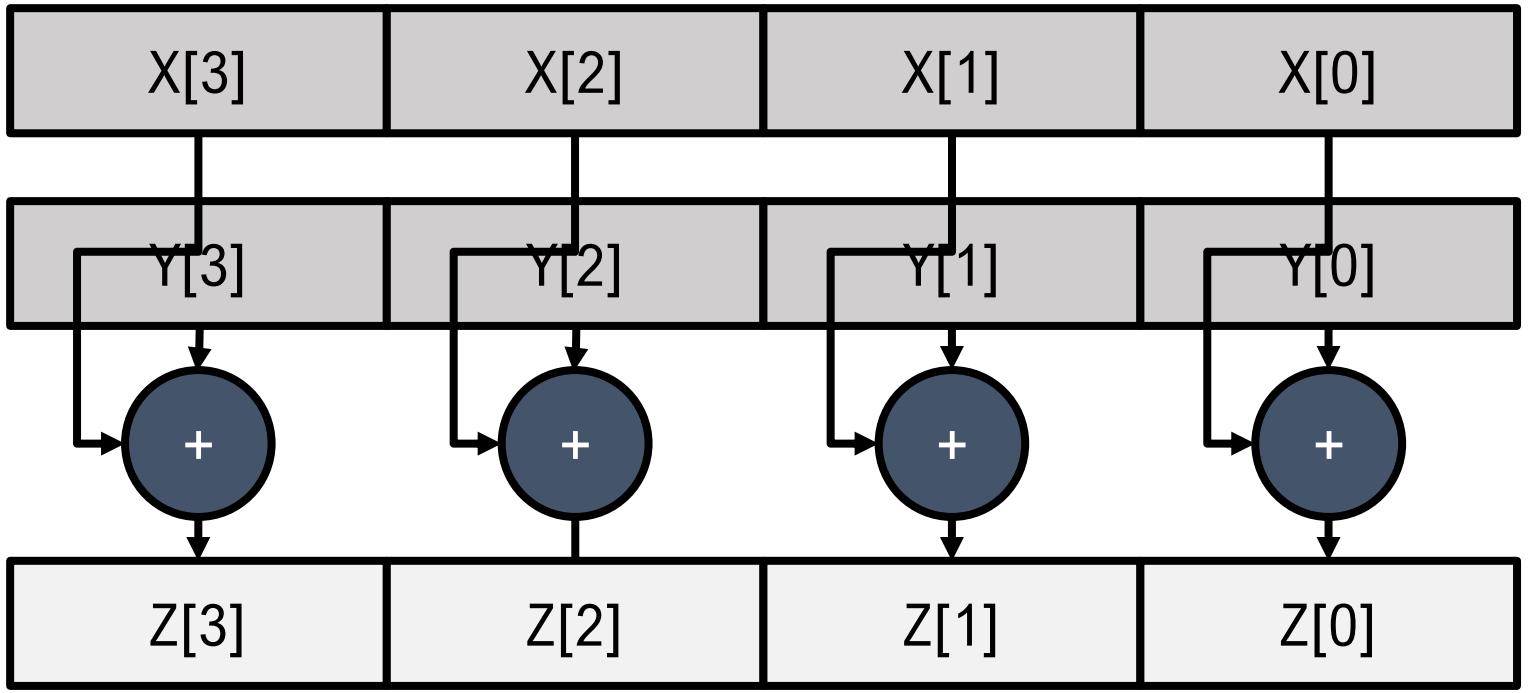
Types of parallelism: SIMD instruction

- an instruction for multiple data (data array) at a single cycle

  for(i=0; i<N; i++)

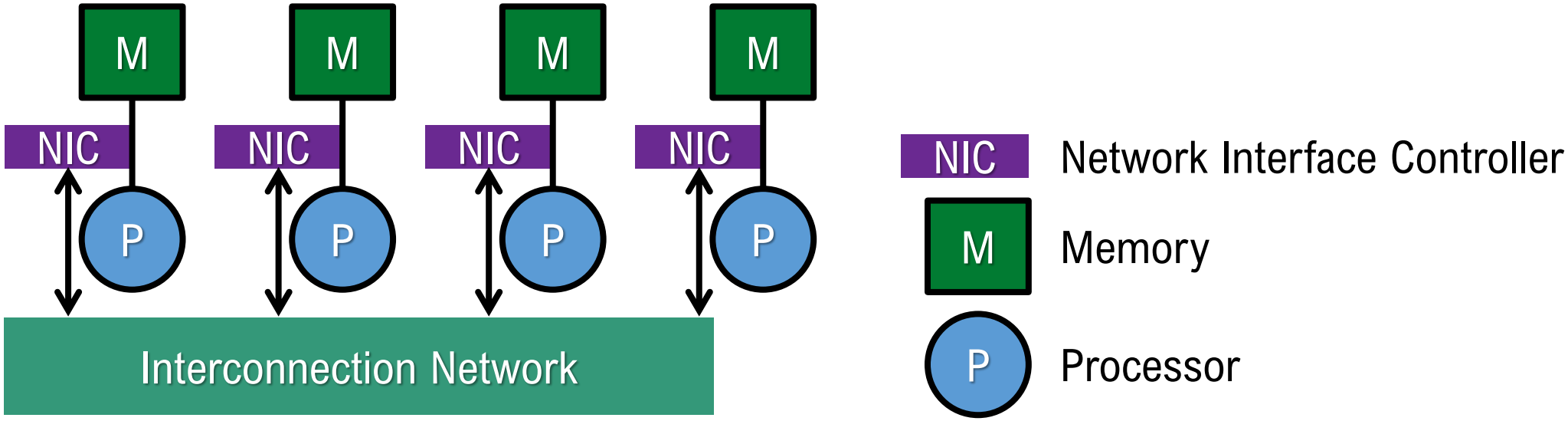
  z[i] = x[i]+y[i]

  - SPARC64 VIIIfx processor (K computer) : 128-bit SIMD (2 double precision can be processed in parallel)
  - SPARC64 XIfx processor (FX100 series) : 256-bit SIMD
  - Intel-AVX512 series: 512-bit SIMD



Distributed memory system

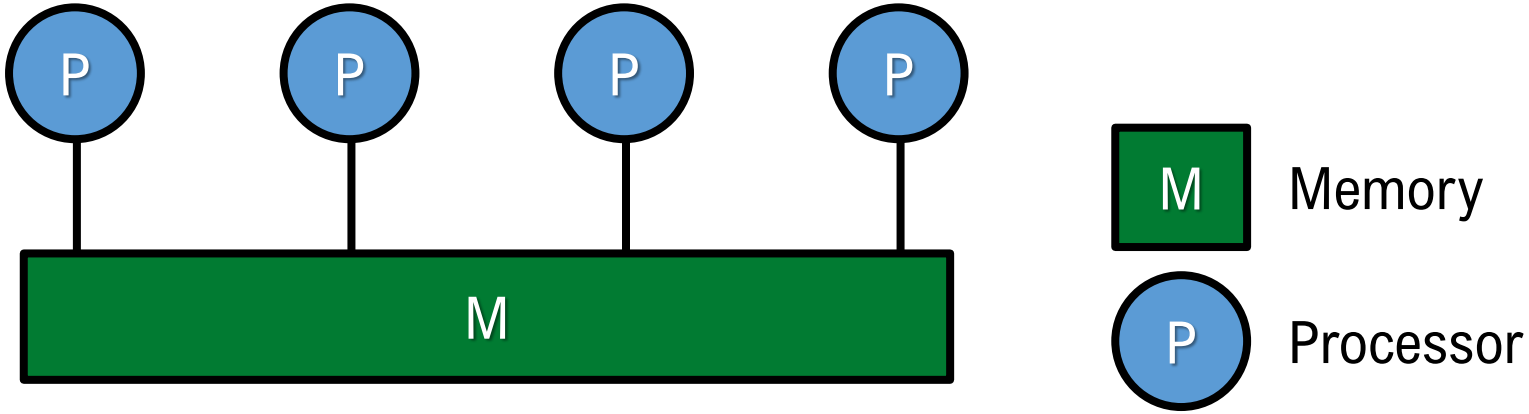
- each processor has its own local address space
- memory is logically or **physically** distributed
- systems, where compute nodes (w/ CPU and memory) are connected via network
- each program on each compute node exchanges data (messages) through network
- expandable
  - Massively Parallel Processor
  - Cluster



Shared memory system

- all processors can access a single address space
- each program (thread) on each compute node reads/writes a memory to exchange data

- Modern CPUs include multi-processor cores and a shared memory



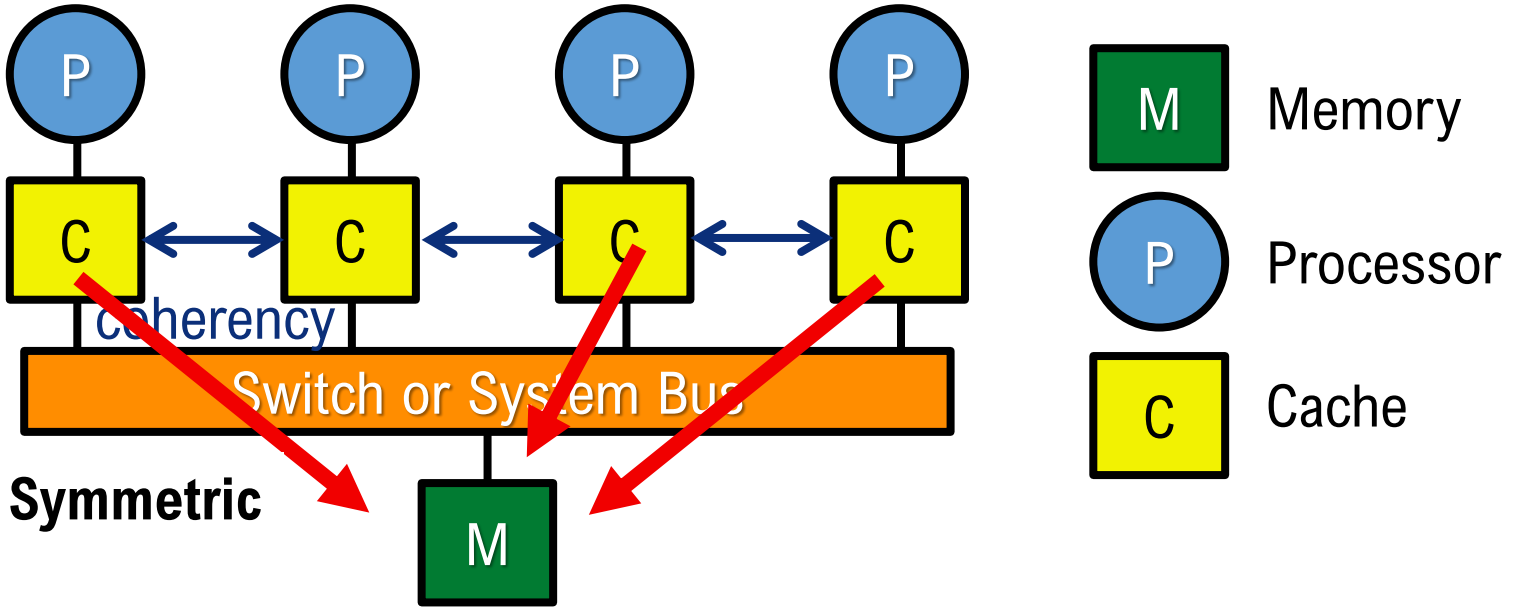
Shared memory system: SMP Symmetric Multi-Processor

- multi-processors are connected to a single, shared main memory
  - multi processors access a (set of) shared memory module(s) via network switch or bus
- all processors are treated equally
- traditional: without cache
- modern: with coherent caches, which keep the data in the caches consistent
- limits on the scalability of SMP, cache coherence and shared objects
- Performance degradation when traffic is concentrated

Fujitsu HPC2500 (2002)

Hitachi SR16000 (2011)

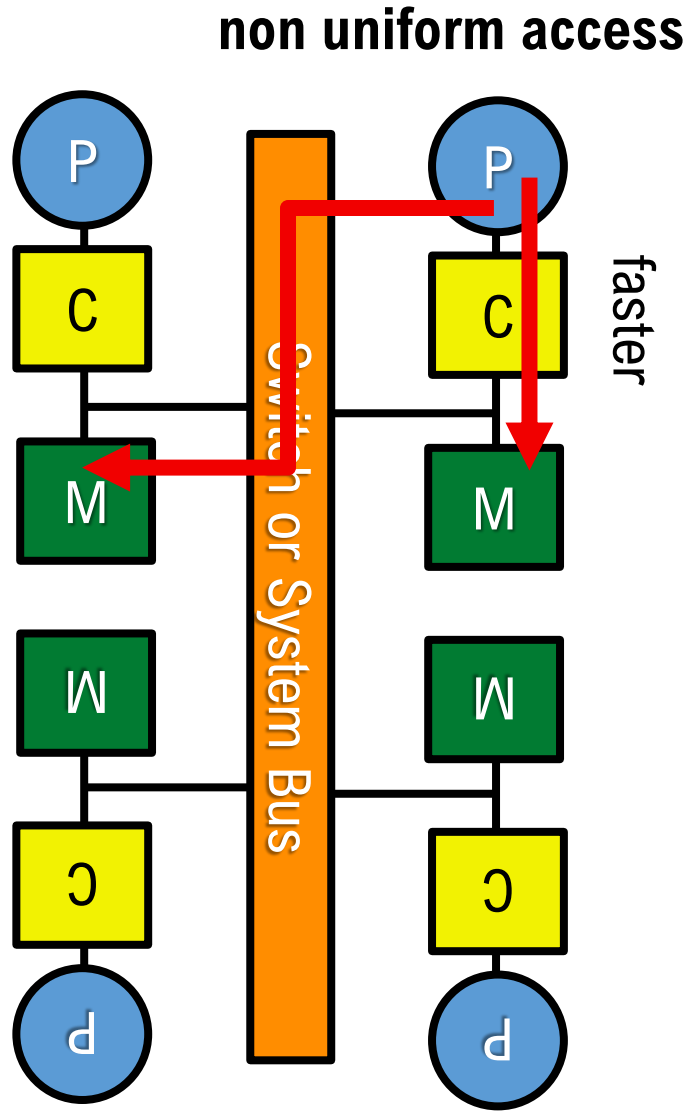
etc..



Shared memory system: NUMA Non-Uniform Memory Access

- a memory module (local memory) dedicated to each CPU
- a CPU can access a memory dedicated to a different CPU via shared bus or switch (remote memory)
- non-symmetric, where access to remote memories takes a longer time than access to local memory

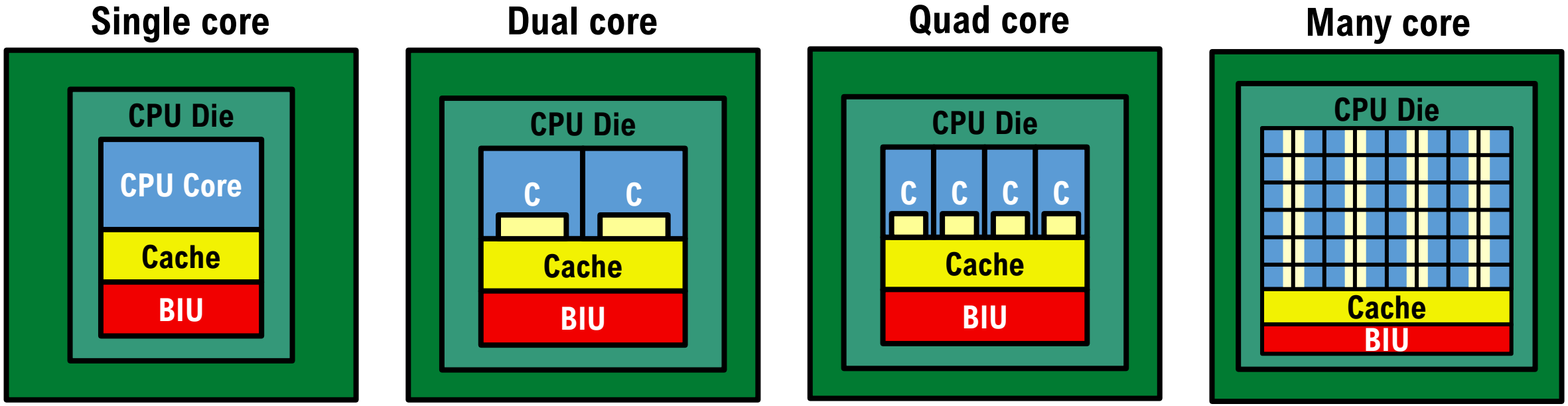
- AMD Opteron Barcelona (2007)



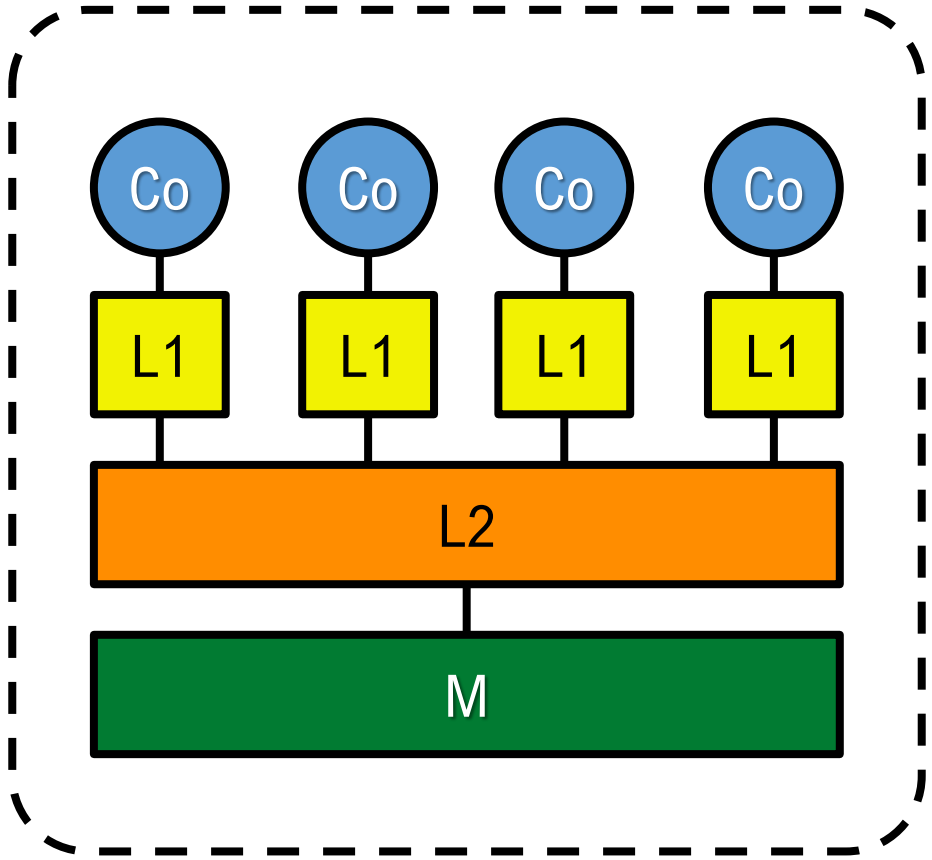
Multi-core processors

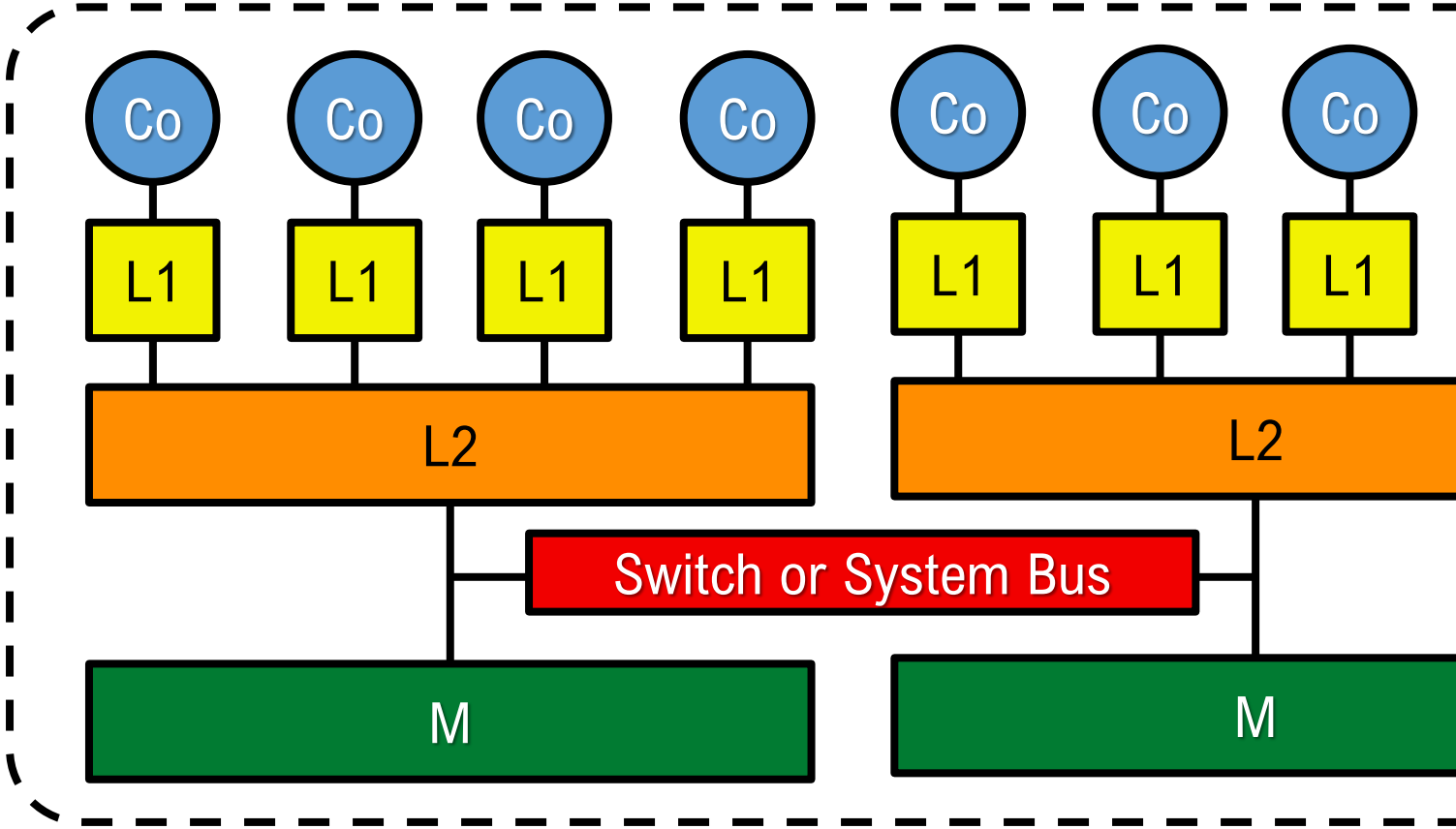
- core is a processing unit
- two or more cores in a computer processor : multi-core processor
  - ex. 8-cores in the SPARC64 VIIIfx processor (K-computer)
  - cores are independent
    - a processor can issue multiple (different/same) instructions from multiple cores
  - inter-core communication:
    - via message passing
    - **via shared-memory**

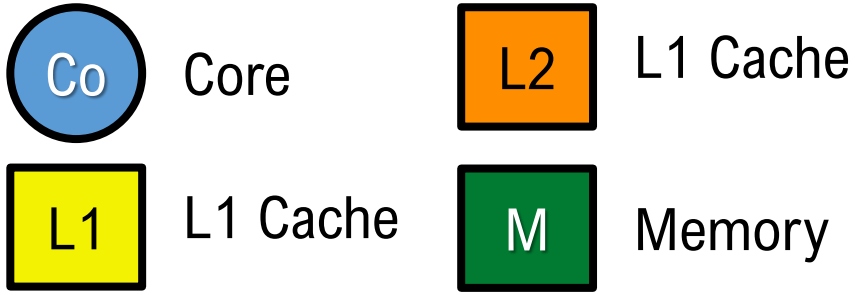
} can be both



Multi-core processors: SMP (SMC?) / NUMA

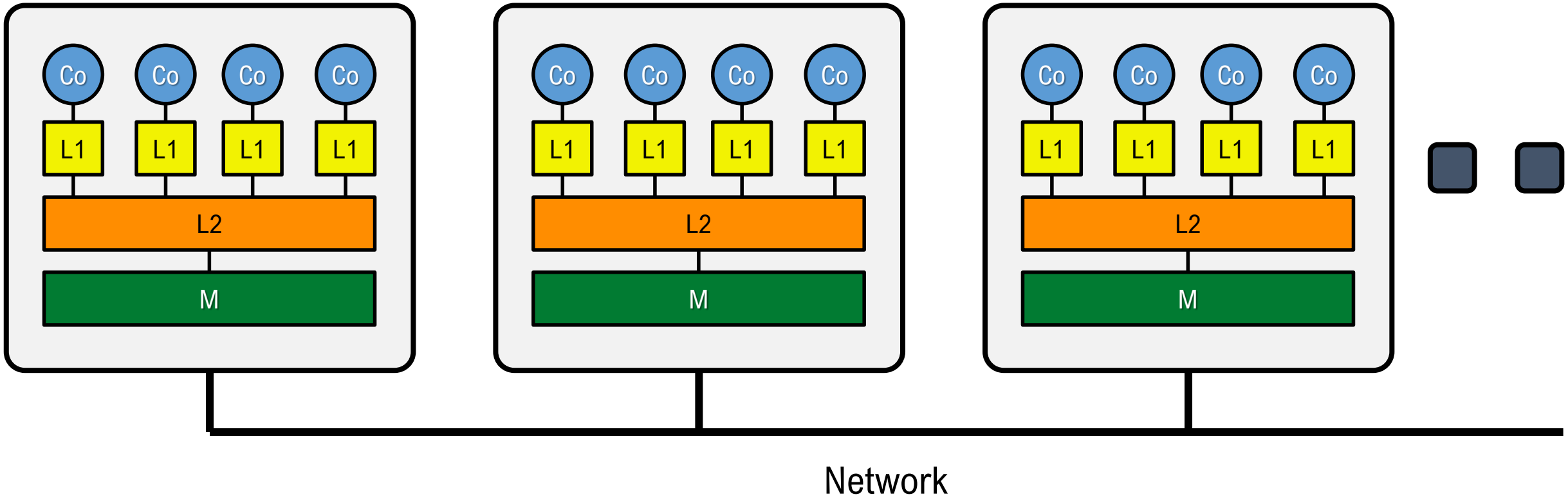






Hybrid of distributed parallel and shared memory systems

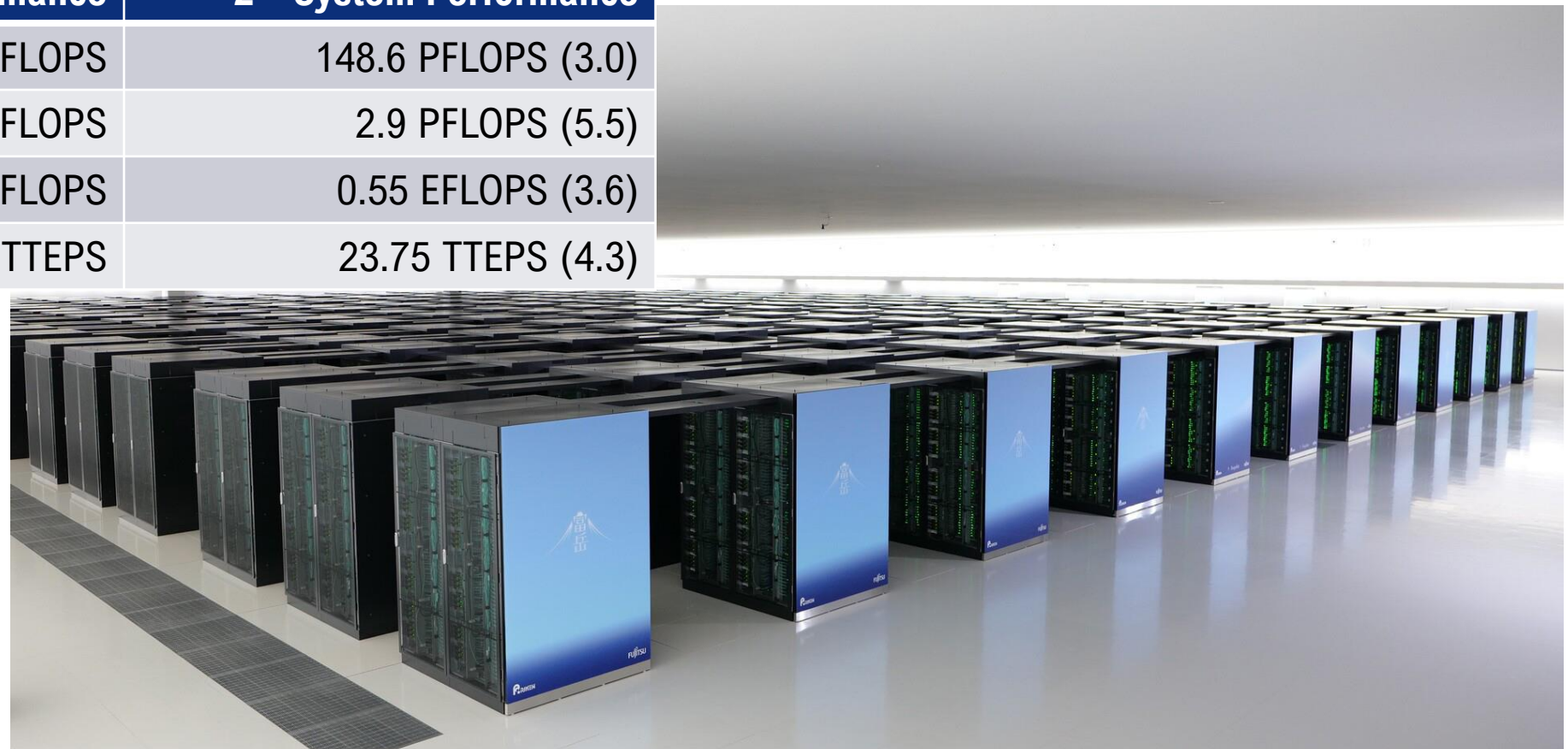
- several (80,000+ in case of K-computer) nodes of shared memory systems are connected as a distributed parallel system
- because of the popularity of the shared memory architecture in a single processor, i.e. a multi-core processor



An example of large-scale parallel systems: Overview of supercomputer Fugaku

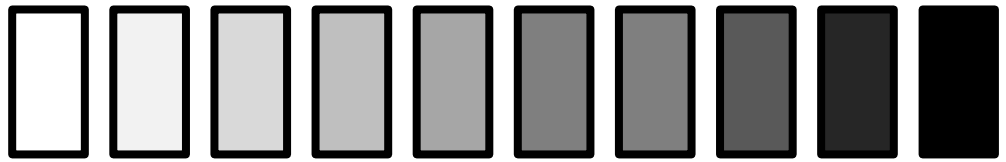
- A supercomputer installed at RIKEN Center for computational science
- Massively parallel system with 158,978 **general purpose CPUs**
- Ranked #1 in the 4 rankings announced in Nov. 2020

Ranking	Performance	2nd System Performance
TOP500	442.01 PFLOPS	148.6 PFLOPS (3.0)
HPGC	16.00 PFLOPS	2.9 PFLOPS (5.5)
HPL-AI	2.00 EFLOPS	0.55 EFLOPS (3.6)
Graph500	102.05 TTEPS	23.75 TTEPS (4.3)



Specification of supercomputer Fugaku (& K)

Specification of supercomputer Fugaku	
CPU Technology	
# of Cores in CPU	
CPU Clock	
Theoretical Peak	
Node Cache	
Memory Technology	
Memory Capacity	
Memory Bandwidth	1024 GB/s
Network	TofuD, 28 Gbps x 2 lane x 10 port
# of nodes	158,978 nodes



10 racks ≒ K computer

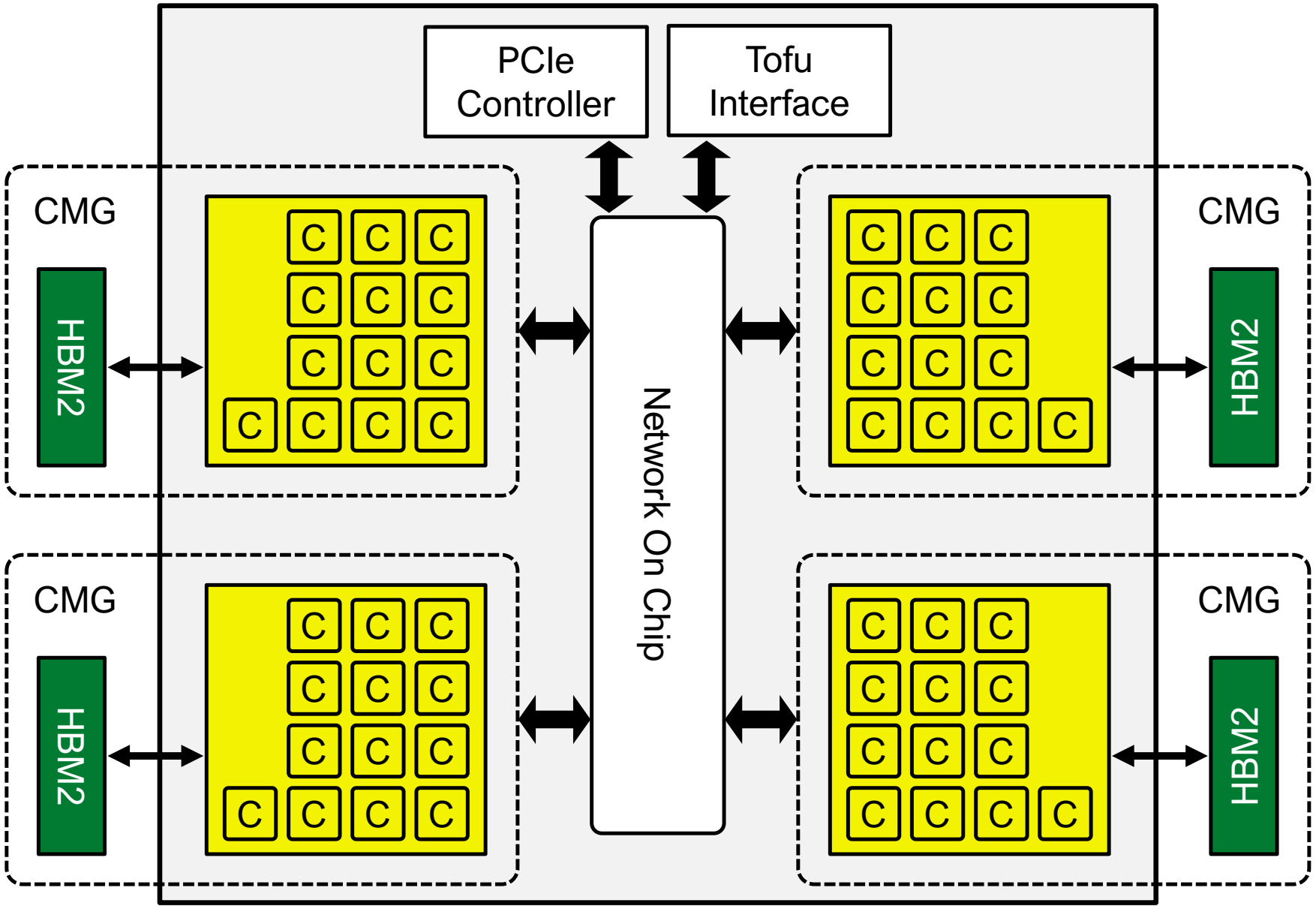
Specification of K computer	
ogy	SPARC64 VIIIfx
PU	8 cores
ock	2 GHz
eak	128Gflops
che	L1 32 KB / core
	L2 6 MB / node
ogy	DDR3
city	16 GB
Memory Bandwidth	64 GB/s
Network	Tofu 6-dimentional torus, 5GB/s (bi-direction)
# of nodes	82944 (88128, including IO-nodes)

K computer

A64FX: Node Overview

C: Core
CMG: Core Memory Group
HBM: High Bandwidth Memory

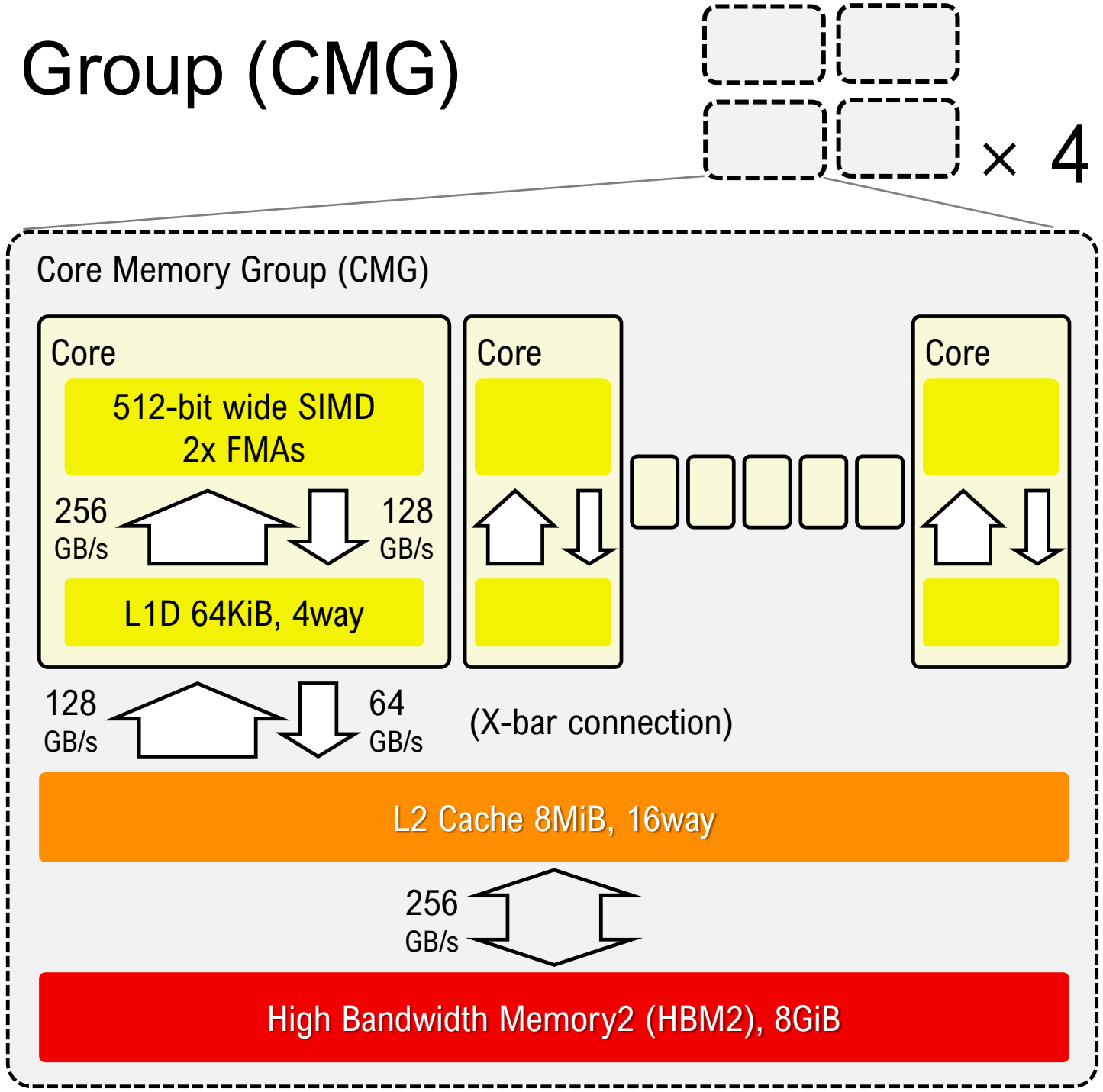
- SVE 512-bit wide SIMD
- FP64/FP32/FP16
- 12+1 cores in a CMG
  - an assistant core in each CMG
- 4 CMG in a Node
  - 48 + 2/4 core
- HBM2 32GiB/Node
  - 8GiB/CMG
  - 1024 GB/s
- Ring Network, 128 GB/s x 2
- TofuD NIC, 6.8 GB/s x 6
  - 6 simultaneously transmit directions



A64FX: Core Memory Group (CMG)

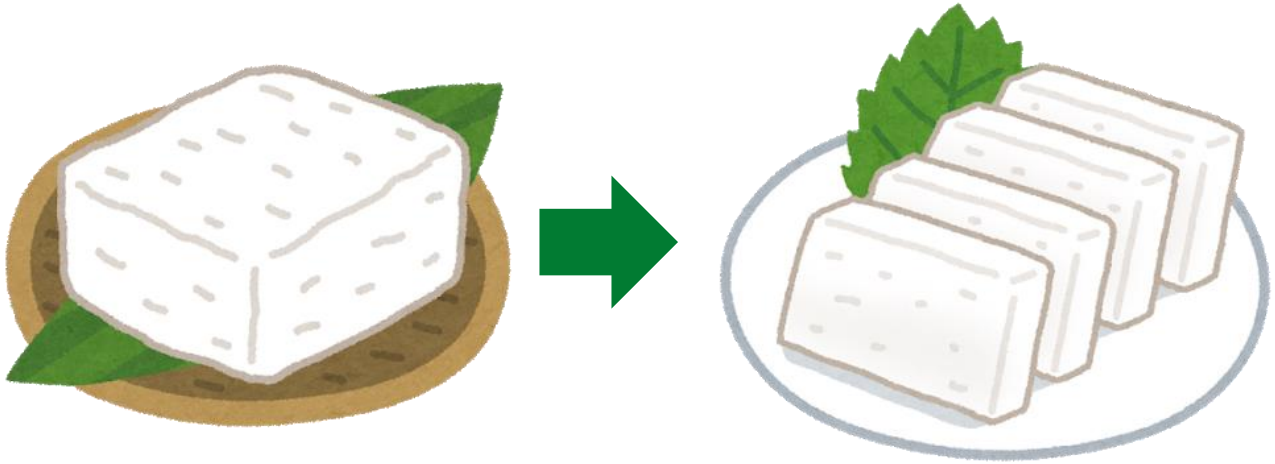
- 2x 512-bit wide SIMD, 4x ALUs, Predicate Operation
- 2x 512-bit wide SIMD load or 512-bit wide SIMD store
- L1D cache (/core) : 64 KiB, 4 ways, “Combined Gather” on L1
- L2D cache (/CMG): 8MiB
  - X-bar connection in a CMG
- 4 CMGs support cache coherency by ccNUMA with on-chip directory (256 GB/s x 2 for inter-CMGs)
- Memory controller for HBM2

※ L1/L2 cache bandwidths are for 2.0GHz

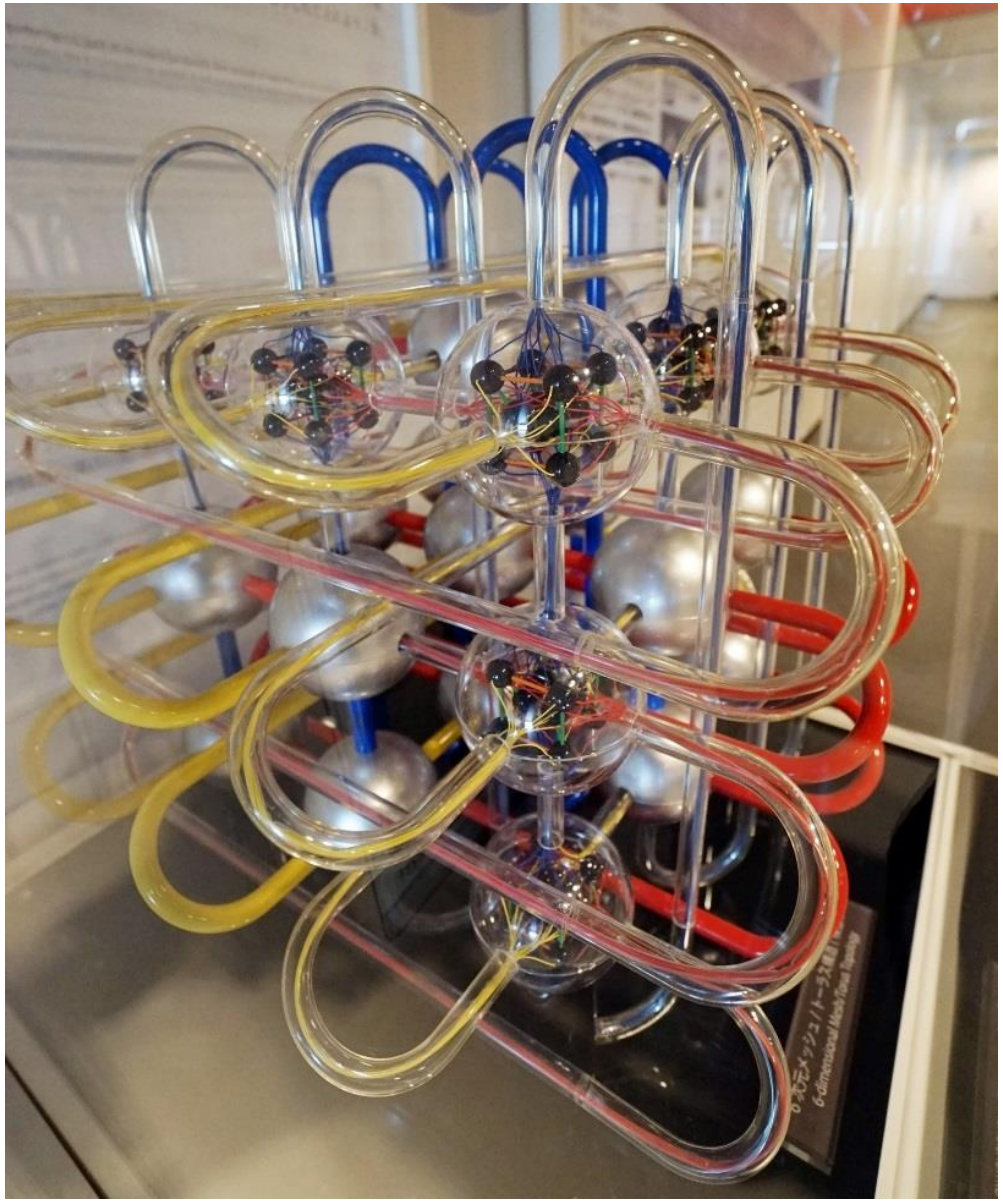


Tofu Interconnect D (TofuD)

- Tofu interconnect series
  - High scalable and fault tolerant 6D mesh/torus network for large scale systems
  - Arbitrary 3-Dimentional **torus** topology can be extracted from 48x36x48 (current maximum for a user), whereas a general torus network will be **mesh** if you extract a part of it



Tofu (豆腐) is Tofu even after cut as you like.
TofuD is torus even after cut ☺



Summary: parallelism in modern HPC systems

- Multi-nodes connected by network
  - multi-processors (multi-sockets) in a single node
    - multi-cores in a single processor
      - SIMD instructions in a single core
        - pipelined

} automatically parallelized by compilers and hardware !

※ you can help compilers to generate more efficient program, even you can parallelize your code on these levels

- A programming model for a level of parallel architectural level
- Hybrid of parallel programming models for a whole system

- Discuss parallel programming model for these levels+

Some important concepts about parallel programming

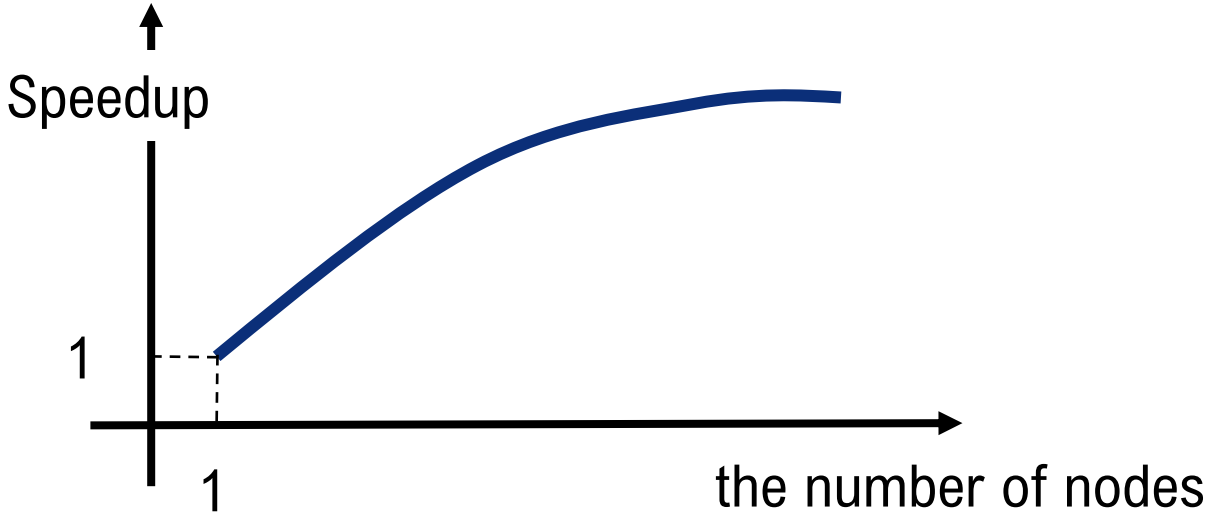
- Speedup
- Amdahl's law
- Weak scaling vs Strong scaling

Speedup

- the relative performance of two systems processing the same program
  - typically, the relative performance of parallel and serial executions

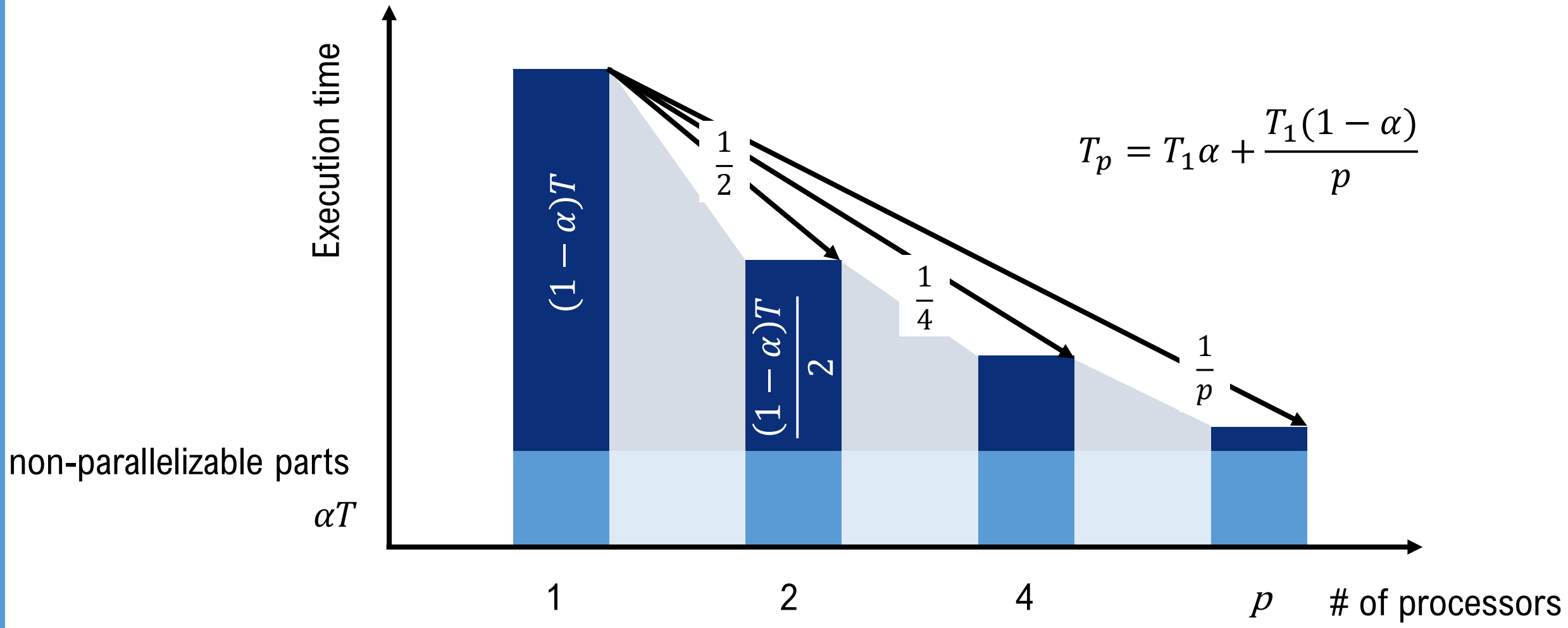
$\frac{T_1}{T_p}$ execution time w/ 1 processor / execution time w/ p processors

- If we use 2 processors and the execution time becomes the half of the 1 processor case, then the speedup is “2”



Amdahl's law

- Total execution time: T_1 on a single processor
- Total execution time: T_p on p processors
- α is the ratio of non-parallelizable part
- P processors take $T_1\alpha$ (sec) for the part
- The rest can be parallelized: $\frac{T_1(1-\alpha)}{p}$



$$T_p = T_1\alpha + \frac{T_1(1-\alpha)}{p}$$

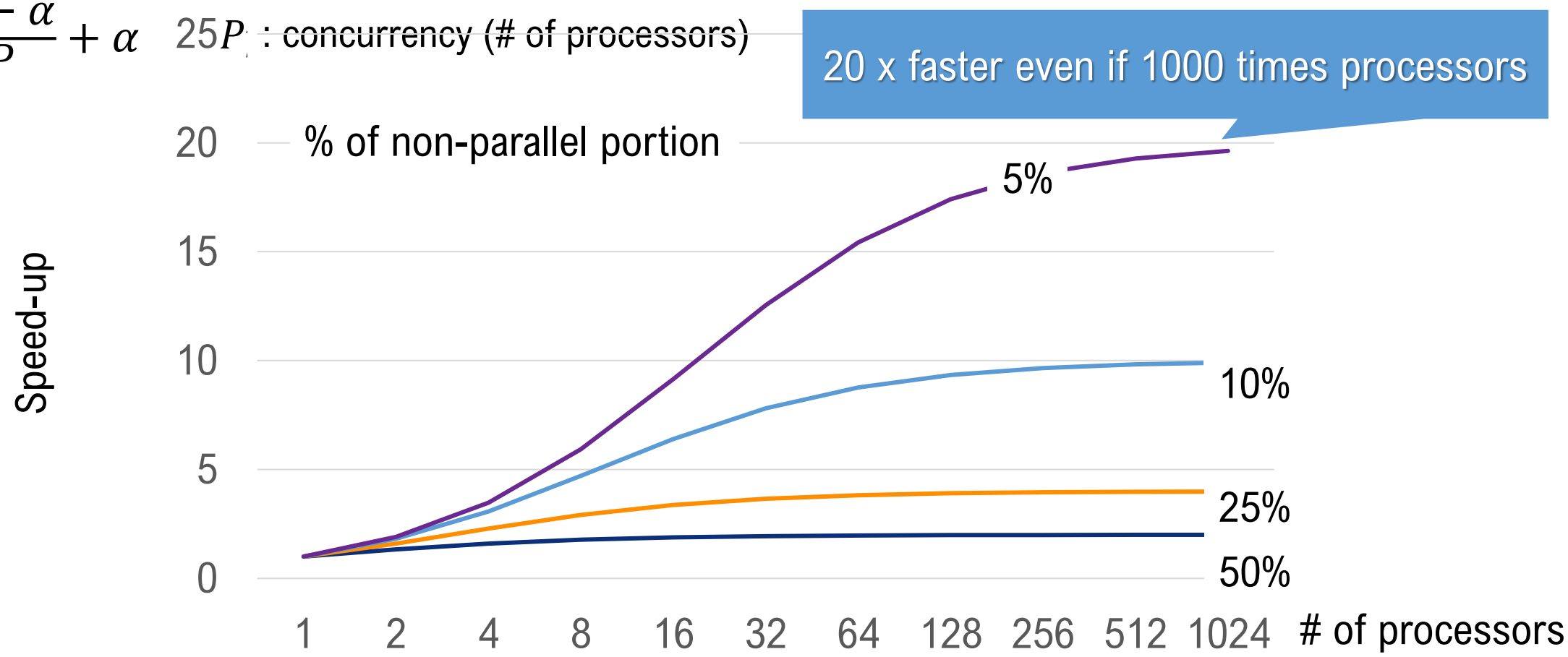
Amdahl's law

- The speed-up from parallelization
  - ✗ 2 processors ⇒ 2 times faster

$$S(s) = \frac{1}{\frac{1-\alpha}{P} + \alpha}$$

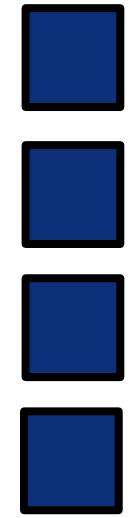
α the fraction of running time a program spends on non-parallelizable parts

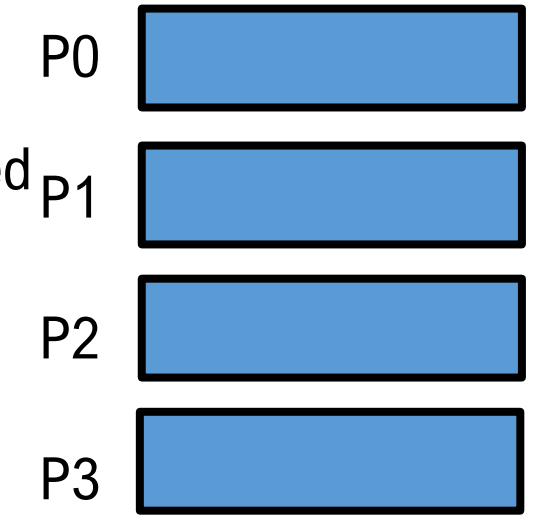
P : concurrency (# of processors)



Weak scaling vs Strong scaling

- We do not have to solve the program size of a small system for large systems
  - Parallelism : Faster time to solution / **larger computing problems(scalability)**
- **Strong scaling**
  - Fixed problem size while the number of processors are increased
  - problem size for each processor becomes smaller
  - Amount of communication between processors may be smaller or stay constant or grow
  - Limited scalability due to Amdahl's low
- **Weak scaling**
  - Fixed problem size for each processor
  - (Total) problem size increases when the number of processors are increased
  - Amount of communication between processors remains constant or grows
    - Note: Communication overhead may grow even the amount remains constant, because of synchronization overhead, etc..





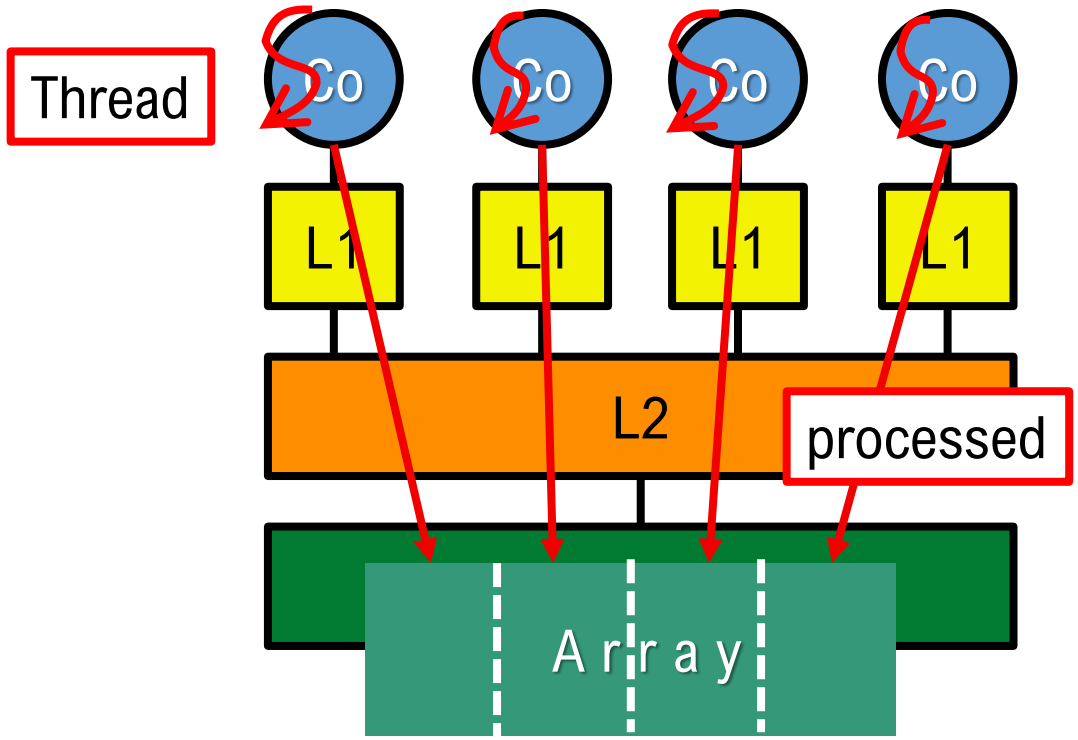
Parallelization and parallel programming

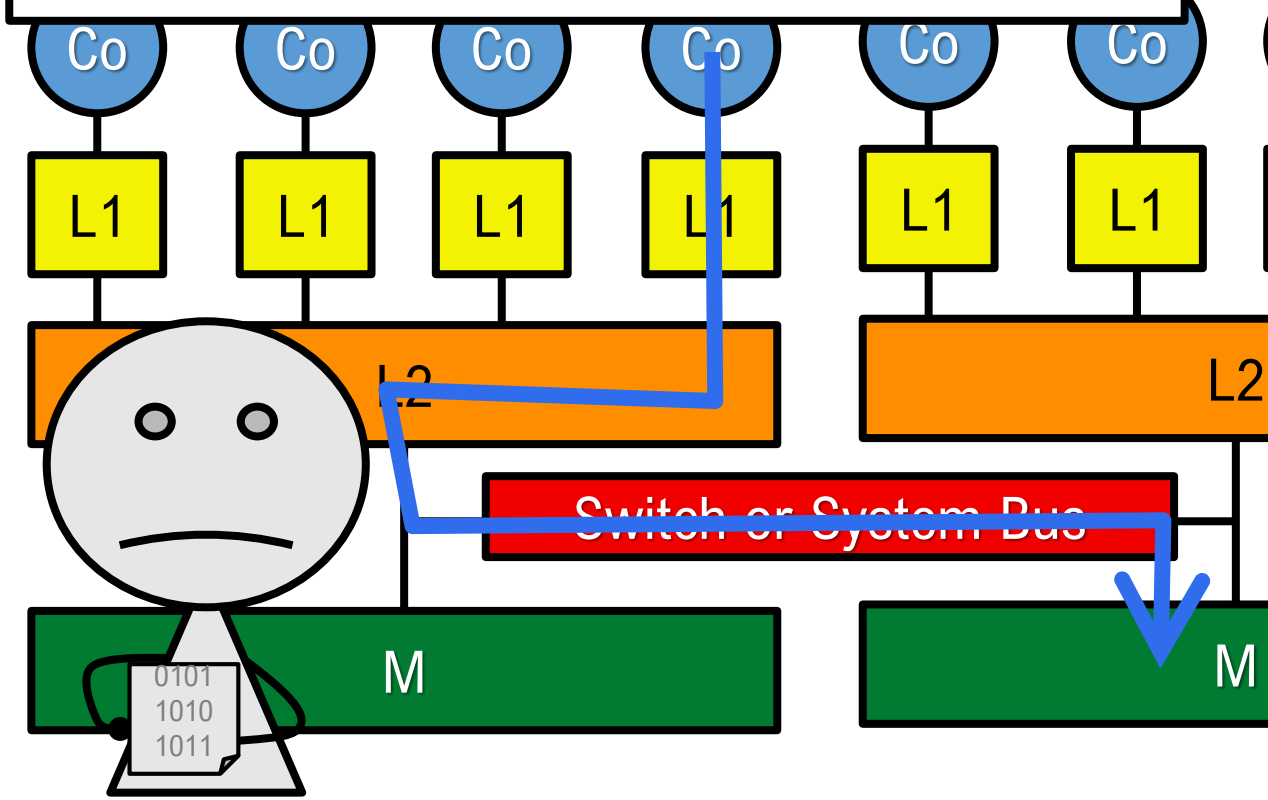
- Shared memory programming
  - Overview
  - OpenMP
- Distributed parallel programming, Message Passing
  - Overview
  - MPI
- Hybrid programming
  - OpenMP+MPI

Shared memory programming model

- Threads share a common address space
- on the shared memory architectures
- Easy to program (/extend) from a serial code

※ Note:
Process: independent, separate memory space
Thread: subsets of a process, shared memory space. Two or more threads can share a core (Hyperthreading, simultaneous multithreading)

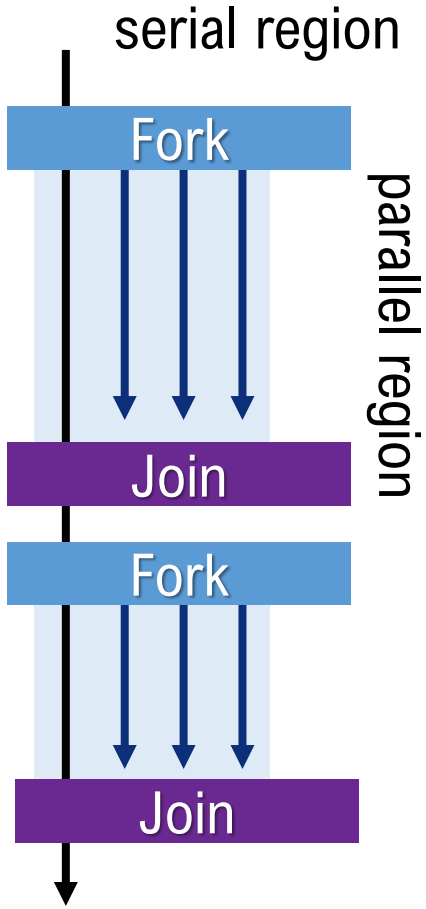




Shared memory programming model: OpenMP

- Most popular parallel programming language (and library) for the shared memory programming
- "Fork-Join" execution model
  - A *parent* thread calls "**Fork**" to create new threads
    - The parent thread continues operation, the children threads also start operation
  - "**Join**" is called by both the parent and children threads
    - Children exit
    - Parent waits until all children join
    - Parent continues operation (serial)
- Directive based
  - insert directives into C/fortran

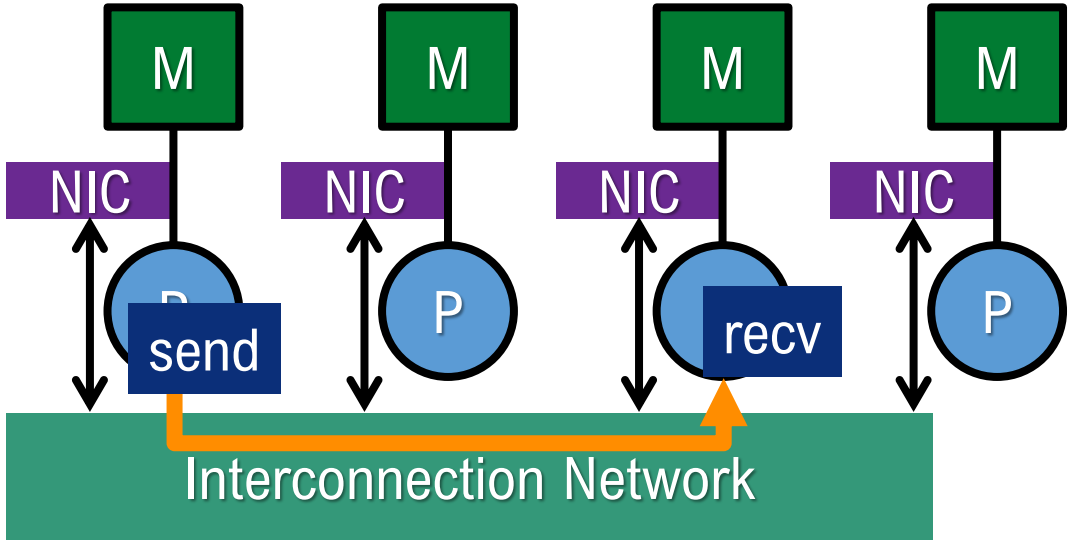
```
PROGRAM TEST
print *,"Thanks"
!$OMP PARALLEL
print *,"Many Thanks"
!$OMP END PARALLEL
END PROGRAM TEST
```



Distributed parallel programming model, Message Passing

- In distributed parallel systems, each processor can not access all data
- Processors must access non-local data by *communication*
  - Message passing Interface (MPI)
  - Parallel Virtual Machine (PVM)
  - etc..
- Applications must be parallelized explicitly
  - work mapping
  - data distribution
- Scalable from the viewpoint of construction
  - Just increase the number of nodes

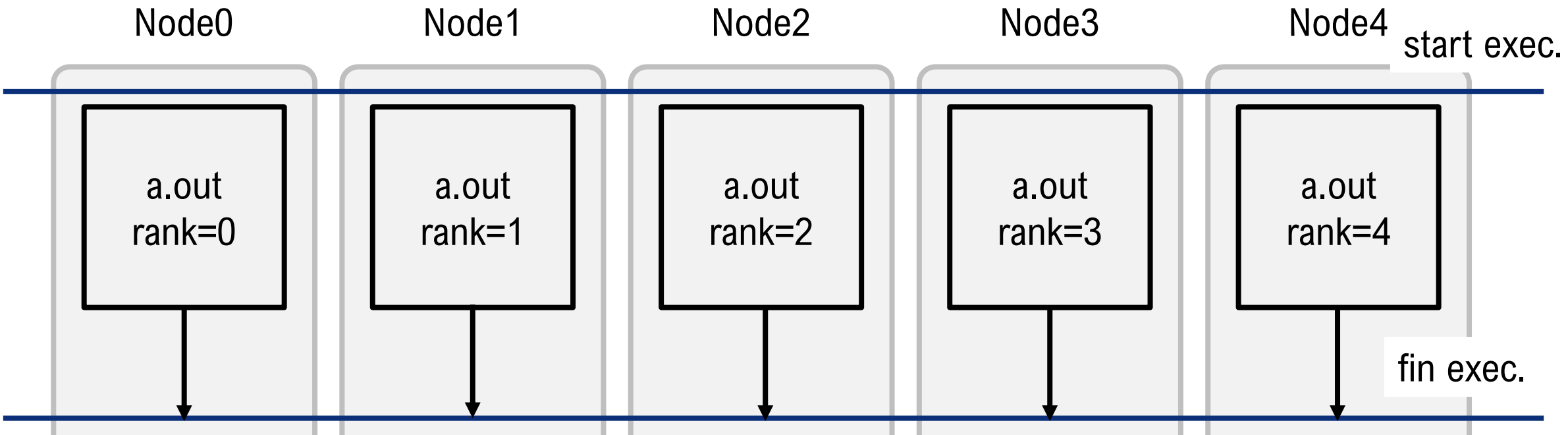
- Note: Distributed parallel programming model is available on shared memory systems



MPI : Message Passing Interface

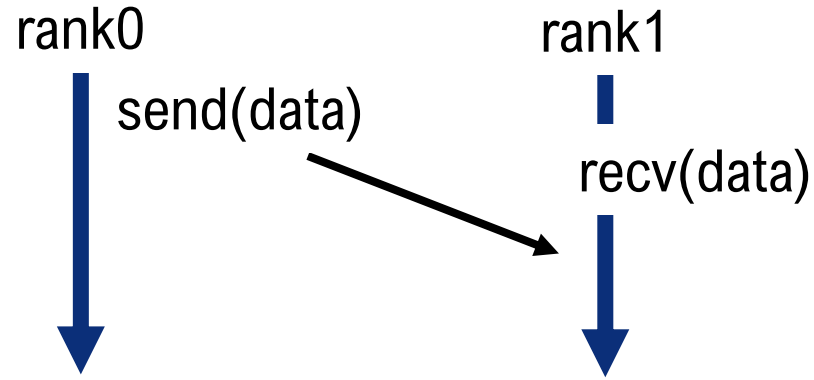
Note: MPI is not a programming language. MPI is a message passing interface specification.

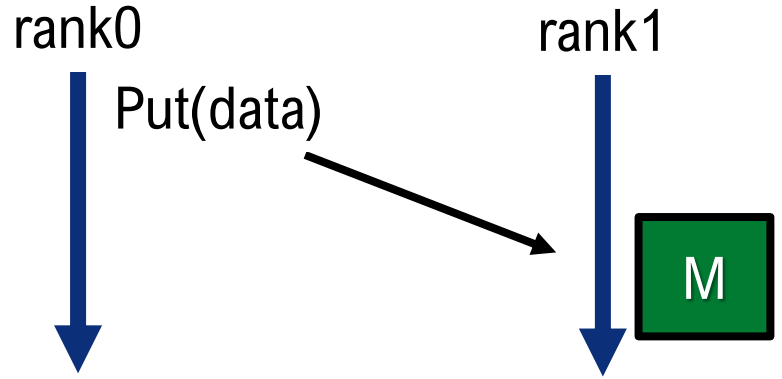
- de fact standard for parallel programming for distributed parallel systems
- SPMD programming model
  - SI**MD** : Single Instruction Multiple Data
  - MI**MD** : Multiple Instruction Multiple Data
  - SPMD: Single **Program** Multiple Data
    - a same binary runs on multiple nodes to process multiple data
    - use if (rank=**) to assign a special work on a certain process



MPI: communication types

- Cooperative operations
  - cooperatively exchanged in message passing
    - receiver explicitly allocate memory space to receive
  - explicitly sent by a process and received by another
  - communication and synchronization are combined
- One-sided operations
  - remote memory reads/writes
  - only one process needs to explicitly participate
  - communication and synchronization are not combined
    - faster
  - Programmers must take care about local memory control





MPI: Communication types, from a different perspective

- Pairwise (point-to-point) communication
  - communication between 2 processes
    - Send/Recv
- Collective communication
  - communication between multiple processes
    - a group of all processes
    - a group of some processes
  - ex: send a data from rank-0 to all processes
  - rank-0 receives data from all other processes

MPI : point-to-point communication

- rank=0 sends a number to rank=1
- rank=1 receives a number from rank=0, and print the number

```c
#include <mpi.h>
#include <stdio.h>
int main(int argc, char *argv[]) {
    int nprocs, myrank;
    double number;

    MPI_Init(&argc, &argv);                    // Initialize the MPI execution environment
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs); // Get the number of processes
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank); // Get the rank of the calling process
    if (myrank == 0) {
        number = 1.0;
        MPI_Send(&number, 1, MPI_DOUBLE, 1, 0, MPI_COMM_WORLD);
    }else if (myrank == 1) {
        MPI_Recv(&number, 1, MPI_DOUBLE, 1, 1, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
        printf("recv: %f\n", number);
    }
    MPI_Finalize();                            // Finalize the MPI execution environment
}
```

MPI : point-to-point communication

```
MPI_Send(&number,          const void*   initial address of send buffer
         1,                int           the number of elements
         MPI_DOUBLE,       MPI_Datatype  datatype of each element
         1,                int           rank of destination
         0,                int           message tag, will be used to differentiate messages
         MPI_COMM_WORLD);  MPI_Comm      communicator, which describes a group of processors
                                         MPI_COMM_WORLD is the group of all processors in your job

MPI_Recv(&number,          const void*   initial address of recieve buffer
         1,                int           the number of elements
         MPI_DOUBLE,       MPI_Datatype  datatype of each element
         0,                int           rank of source
         0,                int           message tag
         MPI_COMM_WORLD,   MPI_Comm      communicator
         MPI_STATUS_IGNORE); MPI_Status  a structure including a status of a reception
```

MPI: collective communication

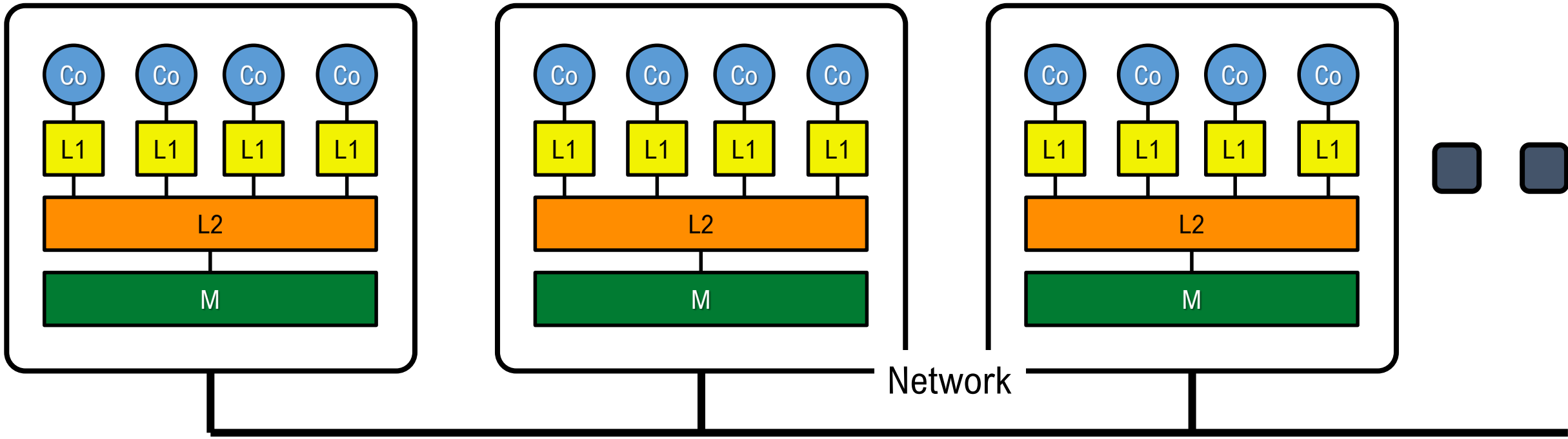
- rank=0 sends “number” to all other processes

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char *argv[]) {
   int nprocs, myrank;
   double number;

   MPI_Init(&argc, &argv);                  // Initialize the MPI execution environment
   MPI_Comm_size(MPI_COMM_WORLD, &nprocs); // Get the number of processes
   MPI_Comm_rank(MPI_COMM_WORLD, &myrank); // Get the rank of the calling process

   if(myrank == 0) number = 1.23;
   else            number = 3.21;

   MPI_Bcast(&number, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);

   printf(“recv: %f\n”, number);

   MPI_Finalize();                          // Finalize the MPI execution environment
}
```

MPI: collective communication

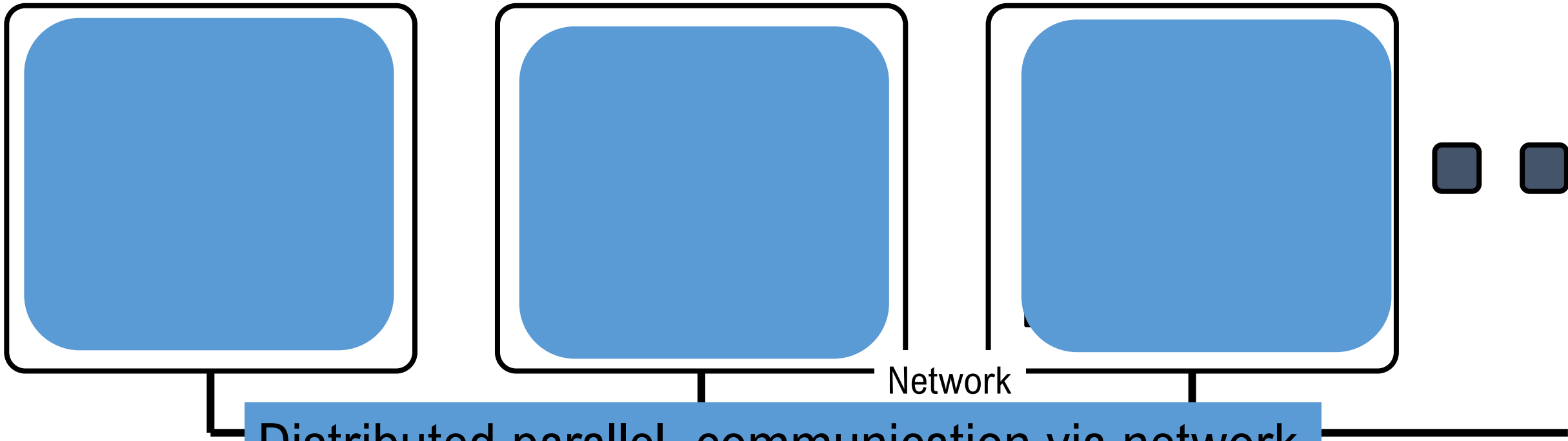
`MPI_Bcast(&number,`	`const void*`	initial address of send buffer
`1,`	`int`	the number of elements
`MPI_DOUBLE,`	`MPI_Datatype`	datatype of each element
`1,`	`int`	rank of root (any process can be a root)
`MPI_COMM_WORLD);`	`MPI_Comm`	communicator

Hybrid of shared memory and distributed parallel



- 2 possible choices of programming models
  - **Hybrid of shared memory and distributed parallel programming models**
    - **OpenMP + MPI (Today's focus)**
  - distributed parallel programming model
    - flat-MPI (remember! sometimes, this is not bad choice)

Hybrid of shared memory and distributed parallel



- 2 possible choices of programming models
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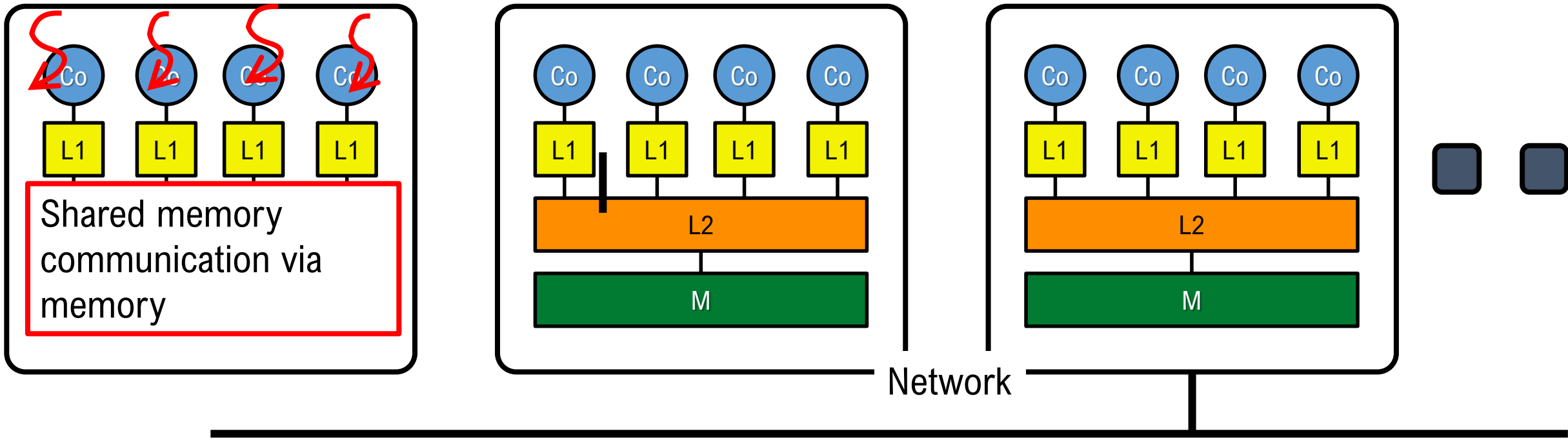
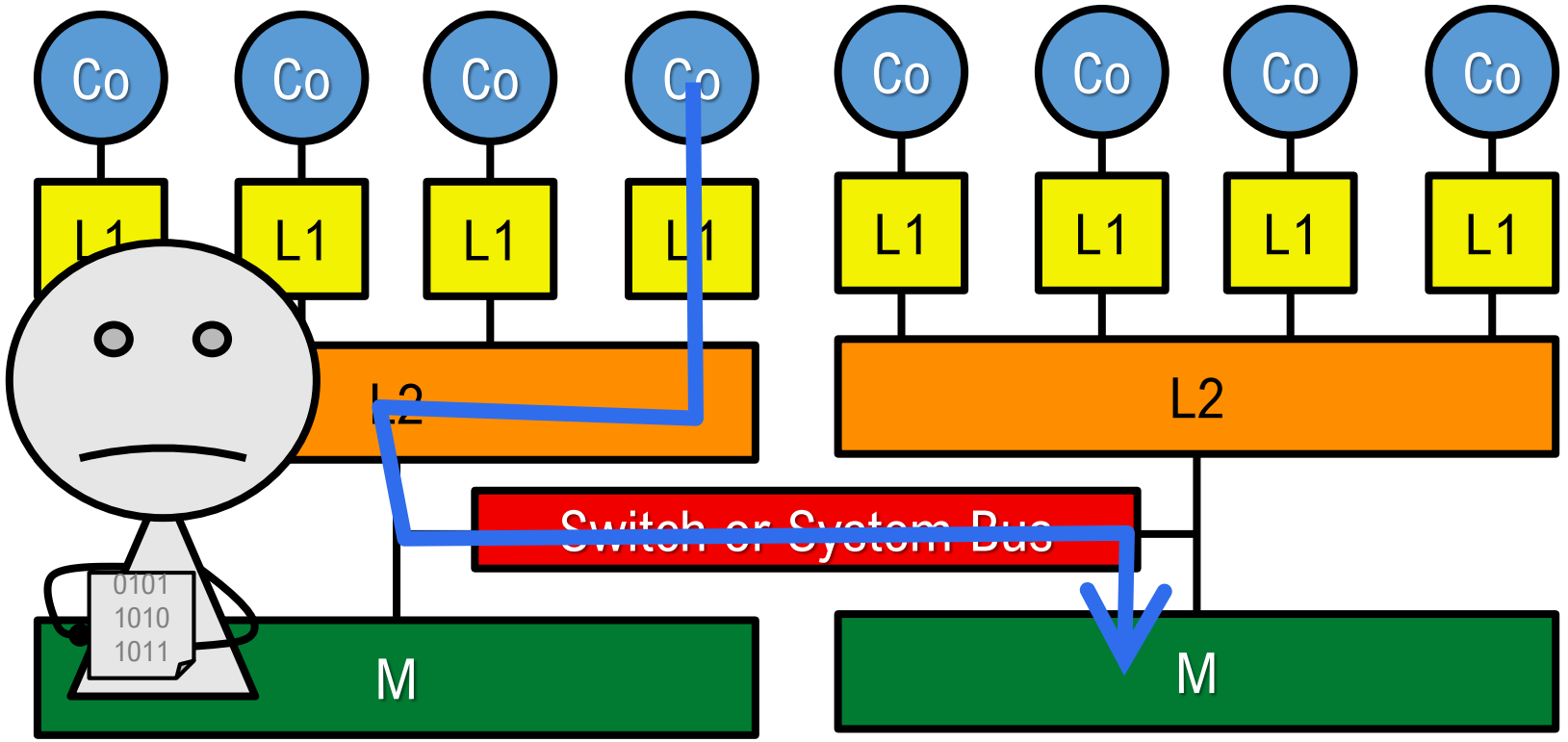
Hybrid of shared memory and distributed parallel



- 2 possible choices of programming models
  - **Hybrid of shared memory and distributed parallel programming models**
    - **OpenMP + MPI**
  - distributed parallel programming model
    - flat-MPI (remember! sometimes, this is not bad choice)

Hybrid of shared memory and distributed parallel

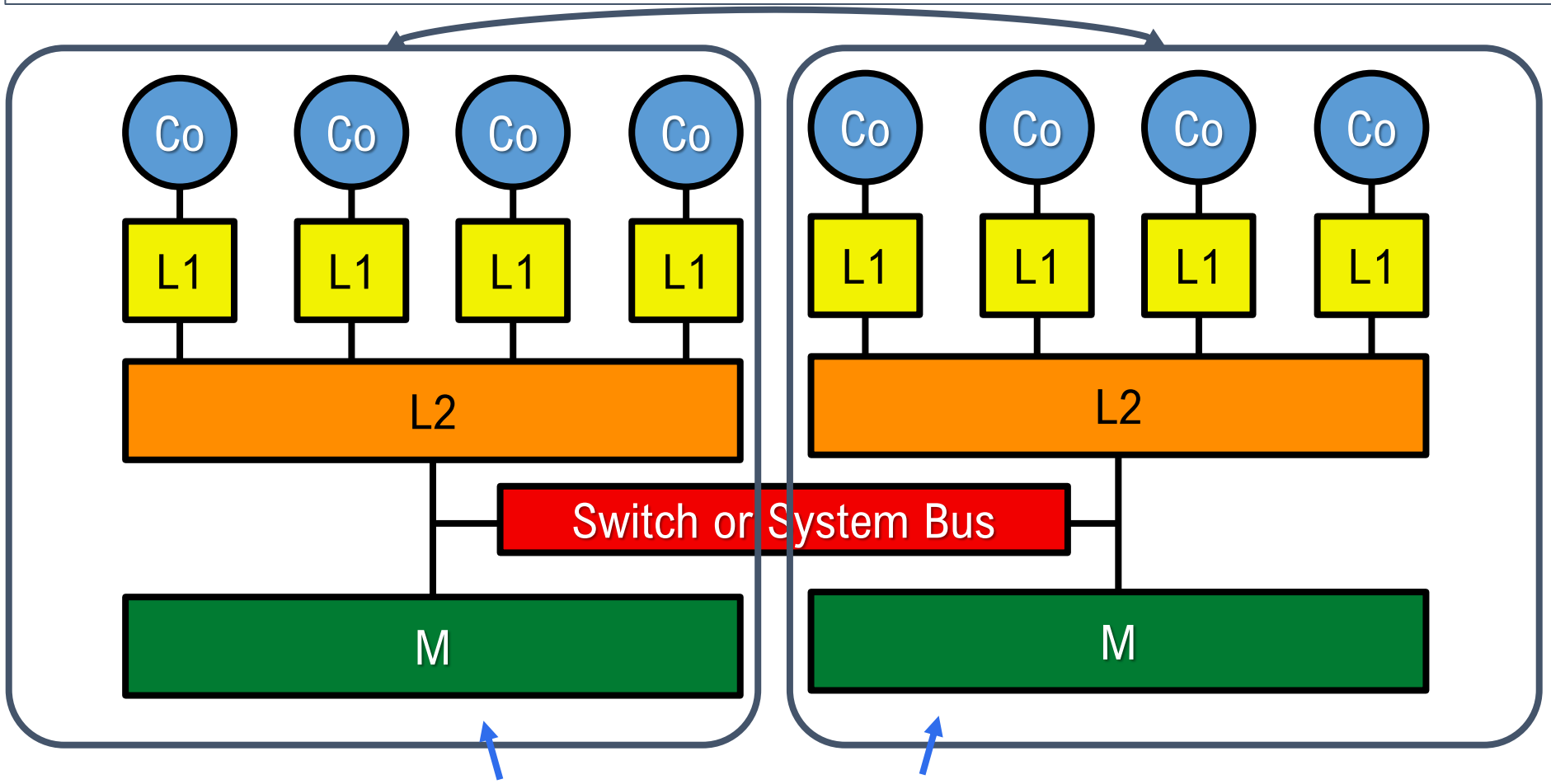
- For NUMA (ex. 2-CPUs in a node), shared memory programming model has “non-local data access” problem

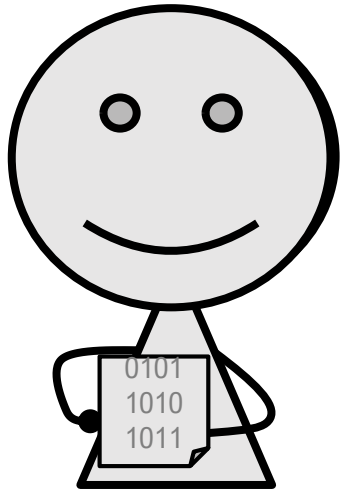


Hybrid of shared memory and distributed parallel

- For NUMA, shared memory programming model has “non-local data access” problem

Distributed parallel programming model between sets of shared memory cores

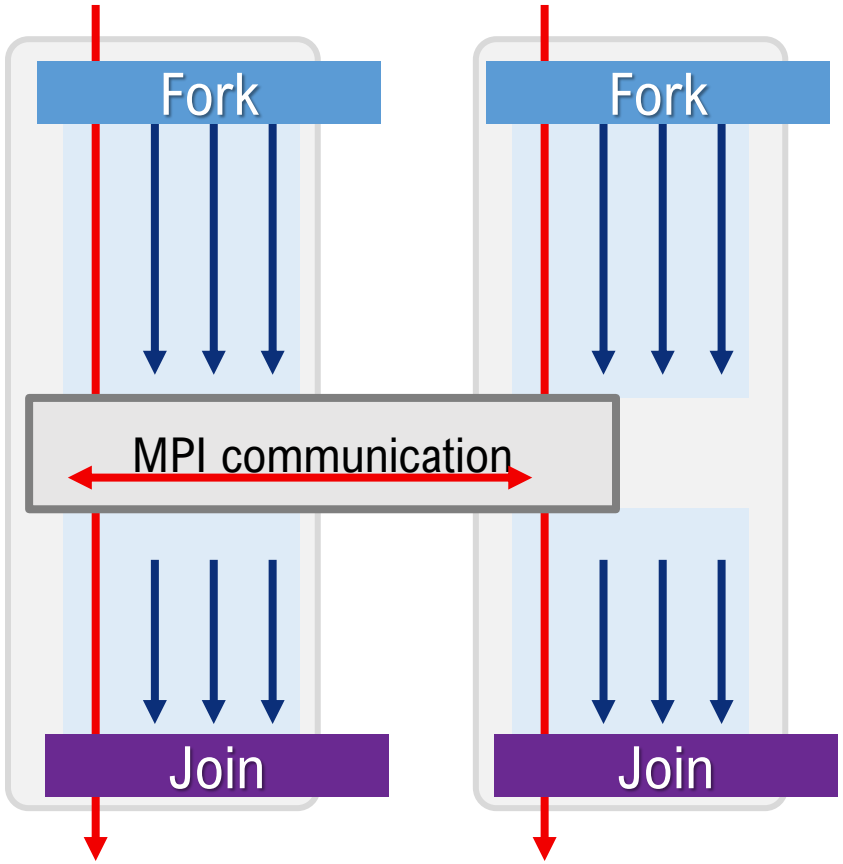




Shared memory programming model inside a set of shared cores

Hybrid of OpenMP+MPI

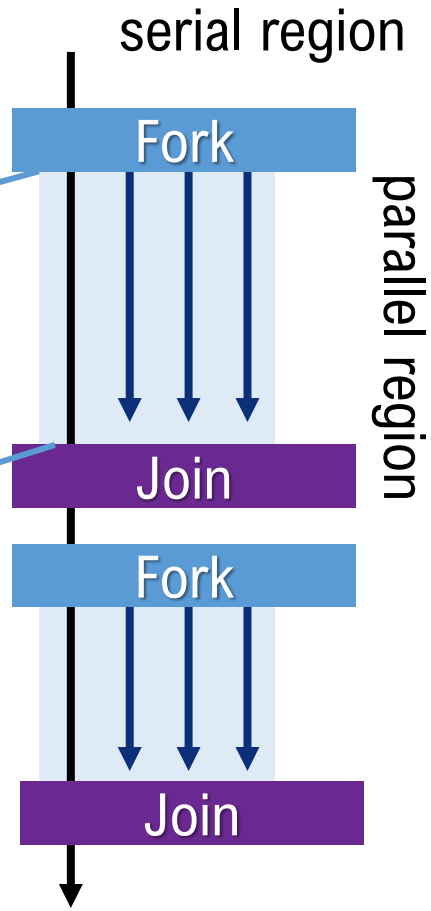
- MPI describes parallelism between processes
- OpenMP provides a shared memory model within a process



Hybrid of OpenMP+MPI

- MPI describes parallelism between processes
- OpenMP provides a shared memory model within a process
- After the MPI_Init_thread, you can fork threads wherever you need

```
MPI_Init_thread(&argc, &argv, MPI_THREAD_SINGLE, &prov);
MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);

#pragma omp parallel default(shared) private(iam, np)
{
    np = omp_get_num_threads();
    iam = omp_get_thread_num();
    printf("Hybrid: Hello from thread %d out of %d from process %d out of %d¥n",
           iam, np, rank, numprocs);
}
```



Hybrid of OpenMP+MPI

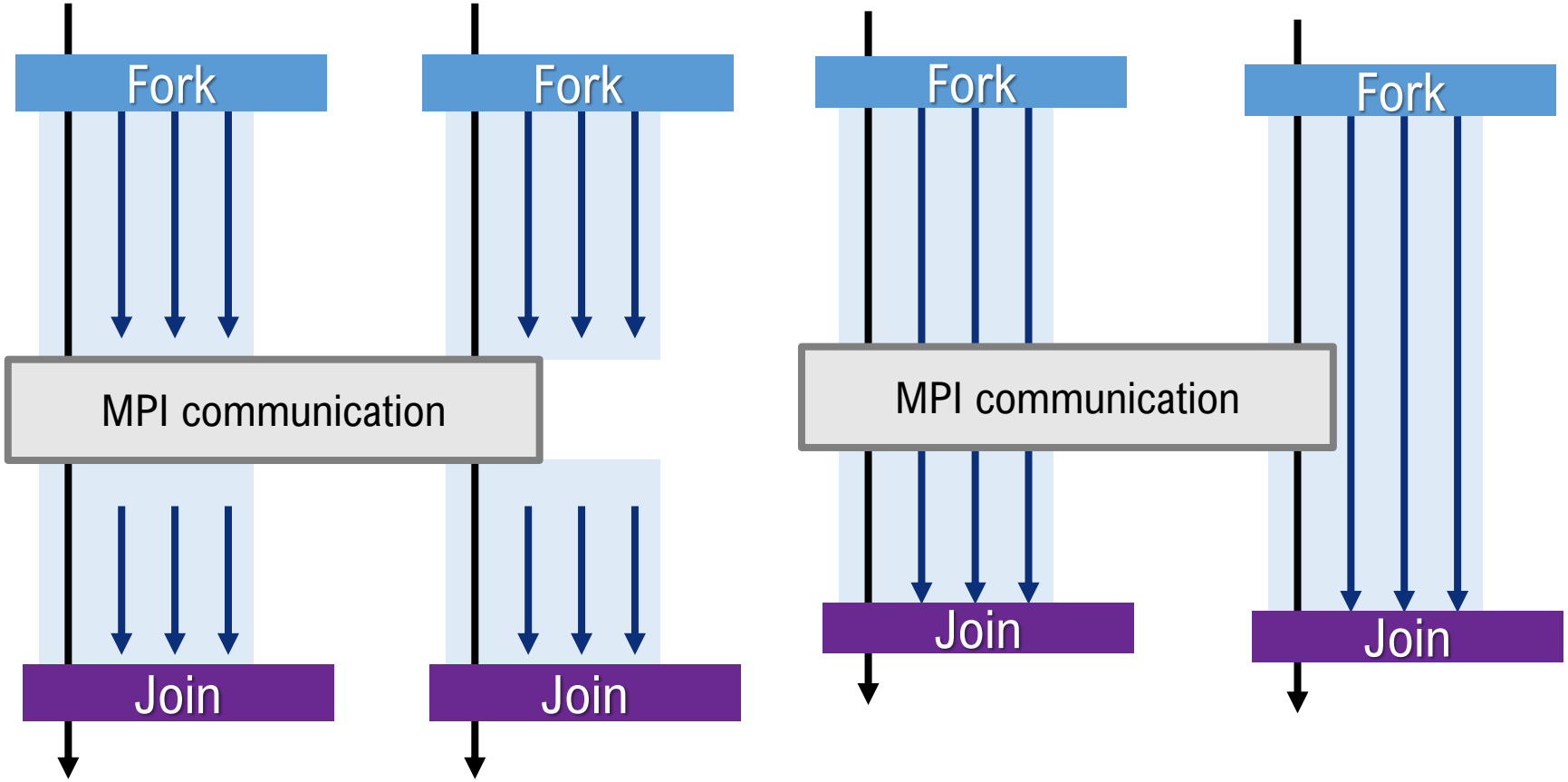
- MPI specification defines four levels of hybrid parallelism to be used with OpenMP-programming
  - MPI implementation do NOT always support all of them ☹

  - MPI_THREAD_SINGLE
    - Only one thread will call communication interface at once
  - MPI_THREAD_FUNNELED
    - The process may be multi-threaded, but only the main thread will make MPI calls (all MPI calls are funneled to the main thread).
  - MPI_THREAD_SERIALIZED
    - The process may be multi-threaded, and multiple threads may make MPI calls, but only one at a time: MPI calls are not made concurrently from two distinct threads (all MPI calls are serialized).
  - MPI_THREAD_MULTIPLE
    - Multiple threads may call MPI, with no restrictions.

https://www.mpich.org/static/docs/latest/www3/MPI_Init_thread.html

Hybrid of OpenMP+MPI: Overlapping communication and computation

- The hybrid of OpenMP+MPI allows us to overlap communication and computation
- The threads which do not call MPI functions can continue to other works (not communication)



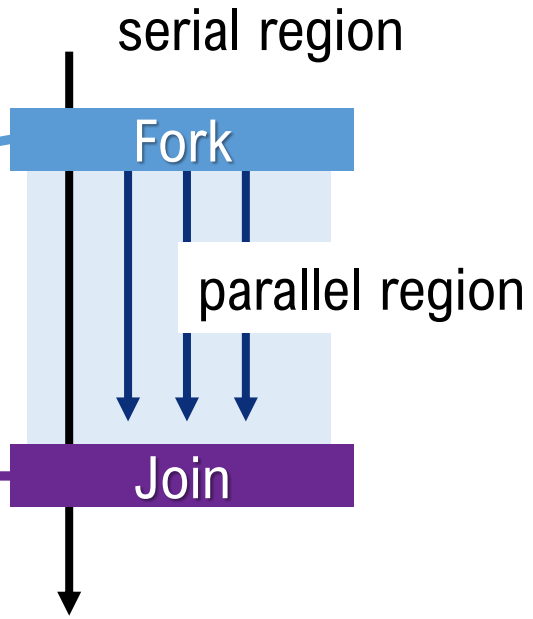

```
# pragma omp parallel
{
 // computation
    …..
#pragma omp single
  MPI_function();

….
}
```

Hands-on Practice

OpenMP: Hello world

- The directive to fork threads is #pragma omp parallel
- The threads join at the end of the region

```
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
#pragma omp parallel
{
  printf("Hello world\n");
}
}
```



Exercise: Hello world (OpenMP)

- write the hello world code, compile and run with 12 threads
  - compile:

    $ fccpx -Kfast,openmp <your-source-code.c>
  - execution: see next page
- To set the number of threads, set the environmental variable OMP_NUM_THREADS
  - for example, **export OMP_NUM_THREADS=12**
  - Edit your job-script and insert the command to set the environmental variable
- Check the result
  - *may be,* you can find “Hello world” repeated 12 times

```
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
#pragma omp parallel
{
  printf("Hello world\n");
}
}
```

Exercise: Hello world (OpenMP)

- write a job script

```
#!/bin/bash
#PJM -L "node=1"
#PJM -L "rscunit=rscunit_ft01"
#PJM -L "rscgrp=small"
#PJM -L "elapse=0:10:00"
#PJM -S

#------- Program execution -------#
export OMP_NUM_THREADS=<your number of threads>
./<your binary>
```

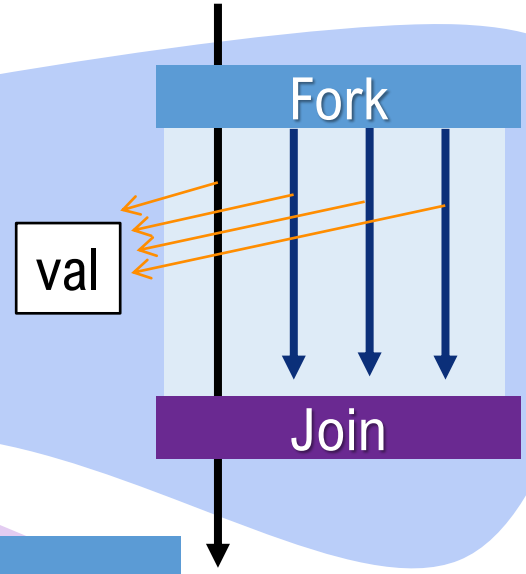
- submit your job

$ pjsub <your-job-script-file.sh>

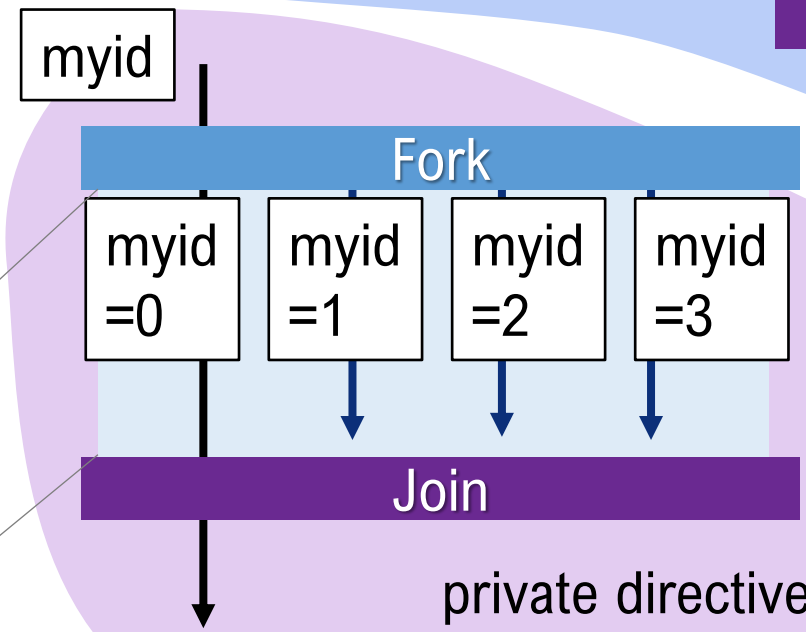
OpenMP: private data and shared data

- The basic idea of the shared programming model is that variables are shared by default, i.e. thread can read/write arbitrary variables
  - sometimes, threads need their own “private” workspace
- By using *private* clause, you can make a separate copy for each thread

default: all threads access all variables




```
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myid;

#pragma omp parallel private(myid)
{
  myid = omp_get_thread_num();
  printf("Hello world I'm %d\n",myid);
}
}
```



private directive enable us to make the copies of the variables

OpenMP: private data and shared data (FYI)

- private: each thread has its own instance of a variable
- firstprivate: each thread has its own instance of a variable. The variable must be initialized before the parallel region. At the beginning of the parallel region, the variables in all threads have a same initial value.
- lastprivate: : each thread has its own instance of a variable. The final value can be transmitted to the shared variable outside the parallel region.
- shared(default) : variable(s) can be shared among all threads. If you don’t specify any data type, then the variables should be shared in the parallel region.

Exercise: Hello world from who?

- write, compile and run the following code w/ 12 threads

```
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myid;

#pragma omp parallel private(myid)
{
  myid = omp_get_thread_num();
  printf("Hello world I'm %d\n",myid);
}
}
```

Note

- omp_get_thread_num() is a function to obtain its thread-id.
- Another important function is omp_get_num_threads(), which gives the number of threads in the region.

OpenMP: set the number of threads

- You've already learned the way to specify the number of threads by using the environmental variable OMP_NUM_THREADS, omp_set_num_threads(num) also allow us to set the number of threads.

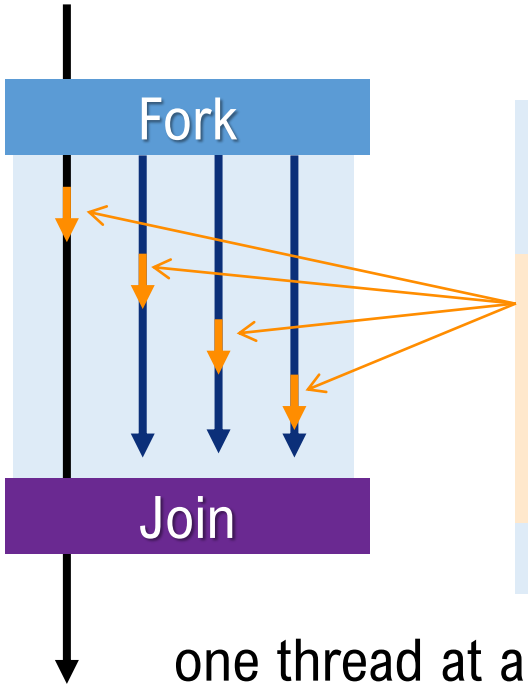
```
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myid;
  int nthreads;

  omp_set_num_threads(4);
#pragma omp parallel private(myid, nthreads)
{
  myid     = omp_get_thread_num();
  nthreads = omp_get_num_threads();
  printf("Hello world I'm %d of %d\n",myid, nthreads);
}
}
```

Exercise: the number of threads

- write, compile and run the code at the previous slide by specifying **OMP_NUM_THREADS=12** at the job-script
- check the results
  - how many threads can you find?

OpenMP: synchronization

- The synchronization directives allow us to control the order of execution of threads
- #pragma omp barrier: synchronizes all threads in the parallel region; all threads pause at the barrier, until all threads execute the barrier
- #pragma omp critical: specifies mutual exclusion. Only one thread at a time can enter a critical region




```
#pragma omp parallel
{
   ...
#pragma omp critical
{
  jobcall(A, B, n);
}
}
```

one thread at a time

- #pragma omp atomic: Only one thread at a time can update the specified variable

Exercise: synchronization

- write, compile and run the following two codes w/ 28 threads, and compare the results

```c
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myid;
  int val;

  val = 1000;
#pragma omp parallel private(myid) shared(val)
{
  myid     = omp_get_thread_num();
  printf("myid = %d, val = %d\n",myid,val);
  if(myid==0){
    val = myid;
  }
  printf("myid = %d, val = %d\n",myid,val);
}
}
```

```c
#include<omp.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myid;
  int val;

  val = 1000;
#pragma omp parallel private(myid) shared(val)
{
  myid     = omp_get_thread_num();
  printf("myid = %d, val = %d\n",myid,val);
  if(myid==0){
    val = myid;
  }
#pragma omp barrier
  printf("myid = %d, val = %d\n",myid,val);
}
}
```

OpenMP: loop

- loop work-sharing is a typical way to share workloads by threads to speed-up!
- scheduling and work-assignment can be specified by clauses such as *schedule*

```
#include<omp.h>
#include<stdio.h>
#include<stdlib.h>

#define N 1000

int main(int argc, char **argv)
{
  int i;
  double rmax;
  double A[N], B[N];

  rmax = 1.0/(double)RAND_MAX;

  for(i=0; i<N; i++) A[i] = ((double)random())*rmax;
  for(i=0; i<N; i++) B[i] = ((double)random())*rmax;


#pragma omp parallel private(i)
{
#pragma omp for
  for(i=0; i<N; i++){
    A[i] = A[i]+B[i];
  }
}

}
```

Note: these are equivalent

```
#pragma omp parallel for
  for(i=0; i<N; i++){
    A[i] = A[i]+B[i];
  }
```

loop index “i” is private by default in *parallel for*

OpenMP: reduction

- Standard reduction expressions such as +, max, min, can be defined in the reduction clause. *reduction(op: list)*
- If the reduction is declared, local copies of *"list"* are made in all threads, local results are stored in the local copies, and the local copies are reduced into a single shared value.

```
#pragma omp parallel for reduction(+:total_sum)
for(i=0; i<N; i++){
  total_sum += A[i];
}
```

these are equivalent

```
#include<omp.h>
#include<stdio.h>
#include<stdlib.h>

#define N 1000

int main(int argc, char **argv)
{
  int i;
  double rmax, sum, total_sum;
  double A[N];

  rmax = 1.0/(double)RAND_MAX;

  for(i=0; i<N; i++) A[i] = ((double)random())*rmax;

  total_sum = 0.0;
#pragma omp parallel private(i, sum) shared(total_sum)
{
  sum = 0.0;
#pragma omp for
  for(i=0; i<N; i++){
    sum += A[i];
  }
  printf("%f\n",sum);
#pragma omp atomic
  total_sum += sum;
}

printf("total sum = %f\n",total_sum);
}
```

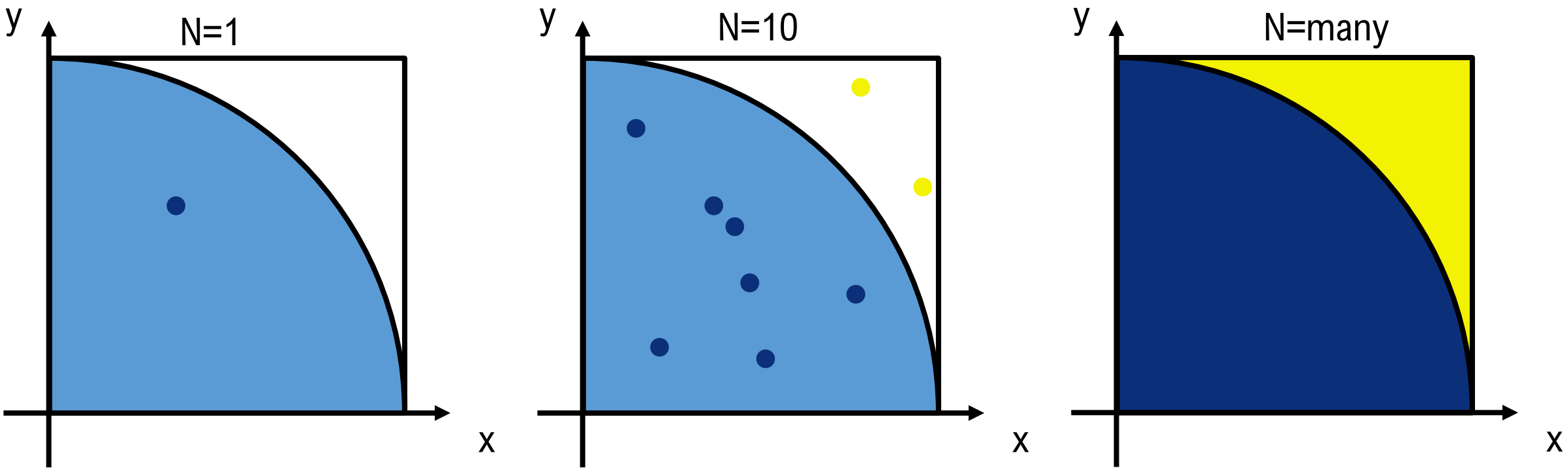
Exercise: parallelize the pi code by using OpenMP

and check execution time by changing the number of threads, 1, 2, 14, 28

```
#include<stdio.h>
#include<stdlib.h>
#include<omp.h>

#define N 100000000
double mytime();

int main(int argc, char **argv)
{
  int i, n, seed;
  double x, y;
  double t0, t1;
  struct drand48_data drand_buf;

  t0 = mytime();

  seed = 0;
  srand48_r (seed, &drand_buf);

  n = 0;
  for(i=0; i<N; i++){
    drand48_r (&drand_buf, &x);
    drand48_r (&drand_buf, &y);

    if(x*x + y*y < 1.0){
      n++;
    }
  }

  t1 = mytime();
  printf("pi = %f time=%f¥n",4.0*(double)n/(double)N,
t1-t0);

}

double mytime()
{
  struct timeval tv;
  gettimeofday(&tv, NULL);
  return tv.tv_sec + tv.tv_usec*1e-6;
}
```

Exercise: parallelize the pi code (FYI)

- Compute pi using Monte Carlo method
  - generate N sets of two random numbers of [0, 1] : (x,y)
  - if (x, y) is in the inside of quadrant of radius 1, then n++
  - the ratio of n/N approximates the area of the quadrant
    - n/N = (1*1*pi)/4
    - pi = 4*n/N



Exercise: parallelize the pi code

- Hints:
  - drand_buf, seed, must be “private”

MPI (review) : Message Passing Interface

- MPI is not a programming language.
- MPI is a message passing interface specification.
- Programmers call MPI functions to communicate
- MPI_Init function initializes the MPI execution environment. All other MPI functions must be called **after** the MPI_Init
- MPI_Finalize function finalizes the MPI execution environment. All processes must call this before exiting.

```c
#include<mpi.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  MPI_Init(&argc, &argv);
  /* starts MPI */

  printf("Hello world\n");

  MPI_Finalize();
  /* exits MPI */
  return 0;
}
```

MPI: Hello world

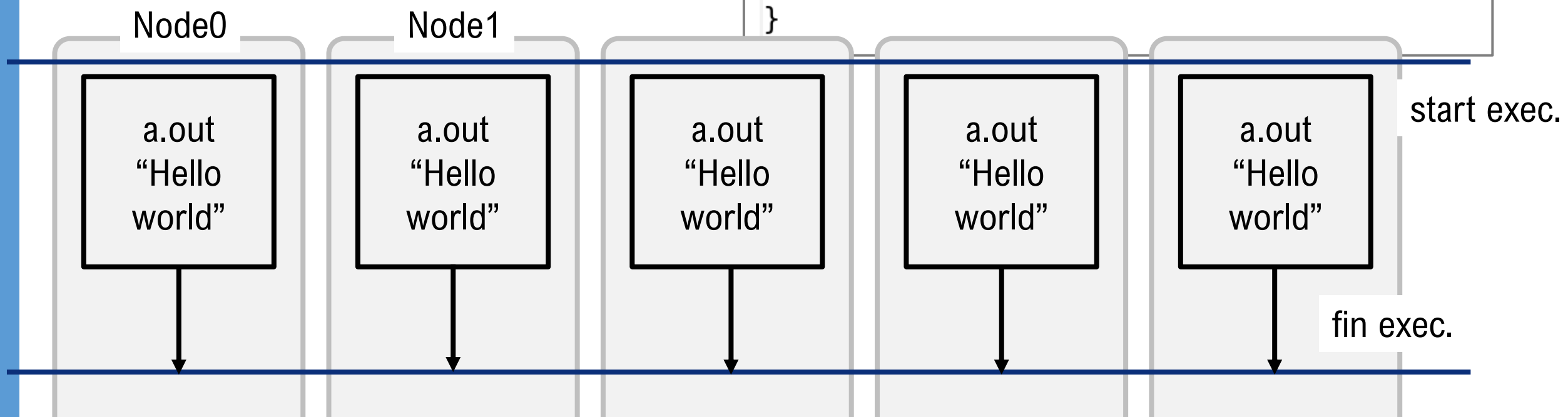
- MPI programs must be launched by a command for execution such as mpirun, mpiexe:

$ mpiexec.hydra –n *num your_binary*

- This runs *num* copies of *your_binary*

```c
#include<mpi.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  MPI_Init(&argc, &argv);
  /* starts MPI */

  printf("Hello world\n");

  MPI_Finalize();
  /* exits MPI */
  return 0;
}
```

includes MPI definitions and types



MPI: Hello world from who?

- MPI library provides functions to give
  - ID number (rank) of a specific process
  - the number of processes in a program
- MPI_Comm_rank gives the rank of the calling process in the communicator (MPI_COMM_WORLD)
- MPI_Comm_size gives the number of processes in the communicator.

Note: *Communicator* contains a list of processes attending a program. MPI_COMM_WORLD is the default communicator

```c
#include<mpi.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myrank, nprocs;

  MPI_Init(&argc, &argv);

  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  /* gets the ID number of "this" process */

  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
  /* gets the number of processes */

  printf("I'm number %d of %d processors\n",myrank, nprocs);

  MPI_Finalize();

  return 0;
}
```

Exercise: Hello world from who (MPI)

- write the hello world from who code in the previous page, compile and run with 4 processes

Here is an example of a jobscript

```
#!/bin/bash
#PJM -L "node=1"
#PJM -L "rscunit=rscunit_ft01"
#PJM -L "rscgrp=small"
#PJM -L "elapse=0:10:00“
#PJM --mpi "max-proc-per-node=4"
#PJM -S

#------- Program execution -------#
mpiexec -n 4 ./<your binary>
```

MPI: Synchronization

- MPI also provides a function to synchronize all processes in a communicator, MPI_Barrier

```c
#include<mpi.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myrank, nprocs;

  MPI_Init(&argc, &argv);

  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

  MPI_Barrier(MPI_COMM_WORLD);
  /* Blocks until all processes in the communicator have
     reached this routine. */

  printf("I'm number %d of %d processors\n",myrank, nprocs);

  MPI_Finalize();

  return 0;
}
```

MPI: Pairwise communication

- MPI_Send sends the buffer to the specified rank (dest)
- MPI_Recv receives the buffer from the specified rank (source)

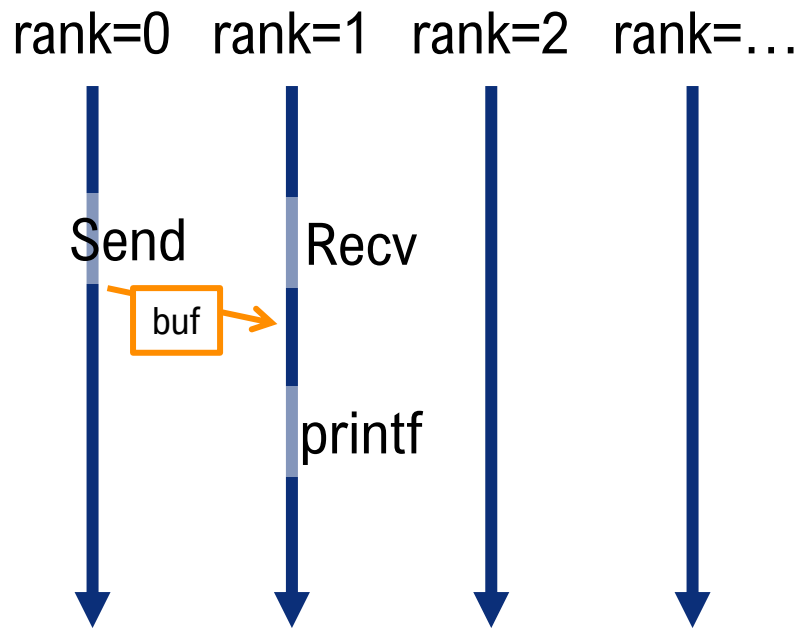
```
int MPI_Send(const void *buf, int count, MPI_Datatype datatype, int dest, int tag,
             MPI_Comm comm)

int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag,
             MPI_Comm comm, MPI_Status *status)
```

- **buf:** the pointer to buffer to be sent/received
- **count**: the number of elements in the buffer
- **datatype**: MPI_INT, MPI_LONG, MPI_FLOAT, MPI_DOUBLE, …
- **dest/source**: rank of destination/source
- **tag**: message tag
- **comm**: communicator

Remarks: If there is no corresponding MPI_Recv function call in *dest* processes, MPI_Send can never be success, and never finish. vice, sersa

MPI: Pairwise communication

```c
#include<mpi.h>
#include<stdio.h>

int main(int argc, char **argv)
{
  int myrank, nprocs;
  int yourrank;
  MPI_Status stat;

  MPI_Init(&argc, &argv);

  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

  if(myrank==0){
    MPI_Send(&myrank, 1, MPI_INT, 1, 123, MPI_COMM_WORLD);
  }else if(myrank==1){
    MPI_Recv(&yourrank, 1, MPI_INT, 0, 123, MPI_COMM_WORLD, &stat);
    printf("I'm number %d, I've received %d\n",myrank, yourrank);
  }

  MPI_Finalize();

  return 0;
}
```



Exercise: Pairwise communication

- write, compile and run the code in the previous page with 2 processes

- modify the code in the previous page to perform the following communication:

  rank-0 sends an integer to rank-1

  rank-2 sends an integer to rank-3

  …

  rank-n sends an integer to rank-(n+1)

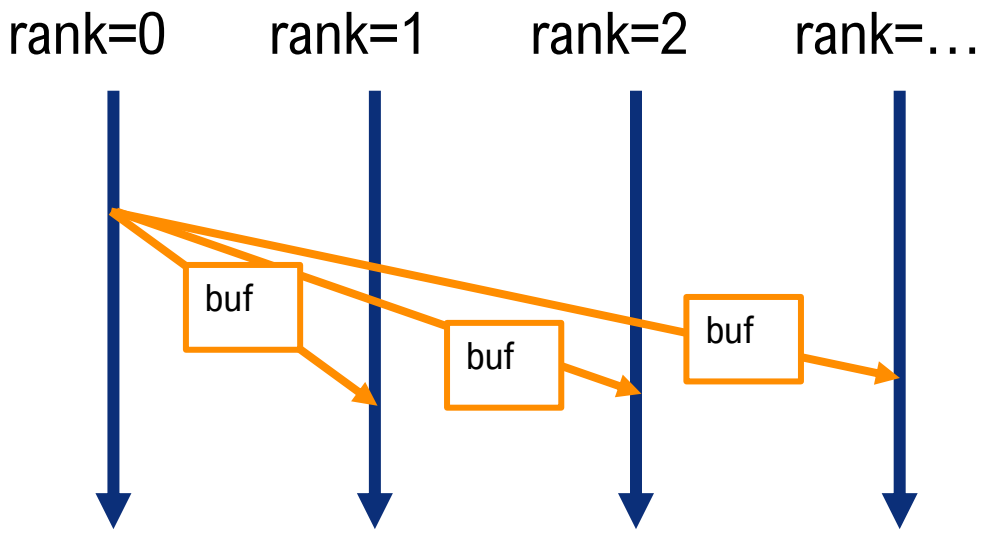
  and run the program with 10, 11, and 24 processes

MPI: Collective communication bcast

- Collective communication involves all processes in a communicator
  - we've already learned MPI_Barrier (MPI_COMM_WORLD), which is a kind of collective communication to make all processes synchronize
- MPI_Bcast broadcasts a buffer from a process to all processes

```
int MPI_Bcast(const void *buf, int count, MPI_Datatype datatype,
              int root, MPI_COMM comm);
```

  - **root** is the rank of broadcast root. All processes can be root



MPI: Collective communication reduction

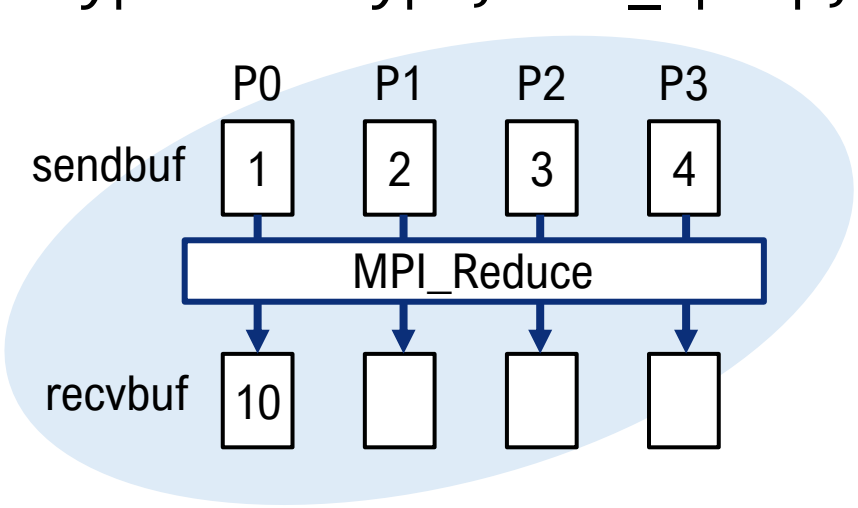
- MPI_Reduce reduces the values on all processes to a single value

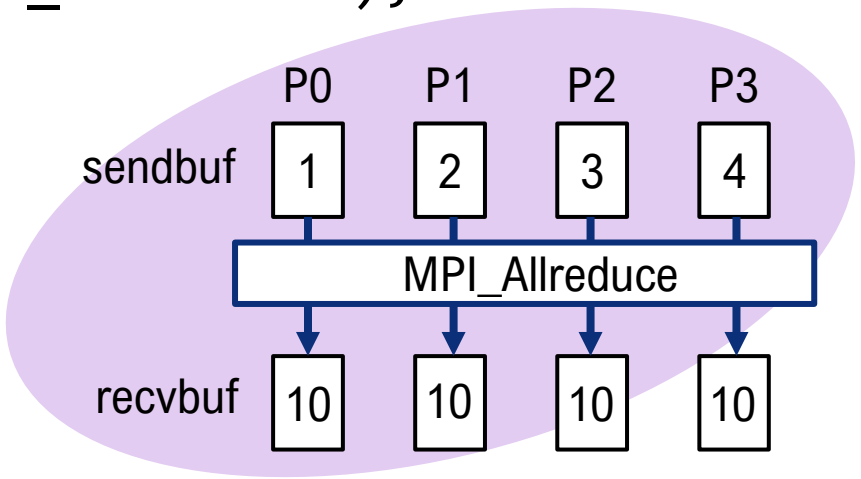
```
int MPI_Reduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype
datatype, MPI_Op op, int root, MPI_COMM comm);
```

  - **sendbuf**, **recvbuf**: address of send/recv buffer
  - **op**: reduce operation (MPI_SUM, MPI_MAX, MPI_MIN, etc)
  - **root**: rank of root process

- MPI_Allreduce reduce the values on all processors to a single value, and share the value among all processors

```
int MPI_Allreduce(void *sendbuf, void *recvbuf, int count,
MPI_Datatype datatype, MPI_Op op, MPI_COMM comm);
```





Exercise: Collective communication

- Write, compile and run the code->
- Replace MPI_Reduce with MPI_Allreduce, and compare the results

```
#include<mpi.h>
int main(int argc, char **argv)
{
  int        send[2], recv[2];
  int        myrank;
  MPI_Status stat;

  MPI_Init(&argc, &argv);

  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

  send[0] = myrank*10+1;
  send[1] = myrank*20+1;

  printf("rank %d sends %d, and %d\n",myrank, send[0], send[1]);

  MPI_Reduce(send, recv, 2, MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);

  if(myrank==0){
    printf("recv[0] is %d, recv[1] is %d\n",recv[0],recv[1]);
  }

  MPI_Finalize();

  return 0;
}
```

Exercise:

- prepare an integer array of size 3
- substitute your favorite numbers to the array at rank-0
- share the favorite numbers to all processes
  1) by using MPI_Send/Recv
  2) by using MPI_Bcast
  3) by using MPI_Allreduce
- run the three program (all with 28 processors) and check if the numbers can be shared successfully

References:

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- “Structured Parallel Programming: Patterns for Efficient Computation,” Michael McCool, Arch Robinson, James Reinders
- MPI and Hybrid Programming Models William Gropp
- https://www.openmp.org/wp-content/uploads/omp-hands-on-SC08.pdf