HELP US ALL STAY HEALTHY

SIX SIMPLE TIPS

Maintain 1.5 metres distance between yourself and others where possible

Cough and sneeze into your elbow or a tissue (not your hands)

Avoid shaking hands

Put used tissues in the bin

Wash hands with soap and warm water or use an alcohol-based hand sanitiser after you cough or sneeze

Do not touch your face

IF YOU ARE UNWELL AND WORRIED ABOUT COVID-19:

- Call the National Coronavirus Helpline: 1800 020 080
- Call your usual GP for advice
- Call the UWA Medical Centre for advice: 6488 2118

UWA FAQs:
uwa.edu.au/coronavirus

Report COVID-19 hazards and suspected/confirmed cases via RiskWare:
uwa.edu.au/riskware

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High-Performance Computing

Lecture 2 Introduction to Parallel Programming and OpenMP

CITS5507

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Acknowledgement: The lecture slides are adapted from many online sources.

Outline

- Parallel Programming
  - ✓ Why, What and How
- Parallel Architectures
  - ✓ SISD, SIMD, MIMD
  - ✓ CPU v.s. GPU, Cluster v.s. Multicores
- Shared and Distributed Memory Systems
  - ✓ OpenMP and MPI
- Introduction to OpenMP
  - ✓ What is OpenMP
  - ✓ Hello World Example
  - ✓ Loop Example

Why Parallel Programming

- **To solve larger problems**
  - many applications need significantly more memory than a regular PC can provide/handle
  - many computers, or “nodes” can be combined into a cluster

- **To solve problems faster**
  - despite of many advances in computer hardware, many applications are running slower and slower
    - ✓ databases having to handle more and more data
    - ✓ working on more accurate solutions

- **Make use of less powerful hardware**

Parallel Programming Analogy

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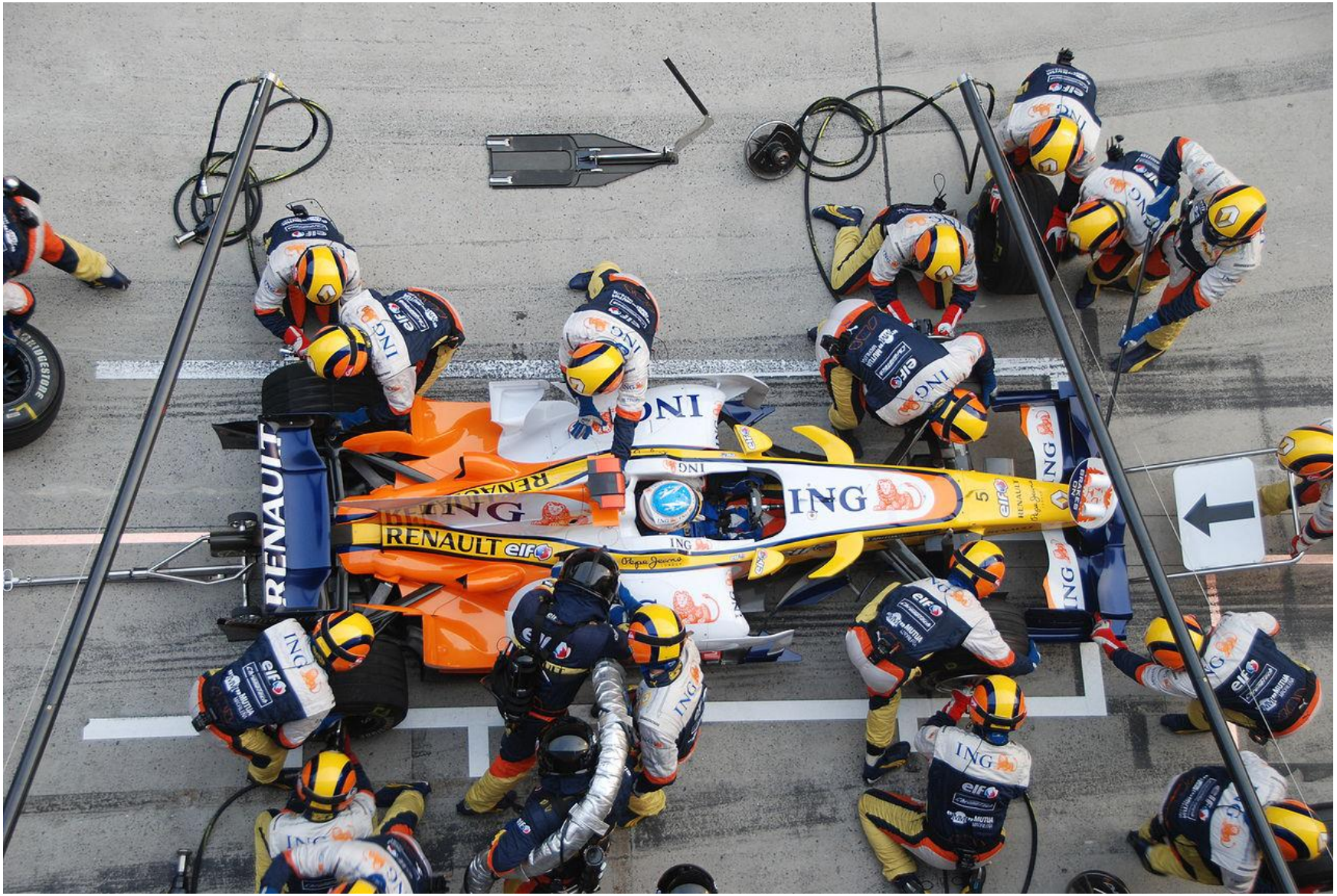
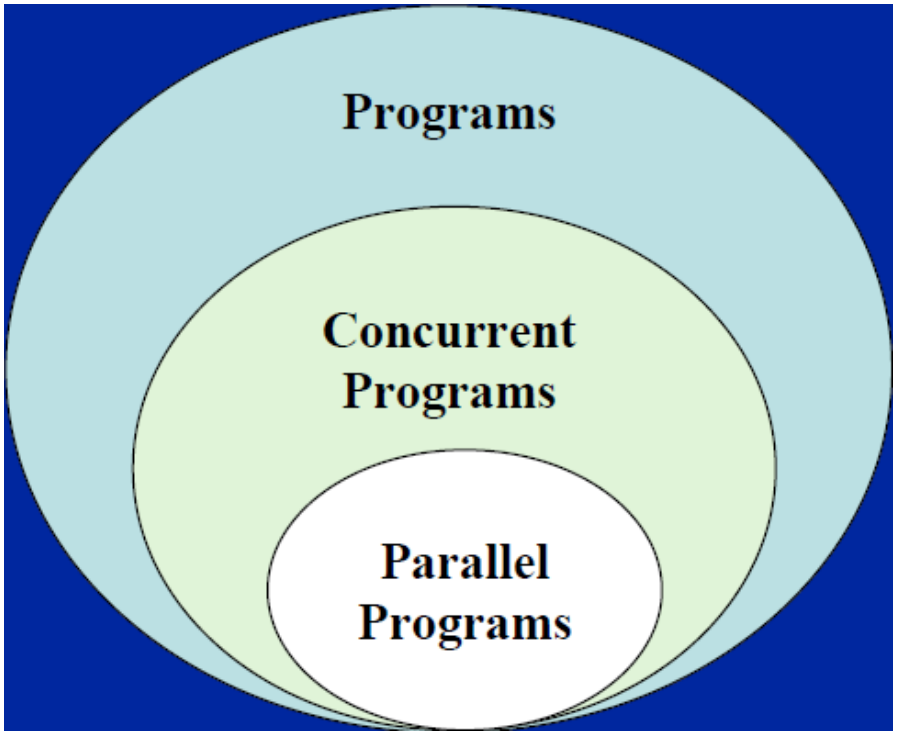


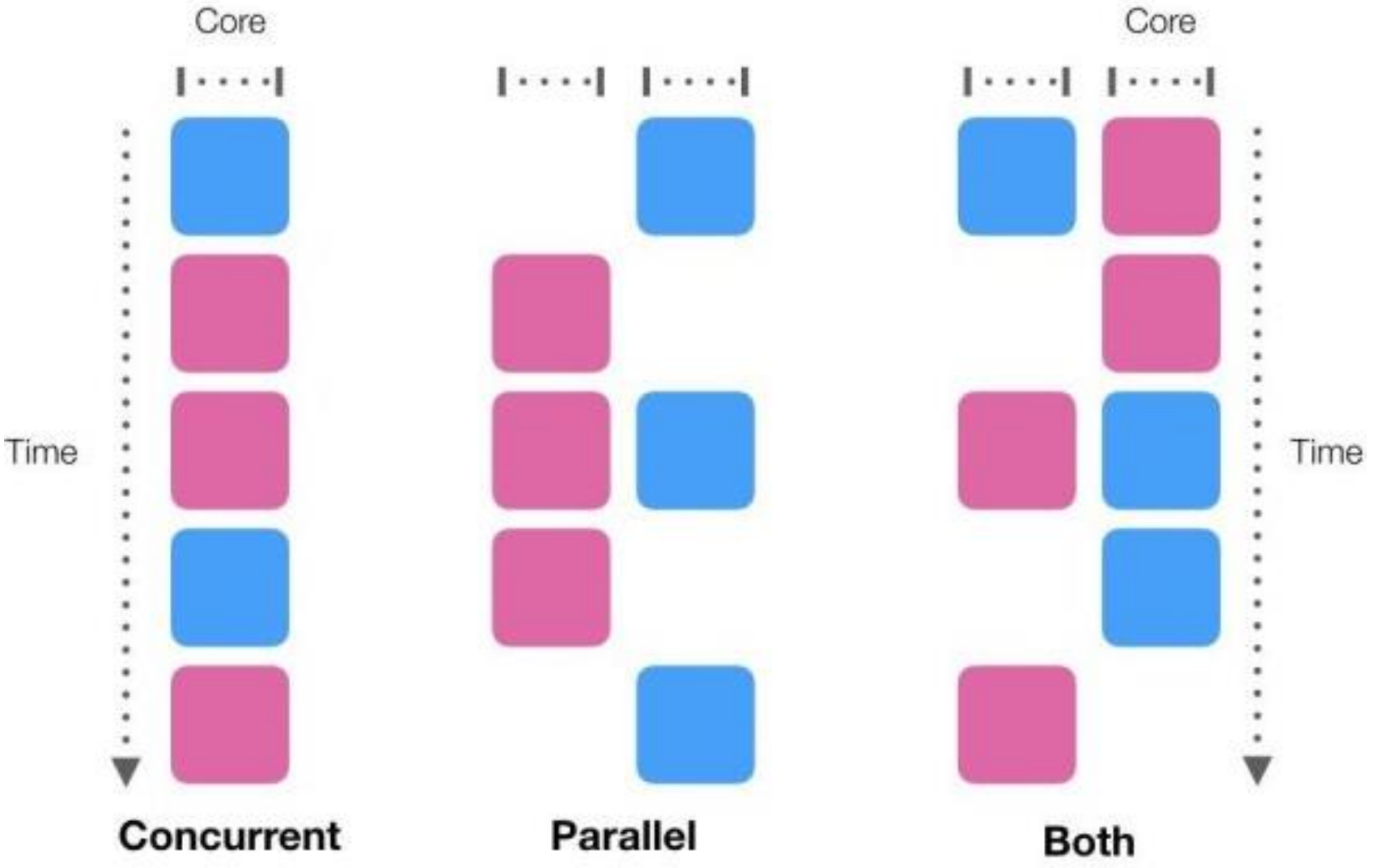
Concurrent and Parallel Programs

Two important definitions:

- Concurrency: A condition of a system in which multiple tasks are logically active at one time.
- Parallelism: A condition of a system in which multiple tasks are actually active at one time.

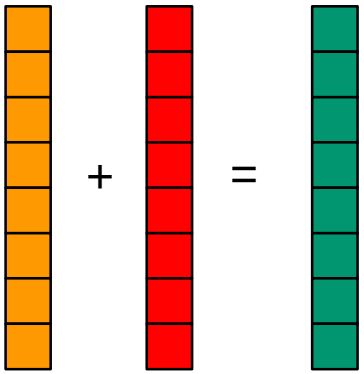


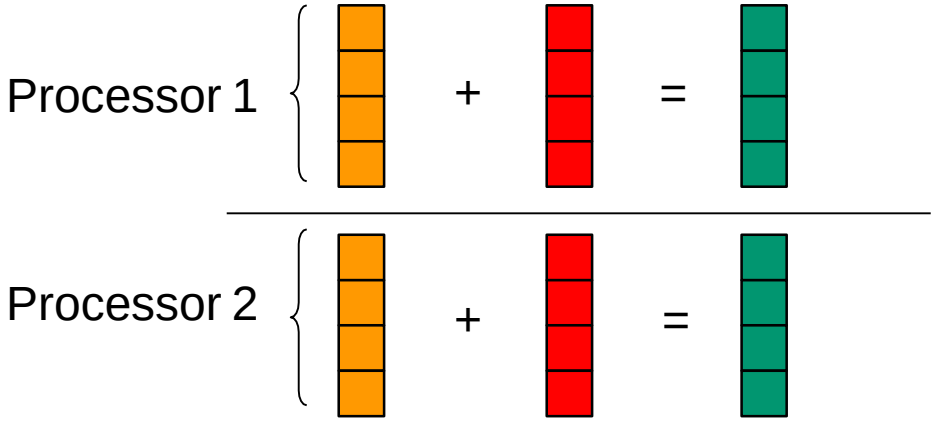
(Lecture 1) Concurrency v.s. Parallelism



Parallel Programming

- **Exploit concurrency**
  - Internet: client and server are independent, interacting applications
  - Searching an element: distribute the search database onto multiple processors
  - Adding two arrays of integers:





Parallel Programming (Continued)

- **Scalar product:**

$$s = \sum_{i=0}^{N-1} a[i] * b[i]$$

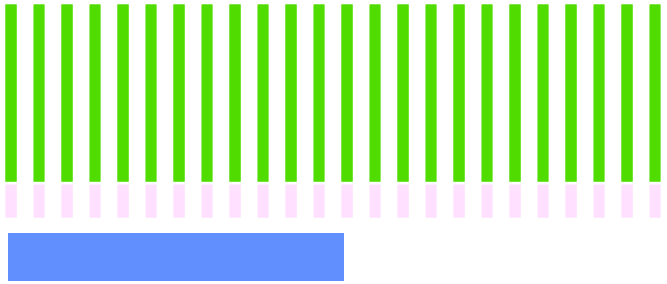
- **Parallel algorithm**

$$s = \sum_{i=0}^{N/2-1} a[i] * b[i] + \sum_{i=N/2}^{N-1} a[i] * b[i]$$

Parallel Programming Process

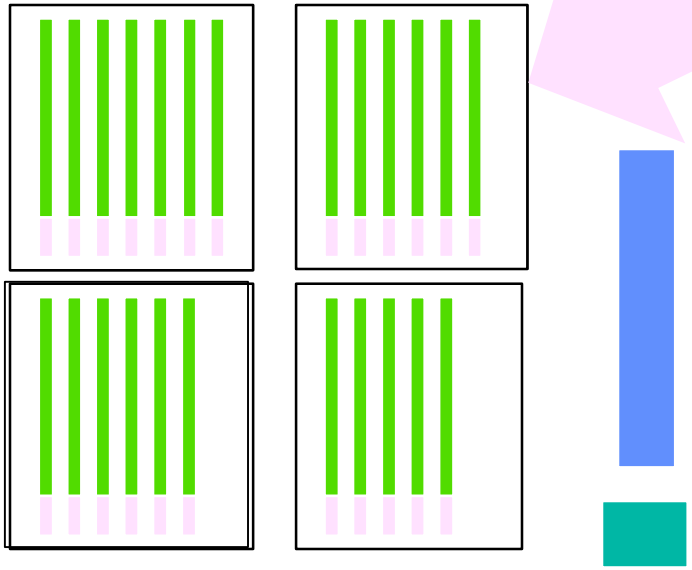
Original Problem

Find Concurrency



Tasks, shared and local data

Algorithm strategy



Units of execution + new shared data for extracted dependencies

Implementation strategy

```
Program SPMD_Emb_Par ()
Program SPMD_Emb_Par ()
Program SPMD_Emb_Par ()
Program SPMD_Emb_Par ()
{
TYPE *tmp, *func();
global_array Data(TYPE);
global_array Res(TYPE);
int Num = get_num_procs();
int id = get_proc_id();
if (id==0) setup_problem(N, Data);
for (int I= ID; I<N;I=I+Num){
tmp = func(I, Data);
Res.accumulate( tmp);
}
}
```

Job Scheduling

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- Integral to parallel computing
  - ✓ assign tasks to cores
- Job scheduling also used in
  - ✓ batch jobs,
  - ✓ multiple users,
  - ✓ resource sharing,
  - ✓ system monitoring

Realistic Expectations

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- Ex. – Your program takes 20 days to run
- 95% can be parallelized
- 5% cannot (serial)
- What is the fastest this code can run?
  - ✓ As many CPU's as you want!

1 day!

Amdahl's Law

- Hardware speed measured in FLOPS
  - ✓ FLOPS: Floating Point Operation Per Second

Disadvantages and Issues

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- No free lunch - can't just "turn on" parallel
  - ✓ It's a lot more complex to implement
- Parallel programming requires work
  - ✓ Code modification – **always**
  - ✓ Algorithm modification – often
  - ✓ New sneaky **bugs** – you bet
- Speedup limited by many factors
- **Not everything benefits**
  - ✓ Many problems must be solved sequentially (e.g. protein folding)
  - ✓ Interactive stuff

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Computer Architectures

- As you consider parallel programming understanding the **underlying architecture** is important (review Lecture 1).

- Performance is affected by hardware configuration
  - ✓ Memory or CPU architecture
  - ✓ Numbers of cores/processor
  - ✓ Network speed and architecture

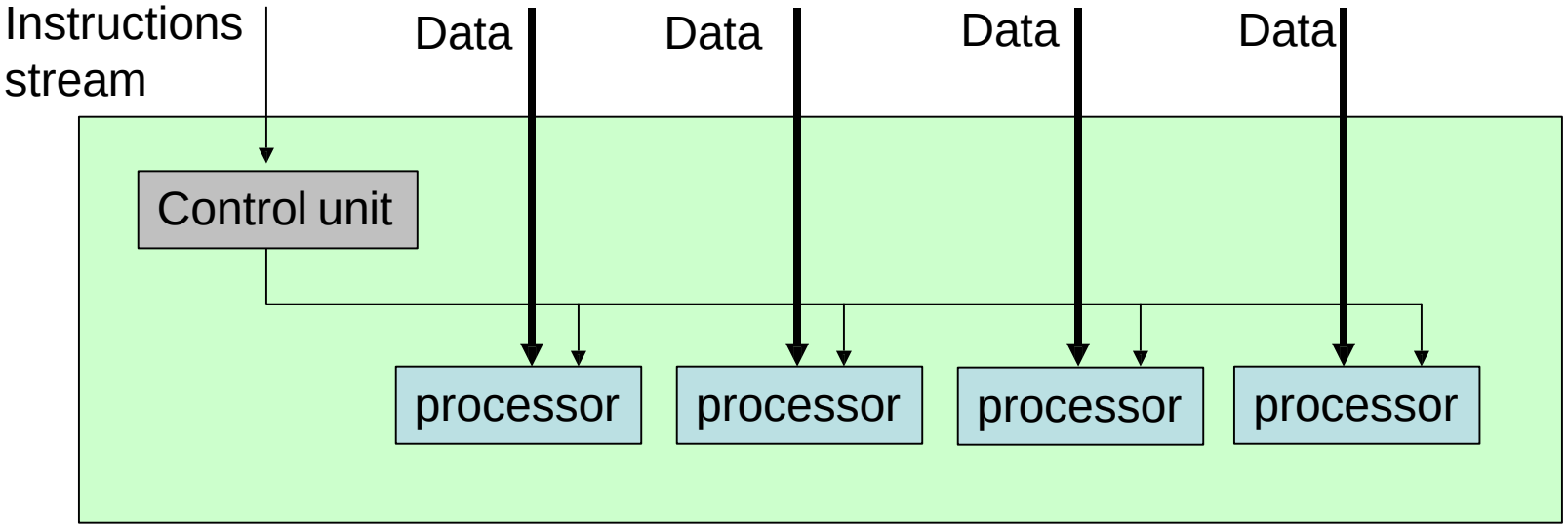
Classification of Parallel Architectures

Flynn's Taxonomy

- SISD: Single instruction single data
  - Classical von Neumann architecture
- SIMD: Single instruction multiple data
- MISD: Multiple instructions single data
  - Non existent, just listed for completeness
- MIMD: Multiple instructions multiple data
  - Most common and general parallel machine

Single Instruction Multiple Data (SIMD)

- Also known as array/vector-processors
- A single instruction stream is broadcasted to multiple processors, each having its own data stream
  - Still used in graphics cards (i.e. GPUs) today
  - CPUs can also support SIMD (e.g. AVX-512)



Multiple Instructions Multiple Data (MIMD)

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- Each processor has its own instruction stream and input data
- Very general case
  - every other scenario can be mapped to MIMD
- Further breakdown of MIMD usually based on the memory organisation
  - Shared memory systems
  - Distributed memory systems

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GPU Architectures

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- Like a multi-core CPU, but with thousands of cores
- Has its own memory to calculate with
- GPU advantages
  - ✓ higher computation power than CPUs
  - ✓ can be thousands of simultaneous calculations
  - ✓ relatively cheap in terms of FLOPS or cores per $
- Modern GPU frameworks
  - ✓ CUDA: Proprietary, easy to use, sponsored by NVIDIA and only runs on their cards
  - ✓ OpenCL: Open, a bit harder to use, runs on both AMD and NVIDIA GPUs; also can run on CPUs

CPU or GPU? Cluster or Multicore?

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- CPU or GPU?
  - ✓ CPU: Easier to program for, has much more powerful individual cores
  - ✓ GPU: Trickier to program for, thousands of relatively weak cores

- Cluster or Multicore?
  - ✓ Multicore: All the cores are in a single computer, usually shared memory.
  - ✓ Cluster: Many computers linked together, each with individual memory.

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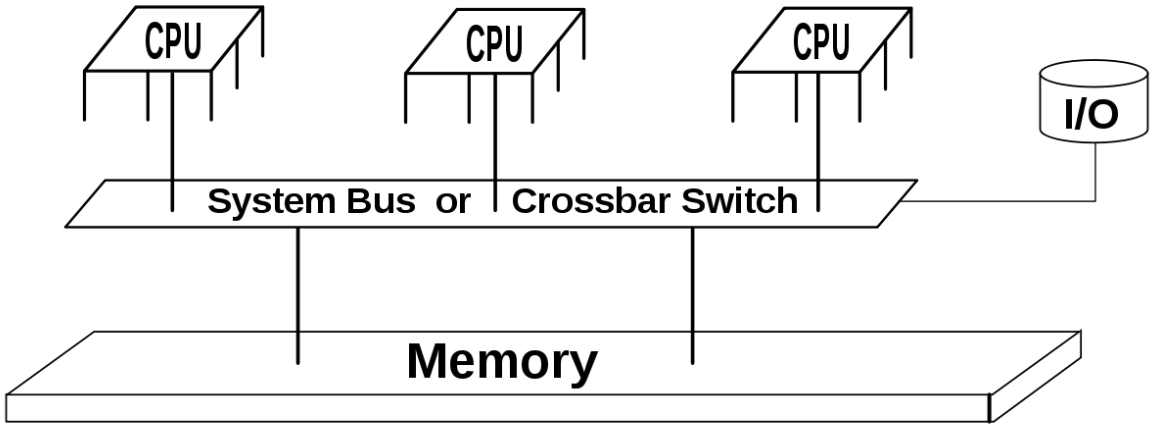
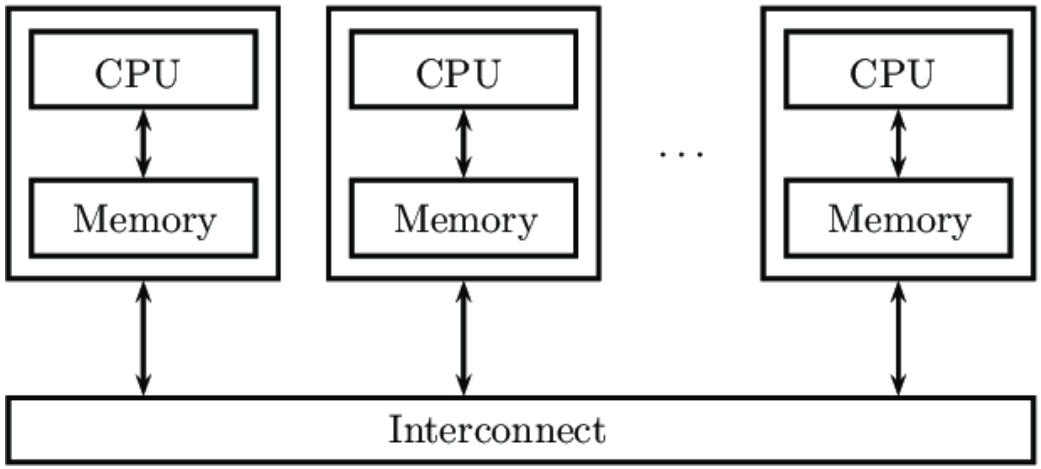
Shared and Distributed Memory Systems





Shared Memory Systems

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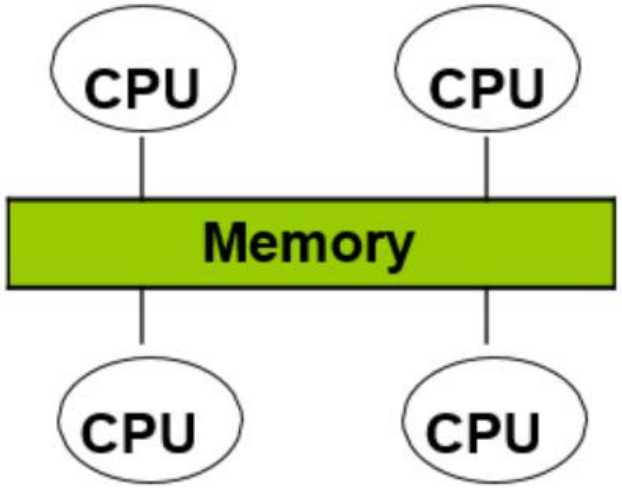
- All processes have access to the same address space
  - A computer/machine with more than one processor
- Data exchange between processes by writing/reading shared variables
  - Shared memory systems are easy to program
  - Popular programming interface: OpenMP
- Two versions of shared memory systems available today
  - Symmetric multiprocessors (SMP)
  - Non-uniform memory access (NUMA) architectures

Symmetric Multi-Processors (SMPs)

- All processors share the same physical main memory

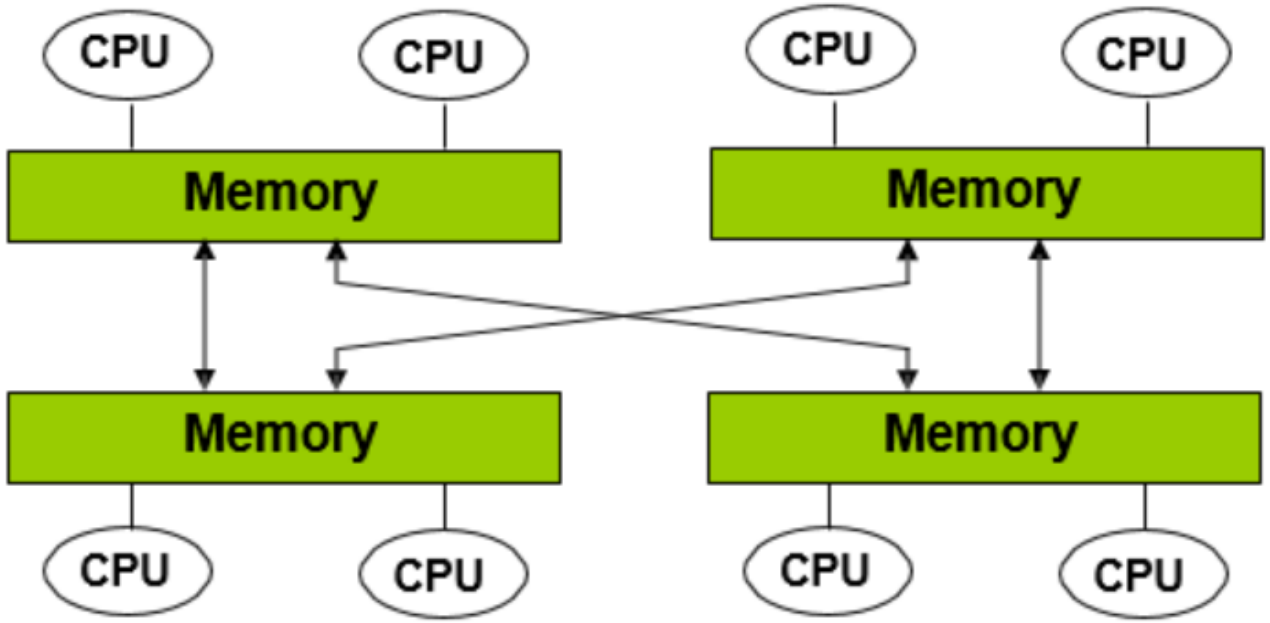


- Memory bandwidth per processor is a limiting factor for this type of architecture

- Typical size: 2-32 processors

NUMA Architectures

- Some memory is closer to a certain processor than other memory
  - The whole memory is still addressable from all processors
  - Depending on what data item a processor retrieves, the access time might vary strongly

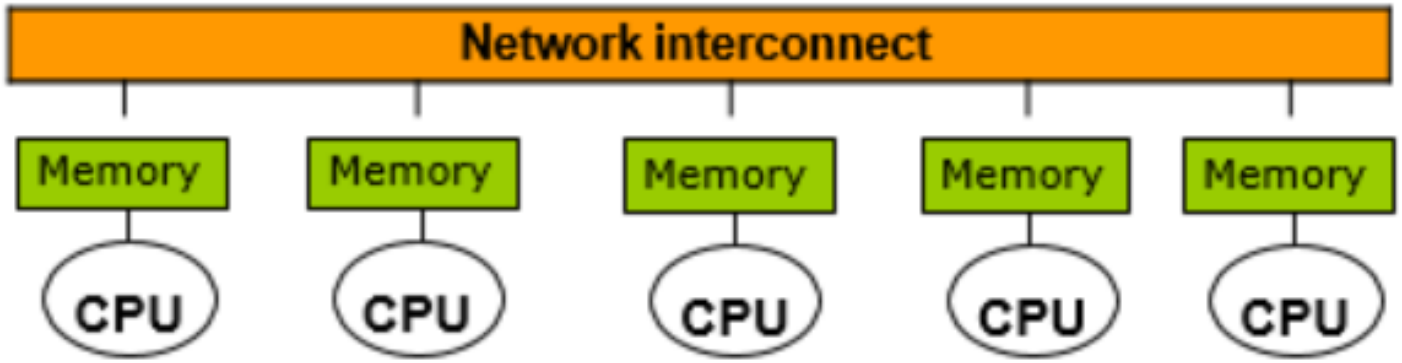


NUMA Architectures (Continued)

- Reduces the memory bottleneck compared to SMPs
- More difficult to program efficiently
  - E.g. first touch policy: data item will be located in the memory of the processor which uses a data item first
- To reduce effects of non-uniform memory access, caches are often used
  - ccNUMA: cache-coherent non-uniform memory access architectures
- Example: SGI Origin with 512 processors

Distributed Memory Machines

- Each processor has its own address space
- Communication between processes by explicit data exchange
  - Sockets (a term in computer network)
  - Message passing (this unit covers in the 2nd half)
  - Remote procedure call/remote method invocation



Distributed Memory Machines (Continued)

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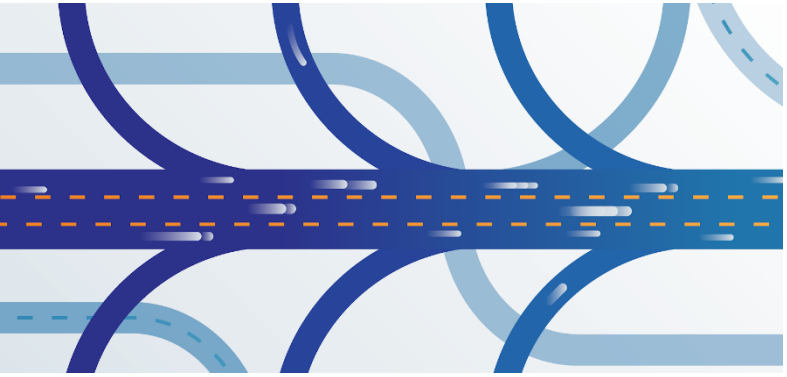
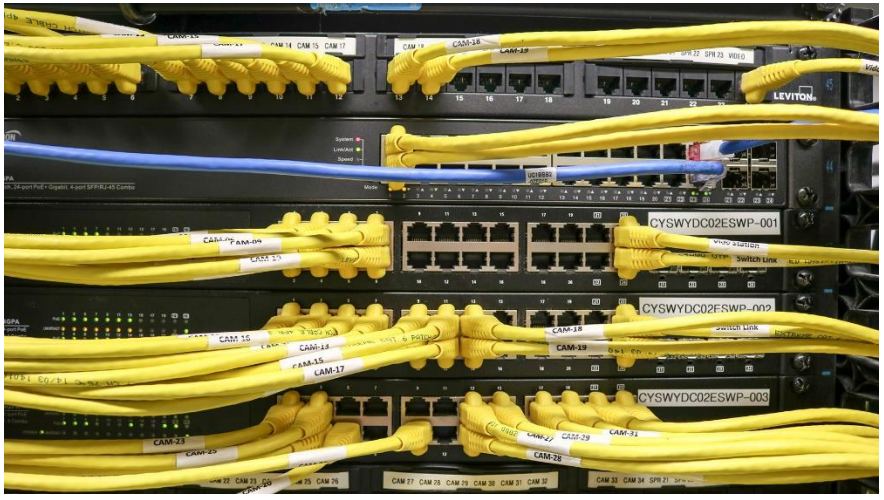
- Performance of a distributed memory machine strongly depends on the quality of the network interconnect and the topology of the network interconnect
  - Of-the-shelf technology: fast-Ethernet, gigabit-Ethernet
  - Specialised interconnects: Myrinet, **Infiniband**, Quadrics, 10G Ethernet…





Distributed Memory Machines (Continued)

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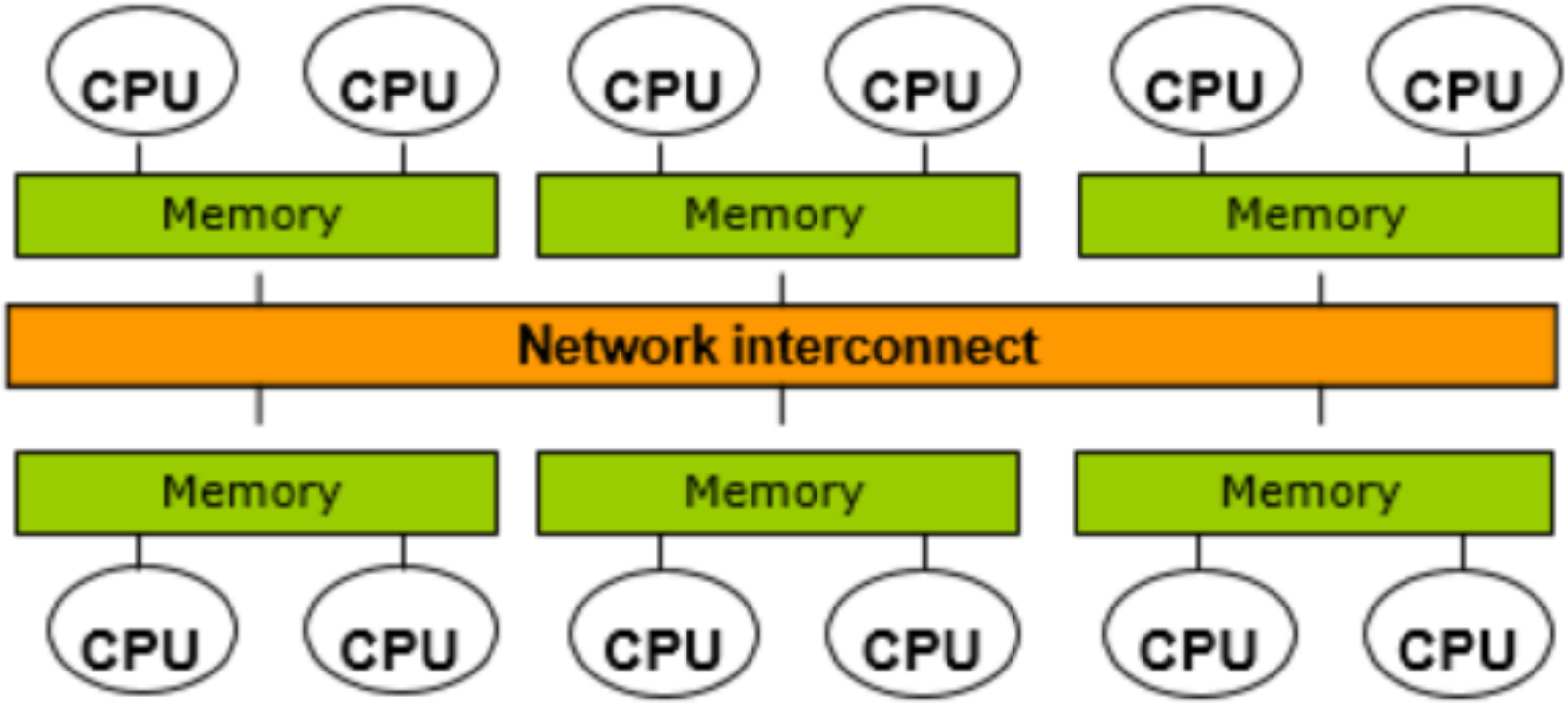
- Two classes of distributed memory machines:
  - Massively parallel processing systems (MPPs)
    - Tightly coupled environment
    - Single system image (specialised OS)
  - Clusters: of-the-shelf hardware/software components
    - Intel Pentium, AMD Opteron, etc.
    - Standard operating systems such as LINUX, Windows, BSD UNIX

Hybrid systems

- E.g. clusters of multi-processor nodes

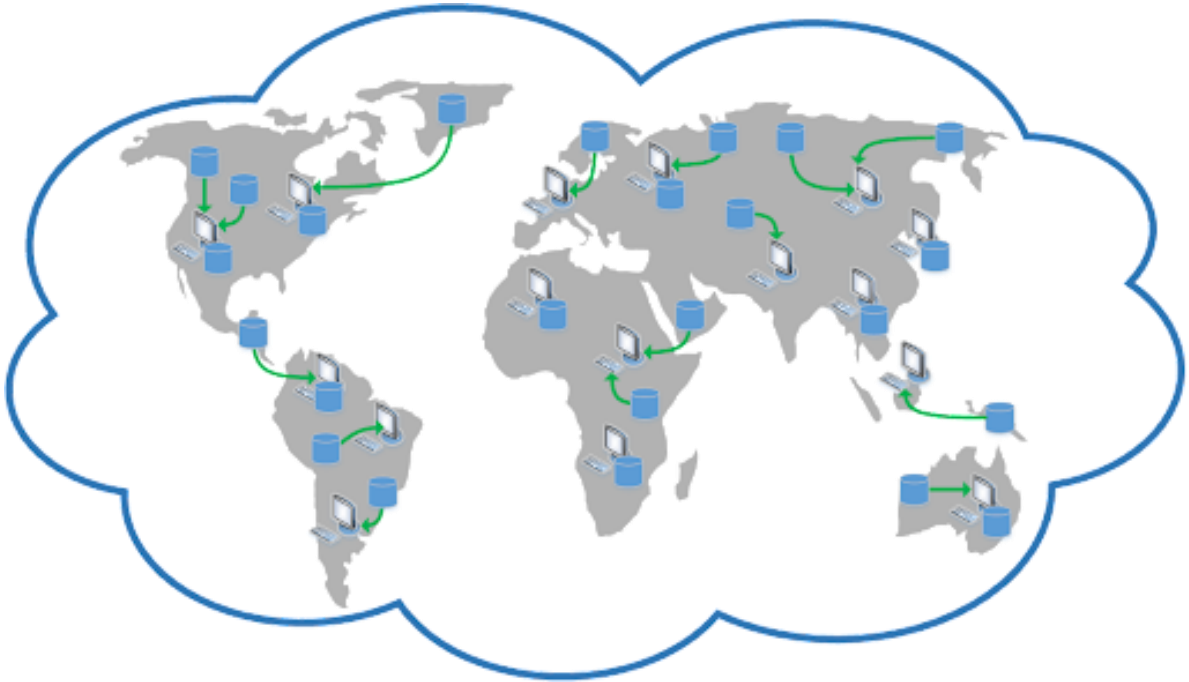


OpenMP and MPI

- **Message Passing Interface (MPI)–designed for distributed memory**
  - Multiple systems
  - Send/receive messages
- **OpenMP (Open Multi-Processing)–designed for shared memory**
  - Single system with multiple cores
  - One thread/core sharing memory
- **C, C++, and Fortran**
- **There are other options**
  - Interpreted languages with multithreading
    - Python, R, matlab (have OpenMP & MPI underneath)
  - CUDA, OpenACC (GPUs)
  - Pthreads, Intel Cilk Plus (multithreading)
  - OpenCL, Chapel, Co-array Fortran, Unified Parallel C (UPC)

Grid

- “Evaluation” of distributed memory machines and distributed computing
- Several (parallel) machines connected by wide-area links (typically the internet)
  - Machines are in different administrative domains



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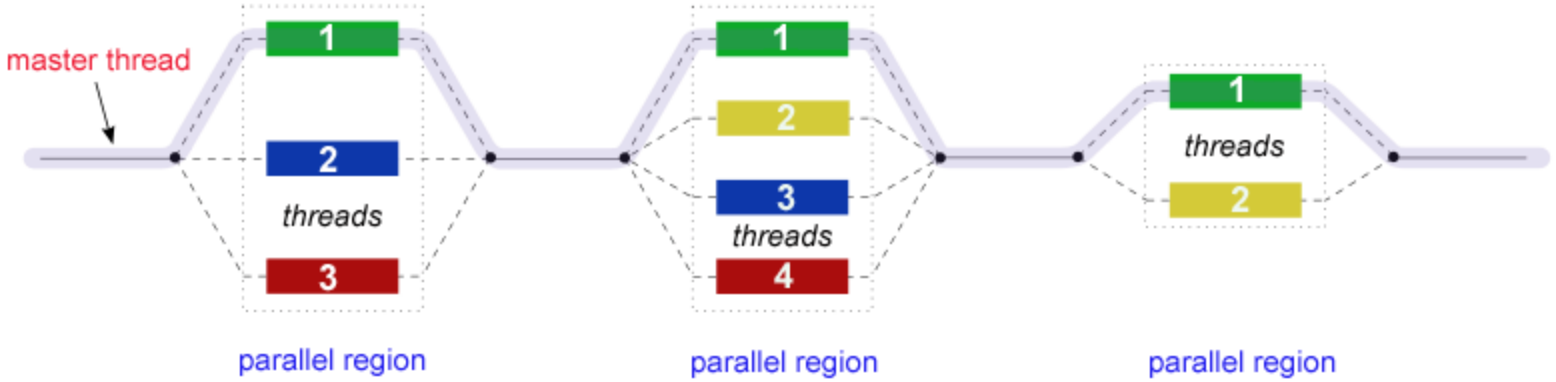
OpenMP

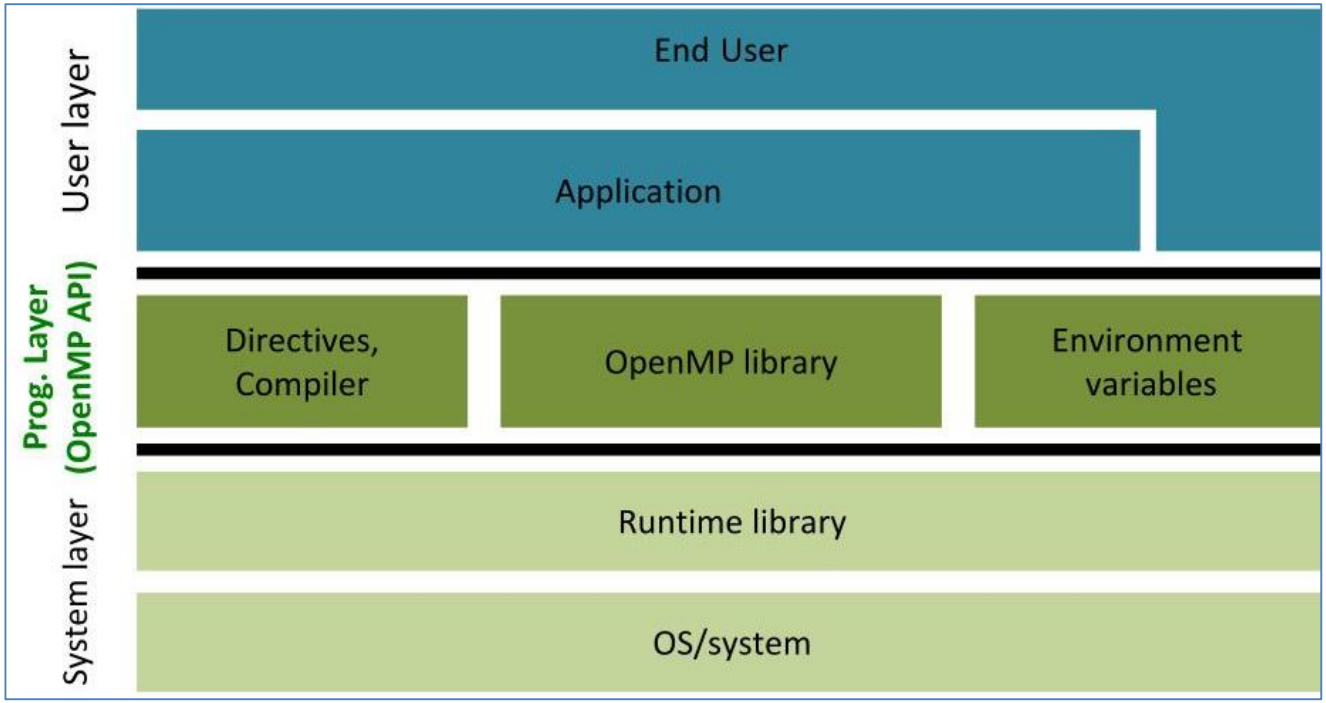
- **What is it?**
  - Open Multi-Processing
  - Completely independent from MPI
  - Multi-*threaded* parallelism
- **Standard since 1997**
  - Defined and endorsed by the major players
- **Fortran, C, C++**
- **Requires compiler to support OpenMP**
  - Nearly all do
- **For shared memory machines**
  - Limited by available memory
  - Some compilers support GPUs

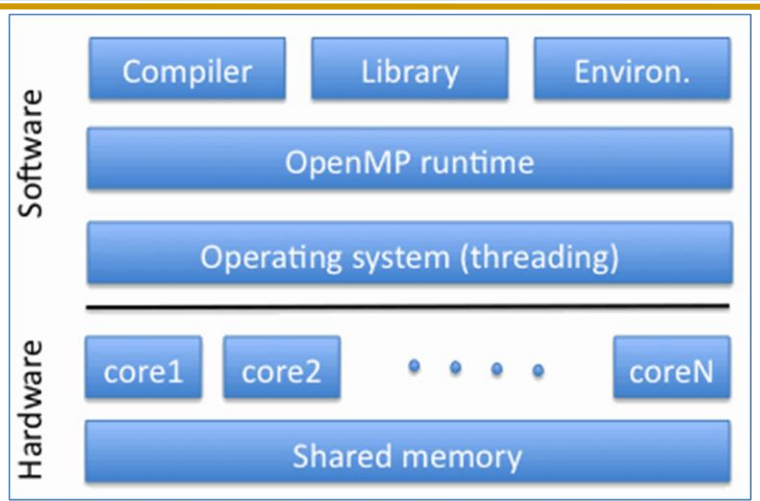
OpenMP (Continued)

- OpenMP is one of the most common parallel programming models in use today.
- It is relatively easy to use which makes a great language to start with when learning to write parallel programs.



OpenMP Solution Stack





Preprocessor Directives

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- Preprocessor directives tell the compiler what to do
- Always start with #
- You've already seen one:

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

- OpenMP directives tell the compiler to add machine code for parallel execution of the following block

```
#pragma omp parallel
```

- "Run this next set of instructions in parallel"

Some OpenMP Subroutines

```
int omp_get_max_threads()
```

- Returns max possible (generally set by OMP_NUM_THREADS)

```
int omp_get_num_threads()
```

- Returns number of threads in current team

```
int omp_get_thread_num()
```

- Returns thread id of calling thread
- Between 0 and omp_get_num_threads-1

(Lecture 1) Process and Thread

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- A process can be considered as an independent execution environment in a computer system.
- There are usually many processes in a system at any time, each with its own memory space.
- Each process executes a sequence of instructions (the machine language program).
- Threads are also independent execution environments, but with a shared memory space (or address space).

Process vs. Thread

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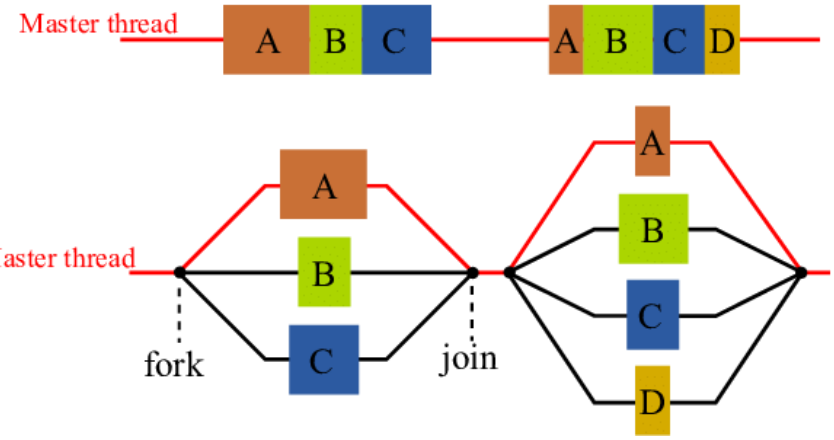
- MPI = Process, OpenMP = Thread
- Program starts with a single process
- Processes have their own (private) memory space
- A process can create one or more threads
- Threads created by a process share its memory space
  - ✓ Read and write to same memory addresses
  - ✓ Share same process ids and file descriptors
- Each thread has a unique instruction counter and stack pointer
  - ✓ A thread can have private storage on the stack

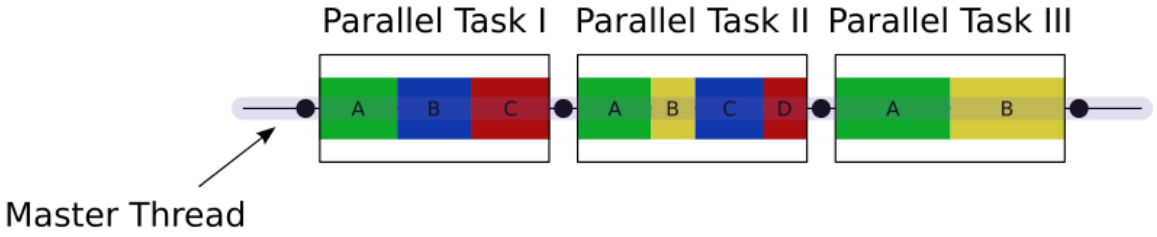
Hyperthreading

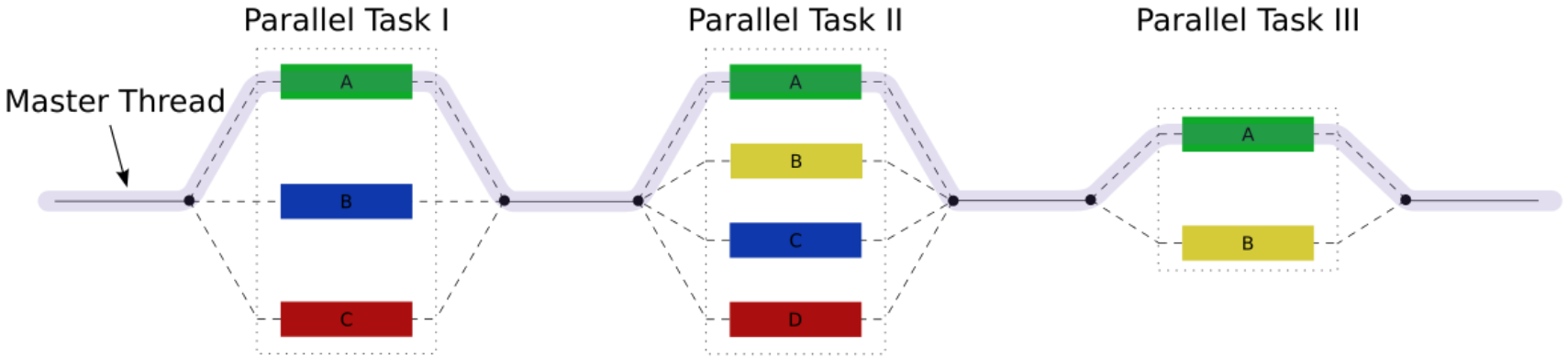
- Hyperthreading is an Intel technology that treats each physical core as two logical cores.
- Two threads are executed at the same time (logically) on the same core.
- Hyperthreading schedules two threads to every core.
- The purpose of hyperthreading is to improve the throughput (processing more per unit time).

OpenMP Fork-Join Model

- Automatically distributes work
- Fork-Join Model







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OpenMP: Hello World Example

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```
#include <omp.h>  //<-- necessary header file for OpenMP API
#include <stdio.h>

int main(int argc, char *argv[]){

  printf("OpenMP running with %d threads\n", omp_get_max_threads());

#pragma omp parallel
  {
    //Code here will be executed by all threads
    printf("Hello World from thread %d\n", omp_get_thread_num());
  }

  return 0;
}
```

Running OpenMP Hello World

```
[vagrant@kaya2]$ module load gcc
[vagrant@kaya2]$ gcc -fopenmp hello_world_omp.c -o hello_world_omp
```

Compiler flag to enable OpenMP
(-fopenmp for gcc)

Environment variable defining max threads

```
[vagrant@kaya2]$ export OMP_NUM_THREADS=4
[vagrant@kaya2]$ ./hello_world_omp
OpenMP running with 4 threads
 Hello World from thread 1
 Hello World from thread 0
 Hello World from thread 2
 Hello World from thread 3
```

- OMP_NUM_THREADS defines run time number of threads can be set in code as well using: omp_set_num_threads()
- OpenMP may try to use all available CPUs if not set (on cluster–always set it!)

Threads Run Independently

```
#pragma omp parallel
  {
    //Code here will be executed by all threads
    printf("Hello World from thread %d\n", omp_get_thread_num());
  }
```

- There is only one thread until the parallel directive is encountered.
- Thread 0 is usually the master thread (that spawns the other threads).
- The parallel region is enclosed in curly brackets.
- There is an implied barrier at the end of the parallel region.

What is a Barrier?

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- A barrier is a place in the process where all threads must reach before further processing occurs.
- Barriers are sometime implicit.
- Barriers are expensive in terms of run time performance. A typical barrier may take hundreds of clock cycles to ensure that all threads have reached the barrier.
- It is better to remove barriers, but this is fraught with danger.

A Variation of OpenMP Hello World

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```
#include <omp.h>  //<-- necessary header file for OpenMP API
#include <stdio.h>
#include <unistd.h>
int main(int argc, char *argv[]){

  printf("OpenMP running with %d threads\n", omp_get_max_threads());

#pragma omp parallel
  {
    //Code here will be executed by all threads
    if(omp_get_thread_num()==3) sleep(1);
    printf("Hello World from thread %d\n", omp_get_thread_num());
  }

  return 0;
}
```

Outline

- Parallel Programming
  - ✓ Why, What and How
- Parallel Architectures
  - ✓ SISD, SIMD, MIMD
  - ✓ CPU v.s. GPU, Cluster v.s. Multicores
- Shared and Distributed Memory Systems
  - ✓ OpenMP and MPI
- Introduction to OpenMP
  - ✓ What is OpenMP
  - ✓ Hello World Example
  - ✓ Loop Example

The Loop Worksharing Construct

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- The loop worksharing construct splits up loop iterations among the threads in a team.

```
#pragma omp parallel
  {
    #pragma omp for
        for(i=0; i<N; i++){
           do_something(i);
        }
  }
```

```
#pragma omp parallel
  {
    #pragma omp for
        for(i=0; i<N; i++){
           c[i] = a[i]+b[i];
        }
  }
```

Sequential code

```
for(i=0; i<N; i++){
   c[i] = a[i]+b[i];
}
```

References

- Readings
  - Hyperthreading
  - A Hands-on Introduction to OpenMP

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