高能所计算中心 IHEP Computing Center

中国科学院高能物理研究所
Institute of High Energy Physics, Chinese Academy of Sciences

高能物理计算暑期学校 IHEP School of Computing

高能物理中的高性能计算技术

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IHEP School of Computing 2023, 2023.8.16-18

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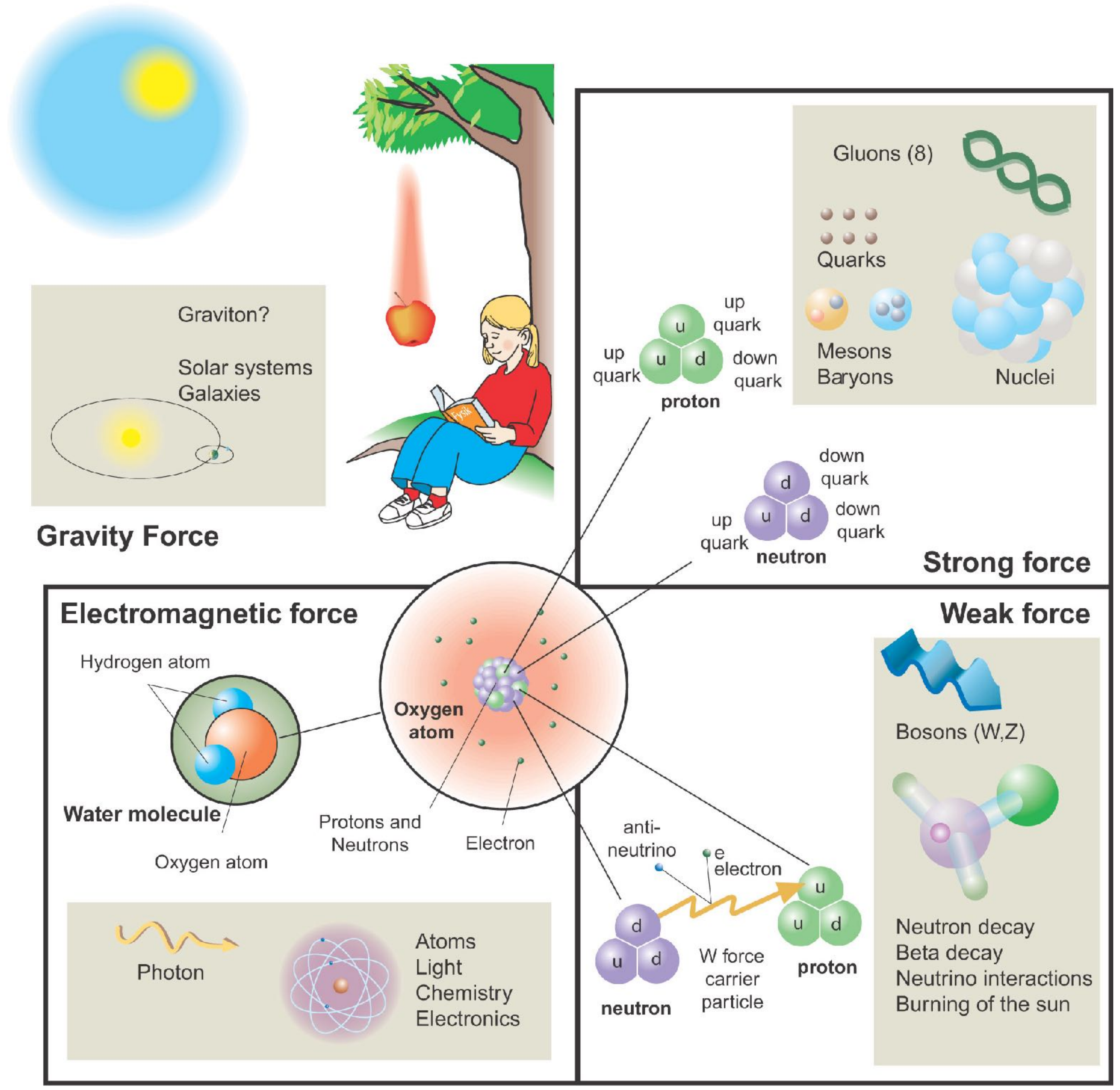


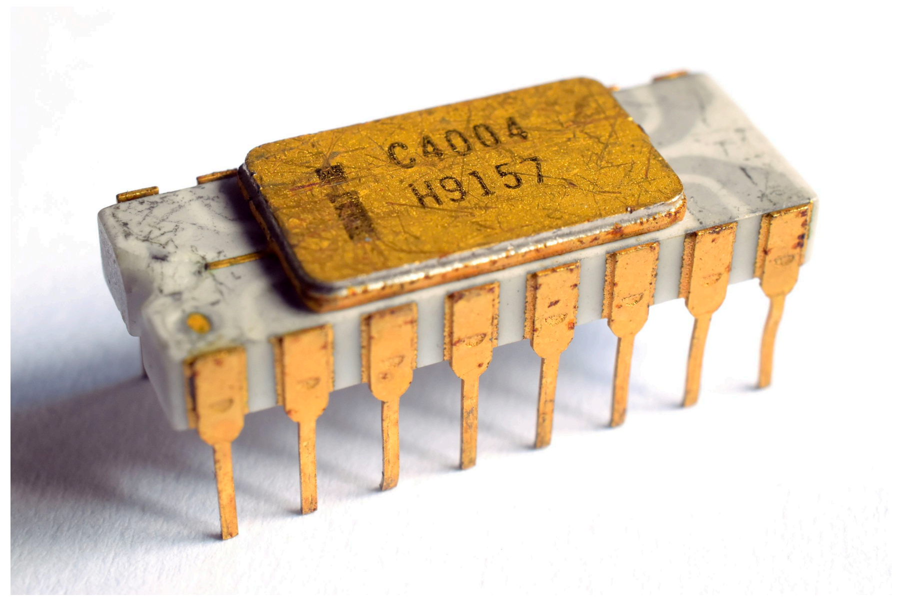
Standard Model

Weinberg–Salam theory

Electromagnetic interaction
Weak interaction

Quantum Chromodynamics

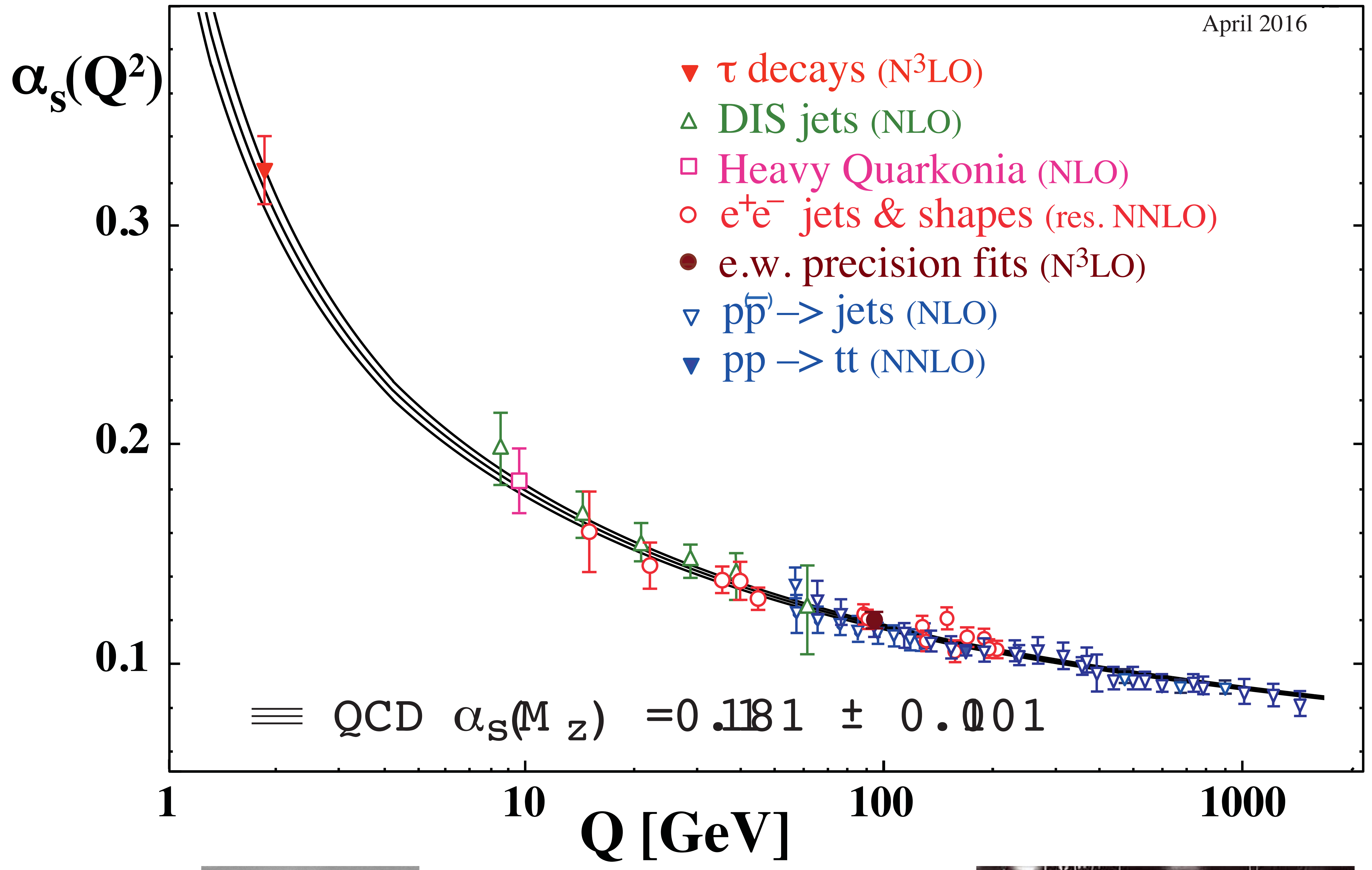
Strong interaction



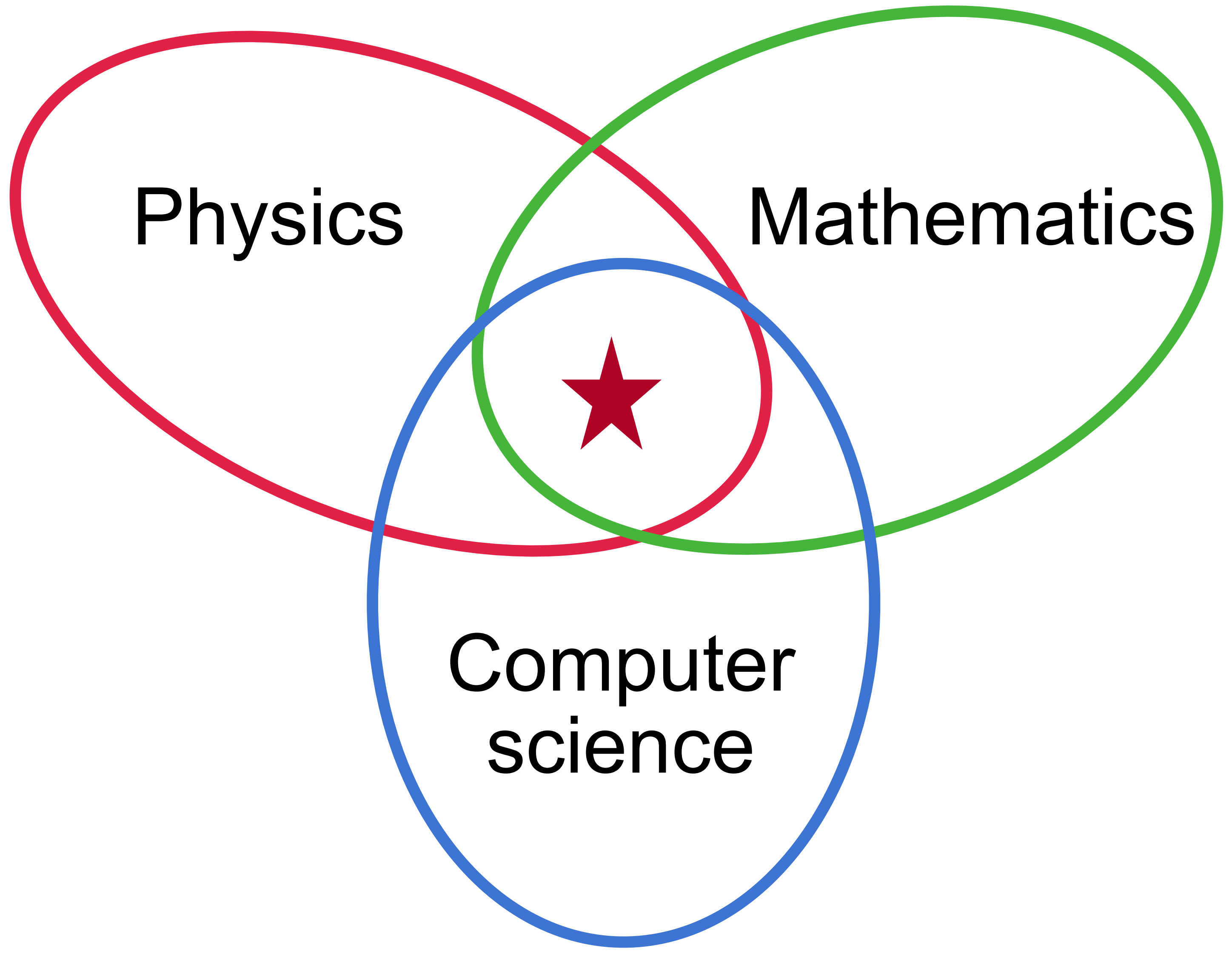
classical computer

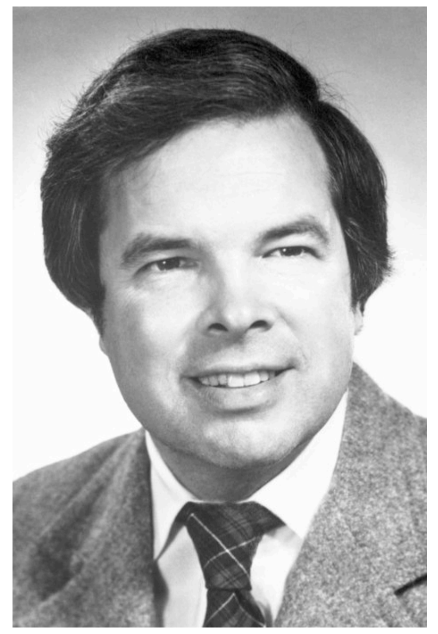
quantum computer

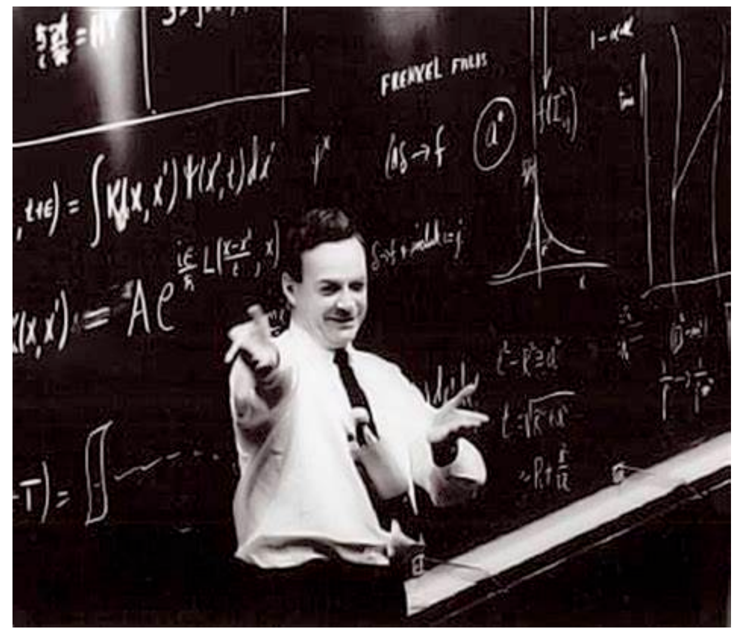
Introduction



- analytical method at high energy
- numerical **Monte Carlo** method at low energy







Introduction

Computational Task	Current Usage	2025 Usage	Current Storage (Disk)	2025 Storage (Disk)	2025 Network Requirements (WAN)
Accelerator Modeling	$\sim$ 10M – 100M core-hrs/yr	$\sim$ 10G – 100G core-hrs/yr			
Computational Cosmology	$\sim$ 100M – 1G core-hrs/yr	$\sim$ 100G – 1000G core-hrs/yr	$\sim$10PB	>100PB	300Gb/s (burst)
Lattice QCD	$\sim$1G core-hrs/yr	$\sim$ 100G – 1000G core-hrs/yr	$\sim$1PB	>10PB	
Theory	$\sim$ 1M – 10M core-hrs/yr	$\sim$ 100M – 1G core-hrs/yr			
Cosmic Frontier Experiments	$\sim$ 10M – 100M core-hrs/yr	$\sim$ 1G – 10G core-hrs/yr	$\sim$1PB	10 – 100PB	
Energy Frontier Experiments	$\sim$ 100M core-hrs/yr	$\sim$ 10G – 100G core-hrs/yr	$\sim$1PB	>100PB	300Gb/s
Intensity Frontier Experiments	$\sim$ 10M core-hrs/yr	$\sim$ 100M – 1G core-hrs/yr	$\sim$1PB	10 – 100PB	300Gb/s

ASCR/HEP Exascale Report [arXiv:1603.09303]

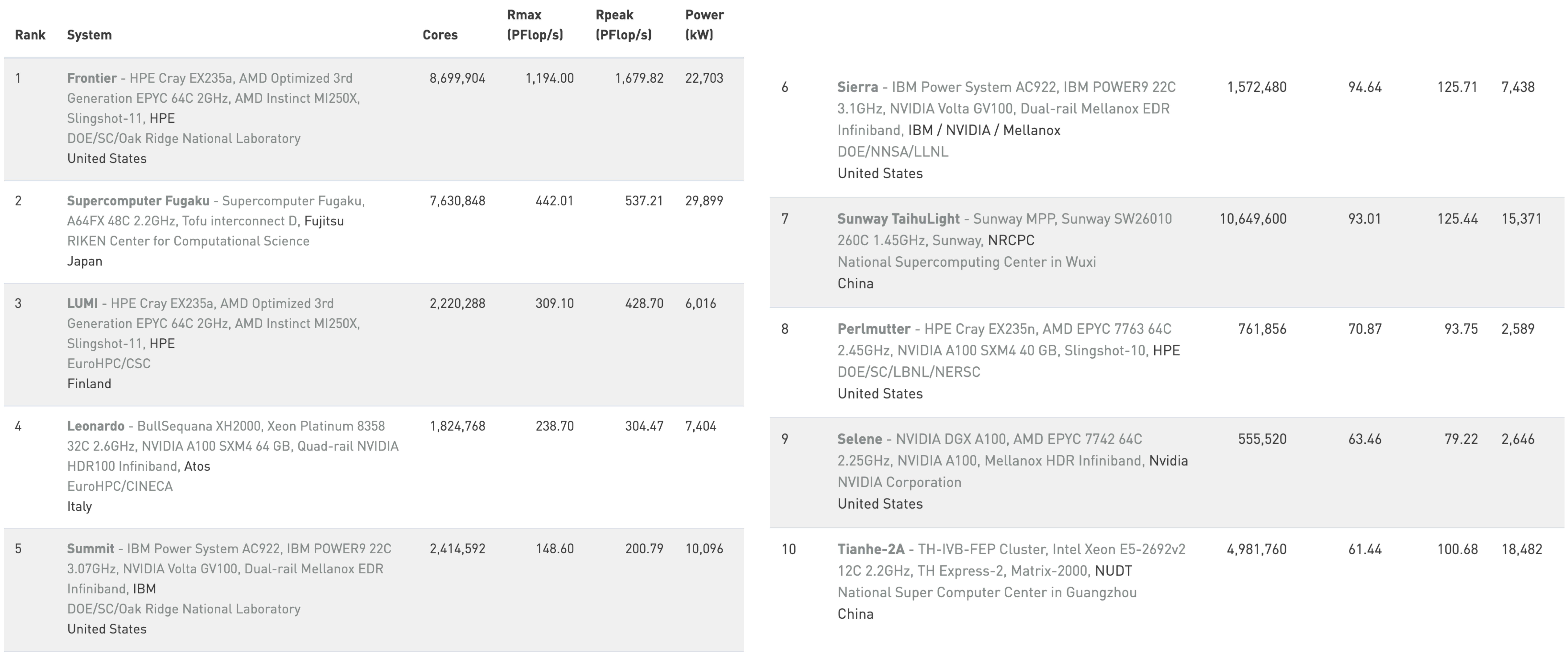
Introduction

my definition

High Performance Computing $\approx$ Numerical Linear Algebra on Supercomputers

High performance computers and supercomputers

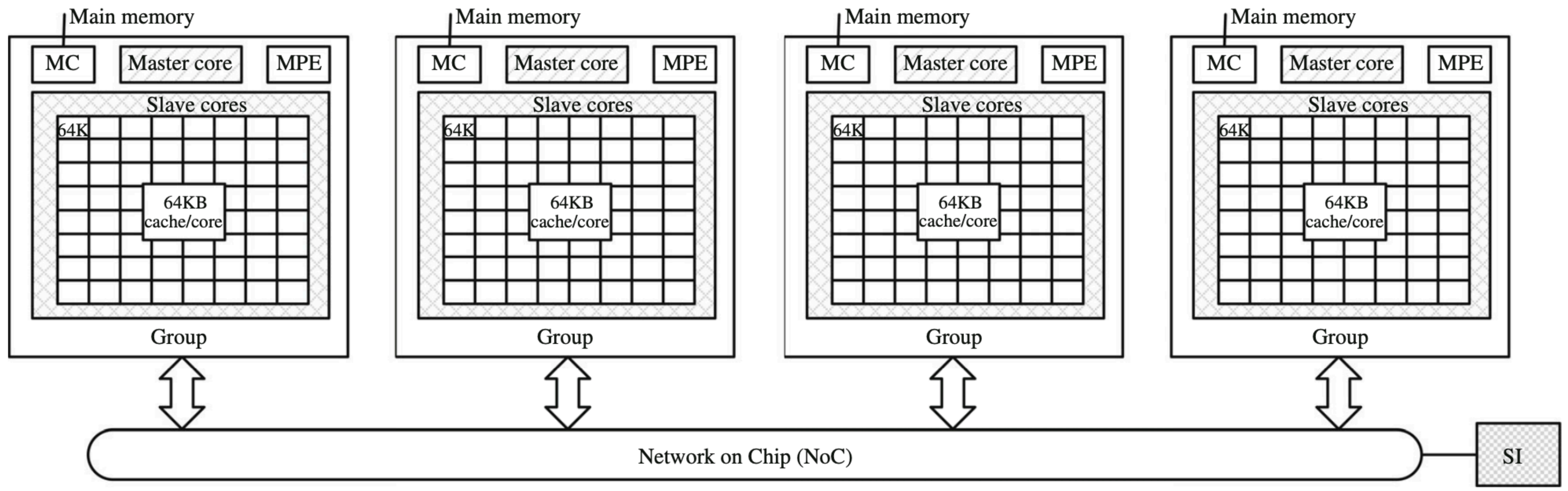
https://www.top500.org/lists/top500/2023/06/



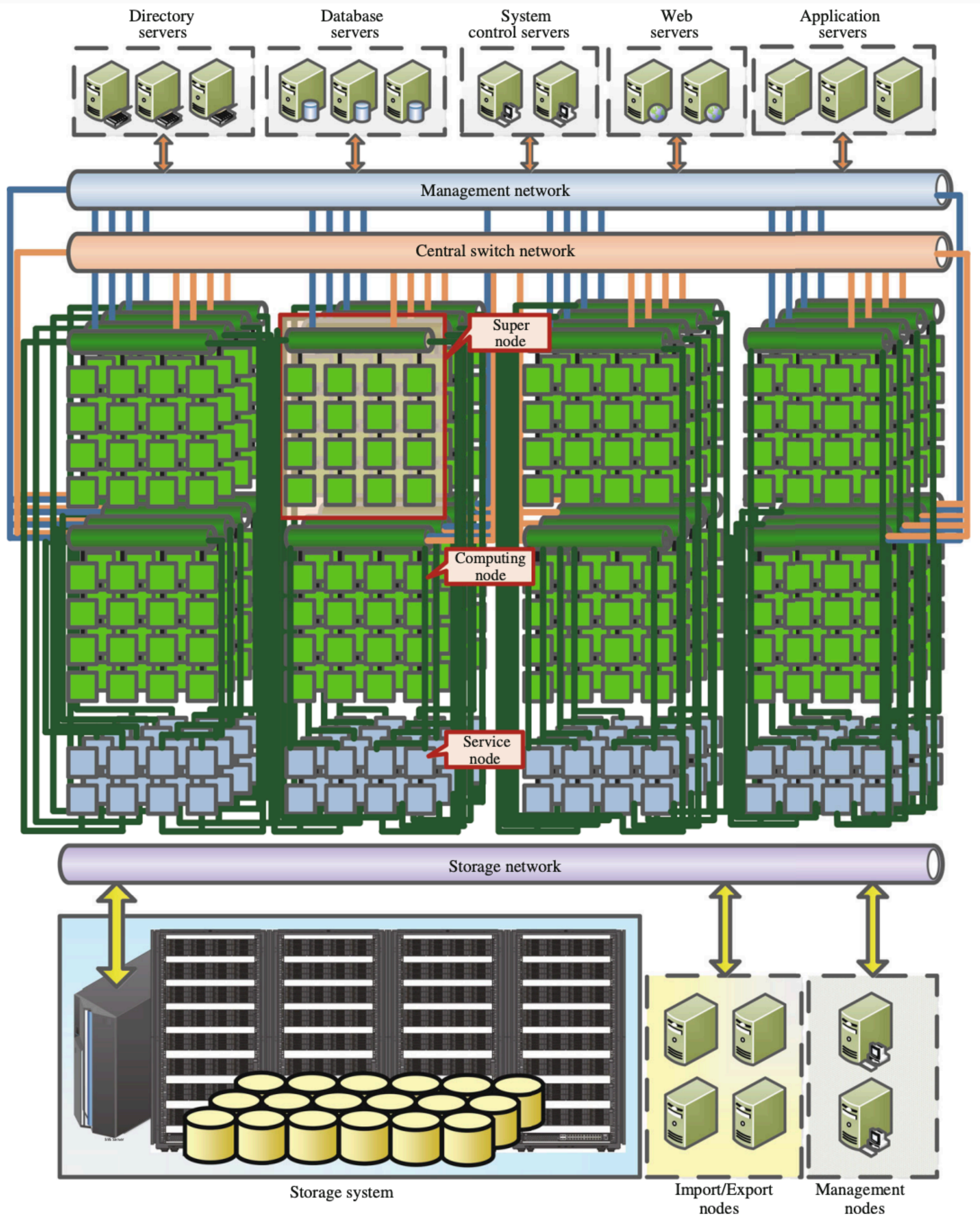
Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
4	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
5	**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	148.60	200.79	10,096
6	**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	94.64	125.71	7,438
7	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93.01	125.44	15,371
8	**Perlmutter** - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE DOE/SC/LBNL/NERSC United States	761,856	70.87	93.75	2,589
9	**Selene** - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63.46	79.22	2,646
10	**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	61.44	100.68	18,482

High performance computers and supercomputers

Supercomputer example: Sunway TaihuLight

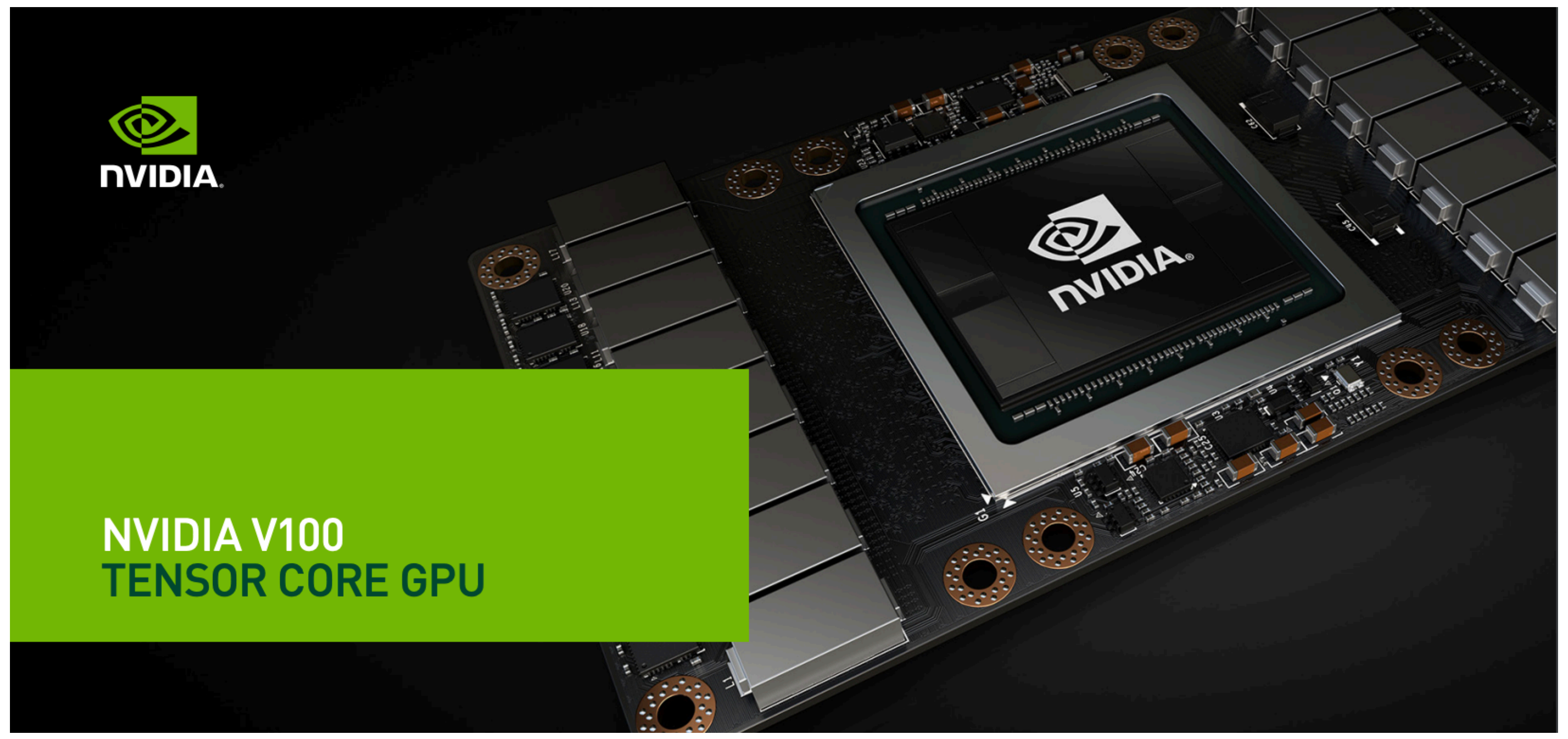


Fu, H., Liao, J., Yang, J. *et al.,* Sci. China Inf. Sci. **59,** 072001 (2016).

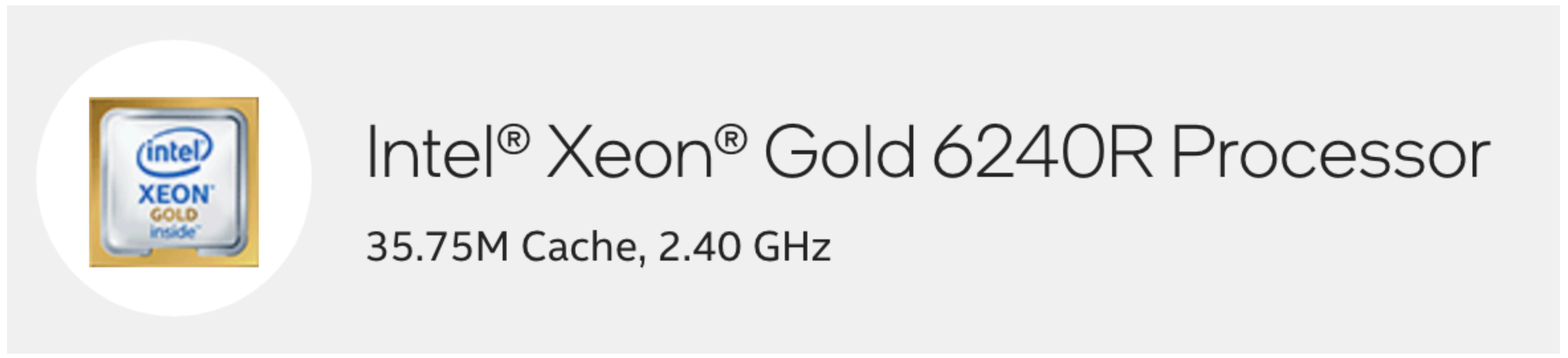


High performance computers and supercomputers

High performance clusters at IHEP



Nvidia V100 GPU: $\approx$ 300 cards



x86 CPU: $\approx O(10000)$ cores

ARM CPU: $\approx O(10000)$ cores

High performance computers and supercomputers

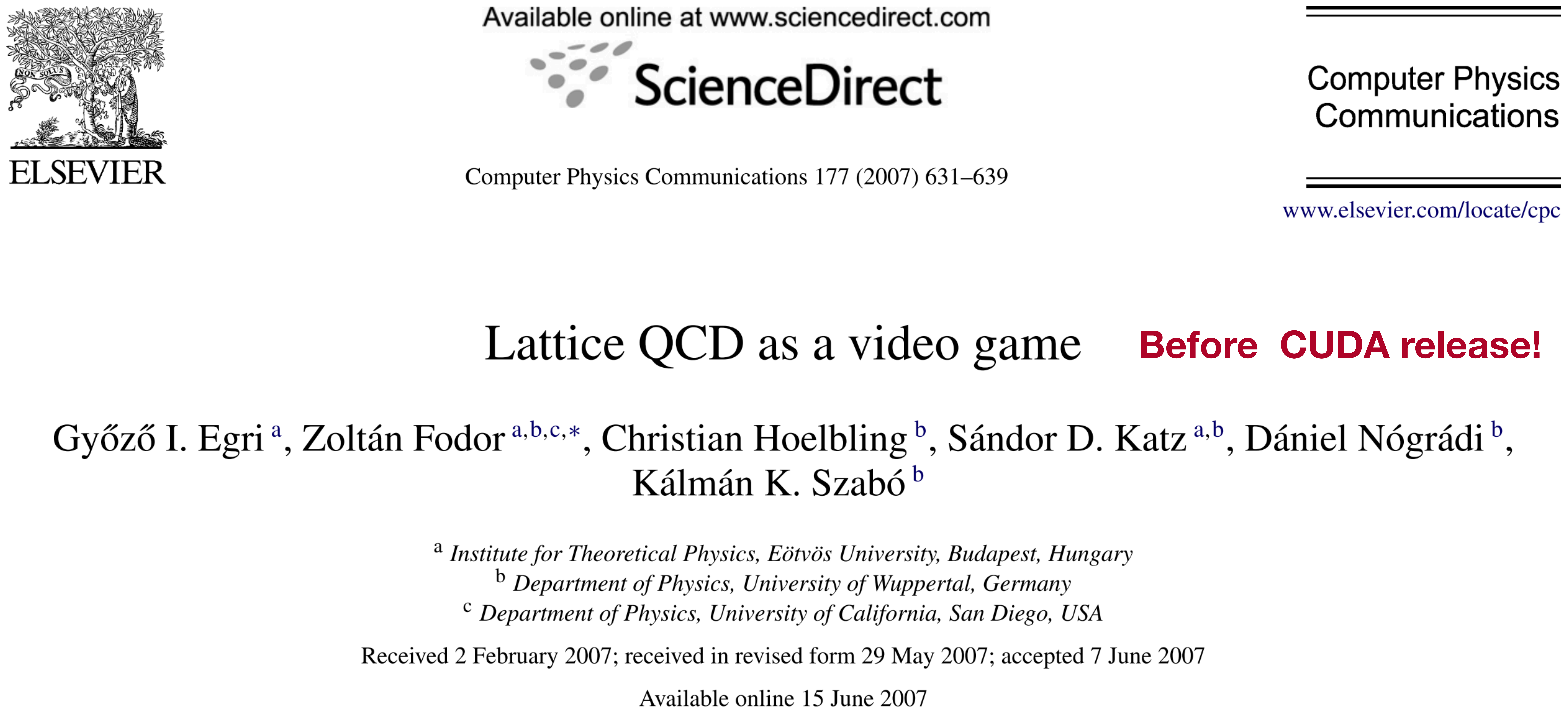
Example in HEP: LQCD with HPC

- Decades ago - customized processors
- QCDOC (QCD On a Chip)

- Nowadays - supercomputers / clusters
- TOP 500

QCDOC Asic, 1 Gflop/s

- LQCD awarded 1995,1998,2006 Goldon Bell Prize and 2018 finalist



Available online at www.sciencedirect.com

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Computer Physics Communications 177 (2007) 631–639

Computer Physics Communications

www.elsevier.com/locate/cpc

Lattice QCD as a video game

Before CUDA release!

Győző I. Egri [a], Zoltán Fodor [a,b,c,*], Christian Hoelbling [b], Sándor D. Katz [a,b], Dániel Nógrádi [b], Kálmán K. Szabó [b]

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[b] *Department of Physics, University of Wuppertal, Germany*
[c] *Department of Physics, University of California, San Diego, USA*

Received 2 February 2007; received in revised form 29 May 2007; accepted 7 June 2007

Available online 15 June 2007

Parallel programming models

Common programming language in HPC

- Fortran (Formula Translation)
  - Oldest high level programming language, first compiler released in 1957
  - Designed for numerical and scientific computing
  - Highly efficient, still widely used in high performance computing today
- C
  - Flexible, efficient, …
- C++
  - Efficient, abstract, multi-paradigm (procedural, object oriented, functional)
- Assembly
  - Highly efficient but not portable across different processor architecture
- Python
  - Slow in python itself, but with great library such as Scipy, very suitable for data processing, analysis and visualization

Parallel programming models

MPI + X model (**cluster level + node level + processor level + instruction level**)

- MPI (Message Passing Interface)
  - MPI is a communication protocol for programming parallel computers
  - The dominant programming model in high performance computing today
  - Support point-to-point and collective communication
  - MPI version 1.0 standard released in 1994
  - Directly callable from C, C++, Fortran
  - Very suitable for **distributed memory system**, therefore supported by all kinds of supercomputers
- Major implementation
  - MPICH (https://www.mpich.org/)
  - Open MPI (https://www.open-mpi.org/)
  - Many others derived from MPICH and Open MPI, such as Intel MPI, Cray MPI, IBM Spectrum MPI

Parallel programming models

MPI Basics

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

int main(int argc, char** argv) {
    // Initialize the MPI environment
    MPI_Init(&argc, &argv);

    // Get the number of processes
    int size;
    MPI_Comm_size(MPI_COMM_WORLD, &size);

    // Get the rank of the process
    int rank;
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    // Get the name of the processor
    char processor_name[MPI_MAX_PROCESSOR_NAME];
    int name_len;
    MPI_Get_processor_name(processor_name, &name_len);

    // Print off a hello world message
    printf("Hello world from processor %s, rank %d out of %d processors\n",
            processor_name, rank, size);

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

- Compile: `mpicc hello_world.c -o hello_world`
- Run: `mpirun -np 4 hello_world`
- NOTE: MPI is a library and mpicc is not a compiler, it is a wrapper over regular C compiler
- Use `mpicc -show` to see the compile and link flags
- **`gcc -I /path to MPI/include -L /path to MPI/lib -lmpi`**

output

```
Hello world from processor ui03.hep.ustc.edu.cn, rank 1 out of 4 processors
Hello world from processor ui03.hep.ustc.edu.cn, rank 2 out of 4 processors
Hello world from processor ui03.hep.ustc.edu.cn, rank 3 out of 4 processors
Hello world from processor ui03.hep.ustc.edu.cn, rank 0 out of 4 processors
```

Parallel programming models

MPI Basics (point-to-point communication)

- Total 400+ APIs

```
MPI_Send(
    void* data,
    int count,
    MPI_Datatype datatype,
    int destination,
    int tag,
    MPI_Comm communicator)
```

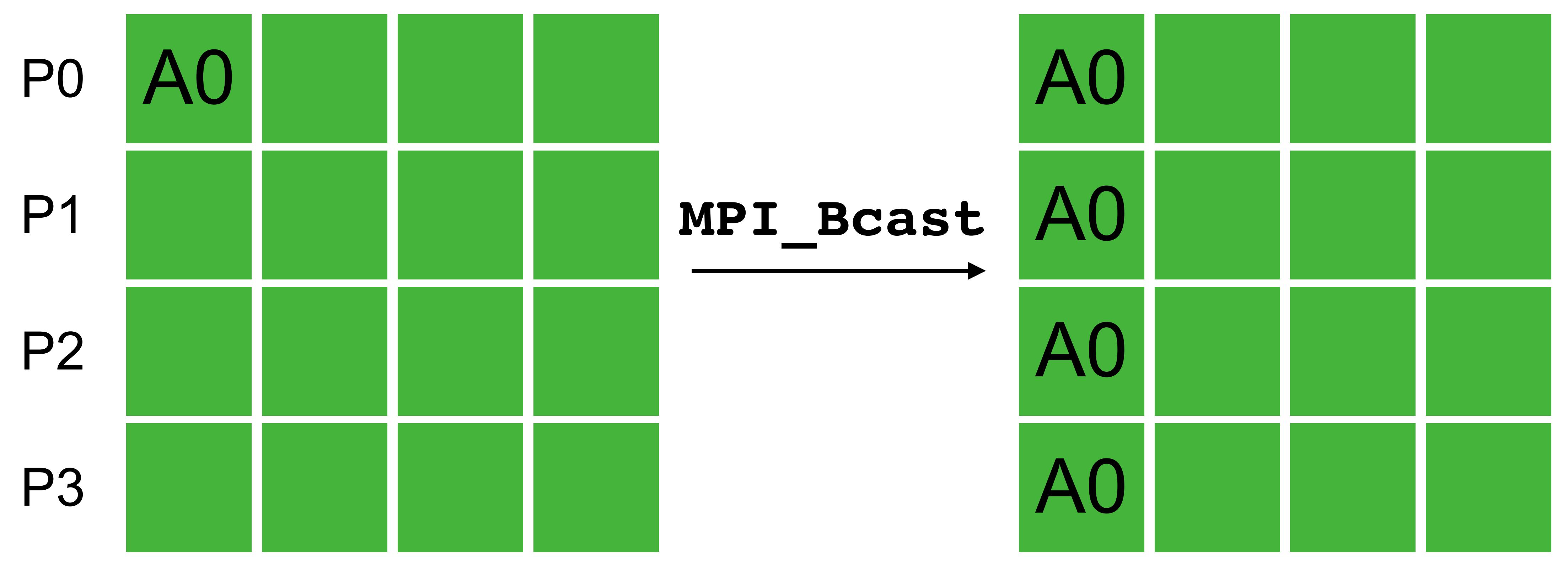
```
MPI_Recv(
    void* data,
    int count,
    MPI_Datatype datatype,
    int source,
    int tag,
    MPI_Comm communicator,
    MPI_Status* status)
```

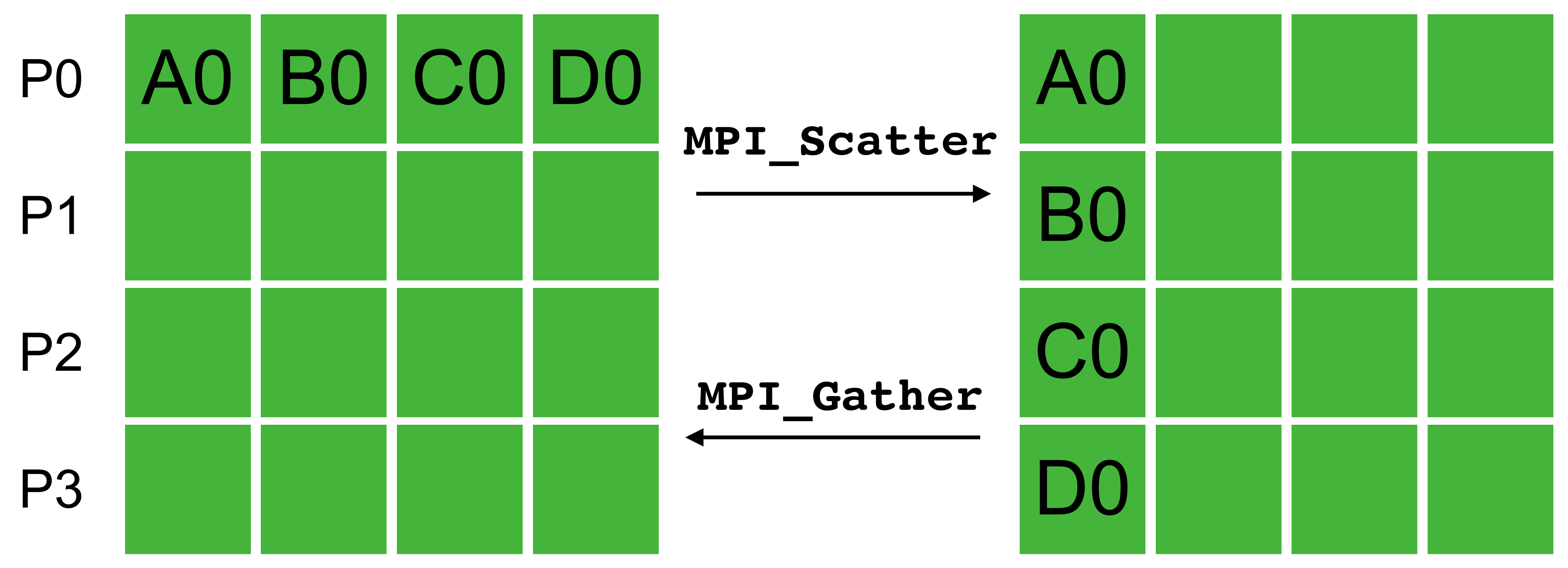
```
int world_rank;
MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);
int world_size;
MPI_Comm_size(MPI_COMM_WORLD, &world_size);

int number;
if (world_rank == 0) {
    number = -1;
    MPI_Send(&number, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
} else if (world_rank == 1) {
    MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
    printf("Process 1 received number %d from process 0\n",
           number);
}
```

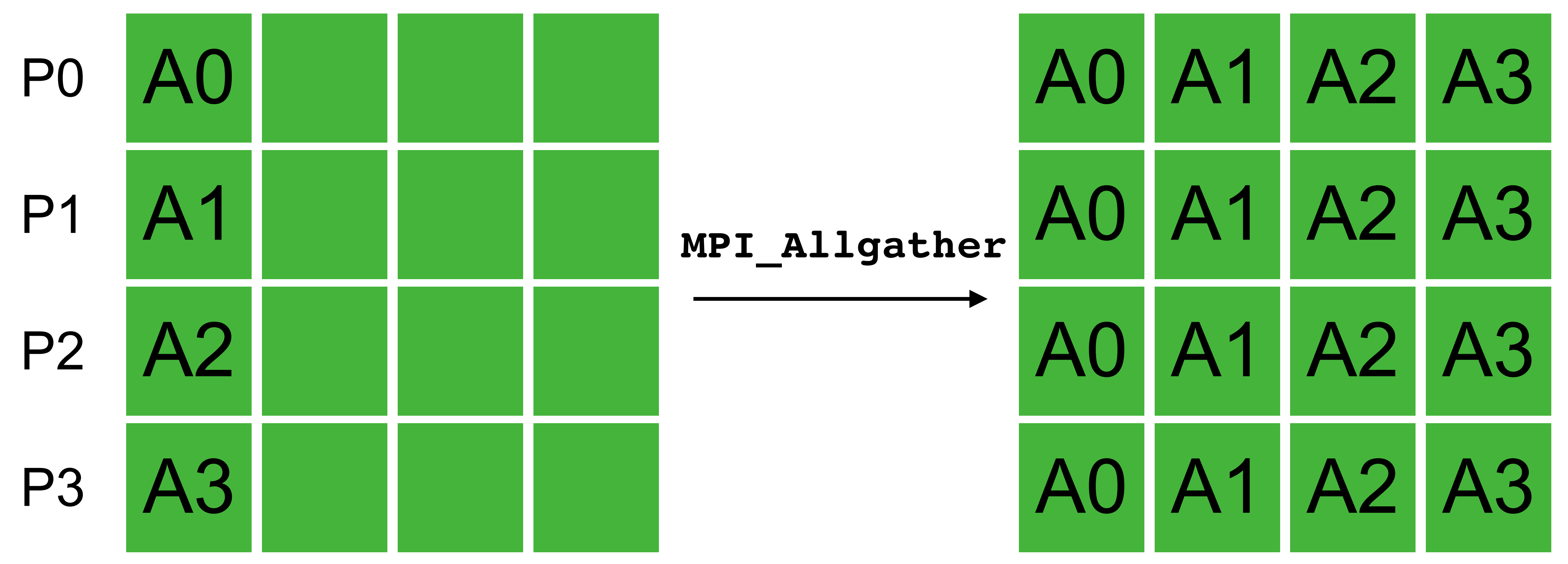
Parallel programming models

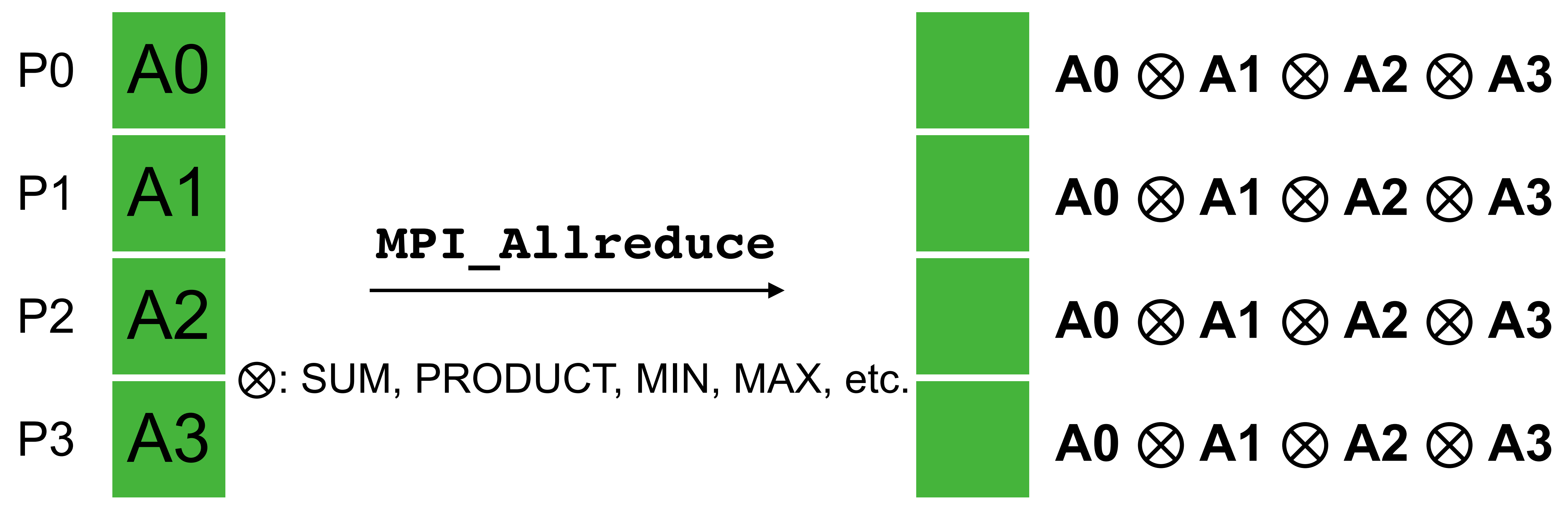
MPI Basics (collective communication)

- Total 400+ APIs





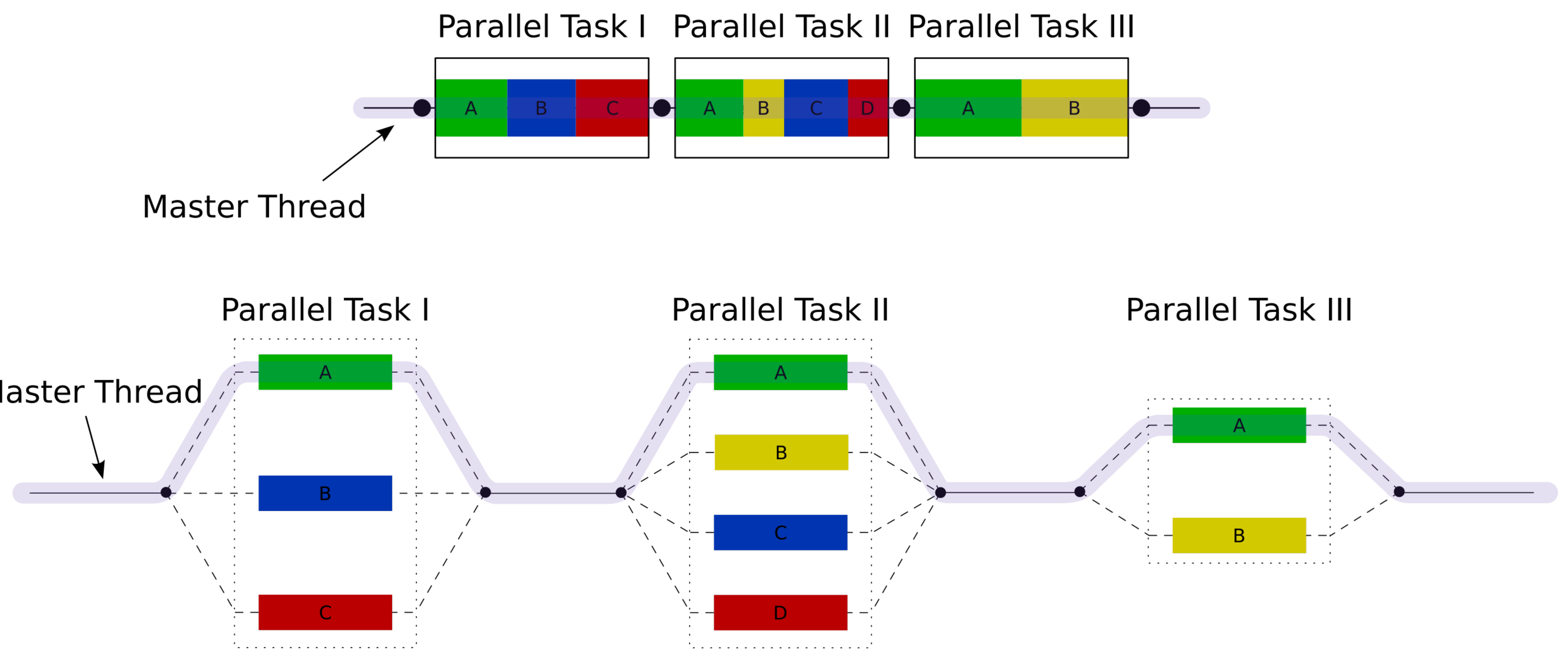




Parallel programming models

OpenMP (Open Multi-Processing)

- Pros
  - API that supports various instruction set architectures, operating system, and C, C++, Fortran
  - First standard released in 1997
  - Compiler directive based
  - Simple, flexible, portable, scalable
  - Easy to modify existing serial code into parallel
  - OpenMP 4.0 and later version support GPUs
- Cons
  - Multi-threading programming is easy to implement but hard to debug in general
  - Need to deal with **race condition** very carefully
  - Only used for parallelism **within a node**
- Major implementation
  - GCC, Intel, Clang



source: wikipedia

Parallel programming models

OpenMP hello world example

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

int main(int argc, char **argv) {
#pragma omp parallel
  {
    int threads_total = omp_get_num_threads();
    int thread_id = omp_get_thread_num();
    printf("Hello, world from thread %d,"
           "out of %d threads.\n ",
           thread_id,
           threads_total);
  }
  return 0;
}
```

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

int main(int argc, char **argv) {
  const int N = 1000000;
  int a[N];

#pragma omp parallel for
  for (int i = 0; i < N; i++) {
    a[i] = sin(i);
  }

  return 0;
}
```

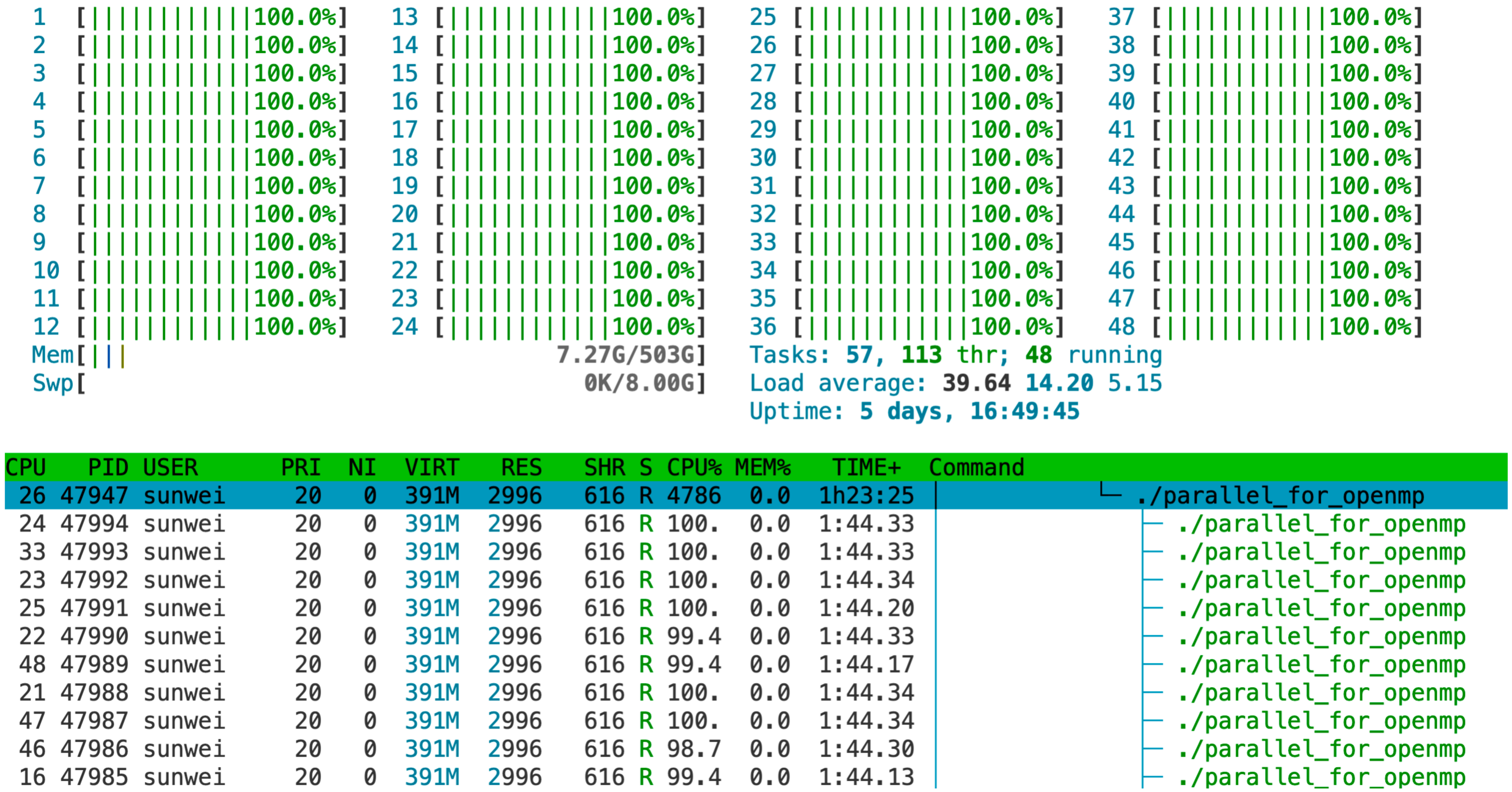
Compile: `gcc -fopenmp hello_world.c -o hello_world`

Run: `./hello_world` # use all cores / hardware threads available on single node

`OMP_NUM_THREADS=4 ./hello_world` # use 4 cores / hardware threads

Parallel programming models

OpenMP program monitored with htop



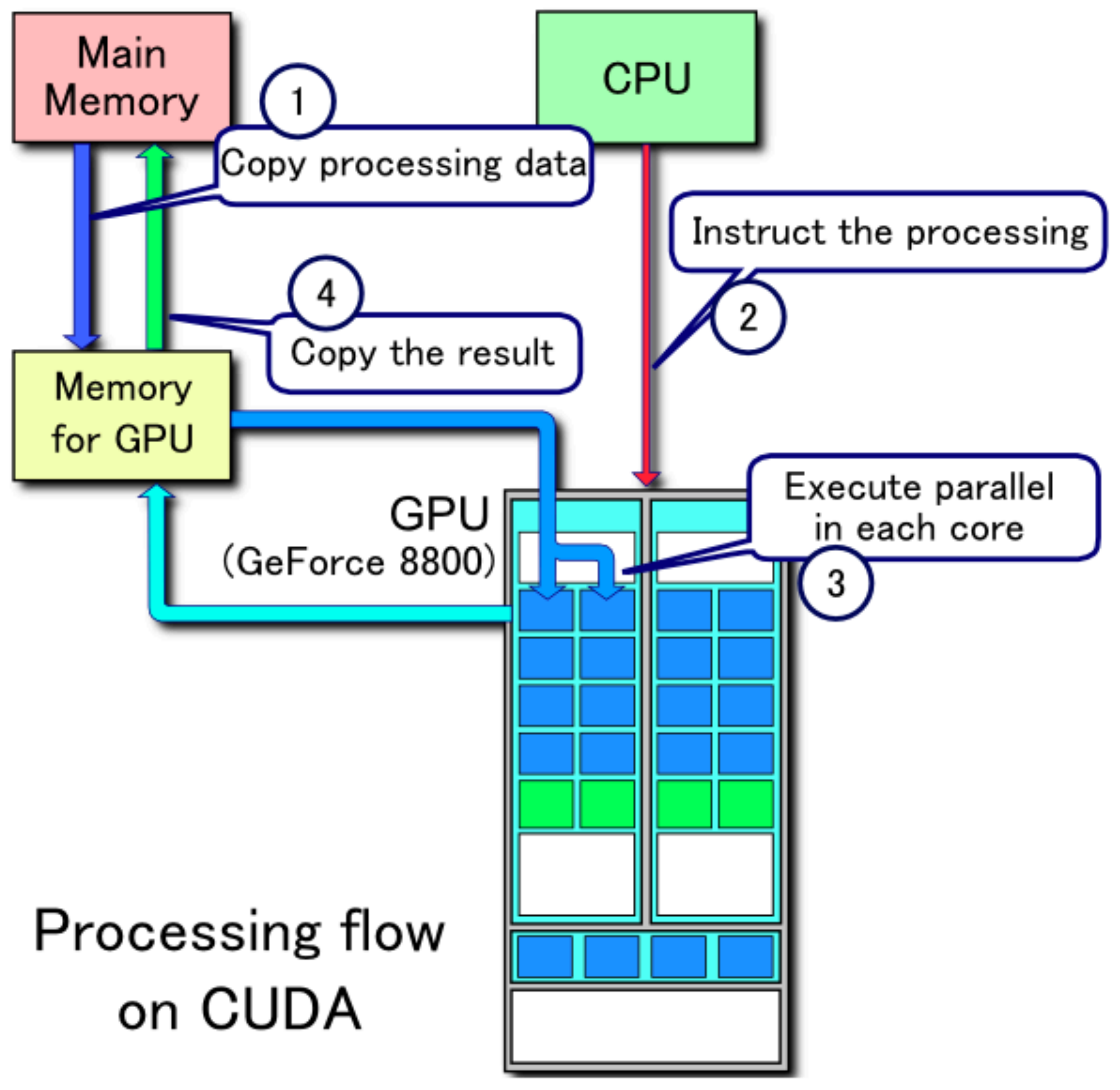
```
  1  [||||||||||||100.0%]   13 [||||||||||||100.0%]   25 [||||||||||||100.0%]   37 [||||||||||||100.0%]
  2  [||||||||||||100.0%]   14 [||||||||||||100.0%]   26 [||||||||||||100.0%]   38 [||||||||||||100.0%]
  3  [||||||||||||100.0%]   15 [||||||||||||100.0%]   27 [||||||||||||100.0%]   39 [||||||||||||100.0%]
  4  [||||||||||||100.0%]   16 [||||||||||||100.0%]   28 [||||||||||||100.0%]   40 [||||||||||||100.0%]
  5  [||||||||||||100.0%]   17 [||||||||||||100.0%]   29 [||||||||||||100.0%]   41 [||||||||||||100.0%]
  6  [||||||||||||100.0%]   18 [||||||||||||100.0%]   30 [||||||||||||100.0%]   42 [||||||||||||100.0%]
  7  [||||||||||||100.0%]   19 [||||||||||||100.0%]   31 [||||||||||||100.0%]   43 [||||||||||||100.0%]
  8  [||||||||||||100.0%]   20 [||||||||||||100.0%]   32 [||||||||||||100.0%]   44 [||||||||||||100.0%]
  9  [||||||||||||100.0%]   21 [||||||||||||100.0%]   33 [||||||||||||100.0%]   45 [||||||||||||100.0%]
  10 [||||||||||||100.0%]   22 [||||||||||||100.0%]   34 [||||||||||||100.0%]   46 [||||||||||||100.0%]
  11 [||||||||||||100.0%]   23 [||||||||||||100.0%]   35 [||||||||||||100.0%]   47 [||||||||||||100.0%]
  12 [||||||||||||100.0%]   24 [||||||||||||100.0%]   36 [||||||||||||100.0%]   48 [||||||||||||100.0%]
  Mem[|||                                 7.27G/503G]   Tasks: 57, 113 thr; 48 running
  Swp[                                     0K/8.00G]   Load average: 39.64 14.20 5.15
                                                        Uptime: 5 days, 16:49:45

CPU   PID USER       PRI  NI  VIRT   RES    SHR S CPU% MEM%   TIME+  Command
 26 47947 sunwei      20   0  391M  2996    616 R 4786  0.0  1h23:25 │         └─ ./parallel_for_openmp
 24 47994 sunwei      20   0  391M  2996    616 R 100.  0.0  1:44.33 │            ├─ ./parallel_for_openmp
 33 47993 sunwei      20   0  391M  2996    616 R 100.  0.0  1:44.33 │            ├─ ./parallel_for_openmp
 23 47992 sunwei      20   0  391M  2996    616 R 100.  0.0  1:44.34 │            ├─ ./parallel_for_openmp
 25 47991 sunwei      20   0  391M  2996    616 R 100.  0.0  1:44.20 │            ├─ ./parallel_for_openmp
 22 47990 sunwei      20   0  391M  2996    616 R 99.4  0.0  1:44.33 │            ├─ ./parallel_for_openmp
 48 47989 sunwei      20   0  391M  2996    616 R 99.4  0.0  1:44.17 │            ├─ ./parallel_for_openmp
 21 47988 sunwei      20   0  391M  2996    616 R 100.  0.0  1:44.34 │            ├─ ./parallel_for_openmp
 47 47987 sunwei      20   0  391M  2996    616 R 100.  0.0  1:44.34 │            ├─ ./parallel_for_openmp
 46 47986 sunwei      20   0  391M  2996    616 R 98.7  0.0  1:44.30 │            ├─ ./parallel_for_openmp
 16 47985 sunwei      20   0  391M  2996    616 R 99.4  0.0  1:44.13 │            ├─ ./parallel_for_openmp
```

Parallel programming models

Details in Friday's lectures

CUDA for GPU computing

- CUDA (Compute Unified Device Architecture)
  - CUDA is a parallel programming framework and API for general purpose GPU (GPGPU) computing
  - Developed by Nvidia and support Nvidia's GPUs
  - Supported Tesla -> Fermi -> Kepler -> Maxwell -> Pascal -> Volta -> Turing -> Ampere -> Hopper
  - Directly callable from C, C++, Fortran
  - Need CUDA Toolkit to compile
  - Free but not open source
  - Multi-node GPU programming with CUDA-aware MPI
  - The HIP (Heterogeneous Interface for Portability) developed by AMD can is portable both for AMD and Nvidia's GPUs, and also free and open source

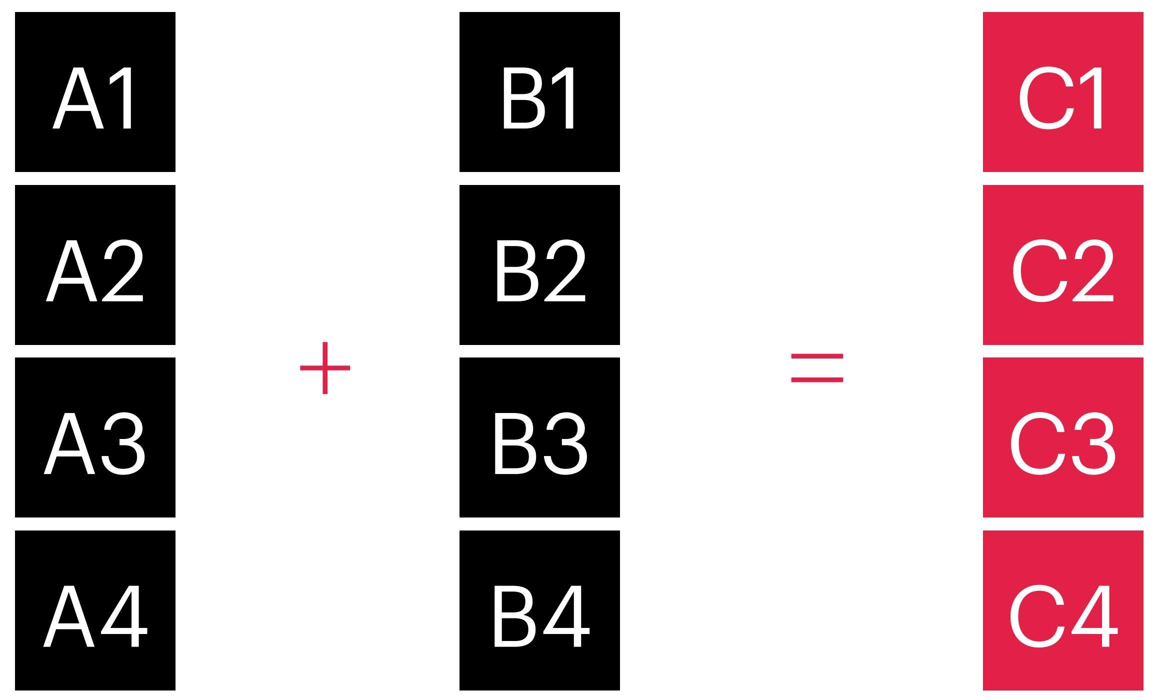


source: wikipedia

Parallel programming models

SIMD (Single Instruction Multiple Data)

- Vectorization: supported by x86 (SSE, AVX, AVX2, AVX512 etc.), Arm (NEON, SVE), PowerPC (AltiVec) etc.
- Implementation: optimized math libraries (such as Intel MKL), inline assembly, intrinsic function



Parallel programming models

SIMD with intrinsic functions

No explicit SIMD

```
void add(float* out, const float* input1, const float* input2, int N)
{
    for(int i=0; i<N; i++){
       out[i] = input1[i] + input2[i];
    }
}
```

x86 AVX SIMD

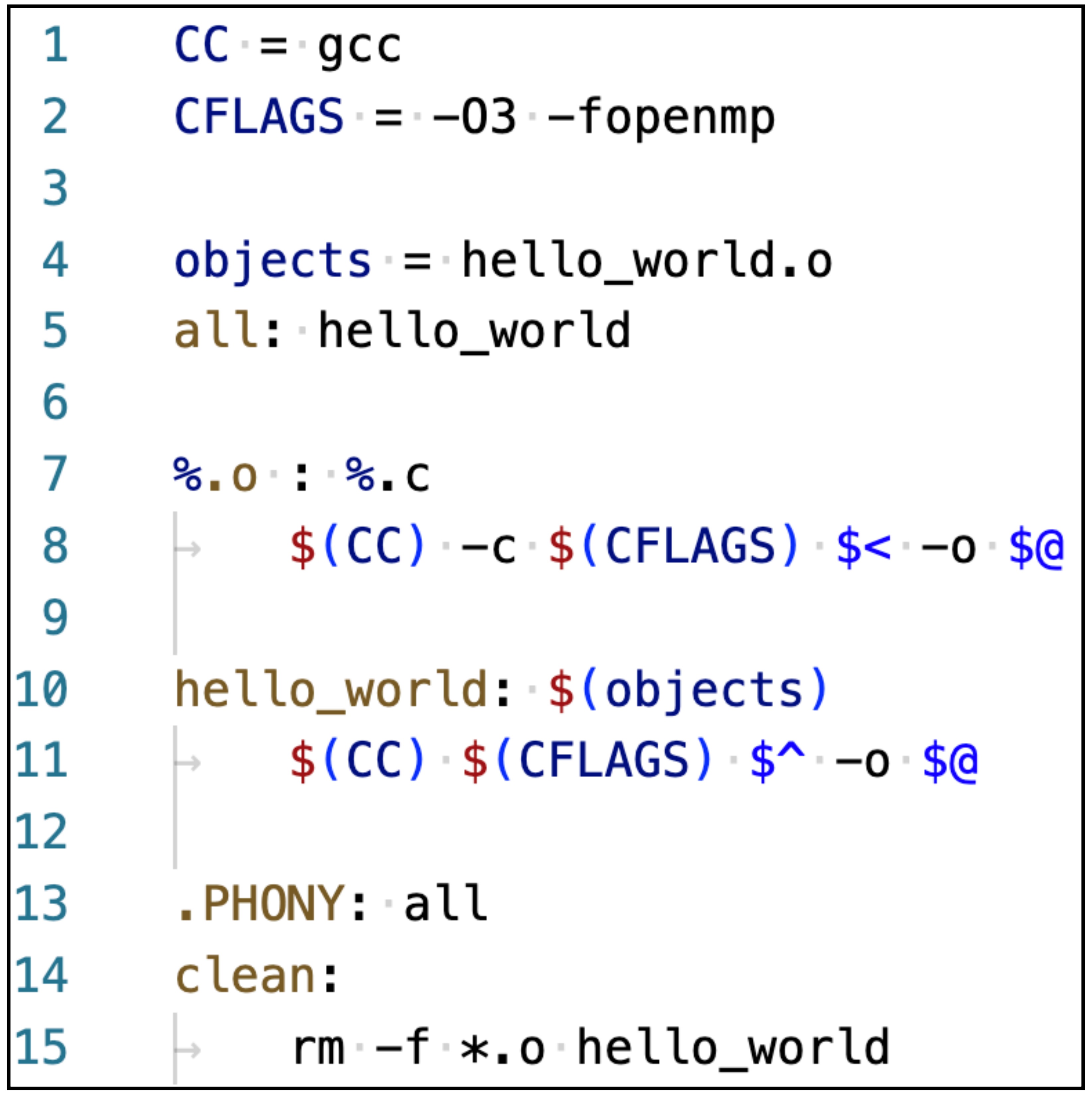
```
#include<immintrin.h>
//compile: g++ -O3 -mavx -o exe src.c

void add_avx(float* out, const float* input1,
            const float* input2, int N)
{
    for(int i=0; i<N; i+=8){
        __m256 v1 = _mm256_load_ps(input1+i);
        __m256 v2 = _mm256_load_ps(input2+i);

        __m256 v0 = _mm256_add_ps(v1, v2);
        _mm256_store_ps(out+i, v0);
    }
}
```

ARM NEON SIMD

```
#include<arm_neon.h>
//compile: g++ -O3 -march=armv8-a -o exe src.c

void add_neon(float* out, const float* input1,
             const float* input2, int N)
{
    for(int i=0; i<N; i+=4){
        float32x4_t v1 = vld1q_f32(input1+i);
        float32x4_t v2 = vld1q_f32(input2+i);

        float32x4_t v0 = vaddq_f32(v1, v2);
        vst1q_f32(out+i, v0);
    }
}
```

Parallel programming models

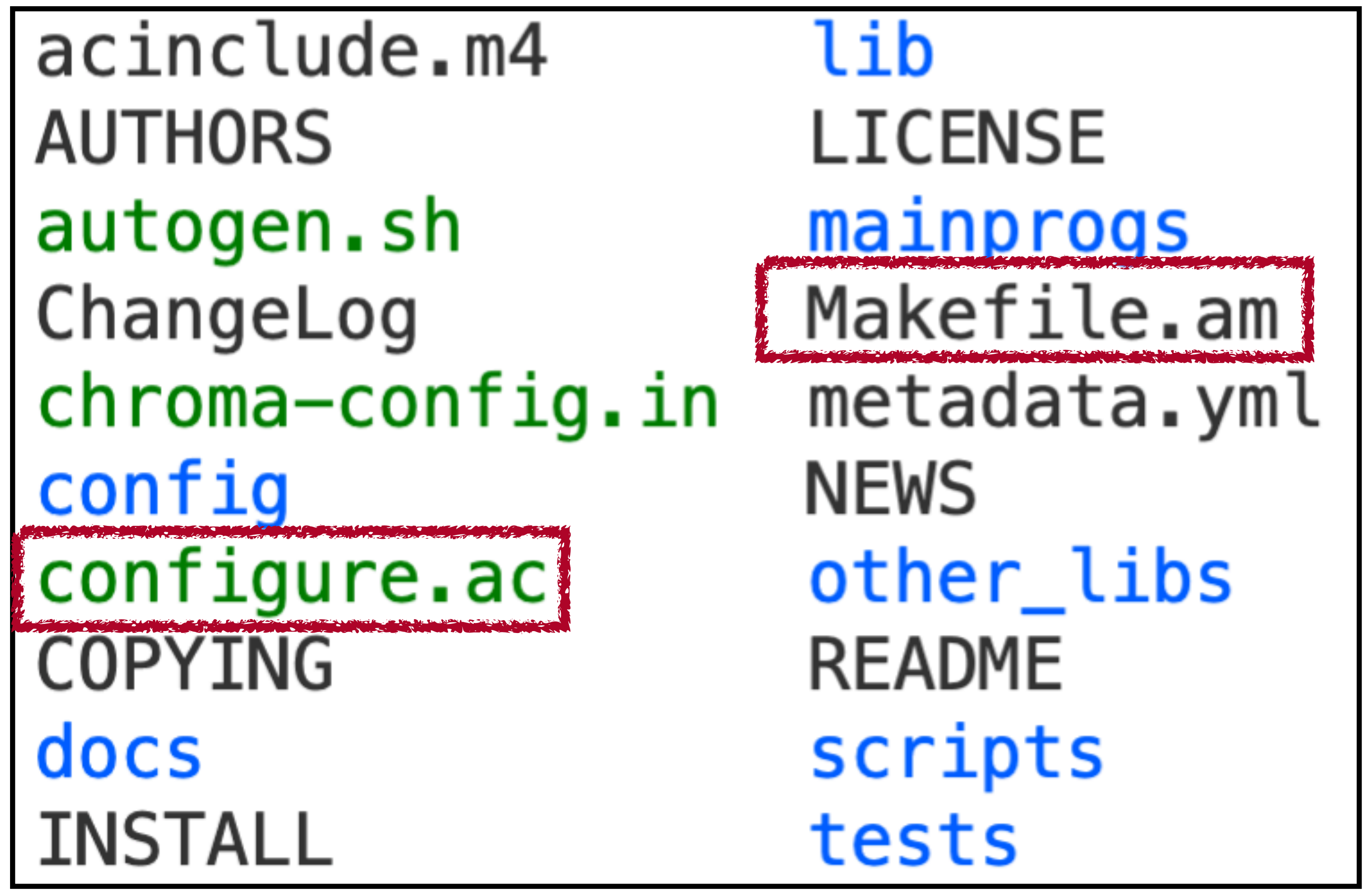
Software build tools



```
CC = gcc
CFLAGS = -O3 -fopenmp

objects = hello_world.o
all: hello_world

%.o : %.c
	$(CC) -c $(CFLAGS) $< -o $@

hello_world: $(objects)
	$(CC) $(CFLAGS) $^ -o $@

.PHONY: all
clean:
	rm -f *.o hello_world
```

Makefile

Build: **`make`**



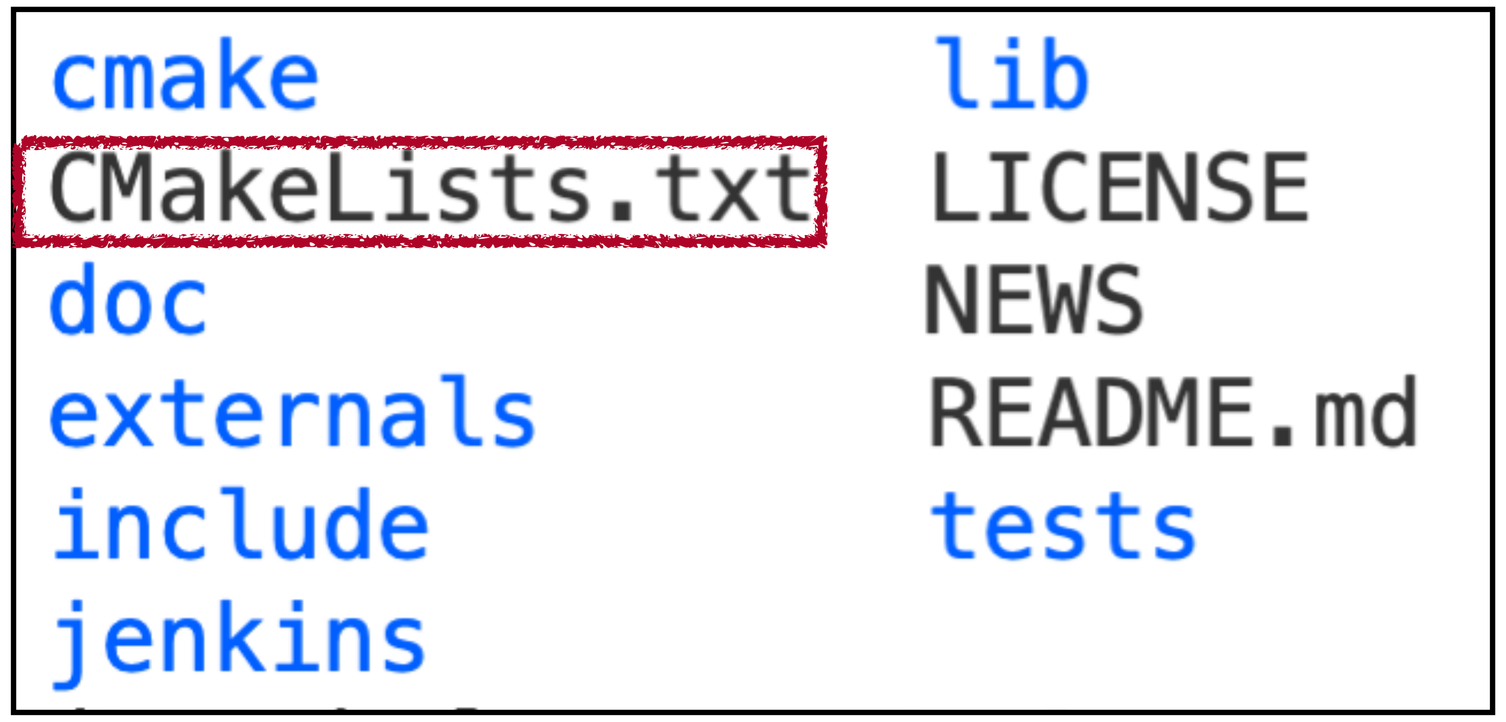
```
acinclude.m4       lib
AUTHORS            LICENSE
autogen.sh         mainprogs
ChangeLog          Makefile.am
chroma-config.in   metadata.yml
config             NEWS
configure.ac       other_libs
COPYING            README
docs               scripts
INSTALL            tests
```

GNU Autotools

Build: **`autoreconf`**

`./configure`

`make && make install`



```
cmake            lib
CMakeLists.txt   LICENSE
doc              NEWS
externals        README.md
include          tests
jenkins
```

CMake

Build: **`mkdir build && cd build`**

`cmake ..`

`make && make install`

Summary and tips

- Covered basics of high performance computing programming model and tools widely used in high energy physics
- **Tips:**
  - **Select the right programming model and tools before writing the code**
  - **Correctness is the top priority, NOT performance at the beginning of the software development**
  - **Use well established and tested libraries, do NOT reinvent the wheels unless you know what you are doing**
  - **Use version control system such as git for code development, use github or gitlab for collaborative development**

Hands-on exercises

- MPI
  1. Hello world
  2. Compute π with formula $\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \dots$
- OpenMP
  1. Compute π