

# Practical aspects of HPC

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Introduction to High-Performance Computing with Python

The Cyprus Institute — 11<sup>th</sup> June 2025

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Giannis Koutsou,

Computation-based Science and Technology Research Center,

The Cyprus Institute

# Outline

## Supercomputing basics

- High-performance Computing and parallel computing
- Why the need for parallelism

## Top500 trends

- Multiprocessors
- Accelerators

## Landscape

- EuroHPC systems



# High-performance computing

*"The use of supercomputers to solve complex computational tasks"*



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- Parallelism as we understand it today: distributed and shared memory, message passing, etc.



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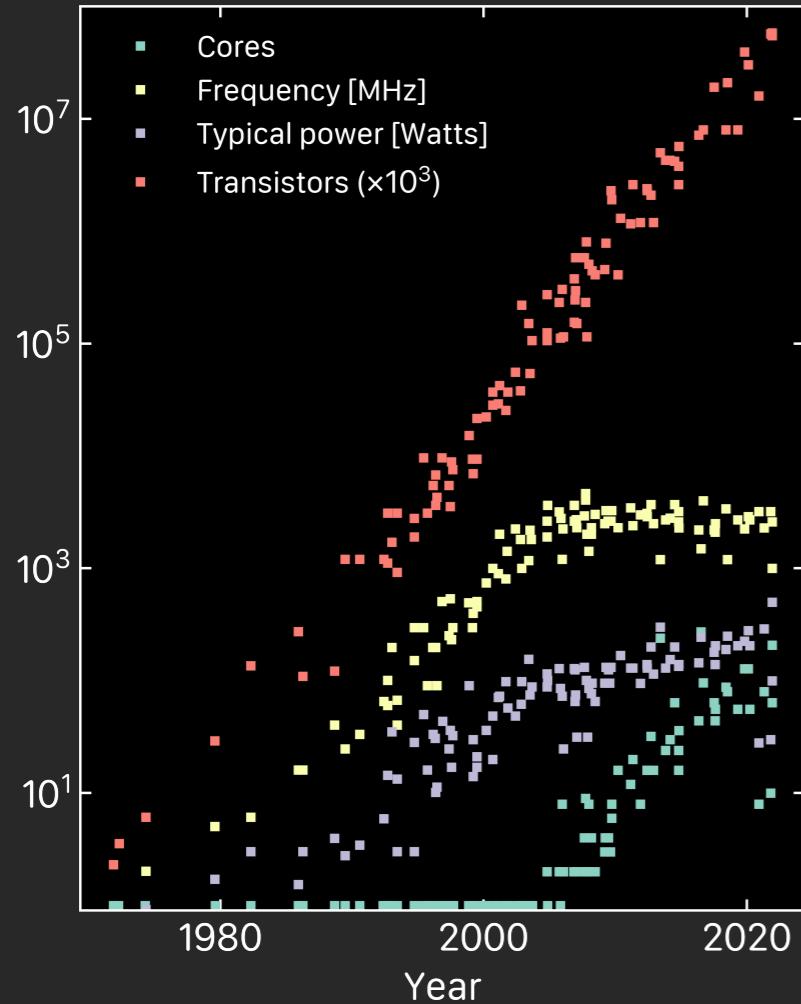
- Parallelism as we understand it today: distributed and shared memory, message passing, etc.

2010s onwards — Heterogeneous supercomputers

- Many sockets per node; co-processors, e.g. GPUs, potentially multiple architectures within same system



# Supercomputing means Parallel Computing



No Dennard scaling after  $\sim 2005$

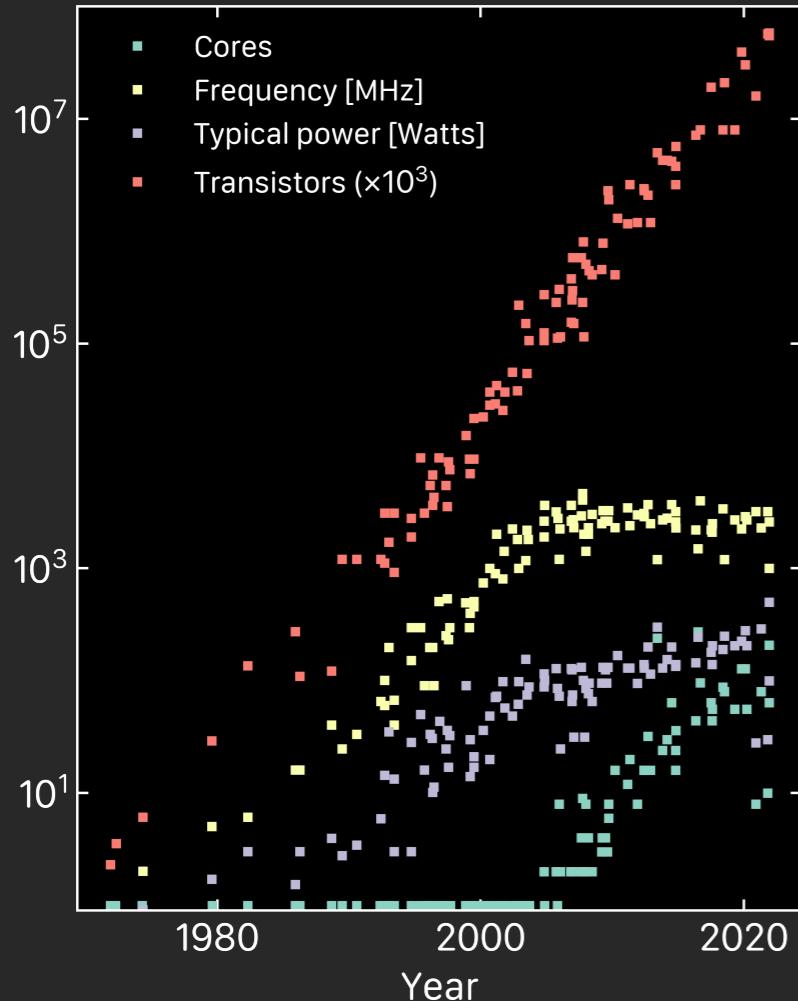
- $P \propto A f V^2$  ( $P$ : power,  $A$ : area,  $f$ : freq.,  $V$ : voltage)
- Roughly, as transistors get smaller, the *power density* stays constant
- This efficiency was typically used towards increasing frequency

Moore's law?

- A statement about *transistor count*
- So far seems to hold

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⇒ Efficiencies are now used to increase parallelism rather than frequency

- HPC now means more parallel hardware, rather than faster scalar hardware
- HPC primarily deals with tackling the challenges of parallelism, from all aspects (hardware, software, algorithmic, etc.)

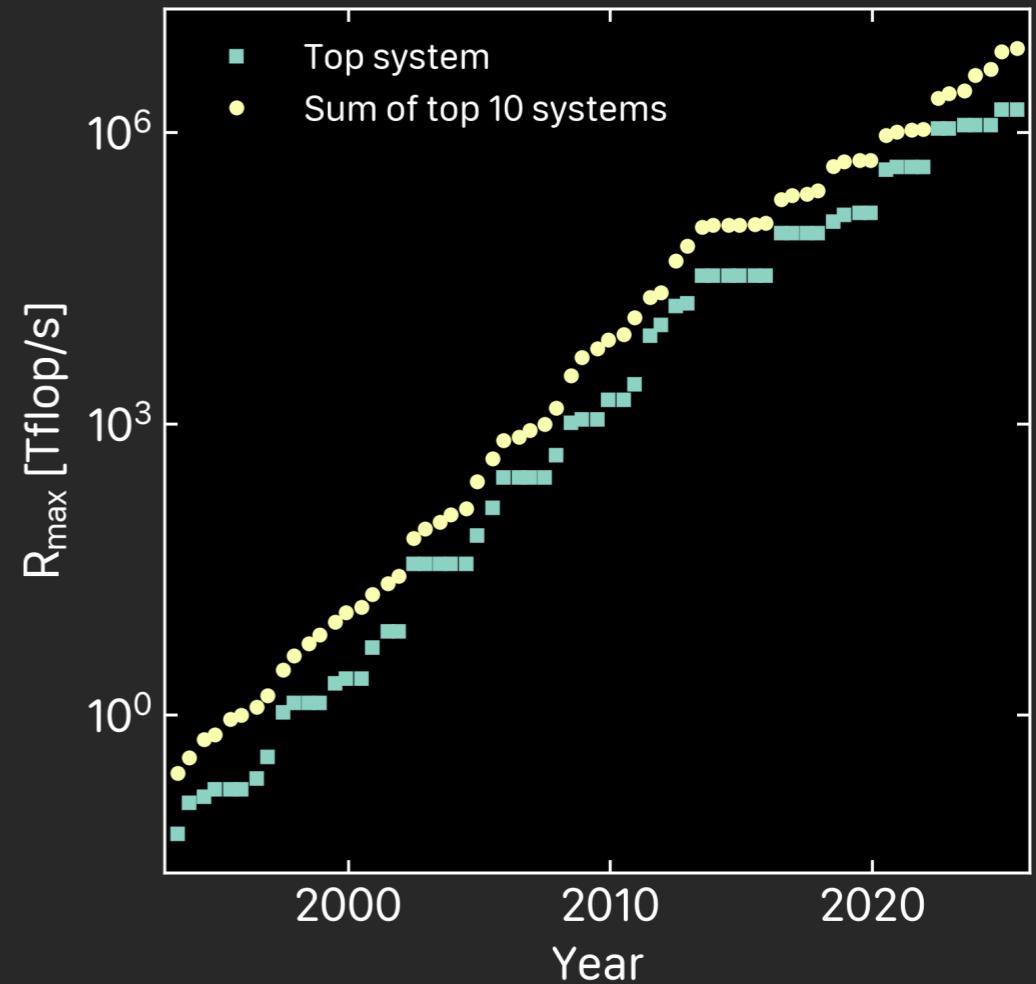
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# Evolution of Supercomputing

## The "Top500" list

- Ranked list of top 500 supercomputers populated twice per year
- Data shown here since 1993
- Shown is High-Performance Linpack (HPL) performance achieved

⇒ Shows that exponential increase has been maintained



<https://www.top500.org>

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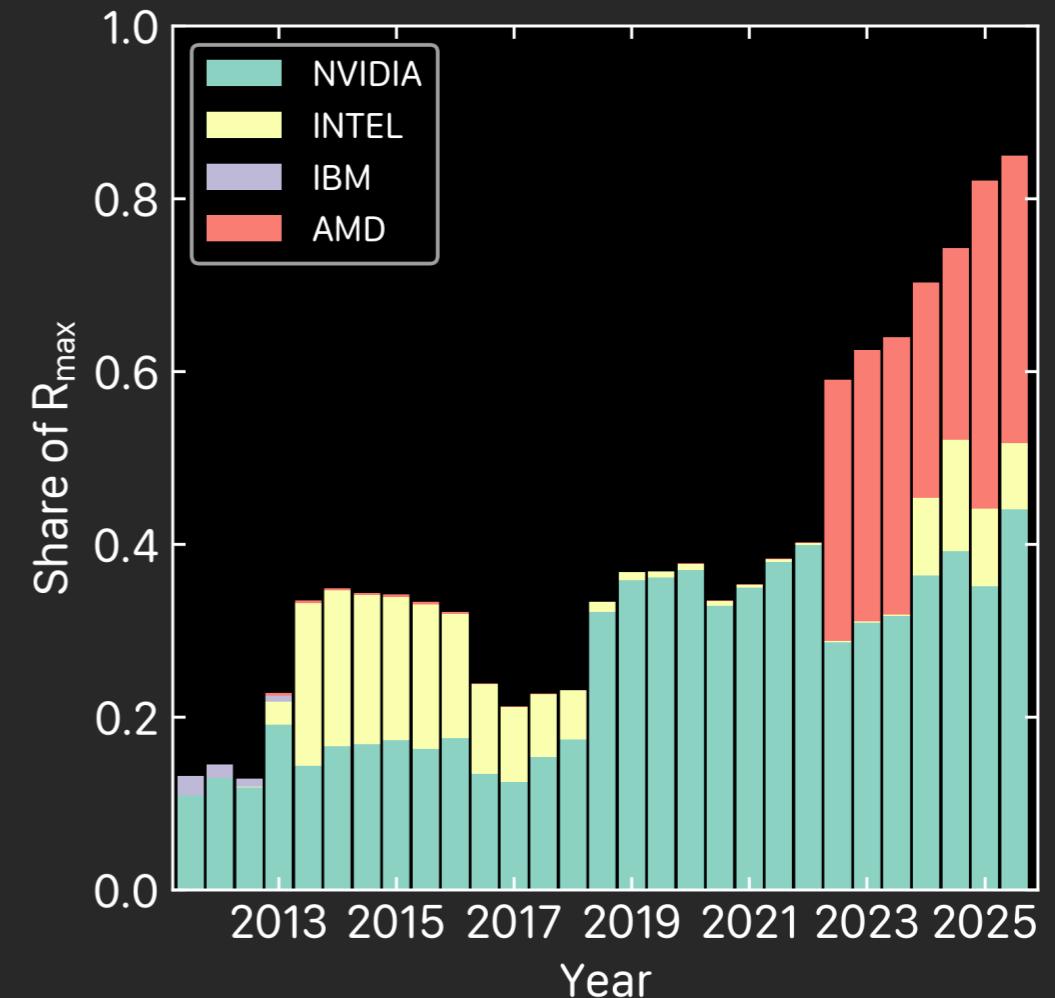
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- Proliferation of accelerators
  - Latest AMD accelerators are Instinct GPUs
  - Intel between 2012 and 2017 includes Xeon Phi
  - IBM accelerators refer to IBM Cell

⇒ Since 2021, more than half of performance over Top500 now from accelerated systems



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# Parallel computing as the main paradigm

High performance computing means parallel computing

- Technology trends mean parallelism is essential for advanced computing

# Parallel computing as the main paradigm

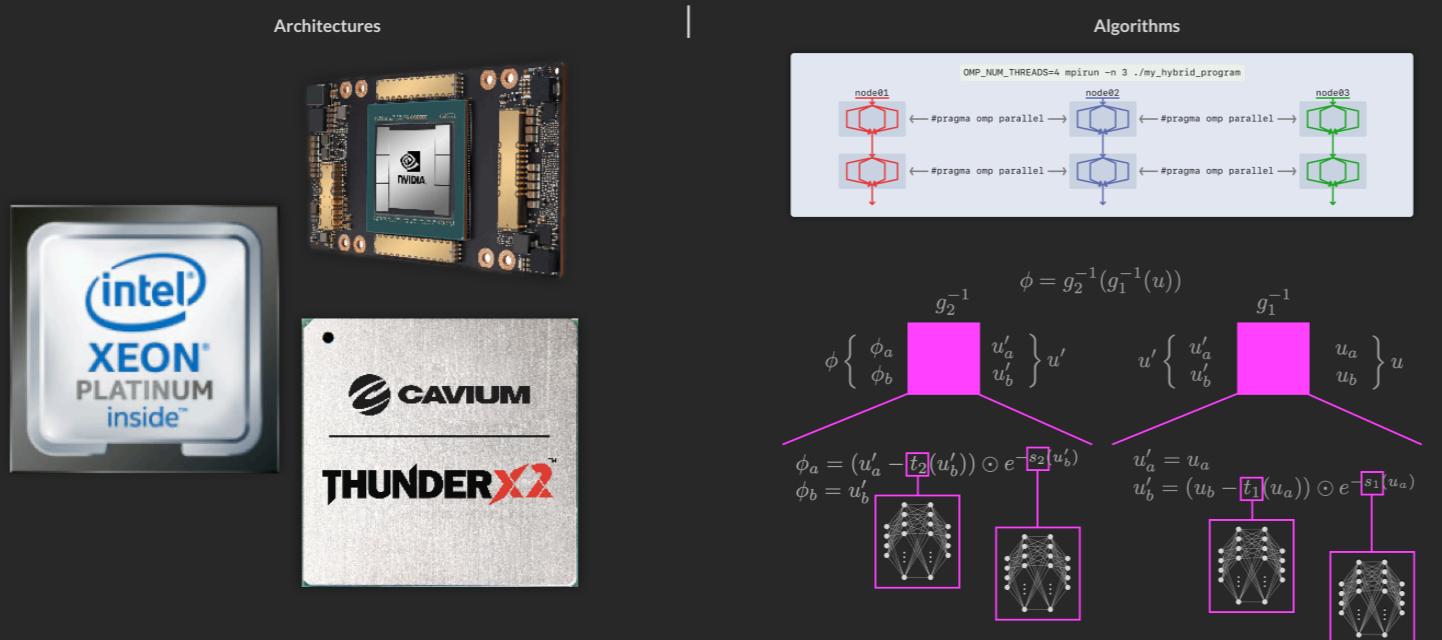
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# Parallel computing as the main paradigm

## High performance computing means parallel computing

- Technology trends mean parallelism is essential for advanced computing
- Practitioners of computational science and engineering benefit from knowledge of concepts and challenges of parallel computing
  - Architectures and their characteristics
  - Algorithms and how amenable they are to parallelisation
  - Performance metrics and their significance, e.g. sustained and peak floating point performance, bandwidth, scalability



# Capacity vs Capability

How do we "spend" parallelism?

- *Capacity computing*
  - Improve time-to-solution of a problem that can also run on less number of processes
  - E.g. solve many small problems
- *Capability computing*
  - Solve a problem that was *impossible* to solve on less processes
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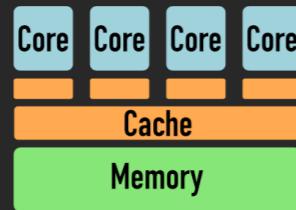
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# Shared vs Distributed memory paradigm

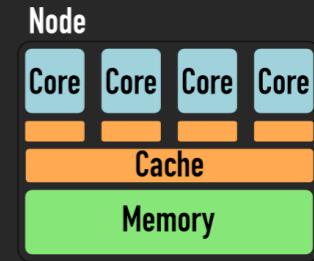
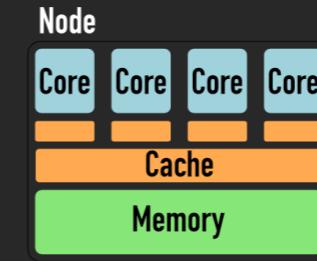
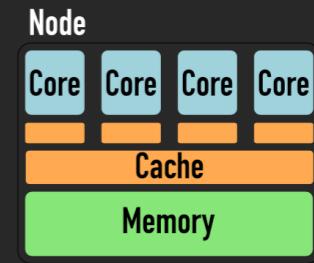
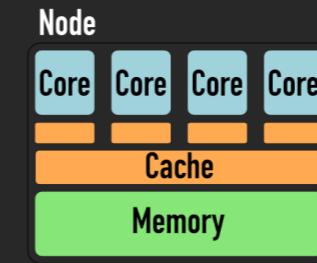
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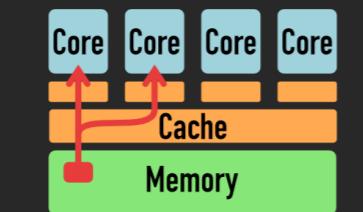
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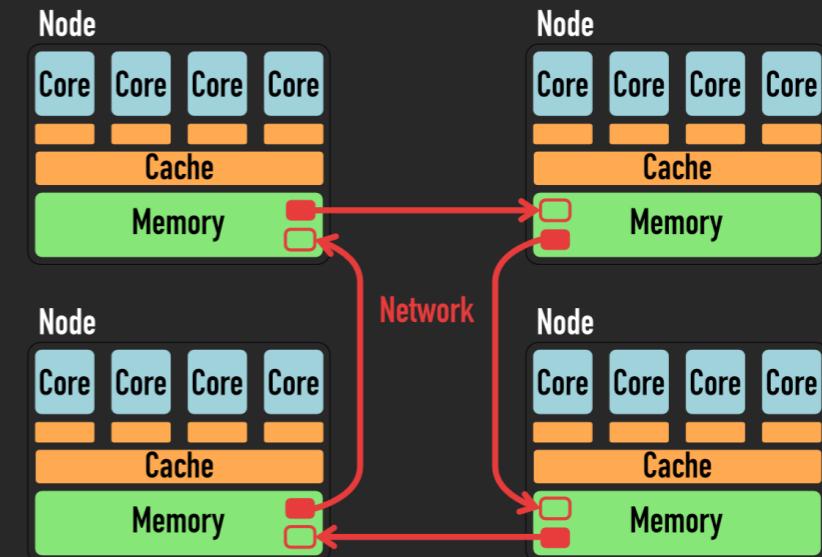
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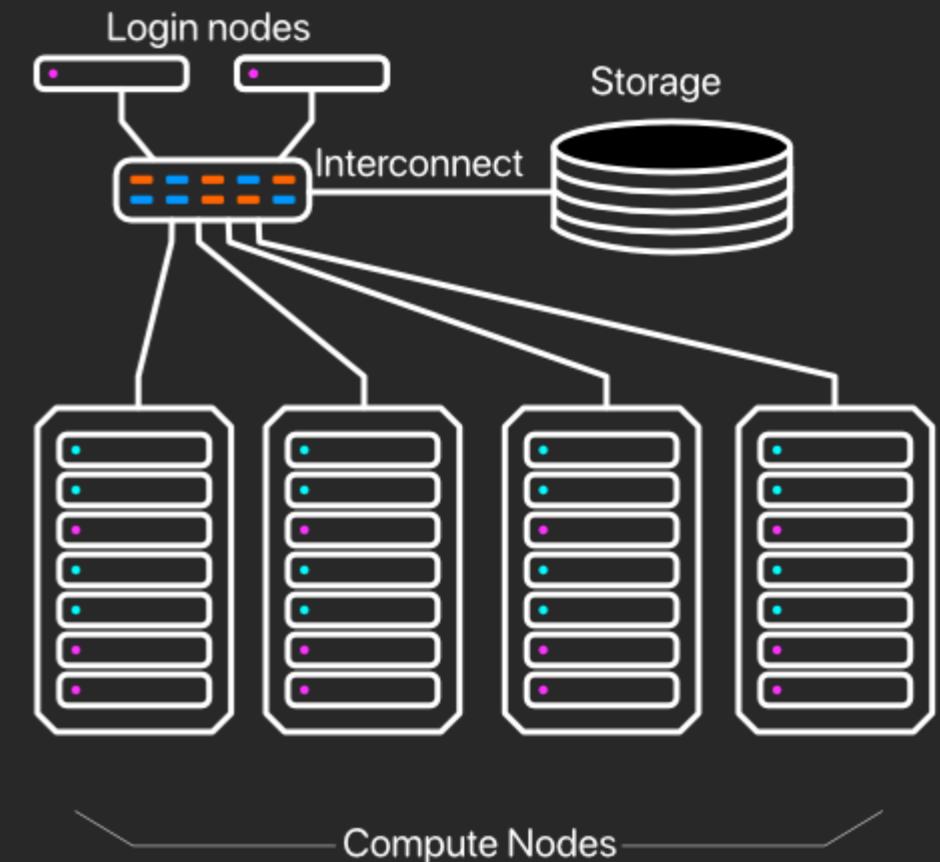
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Data shared via explicit communication over a network

# A User's View of a Supercomputer

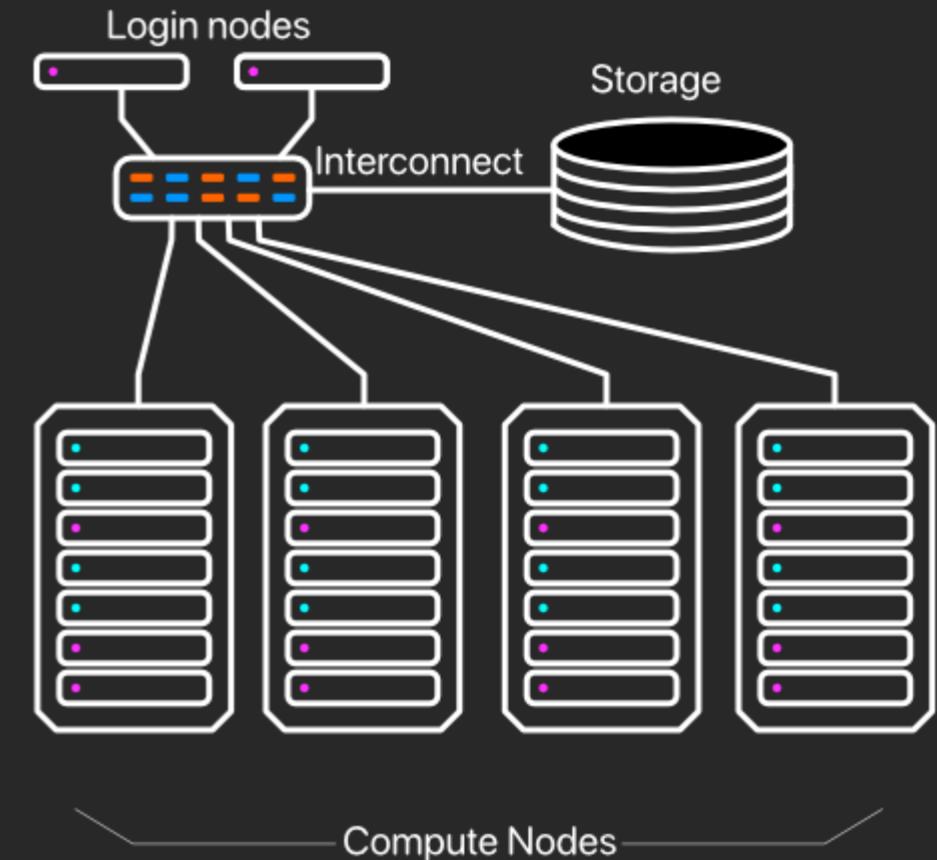
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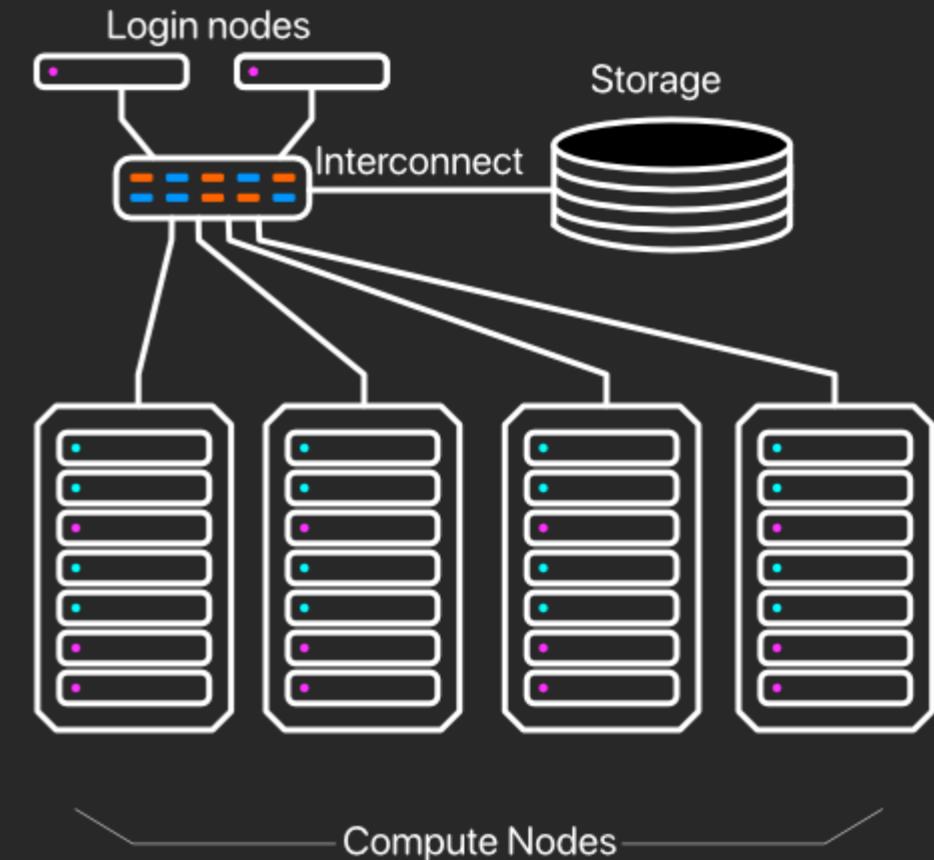
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  - Memory (i.e. RAM)
  - Some storage and/or NVMe
  - Network interfaces, possibly separate between management and workload



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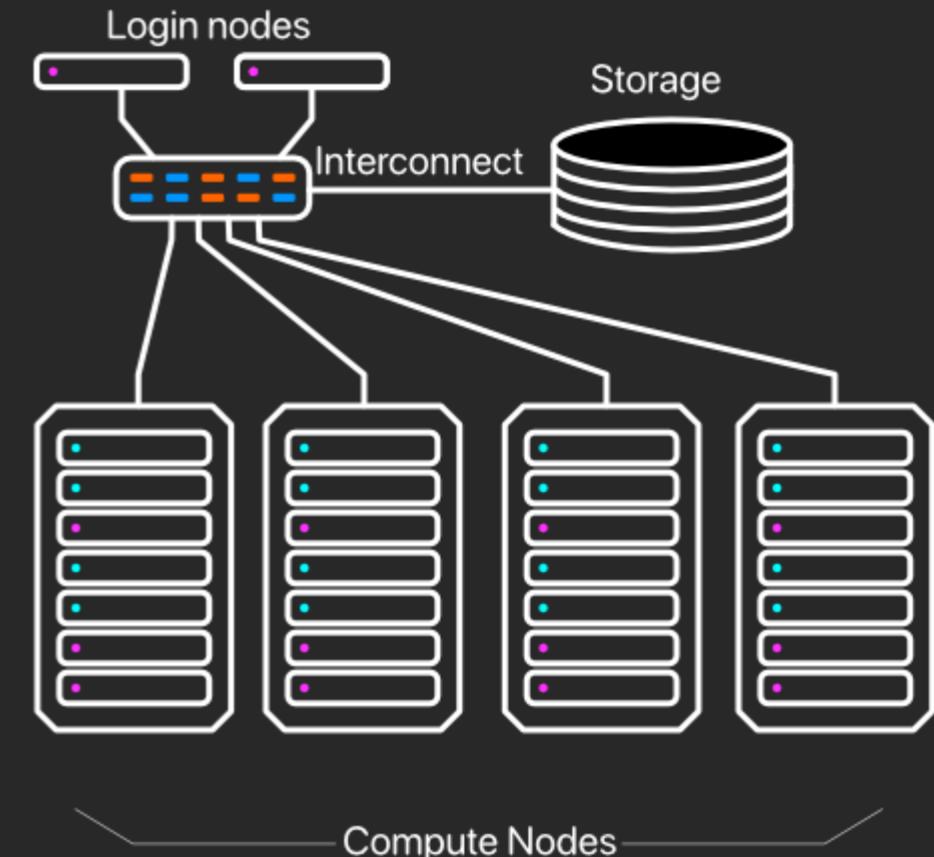
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  - Interfaces on nodes
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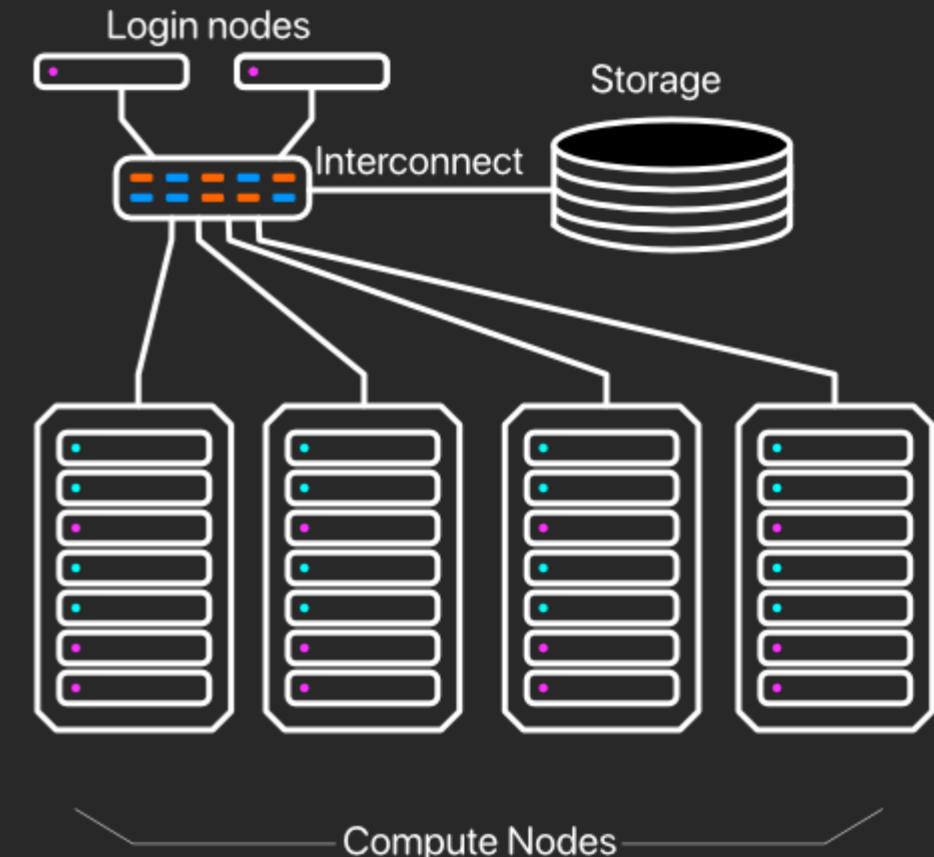
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- Storage
  - Still predominantly spinning disks
  - Solid state drives are emerging for smaller scratch space
  - Tape systems for archiving



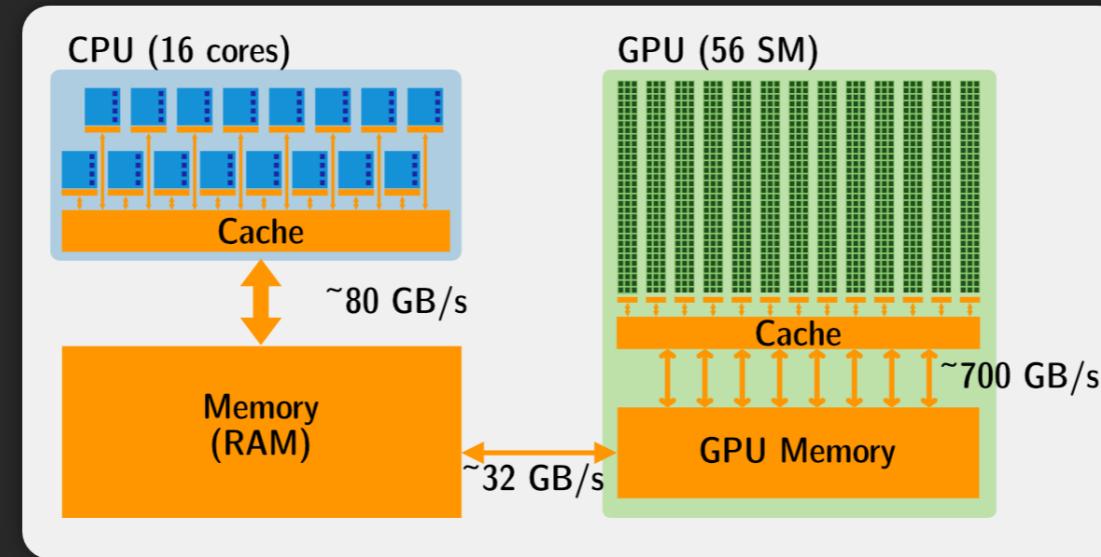
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- Storage
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  - Solid state drives are emerging for smaller scratch space
  - Tape systems for archiving
- Front-end nodes
  - For user access
  - Compiling, submitting jobs, etc.



# Accelerators and Their Characteristics



## CPU

- Large area devoted to control
- Less area devoted to ALUs
- Larger memory and caches
- Moderate bandwidth to memory
- Optimized for serial execution

## GPU

- Less area devoted to control
- More area devoted to ALUs
- Smaller memory and caches
- Higher bandwidth to memory
- Optimized for parallel execution

# Accelerators and Their Characteristics

## Computing devices

Most supercomputers have compute nodes equipped with a co-processor, typically a general purpose GPU

- CPU architecture
  - Optimized for handling a diverse ranged of instructions on multiple data
  - Reliance on prefetching
  - Some availability of SIMD floating point units
- GPU architecture
  - Optimized for *throughput*, i.e. applying the same operation on multiple data
  - Reliance on very wide SIMD units

# Accelerators and Their Characteristics

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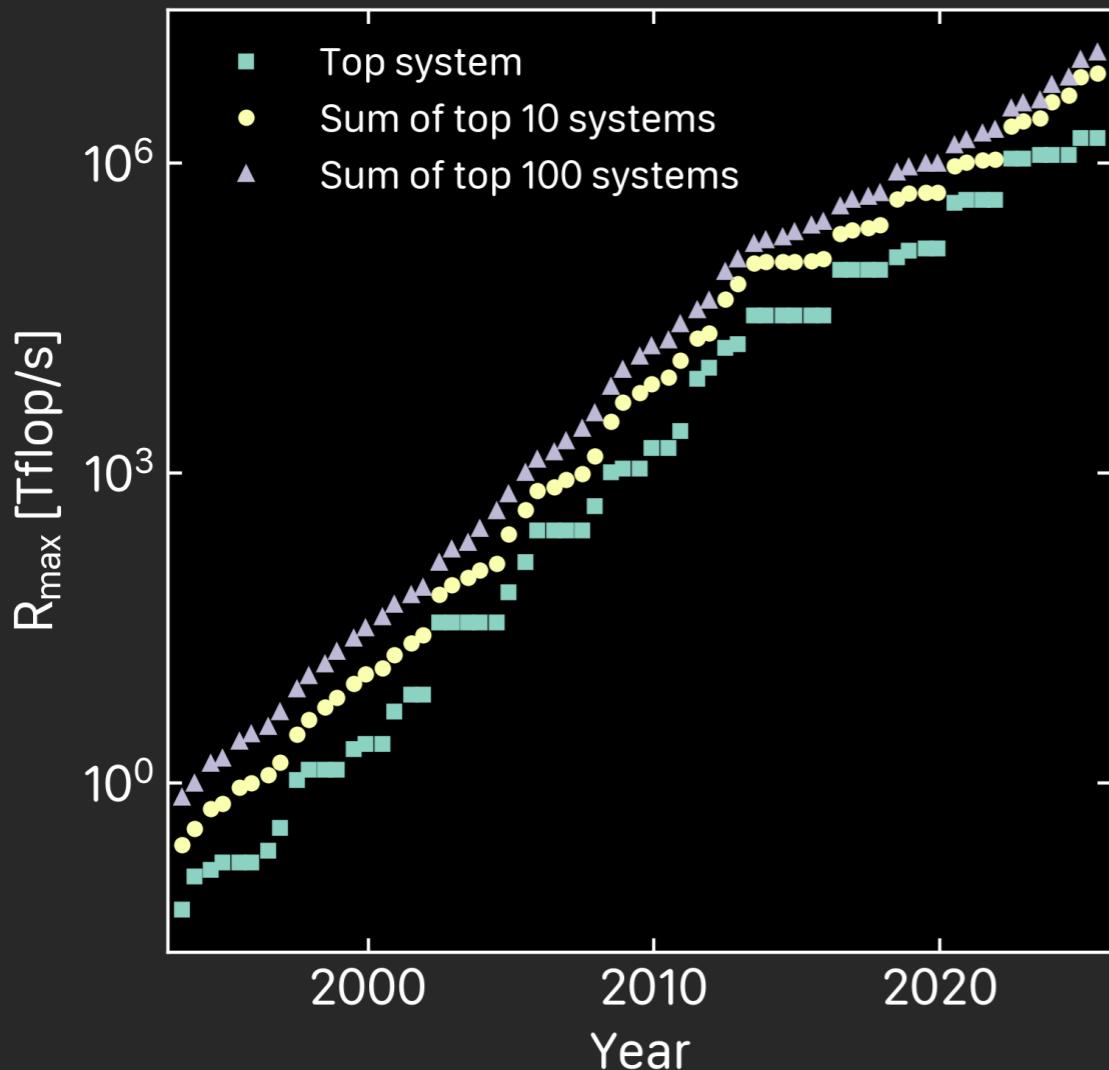
CPU architectures and main characteristics

- Intel Xeon and AMD EPYC (x86), various ARM implementations, and IBM Power
- O(10) cores per CPU (nowadays: 128), 2 - 4 CPUs per node
- Memory bandwidth of ~50-100 GBytes/s
- Theoretical peak floating point performance ~30-50 Gflop/s per core

GPU architectures and main characteristics

- NVIDIA Data Center GPUs and AMD Instinct
- O(1000) "cores" or Arithmetic and Logical Unit (ALUs). 2 - 6 GPUs per node
- Memory bandwidth of O(1000) GBytes/s
- Theoretical peak floating point performance ~50 Tflop/s per GPU

# State of Supercomputer Landscape



- Classification according to *sustained* floating point performance
- Run High Performance Linpack (HPL) on whole system
- <https://www.top500.org> Latest list: **June 2025**
  - Top two system: US, AMD GPU-based system, 1.7 and 1.3 Eflop/s sustained
  - Top in Europe: DE, 4<sup>th</sup> overall, GPUs (NVIDIA GH200), 793 Pflop/s sustained
  - **8** out of top 10 equipped with GPUs, either NVIDIA or AMD, +1 with Intel GPUs

# State of Supercomputer Landscape

## Notable supercomputers in Europe



Lumi - CSC, FI

- HPE Cray EX235a, AMD EPYC CPUs, AMD Instinct MI250X GPUs
- ~430 Pflop/s theoretical peak

Leonardo - CINECA, IT

- BullSequana XH2000, Intel Xeon CPUs, NVIDIA A100 GPUs
- ~300 Pflop/s theoretical peak



# State of Supercomputer Landscape

## Notable supercomputers in Europe



Adastra - GENCI, FR

- HPE Cray EX235a, AMD EPYC CPUs, AMD Instinct MI250X GPUs
- ~60 Pflop/s theoretical peak

Jupiter - JSC, DE

- NVIDIA Grace Hopper Superchips (ARM G100 CPU + H200 GPU)
- ~ 930 Pflop/s theoretical peak (partial system)
- >1 Eflop/s expected on full system



# State of Supercomputer Landscape

## Notable supercomputers in Europe



Alps - CSCS, CH

- NVIDIA Grace CPUs, NVIDIA Hopper (H100) GPUs
- ~575 Pflop/s theoretical peak

MareNostrum 5 - BSC, ES

- Bull, four main partitions including Intel CPUs and NVIDIA H100 GPUs
- GPU partition: 250 Pflop/s theoretical peak



# Accessing Supercomputing Resources

In Europe, these systems also made available via a single, centralized allocation process

Access via so-called EuroHPC calls

- Technical review: need to show that methods and software are appropriate for the underlying architecture. Scaling and performance analysis required.
- Scientific review: peer-review of the proposed science.
- $O(100)$  core-hours for individual projects within "Extreme Scale Allocations"
- $O(10)$  core-hours for individual projects within regular allocations

Smaller-scale access available nationally

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→ National Competence Centers

- Facilitate access to HPC resources
- Training, consulting, networking

# Summary

## Supercomputing architectures today

- Commodity components
- Specialized integration
- Massively parallel
- Heterogeneous; most of the performance is provided by accelerators

## Main challenge is exploiting parallelism

- Need a good understanding of the application
- ... and of the characteristics of the underlying architecture

## World's largest systems are open-access

- EuroHPC systems are open for applications from all participating members
- National Competence Centers here to facilitate access
- Expect Exascale in EU this year. Systems in France and Jupiter at Jülich, Germany



# Introduction to distributed memory parallel computing

## Examples with mpi4py

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## Parallel programming

- Distributed memory paradigm
- Main features and relation to shared memory parallelism

## MPI Introduction

- The MPI standard and development workflow
- Using MPI with Python
- Hands-on examples

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1. PDF from github: <https://github.com/CaSToRC-CyI/EuroCC-Intermediate-Training-2024>
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## Exercises

- Available on github:
  - <https://github.com/CaSToRC-CyI/EuroCC-Intermediate-Training-2024>
- On common storage on "Cyclone"
  - /nvme/scratch/edu27/MPI/

# The Message Passing Interface

- MPI: An Application Programmer Interface (API)
  - A *library specification*; determines functions, their names and arguments, and their functionality
- A *de facto* standard for programming *distributed memory* systems
- Current specification is version 4 (MPI-4.0), released June 9, 2021
  - For most systems you can reliably assume MPI-3.1 is in place
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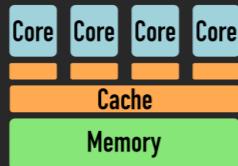
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## Distributed memory programming

- Each process has its own memory domain
- MPI functions facilitate:
  - Obtaining environment information about the running process, e.g., process id, number of processes, etc.
  - Achieving *communication* between processes, e.g. synchronization, copying of data, etc.

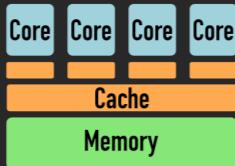
# Shared memory

- Multiple processes share common memory (common *memory address space*)
- E.g. multi-core CPU, multi-socket node, GPU threads, etc.
- Programming models: OpenMP, pthreads, MPI, CUDA (sort of)

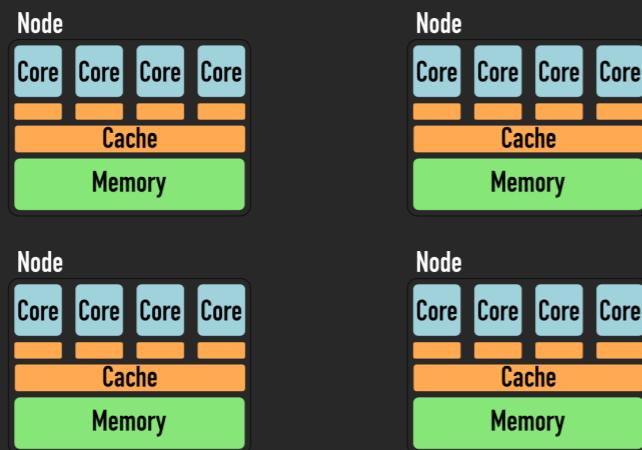


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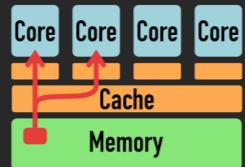
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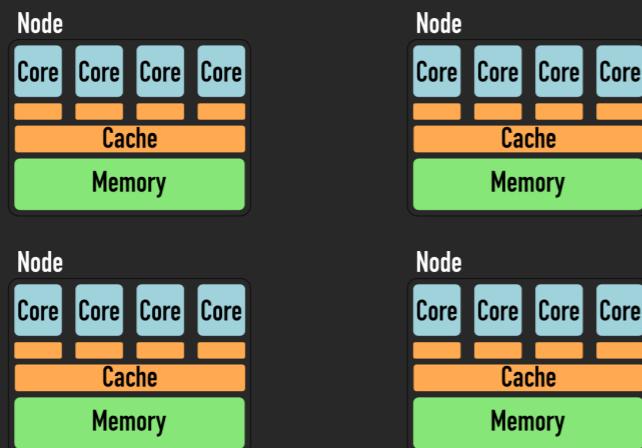
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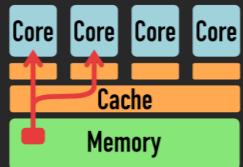
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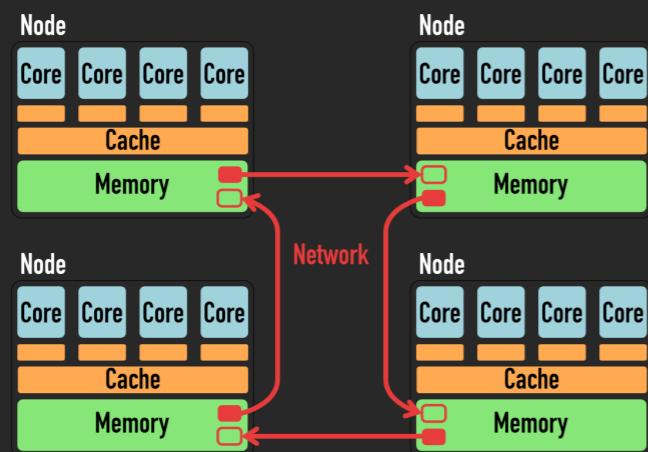
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# Distributed memory



Data shared via explicit communication over a network

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ssh node01 python my_script.py &
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`my_script.py` will run on each node identically

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- Depending on the system, instead of `mpirun` you may be required `mpiexec` or `srun` which take similar (but not identical) arguments

# Linking against MPI/loading MPI modules

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- We would also need to link against MPI libraries; precise invocation depends on the compiler, the MPI implementation used, its version, etc., e.g.:

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mpicc -o my_mpi_program my_mpi_program.c
```

- For our Python examples, we will use a Python module, `mpi4py`, which implements the MPI API

```
import mpi4py
```

or, more commonly

```
from mpi4py import MPI
```

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```
#include <mpi.h>

int
main(int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    /*
     ...
     ...
     ...
    */
    MPI_Finalize();
    return 0;
}
```

# Initialization

- Two functions you will almost always call
  - `MPI_Comm_size()` or `MPI.COMM_WORLD.Get_size()`: gives the number of parallel process running ( $n_{\text{proc}}$ )
  - `MPI_Comm_rank()` or `MPI.COMM_WORLD.Get_rank()`: determines the *rank* of the process, i.e. a unique number between 0 and  $n_{\text{proc}} - 1$  that identifies the calling process
- A complete example:

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

int
main(int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    int nproc, rank;
    MPI_Comm_size(MPI_COMM_WORLD, &nproc);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    printf(" This is rank = %d of nproc = %d\n", rank, nproc);
    MPI_Finalize();
    return 0;
}
```

```
from mpi4py import MPI
nproc = MPI.COMM_WORLD.Get_size()
rank = MPI.COMM_WORLD.Get_rank()
print(f" This is rank = {rank} of nproc = {nproc}")
```

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}
```

```
from mpi4py import MPI

nproc = MPI.COMM_WORLD.Get_size()
rank = MPI.COMM_WORLD.Get_rank()
print(f" This is rank = {rank} of nproc = {nproc}")
```

- `MPI_COMM_WORLD` or `MPI.COMM_WORLD` is an *MPI communicator*
  - A user can partition processes into subgroups, defining *custom communicators* (not covered here)
  - *By default*, the initial communicator is `COMM_WORLD`, i.e. all processes in one communicator

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  - A user can partition processes into subgroups, defining *custom communicators* (not covered here)
  - *By default*, the initial communicator is `COMM_WORLD`, i.e. all processes in one communicator

- **No assumptions** can safely be made about the order in which the `printf()` statements occur, i.e. the order in which each process prints is **practically random**

# Initialization

- Compiling and running the previous program (assuming it is saved as `example.c` or `example.py`)

```
[user@front02 ~]$ mpicc -o example example.c
[user@front02 ~]$ mpirun -n 5 example
This is rank = 3 of nproc = 5
This is rank = 1 of nproc = 5
This is rank = 2 of nproc = 5
This is rank = 4 of nproc = 5
This is rank = 0 of nproc = 5
```

```
[user@front02 ~]$ mpirun -n 5 python example.py
This is rank = 3 of nproc = 5
This is rank = 1 of nproc = 5
This is rank = 2 of nproc = 5
This is rank = 4 of nproc = 5
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```

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```

```
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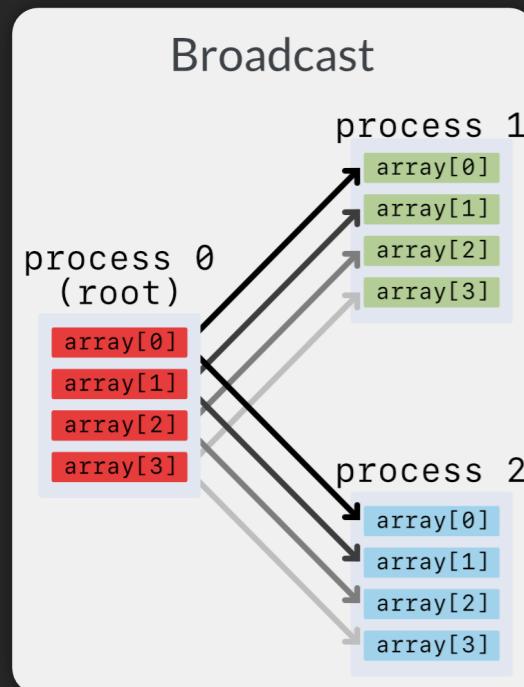
- Note that the order is random
- Unless any *explicit synchronization* is implemented, the order in which each process calls the print statement is unpredictable
- Most *collective operations* implicitly synchronize the processes

# Collective operations

- The first set of communication functions we will look at are *collective operations*
- Collective: all processes must be involved in the operation (as opposed to *point-to-point* communications)
- Examples (this list is not exhaustive!):
  - Broadcast a variable from one process to all processes (Broadcast)
  - Distribute elements of an array on one process to multiple processes (Scatter)
  - Collect elements of arrays scattered over processes into a single process (Gather)
  - Sum a variable over all processes (Reduction)

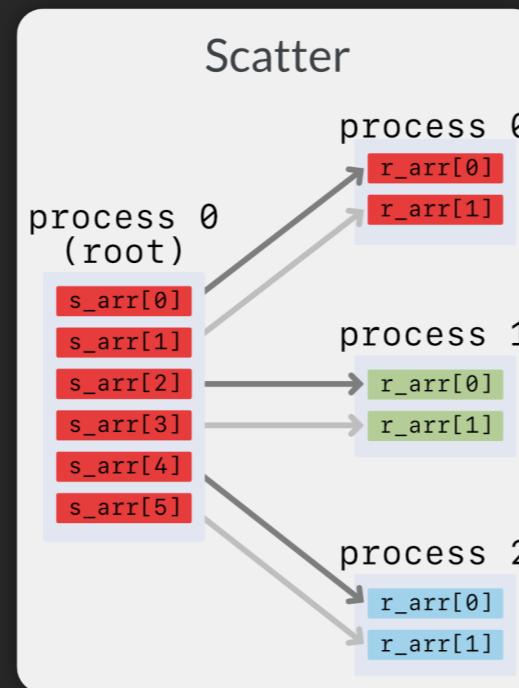
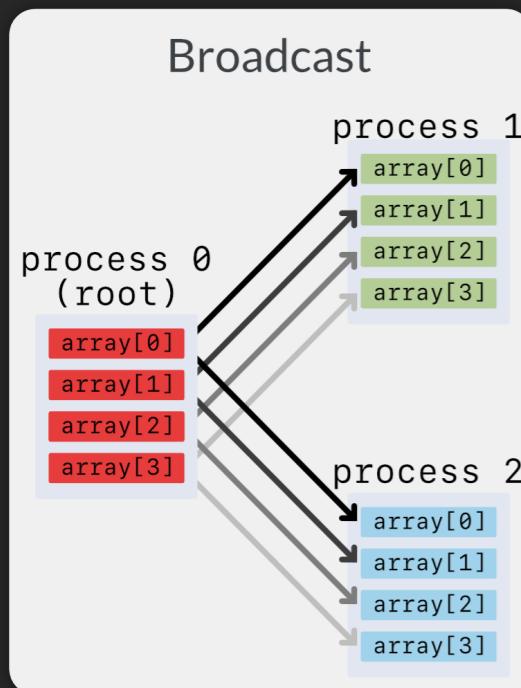
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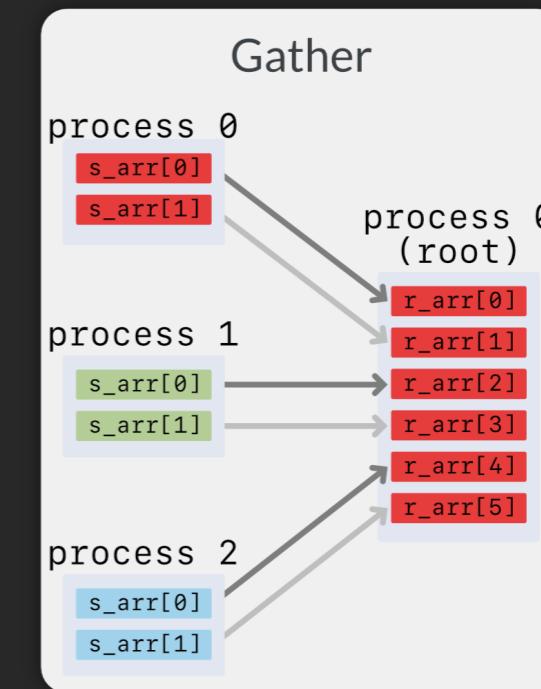
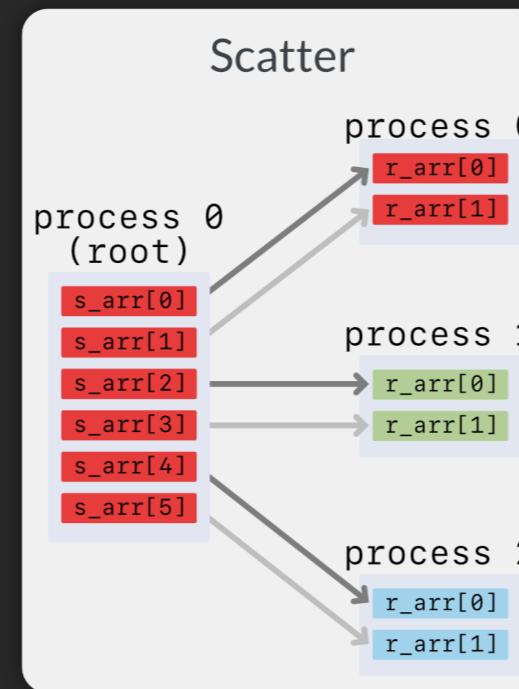
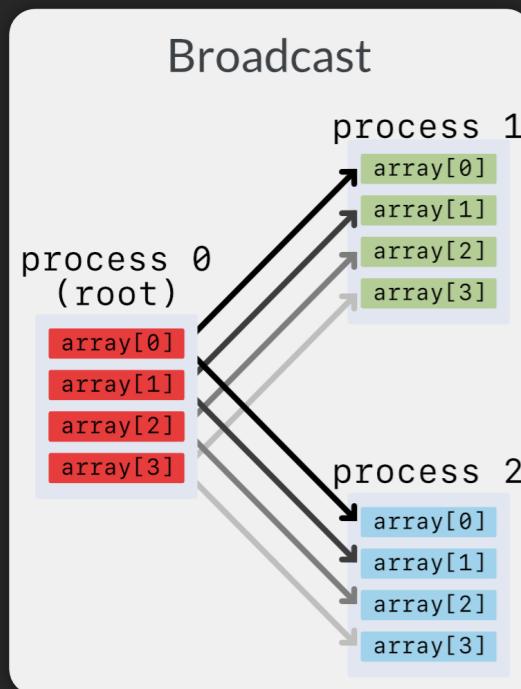
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# Collective operations: Broadcast

Broadcast:

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MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm);
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- In C, we can pass a scalar by using its memory address (2<sup>nd</sup> example above). In Python, we can use zero-dimensional numpy array for this
- Full list of types available in MPI documentation. E.g. see: <https://www.mpich.org/static/docs/latest/www3/Constants.html>

# Collective operations: Scatter

- Scatter:

```
MPI_Scatter(  
    const void *sendbuf, int sendcount, MPI_Datatype sendtype,  
    void *recvbuf, int recvcount, MPI_Datatype recvtype,  
    int root, MPI_Comm comm  
)
```

```
MPI.COMM_WORLD.Scatter(  
    sendbuf: BufSpec, recvbuf: BufSpec, root: int = 0  
)
```

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MPI.COMM_WORLD.Scatter(  
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)
```

- sendcount is the number of elements to be sent to *each* process
- sendbuf is only relevant in the root process

- Example: distribute a 12-element array from process 0, assuming 3 processes in total (including root)

```
double arr_all[12]; /* ← this only needs to be defined on process with rank = 0 */  
double arr_proc[4];  
MPI_Scatter(arr_all, 4, MPI_DOUBLE, arr_proc, 4, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

```
arr_all = np.random.rand(12)  
arr_proc = np.zeros([4])  
MPI.COMM_WORLD.Scatter(arr_all, arr_proc, root = 0)
```

# Collective operations: Scatter

- Scatter:

```
MPI_Scatter(  
    const void *sendbuf, int sendcount, MPI_Datatype sendtype,  
    void *recvbuf, int recvcount, MPI_Datatype recvtype,  
    int root, MPI_Comm comm  
)
```

```
MPI.COMM_WORLD.Scatter(  
    sendbuf: BufSpec, recvbuf: BufSpec, root: int = 0  
)
```

- *Example:* distribute each element of a 4-element array to 4 processes in total (including root)

```
double arr[4]; /* ← this only needs to be defined on process with rank = 0 */  
double element;  
MPI_Scatter(arr, 1, MPI_DOUBLE, &element, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

```
arr = np.random.rand(4)  
element = np.zeros([])  
MPI.COMM_WORLD.Scatter(arr, element, root = 0)
```

# Collective operations: Scatter

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```
MPI_Scatter(  
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```
double arr[4]; /* ← this only needs to be defined on process with rank = 0 */  
double element;  
MPI_Scatter(arr, 1, MPI_DOUBLE, &element, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

```
arr = np.random.rand(4)  
element = np.zeros([])  
MPI.COMM_WORLD.Scatter(arr, element, root = 0)
```

**Note:** the initialization of `element` as a zero-dimensional array

# Collective operations: Gather

- Gather:

```
MPI_Gather(  
    const void *sendbuf, int sendcount, MPI_Datatype sendtype,  
    void *recvbuf, int recvcount, MPI_Datatype recvtype, int root,  
    MPI_Comm comm  
)
```

# Collective operations: Gather

- Gather:

```
MPI_Gather(  
    const void *sendbuf, int sendcount, MPI_Datatype sendtype,  
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    MPI_Comm comm  
)
```

- `recvcount` is the number of elements to be received by *each* process

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)
```

- `recvcount` is the number of elements to be received by *each* process
- `recvbuf` is only relevant in the root process

# Collective operations: Gather

- Gather:

```
MPI_Gather(  
    const void *sendbuf, int sendcount, MPI_Datatype sendtype,  
    void *recvbuf, int recvcount, MPI_Datatype recvtype, int root,  
    MPI_Comm comm  
)
```

- *Example:* collect a 9-element array at process 0, by concatenating 3 elements from each of 3 processes in total (including root)

```
double arr_all[9]; /* ← this only needs to be defined on process with rank = 0 */  
double arr_proc[3];  
MPI_Gather(arr_proc, 3, MPI_DOUBLE, arr_all, 3, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

```
arr_all = np.zeros([9])  
arr_proc = np.random.rand(3)  
MPI.COMM_WORLD.Gather(arr_proc, arr_all, root = 0)
```

# Collective operations: Gather

- Gather:

```
MPI_Gather(  
    const void *sendbuf, int sendcount, MPI_Datatype sendtype,  
    void *recvbuf, int recvcount, MPI_Datatype recvtype, int root,  
    MPI_Comm comm  
)
```

- *Example:* collect a 4-element array at process 0, by concatenating an element from each of 4 processes in total (including root)

```
double arr[4]; /* ← this only needs to be defined on process with rank = 0 */  
double element;  
MPI_Gather(&element, 1, MPI_DOUBLE, arr, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

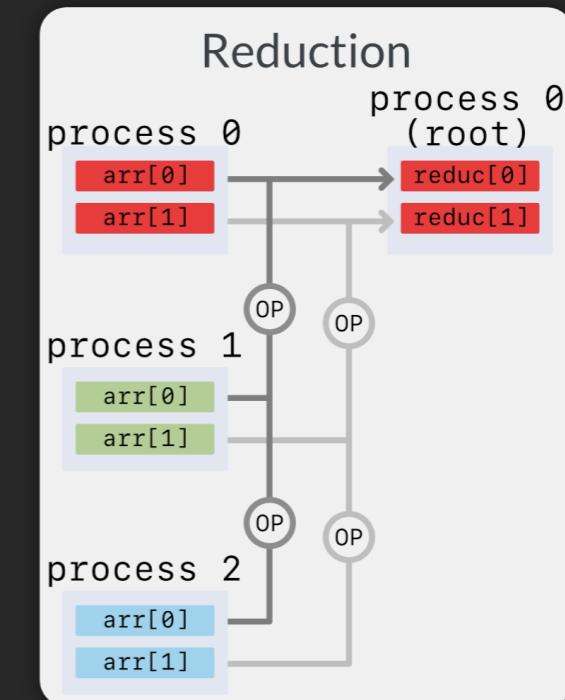
```
arr = np.zeros([4])  
element = np.random.rand(1)  
MPI.COMM_WORLD.Gather(element, arr, root = 0)
```

# Collective operations: Reduction

- Reduction:

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

```
MPI.COMM_WORLD.Reduce(  
    sendbuf: BufSpec, recvbuf: BufSpec,  
    op: Op = SUM, root: int = 0  
)
```



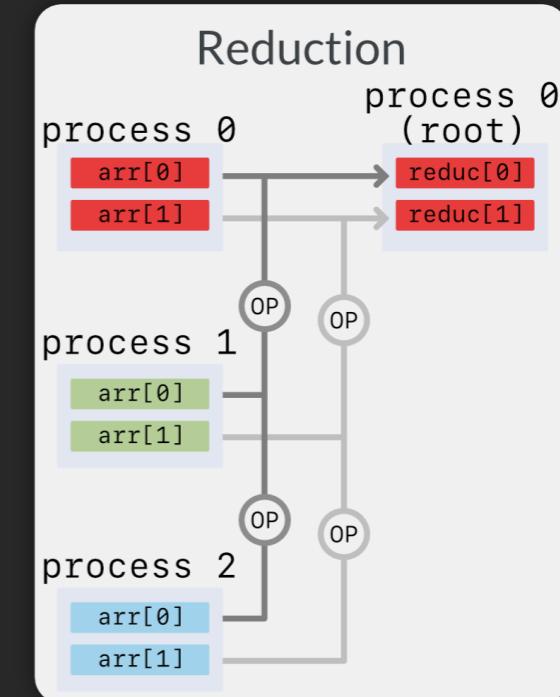
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MPI.COMM_WORLD.Reduce(  
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)
```

- Notes:
  - `Op` is an operation, e.g. `MPI.SUM`, `MPI.PROD`, etc. (`MPI_SUM` and `MPI_PROD` in C)
  - In C note the need for specifying the datatype and `count`, the number of elements of the arrays
  - The operation is over all processes in `comm`, in this case `COMM_WORLD`



# Collective operations: Reduction

- Reduction:

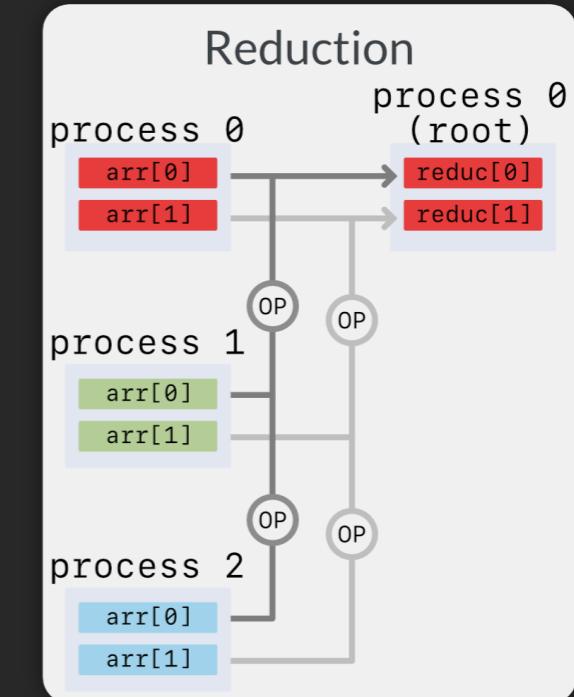
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    MPI_Comm comm  
)
```

```
MPI.COMM_WORLD.Reduce(  
    sendbuf: BufSpec, recvbuf: BufSpec,  
    op: Op = SUM, root: int = 0  
)
```

- Example:* Sum each element of a 3-element array over all processes

```
double s_arr[3];  
double r_arr[3]; /* ← only needs to      *  
                  *      be defined on root */  
MPI_Reduce(s_arr, r_arr, 3, MPI_DOUBLE,  
           MPI_SUM, 0, MPI_COMM_WORLD);
```

```
s_arr = np.random.rand(3)  
r_arr = np.zeros([3])  
MPI.COMM_WORLD.Reduce(s_arr, r_arr, MPI.SUM, root = 0)
```



# Collective operations: Reduction

- Reduction:

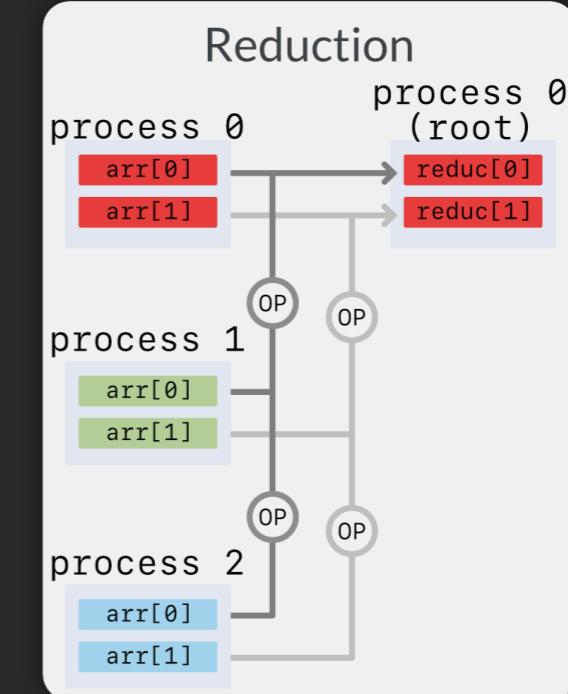
```
MPI_Reduce(  
    const void *sendbuf, void *recvbuf, int count,  
    MPI_Datatype datatype, MPI_Op op, int root,  
    MPI_Comm comm  
)
```

```
MPI.COMM_WORLD.Reduce(  
    sendbuf: BufSpec, recvbuf: BufSpec,  
    op: Op = SUM, root: int = 0  
)
```

- Example: Sum variable var over all processes

```
double var;  
double sum; /* ← only needs to      *  
             *      be defined on root */  
MPI_Reduce(&var, &sum, 1, MPI_DOUBLE,  
           MPI_SUM, 0, MPI_COMM_WORLD);
```

```
var = np.random.rand(1)  
sum = np.zeros([])  
MPI.COMM_WORLD.Reduce(var, sum, MPI.SUM, root = 0)
```



# Collective operations

## Some additional notes on variants of the collectives we have covered

- `Scatterv()` and `Gatherv()`
  - Allow specifying *varying* number of elements to be distributed or collected to or from the process pool
  - Need specifying additional arguments containing offsets of the send or receive buffer

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  - Same as `Reduce()`, but result is placed on all processes in the pool
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  - For some functions, can replace the send or receive buffer with MPI.IN\_PLACE (MPI\_IN\_PLACE in C)  
→ which buffer depends on the specific MPI function
  - Instructs MPI to use the **same** buffer for receive and send
  - E.g. below, the sum will be placed in var of the root process (process with rank = 0):

```
var = np.random.rand(1)
if rank != 0:
    MPI.COMM_WORLD.Reduce(var, None, MPI.SUM, root = 0)
else:
    MPI.COMM_WORLD.Reduce(MPI.IN_PLACE, var, MPI.SUM, root = 0)
```

# Point-to-point communication

- Communications that involve transfer of data between two processes

# Point-to-point communication

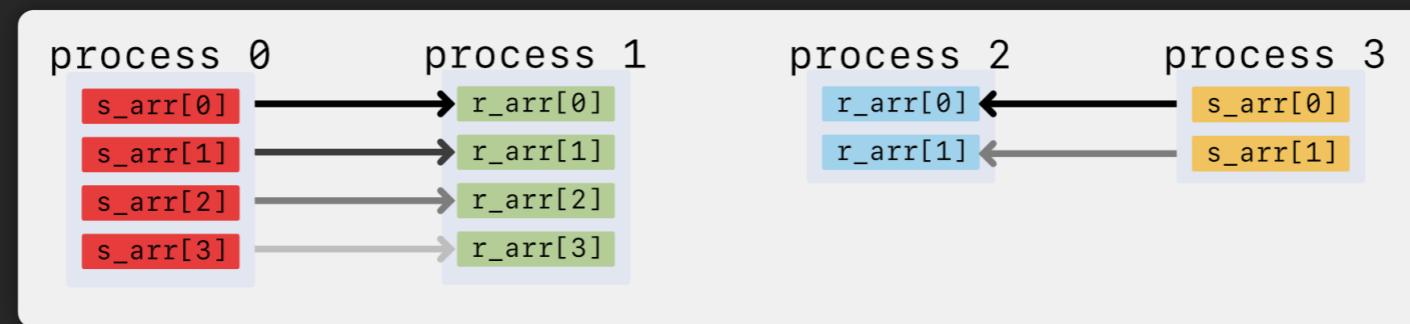
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  - Posting a receive which does not have a matching send

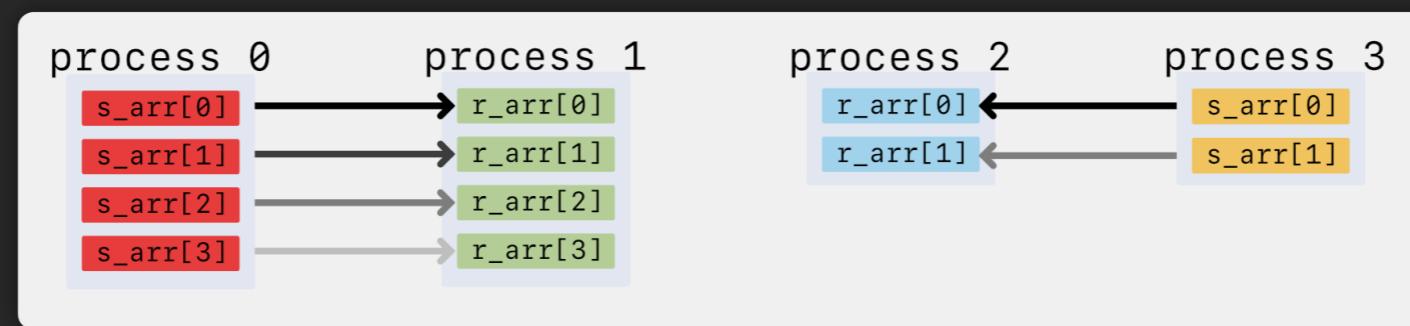
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Two point-to-point communications are depicted above  
↳ between i) process 0 and 1 and between ii) process 2 and 3

# Point-to-point communication

- Send/Receive

```
MPI.COMM_WORLD.Send(buf: BufSpec, dest: int, tag: int = 0)
MPI.COMM_WORLD.Recv(buf: BufSpec, source: int = ANY_SOURCE, tag: int = ANY_TAG, status: Status = None)
```

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- Note the need to specify a source and destination rank

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- The `tag` variable tags the message. In the receiving process, it must match what the sender specified, or can be set to `MPI.ANY_TAG`
- Use of `MPI.ANY_SOURCE` in `Recv()` means "accept data from any source"
- `status` can be used to query the result of the receive (e.g. how many elements were received). We will leave to its default value, `None`, which ignores the status

# Point-to-point communication

- Send/Receive; a trivial example



# Point-to-point communication

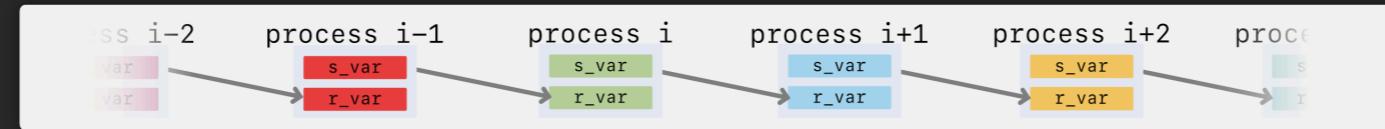
- Send/Receive; a trivial example



```
s_arr = np.random.rand(4)
r_arr = np.zeros([4])
if rank == i:
    MPI.COMM_WORLD.Send(s_arr, j)
if rank == j:
    MPI.COMM_WORLD.Recv(r_arr, i)
```

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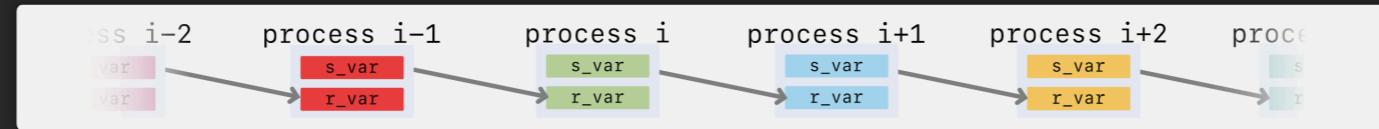
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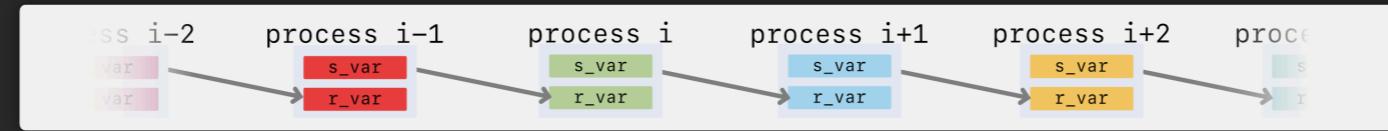
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  - Inelegant, obscure, and error-prone

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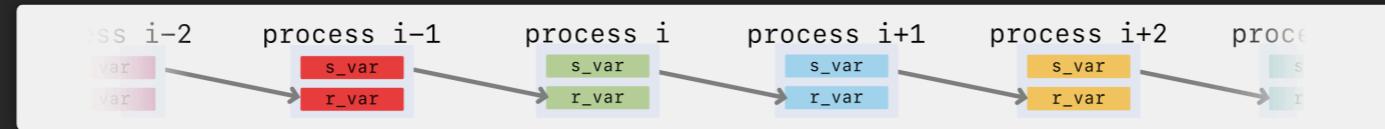


- A more efficient and elegant solution is to use `Sendrecv()`:

```
MPI.COMM_WORLD.Sendrecv(  
    sendbuf: BufSpec, dest: int, sendtag: int = 0,  
    recvbuf: BufSpec, source: int = ANY_SOURCE, recvtag: int = ANY_TAG,  
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- For the depicted example:

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Note: lower-case versions of `send()` and `recv()`

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  - The function `wait()` is used to block until the operation has complete

```
request = MPI.COMM_WORLD.Isend(sendbuf, destrank);
/*
 * More code can come here, provided it
 * does not modify sendbuf, which is
 * assumed to be "in-flight"
 */
request.wait()
```

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- Note that if you have modified `ex${n}.py` correctly, the job should complete in **less than one minute**

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- The MPI functions demonstrated in each exercise are:
  - ex01: Use of `Get_rank()` and `Get_size()`
  - ex02: Use of `Bcast()`, `Scatter()`, and `Reduce()`
  - ex03: Use of `Gather()`
  - ex04: Use of `Bcast()`, `Scatter()`, `Sendrecv()`, and `Gather()`

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- The MPI functions demonstrated in each exercise are:
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  - ex02: Use of `Bcast()`, `Scatter()`, and `Reduce()`
  - ex03: Use of `Gather()`
  - ex04: Use of `Bcast()`, `Scatter()`, `Sendrecv()`, and `Gather()`
- All exercises have been tested with specific versions of OpenMPI, the GNU Compiler, and numpy and mpi4py. Please use:

```
module load SciPy-bundle/2024.05-gfbf-2024a mpi4py/4.0.1-gompi-2024a
```

for all exercises.

# Exercises

## Ex01

- Modify ex01.py to call Get\_size() and Get\_rank() appropriately

```
# TODO: call the appropriate MPI functions here
#
rank = # TODO
size = # TODO
```

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```

- A job script has been prepared to run ex01:

```
[user@front02 ex01]$ cat sub-ex01.sh
#!/bin/bash
#SBATCH --job-name=ex01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --ntasks-per-node=4
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00
#SBATCH --reservation=edu27
#SBATCH -A edu27
module load SciPy-bundle/2024.05-gfbf-2024a mpi4py/4.0.1-gompi-2024a
mpirun python ex01.py
```

# Exercises

## Ex01

- Modify ex01.py to call Get\_size() and Get\_rank() appropriately

```
# TODO: call the appropriate MPI functions here
#
rank = # TODO
size = # TODO
```

- A job script has been prepared to run ex01:

```
[user@front02 ex01]$ cat sub-ex01.sh
#!/bin/bash
#SBATCH --job-name=ex01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --ntasks-per-node=4
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00
#SBATCH --reservation=edu27
#SBATCH -A edu27
module load SciPy-bundle/2024.05-gfbf-2024a mpi4py/4.0.1-gompi-2024a
mpirun python ex01.py
```

- 2 nodes, 8 processes, meaning 4 processes per node

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#
rank = # TODO
size = # TODO
```

- A job script has been prepared to run ex01:

```
[user@front02 ex01]$ cat sub-ex01.sh
#!/bin/bash
#SBATCH --job-name=01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --ntasks-per-node=4
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00
#SBATCH --reservation=edu27
#SBATCH -A edu27
module load SciPy-bundle/2024.05-gfbf-2024a mpi4py/4.0.1-gompi-2024a
mpirun python ex01.py
```

- 2 nodes, 8 processes, meaning 4 processes per node
- program output will be redirected to file ex01-output.txt

# Exercises

## Ex01

- Modify ex01.py to call Get\_size() and Get\_rank() appropriately

```
# TODO: call the appropriate MPI functions here
#
rank = # TODO
size = # TODO
```

- A job script has been prepared to run ex01:

```
[user@front02 ex01]$ cat sub-ex01.sh
#!/bin/bash
#SBATCH --job-name=ex01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --ntasks-per-node=4
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00
#SBATCH --reservation=edu27
#SBATCH -A edu27
module load SciPy-bundle/2024.05-gfbf-2024a mpi4py/4.0.1-gompi-2024a
mpirun python ex01.py
```

- 2 nodes, 8 processes, meaning 4 processes per node
- program output will be redirected to file ex01-output.txt
- requests 1 minute. If not done by then, the scheduler will kill the job

# Exercises

## Ex01

- Submit the job script:

```
[user@front02 ex01]$ sbatch sub-ex01.sh
Submitted batch job 69711
[user@front02 ex01]$
```

# Exercises

## Ex01

- Submit the job script:

```
[user@front02 ex01]$ sbatch sub-ex01.sh
Submitted batch job 69711
[user@front02 ex01]$
```

- Check status of job:

```
[user@front02 ex01]$ squeue -u $USER
JOBID PARTITION      NAME      USER ST      TIME   NODES NODELIST(REASON)
69712      cpu      01      user  R      0:00      2  cn[01-02]
[user@front02 ex01]$
```

# Exercises

## Ex01

- Submit the job script:

```
[user@front02 ex01]$ sbatch sub-ex01.sh
Submitted batch job 69711
[user@front02 ex01]$
```

- Check status of job:

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JOBID PARTITION      NAME      USER ST      TIME   NODES NODELIST(REASON)
69712      cpu      01      user R      0:00      2 cn[01-02]
[user@front02 ex01]$
```

- If status is **CF**, i.e. "configuring", you have been allocated nodes that were in power-saving mode and are now booting. It may take several minutes until they boot.

# Exercises

## Ex01

- Submit the job script:

```
[user@front02 ex01]$ sbatch sub-ex01.sh
Submitted batch job 69711
[user@front02 ex01]$
```

- Check status of job:

```
[user@front02 ex01]$ squeue -u $USER
JOBID PARTITION      NAME      USER ST      TIME   NODES NODELIST(REASON)
69712      cpu      01      user    R      0:00      2 cn[01-02]
[user@front02 ex01]$
```

- If status is `CF`, i.e. "configuring", you have been allocated nodes that were in power-saving mode and are now booting. It may take several minutes until they boot.
- Otherwise, the job runs very quickly. You may see no output above if the job has finished:

```
[user@front02 ex01]$ squeue -u $USER
JOBID PARTITION      NAME      USER ST      TIME   NODES NODELIST(REASON)
[user@front02 ex01]$
```

# Exercises

## Ex01

- If done, the file ex01-output.txt should have been created
- Inspect the file:

```
[user@front02 ex01]$ cat ex01-output.txt
This is rank = 2 of nproc = 8 on node: cn03
This is rank = 3 of nproc = 8 on node: cn03
This is rank = 4 of nproc = 8 on node: cn03
This is rank = 5 of nproc = 8 on node: cn03
This is rank = 6 of nproc = 8 on node: cn13
This is rank = 0 of nproc = 8 on node: cn13
This is rank = 1 of nproc = 8 on node: cn13
This is rank = 7 of nproc = 8 on node: cn13
[user@front02 ex01]$
```

# Exercises

## Ex01

- If done, the file `ex01-output.txt` should have been created
- Inspect the file:

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This is rank = 6 of nproc = 8 on node: cn13
This is rank = 0 of nproc = 8 on node: cn13
This is rank = 1 of nproc = 8 on node: cn13
This is rank = 7 of nproc = 8 on node: cn13
[user@front02 ex01]$
```

- Note the order is nondeterministic; whichever process reaches the print statement first prints

# Exercises

## Ex02

- ex02.py demonstrates the use of Scatter() and Reduce()
- The file with name array.txt includes 55,440 floating point numbers, one per line:

```
[user@front02 ex02]$ head array.txt
7.913676052329088328e-01
1.879167007836126668e-01
2.343674804515035737e-01
4.707043244181141617e-02
6.272795840838938375e-01
2.725799268304553991e-01
5.803516013116442052e-01
2.356271465482765448e-01
2.982738904468156260e-01
5.372364132030218453e-01
[ikoutsou@front02 ex02]$
```

# Exercises

## Ex02

- We would like:

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  - The root process to read all elements into an array `array[]`

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  - The root process to read all elements into an array `array[]`
  - The root process to *broadcast* the total number of elements of the array, `ntot`
  - Each process to initialize an empty array `sub[]` with number of elements `nloc = ntot / size`

# Exercises

## Ex02

- We would like:
  - The root process to read all elements into an array `array[]`
  - The root process to *broadcast* the total number of elements of the array, `ntot`
  - Each process to initialize an empty array `sub[]` with number of elements `nloc = ntot / size`
  - The root process to scatter the elements of array `array[]` to all processes
    - ↳ Each process should receive `nloc` elements

# Exercises

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  - Each process to sum its local elements, storing the result into `sum_loc`

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  - To use a reduction operation to obtain the grand total over all 55,440 elements in the root rank

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- Look at `ex02.py`. You **only need to complete some parts**, as instructed by the comments with `TODO`

# Exercises

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    - ↳ Each process should receive `nloc` elements
  - Each process to sum its local elements, storing the result into `sum_loc`
  - To use a reduction operation to obtain the grand total over all 55,440 elements in the root rank
- Look at `ex02.py`. You **only need to complete some parts**, as instructed by the comments with `TODO`
- The correct result, which will be in `ex02-output.txt` should be:

```
Sum: 27777.25711
```

# Exercises

## Ex03

- This exercise demonstrates `Gather()`
- A file `filenames.txt` includes the filenames of 8 files:

```
[user@front02 ex03]$ cat filenames.txt  
00.txt  
01.txt  
02.txt  
03.txt  
04.txt  
05.txt  
06.txt  
07.txt  
[user@front02 ex03]$
```

# Exercises

## Ex03

- This exercise demonstrates Gather()
- A file `filenames.txt` includes the filenames of 8 files:

```
[user@front02 ex03]$ cat filenames.txt  
00.txt  
01.txt  
02.txt  
03.txt  
04.txt  
05.txt  
06.txt  
07.txt  
[user@front02 ex03]$
```

- In `ex03.py`, the root process (process with `rank = 0`) reads the filenames and scatters one to each process

# Exercises

## Ex03

- This exercise demonstrates Gather()
- A file `filenames.txt` includes the filenames of 8 files:

```
[user@front02 ex03]$ cat filenames.txt  
00.txt  
01.txt  
02.txt  
03.txt  
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06.txt  
07.txt  
[user@front02 ex03]$
```

- In `ex03.py`, the root process (process with `rank = 0`) reads the filenames and scatters one to each process
- Each process then computes the Fletcher 32 checksum of one file

# Exercises

## Ex03

- This exercise demonstrates `Gather()`
- A file `filenames.txt` includes the filenames of 8 files:

```
[user@front02 ex03]$ cat filenames.txt  
00.txt  
01.txt  
02.txt  
03.txt  
04.txt  
05.txt  
06.txt  
07.txt  
[user@front02 ex03]$
```

- In `ex03.py`, the root process (process with `rank = 0`) reads the filenames and scatters one to each process
- Each process then computes the Fletcher 32 checksum of one file
- You need to write an appropriate `Gather()` operation to collect the checksums into the root process such that it prints them correctly

# Exercises

## Ex03

- If done correctly, ex03-output.txt should include the following output:

```
[user@front02 ex03]$ cat ex03-output.txt
[user@front02 ex03]$
00.txt → 04D70552
01.txt → 19708CD4
02.txt → ED737A1C
03.txt → 0C40E2D2
04.txt → F7BDE74D
05.txt → 562DDD6C
06.txt → 6F2CD2F1
07.txt → 016DB6C6
[user@front02 ex03]$
```

# Exercises

## Ex04

- In this exercise, a large array of 55,440 elements is read by rank 0 (`ntot = 55400`)

# Exercises

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- In this exercise, a large array of 55,440 elements is read by rank 0 (`ntot = 55400`)
- Our objective is to compute a second order discrete derivative of the data:

```
deriv[i] = array[i-1] + array[i+1] - 2*array[i]
```

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  - Now your program can proceed to correctly compute the derivative:

```
deriv_loc[i] = sub[i-1] - 2*sub[i] + sub[i+1]
```

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deriv_loc[i] = sub[i-1] - 2*sub[i] + sub[i+1]
```

- Use a `Gather()` to collect the full array of the derivative into the root process (rank = 0). The root process will then write the array to a new file `deriv.txt`

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deriv_loc[i] = sub[i-1] - 2*sub[i] + sub[i+1]
```

- Use a `Gather()` to collect the full array of the derivative into the root process (rank = 0). The root process will then write the array to a new file `deriv.txt`
- If done correctly, `deriv.txt` will contain all zeros, except for the first and last element

# Exercises

## Ex04

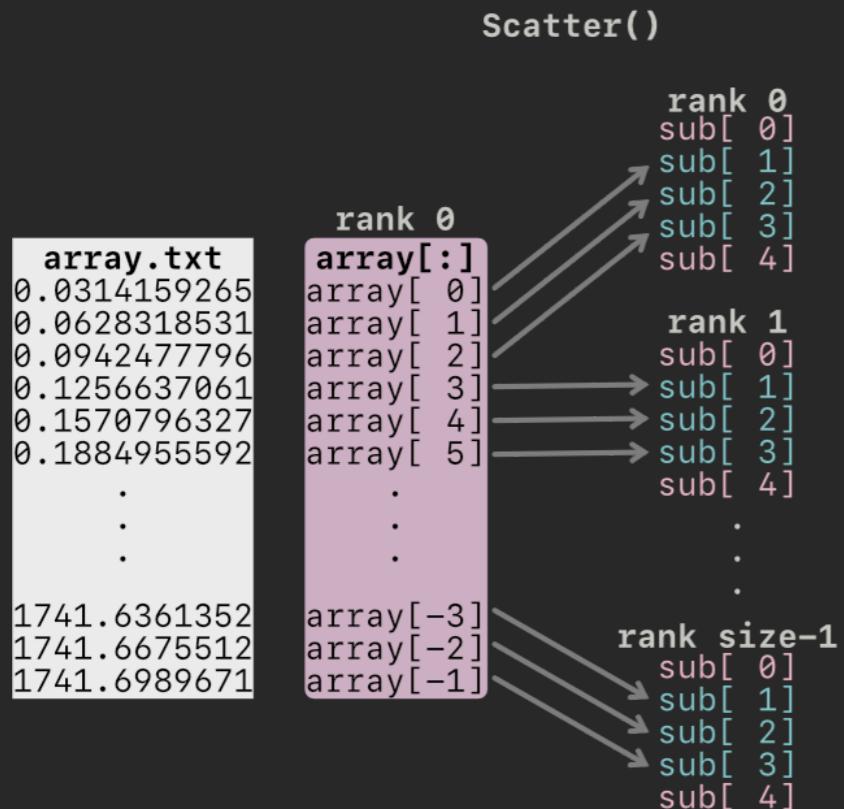
# Exercises

## Ex04

rank 0	
<b>array.txt</b>	<b>array[::]</b>
0.0314159265	array[ 0]
0.0628318531	array[ 1]
0.0942477796	array[ 2]
0.1256637061	array[ 3]
0.1570796327	array[ 4]
0.1884955592	array[ 5]
.	.
.	.
.	.
1741.6361352	array[-3]
1741.6675512	array[-2]
1741.6989671	array[-1]

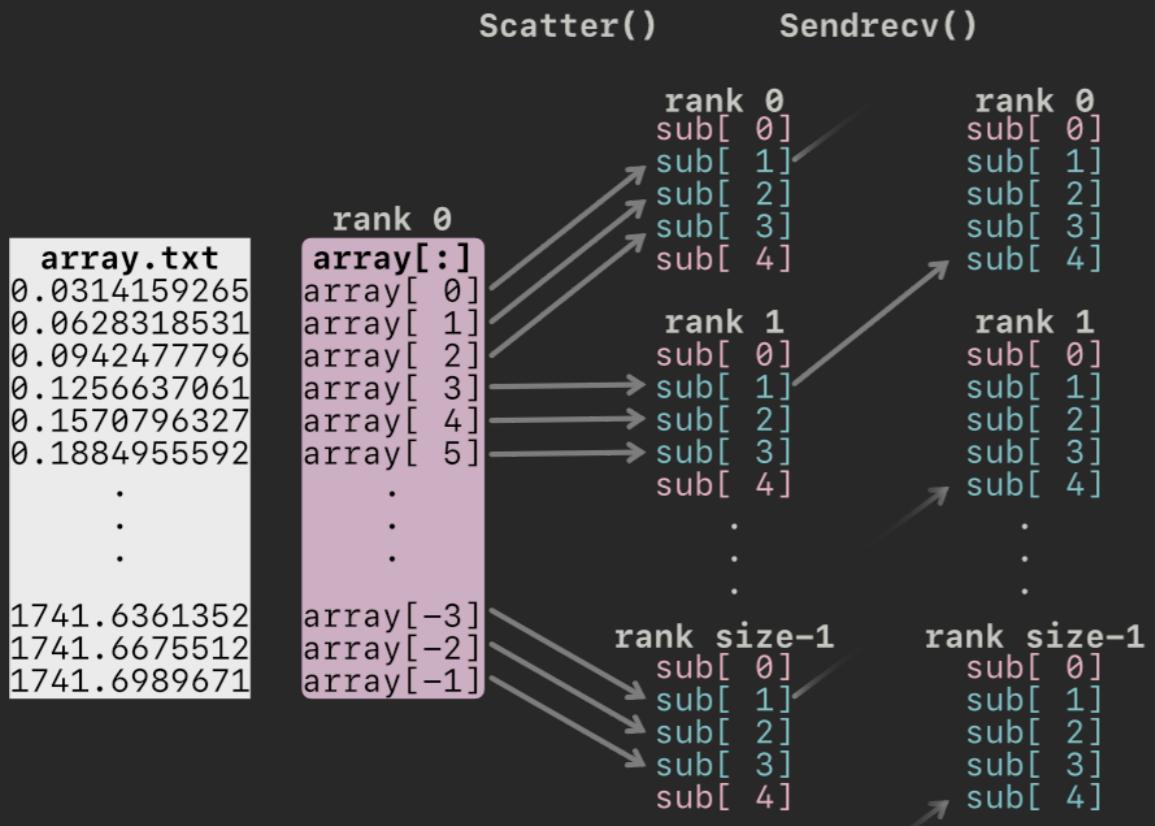
# Exercises

## Ex04



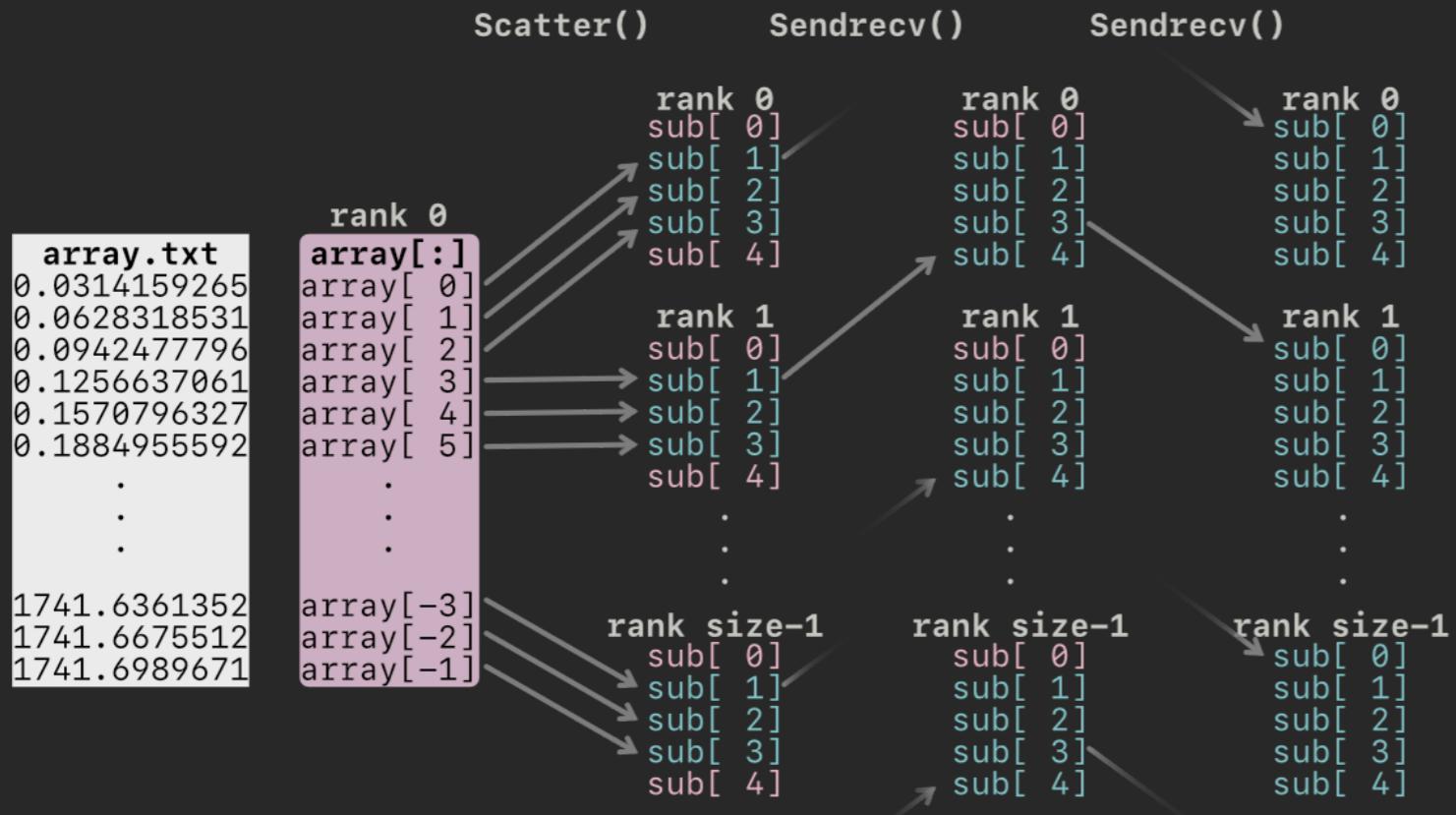
# Exercises

## Ex04



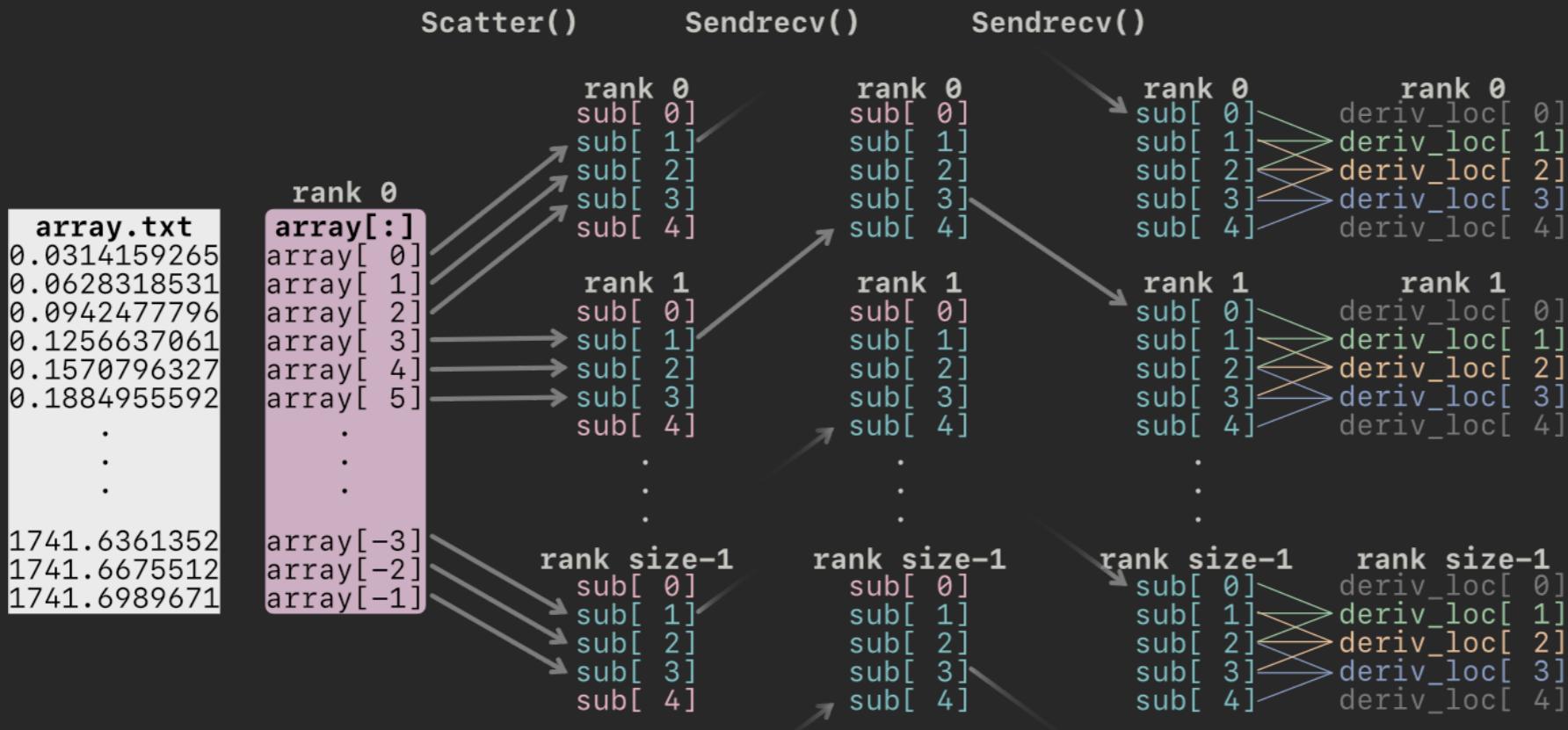
# Exercises

## Ex04



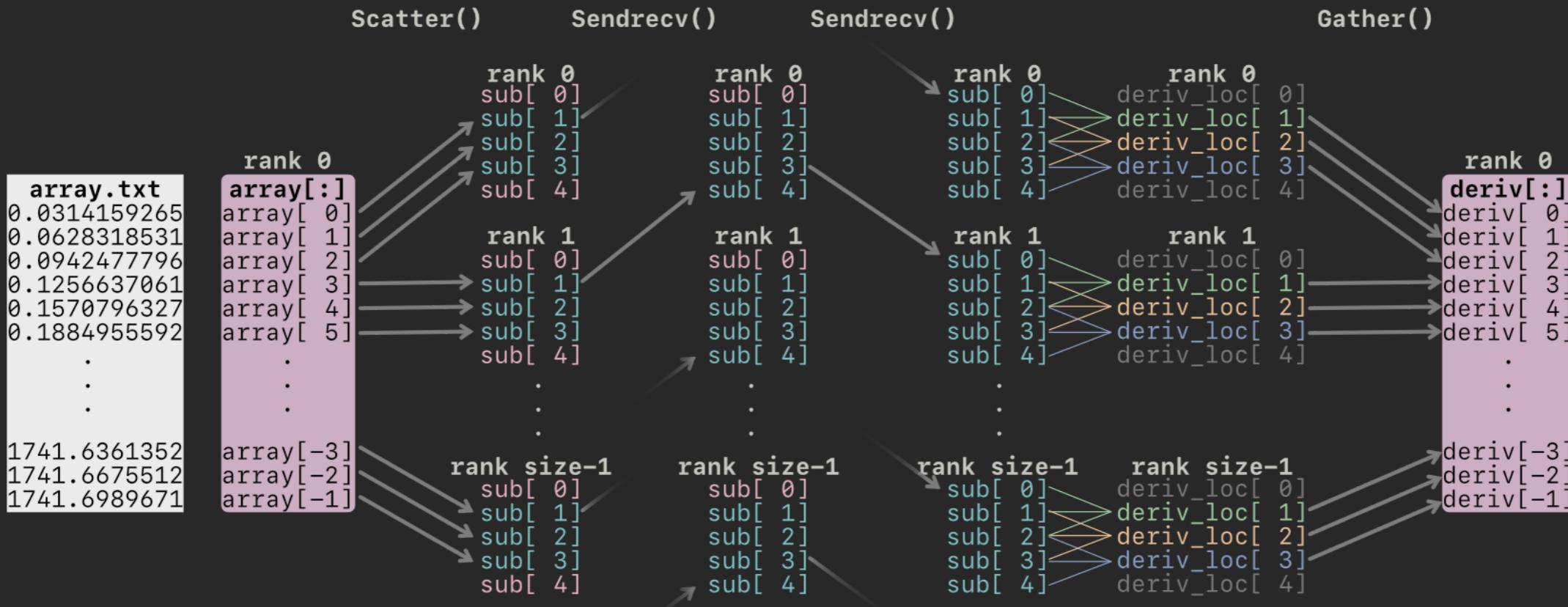
# Exercises

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## Ex04

