Practical aspects of HPC

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Introduction to High-Performance Computing with Python

The Cyprus Intitute — 11^{th} 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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(Super)Computing evolution

1940s — First computers, e.g. ENIAC

- are effectively supercomputers — expensive to buy and operate; large footprint

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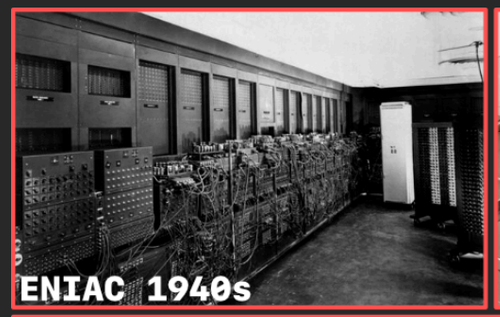
- parallelism emerges: vectorization, parallel instructions



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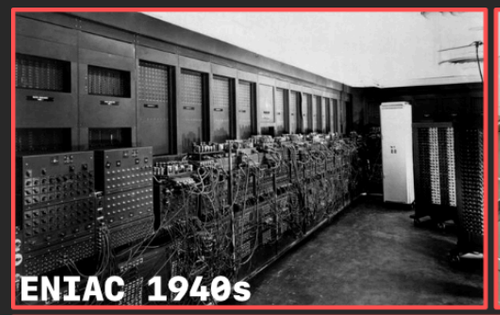
- Parallelism as we understand it today: distributed and shared memory, message passing, etc.



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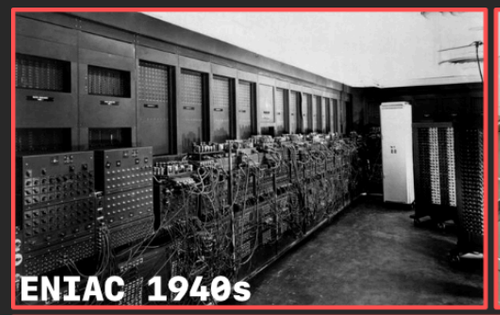
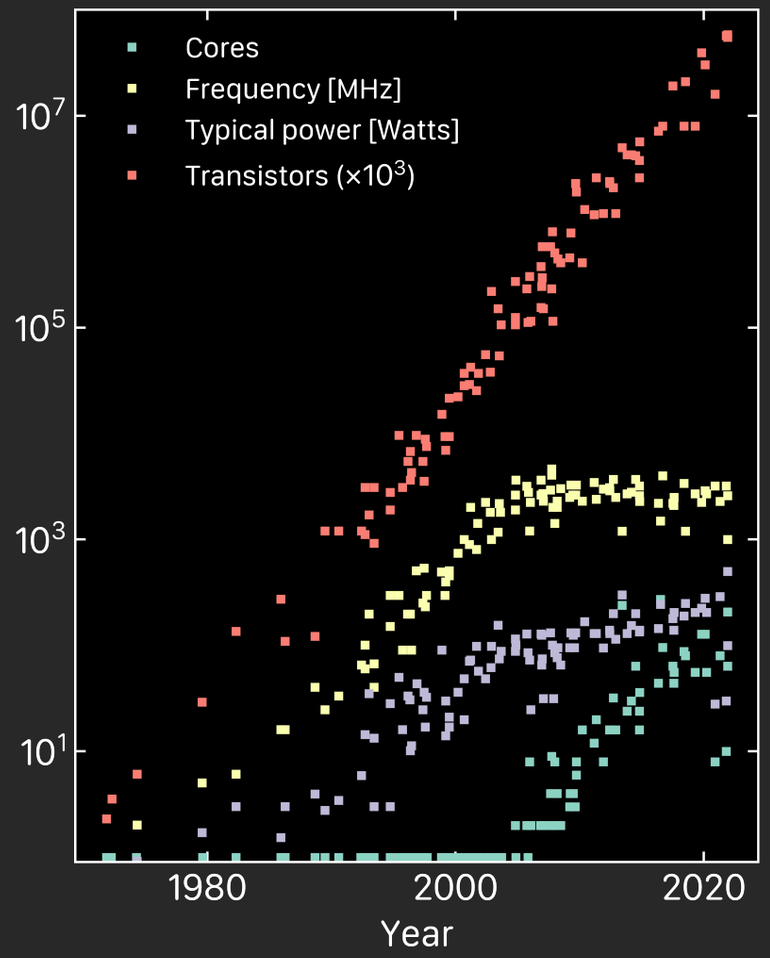
2010s onwards — Heterogeneous supercomputers

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



Supercomputing means Parallel Computing



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No *Dennard scaling* after ~2005

- $\mathrm{P} \propto A \mathrm{f} V^2$ (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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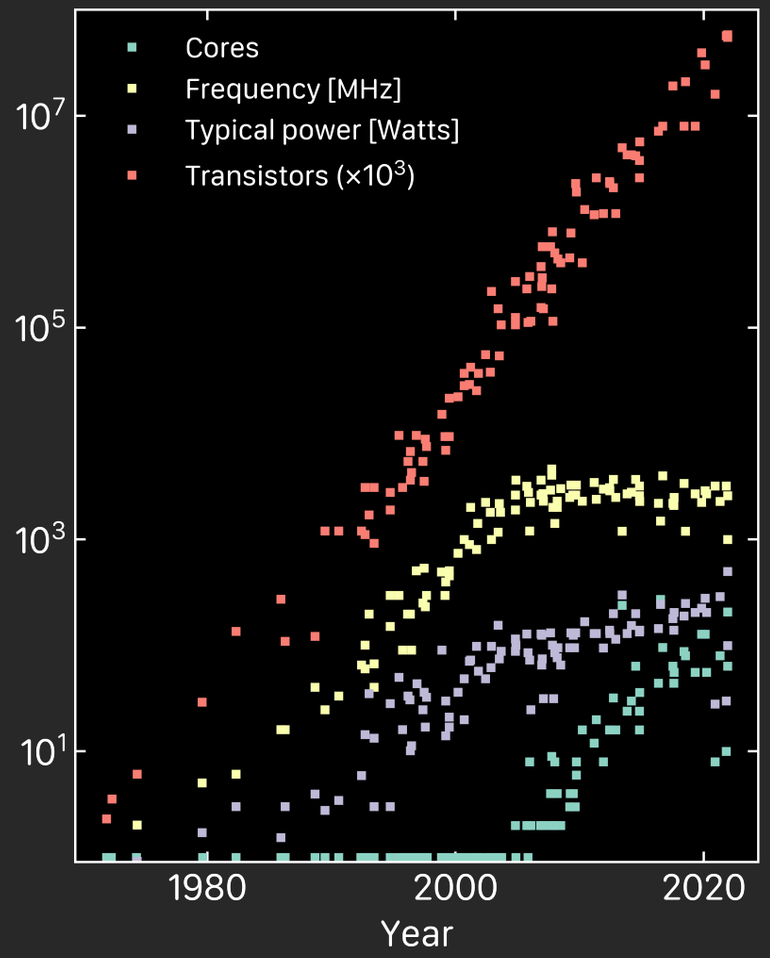

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⇒ Efficiencies are now used to increase parallelism rather than frequency

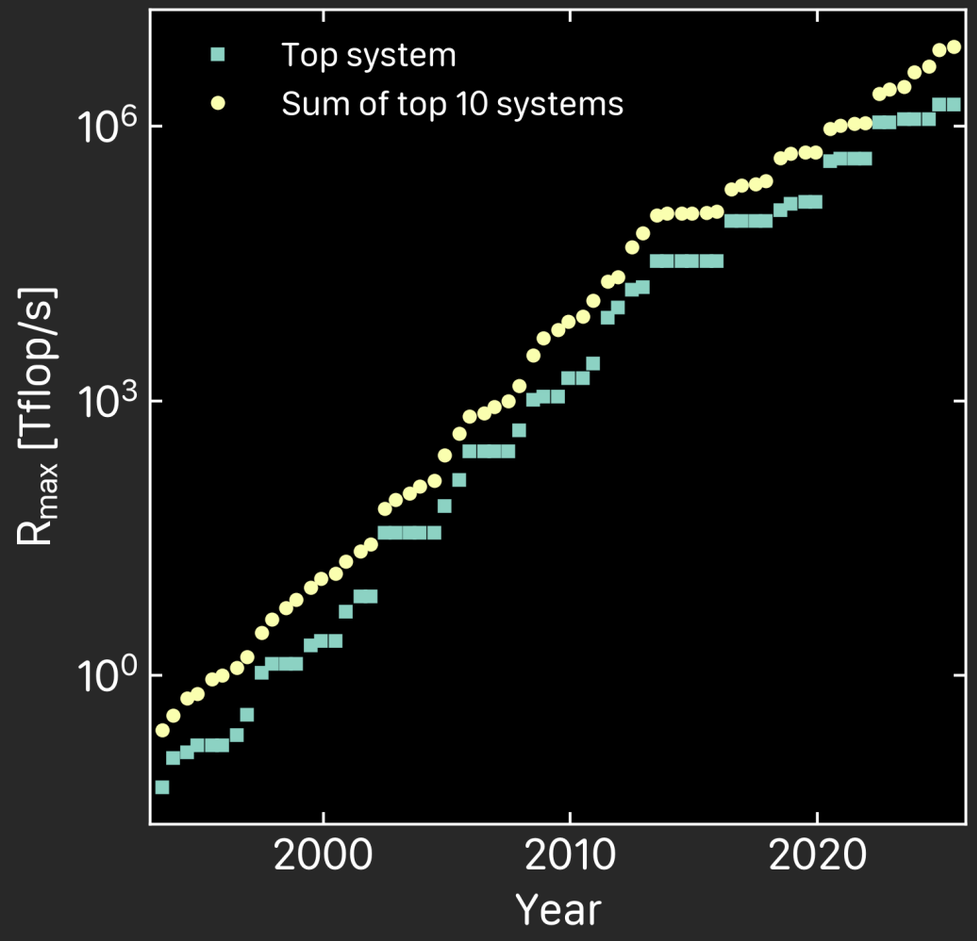
- HPC now means more parallel hardware, rather than faster scalar hardware
- HPC primarily deals with tackling the challenges of parallelism, from all aspects (hardware, software, algorithmic, etc.)

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



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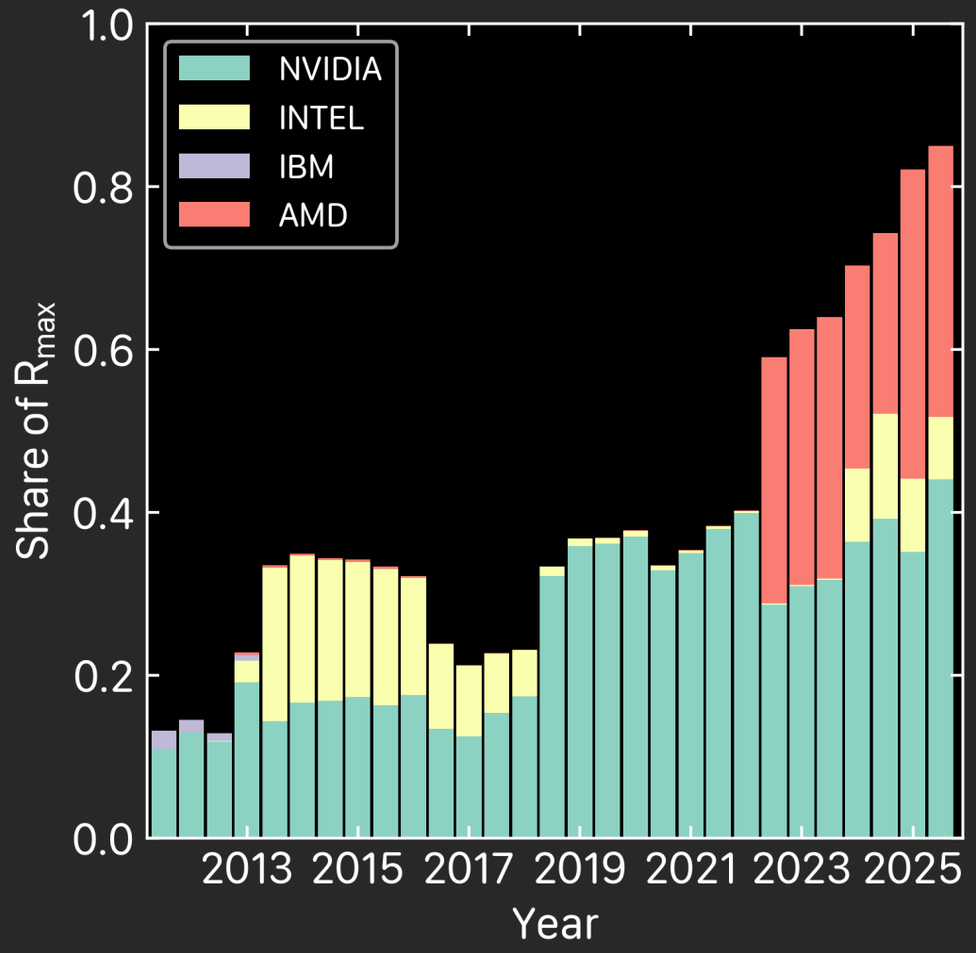
- Proliferation of accelerators
  - Latest AMD accelerators are Instinct GPUs
  - Intel between 2012 and 2017 includes Xeon Phi
  - IBM accelerators refer to IBM Cell

⇒ 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

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- Practitioners of computational science and engineering benefit from knowledge of concepts and challenges of parallel computing

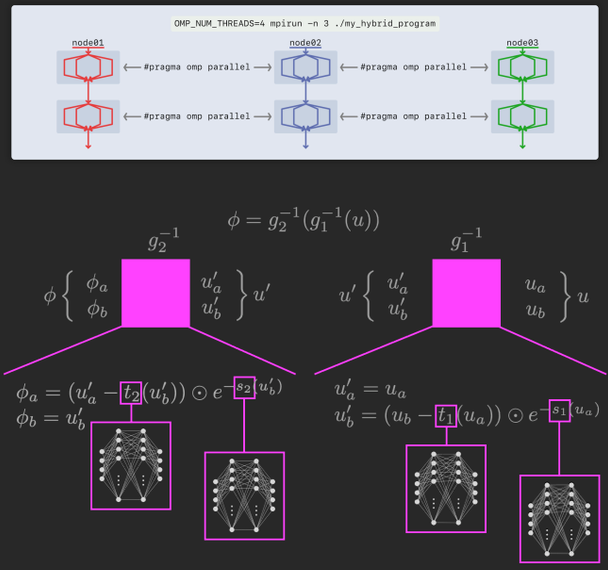
Parallel computing as the main paradigm

High performance computing means parallel computing

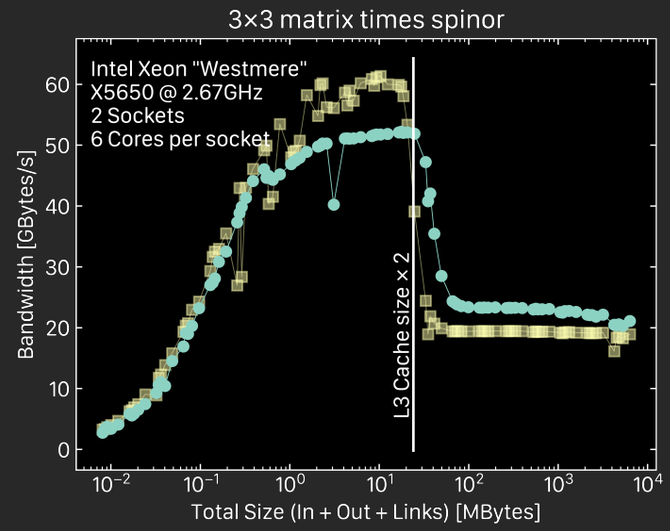
- Technology trends mean parallelism is essential for advanced computing
- Practitioners of computational science and engineering benefit from knowledge of concepts and challenges of parallel computing
  - Architectures and their characteristics
  - Algorithms and how amenable they are to parallelisation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

Architectures

Algorithms



Performance metrics



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
  - E.g. solve a problem using $\mathbb{N}$ nodes, that cannot fit in memory of less nodes

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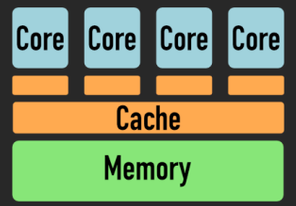
More "*capacity*-like"

More "*capability*-like"

Shared vs Distributed memory paradigm

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



Distributed memory

- Processes have distinct memory domains (different *memory address space*)
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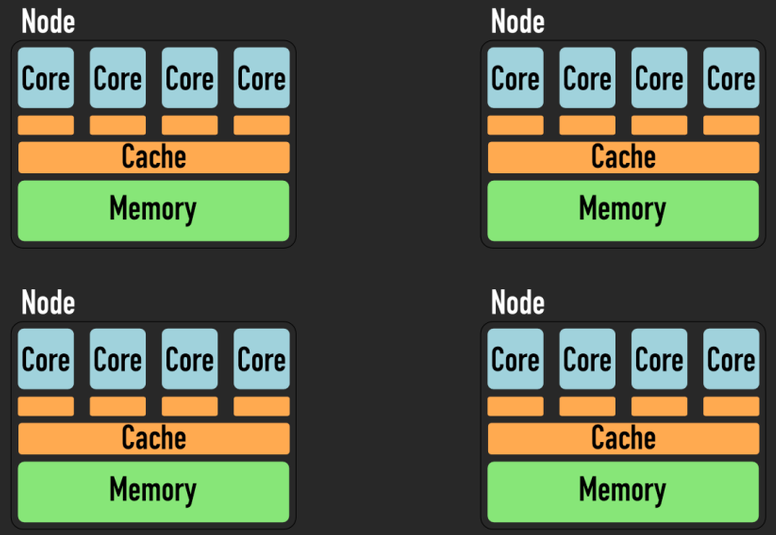

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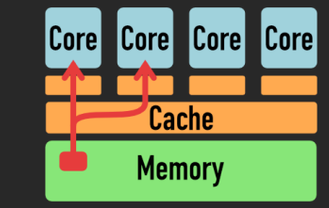

Data shared via memory

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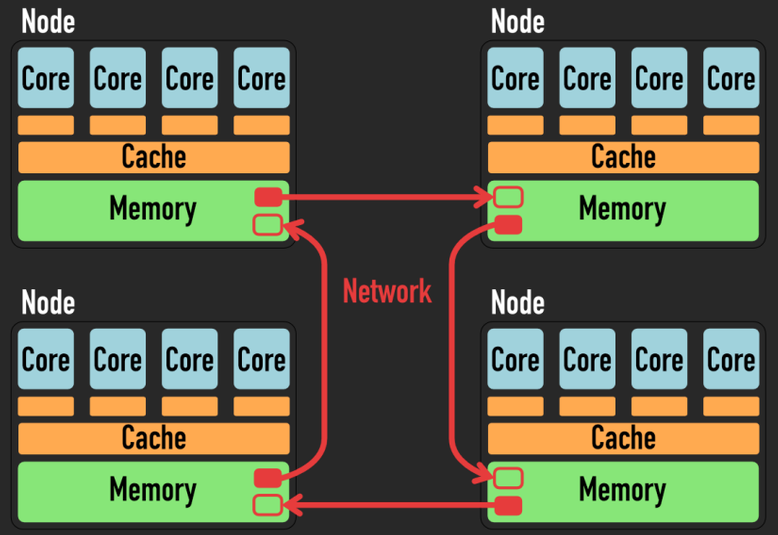
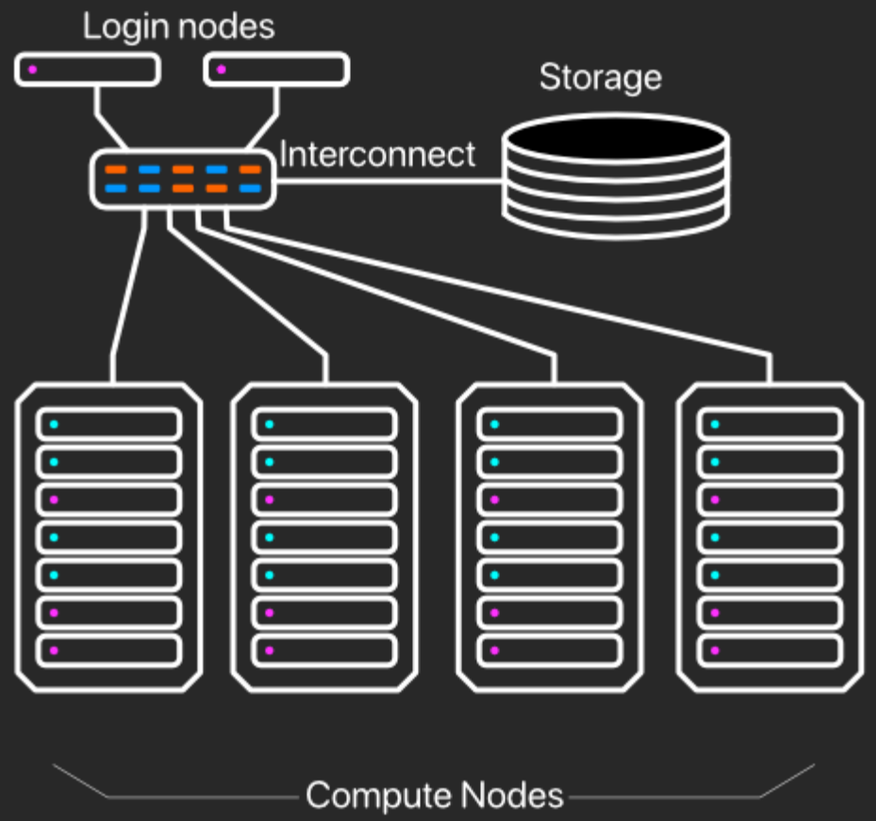


Data shared via explicit communication over a network

A User's View of a Supercomputer

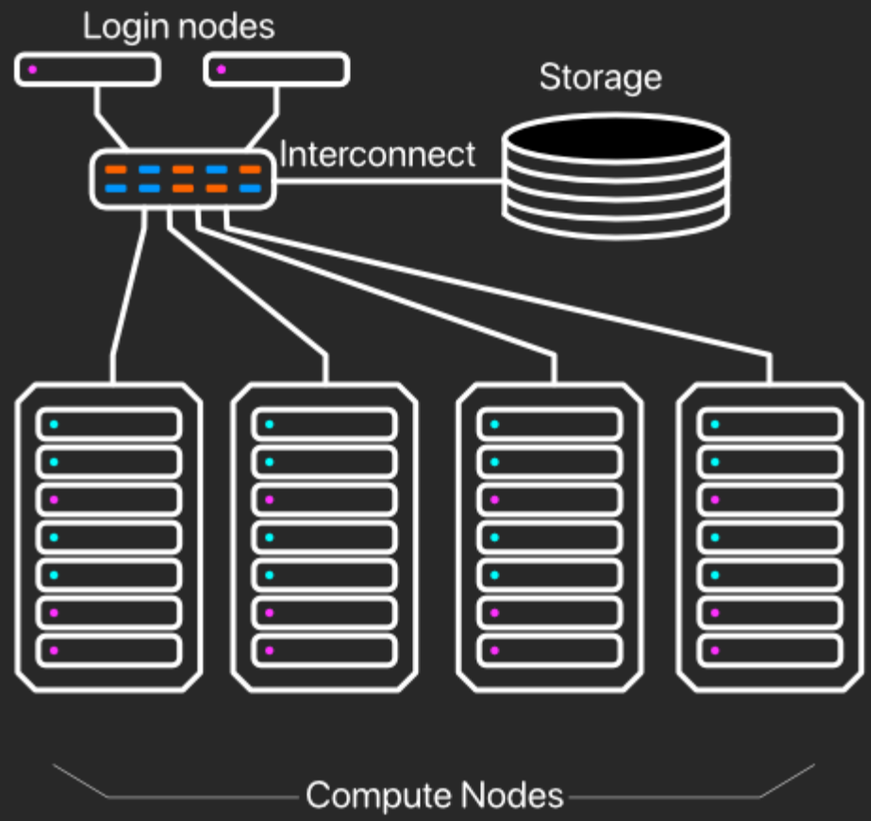
Components



A User's View of a Supercomputer

Components

- Compute Nodes
  - Computational units - CPU and potentially a co-processor, e.g. a GPU
  - Memory (i.e. RAM)
  - Some storage and/or NVMe
  - Network interfaces, possibly separate between management and workload



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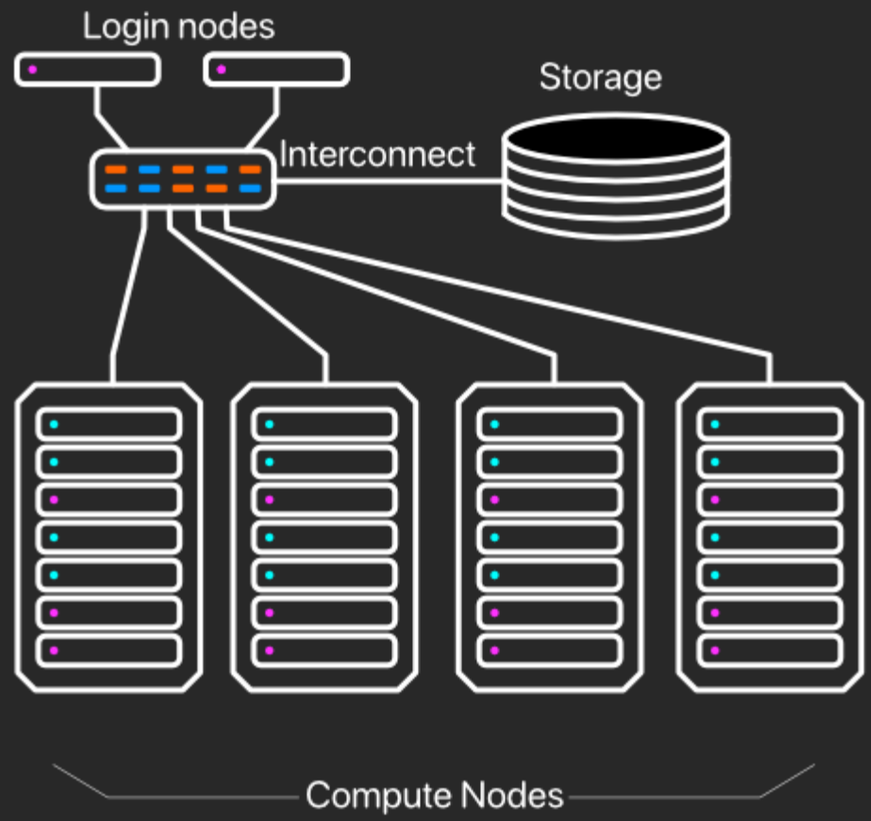

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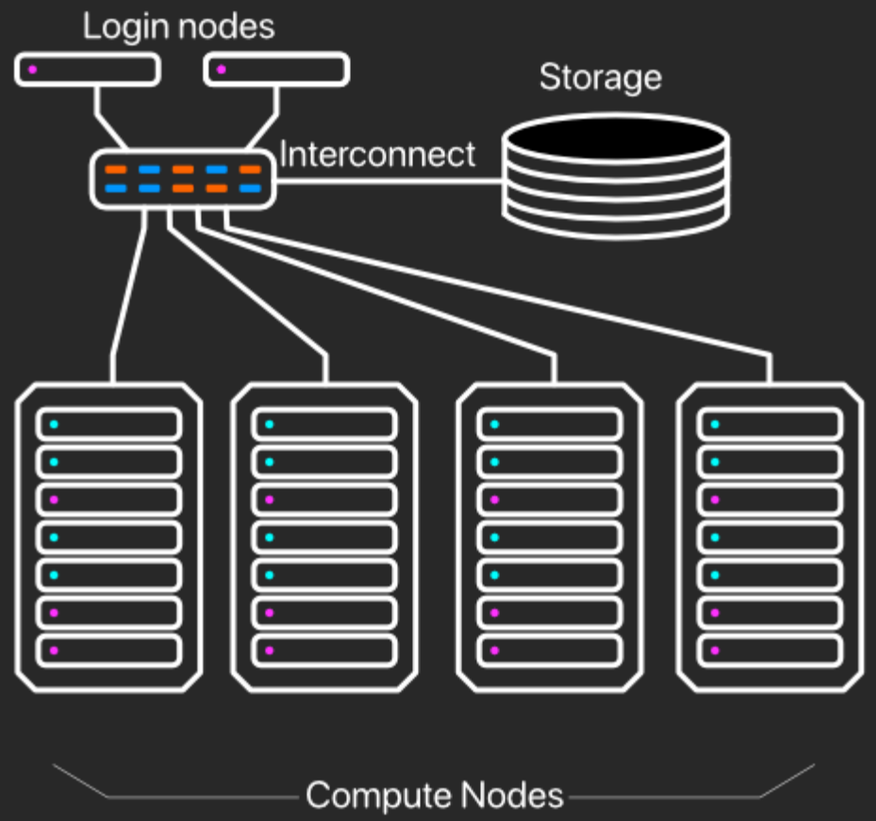
  - Solid state drives are emerging for smaller scratch space
  - Tape systems for archiving



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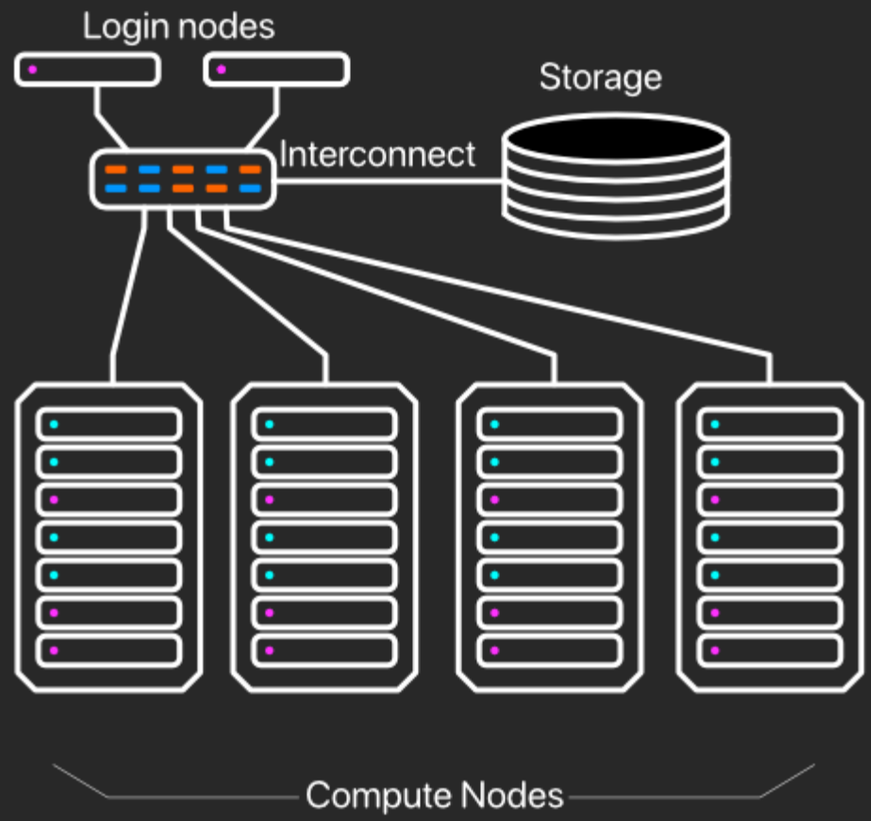
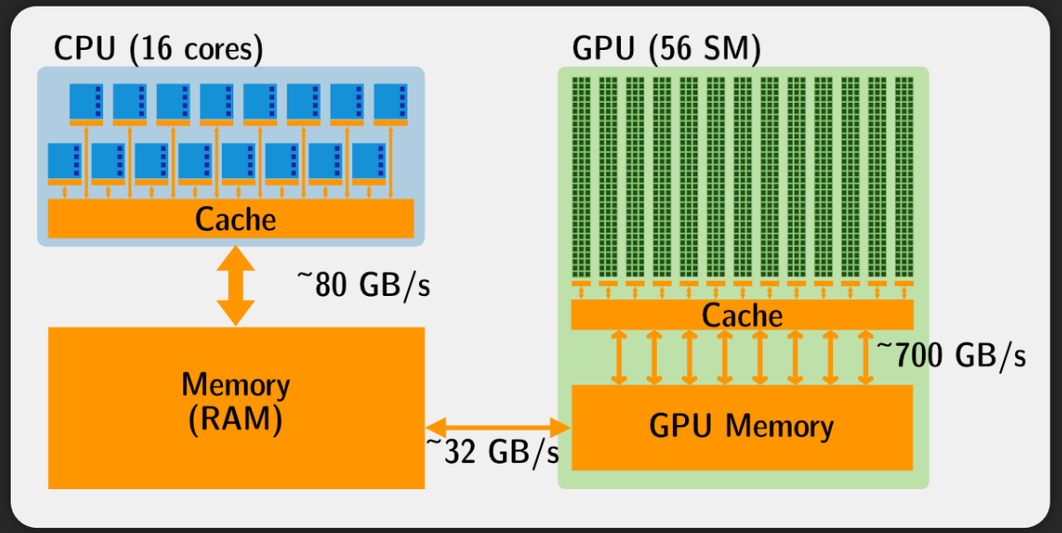
- Front-end nodes
  - For user access
  - Compiling, submitting jobs, etc.



Accelerators and Their Characteristics



CPU

- Large area devoted to control
- Less are 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

Computing devices

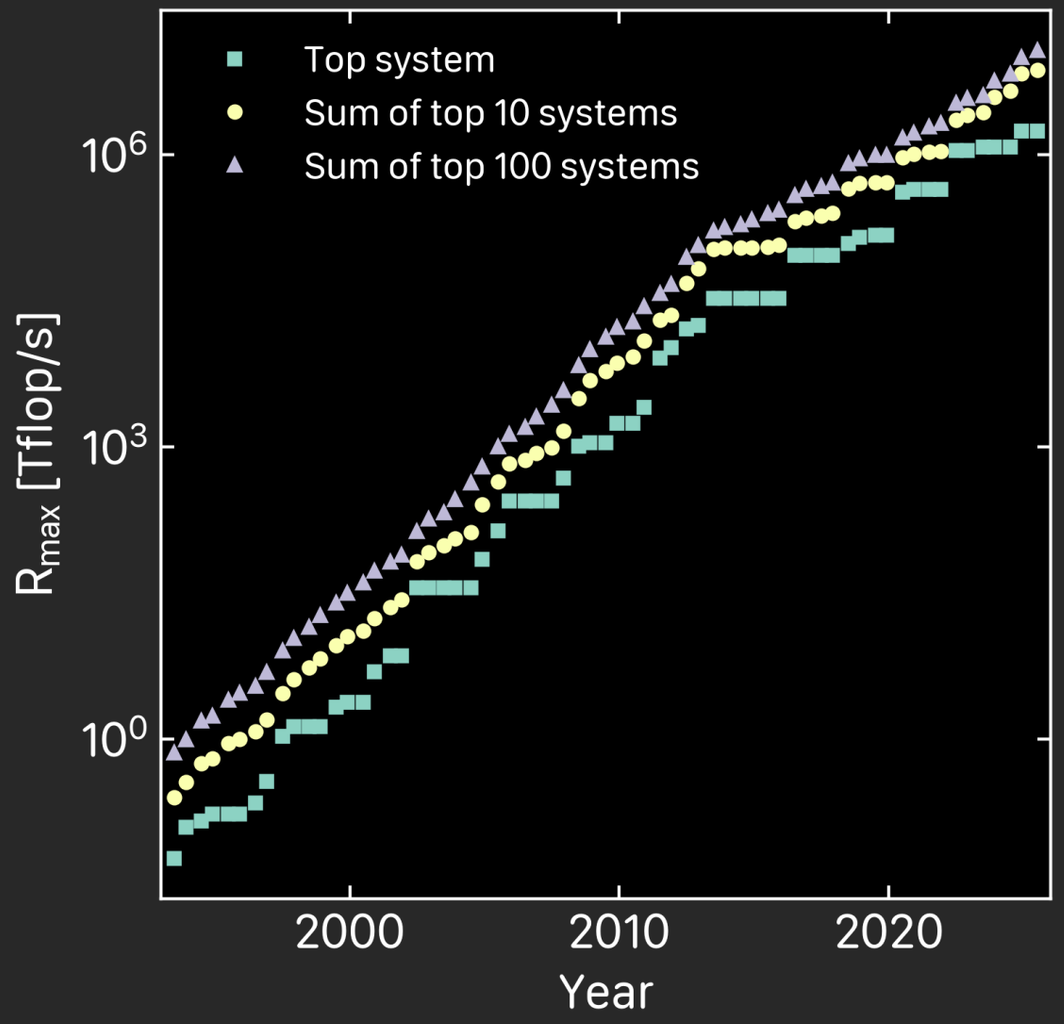
CPU architectures and main characteristics

- 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^{th} 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

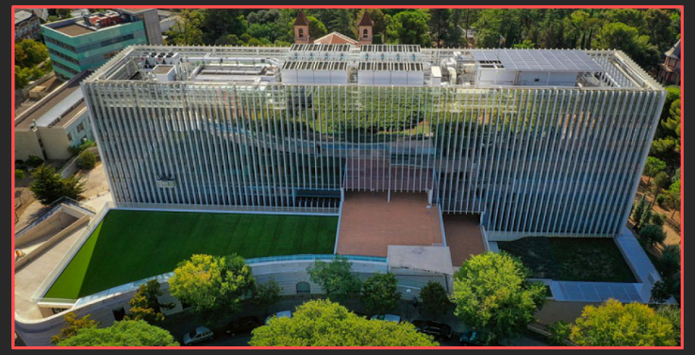
Notable supercomputers in Europe

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.
- $\mathrm{O}(100)$ core-hours for individual projects within "Extreme Scale Allocations"
- $\mathrm{O}(10)$ core-hours for individual projects within regular allocations

Smaller-scale access available nationally

- Depends on national mechanisms for access
- Usually follows same approach of technical and scientific review

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$\longrightarrow$ 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 Pyton
- Hands-on examples

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1. PDF from github: https://github.com/CaSToRC-CyI/EuroCC-HPC-with-Python-2025
2. Via browser: https://slides.koutsou.net/EuroCC-2025-06-11/

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Exercises

- Available on github:
  - https://github.com/CaSToRC-CyI/EuroCC-HPC-with-Python-2025
- 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
- Several free (open) or vendor-provided implementations, e.g.:
  - Mvapich
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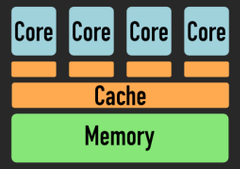
Distributed memory programming

- 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



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- E.g. multi-core CPU, multi-socket node, GPU threads, etc.
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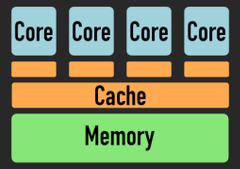

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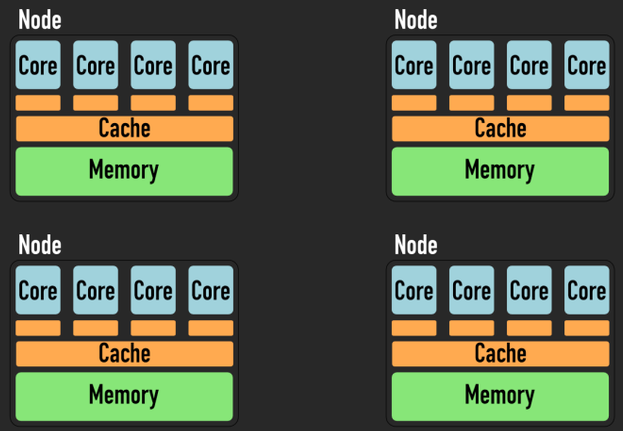

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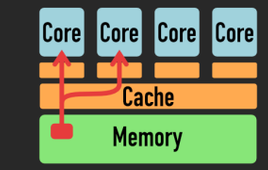

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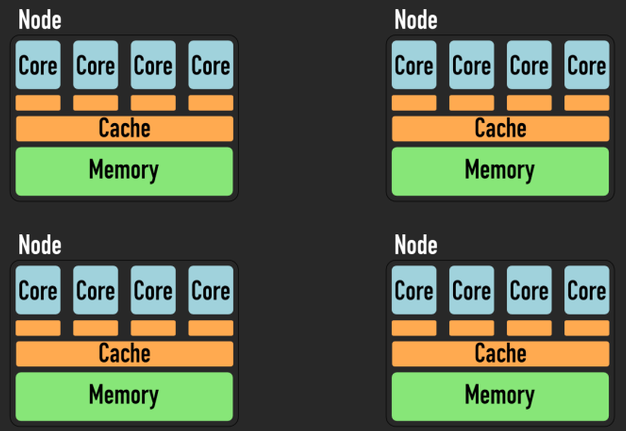

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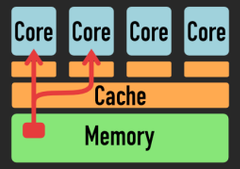

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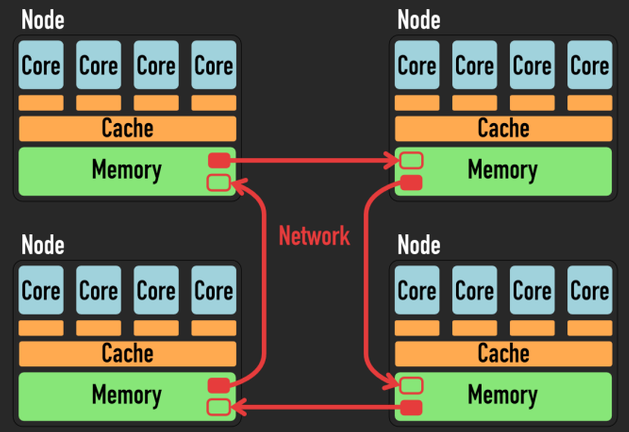

Data shared via explicit communication over a network

- Processes have distinct memory domains (different *memory address space*)
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Running a program in parallel

- Trivially, in Linux it is simple to run a program in parallel

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ssh node01 python my_script.py &
ssh node02 python my_script.py &
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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

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- 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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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_{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:

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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);
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- 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
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```

```
[user@front02 ~]$ mpirun -n 5 python example.py
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- 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)
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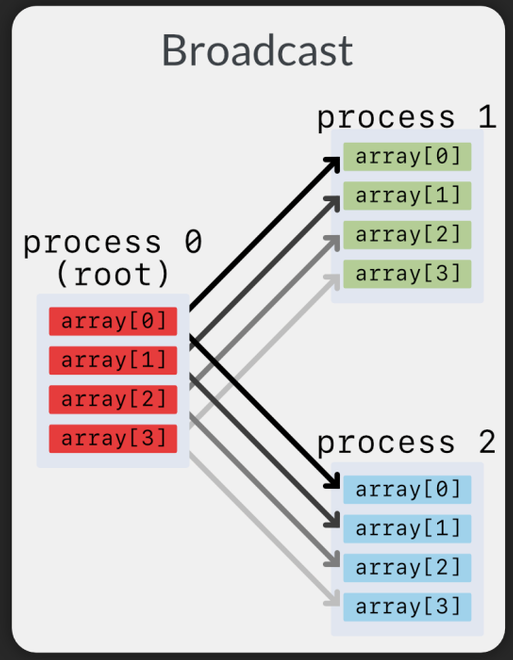

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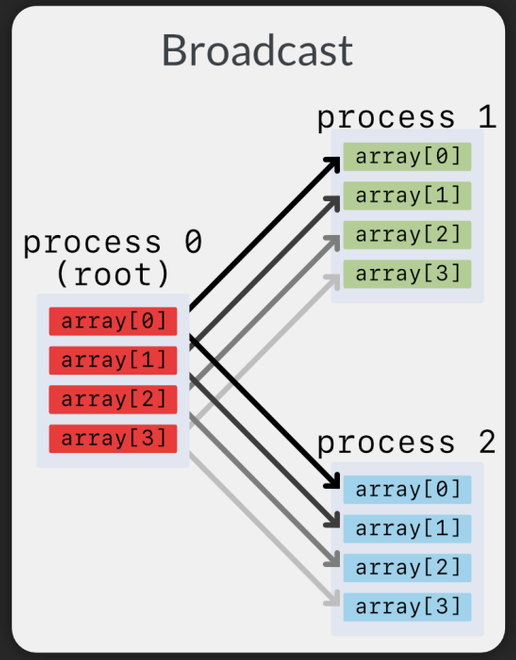

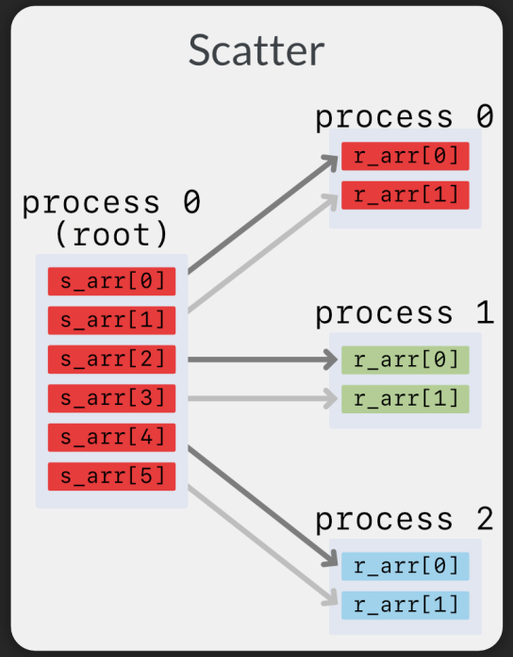

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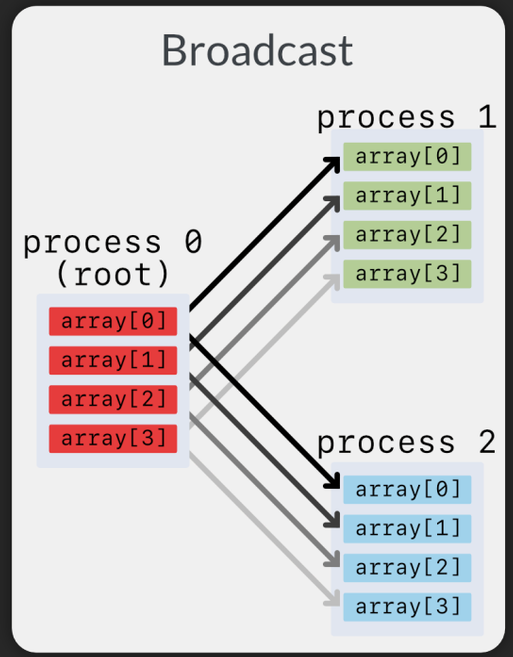

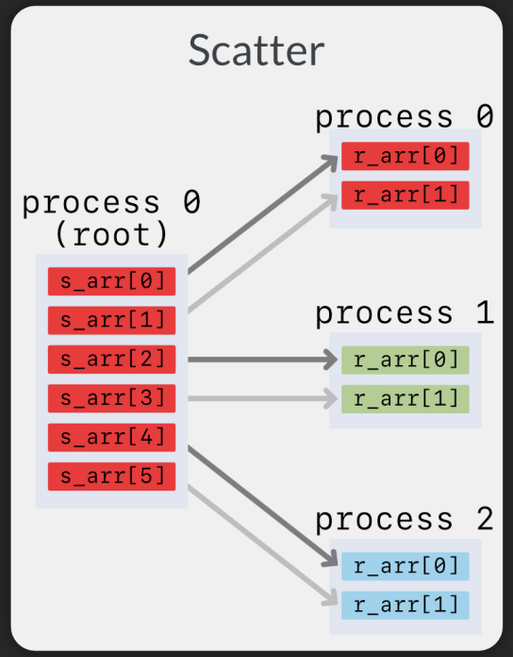

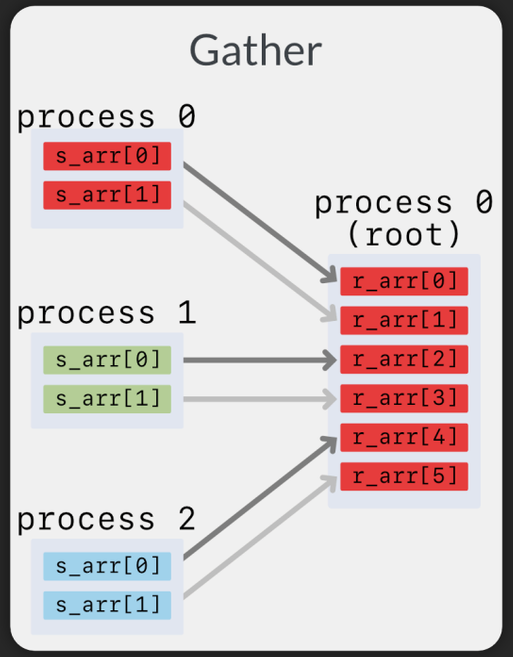

Collective operations: Broadcast

Broadcast:

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- In C, we can pass a scalar by using its memory address (2^{nd} example above). In Python, we can use zero-dimensional numpy array for this

Collective operations: Broadcast

Broadcast:

```
MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm);
```

```
MPI.COMM_WORLD.Bcast(buf: BufSpec, root: int = 0)
```

- *Example*: Broadcast from rank 0 (root), the four-element, double precision array `arr[]`

  ```
  MPI_Bcast(arr, 4, MPI_DOUBLE, 0, MPI_COMM_WORLD);
  ```

  ```
  MPI.COMM_WORLD.Bcast(arr, 0)
  ```

- *Example*: Broadcast from rank 0 (root), the scalar integer variable `var`

  ```
  MPI_Bcast(&var, 1, MPI_INT, 0, MPI_COMM_WORLD);
  ```

  ```
  var = np.array(var)
  MPI.COMM_WORLD.Bcast(var, 0)
  ```

- In C, the `MPI_Datatype` is used to estimate the size in bytes that need to be transferred. In Python this can be deduced from the variable
- In C, we can pass a scalar by using its memory address (2^{nd} 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
                     )
```

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
                     )
```

  - `sendcount` is the number of elements to be sent to *each* process

Collective operations: Scatter

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```
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
                     )
```

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

Collective operations: Scatter

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```
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
                    )
```

  - `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

- 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)
```

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,
        void *recvbuf, int recvcount, MPI_Datatype recvtype, int root,
        MPI_Comm comm
        )
```

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

  - `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);
```

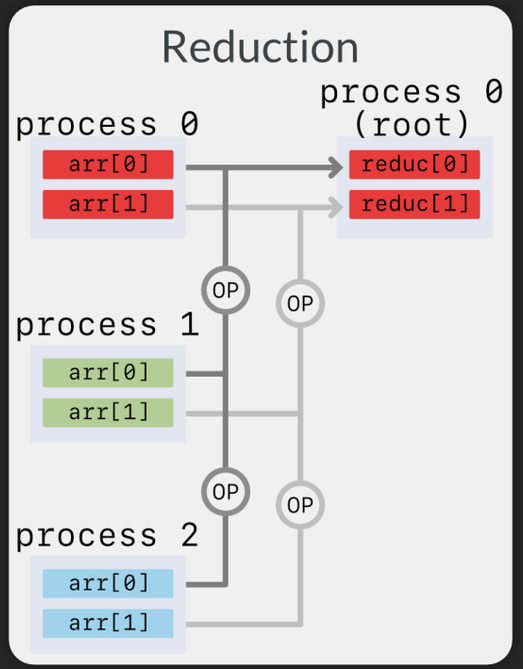
```
arr = np.zeros([4])
element = np.random.rand(1)
MPI.COMM_WORLD.Gather(element, arr, root = 0)
```

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
                      )
```



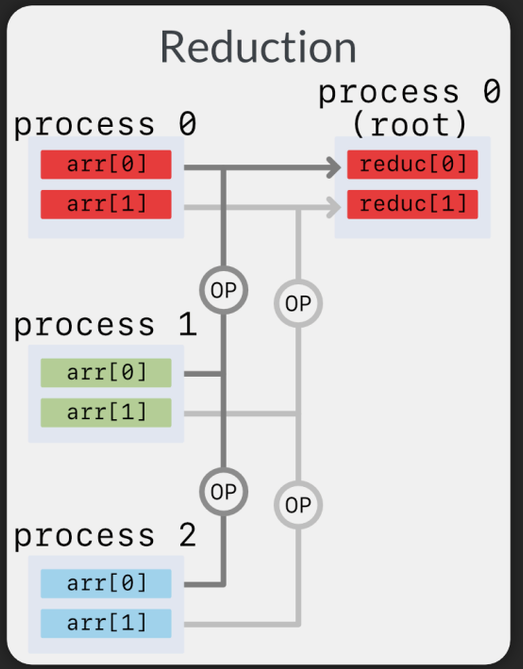
Collective operations: Reduction

- 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
                      )
```

- 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:

```
MPI_Reduce(
          const void *sendbuf, void *recvbuf, int count,
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          )
```
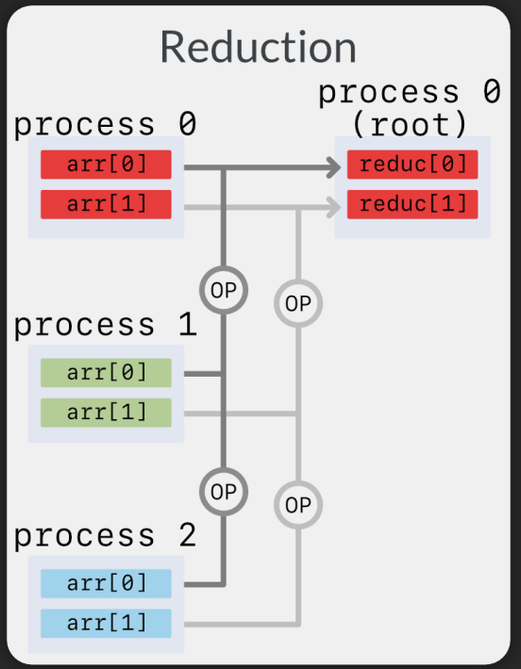

```
MPI.COMM_WORLD.Reduce(
                      sendbuf: BufSpec, recvbuf: BufSpec,
                      op: Op = SUM, root: int = 0
                      )
```

- *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:

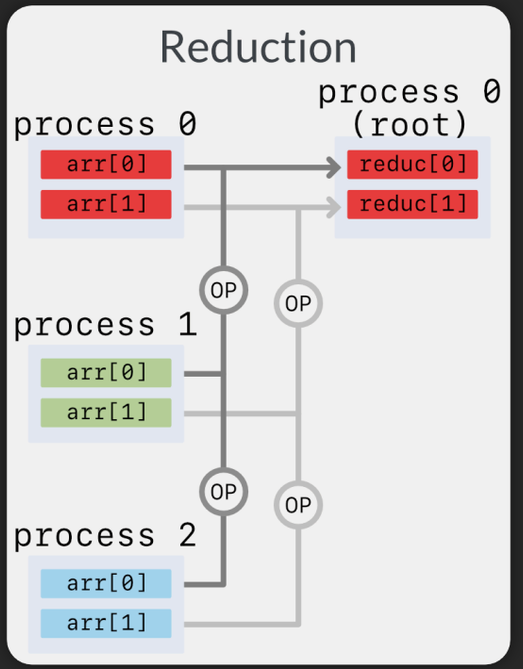
```
MPI_Reduce(
          const void *sendbuf, void *recvbuf, int count,
          MPI_Datatype datatype, MPI_Op op, int root,
          MPI_Comm comm
          )
```

```
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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- `Scatterv()` and `Gatherv()`
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  - Result is equivalent to `Reduce()` followed by an `Bcast()`

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  - For some functions, can replace the send or receive buffer with `MPI.IN_PLACE` (`MPI_IN_PLACE` in C)
    $\longrightarrow$ 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

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- Most common case: send/receive
  - The sender process issues a send operation
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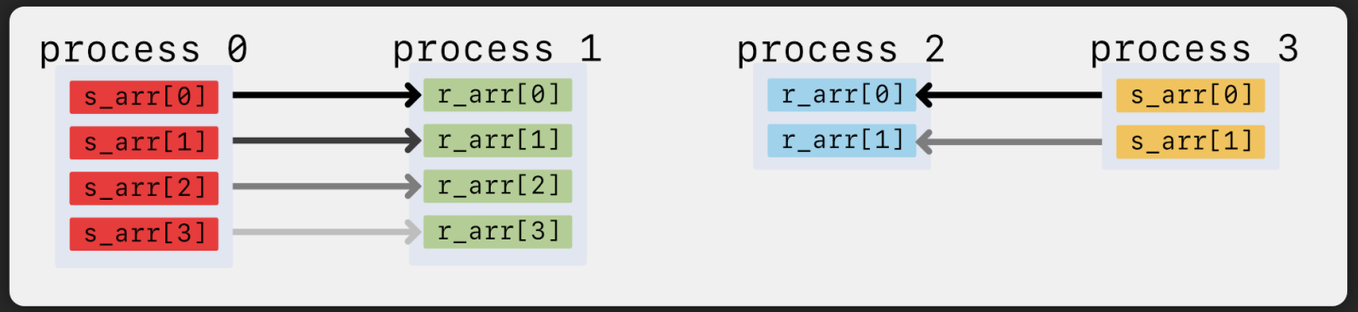

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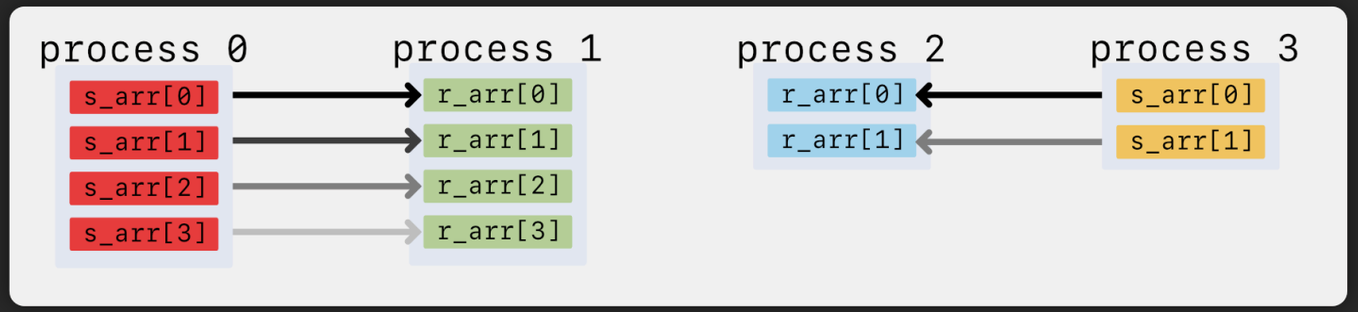

Two point-to-point communications are depicted above
↳ between i) process 0 and 1 and between ii) process 2 and 3

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

Point-to-point communication

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```
MPI.COMM_WORLD.Send(buf: BufSpec, dest: int, tag: int = 0)
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```

- Note the need to specify a source and destination rank
- The `tag` variables tags the message. In the receiving process, it must match what the sender specified, or can be set to `MPI.ANY_TAG`

Point-to-point communication

- Send/Receive

```
MPI.COMM_WORLD.Send(buf: BufSpec, dest: int, tag: int = 0)
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```

- Note the need to specify a source and destination rank
- The `tag` variables 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"

Point-to-point communication

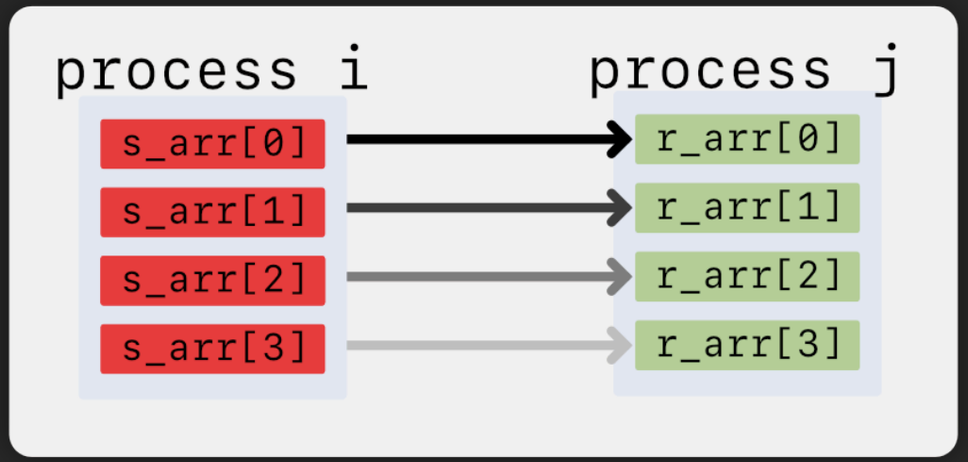
- Send/Receive

```
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)
```

- Note the need to specify a source and destination rank
- The `tag` variables 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

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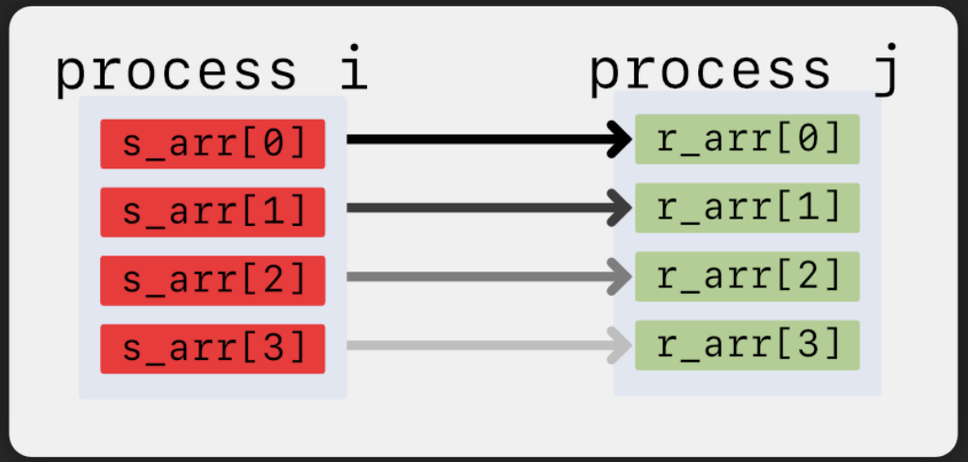
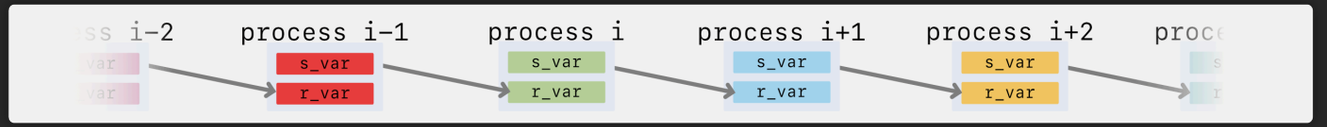



```
s_arr = np.random.rand(4)
r_arr = np.zeros([4])
if rank == i:
    MPI.COMM_WORLD.Send(s_arr, j)
if rank == j:
    MPI.COMM_WORLD.Recv(r_arr, i)
```

Point-to-point communication

- It is common in parallel applications to require that every process communicates with another process, e.g. a neighboring process



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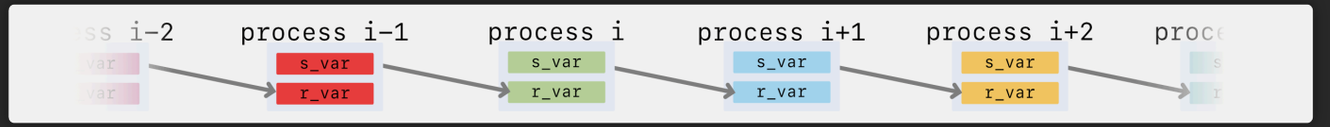

- This will not work:

```
MPI.COMM_WORLD.Send(s_var, rank+1);
MPI.COMM_WORLD.Recv(r_var, rank-1);
```

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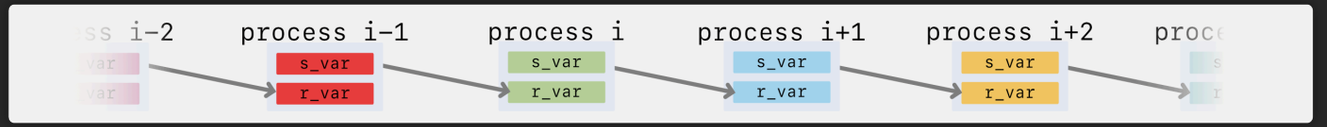

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  - an `Recv()` can only be posted once an `Send()` completes
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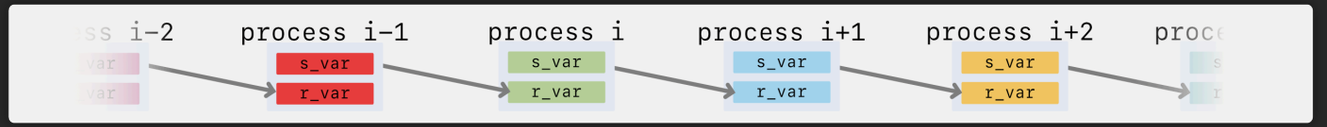

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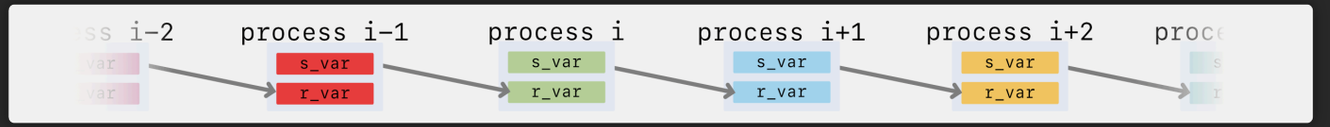

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```

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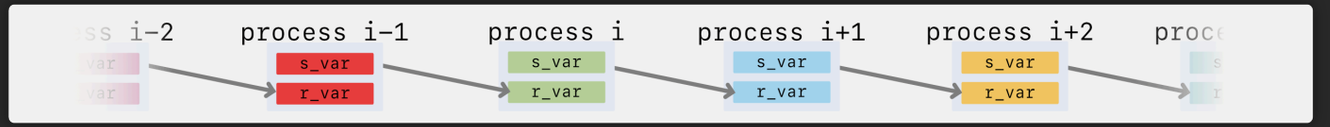
  - an `Recv()` can only be posted once an `Send()` completes
  - an `Send()` can only complete if a matching `Recv()` is posted
- One can serialize the communications, i.e. use a loop to determine the order of send/receives
  - Serializes communications that would otherwise be done faster in parallel

Point-to-point communication

- It is common in parallel applications to require that every process communicates with another process, e.g. a neighboring process



- This will not work:

```
MPI.COMM_WORLD.Send(s_var, rank+1);
MPI.COMM_WORLD.Recv(r_var, rank-1);
```

- It results in a deadlock:
  - an `Recv()` can only be posted once an `Send()` completes
  - an `Send()` can only complete if a matching `Recv()` is posted
- One can serialize the communications, i.e. use a loop to determine the order of send/receives
  - Serializes communications that would otherwise be done faster in parallel
  - Inelegant, obscure, and error-prone

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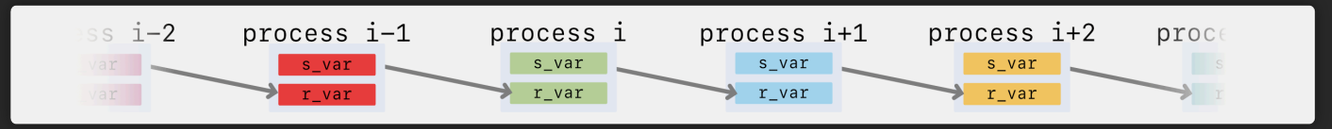

- A more efficient and elegant solution is to use `Sendrecv()`:

```
MPI.COMM_WORLD.Sendrecv(
    sendbuf: BufSpec, dest: int, sendtag: int = 0,
    recvbuf: BufSpec, source: int = ANY_SOURCE, recvtag: int = ANY_TAG,
    status: Status = None
)
```

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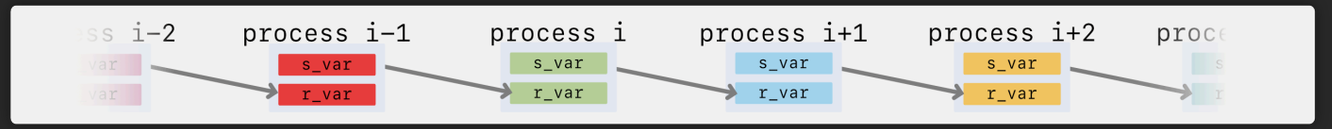

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    sendbuf: BufSpec, dest: int, sendtag: int = 0,
    recvbuf: BufSpec, source: int = ANY_SOURCE, recvtag: int = ANY_TAG,
    status: Status = None
)
```

- For the depicted example:

```
MPI.COMM_WORLD.Sendrecv(s_var, rank+1, 0, r_var, rank-1)
```

Point-to-point communications

Some additional notes on variants of the point-to-point communications we have covered

Point-to-point communications

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- Some MPI functions allow omitting the mandatory buffer argument. The buffer is returned instead, e.g.:

```
s_arr = np.random.rand(4)
if rank == i:
    MPI.COMM_WORLD.send(s_arr, j)
if rank == j:
    r_arr = MPI.COMM_WORLD.recv(source = i)
```

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

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- `Isend()` and `Irecv()`
    - *Non-blocking* variants. The `I` stands for "immediate"

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  - *Non-blocking* variants. The `I` stands for "immediate"
  - Functions return immediately, i.e. the functions don't block waiting for `sendbuf` to be sent or `recvbuf` to be received
  - 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()
```

Exercises

Exercises

```
cp -r /nvme/scratch/edu27/MPI/ex?? .
```

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- Each folder includes (where `${n}` below is the exercise number, i.e. `01`, `02`, etc.):
  - A `.py` source code file (`ex${n}.py`)
  - A submit script (`sub-ex${n}.sh`)

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  - A `.py` source code file (`ex${n}.py`)
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- Our workflow will typically be:
  - Modify `ex${n}.py` as instructed
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  - Look at the output, which can be found in `ex${n}-output.txt`

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  - Modify `ex${n}.py` as instructed
  - Submit the job script `sbatch sub-ex${n}.sh`
  - Look at the output, which can be found in `ex${n}-output.txt`
- Note that if you have modified `ex${n}.py` correctly, the job should complete in less than one minute

Exercises

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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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  - `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
```

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=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
```

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=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

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=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=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`
  - 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:

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

```
[user@front02 ex01]$ cat ex01-output.txt
This is rank = 2 of nproc = 8 on node: cn03
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This is rank = 4 of nproc = 8 on node: cn03
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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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- We would like:
  - The root process to read all elements into an array `array[]`

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  - The root process to *broadcast* the total number of elements of the array, `ntot`

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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`

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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  - The root process to *broadcast* the total number of elements of the array, `ntot`
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  - Each process to sum its local elements, storing the result into `sum_loc`

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  - 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

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  - 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`

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
  - 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
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

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

Ex04

- 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]
```

Exercises

Ex04

- 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]
```

- The goal is to do this *in parallel*, such that each rank computed it for a *subset of the data*

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- We will proceed as follows:

Exercises

Ex04

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

- The goal is to do this *in parallel*, such that each rank computed it for a *subset of the data*
- We will proceed as follows:
  - The array in each rank has two additional elements, `sub = np.empty(shape=(nloc+2))`, where `nloc = ntot / size`

Exercises

Ex04

- In this exercise, a large array of 55,440 elements is read by rank 0 (`ntot = 55400`)
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```
deriv[i] = array[i-1] + array[i+1] - 2*array[i]
```

- The goal is to do this *in parallel*, such that each rank computed it for a *subset of the data*
- We will proceed as follows:
  - The array in each rank has two additional elements, `sub = np.empty(shape=(nloc+2))`, where `nloc = ntot / size`
  - Add a missing `Scatter()` to distribute to each processes the corresponding `nloc` elements. These should be received in `sub[1:-1]` of each rank

Exercises

Ex04

- 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]
```

- The goal is to do this *in parallel*, such that each rank computed it for a *subset of the data*
- We will proceed as follows:
  - The array in each rank has two additional elements, `sub = np.empty(shape=(nloc+2))`, where `nloc = ntot / size`
  - Add a missing `Scatter()` to distribute to each processes the corresponding `nloc` elements. These should be received in `sub[1:-1]` of each rank
  - Use `Sendrecv()` to fill the first and last elements element of `sub[]`, i.e. `sub[0]` and `sub[-1]`, with the corresponding elements of the neighboring ranks, needed to carry out the derivative

Exercises

Ex04

- In this exercise, a large array of 55,440 elements is read by rank 0 (`ntot = 55400`)
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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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- If done correctly, `deriv.txt` will contain all zeros, except for the first and last element

Exercises

Ex04

Exercises

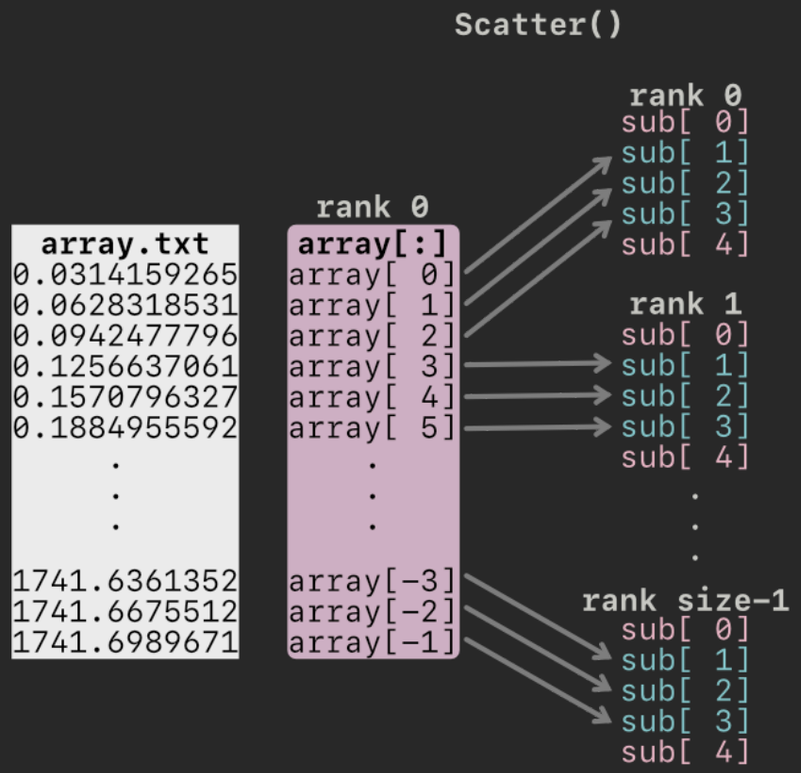
Ex04

array.txt
0.0314159265
0.0628318531
0.0942477796
0.1256637061
0.1570796327
0.1884955592
.
.
.
1741.6361352
1741.6675512
1741.6989671

rank 0
array[:]
array[0]
array[1]
array[2]
array[3]
array[4]
array[5]
.
.
.
array[-3]
array[-2]
array[-1]

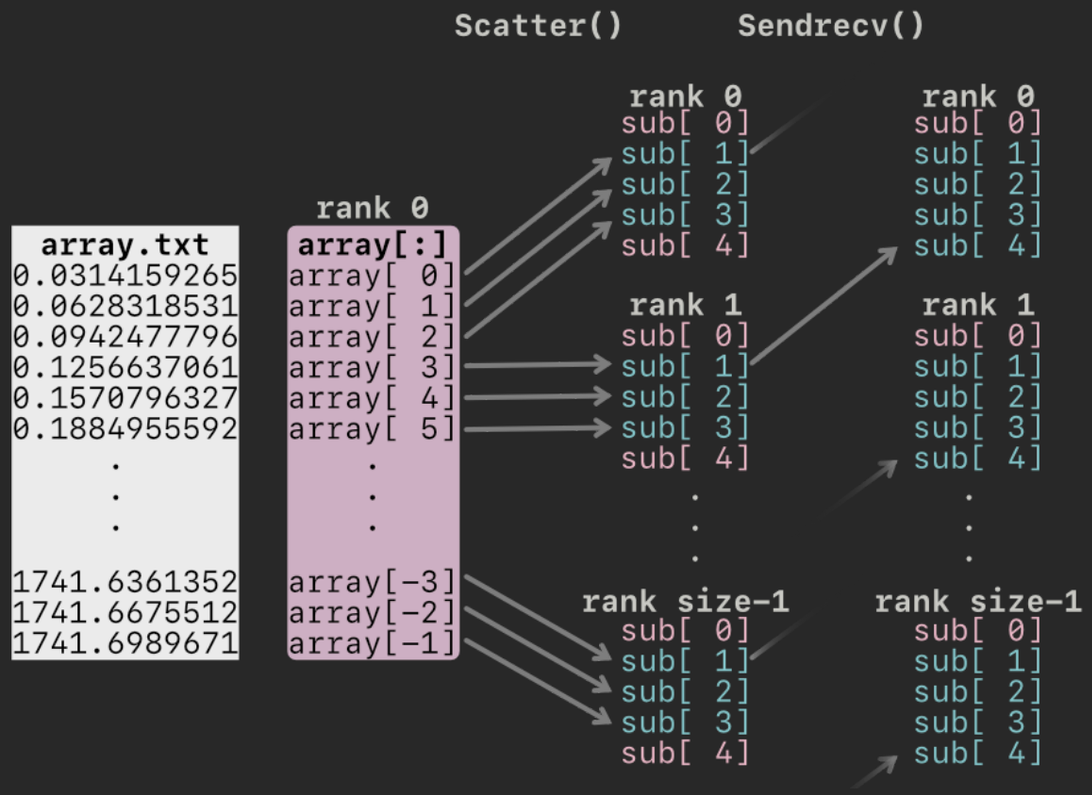
Exercises

Ex04



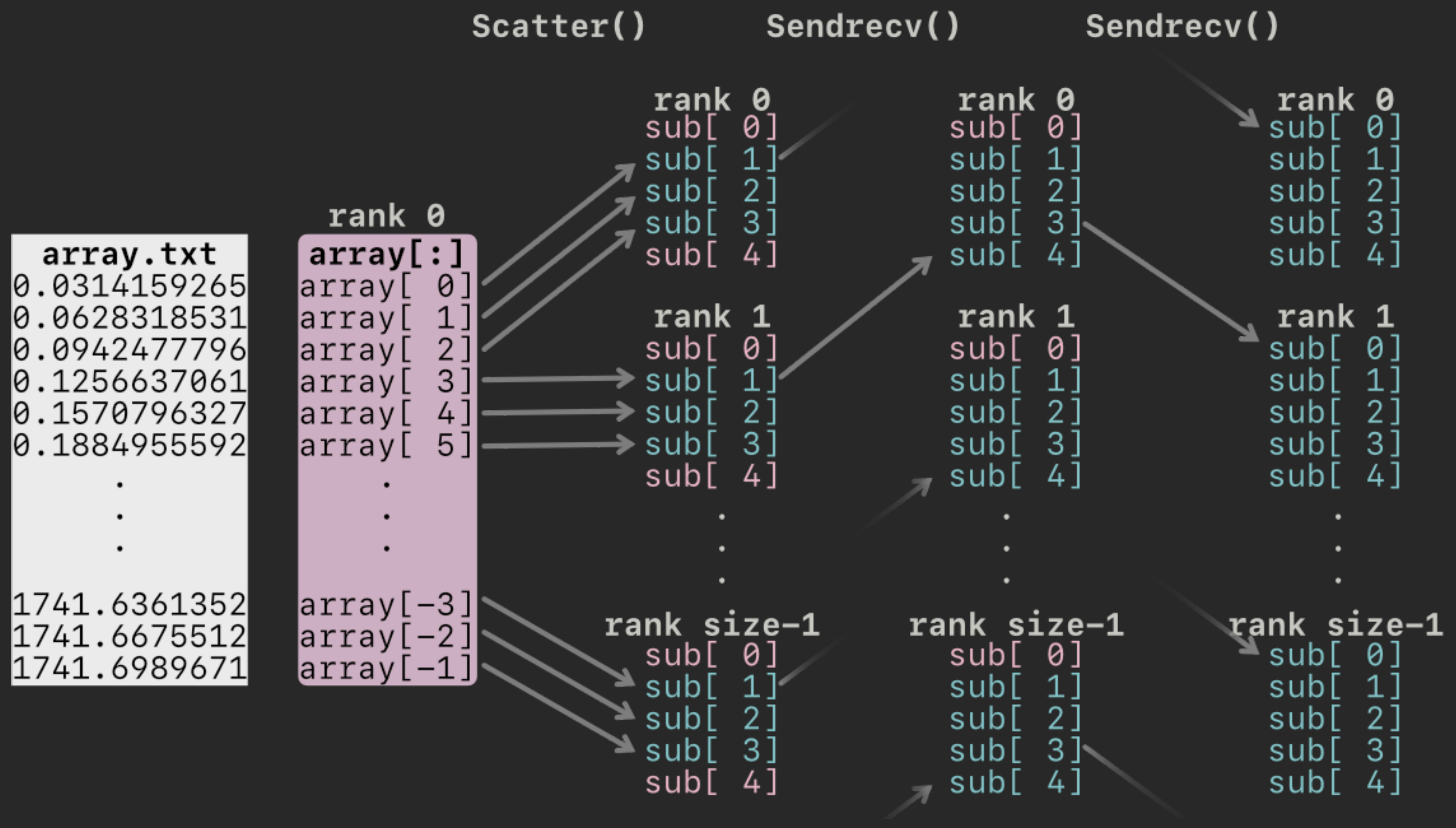
Exercises

Ex04



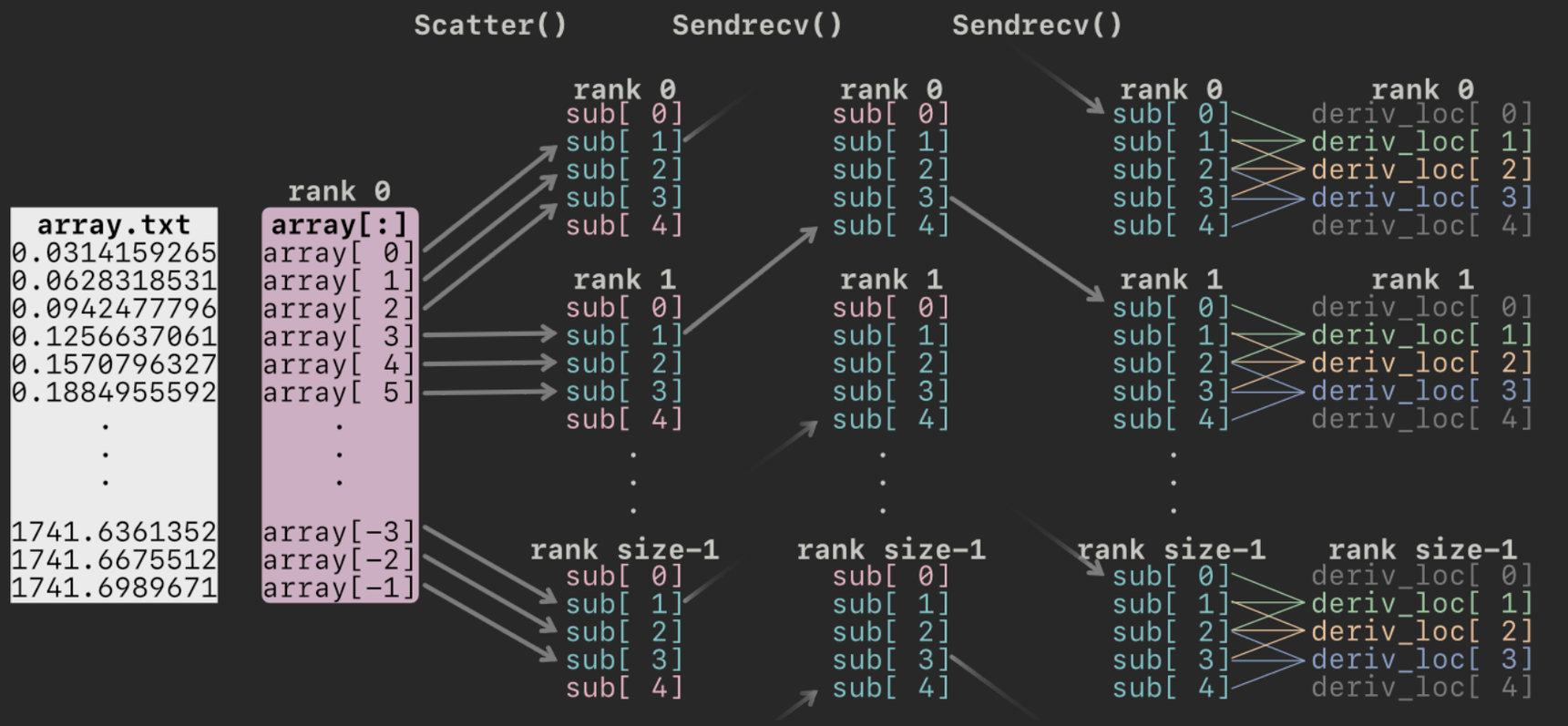
Exercises

Ex04



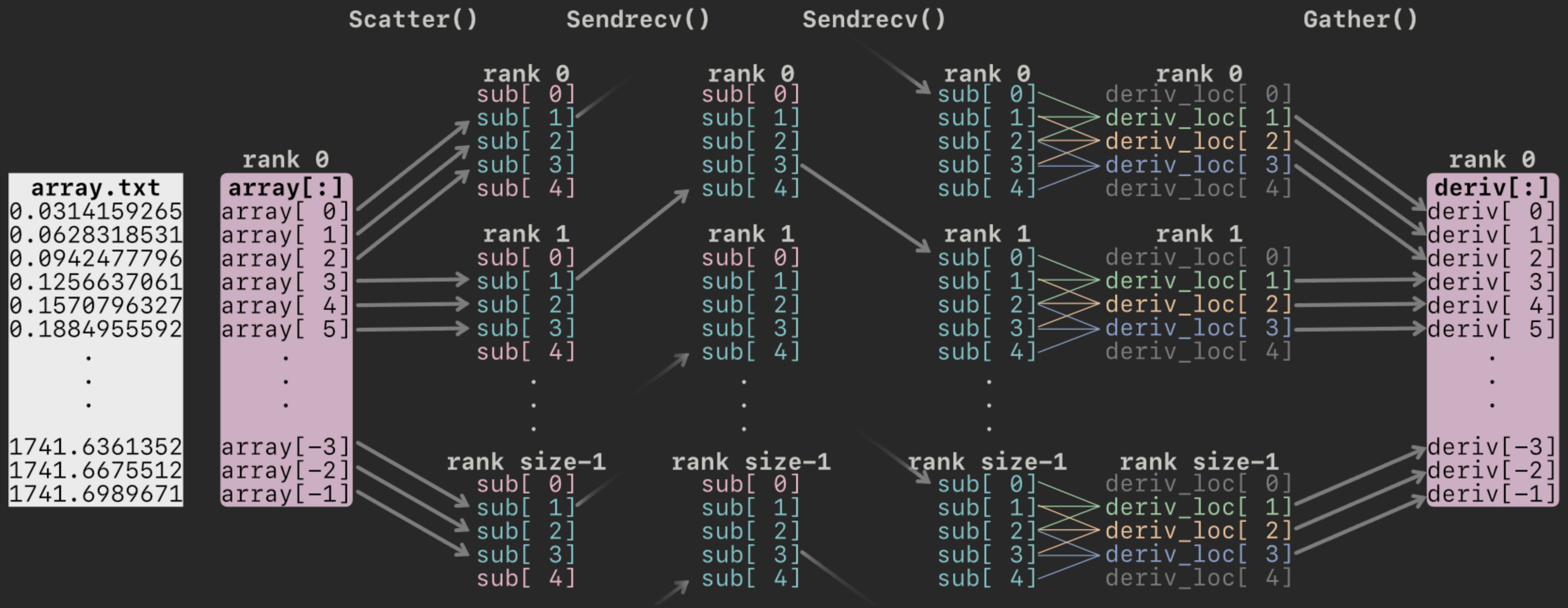
Exercises

Ex04



Exercises

Ex04



Exercises

Ex04