Introduction to High Performance Computing

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SDS406 – Fall semester, 2024 - 2025

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L08: Distributed memory parallel programming, 18th November 2024

Outline

Parallel programming

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

MPI Introduction

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

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.:
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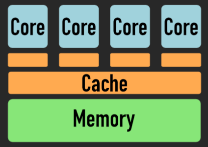
Distributed memory programming

- 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 vs Distributed memory paradigm

Shared memory



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- E.g. multi-core CPU, multi-socket node, GPU threads, etc.
- Programming models: OpenMP, pthreads, MPI, CUDA (sort of)

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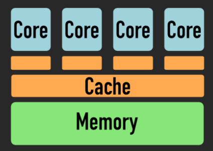

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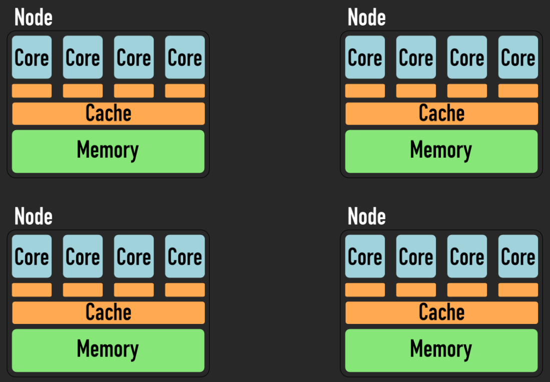

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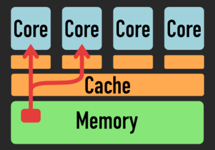

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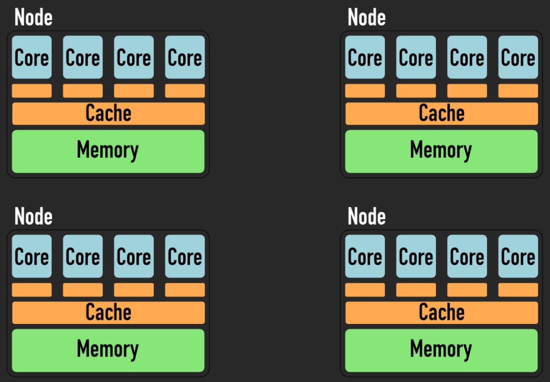

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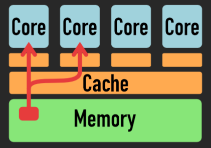

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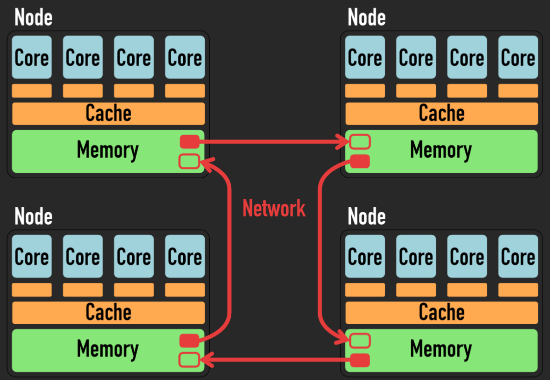

Data shared via explicit communication over a network

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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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- 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 Python, a Python module, `mpi4py`, implements the MPI API

  ```
  import mpi4py
  ```

  or, more commonly

  ```
  from mpi4py import MPI
  ```

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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_{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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#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);
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```python
from mpi4py import MPI

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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
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- 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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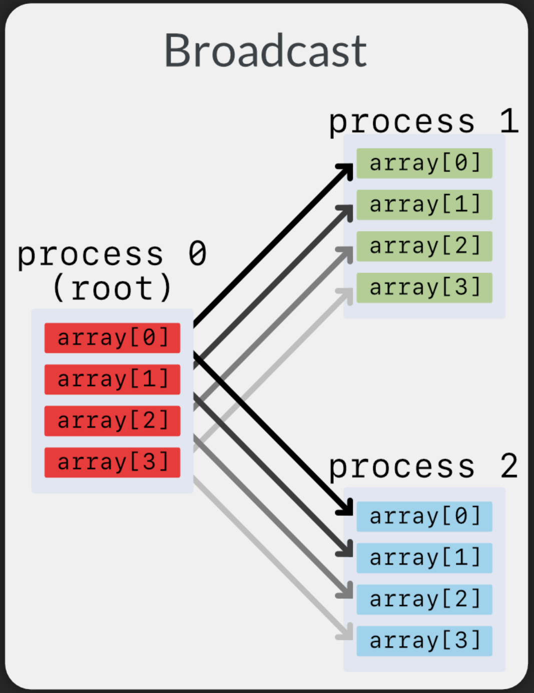

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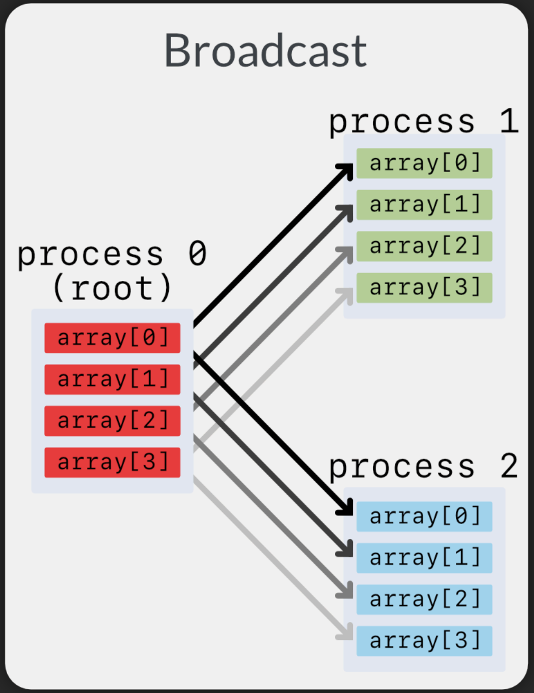

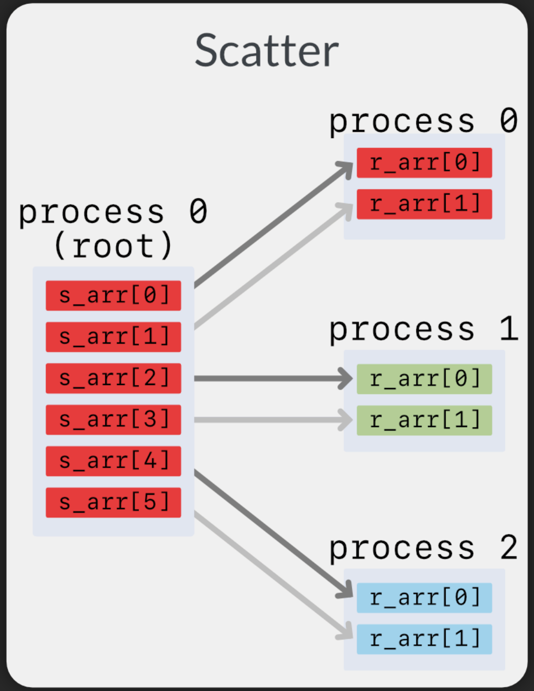

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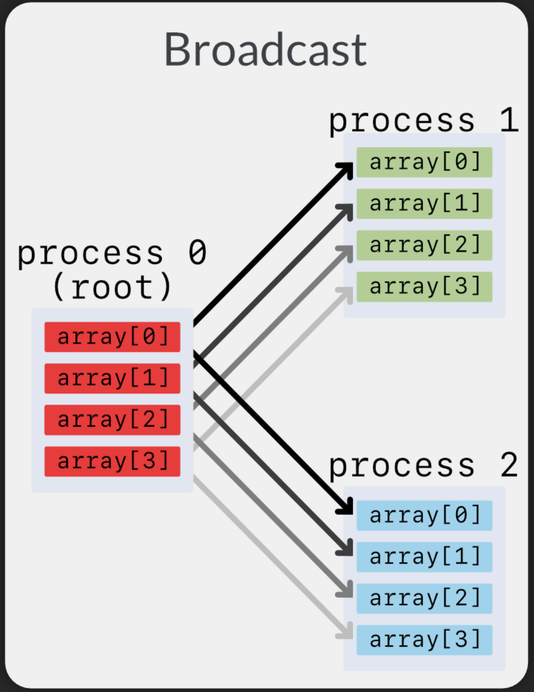

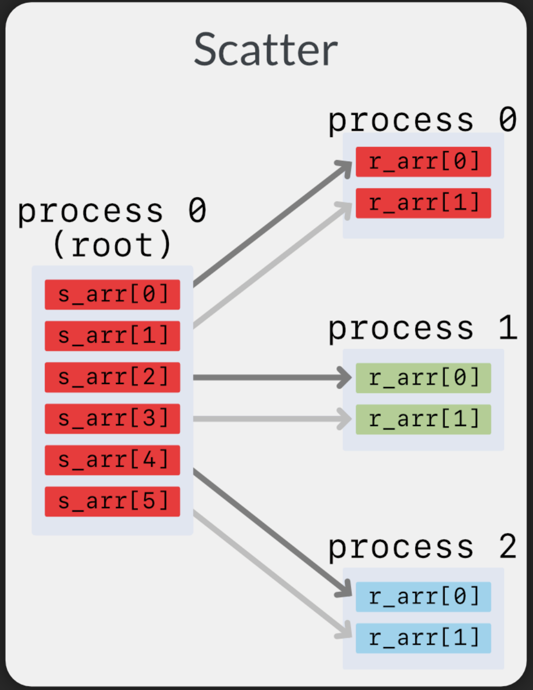

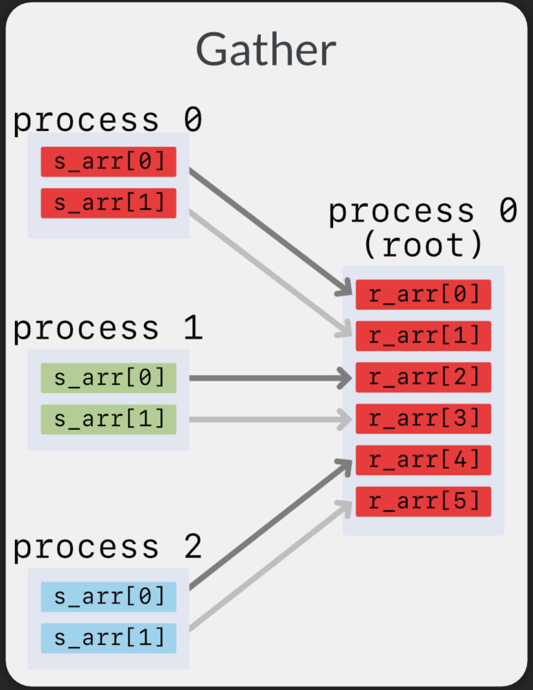

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- In C, we can pass a scalar by using its memory address (second example above). In Python, we can use zero-dimensional numpy array for this

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```

- *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 important since MPI uses it 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 (second 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

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          int root, MPI_Comm comm
          );
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```
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                     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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          const void *sendbuf, int sendcount, MPI_Datatype sendtype,
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          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);
```

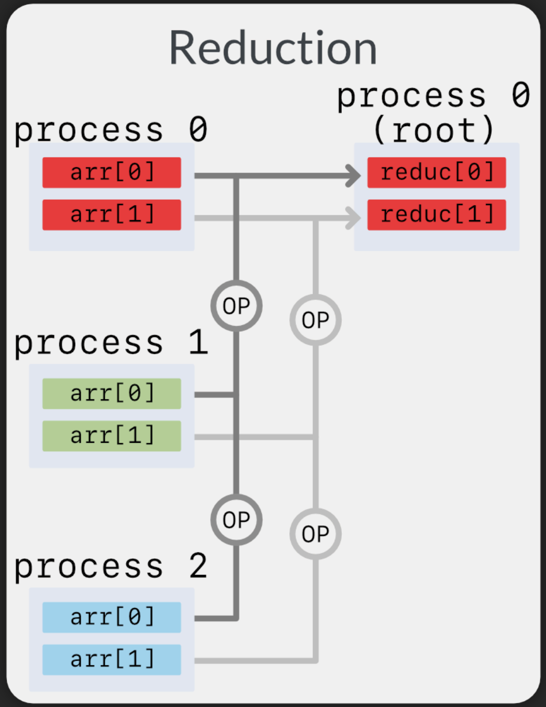
```
arr = np.zeros([4])
element = np.random.rand(1)
MPI.COMM_WORLD.Gather(element, arr, root = 0)
```

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
                      )
```



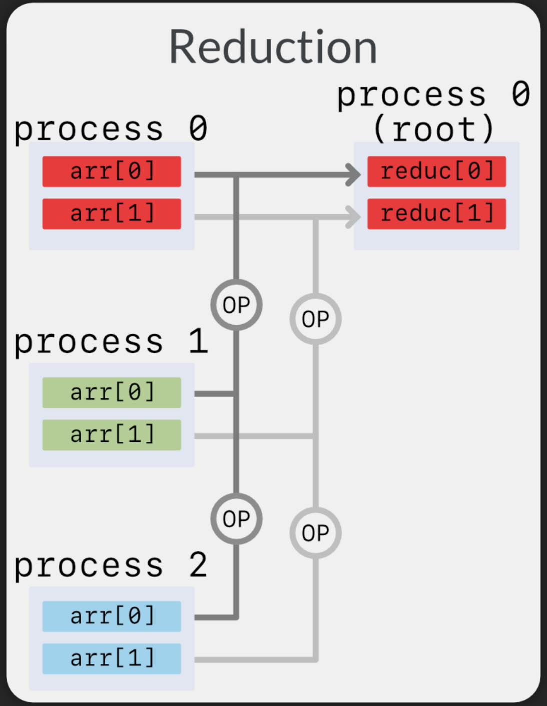
Collective operations: Reduction

- 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 Python)
  - 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:

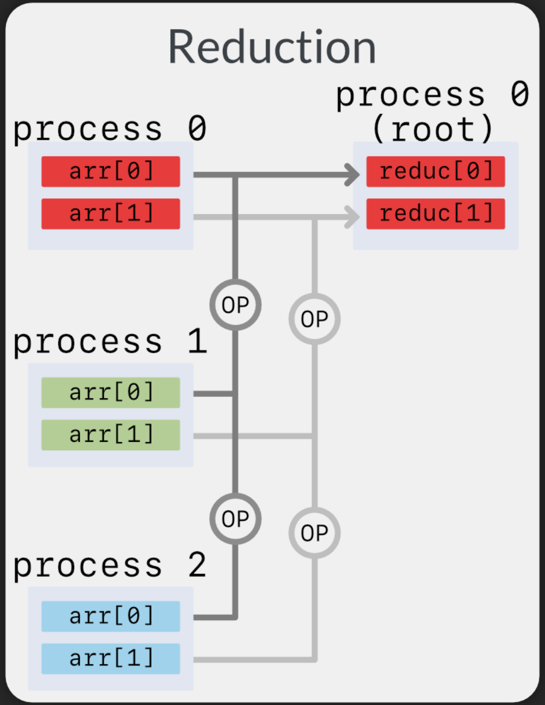
```
MPI_Reduce(
           const void *sendbuf, void *recvbuf, int count,
           MPI_Datatype datatype, MPI_Op op, int root,
           MPI_Comm comm
           )
```

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

- *Example*: Sum 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:

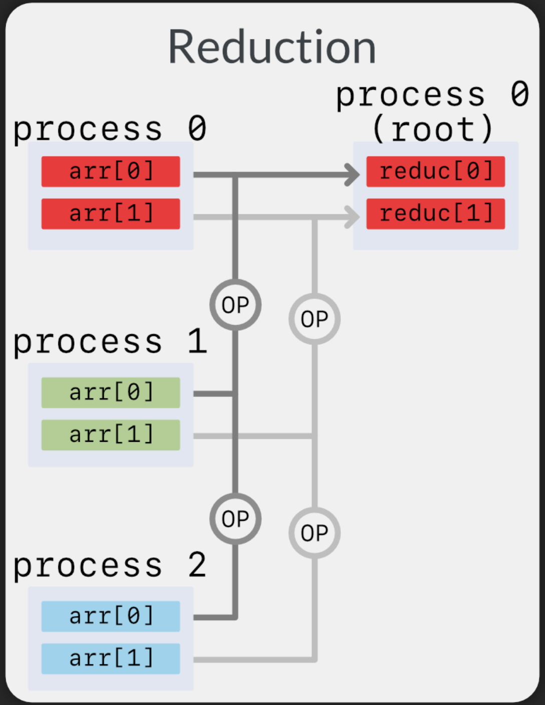
```
MPI_Reduce(
           const void *sendbuf, void *recvbuf, int count,
           MPI_Datatype datatype, MPI_Op op, int root,
           MPI_Comm comm
           )
```

```
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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  - Need specifying additional arguments containing offsets of the send or receive buffer
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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`):

```
if(rank != 0) {
    MPI_Reduce(&var, null, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
} else {
    MPI_Reduce(MPI_IN_PLACE, &var, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
}
```

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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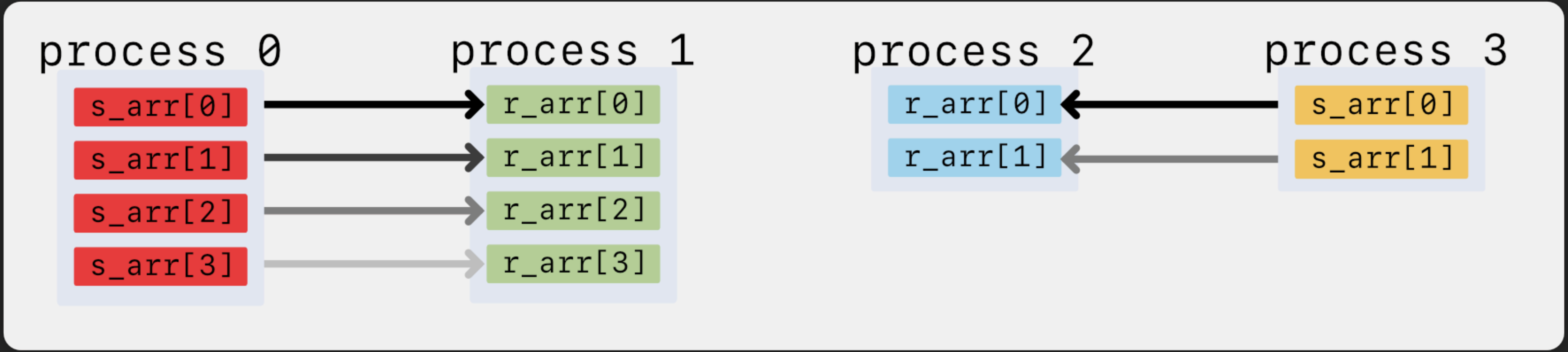

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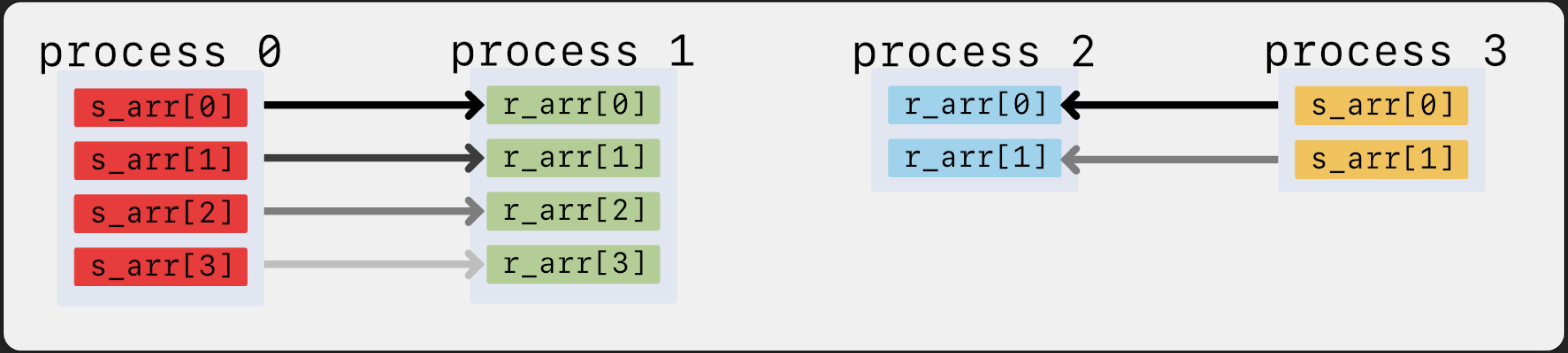

Two point-to-point communications are depicted above
↳ between i) process 0 and 1 and between ii) process 2 and 3

Point-to-point communication

- Send/Receive

```
MPI_Send(void *buf, int n, MPI_Datatype type, int dest, int tag, MPI_Comm comm)
MPI_Recv(void *buf, int n, MPI_Datatype type, int srce, int tag, MPI_Comm comm, MPI_Status *status)
```

```
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)
```

Point-to-point communication

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- Note the need to specify a source and destination rank

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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` (`MPI.ANY_TAG` in Python)

Point-to-point communication

- Send/Receive

```
MPI_Send(void *buf, int n, MPI_Datatype type, int dest, int tag, MPI_Comm comm)
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```
MPI.COMM_WORLD.Send(buf: BufSpec, dest: int, tag: int = 0)
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- Use of `MPI_ANY_SOURCE` (`MPI.ANY_SOURCE` in Python) in `Recv()` means "accept data from any source"

Point-to-point communication

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MPI_Send(void *buf, int n, MPI_Datatype type, int dest, int tag, MPI_Comm comm)
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```
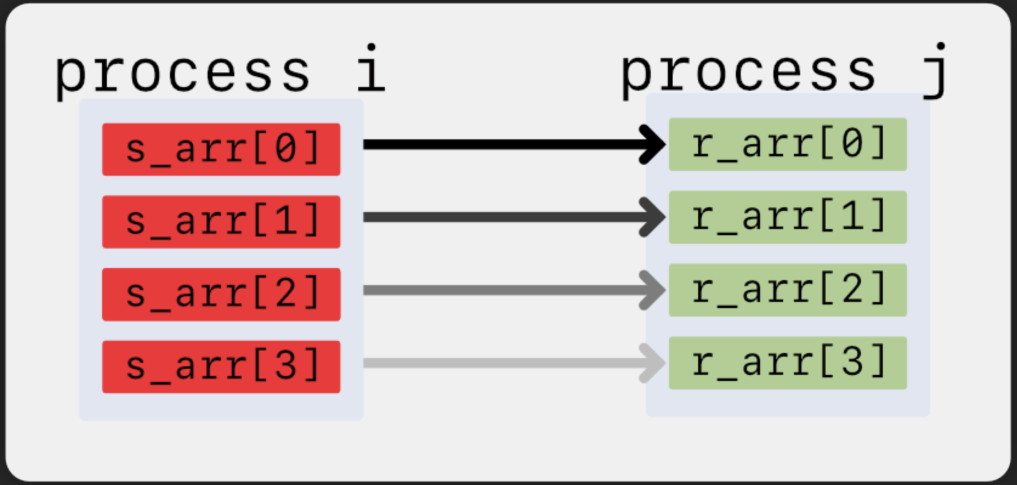

```
MPI.COMM_WORLD.Send(buf: BufSpec, dest: int, tag: int = 0)
MPI.COMM_WORLD.Recv(buf: BufSpec, source: int = ANY_SOURCE, tag: int = ANY_TAG, status: Status = None)
```

- 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` (`MPI.ANY_TAG` in Python)
- Use of `MPI_ANY_SOURCE` (`MPI.ANY_SOURCE` in Python) 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 set to `MPI_STATUS_IGNORE`

Point-to-point communication

- Send/Receive; a trivial example



Point-to-point communication

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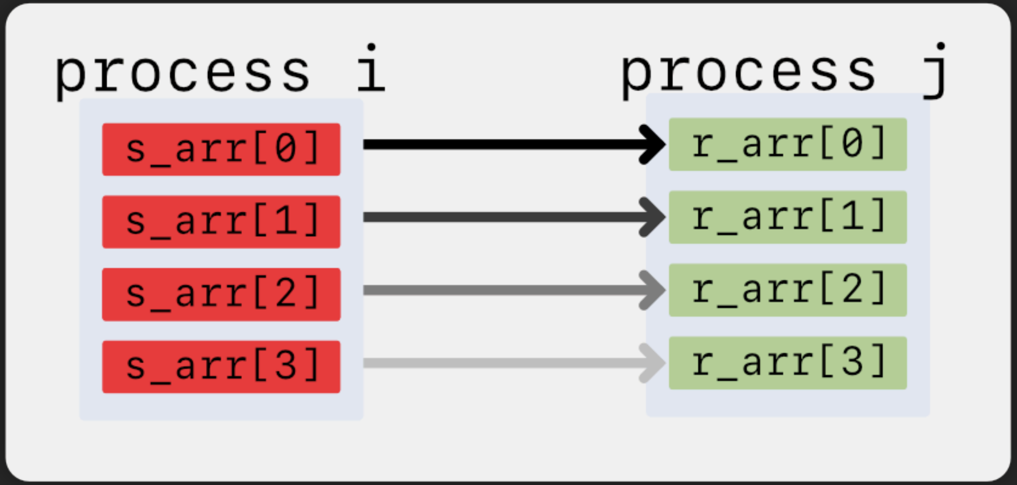
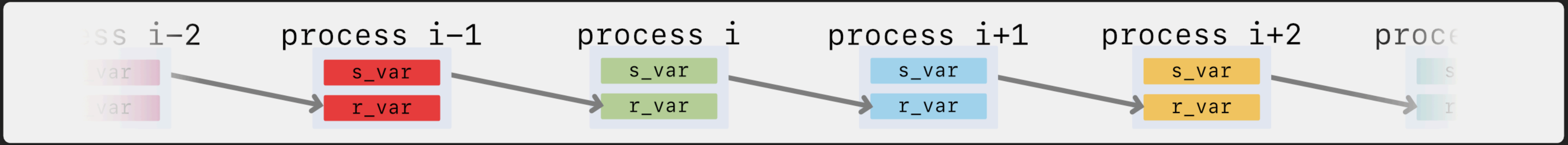


```
if(rank == i) {
  MPI_Send(s_arr, 4, MPI_DOUBLE, j, 0, MPI_COMM_WORLD);
}
if(rank == j) {
  MPI_Recv(r_arr, 4, MPI_DOUBLE, i, MPI_ANY_TAG, MPI_COMM_WORLD, MPI_S
}
```

```
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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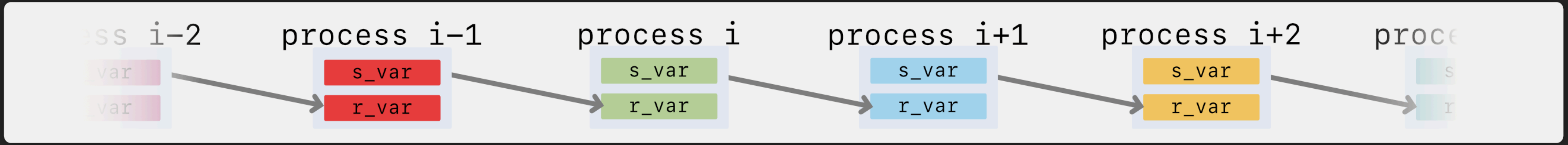

- This will not work:

```
MPI_Send(&s_var, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
MPI_Recv(&r_var, 1, MPI_DOUBLE, rank-1, MPI_ANY_TAG, MPI_COMM_WORLD, M
```

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

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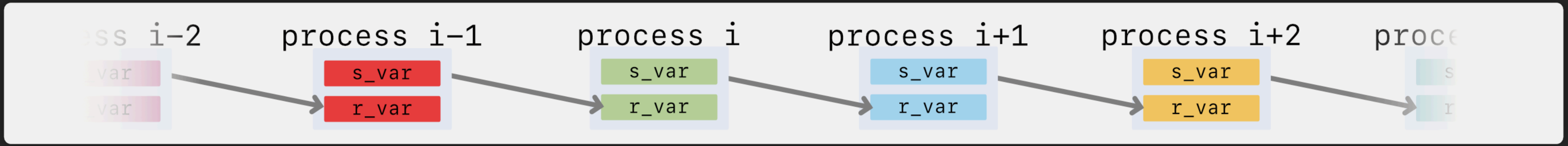

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```

```
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

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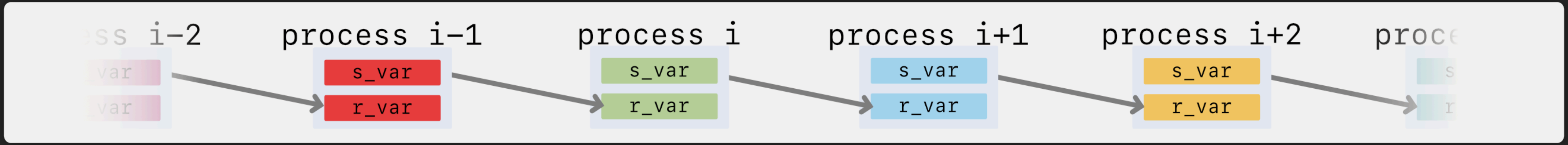

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```

- 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

Point-to-point communication

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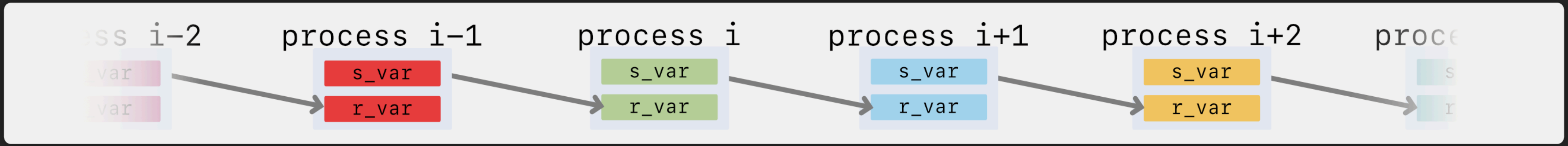

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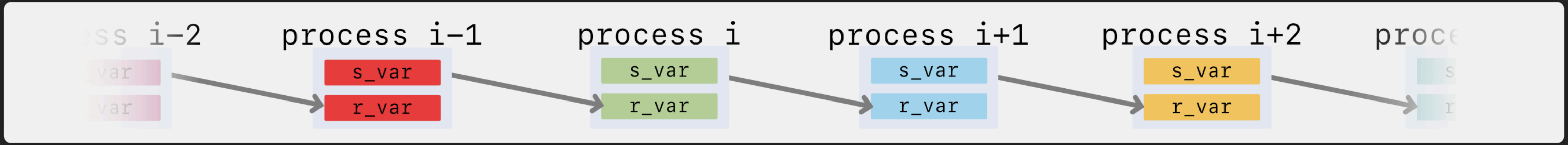
- It results in a deadlock:
  - an `Recv()` can only be posted once an `Send()` completes
  - an `Send()` can only complete if a matching `Recv()` is posted
- One can serialize the communications, i.e. use a loop to determine the order of send/receives
  - Serializes communications that would otherwise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

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_Send(&s_var, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
MPI_Recv(&r_var, 1, MPI_DOUBLE, rank-1, MPI_ANY_TAG, MPI_COMM_WORLD, M
```

```
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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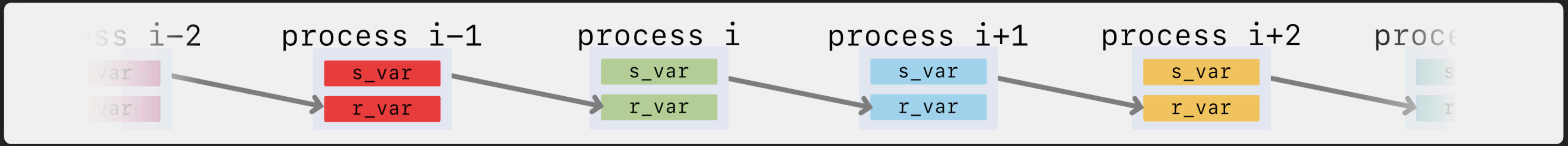

- A more efficient and elegant solution is to use `Sendrecv()`:

```
MPI_Sendrecv(void *sendbuf, int sendcount, MPI_Datatype sendtype, int dest, int sendtag,
             void *recvbuf, int recvcount, MPI_Datatype recvtype, int srce, int recvtag,
             MPI_Comm comm, MPI_Status *status)
```

```
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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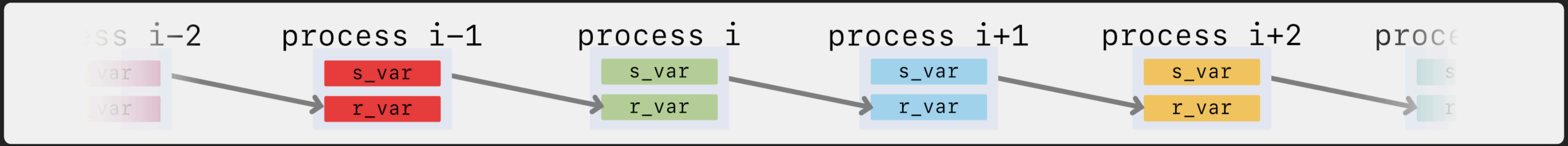

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             MPI_Comm comm, MPI_Status *status)
```

```
MPI.COMM_WORLD.Sendrecv(
    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_Sendrecv(&s_var, 1, MPI_DOUBLE, rank+1, 0,
             &r_var, 1, MPI_DOUBLE, rank-1, MPI_ANY_TAG,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Point-to-point communications

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

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

Point-to-point communications

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- `MPI_Isend()` and `MPI_Irecv()`
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  - The function `MPI_Wait()` is used to block until the operation has complete

```
MPI_Isend(sendbuf, ..., request);
  /*
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   * does not modify sendbuf, which is
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```

- `MPI_Sendrecv_replace()`
    - Like `MPI_Sendrecv()` but with a single `buf` rather than separate `sendbuf` and `recvbuf`

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

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

- `MPI_Sendrecv_replace()`
  - Like `MPI_Sendrecv()` but with a single `buf` rather than separate `sendbuf` and `recvbuf`
    ↳ The receive message overwrites the send message

Exercises

Exercises

```
cp -r /onyx/data/sds406f24/l08/ex?? .
```

- Exercises follow a common structure

Exercises

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

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    - A `.c` source code file (`ex${n}.c`)
    - A submit script (`sub-ex${n}.sh`)
- Our workflow will typically be:
    - Modify `ex${n}.c` as instructed
    - Compile the program with `mpicc`
    - Submit the job script `sbatch sub-ex${n}.sh`
    - Look at the output, which can be found in `ex${n}-output.txt`

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  - Compile the program with `mpicc`
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  - Look at the output, which can be found in `ex${n}-output.txt`
- Note that if you have modified `ex${n}.c` correctly, the job should complete in less than one minute

Exercises

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- Exercises are mostly complete but require some minor modifications by you
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- The MPI functions demonstrated in each exercise are:
    - `ex01`: Use of `Comm_rank()` and `Comm_size()`
    - `ex02`: Use of `Bcast()`, `Scatter()`, and `Reduce()`
    - `ex03`: Use of `Gather()`
    - `ex04`: Use of `Bcast()`, `Scatter()`, `Sendrecv()`, and `Gather()`

Exercises

- Exercises are mostly complete but require some minor modifications by you
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- The MPI functions demonstrated in each exercise are:
  - `ex01`: Use of `Comm_rank()` and `Comm_size()`
  - `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 and the GNU Compiler. Please use:

  ```
  module load gompi/2023a
  ```

  for all exercises.

Exercises

Ex01

- Modify `ex01.c` to call `MPI_Comm_size()` and `MPI_Comm_rank()` appropriately

```
/*
 * TODO: call the appropriate MPI functions here
 */
```

Exercises

Ex01

- Modify `ex01.c` to call `MPI_Comm_size()` and `MPI_Comm_rank()` appropriately

```
/*
 * TODO: call the appropriate MPI functions here
 */
```

- Compile

  ```
  mpicc -o ex01 ex01.c
  ```

Exercises

Ex01

- Modify `ex01.c` to call `MPI_Comm_size()` and `MPI_Comm_rank()` appropriately

```
/*
 * TODO: call the appropriate MPI functions here
 */
```

- Compile

  ```
  mpicc -o ex01 ex01.c
  ```

- 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 --partition=p100
  #SBATCH -A sds406f24

  module load gompi/2023a
  mpirun ex01
  ```

Exercises

Ex01

- Modify `ex01.c` to call `MPI_Comm_size()` and `MPI_Comm_rank()` appropriately

```
/*
 * TODO: call the appropriate MPI functions here
 */
```

- Compile

  ```
  mpicc -o ex01 ex01.c
  ```

- 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 --partition=p100
  #SBATCH -A sds406f24

  module load gompi/2023a
  mpirun ex01
  ```

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

Exercises

Ex01

- Modify `ex01.c` to call `MPI_Comm_size()` and `MPI_Comm_rank()` appropriately

```
/*
 * TODO: call the appropriate MPI functions here
 */
```

- Compile

  ```
  mpicc -o ex01 ex01.c
  ```

- 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 --partition=p100
  #SBATCH -A sds406f24

  module load gompi/2023a
  mpirun ex01
  ```

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

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]$
```

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

Exercises

Ex01

- Submit the job script:

```
[user@front02 ex01]$ sbatch sub-ex01.sh
Submitted batch job 69711
[user@front02 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 = 0 of nproc = 8 on node: cyc06
This is rank = 2 of nproc = 8 on node: cyc06
This is rank = 3 of nproc = 8 on node: cyc06
This is rank = 5 of nproc = 8 on node: cyc07
This is rank = 6 of nproc = 8 on node: cyc07
This is rank = 1 of nproc = 8 on node: cyc06
This is rank = 7 of nproc = 8 on node: cyc07
This is rank = 4 of nproc = 8 on node: cyc07
[user@front02 ex01]$
```

Exercises

Ex01

- Submit the job script:

```
[user@front02 ex01]$ sbatch sub-ex01.sh
Submitted batch job 69711
[user@front02 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 = 0 of nproc = 8 on node: cyc06
This is rank = 2 of nproc = 8 on node: cyc06
This is rank = 3 of nproc = 8 on node: cyc06
This is rank = 5 of nproc = 8 on node: cyc07
This is rank = 6 of nproc = 8 on node: cyc07
This is rank = 1 of nproc = 8 on node: cyc06
This is rank = 7 of nproc = 8 on node: cyc07
This is rank = 4 of nproc = 8 on node: cyc07
[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:

Exercises

Ex02

- We would like:
    - The root process to read all elements into an array `array[]`

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`

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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

Ex02

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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`
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      ↳ Each process should receive `nloc` elements
    - Each process to sum its local elements, storing the result into `sum_loc`

Exercises

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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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    - 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`

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.c`, 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.c`, 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.c`, 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

- See also `ex03-scalar.c`, which implements the same but with no parallelism,

```
[user@front02 ex03]$ srun -n 1 -p p100 ./ex03-scalar filenames.txt
   * 00.txt → 04D70552
   * 01.txt → 19708CD4
   * 02.txt → ED737A1C
   * 03.txt → 0C40E2D2
   * 04.txt → F7BDE74D
   * 05.txt → 562DDD6C
   * 06.txt → 6F2CD2F1
   * 07.txt → 016DB6C6
   Done 8 files in t = 12.953475 sec
[user@front02 ex03]$
```

Exercises

Ex04

- In this exercise, a large array of 17,463,600 elements is read by rank 0 (`n_arr = 17463600`)

Exercises

Ex04

- In this exercise, a large array of 17,463,600 elements is read by rank 0 (`n_arr = 17463600`)
- Our objective is to compute a second order discrete derivative of the data:

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

Exercises

Ex04

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- We will proceed as follows:

Exercises

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- 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, `arr_loc[n_loc+2]`, where `n_loc = n_arr / nproc`

Exercises

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- 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, `arr_loc[n_loc+2]`, where `n_loc = n_arr / nproc`
  - Add a missing `Scatter()` to distribute to each processes the corresponding `n_loc` elements. These should be received in `arr_loc[1:-1]` of each rank

Exercises

Ex04

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```
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```

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  - Add a missing `Scatter()` to distribute to each processes the corresponding `n_loc` elements. These should be received in `arr_loc[1:-1]` of each rank
  - Use `Sendrecv()` to fill the first and last elements element of `arr_loc[]`, i.e. `arr_loc[0]` and `arr_loc[n_loc+1]`, with the corresponding elements of the neighboring ranks, needed to carry out the derivative

Exercises

Ex04

- In this exercise, a large array of 17,463,600 elements is read by rank 0 (`n_arr = 17463600`)
- Our objective is to compute a second order discrete derivative of the data:

`deriv[i] = arr[i-1] + arr[i+1] - 2*arr[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, `arr_loc[n_loc+2]`, where `n_loc = n_arr / nproc`
  - Add a missing `Scatter()` to distribute to each processes the corresponding `n_loc` elements. These should be received in `arr_loc[1:-1]` of each rank
  - Use `Sendrecv()` to fill the first and last elements element of `arr_loc[]`, i.e. `arr_loc[0]` and `arr_loc[n_loc+1]`, with the corresponding elements of the neighboring ranks, needed to carry out the derivative
  - Now your program can proceed to correctly compute the derivative:

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

Exercises

Ex04

- In this exercise, a large array of 17,463,600 elements is read by rank 0 (`n_arr = 17463600`)
- Our objective is to compute a second order discrete derivative of the data:

  `deriv[i] = arr[i-1] + arr[i+1] - 2*arr[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, `arr_loc[n_loc+2]`, where `n_loc = n_arr / nproc`
  - Add a missing `Scatter()` to distribute to each processes the corresponding `n_loc` elements. These should be received in `arr_loc[1:-1]` of each rank
  - Use `Sendrecv()` to fill the first and last elements element of `arr_loc[]`, i.e. `arr_loc[0]` and `arr_loc[n_loc+1]`, with the corresponding elements of the neighboring ranks, needed to carry out the derivative
  - Now your program can proceed to correctly compute the derivative:

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

Exercises

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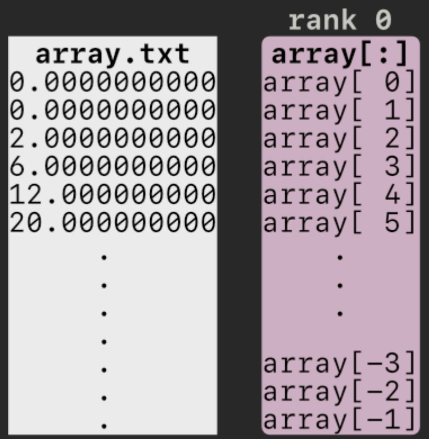
  - Use a `Gather()` to collect the full array of the derivative into the root process (`rank` = 0). The root process will then write the array to a new file `deriv.txt`
- If done correctly, `deriv.txt` will contain all `+2.000000`, except for the first and last element

Exercises

Ex04

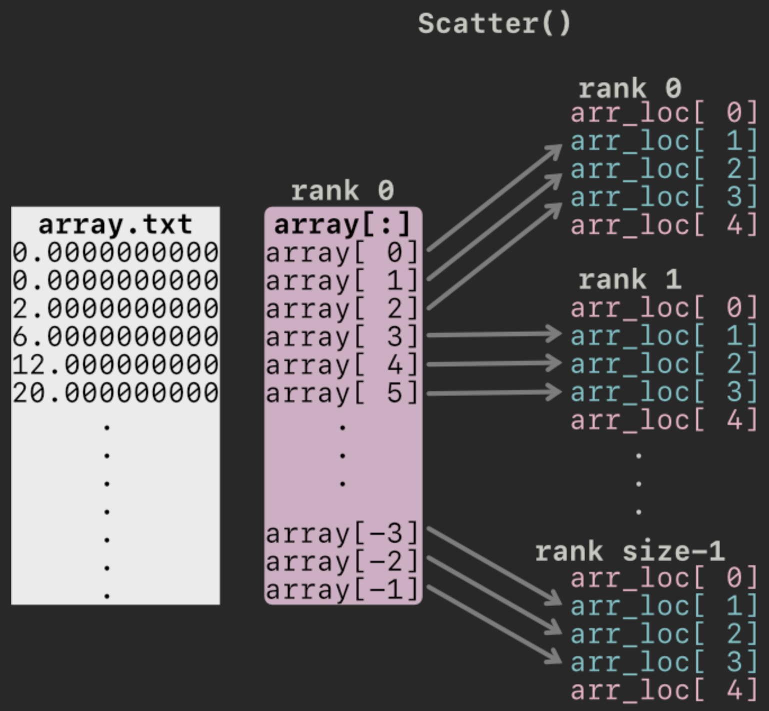
Exercises

Ex04



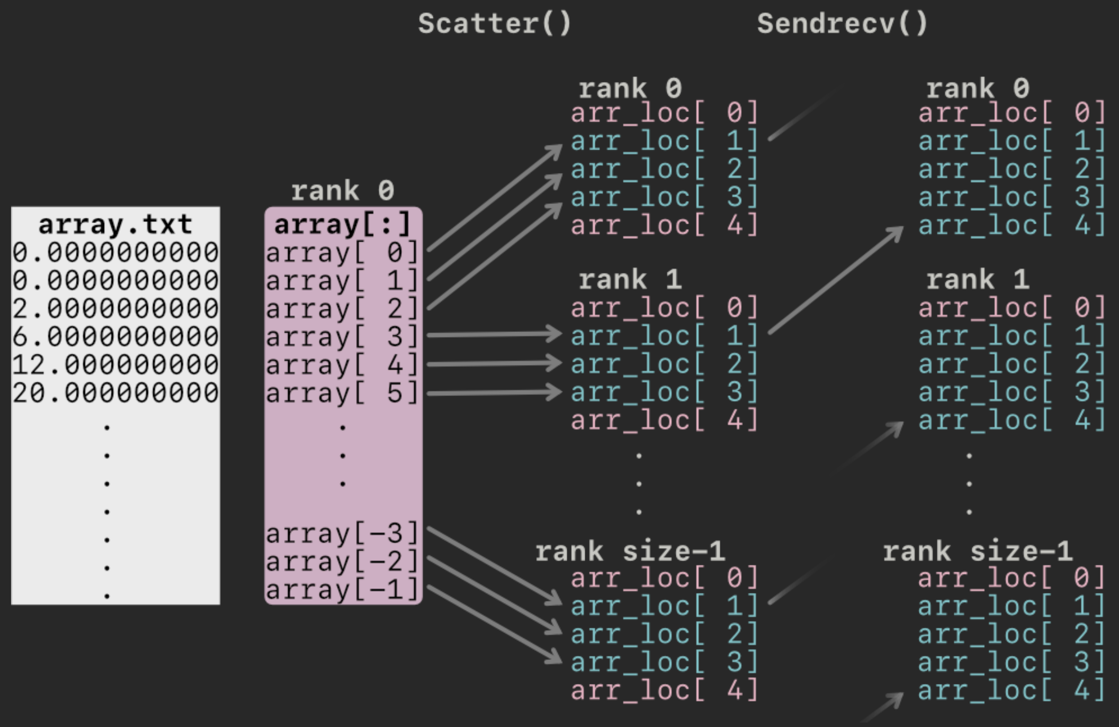
Exercises

Ex04



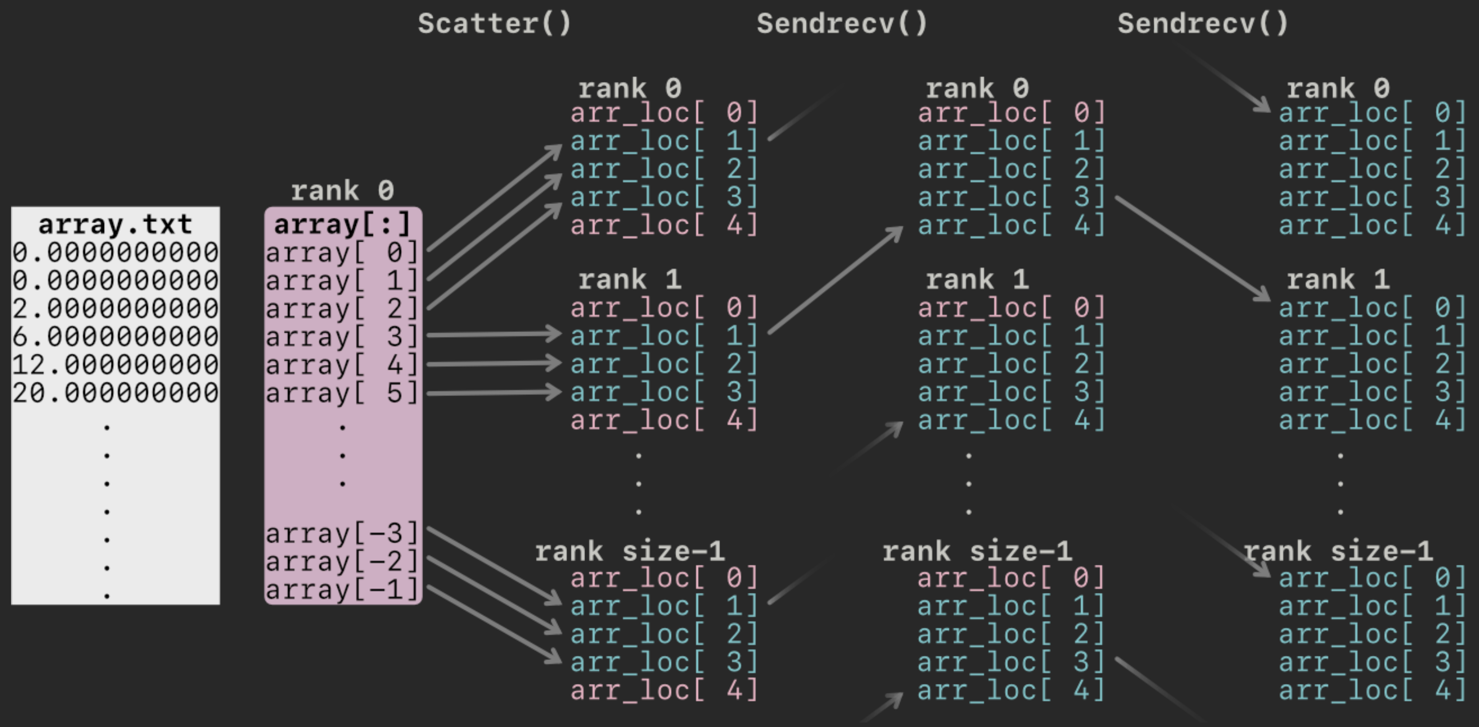
Exercises

Ex04



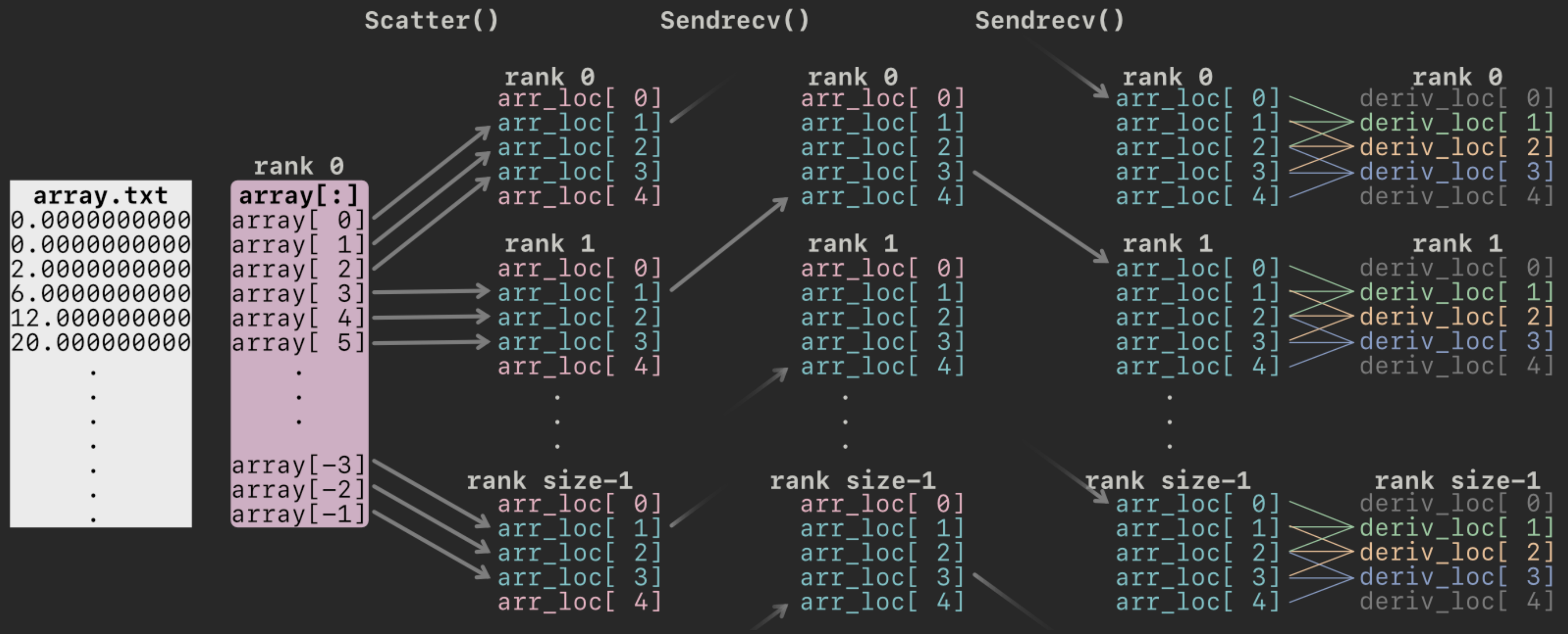
Exercises

Ex04



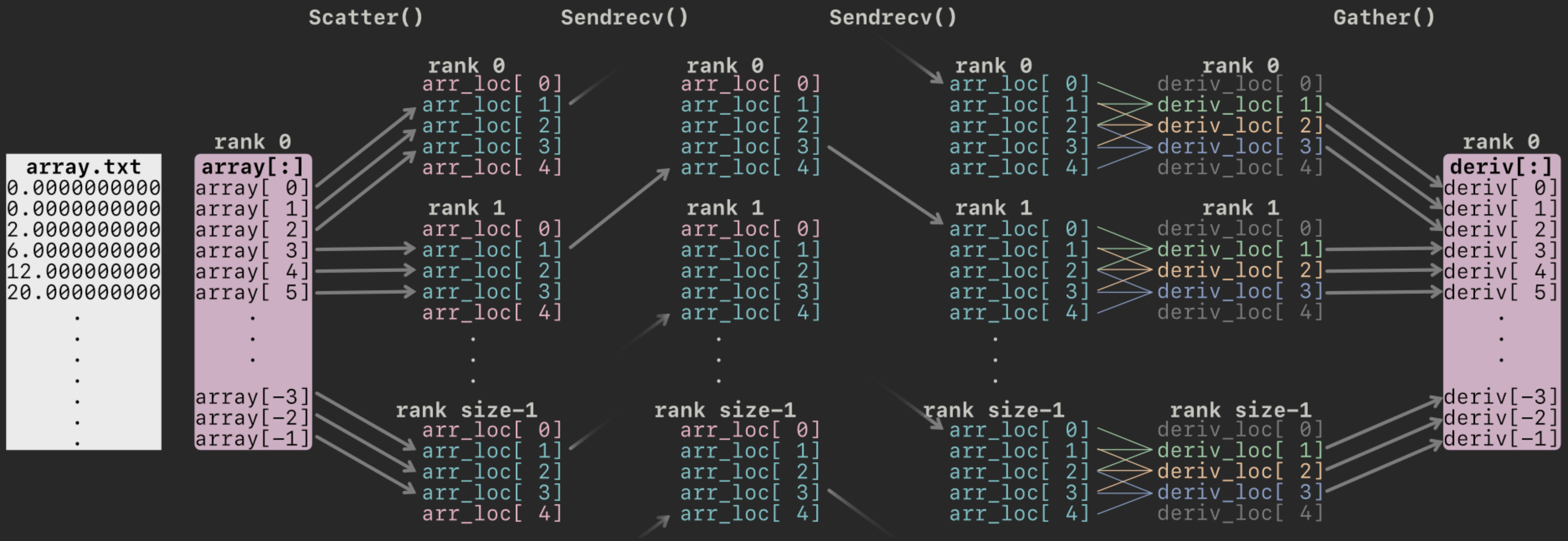
Exercises

Ex04



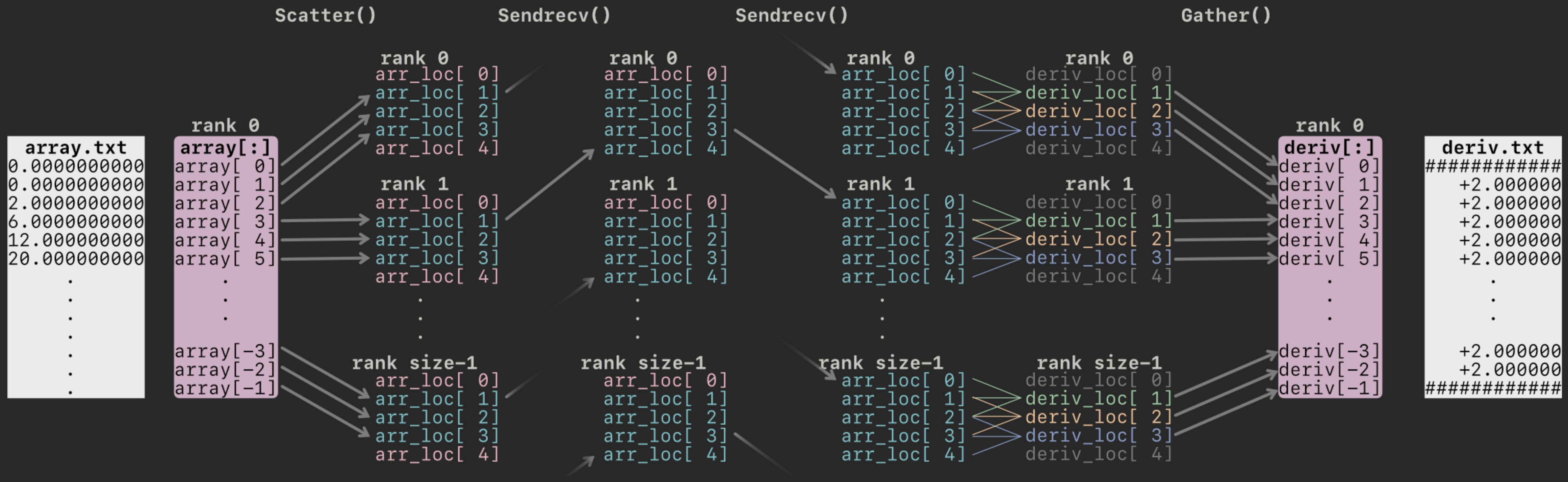
Exercises

Ex04



Exercises

Ex04


Scatter()
Sendrecv()
Sendrecv()
Gather()
array.txt
0.0000000000
0.0000000000
2.0000000000
6.0000000000
12.000000000
20.000000000
rank 0
array[:]
array[0]
array[1]
array[2]
array[3]
array[4]
array[5]
array[-3]
array[-2]
array[-1]
rank 0
rank 1
rank size-1
arr_loc[0]
arr_loc[1]
arr_loc[2]
arr_loc[3]
arr_loc[4]
deriv_loc[0]
deriv_loc[1]
deriv_loc[2]
deriv_loc[3]
deriv_loc[4]
rank 0
deriv[:]
deriv[0]
deriv[1]
deriv[2]
deriv[3]
deriv[4]
deriv[5]
deriv[-3]
deriv[-2]
deriv[-1]
deriv.txt
###########
+2.000000
+2.000000
+2.000000
+2.000000
+2.000000
+2.000000
+2.000000
###########