HPC Intermediate Training Event

EuroCC Training, 19th April 2021

MPI, OpenMP, and Hybrid Programming

Outline

- Overview of the Message Passing Interface (MPI)
- Basics of MPI
 - Distributed memory paradigm (as compared to shared memory)
 - Start-up and initialization
- Synchronization
- Collectives
- Point-to-point communication

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:
 - version 3.1 (MPI-3.1), since June 2015
 - o Release Candidate for version 4.0 (MPI-4.0) as of November 2020
- Several free (open) or vendor-provided implementations, e.g.:
 - Mvapich
 - OpenMPI
 - IntelMPI

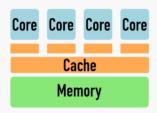
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Distributed memory programming

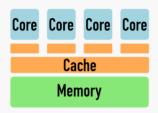
- Each process has its own memory domain
- MPI functions facilitate:
 - Obtaining environment information about the running process, e.g., process id, number of processes, etc.
 - Achieving *communication* between processes, e.g. synchronization, copying of data, etc.

Shared memory



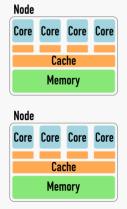
- Multiple processes share common memory (common *memory address space*)
- E.g. multi-core CPU, multi-socket node, GPU threads, etc.
- Programming models: OpenMP, pthreads, MPI, CUDA (sort of)

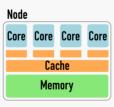
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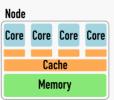


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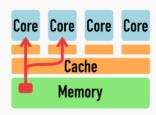






- Processes have distinct memory domains (different memory address space)
- E.g. multiple nodes within a cluster, multiple GPUs within a node
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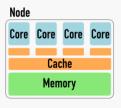
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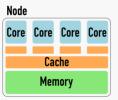


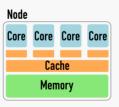
Data shared via memory

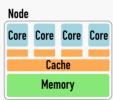
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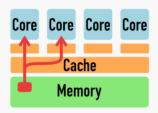






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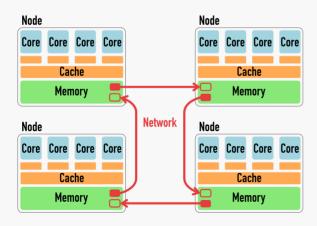


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ssh node01 /my_program & ssh node02 /my_program & ssh node03 /my_program &
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• Depending on the system, instead of mpirun you may be required mpiexec or srun which take similar (but not identical) arguments

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• Need to link against MPI libraries; precise invocation depends on the compiler, the MPI implementation used, its version, etc., e.g.:

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• Thankfully, knowing the locations of the MPI library and include files is never needed in practice; implementations come with wrappers that set the appropriate include paths and linker options:

mpicc -o my_mpi_program my_mpi_program.c

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```
#include <mpi.h>
int
main(int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    /*
    ...
    ...
    ...
    //
    MPI_Finalize();
    return 0;
}
```

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

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

int
main(int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    int nproc, rank;
    MPI_Comm_size(MPI_COMM_WORLD, &nproc);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    printf(" This is rank = %d of nproc = %d\n", rank, nproc);
    MPI_Finalize();
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- MPI_COMM_WORLD is an MPI communicator. This specific communicator is the default communicator, defined in mpi.h, and trivially specifies all processes
- A user can partition processes into subgroups by defining custom communicators, but this will not be covered here

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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

```
[user@front01 ~]$ mpircu -o example example.c

[user@front01 ~]$ mpirun -n 5 example

This is rank = 3 of nproc = 5

This is rank = 1 of nproc = 5

This is rank = 2 of nproc = 5

This is rank = 4 of nproc = 5

This is rank = 0 of nproc = 5
```

• Compiling and running the previous program (assuming it is saved as example.c)

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[user@front01 ~]$ mpicc -o example example.c

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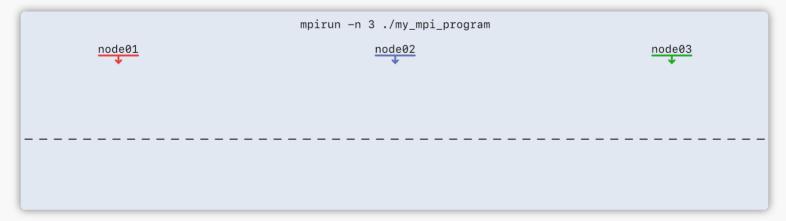
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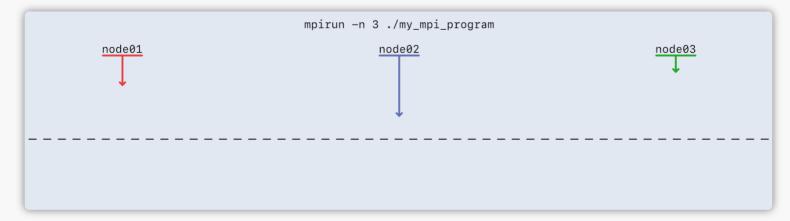
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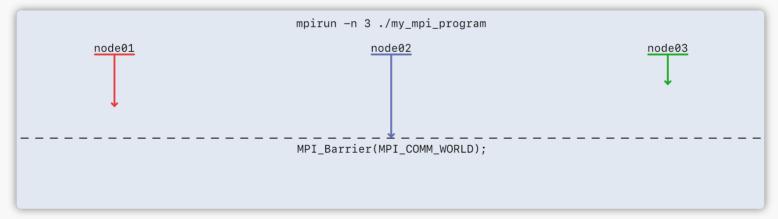
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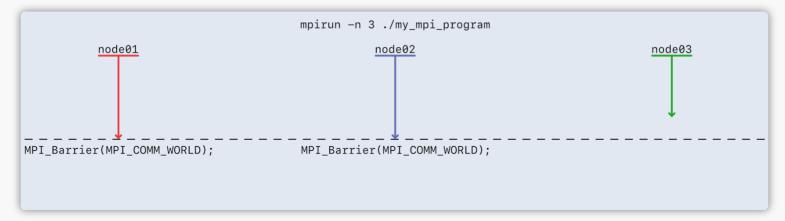
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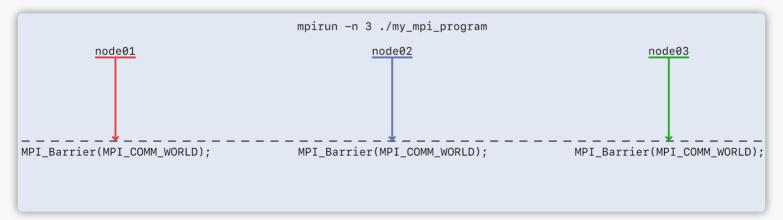
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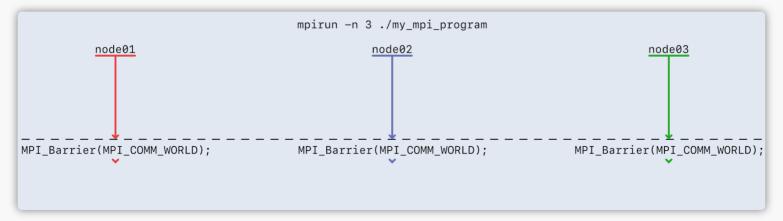
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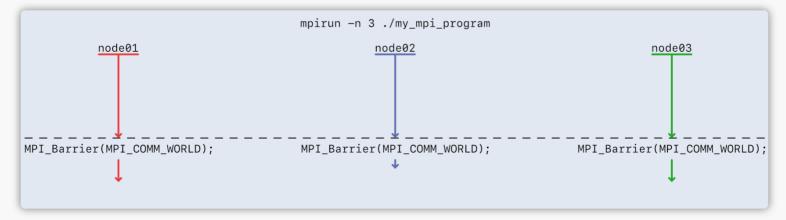
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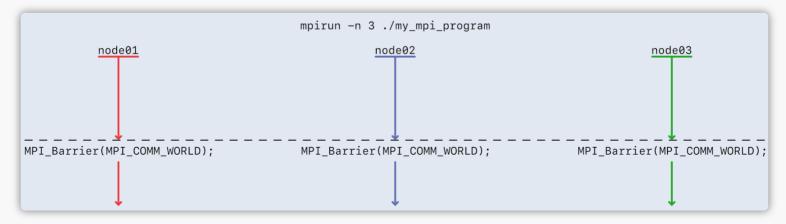
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- The first set of communication functions we will look at are *collective operations*
- Collective: all processes must be involved in the operation (as opposed to *point-to-point* communications)
- Examples (this list is not exhaustive!):
 - Broadcast 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)
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- Full list of types available in MPI documentation. E.g. see: https://www.mpich.org/static/docs/latest/www3/Constants.html

• Scatter:

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

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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);</pre>
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• 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);</pre>
```

• Gather:

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

• Gather:

```
MPI_Gather(
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    void *recvbuf, int recvcount, MPI_Datatype recvtype, int root,
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- recvcount is the number of elements to be received by each process
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- 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);</pre>
```

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```
MPI_Gather(
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MPI_Gather(arr_proc, 3, MPI_DOUBLE, arr_all, 3, MPI_DOUBLE, 0, MPI_COMM_WORLD);</pre>
```

• *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);</pre>
```

• Reduction:

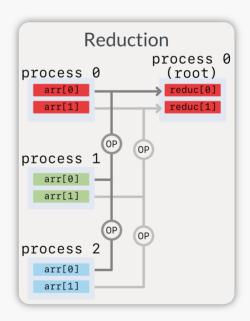
```
MPI_Reduce(
    const void *sendbuf, void *recvbuf, int count,
    MPI_Datatype datatype, MPI_Op op, int root,
    MPI_Comm comm
)
```

• Reduction:

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

• Notes:

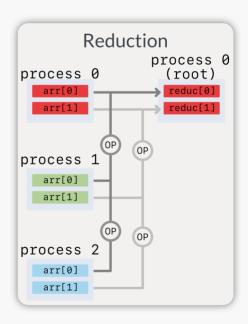
- MPI_Op is an operation, e.g. MPI_SUM, MPI_PROD, etc.
- The correct result of the operation depends on specifying the datatype correctly
- count is the number of elements of the arrays and is the same for send and receive, e.g. in the example on the right, count == 2
- The operation is over all processes in comm



Reduction:

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

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



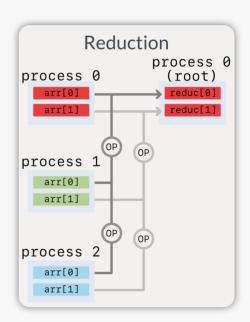
Reduction:

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

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

• 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);
```



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 - Allow specifying *varying* number of elements to be distributed or collected to or from the process pool
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 → which buffer depends on the specific MPI function
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 - \circ E.g. below, the sum will be placed in var of the root process (process with rank == 0):

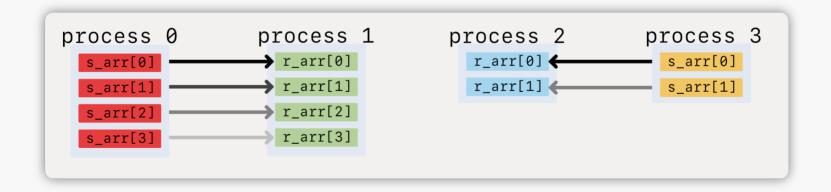
```
if(rank != 0) {
    MPI_Reduce(&var, null, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
} else {
    MPI_Reduce(MPI_IN_PLACE, &var, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
}
```

• Communications that involve transfer of data between two processes

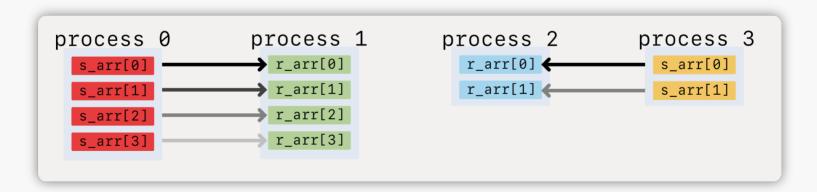
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Two point-to-point communications are depicted above → between i) process 0 and 1 and between ii) process 2 and 3

• 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)

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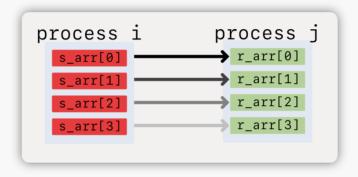
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- Use of MPI_ANY_SOURCE in MPI_Recv() means "accept data from any source"
- status can be used to query the result of the receive (e.g. how many elements were received). We
 will use MPI_STATUS_IGNORE in place of status, which ignores the status

• Send/Receive; a trivial example



• Send/Receive; a trivial example



```
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_STATUS_IGNORE);
}
```

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



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```
MPI_Send(&s_var, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
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- It results in a deadlock:
 - o an MPI_Recv() can only be posted once an MPI_Send() completes
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 - Serializes communications that may be done faster in parallel
 - o Inelegant, obscure, and error-prone

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A more efficient and elegant solution is to use MPI_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)
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• A more efficient and elegant solution is to use MPI_Sendrecv():

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```

• 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);
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```
MPI_Isend(sendbuf, ..., request);

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* More code can come here, provided it

* 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

 The receive message overwrites the send message

cp -r /onyx/data/edu12/mpi/ex .

• Exercises follow a common structure

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 - Look at the output, which can be found in ex\${n}-output.txt

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

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ex01: Use of MPI_Comm_rank() and MPI_Comm_size()
```

- o ex02: Use of MPI_Barrier()
- o ex03: Use of MPI Bcast()
- o ex04: Use of MPI Scatter()
- o ex05: Use of MPI_Scatter() and MPI_Gather()
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- o ex08: Use of MPI_Sendrecv()
- All exercises have been tested with OpenMPI and the GNU Compiler. Please use:

module load gompi

for all exercises.

Ex01

• Modify ex01.c to call MPI_Comm_size() and MPI_Comm_rank() with the appropriate arguments

```
int nproc, rank;
/*
* TODO: call `MPI_Comm_size()' and `MPI_Comm_rank()' with the
* appropriate arguments
*/
MPI_Comm_size(/* TODO */);
MPI_Comm_rank(/* TODO */);
```

Ex01

• Modify ex01.c to call MPI_Comm_size() and MPI_Comm_rank() with the appropriate arguments

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* appropriate arguments
*/
MPI_Comm_size(/* TODO */);
MPI_Comm_rank(/* TODO */);
```

• To compile, type make. Remember to first load the appropriate module (gompi):

```
[user@front01 ex01]$ module load gompi
[user@front01 ex01]$ make
mpicc -c ex01.c
mpicc -o ex01 ex01.o
[user@front01 ex01]$
```

Ex01

• A job script has been prepared to run ex01:

```
[user@front01 ex01]$ cat sub-01.sh
#!/bin/bash
#SBATCH --job-name=01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00

module load gompi
mpirun /ex01
```

Ex01

• A job script has been prepared to run ex01:

```
[user@front01 ex01]$ cat sub-01.sh
#!/bin/bash
#SBATCH --job-name=01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00

module load gompi
mpirun //ex01
```

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

Ex01

• A job script has been prepared to run ex01:

```
[user@front01 ex01]$ cat sub-01.sh
#!/bin/bash
#SBATCH --job-name=01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00

module load gompi
mpirun /ex01
```

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

Ex01

• A job script has been prepared to run ex01:

```
[user@front01 ex01]$ cat sub-01.sh
#!/bin/bash
#SBATCH --job-name=01
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --output=ex01-output.txt
#SBATCH --time=00:01:00

module load gompi
mpirun /ex01
```

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

Ex01

• Submit the job script:

[user@front01 ex01]\$ sbatch sub-01.sh Submitted batch job 69711 [user@front01 ex01]\$

Ex01

• Submit the job script:

```
[user@front01 ex01]$ sbatch sub-01.sh
Submitted batch job 69711
[user@front01 ex01]$
```

• Check status of job:

```
[user@front01 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@front01 ex01]$
```

Ex01

• Submit the job script:

```
[user@front01 ex01]$ sbatch sub-01.sh
Submitted batch job 69711
[user@front01 ex01]$
```

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[user@front01 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@front01 ex01]$
```

• The job runs very quickly. You may see no output above if the job has finished:

```
[user@front01 ex01]$ squeue -u $USER

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

[user@front01 ex01]$
```

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

```
[user@front01 ex01]$ cat ex01-output.txt
This is rank = 3 of nproc = 8 on node: cn01
This is rank = 0 of nproc = 8 on node: cn01
This is rank = 1 of nproc = 8 on node: cn01
This is rank = 2 of nproc = 8 on node: cn01
This is rank = 7 of nproc = 8 on node: cn02
This is rank = 5 of nproc = 8 on node: cn02
This is rank = 6 of nproc = 8 on node: cn02
This is rank = 4 of nproc = 8 on node: cn02
[user@front01 ex01]$
```

Ex01

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

```
[user@front01 ex01]$ cat ex01-output.txt
This is rank = 3 of nproc = 8 on node: cn01
This is rank = 0 of nproc = 8 on node: cn01
This is rank = 1 of nproc = 8 on node: cn01
This is rank = 2 of nproc = 8 on node: cn01
This is rank = 7 of nproc = 8 on node: cn02
This is rank = 5 of nproc = 8 on node: cn02
This is rank = 6 of nproc = 8 on node: cn02
This is rank = 4 of nproc = 8 on node: cn02
[user@front01 ex01]$
```

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

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

```
[user@front01 ex01]$ cat ex01-output.txt
This is rank = 3 of nproc = 8 on node: cn01
This is rank = 0 of nproc = 8 on node: cn01
This is rank = 1 of nproc = 8 on node: cn01
This is rank = 2 of nproc = 8 on node: cn01
This is rank = 7 of nproc = 8 on node: cn02
This is rank = 5 of nproc = 8 on node: cn02
This is rank = 6 of nproc = 8 on node: cn02
This is rank = 4 of nproc = 8 on node: cn02
[user@front01 ex01]$
```

- Note the order is nondeterministic; whichever process reaches the print statement first prints
- We can use synchronization to serialize the print statements and ensure the correct order

- ex02.c is similar to ex01.c
- A for-loop is included over the print statement:

```
/*
* TODO: add an MPI_Barrier() to ensure the ranks print in-order
*/
for(int i=0; i<nproc; i++) {
    if(rank == i)
        printf(" This is rank = %d of nproc = %d on node: %s\n", rank, nproc, hname);
}</pre>
```

Ex02

- ex02.c is similar to ex01.c
- A for-loop is included over the print statement:

```
/*
  * TODO: add an MPI_Barrier() to ensure the ranks print in-order
  */
for(int i=0; i<nproc; i++) {
    if(rank == i)
        printf(" This is rank = %d of nproc = %d on node: %s\n", rank, nproc, hname);
}</pre>
```

• Study the code and carefully place an MPI_Barrier() so that the print statements will be executed in rank ordered

- ex02.c is similar to ex01.c
- A for-loop is included over the print statement:

```
/*
* TODO: add an MPI_Barrier() to ensure the ranks print in-order
*/
for(int i=0; i<nproc; i++) {
    if(rank == i)
        printf(" This is rank = %d of nproc = %d on node: %s\n", rank, nproc, hname);
}</pre>
```

- Study the code and carefully place an MPI_Barrier() so that the print statements will be executed in rank ordered
- As before, when done:
 - o use make to compile and
 - o sbatch sub-02.sh to submit the prepared job script

Ex02

• Inspect the file ex02-output.txt:

```
[user@front01 ex02]$ cat ex02-output.txt
This is rank = 0 of nproc = 8 on node: cn01
This is rank = 1 of nproc = 8 on node: cn01
This is rank = 2 of nproc = 8 on node: cn01
This is rank = 3 of nproc = 8 on node: cn01
This is rank = 4 of nproc = 8 on node: cn02
This is rank = 5 of nproc = 8 on node: cn02
This is rank = 6 of nproc = 8 on node: cn02
This is rank = 7 of nproc = 8 on node: cn02
[user@front01 ex02]$
```

Ex02

• Inspect the file ex02-output.txt:

```
[user@front01 ex02]$ cat ex02-output.txt
This is rank = 0 of nproc = 8 on node: cn01
This is rank = 1 of nproc = 8 on node: cn01
This is rank = 2 of nproc = 8 on node: cn01
This is rank = 3 of nproc = 8 on node: cn01
This is rank = 4 of nproc = 8 on node: cn02
This is rank = 5 of nproc = 8 on node: cn02
This is rank = 6 of nproc = 8 on node: cn02
This is rank = 7 of nproc = 8 on node: cn02
[user@front01 ex02]$
```

• The print statements should appear in rank order

Ex03

- This exercise demonstrates MPI_Bcast()
- A file data.txt is included:

[user@front01 ex03]\$ cat data.txt 3.14159265359
[user@front01 ex03]\$

Ex03

- This exercise demonstrates MPI_Bcast()
- A file data.txt is included:

```
[user@front01 ex03]$ cat data.txt 3.14159265359
[user@front01 ex03]$
```

• In ex03.c, the root process (process with rank == 0) calls the readline() function to read the single line from the file

- This exercise demonstrates MPI Bcast()
- A file data.txt is included:

```
[user@front01 ex03]$ cat data.txt
3.14159265359
[user@front01 ex03]$
```

- In ex03.c, the root process (process with rank == 0) calls the readline() function to read the single line from the file
- Your task is to use a MPI_Bcast() to broadcast the variable read to all processes:

```
* TODO: add an MPI_Bcast() with the appropriate arguments to
* broadcast variable `val' from the root process to all processes
*/
MPI_Bcast(/* TODO */);
```

Ex03

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

```
[user@front01 ex03]$ cat ex03-output.txt

This is rank = 7 of nproc = 8 on node: cn02 | Got from root var = 3.141593

This is rank = 6 of nproc = 8 on node: cn02 | Got from root var = 3.141593

This is rank = 5 of nproc = 8 on node: cn02 | Got from root var = 3.141593

This is rank = 4 of nproc = 8 on node: cn02 | Got from root var = 3.141593

This is rank = 3 of nproc = 8 on node: cn01 | Got from root var = 3.141593

This is rank = 0 of nproc = 8 on node: cn01 | Got from root var = 3.141593

This is rank = 2 of nproc = 8 on node: cn01 | Got from root var = 3.141593

This is rank = 1 of nproc = 8 on node: cn01 | Got from root var = 3.141593

[user@front01 ex03]$
```

With the order being undetermined also in this case

Ex04

- This exercise demonstrates the scatter operation
- The file data.txt now includes eight lines:

[user@front01 ex04]\$ cat data.txt
0.42816572487
0.57721566490
0.66274341935
0.69314718056
1.41421356237
1.61803398875
2.71828182846
3.14159265359
[user@front01 ex04]\$

Ex04

- This exercise demonstrates the scatter operation
- The file data.txt now includes eight lines:

```
[user@front01 ex04]$ cat data.txt
0.42816572487
0.57721566490
0.66274341935
0.69314718056
1.41421356237
1.61803398875
2.71828182846
3.14159265359
[user@front01 ex04]$
```

• The root process reads the eight lines into the eight-element double precision array vals[] using the function readlines()

```
/*
 * root process: read `n' lines of "data.txt" into array `vars[]'
 */
int nelems = 8;
double vars[nelems];
if(rank == 0) {
    char fname[] = "data.txt";
    readlines(nelems, vars, fname);
}
```

Ex04

• Your task is to scatter the array vals[] so that each of the eight processes receives one element of the array into variable var:

```
double var;
/*
 * TODO: use an MPI_Scatter() to distribute the elements of `vars[]'
 * to the processes, one element for each process. Assume the number
 * of processes is the same as the number of elements.
 */
MPI_Scatter(/* TODO */);
```

Ex04

• Your task is to scatter the array vals[] so that each of the eight processes receives one element of the array into variable var:

```
double var;
/*
 * TODO: use an MPI_Scatter() to distribute the elements of `vars[]'
 * to the processes, one element for each process. Assume the number
 * of processes is the same as the number of elements.
 */
MPI_Scatter(/* TODO */);
```

• Once done, compile (make) and submit the job script (sbatch sub-04.sh)

Ex04

• Your task is to scatter the array vals[] so that each of the eight processes receives one element of the array into variable var:

```
double var;
/*
 * TODO: use an MPI_Scatter() to distribute the elements of `vars[]'
 * to the processes, one element for each process. Assume the number
 * of processes is the same as the number of elements.
 */
MPI_Scatter(/* TODO */);
```

- Once done, compile (make) and submit the job script (sbatch sub-04.sh)
- If done correctly, you should see the following in ex04-output.txt:

```
[user@front01 ex04]$ cat ex04-output.txt

This is rank = 2 of nproc = 8 on node: cn01 | Got from root var = 0.662743

This is rank = 3 of nproc = 8 on node: cn01 | Got from root var = 0.693147

This is rank = 1 of nproc = 8 on node: cn01 | Got from root var = 0.577216

This is rank = 4 of nproc = 8 on node: cn02 | Got from root var = 1.414214

This is rank = 5 of nproc = 8 on node: cn02 | Got from root var = 1.618034

This is rank = 6 of nproc = 8 on node: cn02 | Got from root var = 2.718282

This is rank = 0 of nproc = 8 on node: cn01 | Got from root var = 0.428166

This is rank = 7 of nproc = 8 on node: cn02 | Got from root var = 3.141593

[user@front01 ex04]$
```

Ex04

 Your task is to scatter the array vals[] so that each of the eight processes receives one element of the array into variable var:

```
double var;
/*
 * TODO: use an MPI_Scatter() to distribute the elements of `vars[]'
 * to the processes, one element for each process. Assume the number
 * of processes is the same as the number of elements.
 */
MPI_Scatter(/* TODO */);
```

- Once done, compile (make) and submit the job script (sbatch sub-04.sh)
- If done correctly, you should see the following in ex04-output.txt:

```
[user@front01 ex04]$ cat ex04-output.txt
This is rank = 2 of nproc = 8 on node: cn01 | Got from root var = 0.662743
This is rank = 3 of nproc = 8 on node: cn01 | Got from root var = 0.693147
This is rank = 1 of nproc = 8 on node: cn01 | Got from root var = 0.577216
This is rank = 4 of nproc = 8 on node: cn02 | Got from root var = 1.414214
This is rank = 5 of nproc = 8 on node: cn02 | Got from root var = 1.618034
This is rank = 6 of nproc = 8 on node: cn02 | Got from root var = 2.718282
This is rank = 0 of nproc = 8 on node: cn01 | Got from root var = 0.428166
This is rank = 7 of nproc = 8 on node: cn02 | Got from root var = 3.141593
[user@front01 ex04]$
```

• Pro tip: you can sort the output by piping through sort, i.e. cat ex04-output.txt | sort

- This exercise demonstrates the gather operation
- The exercise starts like ex04:
 - The root process reads the eight values from data.txt and stores them in vars[]

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 - The root process reads the eight values from data.txt and stores them in vars[]
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 - The elements of vars[] to be scattered, one element to each of eight processes (same as ex04)

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- The exercise starts like ex04:
 - The root process reads the eight values from data.txt and stores them in vars[]
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 - The elements of vars[] to be scattered, one element to each of eight processes (same as ex04)
 - o Each process to divide its element, stored in var, by two

- This exercise demonstrates the gather operation
- The exercise starts like ex04:
 - The root process reads the eight values from data.txt and stores them in vars[]
- We would like:
 - The elements of vars[] to be scattered, one element to each of eight processes (same as ex04)
 - o Each process to divide its element, stored in var, by two
 - The process' var variables to be gathered back into vars[] of the root process

- This exercise demonstrates the gather operation
- The exercise starts like ex04:
 - The root process reads the eight values from data.txt and stores them in vars[]
- We would like:
 - The elements of vars[] to be scattered, one element to each of eight processes (same as ex04)
 - Each process to divide its element, stored in var, by two
 - The process' var variables to be gathered back into vars[] of the root process

```
/* TODO: use an MPI_Scatter() to distribute the elements of `vars[]'

* to the processes, one element for each process. Assume the number

* of processes is the same as the number of elements. Same as in

* exercise ex04.

*/

MPI_Scatter(/* TODO */);

/* Divide by two on each rank */

var = var*0.5;

/* TODO: use an MPI_Gather() to collect `var' from each rank to the

* array `vars[]' on the root process

*/

MPI_Gather(/* TODO */);
```

Ex05

• At the end, the root process prints all elements of vars[]

```
/*
 * root process: print the elements of `vars[]' obtained via the
 * `MPI_Gather()'
 */
if(rank == 0)
    for(int i=0; i<nelems; i++)
        printf(" vars[%d] = %lf\n", i, vars[i]);</pre>
```

Ex05

• At the end, the root process prints all elements of vars[]

```
/*
 * root process: print the elements of `vars[]' obtained via the
 * `MPI_Gather()'
 */
if(rank == 0)
    for(int i=0; i<nelems; i++)
        printf(" vars[%d] = %lf\n", i, vars[i]);</pre>
```

• Inspect the output ex05-output.txt and ensure the result is correct:

```
[user@front01 ex05]$ cat ex05-output.txt
vars[0] = 0.214083
vars[1] = 0.288608
vars[2] = 0.331372
vars[3] = 0.346574
vars[4] = 0.707107
vars[5] = 0.809017
vars[6] = 1.359141
vars[7] = 1.570796
[user@front01 ex05]$
```

- This exercise demonstrates the reduction operation
- data.txt is now a file with 2520 random numbers, one per line (nelems = 2520)

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- We would like:

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- data.txt is now a file with 2520 random numbers, one per line (nelems = 2520)
- We would like:
 - The root process to read all elements into an array vars[]

- This exercise demonstrates the reduction operation
- data.txt is now a file with 2520 random numbers, one per line (nelems = 2520)
- We would like:
 - The root process to read all elements into an array vars[]
 - The elements to be scattered to all processes
 Each process should receive nelems_loc = nelems / nproc elements

- This exercise demonstrates the reduction operation
- data.txt is now a file with 2520 random numbers, one per line (nelems = 2520)
- We would like:
 - The root process to read all elements into an array vars[]
 - The elements to be scattered to all processes
 Each process should receive nelems_loc = nelems / nproc elements
 - Each process to sum its local elements, storing the result into sum_loc

- This exercise demonstrates the reduction operation
- data.txt is now a file with 2520 random numbers, one per line (nelems = 2520)
- We would like:
 - The root process to read all elements into an array vars[]
 - The elements to be scattered to all processes
 Each process should receive nelems_loc = nelems / nproc elements
 - Each process to sum its local elements, storing the result into sum_loc
 - o To use a reduction operation to obtain the grand total over all 2520 elements

- This exercise demonstrates the reduction operation
- data.txt is now a file with 2520 random numbers, one per line (nelems = 2520)
- We would like:
 - The root process to read all elements into an array vars[]
 - The elements to be scattered to all processes
 Each process should receive nelems_loc = nelems / nproc 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 2520 elements
- Note that in ex06.c we explicitly check that the number of processes divides the number of elements in data.txt:

```
/*
    * Abort if the number of processes does not divide `nelems' exactly
    */
int nelems = 2520;
if(nelems % nproc != 0) {
    fprintf(stderr, " nelems = %d not divisible by nproc = %d\n", nelems, nproc);
    MPI_Abort(MPI_COMM_WORLD, 1);
}
```

Ex06

• Your TODOs are to complete the scatter and reduction operations:

```
/*
   * TODO: use an MPI_Scatter() to distribute the elements of `vars[]'
   * to each process' `vars_loc[]' array
   */
MPI_Scatter(/* TODO */);

/*
   * `sum_loc' holds the sum over each process' local elements
   */
double sum_loc = 0;
for(int i=0; i<nelems_loc; i++)
sum_loc += vars_loc[i];

/*
   * TODO: use an MPI_Reduce() to sum `sum_loc' over all processes and
   * store in `sum' of the root process
   */
double sum;
MPI_Reduce(/* TODO */);
```

Ex06

• The root process prints the result at the end. If correct, you should see:

[user@front01 ex06]\$ cat ex06-output.txt Used 8 processes, sum = 1266.960662 [user@front01 ex06]\$

Ex06

• The root process prints the result at the end. If correct, you should see:

[user@front01 ex06]\$ cat ex06-output.txt Used 8 processes, sum = 1266.960662 [user@front01 ex06]\$

• Note that ex06.c allows running with any number of processes which divide 2520 exactly

Ex06

• The root process prints the result at the end. If correct, you should see:

[user@front01 ex06]\$ cat ex06-output.txt Used 8 processes, sum = 1266.960662 [user@front01 ex06]\$

- Note that ex06.c allows running with any number of processes which divide 2520 exactly
- Try, for example, modifying sub-06.sh to use 40 processes (20 per node)

Ex06

• The root process prints the result at the end. If correct, you should see:

```
[user@front01 ex06]$ cat ex06-output.txt
Used 8 processes, sum = 1266.960662
[user@front01 ex06]$
```

- Note that ex06.c allows running with any number of processes which divide 2520 exactly
- Try, for example, modifying sub-06.sh to use 40 processes (20 per node)
- You should see an identical sum:

```
[user@front01 ex06]$ cat ex06-output.txt
Used 40 processes, sum = 1266.960662
[user@front01 ex06]$
```

- This exercise demonstrates MPI_Send() and MPI_Recv()
- data.txt is the same as in ex04, with eight elements:

```
[user@front01 ex07]$ cat data.txt
0.42816572487
0.57721566490
0.66274341935
0.69314718056
1.41421356237
1.61803398875
2.71828182846
3.14159265359
[user@front01 ex07]$
```

Ex07

- This exercise demonstrates MPI_Send() and MPI_Recv()
- data.txt is the same as in ex04, with eight elements:

```
[user@front01 ex07]$ cat data.txt
0.42816572487
0.57721566490
0.66274341935
0.69314718056
1.41421356237
1.61803398875
2.71828182846
3.14159265359
[user@front01 ex07]$
```

• All elements are read by the root process into array vars[]

- This exercise demonstrates MPI_Send() and MPI_Recv()
- data.txt is the same as in ex04, with eight elements:

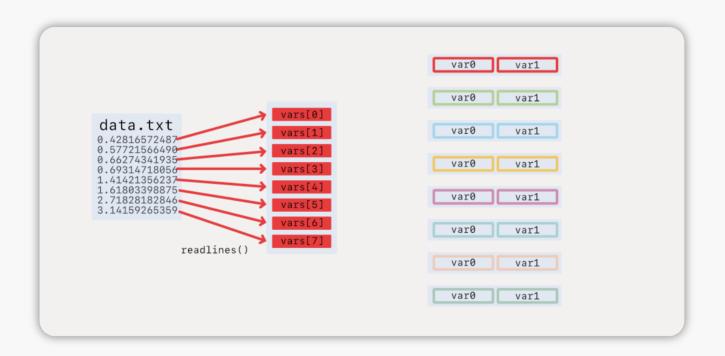
```
[user@front01 ex07]$ cat data.txt
0.42816572487
0.57721566490
0.66274341935
0.69314718056
1.41421356237
1.61803398875
2.71828182846
3.14159265359
[user@front01 ex07]$
```

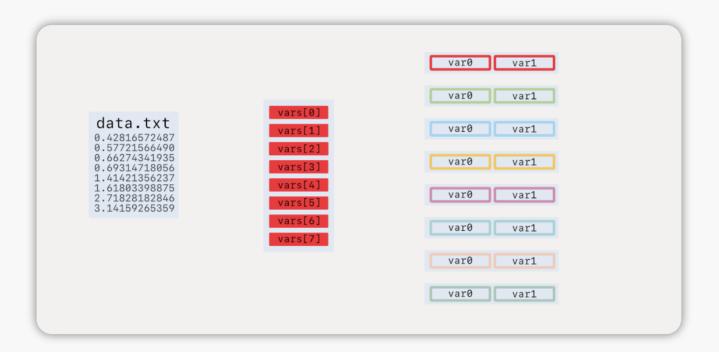
- All elements are read by the root process into array vars[]
- The elements are then scattered, one to each process, and stored in variable var0

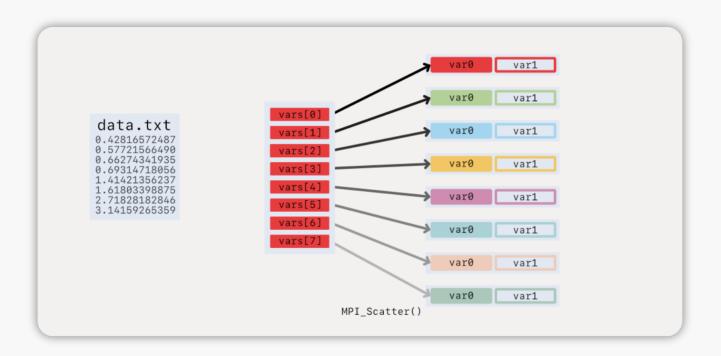
- This exercise demonstrates MPI_Send() and MPI_Recv()
- data.txt is the same as in ex04, with eight elements:

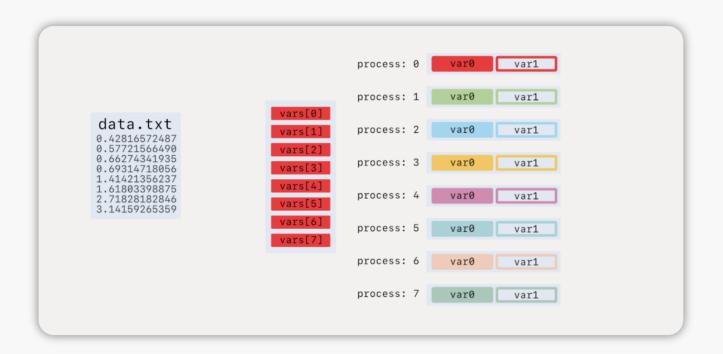
```
[user@front01 ex07]$ cat data.txt
0.42816572487
0.57721566490
0.66274341935
0.69314718056
1.41421356237
1.61803398875
2.71828182846
3.14159265359
[user@front01 ex07]$
```

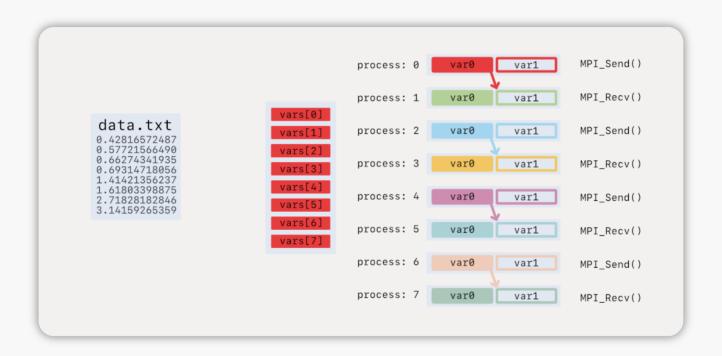
- All elements are read by the root process into array vars[]
- The elements are then scattered, one to each process, and stored in variable var0
- Using MPI_Send() and MPI_Recv(), We would like that:
 - All processes with even ranks store in variable var1 the value of var0 corresponding to their next odd rank
 - All processes with odd ranks store in variable var1 the value of var0 corresponding to their previous even rank

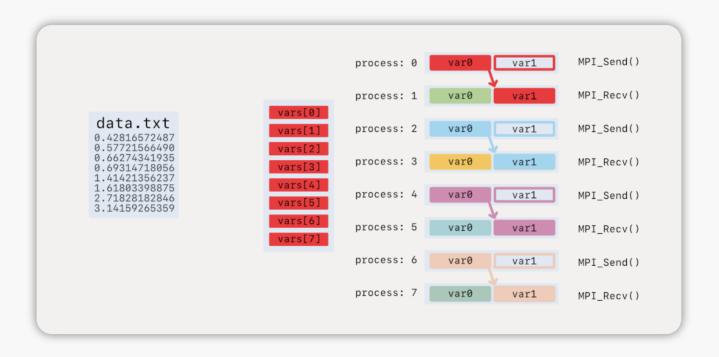


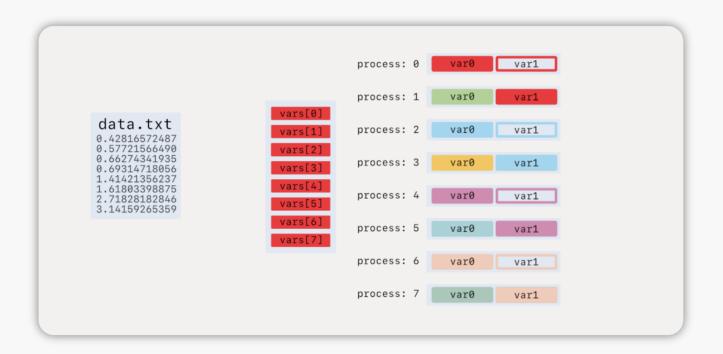


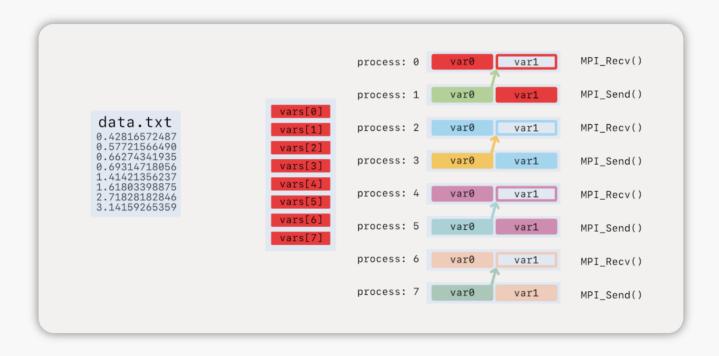


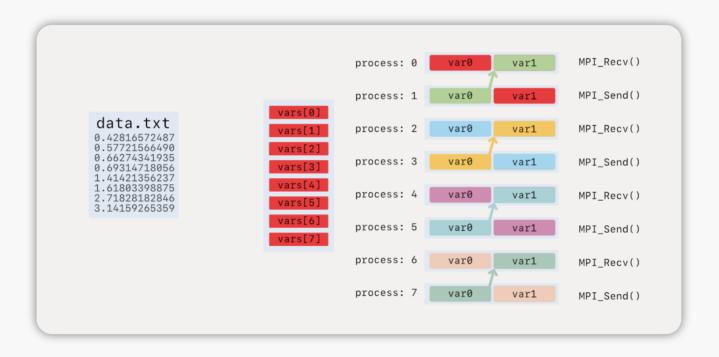


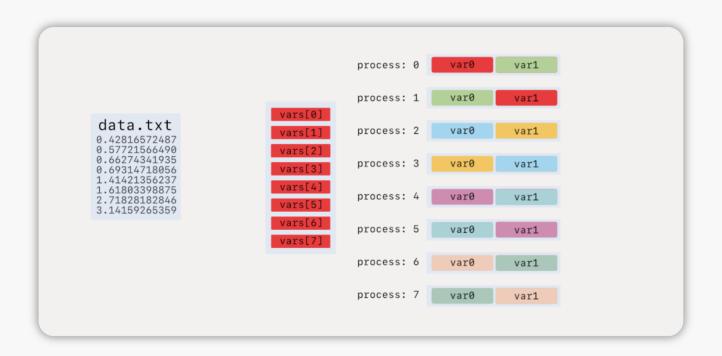












Ex07

• The TODOs are for completing the arguments of the MPI_Recv()s and MPI_Send()s

```
double var1;
* TODO: Use `MPI_Send()' and `MPI_Recv()' appropriately, so that
* `var0' of each even rank is copied into `var1' of the next odd
* rank
*/
if(rank \% 2 == 0) {
  MPI_Send(/* TODO */);
} else {
  MPI_Recv(/* TODO */);
* TODO: Use `MPI_Send()' and `MPI_Recv()' appropriately, so that
* `var0' of each odd rank is copied into `var1' of the previous
* even rank
*/
if(rank \% 2 == 1) {
  MPI_Send(/* TODO */);
} else {
  MPI_Recv(/* TODO */);
```

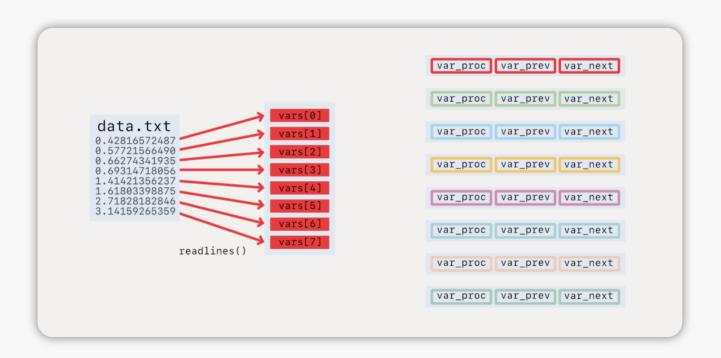
Ex07

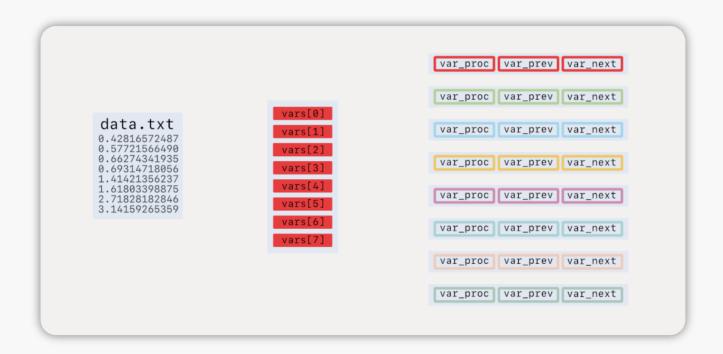
• The correct output should look like this:

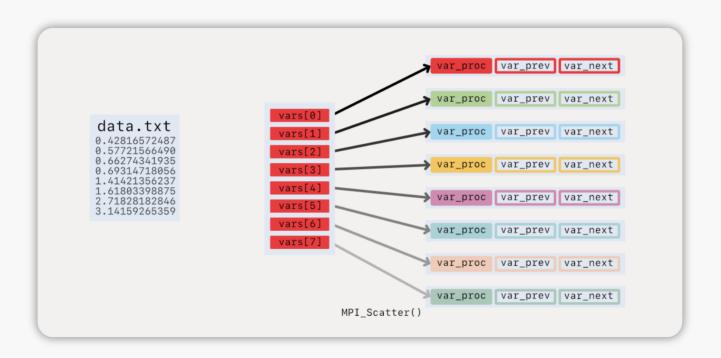
- This exercise demonstrates the use of MPI_Sendrecv()
- The same data.txt with eight elements is used as before
- The elements are read by the root process and scattered to all processes as before

- This exercise demonstrates the use of MPI_Sendrecv()
- The same data.txt with eight elements is used as before
- The elements are read by the root process and scattered to all processes as before
- Now each process has three variables:
 - o var_proc contains the element received from the scatter
 - var_next is to contain var_proc of the next process
 - var_prev is to contain var_proc of the previous process

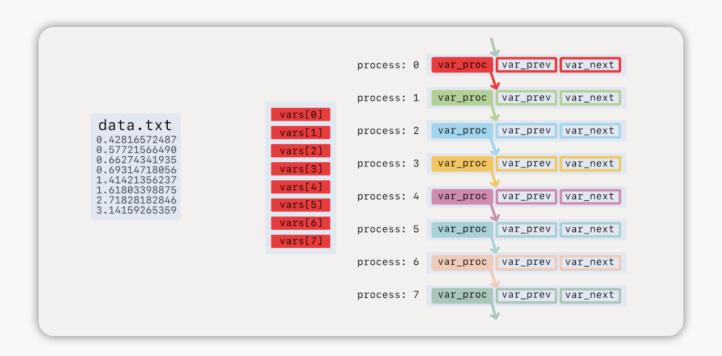
- This exercise demonstrates the use of MPI_Sendrecv()
- The same data.txt with eight elements is used as before
- The elements are read by the root process and scattered to all processes as before
- Now each process has three variables:
 - o var_proc contains the element received from the scatter
 - var_next is to contain var_proc of the next process
 - o var_prev is to contain var_proc of the previous process
- Use two MPI Sendrecv() to achieve this

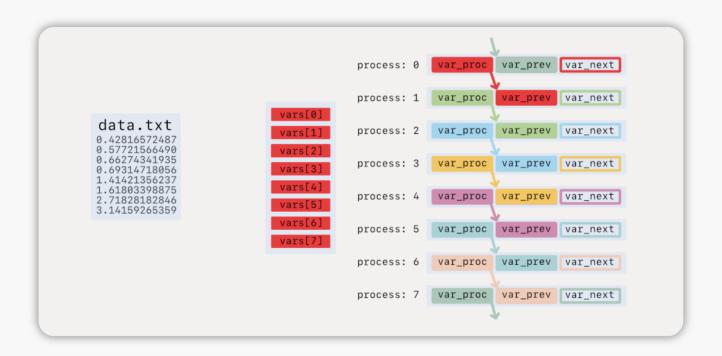




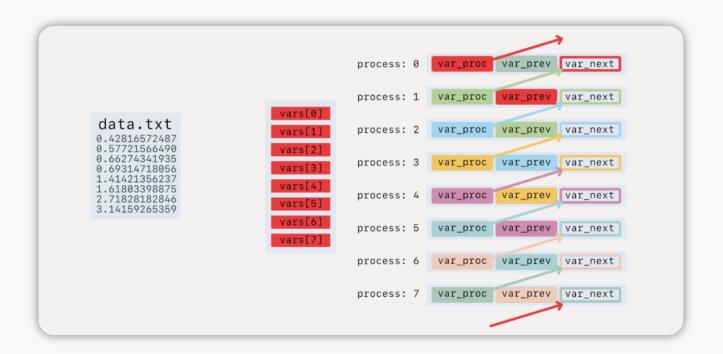


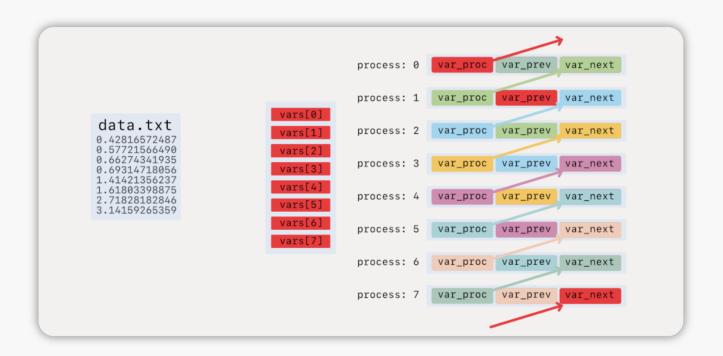
```
var_proc var_prev var_next
                                        process: 0
                                                     var_proc var_prev var_next
                                        process: 1
                            vars[0]
data.txt
                                                    var_proc var_prev var_next
                            vars[1]
                                        process: 2
0.42816572487
0.57721566490
                            vars[2]
0.66274341935
                                                     var_proc var_prev var_next
                                        process: 3
                            vars[3]
0.69314718056
1.41421356237
                            vars[4]
1.61803398875
                                                    var_proc var_prev var_next
                                        process: 4
2.71828182846
                            vars[5]
3.14159265359
                            vars[6]
                                                     var_proc var_prev var_next
                                        process: 5
                            vars[7]
                                                     var_proc var_prev var_next
                                        process: 6
                                        process: 7
                                                    var_proc var_prev var_next
```





```
var_prev var_next
                                         process: 0
                                                     var_proc
                                                               var_prev    var_next
                                         process: 1
                                                     var_proc
                            vars[0]
data.txt
                                                     var_proc var_prev var_next
                            vars[1]
                                        process: 2
0.42816572487
0.57721566490
                            vars[2]
0.66274341935
                                                     var_proc var_prev var_next
                                        process: 3
                            vars[3]
0.69314718056
1.41421356237
                            vars[4]
1.61803398875
                                                               var_prev var_next
                                                     var_proc
                                        process: 4
2.71828182846
                            vars[5]
3.14159265359
                            vars[6]
                                                               var_prev
                                         process: 5
                                                     var_proc
                                                                         var_next
                            vars[7]
                                                               var_prev var_next
                                                     var_proc
                                         process: 6
                                         process: 7
                                                     var_proc var_prev var_next
```





```
process: 0
                                                     var_proc
                                                              var_prev
                                                                        var_next
                                                                        var_next
                                                     var_proc
                                                               var_prev
                                        process: 1
                            vars[0]
data.txt
                                                    var_proc var_prev var_next
                            vars[1]
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0.42816572487
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                                        process: 3
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                                                              var_prev var_next
                                                     var_proc
                                        process: 4
2.71828182846
                            vars[5]
3.14159265359
                            vars[6]
                                                               var_prev
                                        process: 5
                                                     var_proc
                                                                        var_next
                            vars[7]
                                                              var_prev var_next
                                                     var_proc
                                        process: 6
                                        process: 7
                                                    var_proc var_prev
                                                                        var_next
```

Ex08

• The TODOs are for completing the arguments of the MPI_Sendrecv()s

```
double var_next, var_prev;
/*
* TODO: Use `MPI_Sendrecv()' appropriately, so that `var_proc' of
* each rank is copied into `var_prev' of the next rank. Assume
* periodicity of ranks, i.e. if the sender is the last process
* ( rank == nproc - 1') then send to the first process ( rank ==
* 0')
*/
MPI_Sendrecv(/* TODO */);
/*
* TODO: Use `MPI_Sendrecv()' appropriately, so that `var_proc' of
* each rank is copied into `var_next' of the previous rank. Assume
* periodicity of ranks, i.e. if the sender is the first process
* ( rank == 0') then send to the last process ( rank == nproc - 1')
*/
MPI_Sendrecv(/* TODO */);
```

Ex08

• The correct output should look like this:

```
[user@front01 ex08]$ cat ex08-output.txt | sort

This is rank = 0 of nproc = 8 on node: cn01 | var_proc = 0.428166 | var_prev = 3.141593 | var_next = 0.577216

This is rank = 1 of nproc = 8 on node: cn01 | var_proc = 0.577216 | var_prev = 0.428166 | var_prev = 0.428166 | var_next = 0.662743

This is rank = 2 of nproc = 8 on node: cn01 | var_proc = 0.662743 | var_prev = 0.577216 | var_next = 0.662743 | var_next = 0.693147

This is rank = 3 of nproc = 8 on node: cn02 | var_proc = 0.693147 | var_prev = 0.662743 | var_next = 1.414214 | var_prev = 0.693147 | var_prev = 1.618034 | var_prev = 2.718282 | var_prev = 2
```

Combining OpenMP and MPI

- OpenMP parallelism within node
- MPI parallelism between nodes

Why?

- Better control of granularity
- Easier to parallelize across domains not divisible by number of processes available
- Allows for controlling parallelism in less parallelizable regions (e.g. I/O)

Types of hybrid parallelism

- Only master thread calls MPI
 - No MPI calls within OpenMP parallel regions
 - o May be permitted in an OpenMP Master region
- Any thread calls MPI
 - Serialized
 - If multiple threads call MPI, there are mechanisms to serialize the calls
 - Concurrently
 - MPI thread-safety level permits concurrently calling MPI

Thread awareness in MPI

int MPI_Init_thread(int *argc, char ***argv, int required, int *provided)

- MPI_Init_thread() instead of MPI_Init()
- required is the level of thread-safety required (input)
- provided is the level of thread-safety this implementation of MPI can provide (output)
- One of:
 - MPI_THREAD_SINGLE, no thread-safety assumed. Equivalent to MPI_Init()
 - MPI_THREAD_FUNNELED, it is assumed only one thread will call MPI functions
 - MPI_THREAD_SERIALIZED, multiple threads might call MPI, but serialized
 - MPI_THREAD_MULTIPLE, any thread can call MPI, even concurrently with other threads

- We will cover using *single mode*
 - o Parallel regions can exist in a program
 - o MPI is called outside of the parallel regions

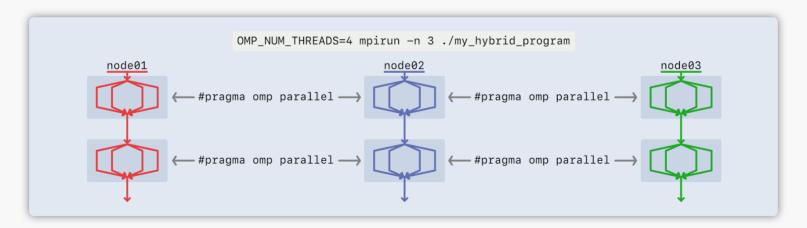
- See ex09
- MPI_Comm_rank() and MPI_Comm_size() are called outside parallel regions
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Dot product using hybrid MPI/OpenMP

- ex10 implements a vector dot-product using MPI and OpenMP
- Investigate the timing as you vary the number of threads per process and total number of processes