Practical hints for the NAISS MPI course

Connecting

COSMOS @ LUNARC

Obtaining Passwords and setting up two factor authentication

Once your COSMOs account has been created, you can set your password in the self service portal. This is described in:

https://lunarc-documentation.readthedocs.io/en/latest/getting_started/login_password/

A step-by-step guide on how to set up the pocket pass authentiacator is provided on:

https://lunarc-documentation.readthedocs.io/en/latest/getting_started/authenticator_howto/

V**ery important** is to perform the step 5, which is often missed

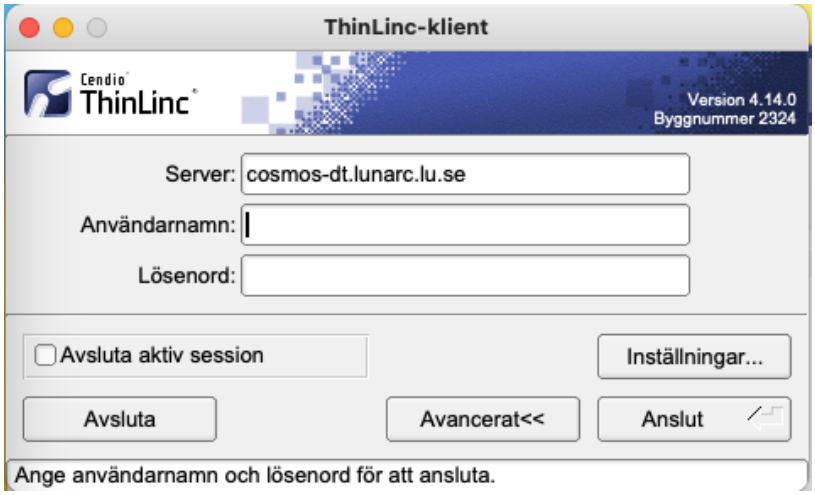
The LUNARC FAQ on login can also be helpful when resolving connection issues:

https://lunarc-documentation.readthedocs.io/en/latest/manual/faq/manual_faq_login/

Connection option 1 (suggested)

Install the Thinlinc client for your OS (https://www.cendio.com/thinlinc/download)

Use the server name: **cosmos-dt.lunarc.lu.se**
and the username/password you got from LUNARC



More detailed information can be found here: https://lunarc-documentation.readthedocs.io/en/latest/getting_started/using_hpc_desktop/

If that step is succesful, you get prompted for an OTP, which is in the pocket pass app on your smart phone.

Connection option 2

Open a terminal (on some windows systems you might need an emulator) on your local system and connect via ssh. Use the server name: **cosmos.lunarc.lu.se**
and the username/password you got from LUNARC:

```
ssh cosmos.lunarc.lu.se -l username
```

If that step is succesful, you get prompted for an OTP, which is in the pocket pass app on your smart phone.

Running and building MPI codes

For the following you should open a terminal window inside the HPC desktop and work at the command line prompt. A number of editors are available on COSMOS to edit code, scripts etc. For beginners **nano** is a good choice. It is easy to use and sufficiently powerful for this course.

Setting up the environment

For the practical parts of the course we are using the GCC compiler suite and the OpenMPI MPI library. To get a modern GCC version of these, we recommend loading the foss/2024a module:

module load foss/2024a

When doing the course in Python, you also need to get access to Python with MPI4PY. In addition to foss/2024a, you need to additionally load the following:

```
module load Python/3.12.3
module load SciPy-bundle/2024.05
module load mpi4py/4.0.1
```

This will provide you with Python 3.12.3, including NumPy, SciPy, MPI4Py.

Getting the templates

We need to obtain the distribution

```
git clone https://github.com/MPI-course-collaboration/MPI-course.git
cd MPI-course/
```

If you need to refresh, e.g. due to updates, please do

```
git pull origin
```

Lecture notes

The repository contains PDFs of the course's lectures. They are located in the directory Lectures of the repository. There is a separate directory for each day of teaching.

Compiling code (not relevant for participants doing Python)

This section applies to Fortran and C/C++ users. When using Python you do not need to compile code.
To compile MPI code it is customary to utilise wrapper scripts. These call the underlying compiler and tell it where to look for MPI headers files and libraries.

```
cd Templates/Day_1/RunningCode/
```

Fortran compilation

With OpenMPI Fortran code is compiled with **mpifort**. Use the compiler options of the underlying Fortran compiler, gfortran in this case:

```
mpifort -O3 -march=native -o mpihello hello_mpi.f90
```

C/C++ code compilation

With OpenMPI, C code is compiled with **mpicc**. Use the compiler options of the underlying Fortran compiler, gfortran in this case:

```
mpicc -O3 -march=native -o mpihello hello_mpi.c
```

For C++ code the wrapper **mpiCC** can be utilised.

Submission script (Relevant for Fortran, C, C++ and Python)

To get performance out of an MPI code, it is crucial to have dedicated hardware. In a cluster environment this requires running on one or more backend nodes using a batch scheduler. Within NAISS we use SLURM.
Sample scripts for the use on COSMOS are provided in the subdirectory named

- LUNARC

Running script

Copy the relevant sample script into the current directory

- C, C++, Fortran
  - **cp LUNARC/run_hello_lunarc.sh run_hello.sh**
- Python
  - **cp LUNARC/run_hello_python_lunarc.sh run_hello_python_lunarc.sh**

and add the **accounting string** (mandatory) and **reservation** name to the script.

```
#SBATCH -A lu2025-7-75
```

To get a faster turnaround, we recommend using the relevant reservation name string for each day:

```
#SBATCH --reservation=mpi-course-1day
##SBATCH --reservation=mpi-course-2day
##SBATCH --reservation=mpi-course-3day
##SBATCH --reservation=mpi-course-4day
```

You may use nano or another editor of your liking. It is best practise to set up the environment inside the script. The task count is set with the line

#SBATCH --tasks-per-node=4

(in the example above, for 4 tasks).

For MPI running the crucial line is the last row of the script. For compiled code, to run an executable named **mpihello** this looks like

mpirun --bind-to core mpihello

For Python scripts, running a Python script named run_hello_python.sh this looks like

mpirun --bind-to core python3 hello_mpi.py

Submit

sbatch run_hello.sh

Monitor job progress with

squeue -u *userid*

If successful you get an output file of the form: **result_mpihello_10597613.out.** The number is the unique job number.

Hello World code

Change directory

cd ../HelloWorld

Copy your submission script(s)

cp ../RunningCode/run_hello*.sh .

Write code in C, Fortran or Python to query the size of a communicator and the rank number

Compile the code in case of C and Fortran

Run the code in the batch system

Point-to-Point communication - calculate Pi

Change into the directory

cd MPI-course/Templates/Day_2/CalculatingPi

Within the directories **C/**, **Fortran/** and **Python/** we provide you with a working serial code. Choose a programming language and copy the relevant code, e.g.:

cp C/pi_square_serial.c pi_square.c
cp Fortran/pi_square_serial.f90 pi_square.f90
cp Python/pi_square_serial.py pi_square.py

Check that you can run the serial code and that it produces correct results. Parallelise the code using MPI.

Steps to be taken for the exercise:

- Initialize MPI
- Query the properties of the MPI ranks (size, and each process's rank)
- Divide up the work among the ranks
- Aggregate partial results
- Finalize the program

Message around a ring

Start in the folder with the material

cd MPI-course/Templates/Day_2/MessageAroundRing

We have template codes for C, Fortran and Python

Fortran

Go into the Fortran folder

cd Fortran

Copy the file: **ringsend.f90** and open the copy. Do not work in the original file.

Base communicator

The code has a subroutine **setup_mpi**, which

- Sets up base communicator **my_world**
- Returns a handle to the base communicator
- Returns the rank in base communicator
- Returns the size of base communicator

Search for "*Implement base communicator here*" and implement the functionality

Neighbours

Each task needs neighbours up- and down-stream. This is with periodic boundaries. The highest ranking task has rank zero as up neighbour, while rank zero has the highest ranking task as down neighbour.
Implement this after the comment "*Implement neighbours here*".

Data exchange

The actual exchange is to be implemented in the subroutine **exchange**. Implement it with either MPI_Ssend or MPI_Issend to make sure it is correct. Once it is correct change for MPI_Send or MPI_Isend.
Implement this after the comment "*Implement data exchange here*"
The data exchange needs to be executed more than once, for the messages to reach back their origin. Implement this in the main program at the comment "*Implement the travel around the ring here*"

Shutdown

The MPI library needs closing down. Implement this in the subroutine **shutdown_mpi**.
Implement this after the comment "*Implement shutdown of MPI library*"

C

Go into the C folder

cd C

Copy the file: **ringsend.c** and open the copy. Do not work in the original file.

Base communicator

The code has a function **setup_mpi**, which

- Sets up base communicator **my_world**
- Returns a handle to the base communicator
- Returns the rank in base communicator
- Returns the size of base communicator

Search for "*Implement base communicator here*" and implement the functionality

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Shutdown

The MPI library needs closing down. Implement this in the function **shutdown_mpi**.
Implement this after the comment "*Implement shutdown of MPI library*"

Python

Go into the Python folder

cd Python

Copy the file: **ringsend.py** and open the copy. Do not work in the original file.

Base communicator

To set up the MPI communication, the code needs to

- Sets up base communicator **my_world**
- Provide a handle to the base communicator
- Query the rank in base communicator
- Query the size of base communicator

Search for "*Implement base communicator here*" and implement the functionality

Neighbours

Each task needs neighbours up- and down-stream. This is with periodic boundaries. The highest ranking task has rank zero as up neighbour, while rank zero has the highest ranking task as down neighbour.
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Implement this after the comment "*Implement data exchange here*"
The data exchange needs to be executed more than once, for the messages to reach back their origin. Implement this in the main program at the comment "*Implement the travel around the ring here*"

Shutdown

This is not required with MPI4PY

Collective communication

Templates for the collective calls are provided in the subdirectory:

MPI-course/Templates/Day_2/Collectives/Examples

and a 2D integration example can be found in:

MPI-course/Templates/Day_2/Collectives/Integration2D

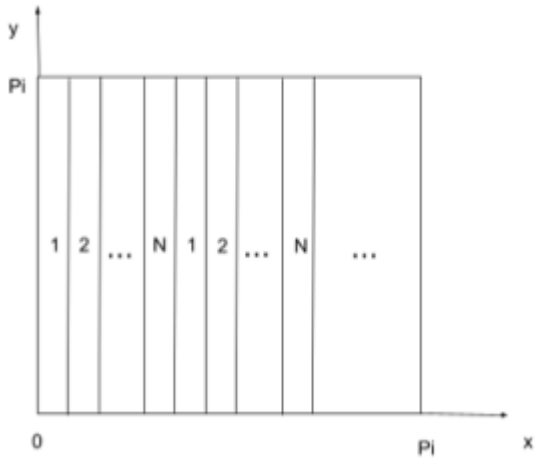
of your cloned repository with the C/Fortran examples. In the Readme.md file, you can find instructions on how to run the templates by using a Makefile.

2D Integration

In this example you will calculate the double integral:

$$\int_0^{\pi}\int_0^{\pi} sin(x + y)dxdy = 0$$

One way to parallelize this calculation is as follows. We start by discretizing the range in both x and y into bins of equal size. This will create a grid of *nxn* bins where *n* is an input parameter provided by the user. We can parallelize the code in one direction only, for instance in the “x” direction. In this case, the first bin in “x” will be computed by process 1, the second bin by process 2, and so on up to the process N. This procedure will be repeated until the last bin n is computed, see the figure below.



Notice that during the computation of each bin in “x” you can perform the regular (not parallel) integration in “y” over the entire range 0<y<π. As a first approximation, we can take the “volume” generated by each grid element (i,j) being equal to $\sin(x_i+y_j)\Delta x\Delta y$, with $\Delta x=/n$, $\Delta y=/n$ and x_i,y_j being the center of the grid element. Each process can accumulate a local value of the integral which can be “reduced” into a total integral value.

This problem is useful for two reasons, first we know the exact value of the integral (0) and second because it includes a double integral, the computation is heavier enough to detect the effects of a parallel implementation.

Splitting communicators

- Write a program that splits the processes of MPI_COMM_WORLD into two sub-groups based on whether the process ranks are even or odd.
- Calculate the average over rank numbers in both the split and the global communicators.
- Rank 0 (in the global as well as the sub-communicators) should print out the results.
- You should implement using only one reduction operation for each average value that is going to be printed out.

Sending derived data types in C and Fortran

Point to point communication

In the template section you find a C and Fortran template with a derived data type named **ri_pair**. The derived data type consists out of a double and a default integer number. The provided template initialises MPI and has the code to transfer a derived data type (Fortran/C) from rank 1 to rank 0.
We recommend copying the template before starting modifying. It is your task to create an MPI_Datatype suitable for transferring the data in a single call.

Advanced exercise: user reduction

If you succeeded in creating the MPI_Datatype, you can implement a user reduction, which

- Sums the double element
- Determines the maximum of the integer element

over all tasks involved in the collective.

Sample solutions

Sample solutions are provided for a code which does the point to point transfer as well as the reduction. The sample solution does not implement a pad and is not suitable to transfer arrays of **ri_pair** elements.

Sending NumPy-objects in Python

In the template section you find a Python template for transferring NumPy objects using MPI collectives. The purpose of the code is to calculate the dot product of two vectors using Scatter and Reduce.

Performance lab

Exercise instructions, are on the slides.