Message Passing with MPI

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Compiling and running MPI code on COSMOS at LUNARC

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Overview

- Connecting to COSMOS using Lunarc HPC desktop
- The Lunarc module environment
- Building MPI executables on Lunarc systems
- Executing MPI jobs on Lunarc systems
- Write your first MPI program

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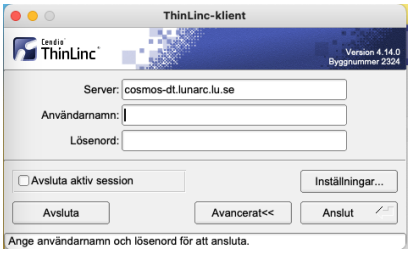
Connecting to Aurora: Lunarc HPC Desktop

- Download and install the client from: http://www.cendio.com/downloads/clients/
- Launch the client
- Enter ”cosmos-dt.lunarc.lu.se" in the server field.
- Enter your user-id & password
- Click [Connect]
- Enter the one time password from your PocketPass app



Detailed descriptions:

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

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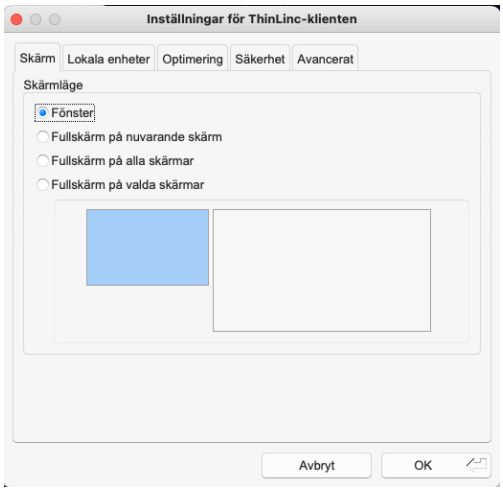
Some Useful Tricks

- Disable “fullscreen” before connecting
- F8 (fn F8 on MBP) during a DT session could be your friend



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Building MPI executables

C, C++ and Fortran

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Building MPI executables

- You use standard compilers (e.g. Intel, GCC, …) to compile the source
- Link against the MPI library to build an MPI executable
- LUNARC/NAISS systems use modules to make these steps convenient

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Quick primer to modules

- Show all available modules
  ```
  module spider
  ```
- Load a recent foss toolchain (GCC 13.3.0, OpenMPI 5.0.3, …)
  ```
  module load foss/2024a
  ```
- We also provide Intel toolchains
- To get rid of all modules
  ```
  module purge
  ```

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Hands on: Compiling MPI with OpenMPI

- Compile and link your code using wrapper scripts

Language	Command
Fortran	`mpifort`
C	`mpicc`
C++	`mpiCC`

- The wrappers will call the compiler and tell is about the MPI-lib
- For a `foss` toolchain they will call `gcc`, `g++` or `gfortran`

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Example: Fortran source with OpenMPI

- Can use options of underlying compiler

- Example:

```
mpifort -O3 -march=native -o program program.f90
```

  - takes the source: `program.f90`
  - calls gfortran compiler
  - creates an executable: `program`
  - uses optimisation level: `O3`
  - optimises for present architecture (instruction set)

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Example: C-source with OpenMPI

- Can use options of underlying compiler
- Example:

```
mpicc -O3 -march=native -o program program.c
```

  - takes the source: `program.f90`
  - calls gcc compiler
  - creates an executable: `program`
  - uses optimisation level: O3
  - optimises for present architecture (instruction set)

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Cmake

- CMake has a utility: **FindMPI**
  - locate the MPI library
  - set up compiler and linker flags
- FindMPI set up the following Cmake variables (v 2.8.12)
  - `MPI_<lang>_FOUND`
  - `MPI_<lang>_COMPILER`
  - `MPI_<lang>_INCLUDE_PATH`
  - `MPI_<lang>_LINK_FLAGS`
  - `MPI_<lang>_COMPILE_FLAGS`
  - `MPI_<lang>_LIBRARIES`
- `<lang> is one of C, CXX and Fortran`

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CMake example for MPI in Fortran

```
project(mpihello)
enable_language(Fortran)
include(FindMPI)
add_executable(mpihello.x mpihello.f90)

target_include_directories(mpihello.x
                   PUBLIC "${MPI_Fortran_INCLUDE_PATH}")
target_link_libraries(mpihello.x "${MPI_Fortran_LIBRARIES}")
set(CMAKE_Fortran_FLAGS
        "${CMAKE_Fortran_FLAGS} ${MPI_Fortran_COMPILE_FLAGS}")
set(CMAKE_EXE_LINKER_FLAGS
        "${CMAKE_EXE_LINKER_FLAGS} ${MPI_Fortran_LINK_FLAGS}")
```

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Running MPI programs

- Make sure the modules (compiler and MPI library) used for building the executable are loaded (shared objects!)
- Message passing jobs need to run inside the batch submission system
- Batch submission systems are vital for running message passing applications
- Expect a similar set-up on any well managed service
- Use the course account for quick turn around of jobs

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Standard MPI job
Run executable: `processor_mpi`

```
#!/bin/bash
#SBATCH -N 2                    # number of nodes
#SBATCH --tasks-per-node=48     # number of processes per node
#SBATCH -t 00:05:00             # job-time – here 5 min
#SBATCH -J data_process         # name of job
#SBATCH -o process_mpi_%j.out   # output file
#SBATCH -e process_mpi_%j.err   # error messages
#SBATCH -A lu2025-7-75          # only for the course
#SBATCH --reservation=mpi-course-1day # only for the course – change for other course days

cat $0
module purge
module load foss/2024a
mpirun --bind-to core ./processor_mpi       #run the program
```

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Running MPI4PY scripts

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We need a few extra modules

- Load a recent foss toolchain (GCC 13.3.0, OpenMPI 5.0.3, …)

```
module load foss/2024a
```

- We need Python, NumPy, SciPy, MPI4PY

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

- To get rid of all modules

```
module purge
```

- Required in jobscript

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Standard MPI4PY job
Run executable: `processor_mpi.py`

```
#!/bin/bash
#SBATCH -N 2                    # number of nodes
#SBATCH --tasks-per-node=48     # number of processes per node
#SBATCH -t 00:05:00             # job-time – here 5 min
#SBATCH -J data_process         # name of job
#SBATCH -o process_mpi_%j.out   # output file
#SBATCH -e process_mpi_%j.err   # error messages
#SBATCH -A lu2025-7-75          # only for the course
#SBATCH --reservation=mpi-course-1day # only for the course – update as needed

cat $0
module purge
module load foss/2024a
module load Python/3.12.3 SciPy-bundle/2024.05 mpi4py/4.0.1
mpirun --bind-to core python3 ./processor_mpi        #run the python script
```

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Interacting with SLURM

Submission, queue monitoring and modification

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Submission with `sbatch`

- Use sbatch to submit your job script to the job-queue
- Example:

```
[fred@cosmos Timetest]$ sbatch runjob.sh
Submitted batch job 7197
```

- Submit script "`runjob.sh`"
- Successful submission returns a job-id number

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Monitoring the queue with `squeue`

- Use **squeue** to monitor the job queue

```
JOBID  PARTITION    NAME   USER  ST   TIME  NODES NODELIST(REASON)
  7303   lu48   hybrid_n   fred  PD   0:00     32 (Priority)
  7302   lu48   hybrid_n   fred  PD   0:00     32 (Priority)
  7301   lu48   hybrid_n   fred  PD   0:00     32 (Resources)
  7304   lu48   preproce   karl  PD   0:00      6 (Priority)
  7300   lu48   hybrid_n   fred   R   0:24     32 cn[001-032]
  7305   lu48   preproce   karl   R   0:37      6 cn[081-086]
  7306   lu48   hybrid_n   fred   R   0:37      6 cn[081-086]
  7307   lu48   testsimu   sven   R   0:07      1 cn081
```

- Typically lots of output – use options of `squeue` to filter

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Options of `squeue`

- Showing jobs for a specific user

```
squeue -u fred
```

will show the jobs of user "`fred`" only

- Option `--start` gives the estimated job start time
  - This can shift in either direction

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Deleting jobs with `scancel`

- You can cancel a queued or running job
- Determine job-id, e.g. with `squeue`
- Use scancel

```
scancel 7103
```

  - terminates job 7103, if running
  - removes from the queue

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Exercise

- See the section “Running and building MPI codes” in the practicalities document
- Make sure you can
  - Connect to COSMOS
  - Compile C and/or Fortran code
  - Interact with SLURM
  - Run MPI code (C, Fortran and/or Python)

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