Uni.lu HPC School 2018

PS5: Parallel computations with OpenMP/MPI

Uni.lu High Performance Computing (HPC) Team

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Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: http://hpc.uni.lu/hpc-school/

PS5 tutorial sources: ulhpc-tutorials.rtfd.io/en/latest/parallel/basics/

Summary

Main Objectives of this Session

- See how to run **threaded parallel OpenMP** programs
- See how to **use the MPI suits** available on the UL HPC platform:
  - ↪ Intel MPI and the Intel MKL
  - ↪ OpenMPI
  - ↪ MVAPICH2
- **Build** and **run** OpenMP and/or MPI code
  - ↪ interactive and passive (through **launcher**) jobs

- **Test cases** on reference parallel and distributed **benchmarks**:
  - ↪ OSU micro-benchmarks:
    - ✓ measure the performances of various MPI operations
  - ↪ High-Performance Linpack (HPL)
  - ↪ Hybrid High Performance Conjugate Gradients (HPCG)

Summary

OpenMP

- OpenMP: Open Multi-Processing
  - ↪ popular parallel programming model for multi-threaded applications.
  - ↪ API for **multi-platform shared memory multiprocessing**
    - ✓ in C, C++, and Fortran
    - ✓ on most platforms, instruction set architectures and OS.
  - ↪ Parallelism accomplished **exclusively** through the use of threads.
    - ✓ **Thread**: smallest unit of processing that can be scheduled by an OS
  - ↪ **#threads ≃ number of machine processors/cores**.
    - ✓ `OMP_NUM_THREADS` (if present): **initial max** number of threads;

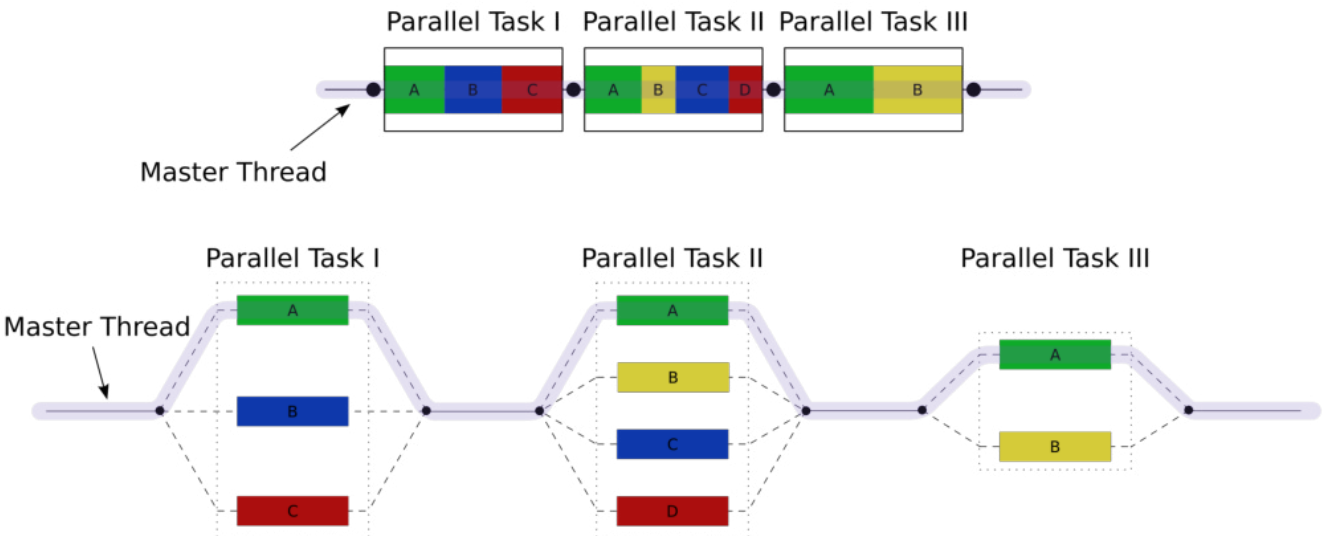
OpenMP

https://www.openmp.org/

- Reference website
- **Latest version: 5.0** (Nov 2018) – specifications

OpenMP Programming Model

- Explicit (not automatic) programming model
  - ↪ may mean taking a serial program & insert compiler directives. . . .
- **Fork-Join** model of parallel execution
  - ↪ **FORK**: **master** thread creates a **team** of parallel threads.
  - ↪ **JOIN**: team threads complete statements in parallel regions
    - ✓ then they synchronize & terminate, leaving only the master thread.



OpenMP on UL HPC platform

- Rely on Environment Modules **once** on a computing node
- Comes part of the `intel` or the `foss` toolchains modules

Toolchain	Compilation command
`toolchain/intel`	`icc -qopenmp [...]`
`toolchain/foss`	`gcc -fopenmp [...]`

Reservation

- You will probably want to compile/test within an **interactive job**
  - ↪ **Ex**: 4 threads (core) on 1 node

```
# SLURM -- Iris cluster
(access)$> srun -p interactive --ntasks-per-node=1 -c 4 --pty bash

# OAR --  gaia, chaos cluster
(access)$> oarsub -I -l nodes=1/core=4,walltime=4
```

OpenMP with OAR

- Reservation has to match the required number of OpenMP threads:
  ↪ **Ex**: `oarsub -l nodes=1/core=4[...]`

```
#!/bin/bash -l
#OAR -l nodes=1/core=4,walltime=1

export OMP_NUM_THREADS=$(cat $OAR_NODEFILE| wc -l)

# Use the RESIF build modules of the UL HPC platform
if [ -f  /etc/profile ]; then
   .  /etc/profile
fi
# Load the {intel | foss} toolchain and whatever module(s) you need
module purge
module load toolchain/intel # or toolchain/foss

path/to/your/openmp_program
```

OpenMP with Slurm

sbatch/srun option	Description
`--ntasks-per-node=1`	**single** task per node
`-c <T>`	number of OpenMP threads

```
#!/bin/bash -l
#SBATCH --ntasks-per-node=1     # more explicit than '-n 1'
#SBATCH -c 28       # number of CPU cores / OpenMP threads per task
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch
if [ -f  /etc/profile ]; then
   .  /etc/profile
fi
# Load the {intel | foss} toolchain and whatever module(s) you need
module purge
module load toolchain/intel # or toolchain/foss
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
srun /path/to/your/openmp_program
```

Hands-on 1: Parallel OpenMP jobs

Your Turn!

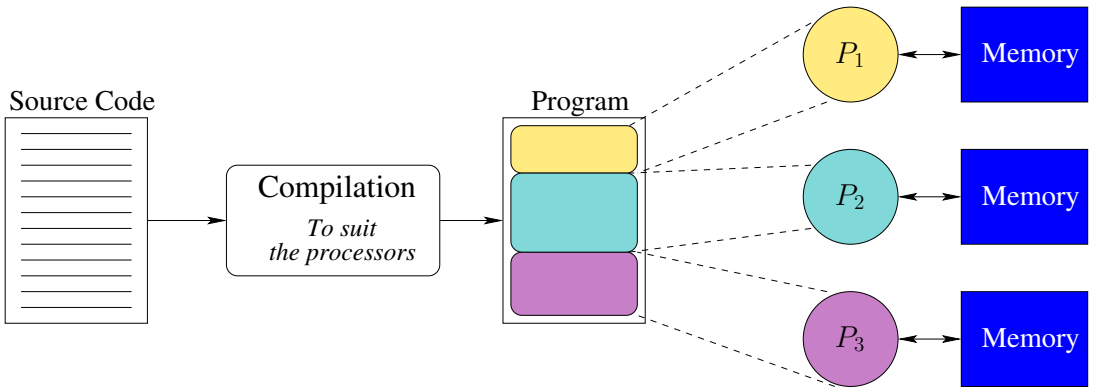
Hands-on 1

ulhpc-tutorials.rtfd.io/en/latest/parallel/basics/#parallel-openmp-jobs

- **Reserve** an **interactive** job to launch 4 OpenMP threads
- Check and **compile** `src/hello_openmp.c`
  - ↪ against both toolchains `bin/[intel_]hello_openmp`
- **execute** the generated binaries
  - ↪ set `$OMP_NUM_THREADS`
- prepare a **launcher script** `runs/launcher.OpenMP.sh`
- repeat on a more serious program `src/matrix_mult_openmp.c`
  - ↪ `bin/[intel_]matrix_mult_openmp`
- (eventually) OpenMP DataRaceBench suite

Summary

SPMD Programming model

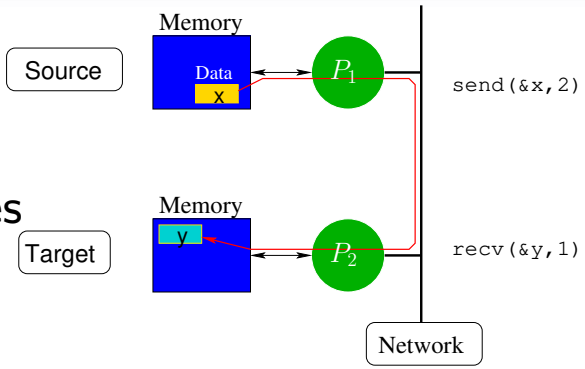


- SPMD: **Simple Program, Multiple Data**
  - ↪ same programs for each processors
    - ✓ executed at independent points
  - ↪ processes identified by a rank
    - ✓ each process knows the piece of code he works on
    - ✓ common in master-worker computations

```
if (my_rank == 0) { /* master */
    //... load input and dispatch ...
} else { /* workers */
    //... wait for data and compute ...
}
```

MPI (Message Passing Interface)

- **Message Passing Model**:
  - ↪ each "processor" runs a process
  - ↪ processes communicate by exchanging messages
    - ✓ *analogy*: **mail**



Message Passing Interface (MPI) Standard

- **Goal**:
  - ↪ **portable**, **efficient** & **flexible** standard for message passing
  - ↪ industry standard
- Reference website https://www.mpi-forum.org/
- **Latest version: 3.1** (June 2015) – specifications

MPI on UL HPC platform

- Rely on Environment Modules **once** on a computing node
  ↪ then you can search for MPI suites available: `module avail mpi`

MPI Suite	Version	`module load...`	Compiler
Intel MPI	18.0.1	`toolchain/intel`	C: `mpiicc`; C++: `mpiicpc`
OpenMPI	2.1.3	`mpi/OpenMPI`	C: `mpicc`; C++: `mpic++`
MVAPICH2	2.3a	`mpi/MVAPICH2`	C: `mpicc`; C++: `mpic++`

MPI on UL HPC platform

- Rely on Environment Modules **once** on a computing node
  ↪ then you can search for MPI suites available: `module avail mpi`

MPI Suite	Version	`module load...`	Compiler
Intel MPI	18.0.1	`toolchain/intel`	C: `mpiicc`; C++: `mpiicpc`
OpenMPI	2.1.3	`mpi/OpenMPI`	C: `mpicc`; C++: `mpic++`
MVAPICH2	2.3a	`mpi/MVAPICH2`	C: `mpicc`; C++: `mpic++`

MPI Suite	Compilation command (in C)
Intel MPI	`mpiicc -Wall [-qopenmp] [-xhost] -O2 [...]`
OpenMPI	`mpicc -Wall [-fopenmp] -O2 [...]`
MVAPICH2	`mpicc -Wall [-fopenmp] -O2 [...]`

Reservation

- You will probably want to compile/test within an **interactive job**
  - ↪ **Ex**: 1 core on two **different** nodes

```
# SLURM -- Iris cluster
(access)$> srun -p interactive -N 2 --ntasks-per-node 1 --pty bash

# OAR --  gaia, chaos cluster
(access)$> oarsub -I -l nodes=2/core=1,walltime=4
```

- Then you can search for MPI suites available

```
(node)$> module avail mpi
```

MPI with OAR

- Reservation has to match the required number of MPI processes:
  - ↪ **Ex**: `oarsub -l nodes=2/core=12[...]`
- Running MPI code using traditional `mpirun`

```
# Intel MPI
$> module load toolchain/intel
# ONLY on moonshot node have no IB card: export I_MPI_FABRICS=tcp
$> mpirun -hostfile $OAR_NODEFILE ...
```

MPI with OAR

- Reservation has to match the required number of MPI processes:
  - ↪ **Ex**: `oarsub -l nodes=2/core=12[...]`
- Running MPI code using traditional `mpirun`

```
# Intel MPI
$> module load toolchain/intel
# ONLY on moonshot node have no IB card: export I_MPI_FABRICS=tcp
$> mpirun -hostfile $OAR_NODEFILE ...
```

```
# OpenMPI
$> module load mpi/OpenMPI
$> mpirun -hostfile $OAR_NODEFILE -x PATH -x LD_LIBRARY_PATH ...
```

MPI with OAR

- Reservation has to match the required number of MPI processes:
  - ↪ **Ex**: `oarsub -l nodes=2/core=12[...]`
- Running MPI code using traditional `mpirun`

```
# Intel MPI
$> module load toolchain/intel
# ONLY on moonshot node have no IB card: export I_MPI_FABRICS=tcp
$> mpirun -hostfile $OAR_NODEFILE ...
```

```
# OpenMPI
$> module load mpi/OpenMPI
$> mpirun -hostfile $OAR_NODEFILE -x PATH -x LD_LIBRARY_PATH ...
```

```
# MVAPICH2
$> module load mpi/MVAPICH2
$>-launcher ssh -launcher-exec /usr/bin/oarsh -f $OAR_NODEFILE ...
```

MPI launchers (OAR) Github

```
$> oarsub -S <scriptname>          # -S: interpret #OAR comments
```

```
#!/bin/bash -l
#OAR -l nodes=2/core=6,walltime=1
if [ -f  /etc/profile ]; then
    .  /etc/profile
fi
# Load the intel toolchain and whatever MPI module you need
module purge && module load toolchain/intel # or mpi/{OpenMPI|MVAPICH2}
# ONLY on moonshot node that have no IB card: export I_MPI_FABRICS=tcp

### Intel MPI
mpirun -hostfile $OAR_NODEFILE mpi_program
### OpenMPI
mpirun -hostfile $OAR_NODEFILE -x PATH -x LD_LIBRARY_PATH mpi_program
### MVAPICH2
mpirun -launcher ssh -launcher-exec /usr/bin/oarsh \
       -f $OAR_NODEFILE mpi_program
```

MPI with Slurm

sbatch/srun option	Description
`-N <N>`	number of **distributed** nodes
`--ntasks-per-node=<N>`	number of **MPI processes** per node
`-c 1`	(default) set a **single** thread per MPI process
`-c <T>`	number of OpenMP threads for hybrid runs

- SLURM able to directly launch MPI tasks (_recommended_)
  - ↪ . . . and initialize of MPI communications
  - ↪ via Process Management Interface (PMI) [v2]

```
$> srun -n $SLURM_NTASKS /path/to/mpiprog
```

MPI launcher (Slurm) Docs

```
$> sbatch [-p batch] <scriptname>
```

```
#!/bin/bash -l
#SBATCH -N 2                    # Use 2 nodes
#SBATCH --ntasks-per-node=28  # Number of MPI process per node
#SBATCH -c 1      # threads per MPI process (1 unless hybrid code)
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

if [ -f  /etc/profile ]; then
    .  /etc/profile
fi
# Load the intel toolchain and whatever MPI module you need
module purge
module load toolchain/intel # or mpi/{OpenMPI|MVAPICH2}
# export I_MPI_PMI_LIBRARY=/usr/lib64/libpmi.so
srun -n $SLURM_NTASKS /path/to/your/mpi_program
```

Hands-on 2: MPI jobs

Your Turn!

Hands-on 2

ulhpc-tutorials.rtfd.io/en/latest/parallel/basics/#paralleldistributed-mpi-jobs

- **Reserve** an **interactive** job to launch 6 MPI processes
  - ↪ across two nodes (2x3), for 30 minutes
- Check and **compile** `src/hello_mpi.c`
  - ↪ `bin/{openmpi,intel,mvapich2}_hello_mpi`
- **execute** the generated binaries
- prepare a **launcher script** `runs/launcher.MPI.sh`
- repeat on a more serious program `src/matrix_mult_mpi.c`
  - ↪ `bin/{openmpi,intel,mvapich2}_matrix_mult_mpi`

Summary

Hybrid OpenMP+MPI Programs

MPI Suite	`module load...`	Compilation command (C)
Intel MPI	`toolchain/intel`	`mpiicc -Wall -qopenmp [-xhost] -O2 [...]`
OpenMPI	`mpi/OpenMPI`	`mpicc -Wall -fopenmp -O2 [...]`
MVAPICH2	`mpi/MVAPICH2`	`mpicc -Wall -fopenmp -O2 [...]`

- adapt (and share) `OMP_NUM_THREADS` environment variable
- **(Slurm only)**: adapt `-c <T>`: number of OpenMP threads
- **(OAR only)**: you have to take the following elements into account:
  - ↪ compute accurately MPI processes per node `<PPN>`
  - ↪ pass it to `mpirun`:
    - ✓ OpenMPI: `mpirun -npernode <PPN> -np <N>`
    - ✓ Intel MPI: `mpirun -perhost <PPN> -np <N>`
    - ✓ MVAPICH2: `mpirun -ppn <PPN> -np <N>`
  - ↪ (_Intel MPI only_): `I_MPI_PIN_DOMAIN=omp`
  - ↪ (_MVAPICH2 only_) `MV2_ENABLE_AFFINITY=0`

Hybrid OpenMP+MPI with OAR

```
### Intel MPI
mpirun -perhost ${NPERNODE:=1} -np ${NP} \
       -genv OMP_NUM_THREADS=${OMP_NUM_THREADS} \
       -genv I_MPI_PIN_DOMAIN=omp \
       -hostfile $OAR_NODEFILE  hybrid_program
```

Hybrid OpenMP+MPI with OAR

```
### Intel MPI
mpirun -perhost ${NPERNODE:=1} -np ${NP} \
       -genv OMP_NUM_THREADS=${OMP_NUM_THREADS} \
       -genv I_MPI_PIN_DOMAIN=omp \
       -hostfile $OAR_NODEFILE  hybrid_program
```

```
### OpenMPI
mpirun -npernode ${NPERNODE:=1} -np ${NP} \
       -x OMP_NUM_THREADS -x PATH-x LD_LIBRARY_PATH \
       -hostfile $OAR_NODEFILE  hybrid_program
```

Hybrid OpenMP+MPI with OAR

```
### Intel MPI
mpirun -perhost ${NPERNODE:=1} -np ${NP} \
       -genv OMP_NUM_THREADS=${OMP_NUM_THREADS} \
       -genv I_MPI_PIN_DOMAIN=omp \
       -hostfile $OAR_NODEFILE  hybrid_program
```

```
### OpenMPI
mpirun -npernode ${NPERNODE:=1} -np ${NP} \
       -x OMP_NUM_THREADS -x PATH-x LD_LIBRARY_PATH \
       -hostfile $OAR_NODEFILE  hybrid_program
```

```
### MVAPICH2
export MV2_ENABLE_AFFINITY=0
mpirun -ppn ${NPERNODE:=1} -np ${NP} \
       -genv OMP_NUM_THREADS=${OMP_NUM_THREADS} \
       -launcher ssh -launcher-exec /usr/bin/oarsh \
       -f $MACHINEFILE  hybrid_program
```

Hybrid OpenMP+MPI with Slurm

```
#!/bin/bash -l
#SBATCH -N 2                        # Use 2 nodes
#SBATCH --ntasks-per-node=1    # Number of MPI process per node
#SBATCH -c 4                  # Number of OpenMP threads per MPI process
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

if [ -f  /etc/profile ]; then
    .  /etc/profile
fi
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}

# Load the intel toolchain and whatever MPI module you need
module purge
module load toolchain/intel    # or mpi/{OpenMPI|MVAPICH2}
# export I_MPI_PMI_LIBRARY=/usr/lib64/libpmi.so
srun -n $SLURM_NTASKS /path/to/your/hybrid_program
```

Hands-on 3: Hybrid OpenMP+MPI

Your Turn!

Hands-on 3

ulhpc-tutorials.rtfd.io/en/latest/parallel/basics/#hybrid-openmpmpi-programs

- **Reserve** an **interactive** job to launch
  - ↪ 2 MPI processes (on 2 nodes) / 4 OpenMP threads
- Check and **compile** `src/hello_hybrid.c`
  - ↪ `bin/{openmpi,intel,mvapich2}_hello_hybrid`
- **execute** the generated binaries
  - ↪ set `$OMP_NUM_THREADS`
  - ↪ compute `$NPERHOST`
- prepare a **launcher script** `runs/launcher.hybrid.sh`

Summary

HPC Interconnect Benchmarking

OSU Micro-Benchmarks Instructions

ulhpc-tutorials.rtfd.io/en/latest/parallel/mpi/OSU_MicroBenchmarks/

- **Pre-requisites**: get an interactive job for compilation

```
### Iris cluster
(access)$> srun -p interactive -N 2 --ntasks-per-node 1 --pty bash
# aliased/short version: 'si -N 2 --ntasks-per-node 1'
# best-effort mode :    append '--qos qos-best-effort'
# within a reservation: append '--reservation <name>'
```

```
### Gaia, chaos cluster
(access)$> oarsub -I -l nodes=2/core=1,walltime=4
# best-effort mode :    append '-t besteffort'
# within a reservation: append '-t inner=<containerID>'
```

OSU micro-benchmarks

http://mvapich.cse.ohio-state.edu/benchmarks/

- We will build **version 5.5 of the OSU micro-benchmarks**
- Focusing on (only) two one-sided benchmarks:
  - ↪ `osu_get_latency` - Latency Test
  - ↪ `osu_get_bw` - Bandwidth Test

Building the Benchmarks

Your Turn!

Hands-on 4

ulhpc-tutorials.rtfd.io/en/latest/parallel/mpi/OSU_MicroBenchmarks/

- Get the sources
- Uncompress them
- Compilation based on
  - ↪ **Intel MPI**
  - ↪ **Open MPI**
  - ↪ **Open MPI** over Ethernet interface
    - ✓ highlight performance drops compared to Infiniband

Building the Benchmarks

```
$> configure -prefix=<path>; make && make install
```

- Based on Autotools/Automake
  - ↪ **Rely on `--prefix=$(pwd)`** to state where to install
  - ↪ sometimes being in a separate build directory raise issues!
    - ✓ Ex: *osu_util.h: No such file or directory* (missing header)
    - ✓ then you have to play with `CFLAGS=-I<path>` (or `LDPATH`)

```
$> mkdir <builddir> && cd <builddir>
$> ../src/configure [CC=<compiler>] --prefix=$(pwd)
$> make && make install
```

Building the Benchmarks

```
$> configure -prefix=<path>; make && make install
```

- Based on Autotools/Automake
  - ↪ **Rely on `--prefix=$(pwd)`** to state where to install
  - ↪ sometimes being in a separate build directory raise issues!
    - ✓ Ex: *osu_util.h: No such file or directory* (missing header)
    - ✓ then you have to play with `CFLAGS=-I<path>` (or `LDPATH`)

```
$> mkdir <builddir> && cd <builddir>
$> ../src/configure [CC=<compiler>] --prefix=$(pwd)
$> make && make install
```

- Now common to have CMake based software

```
$> cmake ../src/
$> make && make install
```

Running the Benchmarks

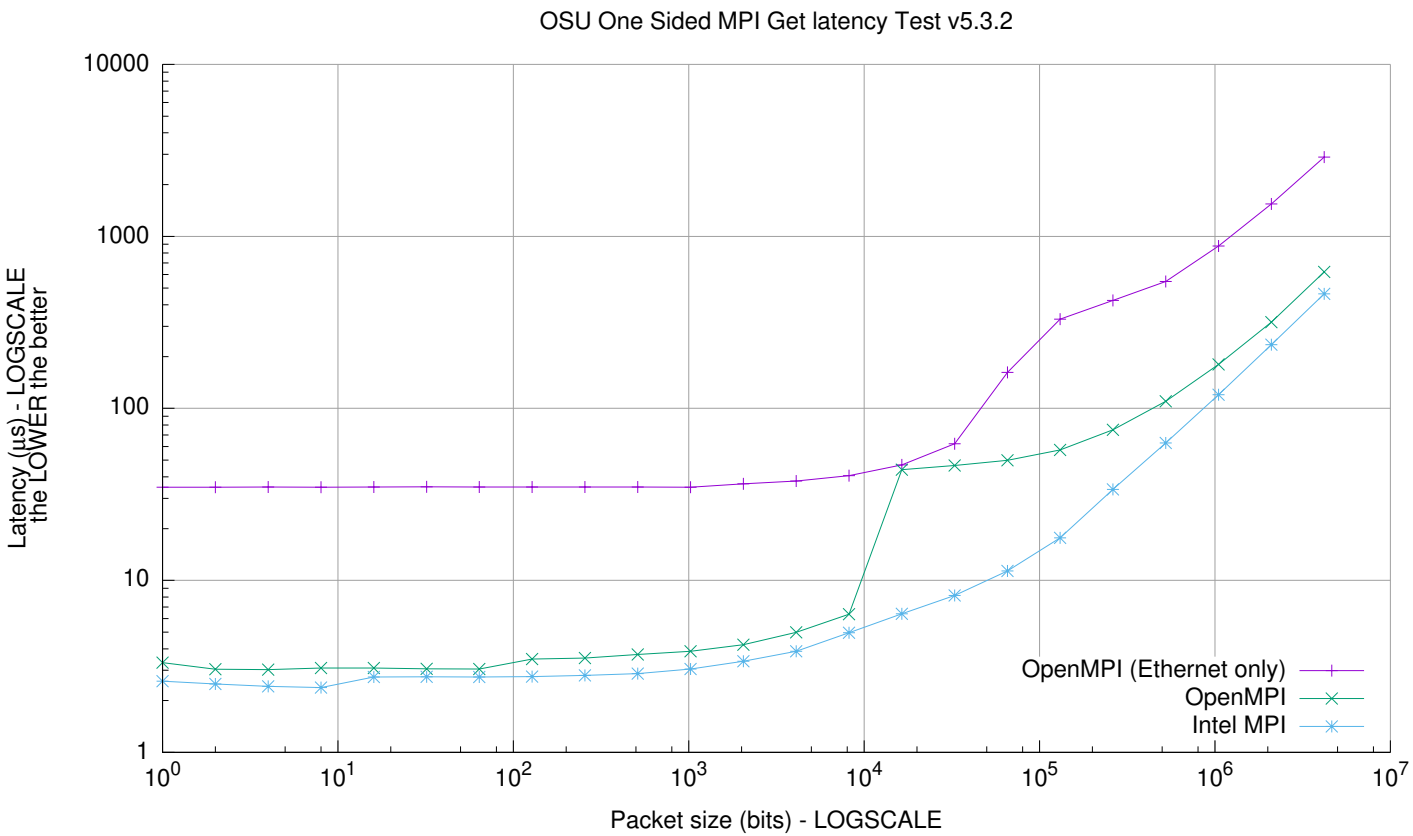
Your Turn!

- Build directory:
  `libexec/osu-micro-benchmarks/mpi/one-sided/`
- Prepare a batch launcher
  - ↪ copy and adapt the default SLURM launcher
- Run it in batch mode

```
$> cd ~/tutorials/OSU-MicroBenchmarks/runs
### On iris
$> sbatch ./launcher-OSU.intel.sh osu_get_bw
$> sbatch ./launcher-OSU.intel.sh osu_get_latency
### On gaia, chaos
$> oarsub -S ./launcher-OSU.intel.sh
```

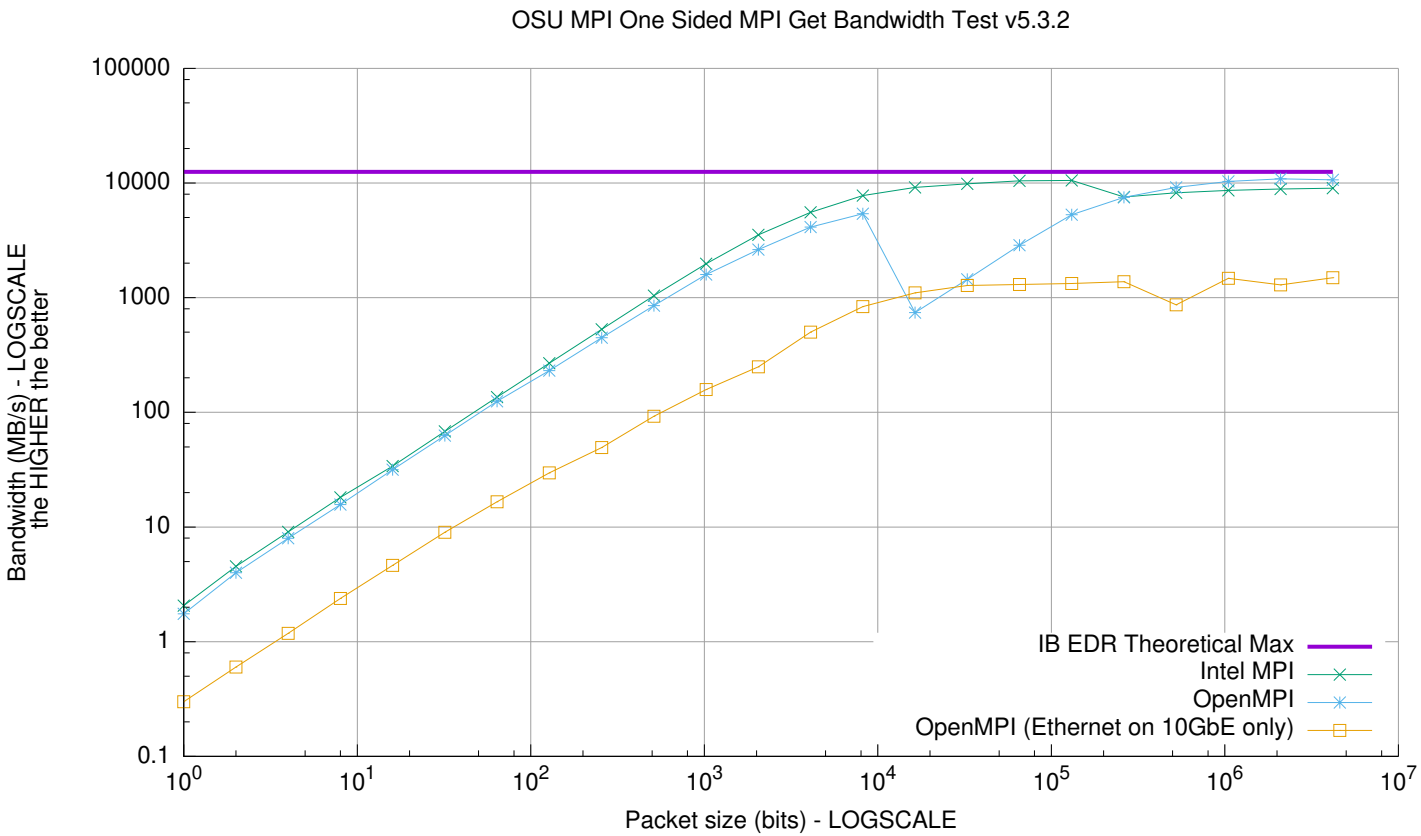
Interconnect Performances

- Based on OSU Micro-benchmarks



Interconnect Performances

- Based on OSU Micro-benchmarks



Summary

High-Performance Linpack (HPL)

HPL Instructions

ulhpc-tutorials.rtfd.io/en/latest/parallel/mpi/HPL/

- **Pre-requisites**: get an interactive job for compilation
  - ↪ **Q**: justify the difference with the job request made for OSU.

```
### Iris cluster
(access)$> srun -p interactive -n 14 --pty bash
# aliased/short version: 'si -n 14'
# best-effort mode :    append '--qos qos-best-effort'
# within a reservation: append '--reservation <name>'
```

```
### Gaia, chaos cluster
(access)$> oarsub -I -l nodes=1/core=6,walltime=4
# best-effort mode :    append '-t besteffort'
# within a reservation: append '-t inner=<containerID>'
```

High-Performance Linpack (HPL)

http://www.netlib.org/benchmark/hpl/

- Portable implem. of High-Performance Linpack (HPL) Benchmark
  - ↪ for Distributed-Memory Computers
  - ↪ *reference* benchmark for ranking the Top500 list
- We will build **version 2.2 of the HPL**
  - ↪ Focusing (only) on Intel MPI+MKL build
  - ↪ **Pre-requisites**:
    - ✓ clone ULHPC/tutorials and ULHPC/launcher-scripts repositories
    - ✓ preparing your working directory

Building HPL

Your Turn!

Hands-on 4

ulhpc-tutorials.rtfd.io/en/latest/parallel/mpi/HPL/

- Get the sources
- Uncompress them
- Compilation based on the **Intel MPI** suit
  - ↪ Prepare and adapt `src/hpl-2.2/Make.intel64`
- Compile it !

Building HPL

```
$> cd ~/tutorials/HPL/src/hpl-2.2
$> cp setup/Make.Linux_Intel64 Make.intel64
$> vim Make.intel64
# [...] change TOPdir and MP{dir,inc,lib} (at least)
$> make arch=intel64 clean_arch_all
$> make arch=intel64
```

Preparing the HPL Benchmark Run

Your Turn!

- Build directory: `bin/intel64`
- Prepare a batch launcher
  - ↪ copy and adapt the default SLURM launcher
- Prepare an input `HPL.dat` file
  - ↪ use Tuning HPC Online for some default settings

- **Main HPL parameters constraints**
  - ↪ `PxQ = <nodes>*<cores> = $SLURM_NTASKS`
  - ↪ Problem size: `N` (to be as large as possible)
    - ✓ $\texttt{N} = \alpha\sqrt{\#nodes * RAM * 1024}$ where RAM is expressed in GiB
  - ↪ `NB`: depends on processor architecture (Ex: Intel MKL notes)
    - ✓ `NB = 192` on `iris` cluster

Example HPL.dat

```
HPLinpack benchmark input file
Innovative Computing Laboratory, University of Tennessee
HPL.out      output file name (if any)
6            device out (6=stdout,7=stderr,file)
1            # of problems sizes (N)
24650        Ns
1            # of NBs
192          NBs
0            PMAP process mapping (0=Row-,1=Column-major)
2            # of process grids (P x Q)
2 4          Ps
14 7         Qs
[...]
```

- Targeting 1 node in this case on 2 sets of parameters (PxQ = 28)

	N	NB	P	Q
Run 1	24650	192	2	14
Run 2	24650	192	4	7

HPL Benchmark [batch] Runs

- Adapt the default SLURM launcher
- Run it

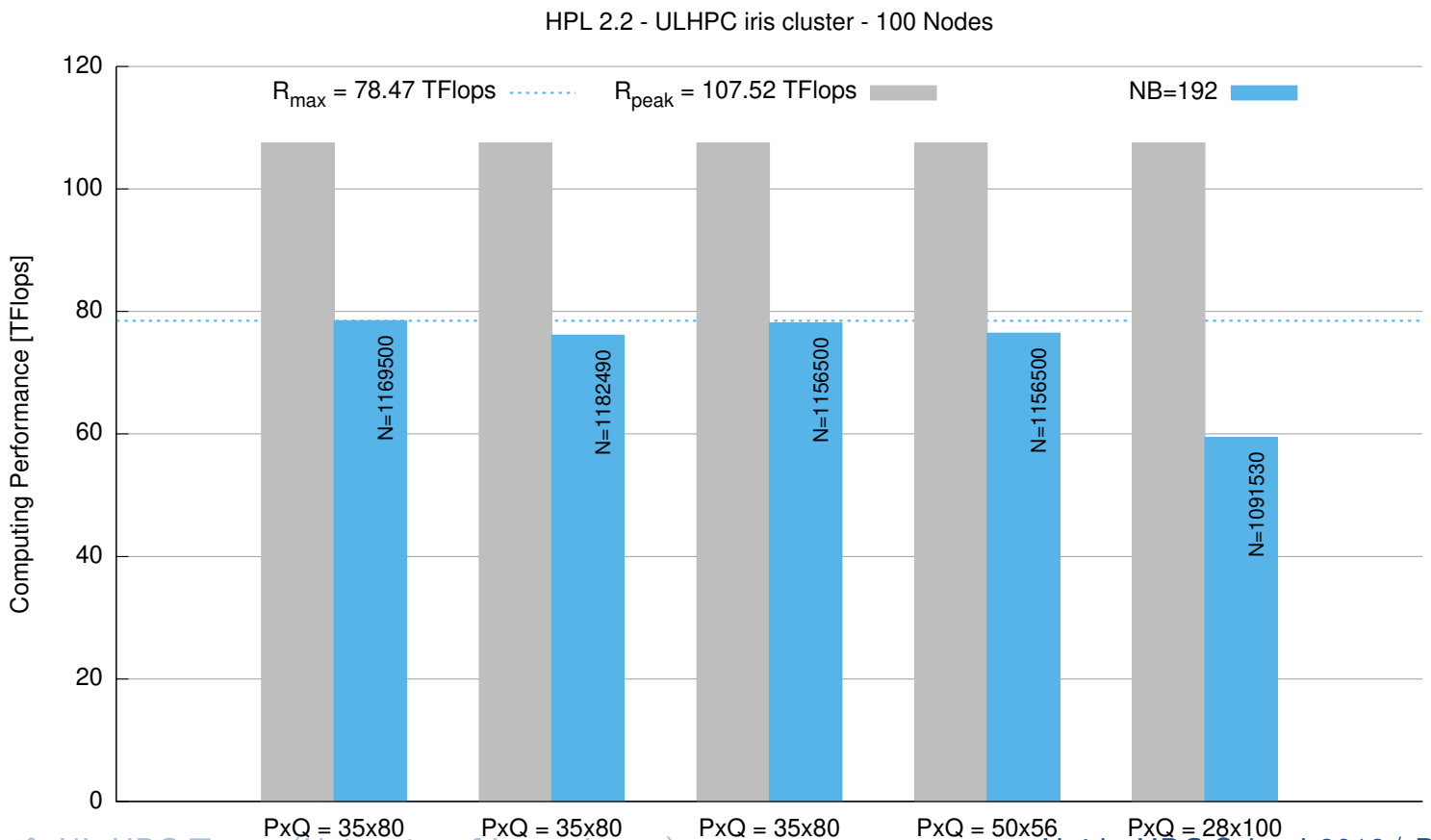
```
$> cd ~/tutorials/HPL/runs
$> cp ../ref.ulhpc.d/HPL.dat .
### On iris
$> sbatch ./launcher-HPL.intel.sh
### On gaia, chaos
$> oarsub -S ./launcher-HPL.intel.sh
```

- Grab the HPL results from the output logs

```
# T/V     N       NB      P     Q    Time       Gflops
$> grep WR slurm-2758.out
WR11C2R4  24650   192     2     14   13.51      7.392e+02
WR11C2R4  24650   192     4      7   12.69      7.869e+02
```

Computing Performances / HPL

- Based on High-Performance Linpack (HPL)
  - ↪ reference benchmark for Top 500



Questions?

http://hpc.uni.lu

High Performance Computing @ uni.lu

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