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;
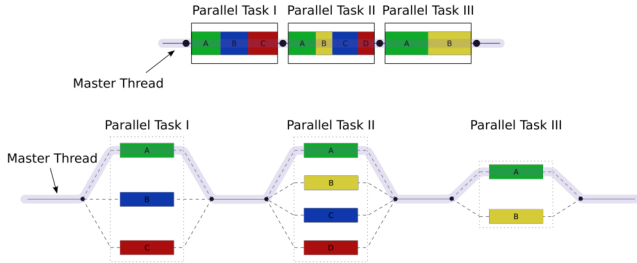

OpenMP
https://www.openmp.org/

- Reference website
- **Latest version: 4.5** (Nov 2015) – 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[...]`

```bash
#!/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

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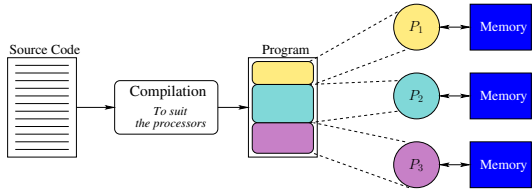
- SPMD: **Simple Program, Multiple Data**
  - ↪ same programs for each processors
    - ✓ executed at independent points
  - ↪ processes identified by a rank
    - ✓ each process knows the piece of code he works on
    - ✓ common in master-worker computations

```
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**
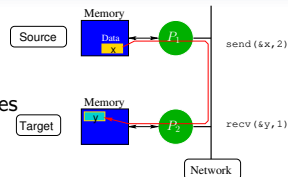
Message Passing Interface (MPI) Standard

- **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	17.0.1	`toolchain/intel`	C: `mpiicc`; C++: `mpiicpc`
OpenMPI	2.1.1	`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	17.0.1	`toolchain/intel`	C: `mpiicc`; C++: `mpiicpc`
OpenMPI	2.1.1	`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
```

```bash
#!/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

```bash
#!/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 5.4 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
```
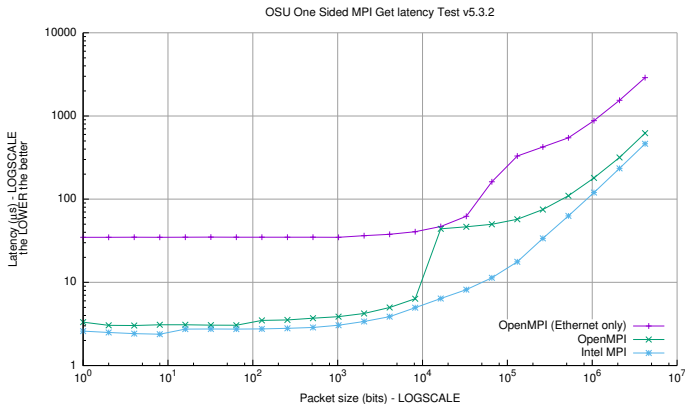
Running the Benchmarks

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
```
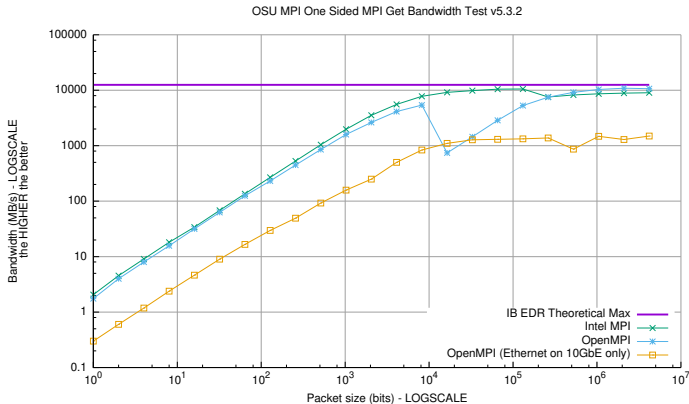
Interconnect Performances

- Based on OSU Micro-benchmarks

OSU One Sided MPI Get latency Test v5.3.2

Interconnect Performances

- Based on OSU Micro-benchmarks

OSU MPI One Sided MPI Get Bandwidth Test v5.3.2

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)
    - ✓ $N = \alpha\sqrt{\#nodes * RAM * 1024}$ 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
```
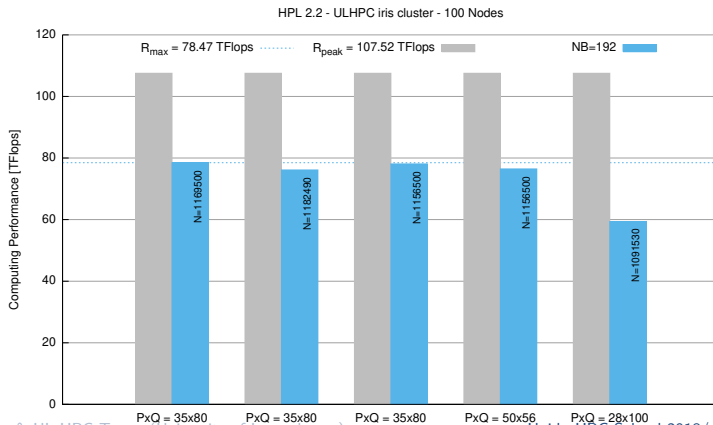
- Grab the HPL results from the output logs

```
# 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

HPL 2.2 - ULHPC iris cluster - 100 Nodes

Questions?

High Performance Computing @ uni.lu

Prof. Pascal Bouvry
Dr. Sebastien Varrette
Valentin Plugaru
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1 **Introduction**

2 **Threaded Parallel OpenMP Jobs**

3 **Parallel/distributed MPI Jobs**

4 **Hybrid OpenMP+MPI Jobs**

5 **OSU Micro-Benchmarks**

6 **High-Performance Linpack (HPL)**

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