Uni.lu HPC School 2019

PS5a: Scalable Science I: Parallel computations with OpenMP/MPI



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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/

PS5a tutorial sources:

ulhpc-tutorials.rtfd.io/en/latest/parallel/basics/









2019















Summary

- Introduction
- 2 Threaded Parallel OpenMP Jobs
- Parallel/distributed MPI Jobs
- 4 Hybrid OpenMP+MPI Jobs
- 5 OSU Micro-Benchmarks
- 6 High-Performance Linpack (HPL)





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:

 - \hookrightarrow 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)





Threaded Parallel OpenMP Jobs

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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.
 - \hookrightarrow Parallelism accomplished **exclusively** through the use of threads.
 - √ Thread: smallest unit of processing that can be scheduled by an OS
 - \hookrightarrow #threads \simeq number of machine processors/cores.
 - ✓ OMP_NUM_THREADS (if present): initial max number of threads;

OpenMP

https://www.openmp.org/

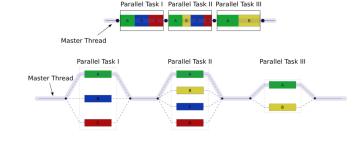
- Reference website
- Latest version: 5.0 (Nov 2018) specifications





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
 - $\checkmark\,$ 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 toolchain/foss	<pre>icc -qopenmp [] gcc -fopenmp []</pre>





Reservation

- # 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:

```
#!/bin/bash -l
#OAR -l nodes=1/core=4, walltime=1
export OMP NUM THREADS=$(cat $OAR NODEFILE| wc -1)
# 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
                        number of OpenMP threads
-c < T >
```

```
#!/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 -- gos=gos-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
- 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





Parallel/distributed MPI Jobs

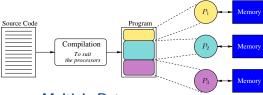
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SPMD Programming model



- 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

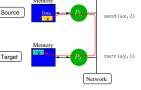
```
if (my rank == 0) \{ /* master */
  //... load input and dispatch ...
 else { /* workers */
  //... wait for data and compute ...
```





MPI (Message Passing Interface)

- Message Passing Model:
 - \hookrightarrow each "processor" runs a process



Message Passing Interface (MPI) Standard

- Goal:
 - → portable, efficient & flexible standard for message passing
- 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
 - \hookrightarrow 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

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MVAPICH2	2.3a	mpi/MVAPICH2	C: mpicc; C++: mpic++

MPI Suite	Compila	tion co	mmand (in C)
Intel MPI OpenMPI MVAPICH2	mpicc	-Wall	[-qopenmp] [-fopenmp] [-fopenmp]	





Reservation

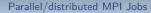
You will probably want to compile/test within an interactive job
 Ex: 1 core on two different nodes

```
# 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:
- 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

MPI with OAR

- Reservation has to match the required number of MPI processes:
- 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 ...
```

```
$> 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:
- 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 ...

MVAPTCH2

- \$> 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
#DAR -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
### Tn.t.e.1. MPT
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>ntasks-per-node=<n> -c 1 -c <t></t></n></n>	number of distributed nodes number of MPI processes per node (default) set a single thread per MPI process number of OpenMP threads for hybrid runs

- SLURM able to directly launch MPI tasks (recommended)
 - \hookrightarrow ... and initialize of MPI communications

 - \$> 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 (2×3), for 30 minutes
- execute the generated binaries
- prepare a launcher script runs/launcher.MPI.sh





Hybrid OpenMP+MPI Jobs

Summary

- 4 Hybrid OpenMP+MPI Jobs
- OSU Micro-Benchmarks





Hybrid OpenMP+MPI Programs

MPI Suite	module load	Compilation command (C)
Intel MPI OpenMPI MVAPICH2	toolchain/intel mpi/OpenMPI mpi/MVAPICH2	<pre>mpiicc -Wall -qopenmp [-xhost] -02 [] mpicc -Wall -fopenmp -02 [] mpicc -Wall -fopenmp -02 []</pre>

- 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:
 - \hookrightarrow compute accurately MPI processes per node <PPN>
 - \hookrightarrow pass it to mpirun:
 - ✓ OpenMPI: mpirun -npernode <PPN> -np <N>
 - ✓ Intel MPI: mpirun -perhost <PPN> -np <N>
 - √ MVAPICH2: mpirun -ppn <PPN> -np <N>

 - → (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
mpirum -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
```





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 --t.i.me=0-01:00:00
#SBATCH -p batch
#SBATCH -- gos=gos-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





OSU Micro-Benchmarks

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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 -1 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:
 - $\hookrightarrow \ \mathtt{osu_get_latency} \ \mathtt{-} \ \mathsf{Latency} \ \mathsf{Test}$
 - $\hookrightarrow \ \mathtt{osu_get_bw} \ \mathtt{-} \ \mathsf{Bandwidth} \ \mathsf{Test}$





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
 - \hookrightarrow 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
```

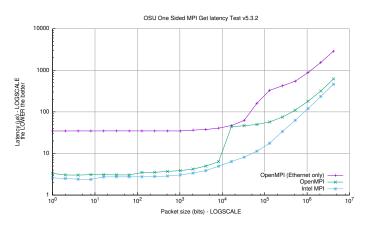
\$> oarsub -S ./launcher-OSU.intel.sh





Interconnect Performances

Based on OSU Micro-benchmarks

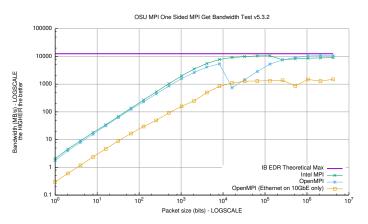






Interconnect Performances

Based on OSU Micro-benchmarks







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High-Performance Linpack (HPL)

HPL Instructions

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

- Pre-requisites: get an interactive job for compilation
 - $\,\hookrightarrow\,$ $\boldsymbol{Q}:$ 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
- 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
- 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
- Prepare an input HPL.dat file
 - \hookrightarrow 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)
 - \checkmark N = $\alpha\sqrt{\#nodes*RAM*1024}$ where RAM is expressed in GiB
 - $\hookrightarrow\,$ 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)
             device out (6=stdout,7=stderr,file)
6
             # of problems sizes (N)
24650
             Ns
             # of NBs
192
             NBs
             PMAP process mapping (0=Row-,1=Column-major)
             # of process grids (P \times Q)
2 4
             Ps
14 7
             Qs
[...]
```

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

	N	NB	Р	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

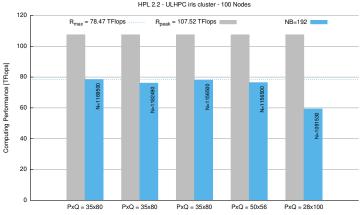
WR11C2R4 24650 192 4 7 12.69 7.869e+02
```





Computing Performances / HPL

- Based on High-Performance Linpack (HPL)





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