Tutorial 1 Parallel Computer Architecture and Slurm

CS3210 - 23/24 Semester 1

Learning Outcomes

Part 1: Tutorial

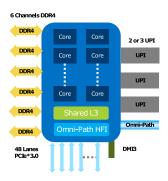
- 1. Recall the various levels of parallelism
- 2. Understand and apply the Flynn's taxonomy of computer architectures
- 3. Understand the various ways memory can be organized

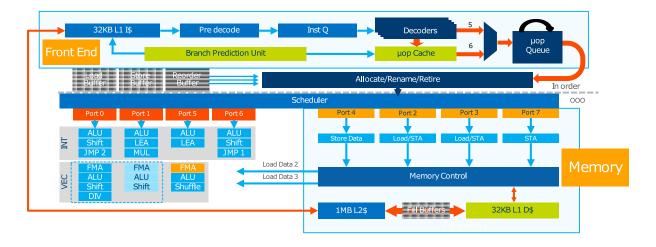
Part 2 and 3: Lab

- 4. Understand the hardware configuration of our lab cluster
- 5. Set-up and run applications on our lab cluster using Slurm

Part 1: Tutorial on Parallel Computing Architectures

1. (Levels of Parallelism) A simplified diagram of the Intel Xeon Scalable processor family and its microarchitecture diagram is reproduced below





Briefly discuss and identify the various forms of parallelism that are supported by this processor chip.



Useful information on Intel Xeon Scalable

- https://software.intel.com/en-us/articles/intel-xeon-processor-scalable-family-technical-overview
- https://www.intel.com/content/dam/www/public/us/en/documents/ product-briefs/xeon-scalable-platform-brief.pdf (page 9)

Solution:

- Instruction-level μ ops and superscalar execution. Out-of-order execution allows us to maximize our CPU's cycles by running other instructions that do not violate data dependencies while another instruction is waiting to complete.
- Thread-level Hyperthreading (SMT) 2 threads per core
- Processor-level
 - Shared memory Intel UltraPath Interconnect (point to point processor interconnect)
 NUMA (ccNUMA?)
 - Distributed Intel Omni-Path Architecture
- 2. **(Flynn's Taxonomy)** For each of the following scenarios, classify them according to Flynn's taxonomy (i.e. SISD, SIMD, MISD, MIMD) and provide a brief (say, one line) justification
 - (a) A personal computer from the 1980s

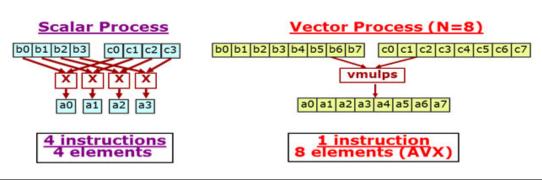
Solution: SISD. Almost all computers in the era are **uniprocessor systems**, capable of only executing one instruction stream on a single data stream.

(b) A laptop with a multi-core processor

Solution: MIMD. Each core can potentially execute a different thread, which can operate on different data streams.

(c) Intel's AVX instruction set

Solution: SIMD. One instruction stream (e.g. **vmulps**) operating on different sets of data at the same time.



(d) A uniprocessor (i.e. single core) with pipelining (ILP)

Solution: SISD. Despite the presence of pipelining, it is still executing the same instruction and data stream. Viz: different instructions, but coming from the same program!

(e) Students attempting the same exam in an exam hall

Solution: MISD. The "exam script" (data) is the same for all students, but they are working on different parts of the exam paper in any single moment (multiple instruction streams).

- 3. (Memory + Multi-core Architecture) For each of the following questions, indicate whether the statement is true or false. Briefly justify your answer.
 - (a) Shared-memory system implies a UMA architecture.

Solution: False. There's NUMA and COMA architectures in shared-memory systems.

(b) On a NUMA architecture, the actual location of data (i.e. on which node) has no impact for a distributed shared-memory program.

Solution: False. Non-uniform accesses, but shared memory. Memory is physically distributed across all PUs (but seen as one), and where the data is located might translate in different overheads in accessing it when running one of the distributed tasks. A distributed task accesses local data (which might be stored on a memory that has a longer access time due to NUMA shared memory), and transferes data to other task (which might not be an actual transfer since the memory is shared, but it might have longer access time for the new task)

(c) In the hierarchical design of multicore architecture, the memory organization is hybrid (distributed-shared memory)

Solution: True, but students might argue for false as well. Pay attention to their justification, and discuss on the spot. True because if you see the memory as being cache + memory, you can argue that cache is distributed memory, while you still have some shared memory (shared caches and/or shared memory). False because you only focus on the memory (ignore cache), and it is not guaranted that the architecture has shared memory. False can also be if you argue that caches are (usually) cache coherent - so you can consider them shared memory.

- 4. **(Processes and Threads)** For each of the following questions, indicate whether the statement is true or false. Briefly justify your answer.
 - (a) A semaphore can be used to replace a mutex without affecting the correctness of a program.

Solution: True. Initialize to 1. Some changes in the logic of the program might be needed. Note: this answer does not work if we are replacing a semaphore by a mutex (other way around). We cannot signal a pthread mutex that we have not locked, but we can post to a semaphore we have not waited on.

(b) Implementing an algorithm using multiple threads **always** runs faster than implementing the same algorithm using multiple processes.

Solution: False - if there are user-level threads they are mapped to one process and they might end up running slower. Students might argue successfully for true if they refer to pthreads (kernel-level threads), or if they refer to some type of scheduling at the library level for user-level threads. If students said true because overhead of threading is lower than overhead of processes, they will not be awarded marks.

Part 2: Foundation: Parallel and Distributed Computing Lab Cluster

To start using our lab cluster to its full potential, we need to understand the available hardware.

Lab Machines: Physical Layout

The diagram below shows the arrangement of the machines in each workbench at the Parallel Computing Lab at COM1-B1-02. Each of the two computers in a workbench are connected with a switch, as follows:

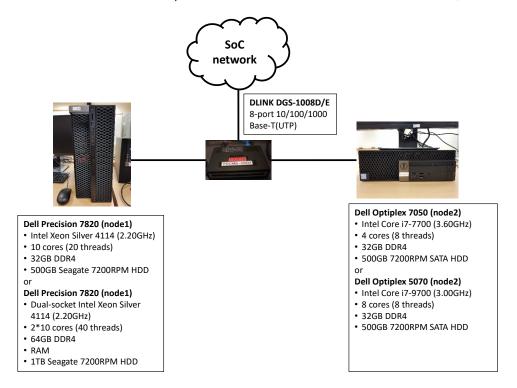


Figure 1: Layout of machines on each workbench

The hostname and the type of node are shown below.

- soctf-pdc-001 soctf-pdc-008: Intel Xeon Silver 4114
- soctf-pdc-009 soctf-pdc-016: Intel Core i7-7700
- soctf-pdc-018 soctf-pdc-019: Dual-socket Intel Xeon Silver 4114
- soctf-pdc-020 soctf-pdc-021: Intel Core i7-9700
- soctf-pdc-022 soctf-pdc-024: Intel Xeon W-2245 (not shown above)



Exercise 1

Please ssh into one of our lab machines as in Lab 1. What is the hardware configuration of the lab machine you are currently connected to? Run:

- \$ lscpu
- \$ lstopo

Some questions (non-exhaustive):

- 1. What is a socket and how many do you have?
- 2. What are, and what are the relationships between CPUs, cores, and threads?
- 3. What are the different levels of cache present and how large are they?

Part 3: Using Slurm Workload Manager (Practical)



Please read this section carefully and try all the exercises.

Please also open our **Slurm Student User Guide** (https://bit.ly/cs3210-slurm-guide).

In case of any conflicting information after this tutorial, the Slurm Student User Guide takes precedence, as it is updated regularly throughout the semester.

What is Slurm? Why does it exist?

So far, you have been running your programs *interactively*. That is, you have been connecting *directly* to a specific machine over ssh, and executing programs on it through an interactive shell (e.g., bash). However, there are a few reasons why running programs interactively **not ideal**:

- "Hogging" the machines: Some students may not be able to run their code in a timely manner. Other
 students could unfairly use a large portion of our available CPU/memory resources by running many
 resource-intensive programs that take a long time to complete. This problem is exacerbated during
 assignments that may need to be executed across multiple machines simultaneously.
- Cannot get accurate performance readings: Students may not be able to get an accurate measurement of how fast their solutions are. If many students are logged into a single node and running their programs simultaneously, all of their programs will seem slower (take more wall-clock time) than if each student had exclusive access to the node for a short period.

To address these problems, a significant number of machines in the Parallel and Distributed Computing Lab are controlled by the **Slurm Workload Manager**. Slurm performs three key functions:

- Fair Job Queue: Students will submit jobs to Slurm through commands such as sbatch and srun.
 These jobs will be placed in a queue and then scheduled to run on the lab machines once enough
 resources are available for the specific job. Every student will get their fair share of time to run their
 programs nobody can hog the machines.
- 2. **Exclusive Access for Performance Measurements:** When a student's job is running on Slirm nodes, no other jobs will run on those nodes. This ensures that any performance measurements can be taken accurately and free from the effects of other users' jobs.
- 3. Running Jobs Across Multiple Machines: Slurm provides a framework to distribute computation across many physical machines, and integrates with existing parallel and distributed computing systems such as OpenMP and MPI.

In fact, NUS SoC uses SLURM across our entire Compute Cluster, as do other major institutions (Harvard, MIT), industry users (NASA, AWS, IBM), and even over half of the top ten supercomputers.



Logging in & Learning About Slurm

As in Lab 1, please ssh into one of our lab machines (soctf-pdc-001, 002, 003. 009, 010, or 011. If you have forgotten how to do so, please refer to the Lab 1 pdf).

Please continue to the next page once you have connected to a lab machine. The following commands will not work unless you are running them on a lab machine.

Step 1: Understanding our Slurm Cluster

Now that we understand the individual lab machines better, let's look at how our Slurm manages our cluster of machines.



Exercise 2

On your lab machine, run the following command and observe the output:

\$ sinfo

Your sinfo output will look similar to this (may not be exactly this exactly)

```
RTITION AVAIL
                                     idle soctf-pdc-[004-008,012-016,018-021,023-024]
                   3:00:00
            uр
s-4114
                                     idle soctf-pdc-[004-008]
                   3:00:00
 7700
                   3:00:00
                                     idle soctf-pdc-[012-016]
            up
                   3:00:00
                                     idle soctf-pdc-[018-019
                                     idle soctf-pdc-[020-021
            uр
                   3:00:00
            uр
```

Figure 2: Possible sinfo output

sinfo lists information about Slurm nodes and **partitions**. A partition is a logical grouping of compute nodes which can each be thought of as a job queue. For example, if a user submits a job to the xs-4114 partition above and asks for a single node, the job can run on any of soctf-pdc-004 to 008. The partition with a "*" symbol is the *default partition* that will be used to run a job if a partition is not explicitly specified.

Notice that we have created **separate partitions for each hardware type**. For example, the xs-4114 partition only contains Intel Xeon Silver 4114 nodes. This allows students to queue jobs to run only on a specific hardware type, which may be useful for performance measurements later on.

Lastly, take note that you *cannot ssh directly to these machines*. This allows for accurate performance measurement as students can be guaranteed that only Slurm-allocated jobs are running on those nodes.

Step 2: Running your first jobs!

We finally have enough information to run our first Slurm job. We can use the srun command to send very simple commands as jobs to the Slurm system.



Exercise 3

Run the following commands and observe the output:

- \$ hostname
- \$ srun hostname

The first command is a normal shell command that executes on your local host machine. You should see it print the name of the machine you are currently logged into. The second command uses srun (think of it as short for "Hey Slurm, please run this") to run the hostname command as a job on the Slurm system.

You should see that the second command prints the hostname of a node *other* than the one you are currently logged into. srun caused Slurm to allocate a node from the cluster to you, and it automatically ran the hostname executable on it, printing the hostname of the allocated node.

Congratulations - you just ran a job on a totally different machine by using Slurm!



Problems with running Slurm in your home directory

You might have seen an error printed by Slurm before it printed the hostname of the allocated node, something like:

slurmstepd-soctf-pdc-004: error: couldn't chdir to '/home/cristina': No such file or directory: going to /tmp instead.

The problem is this:

- 1. Assume you are currently at your home folder (e.g., /home/cristina) in your login node (run the command pwd to get the full current folder name).
- 2. If you run srun hostname, Slurm will execute your job on one of the Slurm nodes, and it will try to **change directory** (cd) to the same folder on that node (e.g., /home/cristina)
- 3. However, your home folder is not present on the Slurm nodes as they are only created when you login directly to that node. Therefore, Slurm will print the error above and change directory to /tmp instead.
- 4. To run a Slurm job without seeing errors, you should always run your jobs from a folder that is shared across all the Slurm nodes. We have created a folder for each of you at /nfs/home/your_username (e.g., /nfs/home/cristina in this example), which is shared across all nodes using a networked file system (NFS).



What you should do to run Slurm jobs without errors:

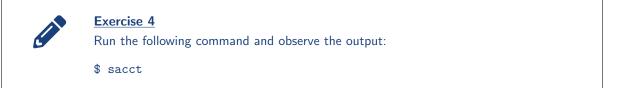
Please cd to your NFS folder before running any Slurm jobs. For instance, in this example (replace cristina with your own username):

\$ cd /nfs/home/cristina

Please note that you can put anything you want in your NFS folder and it will be accessible from any machine, including any of the other login nodes.

We will assume for the rest of this lab that you are running all your Slurm jobs from your NFS folder.

Getting back to running jobs on Slurm – let's actually see what Slurm allocated to us during our previous command.



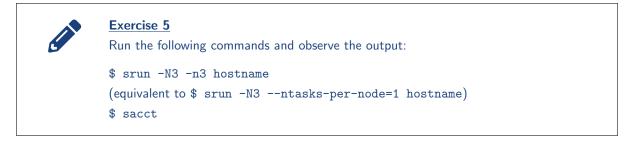
You might see something like this:

JobID	JobName	Partition	Account	AllocCPUS	State	ExitCode
258	hostname	all	staff	20	COMPLETED	0:0

Figure 3: Possible sacct output - your Account should be students, however

sacct shows us our past jobs and the Slurm "accounting" data for them, which tracks how many resources we used. Notice above that we allocated **20 CPUs** (your number may be different: equal to every CPU available in the node we ran on) for our simple hostname job (even though we didn't actually need 20 CPUs worth of computing power). As we had *exclusive access* to the node during our job, no other jobs could have run on it, so we are still "charged" by the Slurm fair-use accounting system for allocating 20 CPUs.

Let's get Slurm to stretch its legs by running our hostname command across multiple nodes.



Notice that this job printed out three *different* hostnames. The fact that we see the output of the hostname commands on our current node implies that Slurm collates all the standard output (and error) streams from the allocated nodes. By using the -N3 option, we have asked Slurm to run our job on 3 separate nodes, and -n3 indicates we want to only run 3 tasks in total (1 per node).

We can also get Slurm to run our jobs on specific partitions, or even specific nodes.



Exercise 6

Run the following command and observe the output:

\$ srun --partition i7-7700 bash -c "lscpu; hostname"

Verify that your job was executed on a node within the i7-7700 partition. We use bash -c to execute multiple commands within one Slurm job.

Choose your favorite hostname from our lab machines (make sure it's managed with Slurm by checking sinfo). Run this command (assuming you chose a hostname of soctf-pdc-0xx):

\$ srun -w soctf-pdc-0xx hostname

Verify that your job was executed on the node you specified.

Step 3: Running real batch jobs with sbatch

While srun is useful for testing and as a component of larger jobs, we rarely submit jobs directly this way. We usually submit jobs using a command like sbatch job.sh, where job.sh is a Slurm batch script written by you. Here are some reasons why:

- srun runs in an **interactive** and **blocking** mode your terminal blocks until the command completes, and you see the output of stdout and stderr in your terminal. sbatch runs in a **batch**, **non-interactive** mode, so you can submit your job and disconnect safely.
- srun requires you to list all your options as command line parameters (e.g., -w soctf-pdc-0xx, --ntasks-per-node=1). sbatch scripts can include all these options as part of the script itself, as we will see soon.

Let's write our first Slurm batch script!



Exercise 7

Create a file in your NFS directory called basic.sh. Observe the code listing below and duplicate it **exactly** into basic.sh. Save the file.



basic.sh

```
#!/bin/bash
#SBATCH --job-name=basic
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --mem=1gb
#SBATCH --time=00:00:30
#SBATCH --output=basic_%j.log
#SBATCH --error=basic_%j.log
#SBATCH --mail-type=ALL
echo "Running basic job!"
echo "We are running on $(hostname)"
echo "Job started at $(date)"
# Actual "job"
sleep 5;
# This is useful to know (in the logs) when the job ends
echo "Job ended at $(date)"
```

Notice that our job script has several lines starting with #SBATCH. These are *Slurm directives* which affect the configuration of our job: these should be mostly self-explanatory given your experience with srun. There are a few new options: --time which is limited to 30 seconds for this job, --job-name which gives your job a human readable name in the queue, and --output which tells Slurm what to call your logfile which has all the printouts from this run.

There are a few crucial points to notice before we finally run our script:



stdout/err file name

We are asking Slurm to collate the script output into a file called basic_%j.log, where Slurm will replace %j with your job ID. If your job ID was 231, your stdout and error will be in basic_231.log.

As the %j variable only applies inside the #SBATCH directives, in the rest of the shell script, the same value is available in the environment variable SLURM_JOB_ID.



Slurm Emails

We set the option --mail-type=ALL. This asks Slurm to send us an email when the job begins, ends, fails, etc. This email system is new for this semester, which allows you to know when your long running jobs (for assignments!) complete.

If you do not want emails, remove this option or set the mail type to NONE. To see other options, see man srun. If you have issues with emails (since this is a new feature), please let us know.

Now we can finally run our job script.



Exercise 8

Run our job script as follows, and be prepared to run a command immediately after:

\$ sbatch basic.sh

Now immediately run this command a few times until your job completes and observe the output:

\$ squeue

(alternatively, try watch -n 0.5 squeue) to auto-run the command every 0.5 seconds.

Finally, locate your logfile inside your NFS directory (use 1s) and look at its contents. If the job ID was 231, we could print the logfile with:

\$ cat basic_231.log

You should observe a few things:

- No output from sbatch: Note that sbatch itself did not write any output to your screen (besides the job ID), which is unlike srun's behavior. All output is redirected to the logfile and ultimately copied to your NFS directory.
- squeue output while waiting: Your job may have to wait for other jobs to complete. If it is waiting only because of a lack of resources (nodes), the REASON column will state "(Resources)". If it is waiting due to other jobs having priority over yours, it will state "(Priority)"
- squeue output while running: You should see your job in the running state ("R" under the "ST" column), and the time it has been executing. You can also see the node assigned to your job under the NODELIST(REASON) columns.

Step 4: Running custom executables with sbatch

In the past few examples, we have only been running executables that are *already pre-installed* on each of the cluster's machines (e.g., hostname, sleep, date, etc). This hides another important detail:

Your executables also must be present on every node Slurm runs your job on.

Let's first create an executable that is not already present on each machine.



Exercise 9

- Download the lab code to your NFS folder via wget https://www.comp.nus.edu.sg/ ~srirams/cs3210/L1_code.zip, then run unzip on it.
- 2. Compile the ex6-cond-example.cpp file into an executable called cond.
- 3. Run the cond executable normally (i.e., ./cond) and ensure that it is working normally as expected.

Since this executable is in your NFS home folder, it is now accessible on every machine!

Now, we will set up a Slurm job to run cond. We will make only very minor changes to the original basic.sh,



Exercise 10

Create a file in your NFS directory called cond.sh. Observe the code listing below and duplicate it into cond.sh. Save the file.



cond.sh

```
#!/bin/bash
#SBATCH --job-name=cond
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --mem=1gb
#SBATCH --time=00:00:30
#SBATCH --output=cond_%j.log
#SBATCH --error=cond_%j.log
#SBATCH --mail-type=ALL

echo "Running cond job!"
echo "We are running on $(hostname)"
echo "Job started at $(date)"
# NOTE: LINE BELOW CHANGED TO RUN COND
./cond
echo "Job ended at $(date)"
```

Ensure that the cond executable is in the same folder. Now, run this job with sbatch cond.sh and look at the output of the logfile (on your NFS directory).

The job should end successfully in approximately 10 seconds or so. Congratulations - you have just run your first custom executable on Slurm!

Step 5: Bringing it all together: Preliminary Performance Evaluation and Optimization

So far, you have experienced Slurm in a guided and structured manner. To conclude this tutorial, you will self-explore some the strengths that Slurm has (exclusive node access for performance evaluation, ease of code execution on different machines, etc) to perform a real task.



Exercise 11

This tutorial should have come with a file called pthread_addsub.cpp, which should also be accessible from https://www.comp.nus.edu.sg/~srirams/cs3210/T1_code.zip. Download that file to your NFS home folder of your current machine.

Compile that file with the command:

\$ g++ -o pthread_addsub pthread_addsub.cpp -pthread

Your goal: Use Slurm to investigate the time taken for the pthread_addsub program to run across all of our lab machine hardware types, and the reasons for what you observe.

Some guiding questions:

- Does this program (with its current settings) run fastest on our i7-7700, i7-9770, Xeon Silver, or Dual-Socket Xeon Silver machines? Why?
- What happens if you change the value of DELAY? Does this trend change or scale differently? Why?
- What happens if you change the value of ADD_THREADS and SUB_THREADS? Does this trend change or scale differently? Why?
- Is there an optimum value of ADD_THREADS and SUB_THREADS for a given type of machine? Why?

Use what you have learnt so far to write the necessary Slurm batch scripts to explore these questions. Consider using time measurement programs such as /usr/bin/time -vvv or time for now.



In case of technical issues

If there is something **operationally wrong** (not debugging related!) with the cluster (e.g., nodes are unexpectedly down, no internet access, your user account doesn't work with Slurm, etc):

Please email Alex (seowalex@u.nus.edu) and cc: Sriram (srirams@comp.nus.edu.sg) and ccristina@comp.nus.edu.sg

Conclusion and Summary

In this section, you have explored most of Slurm's basic features, such as:

- 1. Using sinfo to view partition information.
- 2. Using srun to run simple commands.
- 3. Using sbatch to run more complex jobs.
- 4. Using sacct and squeue to monitor job information.

There is much more to Slurm, and more that we will explore this semester. We will soon we how to use Slurm to run multithreaded/multiprocess code, OpenMP programs, and even distributed MPI programs!

Further reading

- 1. The **Slurm Student User Guide** (https://bit.ly/cs3210-slurm-guide) will contain the most updated information about our node allocations, policies, and advanced Slurm topics.
- 2. The Slurm official quickstart guide (https://slurm.schedmd.com/quickstart.html).
- 3. The man pages for common Slurm commands such as (sacct, sbatch, scancel, \dots) .