Parallel computing infrastructure

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July 25th 2017
Open Source Macroeconomics Laboratory Boot Camp – BFI/UChicago

Outline

- Make first steps on a Linux Cluster
  Login via ssh, remotely, short overview of basic unix commands like cd, pwd, cp, scp,...

- Submit jobs to the queue
  Slurm

- Get lecture notes
  Clone a git repository

https://rcc.uchicago.edu

For this course, we use the Uchicago's **Midway compute cluster**.

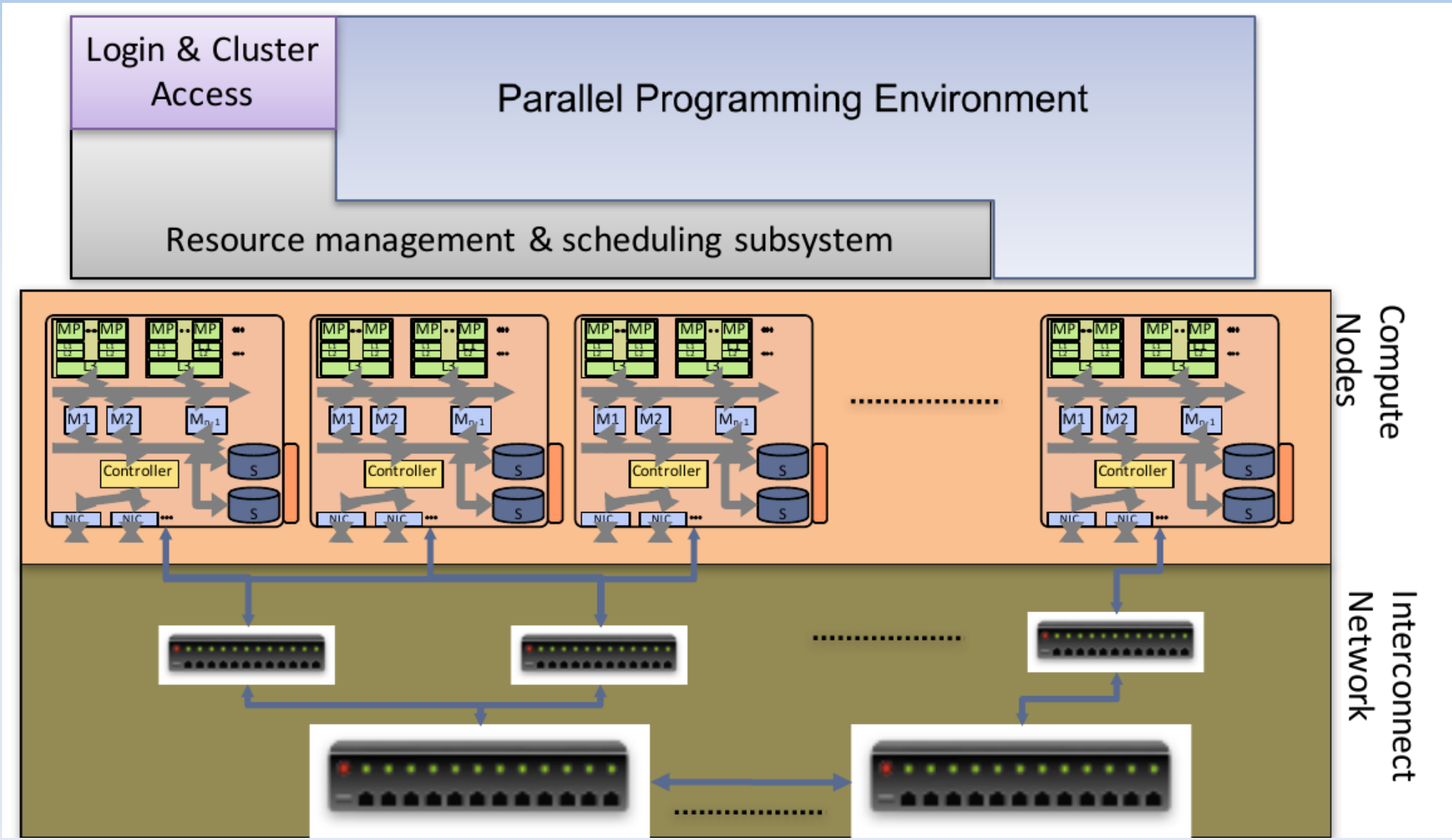
It is managed by the **R**esearch **C**omputing **C**entre

→ Its setup is very similar to any other top system

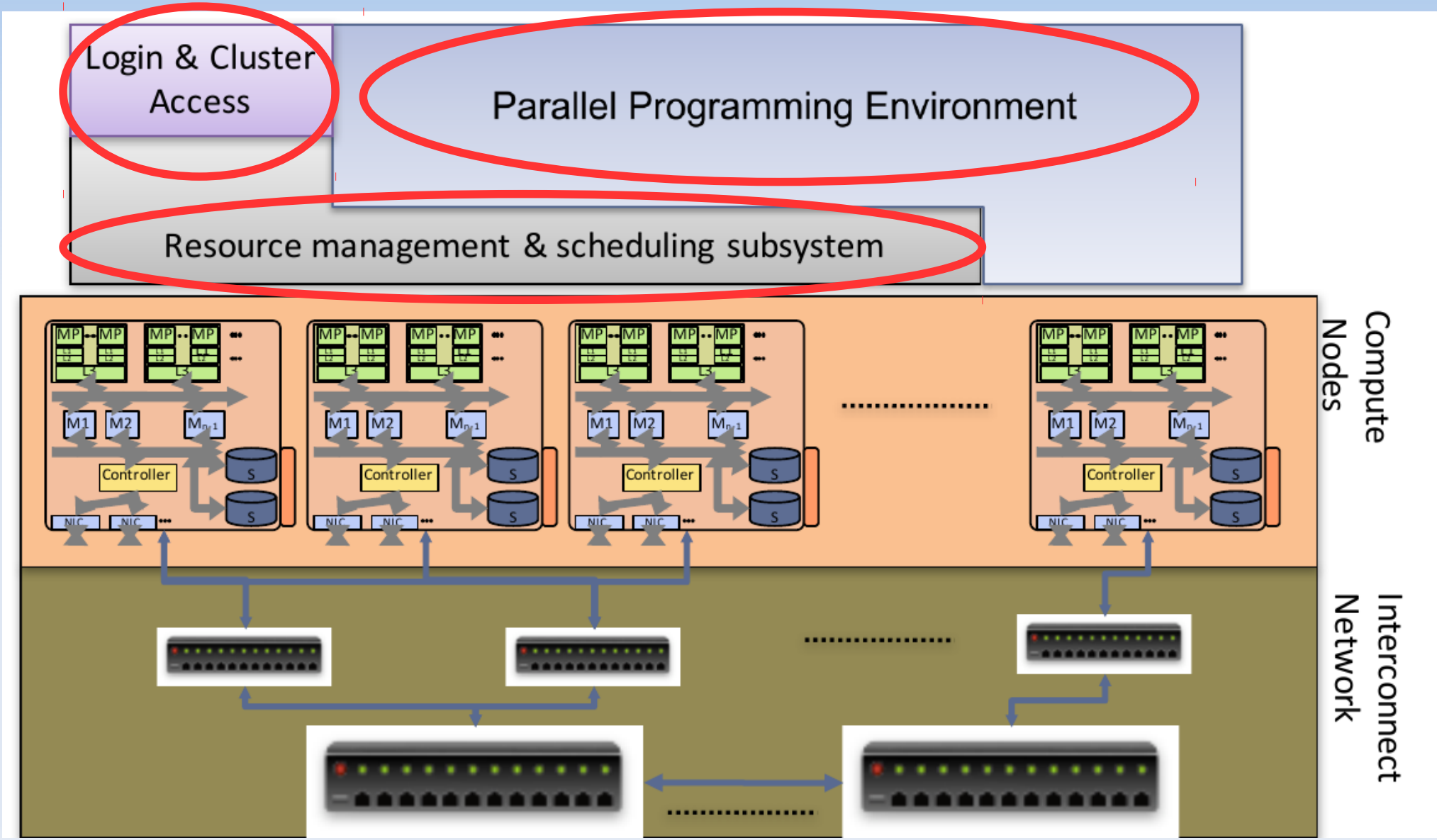
For the RCC Manual see the documentation site at

http://docs.rcc.uchicago.edu

An abstract compute cluster



An abstract compute cluster



The size of a HPC cluster

Credit – https://bluewaters.ncsa.illinois.edu/

Login for participants

- If you don't have an account on Midway request one (infrastructure for this course)
  https://rcc.uchicago.edu/docs/using-midway/index.html

- For MS-Windows users: Download and install Putty
  → http://the.earth.li/~sgtatham/putty/latest/x86/putty.exe

  → Download and install Winscp

  → http://winscp.net/download/winscp576setup.exe

Basic Linux commands (1)

Command	Description
pwd	Print name of current/working directory
cd [Directory]	Change directory (no directory → change to home)
ls [Directory]	List directory contents (no directory → list current)
cat FILE	Concatenate files and print on the standard output
mkdir DIRECTORY	Make directories
mkdir -p DIRECTORY	Make directories, make parent directories as needed
cp SOURCE... DIRECTORY	Copy files and directories
cp -r SOURCE... DIRECTORY	Copy files and directories, copy directories recursively
mv SOURCE... DIRECTORY	Move (rename) files
man COMMAND	An interface to the on-line reference manuals

Basic Linux commands (2)

Command	Description
ssh -X foo@host.com	OpenSSH SSH client (remote login program), access to host.com with user foo
scp foo@host.com:/home/bar ./	Secure copy (remote file copy program), copy file bar from /home on host.com to directory
scp bar foo@host.com:/home/	Secure copy (remote file copy program), copy file bar from the local host to /home on host.com
git clone git@github.com:whatever folder-name	The stupid content tracker, Clone a repository (whatever) into a new directory (folder-name).
git checkout	Checkout a branch or paths to the working tree.

Other clusters – Step-by-Step

- First login, change password and get lecture notes (MS-Windows: Putty, Linux/MacOS: Terminal)

```
> ssh -X USERNAME@midway1.rcc.uchicago.edu
> passwd  #Change password for USERNAME.
  (current) UNIX password:
  Enter new UNIX password:
  Retype new UNIX password:
  Password changed
> git clone ***lecture-folder*** #clone lecture
> cd ***lecture_folder***  #go into folder
> ls # list content of folder
```

Step-by-Step (2)

→ **Perform some basic operations on the cluster**

```
> ssh -X USERNAME@hpc.alphacruncher.net
> pwd
/home/USERNAME
> mkdir -p firstFolder/secondFolder
> ls
FirstFolder
> ls firstFolder
secondFolder
> cd firstFolder
> pwd
/home/USERNAME/firstFolder
> ls
secondFolder
> exit
```

Step-by-Step (3)

- How to copy folders and files to your PC?
- MS-Windows, start WinSCP

  → Host-Name: `midway1.rcc.uchicago.edu`

  → User: `USERNAME`
- Linux/MacOS, replace /YOUR-LOCAL-PATH/

  → with /home/LOCAL-LOGIN-NAME/ for linux

  → with /Users/LOCAL-LOGIN-NAME/ for MacOS

```
>scp -r USERNAME@midway1.rcc.uchicago.edu:/home/simonsch/YOUR-LOCAL-PATH/ .
```

Step-by-Step (4)

- Copy folders and files from your notebook

  create a file named firstFile in firstFolder

  → MS-Windows: use WinSCP to copy the directory back

  → Linux/MacOS

```
>scp -r /YOUR-LOCAL_PATH/firstFolder/FILENAME USERNAME@midway1.rcc.uchicago.edu:
```

- Check that file is there by

```
>ssh -X midway1.rcc.uchicago.edu
> ls
FILENAME
>cat FILENAME  #shows content of file
```

Environment setup

Supporting diverse user community requires supporting diverse tool sets (different vendors, versions of compilers, debuggers, libraries, apps, etc)

User environments are customized via modules system (or softenv)

```
> module avail #shows list of available modules

> module list  #shows list of modules loaded by user

> module load module_name #load a module e.g. compiler

> module unload module_name #unload a module
```

Example – environment setup

```
> vi ~/.bashrc    #here you can setup/store your profile
module load openmpi  #always load this lib upon login
```

Using an editor on a cluster

Compute clusters like Midway's infrastructure have a variety of simple text editors available.

→ vi, vim

```
>vi helloworld.cpp

#include <iostream>

int main()
{
  std::cout << "Hello World!"  << std::endl;

  return 0;
}
```

More low bandwidth editors

Depending on network and preference, you may want to use an editor without a graphical user interface; common options:

- vi/vim
- emacs
- nano

emacs:

Undo: C-_

Find/create file: C-x C-f

Save file: C-x C-s

Exit Emacs: C-x C-c

Quit: C-g

Two modes – insertion and command mode
Insertion mode begins upon an insertion
[ESC] returns to command mode

Command mode options:
:w save
:wq save and exit
:q exit as long as there are no changes
:q! exit without saving

Insertion:
i (insert before cursor)
a (append)

Deletion: x
Motion: h (left) k (up)
j (down) l (right)

Compiling & running code interactively

→ go to OSM_Lab/HPC_day1/code_day_1 → cd OSM_Lab/HPC_day1/code_day_1

If your program is only in one file (a hello-world program, or any simple code that doesn't require external libraries), the compilation is straightforward:

```
> gfortran helloworld.f90 -o helloworld.exe #Fortran
```

```
> g++ helloworld.cpp -o helloworld.exe       #C++
```

Once you produced the executable, you can run it (serial code) by

```
> ./helloworld.exe

> hello
```

Example: ...

*later on, we will also will link in libraries as well as use optimization flags.

Compiling Code with a makefile

In case your program consists of many routines (files), compiling by hand gets very cumbersome

```
> g++  -o abc abc.cpp a.cpp b.cpp c.cpp
```

→ **A makefile is just a set of rules to determine which pieces of a large program need to be recompiled, and issues commands to recompile them**

→ For large programs, it's usually convenient to keep each program unit in a separate file. Keeping all program units in a single file is impractical because a change to a single subroutine requires recompilation of the entire program, which can be time consuming.

→ When changes are made to some of the source files, only the updated files need to be recompiled, although all relevant files must be linked to create the new executable.

Compiling Code with a makefile (2)

Basic makefile structure: a list of rules with the following format:

target ... : prerequisites ...
<TAB> construction-commands

A **“target”** is usually the name of a file that is generated by the program (e.g, executable or object files). It can also be the name of an action to carry out, like “clean”.

A “prerequisite” is a file that is used as input to create the target.

```
# makefile : makes the ABC program

abc : a.o b.o c.o  ### by typing „make“, the makefile generates an executable denotes as „abc“

g++ -o abc a.o b.o c.o

a.o : a.cpp

        g++ -c a.cpp

b.o : b.cpp

        g++ -c b.cpp

c.o : c.cpp

        g++ -c c.cpp

clean :   ### by typing „make clean“, the executable, the *.mod as well as the *.o files are deleted

        rm *.mod *.o abc
```

Compiling Code with a makefile (3)

- By default, the first target listed in the file (the executable abc) is the one that will be created when the make command is issued.
- Since **abc** depends on the files **a.o, b.o** and **c.o**, all of the .o files must exist and be up-to-date. make will take care of checking for them and recreating them if necessary. Let's give it a try!
- Makefiles can include **comments** delimited by hash marks (#).
- A **backslash (\)** can be used at the end of the line to continue a command to the **next physical** line.
- The make utility **compares** the modification time of the target file with the modification times of the prerequisite files.
- Any prerequisite file that has a more recent modification time than its target file forces the target file to be recreated.

→ A lot more can be done with makefiles (beyond the scope of this lecture)

Slurm Workload Manager

http://slurm.schedmd.com/

Simple Linux Utility for Resource Management (SLURM).

Open-source workload manager designed for Linux clusters of all sizes.

Provides three key functions:

1) It allocates exclusive and/or non-exclusive access to resources (computer nodes) to users for some duration of time so they can perform work.

2) It provides a framework for starting, executing, and monitoring work (typically a parallel job) on a set of allocated nodes.

3) It arbitrates contention for resources by managing a queue of pending work.

```
> sbatch submit_helloworld.sh (submit job)
> squeue -u NAME   (status of job)
> scancel JOBID      (cancel job)
```

A minimal „slurm“ file

```
#!/bin/bash -l

#SBATCH --ntasks=1     ## how many cpus used here

#SBATCH --time=01:00:00  ## walltime requested

#SBATCH --output=slurm_test.out ## output file
#SBATCH --error=slurm_test.err     ## error


### executable
./helloworld.exe
```

Run an executalbe on MIDWAY

https://rcc.uchicago.edu/docs/running-jobs/index.html#running-jobs

```
#!/bin/bash
# a sample job submission script to submit an MPI job to the sandyb partition on Midway1

# set the job name to hello
#SBATCH --job-name=hello

# send output to hello-world.out
#SBATCH --output=hello-world.out

# receive an email when job starts, ends, and fails
#SBATCH --mail-type=BEGIN,END,DAIL

# this job requests 1 core. Cores can be selected from various nodes.
#SBATCH --ntasks=1

# there are many partitions on Midway1 and it is important to specify which
# partition you want to run your job on. Not having the following option, the
# sandby partition on Midway1 will be selected as the default partition
#SBATCH --partition=sandyb

# Run the executable (serial code for now)
./helloworld.exe
```

Run on MIDMAY

→ Try NOW on MIDWAY

```
> cd OSM_Lab/HPC_day1/code_day_1

> make -f makefile_cpp

> sbatch submit_midway.sh
```

→What is the output? Play with it a bit.

Nodes available on Midway

Midway1 contains a total of 13,500 cores across 792 nodes, and 1.5 PB of storage.

Midway2 adds 10,696 cores across 382 nodes, and 2.2 PB of storage.

Types of Compute Nodes

The Midway compute cluster is made up of compute nodes with a variety architectures and configurations. A **partition** is a collection of compute nodes that all have the same, or similar, architecture and configuration. Currently, Midway has the following partitions:

Cluster	Partition	Compute cores (CPUs)	Memory	Other configuration details
midway1	westmere	12 x Intel X5675 3.07 GHz	24 GB	
	sandyb	16 x Intel E5-2670 2.6GHz	32 GB	
	bigmem	16 x Intel E5-2670 2.6GHz	256 GB	
		32 x Intel E7-8837 2.67GHz	1 TB	
	gpu	16 x Intel E5-2670 2.6GHz	32 GB	2 x Nvidia M2090 or K20 GPU
		20 x Intel E5-2680v2 2.8GHz	64 GB	2 x Nvidia K40 GPU
	mic	16 x Intel E5-2670 2.6GHz	32 GB	2 x Intel Xeon Phi 5100 coprocessor
	amd	64 x AMD Opteron 6386 SE	256 GB	
	ivyb	20 x Intel E5-2680v2 2.8GHz	64 GB	
midway2	broadwl	28 x Intel E5-2680v4 2.4GHz	64 GB	
	bigmem2	28 x Intel E5-2680v4 @ 2.4 GHz	512 GB	
	gpu2	28 x Intel E5-2680v4 @ 2.4 GHz	64 GB	4 x Nvidia K80 GPU

You can also retrieve a summary of the partitions on Midway using the **sinfo** command:

```
$ sinfo -s
```

In the **sinfo** summary, the right-most number in the "NODES" column gives the total number of nodes in each partition. This summary also lists partitions that are reserved for use by certain labs.

Clone a git repository

```
>ssh -X USERNAME@midway1.rcc.uchicago.edu
```

> git clone …. # clone the git repository

> cd .. # go into the repository

> ls … # check that all is there