CSC4005 Parallel Programming Tutorial 1

Bokai Xu, 119010355@link.cuhk.edu.cn

Tutorial Schedule

- Tuesday 18:00-18:50 TA307
- Wednesday 20:00-20:50 TA307
- Other sessions are cancelled.

Office Hour Schedule

| | Time | Venue |
|---------------------------------------|-----------------------|--|
| Weibin Chen (TA) | 9:00-10:00 Wednesday | SDS office on the floor 4 of ZhiXin building |
| Yihan Liu (TA) | 19:00-20:00 Thursday | Online, zoom id: 613-456- 4907 |
| Yuxuan Liu (TA) | 20:00-21:00 Thursday | Online, zoom id: 394-118- 1035 |
| Bokai Xu and Zhixin Luoyang (USTF) | 21:00-22:00 Wednesday | TA307 |

Outline of Tutorial 1

- About Linux
- Basic Linux Commands
- Development environment
- CSC4005 Virtual Machine setup
- C++ environment for parallel programs
- Compiler for parallel programs
- Run C++ parallel programs
- HPC (High Performance Computing) cluster
- IDE

Why linux

- High performance computing clusters serve multiple users simultaneously, linux works well.
- Linux are very friendly to cpp programming, a lot of cpp libraries provided on linux.
- Linux has a small size and high efficiency.

20% of interviewees told us that they don't know how to use linux. So we add a linux part.

How to use linux?



- What is your purpose to use Linux?
 - We want to utilize the capability of hardwares (like CPU, GPU, hard disk, network ...)
- How to use?
 - Hardware is wrapped by linux kernel, and kernel is wrapped by shell (terminal). Terminal is an interface layer.
 - We can only use terminal.

The Matrix





- The Matrix is a high performance computer, people who live in reality can only interact with the Matrix by using a terminal.
- GUI Desktop is indeed a program running on Linux. It is a enchanced version of terminal. But it is essentially a terminal.

A classical terminal

| | Image: Sec4005-v6 | Ð |
|---------------------------------------|-------------------|-------|
| 🏶 Applications Places | Mon 11:27 🛔 | 1) () |
| | | |
| | | |
| | | |
| | | |
| | | |
| Trasn Fiome CSC4005_2022Fatt_ Demo | | |
| | | |
| | | |
| Visual Studio Code | | |
| | | |
| Terminal | | |
| | | |
| | | |
| | | |
| | 7 | |
| | CENTOS | |
| | | |

A classical terminal



pwd

 Use the pwd command to find out the path of the current working directory (folder) you're in. The command will return an absolute (full) path, which is basically a path of all the directories that starts with a forward slash (/). An example of an absolute path is /home/username.

[csc4005@localhost ~]\$ pwd
/home/csc4005
[csc4005@localhost _lt



• To navigate through the Linux files and directories, use the **cd** command. It requires either the full path or the name of the directory, depending on the current working directory that you're in.

[csc4005@localhost ~]\$ cd ~/Desktop/CSC4005 2022Fall_Demo
[csc4005@localhost CSC4005_2022Fall_Demo]\$

```
[csc4005@localhost CSC4005_2022Fall_Demo]$ cd ..
[csc4005@localhost Desktop]$
```

• The **Is** command is used to view the contents of a directory. By default, this command will display the contents of your current working directory.

| [csc4005 | - @localhost | CSC4005_20 | 022Fall | Demo]\$ | 5 ls | _ | _ | |
|----------|-----------------|------------|---------|----------|------|----------|------|-----------|
| gui_demo | mpi_demo | mpi_gui_d | demo o | penmp_d | lemo | pthread_ | demo | README.md |
| [csc4005 | @localhost | CSC4005_20 | 022Fall | _Demo]\$ | 5 | | | |

Run an executable

- Go to a proper directory
- Make sure you refer to the right executable
- Some program are global (you have to add it to PATH env variable)



Interrupt a program

- so it will kill itself:
- Ctrl+C

```
[csc4005@localhost ~]$ cd /home/csc4005/Desktop/CS(
[csc4005@localhost gui_demo]$ ls
gui_hello gui_hello.cpp hello_gui.png readme.md
[csc4005@localhost gui_demo]$ ./gui_hello
^C
[csc4005@localhost gui_demo]$
```

Kill a process

- pkill [process_name]
- Kill -9 [pid]

htop

| • • • | b 🛅 b | okesyo - | – roc | ot@csc | 4005_s | lurm_r | noc | de_01 | l:~ — | ssh root@ | 10.26.200.22 — |
|---|-----------|---|--|---|--|--|---|-----------------------|--|--|---|
| 1 [2 [3 [4 [5 [6 [7 [8 [9 [10 [Mem[Swp[] | | 0.0%] 3.2%] 0.0%] 0.0%] 5.8%] 0.0%] 0.0%] 1.3%] 0.6%] | 11 12 13 14 15 16 17 18 19 20 | [[[[[[4.30G/ 279M/ | 0.0%] 0.0%] 0.0%] 0.6%] 0.0%] 4.5%] 0.0%] 0.6%] 0.6%] 0.6%] (92.9G] /16.0G] | 21 22 23 24 25 26 27 28 29 30 Tas Loa | [[] [[[[[[[[[[[[]]] | : 140 avera | 0.65 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 | 31 32 33 33 33 34 35 36 37 38 39 40 2 40 2 40 | 0.0%] 0.0%] 0.0%] 0.0%] 0.0%] 0.0%] 0.0%] 0.0%] 0.0%] |
| | | | | | | Upt | im | e: 28 | 3 day | /s(!), 13 | :26:19 |
| PID | USER | PRI | NI | VIRT | RES | SHR | S | CPU% | MEM% | TIME+ | Command |
| 226911 | tidb | 20 | 0 | 3969M | 2169M | 155M | S . | 15.5 | 2.3 | 5h31:28 | bin/tikv-server |
| 227169 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 6.5 | 2.3 | 1:13.49 | bin/tikv-server |
| 133205 | tidb | 20 | 0 | 38388 | 21408 | 2796 | S | 3.9 | 0.0 | 297h | bin/blackbox_exp |
| 22/131 | tidb | 20 | 0 | 3969M | 2169M | 155M | 5 | 3.9 | 2.3 | 0:54.60 | bin/tikv-server |
| 227987 | root | 20 | 0 | 120M | 2756 | 1388 | R | 2.6 | 0.0 | 0:00.67 | htop |
| 227273 | tidb | 20 | 0 | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 31:09.01 | bin/tikv-server |
| 22/165 | tidb | 20 | 0 | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 27:42.12 | bin/tikv-server |
| 226937 | tidb | 20 | 0 | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 27:36.98 | bin/tikv-server |
| 133250 | tidb | 20 | 0 | 38388 | 21408 | 2796 | S | 0.6 | 0.0 | 5h41:55 | bin/blackbox_exp |
| 226927 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 12:36.84 | bin/tikv-server |
| 226928 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 13:11.48 | bin/tikv-server |
| 35055 | root | 9 | -11 | 877M | 3960 | 2716 | S | 0.6 | 0.0 | 0:10.76 | /usr/bin/pulseau |
| 133249 | tidb | 20 | Θ | 38388 | 21408 | 2796 | S | 0.6 | 0.0 | 5h31:42 | bin/blackbox_exp |
| 226940 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 5:28.78 | bin/tikv-server |
| 227123 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 4:18.25 | bin/tikv-server |
| 227248 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 0.6 | 2.3 | 2:05.07 | bin/tikv-server |
| 227249 | tidb | 20 | Θ | 3969M | 2169M | 155M | S | 0.0 | 2.3 | 12:54.55 | bin/tikv-server |
| 133210 | tidb | 20 | Θ | 38388 | 21408 | 2796 | S | 0.0 | 0.0 | 5h36:35 | <pre>bin/blackbox_exp</pre> |
| 133221 | tidb | 20 | 0 | 38388 | 21408 | 2796 | S | 0.0 | 0.0 | 5h22:27 | <pre>bin/blackbox_exp</pre> |
| 133330 | tidb | 20 | 0 | 38388 | 21408 | 2796 | S | 0.0 | 0.0 | 5h20:43 | <pre>bin/blackbox_exp</pre> |
| 122727 | tidh | 20 | 6 | 28388 | 21/08 | 2796 | C | 0 0 | 0 0 | 5630.00 | hin/hlackhov ovn |

ls -lh

| 🖲 😑 💿 bokesyo — root(| @csc40 | 05 | _slurm | _node_01:~ — ssh root@10.26.200.22 — |
|---------------------------------------|---------|------|--------|--------------------------------------|
| [[root@csc4005 slurm node 0 | 1 ~]#] | ls · | -lh | |
| total 3.7G | | | | |
| drwxr-xr-x. 2 root root | 21 Sep | 8 | 14:06 | Desktop |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Documents |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Downloads |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Music |
| -rwxrr 1 root root 34 | 8M Sep | 8 | 08:07 | NVIDIA-Linux-x86_64-515.65.01.run |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Pictures |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Public |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Templates |
| drwxr-xr-x. 2 root root | 6 Sep | 8 | 05:47 | Videos |
| -rw 1 root root 4. | 3K Nov | 25 | 2021 | anaconda-ks.cfg |
| -rwxrr 1 root root 3. | 3G Jul | 29 | 05:31 | cuda_11.7.1_515.65.01_linux.run |
| -rw 1 root root 4. | 3K Nov | 25 | 2021 | original-ks.cfg |
| -rw 1 root root | 8 Sep | 8 | 05:39 | root |
| drwxr-xr-x. 8 root root | 89 Sep | 5 | 21:54 | rpmbuild |
| drwxr-xr-x. 2 root root | 70 Sep | - 7 | 22:58 | slurm_config |
| drwxr-xr-t. 2 root root | 6 Sep | 8 | 05:47 | <pre>thinclient_drives</pre> |
| <pre>[root@csc4005_slurm_node_0</pre> | 1~]# | | | |

ssh

• ssh [user]@[IP]

| [(base) bokesyo@bokesyo-mac ~ % ssh 119010355@10.26.200.21 [119010355@10.26.200.21's password: [ast login: Mon Sep 12 12:21:33 2022 from 10 30 120 43 |
|---|
| <pre>-bash: warning: setlocale: LC_CTYPE: cannot change locale (UTF-8): No such fi or directory [119010355@csc4005_slurm_master ~]\$</pre> |
| |
| |
| |
| |

scp

- Copy files from one machine to another.
- scp [user]@[IP of remote machine]:[source file address on remote machine] [target file address on local machine]
- scp [target file address on local machine] [user]@[IP of remote machine]:[source file address on remote machine]

Suggested Development Environment

| | MPI, pthreads, openMP, GUI | CUDA |
|---|---|-----------------------------------|
| If you are using Windows | Virtual Machine for coding and debug, ssh+HPC cluster for large scale experiment | ssh+HPC cluster for everything |
| If you are using Mac (intel chip) | Virtual Machine for coding and debug, ssh+HPC cluster for large scale experiment | ssh+HPC cluster for everything |
| If you are using Mac (Apple Silicon) | ssh+HPC cluster for everything | ssh+HPC cluster for everything |

CSC4005 Virtual Machine Setup

- You need a virtual machine software
- For windows users:
 - You can use either VirtualBox (free) or VMware Workstation (paid)
- For Mac (intel) users:
 - You can try VMware Fusion Player (free) or VirtualBox (free)
- For Mac (Apple silicon) users:
 - You are suggested to use HPC cluster for everything (we will provide special guidance for you)

C++ libraries on linux

- Compiling parallel programs requires external libraries (previously we only use C++ standard library in CSC3002)
- Install external libraries
 - sudo yum install xxxx
- External libraries are stored in
 - Include directory (.h):
 - /usr/include
 - Library directory (.so binary compiled code):

18 19 20

- /usr/lib
- /usr/lib64

```
mpi_demo > 🚱 mpi_hello.cpp > ...
      #include <mpi.h>
      #include <stdio.h>
      #include <math.h>
      int main(int argc, char** argv)
           int myid, numproces;
           int namelen;
  8
           char processor name[MPI MAX PROCESSOR NAME];
  9
           MPI Init(&argc,&argv);
 10
           MPI Comm rank(MPI COMM WORLD,&myid);
 11
           MPI Comm size(MPI COMM WORLD,&numproces);
 12
           MPI_Get_processor_name(processor_name,&namelen);
 13
           fprintf(stdout, "hello world! Process %d of %d on %s
 14
                   myid,numproces,processor name);
 15
           MPI Finalize();
 16
 17
           return 0;
```

C++ compilers on linux

- Suggested: g++ (for both C and C++)
- Function1: Compilation
 - Make your code binary code for CPU to execute.

• Function2: Linking

• Link your compiled program with external libraries (*.so) to make the program executable. Otherwise some functions will be undefined. Error will occurs.

C++ compilers for CSC4005

We will have four programming projects in CSC4005, all frameworks needed are listed here:

| | compiler | |
|---------------------------------|--------------------------|-----------------------------|
| MPI | mpic++ | It is a wrapped g++ command |
| OpenMP, pthread | g++ | |
| GUI | g++ | |
| CUDA | nvcc | |
| Hybrid Compilation (CUDA & C++) | nvcc & g++ -> g++ linker | |

C++ libraries on linux

- Using external libraries
- When you are writing your MPI parallel programs, you have to include <mpi.h>
- When you compile your mpi code, you should use mpic++ as compiler, it will help you find mpi.h and link mpi runtime library to your program.
- You can also use
- g++ -m64 -O2 -g -pipe -Wall -Wp,-D_FORTIFY_SOURCE=2 -fexceptions -fstackprotector-strong --param=ssp-buffer-size=4 grecord-gcc-switches -m64 -mtune=generic -fPIC -Wl,-z,noexecstack -I/usr/include/mpich-3.2x86_64 -L/usr/lib64/mpich-3.2/lib -lmpicxx -Wl,rpath -Wl,/usr/lib64/mpich-3.2/lib -Wl,--enablenew-dtags -Impi

| mpi_dem | io > 🚱 mpi_hello.cpp > |
|---------|---|
| 1 | #include <mpi.h></mpi.h> |
| 2 | #include <stdio.h></stdio.h> |
| 3 | #include <math.h></math.h> |
| 4 | |
| 5 | <pre>int main(int argc,char** argv)</pre> |
| 6 | { |
| 7 | int myid,numproces; |
| 8 | int namelen; |
| 9 | char processor_name[MPI_MA |
| 10 | <pre>MPI_Init(&argc,&argv);</pre> |
| 11 | MPI_Comm_rank(MPI_COMM_WOR |
| 12 | MPI_Comm_size(MPI_COMM_WOR |
| 13 | MPI_Get_processor_name(pro |
| 14 | fprintf(stdout,"hello worl |
| 15 | myid,numproces,pro |
| 16 | <pre>MPI_Finalize();</pre> |
| 17 | |
| 18 | return 0; |
| 19 | } |
| 20 | |

C++ libraries on linux

g++ -I/usr/include -L/usr/local/lib -L/usr/lib -lglut -IGLU -IGL -lm gui_hello.cpp -o gui_hello

🔄 gui_hello.cpp 🗙 qui_demo > 🚱 qui_hello.cpp > ... #include <GL/glut.h> 2 void display() glClear(GL COLOR BUFFER BIT); glBegin(GL POLYGON); glVertex2f(-0.5,-0.5); glVertex2f(-0.5,0.5); glVertex2f(0.5,0.5); 10 glVertex2f(0.5,-0.5); 11 glEnd(); 12 13 glFlush(); 14 15 16 int main(int argc, char **argv) 17 18 glutInit(&argc,argv); 19 glutCreateWindow("Hello,world!"); 20 glutDisplayFunc(display); 21 glutMainLoop(); 22 23 24 25

C++ parallel program compilation

You need to use CSC4005 VM or HPC cluster to compile.

• If you have finsihed setting up your VM, open Terminal on your VM.



cd ~/Desktop/CSC4005_2022Fall_Demo/mpi_demo # switch to code folder mpic++ mpi_hello.cpp -o mpi_hello # compile command



C++ parallel program compilation

- For those students unable to run a VM, ssh to HPC clusters.
 - ssh 119010355@10.26.200.21 Password: csc4005
 - This is only a test account, we will distribute your own account next week.

mkdir 119010355 # change to your student id cd 119010355 # change to your student id git clone https://github.com/bokesyo/CSC4005_2022Fall_Demo.git # download our demo script chmod -R 777 CSC4005_2022Fall_Demo # make those files executable cd CSC4005_2022Fall_Demo/mpi_demo # switch to code folder mpic++ mpi_hello.cpp -o mpi_hello # compile command • • • • bokesyo – demo@csc4005_slurm_master:~/119010355/CSC4005_2022...

[[demo@csc4005_slurm_master mpi_demo]\$ mpic++ mpi_hello.cpp -o mpi_hello [[demo@csc4005_slurm_master mpi_demo]\$ ls mpi_hello mpi_hello.cpp mpi_walker mpi_walker.cpp readme.md [[demo@csc4005_slurm_master mpi_demo]\$ ls -lh total 148K -rwxrwxr-x. 1 demo demo 29K Sep 13 02:37 mpi_hello -rwxrwxrwx. 1 demo demo 488 Sep 13 02:30 mpi_hello.cpp -rwxrwxrwx. 1 demo demo 100K Sep 13 02:30 mpi_walker -rwxrwxrwx. 1 demo demo 6.0K Sep 13 02:30 mpi_walker.cpp -rwxrwxrwx. 1 demo demo 911 Sep 13 02:30 readme.md [demo@csc4005_slurm_master mpi_demo]\$

Do not kill this terminal!

C++ parallel program compilation

• If no error occurred at compilation step, let's continue.

Run your C++ parallel programming on VM or HPC cluster

• For those students who can use VM

mpirun -np 4 ./mpi_hello

• For those students unable to run a VM

salloc -n4 # request 4 cores on compute nodes to run your compiled program mpirun -np 4 ./mpi_hello



Run your C++ parallel programming on VM or HPC cluster

• If your output contains process 0,1,2,3, let's continue.

Configuration

- 1 login node
 - 20 Intel CPU cores (40 logic cores)
 - 100GB RAM
 - 1 Nvidia Quadro RTX 4000 GPU
- 30+ compute node
 - Each compute node has:
 - 20 Intel CPU cores (40 logic cores)
 - 100GB RAM
 - 1 Nvidia Quadro RTX 4000 GPU

 Topology: one login node (controller) and 30+ compute node.



Cite: https://hpc.ilri.cgiar.org/using-the-cluster

- Scheduler: slurm
- Basic command:
- sbatch
- salloc
- more on Tutorial 2

Cite: https://aws.amazon.com/blogs/hpc/using-the-slurm-rest-api-to-integrate-with-distributed-architectures-on-aws/



- Underlying process:
- Slurm transfers your shell script to compute node (same environment has been configured on each compute node and file system is shared, so your shell script can run on compute node). The output will be stored in a log file. Slurm will reserve the resources you applied for your parallel programs.
- A parallel program can create many processes on the same machine (processes communicate within that machine) or on multiple machines (processes communicate by networks)

- Login node is for you to:
- Use file system (store your code and other files)
- Debug your code
- Compile your code
- Apply for resources and create computing jobs using slurm
- Normal users cannot directly access compute node.

- Your personal directory on HPC cluster controller node
- /nfsmnt/[your student id]/
- You can access your personal files, while others cannot.
- /nfsmnt/ is shared among all nodes (both controller node and compute node) in cluster, when you submit your job, make sure that your program is inside /nfsmnt/[your student id]/. Then compute node can access your program.

About IDE

- 1) For Windows users, if you don't want to waste time on setting up port forwarding/Xming X11 forwarding..., we suggest using CSC4005 Virtual Machine.
- 2) For Mac (Intel chip) users, if you don't want to waste time on setting up port forwarding/XQuartz X11 forwarding..., we suggest using CSC4005 Virtual Machine.
- 3) For Mac (Apple Silicon) users, you can try if our VM can run on your PC, if not, please see special guidance for you on BB/Content/CSC4005 Development Platform.
- 4) For Linux Geeks, you can refer special guidance for you on BB/Content/CSC4005 Development Platform.
- 5) Other cases: You can DIY your development platform~