High Performance Computing (HPC) Club Training Session

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Outline

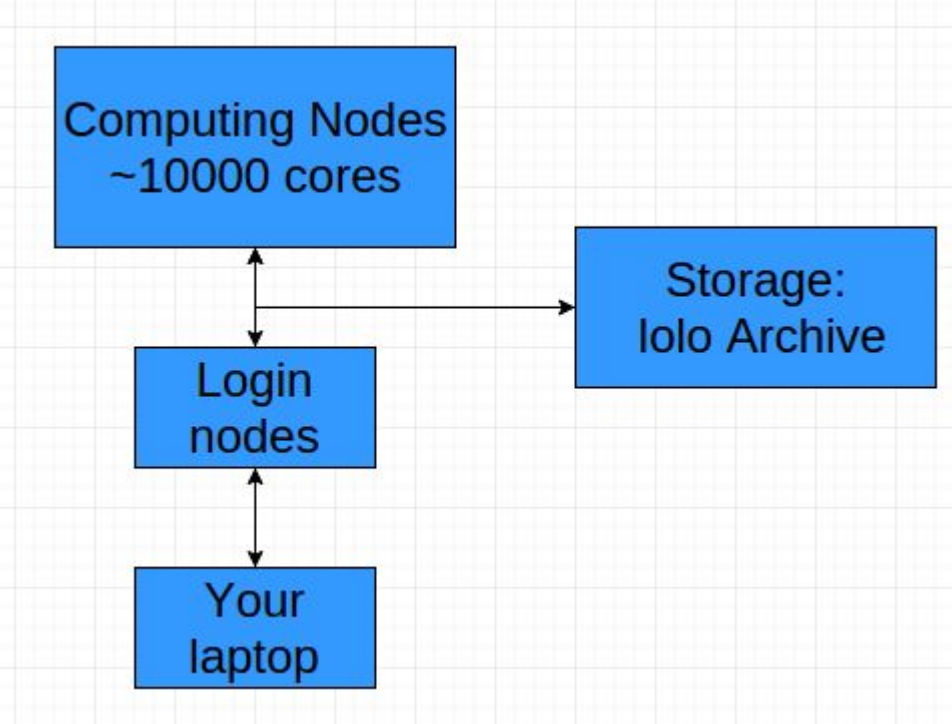
- HPC Club
- The Hyak Supercomputer
- Logging in to Hyak
- Basic Linux Commands
- Transferring Files Between Your PC and Hyak
- Submitting Your Jobs

HPC Club

- High Performance Computing Club (HPCC): http://students.washington.edu/hpcc/
- As a club member, you can have access to thousands of CPU cores on UW Hyak supercomputer
- Become a member:
  http://students.washington.edu/hpcc/getting-started-on-hyak/

Hyak Overview

- A typical **node** has 16 processor **cores** and 128GB of memory
- All the nodes run CentOS 6 Linux
- ~10000 cores in total
- Club members have access to 1028 cores
- Node types
  - Computing nodes
  - Login nodes
    - Submitting jobs
    - Transferring files



Logging in to Hyak

This is essentially remote-accessing a Linux System via SSH protocol

- Need a SSH client program
  - Linux & Mac: just open a terminal
    - Mac: application->utilities->terminal
    - Ubuntu: Search for “terminal” in your applications

usage:ssh [options] user@IP-address

e.g

ssh xsqin@ikt.hyak.uw.edu

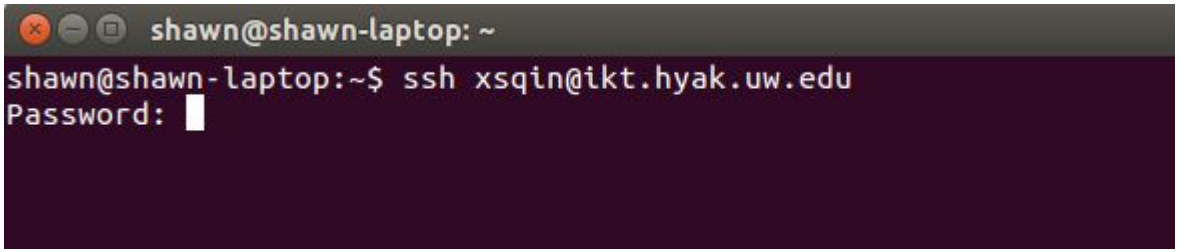
ssh xsqin@americano.amath.washington.edu

ssh shawn@128.95.220.141

Then enter your password and PRN from your token

  - Windows: putty
    - Download: http://www.putty.org/
- More info here:
  http://wiki.cac.washington.edu/display/hyakusers/Logging+In

Logging in to Hyak - Linux and Mac OS



1. Replace “xsqin” with your netid:
2. Enter Password

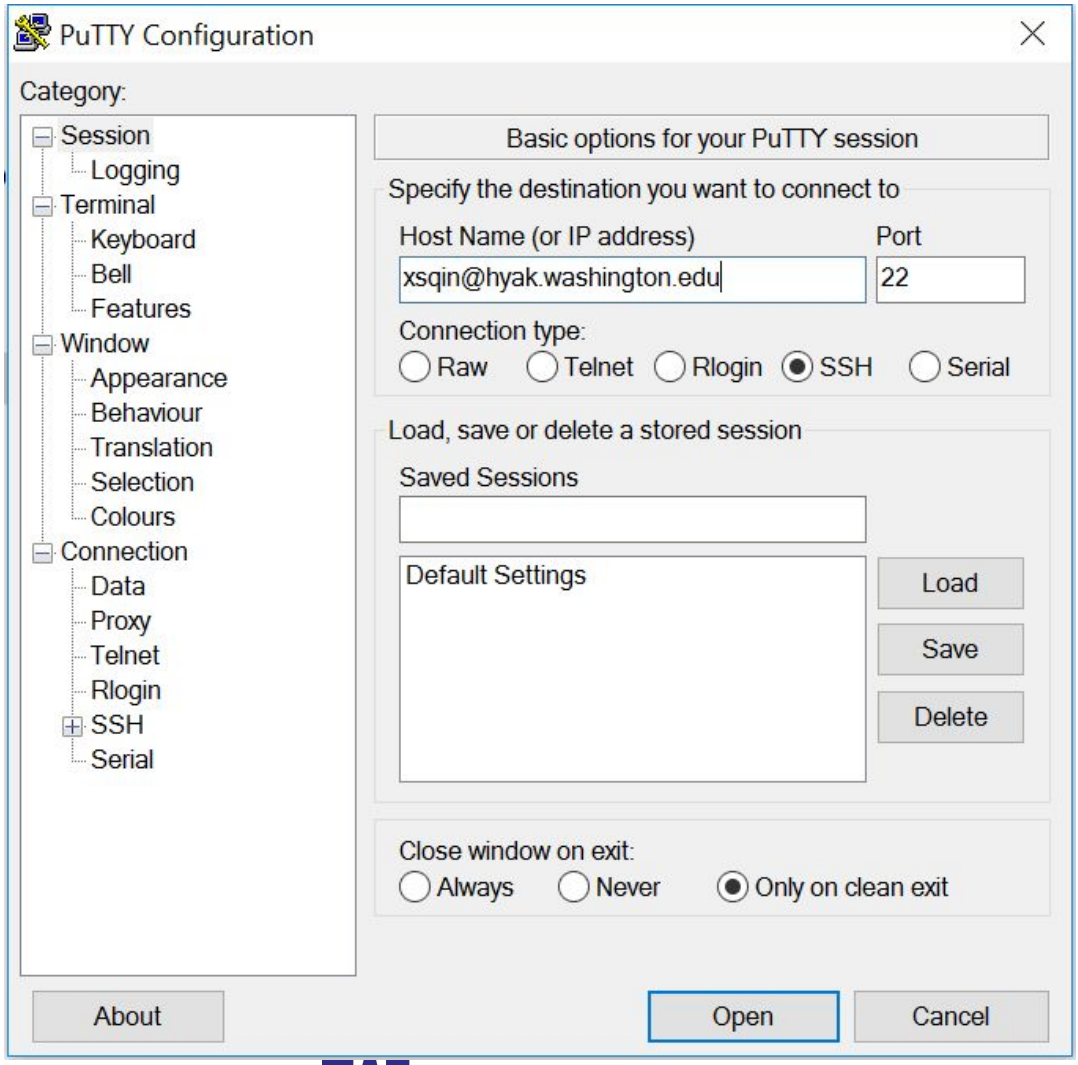
```
shawn@shawn-laptop:~$ ssh xsqin@ikt.hyak.uw.edu
Password:
Enter passcode or select one of the following options:

 1. Duo Push to iOS (XXX-XXX-7529)
 2. Phone call to iOS (XXX-XXX-7529)
```

3. If you have a E-token at hand, follow its instruction and get an 8-digit number. That’s your passcode to use here. Or if you have Duo as 2FA, confirm on your cell phone.

(More info here:https://itconnect.uw.edu/security/uw-netids/2fa/)

Logging in to Hyak - Windows

- putty
  - Enter Host Name and Port number. Then click “Open”
  - A terminal should pop out after you successfully log in.



Logging in to Hyak

```
Last login: Sat May 13 14:38:51 2017 from 128.95.220.134

     ** NOTICE **
     Users need to do all their interactive work, including compiling and
     building software, on the compute nodes (n####) and NOT on the
     head/login node (hyak.washington.edu). The login nodes are for
     interacting with the scheduler and transferring data to and from the
     system.

     Please visit the Hyak User Wiki for more details
     http://wiki.hyak.uw.edu

[xsqin@ikt1 ~]$
```

If you see something like this in your terminal, you are on Hyak.

Note that the prompt should look like netid@ikt1, where ikt is the name of the cluster.

Basic Linux Commands

- Show current directory: pwd
- $HOME directory
- Show contents in current directory: ls [options]
- change current directory: cd + [path]
  - cd absolute_path
  - cd relative_path
- Create a new folder: mkdir folder_name
- Remove a file/folder: rm [options]
- Rename a file/folder: mv old_name new_name

Managing Your Files

- Transfer files from your local desktop to the server
  - Linux & Mac: SCP
    - Usage: scp [options] <source directory> <target directory>
  - Windows: WinSCP
    - Download: https://winscp.net/eng/download.php

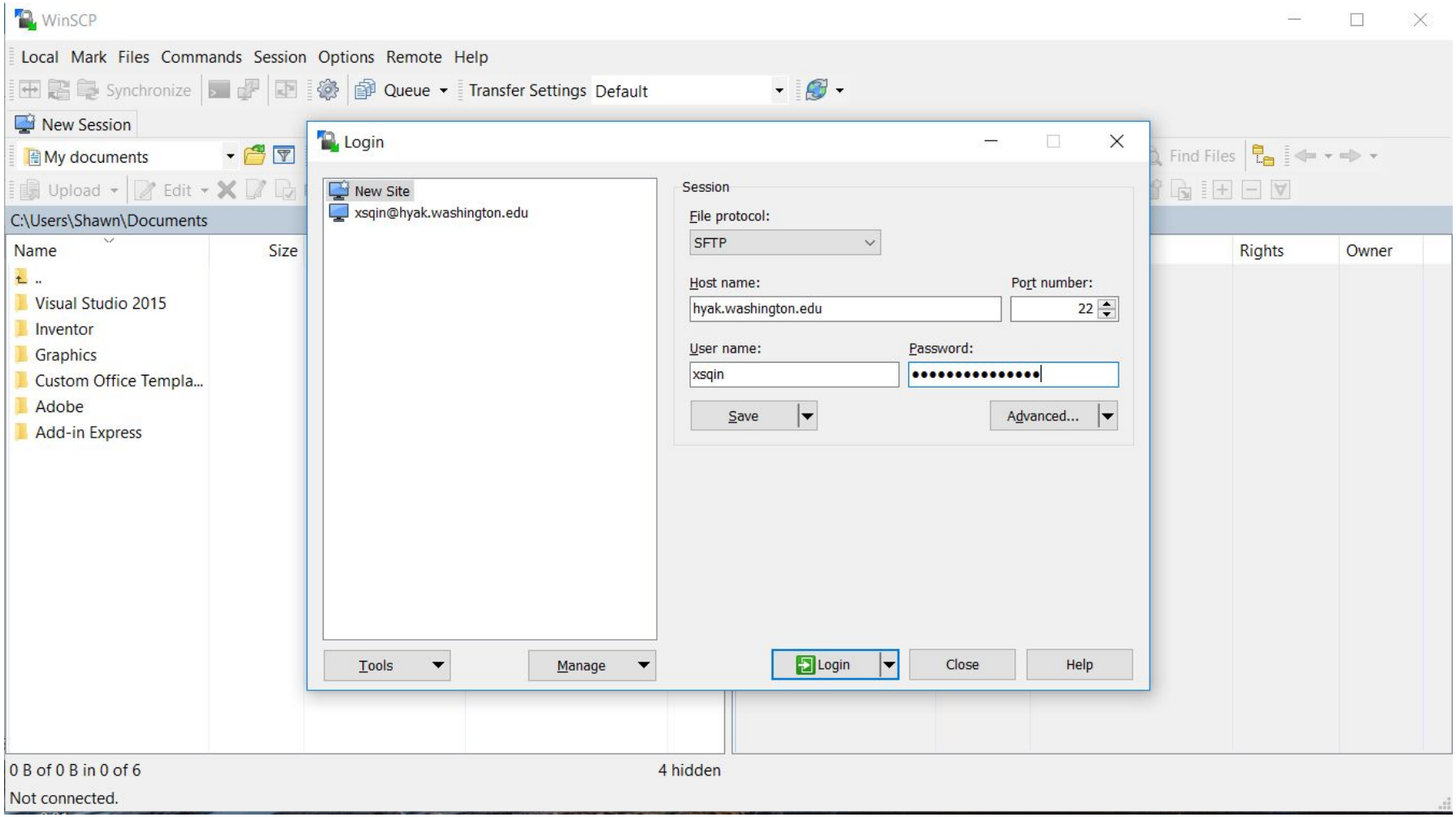
Managing Your Files - Linux and Mac OS

Note that these all these commands should be executed on the remote host (with something like xsqin@dell-inspiron as your terminal prompt, NOT something like xsqin@ikt1):

- **Upload files to Hyak:**
  - $ scp filename user@ikt.hyak.uw.edu:path/to/destination/directory
- **Download files from Hyak to current directory on your machine:**
  - $ scp user@hyak.washington.edu:path/to/file ./

Reference:
http://wiki.cac.washington.edu/display/hyakusers/Managing+your+Files#ManagingyourFiles-TransferringfilesinandoutofHyak–Examples

Managing Your Files - Windows



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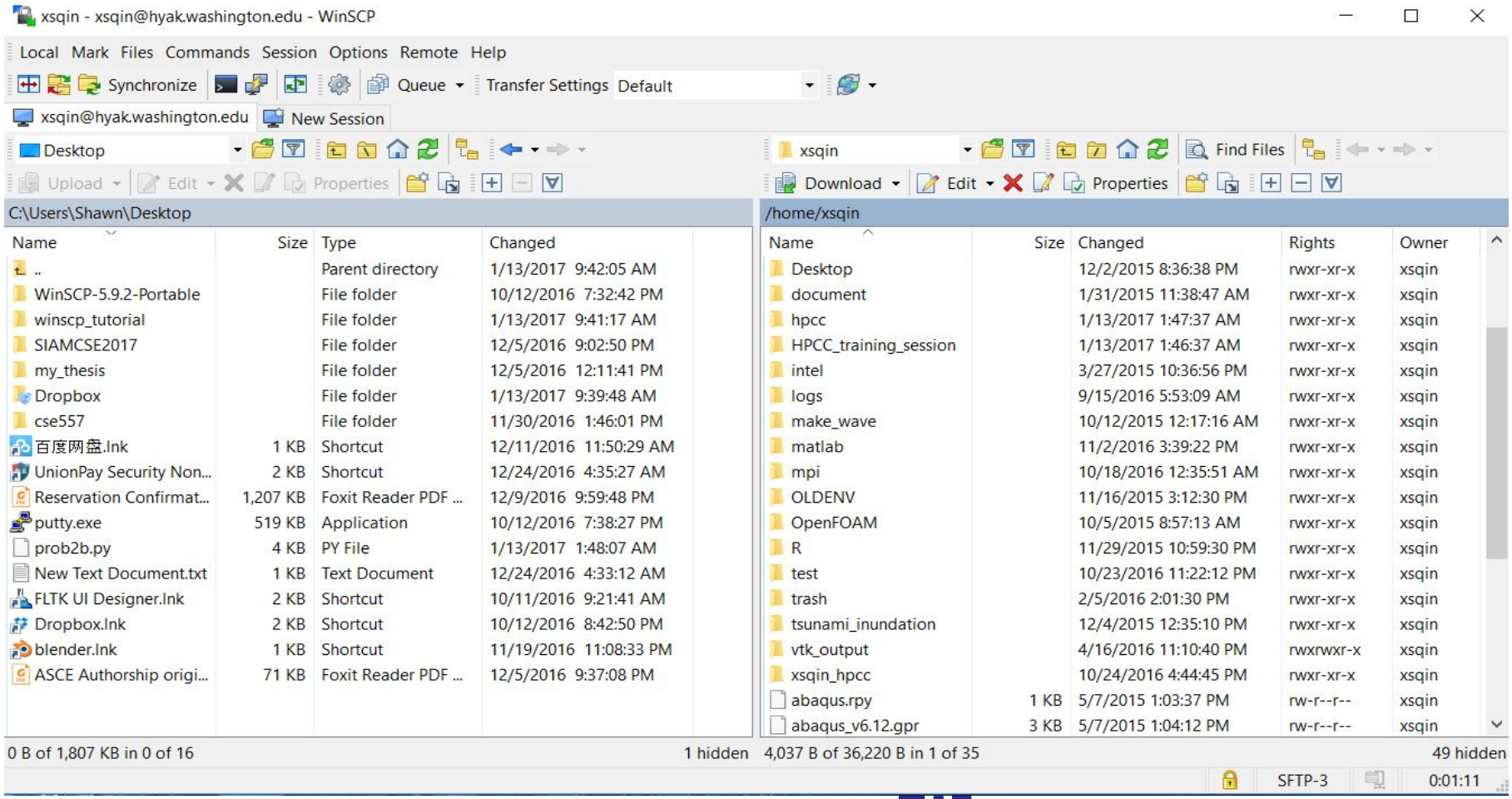
Managing Your Files - Windows

Simply drag files from left to right (upload) or from right to left (download).



Submitting Your Jobs

- Two types of node:
  - login node: for submitting jobs and transferring files. Don't execute heavy tasks (command) on it.
  - computing node: where your jobs are running
- Using qsub to submit your jobs
  - qsub [options] command-for-running-your-job
  - e.g. qsub -I walltime=2:00:00 -I -V matlab compute_norm.m
- Sometimes the options and command-for-running your jobs a

  we need: PBS (Portable Batch System) Jobscripts, which:
  - contains instructions for the scheduler
  - can set up the work environment
  - execute your program
- Reference:

  http://wiki.cac.washington.edu/display/hyakusers/Hyak+Job+Scheduler#HyakJobScheduler-ImportantInformation

Submitting Your Jobs - Hello-world Example

All these code can be accessed at:

https://github.com/xinshengqin/HPCC_training_session/tree/master/hello_world

1. Suppose we create a working directory at $HOME/hello_world on Hyak
2. Let's write a simple hello-world C code, called test.c in this directory:

```c
#include <stdio.h>

int
main (int argc, char *argv[]) {
    printf("%s","Hello world!\n");
    return (0);
}
```

Submitting Your Jobs - Hello-world Example

3. We can compile this code to executable with:

xsqin@ikt1$ c++ test.c -o test

(Note that we should never compile a big project in this way since we are on login node)

4. If we type $ ./test this should print out Hello world! to the standard output. (You can do this here since it's just a tiny program)

5. To execute this program in a submit-job way, we need to create another file as Jobscripts in the same directory. Let's call it run.sh

Submitting Your Jobs - Hello-world Example

run.sh

```
#!/bin/bash
## Specify name of the job, can be renamed to anything your want
#PBS -N hello_world

## Request 16 CPU cores on 1 nodes
#PBS -l nodes=1:ppn=16,mem=10gb,feature=16core,walltime=1:00:00


## Put the output from jobs into the below directory
#PBS -o /usr/lusers/xsqin/hello_world

## Put both the stderr and stdout into a single file
#PBS -j oe

## Specify the working directory for this job
#PBS -d /usr/lusers/xsqin/hello_world

## Specify which group's node your would like to run your job on
#PBS -W group_list=hyak-stf

## Actual command that get executed
./test
```

Submitting Your Jobs - Hello-world Example

6. A line starting with ## is comment.

7. A line starting with # is instruction for the scheduler.

7. There are at least two lines you need to change:

    #PBS -o /usr/lusers/xsqin/hello_world

    #PBS -d /usr/lusers/xsqin/hello_world

    Change these to the path of current directory. You will at least need to change them to /usr/lusers/your_netid/hello_world

8. Submit your job by passing the name of this jobscript to qsub:

    xsqin@ikt1$ qsub run.sh

Submitting Your Jobs - Hello-world Example

9. You should then see something like:

```
[xsqin@ikt1 hello_world]$ qsub run.sh
5866785.mgmt2.hyak.local
[xsqin@ikt1 hello_world]$
```

10. 5866785 is ID of this job. It can be used to query the status of the job.

11. If the job successfully finished, you should see a new file named hello_world.o5866785 in current directory. All output of the program are put in this file. In this case, you should see “Hello world!” in it.

Managing Jobs in Your Queues

- Check the status of your job
  checkjob <job_id>
  qstat -f <job_id>
- Queue Status
  - showq -w qos=<your_group>
  - showq -w user=<your_netid>
  - e.g. showq -w qos=stf

- To cancel a job
  mjobctl -c <job_id>
  qdel <job_id>

More info here:
http://wiki.cac.washington.edu/display/hyakusers/Hyak+Job+Scheduler#HyakJobScheduler-ManagingJobsinYourQueues