Tutorial 1: How to remotely connect to a high performance computer (HPC)

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Notes:

- This tutorial is a demonstration of how to connect to a Linux computer remotely. This computer could be your office Linux workstation that you want to connect to. I will use my research cluster (*xliuws0514.cee.psu.edu*) as an example. Details may vary if you want to connect to other computers. You should consult your HPC user manual or documentation.

- With time, the notion of `HPC` has evolved, especially with the advent of cloud computing services such as Amazon Web Services (AWS), Google Cloud Platform, and Microsoft Azure. This tutorial does not cover how to connect to these cloud services. Computational fluid dynamics (CFD) is one of the targeted use cases of these cloud services and there are many good tutorials online.

1   Introduction

You are not likely (or willing) to work in a hot room with very noisy supercomputers. Instead, you may want to remotely connect to these computers. To access the cluster machines, first you need to get an account (talk to the admin of the computer). In this tutorial, you need to replace the computer name with the one you have access to. This short instruction demonstrates how to connect to a remote machine using *PuTTY*.

For students at Penn State, this tutorial will also cover some basics of how to connect and use the Penn State ICDS ACI machines.

2   SSH connection using *PuTTY*

This tutorial assumes that you are using a local Windows computer. Thus, you need to firstly install a SSH client. If your local computer runs with Linux or Mac OS, it should already have SSH client installed (if not, its installation is very straightforward).

2.1   Download and install *PuTTY*

This is a short guide to get started using *PuTTY*, a SSH client, to access the cluster. If you need more information on how to use PuTTY, please see the official *PuTTY* documentation located at: http://www.chiark.greenend.org.uk/ sgtatham/putty/docs.html

To install PuTTY on your local computer, you need to download a copy from its official website: http://www.chiark.greenend.org.uk/ sgtatham/putty/download.html.

2.2   Login

Launch the installed *PuTTY*, and enter the following information (replace the computer name or IP with your own):

- Host name or IP: *xliuws0514.cee.psu.edu*

- Port: *22*

- Connection type: *SSH*

To avoid the entering of these information every time, you can save them into a session. Next time you only need to load the saved session.
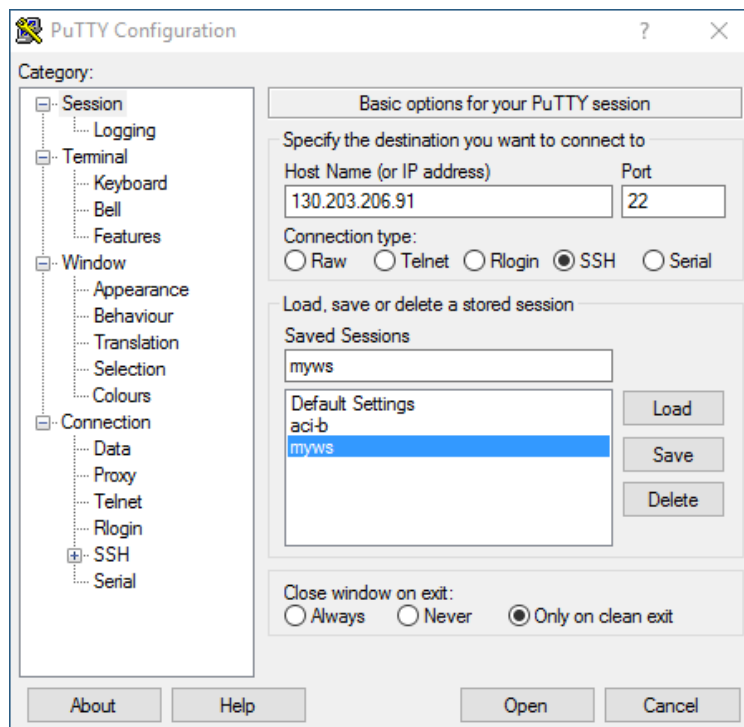

Figure 1: Configuration screen of *PuTTY*

Click "Open", it will connect to the cluster and the following windows will appear. Follow the instruction to input your user name and password. If everything is correct, your login will be successful. As a final note, to log off properly, just type `exit` in the terminal.
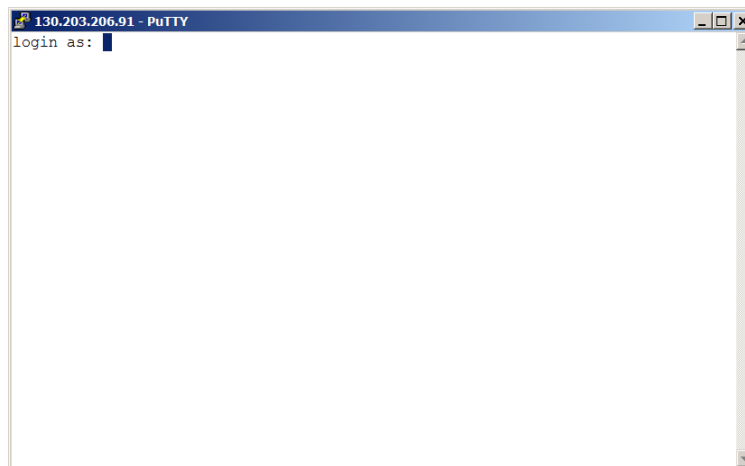

Figure 2: The login screen to type in your user name
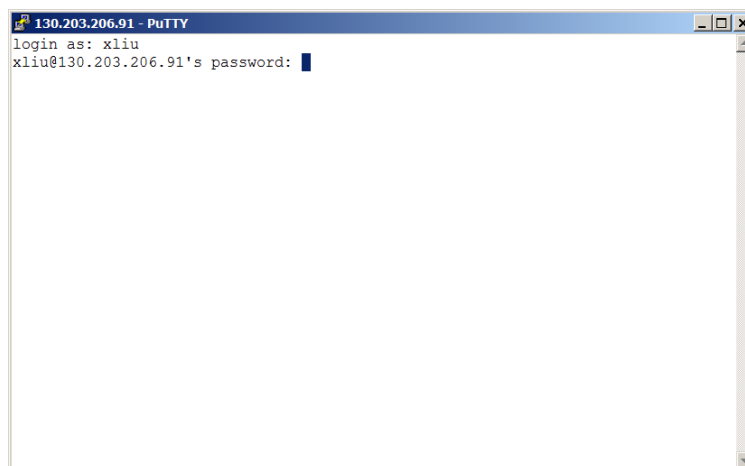

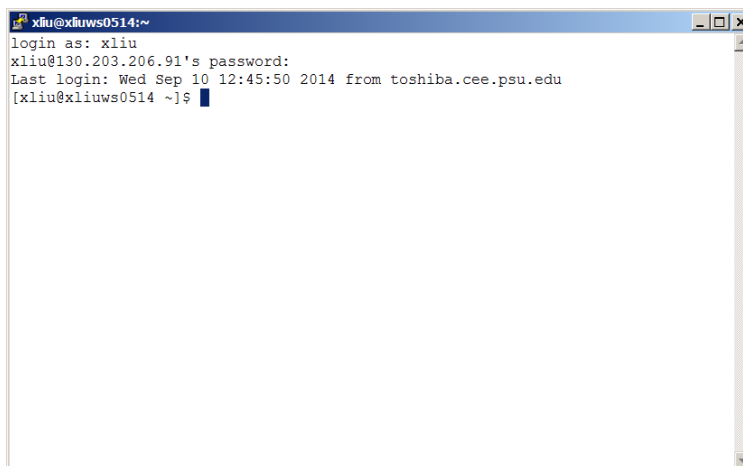Figure 3: The login screen to type in your password

Figure 4: The screen after your successful login

3 Logging into the cluster from other Linux machines using *ssh*

If you have access to other Linux machines, you can login to the cluster using the *ssh* command.

```
[app321@someLinuxBox ~] $ ssh -P 22 app321@somename.hpc.psu.edu
```

The syntax and options for the *ssh* command can be found from its manual by typing `man ssh`. In this case, the option "-P 22" specifies the port number as 22. The default for SSH port is 22. Thus, this option is not necessary. However, if the machine uses a different SSH port, you need to specify.
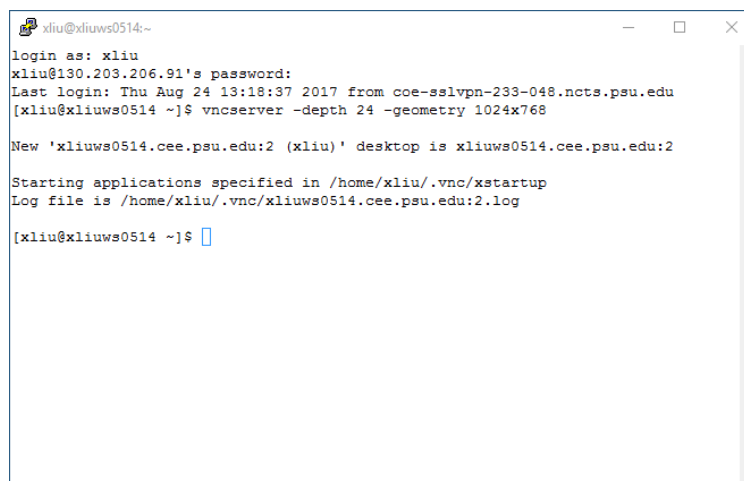
4 Remote desktop connection via VNC

Connection through *PuTTY* is limited to command line, though graphical interface is possible through X11 forwarding. A more convenient way is to use the remote desktop connection via VNC. This part will guide you through setting up the VNC session and connecting to it from a Windows machine. On the Windows machine, *PuTTY* should be installed already. You also need to install a VNC viewer. There are several choices, such as UltraVNC viewer and RealVNC viewer. Free versions, though with less functions and security, are available from their websites. In this tutorial, the RealVNC viewer is demonstrated. You should download and install it on your Windows machine.

The setup and connect through VNC, do the following steps

1. Connect to the Linux machine using $PuTTY$ with your user name and password.

2. On the remote machine, start the VNC server by typing (Figure 5)

   ```
   vncserver -depth 24 -geometry 1024x768
   ```

   Replace 1024x768 with desired resolution. If this is the first time starting vncserver, you'll be asked to setup the password that will be use to connect to the vncserver. It is recommend to setup the password. Otherwise, anybody can connect through the VNC.

Figure 5: Startup of the VNC Server

   Notice what the desktop number is (":2" in this case, yours might be different)
   ```
   New 'xliuws0514.cee.psu.edu:2 (xliu)' desktop is xliuws0514.cee.psu.edu:2
   ```

3. On your Windows machine, launch the RealVNC viewer. Create a new connection through menu "File" − > "New connection". In the pop out window, specify the name of the server as the desktop number you noticed in the previous step, and give it a name. Click "OK" (Figure 6).
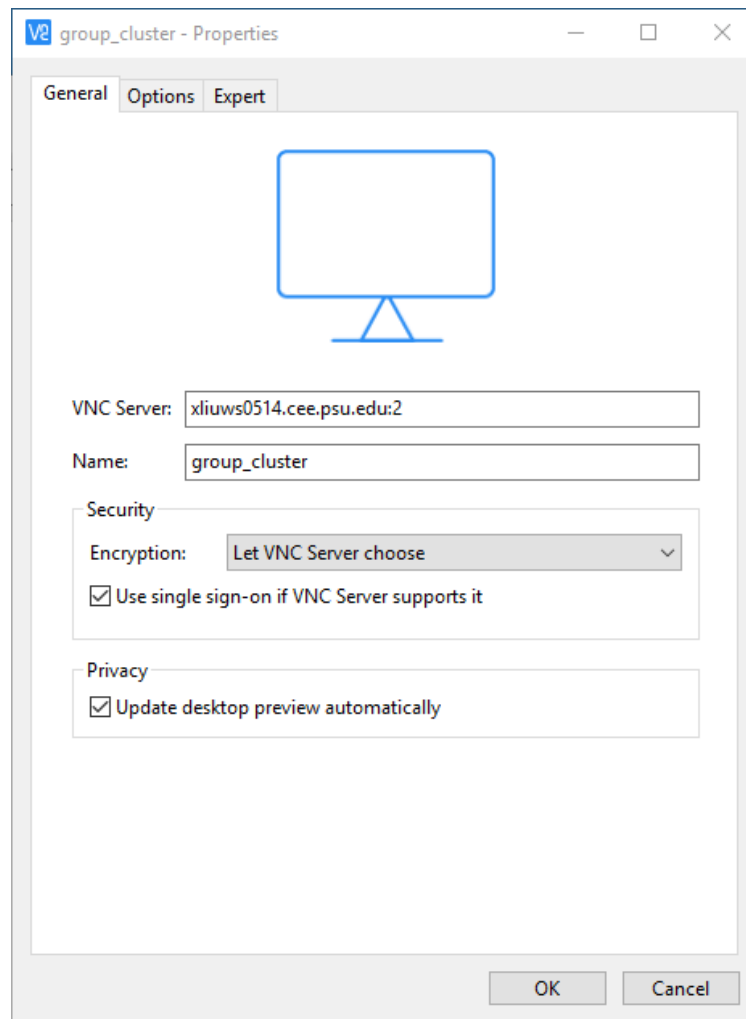
Figure 6: Connect to the VNC Server by launching the VNC viewer on your Windows machine

4. VNC viewer program will ask for the passphrase authentication. Type in the passphase you set for the VNC connection. Click "OK" (Figure 7).
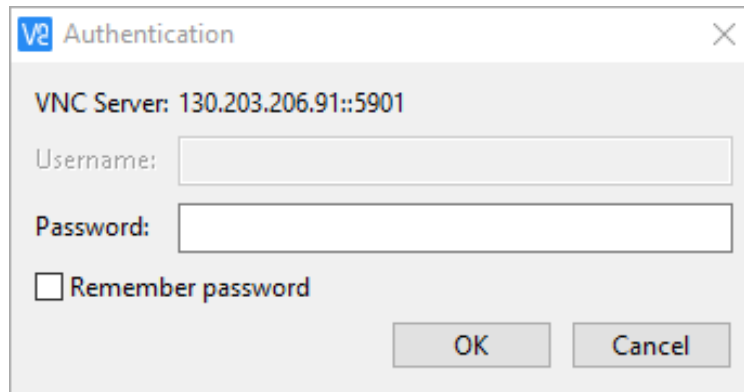
Figure 7: Passphrase authentication for the VNC connection

5. If everything works ok, then the screen of the VNC remote desktop will appear as in Figure 8. You can use the cluster as if you are sitting in front of the machine physically. A useful tip is that you can type the command `vncconfig` and see a new window popup. Leave this window open and you should be able to share the clipboard memory between Linux and Windows. That is convenient to copy and paste between to machines.
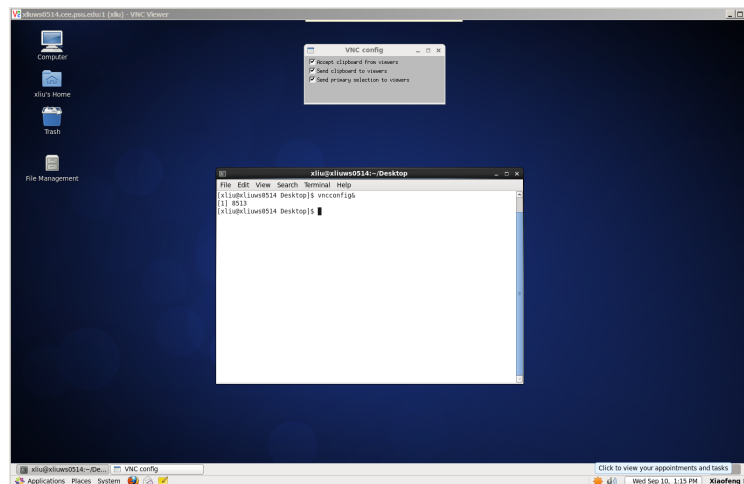

Figure 8: Screen for the VNC connection

5 Moving files to and from the cluster

You may want to move files to and from the cluster. For example, when your simulations are done, you may want to copy the results to your computer for analysis. This section demonstrates how to do this in a secure way.

If you connect to the cluster from a Linux machine, you can use sftp. The following is an example to get a file from the home directory on the cluster:

```
[xliu@SomeLinuxBox ~]$ sftp xliu@xliuws0514.cee.psu.edu
Connecting to xliuws0514.cee.psu.edu...
Password:
sftp> get testfile.txt
Fetching /home/xliu/testfile.txt to testfile.txt
/home/xliu/testfile.txt ...
sftp> quit
```

If you connect to the cluster from a Windows machine, you can also use programs with graphical interfaces, such as the `FileZilla` client. The free client program can be downloaded from its website: https://filezilla-project.org/

1. Launch of the FileZilla program. After the installation, you can launch the FileZilla program and you will see the interface (Figure 9).
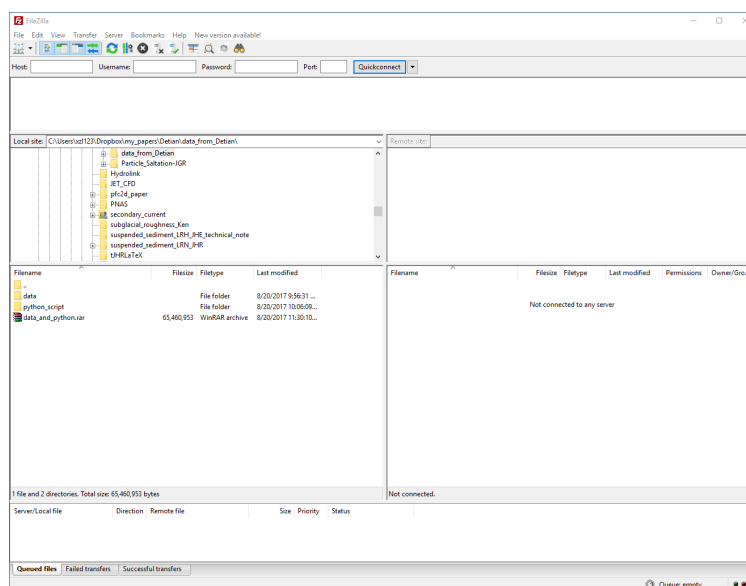

Figure 9: Launch of the FileZilla program

2. Setup a SFTP connection in FileZilla by clicking on the "Site Manager" button on the tool bar. A dialog window will appear as in Figure 10. Type in the following information:

   - Host: xliuws0514.cee.psu.edu

   - Port: 22

- Protocol: SFTP - SSH File Transfer Protocal

- Logon Type: Normal

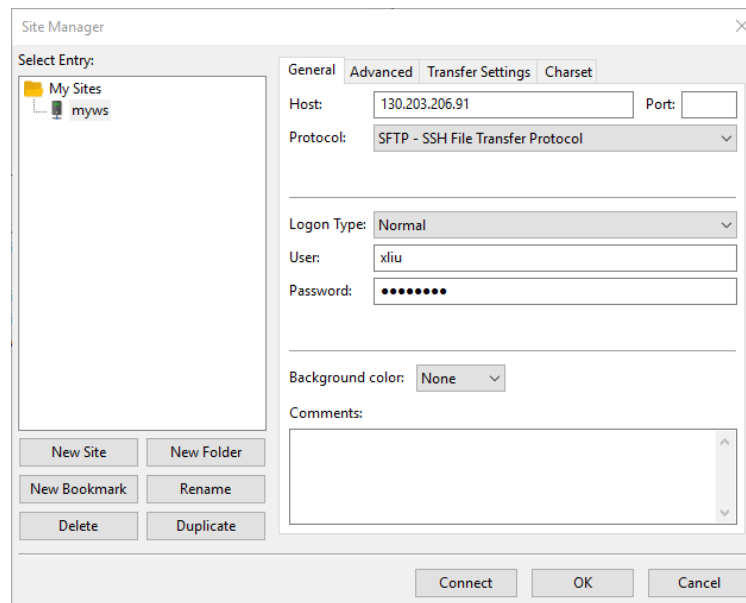- User: `your user name`

- Password: `your password`

Figure 10: Setup of a SFTP connection in FileZilla

3. Click "Connect" and you will be connected to the cluster. By default, FileZilla will go to your home directory (Figure 11). As you can see from the figure, you can transfer files and directories from and to the cluster.
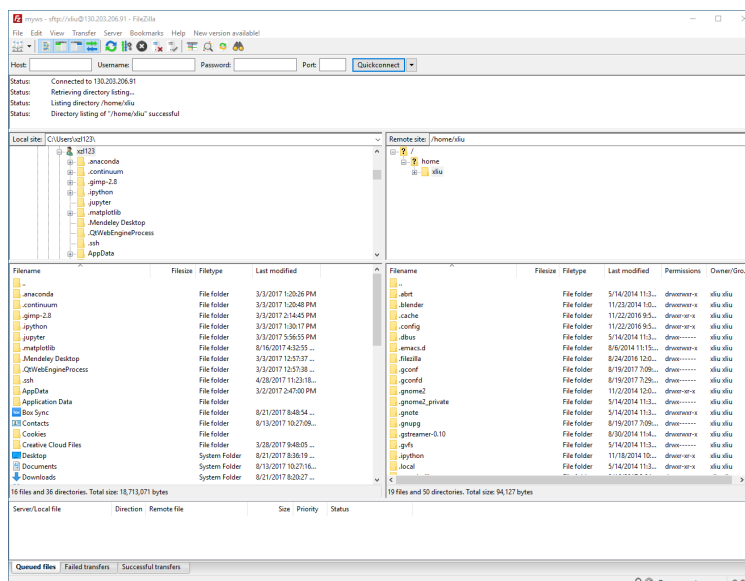
Figure 11: Screen for a connection session in FileZilla

> **Note for using Penn State ICS ACI computers**
>
> You can also use `FileZilla` to transfer files between your local machine and Penn State ICDS computers. The address of the ICDS data nodes is `submit.hpc.psu.edu`. The only difference is when you connect, you will be asked for the Two-Factor Authentication (2FA) approval.

6 Advanced topics

6.1 Penn State ICDS ACI Computing Resources

Presently, Penn State ICDS ACI provides two services: the legacy "Roar" and the new "Roar Collab". This section provides some basic information about them in case you will use their computing facility. The links provided below will get you to the detailed documentation provided by ICDS. They also have regular training workshops that you can attend. The recordings of their past training workshops are also available on their website.

To get started with the supercomputing services "Roar" at Penn State:

https://www.icds.psu.edu/computing-services/getting-started/

To access "Roar Collab" on Open OnDemand: https://www.icds.psu.edu/computing-services/roar-collab/

"Roar Collab" user guide: https://www.icds.psu.edu/roar-collab-user-guide/

To access "Roar Collab": https://portal.hpc.psu.edu

6.2   Generating public/private rsa key pair for automatic login.

Disclaimer: The following information is from the Ubuntu website (all credits go to the original authors):
https://help.ubuntu.com/community/SSH/OpenSSH/Keys.

Please refer to the link above to set up your public and private key pair for automatic login.