Welcome to High Performance Computing at TCU!

About High Performance Computing

The Texas Christian University Advanced Computing Center (TCUACC) provides an environment for high performance computing ideal for small jobs that require a bit more power than your department may have readily available. The TCU primary cluster can be used for batch or MPI workloads.

Citing the Center

Please include the following sentence in any works using center resources.

The author[s] acknowledge the TCU Advanced Computing Center (TCUACC) for providing HPC resources.

Here's how to connect to the cluster using a Mac or PC

Logging in to HPClogin for the first time;

Once you have been assigned access to the HPC cluster, you will use your TCU user account to access the HPC Login node.. The cluster is protected by firewall and you must be connected to the TCU network, either directly or by VPN, to login.

Here's an overview of the process;

- Requesting HPC Access
  - Initiate with TCU Helpdesk
  - HPC New User Survey form
  - Committee review
- Requesting VPN Access
  - Initiate request with helpdesk
  - Install client & connect
    - Login – will not work from within TCU network!
    - MFA with Okta
- Prepare your workstation
  - Windows software
  - Mac software
- Connecting and running applications

Software you will need:

VPN Client *(off-campus)* – This will allow you to connect to TCU's secure VPN, ensuring end-to-end-encryption from your computer to TCU's network.

Terminal Emulation Software

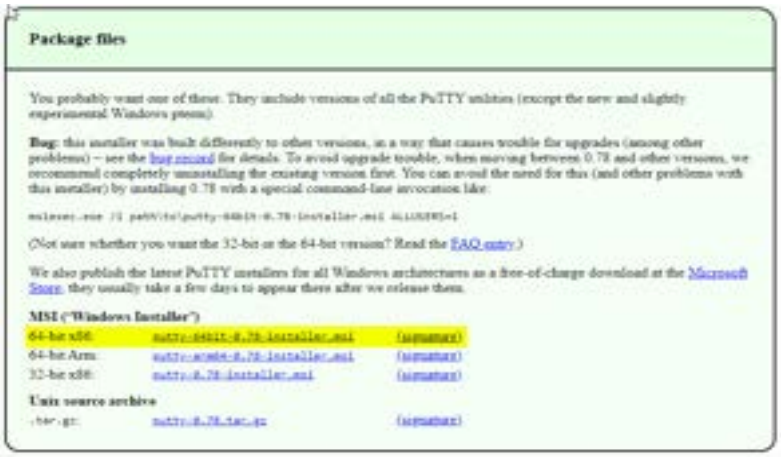
Windows Users

puTTY

puTTY is a text based Windows terminal program that you use to connect to the cluster via SSH.

Official download :
https://www.chiark.greenend.org.uk/~sgtatham/putty/latest.html

Most Windows users will choose the highlighted installer



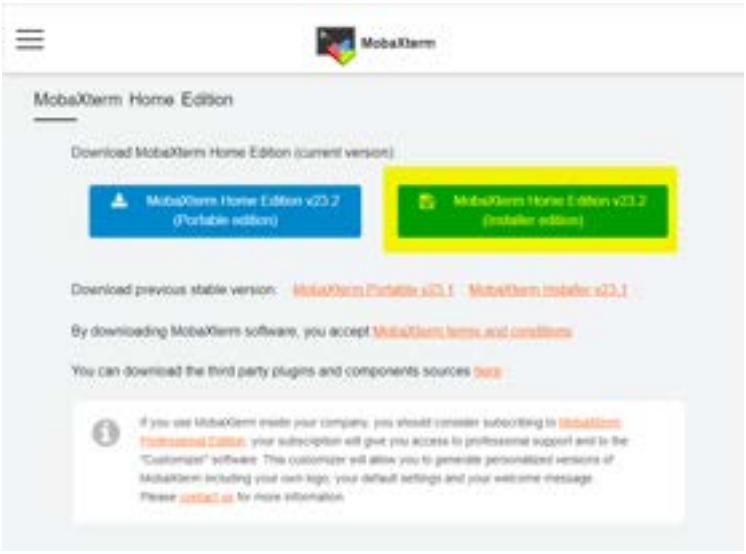
Windows Users

MobaXterm

Enhanced terminal for Windows with X11 server, tabbed SSH client, network tools and much more

Official download:
https://mobaxterm.mobatek.net/download.html

Most Windows users will select the MobaXterm Home edition (installer addition)



Mac Users

XQuartz

The latest versions of macOS or Apple OS X no longer ships with X11.app i.e. XQuartz server.

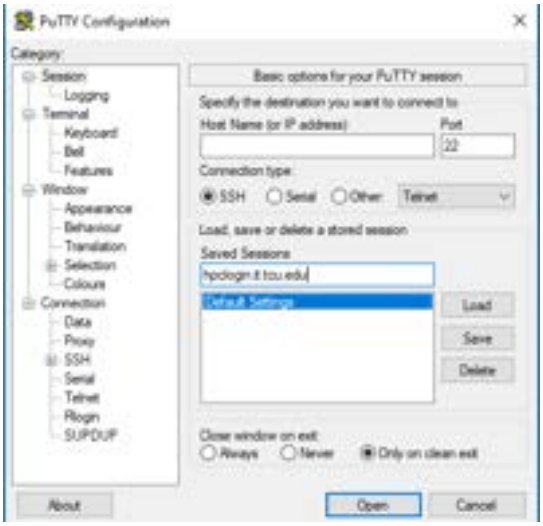
The XQuartz project is an open-source version of the X.Org X Window System that runs on macOS. Together with supporting libraries and Applications, it forms the X11.app that Apple shipped with OS X versions 10.5 through 10.7.

Official download:
https://www.xquartz.org/

Making a terminal connection to the HPC Cluster

Windows Users

Launch puTTY from your start menu. We're going to make a saved connection with a few customizations.



Enter the hostname in the Saved Sessions field and hit the Save button. This will create a saved SSH session to HPCLogin.IT.TCU.EDU that we can use each time we connect. This is all that is required to create the entry, but there are some personalization's that you might want.

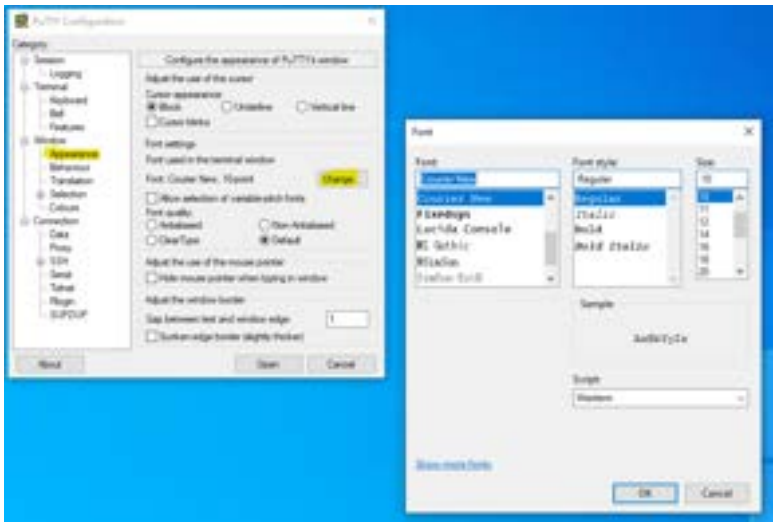
We're going to change the default color scheme to black text on a white background, and make the font bigger for easier visibility. This is a matter of preference and your choice, but you can see how it's done.

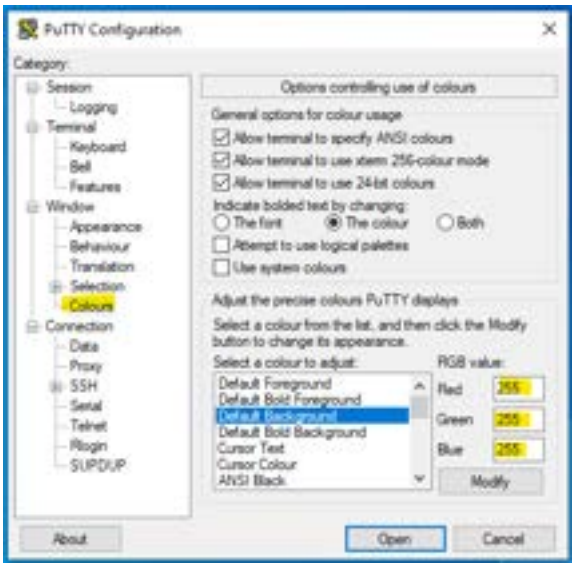
First, we're going to visit the fonts..

In the left column, go ahead and click on Category:Window > Appearance, and then click the Change button in the *Font settings* section.

This opens the font dialogue, where you may select your font, font style, and size.

When you're satisfied with your choices hit OK to complete your selection and close the font dialogue.





Next, we're going to change the color scheme by clicking to Category: Window>Colours.

There are a lot more color properties that you can adjust than we're going to detail here, This is All a matter of preference and your choice, but you can see how it's done.

Each object that you can set a color preference for is listed. Let's first scroll to the Default Background and set the RGB Values as follows to set the background to White

RED	255
GREEN	255
BLUE	255

Don't click any buttons yet, continue on please.

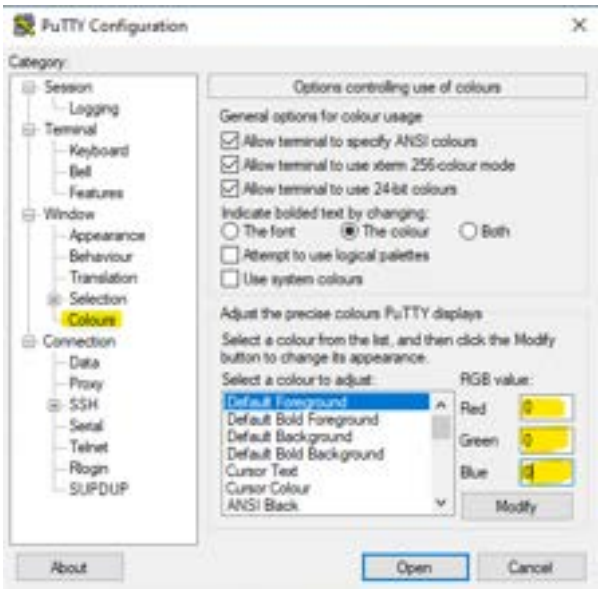
Now we're going to set the type face to black so that it stands out on the white background.

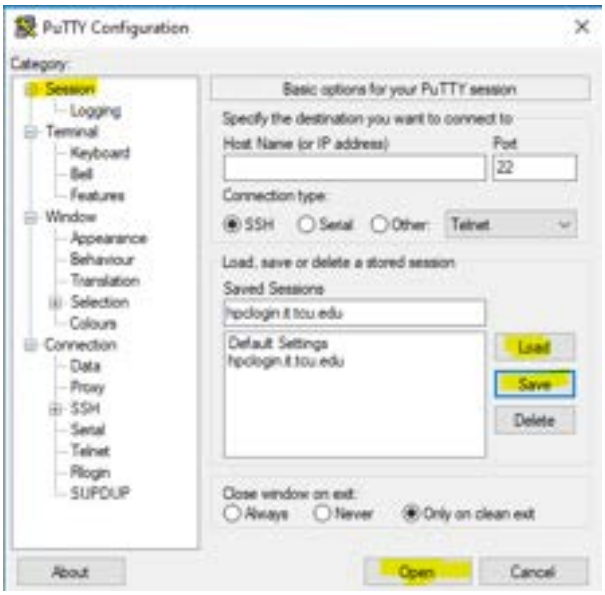
Click to Category: Window>Colours again, and this time we're going to scroll until we find the Default Foreground.

You're going to want to set the RGB values as follows;

RED	0
GREEN	0
BLUE	0

We will need to save these settings with the connection entry.





To save our connection file with all of the preferences we've just configured, click on Category:Session select the **hpclogin.it.tcu.edu** session in the list and hit the Save button. This completes creating your connection file.

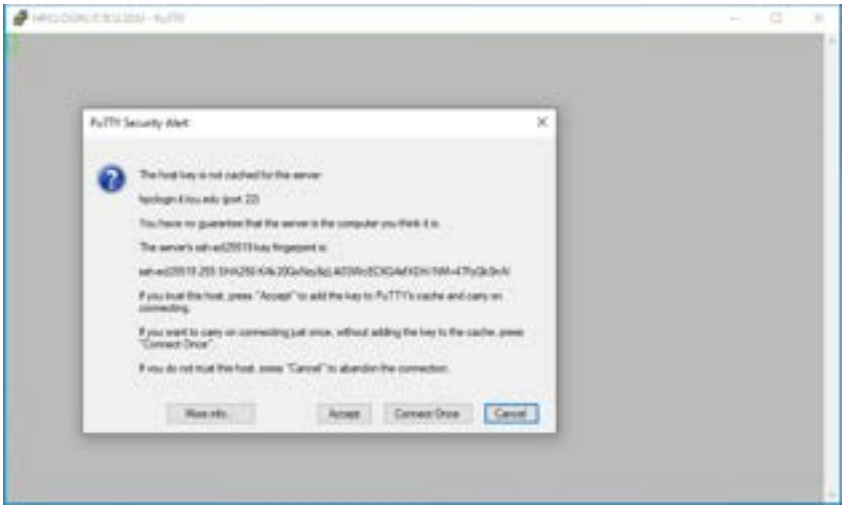
We can now use this to connect to the HPC cluster. If the session name is not in the saved sessions field, you can open it by selecting it and hitting the Load button.

Hit the Open button to connect. This window will close and the terminal window will open.

The first time any SSH client connects to a host, it will display an alert similar to this. This is to verify the identity of the machine you're connecting to

In this case, since we know the host and we in a secure environment, we can trust that the identity of the machine is correct.

You can just click Accept and move on.



Once you have accepted the security key, the host will be saved to your certificate chain and your connection will open to this login screen instead.

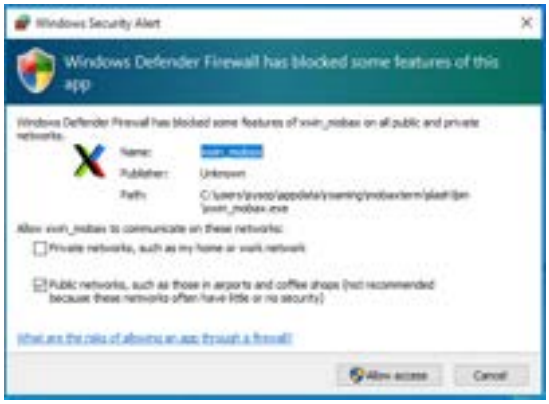
You can login with your TCU ID and password. Once your login is completed you are in a Bash shell and here is where you will do much of your work on the HPC.

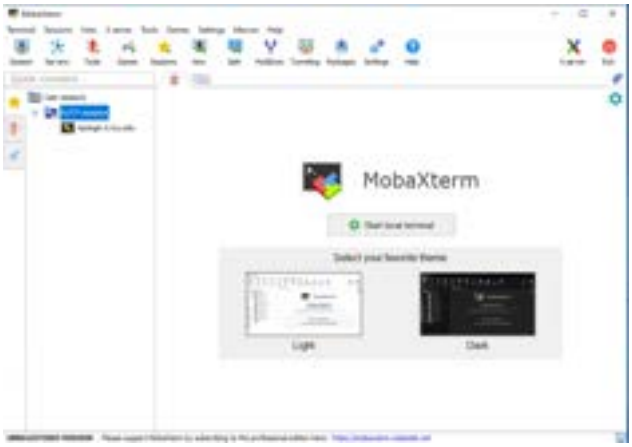
Windows Users

Launch the MobaXterm installer and click through the installation.

Windows Defender Firewall may notify you that it has blocked some features of the app.

If that happens, check the boxes for both public and private networks and click the Allow Access button to continue.





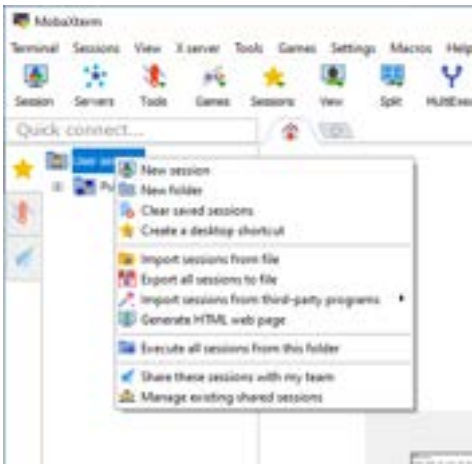
If you've installed and configured puTTY to connect to HPCLogin.it.tcu.edu before launching MobaXterm, it will import the saved connections from puTTY and you only need to select the light or dark theme and you'll be ready to connect.

If you still need to setup your connection to the cluster, the instructions are below.

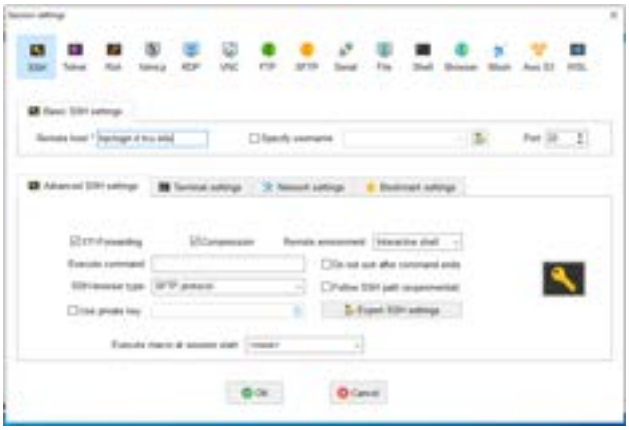
Right-click on the User Sessions folder (slide 1) and select new session.

Left-click SSH and type hpclogin.it.tcu.edu in the Remote host field in the Basic SSH settings section. Click OK to save. (slide 2)

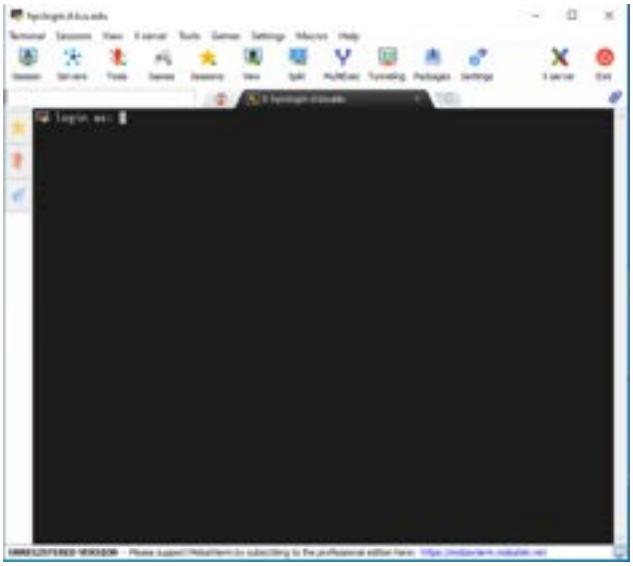
Right-click on the saved connection from your list of user sessions and click connect. Your terminal will launch to a login prompt where you can enter your password and complete your login. (slide 3)



Slide 1.



Slide 2.



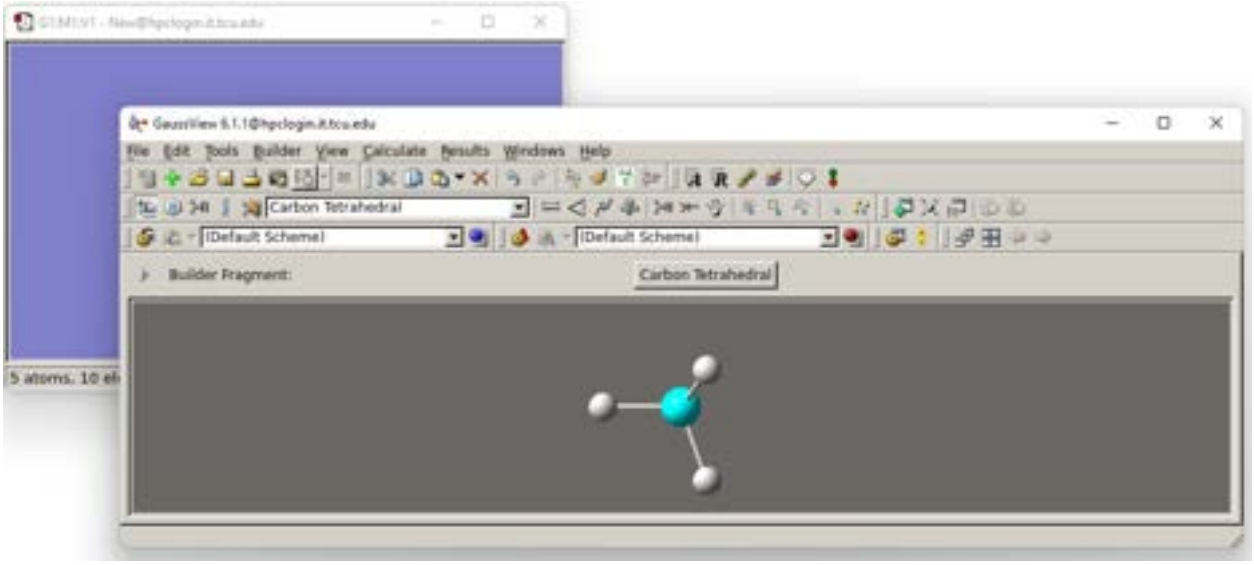
Slide 3.

Connecting to the cluster using MobaXterm is also establishing an SSH connection, but MobaXterm has a built-in X11 server to support X Windows applications such as GaussView6, part of the Guassian toolstack.

X11 apps are launched from the command line in the same way as text based apps but the X11 protocol manages redirecting the display to the remote X11 server on your PC.

When you issue the command to launch your X11 application from your SSH system prompt, the X Windows server is invoked and your program will run with all of it's graphical features.

Once the program has launched, you can continue to run other commands within your SSH terminal session. The X-Windows applications have their own controls for their use and you can generally exit or close the program from one of it's graphical windows.



Mac User

For text-based SSH connections to the cluster, you can use the terminal program that comes included with MacOS. You can find the Terminal in your Mac's Launchpad in the folder labeled "Other".

From the Mac prompt, connect to the cluster by issuing the command ;

ssh -XC <yourID>@hpclogin.it.tcu.edu

The -XC option tells the cluster to redirect X-Windows output to the X11 server on your Mac

For this demonstration, the assumption is made that you will have X-Quartz already installed on your Mac. You don't need to launch X-Quartz, your session will launch it when it's needed as long as your session is launched with the -XC command option.

X11 apps are launched from the command line in the same way as text based apps but the X11 protocol manages redirecting the display to the remote X11 server on your Mac.

When you issue the command to launch your X11 application from your SSH system prompt, the X Windows server is invoked and your program will run with all of it's graphical features.

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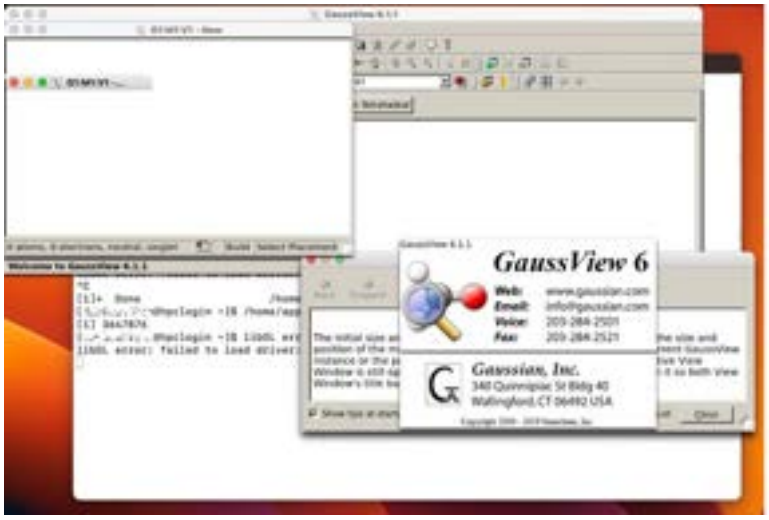

YouTube

Dr. Ben Janesko HPC cluster video series
@benjaminjanesko5940

Be sure to check out these informative videos from Dr. Ben Janesko;

Connecting to the Cluster: https://youtu.be/x7UbvWvfDD0

Running a Gaussian 16 Calculation: https://youtu.be/1m5C90JMEpI

Computing Molecular Electrostatic Potentials: https://youtu.be/ZaEB4neD1sE

Using Python 3 and PySCF: https://youtu.be/a5Blj1DhP9w