**"Talking" to a supercomputer**

**Background**

To run molecular simulations and to train machine learning models, we generally need to use high-performance computer clusters (a.k.a. supercomputers) instead of our regular desktop or laptop machines. These supercomputers are typically located in specialized rooms in remote locations (sometimes even in a different state!). Thus, we need a way to communicate with ("talk to") these computers. **Here we will show how to establish a connection to these supercomputers from your desktop or laptop**. Essentially, we will connect to these supercomputers via internet. But there is one more consideration! Supercomputers only understand UNIX language, so we need to "talk to" them in this language.

**What you need to download.**

***Windows:*** You need to download Putty, which you can get here. Download and run the installer file (.msi). You can simply say yes to all default options. Just pay attention to where the executable (Putty.exe) end up located.

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

***MacOSX***: You do not need to download anything. You can use the built-in Terminal application, which you can find in your Applications/Utilities folder.

**How to connect to the supercomputer.**

To connect to the supercomputer, you essentially need to go through three steps: i) "call" the supercomputer (dial the IP address or the host name of the supercomputer) ii) "tell" the supercomputer who you are (provide your username), iii) "demonstrate" to the supercomputer that you are really you (provide your password). How this is exactly done, looks a bit different depending on whether you are using Putty in Windows or Terminal in MasOSX.

***Windows:*** Run putty.exe. The box shown in Fig. 1 will pop up. You want to keep the default settings Port 22 and SSH (secure shell).

- The hostname of Mines supercomputer is mio.mines.edu, so type this info in the Host Name box.
- RECOMMENDED: With Host Name box filled in, type an "alias" to associate with the hostname (for instance: mio) and click on the Save button.
- Click on the Open button, which will make a window like the one in the Fig. 2 pop up. As soon as the window pops up, it will prompt you for your username. Type your username and press enter. Then the terminal will prompt you for your password. Type your password and press enter. YOU ARE IN!

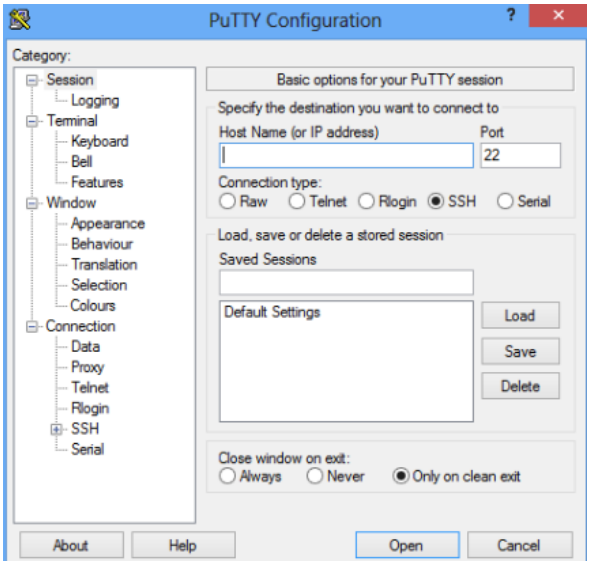


*Figure 1. Appearance of dialog box when you execute Putty*

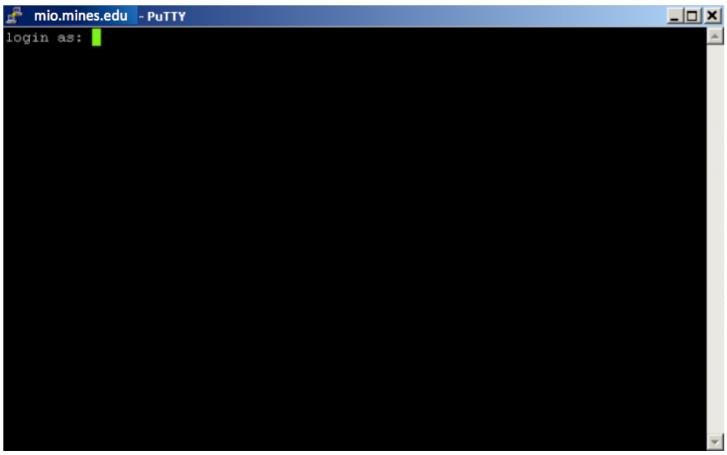


*Figure 2. Appearance of terminal in WIndows once you initiate your connection with Putty*

***MacOSX:*** Go to your applications folder, then to your Utilities folder, then click on Terminal, which will make a window like the one in Fig. 3. pop up. At this point, this window is still providing a UNIX version view of your laptop. But from this window, you can connect to the supercomputer. To do so, simply type ssh username@mio.mines.edu (only make sure to substitute username with you actual username). The terminal will prompt you for your password. Type your password. YOU ARE IN!!!

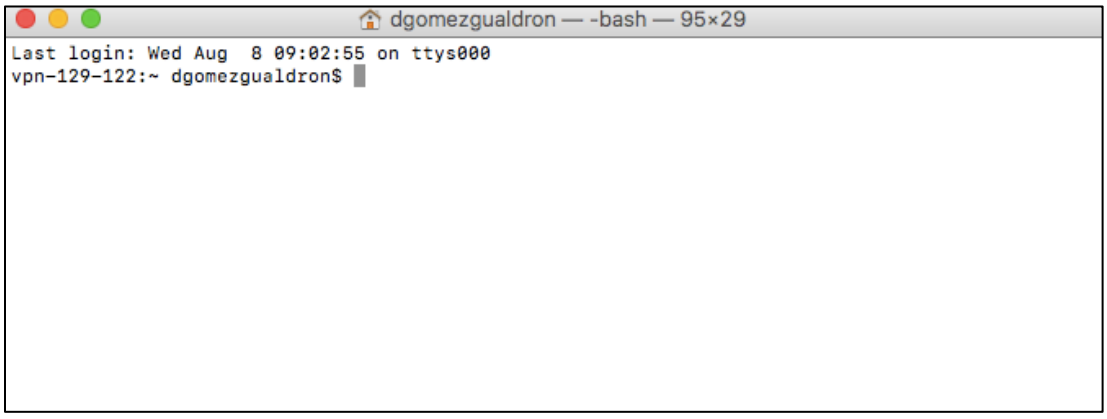


*Figure 3. Appearance of terminal in MacOSX once you initiate your connection with the Terminal utiltiy*