



Accessing the Research Computing Center Resources

Guest Accounts

- Each student has been assigned a Research Computing Center (RCC) guest account.
- By using the guest account each user agrees to the RCC User Policy:
<https://rcc.uchicago.edu/about-rcc/rcc-user-policy>
- Guest accounts will use ssh keys to connect to the RCC compute cluster. You should receive an encrypted 'rccguestXXXX' zip file (where 'XXXX' is a four digit number) by email before the start of the school. The password to decrypt and extract the contents of this zip file will be provided on the first day of the school.

SSH Client Setup – (to be completed by attendees by the end of the 1st day)

Students will need to connect to Midway (the RCC computer cluster) to carry out the hands on exercises. This requires installing an ssh client and using the ssh key in the 'rccguestXXXX' zip file once the password has been provided (see instructions below). Assistance with setting up connections will be provided on the afternoon of the first day of the school. If any issues arise that you are unable to solve, please ask for help to ensure that each student has a working connection by the end of the 1st day.

Macintosh/Linux User Clients

- Macintosh users will have a terminal client installed by default. It is located in Applications → Utilities → Terminal. Verify you can locate the terminal client and add it to your dock. You can easily locate the terminal from the LaunchPad icon located in your Dock. Click the LaunchPad icon and search "terminal". Drag the terminal icon into your dock and close LaunchPad.
- Other client terminals for Mac exist, but will require the user to install them. For example the [iterm2](#) terminal client is an alternative option.
- Mac does not come with X11 server preinstalled. In order to be able to display remote graphical processes from the terminal client, you will need to install X11 server and client libraries, which can be downloaded from the [XQuartz](#) project page. NOTE: Users are encouraged to install the older [2.7.8 version of XQuartz](#), which works with OpenGL applications.

Windows User Clients

- Windows users should install [MobaXterm](#) even if you have previously used Putty. MobaXterm is a more full-featured terminal client that comes integrated with X11 server to allow rendering graphics through X windows on a remote server. MobaXterm also has an sftp tab built in to the client permitting ease of file transfer from remote to local machine.

MobaXterm Install

- Go to The MobaXterm site, and click either the **Download Tab** at the top or the **Get MobaXterm button** on the middle of the page to redirect to the Download page.
- Choose the Free Home Edition of MobaXterm.
- Download the MobaXterm Home (Installer edition) zip file.
- Extract the contents of the zip file by right clicking it and choosing **extract**.
- Locate the MobaXterm_installer.msi file and double click it to install.
- MobaXterm will now be accessible from your Startup menu

VMD

Visualization of molecules will be done with VMD. It is recommended to install VMD on your laptop for best performance, rather than using it over an X11 connection. This installation should also be done by the end of the first day. There are Mac and PC versions available for download on the VMD website:

<http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD>

Connecting to RCC resources

This step is to be done on site when the school commences.

To connect to the remote compute cluster, each participant will need to do the following steps:

Mac/Linux users

- Move the rccguest ssh key zip file to an easily accessible location on your machine.
- Open your terminal client and change directory to where the rccguest ssh key zip file is located.
- Unzip the rccguestXXXX.zip files (where XXXX is the guest number) using the ssh-key file password provided to all participants on the first day.

```
unzip rccguest1234.zip
```

- Descend into the rccguest folder and run the login.sh script by issuing the following:
./login.sh

This script will try to start an -X11 enabled ssh session with midway, if it detects X11 is not currently available it will fall back to a X11 disabled ssh session. If you would like to render remote graphics you will need to follow steps above to instal X11 server.

The login script executes the following command for X11 enabled ssh:

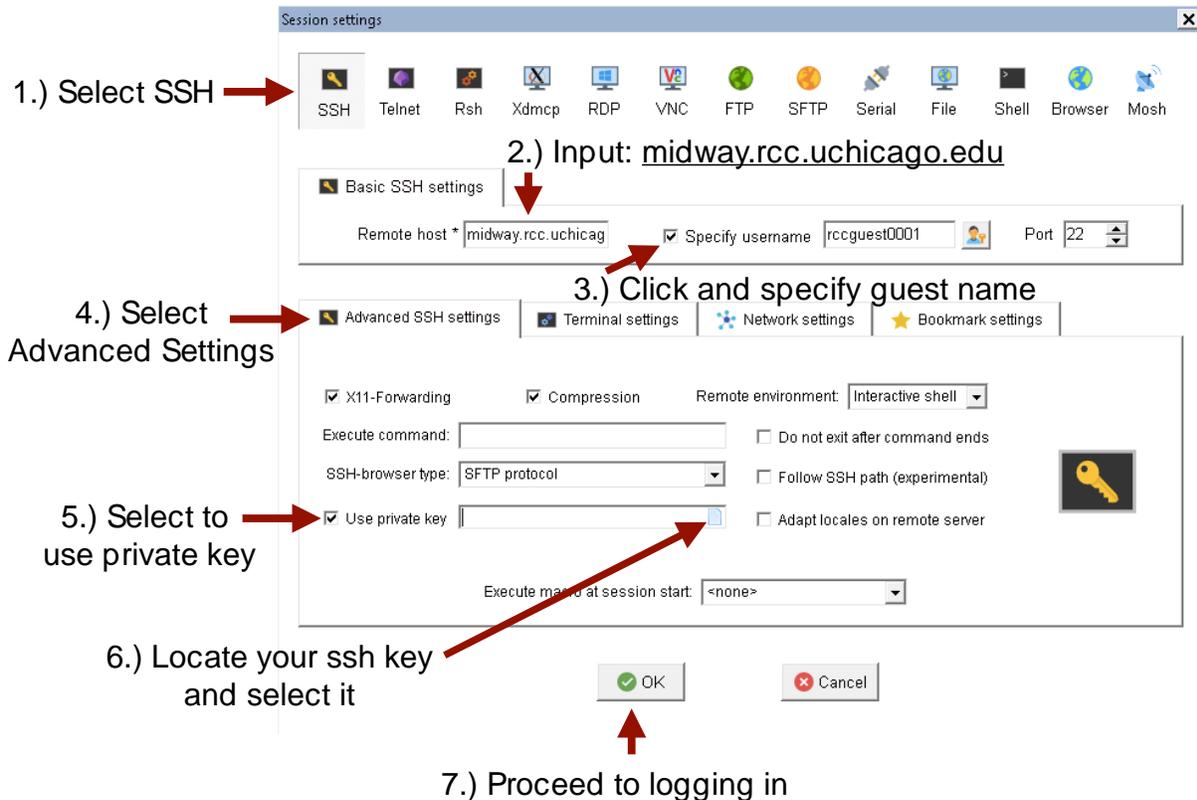
```
ssh -Y -i /PATH_TO_SSHKEY/rccguestxxxx.key rccguestxxxx@midway.rcc.uchicago.edu
```

or if without X11 enabled ssh, the following command is executed:

```
ssh -i /PATH_TO_SSHKEY/rccguestxxxx.key rccguestxxxx@midway.rcc.uchicago.edu
```

Windows users

- Move the rccguest ssh key zip file to an easily accessible location on your machine.
- Open your terminal client (MobaXterm) and click on the Sessions icon at upper left hand corner of the client.
- Then perform the following numbered steps, illustrated in the figure below.
 - 1) Click the SSH tab to expand the SSH login options.
 - 2) In the **Remote host** field input: **midway.rcc.uchicago.edu**
 - 3) Select the **Specify username** button and input your rccguest user name (e.g. rccguest0001)
 - 4) Select the **Advanced SSH Settings** tab.
 - 5) Checkmark the **Use private key** button.
 - 6) Click the icon in the **Use private key field** to locate and select your private ssh key to
 - 7) Proceed to login by clicking the **OK** button.



Accessing the school shared space

- Upon connecting to midway, you will land in your guest user account home directory. This directory contains a README file with useful information about using the compute resources.
- In your home directory there is a soft link to the shared summer school folder (miccom-school). To access this folder simply change directory to it.

```
cd miccom-school
```
- To access your user scratch space, use the environment variable \$SCRATCH

```
cd $SCRATCH
```
- Note: Your home and scratch quotas are 30GB and 100 GB respectively. The shared miccom-school is limited to 1TB.

Transferring files to and from Midway

Mac and Linux users should open their terminal to run the following commands, while Windows users using the MobaXterm client should open a local shell by clicking on the Start local terminal button on the home screen of the MobaXterm client:

To copy a file from your local computer to your home directory on midway:

```
scp -i PATH_TO_SSH-KEY/rccguestXXXX.key local_file rccguestXXXX@midway.rcc.uchicago.edu:~/
```

To copy a directory from your local computer to your home directory on midway:

```
scp -i PATH_TO_SSH-KEY/rccguestXXXX.key local_folder -r rccguestXXXX@midway.rcc.uchicago.edu:~/
```

To copy a file from your home directory on midway to your local computer:

```
scp -i PATH_TO_SSH-KEY/rccguestXXXX.key rccguestXXXX@midway.rcc.uchicago.edu:~/file /local_directory_path
```

To copy a folder from your home directory on midway to your local computer:

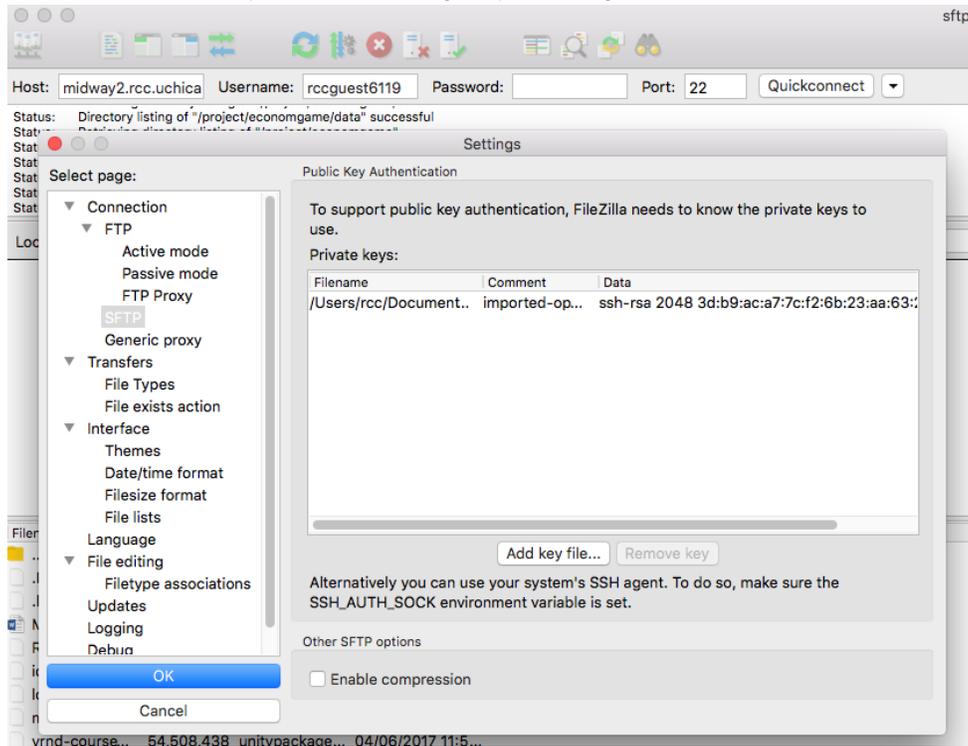
```
scp -i PATH_TO_SSH-KEY/rccguestXXXX.key -r rccguestXXXX@midway.rcc.uchicago.edu:~/folder /local_directory_path
```

On **Windows**, **MAC**, or **Linux** you can use also a GUI-based client tool such as [FileZilla](#) or [Cyberduck](#). Make sure when connecting, that you specify the location of the private ssh-key. MobaXterm has an sftp panel that allows you to drag and drop files between the remote server and your local machine.

The configuration for FileZilla (available for MAC, Linux, and Windows) is provided below and illustrated in the figure that follows.

- **Host:** midway.rcc.uchicago.edu
- **Username:** rccguestXXXX
- **Port:** 22
- **Go to FileZilla -> Settings -> SFTP -> Add key file...**

- Browse for the ssh-key corresponding to your rccguest account:



More information about data transfer on Midway can be found [here](#).

Using Module Installed Software

Software is available by loading the proper module. See [here](#) a full list of the software modules available on the RCC cluster (note that we are using Midway and not Midway2).

Show the list of all available software modules:

- `module avail`

Show the list of available modules for a specific software you are interested (e.g., python):

- `module avail python`

Show the list of currently loaded modules:

- `module list`

Show more information about a specific software package:

- `module show python/3.5.2+intel-16.0`

Load a specific software package version into your environment:

- `module load python/3.5.2+intel-16.0`

-

Unload a specific software package version into your environment:

- `module unload python/3.5.2+intel-16.0`