NSF/DOE Quantum Science Summer School

Introduction to density functional theory

Connecting to MARCC, Maryland Advanced Research Computing Center

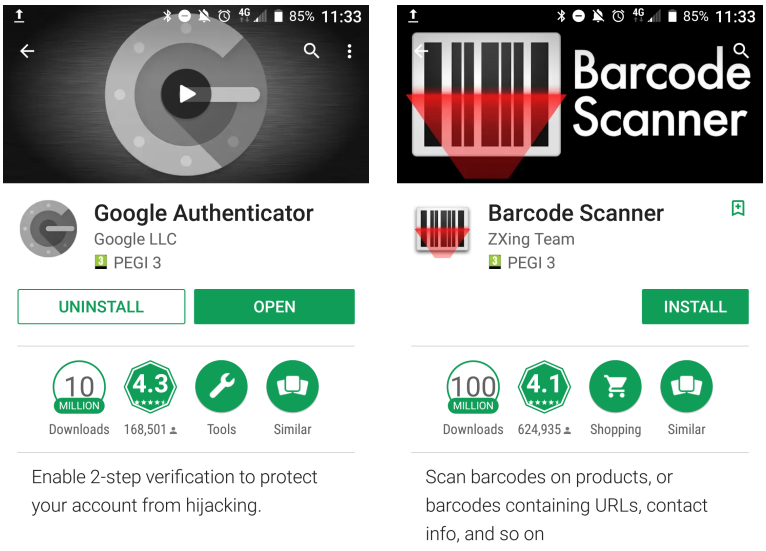
Two-factor authentication

In order to connect to MARCC we need to setup the 'two-factor authentication' protocol.

For this you will need:

- The username sent to you by MARCC via email
- The temporary password sent to you by MARCC via email
- The Google Authenticator

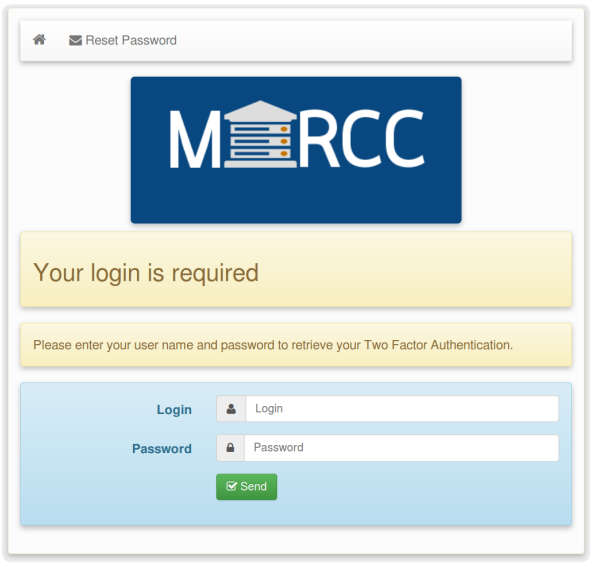
The Google Authenticator can be installed from the Play Store on your mobile device. You will also need a Barcode Scanner. The two apps look as follows:



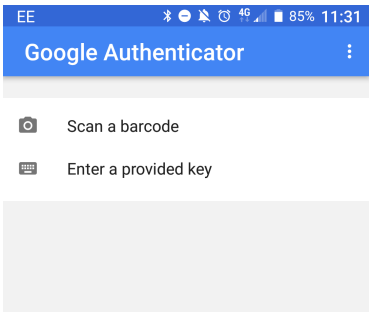
Now open this webpage (just follow the hyperlink):

https://password.marcc.jhu.edu/?action=qrretrieve

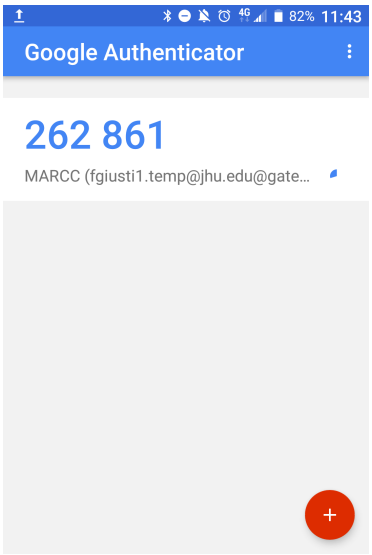
You will be prompted for username and password, here we need to enter the `username` and `password` that we have received by email:



After entering our username and password, the webpage shows a barcode. Here we link the Google Authenticator to our MARCC account by scanning the barcode:



The above steps are performed only once. From now on we can login into MARCC using our username, password, and verification code. The verification code is the number provided by the Google Authenticator, as in the following snapshot:



The standard procedure for logging in is described in Tutorial T1.

Connecting from a Windows machine

If you are using Windows on your laptop/desktop, then in order to connect to MARCC you will need a software that can handle a secure shell (SSH) connection.

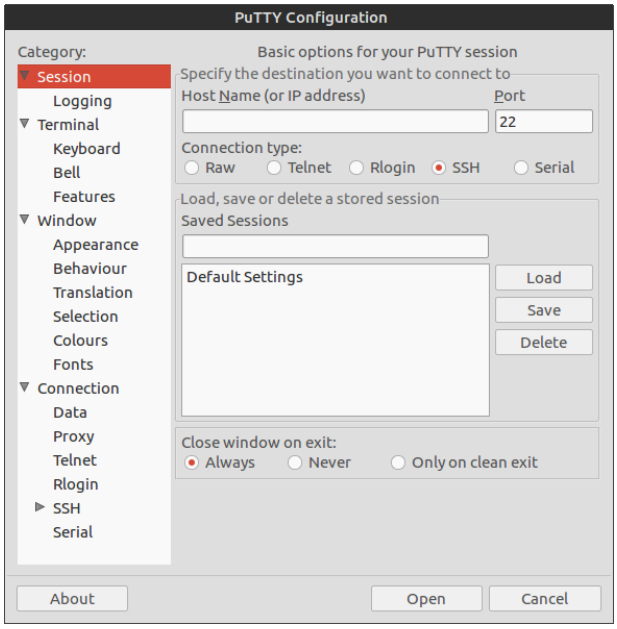
A popular choice is Putty, which can be downloaded from:

http://www.putty.org

If you are unsure whether you have a 32 bit or 64 bit architecture, then the safest option is to download the following executable:

https://the.earth.li/~sgtatham/putty/latest/w32/putty.exe

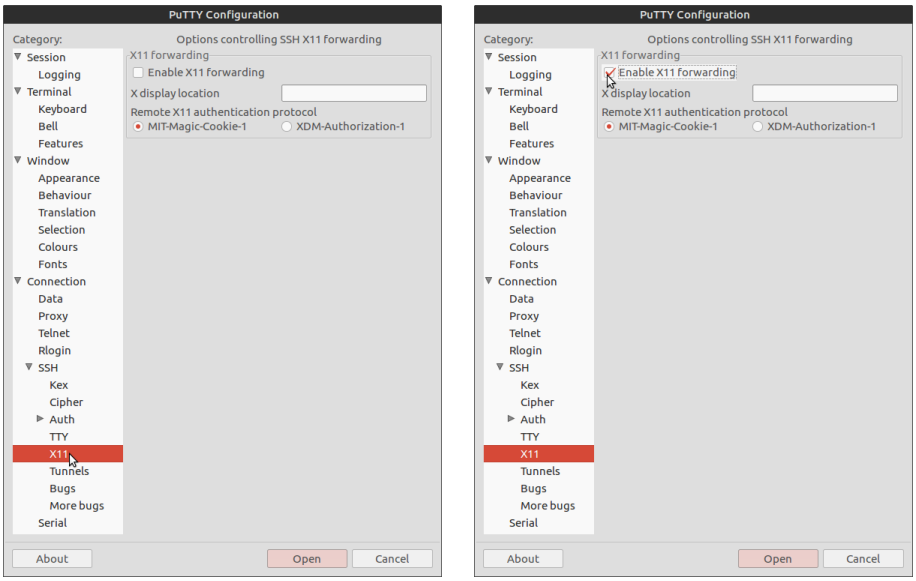
When you execute Putty you will see something like the following:



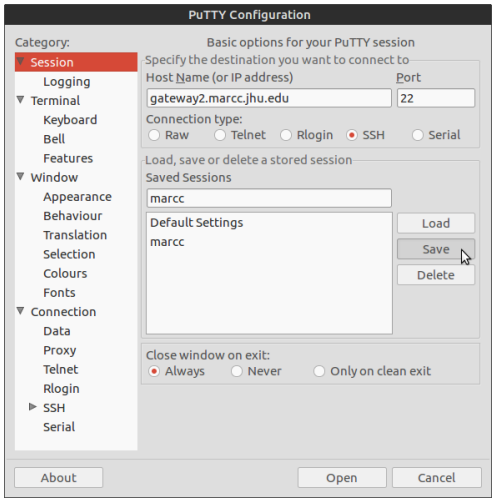
In the field 'Host Name' we enter:

`gateway2.marcc.jhu.edu`

In order to be able to see graphics over this connection, we need to enable 'X11 forwarding'.
For this we proceed as indicated below:



Now we can save these settings, so that next time we will just click on the session name, say 'marcc':



Visualizing graphics from a Windows laptop

In order to visualize graphics when using Putty, your machine must be able to understand the X11 protocol. This can be done by downloading the program Xming.

The installation file can be found at the following link:

https://sourceforge.net/projects/xming/files/Xming/6.9.0.31/Xming-6-9-0-31-setup.exe/download

After installing `Xming` the procedure for running calculations and visualizing graphics on MARCC is as follows:

- Start `Xming`. This application will now run in the background.
- Start `Putty` and open a session.

From this point onward everything works exactly in the same way as for users of Linux or Mac.