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:

M RCC					
Your login is required					
Your logi	in is req	uire	d		
Your logi	in is requ	uire	d word to retrieve your Two Factor Authentication.		
Your logi	in is requ ur user name an Login	uire nd pass	d word to retrieve your Two Factor Authentication.		

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:

EE	¥ ⊖ 🄌 ত 👯 📶 🛢 85% 11:31			
Google Authenticator				
0	Scan a barcode			
	Enter a provided key			

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 down-load the following executable:

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

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

	PuTTY Configuration		
Category: Session Logging ▼ Terminal Keyboard Bell Features ▼ Window	Basic options for your PUTTY session Specify the destination you want to connect to Host Name (or IP address) Port Connection type: Raw Telnet Rlogin SSH Serial Load, save or delete a stored session Saved Sessions		
Appearance Behaviour Translation Selection Colours Fonts V Connection	Default Settings	Load Save Delete	
Proxy Telnet Rlogin ▶ SSH Serial	Close window on exit: • Always Never Only on cle	an exit	
About	Open	Cancel	

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:

	PuTTY Configuration		PuTTY Configuration		
Category:	Options controlling SSH X11 forwarding	Category:	Options controlling SSH X11 forwarding		
▼ Session	-X11 forwarding	▼ Session	X11 forwarding		
Logging	Enable X11 forwarding	Logging	Enable X11 forwarding		
▼ Terminal	X display location	▼ Terminal	ば X display location		
Keyboard	Remote X11 authentication protocol	Keyboard	Remote X11 authentication protocol		
Bell	MIT-Magic-Cookie-1 XDM-Authorization-1	Bell	MIT-Magic-Cookie-1		
Features		Features			
▼ Window		▼ Window			
Appearance		Appearance			
Behaviour		Behaviour			
Translation		Translation			
Selection		Selection			
Colours		Colours			
Fonts		Fonts			
▼ Connection		▼ Connection			
Data		Data			
Proxy		Proxy			
Telnet		Telnet			
Rlogin		Rlogin			
▼ SSH		▼ SSH			
Kex		Kex			
Cipher		Cipher			
Auth		► Auth			
TTY		TTY			
X11		X11			
Tunnels		Tunnels			
Bugs		Bugs			
More bugs		More bugs			
Serial		Serial			
About	Open Cancel	About	Open Cance		

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

	PuTTY Configurati	ion		
Category: Session Logging ▼ Terminal Keyboard Bell Features ♥ Window	Basic options for your PuTTY session Specify the destination you want to connect to Host Name (or IP address) Port gateway2.marcc.jhu.edu 22 Connection type: Raw Raw Telnet Rlogin SSH Load, save or delete a stored session Saved Sessions			
Appearance Behaviour Translation Selection Colours Fonts ▼ Connection Data	marcc Default Settings marcc		Load Save	
Proxy Telnet Rlogin ▶ SSH Serial	Close window on exit: • Always Never Only on clean exit			
About		Open	Cancel	

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.