

NMRbox-General

- *What is NMRbox, what is a VM, what is PaaS, what is the downloadable version of NMRbox?*
- *How do I cite or acknowledge NMRbox?*
- *Are there any advantages of NMRbox as a Platform-as-a-Service (PaaS) over a downloadable version of NMRbox?*
- *When does NMRbox PaaS go off-line for maintenance?*
- *How do I use the terminal, shell, command line?*
- *Why can't I shutdown or reboot NMRbox running as a PaaS?*
- *What do I do if I made the screen resolution very high and cannot change it back?*
- *Why do I get "command not found" when I run my scripts? Why is the current working directory not in the path?*
- *How to deal with high resolution displays on laptops when connecting to NMRbox with RealVNC Viewer?*

NMRbox Account

- *How do I create an NMRbox account?*
- *How do I change or reset my password?*

Virtual Network Computing (VNC)

- *What is a Virtual Network Computing (VNC)?*
- *Why must I use RealVNC Viewer to connect to NMRbox and no other VNC Viewer?*
- *Why do I get a "Either the username was not recognized, or the password was incorrect" message when connecting to my NMRbox VM via RealVNC?*
- *Do I need to start a VNC Server session before connecting to NMRbox with RealVNC Viewer?*
- *How to get the mouse working properly in RealVNC?*
- *How do I view the VNC Viewer Menu / Toolbar?*
- *Does my session close when I exit the RealVNC Viewer?*
- *What if I cannot connect RealVNC Viewer to NMRbox?*
- *How do I change the screen resolution, change the size of the NMRbox window, and work in Full Screen Mode?*
- *Can I use two monitors for my VNC connection?*
- *How do I kill my VNC server session?*
- *Can I print when connected to NMRbox via RealVNC Viewer?*

My Data

- *Is my data safe?*
- *How do I transfer files to/from NMRbox?*

- [Where can I store my files on my NMRbox VM PaaS account?](#)
- [How do I share files with other NMRbox users?](#)
- [Who has access to my data?](#)

NMRbox Software

- [How do I find what software is installed?](#)
- [Can I install programs in my local account?](#)
- [What if a program I want to use is missing from NMRbox?](#)
- [Why does nmrDraw not show my spectrum?](#)
- [Can I use the Ubuntu software installer to add Ubuntu packages?](#)

NMRbox General

What is NMRbox, what is a VM, what is PaaS, what is the downloadable version of NMRbox?

- NMRbox is a virtual machine (VM) running XUbuntu Linux and is pre-configured with a large number of programs for processing and analyzing NMR data as well as many other utilities and programs often used in conjunction with NMR such as SAXS, molecular visualization, etc.
- A virtual machine (VM) is a virtualized operating system configured with installed software and settings just like an ordinary operating system. The VM can be hosted on a personal computer allowing the user to run multiple operating systems concurrently or be hosted on dedicated VM host servers.
- Platform-as-a-Service is where the NMRbox VM is housed on our dedicated VM servers in our high performance computing center and users access their NMRbox VMs by connecting via ssh or more commonly with a full graphical interface through a VNC connection using the free RealVNC Viewer.
- The downloadable version of NMRbox is a VM bundled as a single file for download, often called an OVA file. The OVA file can then be opened with software called a hypervisor, generally Oracle's VirtualBox or VMware's Fusion, Workstation, or Player. There are other hypervisor software programs which may or may not work with NMRbox.
 - Note: We are releasing NMRbox as a PaaS initially and the downloadable version will follow shortly.

[\(top\)](#)

How do I cite or acknowledge NMRbox?

If you utilize NMRbox in your research please cite us by following the instructions from the NMRbox website <https://nmrbox.org/acknowledge-us>.

[\(top\)](#)

Are there any advantages of NMRbox as a Platform-as-a-Service (PaaS) over a downloadable version of NMRbox?

Yes!, there are several significant advantages as outlined here:

- **Ease of installation.** The only thing a User needs to install is a lightweight program called RealVNC Viewer or a ssh client. For a downloadable VM the User must install a hypervisor, such as VirtualBox, install the NMRbox VM, and configure file storage so that it is robust (not always an easy task).
- **Security.** User files are stored on Enterprise class file servers with significant redundancy and Home folders are backed up regularly.
- **Performance.** NMRbox VMs are housed on dedicated VM servers with 36 – 44 compute cores with between 256 and 768 GB of physical RAM and six 10 GB network connections. The data center housing NMRbox servers has a 100 GB network connection to the outside world and 40 GB network fabric between the switches and redundant 10 GB network connections to the VM hosts and storage.
- **Cost.** The use of NMRbox is *free*, including the computational resources and file storage. No need to have your own high-end computers for NMR data processing.
- **Portability.** With the use of RealVNC Viewer a User can connect and disconnect to their NMRbox account while calculations are on-going and Users can connect from wherever they have a network connection. No need to be tied to a Workstation in the lab.
- **Easy migration.** When a new version of NMRbox is released all that is needed to upgrade is shutting down your NMRbox VM server and starting up a new NMRbox server and logging in. In the future Users will be able to manage the process themselves, but initially this will be handled with the help of the NMRbox team.

[\(top\)](#)

When does NMRbox PaaS go off-line for maintenance?

- We will make every effort to not shut-down services to NMRbox VM PaaS, but occasionally the systems will need to be powered off for maintenance. We will make every effort to notify users ahead of time with any scheduled outages and will attempt to perform such maintenance on Monday's at 7:30 AM Eastern Time (New York).

[\(top\)](#)

How do I use the terminal, shell, command line?

The use of a Terminal Emulator (often called “*shell*” or “*terminal*” or “*command line*”) is critical to utilize many of the programs within NMRbox. We have started a document on how to use the terminal which can be found on the Documentation page of the NMRbox website <https://nmrbox.org/documentation>. In addition the sites below are some good sources of information and *Ryans’s Tutorials* has some good tutorials.

- **The Linux Documentation Project (TLDP)**
 - <http://www.tldp.org/guides.html>

A collection of basic to advanced documents covering many aspects. Documents can be viewed on-line, downloaded, or printed.
- **Ryan’s Tutorials. A collection of introductory technology tutorials**
 - <http://ryanstutorials.net/>

A collection of tutorials, but the three most relevant to Linux and the command line are the “*Linux Tutorial*”, “*Bash Scripting*”, and “*Regular Expressions*”.
- **Unix Tutorial for Beginners**
 - <http://www.ee.surrey.ac.uk/Teaching/Unix/>
- **LinuxCommand.org** (Beginners guide to “The Shell” and “Writing Shell Scripts”)

- <http://linuxcommand.org/index.php>
- **Linux Bash Shell Cheat Sheet**
 - http://cli.learncodethehardway.org/bash_cheat_sheet.pdf
- **UNIX Toolbox** (Advanced. Has PDF download for printed versions)
 - <http://cb.vu/unixtoolbox.xhtml>
- **How to Look Like a UNIX Guru** (Advanced)
 - <http://www.cs.usfca.edu/~parrt/course/601/lectures/unix.util.html>

[\(top\)](#)

Why can't I shutdown or reboot NMRbox VM PaaS?

In early versions of NMRbox several users will be sharing a single instance of NMRbox VM and thus we do not want Users to shutdown NMRbox as other Users may have open connections or on-going calculations running. Also, to be honest, we don't want to have to keep restarting NMRbox VMs for Users that accidentally shut them down. In the future we plan on allowing this capability through the NMRbox Website, but for now the ability to shutdown or reboot is restricted. If there is an issue that requires a reboot, please send an email to support@nmrbox.org and the NMRbox team will resolve the issue.

[\(top\)](#)

What do I do if I made the screen resolution very high and cannot change it back?

If you use the resolution-changer script to set a screen resolution much higher than your actual screen resolution you may have a hard time finding your open terminal window to change it back to a lower resolution. There are several potential fixes to this issue:

1. You will notice scroll bars on the sides and bottom of the window - simply move the scroll bars in a systematic way to move around the very large desktop screen to find your open terminal window and re-run resolution-changer to set the resolution to a lower value.
2. From the VNC Viewer Toolbar select the Icon for Full-Screen Mode (the icon with 4 arrows). Optionally hit "F8" and select "Full Screen". In Full Screen Mode you will be able to see your open terminal to re-run the resolution-changer script, although the text will be very small.
3. Right mouse click anywhere on the Wallpaper and select "Open Terminal Here" and then run the resolution-changer script to change to a more appropriate resolution.

[\(top\)](#)

Why do I get "command not found" when I run my scripts? Why is the current working directory not in the path?

In Linux there is a search path that can be shown by opening a terminal window and entering the command "**echo \$PATH**". The output will be a series of directories that are searched when you enter a command. For example, when you type "**find**" from a terminal, locations in the path are searched until the command "**find**" is found and then it is executed (no further searching is done). In the case of "**find**" the command is located in **/usr/bin/find**.

When you create shell scripts for processing data you may simply try to type the name of the script to have the script run. For example, let's say you create a script called **nmrpipe.com**. From a terminal you type "**nmrpipe.com**" and you get a "**command not found**" error. This is because the current working

directory is not in the search path and hence the command `nmrpipe.com` is not found. To resolve this issue add a `./` in front of the script name, `./nmrpipe.com`. The `.` is mapped to the current working directory so typing `./nmrpipe.com` is equivalent to typing the explicit path `/home/nmrbox/username/.../nmrpipe.com` just in a shorthanded way. As a note `..` is mapped to the parent of the current working directory. That is why the command `cd ..` moves up one directory.

In the past many users would add the current working directory to their path. However, we would discourage anyone from doing this for a few reasons.

- It is very easy to type `./` in front of your scripts so very little is gained.
- It ensures you are running the script you think you are running. Imagine a scenario where there is a script called `nmrpipe.com` in the search path and it is searched before the current working directory. Now when you type `nmrpipe.com` you end up running the `nmrpipe.com` script from a different location than the expected current working directory.
- It is security risk. Imagine you accidentally download a malicious program called `ls` which performs some undesirable task and ends by running the real `ls` command. If you perform an `ls` command from a current working directory where the malicious `ls` command was located you would be running the malicious code accidentally, and because it masks itself by running the real `ls` command you may not even realize what you did.
- If you accidentally create a file with the same name as a system command then the system command may not run properly from the directory. Imagine if you accidentally created a file called `mkdir` and the current working directory was in the path. Now when you try to run the command `mkdir` from that directory you would simply get a returned prompt without anything happening making it appear that the `mkdir` command was not working properly.

[\(top\)](#)

How to deal with high resolution displays on laptops when connecting to NMRbox with RealVNC Viewer?

Newer laptops often have very high resolution screens. On Windows and OSX the size of menus, icons, and fonts are scaled to be larger so they are readable. However, when connecting NMRbox VM PaaS the menus, icons, and fonts may be so small they are unreadable. To fix this issue open a terminal and run `resolution-changer` and choose a reasonable resolution for your screen size, which is often considerably less than the actual screen resolution, such as 1920x1080 when using a Retina or 4K laptop. The NMRbox window will be small and hard to read at this point on your high resolution screen. Then go to the RealVNC Viewer Toolbar and select Full Screen or play with the scaling setting to stretch the screen size larger and hence make things easier to view. Note that you may need to select / deselect the `Scale to window size` and `preserve aspect ratio` from the Options window under the `Advanced` window and `Display` tab to optimize your window.

NMRbox Account

[\(top\)](#)

How do I create an NMRbox account?

Go to <https://nmrbox.org> and press "Sign up for an account". A short time after filling out the form the NMRbox team will be in contact with further instructions. We are sorry that we cannot make the NMRbox service available immediately, but we must verify users before granting access for security and legal reasons and it will take some time for your personal VM to be created.

[\(top\)](#)

How do I change or reset my password?

NMRbox passwords are managed by a program called NetWrix Password Manager and is run through the BioScience-CT Network where NMRbox is housed. To change or reset your password go to <https://portal.bioscience-ct.net/pm/> and follow the directions for "Change" or "Reset".

You should have used the site when your account was first created and you enrolled for the first time.

If you are unable to reset a forgotten password you can email support@nmrbox.org and a NMRbox staff member will reset your password manually. Note that this may take a day or two to accomplish as the request will be pushed to the IT professionals that manage the authentication system.

Virtual Network Computing (VNC)

[\(top\)](#)

What is a Virtual Network Computing (VNC)?

VNC is a way to graphically share a desktop including keyboard and mouse events. On Linux the graphical desktop is a virtual display that only the user can access. This allows multiple users to access the same server each with their own graphical display without interfering with each other. VNC has very good performance over even modest network connection speeds as the only information that is transmitted are the changes in the display. VNC was developed in the 1990's by what is now RealVNC. See "Why must I use RealVNC Viewer to connect to NMRbox and no other VNC Viewer?" for additional information.

[\(top\)](#)

Why must I use RealVNC Viewer to connect to NMRbox and no other VNC Viewer?

We are utilizing a commercial VNC server inside NMRbox from the company RealVNC. The commercial version of RealVNC provides several benefits as outlined here, but the only way to connect to NMRbox is with a VNC Viewer from RealVNC.

The good news is that the NMRbox team has purchased licenses for RealVNC server and NMRbox Users only need to download the **free** RealVNC Viewer which runs on almost any device. Note, you do not need to download the VNC server to your local computer.

Benefits of RealVNC server.

- **Free.** RealVNC Viewer is free for all platforms and runs on almost all devices.
- **Full encryption.** All connections with NMRbox are fully encrypted.
- **Single sign-on.** Your NMRbox username and password are used to logon, unlike open-source VNC servers which require the User to create a separate, unsecure, login which resides in the users Home folder.
- **Daemon mode.** There is no need to login via ssh and start a vncserver session manually. VNC server sessions are started automatically when you login via RealVNC Viewer.
- **Built-in file transfer.** Files can be transferred into and out of your NMRbox account from within the RealVNC Viewer program.
- **Local printing.** The default printer on your local computer is mapped to your NMRbox account allowing Users to print from within NMRbox to your local printer.
- **Full screen mode and multiple monitors.** RealVNC supports Full Screen mode with and without scaling and allows the display to span multiple monitors.
- **Performance.** The commercial RealVNC Viewer / Server combination has excellent performance.
- **Persistent sessions.** Once started the VNC server session will remain alive allowing the User to connect and disconnect as often as they like from any location or device.

[\(top\)](#)

Why do I get a "Either the username was not recognized, or the password was incorrect" message when connecting to my NMRbox VM via RealVNC?

Well, the obvious answer is that either the username is not correct or the password is incorrect. However, figuring out which can be difficult. Here are some guidelines on how to resolve the situation.

- Do not continue to login repeatedly with the wrong username or password. After 8 straight unsuccessful login attempts the computer you are using will be blacklisted and it will take a while for the blacklist to be lifted.
- Check that the “Username:” and “Password:” in the *VNC Viewer – Authentication* dialog box, which appears after entering the “VNC Server:” in the *VNC Viewer* dialog box, is correct. By default the “Username:” is set to the username of the current account on your local computer and is generally not your NMRbox username and thus needs to be changed.
- Attempt to **ssh** into the computer to verify the username and password. From Linux or OSX enter the following command from a terminal “**ssh username@username.nmrbox.org**”. From Windows you will need a **ssh** program such as *BitVise Tunnelier*. Note that too many unsuccessful ssh attempts can also cause your computer to be blacklisted, thus don’t try the same wrong username and password over-and-over again.
- Attempt to make a VNC connection from another computer. If your computer was blacklisted the connection will be possible from another computer with a different IP address. The blacklist starts with a 10 second lockout after 8 unsuccessful logins and then grows geometrically. Thus if you wait a while your computer will be removed from the blacklist automatically.
- If you are unable to resolve the issue send an email to support@nmrbox.org for further assistance and provide as much detailed information as possible.

[\(top\)](#)

Do I need to start a VNC Server session before connecting to NMRbox with RealVNC Viewer?

- **No!** With the commercial version of RealVNC that NMRbox is utilizing the VNC server runs as a daemon and a VNC server session is started when the User logs in from the RealVNC Viewer. **In fact, you should never run the command “vncserver” in NMRbox.** See the FAQ on “[How do I end my VNC server session](#)” to kill a VNC server session that was started by accident with vncserver.

[\(top\)](#)

How to get the mouse working properly in RealVNC?

From the RealVNC Viewer program open the Options window by selecting the “Options” button from the VNC Viewer login screen or by pressing the Options icon from the Toolbar (see “[How do I view the VNC Viewer Menu / Toolbar](#)”). Once the Options window is open select the “Advanced” button at the bottom (if the Advanced Mode is already selected the button will say “Basic” and this step is skipped). In Advanced mode select the “Inputs tab”. From here it is difficult to give exact instructions as it is dependent on the operating system you are using and your mouse and hardware. However, by trying different combinations of the mouse settings you should be able to find a selection that makes your mouse or trackpad work as expected inside NMRbox.

It is often advantageous to use a three button mouse rather than a trackpad when using a laptop.

[\(top\)](#)

How do I view the VNC Viewer Menu / Toolbar?

When the VNC Viewer is running there may be a menu at the top/middle of the window that is mostly hidden and all that may be visible is the very bottom of the Toolbar. To reveal the Toolbar hover the mouse over the

area and the Toolbar will reveal itself. It is also possible that the Toolbar is set to not be present from the VNC Viewer Options. If this is the case open the VNC Viewer Options by pressing "F8" from within the program and select "Options" from the menu that appears. Alternatively you can launch the VNC Viewer login window and select the Options button. In the Options dialog select the "Display" tab and check the "Enable toolbar" setting to restore the Toolbar. If only a Basic tab is displayed either select the "Advanced" button and follow the instructions above, or from the Basic tab there is also a "Enable toolbar" checkbox that can be selected.

[\(top\)](#)

Does my session close when I exit the RealVNC Viewer?

No! Once the VNC Server session is started it will remain running until it is either explicitly killed (not generally needed) or the NMRbox server is power cycled. You can connect and disconnect to the same VNC session multiple times and from multiple devices. Calculations that are being performed continue to execute even when the VNC Viewer is disconnected. This can be convenient when using NMRbox from different locations such as work and home.

Note that you can connect to your NMRbox VNC Session multiple times concurrently from the same or different devices. In this case the Desktop environment is shared (all connections will view the exact same screen, including mouse movements).

[\(top\)](#)

What if I cannot connect RealVNC Viewer to NMRbox?

If the VNC Viewer cannot connect to `username.nmrbox.org` there are four likely possibilities;

1. Your internet connection is not functioning or you are mistyping the server name, username, or password.
2. The `username.nmrbox.org` VM is not functioning properly.
3. Your institution is blocking the outgoing port which RealVNC is attempting to use to connect to our servers.
4. You attempted to login repeatedly with the wrong password and your computer has been blacklisted by the VNC server.

Troubleshooting: After verifying that you have an active internet connection attempt to ssh into the NMRbox VM. From OSX or Linux open a terminal and type "`ssh username.nmrbox.org`", without the quotes where username is your username. If you are prompted for a password then the NMRbox VM is alive. From Windows you will need to download a ssh client program if you do not already have one installed. BitVise Tunnelier is a good choice, but there are many others as well. If you cannot ssh to the NMRbox VM please contact the NMRbox team via email at support@nmrbox.org so that we may fix the issue.

If you can ssh successfully, but cannot connect via VNC, then it may be possible that your computer is blacklisted due to too many failed logins or your institution is possibly blocking the outgoing port that VNC is using. If you can connect from a different computer in your institution it is likely that your computer has been blacklisted. Send an email to support@nmrbox.org to have the blacklist removed. To test if your institution is blocking VNC attempt to connect via VNC from outside your institution, such as from your home. You can also send the NMRbox team an email at support@nmrbox.org and we will test the connectivity.

If your institution is blocking the port that VNC is using there are two fixes. The preferred fix is to contact your IT department and ask that they open port 5900 for outbound traffic for your computers. If your IT department is not amendable to this then contact the NMRbox team at support@nmrbox.org and we will work out a solution for you.

[\(top\)](#)

How do I change the screen resolution, change the size of the NMRbox window, and work in Full Screen Mode?

When you connect to NMRbox via RealVNC for the first time the window size will likely be smaller than you desire. There are three ways in which you can make the NMRbox window larger.

- Increase the display resolution. To increase the NMRbox resolution open a terminal by right mouse clicking anywhere in the NMRbox wallpaper and choosing “Open terminal here”. Then run the command “resolution-changer”. This will open a dialog box with many different screen resolutions and aspect ratios. Select the resolution that best matches your screen resolution or the one that best suits your needs and hit “OK”.
 - Note that you can also select the scale by 90% checkbox to reduce the X and Y dimensions by 90%, often helpful when you want NMRbox to be slightly smaller than your whole display.
 - Note that you can also select 2X to double the X dimension if you want to utilize two monitors.
 - Note that if you set the screen resolution larger than your window size vertical and/or horizontal slider bars will appear. However, you can then scale the display to remove the slider bars, although the display will be scaled down.
- Scale to window size. Go to the RealVNC Options and from the “Advanced” menu select the “Display” tab and the “Scale to window size” button.
 - This can be done with or without the “Preserve aspect ratio” button selected based on what you prefer.
 - Note that the resolution will not change, the display will simply be scaled up or down depending on whether the actual resolution was larger or smaller than your initial window size.
- Full screen mode. Full screen mode will scale the NMRbox window to fill your entire screen. It will not preserve the screen resolution. To enter full screen mode go to the RealVNC Toolbar and select the icon with four outward arrows, or go to the Options dialog box and select “Full screen mode”.
 - If you attempt to utilize two monitors than you must be in Full screen mode.

Generally it will take a bit of trial and error to select the combination of screen resolution, scaling, and window size that works best for your needs. Note that if you are using a very high resolution screen it is often helpful to use the resolution changer and set the resolution to a lower value and then scale the window size to enlarge the fonts, menubars, etc. If your screen resolution is very low it is often advantageous to set the resolution higher than your screen and work in Full screen mode to gain more real estate on your display.

[\(top\)](#)

Can I use two monitors for my VNC connection?

Yes, you can have an NMRbox VNC connection use two monitors, but there are a few restrictions. First, the NMRbox display will span two monitors, but they are treated as a single display, not as separate dual displays as is common in Windows and OSX. The other restriction is that the VNC Viewer must be in Full Screen Mode for the display to span multiple monitors.

To setup your NMRbox VNC connection to use two monitors follow these instructions.

1. Use RealVNC Viewer to connect to `username.nmrbox.org` and login.
2. Open a terminal and run “resolution-changer”. Select the desired resolution for a single monitor and then check the 2X “Double Horizontal Width” checkbox.

3. Open the VNC Viewer Options dialog box. If you are in “Basic” mode press the “Advanced” button at the bottom. Once in Advanced mode select the “Expert” tab. Scroll all the way towards the bottom and click “UseAllMonitors”. Change the setting to “True” and hit the “OK” button.
4. From the VNC Viewer Options select Full Screen mode and your NMRbox display should now span across both monitors.
 - a. Note that you may want to play with the “Scale to Window Size” selection under the “Display” tab.
 - b. Note that you will want to change the “UseAllMonitors” setting back to “False” when only using a single monitor.

[\(top\)](#)

How do I kill my VNC server session?

In general there should not be a need to kill a VNC server session. The VNC server remains running indefinitely and the User can connect and disconnect from the VNC Viewer when desired. However, there are times when there may be issues with the VNC server session and it is desirable to kill the session. Follow these instructions if you need to manually kill a VNC server session:

IMPORTANT NOTE: A VNC server session is a Login into the NMRbox VM. Killing the VNC server will log you out of NMRbox and kill any activity running jobs.

1. From within NMRbox open a Terminal or connect via ssh to `username@username.nmrbox.org`
2. Type “kill-vnc-server” and hit Enter.
3. Some text will be displayed with ALL the VNC server sessions that are currently running for username. There should only ever be a single VNC server session per username, but if multiple VNC server sessions are running they all will be shown.
4. Once you decide which VNC server session that needs to be killed enter the Display Port with a colon (e.g. :3).
5. If you are performing this task from within a RealVNC Viewer window the VNC connection will terminate and the VNC Viewer window will close. Simply reconnect with the VNC Viewer and re-login and a new VNC server will start automatically so you can continue your work.

[\(top\)](#)

Can I print when connected to NMRbox via RealVNC Viewer?

Yes! When RealVNC Viewer establishes a connection to NMRbox the default printer on your computer when the connection is created is mapped and set as the default printer inside NMRbox. You can then print to your local printer even though what you are printing is on the remote NMRbox VM server.

My Data

[\(top\)](#)

Is my data safe?

There are several answers to this question depending on perspective as described here:

- **Is the data safe from a mechanical (disk) failure?** NMRbox User Home folders are stored on an Enterprise class file server with redundancy to deal with failures of individual hard drives and even a whole node of the file server. In addition, backups of the Users Home folders occur on a regular basis. While we have confidence in the file server housing Users Home folders and our backup solution we do encourage Users to copy their important files off-line as well. Users can also store their files on `/nmr/archive/username`. This file system is a private cloud file system with a very high level of redundancy and has data stored in three different physical locations and rivals the protection that Fortune 500 companies use to store their data. The downside of the private cloud file system is that the performance is slower than the system where Users Home folders are located.
- **Is the data safe from other NMRbox users?** By default no other NMRbox user has access to your NMRbox Home folder. However, if you change the permissions of your Home folder (***something we strongly advise Users not to do***) then other NMRbox Users may have access to your files. Likewise, the majority of NMRbox team members **do not** have access to Users Home folders except the IT professionals that are in charge of maintaining the infrastructure.
- **Is the data safe from hackers?** The NMRbox team takes protecting the NMRbox VMs from hackers seriously and several mechanisms have been put in place to ensure that the NMRbox VMs are protected. We have had prototype NMRbox VMs running for over two years and have not encountered a breach. However, we cannot guarantee that a breach will not occur. The best protection we can do is to make sure that we have backups of data (which we do) and to encourage Users to not share login information and to use strong passwords (which we are trying to enforce).
- **Is the data safe from myself?** Unlike Windows and OSX, when files are deleted from a terminal they are gone for good and do not end up in a Trash or Recycle Bin. The NMRbox team is creating backups of Users Home folders on a regular basis which may be used to restore data if a User accidentally deletes their files. We also hope to enable file system snapshots in the future which will also provide a mechanism to restore files that are accidentally deleted. However, these backups and snapshots are designed to recover from catastrophic failures of the system and will require significant effort of the NMRbox team to restore. Thus, the NMRbox team will be happy to help a User who accidentally deletes their files, but the restoration may take a day or two and hopefully should not become a regular occurrence. There is also a limited time that a given backup will be kept before it is over-written so it is imperative that you contact the NMRbox team at support@nmrbox.org immediately if you need to restore accidentally deleted files.

[\(top\)](#)

How do I transfer files to/from NMRbox?

- Files can be transferred to and from your NMRbox account with secure copy (scp), with secure copy via a GUI based program such as FileZilla, through the "File Transfer" built-into RealVNC Viewer, or in the near future through Globus. We hope to create a file transfer document in the near future with more detailed information.

[\(top\)](#)

Where can I store my files on my NMRbox VM PaaS account?

There are three locations where users with NMRbox accounts can store their files in NMRbox running as a PaaS.

- **Home Folder**
 - /home/nmrbox/username
 - Home Folders are located on a high performance storage system. The system has fault tolerance with regard to failed components (hard drives) and users home folders are backed up on a regular basis to an external system.
 - Due to limits on how much high performance storage the NMRbox project can afford users *may* be restricted on how much space they can use in their Home Folders.
- **Archive Folder**
 - /nmr/archive/username
 - Archive folders are stored on a private cloud storage system. The system is geo-dispersed and has extreme fault tolerance and can handle a catastrophic failure without the loss of data. The read/write performance for files stored in your Archive Folder is considerably slower than your Home Folder.
- **Public Folder**
 - /public
 - The public folder is readable and writable by all users. By default all files and directories created in /public will be owned by the user and only the user can delete or edit the files. However, they will be readable by all.
 - There is a README file in /public with the following disclosure:

***“This public directory is provided to allow NMRbox users to share files. No provision has been made for retention of files placed herein: users should use their home directories when long term persistence of files is desired.
The nmrbox team reserves the right to remove excessively large files or very old files.
team@nmrbox.org”***

[\(top\)](#)

How do I share files with other NMRbox users?

- By default NMRbox user home folders are only readable by the user and have a default file permission of `drwx-----` or `700`. It is **strongly advised** that users leave their home folder protected and not allow other users to have read access to their home folders.
- To share files with others, users are encouraged to copy files from their home folder to /public. Note however, that /public does not have the same protections as home folders and /nmr/archive/username folders and **SHOULD NOT BE** used as a long term storage of your data.
- If you desire the ability to share your files within your lab group please send us an email at support@nmrbox.org and we will attempt to work with you to accommodate your needs.

[\(top\)](#)

Who has access to my data?

- There are two groups that this question applies to:

- **Other NMRbox Users:** By default the permissions on each Users home folder are set so that no other User has access to their files (**drwx----- or 700**). However, if you change the permission of your home folder to allow **group** or **other** access to your home folder than others may have access to your files. **We strongly suggest that you do not change the default permissions on your home folder** and utilize the /public folder for sharing files or talk with the NMRbox team about setting up a lab group.
- **The NMRbox Team:** In order to maintain the hardware that provides the NMRbox PaaS some members of the NMRbox team need to have access to the file servers that house User data. However, access is limited to the IT professionals that maintain the computing infrastructure and most members of the NMRbox team **do not** have access to Users files.

NMRbox Software

[\(top\)](#)

How do I find what software is installed?

There are three main ways to determine what software programs are installed in a version of NMRbox:

1. From the NMRbox website. Feature is under development and will be available soon.
2. From the program launcher choose nmr-software and the installed software is listed.
3. The software packages in NMRbox are installed in /usr/software. Users can browse the /usr/software directory to view installed programs.

[\(top\)](#)

Can I install programs in my local account?

The short answer is “Yes”. However, if you send an email to support@nmrbox.org we will make an effort to include the program in an upcoming release of NMRbox. If you do install programs in your account we would appreciate being informed as we collect metric information on program usage for the NMR software developers and we can communicate with you as we release new versions of NMRbox with those programs pre-installed in NMRbox.

[\(top\)](#)

What if a program I want to use is missing from NMRbox?

We plan on releasing new versions of NMRbox on a regular schedule and will make efforts to include programs that our Users request. To request that a program be included in NMRbox send an email to support@nmrbox.org. It is also possible to install a program in your Home folder if you need access to the program quickly, however, we would appreciate the opportunity to be informed of programs you are installing in your account.

[\(top\)](#)

Why does nmrDraw not show my spectrum?

There are two known bugs in nmrDraw installed in NMRbox at the moment. We hope to have these resolved in the near future.

- When nmrDraw opens with a loaded spectrum, such as when using the “nmrDraw -in filename” command, the spectrum is loaded but the initial display is blank. Simply hit “d” to display the spectrum or select “draw” from the menu.
- A more insidious bug is that on very fast computers nmrDraw can occasionally not start properly which causes many of the buttons at the top of the nmrDraw window to not function. In this case simply shutdown nmrDraw and restart. nmrDraw will typically start fine the next time you try.

[\(top\)](#)

Can I use the Ubuntu software installer to add Ubuntu packages?

No! If there are Ubuntu software packages that you would like included in NMRbox please send a request to support@nmrbox.org and we will look into adding the package in future releases of NMRbox.