

# NMRBox

## Creating an account:

You need to create an account (register) to use NMRBox. **Also, once you register to have your account created, it may take several days until your account is validated, so you need to register significantly before you need to use NMRBox.**

The NMRBox website is at the following link:

<https://www.nmrbox.org>

On the home page, there is a 'Sign up' button.

Clicking this button will take you to the 'Sign Up' page where you will fill in all of the information for 'User Registration' (there are 'Instructions' on the right-hand side).

Once complete, click the 'Register' button at the bottom of the page.

Before your account is validated, you may receive an email confirming that you have registered and asking for your patience while your account is being validated.

As stated in the 'Instructions', once your account is validated, you will receive an email indicating that fact. You will be assigned a username. You will also be asked to follow a link to 'Set your password online'.

The email will also provide you with a link to the NMRBox documentation, and there is also a helpful 'FAQ' page:

<https://nmrbox.org/pages/documentation>

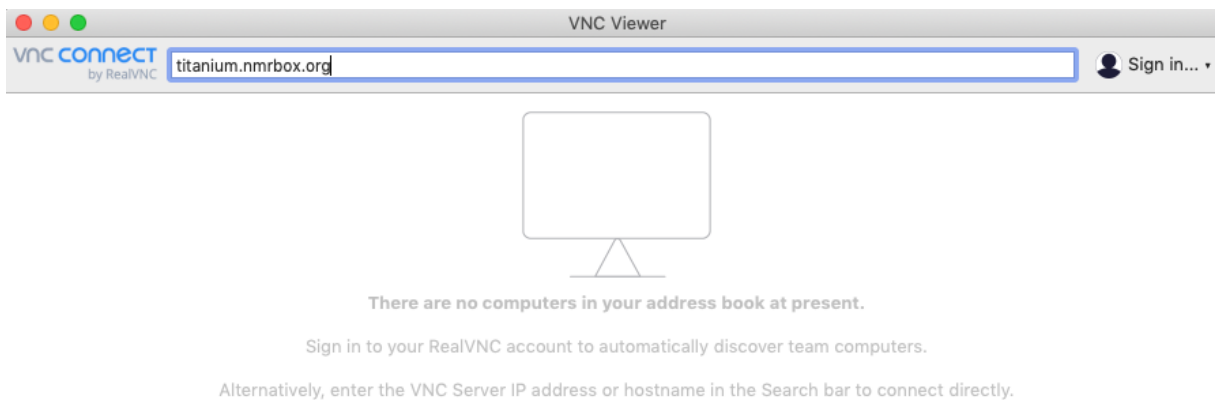
<https://nmrbox.org/faqs>

You can view all of the servers currently running, which you can connect to and use, on the user dashboard page:

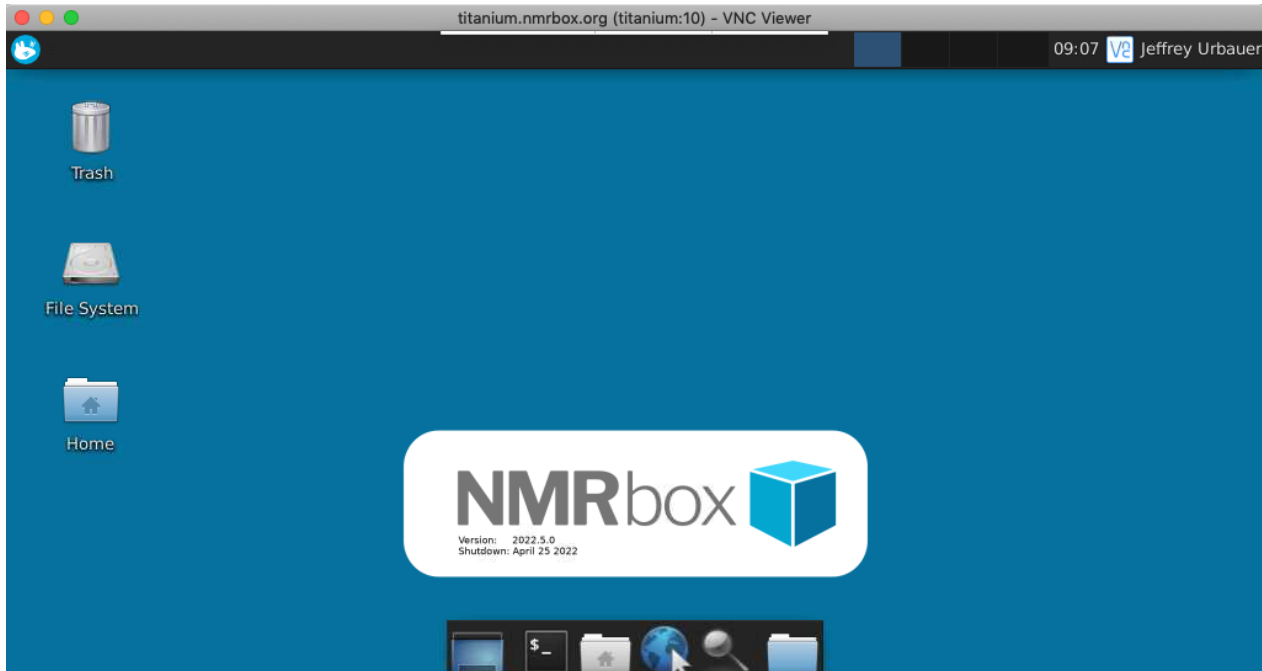
<https://nmrbox.org/user-dashboard>

## Accessing NMRBox using VNC Viewer:

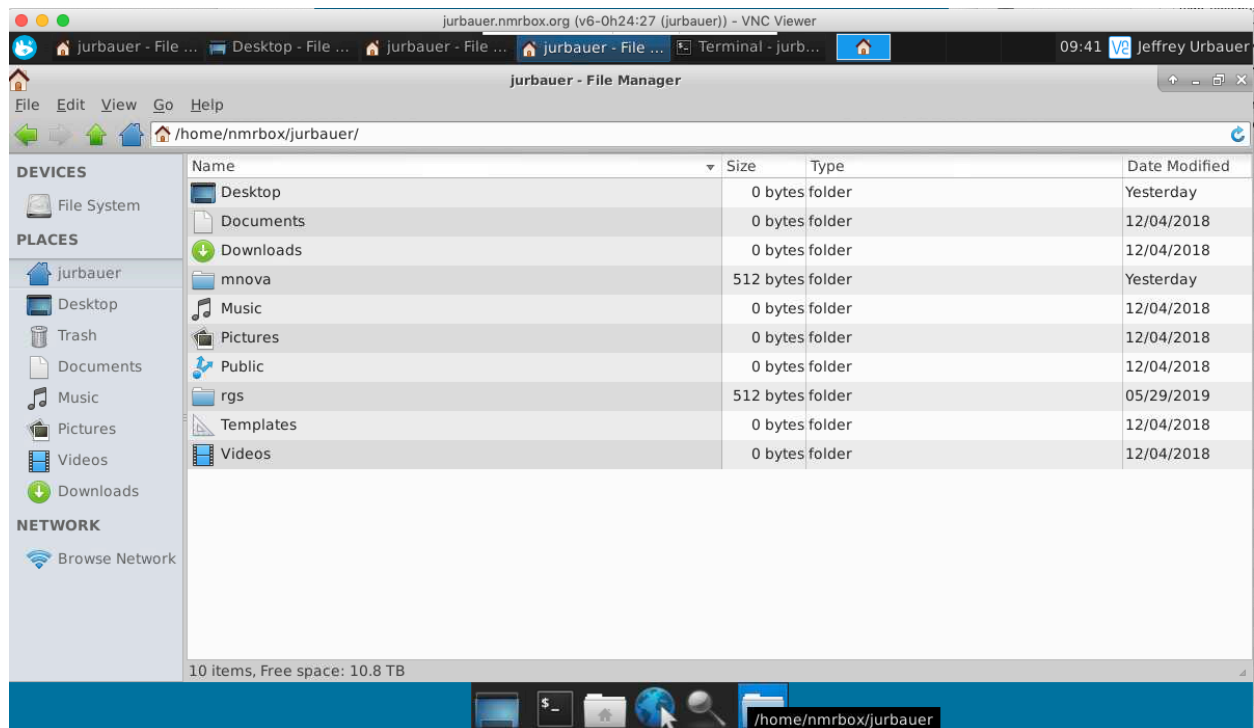
Once you start the VNC Viewer, you can enter the name of one of the active servers in the VNC Viewer address window ('Enter a VNC Server address or search'). Here we accessed the 'titanium' server:



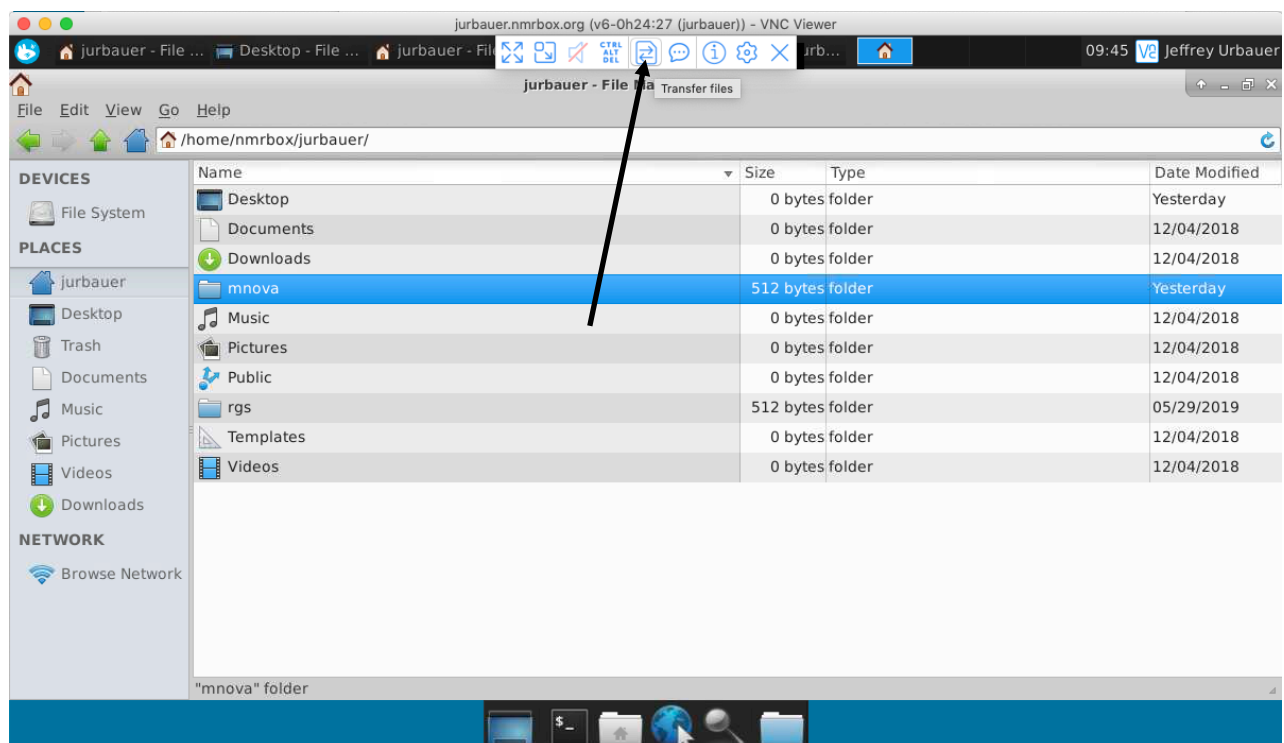
After being prompted for username and password, this will open up the NMRBox main window, as shown below (if you are logging in for the first time, you may be asked some additional questions for security reasons).



If you click on the 'Home' folder (in the NMRBox main window shown above), you'll see the contents of the home folder/directory. In this case, for the user 'jurbauer' ('/home/nmrbox/jurbauer')



Move the cursor up to the center of the top gray bar and a small hidden menu drops down. The icon with the antiparallel arrows allows access (when clicked) to a utility to transfer files. We'll use it in the next section to demonstrate how to transfer files to the NMRBox server from your computer.



## **Transferring files and folders/directories between your computer and NMRBox:**

On the NMRBox website, in the FAQs section, there is a FAQ dealing with transferring files and directories/folders to and from the NMRBox server.

<https://www.nmrbox.org/faqs/file-transfer>

**The fourth option is the easiest, which is using the built-in file/folder/directory transfer protocols in the VNC viewer.** On the following pages are presented VERY detailed examples of transferring a folder containing other folders and files from your computer to NMRBox, and then from NMRBox to your computer, using the built-in VNC utilities. In essence, as presented in the FAQ, the procedure can be reduced to the following:

To transfer files from your computer to the NMRBox:

- hover the cursor near the top gray bar of the NMRBox window
- click on the file transfer icon (antiparallel arrows) in the drop-down menu that appears
- click on the 'Send Files' button in the window that appears
- select the files/folders to send and click the 'OK', 'Open' or equivalent button

To transfer files from your NMRBox account to your computer:

- right click the VNC icon at the top/right of the NMRBox window and select 'File Transfer'
- click the 'Send files' button, and the file/folder selection window appears
- navigate to the files folders you want to transfer, select and click OK
- from the window that appears, select the destination folder on your computer
- click the 'OK', 'Open' or equivalent button

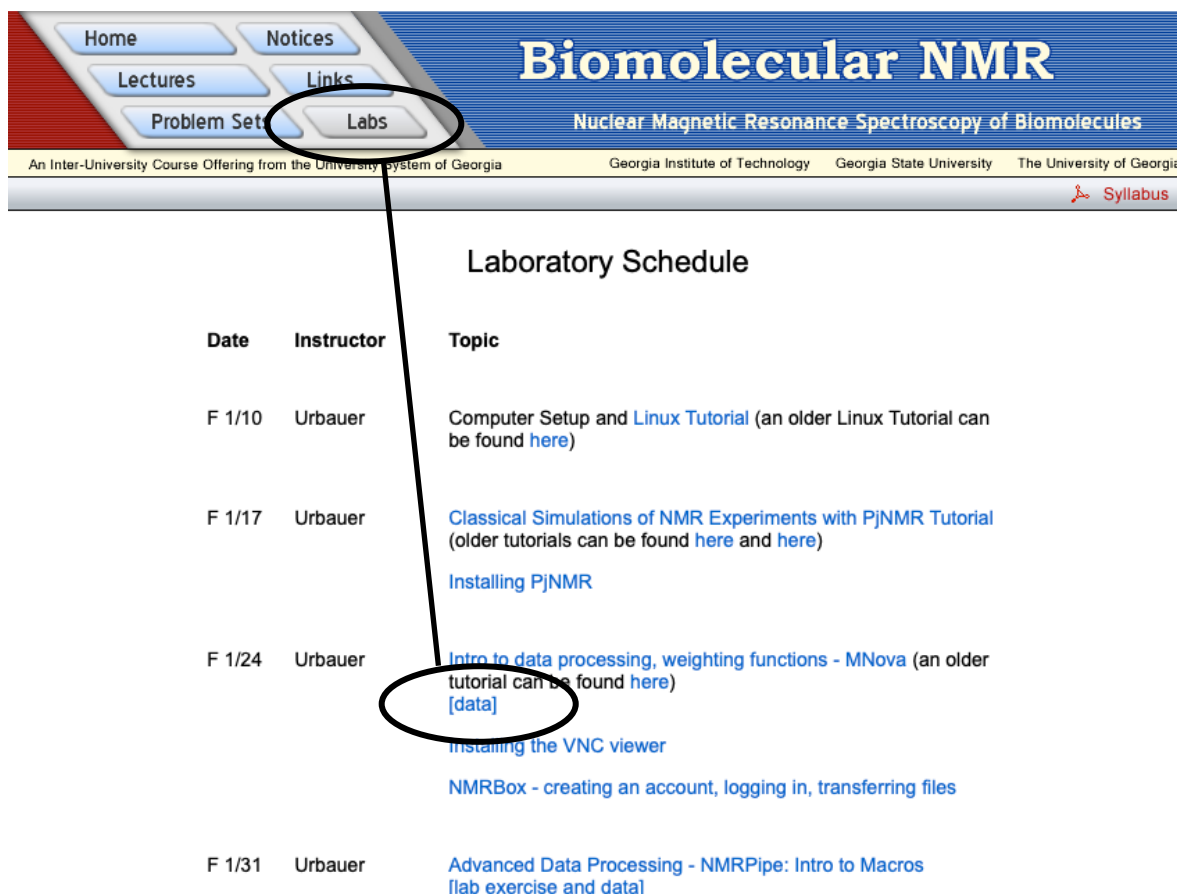
If you are familiar with the UNIX/LINUX command line and transferring files manually, you can use utilities such as 'secure copy' ('scp' and 'scp -r') to copy files and folders between your computer and NMRBox.

You can download and install a graphical file transfer app for your computer. There are actually lots of them to choose from. The app (program) 'Filezilla' is a good one that will run on any platform (and is somewhat recommended by NMRBox). On Apple computers (MacOS), the popular program 'Fetch' is a good one. These allow transfer using secure FTP protocols ('sftp') and are easy to use.

In any case, for our 'Mnova' lab, we'll use the built-in VNC tools for file transfer, and a detailed tutorial on using them to transfer files is below.

## Transferring Mnova data to your NMRBox account:

First, download the data from the course website



**Biomolecular NMR**  
Nuclear Magnetic Resonance Spectroscopy of Biomolecules

An Inter-University Course Offering from the University System of Georgia Georgia Institute of Technology Georgia State University The University of Georgia

[Syllabus](#)

### Laboratory Schedule

Date	Instructor	Topic
F 1/10	Urbauer	Computer Setup and <a href="#">Linux Tutorial</a> (an older Linux Tutorial can be found <a href="#">here</a> )
F 1/17	Urbauer	<a href="#">Classical Simulations of NMR Experiments with PjNMR Tutorial</a> (older tutorials can be found <a href="#">here</a> and <a href="#">here</a> ) <a href="#">Installing PjNMR</a>
F 1/24	Urbauer	<a href="#">Intro to data processing, weighting functions - MNova</a> (an older tutorial can be found <a href="#">here</a> ) <a href="#">[data]</a> <a href="#">Installing the VNC viewer</a> <a href="#">NMRBox - creating an account, logging in, transferring files</a>
F 1/31	Urbauer	<a href="#">Advanced Data Processing - NMRPipe: Intro to Macros</a> [lab exercise and data]

You can put the file anywhere, but, for this tutorial, we'll assume it is on the desktop.

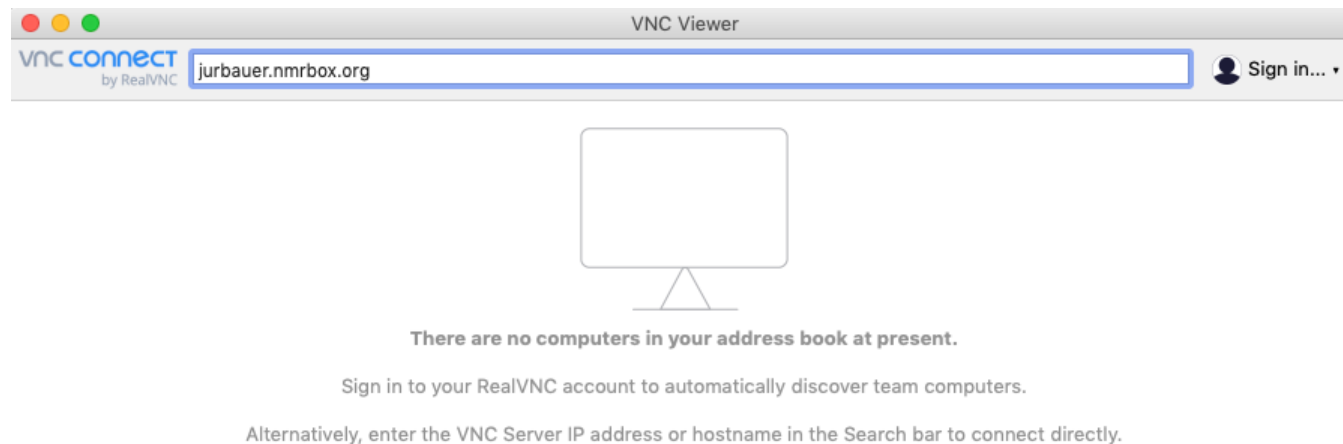
The downloaded file is named 'mnova-data.tar'. Your browser may have already opened/extracted the '.tar' file, in which case you will have a folder called 'mnova-data'. If not, you need to extract the file. You will accomplish this with the 'tar -xf' command, as shown below (for user 'urbauer' using MacOS).

```
roadrunners-MacBook-Pro:~ urbauer$ pwd
/Users/urbauer
roadrunners-MacBook-Pro:~ urbauer$ cd Desktop
roadrunners-MacBook-Pro:Desktop urbauer$ pwd
/Users/urbauer/Desktop
roadrunners-MacBook-Pro:Desktop urbauer$ ls mnova*
mnova-data.tar
roadrunners-MacBook-Pro:Desktop urbauer$ tar -xf mnova-data.tar
roadrunners-MacBook-Pro:Desktop urbauer$ ls mnova*
mnova-data.tar

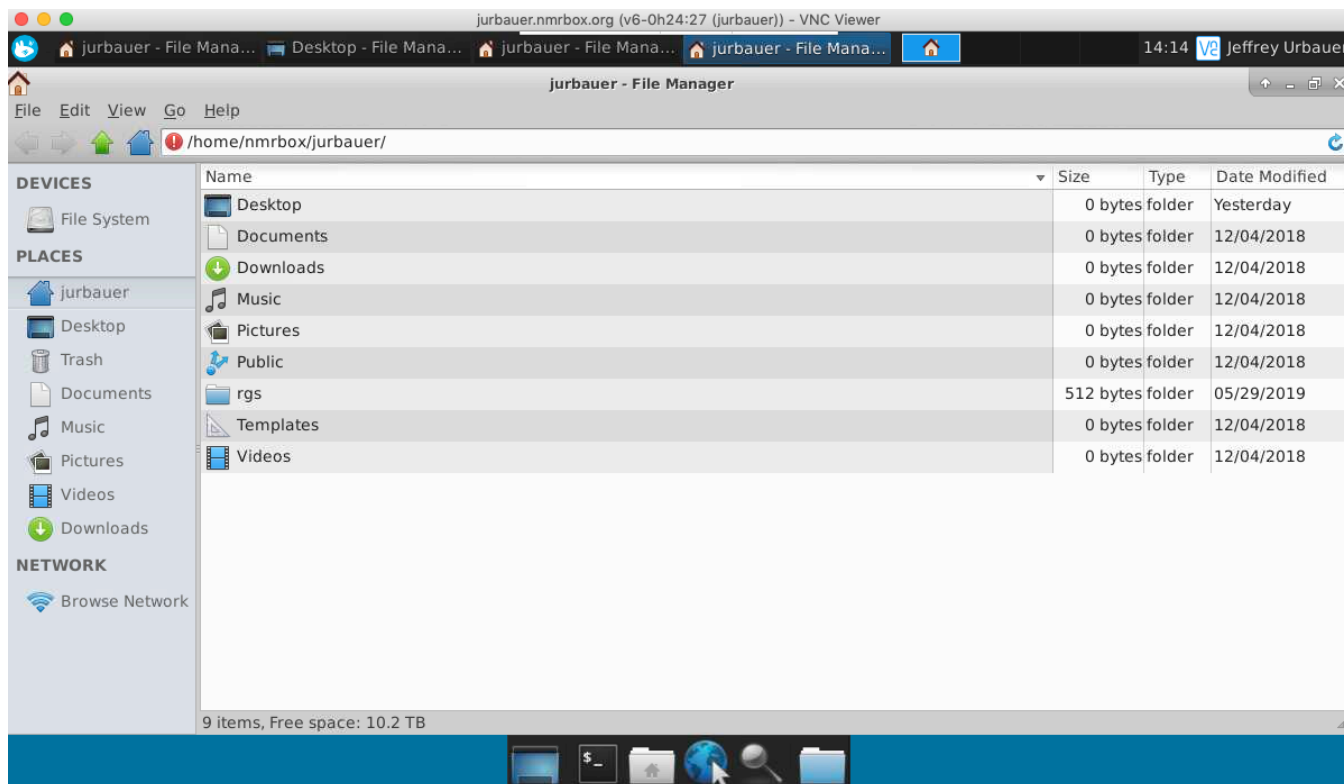
mnova-data:
varian-data-1.fid      varian-data-3.fid
varian-data-2.fid      varian-data-4.fid
roadrunners-MacBook-Pro:Desktop urbauer$
```

Now there is a folder/directory on your desktop called 'mnova-data' that has four subfolders that are Varian spectrometer data directories (Varian 'fid' folders/directories).

In order to move the 'mnova-data' folder to NMRBox, use VNC Viewer to connect to NMRBox. Below, user 'jurbauer' is connecting.

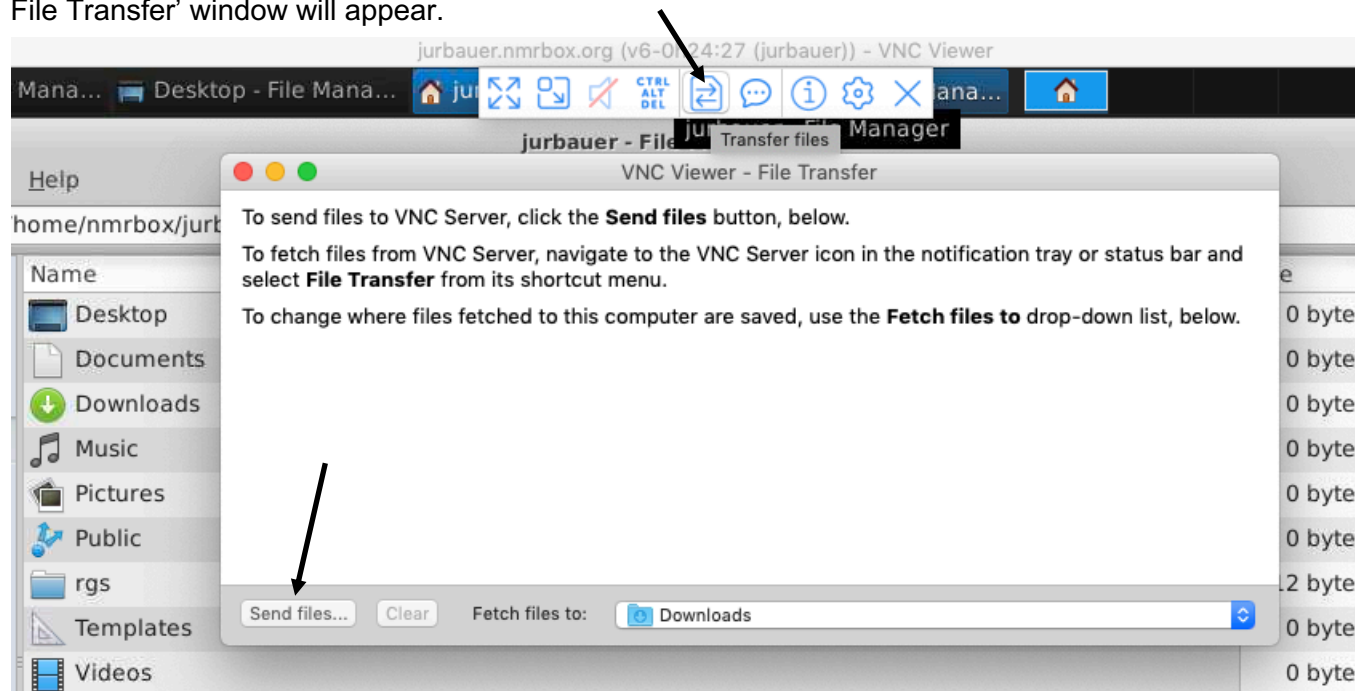


After asking for authentication (password), the NMRBox main window will appear. Shown below is the home folder/directory (/home/nmrbox/jurbauer) for the user 'jurbauer'.



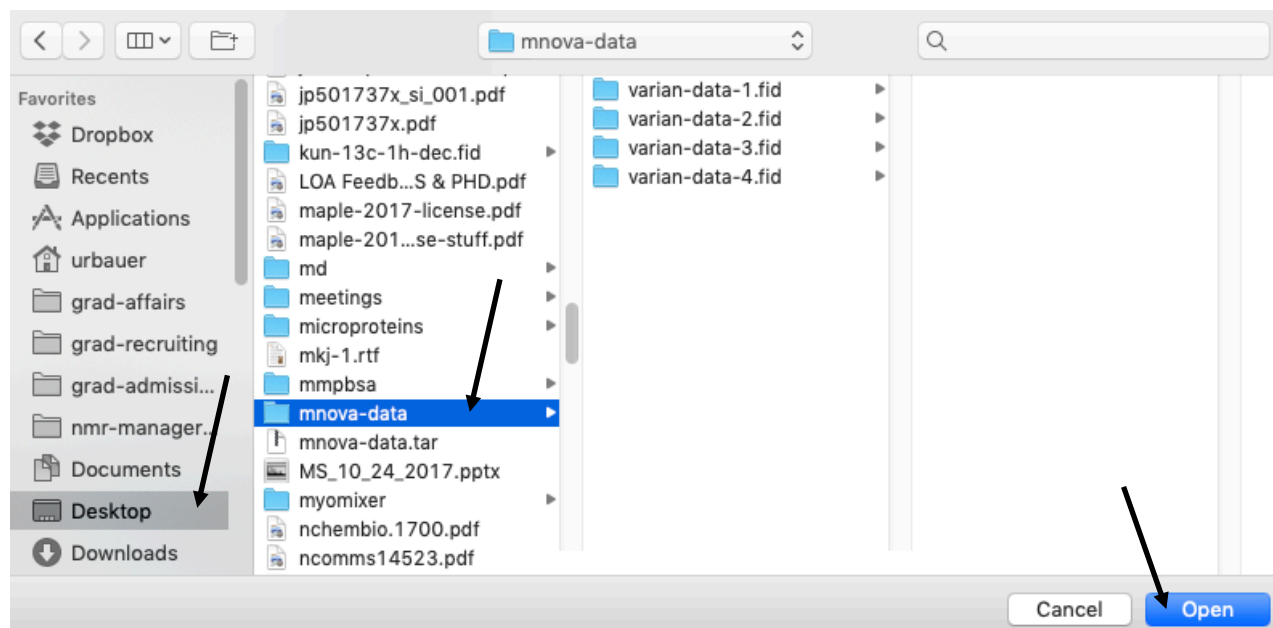
We'll use the built-in file transfer tools in NMRBox/VNC to transfer the files.

First, move the cursor near the top gray bar of the NMRBox window. A small drop-down menu will appear. One of the options will have two antiparallel arrows. **Click on that option** and the 'VNC Viewer File Transfer' window will appear.



We'll want the first option ('send files to VNC Server'), so, at the bottom of the 'VNC Viewer File Transfer' window, **click the 'Send Files....' Button.**

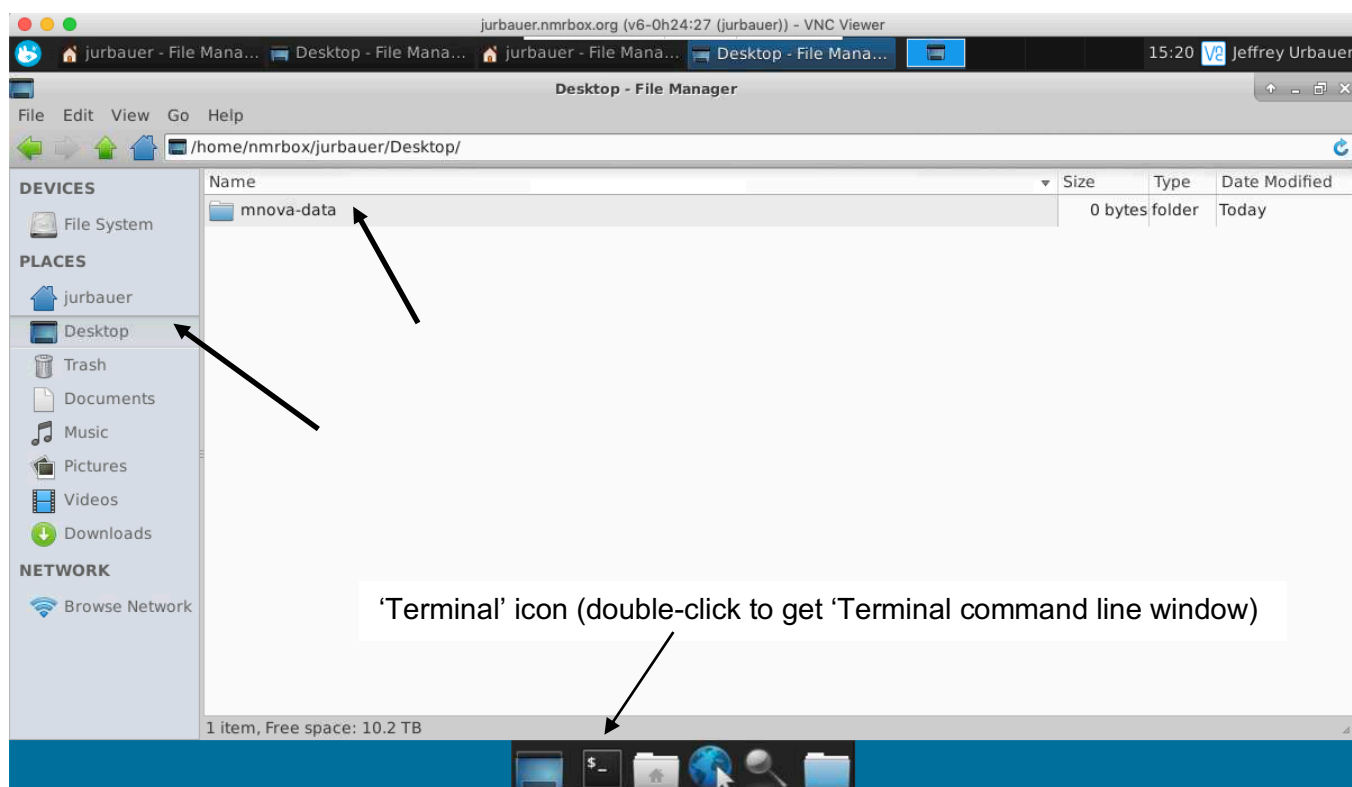
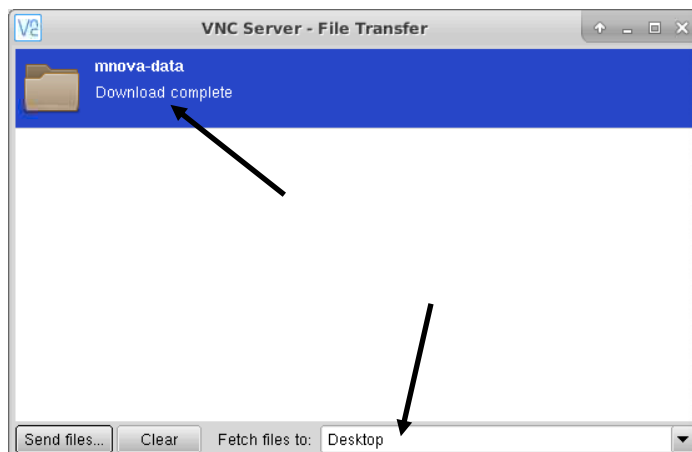
This will bring up a file browser window for your computer filesystem (below, for a MacOS computer). **Select the 'mnova-data' folder on the desktop and click 'Open'.**



A 'VNC SERVER - File Transfer' window will appear, indicating the file transfer was completed ('Download complete'). Also, at the bottom of that window it states where the files were downloaded to (in this case, the NMRBox 'Desktop').

You can close that window.

If we select 'Desktop' on the left side of the main NMRBox window, we'll see the 'mnova-data' folder/directory

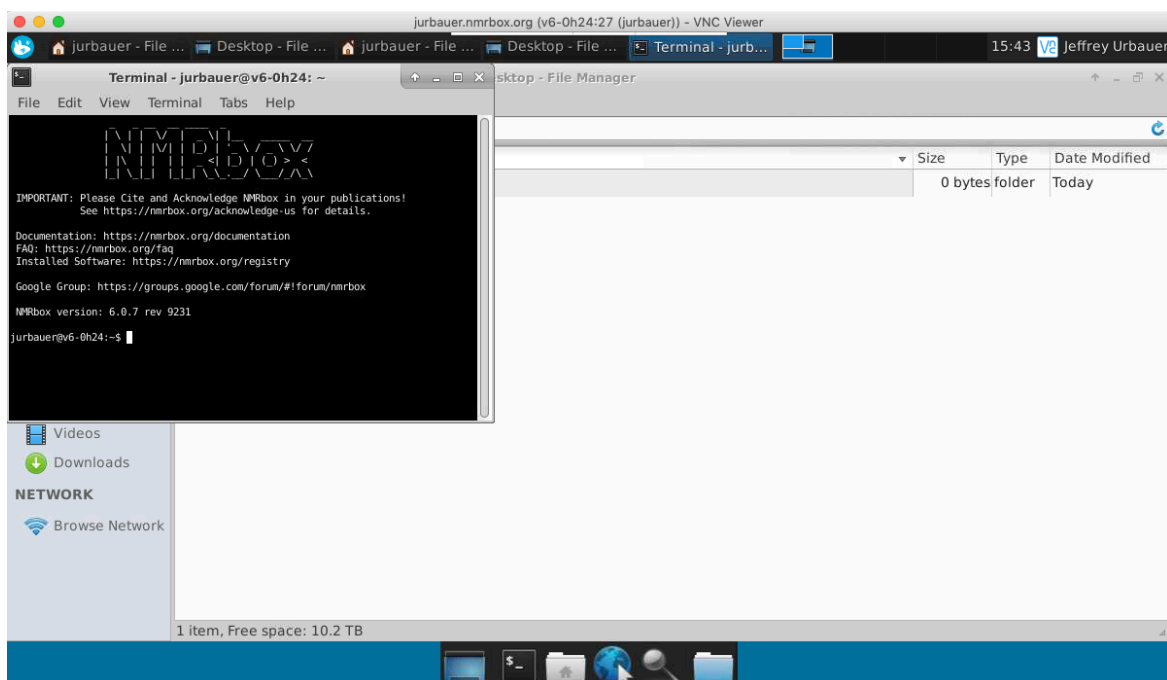


Rather than keep the 'mnova-data' on the Desktop, we'd like to have a main 'mnova' folder in the home directory of this user (/home/nmrbox/jurbauer/mnova) that we can use for our 'mnova' tutorial/exercise, and we'd like to put the 'mnova-data' folder in that folder/directory.

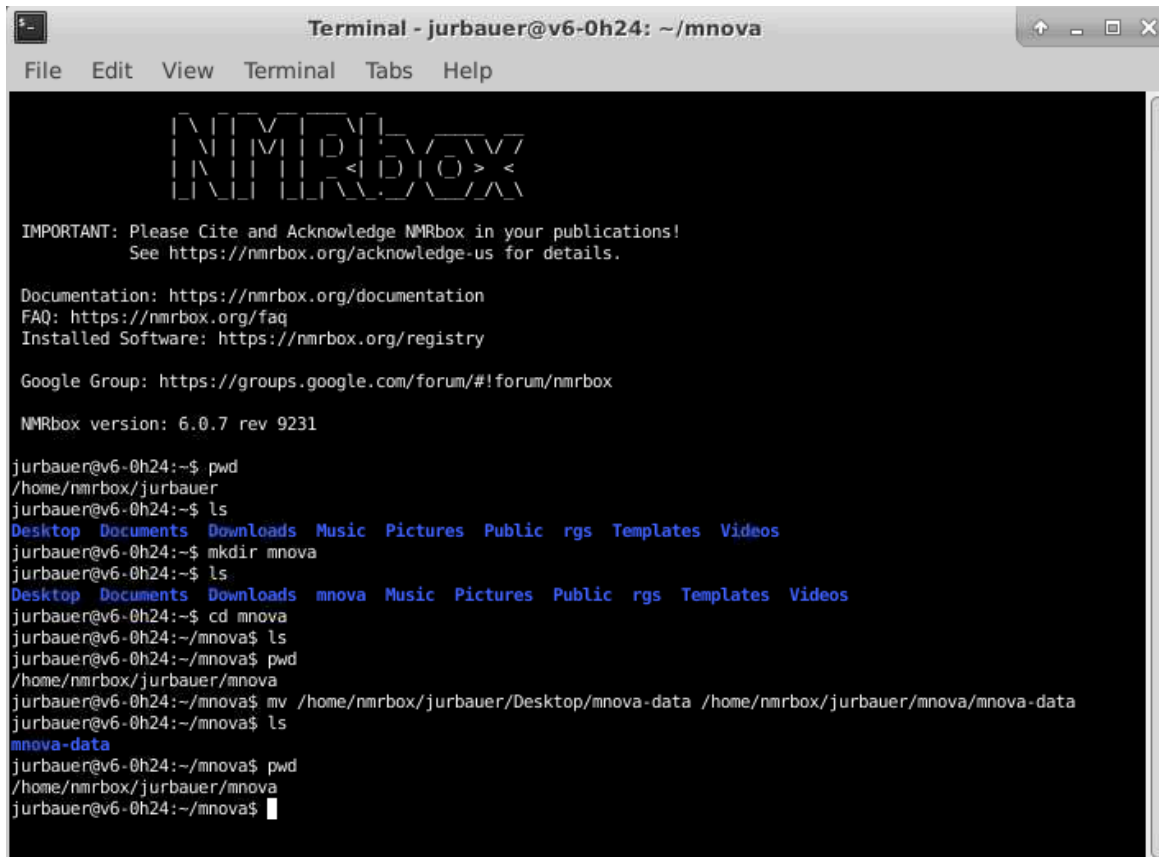
You can go ahead and feel free to use the graphical user interface and do that (just select the 'mnova-data' folder and drag it on top of the home ('jurbauer') directory icon under 'Places' on the left).

Alternatively, you can use the UNIX/LINUX 'Terminal' that is built into NMRBox. You can double-click the 'Terminal' icon at the bottom of the NMRBox window to get the 'Terminal' window.

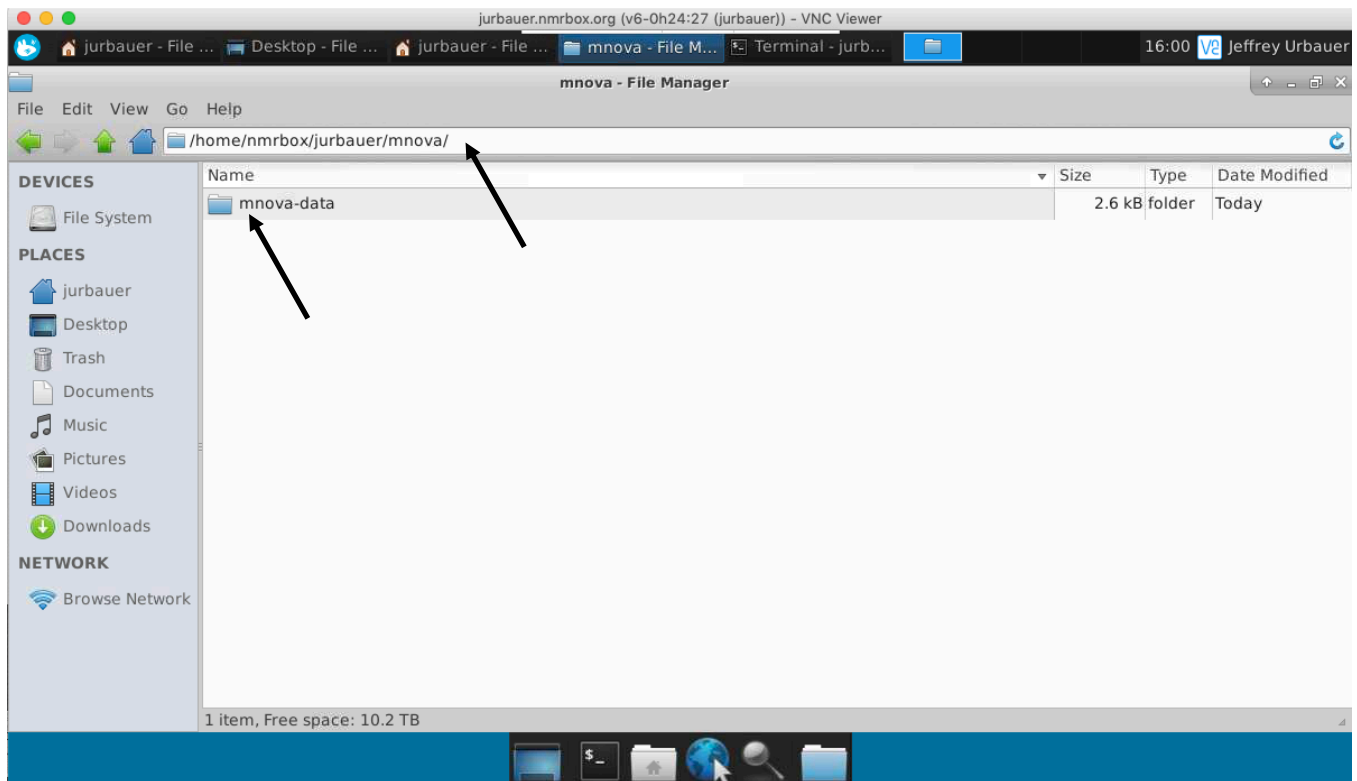




You can move this terminal window around, resize it, etcetera. Below, we enter the commands to create a folder/directory ('mkdir') 'mnova' in the directory/folder '/home/nmrbox/jurbauer'. Then we use the 'mv' command to move the 'mnova-data' folder from the Desktop ('/home/nmrbox/jurbauer/Desktop') to the 'mnova' folder ('/home/nmrbox/jurbauer/mnova').



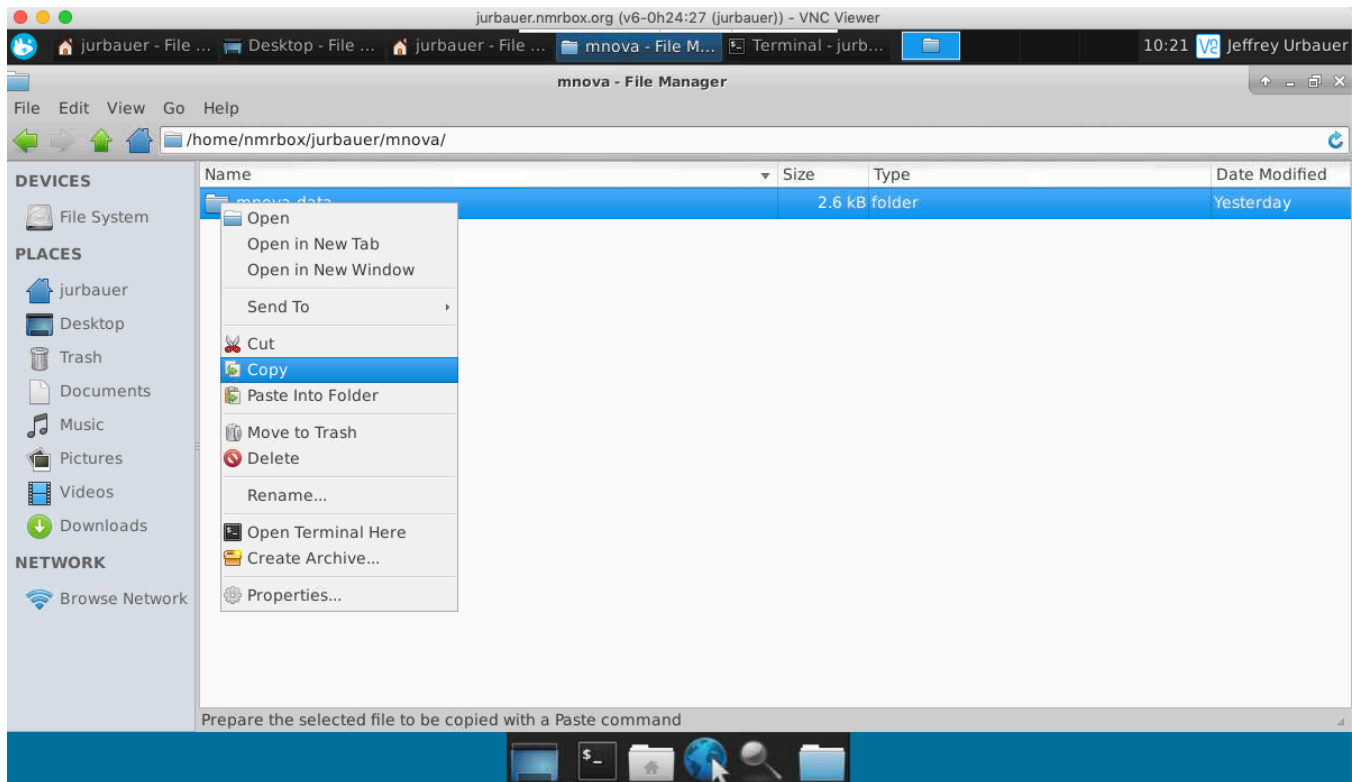
So, now, from the graphical interface, we see a folder/directory 'mnova-data' in the folder/directory '/home/nmrbox/jurbauer/mnova').



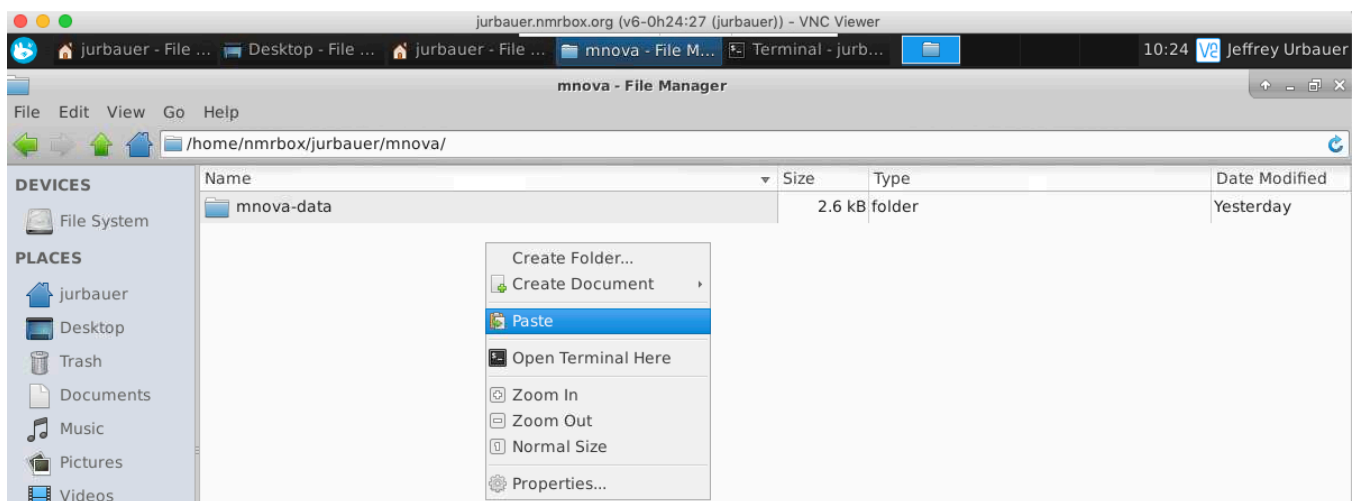
## Transferring data from your NMRBox account to your computer:

Here we'll use the tools available in NMRBox/VNC to transfer files from your account on the NMRBox server back to your computer. First, we'll make a copy of the 'mnova-data' folder/directory, then we'll rename it, then we'll transfer it from your NMRBox server back to your computer.

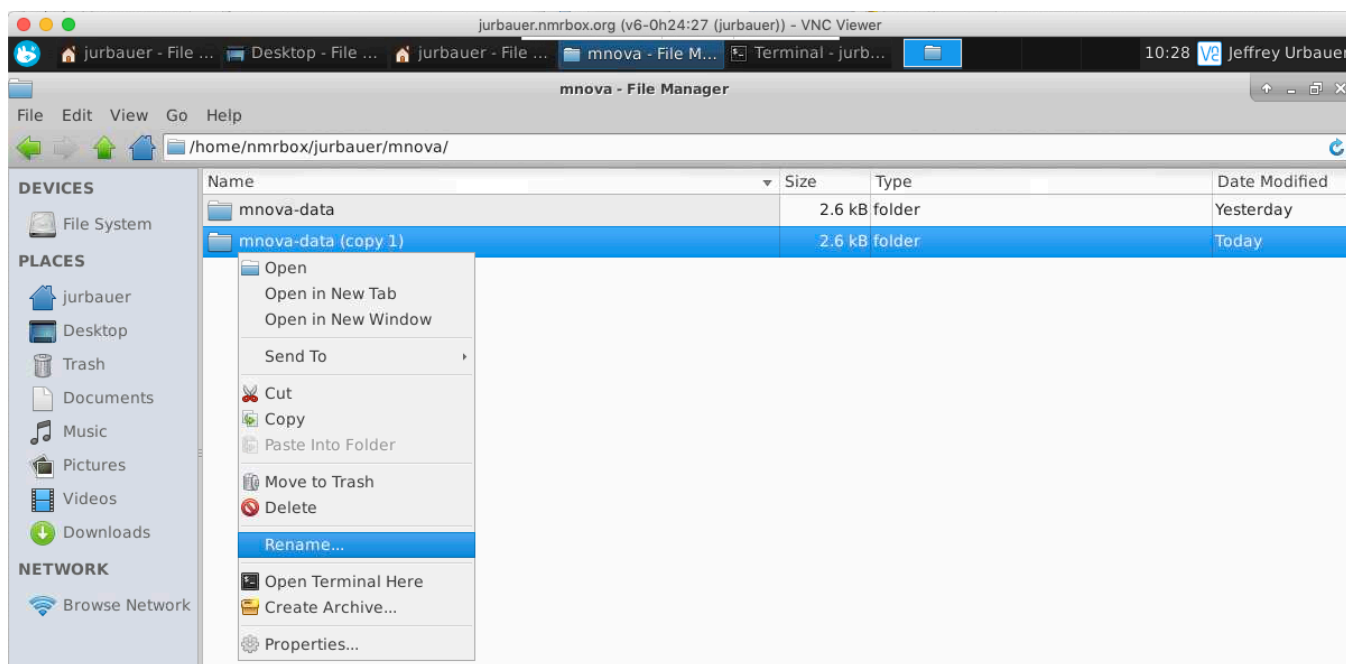
Right-click the 'mnova-data' folder and a menu pops up with a copy option. So, select the copy option. The 'mnova-data' is now copied into a buffer.



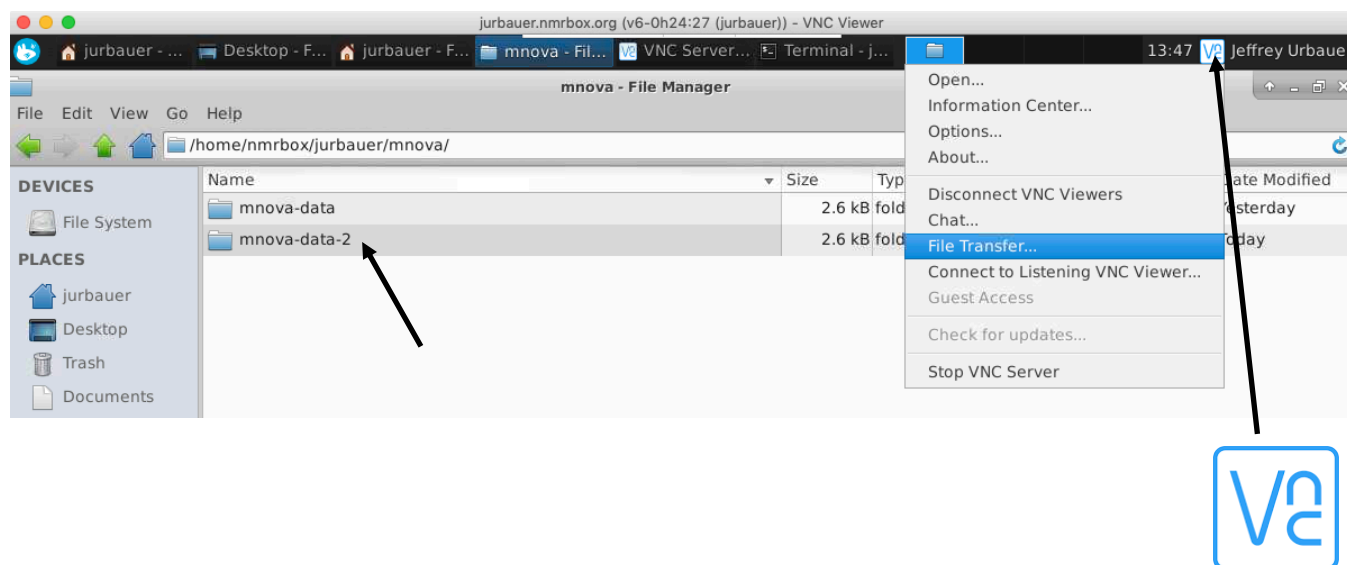
Right-click in the empty space and select the 'paste' option from the menu that appears.



The 'paste' option duplicates the 'mnova-data' folder, and names it 'mnova-data (copy 1)'. Right-click on this new folder, chose the 'rename' option, and a new menu appears that allows you to rename the folder. So, rename it 'mnova-data-2'.



This folder/directory ('/home/nmrbox/jurbauer/mnova') now contains two folders (subdirectories), the original one named 'mnova-data' and the copy named 'mnova-data-2'.

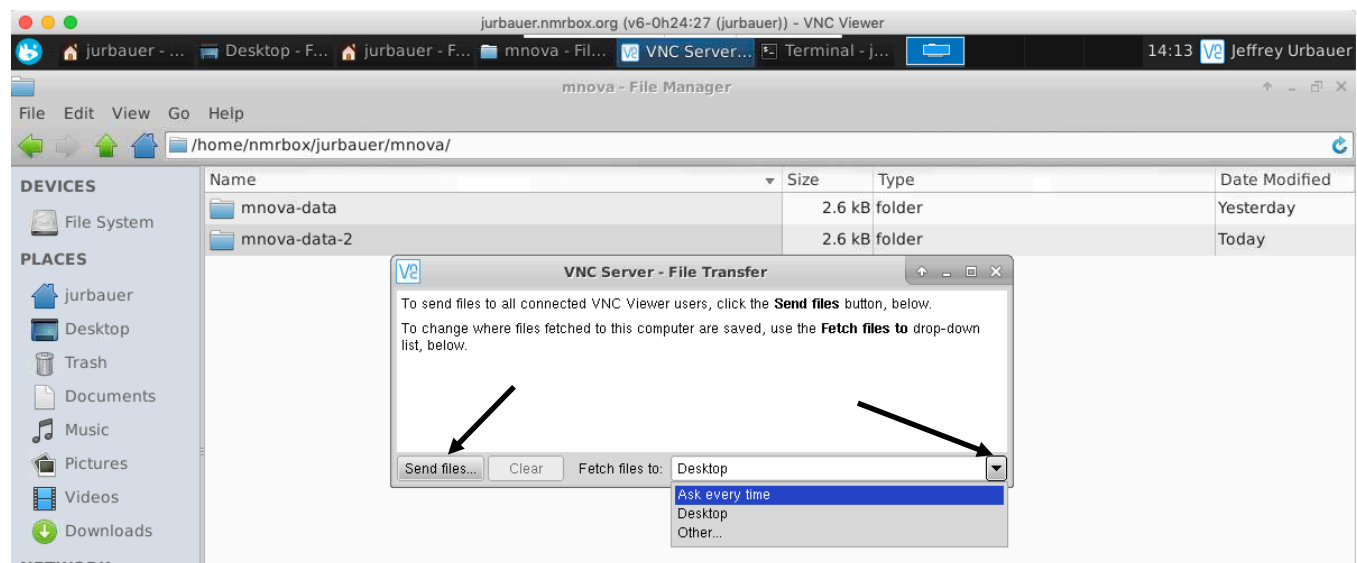


In the upper right hand corner on the top black bar in the NMRBox window is a small "VNC" icon. Right click on that icon, and you'll see a drop-down menu. Select the 'File Transfer' option in order to copy files from your NMRBox account onto your computer.

Once you select the 'File Transfer' option, the 'VNC Server – File Transfer' window appears (below).

At the bottom of this window, on the right, is a drop-down menu for 'Fetch files to:'. Set this to 'Ask every time'. Later, when you actually choose the files to transfer, this allows you to designate precisely where on your computer they will be transferred to.

At the bottom of the window, on the left, is a 'Send files....' button. Click that button.



When you **click 'Send files....'**, a new menu appears that allows you to navigate to the folder/directory that contains the files or folders that you want to transfer. Once you **select 'mnova-data-2'**, the full path to the file ('/home/nmrbox/jurbauer/mnova/mnova-data-2') appears in the 'Path:' window. **Then, click 'OK'**. Because 'Fetch files to:' was set to 'ask every time', a window appears (what the window looks like will depend on the computer that you are using) that allows you to select the destination that the files will be copied to on your computer. That's it.

