

NMR NOTES #19

Recording CD-R Disks with X-CD-Roast

The nmrsun workstations have CD-R/W drives available for storing NMR data to CD. In addition to the operating system Drag-n-Drop interface, which will not burn multisession CDs, there is also the X-CD-Roast software that can burn multisession disks. While this requires more effort than the Drag-n-Drop interface, it allows storing data at different times on the same CD. X-CD-Roast will not burn multisession DVDs, and the DVD driver is missing on the current systems, so DVD burning is best left to the Drag-n-Drop interface. Data in the **/nmrdata** mount points, removable USB media such as memory sticks, as well as home directory space are accessible for burning your CD.

A recordable CD can hold 650-700 MB of data, depending on the media that you use. Since home directory space is limited, it is unlikely that you will be burning a full 650 MB disk at one time. Multisession recording permits you to record a session and access that data, and then go back at some time in the future and add additional sessions to the disk. This process can be repeated until the disk is full. Multisession recording has some overhead associated with it - 22 MB for the first session, and 13 MB for each additional session. Consequently, it does not make sense to add just a few 100K of data to a CD, but once you have 20-30 MB of data to archive, the overhead becomes more acceptable. If you have a large amount of data on remote data storage somewhere, this can be burned in a single session without any additional overhead.

There are three basic steps involved in creating a data CD with your NMR data. The first is to decide what data is to be archived and perhaps to collect it in a single location if it is spread out across several directories. The second step is to create an image of the iso9660 file system that will be burned on the CD when it is recorded. The third step is to actually write the image to the CD. Do not attempt to either write the CD 'on the fly' (one of the option buttons in X-CD-roast) or to run other programs or applications while actually burning the CD. The computer needs all of its clock cycles to keep the CD burner buffer full. This will save you both CD-R media and aggravation. There is nominal provision for buffer underrun protection, and newer systems are faster and more robust, but treat this as emergency prevention rather than something to rely on.

To begin making a data CD, login on to one of the nmrsun system consoles (you cannot run this remotely). It is necessary to access any remote data directories you want to use in order to have the operating system mount them before you try to access them with the CD burner software. Your home directory is automatically mounted when you log in. If you have remote data in the the **/nmrdata** directory, simply open a terminal window and do an **ls** of the pertinent directory to get it mounted. If you want to archive entire directories, you can do so from the xcdroast program directly. If you want to pick and choose the data to archive, it may be easier to create a new directory with only the files you want to archive. This can include subdirectory structure to help organize the data. There is a disk partition, available as **/home1/scratch**, that may be used to collect the data that you want to archive.

Once you have decided on the data to be archived, insert your CD-R disk in the drive and start the CD burner software. This is available on the 'System Tools' menu of the Applications tab, or it can be run from the command line with the **xcdroast &** command. The ampersand (&) is important, because it will run the commands in background, leaving the Linux window available for running other commands. The first time you run Xcdroast, it will complain about the lack of a configuration file. Enter the Setup section and go to the HD Settings tab. At the bottom of the tab, enter **/home1/images** in the path window and click the Add button to add that path to the list of storage directories. select Save Configuration to create a configuration file and Ok to exit the configuration panel. This configuration file will be saved for subsequent invocations of the X-CD-Roast program. The opening screen gives four menu buttons (Setup, Duplicate, Create as well as Exit) - choose the Create CD button. You do not need to change anything in the Setup window.

The Create CD section initially will show information about images already created on the CD-R that you inserted in the drive. If there are previous sessions recorded, they should be shown here. After verifying that the CD-R is correct, you can move down to the Master Tracks button in order to create the list of data files to be archived. The window on the right shows the entire disk directory tree. You can navigate through that tree to locate your data: either in **/nmrdata/<group>**, **/home/<group>/<uname>**, or in **/home1/scratch** if you created a special directory tree for your data. Select the data directory that you want

to archive and press the **Add** button. You will then get a dialog box requesting the path name that you want to use to store the data on the CD. The default is to use the full path name, which isn't normally going to be very useful. You can specify either the root directory (/) of the CD, the last path component, or a custom path. Your choice will be the default for successive directory selections. As an example, suppose that I have service data in a vnmr1 home data directory for userA that I want to archive. The full path that I select in the right hand window may look something like **/home/staff/vnmr1/vnmrsys/data/userA**, and within that directory I would have the actual NMR data files: proton.fid, carbon.fid, dqcosy.fid, etc. After I select the **userA** directory from the tree and choose Add, if I choose the root directory (/) for the path name, then the full path name is removed, and when I look later at the CD, the CD root directory will have proton.fid, carbon.fid, etc. If I choose the last path component, then the CD root directory will have a **userA** directory with the data files contained within it. This is probably the most useful option for most applications. If I choose **Somegroup/UserA** as a custom path, then I specify that the data files in the **userA** directory be placed in a directory **Somegroup/userA** on the CD. You can choose as many different data directories, from various locations, as you want in order to create your session. Furthermore, you can choose a directory from the session list and either remove it or change the pathname that will be used for it on the CD. The only caveat here is that as you create the session, no calculation is done as to how much space is being used. You may want to use the **du_summary** command ahead of time on your data directories to decide how much of your data will fit on a CD. The information box underneath the session window showing used space/available space, is referring to space already recorded on the CD-R that is currently loaded in the drive, not the session you are creating.

Once you have chosen the data for your session, you can move from the **Master Source** tab to the **ISO9660 options** tab. The options that should be selected by default are: Rock Ridge (anonymous), allow 31 character names, Joliet extensions, and allow ISO names starting with a period. Verify that these are selected, and select **Save Defaults** if necessary. Under the **ISO9660 Header** tab, enter a volume ID for your CD. This should not contain any spaces, and the number of characters is limited to 32. You may also enter Publisher and Preparer ID information if you want, and may also choose to save these default values. Next, move to the **Create Session/Image** tab. There will be a delay as the system calculates the size of the session you are attempting to create. The Session Information will show both a size (data CDs) as well as the equivalent time (audio CDs) for the new session as well as the space used and space available on the CD-R. The Create Session window shows the available free space on the disk for creating the ISO9660 image file. This space must be larger than the size of the session. In the window on the right, select Create multisession CD (unless you are creating one large single session disk), Eject after Write, Do not pad tracks (used for audio CDs), and enable Buffer underrun protection. Press the **Master to Image file** button to start creating the ISO9660 disk image file. If you are creating a multisession image, you will get a dialog box asking whether this is the first session of a multisession CD or an additional session. If it is an additional session, it requires that the CD with the prior sessions be loaded before continuing so that the older directory information can be appended to the new session.

After the image file is created, you are ready to actually write it to the CD-R. If this is an additional session on a multisession CD, go back to the **CD/Image Info** button, select update to refresh the information, go back to **Write Tracks** section again. Go to the **Layout Tracks** tab. The window on the right will show the available track image files, and you can select your file and add it to the list of tracks to write. Note that the list of available tracks shows a complete pathname to the image file. . Once you are satisfied with your track selection, you can move to the **Write Tracks** tab either directly or with the **Accept Track Layout** button. Check the **Create Multisession CD** button if this is a multisession track, check the write speed, remove the selection to pad tracks, make sure that the Write mode is Track at Once (TAO) and **NOT** Disk at Once (DAO), and press the **Write Tracks** button to begin recording. If you are recording a multisession disk, there will be a dialog box to confirm that. If there is an error box saying that the media and the session are inconsistent, do not proceed until you refresh the CD information again. Do not do anything to interrupt the writing once you start - it will ruin the CD. After the write is completed, the CD will be ejected. You can re-inset the CD-R in the drive and it should be automatically mounted on the **/media** mount point. All of your sessions should be shown there. When done, do a **cd** to get back to your home directory, unmount your CD-R, remove your image file(s) from **/home1/images** and any temporary data in the **/home1/scratch** directory, exit xcdroast, logout, and you are done. Congratulations!!