

NMR NOTES #5

XL/VXR to UNIX Data Transfer

Moving NMR data from the XL series consoles to the UNIX workstation requires using Varian's LimNet data transfer protocol. This is a fairly limited suite of programs that permits moving a file back and forth between two LimNet nodes. It is not a generic ftp protocol that will communicate with other ethernet nodes. Currently defined LimNet nodes (and their node names) are the XL-200 (XL200), XL-400 (XL400), and XL-200E (XL200E) spectrometers and the Sun Sparc20 workstation nmrsun2 (SUN2). It is not possible to move data directly from an experiment to another node - you must first store the data with the **SVF** command. There are three commands available with LimNet: **EWRITE** to write a file from the local machine to a remote node, **EREAD** to read a file from a remote node to the local machine, and **ELIST** to list a directory on a remote node. The **ELIST** command does not understand UNIX file systems and therefore cannot list a directory on the Sun workstation. **EREAD** and **EWRITE** will not permit overwriting existing files, they can only create new files. Also, the ethernet cards in the spectrometers have a tendency to stop responding periodically, and the only fix is to reboot the spectrometer system. This dictates that normal practice should be to write your data from the spectrometer to the workstation rather than to attempt to read the data from the spectrometer while using the workstation. The LimNet commands require that UNIX file systems be world writable in order to perform transfers to them, and this is not generally considered good practice for user accounts, so there is a temporary directory available on NMRSUN2, /temp, with world writable permissions for this purpose. In order to maintain sufficient space on the disk drives, it is imperative that you treat both DSK3/DSK4 on the spectrometer and /temp on the workstation as TEMPORARY storage and remove your data as soon as possible from those temporary locations. Data on DSK3/DSK4 can be removed as soon as it is written to the workstation. Data on the workstation can be removed as soon as it is converted to your home directory.

Detailed below are two different types of operations that you may want to perform. The first is moving a single NMR data set to the workstation. The second is an example of moving several data sets at once, rather than one at a time as in the first example.

After collecting a single NMR data set, save it to one of the buffer disks, either DSK3 or DSK4 with the **SVF** command:

SVF (DSK3 .MYDATA)

Use the LimNet command EWRITE to write the data from this buffer area to the UNIX workstation:

EWRITE (DSK3 .MYDATA , SUN2 , ' /TEMP/MYDATA ')

There will be a counter that runs and shows the blocks being transferred. No error messages indicate a successful transfer. If there is a network time-out error, then the spectrometer computer needs to be rebooted - reboot it and then retry the data transfer. If the interface failed during the data transfer, then you may get an error indicating a duplicate file name. Repeat the command with a new destination name, since the file that is present on the remote system is only part of your data. Once you have successfully transferred the file, delete it from the scratch disk so that the space is available for someone else.

Move to the UNIX system, login and run a directory list on the **/temp** directory. You should see your data file as **/temp/mydata.5**. All NMR data sets will have the **.5** extension since this is used to store the size of the original Varian file directory. Start Vnmr and use the **convert** command to import your data into the current experiment:

```
convert ('/temp/mydata')
```

At this point you can process, plot, and generally manipulate the data any way you want. If you want to save the data in the UNIX format, however, you must use the **svf** command. This data can then be read back into a Vnmr experiment, but it cannot be moved back to the spectrometer systems. If instead you save and archive the original data file with the **.5** extension, you can move the data back to the spectrometer with LimNet but would have to run the **convert** command again to process the data with Vnmr. In either case, you should remove your data from the temporary directories to make room for other users, and archive the data from your personal account, whether in the UNIX format or the spectrometer format.

Moving multiple data sets is almost as easy as moving a single data set. The procedure is to create a directory, store all of the data to be moved in that directory, transfer the directory, and then unpack the directory on the UNIX end. In order to do this, find the amount of free space on either DSK3 or DSK4 and create a directory large enough to hold your data:

```
FIND (DSK3 .FREE)
```

```
CREATE (DSK3 .UNAME , <freesize> , 1 , 36)
```

Save your NMR data sets in your directory with the **SVF** command, shrink the directory to remove the extra space (There is no reason to move a lot of zeros across the network!), and transfer the file as before:

```
SVF (DSK3 .UNAME .PROTON)
```

```
SVF (DSK3 .UNAME .DQCOSY) . . .
```

```
SHRINK (DSK3 .UNAME)
```

```
EWRITE (DSK3 .UNAME , SUN2 , '/TEMP/UNAME')
```

Now on the UNIX system, it is necessary to unpack this directory before the Vnmr **convert** command can access the individual data sets. Use a UNIX shell, such as the **vnmr** window, and use the **decomp** command to unpack (decompress?) the directory:

```
decomp /temp/uname
```

This will create a UNIX directory called **/temp/uname** with all of the original data sets contained within it: **/temp/uname/proton.5**, **/temp/uname/dqcosy.5**, etc. You can then return to the Vnmr program and use the **convert** command to read any of these data sets for processing. Again, remove both **uname.36** and the **uname** subdirectory from the **/temp** directory to make room for other users' files, and archive your data through your personal directory to one of the magnetic tape drives.