The interaction between XWIN-NMR and UNIX

A basic course
for NMR spectroscopists

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The latest update of Bruker manuals can be found on:

www.bruker.de: click *Downloads -> Documentation*

It is also delivered as `XWIN-NMR` online help:

click *Help -> Other topics -> XWIN-NMR and UNIX*

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Contents

This course has been written for NMR spectroscopists who are using the XWIN-NMR software. It will give the reader a basic understanding of UNIX, the XWIN-NMR directory structure and computer networks. It will also offer help in case of trouble. The material is dedicated to XWIN-NMR versions 3.0 and newer, running on an SGI workstation. Most of it, however, is also valid for older versions of XWIN-NMR.

The following conventions will be used throughout the manual:

times-italic-bold : UNIX command clicked from the toolchest
courier-bold : UNIX commands entered in a UNIX shell
palatino-italic : XWIN-NMR command clicked from the menu
palatino : XWIN-NMR commands entered on the command line
courier : any name, e.g. of a user, a host etc.
italic : a file or directory in UNIX
fila : an example of a file in UNIX
dira : an example of a directory in UNIX
dataseta : an example of a dataset in XWIN-NMR
IRIX >= 6.3 : IRIX 6.3 or newer

Part I

UNIX

toolchest
boot
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the SGI Toolchest

The Toolchest is a small window on the desktop of an SGI workstation.

The Toolchest:

- automatically appears when you log in at a terminal which is directly connected to the workstation
- offers you a list of system tools and applications
- allows you to start tools and applications by mouse click
- can be customized in your personal file *.auxchestrc*
- can be started with the command **`toolchest`** when you are logged in over the network

The Toolchest usually contains the following buttons:

Desktop	- open a `UNIX` shell, log out, customize
Selected	- handle files and directories graphically
Find	- find tools and applications on the local host - find files, hosts, printers etc. network wide
System	- start the system management tools for disks, printers, network, system software, users etc. - restart the window manager, restart the host
Help	- the online books and manual pages

examples of toolchest functions

Open a UNIX window (a UNIX shell):
Desktop -> Open Unix Shell

Open a window with icons for several applications:
Find -> Applications

Open the online books for help on various SGI topics:
Help -> Online Books
-> you can also type **insight**

Install a new user or change an existing user:
System -> System Manager -> Security and Access Control -> User manager [1]
-> you can also type **insight**

Log out:
Desktop -> Log Out
-> you can also type **endsession [-f]**

Shutdown the computer:
System -> System Shutdown
-> you can also type **init 0**

Reboot the computer:
System -> Restart System
-> you can also type **init 6**

1.For IRIX <= 6.2: click *System -> User Manager*

General system information and setup:

System -> System Manager

Switch window auto placement on/off:

Desktop -> Customize -> Windows

Enable remote display permanently: **IRIX >= 6.3**

Desktop -> Customize -> Desktop -> Enable Remote Displ.

-> you can also add **xhost +** to your *.profile* [1]

Change the UNIX default editor (default is jot):

Desktop -> Customize -> Desktop [-> Utilities]

-> you can also type **desktop** in a UNIX shell

Install a new printer:

System -> Printer Manager

-> However, we strongly recommend to use the XWIN-NMR command cfpp to install a new printer [2].

Install system software:

System -> Software Manager

-> this command can be used to install SGI software but not to install Bruker software

A list of all UNIX commands and their manual pages:

Help -> Man Pages

-> each manual page corresponds to the output of the command **man <command>**

1.If you use a csh or tcsh shell then make the entry in the file *.cshrc*

2.For network printing see the XWIN-NMR online help; click *help -> other topics -> network printing*

boot - shutdown - reboot

on SGI

How do you boot an SGI?

If the computer is down and switched on:

- click ***Restart***

If the computer is switched off:

- push the power button to switch it on

How do you reboot an SGI?

Do one of the following:

- click ***System -> Restart System***
- type **`/etc/reboot`**
- type **`init 6`**

How do you shutdown an SGI?

Do one of the following:

- click ***System -> Shut Down System***
- type **`/etc/shutdown`**
- type **`init 0`**

`shutdown` and **`reboot`** send a warning to all logged in users whereas **`init 6`** and **`init 0`** immediately do a shutdown.

If the system hangs (no mouse/keyboard control), you can shutdown the SGI by pushing the power button next to the green light[1]. If this fails, push the power button several times or push the small hidden reset button.

1.The system then tries to properly shutdown as it would do with the command `shutdown`

help in UNIX on SGI

Manual Pages: help on UNIX commands

Do one of the following:

- click ***Help*** `->` ***Man Pages*** or type **`xman`**
  a list of `UNIX` commands appears: click on a command to get help, e.g. click on ***find***
- type **`man <command>`**, e.g. **`man find`**

How do I ... : particular tasks [1]

Click ***Help*** `->` ***How do I...*** and select a question, e.g.:

- Find Software and Applications
- Organize Windows
- Setup Connections with Other Workstations

On-line Books: general information

Click ***Help*** `->` ***Online Books*** or type **`insight`**

Do one of the following:

- select a book e.g: SGI ***EndUser*** `->` ***Desktop Users Guide***
- search for keywords, e.g.: `permissions`, `desktop`, `userid`

1.*How do I...* is available for IRIX >= 6.3

SGI graphical interface

files and directories displayed as icons

Open a directory and show its contents

1. click ***Selected -> File QuickFind*** [1]
2. enter the target directory in the text field
3. double click on the folder icon left of the text field
   -> A new directory window opens, showing icons.

Select one or more icons in a directory window

Do one of the following:

- click one icon
- press the Shift key and click on several icons
- draw a box around a group of icons
  -> All selected icons turn yellow.

Open a file or directory

Double click on the icon.
-> A file is viewed, edited or executed, depending on its type. If it is a directory, it is opened.[2]

Rename a file or directory

1. click on the icon.
2. type the new name in the white rectangle. [3]

Remove a file or directory

1. click on the icon
2. click the right mouse button -> click ***Remove***

1.For IRIX <= 6.2: click ***Selected -> An icon***
2.A file can be an ascii file, an executable program, a tar-file, sub-directory etc.
3.If the name under the icon is not marked by a white rectangle, you have no permission to rename the file.

Change owner or permissions of a file or directory

1. select the icon
2. click the right mouse button -> click ***Permissions***
   -> a new window opens to change owner/permissions

Move a file to a different directory

1. press and hold down the left mouse button on the icon
2. drag the icon into a different directory window

Copy a file to a different directory

1. press and hold down the `Control` key
2. press and hold down the left mouse button on the icon
3. drag the icon into a different directory window

Move a group of files to a different directory

1. select a group of icons
2. press and hold down the left mouse button on one icon
3. drag all selected icons to a different directory window

Place frequently used icons on the desktop

1. open the directory where the icon resides
2. press and hold down the left mouse button on an icon
3. drag the icon onto the desktop [1]

Show details of icons, e.g. date, size, file type

Click ***View -> as List***

More information: ***Help*** -> ***Online Books*** -> ***SGI EndUser*** [2]

1.You can also drag the icon into the Icon Catalog window (*Find -> Icon Catalog*)

basic UNIX commands

on files and directories

- **`pwd`**
  -> print working directory

- **`ls`**
  -> list contents of current directory

- **`cd dira`**
  -> change to directory *dira*

- **`cp fila filb`**
  -> copy the file *fila* to *filb*

- **`mv fila filb`**
  -> move or rename the file *fila* to *filb*

- **`cat fila`**
  -> print the text file *fila* on the screen

- **`more fila`**
  -> print the file *fila* page by page on the screen

- **`rm fila`**
  -> remove the file *fila*

2.For IRIX<= 6.2 click *IRIS Essentials*, for IRIX>= 6.3 click *Desktop User's Guide*

cd

change directory

- **cd**
  -> change to your home directory

- **cd dira**
  -> change to directory *dira*

examples

1.cd /u/data/guest/nmr
-> change to */u/data/guest/nmr*

2.cd dataseta
-> change to */u/data/guest/nmr/dataseta*

3.cd ..
-> change to */u/data/guest/nmr*

4.cd ../../usera/nmr
-> change to */u/data/usera/nmr*

ls

list the contents of a directory

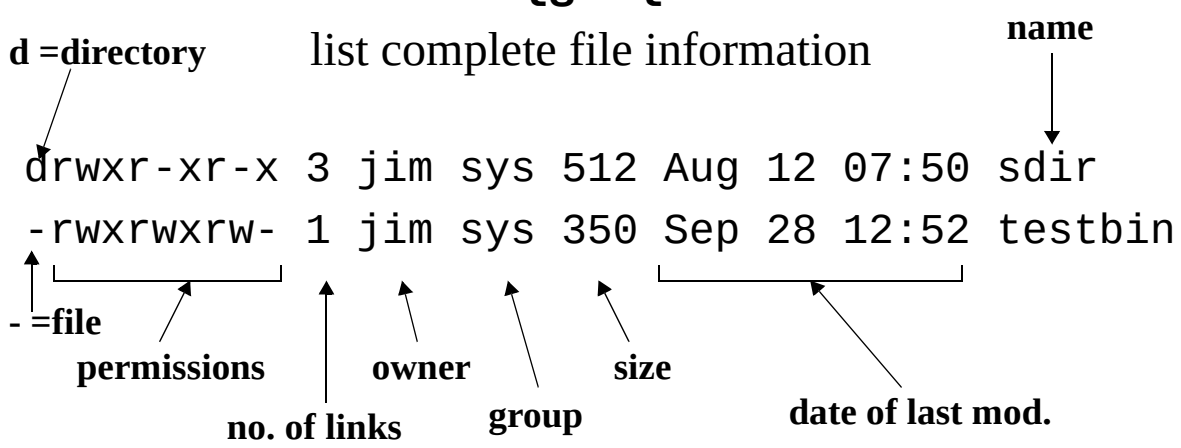
`ls`

list files and sub-directories in current directory

```
sdir testbin
```

`ls -l`

list complete file information



`ls -al`

also list files starting with `.`

```
-rw-r--r-- 1 jim sys 210 Jul 26 14:14 .cshrc
-rw-r--r-- 1 jim sys 149 Jul 26 16:42 .profile
```

`ls -Rl`

also list the contents of all sub-directories

`ls -lt` or **`ls -lrt`**

sort by time of last modification

rm

remove files and/or directories

- **`rm fila`**
  -> remove the file *fila*

- **`rm -r dira`**
  -> remove the directory *dira* including files and subdirectories

- **`rm abc*`**
  -> remove all files beginning with abc

- **`rm -i abc*`**
  -> remove all files beginning with abc interactively. For each file, you are prompted to remove the file or not.

CAUTION: Files which have been deleted under UNIX can not be restored!

Some files, e.g. filenames with special characters, can not be removed with **`'rm filename'`**. You can, however, try to remove them with **`'rm -i *'`** or with **`'rm ./filename'`**.

file permissions

The permissions of a file:

- determine what each user can do with the file
- are represented by a set of characters -, r, w and x or by a set of numbers between 0 and 7:

  1 = x = executable
  2 = w = writable
  4 = r = readable

The numbers 3, 5, 6 and 7 are combinations of 1,2 and 4:

e.g. 7 = 4 + 2 + 1= rwx

Each file has 3 sets of permissions for 3 categories of users:

- the actual owner of the file
- users who have the same group ID as the owner [1]
- users who have a different group ID than the owner

Type **`ls -l filename`** to see the 3 sets of permissions:

e.g. **`ls -l fila`**

```
-rwxrw-r-- 1 jim sys 987 Sep 15 15:08 fila
```

The permissions of the file *fila* are 764:

7 = rwx for the owner `jim`
6 = rw- for all users of the group `sys`
4 = r- - for other users

1.The group attribute of a file can be changed with `chgrp`, the group permissions of a file always refer to the group ID which is shown with `ls -l filename`

chmod

change the permissions of a file or directory

using the character representation

General usage: **`chmod [ugo][=+-][rwx] filename`**

examples

After each example the output of **`ls -l fila`** is shown.

Make *fila* read-only for all users:

`chmod a=r fila` [1]

```
-> -r--r--r-- user group 102 Apr 10 12.20 fila
```

Add the write permission for all users:

`chmod a+w fila`

```
-> -rw-rw-rw- user group 102 Apr 10 12.20 fila
```

Add the execute permission for user (=owner) and group:

`chmod ug+x fila`

```
-> -rwxrwxrw- user group 102 Apr 10 12.20 fila
```

Take away the write permission for others:

`chmod o-w fila`

```
-> -rwxrwxr-- user group 102 Apr 10 12.20 fila
```

Make the directory tree *dira*, including all files and sub-directories, writable for all users:

`chmod -R a+w dira`

1.For IRIX 5.* `chmod +r` and `chmod a+r` set the read perm. for all users, for IRIX 6.* `chmod a+r` sets the read perm. for all users, `chmod +r` sets the read perm. according to `umask`

chmod

set the permissions of a file or directory

using the numerical representation

General usage: **`chmod xxx filename`**

examples

After each example the output of **`ls -l fila`** is shown.

Make *fila* read-only for all users:

```
chmod 444 fila
-> -r--r--r-- user group 102 Apr 10 12.20 fila
```

Make *fila* write-only for all users:

```
chmod 222 fila
-> --w--w--w- user group 102 Apr 10 12.20 fila
```

Make *fila* read/write for the owner, read-only for the group:

```
chmod 640 fila
-> -rw-r----- user group 102 Apr 10 12.20 fila
```

Make *fila* read/write/execute for the owner, read/execute for the group and execute for others:

```
chmod 751 fila
-> -rwxr-x--x user group 102 Apr 10 12.20 fila
```

Make the directory tree *dira*, including all files and sub-directories, readable and searchable for all users:

`chmod -R 555 dira` [1]

1.Note that the x-permission (5=rx) means searchable in case of a directory.

chown/chgrp

change the owner/group of a file or directory

The usage of **chown/chgrp** is shown with examples. The output of **ls -l fila** or **ls -ld dira** shows the result.

Change the owner of the file *fila* to usera:

```
chown usera fila
-> -rw-r--r-- usera system 102 Apr 10 12.20 fila
```

Change the group of the file *fila* to grpa:

```
chgrp grpa fila
-> -rw-r--r-- usera grpa 102 Apr 10 12.20 fila
```

Change the owner of directory tree *dira* to grpa:

```
chown usera dira
-> -rwxr-xr-x usera grpa 512 Apr 10 12.20 dira
```

Change the owner of directory tree *dira*, including all files and sub-directories, to usera:

```
chown -R usera dira
-> -rwxr-xr-x usera grpa 512 Apr 10 12.20 dira
```

Change the owner and group of directory tree *dira*, including all files and sub-directories: [1]

```
touser usera dira
-> -rwxr-xr-x usera grpa 512 Apr 10 12.20 dira
```

touser is a shell script, delivered with XWIN-NMR. It can, for example, be used to change the owner of a dataset:

- type **su - root** to become superuser
- type **cd /u/data/usera/nmr**
- type **touser userb dataseta**

1.The group of dira is set to the group usera belongs to (touser uses chown -R and chgrp -R)

umask

set the initial permissions for file creation

The initial permissions of a file are set according to:

initial permission = creation permission - umask

The creation permissions are:

666 for files created by an editor (e.g. **`vi`**, **`emacs`**)
777 for directories and executables created by a compiler

Each user can set **`umask`** in his *.profile* or *.cshrc*

The superuser can set **`umask`** for all users in the files *etc/profile* and */etc/cshrc* [1]

We recommend `XWIN-NMR` users to set **`umask`** to 002 or 022

examples

In each example a dataset *data1* is created with different values of **`umask`**. You see the output of **`ls -ld data1`**: [2]

- **`umask 000`** -> create *data1* -> permissions 777
  `drwxrwxrwx 1 owner group 10 Jun 7 12:20 data1`
  -> every user can read and write (process) data1
- **`umask 002`** -> create *data1* -> permissions 775
  `drwxrwxr-x 1 owner group 10 Jun 7 12:20 data1`
  -> only the owner and the group can write data1
- **`umask 022`** -> create *data1* -> permissions 755
  `drwxr-xr-x 1 owner group 10 Jun 7 12:20 data1`
  -> only the owner can write data1

1.Each user can overwrite this value by setting the `umask` in his personal *.profile* or *.cshrc*
2.Note that the permission of all subdirectories and files in `data1` are set according to `umask`

more UNIX commands

on files or directories

- **`du [-k] dira`**
  -> disk usage of a directory in number of blocks [Kbytes]

- **`file fila`**
  -> what is the type of the file *fila* (is it ascii, binary etc.)

- **`mkdir dira`**
  -> create the directory *dira*

- **`rm -r dira`**
  -> remove the directory tree *dira* including all files and sub-directories

- **`touch fila`**
  -> set the date of the existing file *fila* or create *fila*

- **`grep stringa fila`**
  -> search for the string stringa in the file *fila*

- **`find dira -name fila -print`**
  -> find the file *fila* in directory tree *dira*

- **`ln [-s] fila filb`** [1]
  -> make a [symbolic] link between *fila* (source) and *filb* (target)

1. Use `ln -s` when *fila* and *filb* reside on different partitions.

filename substitution

In a UNIX shell, you can use the characters *****, **?** and **[]** for filename substitution:

*****	matches any string with zero or more characters
?	matches any single character
[...]	matches any one of the enclosed characters

examples

List all files with the suffix .c:

```
ls *.c
```

List all files which start with a and have 3 characters:

```
ls a??
```

List all files which start with p, q or y:

```
ls [p,q,y]*
```

Search for the string zg30 in all files which start with z and end with p:

```
grep zg30 z*p
```

Search for the string hpdj in all files which start with a, b, c, d or e:

```
grep hpdj [a-e]*
```

grep

search for a string in a text file
show the lines containing this string

normal form

Search for string `stringa` in the file *fila:*

```
grep stringa fila
```

other forms

Search for `stringa` in all files in the current directory:

```
grep stringa *
```

Search in all files which start with `a`,`b`,`c` or `d`:

```
grep stringa [a-d]*
```

Print the lines in *fila* not containing `stringa`:

```
grep -v stringa fila
```

Ignore upper/lower case in `stringa`:

```
grep -i stringa fila
```

Search for `stringa` or `stringb` in the file *fila*:

```
egrep -i "stringa|stringb" fila
```

Search for `stringa` in the output of **`ps -ef`**:

```
ps -ef | grep stringa
```

find

search for files and directories in a directory tree

examples

Search for entries (files and directories) called *fila* in the directory tree *dira*:

```
find dira -name fila -print
```

Search for entries that start with a:

```
find dira -name "a*" -print
```

Search for entries not called *fila*:

```
find dira ! -name fila -print
```

Search for entries newer than the file *fila*:

```
find dira -newer fila -print
```

Search for files bigger than 1000 blocks (512000 bytes) on all local partitions, not on NFS mounted partitions:

```
find / -local -size +1000 -print
```

Run a UNIX command (e.g. **lp** or **rm**) on all entries *fila*:

```
find dira -name fila -exec lp {} \;
```

Delete 2D processed data: *2rr*, *2ir*, *2ri* and *2ii* in */u*:

1. **cd /u/data**
2. **find . -name "2[ir][ri]" -exec rm {} \;**

-> Note that the notation *[ir]* means *i* or *r*.

install new users

on SGI with IRIX >= 6.3

1. click ***System -> System Manager -> Security and Access Control -> User Manager -> Add***
2. enter the root password

-> continue by clicking the ***Next*** button after each step:

3. enter the new `Login Name`
4. enter the `Full Name`
5. click on ***add a password*** -> enter the `password`
6. enter an unused `User ID` [1]
7. accept the default `group` or specify a different one
8. accept the default `home` dir. or specify a different one
9. select the `IRIX shell` of your preference [2]
10. click `OK` to accept the new entry

In step 1, click ***Edit*** instead of ***Add*** to change an existing user

on SGI with IRIX <= 6.2

Click ***System -> User Manager -> Add***

Enter the same information as described for IRIX >= 6.3.

The procedure, however, is slightly different:

- entries are made in one window (no ***Next*** button)
- click on ***open*** instead of ***add*** to change a user entry
- click on ***other*** to install a non default shell (e.g. `bash`)

Important: when computers are in a network, use the same User ID and Group ID for the same user on each host.

1.Type: `cat /etc/passwd` to check if a User ID already exists.
2.For the bash, click *custom* and enter the pathname of the bash, e.g. */bin/bash* or */usr/local/bin/bash*

the file /etc/passwd

user account administration

The file */etc/passwd*:

- contains the complete login account information
- has one line for each user (account) on the system

Each line contains 7 fields separated by colons:

example

```
root:a7hIyuhgY4d7i:0:0:Super-User:/:/bin/csh
lp:*:9:9:Print Spooler Owner:/var/spool/lp:/bin/sh
jr::1021:20:J.Red:/usr/people/jr:/usr/local/bin/bash
guest:oLujnWr:998:20:Guest:/usr/people/guest:/bin/sh
```

meaning of the fields:

1: **Login Name**
2: **Encrypted password**: if empty, the user has no password
3: **User ID** : must be a unique number for each user
4: **Group Id**: must be a unique number for each group
5: **Full Name**: the user's full name, may contain blanks
6: **Home directory**: usually */usr/people/<user>*, but can be different
7: **UNIX shell**: must contain full pathname e.g. */bin/sh* or */bin/bash*

The superuser can change the file */etc/passwd* in order to:

- delete a user's password
- add a `*` in the second field for special users like `lp`, `demos`, `4Dgifts` for security reasons [1]
- change the `UNIX` shell (e.g. to `bash`)

Note that the user `jr` in this example does not have a password. We strongly recommend to give every user a password, also the special users (see user `lp` in the example).

1. There is no password which translates to the encrypted password *.

the file /etc/group

group account information

The file */etc/group*:

- contains the complete information for groups of login accounts
- has one line for each group on the system

Each line contains 4 fields separated by colons:

example

```
root::0:root
user::20:guest,jim
other::995:john,lisa,klp
```

meaning of the fields:

1: **Group Name**
2: **Encrypted group password**: usually empty
3: **Group Id**: must be unique for a group and the same on each host
4: **List of users who belong to this group**: separated by commas

Why are users divided into groups?
You can share your files with users within your group and protect them from all other users.

The file */etc/group* can only be changed by the superuser.

Important: all users who want to run the `XWIN-NMR` automation must be entered in their corresponding group line in */etc/group*. [1]

1.This is NOT done automatically during the installation of a user.

UNIX shells

A UNIX shell:

- is a layer between the operating system and the user.
- offers the user a way to communicate with the o.s.
- is selected upon installation of a new user

Type **`echo $SHELL`** to find out which shell you use!

Different UNIX shells and the files executed during login:

Important differences between shells [2]:

1. how do you set environment variables
   `sh` and `bash`: 1) **`variable=value`**
   2) **`export variable`**
   `csh` and `tcsh`: **`setenv variable value`**
2. `tcsh` and `bash` offer history substitution
   you can use the arrow keys to repeat and modify previously entered commands.

The `bash` is not a standard shell. If it is not installed on your computer get it from the Bruker FTP server [3].

1.The `bash` also executes the file *.bashrc* if it exists.
2.Type `man sh` or `man csh` for more information on these shells.
3.The bash for SGI resides on ftp.bruker.de in the directory */pub/nmr/binarie.indy*

the file .profile

The file *.profile*:

- sets your personal UNIX environment
- is executed every time you log in
- resides in your home directory
- is used in connection with the shells sh and bash

You can edit the file *.profile* and add your personal preferences, e.g.:

```
umask 002
PATH=$PATH:/usr/local/bin
NMR=/u/data/guest/nmr
export PATH NMR
xw() { xwinnmr; }
```

Log out and log in again for your changes to take effect:

- **umask** will be set to 002
- */usr/local/bin* is part of the UNIX search patch
- you can type: **cd $NMR**
  instead of: **cd /u/data/guest/nmr**
- you can type **xw** instead of **xwinnmr**

Note the difference between **NMR**, an environment variable and **xw**, a UNIX function.

For csh and tcsh the file *.cshrc* is used. Note that the setting of environment variables is different (see previous page).

more UNIX commands

for host and user information

- **`id`**
  -> show the user/group name and ID

- **`uname -a`**
  -> show the computer's hostname and `UNIX` version

- **`hostname`**
  -> show the computer's hostname

- **`who`**
  -> who is logged in and since when

- **`df -k`**
  -> show file system and their available disk space

- **`env`**
  -> show all environment variables

- **`passwd`**
  -> change your password

- **`sysinfo`**
  -> unique system identification needed for all Bruker licenses

ps

show the UNIX process table

ps -ef

```
 UID   PID  PPID  C    STIME    TTY   TIME COMD
root   0    0   0  14:01:12   ?    0:01 sched
root   1    1   0  14:01:12   ?    0:00 /etc/init
root 164    1   0  14:01:48   ?    0:00 /usr/etc/nfsd 4
root 270    1   0  14:01:56   ?    0:00 /sbin/cron
 lp  254    1   0  14:01:54   ?    0:00 /usr/lib/lpsched
root 308    1   0  14:01:58   ?    0:00 /usr/diskless/bfsd
demo 312  309  0  14:01:59 pts/2  0:00 /u/prog/cpr/cpr
```

example

ps -ef | grep prog

show all XWIN-NMR processes

```
 UID   PID  PPID  C    STIME    TTY   TIME COMD
demo 758  686  0  17:07:14 pts/1  0:00 /u/prog/cpr/cpr
demo 889  758  0  17:07:24 pts/1  0:00 /u/prog/mod/go
demo 792  758  0  17:07:15 pts/1  0:01 /u/prog/cpr/xcpu
demo 901  811  0  17:09:42 pts/0  0:00 grep prog
```

kill

terminate a UNIX process

e.g. **kill 758 889 792**

Use **kill -9 PID** only if **kill PID** does not kill the process.

lpstat -t

print the printer/plotter status

Use the command **`lpstat -t`**:

- to see if someone is plotting
- in case of plot/print problems

This is the output of **`lpstat -t`** showing:

3 possible problems

```
scheduler is not running
system default destination: hpdj660c
device for hpdj660c: /dev/plp
hpdj660c accepting requests since Sep 19 15:12
printer hpdj660c disabled since Dec 4 12:28
hpdj660c-9 2726 Dec 4 12:23
```

the solutions

- start the scheduler: **`/usr/lib/lpsched`**
- enable the printer: **`/usr/bin/enable hpdj660c`**
- cancel hanging print jobs: **`cancel hpdj660c-9`**

compress, gzip

compression to reduce the size of a file

File compression can be used to:

- save disk space on rarely used files
- reduce network traffic (for **`rcp`**, **`ftp`**, E-mail etc.)

Compress a file: *fila* is replaced by *fila.Z*:

```
compress fila
```

Uncompress a file: *fila.Z* is replaced by *fila*:

```
uncompress fila
```

Compress a file: *fila* is replaced by *fila.gz*:

```
gzip fila
```

Uncompress a file: *fila.gz* is replaced by *fila*:

```
gunzip fila
```

Uncompression does not require the suffix *.Z* or *.gz*

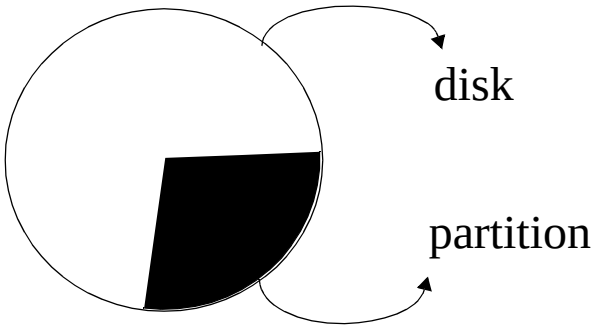
The compression factor depends on the file type (20-70%)
`gzip` gives a better reduction in size than **`compress`**.

If the commands **`gzip`** and **`gunzip`** are not found, then get and install the `gzip` package from the FTP server [1]

Many files on the Bruker FTP server have the extension *.gz*, which means they have been compressed with **`gzip`**.

1.The package `gzip` for SGI resides in ftp.bruker.de in the directory */pub/nmr/binaries.indy*

partition - file system - directory



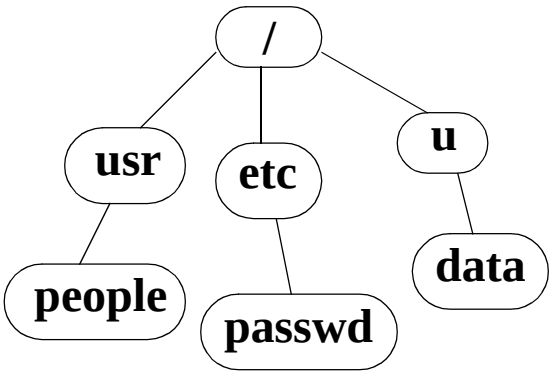
a partition

corresponds to

super block	i-list	data blocks

a file system

which can be mounted on



a directory tree

partition - file system - directory

A partition is a part of a disk; it contains exactly one file system.

A file system is a hierarchical structure on the disk usually containing directories and files.

A directory tree is a representation of a file system, it makes the file system accessible.

Mounting a file system: installing a connection between a file system and a directory tree, which makes the file system accessible.

Show mounted file systems and free space: [1]

type **`df -k`**

This is an example of the output **`df -k`**:

Filesystem	Type	kbytes	use	avail	%use	mounted on
/dev/root	xfs	930000	755734	174265	81%	/
/dev/dsk/dks0d2s7	efs	1030302	790218	240083	77%	/v
host_b:/w	nfs	1016685	376807	639878	37%	/x

Note that the command **`df -k`** only shows a file system when it is mounted.

1.The command `df` will show the disk space in blocks, `df -k` in kbytes.

mount

connect a directory tree to a file system

Connect directory */z* to the corresponding file system:

`mount /dev/dsk/dks0d1s7 /z`

Connect directory */z* according to the file */etc/fstab*:

`mount /z`

Connect */u* on the remote `host_a` to the local */z*:

`mount host_a:/u /z`

-> not that */u* on `host_a` must be exported

Disconnect directory */z* from its file system:

`umount /z`

-> files are still on disk but not accessible

reasons to unmount a file system

You want to do a file system check, e.g. on */z*:

`1.umount /z`

2. **`fsck /dev/dsk/dks0d1s7`** [1]

You want to backup the entire root directory */* except the directory */z* (assuming */z* is a separate file system):

`1.umount /z`

`2.tar cv /`

1.The command `fsck` can only be used for EFS file systems (type `df`). XFS file systems can be repaired with `xfs_repair`

archiving with tar

copy to the default tape, usually DAT

Copy *fila* (file or directory) from disk to tape:

```
tar cv fila
```

Caution: **`tar cv`** destroys the current contents of the tape!

Extract *fila* from tape to disk:

```
tar xv fila
```

List the occurrences of *fila* on the tape:

```
tar tv fila
```

Append *fila* to the end of the archive:

```
tar rv fila
```

-> Caution: do not exceed the end of the tape [1]

Append *fila* if it does not exist on tape or has been modified:

```
tar uv fila
```

Copy the directory-tree *dira* into the tar-file *fila:*

```
tar cvf fila dira
```

Copy to tape with relative pathnames, e.g.:

```
cd /u/data/guest/nmr
tar cv dataseta
```

Copy data with absolute pathnames[2], e.g.:

```
tar cv /u/data/guest/nmr/dataseta
```

1.On some tape drives the End Of Tape handling does not work correctly and data are destroyed.
2.In this case dataseta can only be copied back to the same directory; if it does not exist it will be created.

how to avoid much typing in UNIX

use environment variables, e.g.:

```
NMR=/u/data/usera/nmr
export NMR
```

-> these 2 lines can be entered in your file *.profile*
Type **`cd $NMR`** to go to the corresponding directory.

use UNIX functions, e.g.:

```
data() { cd /u/data/usera/nmr ;}
```
[1]

-> this line can be defined in your file *.profile*
Type **`data`** to execute the function.

use cut and paste

- mark text by holding the left mouse button down
- copy this text by clicking the middle mouse button

use the UNIX shells bash or tcsh

- use the arrow keys up/down to repeat and/or modify previously entered commands
- use the **`Tab`** key to complete commands

use a UNIX shell script

They are described on the next pages.

1.The definition of a UNIX function requires two blanks, one after "{" and one before ";".

UNIX shell scripts

execute a series of UNIX commands

A shell script:

- is an executable text file
- can contain a series of UNIX commands
- can contain control loops and variables

example

scripta displays the date, current directory + contents:

1. edit a file *scripta* and enter:

```
date
pwd
ls
```

2. make *scripta* executable: **chmod a+x scripta**
3. execute the script by typing **./scripta** [1]

When executing *scripta* a possible output is:

```
Wed Jan 3 03:51:07 PST 1996
/usr/people/guest
scripta
fila
```

Note: for csh or tcsh, the first line of the script must be:

```
#! /bin/sh
```

1."./" means: the command resides in the current directory. You can skip the "./" if the current directory is part of the UNIX search path. Type `echo $PATH` to see the UNIX search path.

UNIX shell scripts

the use of parameters and control structures

example

scriptb displays the contents of a pulse program:

1. edit the file scriptb and enter:

```
dir=/u/exp/stan/nmr/lists/pp
cd $dir
cat $1
```

`$dir` = the value of a parameter which is set in the script
`$1` = an argument given to the script when it is executed

2. make the file executable:
   `chmod +x scriptb`

3. execute the script by typing its name and argument e.g.:
   `./scriptb zg30`

Example of a control and loop structure in a shell script: [1]

```
for i in ‘ls *.c‘
do
  if grep strn $i
    then
      rm $i
  fi
done
```

for all files with the extension `.c`

if the file contains the string `strn`

remove the file

1.For more information on control and loop structures type `man sh` or `man test`.

cron - crontab

execute a command daily, weekly

Any UNIX command or program can be executed automatically on a regular basis.

1. check if `cron` is running: **`ps -ef | grep cron`**
   if `cron` is not running: **`sh /etc/init.d/cron start`**

2. create a crontab file using the following syntax:

   ```
   min hour daymo month daywk command
   ```

   `min`: minute (0-59)
   `hour`: hour (0-23)
   `daymo`: day of the month (1-31)
   `month`: month of the year (1-12)
   `daywk`: day of the week (0-6 with 0=Sunday)
   `command`: the command or program to be executed

   Suppose you want to:

   - backup your data at 4.30 am on Tuesday to Friday
   - delete all *core* files at 2 am on Sunday

   Note that the second task needs superuser permissions.

   a) type **`cd`** to go to your home directory
   b) type **`su`** to become superuser
   c) edit the file *fila* and enter the following lines:

   ```
   30 04 * * 2-5 tar cv /u/data/<user>/nmr
   00 02 * * 0   find / -name core -exec rm {} \;
   ```

   d) type **`crontab fila`**

You can skip step b) if all tasks in your crontab file can be done as normal user. Type **`man crontab`** for more information.

function keys in X-windows

set function keys for a winterm

1. type **`cd`** to change to your home directory
2. edit a file named *wkeys*

   enter your personal function keys e.g.:

```
F1(shift):   send("lpstat -t")
F1(control): send("ps -fulp")
F1():        send("ps -ef | grep prog")
F2(shift):   send("cd ‘curd -a‘")
F2(control): send("ftp ftp.bruker.de")
F2():        send("ftp ftp.bruker.com")
```

3. edit the file *.auxchestrc*;

   enter the following line:

```
Menu Desktop
{
  "Wkey" f.exec "xwsh -name winterm -key wkeys"
}
```

4. log out and log in again
5. click on ***Desktop -> Wkey***, which will open a new winterm in which you can use the function keys

Each key can be used for three different commands by using the `Shift` and `Control` modifiers. Note that the order of the lines is important: `key(shift)`, `key(control)`, `key()`.

Type **`man winterm`** for more information on **`winterm`**.

troubleshooting UNIX

things you can do if you have problems on UNIX or XWIN-NMR level

1. always check the available disk space:
   a) type **df**
   b) if the partition / is full:
      - **find / -name core -exec rm {} \;**
      - **cd /usr/adm/crash**
      - **rm *unix* *core***
   c) if another partition, e.g. */x*, is full:
      - **find /x -name core -exec rm {} \;**
      - remove processed data in XWIN-NMR with delp
      - back up raw data and then remove them with dela

2. shutdown and switch off the computer:
   a) shutdown the computer; type **/etc/shutdown**
   b) switch the computer off
   c) switch the computer on, it will boot automatically

3. log in as a different user; if there are no problems now:
   a) save the files in your home directory on a tape
   b) delete the user including the home directory
   c) re-install the user
   d) copy those files you really need back from tape to your home directory

4. If you run IRIX <= 6.2 and see one of the following effects:
   - several ***Toolchest -> System*** functions do not work
   - the icons for the tape, CD, camera, etc, do not appear

   then the object server probably does not run:

   a) open a `UNIX` shell

   b) become superuser; type **`su`**

   `c)chkconfig objectserver on`

   `d)/etc/init.d/cadmin stop`

   `e)/etc/init.d/cadmin clean`

   `f)/etc/init.d/cadmin start`

   `g)/etc/reboot`

5. If the screen is frozen:
   a) press the **`Esc`** key

   b) press 5 keys **`Shift`**-**`Ctrl`**-**`Alt`**-**`F12`**-**`/`** simultaneously where **`/`** is the key left of the `Num Lock` key [1]

   -> this will force a log out

   c) if the system is connected to the network, log in as root via another computer and type **`/etc/reboot`**

   d) push the power button

   -> this will do a proper shutdown

   e) push the small hidden reset button

   -> this will briefly cut off the power

   Caution: if you reboot or shutdown the system, first check who is logged in, type **`who`**

1.This is the / in the numeric pad on the right side of the key board.

Part II

XWIN-NMR

help
directory tree
AU programs
customizing
troubleshooting

help in XWIN-NMR

The complete XWIN-NMR manual and many other documents (e.g. this manual) are available as online help.

click on the Help menu

Click on the XWIN-NMR menu item *Help*. The entries *Contents* and *Index* are organized in hypertext. You can select an item and the corresponding page will be displayed automatically.

Help on any XWIN-NMR acquisition command:
Help -> Acquisition Reference Manual
Help on any XWIN-NMR processing command:
Help -> Processing Reference Manual
The XWIN-NMR Release letters:
Help -> Release Letter
This manual:
Help -> Other topics -> XWIN-NMR and Unix

The programs XWIN-PLOT and ICON-NMR open separate windows with their own *Help* menus.

Frequently Asked Questions on WWW

Start you web browser and enter the following url:
`http://www.bruker.de`
click ***NMR -> Software -> FAQ***

enter xhelp on the command line

All XWIN-NMR help files reside in the directory:

/<xwhome>/prog/docu/english/xwinproc [1]

All files can be displayed by entering xhelp pathname, where pathname is the relative path of the help file, e.g.:

- an XWIN-NMR help file:
  xhelp xwinproc/pdf/tutor1d.pdf
- an ICON-NMR help file:
  xhelp iconman/pdf/routine.pdf
- an XWIN-PLOT help file:
  xhelp xwpman/pdf/xwp.pdf
- an arbitrary pdf file :
  xhelp /usr/people/guest/myfile.pdf

If you often use certain help documents, you can set up a macro with edmac and enter the line: xhelp pathname

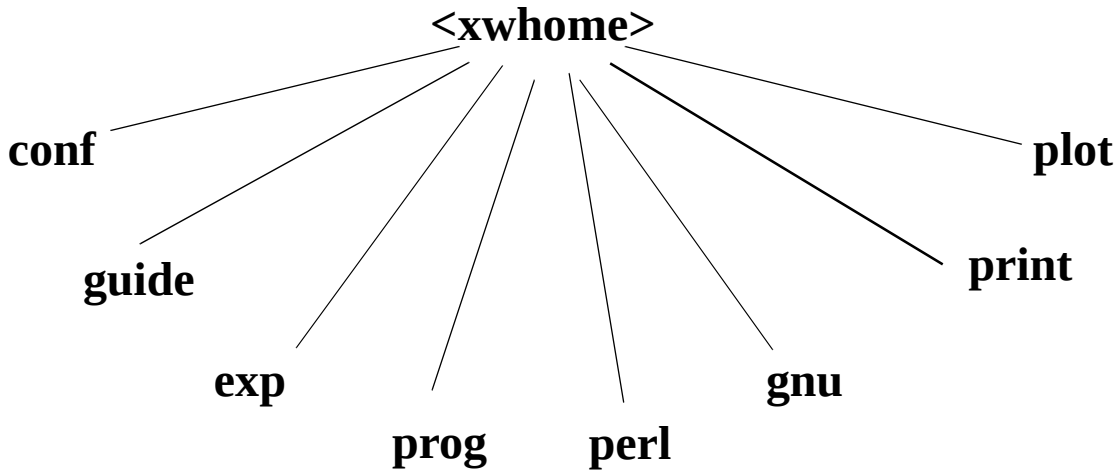
start help from a UNIX shell

If XWIN-NMR does not run you can still use its online help:

1. open a UNIX shell
2. **cd /usr/adobe/Acrobat?.?/bin**
3. **./acroread**
   - click on ***File -> Open***
   - enter the pathname in the Selection field, e.g.:
     /<xwhome>/prog/docu/english/xwinproc/pdf

1. <*xwhome*> is the directory in which XWIN-NMR is installed.

XWIN-NMR directory tree



<xwhome> - the directory where XWIN-NMR is installed
default directory: */u*

conf - spectrometer configuration files
- printer/plotter configuration
- service tools for bsms, acb, hppr, rx22 etc.

guide - NMR-GUIDE installation directory

exp - parameter sets, pulse programs, AU programs, several lists

prog - XWIN-NMR modules and graphics program
- online documentation
- Bruker library AU programs
- Bruker UNIX scripts

perl - perl interpreter for interpreting Perl scripts

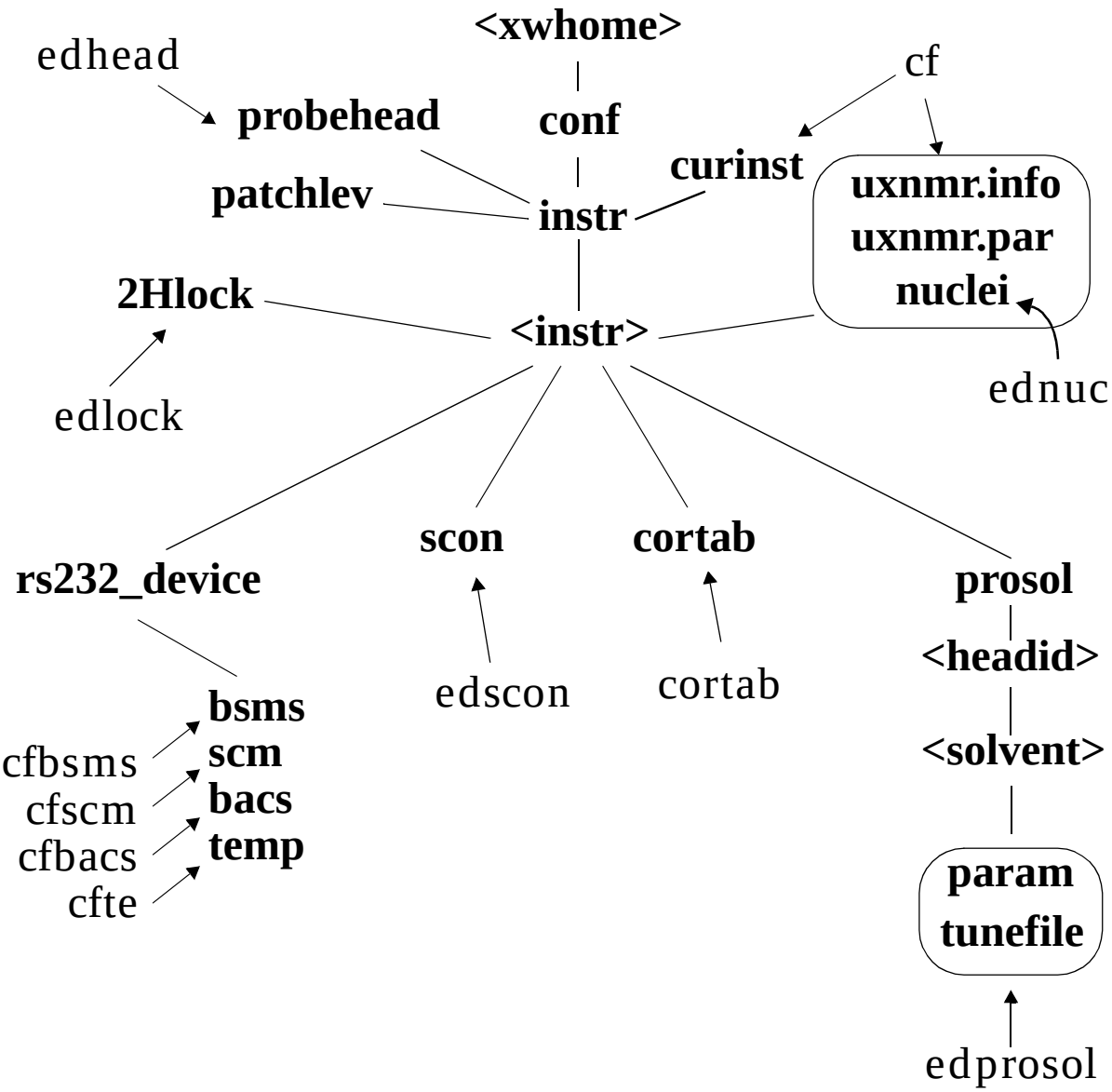
gnu - GNU C-compiler for compiling AU programs

print - programs for laser printers

plot - XWIN-NMR plot programs

directory conf/instr

spectrometer configuration



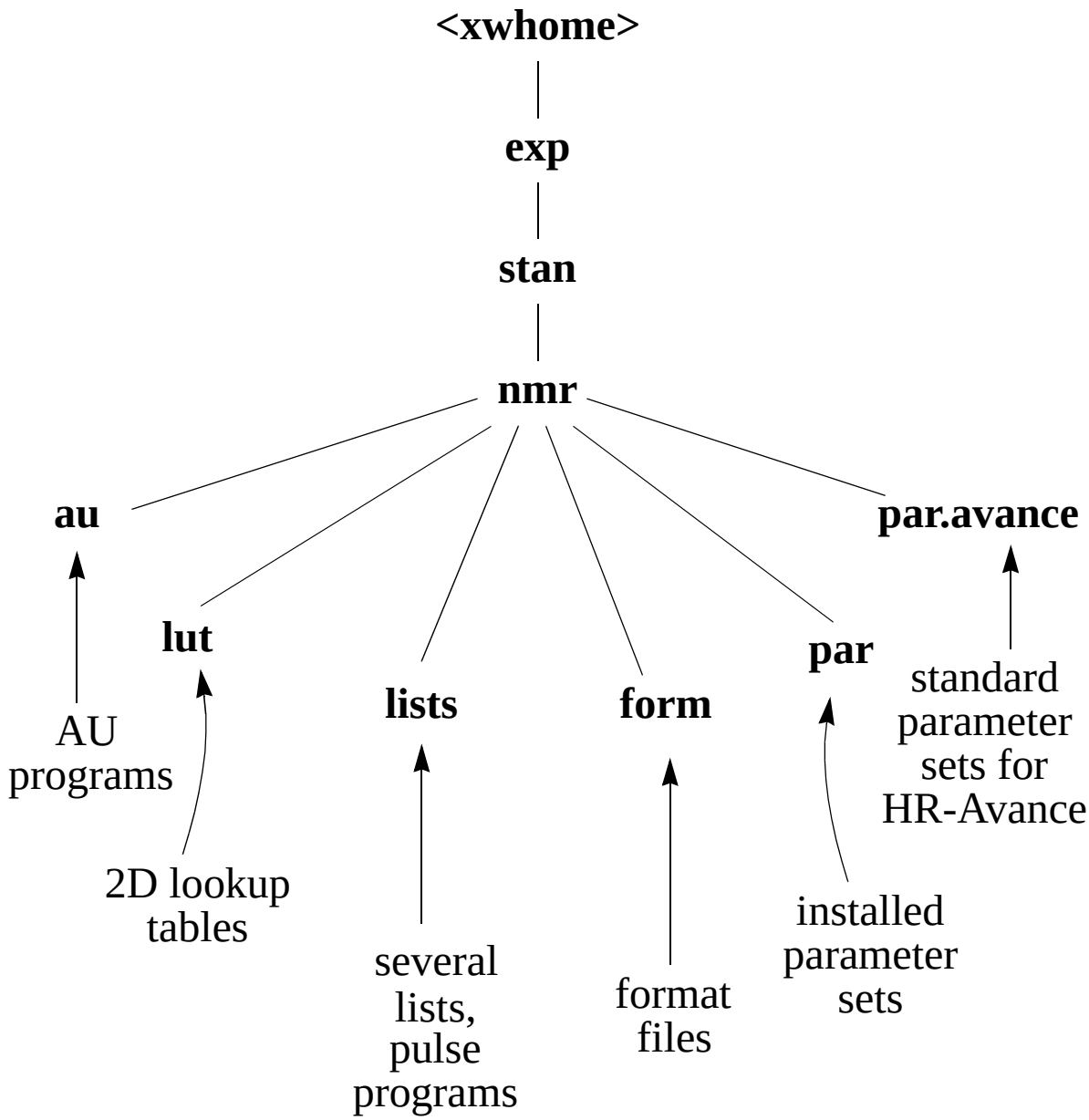
XWIN-NMR commands and the **files** they access

<*instr*> is the instrument name entered during cf

Type **`cat /<xwhome>/conf/instr/curinst`** to view the instrument name

directory exp/stan/nmr

XWIN-NMR experiment files

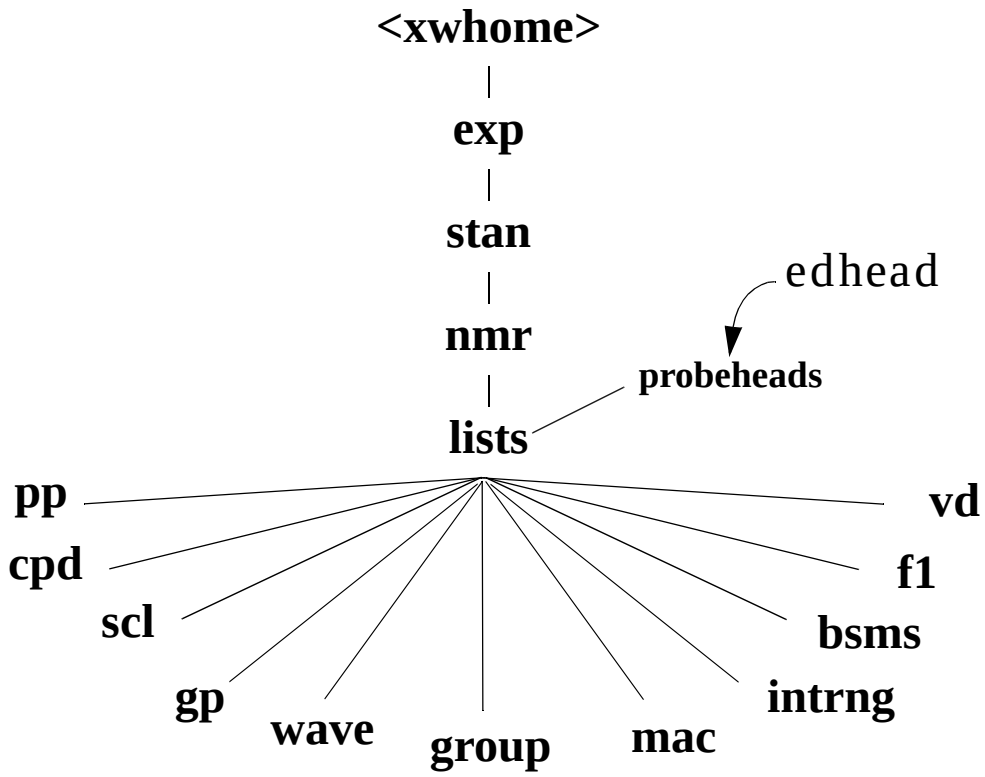


directories containing XWIN-NMR experiment files

The *exp* directory contains both Bruker standard and your own pulse programs, AU programs and parameter sets.

Keep a backup of this directory!

directory exp/stan/nmr/lists

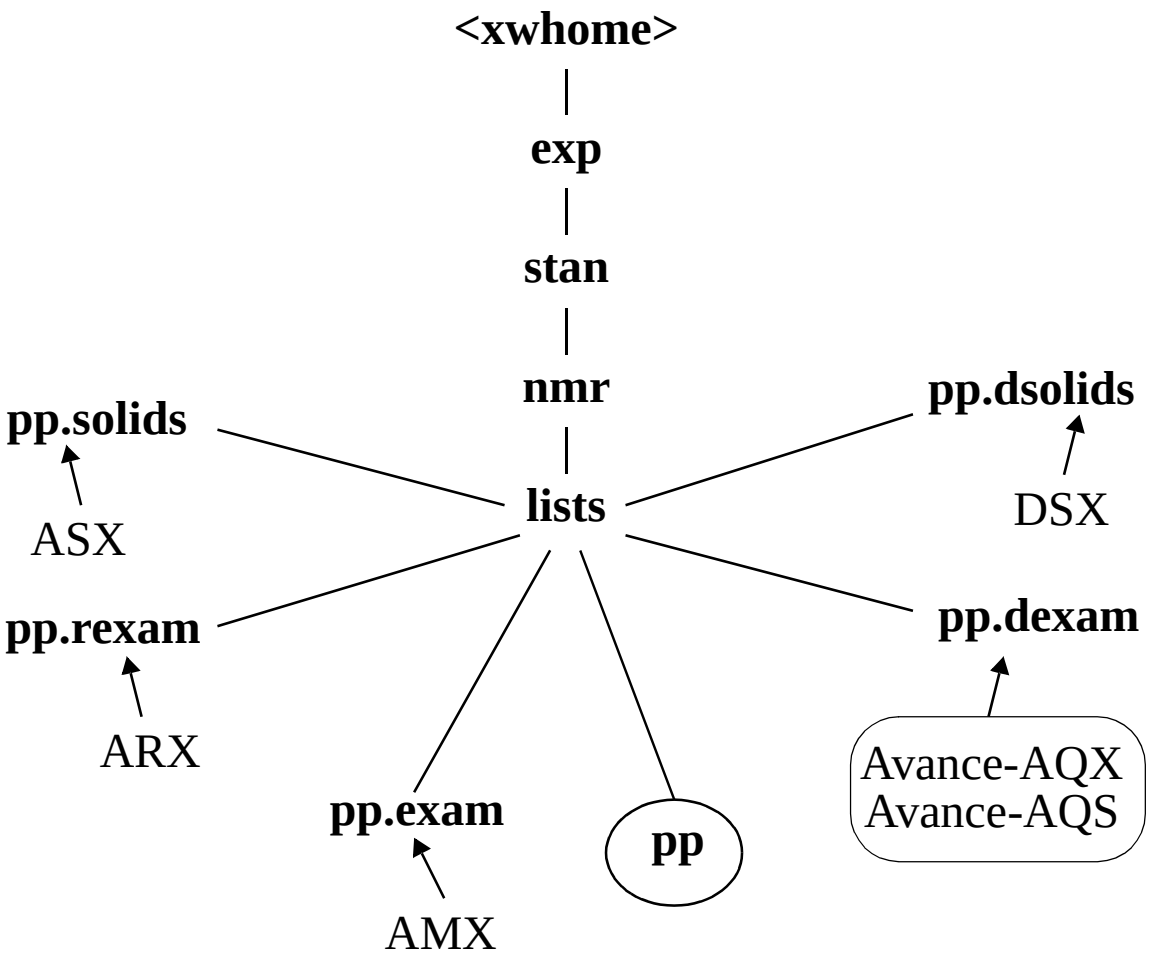


directories containing lists for acquisition

pp:	pulse programs used by `edpul`, `edcpul`, `zg` etc.
cpd:	`cpd` decoupling programs
scl:	scaling region files for PSCAL=`sreg` or `psreg`
gp:	gradient programs
wave:	shape pulses
group:	example and user defined tune files
mac:	macros accessed by `edmac` and `xmac`
intrng:	integral ranges accessed by `rmisc`, `wmisc`
bsms:	shim files accessed by `rsh`, `wsh`, `vish`
f1, vd:	frequency and delay lists accessed by `zg` if used in the pulse program

directory exp/stan/nmr/lists/pp

XWIN-NMR pulse programs



directories containing pulse programs

The directory pp contains the pulse programs which are used in XWIN-NMR by edcpul, as, zg etc.

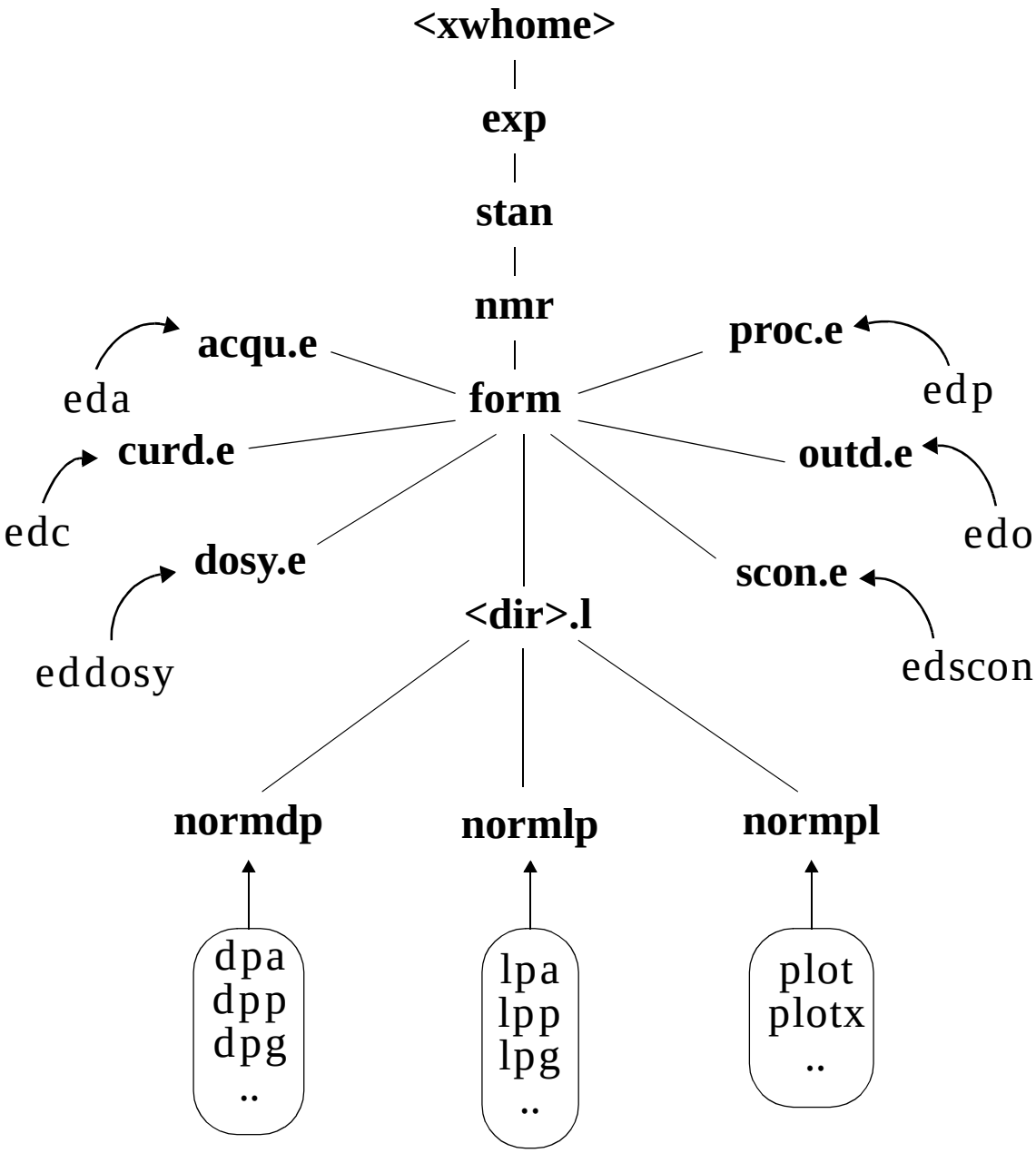
The directories pp.xxxx contain Bruker standard pulse programs for the various spectrometer types.

The command expinstall copies pulse programs from pp.xxxx (depending on the spectrometer type) to pp.

The directory pp also contains all user defined pulse programs.

directory exp/stan/nmr/form

format files



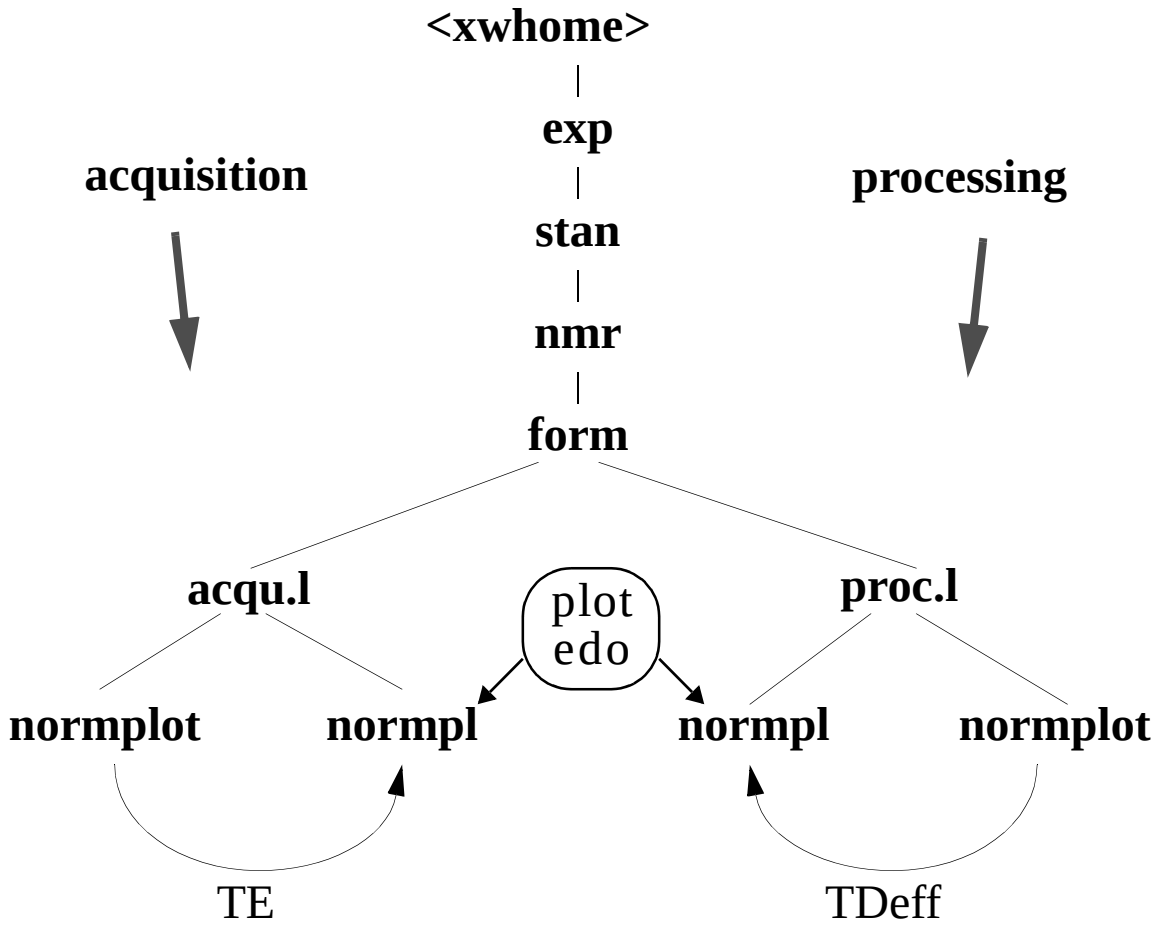
XWIN-NMR commands and the **files** they access

Format files determine the format of a parameter list:

- they can be changed by the NMR Superuser only
- you can add/remove parameters or change comments
- never change relations between parameters!

normpl - normplot

which parameters appear on the plot?



XWIN-NMR commands and the **files** they access

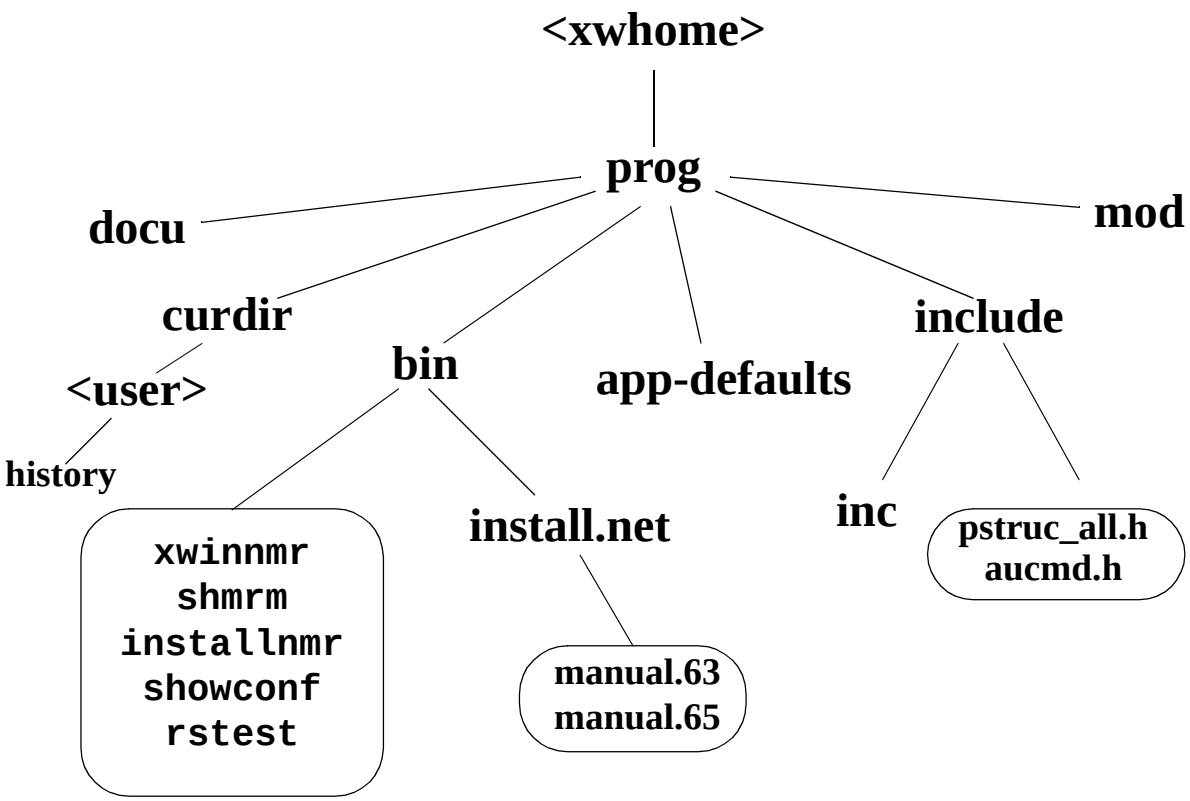
The format file *normpl* contains only a subset of the parameters, *normplot* contains all parameters.

Only the parameters in *normpl* will appear on the plot.

The NMR Superuser can edit *normpl* and add parameters contained in *normplot*, e.g. the processing parameter TDeff or the acquisition parameter TE.

directory prog

XWIN-NMR programs / executables



docu:	online documentation (in PDF format)
curdir/<user>:	XWIN-NMR user specific files, e.g. *history*
bin:	XWIN-NMR binaries and UNIX shell scripts
bin/install.net:	spectrometer network installation files
app-defaults:	resources (e.g. colours) for XWIN-NMR [1]
include:	h-files and command table for AU programs
include/inc:	macros for AU programs
mod:	modules; XWIN-NMR's main executables

1.Ascii files, also for XWIN-PLOT, PARAVISION etc., which can be modified by the NMR Superuser.

Bruker programs executed in UNIX

The following scripts reside in <xwhome>/prog/bin. Normally, you can start them in any directory. If, however, they are not found enter the full pathname, e.g. **/u/prog/bin/shmrm**.

- **installnmr** [1]
  -> install current version, set XWIN-NMR permissions etc.

- **shmrm**
  -> remove all shared memories

- **touser**
  -> set the owner and group of a directory (e.g. a dataset)

- **uxproc**
  -> shows all running or hanging XWIN-NMR processes

- **patchlevel**
  -> show the current XWIN-NMR patchlevel

- **curd**
  -> current XWIN-NMR dataset (usage: **cd 'curd'**)

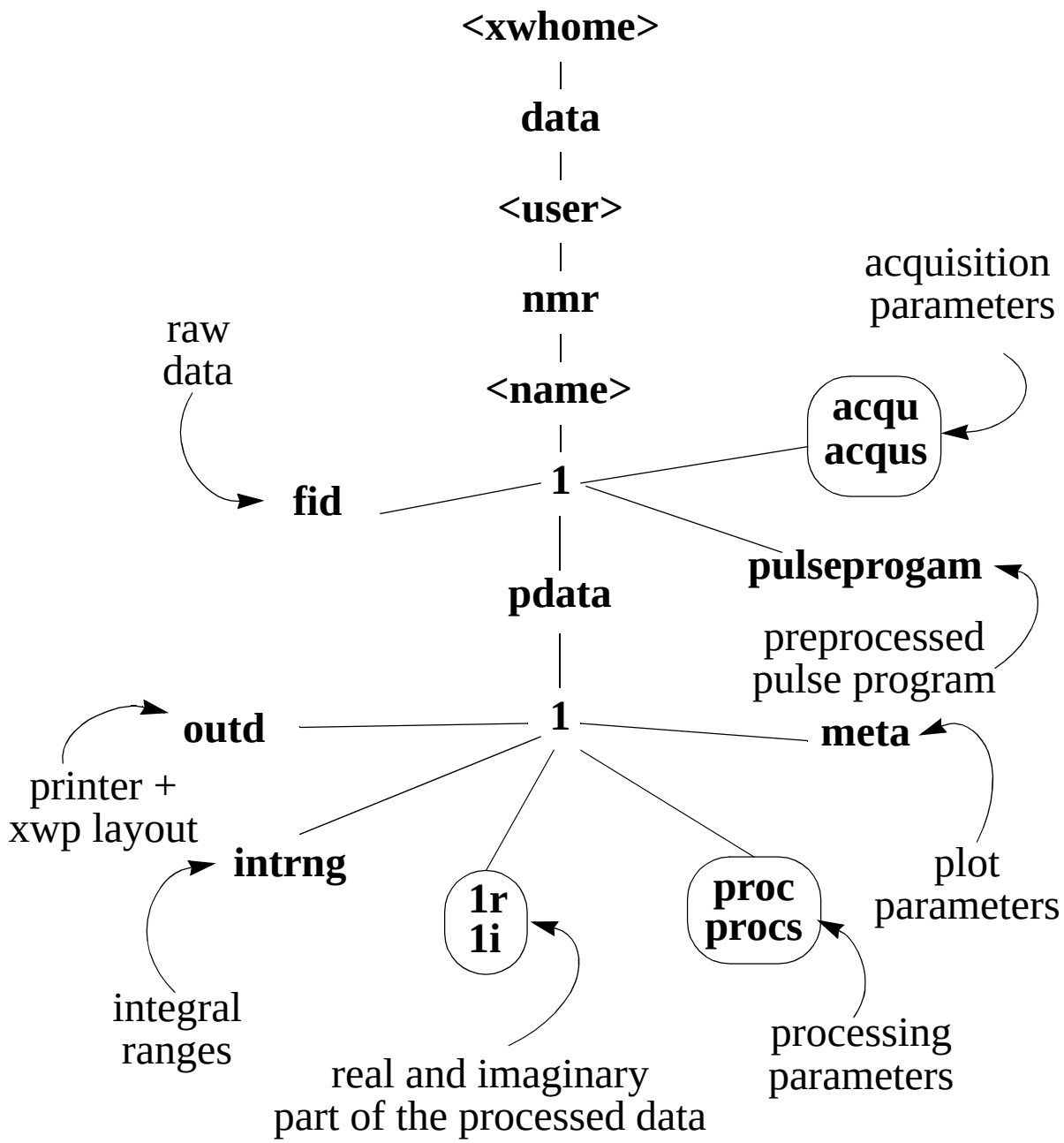
- **reviveccu**
  -> reset the spectrometer CCU

- **showconf**
  -> print the configuration of the workstation and the spectrometer into a file (including cf, **hinv** etc.)

1. installnmr is automatically executed during the installation of XWIN-NMR.

directory data

a 1D dataset



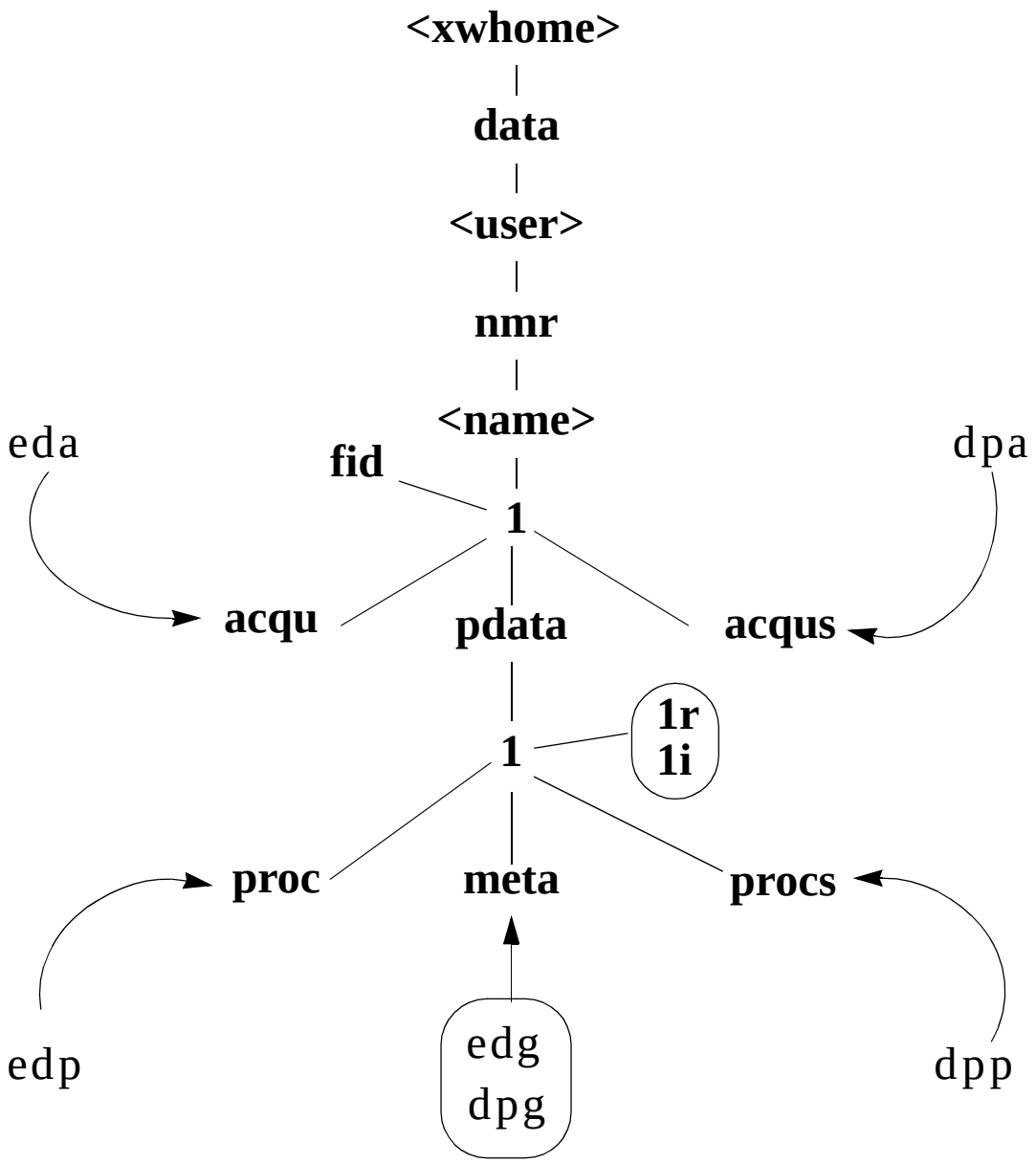
The data files *fid*, *1r*, *1i* are binary files containing integer numbers (the intensities of the data points).

All parameter files are ascii files in JCAMP format.

<xwhome> can be any directory e.g. */u* or */usr/people/guest* and is independent of the `XWIN-NMR` installation path.

directory data

acquisition, processing and status parameters



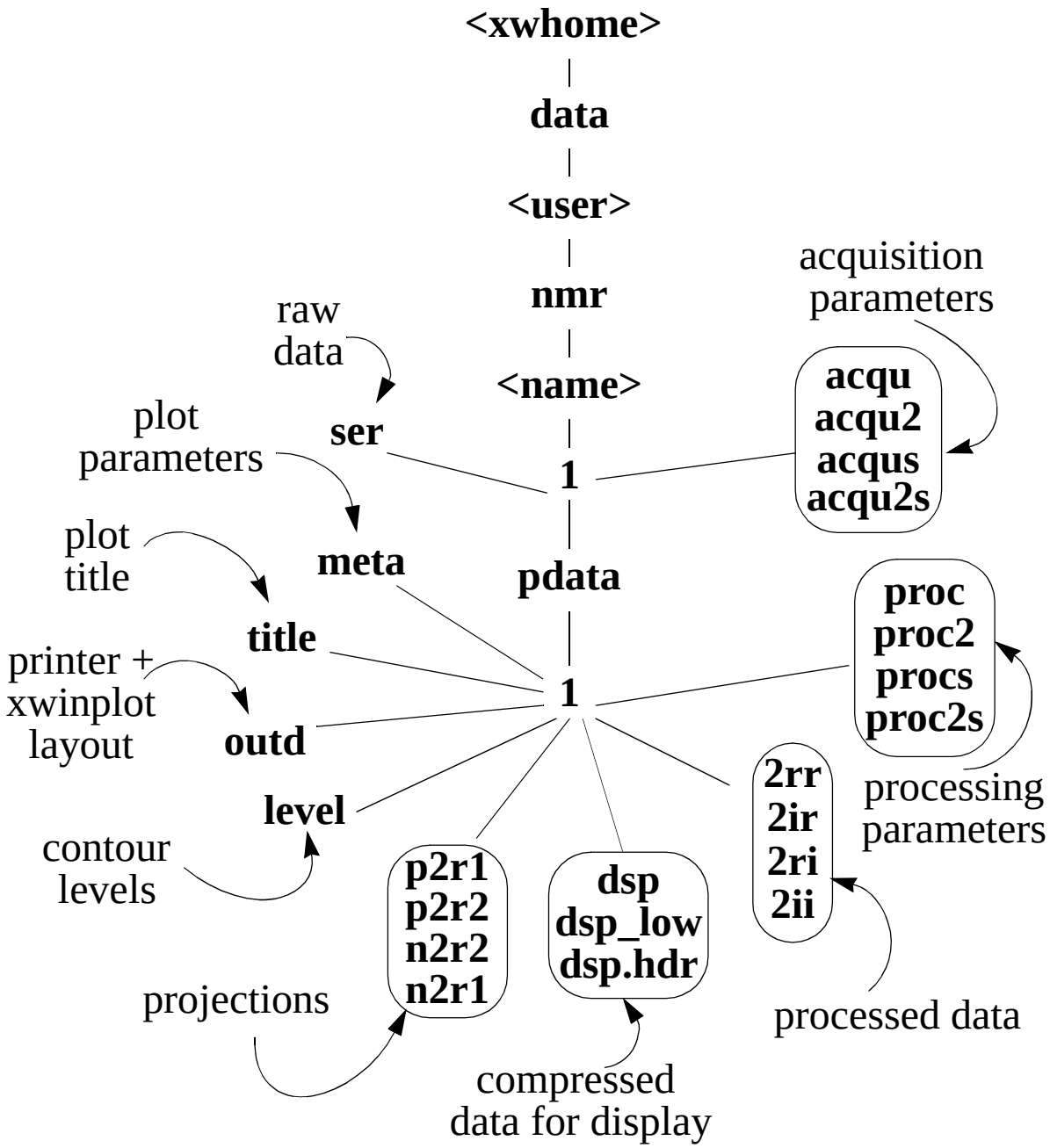
The acquisition parameters in *acqu* are set with eda.

The processing parameters in *proc* are set with edp.

The status parameters in *acqus* (*procs*) can be viewed with dpa (dpp) after acquisition (processing).

directory data

2D dataset



The files *ser*, *2**, *dsp* and *dsplow* are binary files containing integer numbers (the intensities of the data points).

All parameter files and the file *title* are ascii (JCAMP).

The file *level* is binary.

2D dataset

troubleshooting

Sometimes a 2D dataset cannot be displayed in XWIN-NMR; when you try to read the data a graphics restart occurs.

example

Reading the dataset */u/data/usera/nmr/dataseta* fails.
Do the following to solve the problem:

1. open a UNIX window

2. go to the processed data directory:
   cd /u/data/usera/nmr/dataseta/1/pdata/1

3. after each step try to read the data in XWIN-NMR:
   - **rm dsp*** - no information will be lost, XWIN-NMR will automatically create new *dsp* files

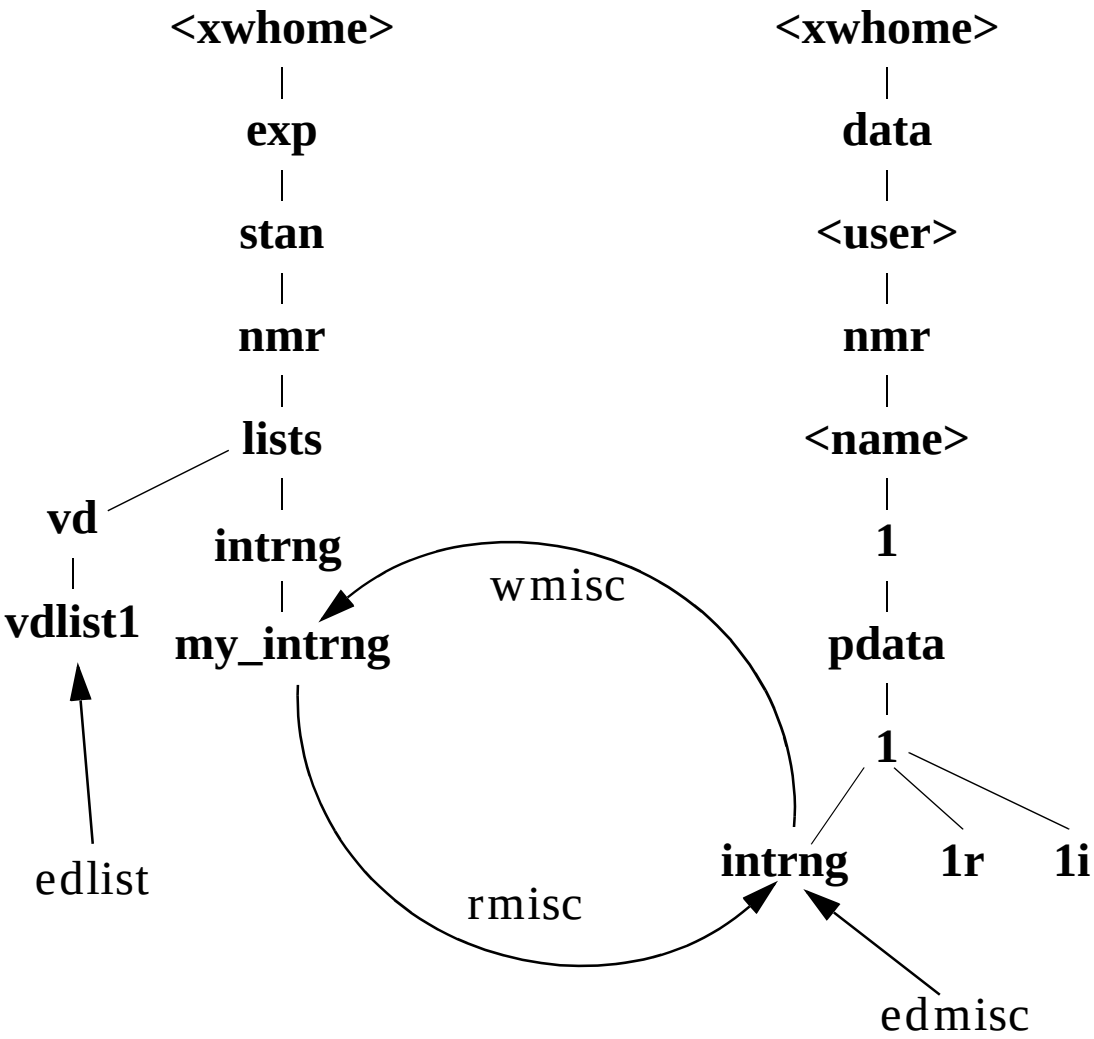
   - **rm level** - you loose your contour levels
     - XWIN-NMR will create a default *level* file
     - change the default levels with edlev

   - **rm 2*** - you loose the processed data
     - re-process the data with xfb

   - **cp /<xwhome>/exp/stan/nmr/par/standard2D/meta ./**
     - or copy any other 2D *meta* file
     - you loose the plot parameters
     - re-define the plot parameters with edg

rmisc/wmisc

read/write a dataset specific list



XWIN-NMR commands and the **files** they access [1]

Note the difference between edmisc and edlist:

- edmisc edits lists specific for one dataset; these lists concern data processing and analysis
- edlist edits lists available for all datasets, these lists mainly concern data acquisition

1.the `misc` commands also handle the files *reg*, *peaklist*, *base_info* and *baslpnts*

rmisc/wmisc

read/write a dataset specific list

example

1. read a dataset, e.g. *dataseta 1 1 /u usera*, enter the *integrate* menu and determine the integrals.

2. click *File -> Save as 'intrng'*
   this stores the integral ranges in the file:
   /u/data/usera/nmr/dataseta/1/pdata/1/intrng

3. type `wmisc intrng my_intrng`
   this copies the file:
   /u/data/usera/nmr/dataseta/1/pdata/1/intrng
   to the file:
   /<xwhome>/exp/stan/nmr/lists/intrng/my_intrng

4. change the dataset, e.g. to: *datasetb 1 1 /u usera*

5. type `rmisc intrng my_intrng`
   this copies the file:
   /<xwhome>/exp/stan/nmr/lists/intrng/my_intrng
   to the file:
   /u/data/usera/nmr/datasetb/1/pdata/1/intrng

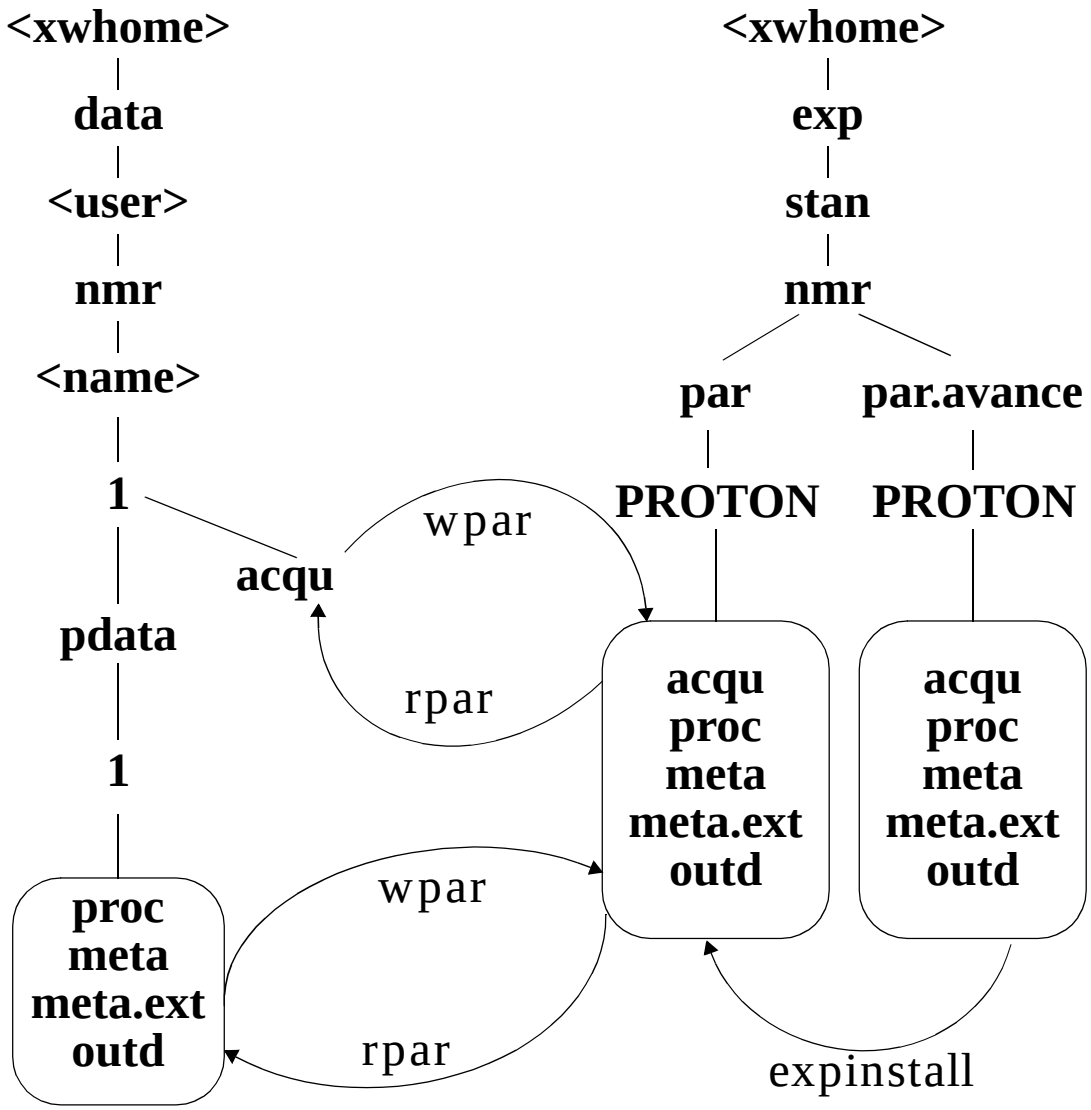
6. enter the *integrate* menu and click *File -> Read 'intrng'*

7. click on *lastscal* to see the integral labels in `AI` (absolute intensity) mode.

The commands `rmisc`, `wmisc` and `edmisc` apply to the following data set specific lists in `XWIN-NMR`: `intrng`, `baslpnts` `base_info`, `peaklist` and `reg`.

rpar - wpar

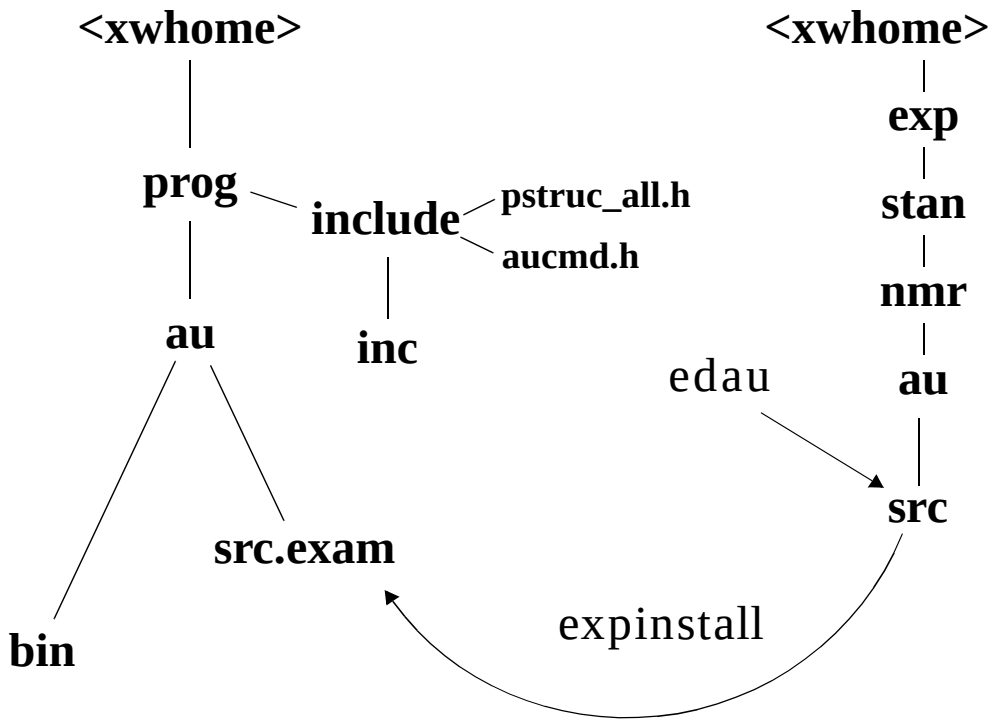
read - write parameter sets



XWIN-NMR commands and the **files** they access

The command rpar reads a parameter set into the current data directory. The command wpar stores a parameter set of the current dataset for general usage. The command expinstall converts Bruker standard parameter sets to the frequency of your spectrometer.

AU programs in XWIN-NMR



XWIN-NMR commands and the **directories** they access

src.exam:	Bruker standard AU programs
src:	installed Bruker and User AU programs
bin:	executables of Bruker and User AU programs
inc:	macros that can be included in AUprograms

For more information on writing and using AU programs click *Help -> Other Topics -> Writing AU programs*

The command expinstall copies all Bruker AU programs

from: */<xwhome>/prog/au/src.exam*

to: */<xwhome>/exp/stan/nmr/au/src*

You can also use the command edau 5 to do this.

After running expinstall, you can use 3 different commands to compile AU programs:

compileall:	compile all AU programs
cplbruk [<name> | all] :	compile Bruker AU programs
cpluser [<name> | all] :	compile user AU programs

The command edau [<name>] allows you to:

- create a user AU program which will be stored in: */<xwhome>/exp/stan/nmr/au/src*
- edit a user AU program or view a Bruker AU program in: */<xwhome>/exp/stan/nmr/au/src*
- compile an AU program and store the executable in: */<xwhome>/prog/au/bin*

The command xau [<name>] compiles an AU program [1] (if necessary) and executes it.

commands and parameters

The ascii file */<xwhome>/prog/include/aucmd.h* shows:

- which XWIN-NMR commands can be used in AU program
- their syntax, e.g. the number of arguments

The ascii file */<xwhome>/prog/include/pstruc_all.h* contains a list of acquisition and processing parameters [2] and can be used to view the type of a parameter (int, float, double etc.)

1.*xau* also compiles all AU programs which are called within an AU program.

2.The file *pstruc_plot.h* contains a list of plot parameters.

macros in XWIN-NMR

execute a series of XWIN-NMR commands

A macro, like an AU program, can execute a series of XWIN-NMR commands.

Differences between macros and AU programs:

- a macro always starts on the foreground dataset [1]
- a macro does not need to be compiled
- a macro cannot execute C language statements

You can create or change a macro by typing edmac <name>

example

1. type edmac my_mac to create/change the macro and enter your macro commands e.g.:

```
ef
apk
sref
abs
autoplot
```

   store the macro and leave the editor
2. execute the macro by typing my_mac or xmac my_mac

All macros are stored in the directory:

/<xwhome>/exp/stan/nmr/lists/mac

1.If you change data sets in a macro, the foreground data set also changes.

setres

the XWIN-NMR user interface

1. start **xwinnmr**
2. type setres [1]

Select the XWIN-NMR layout (standard, extended, uxnmr)

- standard is the default XWIN-NMR layout
- the extended layout contains additional buttons
- uxnmr is the layout of the traditional UXNMR program

Select data field colours e.g. for spectrum, axis etc. [2]

'double click' on the colour names to select a colour

Set XWIN-NMR environment variables:

- Editor: set the XWIN-NMR editor (e.g. **vi**, **xedit**, **jot**)
- Exploc: if set to "xxx", the directory */<xwhome>/exp/xxx* is used instead of */<xwhome>/exp/stan*
- Plotter: printer/plotter used by XWIN-NMR; the entry CURPLOT in edo is ignored from now on
- PlotMsg: switch on/off the plot message after plot
- ZGsafety: switch on/off the warning from the zg command that an existing FID will be overwritten

Switch on/off the history function

The file */<xwhome>/prog/curdir/<user>/history* contains all executed commands and error messages of the current XWIN-NMR session. [3]

1.*setres* information is stored in */usr/people/<user>/.xwinnmr-<hostname>/resources*.
2.Additional colours can be set in */<xwhome>/prog/app-defaults/XWinNmr* or your personal *.Xresources*
3.The *history* file is emptied when you exit and restart XWIN-NMR.

XWIN-NMR resources

colours and function keys

user specific resources

You can define your personal XWIN-NMR function keys:

1. log in as normal user
2. edit the file */usr/people/<user>/.Xresources*
   enter your personal XWIN-NMR function keys e.g.:

```
XWinNmr*cmdline*translations: #override \n\
Ctrl<Key>F2:insert-string("edo") \n\
Shift<Key>F2: insert-string("edp") \n\
<Key>F2: insert-string("eda") \n\
Ctrl<Key>F3: insert-string("xwinplot")
```

3. log out and in again

If you add the string `process-return()`, e.g.:

```
<Key>F2: insert-string("eda") process-return() \n\
```

the command is immediately executed. [1]

The keys F1 and F10 cannot be used for XWIN-NMR. All other keys can be used for 3 different commands, e.g.:

type `Control-F2` to start `edo`
type `Shift-F2` to start `edp`
type `F2` to start `eda`

Important: if you put 3 functions on one key, the order in the file *.Xresources* must be `Ctrl<Key>` - `Shift<Key>` - `<Key>`
No blanks or tabs are allowed at the end of the line.

1.If you add the string `beginning-of-line() kill-to-end-of-line()` before the string `insert-string("")` any characters which already exist on the command line will be removed.

You can define your personal XWIN-NMR menu colours:

- log in as normal user
- edit the file */usr/people/<user>/.Xresources*
  enter your personal XWIN-NMR menu colours e.g:

```
XWinNmr*foreground:darkseagreen
XWinNmr*background: maroon4
XWinNmr*XmText.background: aquamarine
XWinNmr*XmTextField.background: cadet blue
```

- log out and log in again

The colours for XWIN-NMR data field objects (spectrum, axis, background etc.) can only be set with the command setres [1].

You can view a list of available colours with the command **colorview** in a UNIX shell or with setres in XWIN-NMR.

resources for all users

XWIN-NMR resources can also be defined for all users:

1. log in as root
2. edit the file */<xwhome>/prog/app-defaults/XWinNmr*
3. enter function key or colour definitions

The format of the file XWIN-NMR is the same as for the file *.Xresources* (see examples above).

The directory */<xwhome>/prog/app-defaults* contains separate resource files for the different software components like xwinplot, view and pulsedisplay.

1.Double click on the colour name in *setres* to see the colour.

cpan

the XWIN-NMR command panel

The XWIN-NMR command panel cpan allows you to:

- setup a user defined window with XWIN-NMR commands
- give XWIN-NMR commands different names (aliases)
- add short explanations to the commands

How do you set up a command panel?

- type **cd** to go to your home directory
- type **mkdir -p .xwinnmr-xyz/cmdpanels** [1]
  where xyz is the hostname of your host
- type **cd .xwinnmr-xyz/cmdpanels**
- edit a file named *default* [2] and enter for example:

```
TITLE
1D Processing          ------->  title of the cpan window
BUTTON
NEWROW                 ------->  position of the button
ft                     ------->  XWIN-NMR command
fourier                ------->  alias name for command
1D Fourier Transform   ------->  short explanation
BUTTON
SAMEROW                ------->  position of the button
  etc.                 ------->  further entries
END
```

- Note that TITLE, BUTTON etc. are fixed keywords.

Now start XWIN-NMR and enter the command *cpan* [3]

1.You have to do this step only once.
2.*default* is the cpan startup file; you can setup additional files and use the load button in the cpan window
3. *expinstall* -> "Install Bruker Library AU Programs" must have been executed once before using *cpan*

troubleshooting XWIN-NMR

hang-ups and crashes

1. if an XWIN-NMR command has hung up:
   type kill to kill possibly hanging processes

2. if no keyboard or mouse control in XWIN-NMR
   a) move the cursor into the UNIX shell where XWIN-NMR was started
   b) type **^** (control backslash)
   c) answer the question for restart with "no"
   d) type **shmrm**
   e) type **uxproc**
   f) kill any hanging XWIN-NMR processes with:
      kill PID [1] (if this does not work, try **kill -9 PID**)
   g) type **xwinnmr** to restart XWIN-NMR

3. if no keyboard/mouse control on the entire screen
   a) if the computer is on the network, log in from another terminal
   b) perform step ’e’ to ’g’ as described under ’2’
   c) if this does not help, reboot the computer from the remote terminal: type: **/etc/reboot**
   d) if the computer is not on the network, push the power button or, if necessary, the hidden reset button

For more troubleshooting information click *Help - Installation Guide*

1. PID is the first number in the output of uxproc

troubleshooting printing

1. check the plot status in UNIX
   a) type **lpstat -t**
      - is a previous plot hanging?
      - is the printer enabled?
      - is the scheduler running?
   b) solve possible problems as described on page 29

2. switch the printer off and on again

3. only one UNIX processes lpsched should run
   a) type **ps -ef | grep lpsched**
   b) if 2 or more processes lpsched are running:
      - type: **/usr/lib/lpshut**
      - type **ps -ef | grep lpsched**
      - kill remaining lpsched processes: **type kill PID** [1]
      - type **/usr/lib/lpsched** to restart the scheduler
      - check with **lpstat -t** if the scheduler is running

4. check if the printer cable is properly connected

5. remove and re-install the printer
   a) in XWIN-NMR
      - type cfpp
      - click *printer-plotter installation*
      - click *remove printer-plotter*

1.Try kill -9 if kill does not work.

b) if the printer cannot be removed in XWIN-NMR, try in UNIX
   - type **/usr/lib/lpshut**
   - type **/usr/lib/lpadmin -xprintername** (printername is, for instance, hplj4l)
   - type **/usr/lib/lpsched**

c) now re-install the printer in XWIN-NMR
   - type cfpp
   - click *printer-plotter installation*
   - click *install new printer-plotter*

6. If the scheduler cannot be started with **/usr/lib/lpsched**, even after step 3, then reboot the computer; type **/etc/reboot**

7. Check if the RS-232 port is inaccessible
   a) connect the printer to another port
   b) switch the printer off and on again
   c) in XWIN-NMR:
      type cfpp
      click *printer-plotter installation*
      click *change output device of existing printer-plotter*

Part III

NETWORKS

network communication
ftp transfer
spectrometer network
internet
www

network communication

network commands

`host_a`: the computer on which you are logged in
`host_b`: a remote computer in the network

- **`telnet host_b`**
  -> log in on `host_b`, you will be asked for a login name

- **`rlogin host_b`**
  -> log in on `host_b` as current user

- **`rcp fila host_b:/u`**
  -> copy *fila* from `host_a` to `host_b` into directory /u

- **`rcp host_b:/usr/people/guest/fila /u`**
  -> copy *fila* from `host_b` to `host_a` into */u*

- **`rcp -r dira host_b:/u/data/guest/nmr`**
  -> copy the directory tree *dira* from *host_a* to *host_b*

- **`rsh host_b who`**
  -> run the command **`who`** on the remote host *host_b*

- **`cat fila | rsh host_b lp`**
  -> print *fila* on a printer connected to remote host `host_b`

Note that for **`rlogin`**, **`rcp`** and **`rsh`** the remote host must be entered in the file */etc/hosts.equiv* or your personal *.rhosts* file.

network communication

remote login and remote copy with FTP

Differences between **`ftp`** and **`rcp`**:

- **`ftp`** requires a login with password on the remote host
- **`ftp`** does not check */etc/hosts.equiv* or *.rhosts*
- **`ftp`** cannot directly transfer directory trees

examples

1. the file *fila* in */usr/people/demo* on `host_b` is copied to */usr/people/guest* on `host_a`:

   a) log in on host_a as user guest

   b) type **`ftp host_b`**

   ```
   Name: guest                    --> enter a user name
   Password:                      --> enter the password
   ftp> lcd /usr/people/guest --> change local directory (host_a)
   ftp> cd /usr/people/demo   --> change remote directory (host_b)
   ftp> bin                       --> switch to binary mode
   ftp> get fila                  --> get fila from host_b to host_a
   ftp> bye                       --> leave FTP
   ```

2. the file *filb* in */usr/people/guest* on `host_a` is copied to */tmp* on `host_b`:

   a) log in on host_a as user guest

   b) type **`ftp host_b`**

   ```
   Name: guest                    --> enter a user name
   Password:                      --> enter the password
   ftp> lcd /usr/people/guest --> change local directory (host_a)
   ftp> cd /tmp               --> change remote directory (host_b)
   ftp> bin                       --> switch to binary mode
   ftp> put filb          -       --> put filb from host_a to host_b
   ftp> bye                       --> leave FTP
   ```

commands in FTP

`pwd`	print remote current directory
`dir`, **`ls`**	list contents of remote current directory
`cd`	change directory on the remote host
`lcd`	change directory on the local host
`bin`	switch to binary mode
`get fila`	copy the file *fila* from the remote host
`put filb`	copy the file *filb* to the remote host
`prompt`	mget and mput copy all files without asking
`hash`	print a # for each buffer transferred
`mget a*`	copy all files a* from the remote host
`mput a*`	copy all files a* to the remote host
`reget`	continue an interrupted transfer of a file
`help`	show all FTP commands
`help cmd`	help for a specific command
`bye`	leave FTP

Important:

- executable files loose their x-bit during FTP transfer: leave FTP and use **`chmod a+x filename`** to set the x-bit
- binary files must be transferred in binary mode otherwise they will be corrupted. (ascii files can be transferred in binary and ascii mode)

copy directory trees with FTP

FTP cannot directly transfer directories. You can however copy a directory into a tar-file and transfer this tar-file with FTP.

Suppose the user guest:

- is already logged in on host_a
- wants to get the dataset */u/data/guest/nmr/fila* from host_b and copy it to */z/data/guest/nmr* on host_a

1. **`telnet host_b`**
   -> login on host_b, e.g. also as guest
2. **`cd /u/data/guest/nmr`**
   -> change directory on host_b

`3.tar cvf fila.tar fila`
   -> copy the dataset *fila* into the tar-file *fila.tar*

4. **`ftp host_a`**

Name: `guest`	--> enter a user name
Password:	--> enter the password of guest
ftp> `cd /z/data/guest/nmr`	--> go to the target directory
ftp> `bin`	--> switch to binary mode
ftp> `put fila.tar`	--> put the tar-file on host_a
ftp> `bye`	--> leave FTP

`5.rm fila.tar`
   -> remove the tar-file on host_b

6. **`exit`**
   -> go back to host_a
7. **`cd /z/data/guest/nmr`**
   -> change to target directory on host _a
8. **`tar xvf fila.tar`**
   -> unpack the tar-file on host_a

`9.rm fila.tar`
   -> remove the tar-file on host_a

World Wide Web

the internet information service

Bruker offers a large amount of information about hardware, software, applications, employees etc. on the WWW.

Homepage Bruker Germany: `http://www.bruker.de`

From this page you can:

- get a Bruker WWW account:
  -> click ***Register Now***, fill out the form, click ***Submit***

- check the list of Frequently Asked Questions:
  -> click ***NMR -> FAQ***

- check the list of known bugs or send a bug report:
  -> click ***NMR -> Known Bugs***

- read documentation directly from the web:
  -> click ***Downloads -> Documentation***

- download patches from the web:
  -> click ***Downloads -> Update&Patches***

the Bruker FTP server

The Bruker FTP server contains:

- patches for `XWIN-NMR` releases
- Bruker software packages e.g. `Aurelia`, `Xwinplot`
- general software packages e.g. `gzip`, `perl`, `emacs`
- the */incoming* directory to send data or files to Bruker

How do you access the FTP server?

- log in on a computer that is connected to the internet
- type **`ftp ftp.bruker.de`** (Germany)
  or **`ftp ftp.bruker.com`** (USA)
- log in as `anonymous` or `ftp`
- enter your own full E-mail address as password

The most important directory on *ftp.bruker.de* for NMR users is */pub/nmr*. An exact copy of this directory is available on *ftp.bruker.com* as */pub/nmr/mirror.bruker.de*.

Many files on the FTP server have names like: *xyz.tar.gz*. A file with a name like this:

- is a tar-file, which probably contains a software package
- has been compressed with the command **`gzip`**
- must be uncompressed with: **`gunzip xyz.tar.gz`**
- must then be unpacked with: **`tar xvf xyz.tar`**

If **`gunzip`** does not exist on your computer, then get the `gzip` package from the FTP server as described below.

examples

1. get the gzip software package for SGI

   a) **`ftp ftp.bruker.de`**

   Name: `ftp`
   Password: `->` enter your own full Email address
   ftp> `cd /pub/nmr/binaries.indy`
   ftp> `bin`
   ftp> `mget gzip*` (answer each question with `y`)
   ftp> `bye`

   b) install the `gzip` package according to the *readme* file.

2. get all patches for `XWIN-NMR 3.0`

   a) **`ftp ftp.bruker.de`**

   Name: `ftp`
   Password: `->` enter your own full Email address
   ftp> `cd /pub/nmr/xwinnmr/patches/xwinnmr3.0/sgi`
   ftp> `bin`
   ftp> `ls`
   ftp> `get xw30pX.sgi.tar.gz`
   (X is a number greater than 0, the so called patchlevel)
   ftp> `get xw30pX.sgi.readme.txt`
   ftp> `bye`

   b) install the patches according to the file xw30pX.sgi.readme.txt.

You can also get these files from the directory:
/pub/nmr/mirror.bruker.de
on the American FTP server. Usually, it is more efficient to use the server nearest to you.

How to send a data set to Bruker

directly from XWIN-NMR

The XWIN-NMR command smail provides a very easy way send data by Email:

1. start **xwinnmr**
2. go to the data set you want to send (e.g. with search)
3. type smail
4. enter the Email address in the field *Mail to*, e.g.:
   nmr-software-support@bruker.de
5. click on the field *Output data*, enter the data mode
6. optionally fill out the fields *message*, *subject* and *CC* [1]
7. click on *send*

Requirements:

1. you run XWIN-NMR 1.3 or newer [2]
2. Zmail (MediaMail) or Mutt is installed [3]
3. you want to send a 1D data set

If you run an older version of XWIN-NMR or want to send 2D data, pack your data into a tar-file and do one of the following:

- put the tar-file on the FTP server
- convert the tar-file to ascii and send it by Email.

This is described on the next page.

1.In the field CC you can enter further destination Email addresses.
2.In XWIN-NMR 1.3, ICONNMR must be installed. In XWIN-NMR 2.0 *smail* is independent of ICONNMR.
3.Zmail is included in IRIX <= 6.2 but not in IRIX >= 6.3, Mutt is available on the SGI web page.

from a UNIX shell

Suppose you want to send to Bruker the NMR dataset:

/u/data/guest/nmr/exa

Perform the following steps:

1. **`cd /u/data/guest/nmr`**
2. **`tar cvf exa.tar exa`**
   -> this creates the binary tar-file *exa.tar*
3. **`gzip exa.tar`** [1]
   -> this creates the compressed binary tar-file *exa.tar.gz*

There are different ways to send the file *exa.tar.gz* to Bruker, depending on your Internet/Email possibilities.

1. if you have direct Internet access:
   type **`ftp ftp.bruker.de`**
   Name: `ftp`
   Password: `->` enter your own full Email address
   ftp> `cd /incoming`
   ftp> `bin`
   ftp> `put exa.tar.gz`
   ftp> `bye`

2. if you have Email it depends on your Email program:
   a) if it supports binary attachments, e.g. `Zmail`[2]:
      -> send an Email and attach the binary file *exa.tar.gz*
   b) if it doe not support binary attachments: e.g. `elm`:
      - **`uuencode exa.tar.gz exa.tar.gz > exa.asc`**[3]
      - send an Email and include the ascii file *exa.asc*

1.If you do not have `gzip`, get it from the FTP server or use `compress` (this creates a file *exa.tar.Z*)
2.MediaMail is 's version of the graphical Mail interface Zmail
3.The second argument is the name of the binary file which is created when the ascii file is decoded with `uudecode exa.asc`. This can be the same as the name of the input file or any other name.

spectrometer internal network

a network with 2 hosts

All SGI workstations connected to a spectrometer are equipped with 2 ethernet interfaces and support an:

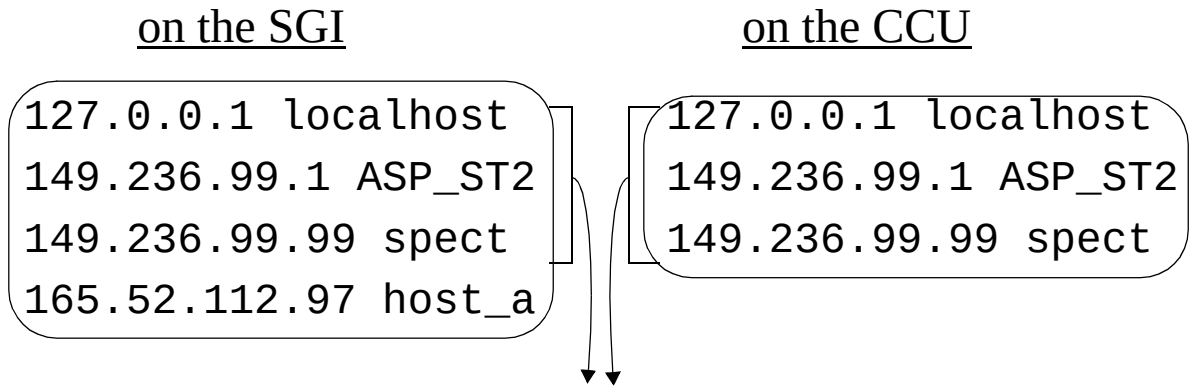
- external network: interface `ec0`
- internal network: interface `ec1`(O2) or `ec2` (indy)

If the SGI is connected to both the external and the internal network, it has 2 hostnames and 2 IP addresses:

- for the external laboratory network the SGI has an IP address corresponding to this network, e.g. 165.52.112.97 and can have any hostname, e.g. `host_a`.
- for the internal spectrometer network the SGI has a fixed IP address: 149.236.99.1 a fixed hostname `ASP_ST2`

The only other host in the internal network is the CCU which has the fixed IP address 149.236.99.99 and hostname spect.

The files */etc/hosts* on these 2 hosts will look like this:



NEVER change or delete these 3 lines

The hostname of the CCU is always spect: you can log in on the CCU by typing **`telnet spect`**

You can, however, define an alias name for the CCU:
edit the file */etc/hosts* on the SGI, append the alias e.g.:

```
149.236.99.99 spect dmx300
```

Now you can type **`telnet dmx300`** to log in on the CCU.

When you configure the spectrometer in XWIN-NMR with cf, you can now enter spect or dmx300 as instrument name.

Important: the alias name for the CCU must be different from the hostname of the SGI workstation or any other host in the external network!

If you have SGI-CCU communication problems, e.g. telnet spect does not work, do the following:

1. open a UNIX shell
2. type **`su - root`** to become superuser
3. type **`reviveccu`**
   -> follow the instructions

If **`reviveccu`** does not solve the problem re-install the Diskless package from the XWIN-NMR CD.

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