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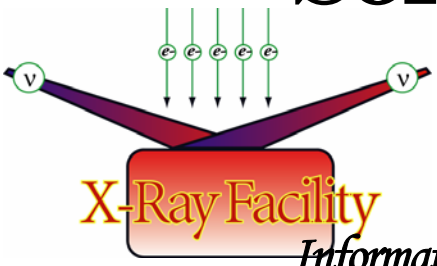
X-Ray Facility Upgrades-2001

XRF Hardware & Software Upgrades



Information regarding X-Ray Facility hardware and software upgrades for year 2001

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XRF Upgrades-2001

Information regarding X-Ray Facility hardware and software upgrades for the year 2001

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Introduction

During the last few months, X-Ray Facility (XRF) has undergone several hardware and software upgrades. This note is intended for updating all the XRF users about the changes and how it will affect the data collection. Please save this Note for future reference. A copy of this Note will be posted in XRF webpage shortly after receiving suggestions and corrections from the users.

Hardware

thr.sb.fsu.edu (128.186.17.77; Silicon Graphics, Irix 5.3)

XRF, effective May 14, 2001, has retired `thr.sb.fsu.edu` (128.186.17.77) the Silicon Graphics Iris Indigo (running under Irix 5.3 operating system). `Thr.sb.fsu.edu` was the computer that controlled the data collection and processing for the R-Axis IIc image plate (IP) detector. The reasons for retiring `thr` are primarily its age (about 8 years) and its obsolete operating system (SGI is no longer supporting Irix 5.3). Secondly, `thr` was the only Iris Indigo in IMB and therefore we won't be able to swap any hardware with another machine in case of failure. Thirdly, Rigaku/MSC, the manufacturer of R-Axis IIc detector, is no longer supporting the operating system or the control software.

Raxis home (`~raxis`) has been restored from `thr.sb.fsu.edu` and it is now available at `/thr/c/raxis` (originally it was `/thr/b/people/raxis`) as an external disk on `ser.sb.fsu.edu`. This will allow, for example, access to Denzo, Scalepack, Mosflm template files, older versions of HKL executables, XRF webpages, etc. External disks on `thr.sb.fsu.edu`: `/thr/c/raxis, /thr/d/raxis, /thr/e/raxis, /thr/f/raxis` with all their data prior to retiring `thr.sb.fsu.edu` (May 14, 2001) are still available except for the fact that they are mounted on other machines. `/thr/c/raxis` and `/thr/d/raxis` are on `ser.sb.fsu.edu` and /`thr/e/raxis` and `/thr/f/raxis` are in `pro.sb.fsu.edu`.

spruce.sb.fsu.edu (128.186.17.60; RedHat Linux 7.0)

We have added an internal DDS-4 tape drive to `spruce.sb.fsu.edu,` the Linux machine (650 MHz Pentium III, 256 Mb memory, 21" monitor, two 34 GB hard disks) that controls marccd data collection and processing. DDS-4 drives can read and write to DDS, DDS2, DDS3 and DDS4 media (tapes). However, it is best to use DDS4 media, which has a native/compressed capacity of 20/40 gigabytes depending upon how much the data will compress (typical IP plate data will compress 40%). All XRF users will be able to read from the tape drive and currently users are NOT allowed to write to the tape. The tape drive status can be checked using the command `mt` and data archived using `tar` command. Typical usage may look like the following:

`mt –f /dev/st0 status` | check the status of the tape drive /dev/st0

`tar tvf /dev/st0` | look at the tape contents

`tar cvf /dev/st0 my_dir` | write contents of `my_dir` to tape

`tar xvRf /dev/st0 parent_dir/my_dir` | extracting `my_dir`

`tar -cvf /dev/st0 my_dir | & tee dds4.listing &` | writing data to a tape at the same time writing the names of those files into another file

Please check with `mt` and `tar` man pages or with Soma, Paul or Mike for further usage. DDS media have a distinctive logo printed on the front cover and on tapes themselves. Shown below are the various DDS media logos:

raccoon.sb.fsu.edu (128.186.17.156; Dell, RedHat Linux 7.0)

We have added a 933 MHz Pentium III Linux machine running Red Hat 7.0 with 21" monitor, 256 MB memory and 40-gigabyte disk space solely for processing of IP and CCD data. `Raccoon.sb.fsu.edu` (located in IMB 406 and next to G3 Mac) has an external DDS3 tape drive, internal CD-ROM drive, and an internal CD-RW drive. `Raccoon` is running `sshd` so all logins and transfers can be done using `secure ssh2 protocol`.

Hard disks

The hard disks on `raccoon` have several partitions and shown below are the important ones:

```
Filesystem           1k-blocks      Used Available Use% Mounted on

/dev/hda9               256667      1008    242407   1% /home

/dev/hda5              3028080    215884   2658376   8% /usr/local

/dev/hda10             8815372        20   8367544   1% /d5

/dev/sda1             17639220   7234608   9508592  44% /d3

/dev/sda2             17639248   7208136   9535088  44% /d4
```

All regular XRF users will have their home directories created in `/home`. Please check with Soma (4-6448) for activating your account with a password and change the password of your choice. All user data should be copied using `sftp` **from** `spruce.sb.fsu.edu` or `anaconda.sb.fsu.edu` **to** `raccoon.sb.fsu.edu` and stored in `/d3, /d4, or /d5`. `Raccoon.sb.fsu.edu` has license to process x-ray data using HKL 1.96.6, Mosflm 6.11, and CCP4. Shortly D*Trek (demo), DPS will be installed in `/usr/local/xray` directory. Once data are transferred to `raccoon`, the user will have the full control and responsibility over their data. The next sections describe how to archive and access user data while on `raccoon`.

Reading from CD-ROM drive/CD-RW Drive:

CD-ROM drive and CD-RW drives can be accessed for data processing and copying by mounting the drives for usage and unmounting after usage. First, place a CD in CD-ROM drive or a CD-R or a CD-RW in CD-RW drive. A typical session might look like the following:

`xray@raccoon[9:28am]~>df -k –l` | check the status local disks

```
/dev/hda10              8815372        20   8367544   1% /d5
/dev/sda1              17639220   7234608   9508592  44% /d3
/dev/sda2              17639248   7208136   9535088  44% /d4
xray@raccoon[9:28am]~>mount   /mnt/cdrom    |mount CD-ROM
xray@raccoon[9:28am]~>df -k –l        |check local disks again
/dev/hda10              8815372        20   8367544   1% /d5
/dev/sda1              17639220   7234608   9508592  44% /d3
/dev/sda2              17639248   7208136   9535088  44% /d4
/dev/hdc                 633432    633432         0 100% /mnt/cdrom
xray@raccoon[9:28am]~>ls -lt  /mnt/cdrom    |check contents of CD-ROM
-r-xr-xr-x    1 root     root     18006000 Oct 26  1999 lysodata002.osc
-r-xr-xr-x    1 root     root     18006000 Oct 26  1999 lysodata001.osc
-r-xr-xr-x    1 root     root      9006000 Oct 26  1999 lysodata_screen002.osc
-r-xr-xr-x    1 root     root      9006000 Oct 26  1999 lysodata_screen001.osc
xray@raccoon[9:28am]~>umount  /mnt/cdrom    |unmount (umount) CD-ROM
```

Repeat the same procedure for CD-RW drive replacing `/mnt/cdrom` by `/mnt/cdrom1`. Remember, however, that CD-R and CD-RW should have data in them for mounting.

Writing to CD-RW Drive:

`Raccoon.sb.fsu.edu` has a CD-RW drive that will allow archiving of your data into a CD-R or CD-RW medium. However, before archiving your data you need to create an ISO 9660 image of your data first and then write that image to the CD-R or CD-RW. We will first create an ISO 9660 image of the directory (for safety do not exceed 600 MB of total space, however, see Splitting Large Directory section below) you want to archive. Then using the command `cdrecord,` we will archive (write) the image to the CD-R or CD-RW. A typical session might look like the following:

```
xray@raccoon[4:49pm]~>cd /d3   |Go to parent directory
xray@raccoon[4:49pm]/d3 >du -sk Images/      |Check size of desired directory for archiving
509656  Images
xray@raccoon[4:49pm]/d3 >mkisofs -l -R -v -o LysImages.raw Images/
     |Make an ISO 9660 filesystem image with RockRidge protocol
```

[-l= long file names; -R= Rock Ridge protocol, -v=verbose, -o=output image name]

```
mkisofs 1.13 (i686-pc-linux-gnu)      |program starts
Scanning Images
```

```
  1.97% done, estimate finish Thu May 31 16:49:36 2001

. . .

..98.26% done, estimate finish Thu May 31 16:50:20 2001

Total rockridge attributes bytes: 6529

. . .

254421 extents written (496 Mb)
```
|Creating an image is complete

```
xray@raccoon[4:55pm]/d3 >ls -lt LysImages.raw
```
|Confirm the presence of the image

```
-rw-r--r--    1 xray     users    521054208 May 31 16:50
LysImages.raw

xray@raccoon[4:55pm]/d3 >cdrecord -v -dummy speed=4 dev=1,0,0
LysImages.img
```
|Check the process with a dummy write; skip this step after few successful write sessions

```
xray@raccoon[4:55pm]/d3 >cdrecord -v speed=4 dev=1,0,0 LysImages.img
```
|Make an archive in CD-R. The command to actually write the CD.

[-v=verbose; speed=4=4x write speed; dev=1,0,0=SCSI number, id number, lun number]

Now try to check whether the archived data is accessible.

```
xray@raccoon[9:28am]~>mount   /mnt/cdrom1

xray@raccoon[9:28am]~>df -k -l

/dev/hda10             8815372        20   8367544   1% /d5

/dev/sda1             17639220   7234608   9508592  44% /d3

/dev/sda2             17639248   7208136   9535088  44% /d4

/dev/scd0               581650    581650         0 100% /mnt/cdrom1

xray@raccoon[9:28am]~>ls -lt         /mnt/cdrom1

-r-xr-xr-x    1 root     root     18006000 Oct 26  1999 mydata002.osc

-r-xr-xr-x    1 root     root     18006000 Oct 26  1999 mydata001.osc

xray@raccoon[9:28am]~>umount  /mnt/cdrom1
```

Take the CD-RW or CD-R from drive, carefully label it and store.

Splitting Large Directory (CD-RW)

One may encounter large data directories that occupy more than 600 MB of space. How does one handle this problem? One-way is to split the directory into ~600 MB of space and write separate CDs. The following section shows how this can be achieved.

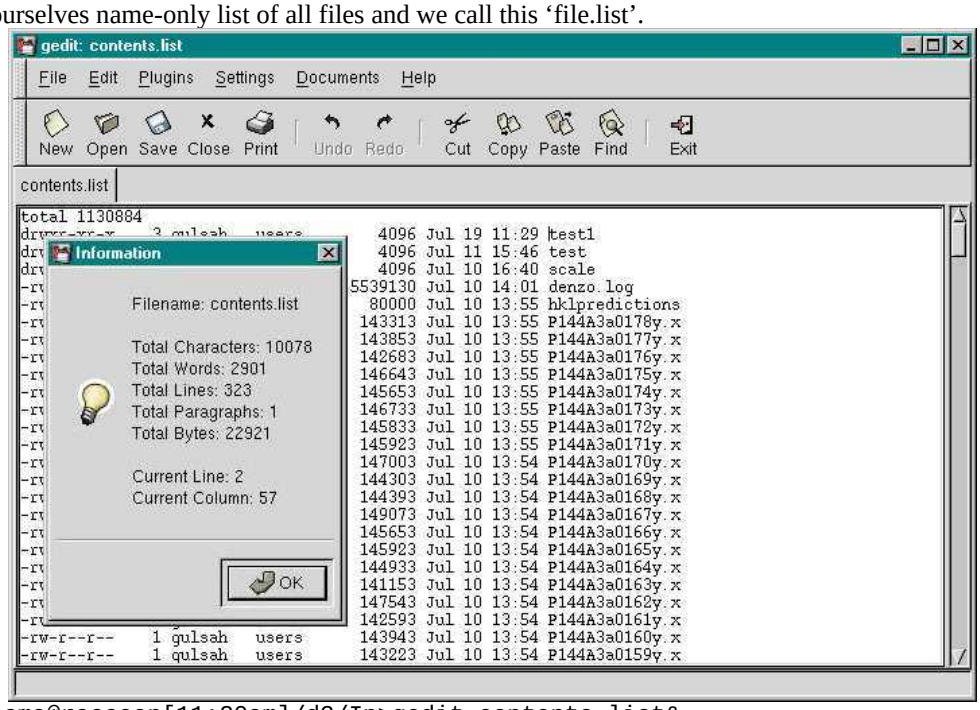
```
soma@raccoon[11:20am]/d3/Ip/>du -ks DKGRA4
```

```
1192408 DKGRA4
```

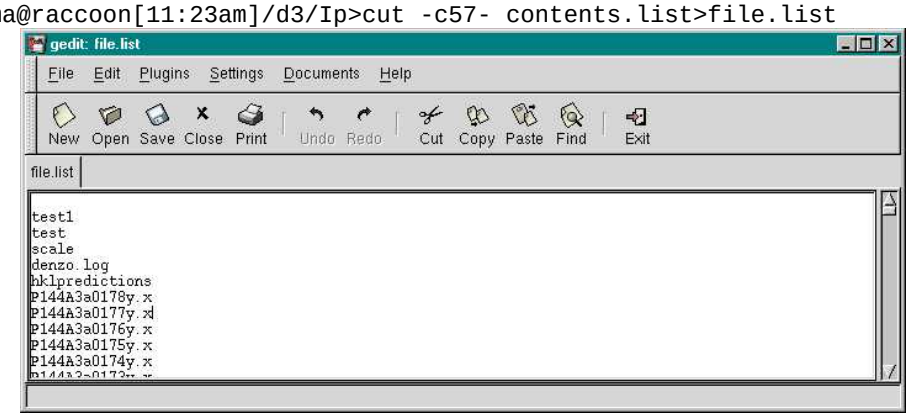
This is obviously more than the capacity of one CD-R media (~650 MB). So move to the directory and first get the listing of all files in the directory and redirect the output to a new file, here it is called, ‘contents.list’

```
soma@raccoon[11:20am]/d3/Ip/>cd DKGRA4
soma@raccoon[11:20am]/d3/Ip/DKGRA4>/bin/ls -lt >contents.list
```

Upon examination of the 'contents.list', one realizes the actual names of the files start at column 57 (use File Info under Edit menu) and higher, so using the 'cut' command we make ourselves name-only list of all files and we call this ‘file.list’.




```
soma@raccoon[11:20am]/d3/Ip>gedit contents.list&
soma@raccoon[11:23am]/d3/Ip>cut -c57- contents.list>file.list
```



Now cut this file.list, assuming all files occupy equal amount of space, into two halves renaming top half as ‘filetop.list’ and bottom half as ‘filebot.list’. Save both the files (‘filetop.list’ and ‘filebot.list’)

```
soma@raccoon[11:23am]/d3/Ip>gedit file.list&
-rw-r--r--    1 soma     users        5004 Aug 10 10:39 file.list
-rw-r--r--    1 soma     users       22921 Aug 10 10:38 contents.list
-rw-r--r--    1 soma     users        2502 Aug 10 10:37 filebot.list
```

```
-rw-r--r--    1 soma     users        2502 Aug 10 10:37 filetop.list
```

Now use the 'mkisofs' command option '–exclude-list' and specify the files to be excluded, here say, filetop.list and this will create an image of only bottom half of the directory DKGRA4, satisfying our objective of keeping the image less than 650 MB.

```
soma@raccoon[11:24am]/d3/Ip>mkisofs -l -R -v -exclude-list
filetop.list -o Dkgra4a.raw DKGRA4/
```

Now make another image, however, this time replace the filebot.list as the excluded file.

```
soma@raccoon[11:24am]/d3/Ip>mkisofs -l -R -v -exclude-list
filebot.list -o Dkgra4a.raw DKGRA4/
```

With the two images, you can create two separate CDs one after another.

Tape drive

Raccoon has an external DDS-3 tape drive. DDS-3 drives can read and write to DDS, DDS2, and DDS3 tapes (and not DDS-4 tapes). However, it is best to use DDS3 media, which has a native/compressed capacity of 12/24 gigabytes depending upon how much the data will compress (typical IP plate data will compress 40%). As discussed earlier for DDS-4 tape drive, command `mt` and `tar` can be used to check the status of the drive and to archive data to the tape.

`mt –f /dev/st0 status` |check the status of the tape drive /dev/st0

`tar -cvf /dev/st0 my_dir/ | & tee dds3.listing &` |writing data to a tape at the same time writing the names of those files into another file

anaconda.sb.fsu.edu (128.186.17.193; Dell, Windows NT 4.0)

R-Axis IIc IP detector is now being controlled by this Dell dual Pentium III 733 MHz Windows NT 4.0 machine with 21" monitor, 768 MB memory, 40 GB of hard disk space. We have installed new software called `CrystalClear` that will control the data collection and processing from R-Axis IIc IP detector. There is a separate x-ray generator control program called `XGControl`, which can be used to start up, control, and shutdown the generator from `anaconda.sb.fsu.edu`. `CrystalClear` needs special license and we have three (3) Crypto Dongle boxes that need to be installed in a parallel port of a Windows NT machine in order for the program to function. One of the Crypto Dongles is installed in `anaconda` and other two can be attached to other machines if needed. Complete functions and capabilities of `CrystalClear` and `XGControl` are too large to cover in this Note. Please consult the on line manual (see below).

Data collection can be initiated by a user after establishing a user and group account in `anaconda.sb.fsu.edu`. We have established individual groups for all PIs who routinely use the XRF, new users or new groups can be added to the list as needed. Please contact Soma for new username and password. StarNet Communications' X terminal application X-Win 32 version 5.1 for NT 4.0 has been installed in `anaconda`. X Win 32 allows Windows NT users to connect to Linux/Unix servers on a local network. SSH.com's SSH Secure Shell version 2.40 is also installed in `anaconda` allowing sftp and ssh login from `anaconda` to `raccoon, spruce, pro, ser, tyr,` and `glu`.

`Anaconda` has a CD-ROM drive and will soon have an internal DDS-4 tape drive that will allow the archiving of data collected in this Windows NT machine.

Software

HKL Suite (XdisplayF, Denzo, Scalepack)

X-Ray Facility has one site license for version 1.96.9 (updated from 1.96.6), one site license for version 1.9.1 and one site license for 1.6.0 (old version). Each version can be used by ten (10) different people or in ten (10) different computers simultaneously. Version 1.96.9 can be run on virtually all platforms, Version 1.96.6 can only be run on Linux machines, Digital Alphas, and SGIs running Irix 6.5 (see Table 1). Version 1.9.1 can be run only on SGIs and is adequate to process image plate data as well as marCCD data sets.

The executable of various versions are located under appropriate directories in several machines (see below) and you are NOT required to copy any of the executable to your home directory to run these programs. Instead, create an alias that points to one of the executables. Remember also to copy a file named '`cr_info`' into your home directory or to the directory where you will process the data, with out this file the program will not run.

```
Alpha version: /tyr/e/users/soma/HKL.1.96.9/
Alpha version: /tyr/e/users/soma/HKL.1.96.6/
Linux version: spruce:/usr/local/xray/HKL.1.96.9/
Linux version: spruce:/usr/local/xray/HKL.1.96.6/
Linux version: rtgpc3:/usr/local/xray/HKL.1.96.9/
Linux version: rtgpc3:/usr/local/xray/HKL.1.96.6/
Linux version: raccoon:/usr/local/xray/HKL.1.96.9/
Linux version: raccoon:/usr/local/xray/HKL.1.96.6/
SGI version :/thr/c/raxis/HKL.1.96.9
SGI version :/thr/c/raxis/Denzo.1.9.1/
SGI version: /thr/c/raxis/Denzo.1.6.0/
SGI version (Irix 6.5): /glu/c/soma/HKL.1.96.6/
```

License

HKL executables will only run on computers that have license to run the program since they are tied to specific hardware found on that computer. The following table shows the list of computers that have licenses to run various versions of HKL suite.

No	Computer (IP address)	HKL.1.96.9	HKL.1.96.6	HKL.1.9.1	HKL.1.6.0
1	arg (128.186.17.65)	Yes	Yes	No	No
2	lys (128.186.17.63)	Yes	Yes	No	No
3	leu (128.186.17.61)	Yes	Yes	No	No
4	tyr (128.186.17.64)	Yes	Yes	No	No
5	rtgpc3 (128.186.17.36)	Yes	Yes	No	No
6	raccoon (128.186.17.60)	Yes	Yes	No	No
7	spruce (128.186.17.156)	Yes	Yes	No	No
8	ser (128.186.17.76)	Yes	No	Yes	Yes
9	his (128.186.17.83)	Yes	No	Yes	Yes
10	pro (128.186.17.84)	Yes	No	Yes	Yes

11	glu ((128.186.17.96)	Yes	Yes	Yes	No
12	gly (128.186.17.87)	Yes	Yes	Yes	No
13	newiris (128.186.17.73)	Yes	Yes	No	No
14	ala (128.186.17.85)	Yes	No	Yes	Yes

Table 1. List of computers with HKL license. ***Orange****: Alphas;* ***Green****: Linux machines;* ***Blue****: common SGIs;* ***Yellow****: Lab SGIs.*

Alias and modifier

Using an alias a user locally runs a program that is physically present in a remote machine without copying the executable. If your default shell is `csh` or `tcsh` then store the following lines in your `.cshrc` or `.tcshrc` file:

alias dzo '/thr/c/raxis/HKL.1.9.1/denzo'

alias xdR '/thr/c/raxis/HKL.1.9.1/xdisp raxis'

alias spo '/thr/c/raxis/HKL.1.9.1/scalepack'

If your default shell is bash then the syntax should look like the following in your .bashrc file:

alias dz='/home/soma/HKL.1.96.9/denzo'

All new versions of HKL require only one display program and the executable for that is '`xdisp`'. In order for the user to display, images collected under different formats, combine `xdisp` with an appropriate modifier. The modifiers and syntax for relevant formats are given below:

`xdisp ␣ raxis ␣ myxtal001.osc` | Regular r-axis data

`xdisp ␣ raxis2n ␣ myxtal001.osc` | New r-axis data (note 2n)

`xdisp ␣ ccd ␣ unsupported-m165 ␣ xtal01.001` | MarCCD165 format

`xdisp ␣ ccd ␣ adsc ␣ unsupported-q4 ␣ xtal01.001` | Quantum 4 format

␣ : indicates a required empty space.

The same modifiers are required while processing the data using denzo with the keyword 'format'. Integrated intensity data files, otherwise known as .x files, can be superimposed on the image data to visually inspect the fit between the observed and calculated. For example, to superimpose the .x file number 15 (myxtal015.x) on data number 15 (myxtal015.osc) follow the syntax:

`xdisp ␣ raxis ␣ myxtal###.osc ␣ 15 ␣ myxtal###.x` | Regular r-axis data

`xdisp ␣ raxis2n ␣ myxtal###.osc ␣ 15 myxtal###.x` | New r-axis data

Crystal Clear & XG Control

`CrystalClear` and `XG Control` are two new Windows NT based programs installed in `anaconda` to collect and process the IP data from R-Axis IIc and to control the generator

respectively. More information about these programs is available on-line manual in xray web page:

http://www.sb.fsu.edu/~xray/Manuals/CCManual130.pdf

http://www.sb.fsu.edu/~xray/Manuals/XGControl.pdf

CCP4

Linux versions of CCP4 version 4.1.1 as well as ccp4-i have been installed in `raccoon`: `/usr/local/xray/CCP4.` All users should include the following line in their `.login` file in order for the environmental variables to be set properly:

```
source /usr/local/xray/CCP4/ccp4-4.1.1/include/ccp4.setup
```

Linux versions of CCP4 version 4.1.1 as well as ccp4-i have also been installed in `spruce`: `/home/marccd/CCP4.` All users should include the following line in their `.login` file in order for the environmental variables to be set properly:

```
source /home/marccd/CCP4/ccp4-4.1.1/include/ccp4.setup
```

Mosflm

Current version of Mosflm (version 6.10a) distributed as a part of CCP4 suite has been installed in `raccoon:/usr/local/xray/CCP4/ccp4-4.1.1/bin/mosflm`. Newer independent version of Mosflm 6.11 has been installed in both raccoon and spruce under the following directories:

`raccoon:/usr/local/xray/Mosflm.6.11`

`spruce:/home/marccd/Mosflm.6.11`

Templates

Several template files needed for processing images with Denzo, Scalepack, and Mosflm are located in the following directory:

`raccoon: /usr/local/xray/Templates`

`spruce: /usr/local/xray/Templates`

`rtgpc3: /usr/local/xray/Templates`

Copy the relevant files like, `auto.dat, auto_mar.dat, auto_chess.dat, scale_simple.com, scale_nomerge.com`, etc., whenever you need them and modify according to your experimental conditions.

Conclusion

With several hardware and software upgrades to the facility there is likely to be some inconvenience and glitches. However, with the improved computing power, number of machines in different platforms as well as installation of several software packages should help the XRF users tremendously. With these additions, the user is going to have more control over data collection, processing, and archiving and therefore more responsibility toward their data. Please send your suggestions and comments to Soma.