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X-Ray Facility Upgrades-2002

XRF Hardware & Software Modifications

*Changes to X-Ray Facility Software &
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Introduction

During October and November 2001, X-Ray Facility (XRF) has moved from its original location to a temporary location in the Dittmer Laboratory of Chemistry (DLC). Then during January 2002 entire IMB including several computers have been moved to Developmental Research School (DRS). These moves have resulted in several changes to the XRF hardware and software at both DLC and DRS. This note is intended to inform the XRF users about all those changes and give suggestions to help with the modifications. 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. Please refer to 2001_XRF_Upgrades for earlier upgrades since this Note covers only modifications related to the move to DLC and DRS.

New Location of XRF in Dittmer Laboratory of Chemistry (DLC229 and DLC239)

The new location of the XRF is shown schematically below.

spruce.chem.fsu.edu (128.186.12.150)(RedHat Linux 7.0)

spruce.sb.fsu.edu has been renamed as spruce.chem.fsu.edu with a new IP address
128.186.12.150. The machine is the same as the original except for the new domain and IP
address. In addition, it is now physically located in DLC 229 and behind a firewall. This
means that the users can access this machine only using secure protocols (e.g., ssh, sftp).

raccoon.chem.fsu.edu (128.186.12.154)(Dell, RHat Linux 7.0)

raccoon.sb.fsu.edu has been renamed as raccoon.chem.fsu.edu with a new IP address
128.186.12.154. Similar to spruce.chem.fsu.edu it is the same machine original machine with
a new domain and IP address and is now physically sitting in DLC 229 and behind a firewall.
Secure protocols are only allowed. All original usernames, home directories and passwords
are retained. Contact Soma (4-6448) if you have questions.

Tapedrive
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%). 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

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

anaconda.chem.fsu.edu (128.186.12.151)(Dell, Win NT 4.0)

anaconda.sb.fsu.edu has been renamed as anaconda.chem.fsu.edu with a new domain and IP
address 128.186.12.151. This machine is behind a firewall and located in DLC239.

`Anaconda` has a CD-ROM drive and has an internal DDS-4 tape drive that will allow the
archiving of data collected in this Windows NT machine using Windows NT back-up protocol
(incompatible with UNIX tar).

Software

HKL Suite 1.97.2 (XdisplayF, Denzo, Scalepack)

Due to the relocation of X-Ray Facility to DLC and the IMB computers to Developmental
Research School (DRS), we obtained two different "new" cr_info files in order to run HKL
suite programs in both these locations. This means that every body has to move their "old"
cr_info file and get the "new" cr_info in order to run the suite. Each version can be used by
ten (10) different people or in ten (10) different computers simultaneously. Versions 1.96.9
and 1.97.2 can be run on virtually all platforms, Linux machines, Compaq Alphas, and SGIs
running Irix 6.5 (see Table 1).

The executables 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.1.97.2/ (New)
Alpha version: /tyr/e/users/soma/HKL.1.96.9/
Alpha version: /tyr/e/users/soma/HKL.1.96.6/
Linux version: rtgpc3:/usr/local/xray/HKL.1.97.2/ (New)
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.1.97.2/ (New)
Linux version: raccoon:/usr/local/xray/HKL.1.96.9/
Linux version: raccoon:/usr/local/xray/HKL.1.96.6/
SGI version: /imb/users/d1/soma/HKL.1.97.2/ (New)
SGI version: /imb/users/d1/soma/HKL.1.96.9/
SGI version (Irix 6.5): /glu/c/soma/HKL.1.97.2/ (New)
SGI version (Irix 6.5): /glu/c/soma/HKL.1.96.9/
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.1.97.2	HKL.1.96.9	HKL.1.96.6	HKL.1.9.1
1	arg (128.186.23.79)	Yes	Yes	Yes	No
2	lys (128.186.23.77)	Yes	Yes	Yes	No
3	leu (128.186.23.76)	Yes	Yes	Yes	No
4	tyr (128.186.23.78)	Yes	Yes	Yes	No
5	rtgpc3 (128.186.23.123)	Yes	Yes	Yes	No
6	raccoon (128.186.12.154)	Yes	Yes	Yes	No
7	ser (128.186.23.120)	Yes	Yes	No	Yes
8	his (128.186.23.122)	Yes	Yes	No	Yes
9	pro (128.186.23.121)	Yes	Yes	No	Yes
10	glu ((128.186.23.112)	Yes	Yes	Yes	Yes
11	newiris (128.186.23.113)	Not Yet	Yes	Yes	No

*Table 1. List of computers with HKL licenses. **Orange**: Alphas; **Green**: Linux machines; **Blue**: common SGIs; **Yellow**: Lab SGIs. All machines now have new IP numbers (Dec. 2001)*

Alias and modifier

Using an alias users locally run 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 dz '/usr/local/xray/HKL.1.97.2/denzo' (or equivalent)

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

alias dz='/imb/users/d1/soma/HKL.1.97.2/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` ♭ `raxis` ♭ `210` ♭ `myxtal001.osc` |Small r-axis format

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

`xdisp` ♭ `raxis2n` ♭ `210` ♭ `myxtal001.osc` |New small r-axis format (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

`CrystalClear` is the new Windows NT based programs installed in `anaconda` to collect and process the IP data from R-Axis IIc and to control the generator. More information about this program is available on-line manual in xray web page:

http://www.sb.fsu.edu/~raxis/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
```

```
tyr: /tyr/e/users/soma/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](#).