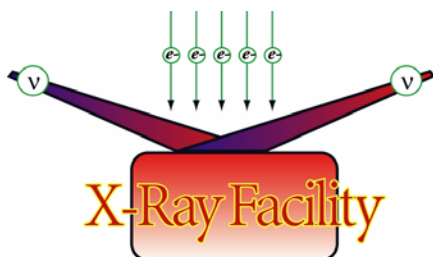


IMB X-Ray Crystallography Facility
410-413 Kasha Laboratory
Florida State University
Tallahassee, FL 32306-4380, USA
Telephone: (850) 645-1333 (Lab) | (850) 644-6448 (Off)
E-mail: soma@sb.fsu.edu
Web: <http://www.sb.fsu.edu/~xray> | <http://www.sb.fsu.edu/~soma>

XRF Upgrades-2003-2004

XRF Hardware & Software Upgrades



*Recent Upgrades to X-Ray Crystallography
Facility Hardware & Software*

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© 2000-2004 Thayumanasamy Somasundaram
414 Kasha Laboratory, Institute of Molecular Biophysics
Florida State University,
Tallahassee, FL 32306-4380
E-mail: soma@sb.fsu.edu • URL: <http://www.sb.fsu.edu/~soma>
URL: <http://www.sb.fsu.edu/~xray>

Phone 850.644.6448 • Fax 850.644.7244
May 10, 2004

XRF Upgrades 2003 - '04

Upgrades to X-Ray Facility Hardware & Software

Introduction

During 2003-04 [X-Ray Crystallography Facility](#) has upgraded and added several pieces of hardware and software. This note is intended to inform the XRF users about all those modifications. Please save this Note for future reference. A copy of this Note will be posted in XRF webpage shortly after receiving suggestions from the users.

Location

XRF Location in Kasha Laboratory (KLB 410-413)

X-ray crystallography facility is now located in the East side of fourth floor of the newly renovated Kasha Laboratory in Institute of Molecular Biophysics (see [Figure 1](#)). It occupies approximately 1200 ft² distributed among KLB 410 (72 ft²), KLB410A (164 ft²), KLB411 (167 ft²), KLB412 (274 ft²), & KLB413 (510 ft²). The Facility has a new telephone number: (850) 645-1333. The picture below schematically shows the XRF layout.

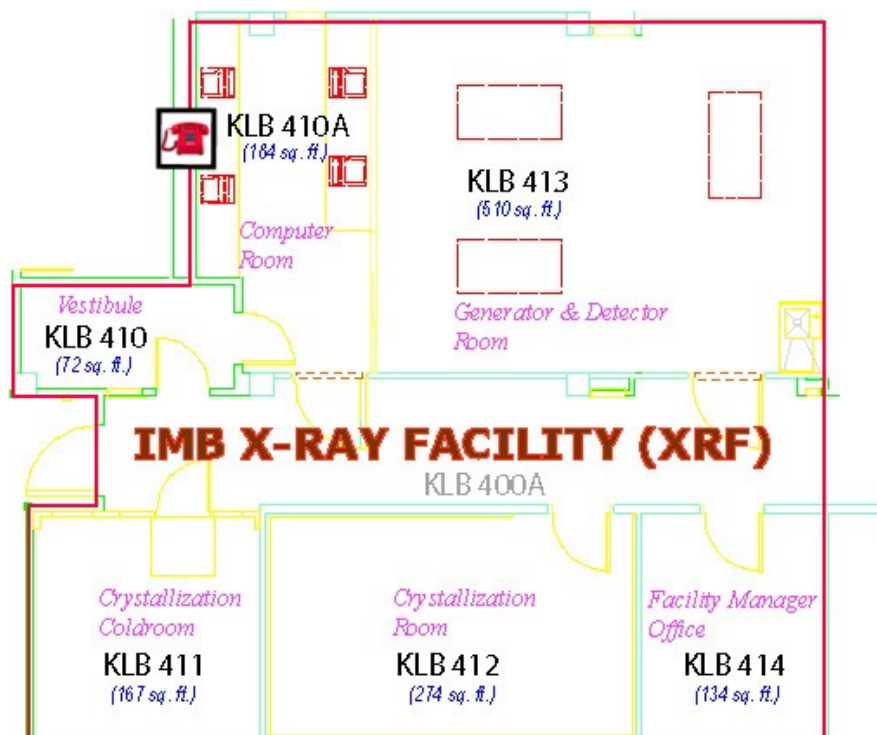


Figure 1 Layout of X-Ray Crystallography Facility

Computers & Computer Accessories

Computer Name, IP Address, & Location

All XRF computers have a new domain-name, IP address and location (see [Table 1](#)). We have added a dual bootable laptop for synchrotron data processing and a desktop for capturing and storing digital images of the crystals. The following table shows the current details of the computers that are available to the Facility users. **Note:** The Windows operating system computers are under two different domains and are indicated in the parenthesis (\\DOMAIN).



Figure 2 Data Processing Computer Raccoon.sb.fsu.edu (KLB 410A)

Name	IP Address	Location	Operating System	Information
Anaconda.sb.fsu.edu (\\XRAY)	128.186.103.102	KLB 410A	Win NT 4.0	R-Axis Iic Controller
Spruce.sb.fsu.edu	128.186.103.109	KLB 410A	RH Linux 8.0 (2.4.18-14 kernel)	MarCCD Controller
Neptune.sb.fsu.edu	128.186.103.106	KLB 410A	RH Linux 7.3 (2.4.20-20 kernel)	Data Processing & Archiving
Raccoon.sb.fsu.edu	128.186.103.108	KLB 410A	RH Linux 7.1 (2.4.20-20 kernel)	Data Processing & Archiving
Tampa.sb.fsu.edu (\\MSHOME)	128.186.103.110	KLB 414	RH Linux 7.3 & Win XP	Data processing Laptop
Phe.sb.fsu.edu (\\IMB2)	128.186.103.107	KLB 412	Win 2000	Digital Crystal Documentation

Table 1 Details of X-Ray Crystallography Facility Computers

XRF offers several options for archiving the user's data, ranging from tapes, CDs, and DVDs both under Windows and Linux environments and are shown in [Table 2](#) below:

Manufacturer & Model	Computer	Operating System	Media	Capacity (native compressed)
Seagate STD624000N	raccoon.sb.fsu.edu (128.186.103.108)	Linux	DDS-3 tape	12 GB 24 GB
Seagate STD1401LW	spruce.sb.fsu.edu (128.186.103.109)	Linux	DDS-4 tape	20 GB 40 GB
Seagate STD1401LW	anaconda.sb.fsu.edu (128.186.103.102)	Windows NT 4.0	DDS-4 tape	20 GB 40 GB
HP 9500 CD-Writer Plus	raccoon.sb.fsu.edu (128.186.103.108)	Linux	CD-R & CD-RW	~ 650-700 MB
Pioneer DVR-A04	neptune.sb.fsu.edu (128.186.103.106)	Linux	DVD-R & DVD-RW	~4.5 – 4.7 GB
Pioneer DVR-A04	anaconda.sb.fsu.edu (128.186.103.102)	Windows NT 4.0	DVD-R & DVD-RW	~4.5 – 4.7 GB

Table 2 Available options for data archiving at IMB XRF

The data collected at the Facility is currently archived in [DDS-3](#) and [DDS-4](#) tapes. Earlier archives were stored in one of the following formats: 4mm DDS tapes, 8mm Exabyte tapes (mostly 8500 or 8500c), ISO 1990 CD-R, and 4mm DDS-3 tapes. In addition to the drives mentioned in [Table 2](#), the facility has access to DLT, ZIP-100, ZIP-250 drives. Due to random-access capability, media reliability, prolonged shelf life, and wide availability, the XRF is encouraging the users to select DVD-R media instead of tapes for future data storage and transport, even though the Facility will continue to support tape drives for several more years.



Figure 3 Maxtor FireWire External Harddrive

[Maxtor](#) Personal Storage [DV3000](#), an 80 GB FireWire (aka, IEEE 1394 & I-link) drive is added recently for collecting data at synchrotrons and quickly transporting the whole data set back home ([Figure 3](#)). The hot-swappable FireWire drive will serve as a fall back option in the event of corrupted or unreadable archived data.

Sony USB + FireWire DVD-Writer (DVD \pm R/RW)



Figure 4 Sony Dual Interface Dual Media DVD Writer

For archiving (backing-up) data at home and retrieving pre-archived data from synchrotrons we have added a new multi-format (DVD \pm R/RW) dual-interface (USB 2.0 & FireWire IEEE1394) external Sony DVD DRX-510UL Writer/Reader ([Figure 4](#)). This drive is capable of reading and writing all the following media:

DVD+R, DVD+RW, DVD-R, DVD-RW, CD-R, and CD-RW (writing)

DVD+R, DVD+RW, DVD-ROM, DVD-R, DVD-RW, CD-ROM, CD-R, and CD-RW (reading)

For compatibility reasons we continue to recommend the use of General-purpose (as opposed to Authoring) 4.7 GB DVD-R and DVD-RW media from Pioneer Electronics for all archiving purposes both at home and while at synchrotrons. More information is available under [Sony DVD Writer](#).

Microscope & Microscope Accessories

Leica S8 APO Microscope & Moticam Digital Camera



Figure5 Leica Microscope with Motic Digital Camera and Documentation Computer

Leica S8 APO Microscope

In January 2004 we have added a Leica S8 Apochromatic Optics (APO) stereo zoom microscope with 1:8 zoom ratio. This microscope has a polarizer and analyzer attachment, a incident light base, a gliding sample stage, an 1x objective, a 10x eye piece and a c-mount photographic attachment for digital documentation ([Figure 5](#)).

Moticam 1300 & Motic Software

Leica microscope has a [Moticam 1300](#) digital CCD camera attached to it and is capable of capturing 1.3 mega pixel images (1280x 1024) of crystals kept under the crossed polarizer. The accompanying [Motic Advanced Images 3.2](#) software allows the capture of a still image or a portion of it at any time and at pre-set intervals of time. Further analysis like measuring

linear dimension, gamma correction, gray scale rendition, etc can also be performed on the images. User's crystal images are stored in phe.sb.fsu.edu in the following directory:

D:\CrystalImages\PI_Name\Project_Name\Date_of_Image_Capture\Image_01.jpg

The top level directory of CrystalImages is a shared folder and anyone with \\IMB2 domain username and password can access is using the following link (under Windows o/s):

<\\phe.sb.fsu.edu\CrystalImages>

Hardware Accessories

Helium Cylinder Auto Switcher



Figure 6 Bio Switch Helium Gas Cylinder Switcher

[Bio Switch](#) is an automated Helium gas cylinder tank switcher ([Figure 6](#)). It has two gas inputs and pressure sensors and one gas output. The first gas input and sensor are connected to the main Helium tank (Primary) and the second sensor and gas input are connected to the second tank (Reserve). The output port is connected to several mirror systems. During the normal operation Helium is supplied from the Primary tank. However, when Helium is depleted from the Primary tank (pressure falls below 10-15 psi), Bio Switch automatically switches the supply to the Reserve tank without flow interruption. An audible alarm notifies that the switch has occurred. Status lamp indicates the identity of the supply cylinder. Depleted cylinder can be replaced at a convenient time without interrupting the gas flow.

Chart Biomed Cryoshipper & Container



Figure 7 Chart-Biomed Cryoshipper and Shipping Container

The facility has acquired a new [Cryoshipper](#) and Shipping Container ([Figure 7](#)) manufactured by [Chart Biomed](#). This dry shipper (aka vapor shipper) will replace the older shipper and is available for all the users of the Facility.

Software

Crystal Clear 1.3.5 SP2

CrystalClear is a Graphical User Interface (GUI) for collecting data from Rigaku/MS-C Axis IIC detector. It provides an unified control over the automated data collection and processing of single crystal data as well as data collection strategy. Underneath the CrystalClear interface lies a powerful compute engine called d*TREK®. D*TREK® was initially designed to handle the volumes of CCD data generated at the APS synchrotron and now it is refined process data at home source. In November 2003 we have upgraded the older CrystalClear version 1.3 to the newer 1.3.5SP2. Details of the newer [CC1.3.5 SP2](#) are available at the Rigaku/MS-C website.

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 3](#) shows the list of computers that have licenses to run various versions of HKL suite.

No	Computer (IP address)	HKL2000	HKL.1.97.9	HKL.1.97.2	HKL.1.96.6
1	Arg (128.186.102.79)	No	Yes	Yes	Yes
2	Lys (128.186.102.77)	No	Yes	Yes	Yes
3	Leu (128.186.102.76)	No	Yes	Yes	Yes
4	Tyr (128.186.102.78)	No	Yes	Yes	Yes
5	Flame (128.186.102.154)	No	Yes	Yes	Yes
6	Raccoon (128.186.103.108)	Yes	Yes	Yes	Yes
7	Neptune (128.186.103.106)	Yes	Yes	Yes	Yes
8	Spruce (128.186.103.109)	No	Yes	Yes	Yes
9	Tampa (128.186.103.110)	No	Yes	Yes	Yes
10	Orlando (128.186.103.165)	Yes	Yes	Yes	Yes
11	Boston (128.186.102.145)	No	Yes	Yes	Yes
12	Miami (128.186.102.136)	No	Yes	Yes	Yes
13	Mozart (128.186.102.139)	No	Yes	Yes	Yes
14	Dallas (128.186.102.135)	Yes	Yes	Yes	Yes
15	Fgf (128.186.103.126)	Yes	Yes	Yes	Yes

Table 3 Computers with HKL licenses. Orange: Computer Resources; Blue: X-Ray Facility; Purple: Individual Lab. Green: Licensed; Red: Not licensed.

Alias and modifier

Users can run a program locally, by invoking an alias, while that program is physically present in a remote machine. Before invoking an alias, however, the user should specify it in their shell-rc file. For example, if your default shell is `cs`h or `tc`sh then, the following line in your `.cshrc` or `.tcshrc` file would specify an alias `dz` to invoke the program `denzo` (please follow the exact syntax):

```
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 (please follow the exact syntax):

```
alias dz=' /imb/users/d1/soma/HKL.1.97.2/denzo ' (or equivalent)
```

In order for the user to display images collected under different formats, combine `xdisp` command with an appropriate modifier. The modifiers for most commonly used formats are given below (*␣*: indicates a blank space):

```
xdisp ␣ raxis2n ␣ myxtal001.osc |R-Axis format
xdisp ␣ raxis2n ␣ 210 ␣ myxtal001.osc |Small R-Axis format
xdisp ␣ ccd ␣ unsupported-m165 ␣ xtal01.001 |MarCCD165 format
xdisp ␣ ccd ␣ adsc ␣ unsupported-q4 ␣ xtal01.001 |Quantum 4 format
xdisp ␣ ccd ␣ unsupported-m225 ␣ xtal01.001 |MarCCD225 format
xdisp ␣ ccd ␣ adsc ␣ unsupported-q210 binned ␣ xtal01.img |Quantum 210 binned 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 ␣ raxis2n ␣ myxtal###.osc ␣ 15 myxtal###.x |R-Axis data + Predictions
```

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/~xray/Manuals/XGControl.pdf>

CCP4

Linux versions of CCP4 version 4.1.1 and 4.2.2 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
```

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
```

XtalView

Current version of XtalView (version 4.1) has been installed in `raccoon`. The executables are in `/usr/local/xray/XtalView`. Please add the following line in your shell-rc file to specify the environment correctly:

```
source /usr/local/xray/XtalView/XtalView.env
```

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
```

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 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](#).