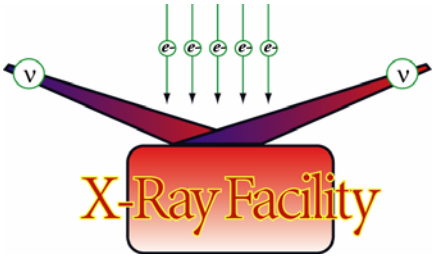
IMB X-Ray Crystallography Facility
410-413 Kasha Laboratory
Florida State University
Tallahassee, FL 32306-4380, USA
Telephone: (850) 644-6448 (Off) | (850) 645-1333 (Lab)
E-mail: soma@sb.fsu.edu
Web: http://www.sb.fsu.edu/~xray | http://www.sb.fsu.edu/~soma

XRF Upgrades-2004-2005

XRF Hardware & Software Upgrades



Recent Upgrades to X-Ray Crystallography Facility Hardware & Software

Table of contents

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
Mar. 10, 2005

XRF Upgrades 2004- ’05

Upgrades to X-Ray Facility Hardware & Software

Version: March 10, 2005; Original: 11102004.

Introduction

The X-Ray Crystallography Facility has recently upgraded or added several pieces of hardware and software. This note is intended to inform the XRF users about all those upgrades. A copy of this Note will be posted in XRF webpage shortly after receiving suggestions from the users. The following is the list of changes that were made recently:

1) Computers: Desktops | Laptop
2) Computer Accessories: Combo FireWire Drive | Veo Observer Camera
3) Cryo Accessories: HC34 Cryo dewar
4) Facility Amenities: Emergency power | UPS Power
5) Software: HKL2000 | CCP4-5.0 | EPMR | Phaser

Computers

Raccoon and Neptune upgrades

Figure1 Data Processing Computer Raccoon.sb.fsu.edu (KLB 410A)

Raccoon and Neptune the main data processing and archiving computers have now additional storage capacity. We have added a Seagate 34 GB SCSI hard disk to each of them. We have added a Belkin USB2 + IEEE1394 comb PCI cards so that external FireWire drives can now

be connected either through FireWire or USB2 connection. We have added a DAT72 (DDS5) internal tape drive. With these additions we support all the five generations of DDS tapes (DDS, DDS2, DDS3, DDS4 and DAT72). The current status is displayed below:

Raccoon (KLB 410A) 128.186.103.108	Neptune (KLB 410A) 128.186.103.106
• Current O/S : RedHat Linux v. 7.1 (Seawolf) & kernel v. 2.4.20-20.7 • 384 MB physical memory • 1.5 GB swap partition • One 20 GB Maxtor IDE hard disk • Two 34 GB (IBM & Seagate) SCSI hard disks • One internal Lite-on IDE CD-ROM drive • One external HP SCSI CD-R/-RW drive • One internal Certance SCSI DAT72 (DDS5) tape drive • Two external FireWire hard drives (Maxtor & Iomega), and • A Belkin Combo USB 2.0 and FireWire card.	• Current O/S: RedHat Linux v. 7.3 (Valhalla) & kernel v. 2.4.20-20.7 • 384 MB physical memory • 1.8 GB swap partition • One 20 GB Maxtor IDE hard disk • One 34 GB Seagate SCSI hard disk • One internal Lite-On IDE CD-ROM drive • One internal Seagate SCSI DDS4 tape drive • One external Seagate SCSI DDS3 tape drive • One Pioneer FireWire DVD-R/-RW drive, and • A Belkin Combo USB 2.0 and FireWire (aka: i-Link, IEEE1394) card.

Laptop (Tampa) upgrades

Tampa, the Dell Latitude Cpx laptop now has additional storage capacity and new Linux operating system. The dual bootable laptop now features Windows XP SP2 and Debian GNU/Linux 3.1 as well as a 60 GB hard disk shared between these two operating systems. The current details of the laptop are listed below:

Tampa (KLB 414) 128.186.103.110

• Current O/S:
  ▪ Debian GNU/Linux v.3.1 and kernel v. 2.4.26 &
  ▪ Windows XP SP2
• 256 MB physical memory | 1.2 GB swap
• One 60 GB SimpleTech IDE hard disk
• One internal Hitachi-LG ATAPI DVD-ROM/CD-R drive
• WD FireWire, 3Com Lan100, Adaptec USB2, and Zoom v.92 modem PC cards

Computer Accessories

The current details for all XRF computers are listed in the table below:

Name (\\DOMAIN)	IP # (Prefix) (128.186.103)	Location (KLB)	Information (Operating System)
Anaconda.sb.fsu.edu (\\XRAY)	.102	410A	R-Axis IIC Controller (Win NT 4.0)
Spruce.sb.fsu.edu	.109	410A	MarCCD Controller (RH Linux 8.0 | Kernel 2.4.18-14)
Neptune.sb.fsu.edu	.106	410A	Data Processing & Archiving (RH Linux 7.3 | Kernel 2.4.20-20)
Raccoon.sb.fsu.edu	.108	410A	Data Processing & Archiving (RH Linux 7.1 | Kernel 2.4.20-20)
Tampa.sb.fsu.edu	.110	414	Laptop (Debian Linux 3.1 & Win XP SP2)
Phe.sb.fsu.edu (\\IMB2)	.107	412	Crystal Documentation (Win 2000 SP4)

Table 1 Details of X-Ray Crystallography Facility Computers

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 | Type	**IP (.sb.fsu.edu | 128.186.103.)**	**Operating System**	**Media / Native Capacity**
Certance CD72LWH-SS | Internal SCSI	raccoon. | .108	Linux	DAT72 tape / 36 GB
HP CD-Writer+ 9200 | External SCSI	raccoon. | .108	Linux	CD-R\-RW / ~700 MB
Seagate STD1401LW | Internal SCSI	neptune. | .106	Linux	DDS4 tape / 20 GB
Seagate STD624000N | External SCSI	neptune. | .106	Linux	DDS3 tape / 12 GB
Pioneer DVR-A04 | External SCSI	neptune. | .106	Linux	DVD-R\-RW/ ~4.6 GB
Seagate STD1401LW | Internal SCSI	spruce. | .109	Linux	DDS4 tape / 20 GB
Seagate STD1401LW | Internal SCSI	anaconda. | .102	Win NT 4.0	DDS4 tape / 20 GB
Pioneer DVR-A04 | Internal SCSI	anaconda. | .102	Win NT 4.0	DVD-R\-RW / ~4.6 GB

Table 2 Available options for data archiving at IMB XRF

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

Figure 2 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 ±R/RW) dual-interface (USB 2.0 & FireWire IEEE1394) external Sony DVD DRX-510UL Writer/Reader. This drive is capable of reading and writing all the following media:

DVD+R\RW, DVD-R\RW, CD-R\RW, and CD-RW (writing); CD-ROM, DVD-ROM (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.

Veo Observer Camera

Veo Observer Camera is a network camera that has a built-in web server that can be accessed by Internet Explorer (only). It has 24 bit digital output with a 640 x 480 pixel size and is pan-tilt capable. XRF has installed one such camera on an experimental basis (in March 2005) to monitor the status of the sample in the Rigaku-Osmic-IP detector set-up. Users have a limited access to the camera functions. Ask Soma for username, password and the protocol for usage. The web address for the VeoXtalCam1 is http://radio.sb.fsu.edu (Works in IE only).

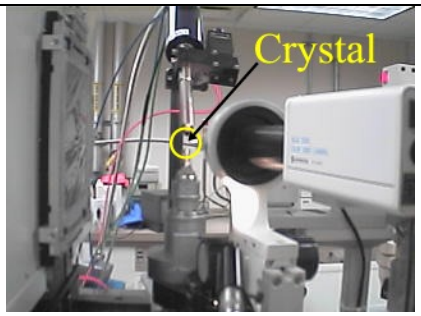
	
Veo Observer Network Camera	Veo Camera snapshot of the sample status

Figure 3 Veo Observer Network Web Camera

Cryo Accessories

Taylor-Wharton HC34 Cryo Dewar

Cryo storage dewar HC34 from Taylor-Wharton is designed specifically to store biological samples including crystals at cryogenic temperatures for long-term (many months). The storage dewar has a 3.6" neck diameter and accommodates six (6) separate 11" cryo canisters. Each canister can accommodate about twenty (20) cryo canes and each cryo cane can accommodate five (5) cryo vials each. Over 500 cryo vial samples can be maintained at cryogenic temperatures for over one hundred (100) days. This cryo dewar is housed in KLB412 and is available to all the members of Structural Biology Program.

Figure 4 Taylor-Wharton HC 34 Cryo Storage Dewar

Amenities

Emergency Generator Power

During the renovation of the Institute in 2003, X-Ray Facility was wired with emergency power sockets that would supply power to mission critical equipments that run on 208 VAC | 20A | 60 Hz | Single Phase. This year we have supplemented the power to include equipments that run on 110 VAC | 20 A | 60 Hz | Single Phase.

Figure 5 Emergency Generator Power Sockets

UPS Power for Cryo Controller

During a power outage cryo controller needs to be powered by, in addition to the emergency generator power, an uninterruptible power supply in order for it to retain the pre-programmed cooling routine. So XRF has added an APC Smart Back UPS Pro 1400 in series with the emergency generator power. During a short power outage the UPS will power the cryo systems and during a pro-longed power outage the generator will power the cryo systems.

Figure 6 Emergency + UPS Power for CryoConroller

Software

HKL2000 and HKL 1.97.9

HKL2000 (v. 0.98.689) and HKL v. 1.97.9 executables are available for XRF machines (*raccoon* and *neptune*) IMB machine (*flame*) and PI machines (*boston, fgf, miami* and *dallas*). Users need to get an updated version of `cr_info` (dated Feb. 2005) from Soma in order to run these programs.

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 `csh` or `tcsh` 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 (***b*** *: indicates a blank space)*:

`xdisp b raxis2n b myxtal001.osc` | R-Axis format

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

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

`xdisp b ccd b unsupported-m225 b xtal01.001` | MarCCD225 format

b *: 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 b raxis2n b myxtal###.osc b 15 myxtal###.x` | R-Axis data + Predictions

CCP4 5.0

Linux versions of CCP4 v. 5.0 and 4.2.2 as well as ccp4-i have been installed in `raccoon` and `neptune`. User should copy the following file in order to run the latest version

```
source /usr/local/xray/CCP4/ccp4-5.0/include/ccp4.setup
```

EPMR 2.5

Version 2.5 of Evolutionary Programming for Molecular Replacement (EPMR) by C.R. Kissinger et al has been installed in `raccoon` and `neptune`. Invoke the program by issuing the following command

```
/usr/local/xray/EPMR/epmr_linux
```

Phaser 1.2

Latest version of Phaser 1.2 from Randy Reed's lab in Cambridge University, England has been installed in `raccoon` and `neptune`. Invoke the program by issuing the following command:

```
/usr/local/xray/Phaser1.2/phaser-linux-1.2/phaser
```

Conclusion

Please send your suggestions and comments for further hardware and software upgrades to Soma.