

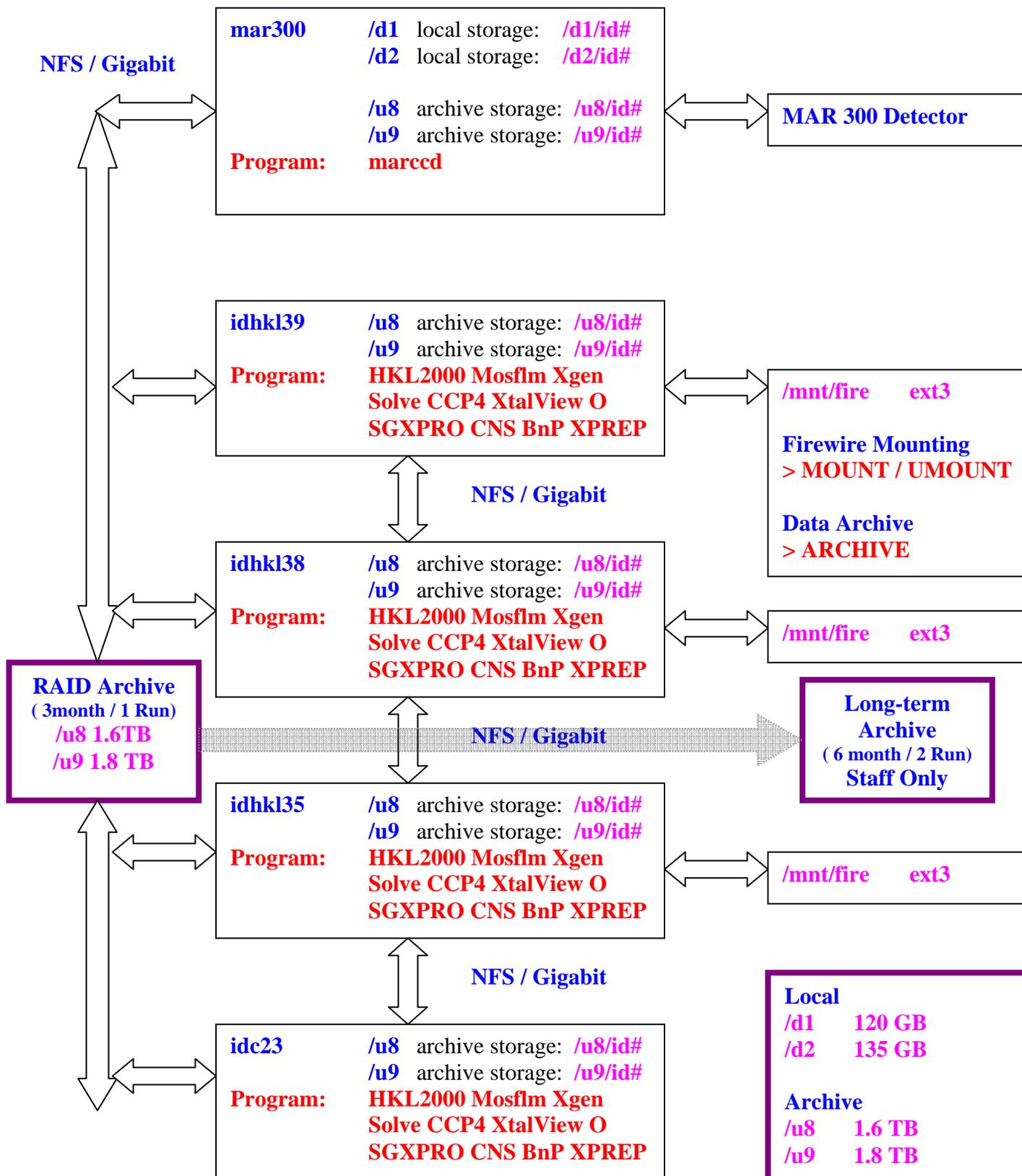


SER-CAT Tutorial

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Computer Disk Structure



Startup Procedure

1. Log into beamline control computer with assigned username and password.
ID beamline: **idc23** (IP: 164.54.208.23)
BM beamline: **bmc93** (IP: 164.54.208.93)
2. Start **MARCCD** program.
 - a. Start shell window from **idc23**
 - b. **\$ slogin mar300** (with the same username and password)
 - c. **\$ marccd** (follow menu flow to start mar server)
 > acquire > remote control > start
3. Start **SERGUI** program.
 - a. Start shell window from **idc23**
 - b. **\$ sergui.py** (most common functions)
 - i. **>Hutch** (wavelength, slit size, transmission, optimization, distance, etc)
 - ii. **>Collect** (collect single, collect strategy, collect run)
 - iii. **>MAD** (periodic table, energy fluorescence scan, f' and f'' analysis)
 - c. Create data archive directory from **> Collect > Archive Directory > Browse**
Example template : **/u9/staff/08_08_05_SERCAT_staff**
4. Start **MOTOR** program.
 - a. Start shell window from **idc23**
 - b. **\$ motor**
5. Mount firewire drive (file system: **EXT3**) as **/mnt/fire** into one of following computers by following **Firewire Drive Mounting Procedure**:
ID beamline: **idhkl35, idhkl38, idhkl39**
BM beamline: **bmhkl68, bmc84**
6. Start automatic data archive script from the machine with firewire drive mounted by following **Data Archive Procedure**.
Example:
From directory: **/u9/staff/08_08_05_SERCAT_staff**
To Directory: **/mnt/fire**
7. Start **HKL2000** program.
 - a. Start shell window from **idc23, idhkl35, idhkl38, idhkl39, bmc93, bmhkl68, bmc84.**
 - b. **\$ HKL2000**

Firewire Drive Mounting Procedure

1. Several beamline data processing computers (**idhkl38, idhkl39, idhkl35, bmhkl68, bmc84**) have the capability for firewire drive mounting.

2. From beamline staff and users' experience, we found out that Firewire drive with **vfat** file system is very unreliable and easy to corrupt.

To protect user's precious data, we will only support user's Firewire drives with file system **ext3.**

3. **idhkl35, idhkl38, and idhkl39, bmhkl68, bmc84** are configured to mount firewire drive **ONLY** with file system **ext3**.

Mounting point: **/mnt/fire**

Mounting steps:

- a. To mount: **\$ MOUNT** **(Notice: Upper case cmd and follow instruction)**
- b. To umount: **\$ UMOUNT**

4. Procedure to reformat user's firewire drive to ext3.

- 1) Login as **root**.
- 2) Connect firewire drive to power supply and wait for the front light turn to green.
- 3) Connect firewire cable to the computer.
- 4) **% rescan-scsi-bus -r** # clean up the scsi bus
- 5) **% /sbin/fdisk /dev/sda** # reformat the drive
 - d** # delete old partition
 - n** # ask for a new partition
 - p** # specify a primary partition
 - 1** # pick cylinder 1 to begin with
 - w** # write out the new partition table
- 6) **% /sbin/mke2fs -j -m0 -LNAME /dev/sda1** # make a filesystem

Data Archive Procedure

Procedure

From data processing computer **idhkl35, idhkl38, idhkl39, bmhkl68, bmc84**

% MOUNT # start automatic **MOUNT** script to mount firewire drive

% ARCHIVE # start automatic **ARCHIVE** scrip to backup data
From directory: **/u9/staff/08_08_05_SERCAT_staff** # user input: from archive directory
To directory: **/mnt/fire** # user input: to mounting point

Notice: ARCHIVE script will keep running every 5 minutes, and will automatically backup user's data from /u1 or /u2 to firewire drive incrementally.

Ctrl^C # stop **ARCHIVE** script after finishing data backup

% UMOUNT # start automatic **UMOUNT** script to unmount drive

Policy

1. Before user leaves the site, it is user's responsibility to backup experimental data and to inform SERCAT staff of the whereabouts of archived data in **/u8 and /u9 RAID** disk.
2. User should follow **Firewire Drive Mounting Procedure** to mount / unmount firewire drive.
3. Archived data will be kept in **/u8 or /u9 RAID** disk for about **3 months (1 run)**.
4. CAT staff will then archive data from **/u8 or /u9 RAID** disk to a long-term storage system (**staff access only**). The archived data will be kept in long-term storage for about **6 months (2 runs)**.
5. **Due to tightened APS firewall policy, user is not able to access data processing computers remotely.** To retrieve archived data in the future, user should provide staff user's institution ftp server IP address, user name, password and large disk space.
6. Occasionally, user may borrow a loan Firewire drive (pre-formatted and 160 GB) from SERCAT. Please leave user name, institution name, and contact information on the assigned log book; and return the drive to staff as soon as possible.

Energy Change and Beam Alignment Procedure

[Any energy change between 6.2 Kev (2 A) and 13.5 Kev (0.92 A)]

- 1) Change energy from **sergui.py** window.
- 2) Enable the experimental hutch and open safety shutter.
- 3) From **sergui.py > hutch** tab, run following optimizations.

Optimize Tune

Program will automatically run scans until the Gaussian peak is found.
Program will automatically move to optimized peak.
No user interaction is necessary.

Optimize Horizontal Slit

Program will automatically run scans until the Gaussian peak is found.
Program will automatically move to optimized peak.
No user interaction is necessary.

Optimize Vertical Slit

Program will automatically run scans until the Gaussian peak is found.
Program will automatically move to optimized peak.
No user interaction is necessary.

If user wants to do large energy change, for example, from 12 keV to 6 keV, user may continue

- 4) Put on the phosphor ball provided by CAT staff and align the ball to the center.
- 5) Tweak the goniostat position to bring the spindle center to beam center
 - i. Reduce slit size to **20x20** and reduce beam transmission to have better view of the beam center profile.
 - ii. From **motor>** window, type command

```
motor> mrel g_hor 10 (+/- 10 to +/- 100 movement)
motor> mrel g_vert 10 (+/- 10 to +/- 100 movement)
```
 - iii. After **align the beam center to the upper horizontal line of cross box**, close the timing shutter, increase slit size to normal 100, and set filter to desired number

MAD Experiment

- 1) Change the energy to the desired heavy atom absorption edge (K_{α} or L_3) energy, which must be between **5 Kev and 20 Kev** and align the beam by following **Energy Change and Beam Alignment Procedure**.
- 2) Put on sample crystal and align it.
- 3) Make sure the Rontec fluorescence detector is aligned (by default) and power supply is **ON**.
- 4) Run fluorescence scan:
 - 1). Change window to **sergui.py>MAD** tab.
 - 2). From **Periodic Table**, choose the desired heavy atom and correct edge.
 - 3). Change the transmission to 20% ~ 50%.
 - 4). Click **Run Scan** and wait until the scan is done (about 1 minute) and the scan plot is displayed. Timing shutter will be automatically closed after scan.
 - 5). Click **Analysis** to run **Benny-Chooch** programs.
 - 6). **Benny-Chooch** window will start automatically to calculate f' and f'' . f' and f'' plots will be displayed for the scan.
 - 7). Close the plot window and “**Hit return to Close**” the **Benny** window. The calculated inflection wavelength, peak wavelength and their f' and f'' will be automatically updated and displayed to the **sergui** window. Type in remote energy about 50 – 100 ev beyond the edge energy in the window to calculate its f' and f'' .
- 5) Change the transmission to desired number for real data collection.
- 6) Setup data collection with calculated inflection, peak and remote energies.
- 7) After data collection and processing, use the program **XPREP** to calculate Patterson map by following **Patterson Map Calculation with Program XPREP**.
- 8) To search multiple heavy atom sites, user may use following programs by **Crystallographic Software**.

sgxpro
BnP

run either solve or shelxd to search heavy atom.
run PHASES and SnB packages GUI

Data Collection

1. Setup file names and archive directory:

From **sergui.py > Collect**,

- a. Create **Sample ID** (file name): lysozyme
Template: lysozyme_1_#.####
- b. Create **Archive Directory**:
Template: /u9/staff/08_08_05_SERCAT_staff

2. Collect Single:

From **sergui.py > Collect > Collect Single**

- a. Set following target values:
 - Transmission**
 - Distance**
 - Omega**
 - Scan Width**
 - Exposure Time**
- b. Click **Collect** to start collecting single frame:
 - What happens: i. Move Distance to target position (take time to move).
 - ii. Move Omega to target position.
 - iii. Start exposure.
- c. Image will be displayed on marccd program and file name will be lysozyme_1_s.####

3. Collect Run of single wavelength data set:

From **sergui.py > Collect > Collect Strategy**

- a. Set following target values:
 - Exposure Time**
 - Starting Angle** (default is 0, click Use Current to change)
 - Scan Width**
 - Number of Frames/Run**
 - Detector Distance** (default is current position, click Use Current to change)
 - Starting Energy** (default is current energy, click Use Current to change)
- b. Click **Generate Runlist**
- c. Go to page **> Collect > Collect Runs**
- d. Click **Collect** to start data collection
- e. Click **Abort** to abort data collection

4. Collect Run of MAD data set:

From **sergui.py > Collect > Collect Strategy**

- a. Set following target values:
 - Exposure Time**
 - Starting Angle** (default is 0, click Use Current to change)
 - Scan Width**
 - Number of Frames/Run**
 - Detector Distance** (default is current position, click Use Current to change)
 - Starting Energy** (default is current energy, click Use Current to change to Peak)
 - Second Energy** (default is disabled, click Use in Data Collection to change to Inflection)

Third Energy

(default is disabled, click Use in Data Collection to change to Remote)

**Inverse Beam
Wedge Size**

(default is No, click Y to enable 180 degree beam inverse)

(Set wedge size for data collection, click Y for Wedge in Angle or Wedge in Energy)

- b. Click **Generate Runlist**
- c. Go to page > **Collect > Collect Runs**
- d. Click **Collect** to start data collection.
- e. Click **Abort** to abort data collection

5. For MAD experiment, make sure the three wavelengths were set correctly for data run.

6. If the beam is dumped during normal data collection,

- 1). Click **Abort**.
- 2). After beam current is restored, open the A shutter on PSS manually.
- 3) Set the correct next frame number and click "Collect" to continue data collection.

Example:

- If beam was dumped at frame #90, user noticed and stopped data collection at frame #94, then next frame number would be #95.
- Frame 90 to frame 94 are empty frames.
- After beam is restored, set the next frame number to 90 to start from the first empty frame. User should not change other Phi, Omega, Kappa values.
- Click **Collect** to start.

Data Reduction

XGEN, HKL2000, MOSFLM were installed in data processing computers **idhkl35, idhkl38, idhkl39, idc23**

Run XGEN:

From data processing computer:

```
bash> cd data-directory           # change into data directory
```

```
bash> xgenproc [-dns] [-cfhipxy<val>] [dirn]
```

i.e. d,n,s are Booleans and the other - options all take values

and an option that doesn't begin with a minus is a directory name

```
-c*)    # specify the number of spots to use  
-d*)    # compress images after processing  
-f*)    # specify a sample image name  
-h*)    # specify the last image number to use  
-i*)    # specify an International Tables #  
-n*)    # means do NOT recenter after indexing  
-p*)    # specify an image prefix  
-s*)    # flip the sign of the stepsize  
-x*)    # specify the beam Xcenter  
-y*)    # specify the beam Ycenter  
*)      # specify the data directory
```

for example:

```
bash> xgenproc -x112.5 -y113           # reset beam center to (112.5, 113)
```

1. XGEN will create directory **xgena** (or **xgenb, ... xgenz**) under data directory.
2. XGEN will automatically run through

Peak search
Autoindexing
Integration
Scaling

3. Even though XGEN can autoindex single image frame as what HKL2000 does, it will work better with multiple data frames (consecutive or separated).
4. XGEN is sensitive to the beam center for successful autoindex. User may change beam center to correct position with parameters.
5. XGEN will create log file **datafilename.xlg** under **xgena**
6. XGEN will create **datafilename.sca** output data as **.sca** format
7. XGEN will create **datafilename.asc** output data with anomalous ON as **.sca** format

Data Reduction

Run HKL2000:

From data processing computer:

```
bash> cd data-directory # change into data directory
```

```
bash> HKL2000
```

If user wants to use special scalepack for different use, please contact staff

```
scalepack16m  
scalepack8m  
scalepackmanyframes  
scalepackribo  
scalepackvirus
```

for example:

scalepack for Virus project

```
bash> cp /usr/local/bin/scalepack /usr/local/bin/scalepacknorm
```

```
bash> cp /usr/local/bin/scalepackvirus /usr/local/bin/scalepack
```

Run Mosfilm:

From data processing computer:

```
bash> cd data-directory # change into data directory
```

For ID beamline data from mar300 detector:

```
bash> ipmosflm # start MOSFLM program  
> detector marccd  
> limits xmin 0 xmax 150 ymin 0 ymax 150 xscan 150 yscan 150  
> template yourdataset.####  
> image 1  
> go
```

For BM beamline data from mar225 detector:

```
bash> ipmosflm # start MOSFLM program  
> detector marccd reversephi # reverse phi convention for BM  
> limits xmin 0 xmax 150 ymin 0 ymax 150 xscan 150 yscan 150  
> template yourdataset.####  
> image 1  
> go
```

Heavy Atom Search, Phasing, Maps

Run SGXPRO:

SGXPRO is an application software suite, developed at University of Georgia, for solving X-ray crystallographic structures of biological macro-molecules.

SGXPEO uses user-friendly GUI for parameter input and is able to run all the procedure as pipeline after user setup.

SGXPRO can be distributed to academic users free.

- 1). Heavy atom sites searching: **SHELXD** and/or **SOLVE**
- 2). Phasing (SAD or MAD): **ISAS** and/or **SOLVE**
- 3). Auto-tracing: **RESOLVE**

Start program: `bash> sgxpro`

Run BnP:

BnP is the Buffalo and Pittsburgh interface, which is combining **SnB** and **Phases** suite for complete protein phasing.

Start program: `bash> BnP`

Run CCP4:

Start program: `bash> ccp4i`

Run CNS:

Start program: `bash> cns_web`

Run O:

Start program: `bash> lin_ono`

Run XtalView:

Start program: `bash> xtalmgr`

FAQ

1. MARCCD program is frozen.

- 1) slogin mar300
- 2) From any shell window, type following command
bash> ps -ax | grep marccd
- 3) Kill the marccd program with shown PID from last command.
bash> kill -9 xxxxx
- 4) Restart marccd program from idc23 computer

2. Remote control box for Phi, Kappa and Z does not work.

- 1) Push down the Phi 0 90 180 270 four buttons at the same time
- 2) From marccd program, take a single exposure.
- 3) After exposure, the remote should be activated and ready to use.

3. Could not find data in archive directory set from marccd program.

- 1) Check the data collection setup, make sure the archive setup is shown like following format.
cp %s /u2/id5/SERCAT/
- 2) Before start the data collection, user must manually create all the directories from shell window. The marccd program can not create directory automatically.

4. Could not mount/umount user's firewire drive.

- 1) Check the Firewire Drive Mounting Procedure.
- 2) Check with staff.

5. When starting sergui.py, error message shows: "Socket connection failed,".

- 1) Go to idc10 computer, from any shell window,
Type: `$camera_server.py`
- 2) If step 1) failed, go to video server box (in beamline rack), power reboot.