

Software for X-ray Scattering Measurement

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Software

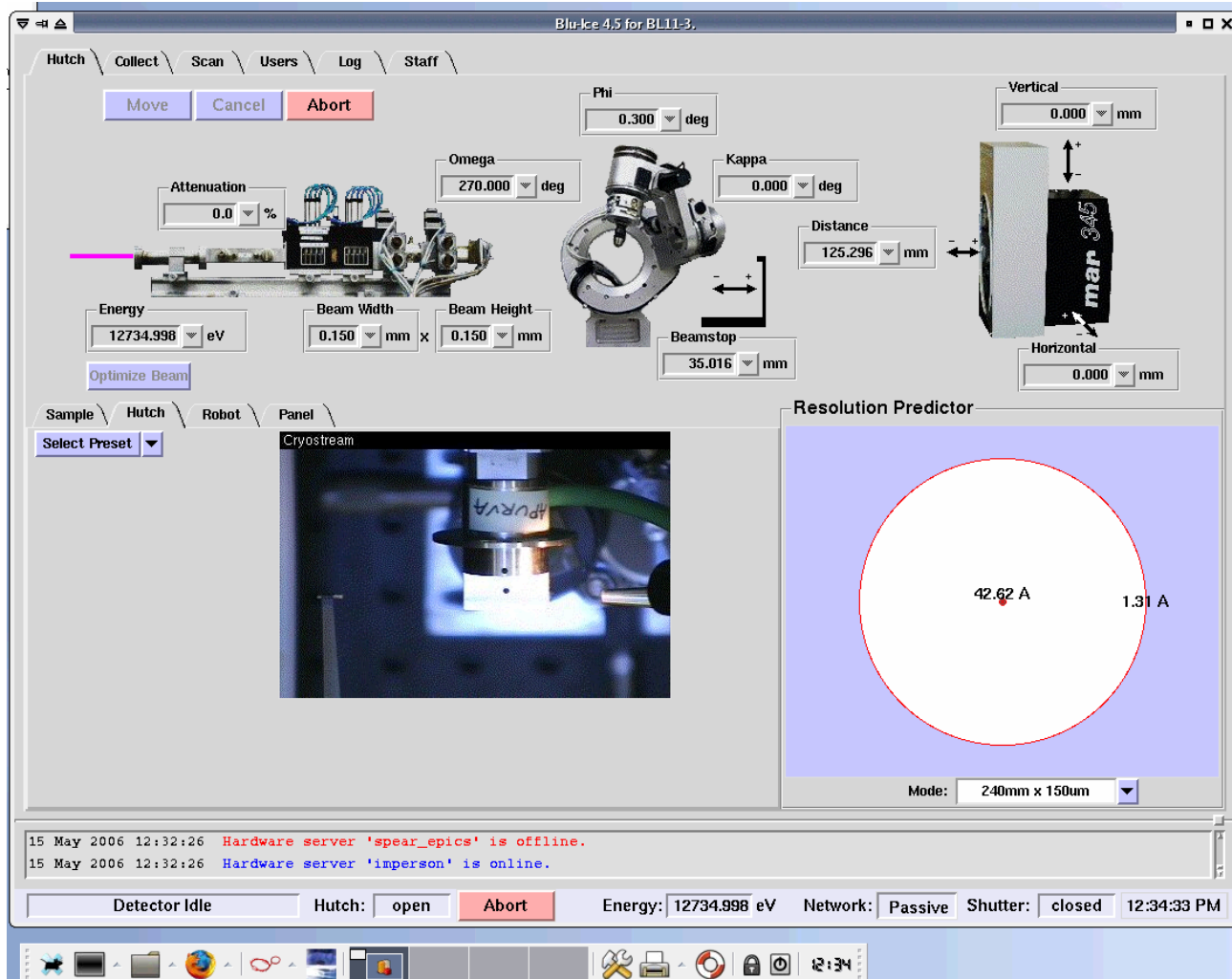
- ◆ Software for SAXS
 - ◆ John Pople will talk about this

- ◆ Software for 2-D WAXS

- ◆ Software for point detector based scattering.

Software for 2-D WAXS

BluIce



BluIce 4.5 for BL11-3

Hutch \ Collect \ Scan \ Users \ Log \ Staff \

Move Cancel Abort

Phi: 0.300 deg

Omega: 270.000 deg

Kappa: 0.000 deg

Attenuation: 0.0 %

Energy: 12734.998 eV

Beam Width: 0.150 mm x 0.150 mm

Beam Height: 0.150 mm

Distance: 125.296 mm

Beamstop: 35.016 mm

Vertical: 0.000 mm

Horizontal: 0.000 mm

Optimize Beam

Sample \ Hutch \ Robot \ Panel \

Select Preset

Cryostream

Resolution Predictor

42.62 A 1.31 A

Mode: 240mm x 150um

15 May 2006 12:32:26 Hardware server 'spear_epics' is offline.
15 May 2006 12:32:26 Hardware server 'imperson' is online.

Detector Idle Hutch: open Abort Energy: 12734.998 eV Network: Passive Shutter: closed 12:34:33 PM



Bluice – Scan tab

Bluice 4.5 for BL11-3

Hutch \ Collect \ Scan \ Users \ Log \ Staff \

File

Definition \ Graph \ Log \

Axes	Points	Start	End	Step		
sample_x	21	-1.00000	1.00000	0.10000	mm	Update
sample_z	21	1.00000	3.00000	0.10000	mm	Update

Detectors
Signal: **i_beamstop**
Reference:

Repeat
Number of scans: 1
Delay between scans: 0.000 s

Timing
Integration Time: 0.100 s
Motor Settling Time: 0.000 s

Files
Directory: ~
Filename root: BL11-3
Scan Number: 122

Scan Control
Scan
Stop

Motor Control
sample_x: -0.40000 mm
sample_z: 2.00000 mm
Move
Cancel
Abort

Foils: Al_1 Al_2 Al_4 Al_8 Al_16 Al_32 Se spareFilter1

100%

```
15 May 2006 12:32:26 Hardware server 'spear_epics' is offline.
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```

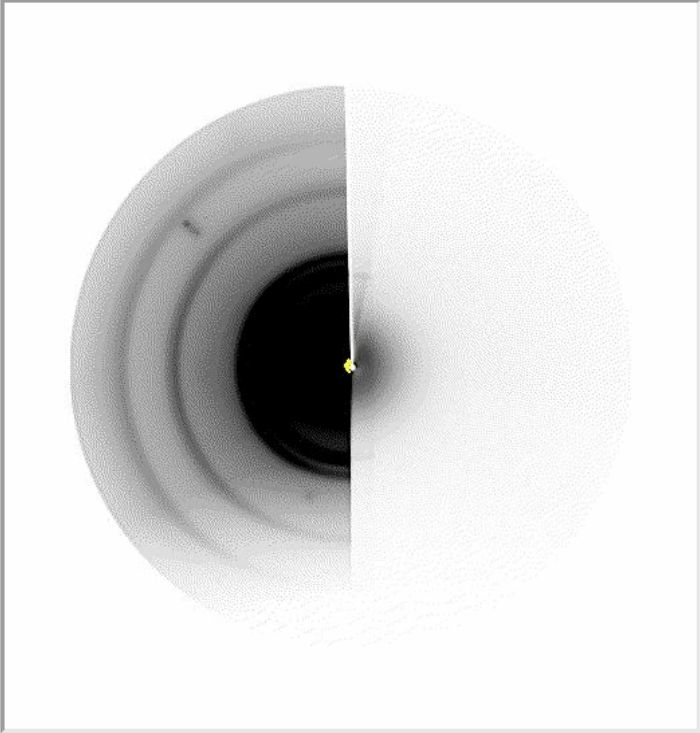
Detector Idle Hutch: open Abort Energy: 12734.998 eV Network: Passive Shutter: closed 12:37:38 PM



Bluice – Collect tab

Blu-ice 4.5 for BL11-3.

Hutch \ Collect \ Scan \ Users \ Log \ Staff \



Brightness: 10000 Zoom: 0.800

File Name: /data/mftoney/rupt/phi0.3_17_06_07.mar2300

Scheduled Scan Setup

Detector: 345mm x 150um
Scan Motor: gonio_phi
Directory: /data/mftoney/rupt
File Root: rupt15

Start Position: -7.00000 Update
Num Points: 5
Step Size: -1.0

Time Interval: 0.00 s
Exposure Time: 1.00 s

Num Sets: 5
Num Images/Set: 1

Start Abort

Status: Stopped Collecting Due to aborted

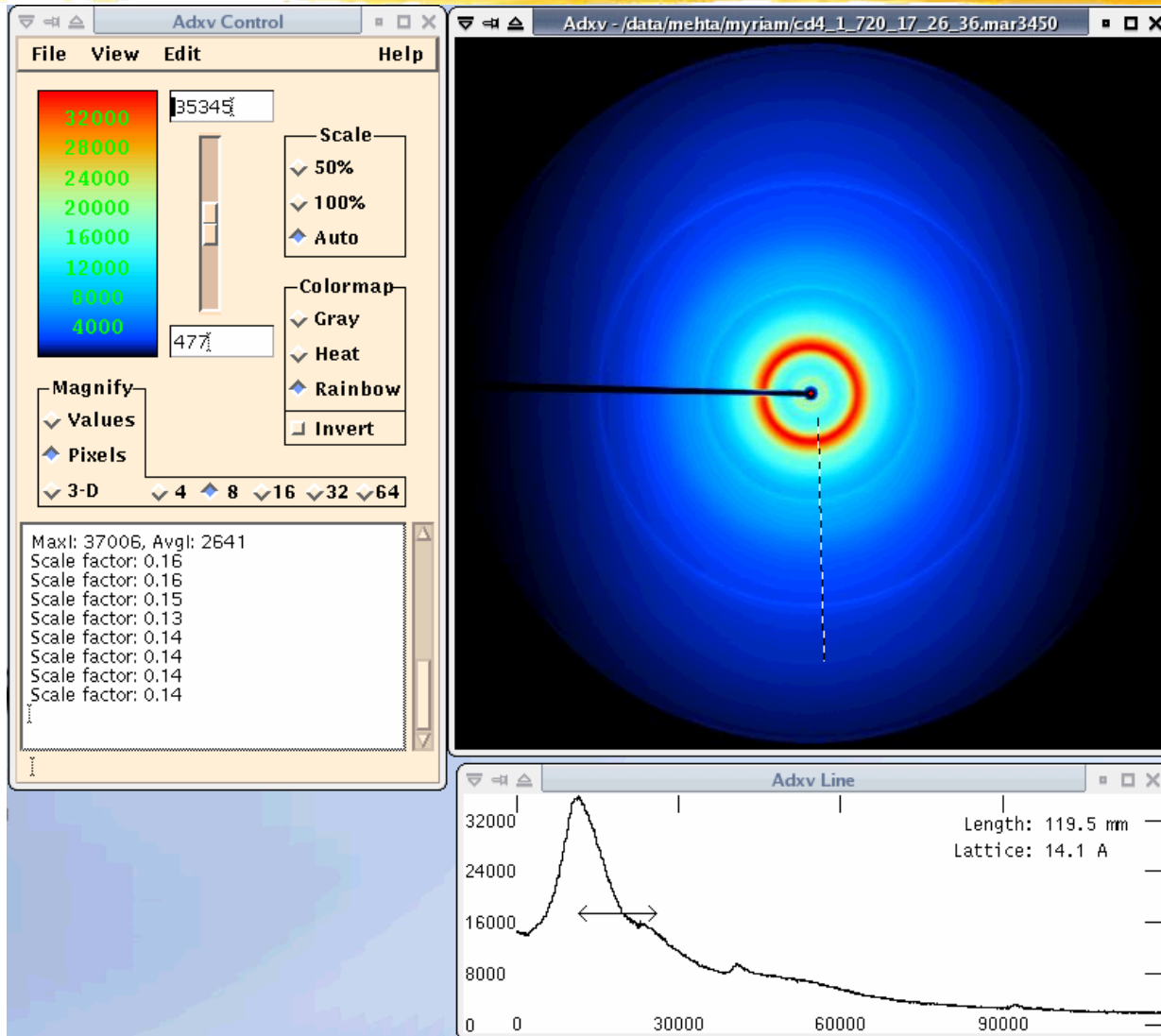
Directory: /data/mehta
Prefix: test Detector: 345mm x 150um
shutter: NULL Time: 1.00 s
Axis: NULL Delta: 1.00 deg

Collect New Image

15 May 2006 12:32:26 Hardware server 'spear_epics' is offline.
15 May 2006 12:32:26 Hardware server 'imperson' is online.

Detector Idle Hutch: open Abort Energy: 12734.998 eV Network: Passive Shutter: closed 01:34:06 PM

Preliminary Analysis



Software for Point Detector

- Architecture –
 - OS – VMS,
 - Super
 - Splot, Scal
- What it Looks Like?
- How to collect data And still get some sleep
 - Running Indirect (batch) files



Operating System

- ◆ Most beamlines have a "PC" and the beamline computer.
- ◆ Beamline Computer runs OpenVMS.
 - ◆ Command line driven. (Like MS-dos)
 - ◆ easy to get online help
 - ◆ Commands not case sensitive.
 - ◆ Will recognize commands even if not fully written out.
 - ◆ Never overwrites files.
- ◆ Beamline computer has two "drives"
 - ◆ \$user1: (default when you login) : indirect files
 - ◆ \$data1: : data files.
- ◆ Beamline computer has four "desktops"



Some VMS Commands

- ◆ `>command/modifier1` (optional) `argument`

- ◆ `>help` (if no argu → will display a menu – unlike unix.)

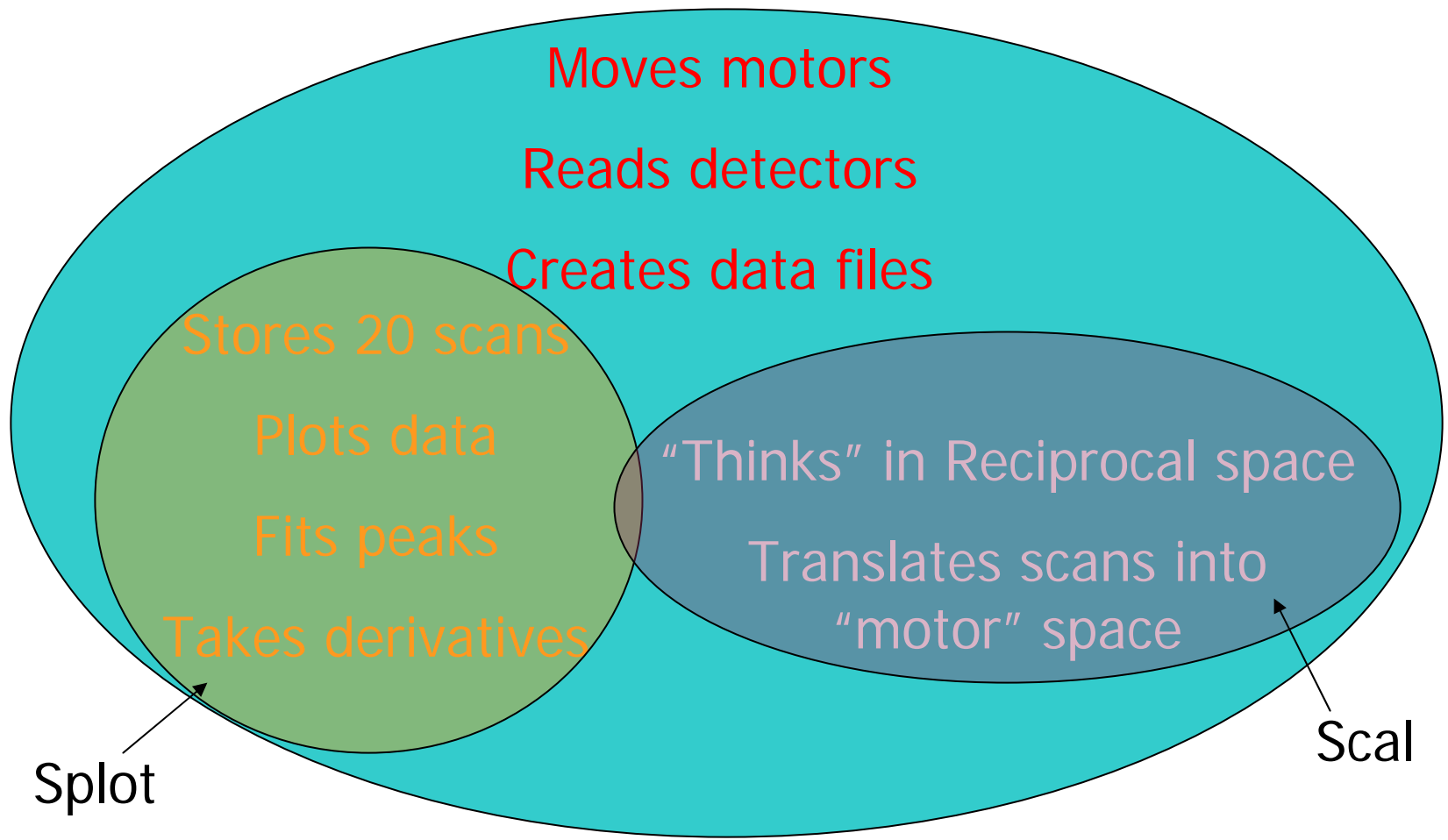
- ◆ `>dir` (e.g. `>dir/since=18-oct-2003 *.his`)

- ◆ `>set default` ⇔ `"cd"` (`>set def $data1:`)

- ◆ `>ftp computer_name` (or IP address)
 - ◆ But most people use **"reflection ftp"** on the PC to transfer data.



Super



Splot

Scal

Two Daughters



Super

- ◆ Command line structure

- ◆ Structure similar to VMS

- ◆ > `command/modifier1` (optional) `argument`

- ◆ > `2theta 42`

- ◆ > `2th/relative 1`

- ◆ Extensive online help

- ◆ > `help command` (if no argument gives the full menu)



More Super details

- ◆ Can scan by just writing out a scan
 - ◆ >Lineup 2theta 0.05 10 21
 - ◆ >Scan m3, 2, 0.01, 10, 1

- ◆ Or run a preprogrammed scan (20 stored)
 - ◆ >Scan 10 (run scan # 10)

- ◆ Three ways of counting
 - ◆ For a fixed time (count/time 1 – 1 sec)
 - ◆ Fixed Dose (count/dose 15 – 100000 monitor ct)
 - ◆ While moving a motor (count/rock theta; ct 21 → θ 2deg once)



"thinking" in Reciprocal Space

- ◆ For Polycrystalline or amorphous samples transformation to Q space is straightforward
- ◆ For a single crystal, Super has to know orientation of the crystal in diffractometer space
 - ◆ Need diffractometer settings for **two non-collinear reflections**.
 - ◆ Need to know the diffraction geometry and restrictions
 - ◆ E.g., 4-circle, kappa, GIXS, fixed omega. Etc
 - ◆ Restrictions imposed by a sample stage – cryostat, for example
- ◆ More in the hands-on sessions

A few Examples of Super Scans

◆ Single motor scan

- ◆ Scan m4 5 .1 10 1 (scan mtr# 4 from 5 to 6)

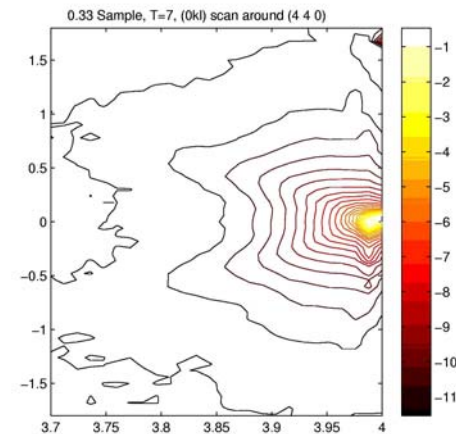
◆ Multiple motor scans

- ◆ Scan s2 1 4 0.02 2 2 0.01 100 21 (scan mtr# 1 from 4 to 6 and mtr# 2 from 2 to 3 – $2\theta - \theta$ scan)
- ◆ 5 motor scan if doing DAFS on single crystals

◆ Reciprocal Lattice Scans

- ◆ Scan I1 2 2 0 3 1 0 100 23 (scan from 220 → 310)
- ◆ Scan k0 8000 2 .001 10000 1 (scan from $Q = 2 \rightarrow 12$)

◆ Energy Scans, Time scans, 2D grid scan....



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- What it Looks Like?



Modes of operation

◆ Setup mode

◆ Interactive

◆ "disposable" filenames
(e.g. junk, align etc.)

◆ Doesn't look for beam
in the hutch before
starting a scan

◆ Data Collection mode

◆ Batch ->
Preprogrammed

◆ "Real" filenames (e.g.,
FAP_t300_x12 etc)

◆ Looks for beam before
and during a scan



Batch files

- ◆ Can list a set of “super” commands in an ascii file (called **indirect** file).
- ◆ Executing the indirect file will execute the listed super commands sequentially
- ◆ Note: the command to execute an indirect file is a super command too.



A Simple indirect file

- ◆ Optimize table
- ◆ Count/rock theta
- ◆ Filename Sample_16may06
- ◆ Scan s2 1 4 .1 2 2 0.05 500 21

Example of another Indirect file

File = **rast1mm.ind**

```
Optimize table

M3n 1
Ind apk 01
M3n 2
Ind apk 02
M3n 3
Ind apk 03
M3n 4
Ind apk 04
.....
```

File = **apk.ind**

```
Scan/beamdump
Count/rock theta
File FAP_t300_x@
Sample Fully ann. Plate T =300, x=@
Set 10 k0 8000 1 0.002 500 21

Scan 10

File align

Count/time

Scan/nobeamdump
```

variable

