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

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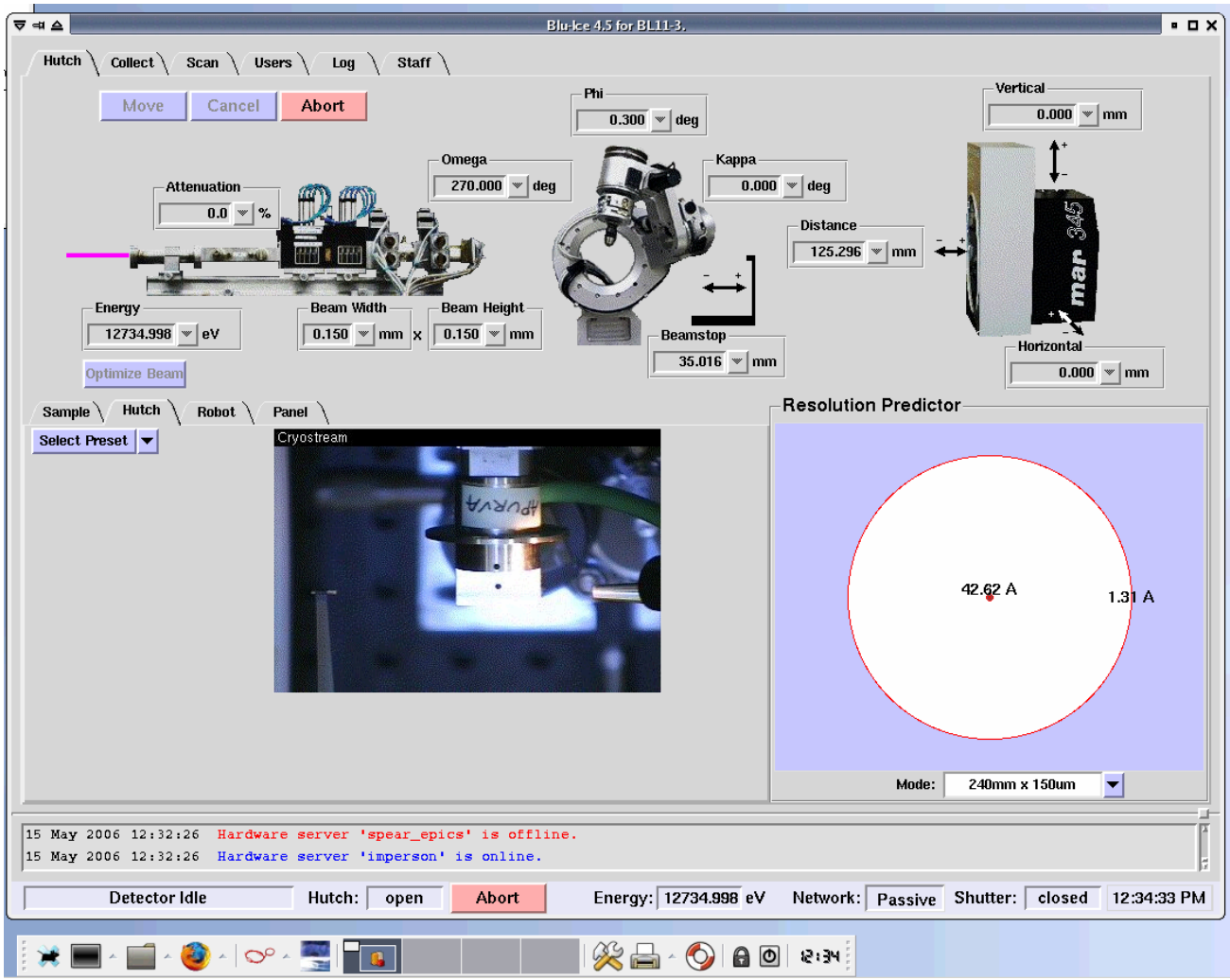
BluIce



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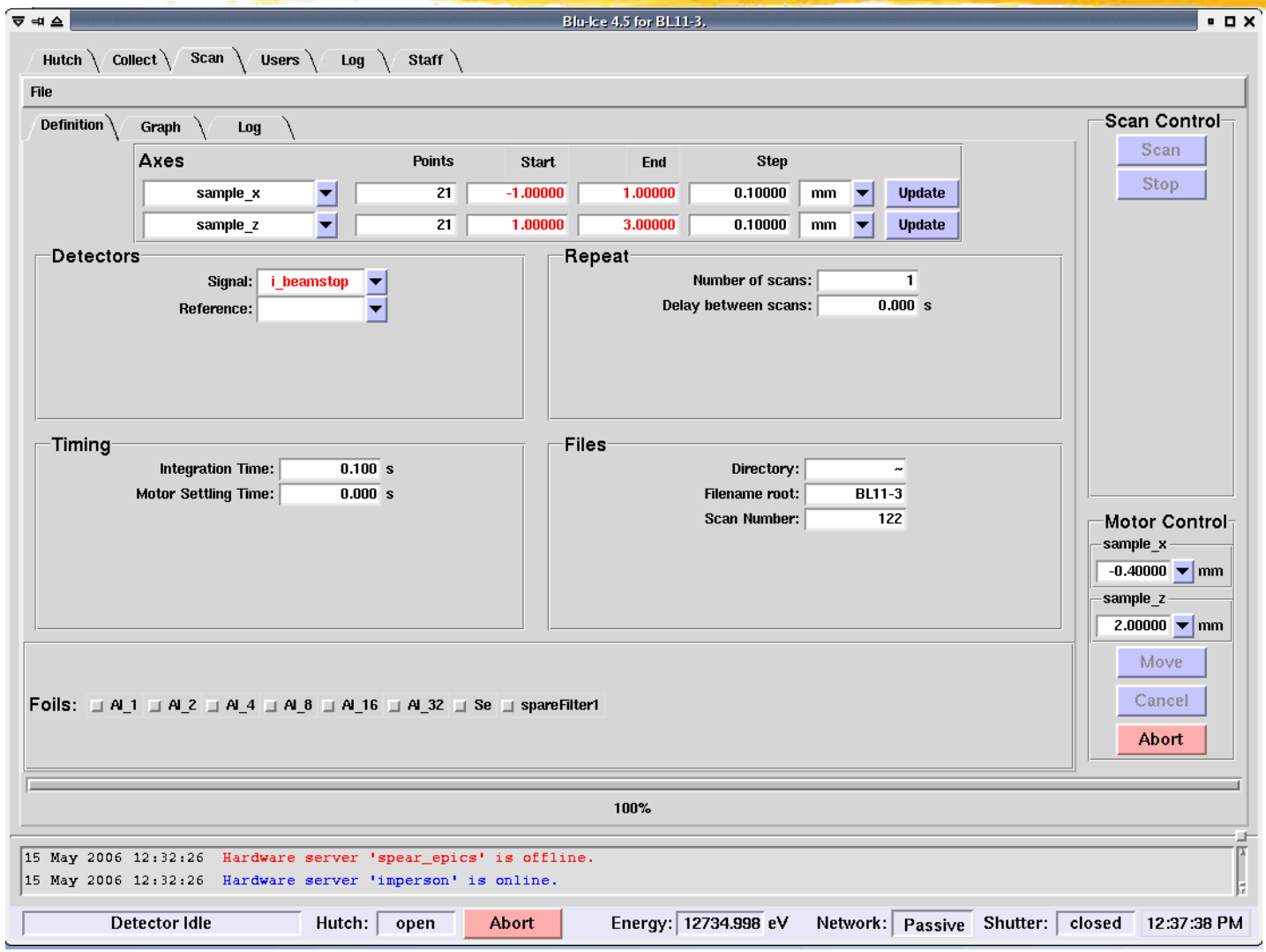
Bluice – Scan tab



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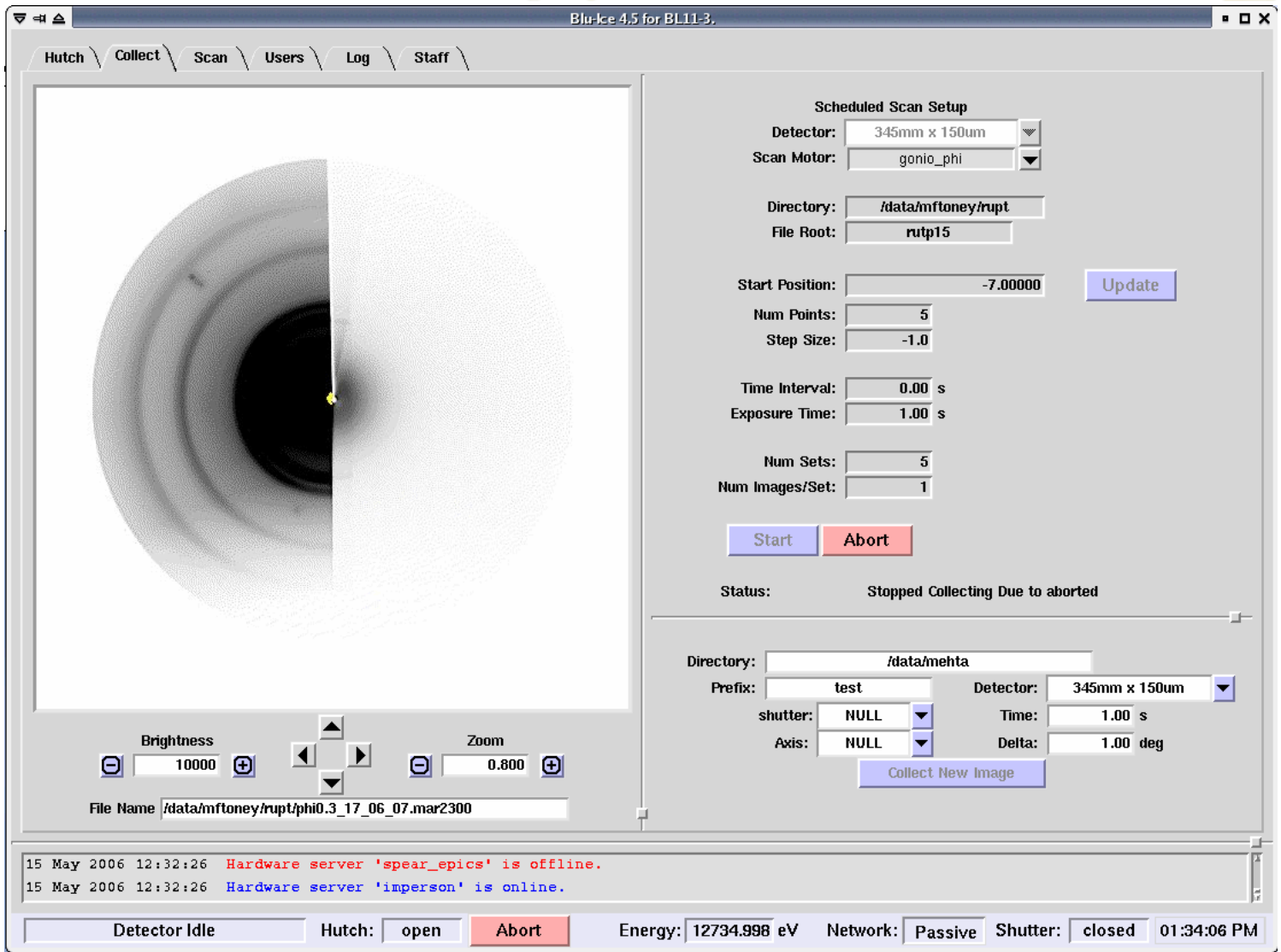
Bluice – Collect tab



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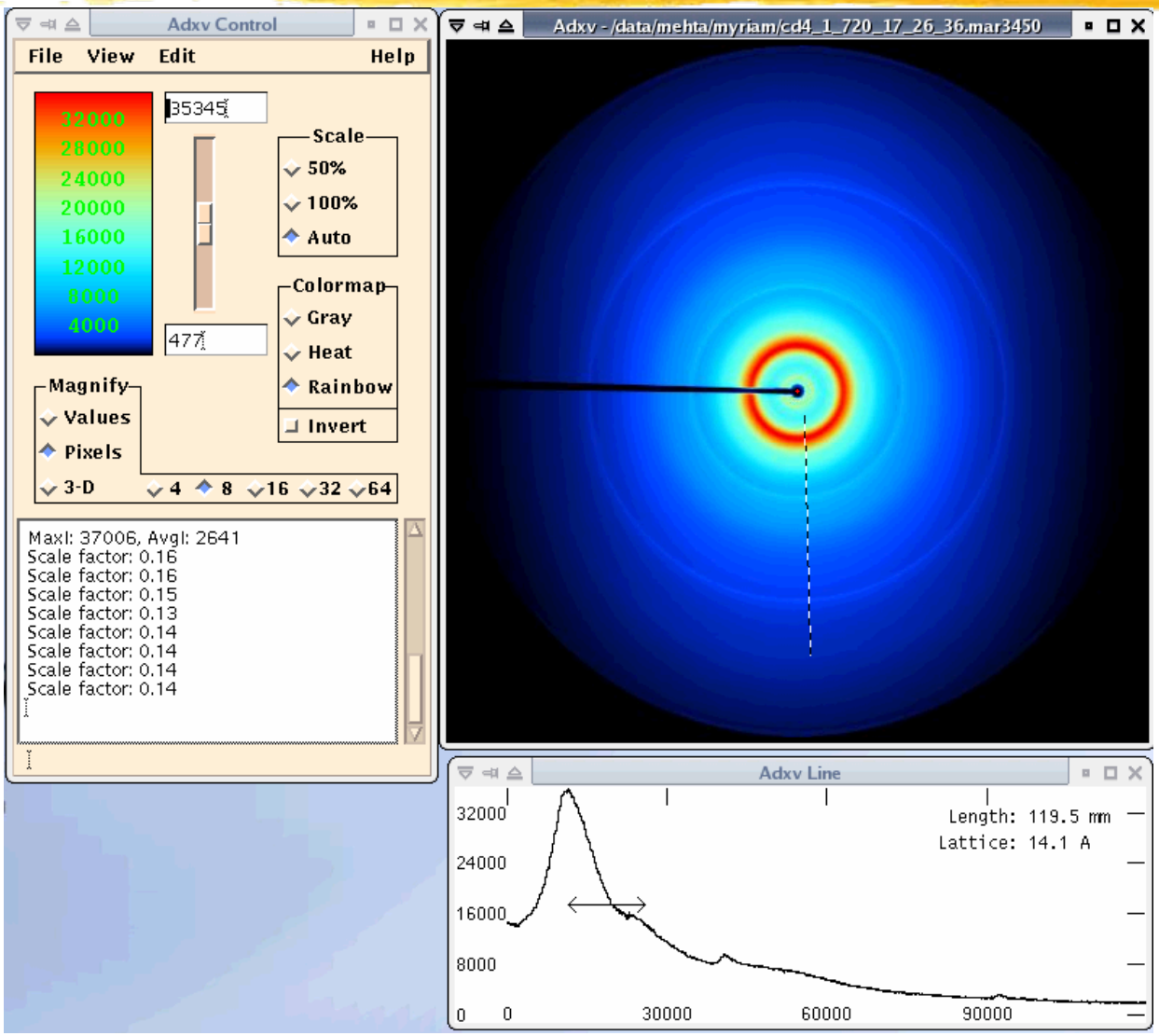
Preliminary Analysis



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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

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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”

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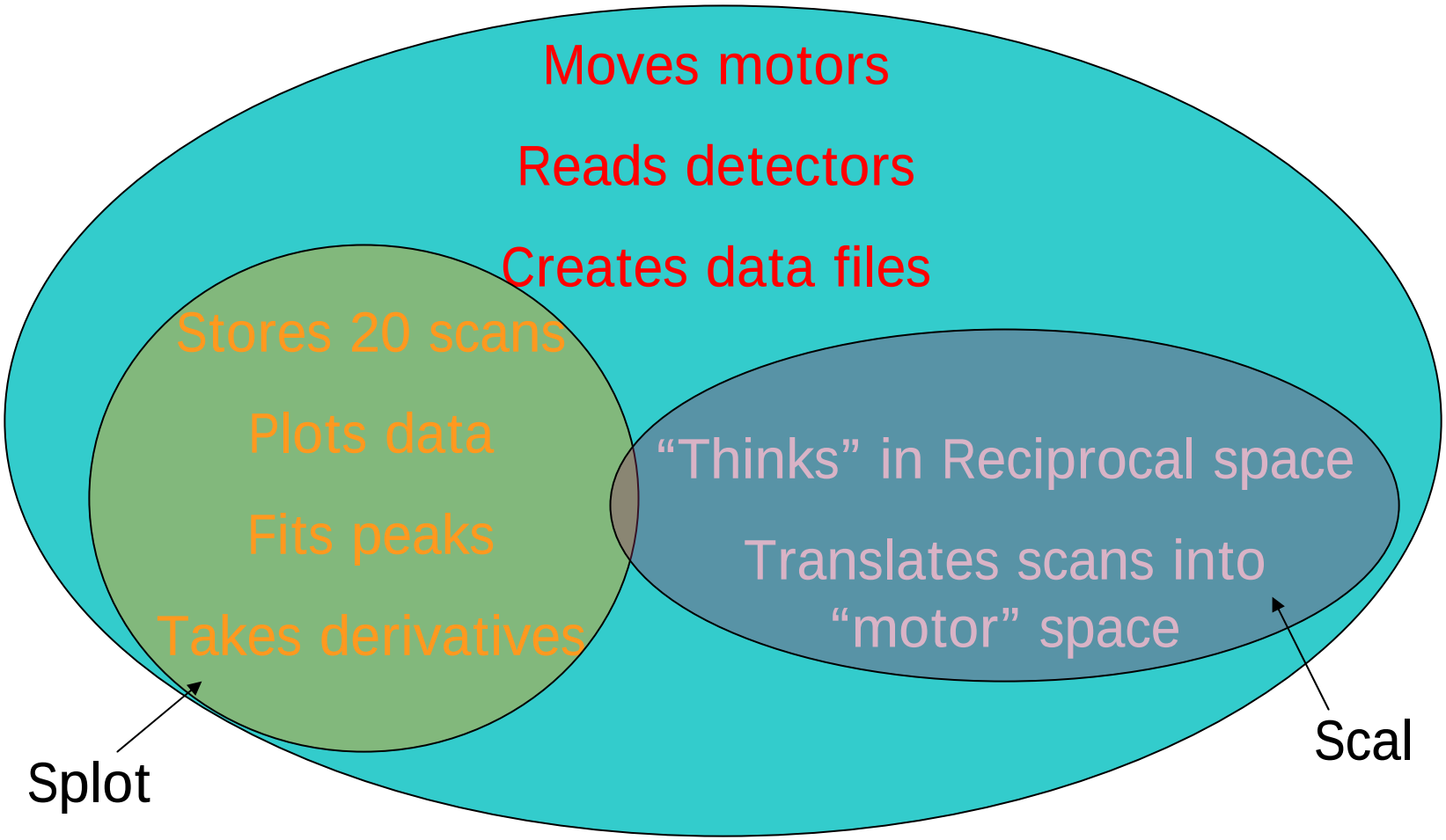
Some VMS Commands

- >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



Two Daughters

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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)

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“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-colinear 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

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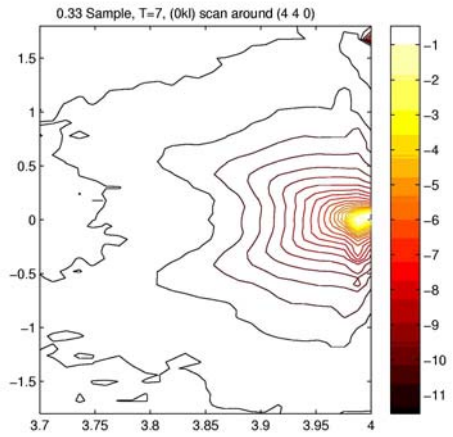
A few Examples of Super Scans

- 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 → 12)
- Energy Scans, Time scans, 2D grid scan....



- What it Looks Like?

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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.

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A Simple indirect file

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

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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

.....
```

variable

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
```