

# Data Management at EBIC: Getting your Data

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# Preparing your experiment (Computing services)

Before arriving at DLS:

- Ensure you have a **fed ID** (user account) and **password**  
Log in to DLS IT systems.  
Get access to the data during and after your experiment.
- Option Data Dispenser  
External hard-disk drive with own power supply.  
Recommended: **USB-3** is faster! (disk must be USB-3, USB-3 cable and use a USB-3 port on the Data Dispenser)

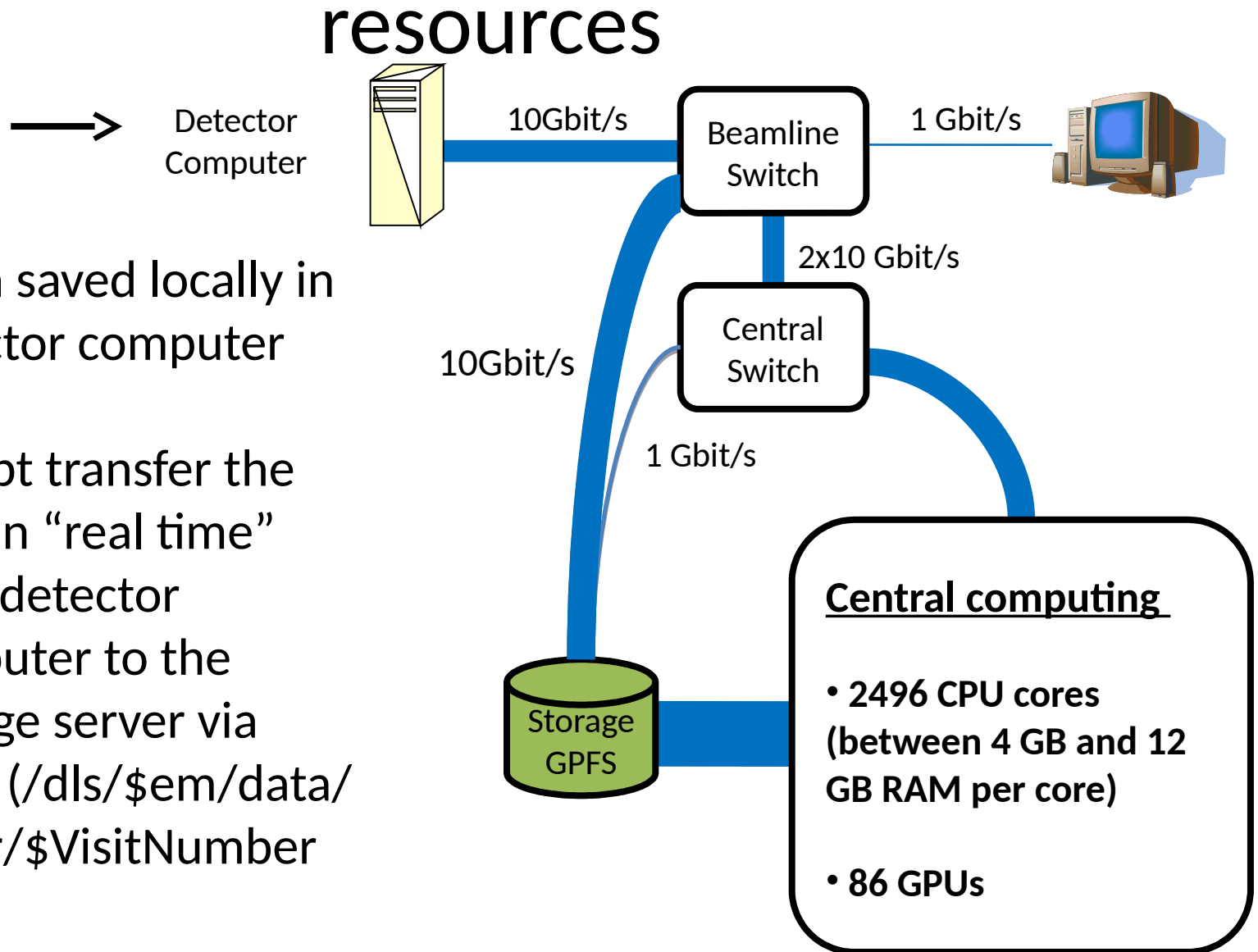
# Visit and proposal

- Proposal: <experiment type><number> e.g em325
- Visit number is Proposal-<visit> e.g em325-1

Note: Some proposal visits are > 100.

- Experiment type is em for Electron Microscopy.
- Experimental data will be in:
  - /dls/\$em/data/\$year/\$VisitNumber with \$em = m02 or m03.
  - You have read access to this area
  - You can process data in the processing subdirectory.

# Outline of current computing resources



- Data saved locally in detector computer

- Script transfer the data in “real time” from detector computer to the storage server via rsync (/dls/\$em/data/\$year/\$VisitNumber )

# Getting data

- At DLS:
  - Data dispenser
- At home institute:
  - **Within 40 days** since session:
    - Data size < 20 GB: ftp, sftp or rsync
    - Data size > 20 GB: **Globus**
  - **After 40 days** since session:
    - Data available on tape only (1 copy)
    - Use **TopCat**

# TopCat

## (icat.diamond.ac.uk)



	Name <input type="text" value="Containing..."/>	Size	Create Time <input type="text" value="From..."/> <input type="text" value="To..."/>	Modified Time <input type="text" value="From..."/> <input type="text" value="To..."/>
<input checked="" type="checkbox"/>	<a href="#">topdir</a>	1.45 kB	2013-06-26 10:55:36	2013-06-26 10:55:36
<input checked="" type="checkbox"/>	<a href="#">dc_sim14</a>	7.46 MB	2013-06-18 19:22:37	2013-06-18 19:22:37
<input checked="" type="checkbox"/>	<a href="#">dc_sim11</a>	7.46 MB	2013-06-18 19:22:37	2013-06-18 19:22:37
<input checked="" type="checkbox"/>	<a href="#">dc_sim13</a>	7.46 MB	2013-06-18 19:22:37	2013-06-18 19:22:37
<input checked="" type="checkbox"/>	<a href="#">dc_sim10</a>	14.93 MB	2013-06-18 19:22:37	2013-06-18 19:22:37
<input checked="" type="checkbox"/>	<a href="#">dc_sim12</a>	7.46 MB	2013-06-18 19:22:36	2013-06-18 19:22:36

# Conclusions (IT Guide)

1

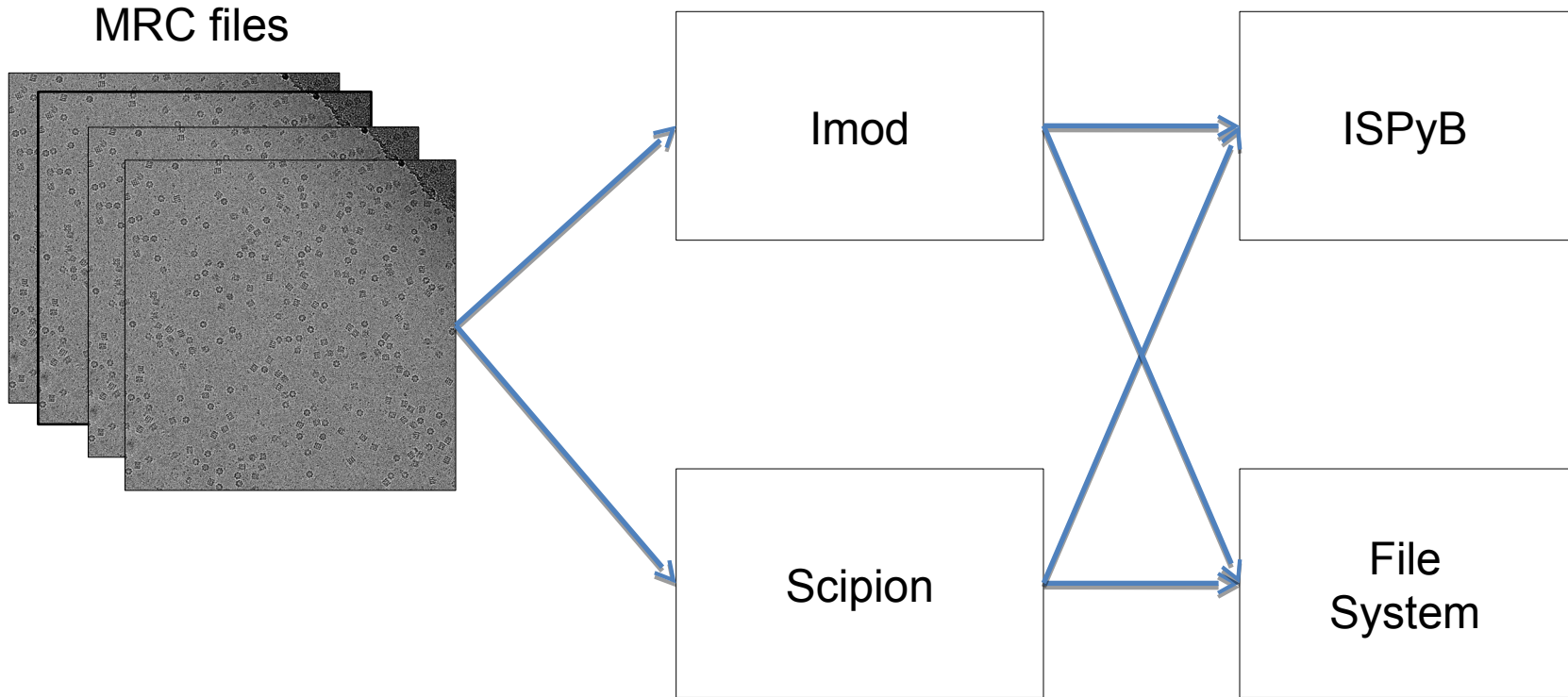


The screenshot shows the Diamond website's navigation structure. At the top is a dark blue header with the Diamond logo and a menu: About Us, For Users, Industry, Public, Science, Beamlines, Careers, More. A search bar is on the right. Below this is a blue banner with the text 'For Users' and a background image of a molecular structure and a diffraction pattern. Underneath the banner is a white navigation bar with links: Users, User Guide, Applying for Beamtime, Diamond Users Committee, FAQ, New User Administration System. A breadcrumb trail below reads 'Users / User Guide / IT User Guide'. On the left is a sidebar with 'In This Section' containing a numbered list of steps from 'Apply for Beamtime' to 'After your Beamtime'. Below this list is a blue button labeled 'IT User Guide'. The main content area is titled 'IT User Guide' and contains four blue boxes with icons and text: 'I am on-site' with 'Access your data', 'I am off-site' with 'Access Diamond desktop', 'Back-up data during your session', and 'Retrieve data after your session'. At the bottom, there are links for 'Bring your own kit', 'Linux help', 'Printing help', and 'Software at Diamond'. Three red numbers with blue arrows indicate navigation steps: '1' points to 'For Users', '2' points to 'User Guide', and '3' points to 'IT User Guide'.

2

3

# Data Processing Automation





# Imod



# Single Particle Analysis

The screenshot displays the SCIPION software interface for a project named "Project TutorialIntro". The interface is divided into several sections:

- Header:** "Project TutorialIntro" with version "devel (2016-08-02) cce98b9" and navigation links for "Protocols" and "Data".
- Left Panel (Navigation):** A tree view under "Protocols SPA" with categories: "Imports" (import movies, micrographs, particles, volumes), "Micrographs" (xmipp3 - optical alignment, grigoriefflab - unblur, grigoriefflab - summovie, xmipp3 - preprocess micrographs, CTF estimation), "Particles" (Picking, Extract, Preprocess, Filter, Mask), "2D" (Align, Classify), "3D" (Initial volume, Preprocess, Refine, Classify, Analysis, Reconstruct), and "Tools".
- Central Panel (Workflow Diagram):** A flowchart showing the analysis steps:
  - PROJECT (blue box)
  - 1. import mics 2 finished (green box)
  - 2. downsample x5 (copy) finished (green box)
  - xmipp3 - ctf estimation finished (green box)
  - xmipp3 - manual-picking (step 1) interactive (yellow box)
  - xmipp3 - auto-picking (step 2) finished (green box)
  - xmipp3 - extract particles finished (green box)
  - relion - 2D classification finished (green box)
- Bottom Panel (Summary):** A section titled "SUMMARY" with tabs for "Summary", "Methods", and "Output Log". It shows input/output details for "xmipp3 - ctf estimation" and a summary of CTF estimation results.

**SUMMARY**  
CTF estimation of 3 micrographs.  
The range of micrograph's experimental defocus was 1.089 - 2.243 microns.

# ISPyB

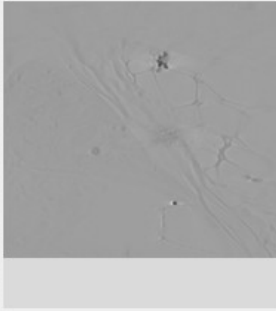
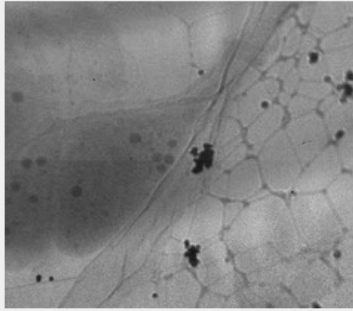
ISPyB » Data Collections » b24 » cm4981-5 - Mozilla Firefox

ISPyB » Data Collecti... x

https://ispyb.diamond.ac.uk/dc/visit/cm4981-5

04-07-2016 16:44:09 - raw/2015\_1206\_Square4\_area2\_tomo1\_4scopyingtesttingmessage3.txrm

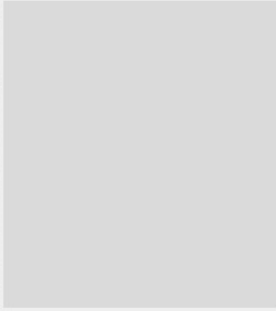
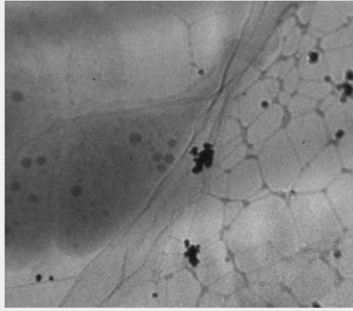
Wavelength: 0.00000Å	Calibrant:
Exposure: 1124s	Resolution: 0.000Å
Beamsize: 20x20µm	
Comment: searchable	



Data Files [Download](#)

04-07-2016 16:40:09 - raw/2015\_1206\_Square4\_area2\_tomo1\_4scopyingtesttingmessage2.txrm

Wavelength: 0.00000Å	Calibrant:
Exposure: 1124s	Resolution: 0.000Å
Beamsize: 20x20µm	
Comment: Click to edit	



Data Files [Download](#)

# Timescales

- Tomography – in testing now
- Single particle analysis – lead developer visiting us later this month