

ICAT use at Diamond

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Diamond Light Source



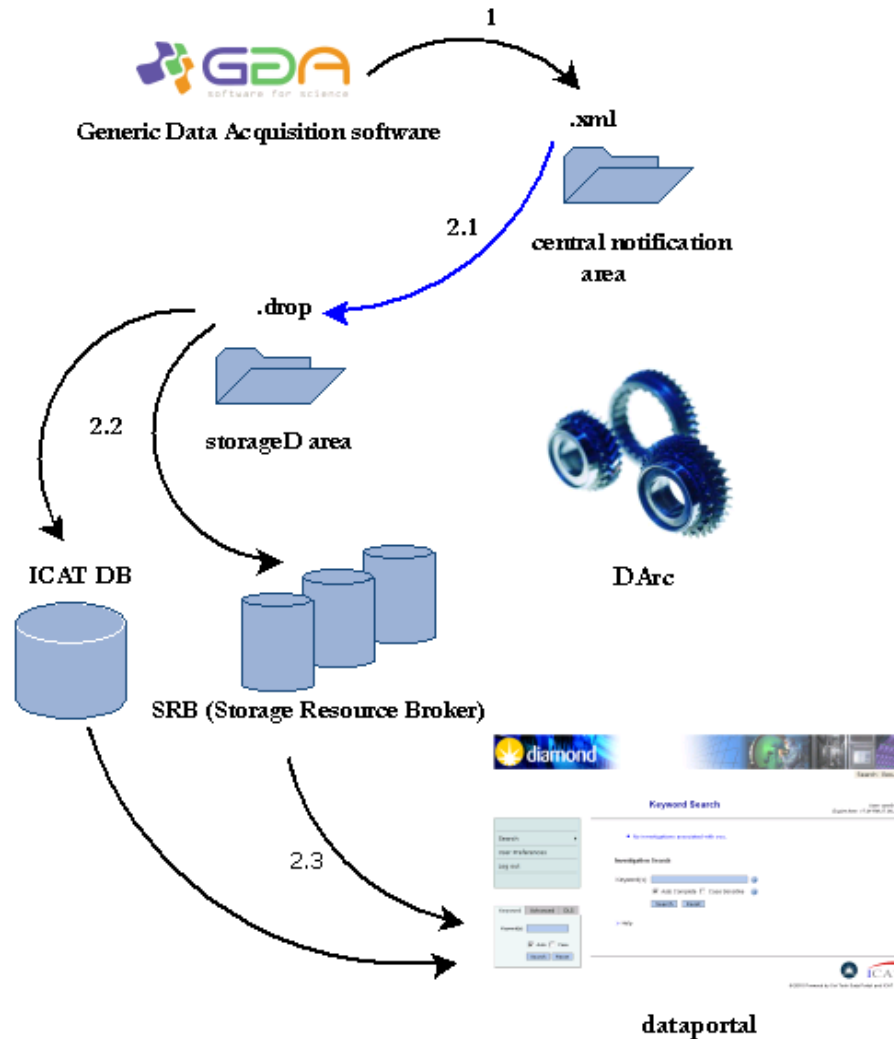
Diamond Light Source



ICAT as a catalogue for archived data

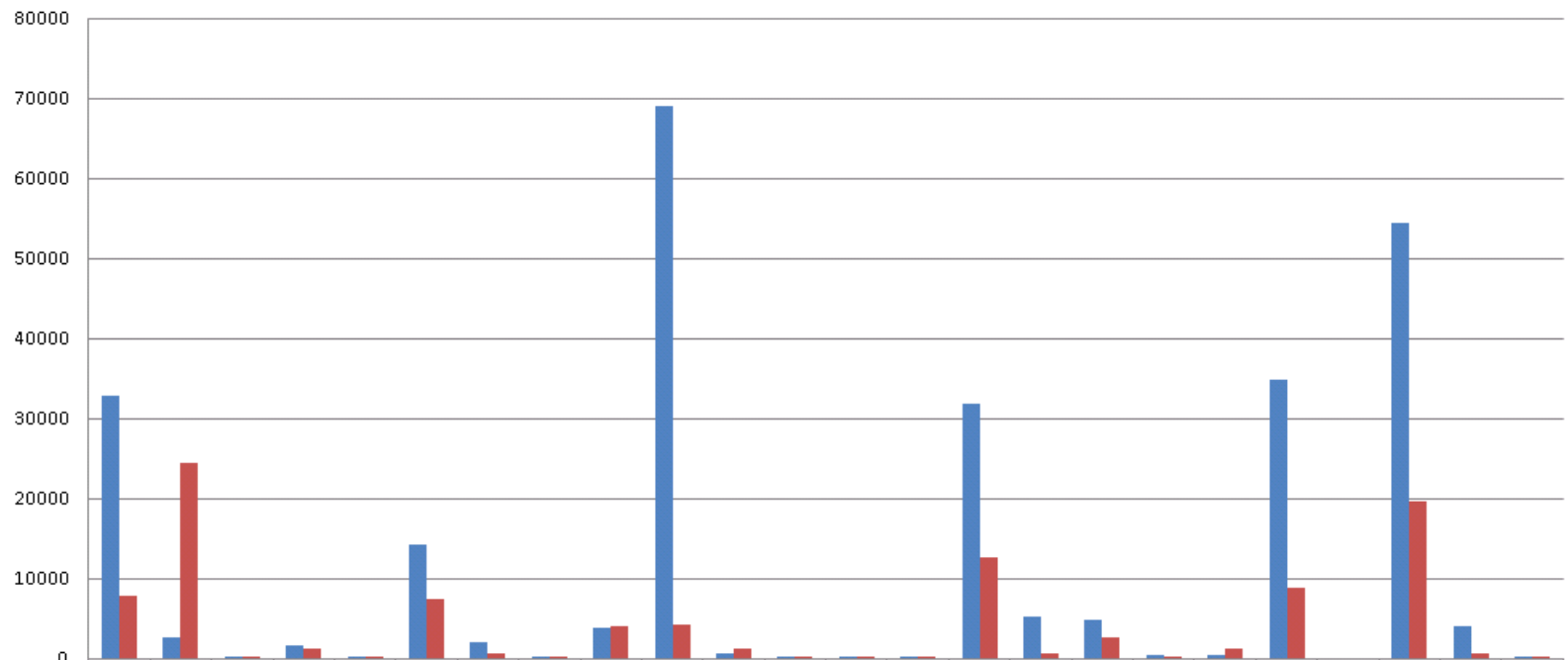


Data archiving – current version



Some statistics

Size and number of files catalogued in ICAT by beamline



Some statistics (cont.)

- Total size ~ 260 Terabytes
- Total number of files ~ 98,497,014 files
- Currently running at 0.5 to 1 Terabyte/day

ICAT integration with SDA



SDA (Scientific Data Analysis)

- A collection of supported, generic and bespoke, RCP views compiled into a number of application or perspectives.
- Views developed by Scientific Software and Data Acquisition teams
 - Plotting
 - ‘simple’ analysis tools
 - Python/Jython tools
 - Eclipse data project
 - File/s viewing
 - Workflow tool
 - ICAT archive explorer and data retrieve

SDA perspectives and views

The screenshot displays the SDA (Software for Data Analysis) interface with several key components:

- File Navigator:** Shows a tree view of the project structure, including folders like 'i05', 'i11', 'I22-NCDReduction', 'MXData', and 'MX-SDA-Training'. A list of data files (DC_0001.cbf to DC_0008.cbf) is visible.
- Image Explorer View:** Displays a grid of diffraction images. A blue selection box highlights a specific image in the top-left corner.
- Dataset Plot:** Shows a 3x3 grid of diffraction images. A green selection box highlights the image in the bottom-left corner.
- Header Dataset Plot:** A table listing metadata for the selected dataset.
- 3D Visualization:** A 3D wireframe model of a detector or sample stage, showing a grid and two vertical axes.

Large blue arrows indicate the flow of information: from the File Navigator to the Image Explorer, from the Image Explorer to the Dataset Plot, and from the Dataset Plot to the 3D visualization.

Key	Value
# Count_cutoff	1220 counts
# Angle_increment	0.30 deg.
# Filter_transmission	1.00
# Silicon sensor, thickness	0.00
numPixels_y	167
numPixels_x	1475
# Flat_field:	(nil)
# N_excluded_pixels =	255
# Detector_distance	0.22270 m
Unknown 1	# 2011-04-19T04:51:31.047
Unknown 0	# Detector: PILATUS 2M, 5/N 24-01...
# Polarization	0.990
Unknown 5	# Image_path: /dls/i04-1/data/2011...
Unknown 4	# Trim_file: p2m0107_E14000_T700...
Unknown 3	# Gain_setting: low gain (vrf = -0.300)
Unknown 2	# Threshold_setting: 7000 eV
# Flux	0.0000
# Tau =	124.0e-09 s
# Start_angle	90.0000 deg.
# Wavelength	0.91730 Å
# Excluded_pixels:	badpix_mask.tif
# Pixel_size	172e-6 m x 172e-6 m
# Exposure_time	0.9964000 s

X position	Y position	Data value	q X (1/Å)	q Y (1/Å)	q Z (1/Å)	2θ (°)	Re
680.5729	738.2269	45.0000	0.2802	0.5349	-0.0267	5.058	10

ICAT Explorer eclipse plugin

- Integrated with the SDA to allow the use of other plugins on user's data files.
- Linked to the ICAT hosted at STFC, webservice V3.3.4
- Security based on fedid/password authentication + HTTPS
- Drag-and-drop to local file system using SFTP
- A step-by-step tutorial cheat sheet
- GENERIC – can be easily customized to be used at any facility (ISIS, ILL, etc)

ICAT Explorer – connection wizard

ICAT Project Wizard - creates a connection to an ICAT database
Wizard to create an ICAT connection to browse datafiles

ICAT site ID:

ICAT site name:

FedId:

Password:

Project name:

SFTP server:

Download directory:

ICAT -

File Edit Navigate Search Project Run Window Help

ICAT Resource

Project Explorer

- data
 - DLS_Archive
 - 2007
 - 2008
 - 2009
 - 2010
 - 2011
 - 2012
 - AllVisits
 - Beamlines
 - B16
 - B23
 - I02
 - 2007
 - 2008
 - 2009
 - 2010
 - 2011
 - 2012
 - CM5697-1 I02 2012-01-02 2012-01-22
 - 0213
 - 0223/gridtest
 - test_1_0001.img 18 MB 2012-02-23 15:21:54
 - test_2_0001.img 18 MB 2012-02-23 15:23:18
 - test_2_0002.img 18 MB 2012-02-23 15:23:20
 - test_2_0003.img 18 MB 2012-02-23 15:23:22
 - test_2_0004.img 18 MB 2012-02-23 15:23:23

Metadata View Dataset Inspector

Key	Value
NAME	test_2_0002.img
CREATION_TIME	2012-02-23 15:23:20
DESCRIPTION	unknown
UNIQUE_ID	
DATASET_ID	769158
LOCATION	/dls/i02/data/2012/cm5697-1/0223/gridtest/test_2_0002.img
MODIFICATION_TIME	2012-02-23 15:23:20
VERSION	1.0

1 items selected



ICAT Explorer – collaborating with the rest of SDA plugins

File Edit Navigate Search Project Run Window Help

Project Explorer File Navigator

DLS_Archive

- 2007
 - EE427-1 i15 2007-10-29 2007-11-10
 - MT428-1 i16 2007-10-29 2007-11-10
 - MT428-2 i16 2007-11-22 2007-11-28
 - MX423-1 i02 2007-10-29 2007-11-10
 - MX424-1 i03 2007-10-29 2007-11-10
 - MX425-1 i04 2007-10-29 2007-11-10
 - NT177-3 i02 2007-09-24 2007-09-26
 - NT20-3 i03 2007-07-24 2007-07-25
 - NT20-4 i02 2007-09-19 2007-09-27
 - NT20-5 i03 2007-10-26 2007-11-03
 - NT20-6 i03 2007-11-30 2007-12-01
 - SI426-1 i06 2007-10-29 2007-11-10
 - SI426-2 i06 2007-11-22 2007-11-28
 - SM430-1 i22 2007-10-29 2007-11-07
 - SP429-1 i18 2007-10-29 2007-11-07
 - SW19-1 i24 2007-06-21 2007-06-24
 - SW19-2 i24 2007-08-08 2007-08-09

i22-34820.nxs 2495.nxs

Name	Class	Dims	Type	Data
HDF5_Version	Attr		STRING	1.8.7
NeXus_version	Attr		STRING	4.2.1
file_name	Attr		STRING	/dls/i22/data/2011/swf
file_time	Attr		STRING	2011-08-06T03:16:15
entry1	NXentry			
Pilatus2M	NXdata			
data	SDS	1, 1, 1679, INT32		double-click to view
Scalars	NXdata			
TfgTimes	NXdata			
instrument	NXinstrument			
user01	NXuser			
entry_identifier	SDS		STRING	34820
program_name	SDS		STRING	GDA 8.14.0
scan_command	SDS		STRING	static readout
scan_dimensions	SDS	1	INT32	1
scan_identifier	SDS		STRING	ab383e84-0eeb-4e6c
title	SDS		STRING	AgBe

Dataset Plot

X position Y position Data value Dataset name

---- ---- ---- data

Metadata View

Key	Value
START_DATE	2007-10-29 09:00:00
END_DATE	2007-11-10 09:00:00
FACILITY	DLS
INSTRUMENT	i15
ID	8632875
INV_NUMBER	EE427

Data axes selection

Name: data; Rank: 4; Dims: [1, 1, 1679, 1475]

Dim	Selection
1	✓ dim:1
2	✓ dim:2
3	✓ dim:3
4	✓ dim:4

2D scatter plot 2D image \gg_{10}

x-axis dim:4

y-axis dim:3

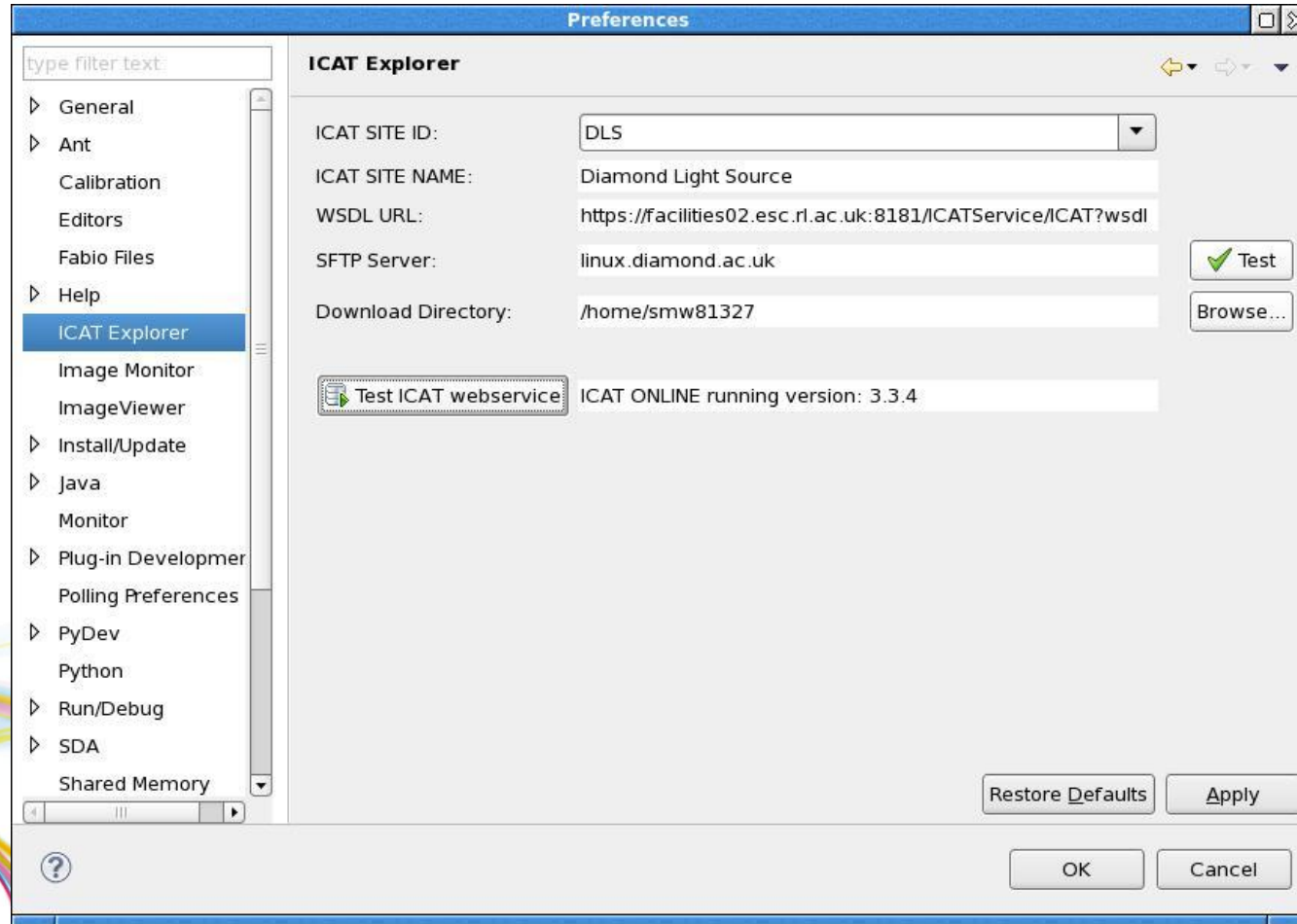
Dataset slicing

Dim	Start position	Start value	Items	Step size
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Side: Dataset Plot

Data Value Colour Mapping: Dataset Plot

ICAT Explorer - customization



Future Possibilities

- DOI, exploring publishing DLS data with DOI
- Integration with workflows:
 - Linking in with future analysis tools
 - Building advanced searches/interactions with DB
 - High level tool to create archive pipeline (Alun can cope with since its as easy as bash but no python)

Working on...

- Admin modes in project explorer: add, delete, modify
- Add search functionality/view
- More enhancements based on users feedback
- Make the code public on GitHub (<https://github.com/>)?