



# ICAT

## A Facility Metadata Catalogue

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November 2013

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# What is ICAT?

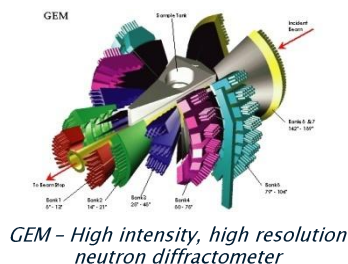
ICAT is a database, with a well defined API that provides a uniform interface to experimental data and a mechanism to link all aspects of research from proposal through to publication.



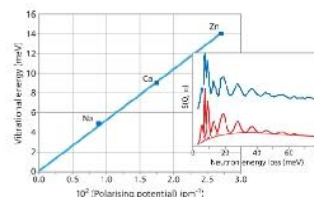
# What is ICAT?



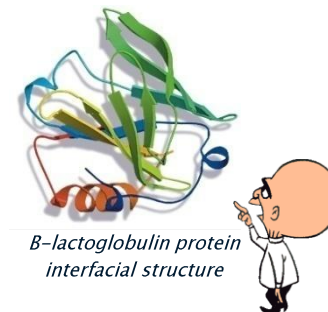
Example ISIS Proposal



GEM - High intensity, high resolution neutron diffractometer



H<sub>2</sub>-(zeolite) vibrational frequencies vs polarising potential of cations



B-lactoglobulin protein interfacial structure

## ICAT

### Proposals

Once awarded beamtime at ISIS, an entry will be created in ICAT that describes your proposed experiment.

### Experiment

Data collected from your experiment will be indexed by ICAT (with additional experimental conditions) and made available to your experimental team

### Analysed Data

You will have the capability to upload any desired analysed data and associate it with your experiments.

### Publication

Using ICAT you will also be able to associate publications to your experiment and even reference data from your publications.



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# Benefits

- Links proposal to data to analysis to publication
- Makes data searchable
- Remote data access
- Assign DOIs to data
- Increased opportunities for data sharing and re-use
- Implements a data policy
- Provenance (Creation, ownership, history)
- Integration with applications
- Relate data to analysis software



# Where is it used?

- STFC (main developer)
  - ISIS pulsed neutron and muon facility
  - CLF (UK national laser facility)
- Diamond
  - UK national synchrotron
- ILL, ESRF, ELETTRA
- Oak Ridge National Laboratory (USA)
  - Spallation Neutron Source, HIFIR
- JET (Fusion)





## Existing Users

# Sign in here



Email:

[Forgot Email?](#)

Password:

[Forgot Password?](#)**Sign In**

Using a public or shared computer? Be sure to sign out when you've finished and close all windows to end your session.

OR

**Sign in with**  **umbrella**



## No online account?


# Register

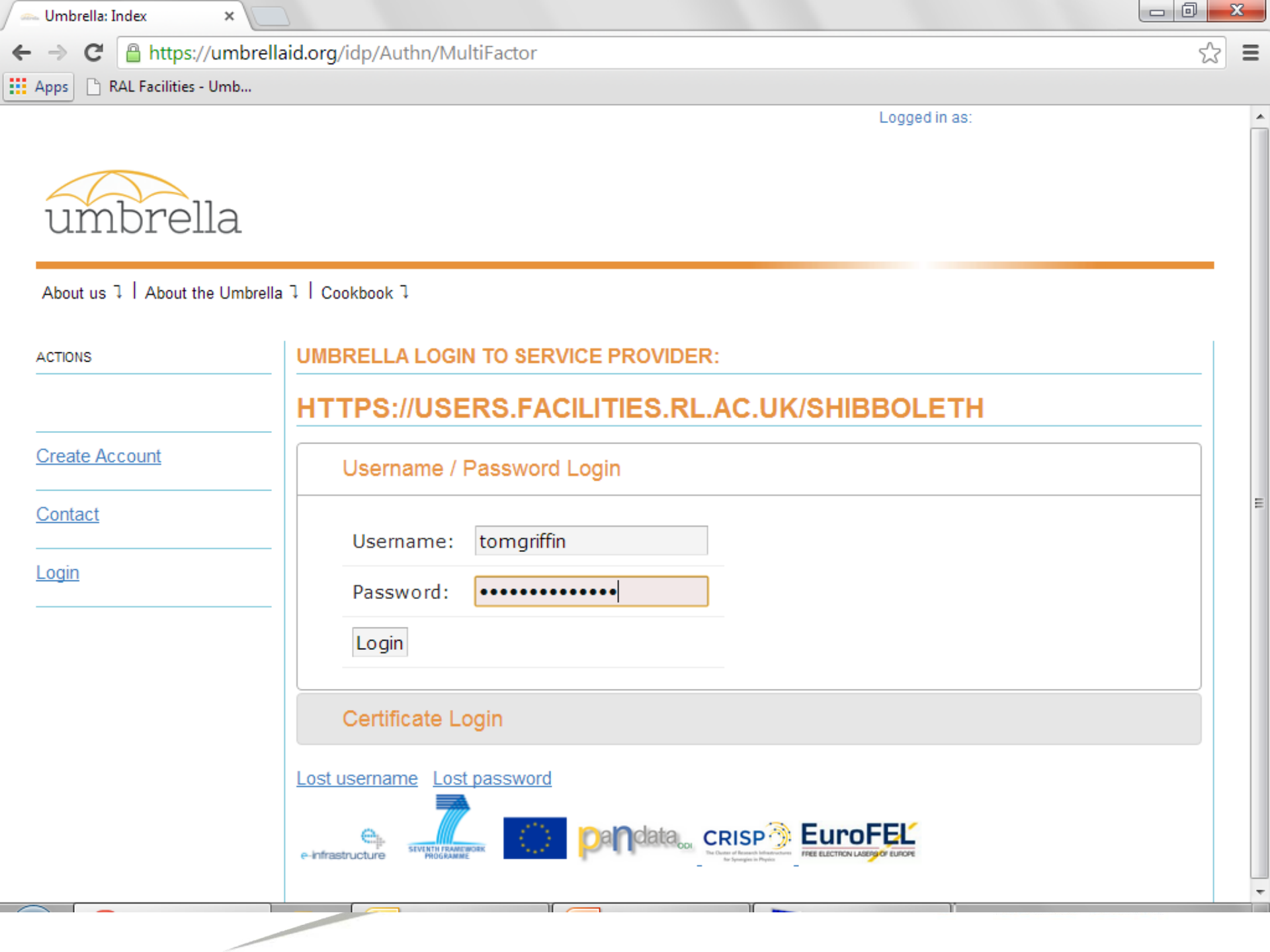
If this is your first time using this website  
please read our

**Terms and Conditions**

before you

**Create a new facility user account  
with us**

If you have an  umbrella account you can link this during sign up.



About us | About the Umbrella | Cookbook

ACTIONS

Create Account

Contact

Login

UMBRELLA LOGIN TO SERVICE PROVIDER:

HTTPS://USERS.FACILITIES.RL.AC.UK/SHIBBOLETH

Username / Password Login

Username: tomgriffin

Password: .....

Login

Certificate Login

Lost username Lost password





## SELECT FACILITY

**ISIS Facility**

Central Laser Facility

Research Complex @  
Harwell

MICE @ RAL



ISIS is a world-leading centre for research in the physical and life sciences at the Rutherford Appleton Laboratory. We support a national and international community of more than 2000 scientists for research into subjects ranging from clean energy and the environment, pharmaceuticals and health care, through to nanotechnology, materials engineering and IT.



## Proposal System

For each experiment at one of our facilities, a proposal outlining the scientific case must be submitted.



## Visits System

Please tell us when you are coming (even if you don't want accommodation or travel) so we can get things like passes ready for you.

Note: If your Principal Investigator has already done this for your group you do not need to do it again.



## Your Details

Please keep your personal details up to date so we can keep in touch. It is especially important you keep your email address up-to-date.





## Facility Safety Test System

Please make sure you have passed the appropriate safety tests before coming to RAL. It is also important that they do not expire just before you arrive or during your visit.

[Take a test »](#)

## Experimental Risk Assessment System

Please ensure that at least one member of the experimental team due to visit ISIS has submitted an ERA for the experiment. This ERA must be approved in plenty of time in order for ISIS staff to properly prepare for your visit.

[Submit an ERA »](#)

## Facility Awareness

Please check you have read the facility awareness pages. You must have ticked to acknowledge you have read and understood the information in order for our staff to grant you access to the halls.

[Read the pages »](#)

## ISIS Data Catalogue

All data produced at ISIS is catalogued into ICAT – the ISIS data catalogue. [What is ICAT and how do I use it?](#)

[Get your data »](#)


TOPCAT web tool for mul

← → ↺

https://data4.isis.stfc.ac.uk/TOPCATWeb.jsp#view///&tab=MyData

☆ ☰

Apps RAL Facilities - Umb...



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icatisis Logout

My DataMy DownloadsSearchBrowse All Data

Get Investigations

Facility Name	Investigation Number	Visit Id	Title	Start Date	End Date
icatisis	13868	1 - HET	YbFe2Ge2 t/ccr cooling 150 mev 5s jaws 40x4...	09/11/2002 00:39	07/10/2003 22:21
icatisis	720206	1 - SXD	Single-Crystal Neutron Diffraction Study on [U(...	12/10/2007 10:55	16/04/2008 18:02
icatisis	820232	1 - CRISP	Magnetic moment of EuO in spin filtering magne...	19/02/2009 13:34	25/02/2009 08:05
icatisis	890086	1 - LOQ	Conformation of poly(3-hexyl thiophene)		
icatisis	1010392	1 - INTER	Smectic Wetting at Nematic Surfaces	19/05/2011 05:23	21/05/2011 09:02
icatisis	1010440	1 - EMU	Muon Spin Relaxation studies of Ni2TCNQ, Ni(T...	12/07/2010 11:55	22/07/2010 09:44
icatisis	1110191	1 - EMU	Source of Electronic Magnetism in Palladium Bio...	07/07/2011 11:36	12/07/2011 09:11
icatisis	1110332	1 - EMU	Motion of Positively Charged Muonium Centres i...	21/05/2011 10:28	26/05/2011 07:22
icatisis	1110334	1 - HRPD	ATOMIC AND MAGNETIC STRUCTURE OF THE ...	13/04/2011 10:07	15/04/2011 09:21
icatisis	1110460	1 - EMU	Spin glass behaviour in the disorder-free geom...	16/03/2011 17:21	24/03/2011 09:06
icatisis	1110529	1 - HIFI	The role of spin fluctuations, disorder and non-...	30/10/2011 10:02	29/05/2012 10:25
icatisis	1120157	1 - EMU	Fluctuating stripes in an insulating hole-doped a...	15/10/2011 11:24	17/07/2012 09:29
icatisis	1120344	1 - EMU	Magnetic Ordering in the Candidate Random Qu...	29/11/2011 11:16	01/12/2011 08:55
icatisis	1193002	1 - LOQ	testing emails- PLEASE IGNORE!!		
icatisis	1193027	1 - LOQ	Testing postal address		

Page 1 of 2

Displaying 1 - 15 of 16

Accessibility | Privacy Policy | Data Policy | Terms Of Use | Complaints Procedure | Feedback

icatisis	1110529	1 - HIFI	The role of spin fluctuations, disorder and non-...	30/10/2011 10:02	29/05/2012 10:25
icatisis	1120157	1 - EMU	Fluctuating stripes in an insulating hole-doped a...	15/10/2011 11:24	17/07/2012 09:29
icatisis	1120344	1 - EMU	Magnetic Ordering in the Candidate Random Qu...	29/11/2011 11:16	01/12/2011 08:55
icatisis	1193002	1 - LOQ	testing emails- PLEASE IGNORE!!		
icatisis	1193027				

## Datafile Window

Download

<input type="checkbox"/>	File Name	File Location	File Size	Format	Format Version	Format Type	Create
Dataset Name: Default (20 Items)							
<input type="checkbox"/>	EMU00024428....	\\isis\inst\$\Instr...	0.944 MB	nexus	4.3.0	HDF4	21/05/2011 10:2
<input type="checkbox"/>	EMU00024429....	\\isis\inst\$\Instr...	1.094 MB	nexus	4.3.0	HDF4	21/05/2011 10:5
<input type="checkbox"/>	EMU00024430....	\\isis\inst\$\Instr...	0.885 MB	nexus	4.3.0	HDF4	21/05/2011 13:1
<input type="checkbox"/>	EMU00024431....	\\isis\inst\$\Instr...	1.038 MB	nexus	4.3.0	HDF4	21/05/2011 13:4
<input type="checkbox"/>	EMU00024432....	\\isis\inst\$\Instr...	1.212 MB	nexus	4.3.0	HDF4	21/05/2011 15:3
<input type="checkbox"/>	EMU00024433....	\\isis\inst\$\Instr...	1.112 MB	nexus	4.3.0	HDF4	21/05/2011 19:0
<input type="checkbox"/>	EMU00024434....	\\isis\inst\$\Instr...	0.887 MB	nexus	4.3.0	HDF4	21/05/2011 21:2
<input type="checkbox"/>	EMU00024435....	\\isis\inst\$\Instr...	1.208 MB	nexus	4.3.0	HDF4	21/05/2011 22:0
<input type="checkbox"/>	EMU00024436....	\\isis\inst\$\Instr...	1.21 MB	nexus	4.3.0	HDF4	22/05/2011 01:2
<input type="checkbox"/>	EMU00024437....	\\isis\inst\$\Instr...	1.257 MB	nexus	4.3.0	HDF4	22/05/2011 04:5
<input type="checkbox"/>	EMU00024438....	\\isis\inst\$\Instr...	1.097 MB	nexus	4.3.0	HDF4	22/05/2011 09:1
<input type="checkbox"/>	EMU00024439....	\\isis\inst\$\Instr...	1.109 MB	nexus	4.3.0	HDF4	22/05/2011 11:4

Page 1 of 5

Displaying 1 - 20 of 82

Show Data Sets Download Investigation

## Investigation Details

Facility: icatisis

Instrument: EMU

Title: Motion of Positive

Investigation No: 1110332

Visit Id: 1 - EMU

Start Date: 21/05/2011 10:28

End Date: 26/05/2011 07:22

Investigators: principal\_experim  
 experimenter - Dr Gurkan Celebi  
 experimenter - Mr Rick Mengyan  
 experimenter - Mr Tom Griffin  
 experimenter - Ms Brittany Baker

## Proposal:

We propose further zero-field muon spin depolarization measurements at temperatures above 300K in order to determine barriers for thermal diffusion of positively charged muonium in ZnO, TiO<sub>2</sub> and other transparent conducting oxides. We have found that the Mu<sup>+</sup> centre undergoes local quantum tunnelling and a site change, but not extended

# Client Applications

- A key requirement for facilities
- Web is not enough (yet?)
- 'ECP' – a way to link Umbrella to these applications
- 'Moonshot' could play a role



# Interfaces - Mantid

The screenshot displays the MantidPlot software interface, titled "MantidPlot - untitled". The main menu bar includes File, Edit, View, Windows, Interfaces, Catalog, and Help. The toolbar contains various icons for file operations, data manipulation, and visualization. The MS Shell Dlg 2 shows the command prompt with the text "0 B It U x^2 x\_2 dß r f".

The Results Log panel shows the following entries:

- CatalogLogin started
- CatalogLogin successful, Duration 1.63 seconds
- CatalogMyDataSearch started
- CatalogMyDataSearch successful, Duration 1.30 seconds
- CatalogGetDataSets started
- CatalogGetDataSets successful, Duration 0.25 seconds
- CatalogGetDataFiles started
- CatalogGetDataFiles successful, Duration 39.94 seconds
- CatalogGetDataFiles successful, Duration 30.94 seconds

The Results: 8 Investigations Found panel displays a table of search results:

	Instrument	Run R
insulating hole-doped antiferromagnet	EMU	26352-
Candidate Random Quantum Spin Chain Sr3CuPtIr1-xO6	EMU	27801-
arged Muonium Centres in Transparent Conducting Oxides	EMU	24428-
Diffraction Study on [U(C5Me5)2(H)(muH)]2	SXD	19913-
natic Surfaces	INTER	9594-9
agnetism in Palladium Bionanoparticles	EMU	24943-
	LOQ	

The Investigation Data panel shows the following data:

Data: 7082 DataFiles found

Name	Location
SXD19913.RAW	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Beam_Current.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Head_MaxPower.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Head_Temp.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_ICPevent.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Sample_MaxPower.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Sample_Setpoint.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Sample_Temp.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_Status.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19913_WCCR.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19914.RAW	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19914_Beam_Current.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19914_Head_MaxPower.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19914_Head_Temp.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...
SXD19914_ICPevent.txt	\\isis\inst\$\Instruments\$\NDXSXD\Instrument\d...

The Workspaces panel shows the following workspaces:

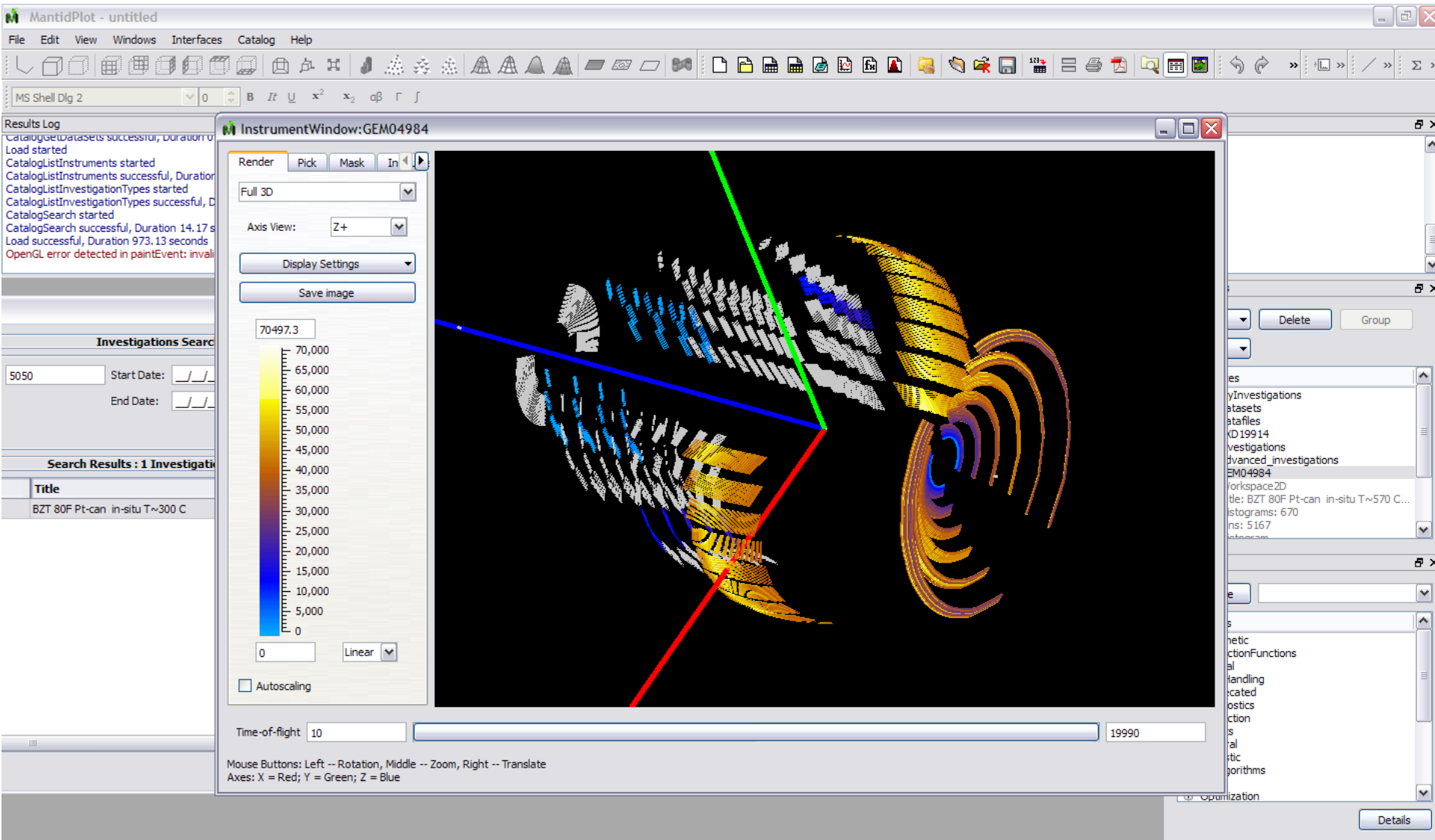
- MyInvestigations
- datasets
- datafiles

The Algorithms panel shows the following algorithms:

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Deprecated
- Diagnostics
- Diffraction
- Events
- General
- Inelastic
- MDAlgorithms
- Muon
- Optimization

The bottom status bar shows the following icons: a series of peaks, a grid, a magnifying glass, a document, a trash can, and a refresh button.

# Interfaces - Mantid



# Summary

- ICAT is a mature solution for facility metadata management
- Enables remote data access and linking between proposals, data, analysis and publications
- Flexible architecture enables integration with differing facility systems and requirements
- API enables integration with other software (analysis)
- Open source project with an active collaboration

