

Mantid & ICAT



About me

```
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```

Agenda

- 1.** Mantid
- 2.** ICAT within Mantid
- 3.** IDS within Mantid
- 4.** Future plans
- 5.** Questions

Mantid

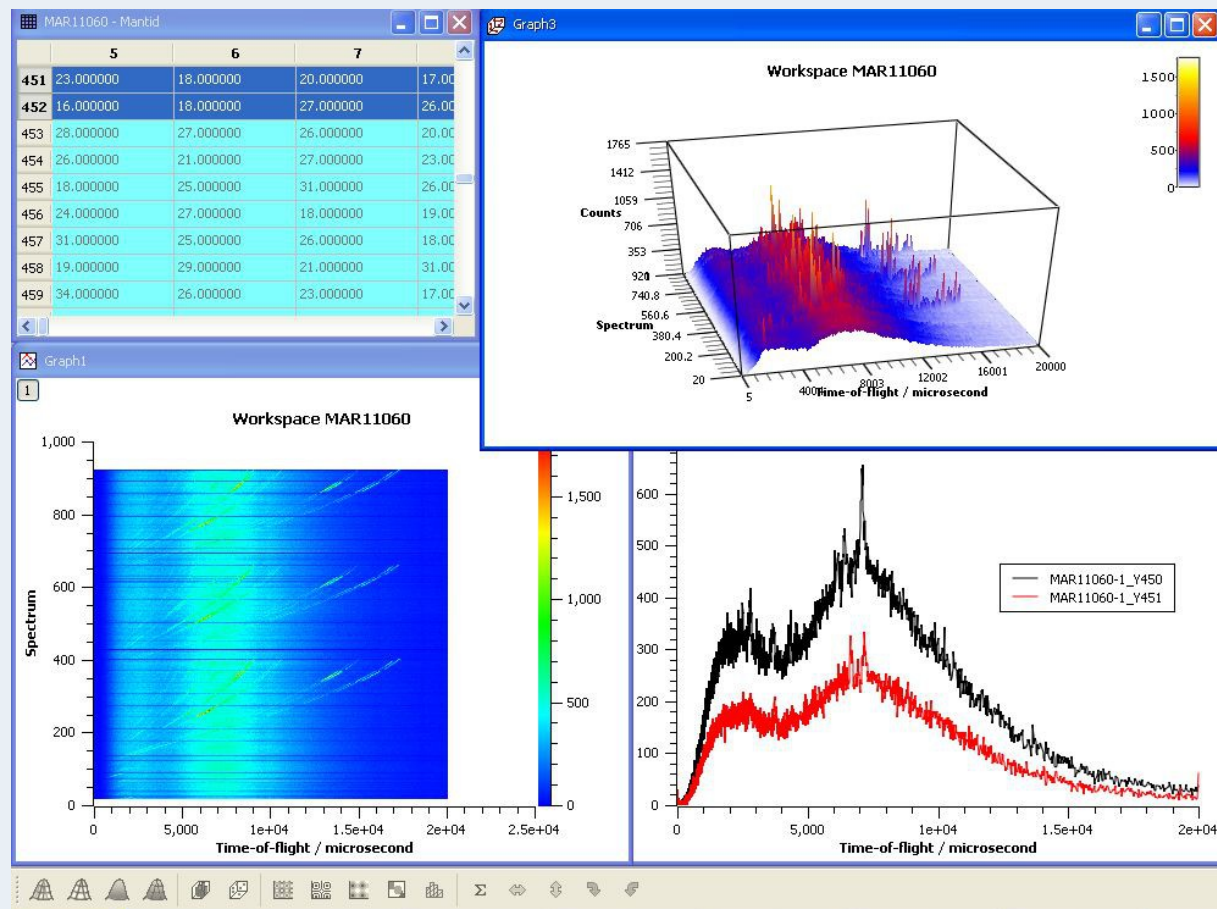
- What is Mantid?
 - Framework that facilitates HPC & visualization and analysis of *neutron* and *muon* data
 - Collaboration between ISIS and SNS
 - Supports various techniques
 - Inelastic (Direct/Indirect)
 - Diffraction
 - Muon
 - Disordered Materials

Mantid

- Features include:
 - Flexible: Instrument/Facility/Technique independent
 - Cross platform (UNIX, Win, OS X)
 - Open source (@mantidproject)
 - Ease of use (Expert -> Visitor)

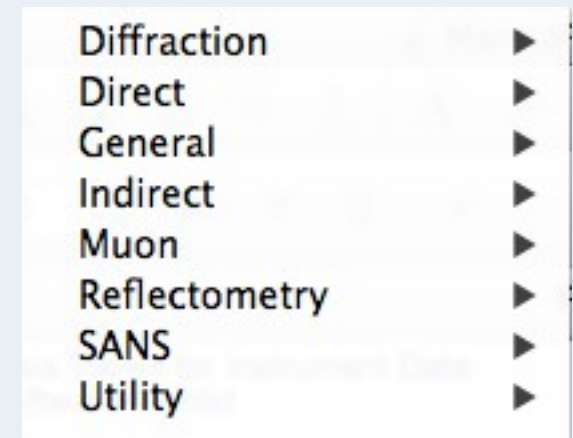
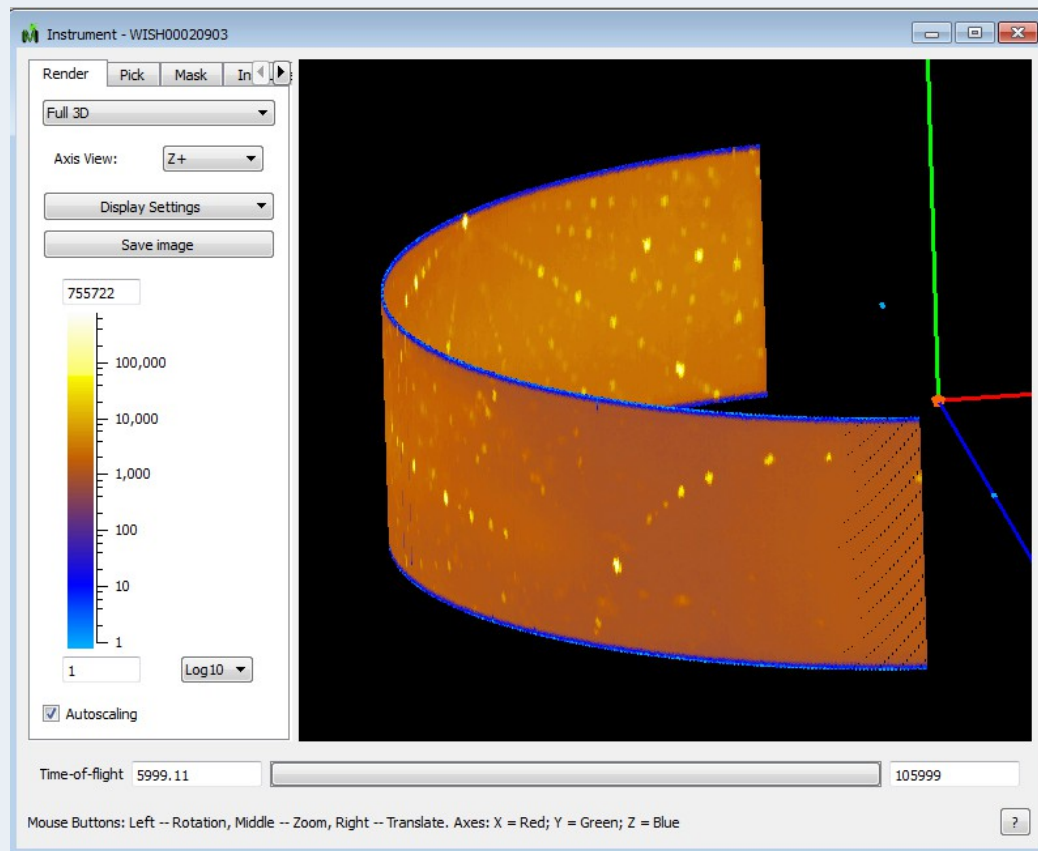
Mantid - visualisations

- MantidPlot



Mantid - visualisations

- Custom interfaces



ICAT within Mantid

- Why is it used?
 - Load data directly from archives
 - Easily access catalogued data
- How is it used?
 - **New** Catalog == **new** adaptor

ICAT within Mantid

- Search parameters

The screenshot shows a 'Catalog search' window with a title bar containing three window control buttons (red, yellow, green) and the text 'Catalog search'. Inside the window, the status 'Currently logged into ISIS' is displayed on the left, and a 'Help' button is on the right. A checked checkbox labeled 'Catalog search' is present. Below this, a search form contains several fields: 'Investigation name' (text input), 'Start date' (date input with slashes and a dropdown arrow), 'Instrument name' (dropdown menu showing 'GEM'), 'End date' (date input with slashes and a dropdown arrow), 'Run range' (text input), 'Keywords' (text input), 'Investigation id' (text input), 'Investigators name' (text input), 'Sample name' (text input), 'Datafile name' (text input), and 'Investigation type' (dropdown menu). At the bottom of the form, there are two checked checkboxes: 'Advanced search' and 'My data only'. To the right of these are 'Reset' and 'Search' buttons. Below the main form, there are two unchecked checkboxes: 'Search results:' and 'Datafiles information:'.

Currently logged into ISIS Help

☒ *Catalog search*

Investigation name: Start date: ...

Instrument name: End date: ...

Run range: Keywords:

Investigation id:

Investigators name: Sample name:

Datafile name: Investigation type:

☒ Advanced search ☒ My data only Reset Search

☐ *Search results:*

☐ *Datafiles information:*

ICAT within Mantid

- Search results

☒ **Search results: 10 investigations found.**

Double click on an investigation to view related datafiles.

Investigation id	Title	Instrument	Run range	Start date ▼	End date
1390019	The structure of the ionic condu...	GEM	62862	2013-05-30	2013-05-30
1390020	Refinement of the ND3 deficit in...	GEM	62855	2013-05-29	2013-05-29
1390046	Undeformed, R242 5x15 mm	GEM	62831, 6303...	2013-05-27	2013-06-11
1390028	Al cylinder with 10% deformation	GEM	62838-62839	2013-05-27	2013-05-28
1390031	Al cylinder with 40% deformation	GEM	62832-62833	2013-05-27	2013-05-27
1390030	Al cylinder with 30% deformation	GEM	62834-62835	2013-05-27	2013-05-27
1390029	Al cylinder with 20% deformation	GEM	62836-62837	2013-05-27	2013-05-27
CAL_GEM_...	Y2O3 pos 5	GEM	62414	2013-05-15	2013-05-15
CAL_GEM_...	Si SRM640c 8mm pos 6	GEM	62410	2013-05-14	2013-05-14
CAL_GEM_...	Empty CCR 4K 15x40 mm	GEM	62402-62409	2013-03-29	2013-05-14

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☐ **Datafiles information:**

ICAT within Mantid

- Investigation datafiles

☒ **Datafiles information: 7 datafiles found.**

Investigation title: The structure of the ionic conductor Ba₃NbMoO_{8.5} (slow cooled) **Instrument:** GEM
Investigation proposal: **Run range:** 62862

<input type="checkbox"/>	Name ▼	Create Time	File size	Description
<input type="checkbox"/>	GEM62862.raw	2013-05-30 07:03:54	35MB	Ba ₃ NbMoO _{8.5} (slow cooled) 817
<input checked="" type="checkbox"/>	GEM62862.nxs	2013-05-30 07:03:54	16MB	
<input type="checkbox"/>	GEM62862.log	2013-05-30 07:03:54	45KB	
<input type="checkbox"/>	GEM62862_Status.txt	2013-05-30 07:03:54	140B	
<input type="checkbox"/>	GEM62862_ICPstatus.txt	2013-05-30 07:03:54	9KB	
<input type="checkbox"/>	GEM62862_ICPevent.txt	2013-05-30 07:03:54	288B	
<input type="checkbox"/>	GEM62862_ICPdebug.txt	2013-05-30 07:03:54	4KB	

Filter type: No filter ▼

Download to...

Load

IDS within Mantid

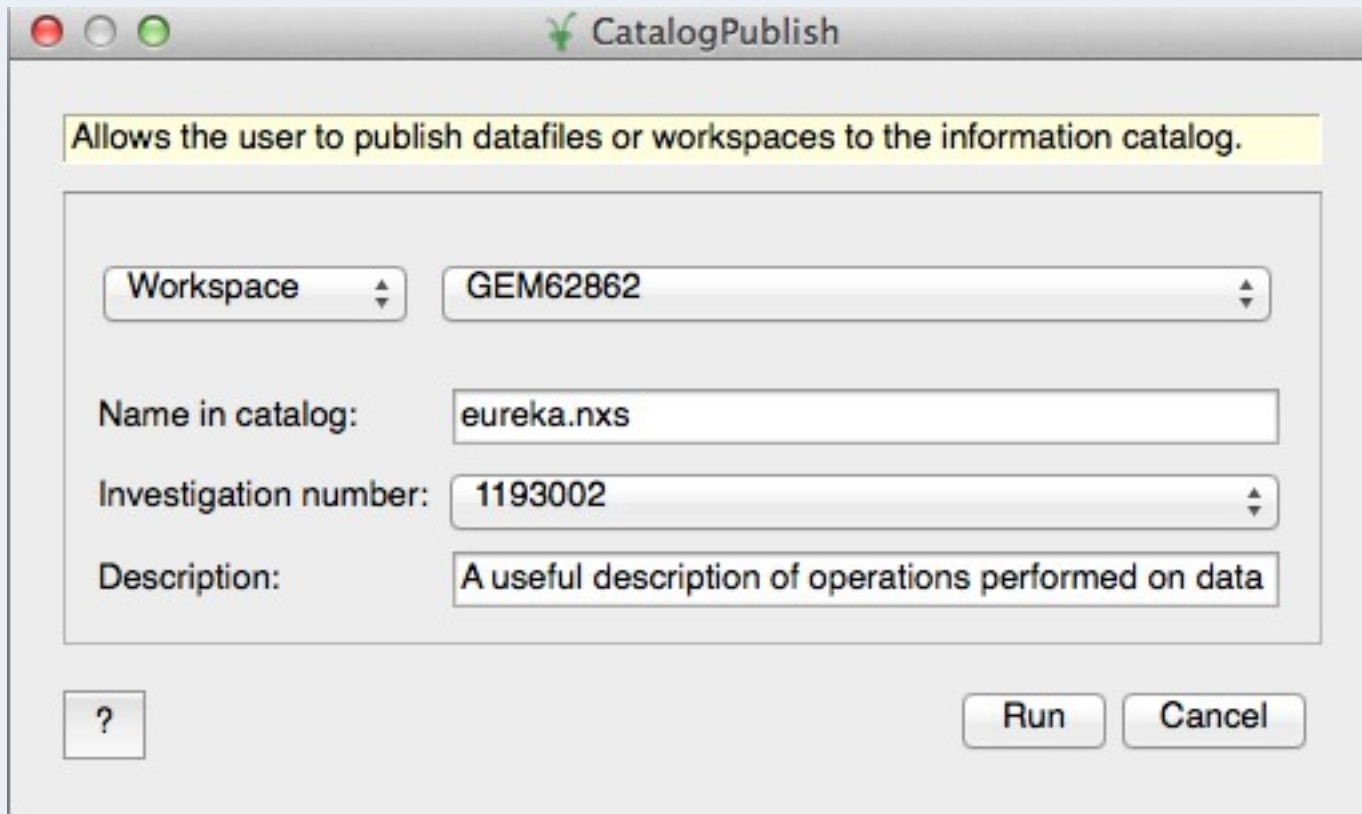
- Downloading (GET)
 - Off-site access
 - Local archive access not required
 - Access latest datafiles

IDS within Mantid

- Publishing (PUT)
 - Share analysed data
 - Automatically upload workspace history

IDS within Mantid

- Publishing GUI



The screenshot shows a macOS-style window titled "CatalogPublish" with a green icon. A yellow tooltip at the top reads: "Allows the user to publish datafiles or workspaces to the information catalog." The main area contains several input fields: a "Workspace" dropdown menu set to "GEM62862", a "Name in catalog:" text field with "eureka.nxs", an "Investigation number:" dropdown menu set to "1193002", and a "Description:" text field with "A useful description of operations performed on data". At the bottom left is a help button with a question mark, and at the bottom right are "Run" and "Cancel" buttons.

Workspace: GEM62862

Name in catalog: eureka.nxs

Investigation number: 1193002

Description: A useful description of operations performed on data

? Run Cancel

Future plans

- Cross facility querying (optional)
 - One query to be sent to each logged in catalog.
 - Results collated on search GUI

Future plans

- DOIs generated for published *public* data

Questions?