TopCAT

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ICAT Workshop - Lund

13th March 2013

Overview

- New setup script
- ICAT 4.2 support
- Parameter searching
- Work in progress
- Future plans
- Links
- Summary

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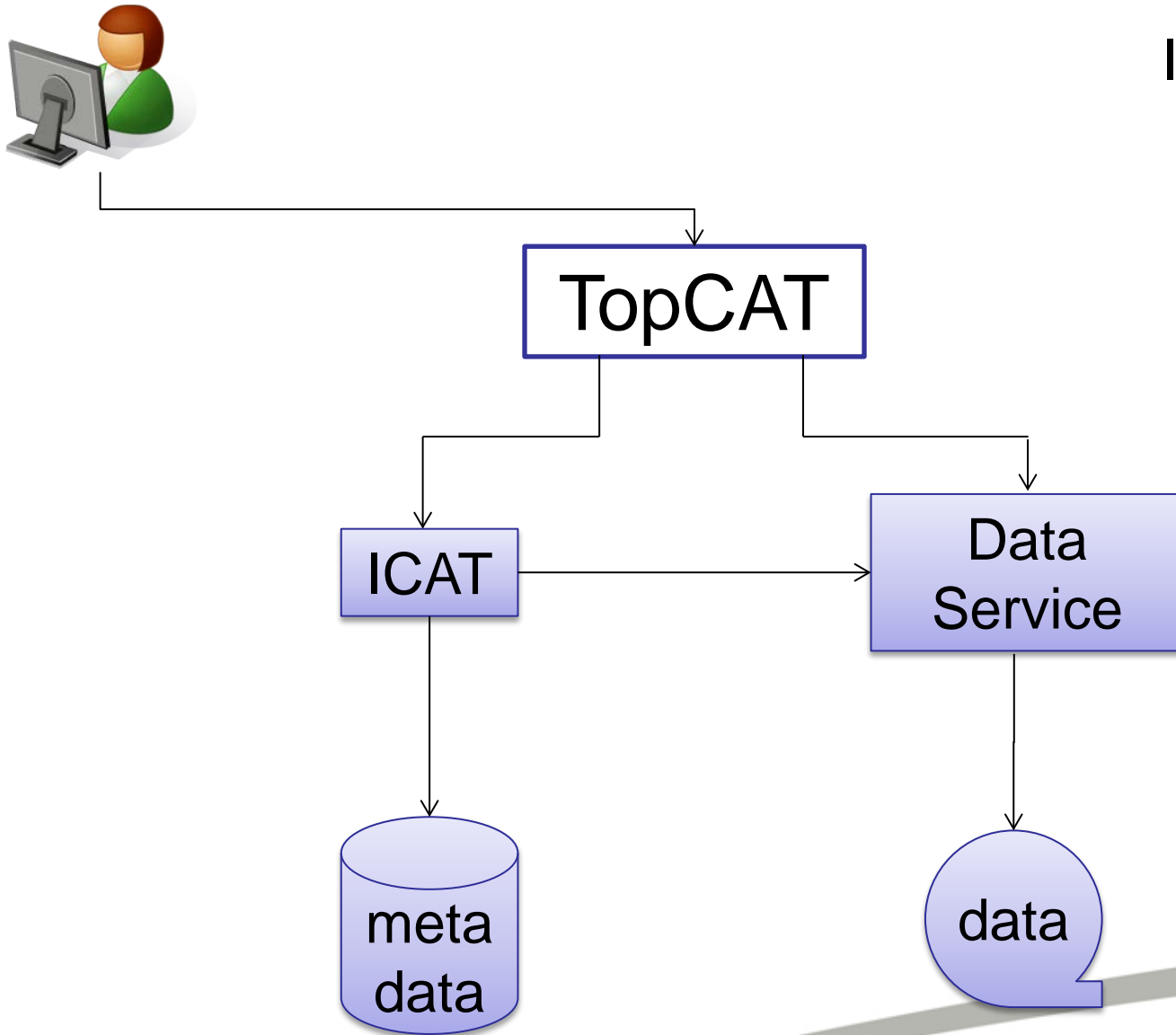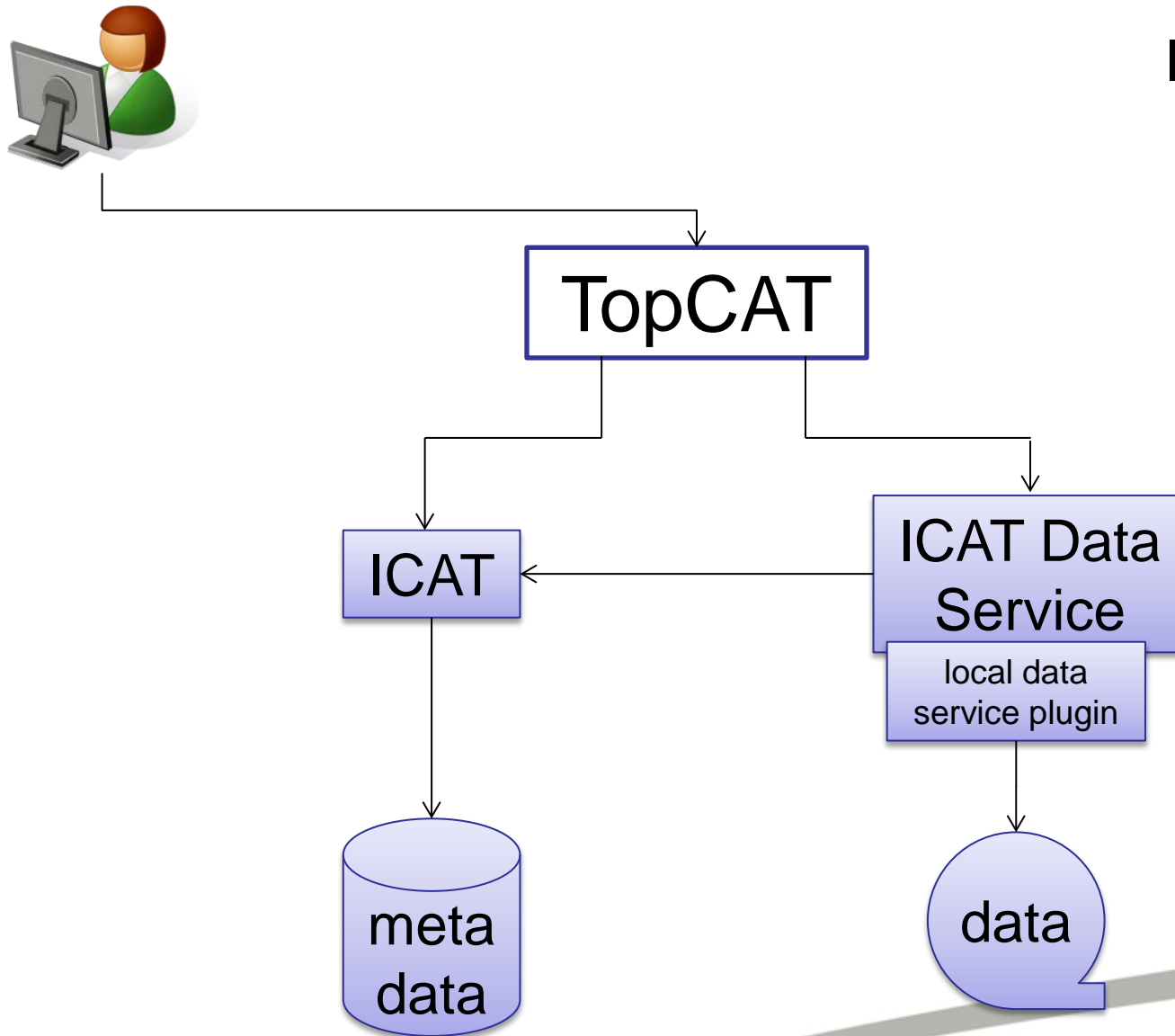Facilities Council

TopCAT

- Provides a web interface to ICAT
- Allows users to search metadata
- Allows searches over multiple ICATS
- Allows users to download data files / data sets

ICAT 3

TopCAT

ICAT

Data
Service

meta
data

data

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ICAT 4

TopCAT

ICAT

ICAT Data Service

local data service plugin

meta data

data

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TopCAT Setup Script

- glasfish.props used for setup configuration

- *.icat used to configure ICAT connections

```
./topcat_setup.py --help

./topcat_setup.py --create

./topcat_setup.py --deploy

./topcat_setup.py --addICAT
```

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ICAT 4.2 Support

- Bug fixes for ICAT 4.2 plugin
- Specify ICAT authentication plugin to use
  - Currently only supports plug-ins that require username and password

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Parameter Searching

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Keywords [_____] Search

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Advanced Search ▼

Parameter Search ▲

Facility
| ISIS 4.2 |

Parameter Name [_____] ▼

| TEMP1 |
| TEMP2 |
| TEMP2 |
| TEMP3 |
| TEMP3 |
| TEMP4 |
| TEMP4 |
| TEMP5 |
| TEMP6 |
| TEMP_1 |
| TEMP_INI |
| TEMP____ |
| TEMP_ini |
| TES |
| TES |

Parameter Units

Parameter Range

Parameter Value

Search Experiment Parameters

Search Data File Parameters

Facilit ▼

Facility Name	Investigation Number	Visit Id	Title	Start Date	End Date

|◄ ◄ Page [____] ► ►|

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Parameter Search ▴

Facility
ISIS 4.2

Parameter Name   TEMP ▾

Parameter Units   [_____] ▾

Parameter Range   --ALL--

Parameter Value   ?
            CELCIUS
            CELSIUS
            degree K

Search Experiment Parameters

Search Data File Parameters   Reset

Facilities Search ▾

Facility Name	Investigation Number	Visit Id	Title	Start Date	End Date

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Keywords [＿＿＿＿＿＿＿＿＿＿] Search

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Parameter Search ▲

Facility
> ISIS 4.2

Parameter Name   TEMP ▼

Parameter Units   degree K ▼

Parameter Range   ☐

Parameter Value   273

Search Experiment Parameters

Search Data File Parameters   Reset

Facilities Search ▼

Facility Name	Investigation Number	Visit Id	Title	Start Date	End Date

|◀ ◀ Page [＿＿] ▶ ▶|

Parameter Searching

- For this to be useful you need
  - a common vocabulary
  - control over new parameter names and units

Work In Progress

- Link to pansoft repository
  - Work being done by ILL
- File upload
  - Makes use of IDS
- Admin interface

Facility Name	Investigation Number	Visit Id	Title	Start Date	End Date
ISIS 4.2	910147	1	Thermochromism in N-salicylideneanilines	2009-06-12 10:13	2009-11-26 00:20
ISIS 4.2	910239	1	Investigations into the solid state structure of [Rh(PiBu3)2(H3BNMe3)]BArF4 and the thermochromic...	2009-06-16 07:00	2011-02-11 17:16
ISIS 4.2	910414	1	Variable Temperature studies of an anomalous proton sponge benzoic acid co-crystal complex	2009-06-21 09:34	2009-07-10 15:05
ISIS 4.2	920360	1	Structural Studies of 9-methyltriptycenes	2009-07-18 09:24	2009-07-29 15:26
ISIS 4.2	920450	1	Neutron Diffraction Studies on Yb3(GaGe)10 compound	2009-07-11 23:47	2009-07-12 01:26
ISIS 4.2	CAL_SXD_2009-07-12T15...	1	CeAuSb2 big xtal T=1.5K rot=+0 j:12,12	2009-07-12 10:02	2009-07-15 00:07
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ISIS 4.2	CAL_SXD_2009-07-16T09...	1	CeCoSi3 lower half screen #1 j:16,16	2009-07-16 08:54	2009-07-16 10:44
ISIS 4.2	CAL_SXD_2009-07-16T11...	1	CeCoSi3 small and thick screen #1 j:16,16	2009-07-16 10:59	2009-07-16 11:12
ISIS 4.2	CAL_SXD_2009-07-16T12...	1	Sq Acid 0.57mm^3 on Al stick 10x10mm beam	2009-07-16 11:28	2009-07-17 12:19
ISIS 4.2	CAL_SXD_2009-07-16T16...	1	d2o ice vi crystal ~1.4 GPa	2009-07-16 15:44	2009-07-16 16:54
ISIS 4.2	CAL_SXD_2009-07-17T10...	1	Al2O3 0.31mm^3 in TiZr gasket VX1 - 2-diamonds	2009-07-17 09:58	2009-07-17 10:41
ISIS 4.2	CAL_SXD_2009-07-17T18...	1	squaric acid 1 mm^3 in panoramic cell	2009-07-17 17:53	2009-07-17 18:35

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Investigation: Variable Temperature studies of an anomalous proton sponge benzoic acid co-crystal complex

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Facility: ISIS 4.2

Instrument: SXD

Title: Variable Temperature studies of an anomalous proton sponge benzoic acid co-crystal complex

Investigation No: 910414

Visit Id: 1

Start Date: 2009-06-21 09:34

End Date: 2009-07-10 15:05

Investigators: principal_experimenter - Professor Chick Chick Wilson

                      experimenter - Mr Andras Kallay

                      experimenter - Professor David David Keen

Proposal:

As part of a long-running programme, we have identified many co-crystallisation systems producing hydrogen-bonded molecular complexes yielding fascinating X-ray diffraction and DFT results. Among the molecular building blocks we utilise in creating these complexes are substituted benzoic acids and a series of so-called proton sponge complexes, of which the archetype is DMAN (dimethylaminonaphthalene). The complex of DMAN with 4-chlorobenzoic acid crystallises in a 1:1 ratio, and produces a unique situation where one DMAN is protonated, the other unprotonated. We aim to investigate this unusual situation of H-atom distribution as a function of T, and also the diffuse scattering, likely to be produced by the local arrangement of the chains of DMAN molecules.

Parameters:

Name	Value	Units
run_number_range	22007-22040	
bcat_inv_str	Kallay/MJG - (Unspecified)	

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Investigation: Variable Temperature studies of an anomalous proton sponge benzoic acid co-crystal complex

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New Data Set Parameters

Data Set Name: [results01]
Data Set Description: [my results]
Data Set Type: [▼]
- etc
- sample/target
- simulation
- special_cal
- experiment_cal
- raw
- processed
- analyzed
- experiment_eng
- laser_shot
- reduced
- experiment_raw
- source_monitoring
- special_user
- unkown

File Name:
File Description:
File Format:

Add

File | Description

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New Data Set Parameters

Data Set Name: [results01]
Data Set Description: [my results]
Data Set Type: [analyzed ▼]

Add A File

File Name: [   ] [Browse...]
File Description: [   ]
File Format: [▼]

[Add File] [Submit] [reset]

File	Description	Format		

Future Plans

- Add redirect to user office to obtain ICAT session id

  - This will be discussed in detail in the PaNdata session

- Modification of access permissions

  - Grant read access to other users

  - Requires ICAT > 4.3

- DOI generation

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Links

- TopCAT the movie

  - http://code.google.com/p/icatproject/downloads/

- PaNdata TopCAT

  - https://pandata.rl.ac.uk/

- ISIS TopCAT

  - https://data.isis.stfc.ac.uk/

- Diamond TopCAT

  - https://icat.diamond.ac.uk/

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Summary

- View meta data from multiple ICATs
- Download data files and data sets
- Compatible with ICAT auth plugins requiring username and password
- Upload of datasets
- Better integration with user office authentication mechanisms

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