ICAT Job Portal

a generic job submission system built on a scientific data catalog

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Use Case

- LSF operate OCTOPUS imaging cluster: lasers coupled to interconnected microscopy stations.
    - a large number of data files
    - applications to process and visualise them
    - interactive program with an easy to use GUI to offer lists of raw and processed datasets and offer the ability to process those datasets
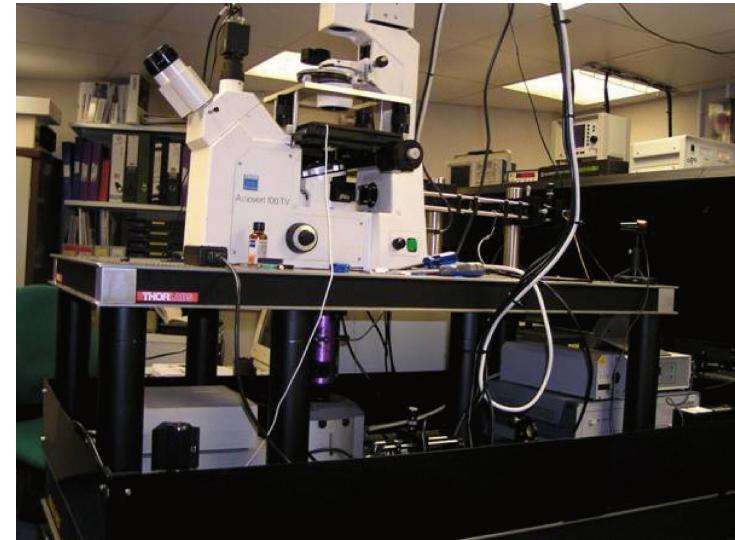
Problems

- Not scalable
    - not backed by a database - GUI had to scan **all** data each time started
    - user needed a machine allocated to him with a personal account - labour intensive

Some Requirements

1. GUI and command line from on and off site.

2. Automated installation of OS and software updates.

3. Centralised user/group management.

4. A file server to store raw data, analysed data and other user data.

5. Consult the metadata to locate the data.

6. Upload and download data.

7. Submit batch jobs to Linux nodes; listing, cancelling and retrieving output.

8. Interactive GUI based analysis/visualisation jobs able to access data.

9. Select and submit multiple datasets for processing through applications.

10. No facility dependence: configurable menus, datasets types, jobs and associated job parameters.

A solution

- Build a batch and interactive job portal on top of STFC's ICAT and IDS
- Implement GUI access via Google Web Toolkit
- Provide command line access via RESTful interface
- Installation and configuration with puppet
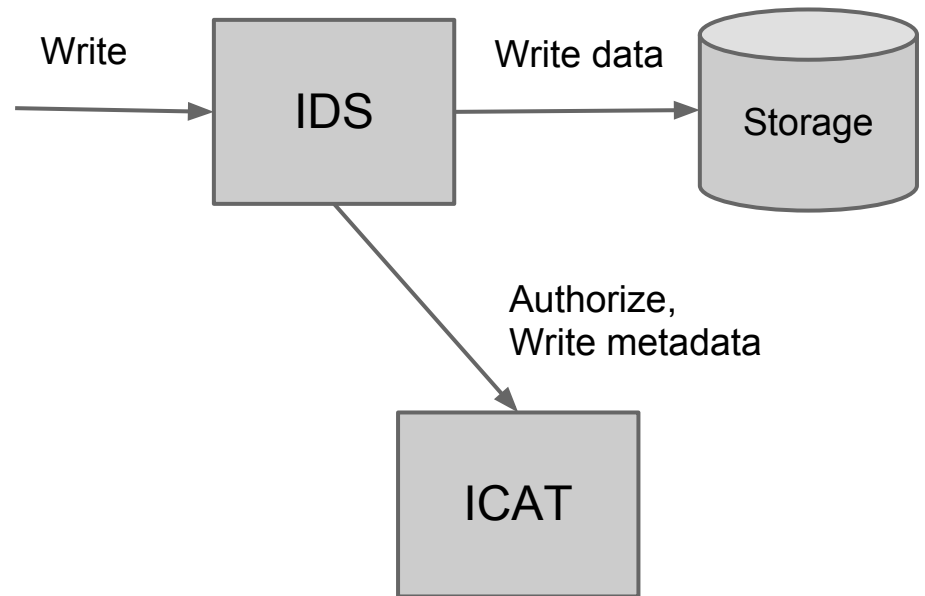- Use other tried, tested, scalable and preferably open source components

ICAT - metadata catalog

- A database designed to support facility data and exposed as a web service
- Uses any eclipselink supported DBMS
  - Tested with Oracle, MySQL and Derby
- Deployed on an application server
  - Such as Glassfish
- Exposed as a web service
  - Very small API
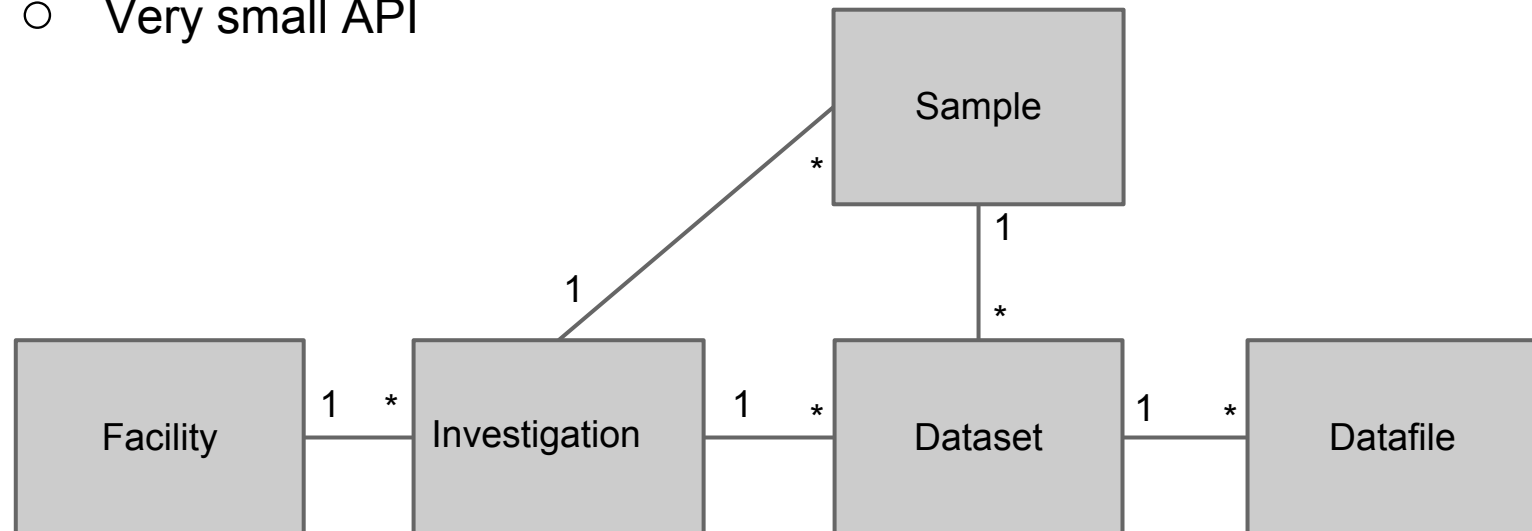
ICAT Data Service (IDS)

This is defined by an interface (RESTful web service) which is able to store files and register their metadata in ICAT.
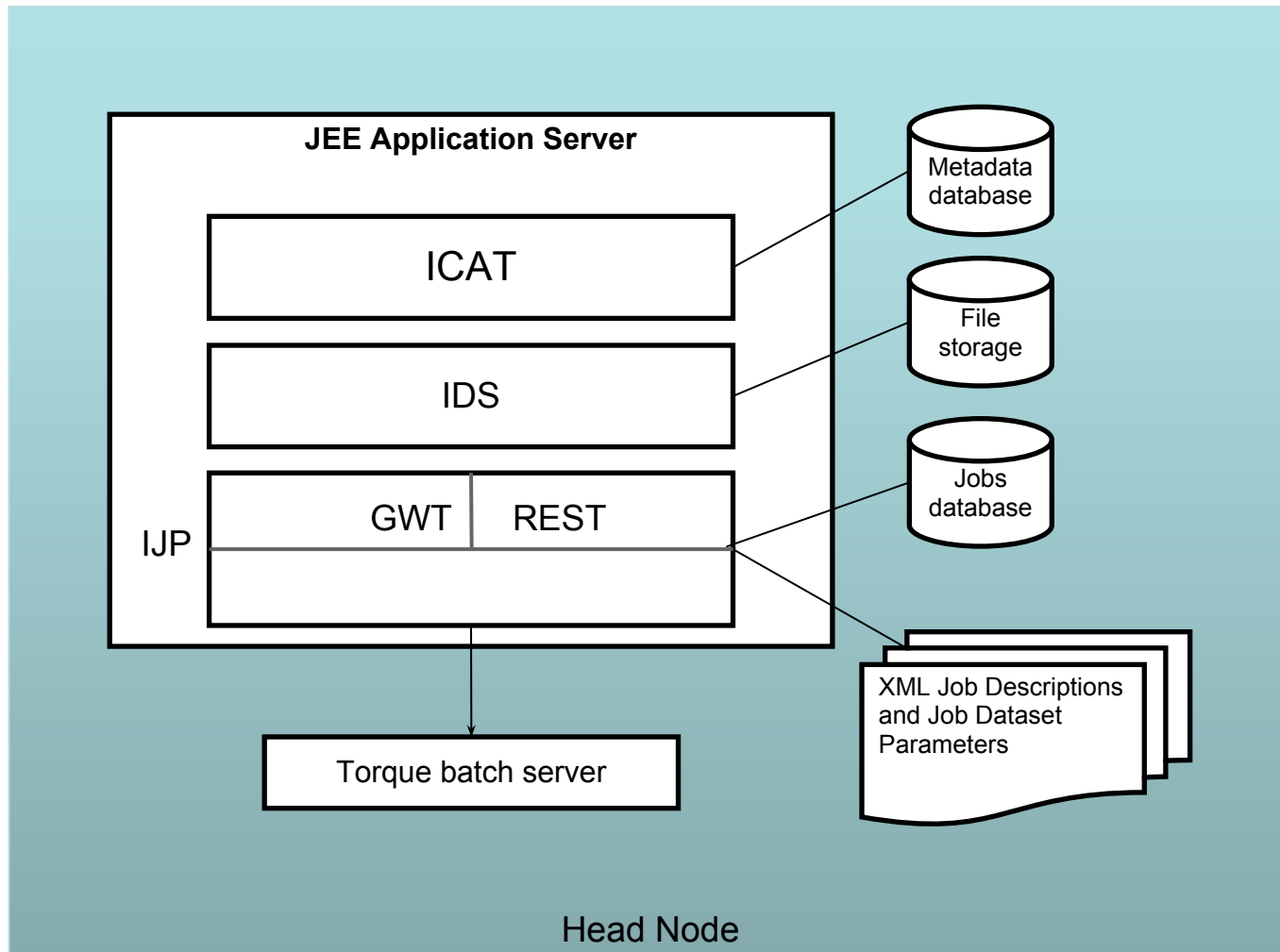
Various implementations depending on needs of facility.

Write → IDS → Write data → Storage

IDS → Authorize, Write metadata → ICAT

ICAT metadata authorization => IDS data authorization

Architecture Overview

User's PC

| Web browser | CLI | | Remote Desktop client |

https   rdp

Head Node

- ICAT Job Portal webapp
  - Submit batch job
- Torque batch server

Assign interactive job

Assign batch job

Worker Node 1

- Prepare job → Facility software
- Run batch job
- Torque worker node

Worker Node n
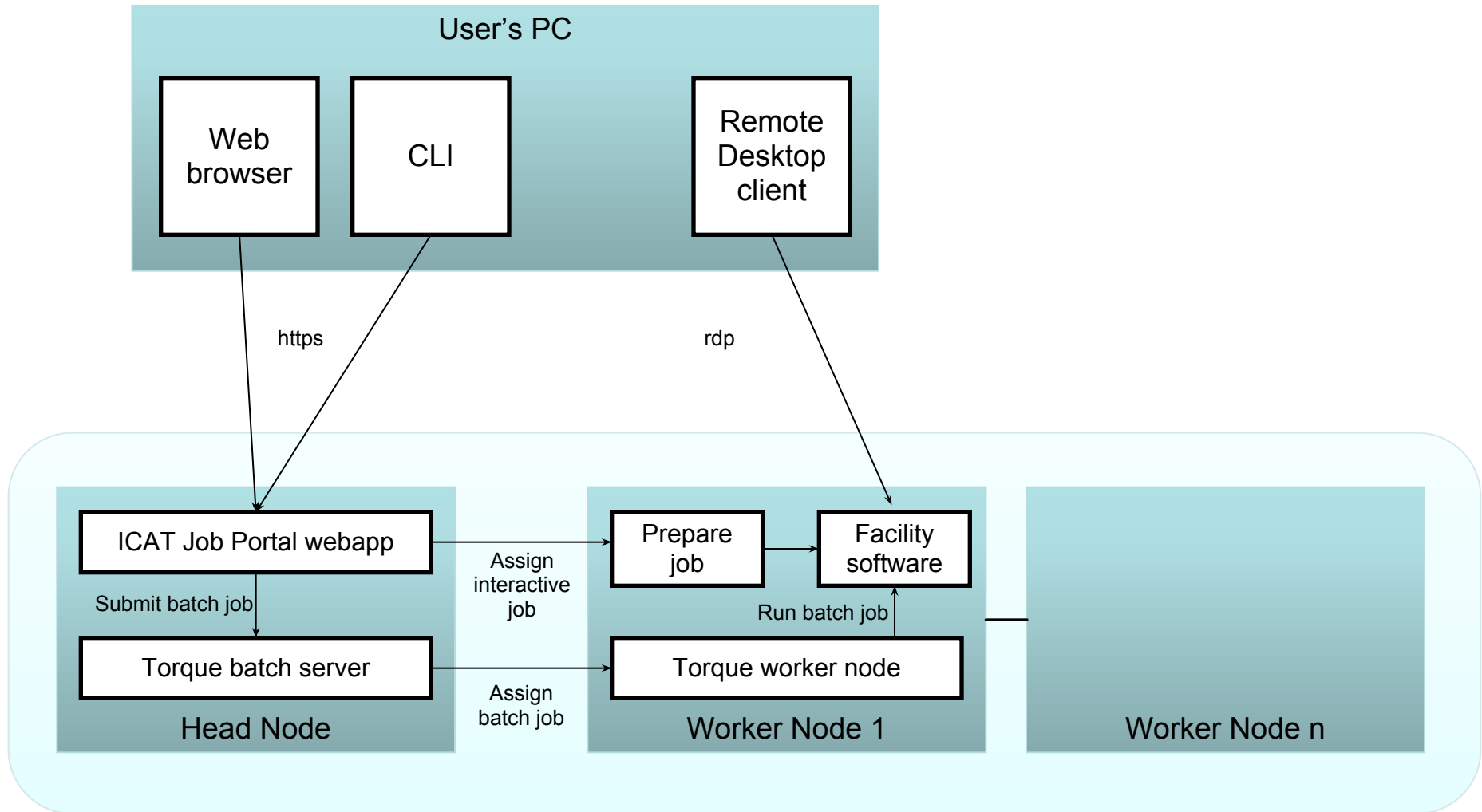
Head Node Architecture

Job Portal Main Panel (Datasets)

Job Options

MSMM Viewer Project Options

View type ⦿ View ○ View beads ○ View whitelights ○ View reg residual frames ○ View reg model frames

Track method [▾]

Show variance image instead of image ☐

Do not load traces ☐

Read features/tracks from hdf5 files (slow) ☐

Set min,max for colour scale [   ]

Regular expression for images in directory [   ]

Do not clean levels/stats [   ] *(default=0) (min=0) (max=10)*

Min number of detected features per frame range of a level/state [   ] *(default=2)*

Threshold for the Chauvenet's outlier test [   ] *(default=2) (min=1) (max=5)*

Set the (real) EM gain by hand [   ]

Quantum efficiency [   ] *(default=0.910000026) (min=-1.0) (max=1.0)*

Set the (real) electron/ADU by hand [   ]

A unique identifier of the EMCCD [   ] *(default=Command:Line)*

Quit immediately after initialisation completes ☐

Add a string to the view window title [   ]

[Submit]   [Close]

Job Status Panel

Multiple Dataset Handling

- Jobs can accept a single or multiple datasets (specified in XML Job Description)

- Multiple datasets can be submitted to a job specified as accepting multiple datasets as input

- A separate batch job can be submitted for each dataset (with a single click)

- With multiple datasets selected, Job Options Form offers only options common to all datasets

Interactive jobs

Configuration

1. Create XML files for each dataset type picking out dataset features relevant to Job Options

2. Create XML Job Descriptions

3. Write applications (or wrappers around existing applications) – loading and saving datasets from IDS and recording provenance in ICAT

```xml
<jobType>
    <name>MSMM Viewer Project</name>
    <executable>/usr/local/msmm/bin/run_msmm_viewer</executable>
    <multiple>false</multiple>
    <type>interactive</type>
    <datasetTypes>project</datasetTypes>
    <jobOptions>
        <name>View</name>
        <groupName>View type</groupName>
        <type>boolean</type>
        <programParameter></programParameter>
        <condition></condition>
    </jobOptions>
    <jobOptions>
    <jobOptions>
        <name>View reg beads</name>
        <groupName>View type</groupName>
        <type>boolean</type>
        <programParameter>--reg-beads</programParameter>
        <condition>numBeadFiles>0 && numChannels>1</condition>
    </jobOptions>
    <jobOptions>
    <jobOptions>
        <name>Track method</name>
        <type>enumeration</type>
        <programParameter>--trackmethod</programParameter>
        <values></values>
        <values>Simple</values>
        <values>SLH</values>
        <values>Biggles</values>
        <values>Simulation</values>
    </jobOptions>
    <jobOptions>
    <jobOptions>
        <name>Regular expression for images in directory</name>
        <type>string</type>
        <programParameter>--image-pattern</programParameter>
    </jobOptions>
    <jobOptions>
        <name>Do not clean levels/stats</name>
        <type>integer</type>
        <programParameter>--Levels.no-clean</programParameter>
        <defaultValue>0</defaultValue>
```

Job Options from XML

XML Job Description on Head Node

Job Options Form in Web Browser

Command Line Interface

- RESTful web service and Python client for job handling
- Alternative to using web browser
- May become preferred interface for some users
- Enables scripted interaction with IJP

```
$> ijp login db username fred password -
password:
d3f58cf7-23fb-4e0a-89bc-292dcc142e20

$> ijp session
User ingest connected to ICAT 4.2.5 at https:
//rclsfserv010.rc-harwell.ac.uk:8181 with 1439
minutes left.

$> ijp jobtype
Available job types are:
view_ingested is interactive
ingest is batch
view_project is interactive
quincy is batch

$> ijp submit ingest gggg
2.rclsfserv010.rc-harwell.ac.uk

$> ijp status
2.rclsfserv010.rc-harwell.ac.uk, R
```

Status

- System as described has been implemented deployed and given to LSF for feedback
  - A number of known deficiencies
  - Documentation very incomplete
  - Apache License Version 2
  - If you want to try it, suggest that you contact us first (dr.s.m.fisher@gmail.com)

Future Developments

- Improvements following user feedback

- Visualisation of Provenance

- Workflow Support

- Software as Data

- Administration console

- Alternative remote desktop mechanism

- Alternative batch systems

- Portability

and finally ...

- The system has the desired functionality and is responsive

- Other STFC facilities and groups are interested in using it

- Going from prototype to a generic, maintainable system took a long time

- Short informal weekly meetings between the developers and LSF have ensured the delivery of the desired product