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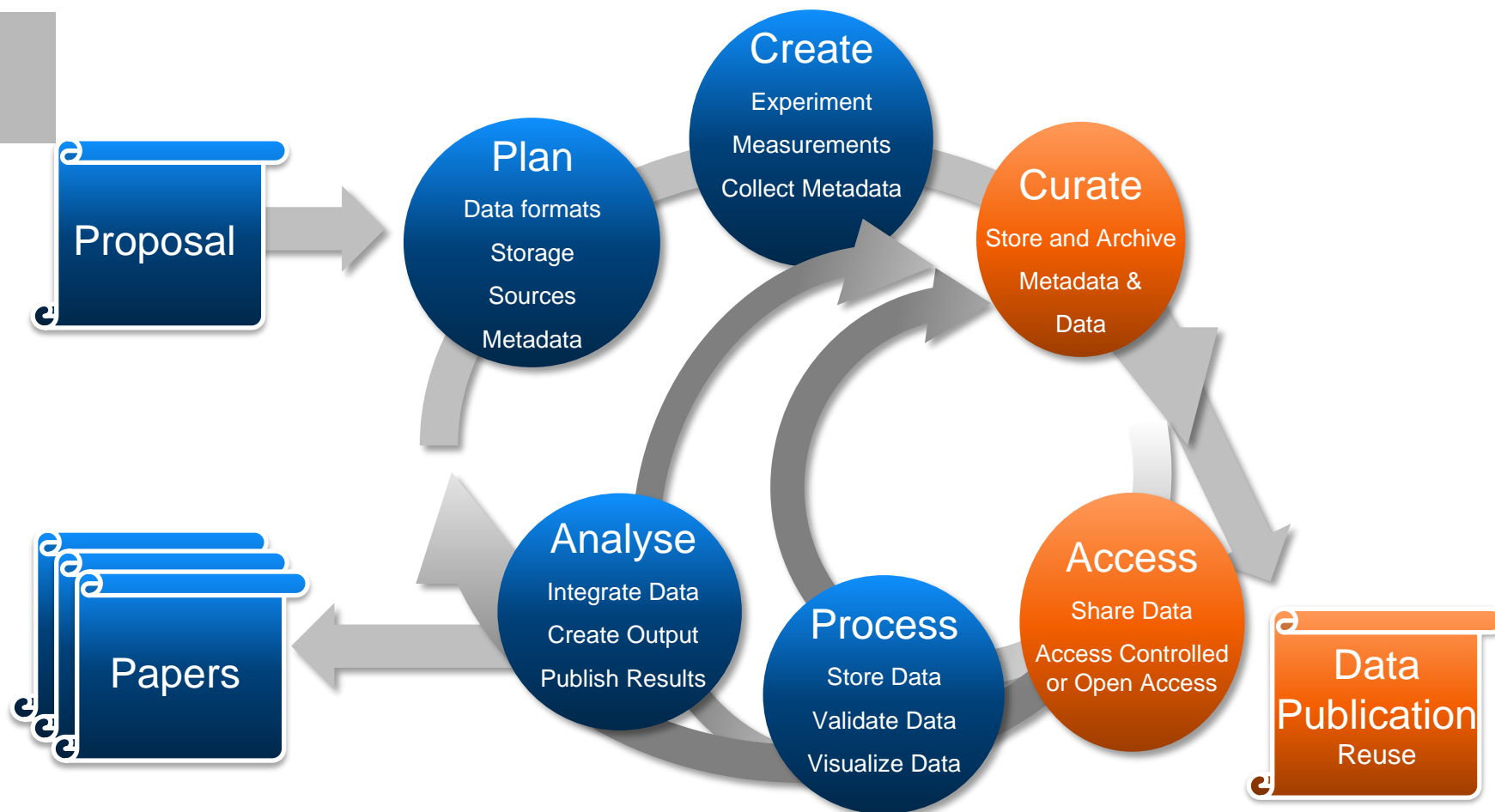
Carlo Minotti (PSI), Stephan Egli (PSI)

SciCat as a Tool for Users and Data Managers

DESY User Meeting,


Satellite Meeting "Science driven data management solutions" - 24/01/22

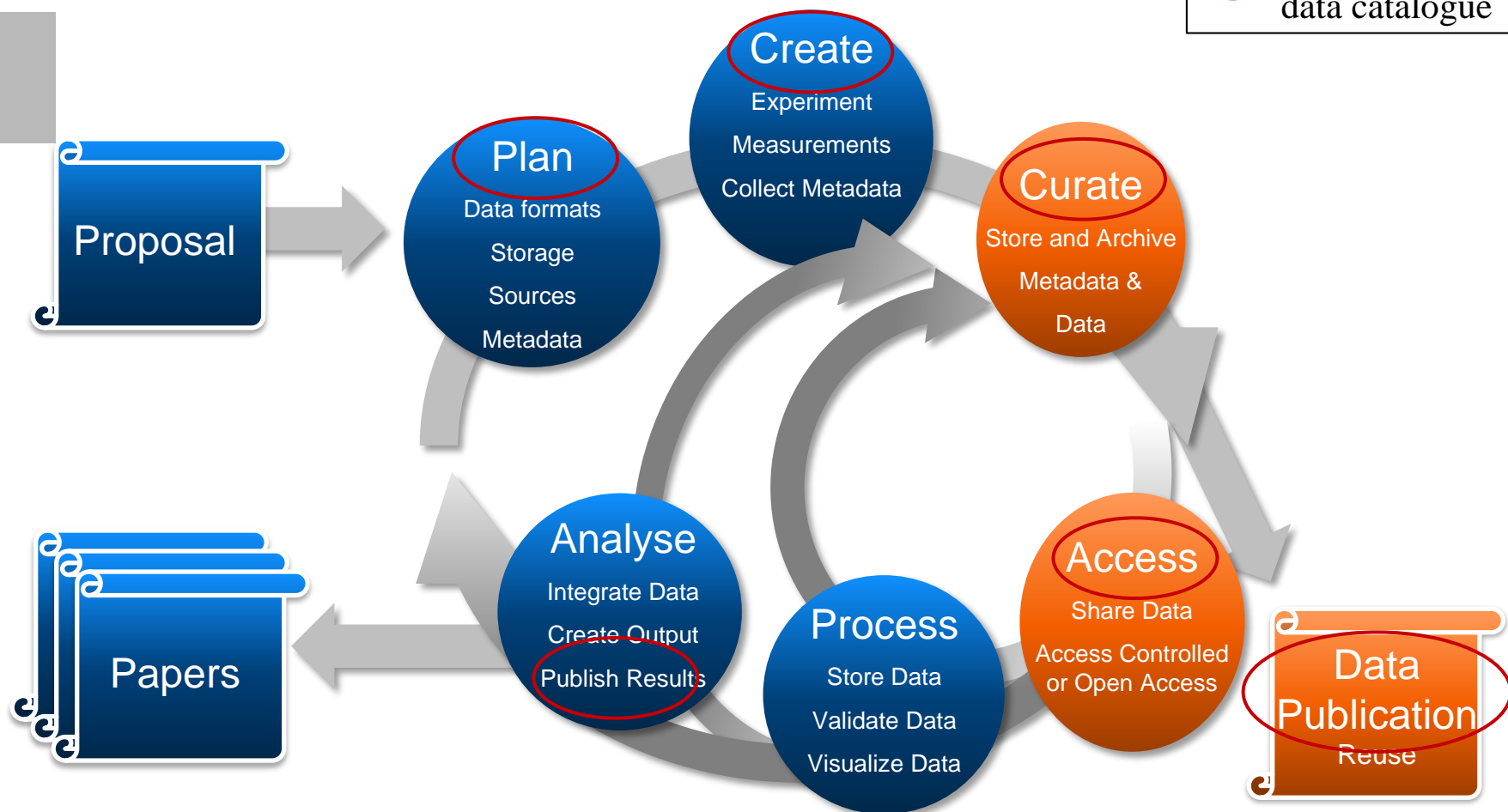
A typical user journey



Where data catalogue is used

legend


 Interaction with
 data catalogue





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Where does SciCat help the Scientists?

- **Organize** the scientific data into datasets
- Annotate the Datasets with **administrative** and **flexible scientific metadata**
- Make the data **searchable/discoverable**
- Provides the infrastructure for **publishing** the data, DOI generation
- Can be used as frontend for **longterm** storage (Archive) solutions of mass data (PB regime)
- Supports both **open access** and **embargoed** data

Discover data via WebUI

User specific data

Archive Interface

Facet search

Search Clear

Text Search

Location

Group

p18788 | 2300

p18762 | 10

p18761 | 49

p18748 | 147

p18675 | 18

My Data Public Data **All** Archivable Retrievable Work In Progress System Error User Error










Items per page: 25 1 - 25 of 111272 |< < > >|

Name	Source Folder	Size	Start Time	Type	Proposal ID	Group	Data Status
029_estaillades1_q01_fw085_ss	...1_fw085_ss	1 TB	2020-12-23 Wed 00:05	derived		p17614	retrievable
020_estaillades1_q01_fw085_us	...1_fw085_us	729 GB	2020-12-23 Wed 00:05	derived		p17614	retrievable
019_estaillades1_q01_fw085_us	...1_fw085_us	376 GB	2020-12-23 Wed 00:05	derived		p17614	retrievable
018_estaillades1_q01_fw085_us	...1_fw085_us	376 GB	2020-12-23 Wed 00:05	derived		p17614	retrievable
031_estaillades1_q01_fw085_ss	...1_fw085_ss	4 TB	2020-12-22 Tue 22:02	derived		p17614	retrievable
20201214_ANAXAM/11_360_	...AM/11_360_	47 GB	2020-12-14 Mon 20:59	raw	unknown	p17896	archivable
20201214_ANAXAM/10_360_	...AM/10_360_	47 GB	2020-12-14 Mon 20:37	raw	unknown	p17896	archivable
09_360/09_360_S13_	...9_360_S13_	47 GB	2020-12-14 Mon 20:09	raw	unknown	p17896	archivable
09_360/09_360_S12_	...9_360_S12_	47 GB	2020-12-14 Mon 20:03	raw	unknown	p17896	archivable
09_360/09_360_S11_	...9_360_S11_	47 GB	2020-12-14 Mon 19:57	raw	unknown	p17896	archivable
09_360/09_360_S10_	...9_360_S10_	47 GB	2020-12-14 Mon 19:52	raw	unknown	p17896	archivable
09_360/09_360_S09_	...9_360_S09_	47 GB	2020-12-14 Mon 19:46	raw	unknown	p17896	archivable
09_360/09_360_S08_	...9_360_S08_	47 GB	2020-12-14 Mon 19:40	raw	unknown	p17896	archivable
09_360/09_360_S07_	...9_360_S07_	47 GB	2020-12-14 Mon 19:35	raw	unknown	p17896	archivable
09_360/09_360_S06_	...9_360_S06_	47 GB	2020-12-14 Mon 19:29	raw	unknown	p17896	archivable

Editing of Metadata

You are editing Published Data record.

Title *
 Real-Time Imaging Reveals Distinct Pore-Scale Dynamics During Transient and Equilibrium Subsurface Multiphase Flow

Creators *
 Catherine Spurin  Tom Bultreys  Maja Rücker  Gaetano Garfi  Christian M. Schlepütz  Vladimir Novak  Steffen Berg  Martin J. Blunt 
 Samuel Krevor 

Publisher *
 PSI

Resource Type *
 derived

Description *
 This published data collection contains five datasets obtained by X-ray tomographic microscopy of a carbonate rock sample 5 mm in diameter and 20 mm in length. Both brine and nitrogen gas are injected into the sample at a total flow rate of 0.1 ml/min (the brine made up 85% of this total flow rate). Data were collected and processed at the TOMCAT beamline X02DA of the Swiss Light Source. The first three datasets contain the scanned volume reconstruction during unsteady-state dynamics, while last two datasets contain the same scanned volume during steady state dynamics.

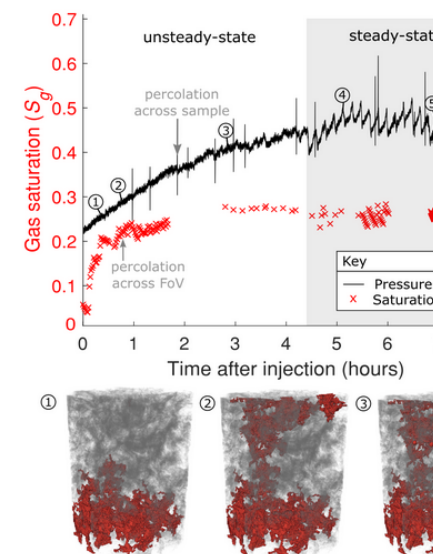
Abstract *
 In the related publication to these data sets, we explore the flow dynamics for two-phase flow in a porous medium (a bioclastic carbonate rock). We use state-of-the-art synchrotron X-ray tomography to capture the fluid dynamics within the pore space, with a scan time of 1 second and a temporal resolution (scan repetition rate) of 2 s. The rock sample was initially saturated with brine (DI water doped with 15%wt. KI) before brine and nitrogen gas were injected simultaneously. As the gas establishes a path through the pore space, the flow dynamics are transient. Eventually, an equilibrium is established, where the gas saturation oscillates about a constant mean value; this is referred to as steady state. There are 5 data sets, 3 of which capture the unsteady state dynamics, and 2 of which capture the steady state dynamics. The images were captured with a voxel size of 2.75 μm^3 . In these data sets we observe that the pore scale dynamics evolve as the macroscopic flow transitions from unsteady state to steady state. We observe that the saturation of the gas plateaus out before the differential pressure across the core. This suggests that gas phase is more mobile during unsteady state.

download link
<https://doi2.psi.ch/datasets/das/work/p17/p17614/Data10/disk1/>

related publications
 C. Spurin, T. Bultreys, M. Rücker, G. Garfi, C. M. Schlepütz, V. Novak, S. Berg, M. J. Blunt, and S. Krevor. Real-Time Imaging Reveals Distinct Pore-Scale Dynamics During Transient and Equilibrium Subsurface Multiphase Flow. Water Resour. Res. 56, 433 (2020). <https://doi.org/10.1029/2020WR028287>

Update Published Data Cancel

Drop a file here
 or
 Browse



Real-Time Imaging Reveals Distinct Pore-Scale Dynamics During Transient and Equilibrium Subsurface Multiphase Flow

Catherine Spurin, Tom Bultreys, Maja Rücker, Gaetano Garfi, Christian M. Schlepütz, Vladimir Novak, Steffen Berg, Martin J. Blunt, Samuel Krevor; PSI (2021)

Abstract

In the related publication to these data sets, we explore the flow dynamics for two-phase flow in a porous medium (a bioclastic carbonate rock). We use state-of-the-art synchrotron X-ray tomography to capture the fluid dynamics within the pore space, with a scan time of 1 second and a temporal resolution (scan repetition rate) of 2 s. The rock sample was initially saturated with brine (DI water doped with 15%wt. KI) before brine and nitrogen gas were injected simultaneously. As the gas establishes a path through the pore space, the flow dynamics are transient. Eventually, an equilibrium is established, where the gas saturation oscillates about a constant mean value; this is referred to as steady state. There are 5 data sets, 3 of which capture the unsteady state dynamics, and 2 of which capture the steady state dynamics. The images were captured with a voxel size of 2.75 μm^3 . In these data sets we observe that the pore scale dynamics evolve as the macroscopic flow transitions from unsteady state to steady state. We observe that the saturation plateaus out before the differential pressure across the core. This suggests that gas phase is more mobile during unsteady state.

Publication details

DOI <https://doi.org/10.16907/46a4d882-4dec-4097-8289-8f6311a4aa36>

Resource Type derived

Related Publications C. Spurin, T. Bultreys, M. Rücker, G. Garfi, C. M. Schlepütz, V. Novak, S. Berg, M. J. Blunt, and S. Krevor. Real-Time Imaging Reveals Distinct Pore-Scale Dynamics During Transient and Equilibrium Subsurface Multiphase Flow. Water Resour. Res. 56, 433 (2020). <https://doi.org/10.1029/2020WR028287>

Datasets

Description This published data collection contains five datasets obtained by X-ray tomographic microscopy of a carbonate rock sample 5 mm in diameter and 20 mm in length. Both brine and nitrogen gas are injected into the sample at a total flow rate of 0.1 ml/min (the brine made up 85% of this total flow rate). Data were collected and processed at the TOMCAT beamline X02DA of the Swiss Light Source. The first three datasets contain the scanned volume reconstruction during unsteady-state dynamics, while last two datasets contain the same scanned volume during steady state dynamics.

20.500.11935/64af1e80-c539-4a90-a051-b7db5e6e714d

20.500.11935/e151f4d6-198a-47e7-ac63-0b258ef36ed3

20.500.11935/441fcd9-fa0c-491c-b102-d114cc841609

20.500.11935/b9782901-be3b-40fe-91d0-3e0a784337c4

20.500.11935/5899a0eb-7e3b-451f-b01e-17ddfc0d0938

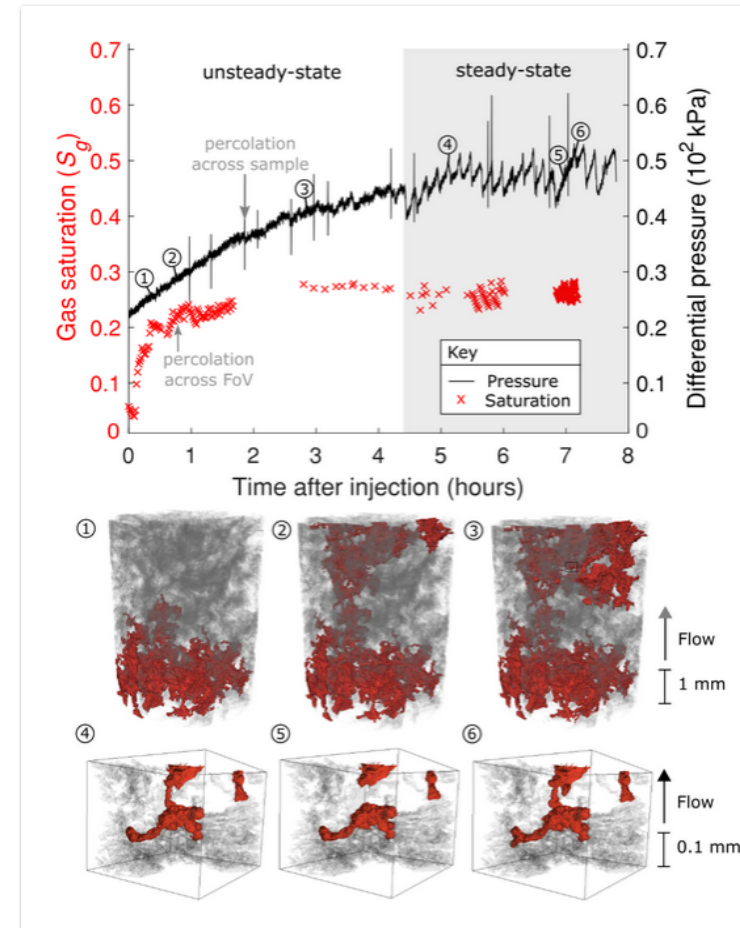
Actions

To access the data associated with this DOI click below and follow the instructions

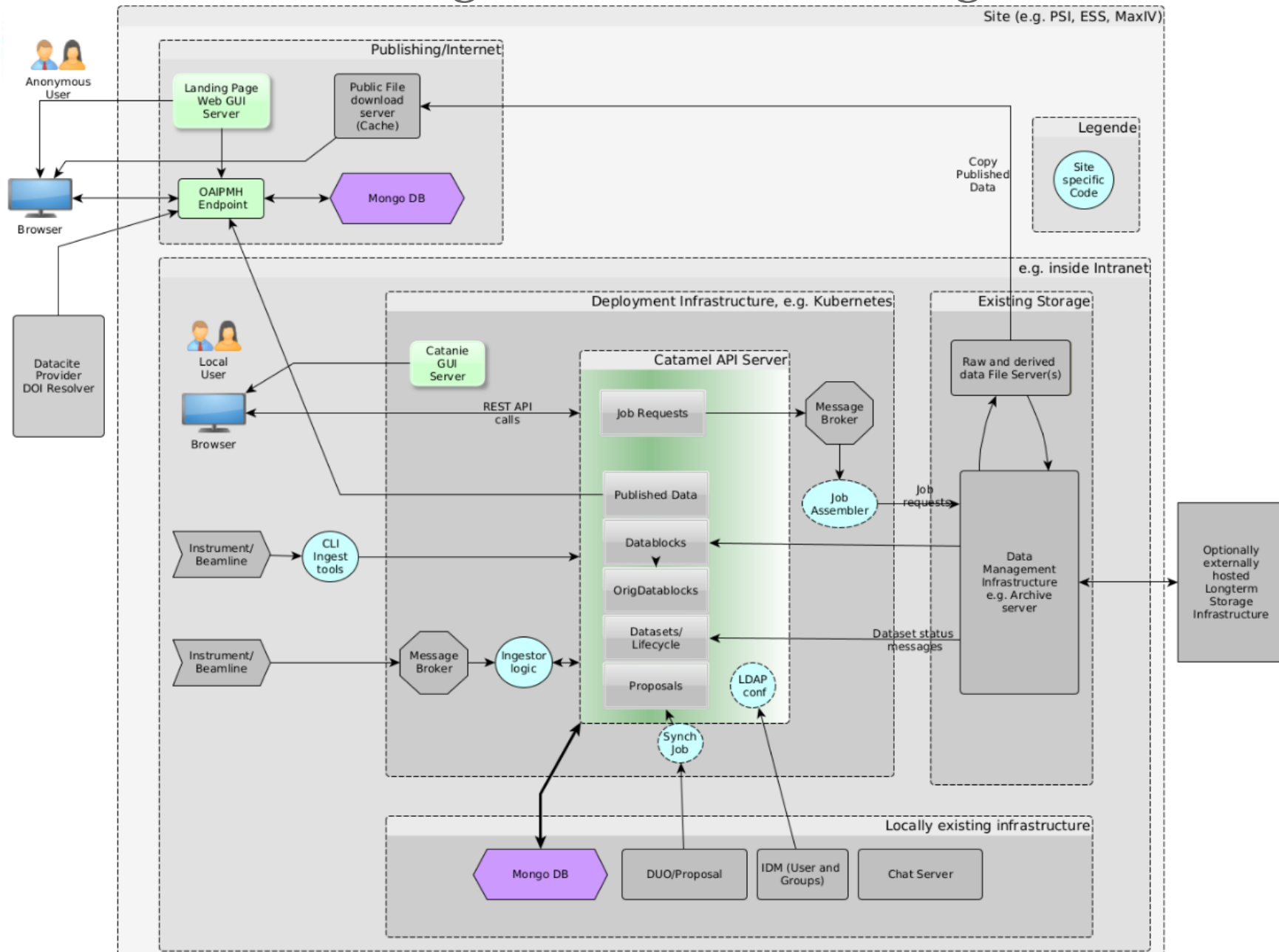
[Access Data](#)



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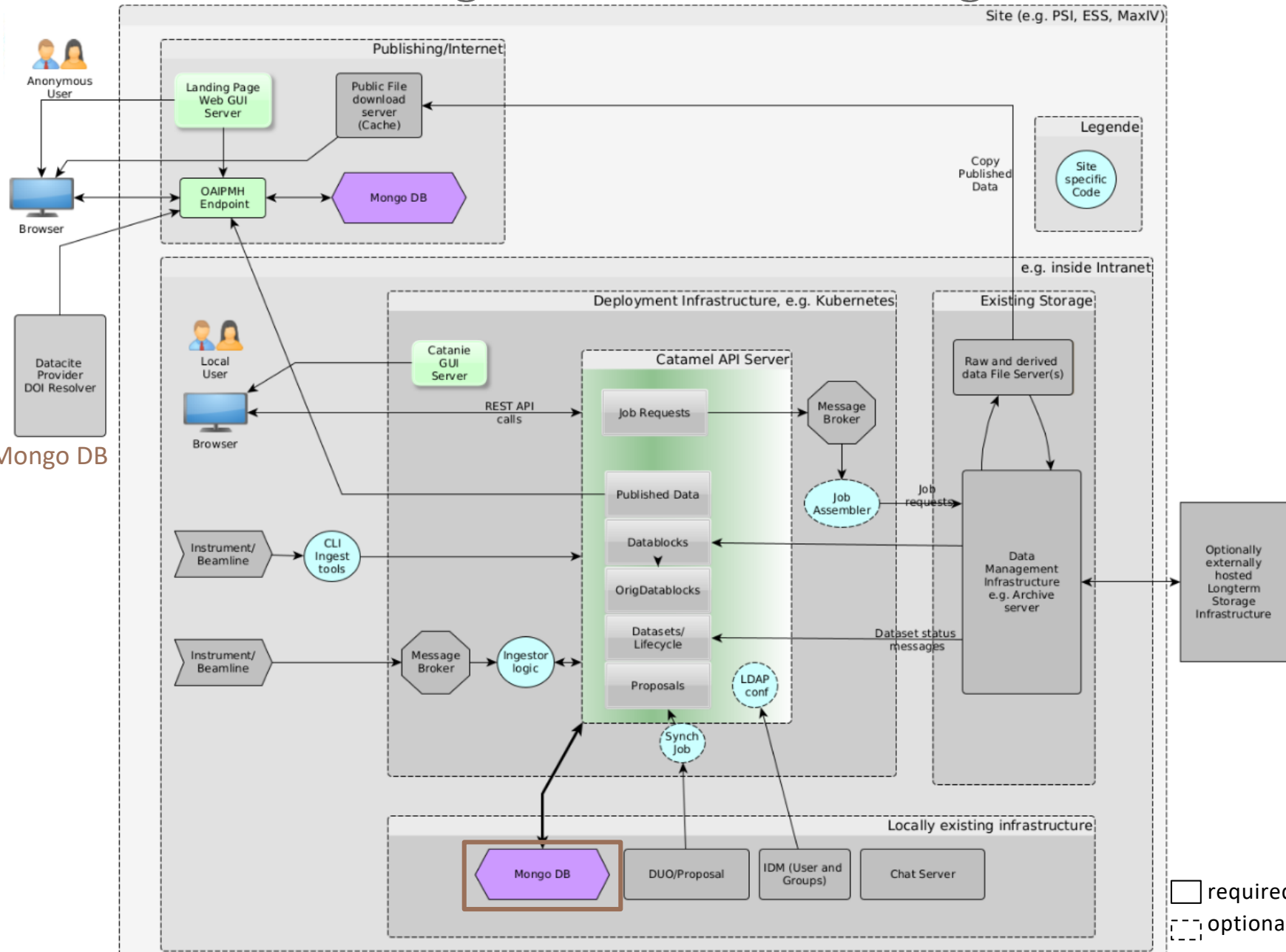


Data Catalog Architecture and Integration



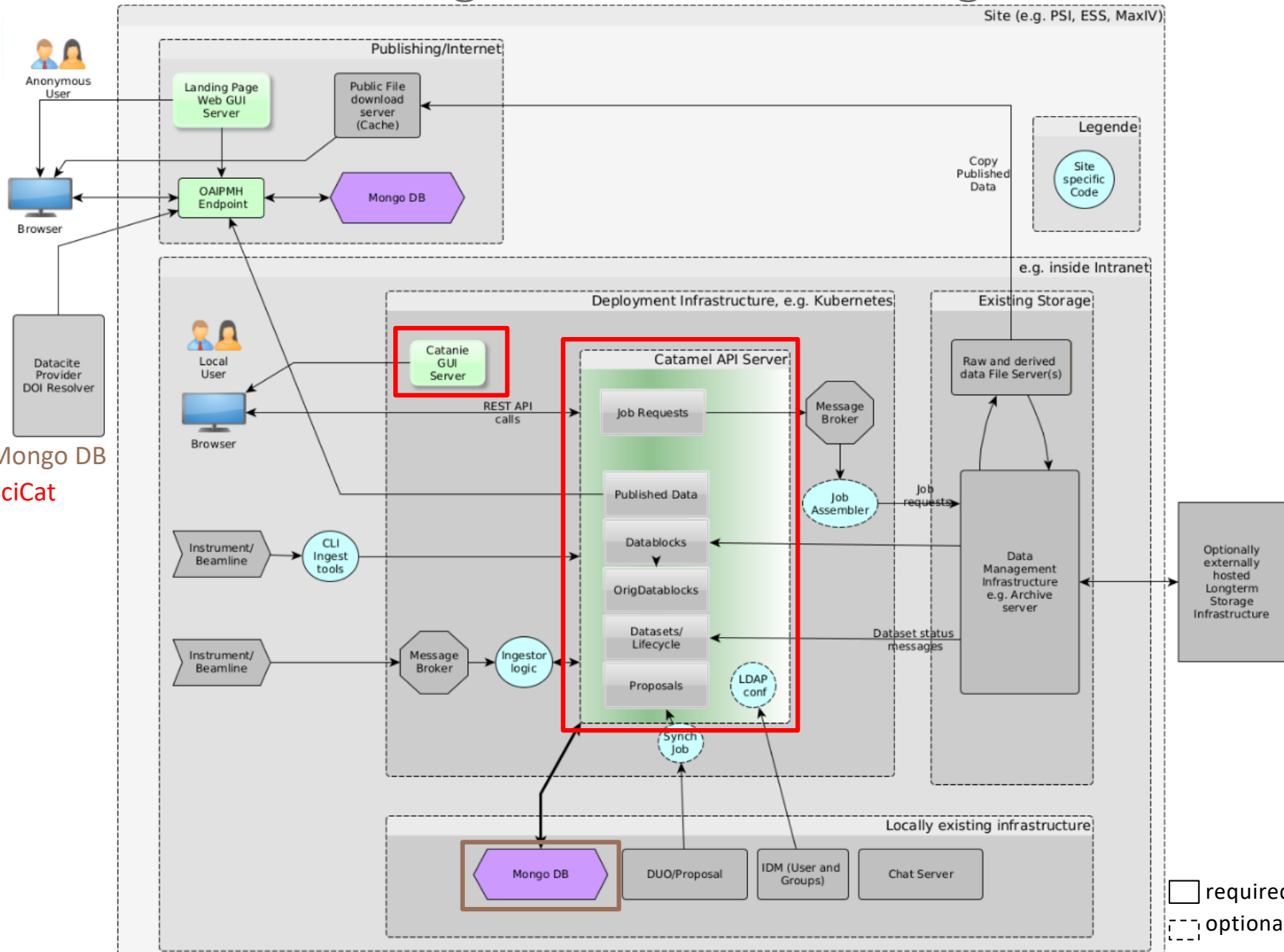
Data Catalog Architecture and Integration

1. Setup Mongo DB





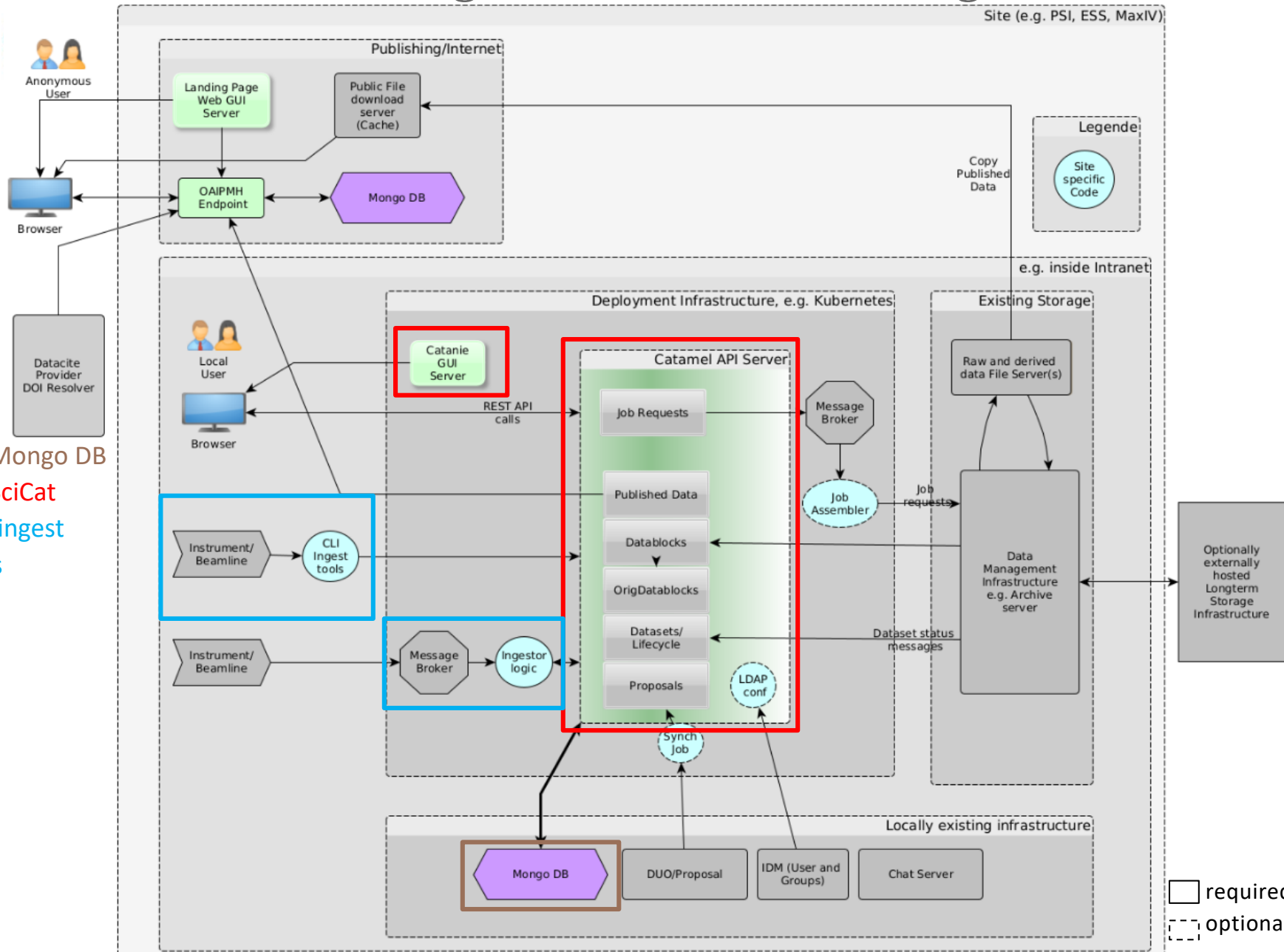
Data Catalog Architecture and Integration



1. Setup Mongo DB
2. Setup SciCat



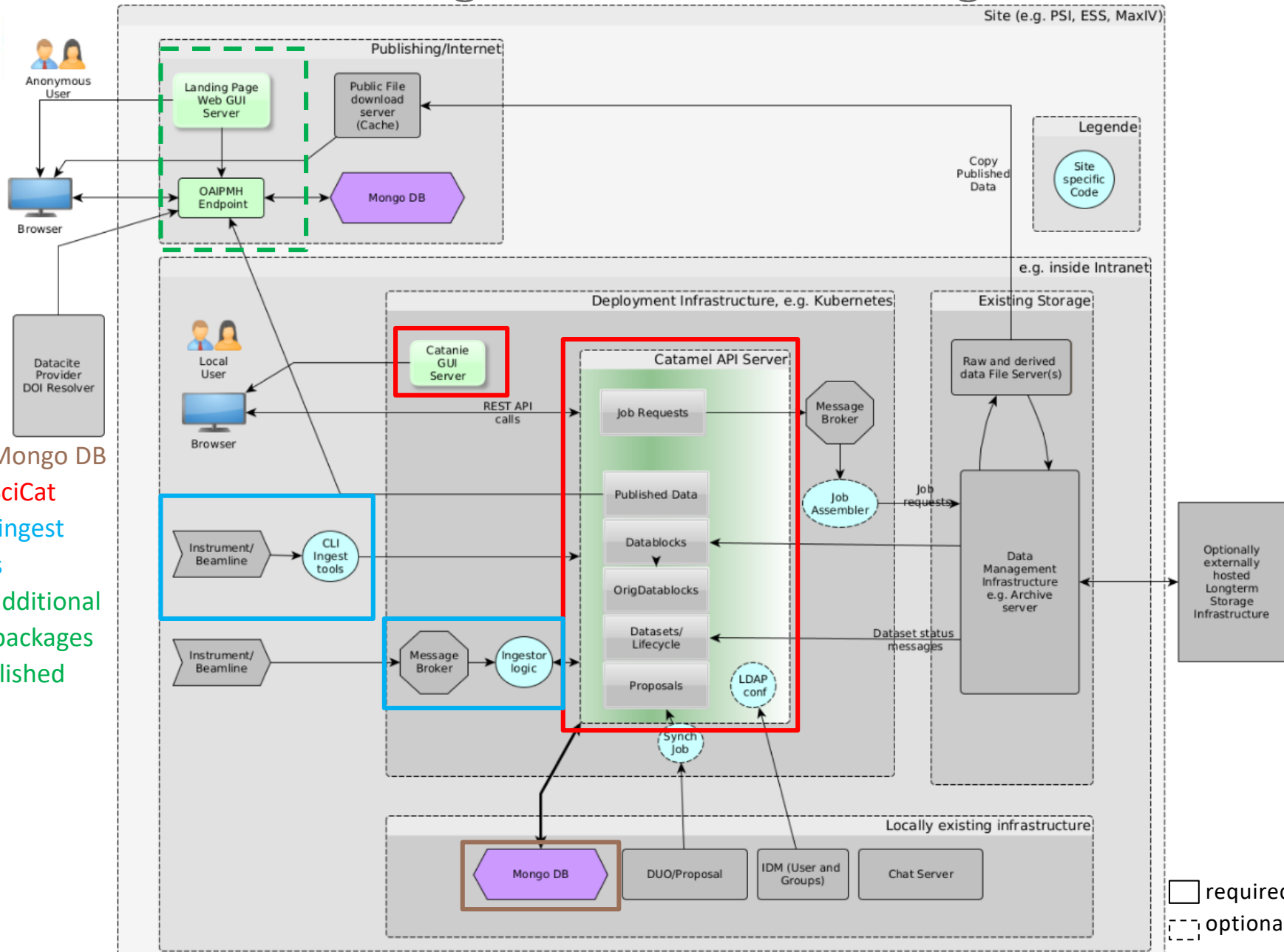
Data Catalog Architecture and Integration





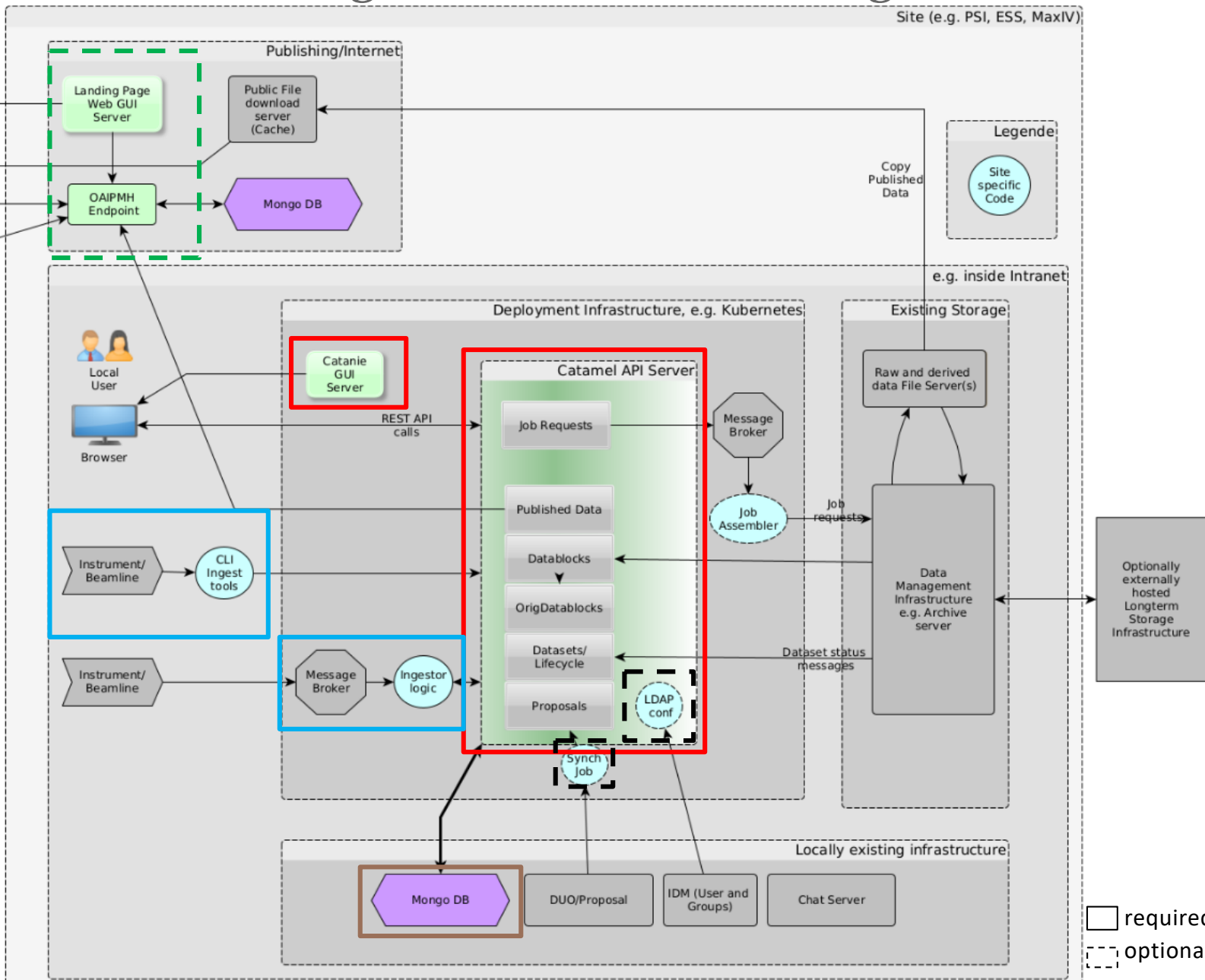
Data Catalog Architecture and Integration

1. Setup Mongo DB
2. Setup SciCat
3. Define ingest process
4. Setup additional SciCat packages for published data



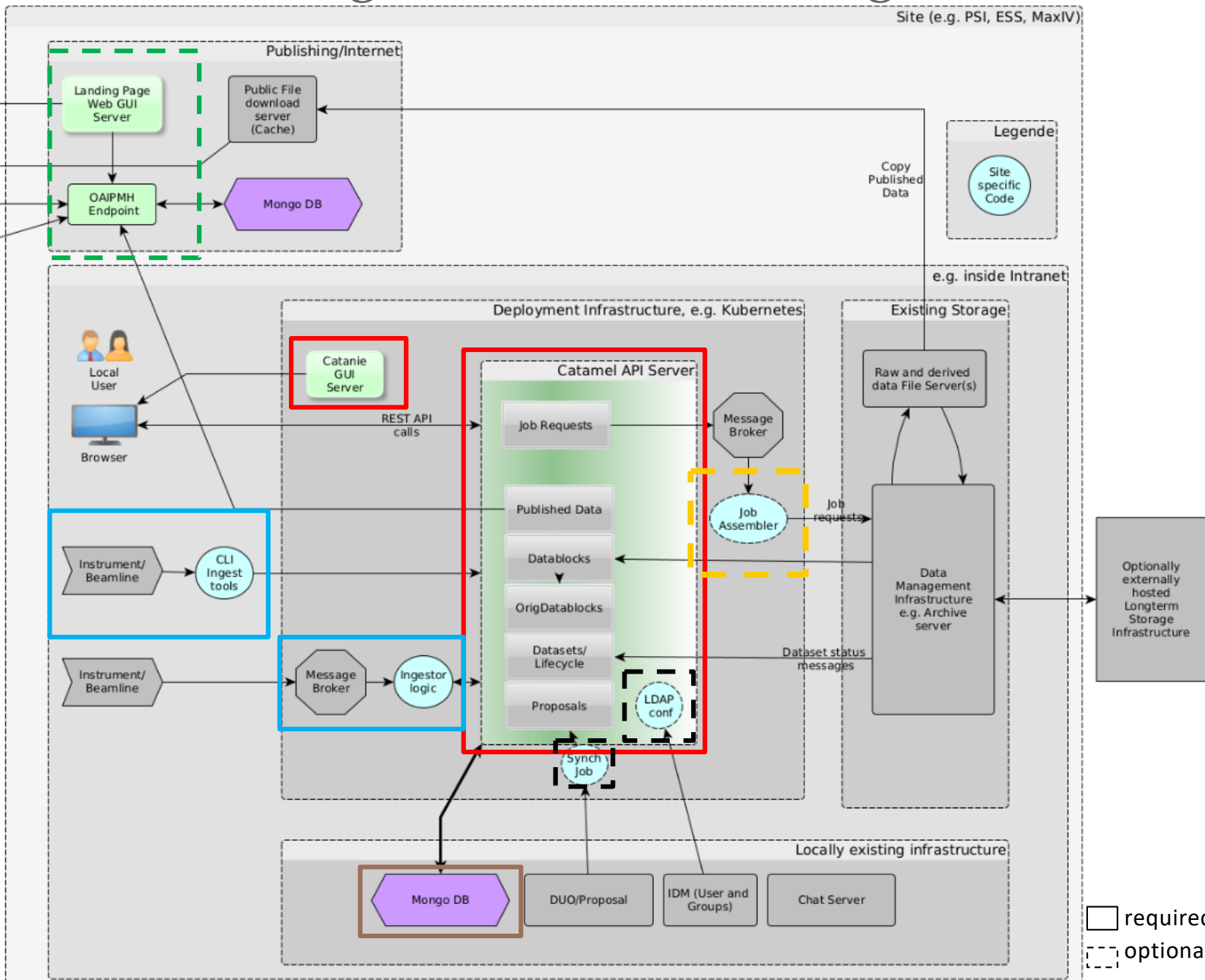
Data Catalog Architecture and Integration

1. Setup Mongo DB
2. Setup SciCat
3. Define ingest process
4. Setup additional SciCat packages for published data
5. Connect to IDM/ proposal system

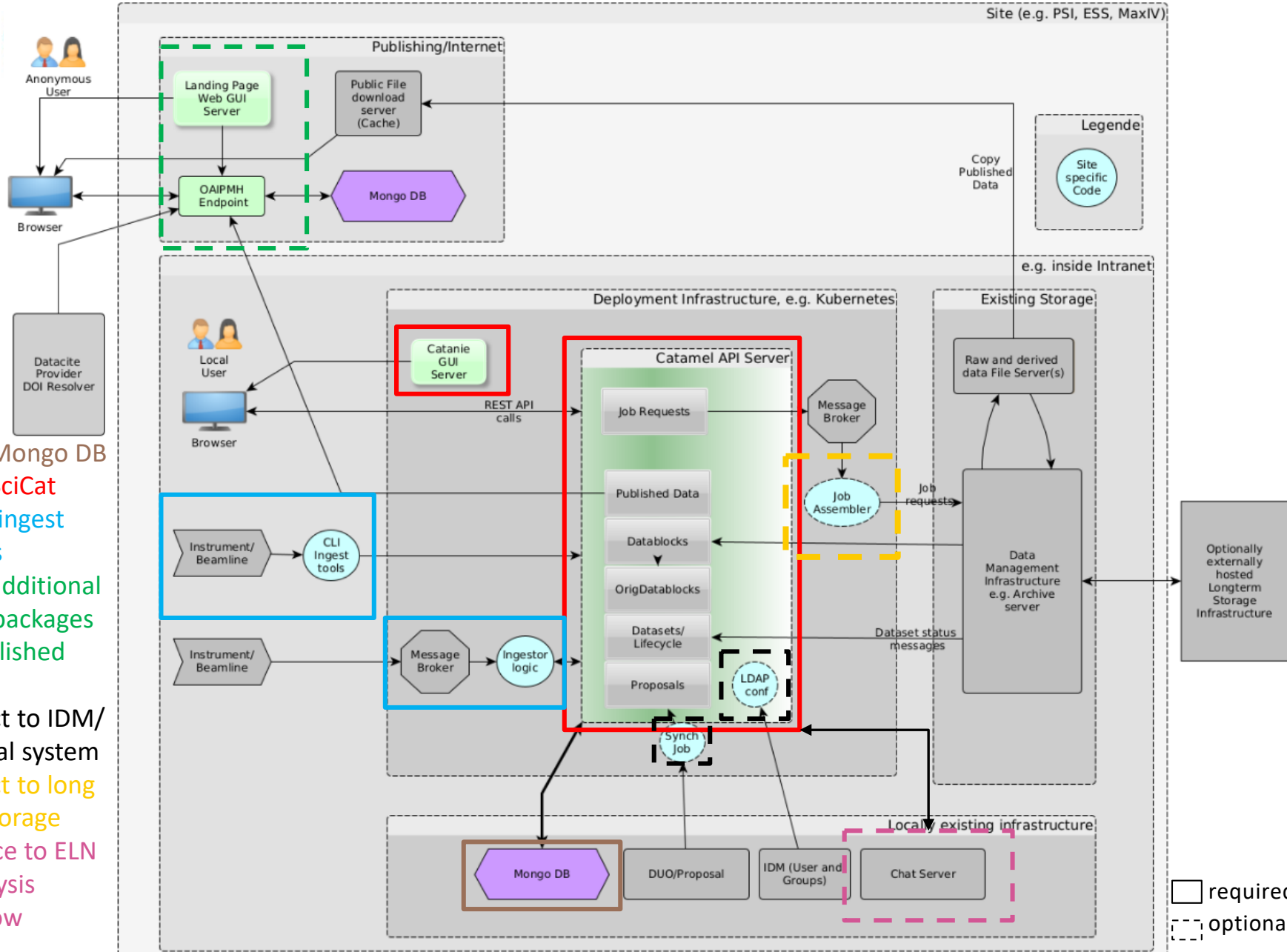


Data Catalog Architecture and Integration

1. Setup Mongo DB
2. Setup SciCat
3. Define ingest process
4. Setup additional SciCat packages for published data
5. Connect to IDM/ proposal system
6. Connect to long term storage



Data Catalog Architecture and Integration



1. Setup Mongo DB
2. Setup SciCat
3. Define ingest process
4. Setup additional SciCat packages for published data
5. Connect to IDM/proposal system
6. Connect to long term storage
7. Interface to ELN or analysis workflow

SciCat

Files for running SciCat with docker-compose.

Steps

1. Clone the repository

```
git clone https://github.com/SciCatProject/scicatlive.git
```

2. Run with the following command inside the directory

```
docker-compose up -d
```

3. SciCat will now be available on <http://localhost>. The Loopback API explorer of catamel is available at <http://localhost/explorer/>, the one for the search-api at <http://localhost/panosc-explorer/>.

Add Your Local Configuration

1. Add your local configuration to [config.local.js](#)
2. Uncomment the `volumes:` line and the line containing `config.local.js` in the catamel service section in [docker-compose.yaml](#) (if commented)
3. Restart the docker containers

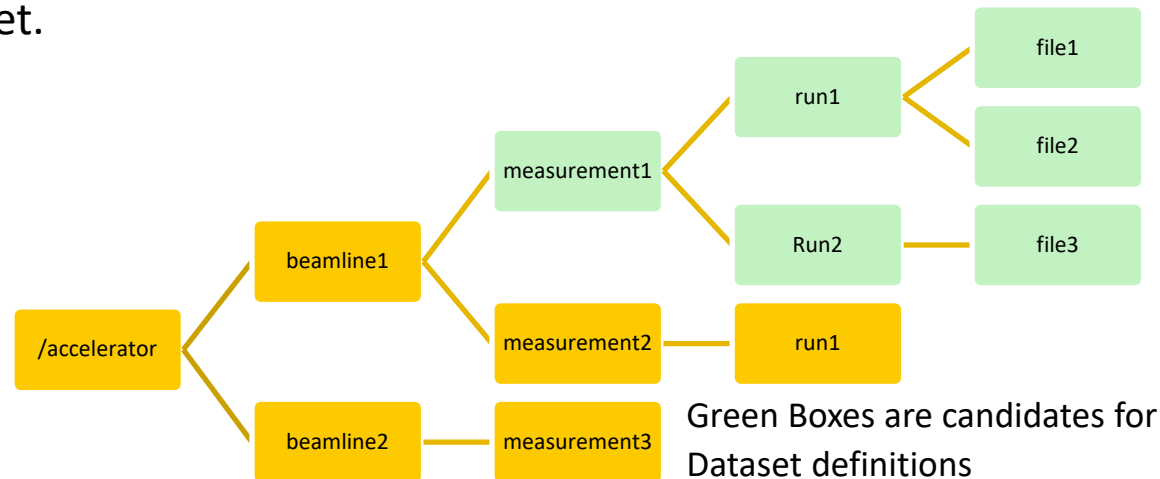
Add LDAP Authentication

1. Add your LDAP configuration to [providers.json](#)
2. Uncomment the `volumes:` line and the line containing `providers.json` in the catamel service section in [docker-compose.yaml](#)
3. Restart the docker containers

<https://github.com/SciCatProject/scicatlive>

Metadata ingestion: 1. start e.g. from existing folder structure to define Datasets

- Datasets are the smallest unit for archiving, retrieving and publication
- Create them by defining a list of files, e.g. for raw data list all the files that logically belong to a measurement/data taking run, or any other criteria. For example: define all the files in the same directory (e.g. measurement1) as part of one dataset.



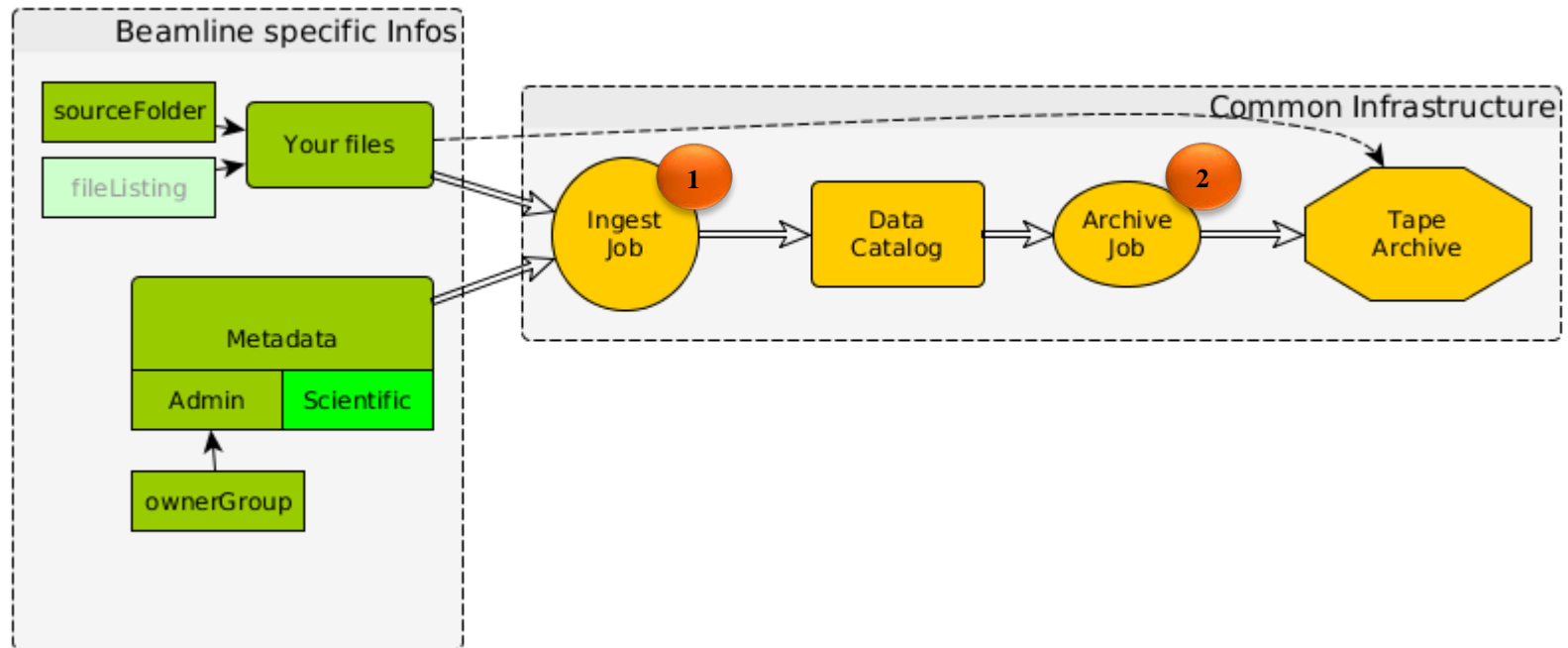
- In addition to “raw” Datasets you can create “derived” datasets containing the results of your analysis derived from the raw data. This ingest step is usually done by the user pursuing the analysis

2. Define Scientific Metadata

- The definition of scientific meta data is fully flexible.
- Ideally following a standard if it exists, e.g. NeXus based HDF5 files, extracted from instrument.
- Example:

```
"scientificMetadata": {  
  "beamlineParameters": {  
    "monostripe": "Ru/C",  
    "ring_current": {  
      "value": 0.402246,  
      "units": "A"  
    },  
    "beam_energy": {  
      "value": 22595,  
      "units": "eV"  
    }  
  },  
  "detectorParameters": {  
    "objective": 20,  
    "scintillator": "LAG 20um",  
    "exposure_time": {  
      "value": 0.4,  
      "units": "s"  
    }  
  }  
}...
```

3. Adding data is a simple (two step) procedure





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Full documentation for users and operators

← → ↺ 🏠

🔒 https://scicatproject.github.io/documentation/

⋮ 📄 ⌕ ⌵

Type to search

[SciCat Overview](#)
> [User Guide](#)
> [Operator Guide](#)
> [Ingestor Guide](#)
> [Developers Guide](#)
[API Documentation](#)

Published with HonKit

☰ A

SciCat Metadata Catalogue

build: passing

Why SciCat ?

See the [SciCat Home Webpage](#) for an overview of how SciCat can help to manage scientific data.

Structure of Documentation

The documentaion is split into the following chapters:

- [User Guide](#) - Users of the system can come here to see screen captures, FAQs and find resources on how to better understand SciCat.
- [Operator Guide](#) - System admins read this part to set up SciCat for their location
- [Ingestor Guide](#) - Instrument responsables read this to understand how data can ge ingested into SciCat either manually or in an automated fashion
- [Developer Guide](#) - Developers who want to contribute to the project should read this chapter.

Electronic Lab Notebook (ELN) integration

- That is a big topic which can easily fill a separate talk
- There are many existing ELN solutions already, often very specialized and tailored for a specific use case or scientific domain.
- Strategy of SciCat to meet the challenges:
 - try to be a «good citizen» in the landscape of existing applications: this means be designed with **easy interfacing** in mind from the start.
 - API centric approach, e.g.: Python SDK
 - Message driven interfacing, loose coupling of components
 - Support for attachments
 - Flexible metadata structure, therefore open to accept new ad-hoc informations from ELNs
- Example of such integrations:
 - SciChat: integrate SciCat API with an existing Matrix/element based chat system
 - SciLog: This is in early state,WIP at PSI, optimized for beamline usage
 - Jupyter Notebooks

Link with SciChat Electronic Logbook

Live commentary and feedback from the experiment can be captured in an electronic logbook and linked to the datasets for reference in data analysis etc.

SciChat | YC7S25

scichat.ess.lu.se/#/room/!UvYHzCBzzpcfEdbXiY:ess

+ tobiasrichter
 V20 K J M
 Explore Filter
 DIRECT MESSAGES
 anderspettersson
 jekabskarklins
 neilvaytet
 Anders LO
 judithhouston
 ROOMS
 Afonso and fredrik...
 fredrikbolmsten an...
 matt.clarke
 SWAP
 WFH Malmö Lunch
 fredrikbolmsten an...
 EFU Team

YC7S25 V20 <2019-11-27>

neilvaytet

Oliver: peterkadletz so i guess one of the th
 have one of the wfm choppers out of phase and see
 you be able to record a few runs with one of the cho
 amounts (a small shift to start with and then increas
 would also be interesting to see how it changes if th
 the second, so maybe also repeat a couple of the me
 chopper being out of phase.

Finally, we also thought we could try some continuous beam scanning. I don't know
 if you are able to get enough flux through when the slits are in place, but it's
 possible, I would like to have a fast scan in a zig-zag or spiral pattern across the
 beam, to see if we can re-create beam profiles in that way.
 We can speak on Monday about details.

(edited)

scicatbot

The file /data/kafka-to-nexus/nicos_00002483.hdf was created. See
https://scicat.ess.lu.se/datasets/20.500.12269%2F2483nicos_00002483.hdf for
 details

nicos_00002483.hdf
 Title: Piaronic f127 10wt%
 Number of events: 2816397
 Min Tot: 0.188 [microseconds]
 Max Tot: 211672.713 [microseconds]

Counts

17500
15000
12500
10000

Counts

10⁴
10³
10²
10¹
10⁰

Counts

10⁴
10³
10²
10¹
10⁰

SciCat | YC7S25

SciCat ESS

scicat.ess.eu/datasets/20.500.12269%2F2482nicos_00002482.hdf

Datasets / 20.500.12269/2482nicos_00002482.hdf /

Details Datafiles Attachments Logbook Lifecycle
 Items per page: 25

Filter

☒ Bot Messages
☒ User Messages
☒ Images

Go to chat

Timestamp	Sender	Entry
2019-12-10, Tue 10:28	oliverlohmann	
2019-12-10, Tue 10:22	jonasnilsson	Oliver: Can you post the current geometry of the V20 have to fix the geometry we are using when re-writing
2019-12-10, Tue 09:45	peterkadletz	In reply to @neilvaytet:ess ok, i'll call around 10:30 if that's ok
2019-12-10, Tue 09:44	neilvaytet	yes ok, i'll call around 10:30 if that's ok
2019-12-10, Tue 09:40	peterkadletz	In reply to @neilvaytet:ess Oliver: peterkadletz so i guess one of the things wfm choppers out of phase and see what the d a few runs with one of the choppers out of pha start with and then increase the shift for the ne how it changes if the first chopper is out of pha couple of the measurements with the other cho Finally, we also thought we could try some con are able to get enough flux through when the s

stephanegli

henrikjohansson

michelebrambilla

Matthew Jones

@Jonas

scicatbot

fredrikbolmsten

judithhouston

robinworacek

Sites using or planning to use SciCat and contact information

- European Spallation Source (Sweden/Denmark)
- Paul Scherrer Institut (Switzerland)
- MaxIV Laboratory (Sweden)
- Advanced Light Source - micro-CT (USA)
- Bundesamt für Materialwirtschaft (Germany)
- Rosalind Franklin Institute (United Kingdom)
- Shanghai Facility SSRF (China)
- Beijing High Energy Photon Source (China)
- Deutsches Elektronen-Synchrotron - PETRA (Germany)
- SOLEIL (France)

- Several of the sites contribute actively to the SciCat codebase

- **Fortnightly developers'/operators' meetings + internal chat channel**
- **Please get in contact for questions about SciCat onboarding at this email address:**
carlo.minotti@psi.ch or max.novelli@ess.eu