

E-Logbook Overview

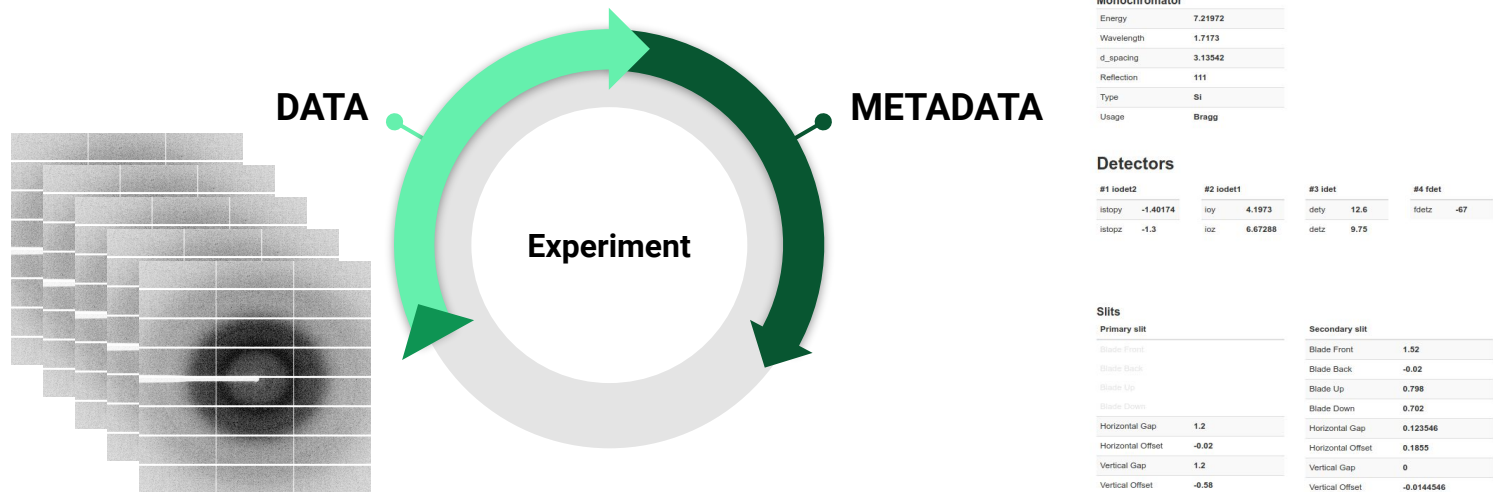
Alex de Maria
Data Manager
Data Analysis Unit
19/May/2021

- Motivation
- Requirements
- Logbook
- Architecture and implementation
- Deployment and risks
- Conclusion

MOTIVATION

“The ultimate goal of FAIR is to optimise the reuse of data”

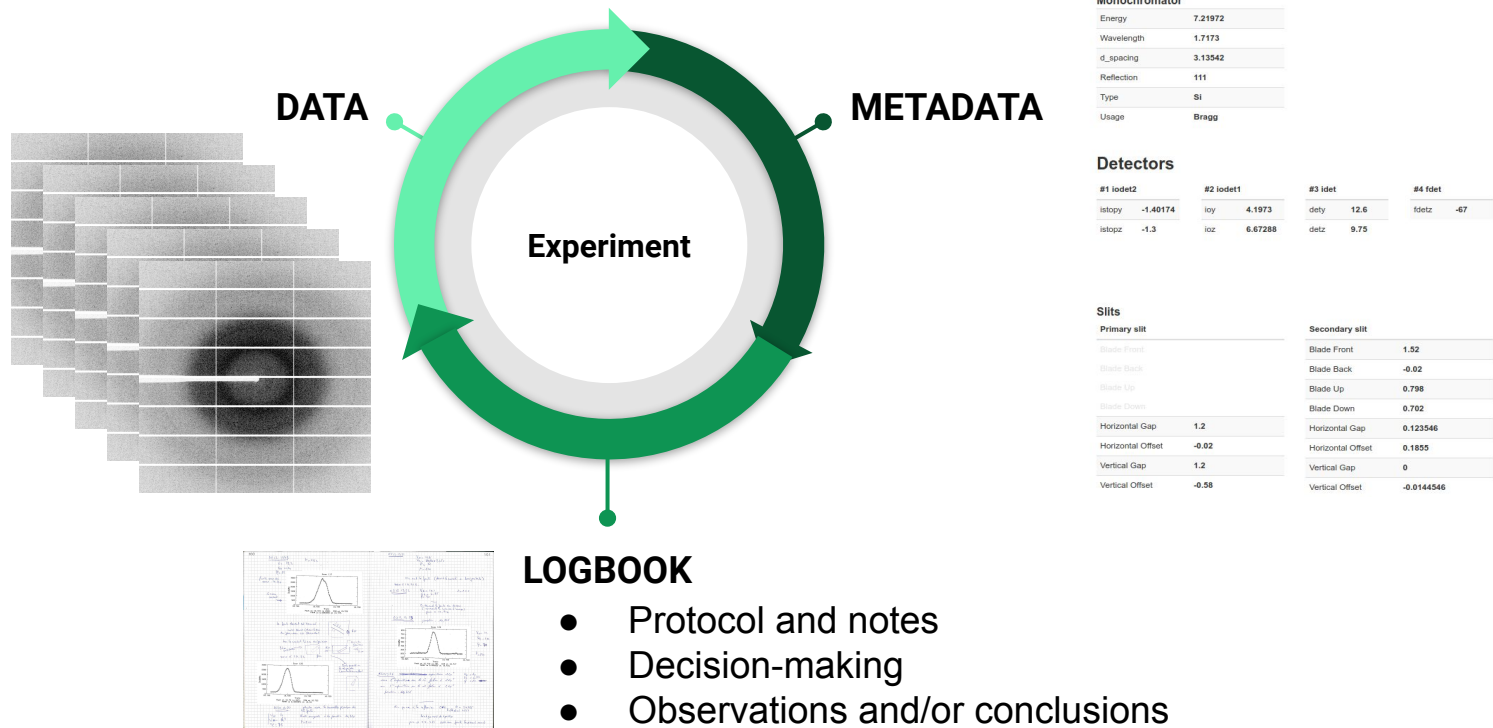
<https://www.go-fair.org/fair-principles>



MOTIVATION

“The ultimate goal of FAIR is to optimise the reuse of data”

<https://www.go-fair.org/fair-principles>



Logbook is considered as a **key feature** in the implementation of the **data policy**

- **Save** the context of experiments on time scale basis
 - Helps scientists in data exploitation/processing
 - Helps scientific community in reusing the data

- Makes experiments easier (or possible) to:
 - **Understand**
 - **Reuse**
 - **Reproduce**

REQUIREMENTS

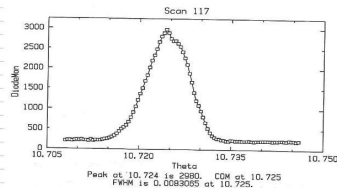
100

0812 1349
 $V_A = 13.3$
 $V_B = 10$
 $\varphi = 85$

$t = 7.5$

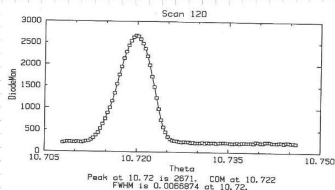
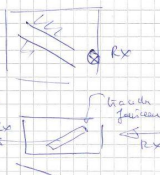
photo prise au max - 10.724

scan avant



la fente devant est ouverte
 c'est d'ailleurs (dans le cas du jeu) est ouverte.

donc le cristal l'air du faisceau
 film vertical
 max à 10.72



soit peut-être la grande conventionnelle



0812 1350

$V_A = 14$
 $V_B = 10.3$
 $\varphi = 78$

photo avec la nouvelle position de la fente.

photo corrigée à la position 10.720

$t = 8.05$

101

0812 1351

$V_A = 10.2$
 $V_B = 20.5 \times 5.15$
 $\varphi = 70$
 $t = 8.06$

On voit la fente (devant le cristal + horizontale)

max à 10.716

0812 1352

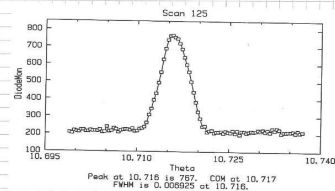
$V_A = 10.1$
 $V_B = 4.95$
 $\varphi = 95$

$t = 8.05$

On déplace la fente du dossier
 (re monte le bras de l'unité)
 pic à 10.716

0812 1353

position : 10.716



$V_A = 10$
 $V_B = 4.92$
 $\varphi = 70$
 $t = 8.05$

0812 1354 ~~avec 5.5~~ exposition 120"
 une 2^{ème} exposition sur le film à 160"
 une 3^{ème} exposition sur le film à 240"
 fonction : 10.716

$V_A = 10$
 $V_B = 4.95$
 $\varphi = 80$

On passe à la réflexion 060 $\theta = 24.865^\circ$
 $2\theta_{max} = 1.4813$

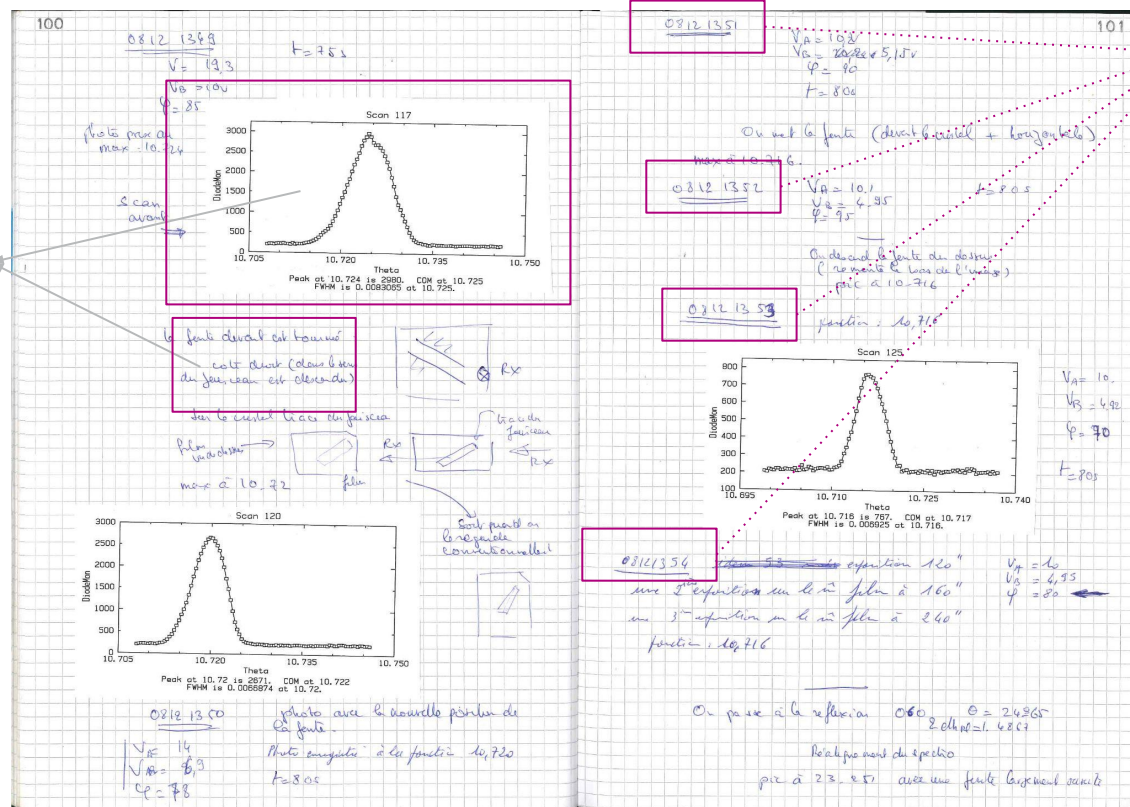
Reajustement du spectre

pic à 23.457 avec une fente large ment ouverte

REQUIREMENTS

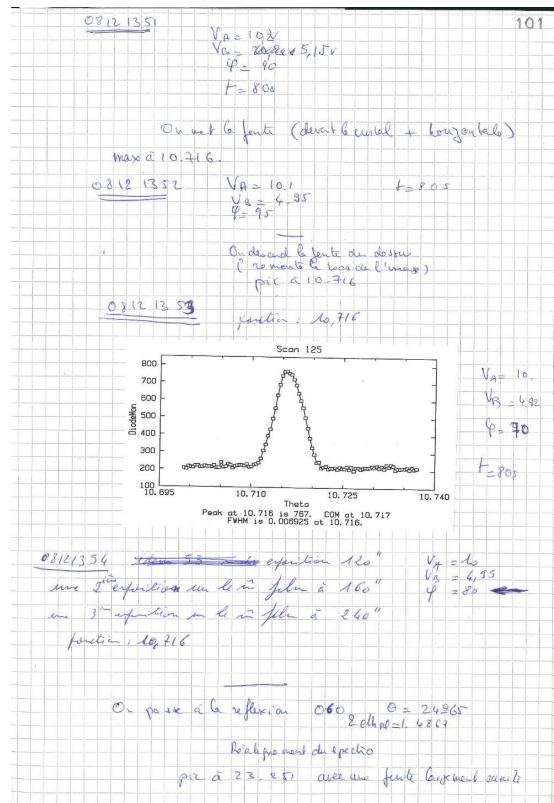
Plots and Text

Time Stamped



Chronological Order

REQUIREMENTS



- A logbook is a **list of entries** (logs or events)
- **Time stamped in chronological** order and **sequential**
- Support rich text and **WYSIWYG** editor
- A logbook can be attached to: beamline, proposal, **session**, dataset, sample, datafile
- **Upload** images and files

Plus:

- Control access. User management and security
- API exposed to be used by users or software (SPEC, Bliss, etc..)
- Support different types of logs. For instance: info, error, debug

REQUIREMENTS

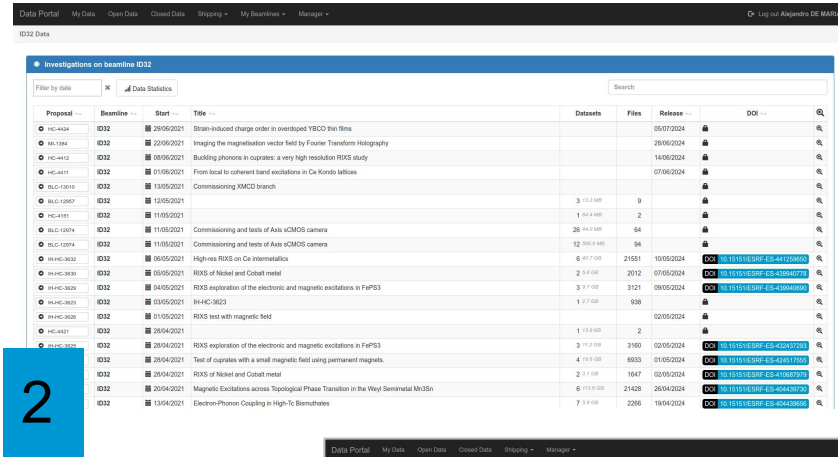
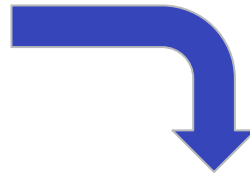
- **Copy/paste** images from other software
- **Version control** for each log
- **Search tool**
- Keep logs forever
- Support the use of **tags**
- Seamless **integration** with the data portal (ICAT)
- Compliant with the **data policy** (e.g: embargo period)

LOGBOOK



ESRF Authentication Service

2

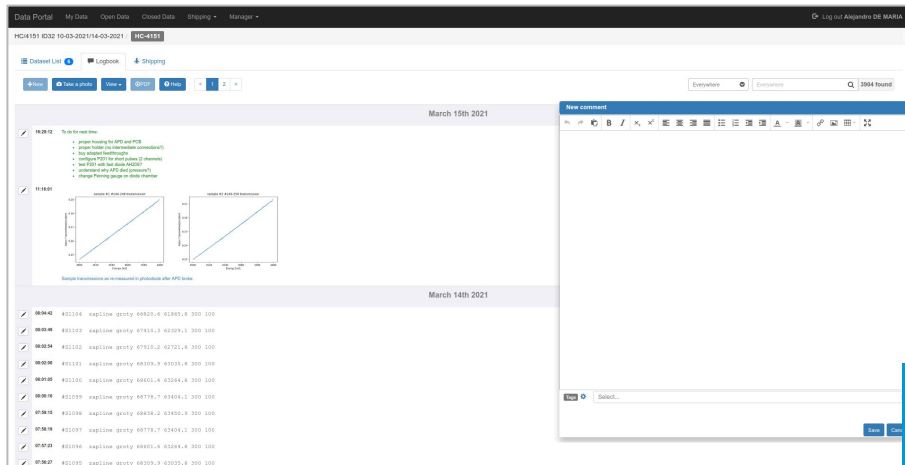


1

<https://data.esrf.fr>

Sign in with SSO

ESRF SS



3

LOGBOOK

Data Portal My Data Open Data Closed Data Shipping ▾ My Beamlines ▾ Manager ▾

Log out Alejandro DE MARIA

BLC-12657 ID32 19/01/2021-29/01/2021 Beamline start-up and commissioning

Dataset List 0

Logbook

Shipping

+ New

Take a photo

View ▾

PDF

Help

Everywhere



Everywhere



70 found

January 28th 2021

- 04:07:32 #S388 zapline groty 38244.5 34597.1 300 100
tracking macro didn't work. Macro stopped.
Kurt takes over at 8:00.
#S389 is the same as #388, but with kd 5 and open slits. But intensity is the same????
last scan of unds calibration
Whole set takes 6 hours
- 03:33:58 #S352 zapline groty 83186.8 75236 300 100
und C, central cone 0.5x0.5, vertical
- 02:37:55 #S293 zapline groty 89255.4 80723.1 300 100
und C, central cone 0.5x0.5, horizontal
- 02:03:46 #S256 zapline groty 77089.5 69722.7 300 100
und A, central cone 0.5x0.5, vertical
- 01:09:27 #S197 zapline groty 85564.2 77385.6 300 100
und A, central cone 0.5x0.5, horizontal
- 00:33:00 #S160 zapline groty 83186.8 75236 300 100

- Simple
- Easy to use
- Automated

LOGBOOK

11:39:53 #S79 ascan ysam -10.4156 -4.41562 20 0.1 launched at Wed Jan 27 11:39:53 2021

Not on sample; 14 mm above it. Recenter and relaunch measurements

11:19:08

```
FOURC> reconfig
```

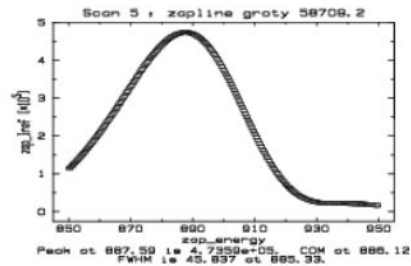
Scans stop on error 'message out of temporary cells'. stops systematically after 20th scan???

11:04:17

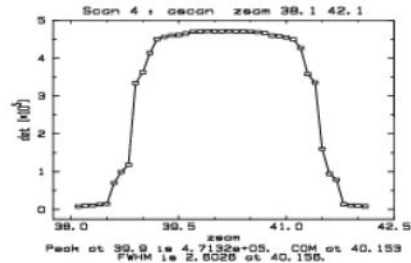
```
FOURC> ksp kd 0 7
```

Problem with intensity through sample, seems very low. Checking gains.

09:14:11



09:11:21



- Keep it small and simple
- Sequential and time stamped

19:44:05 #S104 loopscan 2 1 0 launched at Sun Mar 14 19:44:04 2021

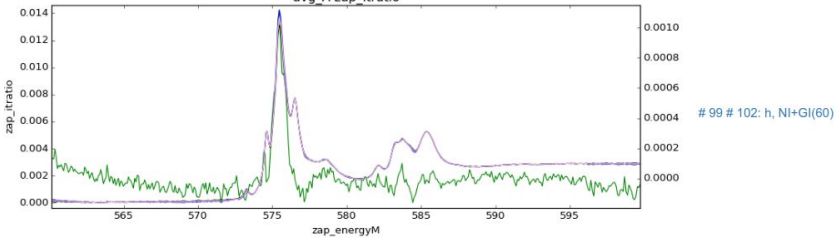
19:41:53 XMCD> qdo /data/id32/inhouse/roberto/ih-hc-3612/id32/macros/CrI3_macros.mac
... 7 command lines more

19:30:56 #S103 ascan sy -5.6495 2.3505 80 0.1 launched at Sun Mar 14 19:30:55 2021

19:30:02 XMCD> umv srot 0

19:29:20 XMCD> wm srot

19:27:13



XMLD out of plane

19:27:13 XMCD> elog_screenshot
... 1 command lines more

19:24:51 #S102 zapline grotv 71637.5 70365.3 450 100

- Simple rich text editor that allows tags

Data Portal
My Data
Open Data
Closed Data
Shipping
Manager
Log out Alejandro DE MARIA

HC/4151 ID32 10-03-2021/14-03-2021 / HC-4151

Dataset List
Logbook
Shipping

+ New
Take a photo
View
PDF
Help
0 new log(s) arrived

16:29:12
To do for next time:

- proper housing for APD and PCB
- proper holder (no intermediate connections?)
- buy adapted feedthroughs
- configure P201 for short pulses (2 channels)
- test P201 with fast diode AH20S?
- understand why APD died (pressure?)
- change Penning gauge on diode chamber

11:16:01

sample #1 #246-248 transmission

sample #2 #246-250 transmission

Sample transmissions as re-measured in photodiode after APD broke.

07:39:50
Undulator C phase shift at gap 28.00

07:01:20
Undulator C phase shift at gap 27.50

06:22:50
Undulator C phase shift at gap 27.00

05:44:13
Undulator C phase shift at gap 26.50

Edit
@Flora YAKHOU-HARRIS - 3 weeks ago

Same sequence but with correct darkcurrent on detector and grid

Tags
Select...

Save
Cancel

00:16:17

OPTICS> New dataset: fe2streptor2_main_root

November 4th 2018

23:59:17

OPTICS> zapxiainmage samy 8.064 7.124 94 samz 25.426 26.056 63 60 0 (zap: #1, spec: #1)

Notify commands

23:58:41

OPTICS> New dataset: fe2streptor2_coarse

23:58:38

OPTICS> New sample: fe2streptor2 ("Fe2 strepto replica 2")

23:58:38

OPTICS> New spec file: /data/visitor/ev280/id21/fe2streptor2/fe2streptor2_spec01/fe2streptor2_spec01.dat

23:58:38

OPTICS> New dataset: fe2streptor2_spec01

23:53:58

no new data collected

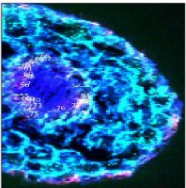
Notify errors

23:50:43

OPTICS> moveE 7.2

23:50:29

OPTICS> Fexanes_ev280



Fe3 prior r3 Sec Root: XANES Points

Comment on a command

23:03:53

OPTICS> New dataset: fe3prior3_sec_root

23:03:26

OPTICS> moveE 7.2

22:55:29

OPTICS> New dataset: fe3prior3_sr_coarse

22:48:31

Annotations

- Created by humans
- Editable

Notifications

- Created by software:
 - Bliss
 - SPEC
 - Flint
- It can only be commented

LOGBOOK

Data Portal My Data Open Data Closed Data Shipping ▾ Manager ▾

AGNES / ID002020 Sample tracking test proposal

Dataset List 0

Logbook

Shipping

+ New

Take a photo

View ▾

PDF

Everywhere

Everywhere



2 found

November 26th 2020



07:30:02



Grenoble City



07:13:01



Hello World!!

places



Tags

- Logs can be tagged
- It allows to:
 - Organize better your data
 - Find your data easier

LOGBOOK

Data Portal My Data Open Data Closed Data Shipping Manager Log out Alejandro DE MARIA

AGNES / ID002020 Sample tracking test proposal

Dataset List Logbook Shipping

+ New Take a photo

Edit

@Alejandro DE MARIA - 18 seconds ago

Grenoble City

Nice city



This log has 2 versions.

Alejandro DE MARIA edited on November 26 07:33 (most recent)

Alejandro DE MARIA created on November 26 07:30

[See all versions](#)

- Read/write access to the **experimental team** until the experiment is **released**
- Read access of the **latest version** to everybody after the release date

Tags

places x

Save

Cancel

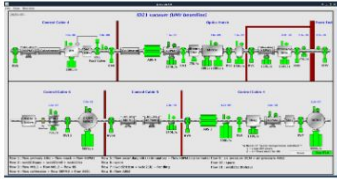
Data Portal
My Data
Open Data
Closed Data
Shipping
Manager

BLC/12581 ID21 21-11-2020/22-11-2020 / BLC-12581

Dataset List 69
Logbook
Shipping

+ New
Take a photo
View
PDF

09:15:45
Macro crashed (problem undulators) at the end of 1st series

09:13:38


19:26:47
we launch the night macro

```
def test_edge_speed():
    speedlist=[0.002,0.003,0.005,0.008,0.01,0.02,0.04,0.05,0.07,0.1,0.004,0.006,0.007,0.009,0.03]
    for speed in speedlist:
        print("Current speed: %d ms " % (speed*1e3))
        newdataset("Cu-K-%dms" % (speed*1e3))
        xanes_edge(8.95,9.2,500,speed,nbliteration=500)
```

19:24:37
NB for Cyril
SESSION_SXM [225]: u42b.velocity=2.4 # ok in idappli
SESSION_SXM [226]: u42b.velocity
Out [226]: 2.5
SESSION_SXM [227]: u42b
Out [227]: AXIS:
name (R): u42b
unit (R): mm
offset (R): 0.00000
backlash (R): 0.00000
sign (R): 1

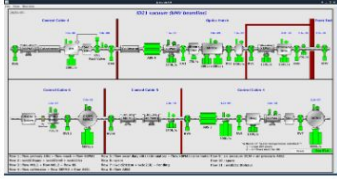
Data Portal
My Data
Open Data
Closed Data
Shipping
Manager

BLC/12581 ID21 21-11-2020/22-11-2020 / BLC-12581

Dataset List 69
Logbook
Shipping

+ New
Take a photo
View
PDF
1 2

09:15:45
Macro crashed (problem undulators) at the end of 1st series

09:13:38


08:08:55
Dataset Cu_K_6ms (Cu_foil) has been stored into ICAT successfully

07:44:11
Dataset Cu_K_4ms (Cu_foil) has been stored into ICAT successfully

06:06:16
Dataset Cu_K_100ms (Cu_foil) has been stored into ICAT successfully

04:34:54
Dataset Cu_K_70ms (Cu_foil) has been stored into ICAT successfully

03:10:43
Dataset Cu_K_50ms (Cu_foil) has been stored into ICAT successfully

01:53:03
Dataset Cu_K_40ms (Cu_foil) has been stored into ICAT successfully

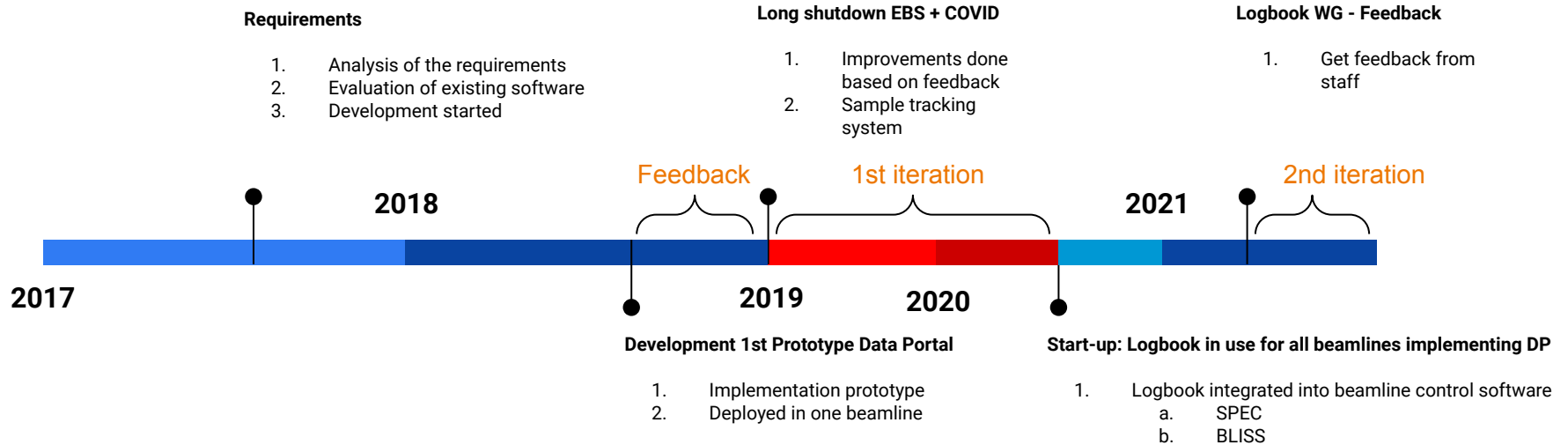
00:41:59
Dataset Cu_K_20ms (Cu_foil) has been stored into ICAT successfully

23:37:28
Dataset Cu_K_10ms (Cu_foil) has been stored into ICAT successfully

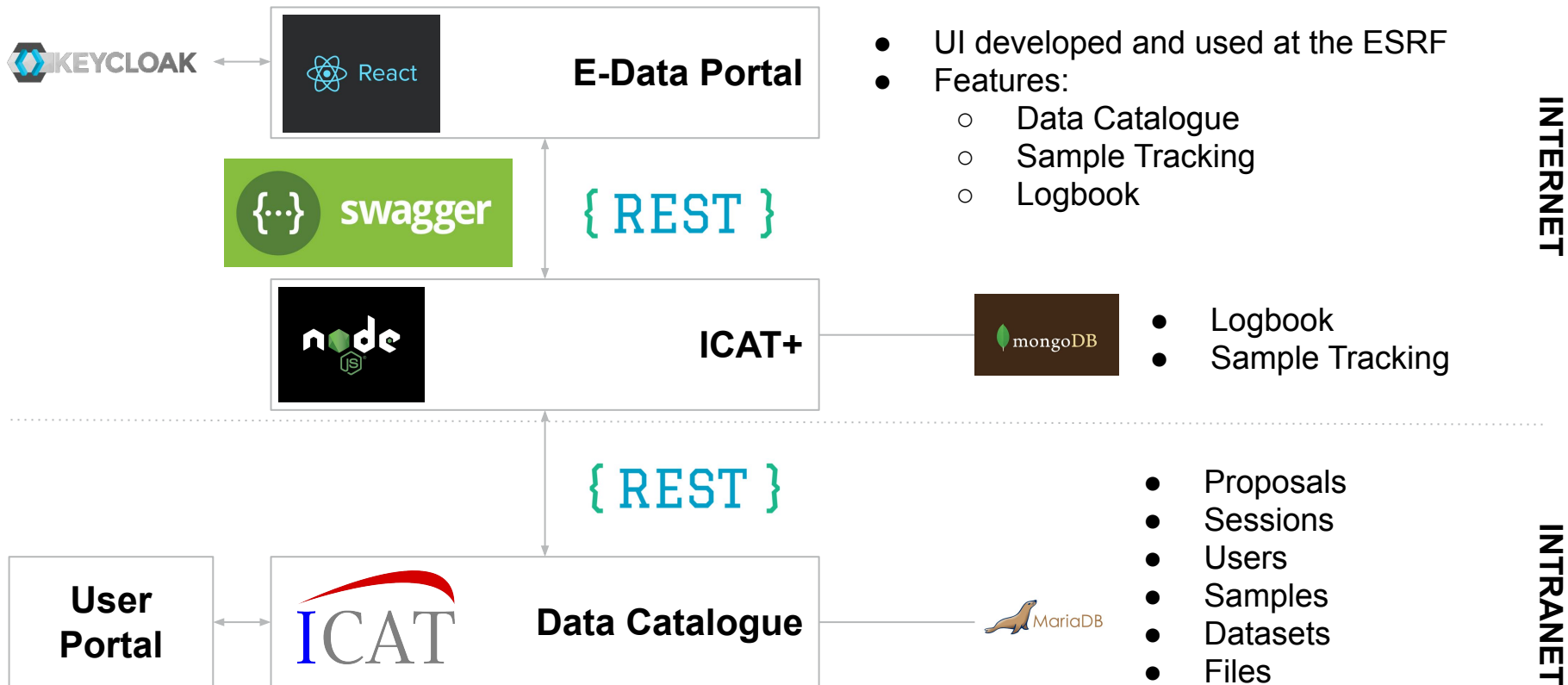
22:39:11
Dataset Cu_K_8ms (Cu_foil) has been stored into ICAT successfully

21:47:09
Dataset Cu_K_5ms (Cu_foil) has been stored into ICAT successfully

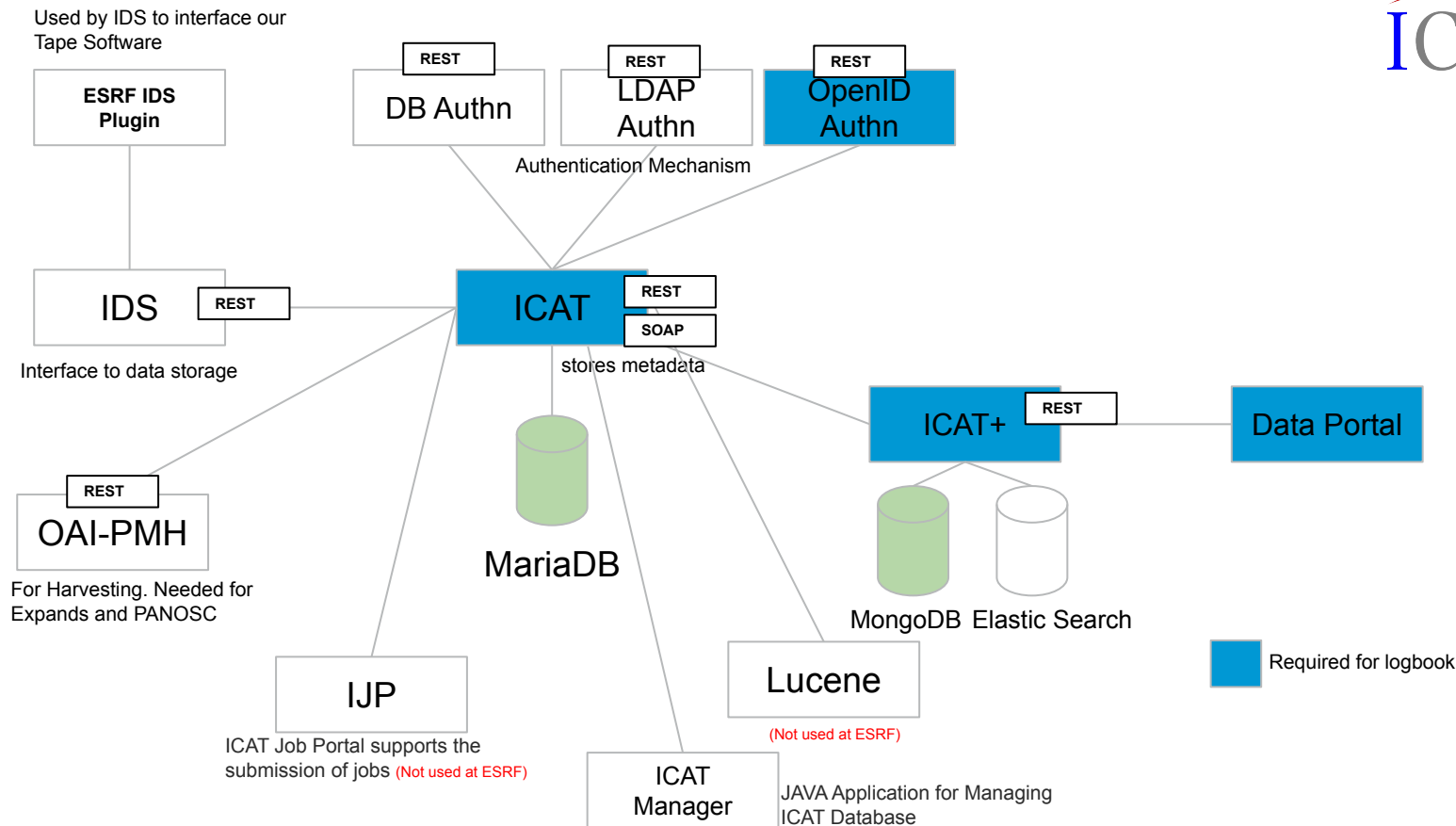
IMPLEMENTATION



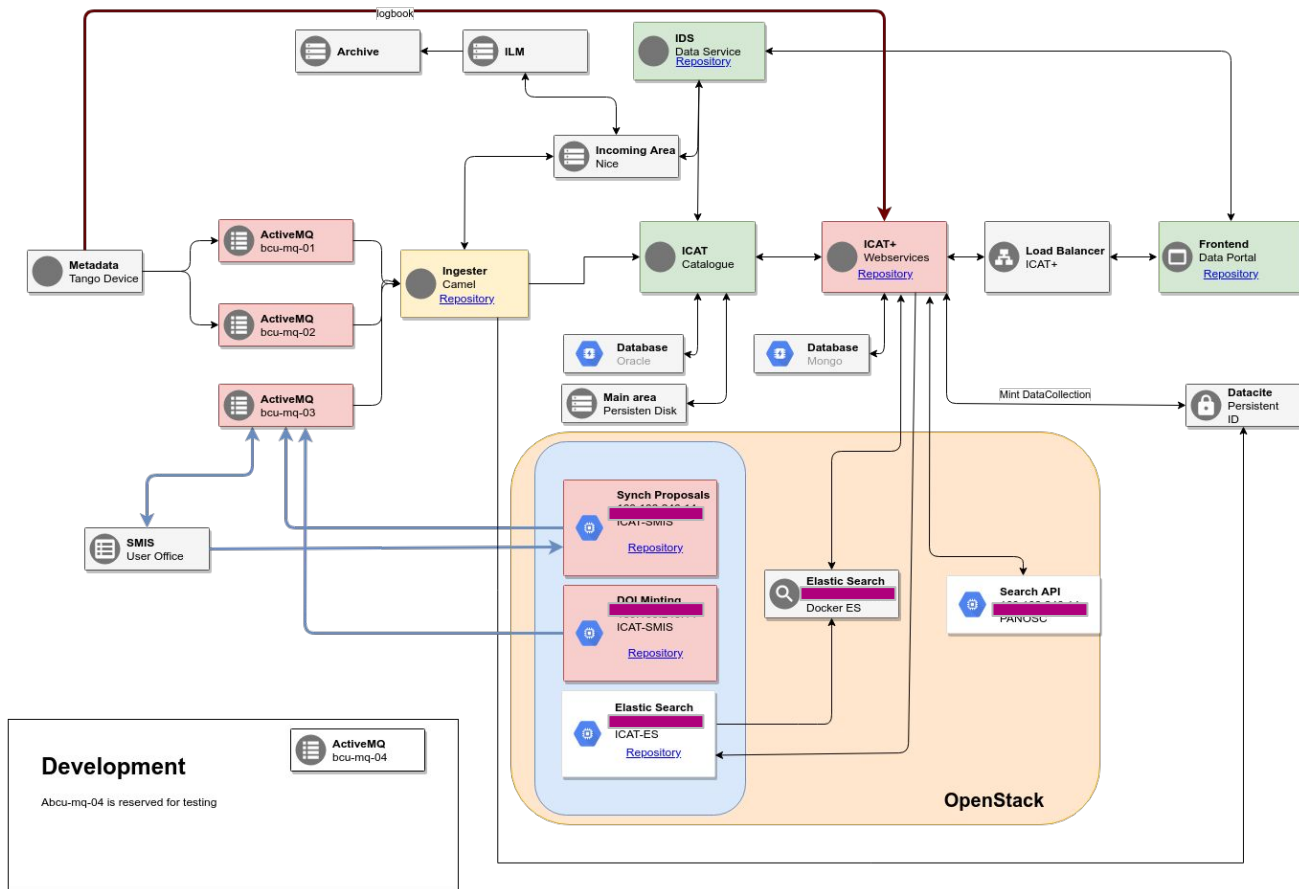
ARCHITECTURE



ARCHITECTURE



ARCHITECTURE



DATA MODEL

Data PortalMy DataOpen DataClosed DataShippingMy BeamlinesManager

Log out Alejandro DE MARIA

HC-4397ID3231/03/2021-06/04/2021 Interdependent charge and magnetic orders and superconducting gap in DyBa2Cu3O6+x thin films

Dataset List0

Logbook

Shipping

+ NewTake a photoViewPDFHelp

<12>

Everywhere

Everywhere

2604 found

April 6th 2021

15:51:05FOURC> codmenu

... 36 command lines more

08:34:57created new dataset: 20210406_end_00

08:34:57FOURC> newvisitor

08:34:49Dataset 20210405_PD2b_03 (PD2b) has been sent to archive. files=927 size=2920256378 bytes

08:34:49Dataset 20210405_PD2b_03 (PD2b) has been stored into ICAT successfully

08:34:30FOURC> shsel

... 3 command lines more

04:13:00#S4 loopscan 230 60 0 launched at Tue Apr 06 04:12:59 2021

00:08:37#S3 loopscan 230 60 0 launched at Tue Apr 06 00:08:37 2021

April 5th 2021

20:04:34#S2 loopscan 230 60 0 launched at Mon Apr 05 20:04:33 2021

16:03:21#S1 loopscan 230 60 0 launched at Mon Apr 05 16:03:20 2021

16:03:17FOURC> eon:prdef last_macro; eoff

DATA MODEL

Data PortalMy DataOpen DataClosed DataShippingMy BeamlinesManager

Log out Alejandro DE MARIA

HC-4397ID3231/03/2021-06/04/2021 Interdependent charge and magnetic orders and superconducting gap in DyBa2Cu3O6+x thin films

Dataset List0

Logbook

Shipping

+ NewTake a photoViewPDFHelp

<12>

Everywhere

Everywhere

2604 found

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08:34:30FOURC> shsel

... 3 command lines more

04:13:00#S4 loopscan 230 60 0 launched at Tue Apr 06 04:12:59 2021

00:08:37#S3 loopscan 230 60 0 launched at Tue Apr 06 00:08:37 2021

April 5th 2021

20:04:34#S2 loopscan 230 60 0 launched at Mon Apr 05 20:04:33 2021

16:03:21#S1 loopscan 230 60 0 launched at Mon Apr 05 16:03:20 2021

16:03:17FOURC> eon:prdef last_macro; eoff

DATA MODEL

08:34:49 Dataset 20210405_PD2b_03 (PD2b) has been sent to archive. files=927 size=2920258378 bytes

system

ingester

```
{
  "id": "6064544ab4469b00228c34bd",
  "tag": [ 2 items ],
  "file": [],
  "investigationName": "HC-4397",
  "investigationId": 404439657,
  "datasetId": null,
  "datasetName": null,
  "title": "",
  "type": "notification",
  "category": "info",
  "filename": null,
  "fileSize": null,
  "username": "Unknown",
  "instrumentName": "id32",
  "software": "ingester",
  "machine": "bcu-mq-01",
  "creationDate": "2021-03-31T10:51:54.000Z",
  "content": [
    {
      "_id": "6064544ab4469b00228c34be",
      "text": "Dataset 20210330_D1_853a_02 (D1_853a) has been sent to archive. files=3282 size=9824117356 bytes",
      "format": "plainText"
    }
  ],
  "previousVersionEvent": null,
  "createdAt": "2021-03-31T10:51:54.151Z",
  "updatedAt": "2021-03-31T10:51:54.151Z",
  "__v": 0,
  "meta": {
    "page": {
      "total": 2615,
      "totalPages": 3,
      "currentPage": 1
    }
  }
}
```

TAGS

Type: notification | annotation
Category : info | error | debug | comment

PlainText
HTML
Markdown

- Officially deployed in August 2020
 - > 20 Beamlines
 - 2M logs (30GB)
- Beamlines are being adapting their macros to send logs in two steps:
 - Integrated in BLISS/SPEC
 - Commands
 - Errors
 - Customization for each technique
 - Configuration
 - Motor positions
 - Etc...
- Very useful for remote experiments (COVID)
- Email sent to users 3 months before logbooks are reased

- Software acceptance
 - Transition from notebook to electronic logbook
 - Fear to made logbook public after embargo
 - Complains/controversy about:
 - Protected logs, e.g. logs can not be removed
 - Change order (or sequence)
 - Google-doc-like solution
- Misuse of the logbook
 - Verbosity
 - **Too little** logs makes logbook **useless**
 - **Too many** logs makes logbook **useless** -> Not a logging tool
 - Not a google doc
- Flexibility: single solution for many different type of experiments (and people)

- It is a tool that allows users to enrich their metadata
- Many scientists are devoting time and effort on enriching their experiments
 - It is a tool with lot of **potential**
- It could be used as a **collaborative tool**
- It is a **new software** and we need:
 - To get experience
 - Improve User eXperience (UX)
 - Implement new features
 - Processed data
 - Retrieve logs by datasets or sample
 - Global search



Thanks for your attention!