



**EUROPEAN
SPALLATION
SOURCE**



Scientific Web Applications

SWAP

PRESENTED BY FREDRIK BOLMSTEN

2022-10-25



Team

Staff & Scope



Fredrik Bolmsten - Section lead



Jekabs Karklins - Software engineer



Max Novelli - Data curation scientist



~~Henrik Johansson - Developer PaNOSC (End December)~~



Martin Trajanovski - Service agreement (End November)

2 recruitments was approved in June., bringing the team to 5 permanent staff.

Development of the user journey in collaboration with the Scientific Activity Division.

User Office Software:

- Proposal system
- Scheduling software
- Statistics
- ...

Data Curation:

- Metadata catalogue
- Electronic logbook
- Scientific data management
- ...

User Office



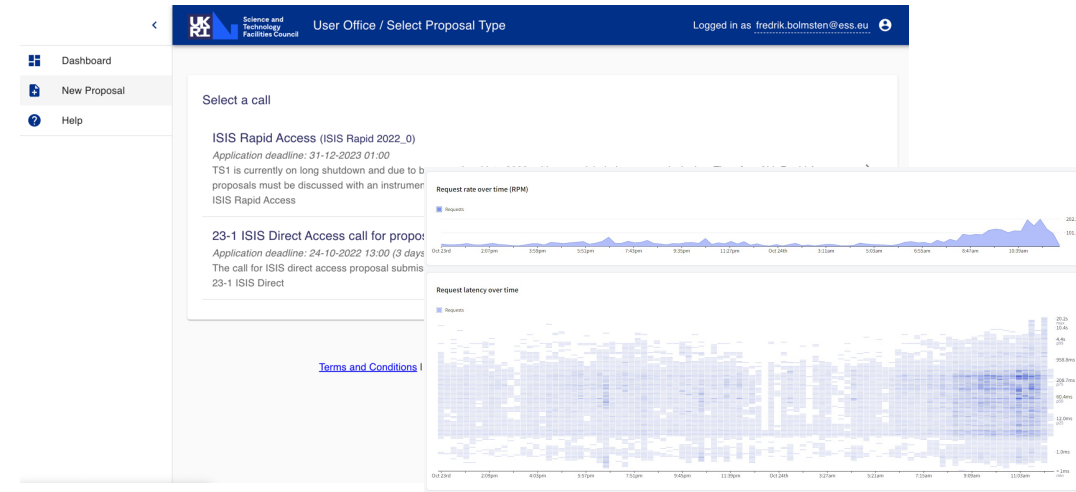
Supporting DEMAX Rolling Access with:

- Proposal submission
- Technical Review
- Scientific Review

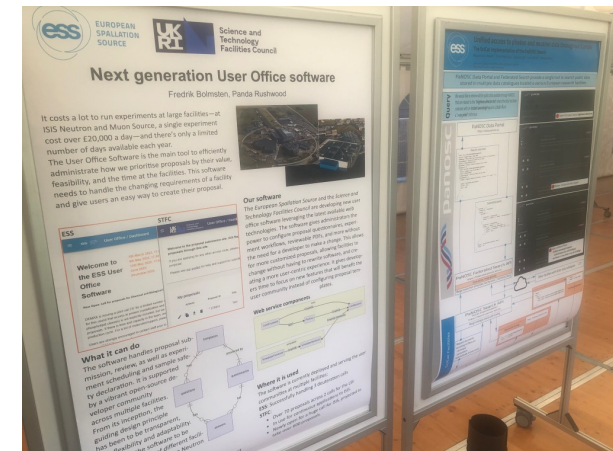
Used for ISIS main call for proposals, received 664 (150 last hour) proposals in October.

New developments:

- OIDC support
- Dynamic PDF's for proposals(STFC)
- SciChat & SciCat & NiCOS integrations
- Settings/Features page
- Antivirus scanning of files(STFC)
- Code refactoring / Mono repository



ISIS Rapid & Direct Calls

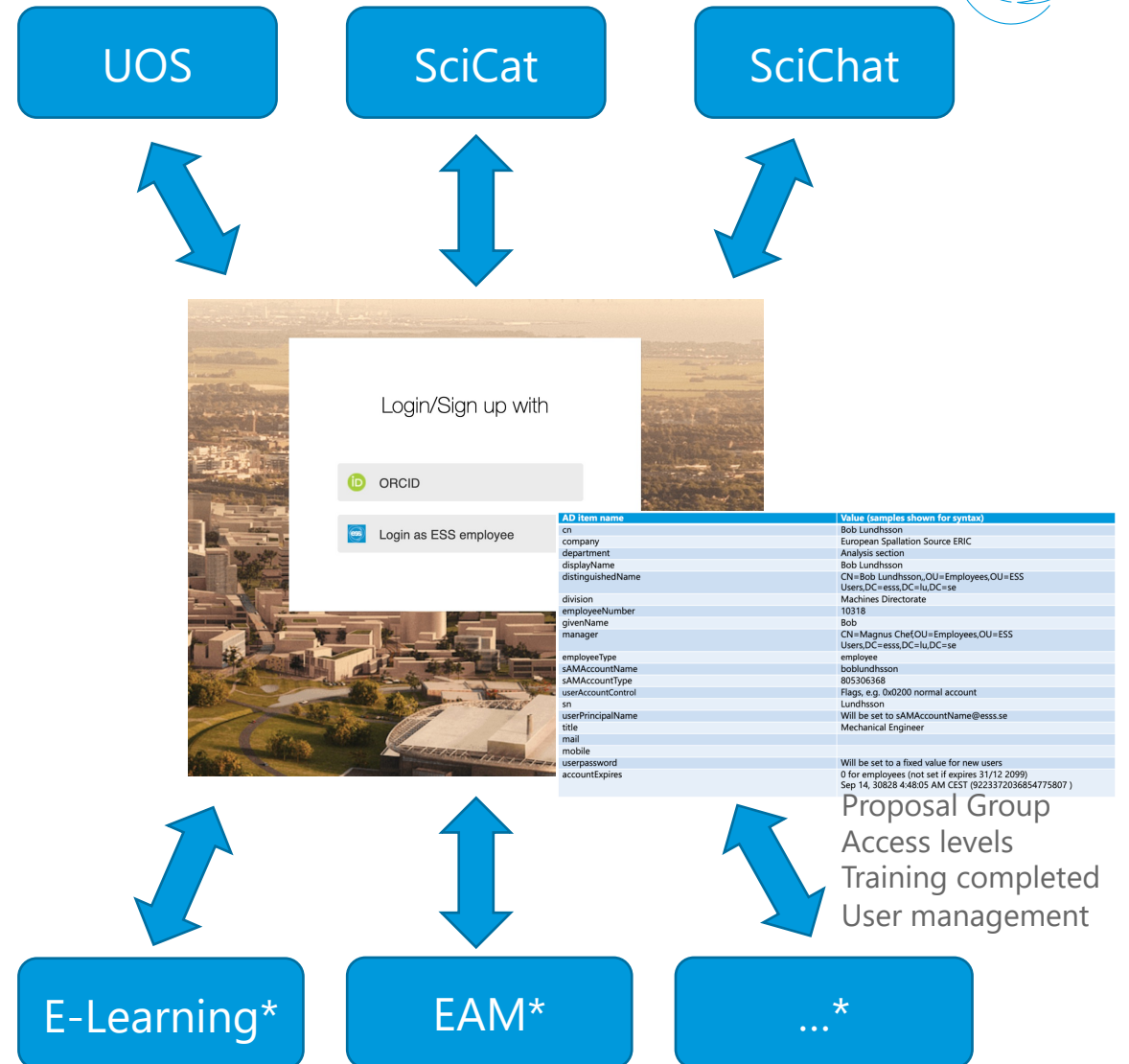
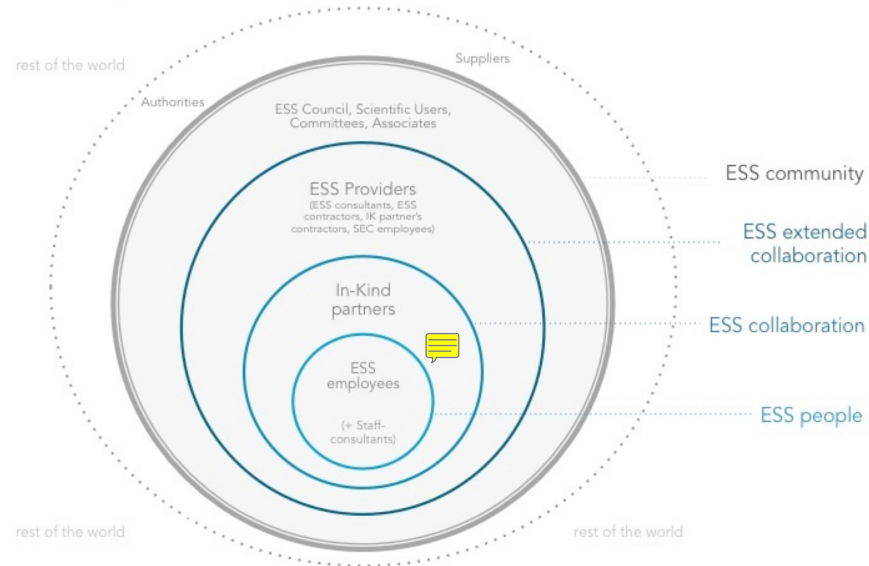


NoBUGS Poster

User Office

OIDC

OpenID Connect (OIDC) is an open authentication protocol that works on top of the OAuth 2.0 framework. Targeted toward consumers, OIDC allows individuals to use single sign-on (SSO) to access relying party sites using OpenID Providers (OPs)



User Office

Dynamic PDF's creation attached to calls



Technique:
Deuteration lab?

Samples

- Details
- Formula
- Properties
- Type
- Container
- ISIS kit
- User kit
- Beamtime
- Availability
- Other info

Sample environment

Temperature: to K
Pressure: to Pa
Magnetic: to T
Other:

Hazards

Only hazards the user has selected appear here.



General information

Science

What is the primary science discipline for research with this sample? Life sciences
Which is the main sub discipline of life sciences? Medicine and pharmaceuticals
What is the primary experimental technique to be used with this sample? Small angle neutron scattering
What societal challenges will research with this sample address? Health

Student

Does the proposed research contribute to a students degree? Yes
Are any of the co-proposers students? No

Industry

academic users funded by industry? No

led by industry? No

research.

tion - DNA nanoparticles (i.e. lipopolyplexes), which
tions

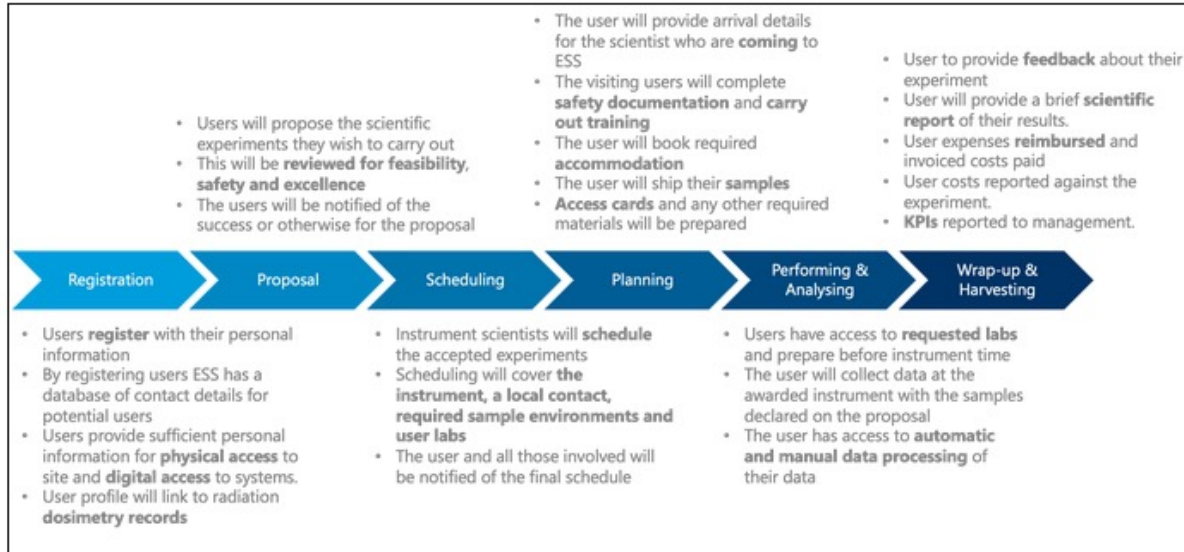
21 DE3) Yes

```
Test
Template contents
{{#> layout}}
<div class="container-fluid">
  <div class="row">
    <div class="col">
      <span class="title">Proposal: {{proposal.title}}</span><br />
      <br />
      <span class="bold">Proposal ID: </span><br />
      {{proposal.proposalId}}<br />
      <br />
      <span class="bold">Brief summary:</span><br />
      {{proposal.abstract}}<br />
      <br />
      <span class="bold">Proposal Team</span><br />
      <br />
      <span class="bold">Principal Investigator:</span><br />
      {{principalInvestigator.firstname}} {{principalInvestigator.lastname}}<br />
      {{principalInvestigator.organisation}}<br />
      {{principalInvestigator.position}}<br />
      <br />
    </div>
  </div>
</div>
```

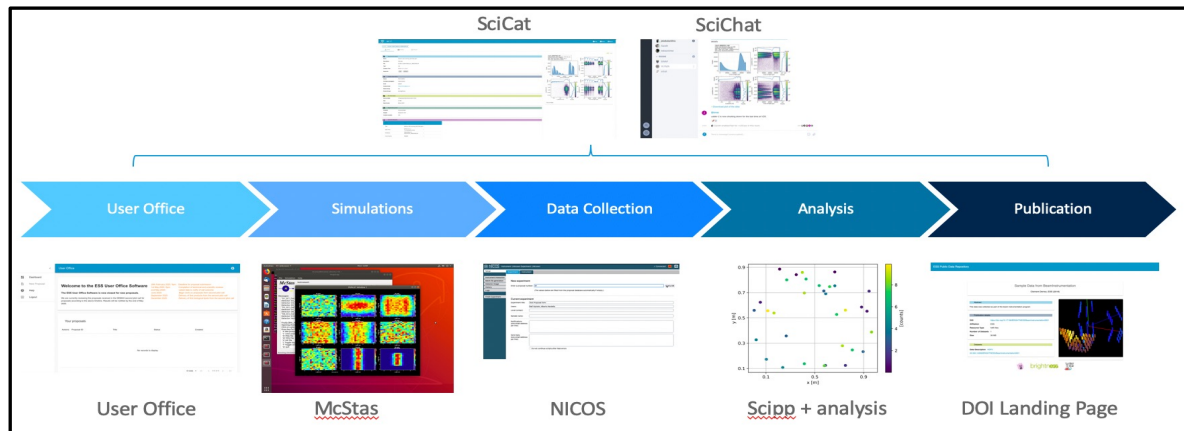

User Journey



User



User Journey in Data



User Journey in Software

Element	Software Solution	Comments
User Registration	User Office Software	Data to be stored in IAM after IAM is procured.
Proposal Submission	User Office Software	How much information should be included in the proposal? Experiment and sample for safety/data management plan?
Technical/Science Review	User Office Software	This includes technical and excellence reviews.
Safety Review	User Office Software	This requires the experiment plan and sample information as input and will have control measures as output.
Experiment Scheduling	User Office Scheduling	This includes collecting user 'bad dates' and scheduling the instrument, sample environment, local contact, on call scientist ...
User ESS Site Training	Learning Management System	Software currently being installed. The completion of training should be required before a visit can be planned.
User Visit Planning	User Office Software	User notifies ESS which scientists are coming and when. Also what arrangements they require ESS to make.
Sample Shipping to ESS	UOS/EAM	Samples shipped to ESS will start a tracking record at this stage.
Sample Registration at ESS	UOS/EAM	Samples brought to ESS will need to be registered for tracking. This is not strictly in the EAM planning.
User Site Access	UOS/IAM/LMS	Complex since requires communication between software
Electronic Logbook	SciChat	Users will be able to record additional metadata as well as messages from the control system and analysis pipelines
User Welcome	User Office Software	The User Office Software should provide sufficient information to facilitate contact at gatehouse and reception (if needed).
On-Site User Training	Learning Management System	Software that will provide required training for users to come on-site
Metadata Catalogue	SciCat	Collect relevant metadata from experiment and provide users with search capabilities and analysis tools.
Sample Tracking	Enterprise Asset Management	EAM will record which samples are exposed to neutrons and which are activated by the experiment.
Sample Information	SciCat	The data collection software should know which samples the user can select, this samples should be stored in SciCat and referenced in datasets
Data Collection	NICOS	The data collection tool that connects with the user office and SciCAT
Data Analysis	Scipp/Jupyter/VISA	
User Cost Reimbursement		Where ESS is covering user cost reimbursement.
User Satisfaction Survey	User Office Software	For reporting and improvement – must be completed within 3 months or user cannot submit another proposal.
Publications	User Office Software	A record of the science published as a result of each proposal.

User Journey



- Users will propose the scientific experiments they wish to carry out
- This will be **reviewed** for **feasibility, safety and excellence**
- The users will be notified of the success or otherwise for the proposal
- The user will provide arrival details for the scientists who are **coming** to ESS
- The visiting users will complete **safety documentation** and **carry out training**
- The user will book required **accommodation**
- The user will ship their **samples**
- **Access cards** and any other required materials will be prepared
- User to provide **feedback**
- User will provide a brief **scientific report** of their results
- User expenses **reimbursed** and invoiced costs paid
- User costs reported against the experiment
- **KPIs** reported to management



- Users **register** with their personal information
- By registering users ESS has a database of contact details for potential users
- Users provide sufficient personal data for **physical access** to site and **digital access** to systems
- User profile will link to radiation **dosimetry records**

- Instrument scientists will **schedule** the accepted experiments
- Scheduling will cover the **instrument, a local contact, required sample environments**
- The user and all those involved will be notified of the final schedule

- User have access to **requested labs** and prepare before instrument time
- The user will collect data at the awarded instrument with the samples declared on the proposal
- The user has access to **automatic and manual data processing** of their data

Data Curation



SciCat is now deployed at more than 6 facilities and with additional interest from the research community.

New developments:

- OIDC Support
- PySciCat: SciCat API for python.
Each endpoint is exposed as python function
- Scitecean: user friendly high level SciCat python library
- Integration in PaNOSC API including scoring and techniques expansion.
- Developing, testing and migration to new SciCat backend.
- Revision of data models in new backend (nest.js).
- Ingestion of legacy data, developing ingestion domain knowledge



Partner facilities

SciCat meeting in Hamburg



PySciCat

ALS, DRAM, SWAP

```
In [13]: import pysciat.client as pyScClient
import pysciat.model as pyScModel
```

Define the ingestion function

```
In [15]: def ingest(local_config, logger):

# loads simulation information from matching json file
logger.info('Loading dataset information from file : {}'.format(local_config.dataset_file_name))
with open(local_config.dataset_file_name, "r") as fh:
    dataset_information = json.load(fh)

# instantiate a pySciCat client
logger.info('Instantiating SciCat client')
logger.info('SciCat instance : {}'.format(local_config.scicat_fields['scicat']['host']))
logger.info('Login as user : {}'.format(local_config.scicat_fields['scicat']['username']))
scClient = pyScClient.SciCatClient(
    base_url=local_config.scicat_fields['scicat']['baseUrl'],
    username=local_config.scicat_fields['scicat']['username'],
    password=local_config.scicat_fields['scicat']['password'],
)

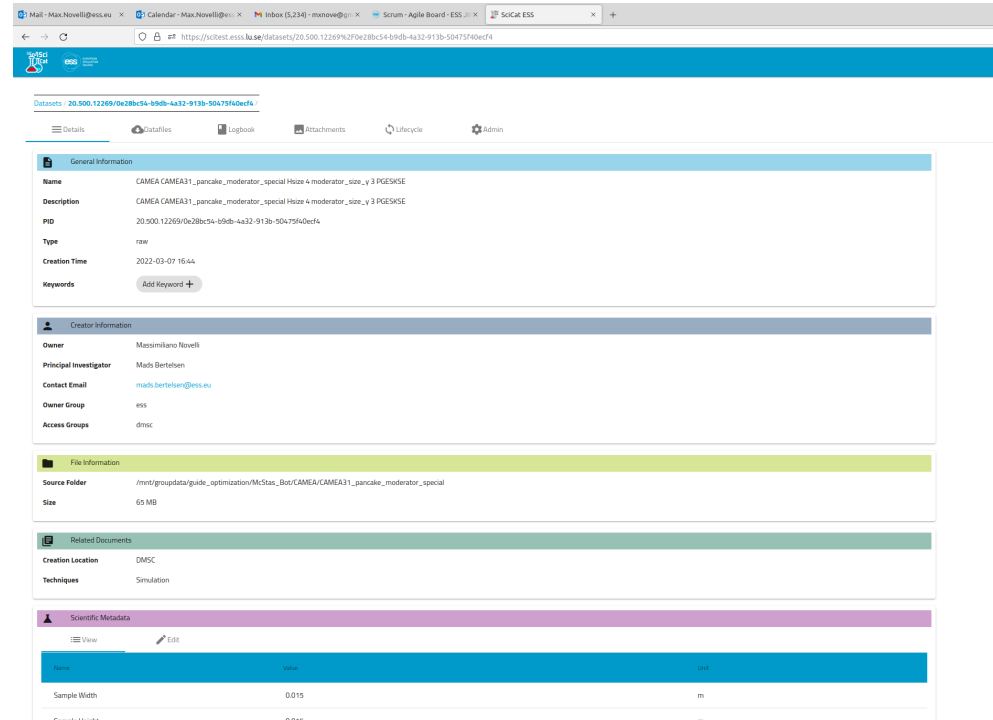
# create an ownable object to be used with all the other models
# all the fields are retrieved directly from the simulation information
logger.info('Instantiate ownable model')
ownable = pyScModel.Ownable(**dataset_information["ownable"])

# create dataset object from the pysciat model
# includes ownable from previous step
logger.info('Instantiating dataset model')
dataset = pyScModel.RawDataset(**dataset_information["dataset"], **ownable.dict())

# create dataset entry in scicat
# it returns the full dataset information, including the dataset pid assigned automatically by scicat
logger.info('Creating dataset on SciCat')
created_dataset = scClient.upload_new_dataset(dataset)
logger.info('Dataset created with pid {}'.format(created_dataset['pid']))

# create origdatablock object from pysciat model
logger.info('Instantiating original datablock')
origDataBlock = pyScModel.OrigDatablock(
    size=dataset_information["orig_datablock"]["size"],
    datasetId=created_dataset["pid"],
    dataFileList=[
        pyScModel.DataFile(**file)
        for file in dataset_information["orig_datablock"]["dataFileList"]
    ],
    **ownable.dict()
)

# create origDatablock associated with dataset in SciCat
# it returns the full object including SciCat id assigned when created
logger.info('Creating original datablock in SciCat')
created_orig_datablock = scClient.upload_dataset_origdatablock(origDataBlock)
logger.info('Original datablock created with internal id {}'.format(created_orig_datablock['_id']))
```

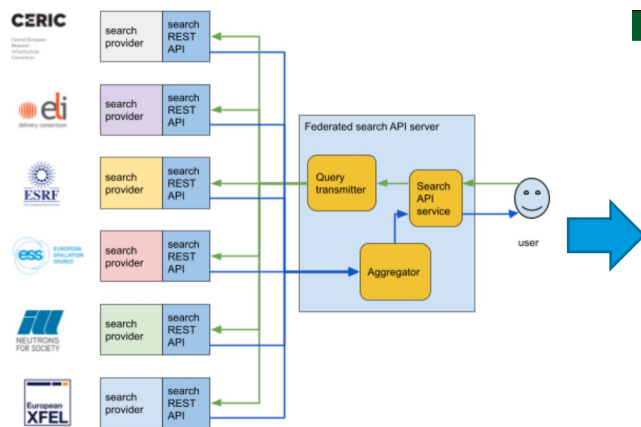


Scitacean approach

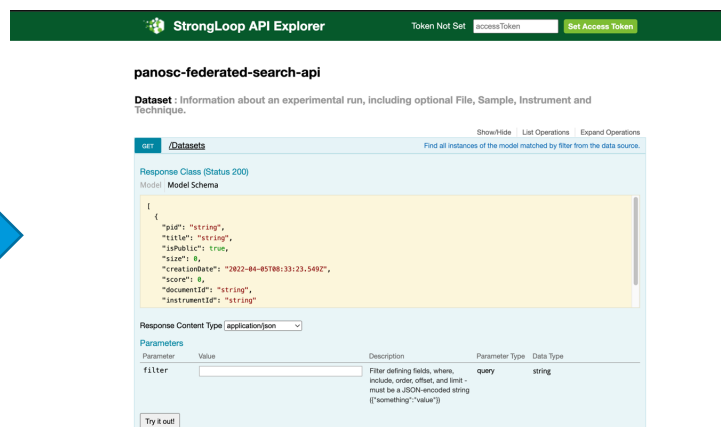
- Dataset creation (local instance)
 - Assign metadata
 - Assign data files
- Dataset sync (upload to production SciCat)
- Dataset retrieval by pid or query
 - Retrieve files

PaNOSC WP3 highlights

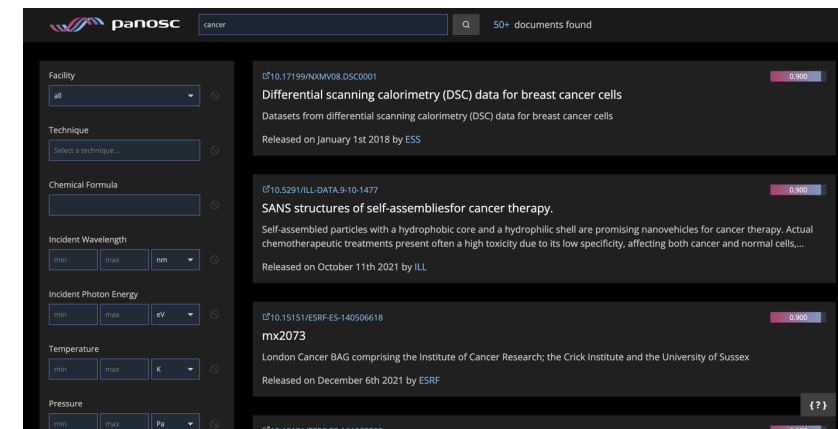
Scoring & techniques & portal



2020: Initial drawing of architecture



2021: Search-API deployed at partner facilities



2022: Federated search-API integrated with PaNOSC portal

PaNOSC Summer School

Proposals & Data curation

As part of the PaNOSC summer school the SWAP team held a presentation regarding proposal writing and data management with the focus on data curation to enable open and FAIR data.

The idea of a future ESS-DMSC summer school has been discussed and a proposal is being drafted.





YMIR

Testing it all

The screenshot displays the YMIR web interface. On the left, a sidebar contains navigation options: Dashboard, New Proposal, Experiment Times, and Help. The main content area shows a proposal titled "I want beamtime 3" with ID 471120. Below the title are sections for "New proposal" (with fields for Title, Abstract, Principal Investigator, and Co-Proposers) and "Samples & Info" (with a question "When do you want to come?" and a Samples field). A chat window is overlaid on the right, showing a list of rooms and a selected room for proposal 471120. The chat content includes a message from a "robot" and a message from "matt.clarke (he/him)".

Below the chat window, a detailed view of the proposal information is shown. It includes a table for "Local contact" and "Users", and a "Sample information" section with fields for name, formula, number of, mass/volume, and identity.

At the bottom right, a summary card for "Proposals / 471120" is displayed, showing "Details", "Datasets", and "Logbook" tabs. The "General Information" section lists the Title as "I want beamtime 3", the Abstract, and the Identifier as "471120". The "Creator Information" section lists the Main proposer and Principal Investigator as "Fredrik Bolmsten".

Resources loaded plan

P6 tracking & JIRA

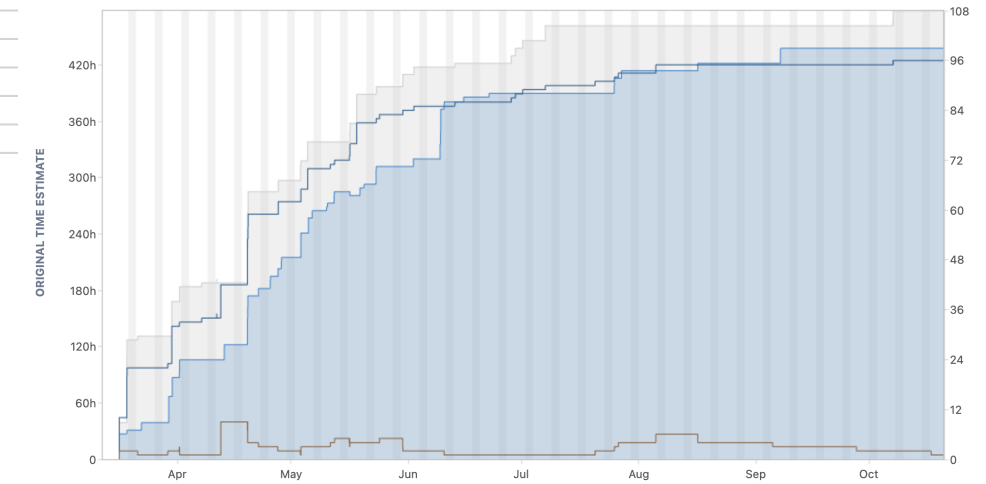


	2022				2023				2024			
	q1	q2	q3	q4	q1	q2	q3	q4	q1	q2	q3	q4
SWAP												
		3	5	5	5	5	5	5	5	5	5	5
Management	1	1	1	1	1	1	1	1	1	1	1	1
Software maintenance - User Office + Scheduler (Software Engineer)	0,2	0,2	0,2	0,2	0,2	0,2	0,2	0,2	0,5	0,5	0,5	0,5
Software maintenance - SciCat (Data Curation officer)	0,2	0,2	0,2	0,2	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
Software maintenance - Electronic logbook, Statistics, Pipelines, Publication	0,1	0,1	0,1	0,1	0,1	0,1	0,1	0,1	0,1	0,1	0,1	0,5
User Support for user office & data management									0,1	0,1	0,1	0,1
Publications storage/statistics/platform (Software Engineer)												
Sample/Shipment tracking (Software Engineer)	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5				
Visitor management + LMS integration (Software Engineer)				0,5	0,5	0,5	0,5	0,5	0,5			
Scheduling (Software Engineer)	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
Sample Safety Review (Software Engineer)												
KPI (Software Engineer)												
End of experiment adminstraion (Feedback form, report, etc..) (Software Engineer)												
Cold commissioning metadata catalogue integration (Data Curation officer)	0,1	0,1	0,5	0,5								
Data Analysis tools integration SciCat (Data Curation officer)												
Jupyter integration (Data Curation officer)												
Electronic logbook for users (Data Curation officer)	0,2	0,2	0,2	0,2								
MxCuBE/ISPyB for NMX (Software Engineer + Data Curation officer)*												
Scientific data/user management (Software Engineer + Data Curation officer)	0,5	0,5	0,5	0,5								
NiCOS integration (Software Engineer + Data Curation officer)												
Total	2,8	2,8	3,2	3,7								

Epic Report

Soft.maint User Office including scheduler

SWAP-2410 Maintenance of user office software [View linked pages](#)

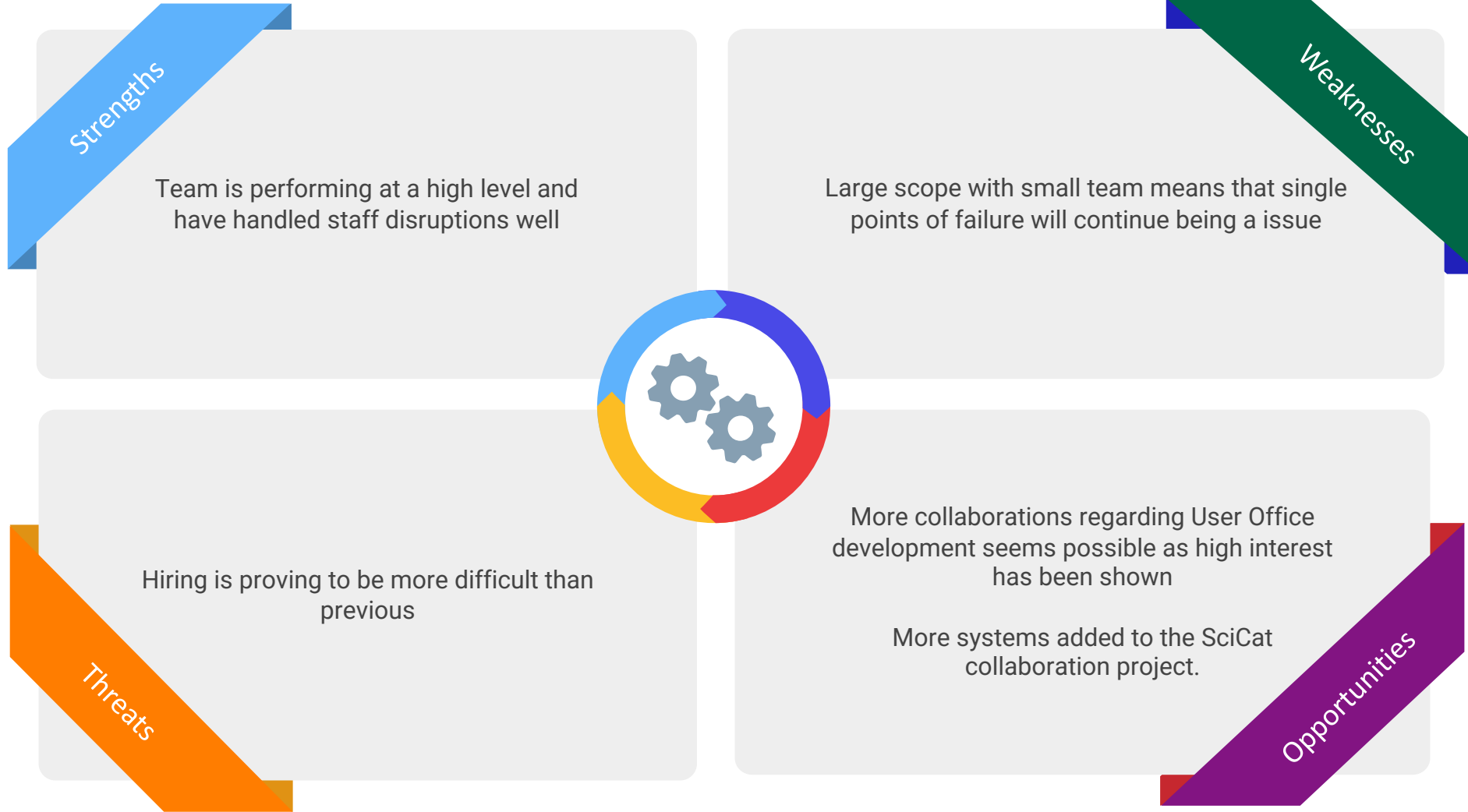


Insights:

- More time spent on maintenance
- Need to move task around due to lack of support
- IAM tasks underestimated



SWOT





Questions?