

Institut Laue-Langevin

Technical Talk
8th of October 2020



The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641.
The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.

Institut Laue-Langevin

- Located in Grenoble, France
- High-flux reactor neutron source
- 40 instruments + 10 test instruments
- First experiments in 1972
- 500 employees
- Usually 3 reactor cycles (50 days each) per year
- Approx 1200 experiments per year
- Approx 2500 scientific visitors per year



Team

Team member	Work Packages	Role
Jamie Hall	WP3, WP4, WP6 (Full time)	Software Developer
Stuart Caunt	WP3, WP4 (Full time)	Software Developer
Philippe le Brouster	WP4, WP6	System Admin
Baptiste Pichot	WP6	System Admin
William Turner	WP4, WP6 (Full time)	System Admin
Gregory Fanjas	WP6 (Full time)	System Admin



The Portal Architecture test experience

- **What went well?**
 - Developed and tested using a test k8s cluster
 - Installation process developed to work with multi-node infra
- **What could go better?**
 - Simplified deployment process that is not dependent on k8s
- **What is the gap between what's in your facility and what the Portal needs?**
 - The current version is far from the final product (only IT1)
 - There are [many use cases](#) still to be accounted for
 - Remote experiments at the ILL have changed the scope of the portal



Facility needs for the Portal

- **Name the features you would prioritise/what does the portal needs in order to run in your facility?**
 - OpenStack provider (VMs)
 - More fine-grained user roles (Instrument Responsibles, Instrument Control, IT Support, etc)
 - Transparent Remote Desktop authentication
 - Instance lifecycle management
 - Support for remote experiments (security groups, scientific support)
 - Admin access (management of instances and sessions)
 - Stakeholder usage statistics (KPIs)
 - Data search and data transfer



COVID-19 and the impact on your team

- **Remote experiments**

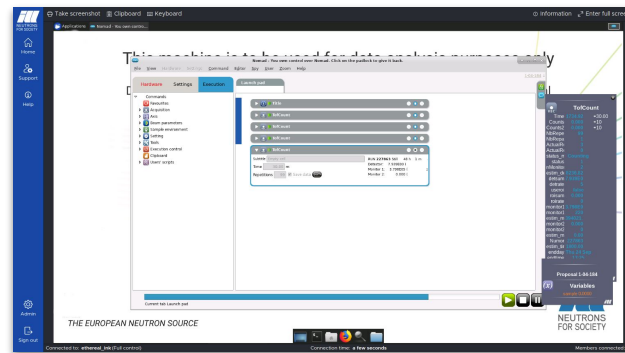
- development focused on ensuring a successful cycle in August
- Extension of existing ILL portal (VISA) to enable this

- **Developing new features**

- Load balancing web-sockets
- Increase compute infrastructure capacity
- Emphasis on security (limiting access to instrument control workstations)
- Enhanced collaboration features and scientific support for users
- Administration interfaces

- **Development of VM Image**

- Scientific data analysis software and instrument control software
- Built automatically and versioned



VISA: Virtual Infrastructure for Scientific Analysis

- **ILL's solution to a data analysis as a service portal**

- Development started three years ago (before PaNOSC started)
- In production since January this year

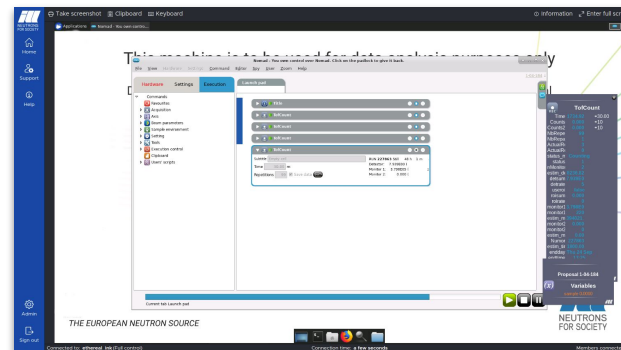
- **Technology**

- OpenStack infrastructure
- Capable of running 400 VMs (current infrastructure)
- Developed in Java 14 and Angular 10 (65k SLOC)

- **Successfully completed a reactor cycle**

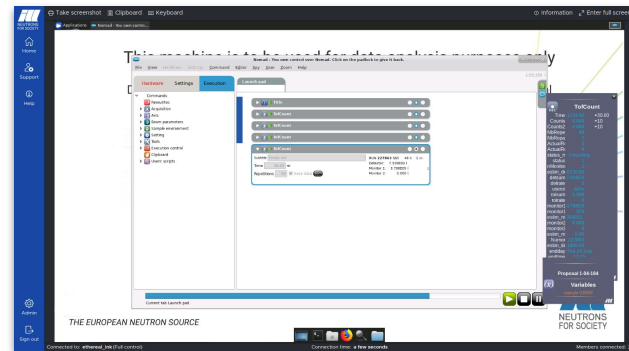
- Remote experiments (250)
- ~1000 VMs created
- 400 active users during the 50 day cycle
- Users from 20 countries
- 10,000+ sessions

- **Users are still active after the cycle**



VISA: Features

- Creation and deletion of linux machines (Ubuntu 18.04)
 - User can choose from predefined *flavours* (CPU & RAM)
 - Scientific and instrument control software is already pre-installed
 - Access to experimental data (NFS)
- Remote Desktop via a browser
 - Apache [Guacamole](#) proxying of RDP via socket.io
- JupyterLab integration (testing)
- Load balanced (containerised deployment using a CI/CD pipeline)
- Sharing machines with other users
 - Enable scientific collaborations
 - Allow for scientific support
- Transparent authentication to remote desktop
 - Developed a custom PAM module using signatures
- OpenID Connect authentication (keycloak)
- Quota management
- Machine lifetime management
 - Automatic deletion after 14 days or 4 days of inactivity
- Role and proposal based security groups (data access and firewall rules)



VISA: Demo

Take screenshot Clipboard Keyboard

Applications Nomad - You own contro...

Home Support Help Admin Sign out

File View Hardware Settings Command Editor Spy User Zoom Help

Hardware Settings Execution Launch pad

Commands

- Favourites
- Acquisition
- Axis
- Beam parameters
- Sample environment
- Setting
- Tools
- Execution control
- Clipboard
- Users' scripts

Launch pad

Commands

- Title
- ToICount
- ToICount
- ToICount
- ToICount

Subtree Empty cell RUN 227863 SHI 48 h 1 m

Detector 7.938E5 Monitor 1: 3.798E5 Monitor 2: 0.000

Time 30.00 m Repetitions 99 Save data

Current tab Launch pad

THE EUROPEAN NEUTRON SOURCE

NEUTRONS FOR SOCIETY

Proposal 1-04-184

Variables

sample 0.0000

Connected to: **etereal_link** (Full control)

Connection time: **a few seconds**

Members connected: **2**

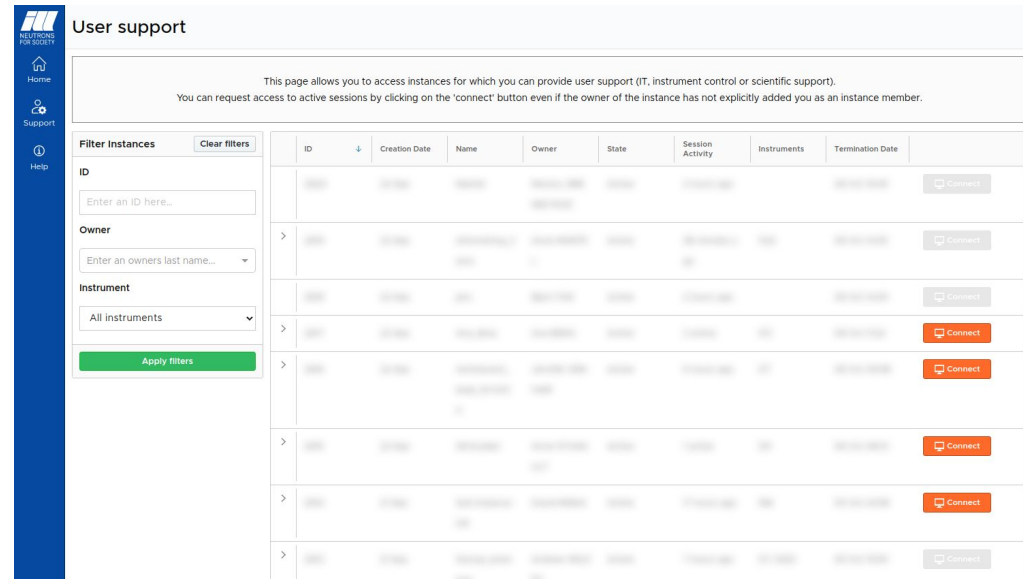
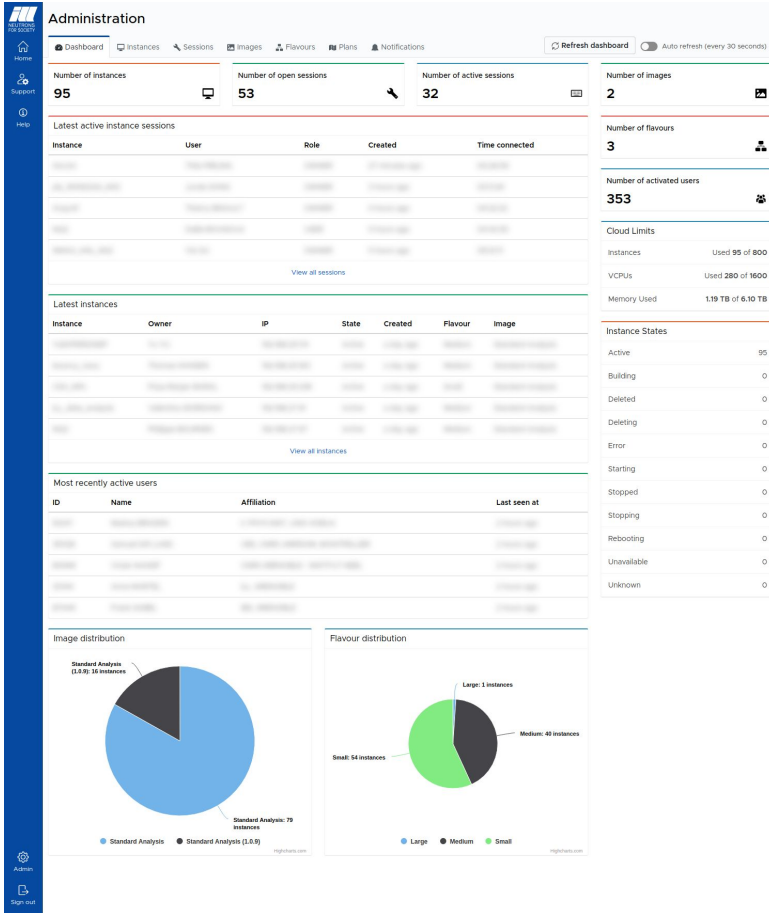
Table of data from the right-hand panel:

ToICount	
Time	1734.92 +30.00
Counts	0.000 +10
Counts2	0.000 +10
NbRepe	99
NbRepa	1
ActualRu	3
ActualRu	0
status_n	0
status	1
nMonitor	2
estim_d4	8438.68
detsum	7.938E5
detrate	5
useroi	None
roisum	0.000
rotate	0
monitor1	3.798E5
monitor1	220
estim_m	394021
monitor2	0.000
monitor2	0
estim_m	0.00
Numer	227863
estim_tr	1900.00
endday	Thu 24 Sep
endtime	14:25



The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641. The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.





The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641. The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.



Compute instances

[CREATE A NEW INSTANCE](#)

My instances

Instances shared with me

Filter instances by experiment...



molecular_analysis

visa-jupyter

8 GB · 2 VCPUs

Instance 202 created on Oct 8, 2020 and due to expire on Oct 22, 2020

active

Connect

Settings

Delete

Remote Desktop

Jupyter (experimental)

No experiments are associated to this instance.



remote_experiment

visa-jupyter

8 GB · 2 VCPUs

Instance 201 created on Oct 8, 2020 and due to expire on Oct 22, 2020

active

Connect

Settings

Delete

No experiments are associated to this instance.

NEUTRONS FOR SOCIETY

Home

Support

Help

Admin

Sign out

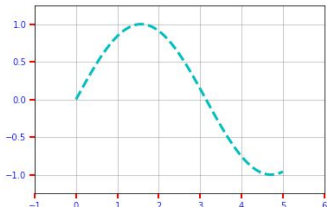
File Edit View Run Kernel Tabs Settings Help

demo.ipynb 2 minutes ago

jupyter-test.ipynb seconds ago

jupyter-test.ipynb demo.ipynb

```
[1]: import numpy as np
import matplotlib.pyplot as plt
fig = plt.figure()
ax = plt.axes()
x = np.linspace(0, 5, 100)
plt.plot(x, np.sin(x), 'c--', linewidth=3)
plt.xlim(-1, 6)
plt.ylim(-1.25, 1.25)
plt.tick_params(axis='both', direction='out', length=6, width=2, labelcolor='b', colors='r', grid_color='gray', grid_alpha=0.5)
plt.grid()
plt.show()
```




[]:

0 2 data-analysis | Idle Mode: Command Ln 1, Col 1 demo.ipynb



The ExPaNDS project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 857641.
The PaNOSC project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 823852.





Take screenshot | Clipboard | Keyboard

Applications | SasView | rbin/bash

Information | Enter full screen

Home

Support

Help

Admin

Sign out

Trash

File Sy...

Home

TEST

SasView

File Edit View Tool Analysis Fitting Window Help

Data Explorer

Data Theory

Data

Load data

Delete Data

Select all

Fit panel - Active Fitting Optimizer: Levenberg Marquardt

No data loaded

Model Fit Options Resolution Polydispersity Magnetism

Model

Category Model name Structure factor

Choose category...

Fit panel - Active Fitting Optimizer: Levenberg Marquardt

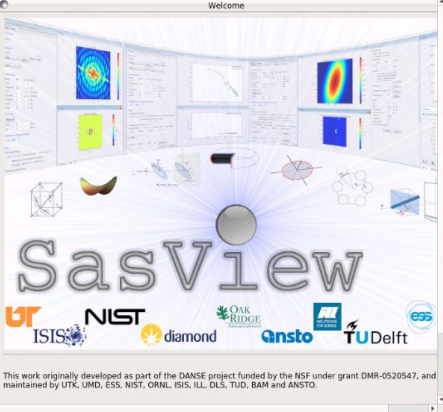
Model Fit Options Resolution Polydispersity Magnetism

Model

Category Model name Structure factor

Choose category...

Welcome



SasView

OR NIST Oak Ridge ISIS diamond Ansto TU Delft ESS

This work originally developed as part of the DANSE project funded by the NSF under grant DMR-0520547, and maintained by UTK, UMD, ESS, NIST, ORNL, ISIS, LL, DLS, TUD, BAM and ANSTO.

Fit panel - Active Fitting Optimizer: Levenberg Marquardt

Model Fit Options Resolution Polydispersity Magnetism

Model

Category Model name Structure factor

Choose category...

Fit panel - Active Fitting Optimizer: Levenberg Marquardt

Model Fit Options Resolution Polydispersity Magnetism

Model

Category Model name Structure factor

Choose category...

Fit panel - Active Fitting Optimizer: Levenberg Marquardt

Model Fit Options Resolution Polydispersity Magnetism

Model

Category Model name Structure factor

Choose category...

THE EUROPEAN NEUTRON SOURCE

Connected to: **ethereal_ink** (Full control)


Connection time: a few seconds

Members connected: 2



The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641.
The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.





Take screenshot Clipboard Keyboard

Applications SasView /bin/bash /bin/bash

Information Enter full screen

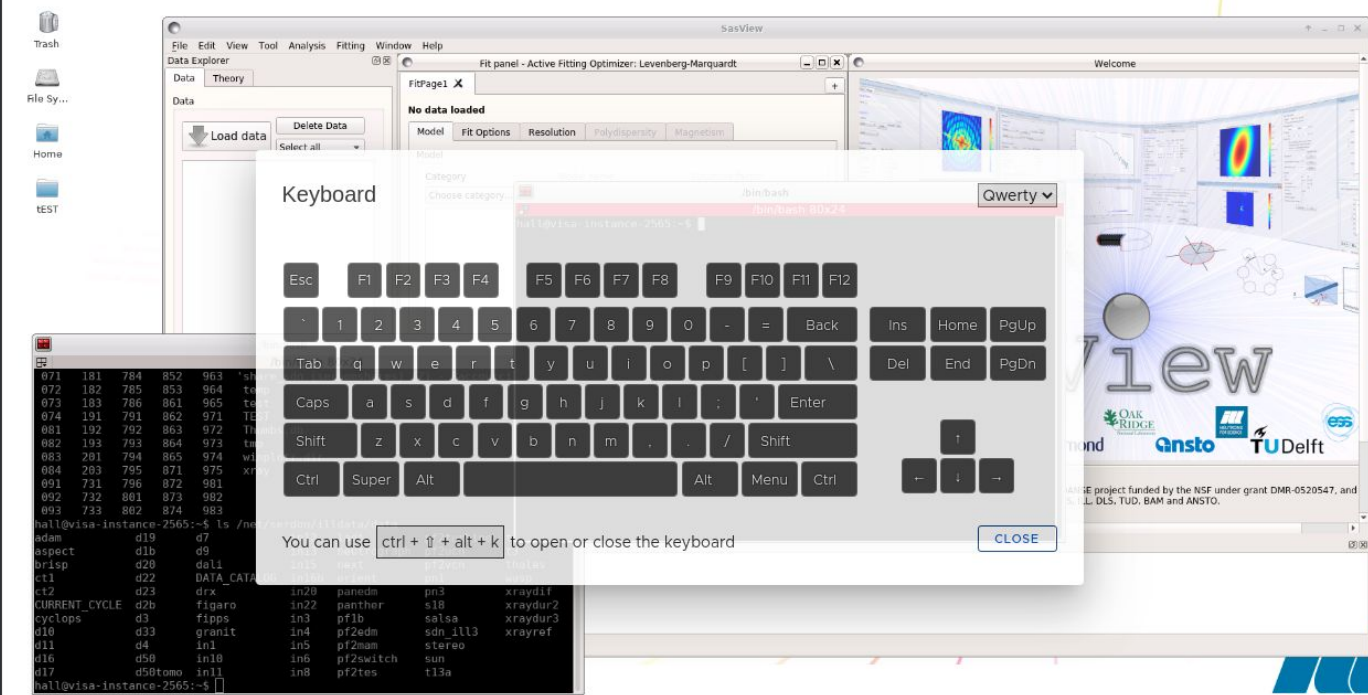
Home

Support

Help

Admin

Sign out



NEUTRONS FOR SOCIETY

Members connected: 1

Connected to: **ethereal_link** (Full control)

Connection time: a few seconds



The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641. The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.



Take screenshot | Clipboard | Keyboard | Information | Enter full screen

Applications | SasView | /bin/bash | /bin/bash

Home | Support | Help

Trash | File Sy... | Home | TEST

SasView

File Edit View Tool Analysis Fitting Window Help

Data Explorer

Data Theory

Data

Load data | Delete Data | Select all

Fit panel - Active Fitting Optimizer: Levenberg-Marquardt

FitPage1

No data loaded

Model Fit Options Resolution Polydispersity Magnetism

Model

Category Model name Structure factor

Choose category...

Request for access

Jamie HALL is requesting access to your instance.

GRANT FULL ACCESS | GRANT READ-ONLY ACCESS | REJECT ACCESS

```

/bin/bash
ll
071 181 784 852 963 'share_sdn (serho
072 182 785 853 964 temp
073 183 786 861 965 test
074 191 791 862 971 TEST
081 192 792 863 972 Thumbs.db
082 193 793 864 973 tmp
083 201 794 865 974 winplotr.dir
084 203 795 871 975 xray
091 731 796 872 981
092 732 881 873 982
093 733 882 874 983
hall@visa-instance-2565:~$ ls /net/serdon/illdata/data
adam d19 d7 in12 ladi pf2turbine t
aspect d1b d9 in13 neutrograph pf2ucn t3
brisp d20 d4i in15 next pf2vcn thales
ct1 d22 DATA_CATALOG in16b orient pn1 wasp
c22 d23 drx in20 panedm pn3 xraydif
CURRENT_CYCLE d2b figaro in22 panther a15 xraydur2
cyclops d3 fipps in3 pf1b salsa xraydur3
d10 d33 granit in4 pf2edm sdn_ill3 xrayref
d11 d4 in1 in5 pf2mem stereo
d16 d50 in10 in6 pf2switch sun
d17 d50tomo in11 in8 pf2tes t13a
hall@visa-instance-2565:~$

```

THE EUROPEAN NEUTRON SOURCE

Connected to: **ethereal_ink** (Full control)

Connection time: a few seconds

Members connected: 1

view

monod ansto TU Delft

ANSE project funded by the NSF under grant DMR-0520547, and S. ILL, DLS, TUD, BAM and ANSTO.

NEUTRONS FOR SOCIETY



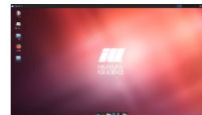
The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641. The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.



VISA Help Centre

Data Analysis, in the cloud.

VISA makes it simple to create compute instances and analyse your experimental data using just your web browser. Welcome to the Help Centre.



Compute Instances

Learn how to create and manage your own compute instances

[What is an instance?](#)

[How do I create and launch an instance?](#)

[How do I manage access to an instance?](#)

[When does my instance expire?](#)

[How do I use the clipboard?](#)

[How do I transfer files on my personal computer?](#)

[How do I provide user support?](#)

[Troubleshooting an instance](#)



Data Analysis

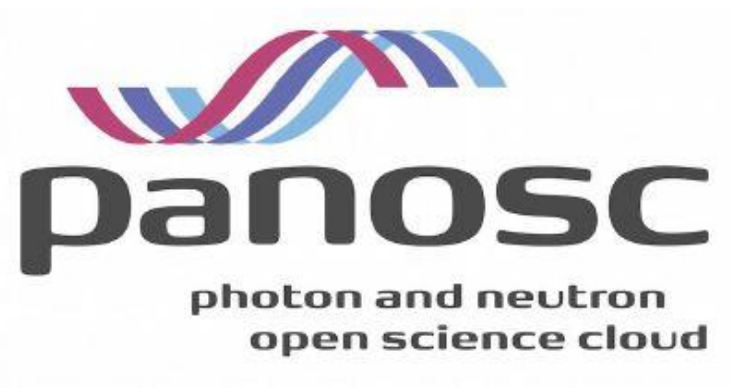
Learn which tools are available to start analysing your experimental data

[Which scientific software is installed?](#)

[How do I access my data?](#)

Still have questions?

Contact the ILL IT service at data@ill.eu for more information.



The ExPaNDS project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 857641.
The PaNOSC project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 823852.

