

Project Deliverable Information Sheet

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Project Coordinator	Andy Götz (andy.gotz@esrf.fr)	
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Authorship	Written by: Jordi Boderà Sempere
	Contributors: Andy Götz, Rudolf Dimper, Jean-Francois Perrin, Hans Fangohr, Florian Gliksohn, Petra Aulin, Thomas Holm Rod, Tobias Richter, Nicoletta Carboni, Roberto Pugliese
	Reviewed by: Andy Götz
	Approved: Andy Götz

List of participants

Participant No.	Participant organisation name	Country
1	European Synchrotron Radiation Facility (ESRF)	France
2	Institut Laue-Langevin (ILL)	France
3	European XFEL (XFEL.EU)	Germany
4	The European Spallation Source (ESS)	Sweden
5	Extreme Light Infrastructure Delivery Consortium (ELI-DC)	Belgium

6	Central European Research Infrastructure Consortium (CERIC-ERIC)	Italy
7	EGI Foundation (EGI.eu)	The Netherlands

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Introduction

This document summarises the progress achieved in the project since the last management report. As such, this document and the ones that follow on months 18, 30 and 42 will complement the four instances of annual workshop reports (months 12, 24, 36 and 48) to provide a regular update on the project, its management and comparing its current status with what was forecasted.

Executive Summary

Overall the project is advancing according to plan. A kick-off meeting attended by all partners and observers took place, a Consortium Agreement was approved and signed by all partners, deliverables proposed in the original proposal are being delivered in time, with the partners engaged in the project, regular meetings, recruitment and continuous activity in our main repository:

<https://github.com/panosc-eu/panosc>

Summary of kick-off meeting

The initial kick-off meeting was organised on 15th and 16th January in Grenoble and the organiser of the event was the ESRF. The event was managed with INDICO (<https://indico.esrf.fr/indico/event/19/>) for registrations of participants, the agenda and presentations.

The kick-off meeting spanned two days, with the first day focusing on introducing the project and work packages and the second day having parallel work sessions for each work package and a meeting of the Executive Board.

Agenda 15th January

Registration and welcome coffee	10:00 - 11:00
Welcome Address by Francesco Sette (Director General - ESRF)	11:00 - 11:15
PaNOSC Overview by Andrew Götz (Primary Coordinator Contact & WP2 leader - ESRF)	11:15 - 11:30
EC View of EOSC by Geert Vancraeynest (Project Officer - European Commission)	11:30 - 11:45
PaNOSC + national RIs by Rudolf Dimper (PaNOSC's Executive Board member - ESRF)	11:45 - 12:00
EOSC-hub by Tiziana Ferrari (PaNOSC's Executive Board - EGI)	12:00 - 12:15
PaNOSC Users: Coherent diffraction + training by Vincent Favre-Nicolin (Scientists and HERCULES director - ESRF)	12:15 - 12:30

PaNOSC Users: a neutron user's view of data and metadata by Andrew Jackson (Scientist - ESS)	12:30 - 12:45
PaNOSC Users: Laser users - vision for ELI by Florian Gliksohn (Associate director - ELI-DC)	12:45 - 13:00
Lunch	13:00 - 14:00
WP1 - Management by Jordi Bodega (WP1 leader - ESRF)	14:00 - 14:20
WP2 - Data Policy by Andrew Götz (WP2 leader - ESRF)	14:20 - 14:40
Identity management by Christos KANELLOPOULOS (GÉANT)	14:40 - 15:00
WP3 - Metadata Catalogues by Tobias Richter (WP3 leader - ESS)	15:00 - 15:20
WP4 - Data Analysis as a Service by Hans Fangohr (WP4 leader - XFEL)	15:20 - 15:40
Jupyter ecosystem by Thomas Kluyver (XFEL)	15:40 - 16:20
WP5 - Virtual X-Ray and Neutron Laboratory (VYNIL) by Carsten Fortmann-Grote (WP5 leader - XFEL)	16:20 - 16:40
WP6 - EOSC Integration by Jean-François Perrin (WP6 leader - ILL)	16:40 - 17:00
WP7 - Sustainability by Ornela de Giacomo (Deputy Executive Director - CERIC-ERIC)	17:00 - 17:20
WP8 - Staff and user training by Thomas Rod (WP8 leader - ESS)	17:20 - 17:40
WP9 - Outreach/communication and dissemination/impact by Nicoletta Carboni (WP9 leader - CERIC-ERIC)	17:40 - 18:00
Dinner	From 19:00

Summary of the 15th January

The morning of the first day started with a short welcome address by Francesco Sette, highlighting how much IT is enabling top-quality science and allowing researchers to accomplish their work.

This was followed by an overview of PaNOSC by Andy Götz who provided key information on the objectives of the project. He explained how PaNOSC was part of the Open Science movement which is happening worldwide and that the outcomes of PaNOSC will help make the science in the partner institutes more open and reproducible. PaNOSC is one of the cluster projects making up EOSC and a successful outcome to PaNOSC will also mean a successful EOSC.

Geert Vancraeynest followed with a presentation about the vision that the European Commission has of the EOSC and how PaNOSC should contribute to co-create it turning FAIR into a reality. Rudolf Dimper presented the PaNOSC's stakeholders (other funded projects, e-infrastructures, national RIs and the INFRAEOSC-05b call) and community (LEAPS and LENS). He emphasised how PaNOSC is part of a larger community and needs to work

closely with the other members of the community especially the photon and neutron sources.

Tiziana Ferrari continued with a presentation on EGI's contribution to ensure PaNOSC integrates into the EOSC via the EOSC-hub project. The following services will be provided by the e-infrastructures to PaNOSC as part of the EOSC-hub: Jupyter notebook service, data transfer service, federated cloud and data discovery and archiving. All these services will be integrated with the PaNOSC AAI solution umbrellaID which will be based on eduTeams from Géant.

The morning was completed by three presentations covering the user needs for PaNOSC. The photon users' needs for tomography and coherent diffraction imaging were presented by Vincent Favre-Nicolas (data scientist and Director of the Hercules School). Vincent presented the need for highly optimised algorithms to address the data challenges of the EBS (the new ESRF accelerator) in Coherent Diffraction Imaging (CDI). He demonstrated how Jupyter notebooks can be used to run software for CDI data reduction. He noted that CDI software is compatible with the Nexus format (the chosen PaNOSC standard) for CDI NXcdi_ptycho. Finally he explained, in his role as Hercules director, that the Hercules school could be used to promote and encourage data management for Open Science by training young scientists.

Andrew Jackson (ESS scientist) presented the Neutron users view. He explained the different kinds of data and metadata they deal with in the workflow of neutron experiments. Electronic logbooks are an essential tool nowadays. He explained the use of the Nexus format NXcanSAS for storing SANS data. Open Data and Open Science are not strong drivers for neutron users however they want reliable and reproducible data with tools for rapid analysis. He concluded with the challenges for PaNOSC which is to enhance the ability of scientists to share data in order to meet legislation.

The morning session wrapped up with a presentation the view for Lasers presented by Florian Gliksohn, ELI-DC associate director. He explained the general data workflow at ELI and the core principles foreseen for the future ELI ERIC data policy, which are close to the PaNdata data policy. PaNOSC is very timely for ELI given that this infrastructure is now transitioning to early operations and will require to work on all areas covered by the project.

After lunch the afternoon focused on the individual work packages:

Jordi Boderà presented WP1 - Management, focusing on the goals of the work package (ensuring good communication, coordination, reporting, monitoring and control), introducing its management structure and management approach. An example of a possible report that could be provided to the Executive Board was shown. At the end of the session the top pending actions for the work package at the time were raised (detailed project plan, risk management, KPIs for monitoring and signature of the Consortium Agreement).

Andy Gotz presented WP2 - Data Policy, covering the objectives which include harmonisation of PaN data policies, adoption of common open

standards, registering of data repositories with standards bodies and publishers, stewardship of data, best practices for implementing data policies and guidelines for handling huge datasets. WP2 will define KPIs for data policies, how to be compliant with GDPR, and develop tools for generating and managing Data Management Plans (DMPs). The goal of WP2 is to update the PaN data policies to be aligned with the FAIR principles. This is essential if PaNOSC and EOSC want to make FAIR data reality.

Tobias Richter presented WP3 - Metadata Catalogues. He gave an overview of the expectations on a good data catalogue and how the activities in the work package will help the facilities to make their catalogues (where they exist today) better and allow a more FAIR exposure of their data. The main strands of tasks would include capturing metadata at the experimental stations, exposing that metadata to the wider scientific communities in line with the data policies via the EOSC and enhance the community definitions for metadata (NeXus). Tobias also stressed that the route via the (public) data, through the data catalogues, is a promising one into further EOSC services that may be offered by partners, such as file access, migration or access to computing and analysis resources.

Hans Fangohr presented WP4 - Data Analysis as a Service. He outlined the data analysis vision of the project: to provide data analysis capabilities as an EOSC service. In particular he explained the two technologies mentioned in the proposal:

- (i) The use of a remote desktop client in a browser (VISA) connected to a virtual machine somewhere in the cloud or a facility, and
- (ii) The use of Jupyter Notebooks as an interactive environment for data analysis.

Hans Fangohr also demonstrated an example of a reproducible publication where together with the manuscript, a GitHub repository is published, which contains notebooks that - when executed - create the figures and data shown in the paper. The project aims to make creation of such reproducible publications more easily possible.

Thomas Kluyver made a break from work package presentations to introduce the Jupyter ecosystem, and provide all participants an introductory overview of important components such as the classic notebook, nbconvert, nbval and nbmerge.

Carsten Fortmann-Grote presented WP5 - VIRTUAL X-RAY and Neutron Laboratory (VYNIL). He explained the general approach to developing a simulation platform for P&N science suitable for various kinds of user interfaces. A set of application-programming interfaces (APIs) will be developed which connect the user to advanced simulation codes for photon and neutron propagation, sample interaction, signal generation and signal processing. In this way, a virtual laboratory will be realized. Some simulation codes and frameworks which will be used to implement a prototype of ViNYL were mentioned and connections to other work packages, in particular WP4 and WP8, were explained.

Jean-François Perrin presented WP6 - EOSC Integration. He presented the different objectives of the work package and highlighted the support role of this WP for the other activities of PaNOSC. This work should provide the building blocks for the infrastructure integration of WP3, 4 and 5. As illustrated during the meeting, this WP should promptly address the

question of the AAI integration in EOSC and provide data transfer solution depending on the size of the data. These technical solutions being core to the integration of the PaNOSC data access and data analyses services in EOSC.

By liaising with the other organisations or projects participating to the EOSC construction, this WP should also ensure that the need of the community are well understood and taken into account.

Ornela de Giacomo presented WP7 - Sustainability. The presentation started with an explanation of the WP describing the specific tasks and their relation. The goal of this WP is to create a sustainability plan for PaNOSC. Two major aspect have been highlighted in order to reach this goal: the connection with the principal stakeholders (list them and collect their feedback is the objective of the task 7.1) and the strong connection with the other WPs, e.g. WP2 - Data Policy and Stewardship as this will affect the storage and computing resources maintenance costs which in turn will affect the long term sustainability of PaNOSC. With this in mind the work package will study the cost per partner for maintaining the infrastructure required for providing FAIR data and explore different scenarios for financing the long term costs. The long term sustainability plan of the PaNOSC infrastructure will balance the viewpoints of the different stakeholders.

Thomas H. Rod presented WP8 - Staff and user training, giving an overview of the schedule for the work package, which essentially continues of three components

- 1) migration of the e-learning platform, e-neutrons.org, to ESS and extension of it to cater for the needs of PaNOSC and its partners,
- 2) training of staff to create courses, and
- 3) development of courses and training of users.

It was noted that the work package essentially is driven by only two partners, namely ELI and ESS, and that it depends on results from WP4 and 5 and that milestones have been introduced to mitigate the risks associated with those dependencies. The functionality and components of the e-learning platform were discussed.

Nicoletta Carboni presented WP9 - Outreach/communication and dissemination/impact, introducing the activities foreseen in the first year of the project in the frame of WP9, including the set up of the tools for internal and external communication (repositories, social media accounts, shared calendar, etc.), the realization of the new project's logo and visual identity, the design, publication and content population of the website, and the preparation of the project's communication strategy. A draft structure of the latter was presented.

Agenda 16th January

WP1 - Management	08:30 - 09:30
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Jupyter latest developments			09:30 – 10:30
Coffee break			10:30 – 11:30
WP6 – EOSC Integration	WP8 – User and Staff Training	Executive Board Meeting	11:00 – 12:30
WP2 – Data Policy	WP7 – Sustainability	WP9 – Outreach /communication and dissemination/impact	12:30 – 13:00
Lunch			13:00 – 14:00
WP4 – Data Analysis as a Service	WP3 – Metadata Catalogues	WP5 – Virtual X-Ray and Neutron Laboratory (VYNIL)	14:00 – 16:00
Coffee break			16:00 – 16:30
Next steps			16:30 – 17:30

Summary of the 16th January

The session was organised in working sessions rather than presentations, this meant that parallel sessions were scheduled and that engagement between the work package leaders, work package contributors and other stakeholders was sought after.

Jordi Boderá started with the WP1 – Management session, which covered the following topics:

- Approach to submit deliverables
 - Each WP leader responsible for their deliverables
 - Aim to have each one quality reviewed by someone else and submit it in advance
 - Internal products that are in fact precursors from deliverables are a good idea
 - A more detailed planning including internal products was requested
 - A quick view of the 44 deliverables and their distribution over time and work packages was shown as well
- Risk management

- o Each work package to look at the risk affecting their area, with shared risks brought up to Project Management Committee meetings
 - o Agreement to review and assess risks regularly
- Communication
 - o Mailing lists and how to be involved
 - o GitHub to share information and documentation
- Control
 - o Broad agreement on using the report showed the previous afternoon
 - o Key Performance Indicators could be used too
- Observers
 - o How to deal with observers was a hot topic, in particular there was much interest regarding the possibility of working together with the EXPaNDS proposal team if they were to become a EU-funded project
- The first deliverable (D1.1 Project Initiation Documentation) was also introduced

Jupyter latest developments:

Sylvain Corlay from Quantstack gave an overview of recent developments in the Jupyter Project and Jupyter Ecosystem. He introduced JupyterLab, the next generation Jupyter interface, Jupyter Lab extensions and Widgets. These allow to create a windows-based interface inside the browser that users can modify for their needs, and where multiple windows can show different but synchronised views of the same data. He also introduced Voila, a new project that strips out (or hides) the code that drives a Jupyter notebook, and has great potential for presenting complex data sets in an interactive or explorable version to a non-expert audience, such as managers or the public.

WP2 Parallel session - was well attended with over 20 people from ESFRI and national sites. Attendees expressed a strong interest to learn from the sites who have already implemented a data policy. CERIC is leading the task of gathering best practices. New areas to be addressed in the data policy framework are FAIR, processed data, logbooks (as metadata), national data policies, DOIs for instruments, and GDPR for scientific data. WP2 will seek help from the FAIRsFAIR project and other initiatives around FAIR data in the EOSC.

The session on WP3 was attended by representatives from all partners as well as observers from national facilities, namely the Paul Scherrer Institute, Diamond Light Source and Helmholtz Zentrum Berlin. All partners presented an overview of their background relevant to the work package and tasks. Staff planning and hires were discussed as well as existing data policies, catalogues, practises around generation of DOIs, capture of metadata from experiments and adoption of community standard file formats. The representatives agreed on using GitHub as open development platform. Activities would be as collaborative as reasonably possible to make best use of the collective experiences and to meet all requirements. To that end monthly and additional topical teleconference would be help between all partners. Every partner is responsible for nominating the staff on WP3 to the corresponding mailing list. Partners without current representation on the NeXus file format committee would strive to join the committee.

Finally Claudia Martens from B2Find presented the options offered by that repository, which would jumpstart some of the early tasks.

Hans Fangohr outlined a vision for WP4 where remote controllable virtual machines can be used to analyse data using software of any type running on any operating system - a technology pioneered by ILL - and where Jupyter Notebooks are used as a better (but less generic) infrastructure for new data analysis processes, and where the current data analysis software can be ported to notebooks with modest effort.

WP5 presentation was split in two parts. In the first part, every participant introduced himself and summarized his scientific background and simulation code projects. The second part saw a sequence of short presentations on the various simulation code projects which will form the basis for the Virtual Laboratory: The x-ray optics design and simulation framework Oasys, the photon experiment simulation platform SIMEX and the neutron ray-tracing platform McStass. The milestones and deliverables as well as tasks were revisited. It was discussed that the WP leadership will intermittently be executed by M. Sanchez-Rio from ESRF after the departure of C. Fortmann-Grote from EuXFEL at the end of February. In the meantime, C. Fortmann-Grote has returned to EuXFEL on a 10% part time employment and has resumed the WP leadership.

Jean-François Perrin chaired the session on WP6 and introduced the different challenges that represent the integration with EOSC. This session continued with presentations from the e-infrastructure providers: EGI presented the EOSC-Hub service catalogue and solutions to transfer data, GEANT presented the EudTEAMS solution from a technical perspective and how it could fit the Photon and Neutron community needs and finally STFC presented its solution for data archiving. These presentations were followed by discussions with the attendees on the organisation of the work: fortnightly video meeting, sharing of the tasks, immediate road map and reporting.

Ornela De Giacomo presented the action plan for WP7 on behalf of the WP leader, Roberto Pugliese. The detailed action plan for every task has been discussed with the partners, in view of the timely achievement of milestones and deliverables. A first list of "stakeholder's types" has been shown as an example, in order to reach the first milestone of this work package in month 6: MS7.1 - Stakeholders list. Finally, the working session was closed with a discussion, based on the experience of previous projects, on the importance of developing contents in close collaboration with the other workpackages, since many technical and policy decisions have a direct effect on the sustainability of the EOSC.

Representatives for each of the partners attended the parallel session for WP8 which started with a round-the-table where each participant presented themselves. This was followed by a discussion of what each partner expects from the work package and which training activities for staff and users they currently have at their respective facilities. Based on this discussion it can be concluded that none of the partners have significant training activities or focus on it, with the exception of the HERCULES school in Grenoble, which is supported by ESRF, ILL, XFEL, and CERIC ERIC through Elettra. It was also realized that it was not yet settled who will be the work package representative for many of the partners. The meeting

continued with a discussion of each of the tasks in the work package, management of the work package, and the next steps. It was agreed that we should have annual meetings in connection with the PaNOSC annual meetings, a video conference in between those meetings, and then meetings between partners when needed. Given that ESS and ELI carries most of the effort in the work package, particularly in the beginning, this level of activity was deemed sufficient.

Moreover, it was agreed to try get Jupyter integrated into the e-learning platform as early as possible in order to accommodate for data analysis from WP4 so that the e-learning platform will become more appealing for scientists. This should be part of the plan to be developed with WP4 (MS8.1).

For the staff training activities, which starts in 2020, each partner should get feedback from their respective facility on which course they would like to have in the e-learning platform and find out who of their colleagues should be involved. ESS can help with the actual implementation but a joint course for staff from all partners should also be organized for early 2020.

CERIC should figure out, which activities similar to WP8 exist in other clusters and then clarification on budget for summer schools and video tutorials were warranted.

On the 2nd day of the meeting, a session dedicated specifically to the WP9 focused on the best ways to proceed with the implementation of the communications activities described during the 1st day.

With reference to communication strategy and the website, participants agreed on the structures proposed on Day 1 of the kick-off meeting. A time schedule for the preparation of the content for the website was also presented.

For what concerns social media, it has been agreed that the PaNOSC twitter account will be managed by both ESRF and CERIC-ERIC, and that the Google account panosc_eu@gmail.com would be created, connecting it to a dedicated YouTube channel, which will be used to upload and share video content, in particular related to training modules developed in WP8.

Participants also agreed to set-up a shared calendar on Google (to be embedded in the PaNOSC future website), allowing all partners to see past and upcoming events, and to keep it up to date.

Finally, the discussion focused on the possible internal repositories to be used for documents' storage and internal communication. Participants proposed a set of options, such as GitHub, CERIC drive, Google drive, Confluence / Jira, to then continue the discussion after the meeting, to further explore their functionalities and suitability according to the need of the project and the partners.

Summary of Executive Board meetings

First meeting

The first meeting of the Executive Board (EB) took place during the second day of the kick-off meeting. Following a summary of the formal role of the EB, the chair for the forthcoming year was elected (R. Dimper - ESRF). One

of the roles of the chair will be to interact closely with the EOSC governance instances representing the PaNOSC consortium and clarifying the link between PaNOSC and the EOSC. The meeting continued with a report from the Project Coordinator about the status of the project and the planning for the deliverables. The EB proposed to advance the deadline for some of the deliverables to avoid too many of them becoming due at the same time. AOB subjects included a discussion on the GDPR, the change of the WP5-leader, status of the consortium agreement, and the first annual general meeting to be held in autumn of 2019.

Second meeting

The second EB meeting took place on 29 April 2019. Six out of the seven partners were present during the video conference. The project coordinator presented the project status and noted that it was difficult following up the progress of the WPs. Additional milestones before the deadlines for the deliverables would help to monitor progress. The EB discussed the requirement to synchronise actions with the recently approved ExPaNDS project and how to ensure that there is strong user involvement. The next annual meeting will take place on 21 and 22 October, possibly followed by WP meetings on 23 and 24 October. This annual meeting will also allow to have the next face to face meeting of the EB on 22 October during which the EB chair for the next year will have to be elected. The following recommendations were unanimously approved by the EB:

1. The EB requests all WPs to provide intermediate milestones to allow WP1 to follow progress or lack of it.
2. The EB requests partners who are in charge of WPs and where the WP leader is not available (WP5, WP7) to formally provide an action plan.
3. The EB requests the PaNOSC PMC to develop a plan how to engage with users and others projects of the PaNOSC and EOSC services.
4. The EB requests increased involvement in the PaNOSC PMC and WP follow-up of risks, milestones, tasks, etc. by all partners.
5. The EB requests the PaNOSC PMC to liaise with FAIRsFAIR as the preferred FAIR expert.

The EB wishes to have the next EB meeting during the 2nd day of the annual meeting, i.e. on 22nd October, from 16:00 to 18:00, without any overlap with other activities during the annual meeting.

Summary of Project Management

Committee meetings

Regular meetings have been taking place between the work package leaders and representatives from each one of the PaNOSC's partners since October. These meetings are documented in GitHub:

<https://github.com/panosc-eu/panosc/tree/master/Work%20Packages/WP1%20Management/Meetings>

Meetings before the project started

The first four meetings took place before December 2018, when PaNOSC had

not yet started but it was clear that the project will be funded and start soon.

15th October 2018

In this meeting we agreed to start work on the Consortium Agreement and prepare the Kick-off meeting.

12th November 2018

We decided to start documenting stakeholders for the project, created an issue log in GitHub (<https://github.com/panosc-eu/panosc/issues>) and agreed to produce a letter of support for the ExPaNDs proposal.

19th November 2018

Work started on formally nominating Executive Board and Project Management Committee members, and further details for the Kick-off meeting agreed.

28th November 2018

Some names were confirmed for the Executive Board and the agenda for the kick-off meeting started to take shape.

Meetings before the Kick-off meeting

5th December 2018

We shared the information of an upcoming change in our project officer and the fact that the WP5 leader would be changing jobs. Attendees reported work in the first deliverable (D1.1) due end of January 2019, draft Consortium Agreement, PaNOSC's website requirements, Kick-off meeting registration and a press release to announce the start of the project.

12th December 2018

We shared information of our new project officer, continued work on the Consortium Agreement and updated the timetable for the Kick-off meeting, asking everyone who intended to attend to register during the week. News about the ESFRI meeting in London 30th January 2019 were also shared.

19th December 2018

This was the last video conference meeting of 2018 and we were happy to report positive feedback from several partners regarding the Consortium Agreement. Plenty of partners started recruitment processes, so positions for PaNOSC could be filled. It was decided who would be interim WP5 leader once the current leader leaves his position.

9th January 2019

This was the first meeting of 2019 and the last before the face-to-face kick-off meeting scheduled for 15th and 16th January. The final agenda for the kick-off meeting was reviewed and mailing lists were discussed

Meetings after the Kick-off meeting

23rd January 2019

During the first meeting after the kick-off we talked about the follow-up actions, like GDPR. We also explained progress on the upcoming deliverable (Project Initiation Documentation) and requests for support to review it. Outstanding issues were reviewed (many were closed during the kick-off) and WP9 leader explained problems with the website call for tender that delayed the start of the work by a few weeks.

29th January 2019

Risks identified were formally assigned to the related work package leaders, we discussed about software storage and licensing. The meeting was a bit shorter than usual as many recurrent attendees couldn't make it due to the ESFRI meeting in London.

6th February 2019

This meeting started with a long briefing about the ESFRI meeting in London and was followed by an update on progress achieved for the deliverable PaNOSC's repository for internal communication. It was decided to keep the Project Initiation Documentation up-to-date so it remains a good reference point for the project. It was agreed to decide how to deal with observers once confirmation is received regarding the financing of EXPaNDS.

13th February 2019

Initial conversations to plan the first annual meeting for PaNOSC took place. It was reported that PaNOSC will not use Confluence for the time being after reviewing the tool. Initial agreement was reached regarding the Consortium Agreement, so copies could now be sent to all partners. In this meeting it was also agreed to move to bi-weekly meetings rather than weekly.

27th February 2019

The meeting started with an update regarding the PaNOSC's repository for internal communication due at the end of the week. The news of EXPaNDS funding were also shared. It was also agreed that existing software projects will continue with their current license model and new software will use MIT license or similar.

13th March 2019

The PaNOSC calendar in Google was presented so it will be easier to keep track of all PaNOSC related events. We shared the news that most of the partners had signed the Consortium Agreement and urged the remaining to sign.

27th March 2019

We used this meeting to remind all partners of the upcoming Deliverables and Milestones. Work Package leaders were also reminded to add in GitHub the minutes of their meetings. Further details were clarified for the 1st annual meeting that will take place in Trieste.

10th April 2019

Draft versions of the upcoming deliverables (Mid-Year Report and Data Management Plan) were uploaded to Google docs, so all partners can easily collaborate.

9th May 2019

Support to complete D1.2 (Mid-Year Report) was requested to WP leaders and a walkthrough the new website for PaNOSC done, however feedback was still required. Feedback regarding a video-conference Executive Board meeting was provided.

22nd May 2019

WP leaders were reminded again of the required support to complete the deliverables due end of May. WP leaders were also reminded of upcoming milestones. It was also decided to create a more detailed planning for PaNOSC including "internal milestones" so it would be easier to follow-up project progress.

Recruitment progress

All partners in PaNOSC have undergone recruitment processes to resource the PaNOSC project:

Partner	Staff	Position	WP	Start Date	Notes
ESRF	M.Chaillet	s/w developer	WP 3	permanent	
ESRF	A.de Maria	data manager	WP 3	permanent	
ESRF	T.Vincent	s/w developer	WP 4	permanent	
ESRF	A.Sole	data scientist	WP 3 WP 4	permanent	
ESRF	J.Bodera	project manager	WP 1	permanent	
ESRF	R.Dimper	EB member	all	permanent	
ESRF	A.Götz	coordinator	all	permanent	
ILL	J-F. Perrin	WP6 leader	WP2, WP6, WP7	permanent	
ILL	J. Hall	s/w developer	WP3, WP4, WP6	permanent	
ILL	S. Caunt	s/w developer	WP3, WP4	permanent	
ILL	W. Turner	s/w developer	WP4	Sep 2019	
ILL	P. Le Brouster	System admin	WP6	March 2019	
XFEL.EU	Robert Rosca	Software Engineer	WP4	Jan 2019	
XFEL.EU	Carsten Fortmann- Grote	Scientist	WP5	May 2019	10% FTE
XFEL.EU	Juncheng E	Scientist for Photon Experiment Simulations	WP5	TBC	
XFEL.EU	F. Fangohr	WP leader	WP4	permanent	
ESS	Mads Bertelsen	Post Doc	WP5 WP8	Jan 2019	

ESS	Ashok Nulguda	HPC system administrator	WP4 WP6 WP8	August 2019	
ESS	Gareth Murphy	Data Scientist	WP3	permanent	
ESS	Linda Udby	Associate Professor UCPH	WP8	Secondment agreement with UCPH	
ESS	Peter Willendrup	Senior Research Engineer DTU	WP8	Secondment agreement with DTU	
ESS	Tobias Richter	Group Leader	WP3	permanent	
ELI-DC	Jan Pernet	Financial officer	WP1	permanent	ELI-DC employee
ELI-DC	David Bereczkei	Financial officer	WP1	permanent	ELI-ALPS employee
ELI-DC	F. Gliksohn	Deputy Director	WP2	permanent	ELI-DC employee
ELI-DC	Tamás Gaizer	Head of IT	WP3, WP6	permanent	ELI-ALPS employee
ELI-DC	Jakub Grosz	Virtual reality specialist	WP4	permanent	ELI Beamlines employee
ELI-DC	Mariana Danielova	Virtual reality specialist	WP4	permanent	ELI Beamlines employee
ELI-DC	Kahaly Mousomi	Theoretician	WP5	permanent	ELI-ALPS employee
ELI-DC	Zsolt Léczi	Theoretician	WP5	permanent	ELI-ALPS employee
CERIC-ERIC	J. Kolar	General Director, GB Member	all	permanent	
CERIC-ERIC	O. De Giacomo	Deputy Director, contributor	WP 2, WP 7	permanent	
CERIC-ERIC	N. Carboni	Senior Communication Officer, WP 9 leader	WP 9	permanent	
CERIC-	D.	Project Officer,	WP 1,	permanent	

ERIC	Roccella	contributor	WP 2, WP 7		
CERIC-ERIC	R. Pugliese	Head of IT, technical coordinator for CERIC-ERIC, WP 7 leader	all	permanent	
CERIC-ERIC	E. Coghetto	Database & Web Developer	WP 3, WP 9	Apr 2019	
CERIC-ERIC	M. De Simone	System Administrator	WP 3, WP 4, WP 6, WP 8, WP 9	May 2019	
CERIC-ERIC	A. Olivo	Software Engineer	WP 2, WP 3, WP 9	Feb 2019	
CERIC-ERIC	A. Hafner	Computational Scientist	WP 5, WP 9	Jun 2019	
CERIC-ERIC	C. E. Sanchez Dos Reis	Software Engineer	WP 4, WP 9	Apr 2019	

Progress of work packages

Work Package 1: Management

The team of the Management work package has been busy ensuring that communication is working between all the work packages and partners, in particular:

- Organising the Project Management Committee meetings and issues notes of them
- Maintaining mailing lists
- Encouraging the use of the issue log in GitHub, reviewing it often
- Reminding partners of upcoming deliverables and milestones
- Interacts and informs the Executive Board of the project status

The Consortium Agreement was finalised and signed by all partners.

WP1 led the effort for its deliverables during this period (the Project Initiation Documentation, Data Management Plan and this Mid-year summary).

Overall the Management work package is working well, however continuous

monitoring and support must carry on to ensure that the PaNOSC project continues under control and delivers its objectives.

Work Package 2: Data Policy and Stewardship

Progress so far includes an analysis of the existing data policies (ILL, ESRF, EU-XFEL, CERIC-ERIC, ESS) for the common points, and areas which need to be addressed compared to the PaN-data data policy (the basis of all the existing data policies). Started to compile the Lessons Learned from the existing sites in a document to help other sites implement their data policy. Three video meetings have been held so far with a fourth planned. Minutes are on GitHub. Most of the meetings have been dedicated to analysing the existing policies. ESS attended the FAIRsFAIR on behalf of WP2 and started discussions with them. PaNOSC and FAIRsFAIR plan to sign an MOU of collaboration. ESRF published a paper in the May issue of Synchrotron Radiation News¹ on the implementation of their data policy.

Work Package 3: Data Catalog Services

Recruitment for WP3 is more or less complete. Two tasks are actively running, in agreement with the plan. The development of a search and discovery API that allows domain specific metadata searches is well underway. Existing public APIs are being surveyed, the query capabilities offered by the facilities that provide them are being compared against this and the requirements needed for the WP deliverables as well as the desired optional features are discussed. A second face to face meeting, held end of May at ESS in Copenhagen, was attended by all partners and made good progress towards a common vision of the work programme. The task to examine and extend the NeXus ontology has been started as well. A list of scientific techniques at photon and neutron facilities has been compiled. In an effort to understand the diversity and commonalities between existing data files, the partners agreed to share and disseminate examples from all facilities. Future face to face meetings have been agreed to plan in more detail for the upcoming milestones.

Work Package 4: Data Analysis Services

Recruiting staff for WP4 is ongoing. A two-weekly video conference has been arranged for WP4. Amongst topics of the conferences are presentations to help the complementary facilities to understand the respective requirements and technical abilities. Preparations for the questionnaire deliverable are underway; this will help to formalise and prioritise data analysis related work across the partners. A first workshop for WP4 is arranged for 25 to 27 June 2019 at European XFEL.

¹ <https://doi.org/10.1080/08940886.2019.1608119>

Work Package 5: Virtual Neutron and x-ray Laboratory (VINYL)

Hiring:

EuXFEL: One FTE has signed a contract and will join EuXFEL to work on WP5 in July 2019. C. Fortmann-Grote has left as a FTE on Feb. 28 2019 and now works as a 10% part time employee since May 1st 2019.

ESRF: One software engineer (Th. Vallois) started on Feb. 4th and left on March 1st. The position remains open.

ESS: Mads Bertelsen started as a postdoc on Jan. 1st to work in WP5.

CERIC-ERIC: One FTE hired from June 17 to work in WP5 and WP9.

ELI: No hirings.

Activities:

EuXFEL:

Due to the change in personnel, not much work has been performed at EuXFEL in WP5. The simulation platform SIMEX was added to the Pandata Software Catalogue in fulfillment of PANOSC milestone MS5.1 in April 2019. All other software packages which are foreseen to be employed in WP5 had already been added to the Pandata Software Catalogue, previously. Current activities are mainly concerned with planning the software developmental tasks required to employ the openPMD metadata standard (D5.1) and API harmonization for Task 5.1 and Deliverable D5.2. Example notebooks are currently updated to take into account user feedback and for Deliverable D5.3

ESRF:

Due to the unexpected departure of the hired software engineer, most planned work for the x-ray optics design and simulation platform Oasys has stalled and not reached the expected state.

ESRF has organised the First Oasys School (14-16 May 2019) with the support of PaNOSC. A report is in preparation. The material of the course is available at github.com/oasys-kit/oasys_school.

ESS

A python interface to the neutron x-ray tracing platform McStas was implemented and is now in a state that can be used for production simulation runs. Configuration, execution, and analysis of a virtual neutron powder diffraction experiment were demonstrated using the Jupyter notebook. Examples can be found at <https://github.com/PaNOSC-ViNYL/McStasScript>.

This marks important steps in fulfillment of Task T5.3 and Deliverables D5.2 and D5.3.

ELI: nothing to report

CERIC-ERIC: nothing to report

From June on, biweekly meetings on Mondays at 1pm will take place to exchange progress updates and to coordinate common efforts.

Work Package 6: EOSC integration

The WP has set up fortnightly video conferences since the kick-off of the project. They have been mainly dedicated to identify technical solutions to address data transfer. Three main use cases have been identified (transfer by users to their home laboratories, transfer to data analyses services offered by 3rd party organisations and transfer to archive centres), technical solutions have been presented and discussed. In the next steps, these solutions will be set up to access RIs data repository and explored from technical and functional perspectives.

A second achievement is the setup of an eduTEAMS pilot to support the infrastructure of the photon and neutron AAI community needs. This pilot and the partnership with GEANT have been presented and discussed during the annual UmbrellaID meeting. The feedback from the UmbrellaID team (all the European photon and neutron facilities) was extremely positive; we are now proceeding to a vote of the partners to formally adopt the EduTEAMS platform for the AAI needs of the community.

Recruitment for most of the RIs partners are still ongoing mainly due to the shortage of system administrator professionals in Europe. In order not to delay the work, ILL has temporarily taken the lead of the tasks where the planned leaders had faced difficulties to recruit.

Work Package 7: Sustainability

Apart from the kick-off meeting, the work package efforts till now have been fully dedicated to the stakeholder list preparation. A first document with the purpose to define first the stakeholders' classes and then the list of specific stakeholders of the PaNOSC project was prepared. The document developed by CERIC-ERIC included a questionnaire to collect feedback from all the project partner and observers. The results of the feedback received will be used by CERIC-ERIC to complete the first version of the stakeholder database that will be published on the internal repository.

The first version of the stakeholder database (milestone MS7.1) will be further refined as the project proceeds using the selected iterative approach reflecting the Deming cycle (plan - do - check - act).

Work Package 8: Staff and User Training

Apart from the kick-off meeting, the work package formally first started in month 4 with Task 8.1. Task 8.1 primarily depends on ESS and staff that ESS has seconded from University of Copenhagen and Technical University of Denmark, and therefore ESS has started to have weekly meetings internally involving the seconded staff as well as staff from the ESS Data Systems and Technologies Group and the ESS Data Reduction, Analysis and Modelling group at ESS. Minutes from those meetings are placed in the WP8 folder in the PaNOSC repository on GitHub. The meetings concerns the migration of the e-neutrons.org e-learning platform to ESS and a first plan has been drafted for how to handle this. A first set of meetings with the leaders of work package 4 and 8 has also taken place and it has been decided that the WP8 leader will draft a joint WP4, 5, and 8 plan, which then will constitute both MS8.1 and MS8.2.

Work Package 9: Outreach/Communication and Dissemination/Impact

During the first six months of the project, WP9 firstly focused on setting up the tools to ensure a proper flow of information within the partnership, as well as between the project partners and the PaN community, other EOSC clusters and the wider community of EOSC stakeholders.

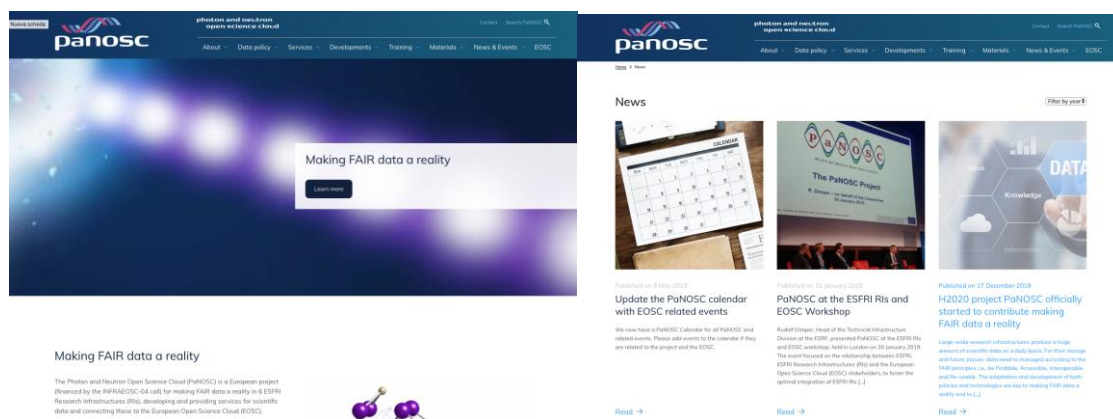
Deliverable 9.3 - "PaNOSC repository for internal communications" was published in this respect at the end of February 2019. The document describes the various tools adopted by PaNOSC for managing the documentation of the project, and provides instructions on how to use them. Such tools include:

- Open source **GitHub repository** for the storage of project's documents and the management of the project and its team. Three repositories have been created:
 - **PaNOSC** (<https://github.com/panosc-eu/panosc>), used for common issues and general information about the project;
 - **Wiki** (<https://github.com/panosc-eu/panosc/wiki>), with basic information about the project, its partners and its scope, which is used as the temporary project's website until the official one is published;
 - **Issues** (<https://github.com/panosc-eu/panosc/issues>), used for discussion on all PaNOSC issues.
- **Google Drive and Docs** is used through a PaNOSC Google account, to store and share working documents, and to edit them collaboratively.
- The **CERIC drive** is a reserved area accessible by all partners, to

store and share confidential documents related to the project.

The **new logo and visual identity** of the project have been developed, also in view of the publication of the new project's website, which is foreseen by the end of May 2019. A visual identity manual will be available by the end of the same month, whereas most templates for the realization of the project's **promotional material** (.ppt, rollups, poster, etc.) have been designed and shared with the partners.

With reference to the **website** (see some images below), technical specifications have been defined according to the communication needs of the project, and a supplier has been selected for its development. Content is currently being drafted and progressively published in the beta version of the website.



A **shared Google calendar** has been created and shared with all partners, who have permissions to update it with information about upcoming PanOSC and EOSC-related events. Such calendar will be embedded directly in the "News & Events" section of the website.

PanOSC is also on **social media** with the Twitter account @Panosc_eu, to promote the project to all target audiences, and to share useful information for the partners and PanOSC/EOSC stakeholders about latest project's achievements, opportunities and upcoming events, relevant publications on FAIR data and the EOSC, etc.

Contacts with communications officers from the partners and **other EOSC clusters** have been taken, starting to give shape to a network of communicators cooperating for the promotion of the advancements in the work conducted towards the construction of the EOSC by research infrastructures throughout Europe.

In addition, staff and managers from PanOSC partners attended a number of **events** to introduce PanOSC to different audiences (including RIs technical

staff and managers, policy makers, researchers and service providers), and to discuss future plans and developments. Attended events in which PaNOSC speakers were actively present include:

- ESFRI RIs and EOSC Workshop, 30 January 2019, London - UK
- ESCAPE kick-off meeting, 7-8 February 2019, Paris - France
- SSHOC kick-off meeting, 11-12 March 2019, Utrecht - The Netherlands
- FAIRsFAIR kick-off meeting, 14-15 March 2019, Amsterdam - The Netherlands
- EOSC-hub week, 10-12 April 2019, Prague - Czech Republic
- EGI Conference, 6-8 May 2019, Amsterdam - The Netherlands

A possible participation in ESOF 2020 in Trieste is being discussed for the outreach to the wider public, with a panel with representatives from all EOSC clusters, to present the EOSC and the expected results for European research infrastructures active in the fields of environment, materials science, life sciences, astronomy and social sciences.

By the end of June 2019, the communication strategy of the project will be published, which includes an overview of the main project's communication goals and objectives, the main target audiences and key messages, as well as a more detailed plan of actions to inform and engage PaNOSC stakeholders in the next four years of the project. The strategy and the annexed communication plan will be working documents, which will be regularly updated and adapted to the needs of the partnership, the project and the EOSC.

Comparison between actual and forecasted project status

At this point in time, the project is advancing as planned. The project team is completing on time its deliverables without any indication that is overspending the allocated resources.

Milestone Deliverable Id	or	Name	Due date	Completed
D1.1		Project Initiation Documentation	M2	YES
MS1.1		Project Initiation Stage completed	M2	YES

D9.3	Repository for internal communication	M3	YES
D9.2	PaNOSC's website	M6	Planned 31/05/2019
MS9.1	PaNOSC's website ready	M6	Planned 31/05/2019
MS5.1	Simulation codes in PaNData Software Catalog	M6	YES
MS7.1	Stakeholder database ready	M6	Coming soon
MS8.1	Joint WP4 and WP8 plan	M6	YES
SM8.2	Joint WP5 and WP8 plan	M6	YES
D1.2	Mid-Year summary	M6	YES
D1.4	Data management plan	M6	Planned 31/05/2019

Recruiting at the different partners in order to support the PaNOSC project is still ongoing and a little bit behind schedule, however we do not expect at this time this to negatively affect the project and its timescales.

Next steps

The first annual workshop for PaNOSC is being planned, with the date of and location confirmed (Trieste during week 43 of 2019).

We expect to have completed most of the recruitment by month 9 (August 2019), so all consortium partners can focus on delivering PaNOSC.

ExPaNDS, the companion project to PanOSC, has received financing from the EU. ExPaNDS has the same objectives as PaNOSC but for national photon and neutron sources. The two projects depend on each other and will work closely together to serve a common community. ExPaNDS officially kicks off in September but discussions on how to work together have already started.

Appendix I: Governance bodies

The organisational structure for the project will comprise the following bodies.

- **Executive Board** as the ultimate decision-making body of PaNOSC.
- **Project Management Committee** as the supervisory body for the execution of the Project which shall report to and be accountable to the Executive Board.

Each member partner participating in PaNOSC (ESRF, ILL, XFEL.EU, ESS, ELI-DC, CERIC-ERIC and EGI) will appoint a member for the Executive Board and Project Management Committee, being present at all of the meetings of these two bodies and appoint a substitute or a proxy when required.

The members of these two governing bodies of PaNOSC will always be available in GitHub, however at the time of writing (April 2019), the membership is:

Partner	Project Management Committee (PMC)	Executive Board (EB)
ESRF	Andy Götz	Rudolf Dimper
ILL	Jean-Francois Perrin	Mark Johnson
EuXFEL	Hans Fangohr	Thomas Tschentscher
ELI-DC	Florian Gliksohn	Allen Weeks
ESS	Petra Aulin	Jonathan Taylor
CERIC-ERIC	Dario Roccella	Jana Kolar
EGI	Diego Scardaci	Tiziana Ferrari

There will be as well the Project Manager and the Project Support Team assisting the Coordinator and each Work Package will have a leader in charge of coordinating and delivering the work agreed in the PaNOSC proposal, feeding back status information to the Project Management Committee.