

Academic Computer Centre CYFRONET AGH



Roksana Wilk, ACC Cyfronet AGH

Head of Data Processing Laboratory, Cyfronet's EOSC and Open Science affairs rep

Skills and competences in Open Science

Academic Computer Centre Cyfronet AGH

- The largest Polish Academic Computer Centre
 - 50 years of experience in IT provision
 - Centre of excellence in HPC, Grid and Cloud Computing
 - Home for Athena, Ares and Prometheus supercomputers
 - LUMI consortium partner (EuroHPC pre-exascale supercomputer #3 on TOP500)
- Legal status: an autonomous within AGH University of Science and Technology
- Staff: 180+, ca. 80 in R&D
- Leader of PLGrid: Polish Grid and Cloud Infrastructure for Science
- NGI Coordination in EGI e-Infrastructure





Academic Computer Centre Cyfronet AGH

Prometheus

2.40 PFLOPS

53 568 cores

From 2015 to 2021 1st HPC system in Poland (475th on Top 500, 38th in 2015)



Athena

7.71 PFLOPS

384 A100 GPGPUs

1st HPC system in Poland (since 2022, 105th on Top500)

9th on Green500

Ares

4.00 PFLOPS

38 112 cores

290th on Top 500







Computing portals and frameworks

OneData

PLG-Data

Rimrock

InSilicoLab



ATACENO



Storage

60+ PB



hierarchical data management

Research & Development

distributed computing environments

computing acceleration

machine learning

software development & optimization



Data Centres

3 independent data centres

dedicated backbone links

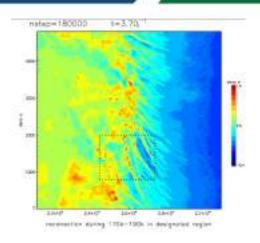
Computational Cloud

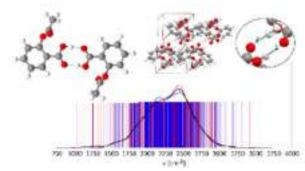
based on OpenStack

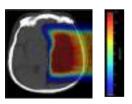


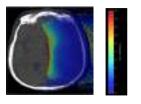
Usage examples

- Astrophysics: users' own code
 - Particle in Cell written in Fortran
 - Production runs 9600 cores
 - One run up to 460 800 h CPU time 53 years
- Chemistry: CPMD, CP2k, Jaguar, Gaussian
 - Importance of hydrogen bonds in biomolecules
 - Jobs: 24-240 cores
 - Hundreds of thousands of jobs with walltime < 1 h</p>
 - Efficient usage resources through backfill
- Biophysics: Proton therapy
 - Monte Carlo simulations of a proton beam
 - Monte-Carlo based treatment planning
 - O Jobs:
 - thousands of jobs with MC simulations (hours on hundreds of nodes)
 - Interactive large data processing with Jupyter noteboooks









Usage examples – AGH students scientific associations

AGH Racing – Formula Student





 AGH Solarboat – Solar Sport One and Monaco Solar & Energy Boat Challenge





Open Publications

SKILLS & EXPERIENCE



PLGrid - infrastructure for (open) science

Welcome to the PLGrid portal!

At this point you can prepare to use the PLGrid infrastructure - create affiliaiton, apply for a service or a grant. We encourage you to use PLGrid user manual.]

If it is necessary to contact Infrastructure employees, we recommend creating message in the system Helpdesk PLGrid.]

The most important functionalities



Affiliation

The PLGrid infrastructure provides resources to people associated with polish science. Enter the scientific unit under which you conduct the research. Then select whether you are an employee or if you work with some of employees (e.g. as a student or a PhD student).



Services

To be able to use the resources, select the services that interest you (big data, storage, cloud computing, social tools), ways to access them and additional services, which will improve the use of the Infrastructure.



Teams

In order to request a proper grant, create a team that reflects the research group with which you want to share the grant. The team can be one person team.



Grants

The use of resources takes place within grants -contracts for the use of resources, defining the parameters of the resources made available. Apply for a grant, provide the research topics and technical parameters of the grant.





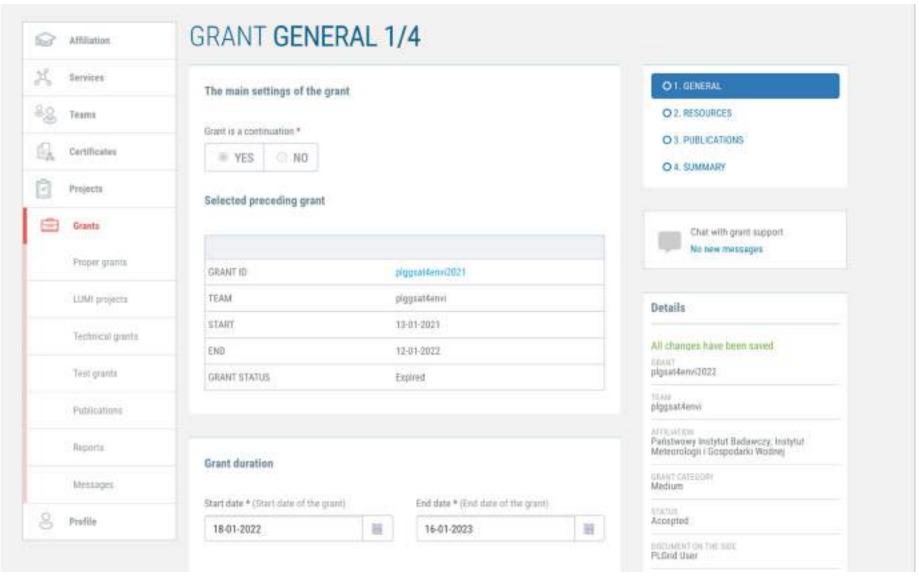


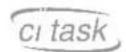






PLGrid - infrastructure for (open) science





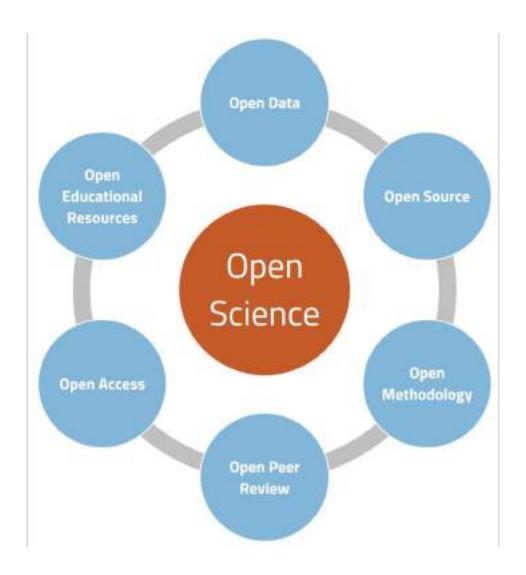








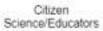




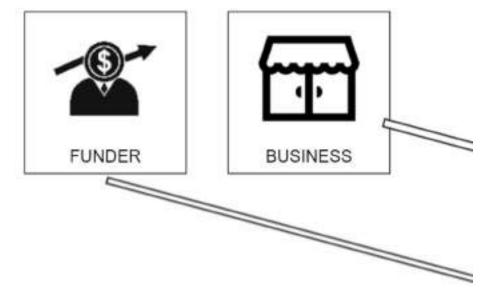


WHO ARE YOU? I AM A...













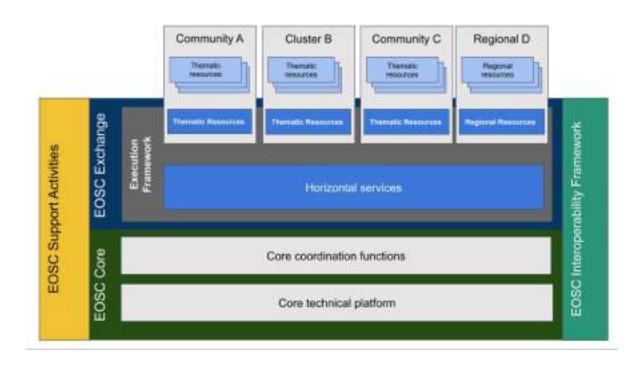




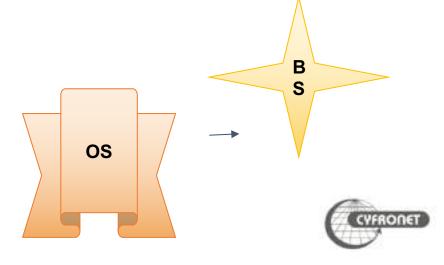


- Supporting tools →
- Features and operation ->
- Knowledge and skills





- Supporting tools →
- Features and operation ->
- Knowledge and skills















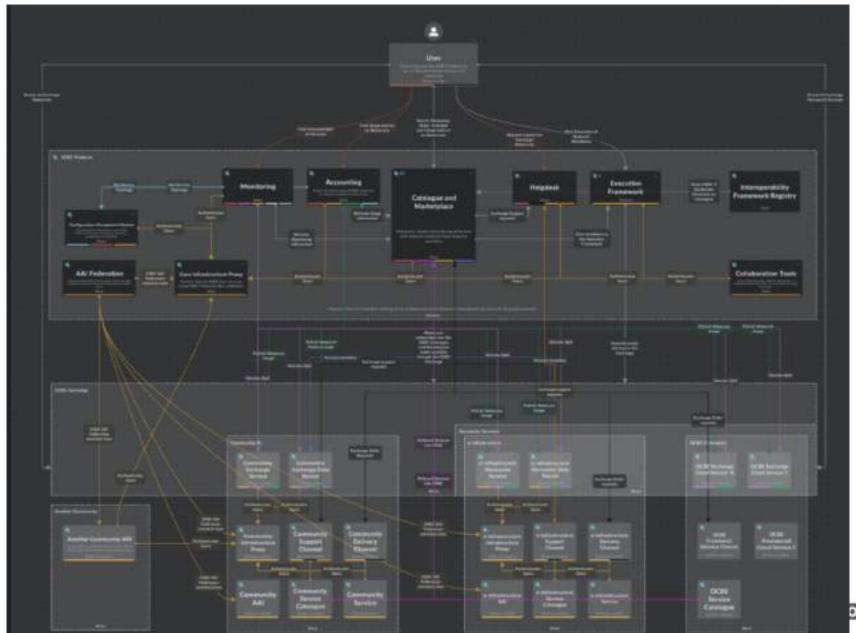




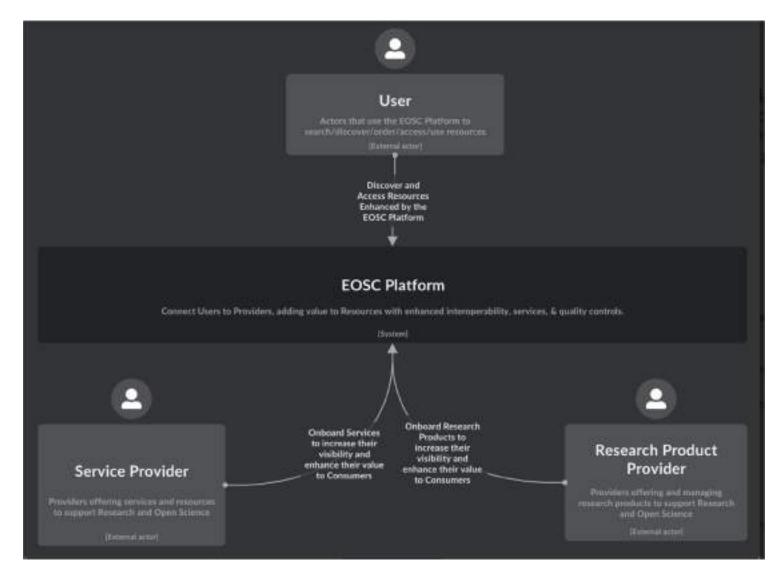




And again

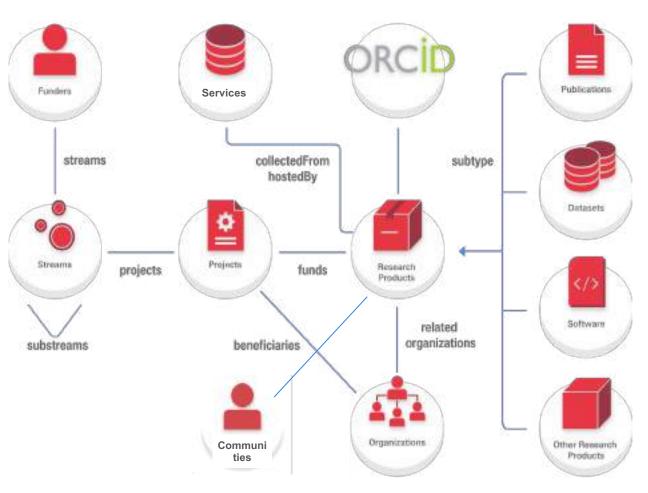








Research products (EOSC RDGraph - Data model)





- 1. RAiD handle: a persistent, unique string of numbers, minted via the RAiD API.
- 2. The metadata envelope records time/date stamped PIDs for
 - Funders
 - Organisations
 - Collaborators
 - Tools and Services
 - Data

Source https://www.raid.org.au Requirements from WP4





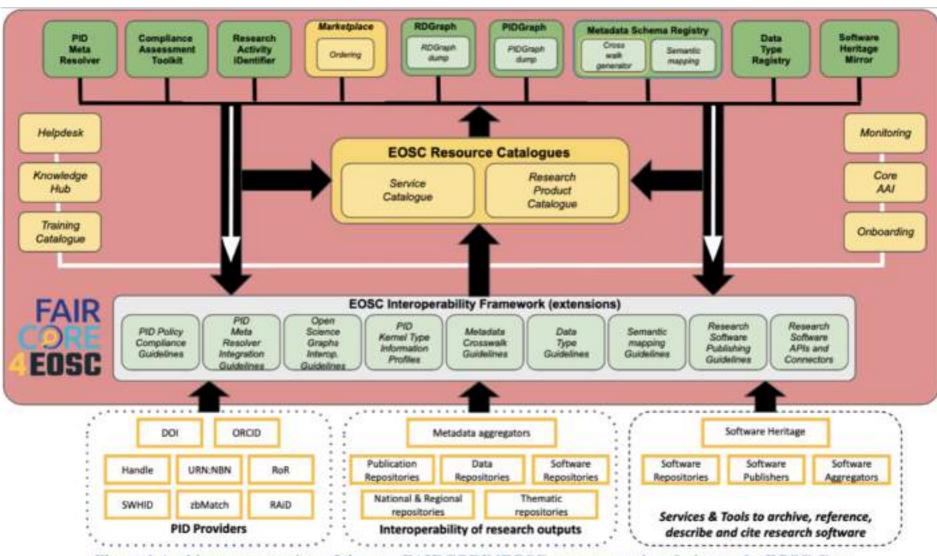
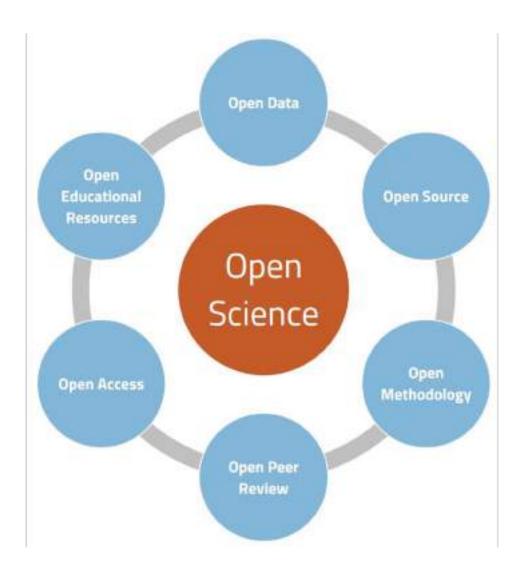


Figure 1 Architecture overview of the new FAIRCORE4EOSC components in relation to the EOSC-Core



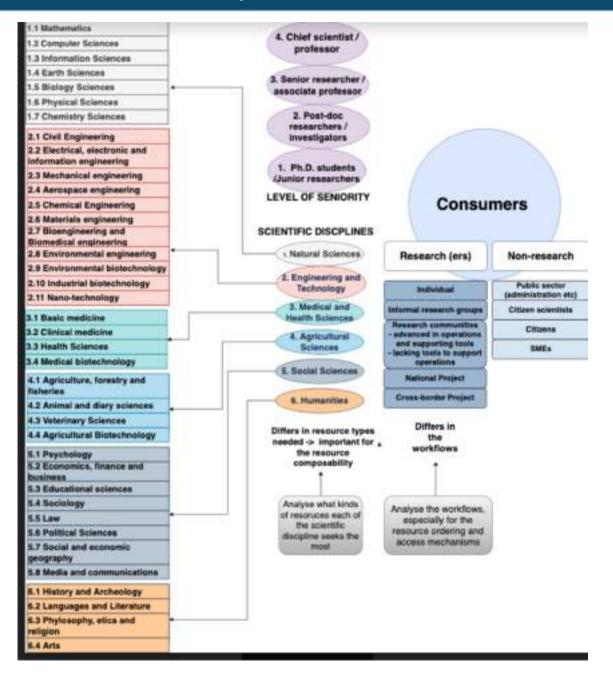






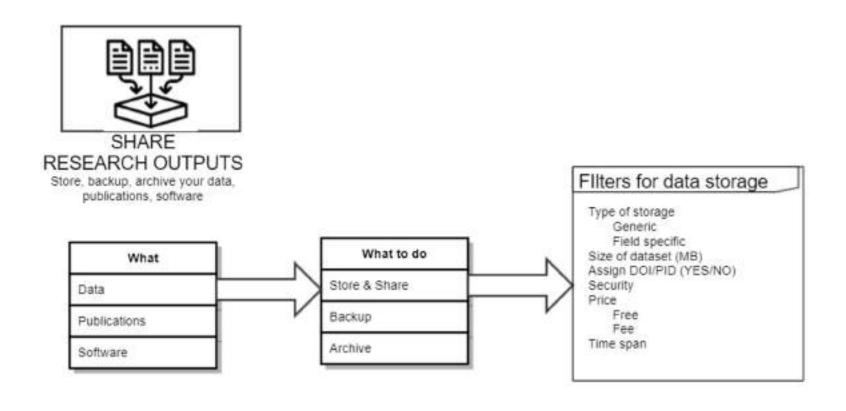


Consumers of Open Science



They come in as many flavours as you can imagine







It's not all...

PROCESSING

- Capabilities needed: transfer, compute (possibly external), processing tool, storage (possibly external)
- What matters for this goal:
 - For storage:
 - Size of the dataset
 - Time of retention
- PUBLISHING YOUR DATASET
 - Capabilities needed: publishing service
 - What matters for this goal:
 - Size of the dataset
 - DOI
 - free/not free
 - Domain
 - Security (anonymise personal data/licence)
- ANONYMISATION
- MOVE/STORAGE YOUR (BIG) DATA (place where I can keep my data to use it during my processing)
 - o Capabilities needed: transfer, storage

- USE EFFICIENT COMPUTING RESOURCES
 - Capabilities needed: computing, storage (possibly external)
- DISCOVER/RE-USE DATA
- MAKE YOUR REPOSITORY FINDABLE IN OPEN SCIENCE
 - Capabilities needed: data sources
 - What matters for this goal:
 - Connecting of metadata?
- DATA MANAGEMENT
- PRODUCE DATA (physical instruments)



