PaNOSC + ExPaNDS tools for scientists + science clusters

Andy Götz (ESRF, PaNOSC coordinator)

PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

Talk outline

1. Science clusters tools and platforms
2. PaN Tools for visualization, processing, remote analysis
3. PaN Training platforms
4. PaN DMPs

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Science Clusters are providers + consumers of Tools + Platforms

Category	EOSC-Life	ENVRI-FAIR	ESCAPE	PaNOSC	SSHOC
AAI	LS-AAI		IAM & existing X509 infrastructure	UmbrellaId	AARC BPA implementations
Data Repositories	Covid portal FAIRsharing catalog	Certified data centers at RI level ENVRI-Hub	HEP Open Data Portal Virtual observatory Software catalogues	ICAT + Scicat Federated search, Human Organ Atlas Software catalogue,	> 40 certified data centres (CTS)
Metadata standards	Fairsharing.org Bioschemas.org	DCAT-AP	FITS	Nexus/HDF5	CMDI, DDI
Data transfer	Globus, http, rsync	https	FTS (http, gridftp), EUDAT solutions	Globus, http, rsync	http, smtp
Training platforms	TESS	ENVRI Training Catalogue	Summer schools, training material in OSSR	Moodle + TESS	SSH Training Toolkit
Tools used / developed	DS-Wizard Galaxy WorkflowHub.eu	FIP, KB, ENVRI-Hub, Jupyter, VRE	Data Lake, OSSR, VO tools, VRE, Jupyter, etc. Citizen Science platforms	DS-Wizard, Jupyter, H5Web, VISA, VINYL,	SSH Open Marketplace; Virtual Collection Registry; Jupyter

Active Data Management Plans

1. **ExPaNDS and PaNOSC have adopted active DMPs**
2. **Active DMPs are updated at different phases of the project**
3. **ESS and ESRF have chosen to use DS Wizard developed by Elixir**
4. **Example of implementation @ ESRF**
    1. Automatically generates a DMP automatically for every proposal
    2. 50 out of 82 questions are automatically filled in from DP/User/Data Portals
    3. DMPs offer a structured way to communicate information
    4. Users can use the DMP for satisfy funders requirements
    5. Next step is to use the DMPs to ensure users can manage their **data**

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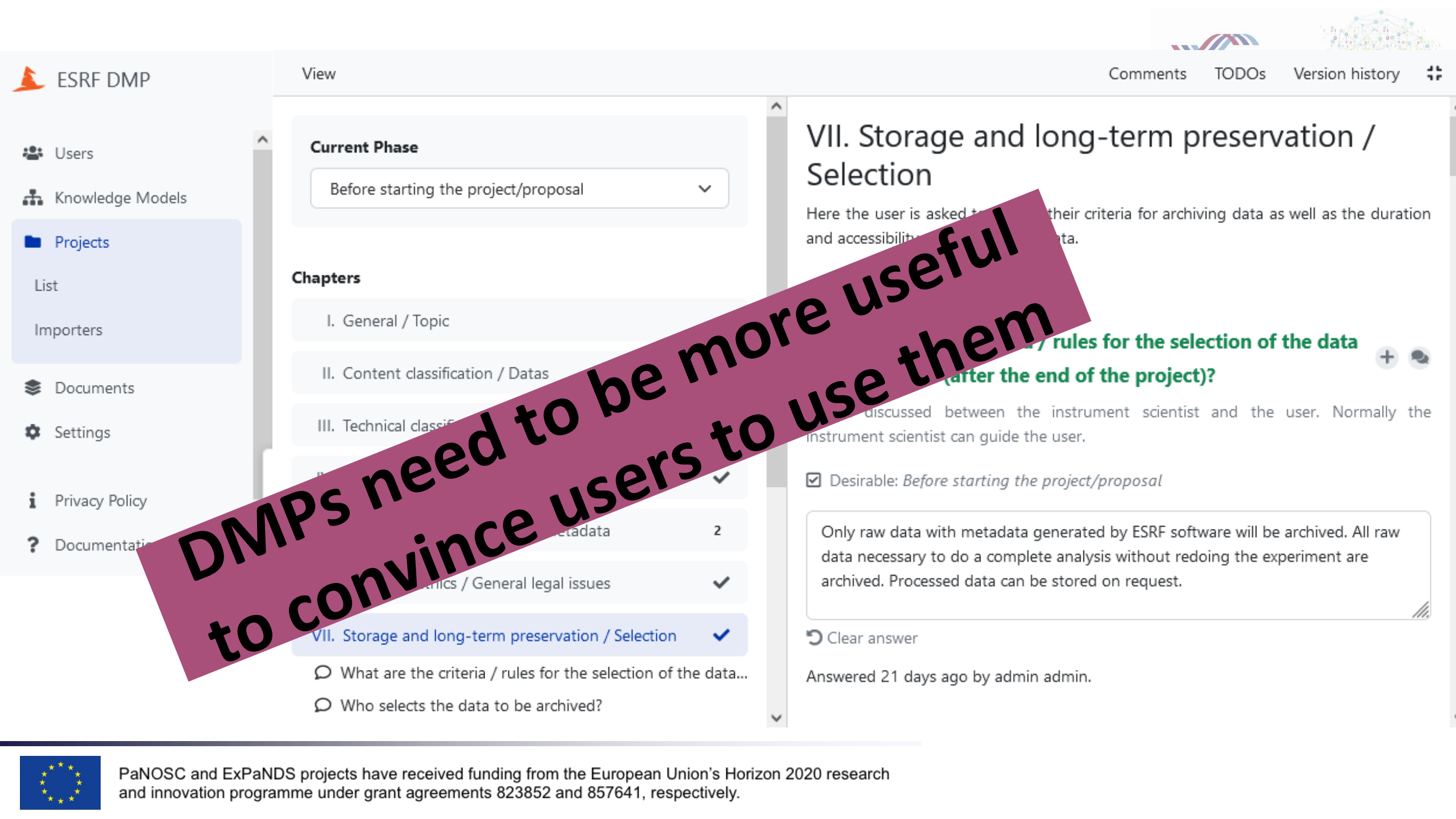

DMPs need to be more useful to convince users to use them

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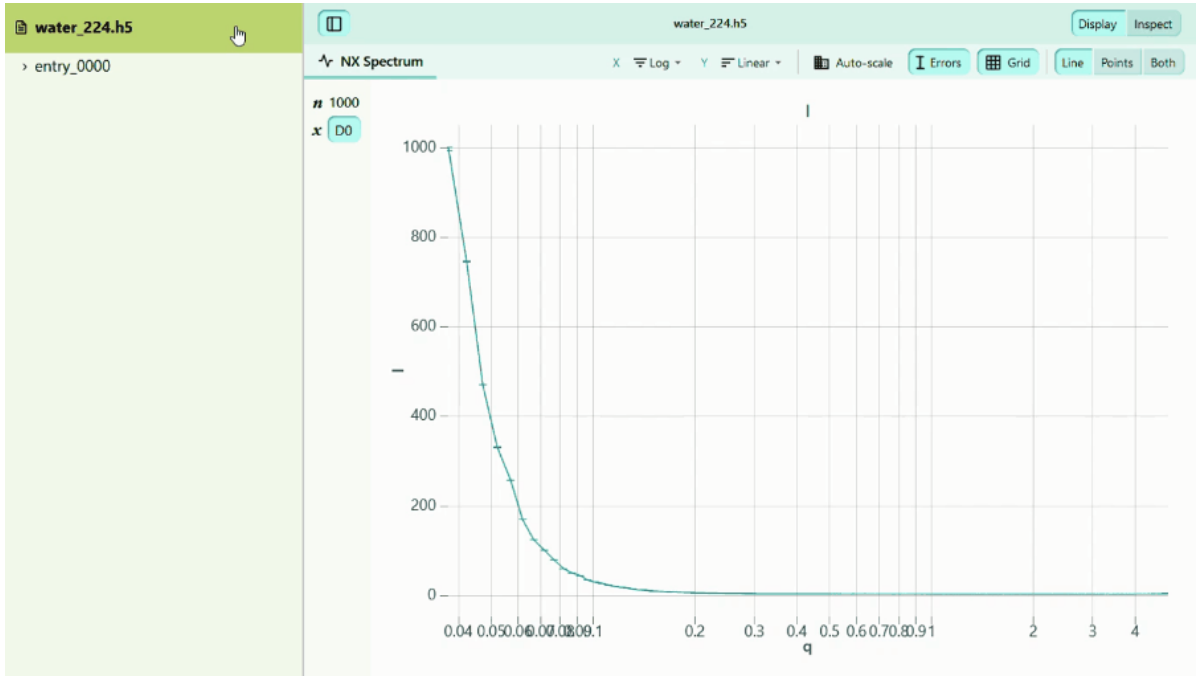
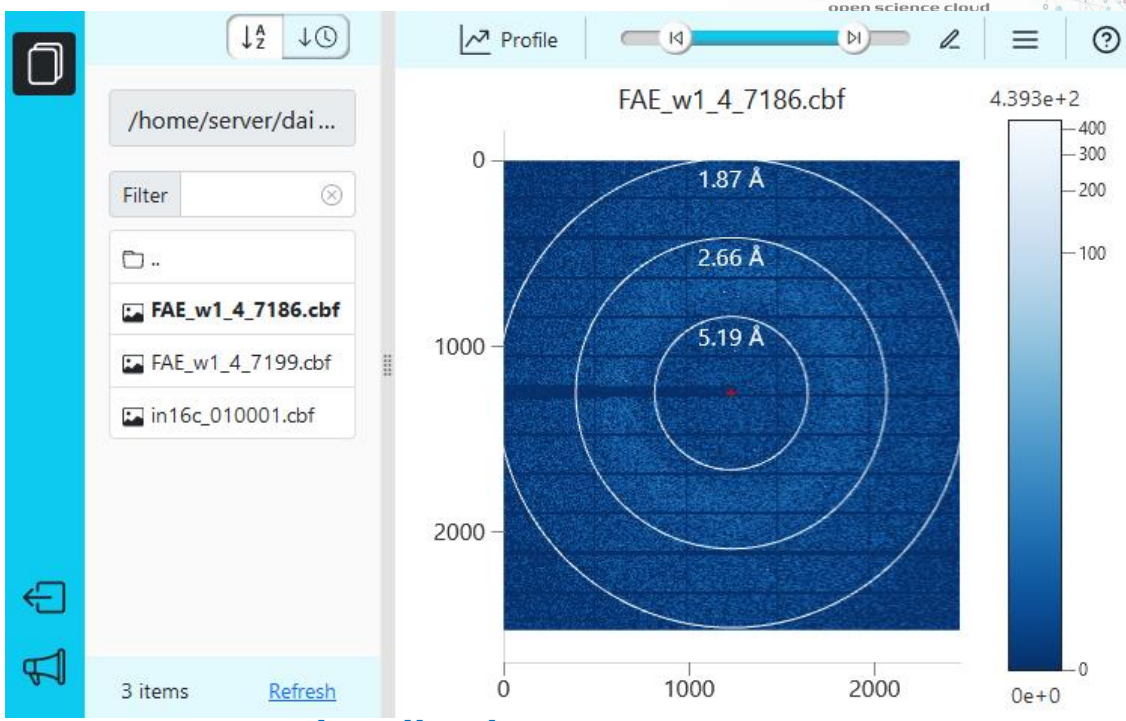
H5Web Visualization Ecosystem



Generic HDF5 file viewer



Visualization components

- Integrated into **ESRF data portal**, for viewing files generated during experiments
- Available as **JupyterLab** and **VS Code extensions**, and soon as part of stand-alone web service, **myHDF5**, for viewing local and hosted HDF5 files

Used in various web applications at ESRF including:

- **Braggy**, diffraction image viewer (screenshot above)
- **Daiquiri**, beamline control and data acquisition software

https://github.com/silx-kit/h5web

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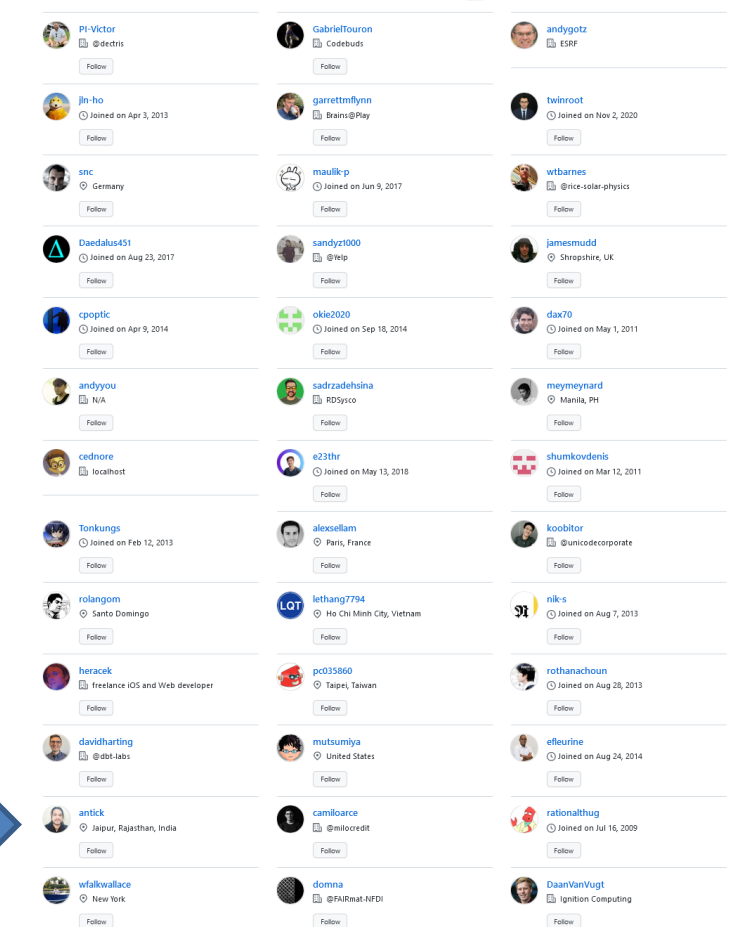
H5Web
H5Web | 1,238 installs | ★★★★★ (3) | Free

H5Web Visualization Ecosystem

- Visualisation in the web is a common requirement for many tools
- H5Web provides a modular solution for plotting in ReactJS applications
- H5Web has been welcomed by many communities e.g. photon + neutron science, neuroscience, astronomy, space, microscopy, materials science, environment, commercial companies …

GitHub **STARGAZERS**



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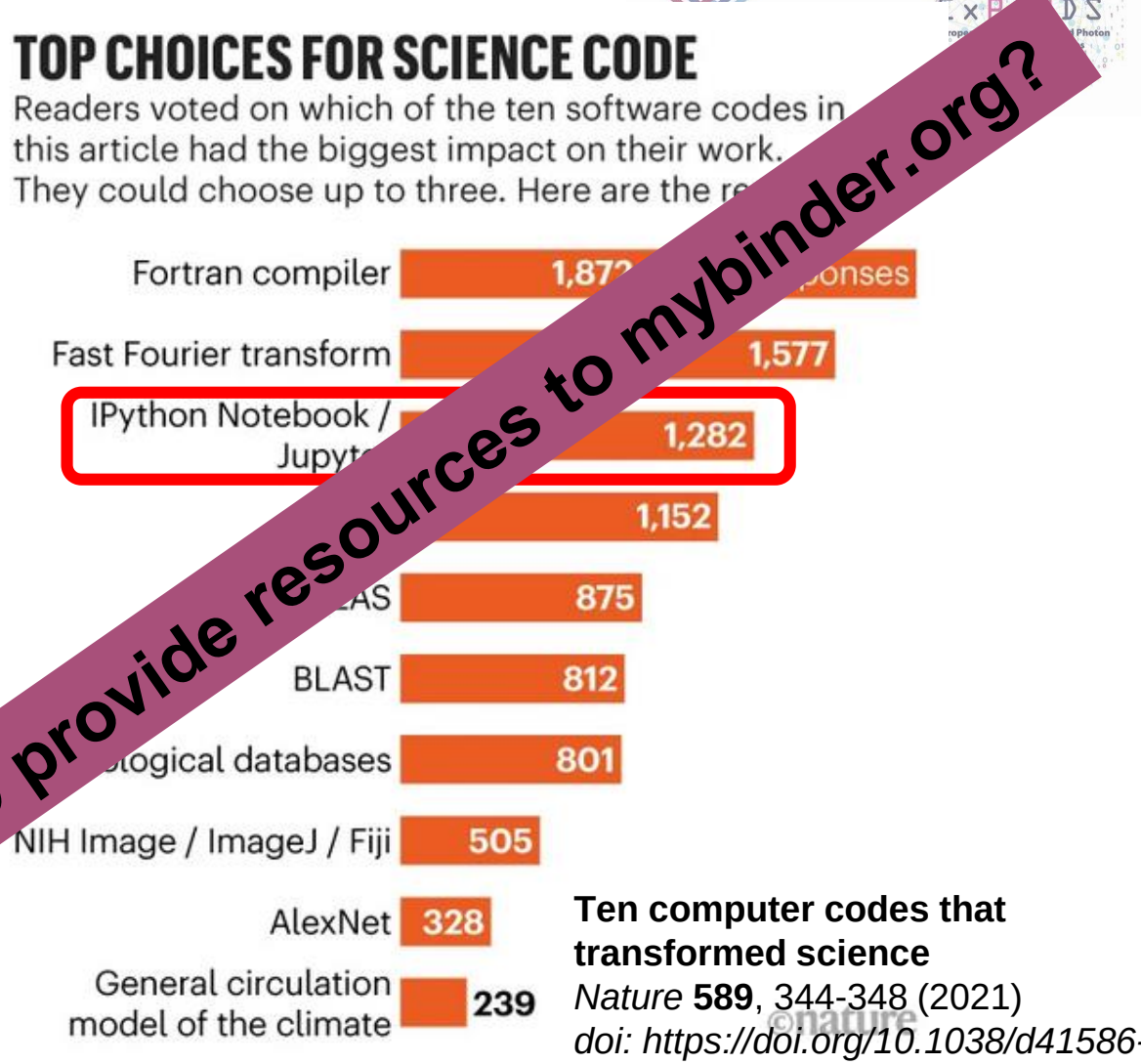
Support for Jupyter notebooks

- **Jupyter service** now available at all PaNOSC and most ExPaNDS sites
- **Jupyter on Slurm** service developed: https://github.com/silx-kit/jupyterhub_moss/
- **H5Web** Jupyterlab plugin developed
- **VISA** provides Jupyter service
- **PaN e-learning** platform provides Jupyter as a service
- **PaNOSC summer school** trained particip… to program in Python using Jupyter
- **EGI** provided Jupyter and Binder as a …ervice

Will EOSC provide resources to mybinder.org?



Ten computer codes that transformed science
Nature **589**, 344-348 (2021)
doi: https://doi.org/10.1038/d41586-021-00075-2

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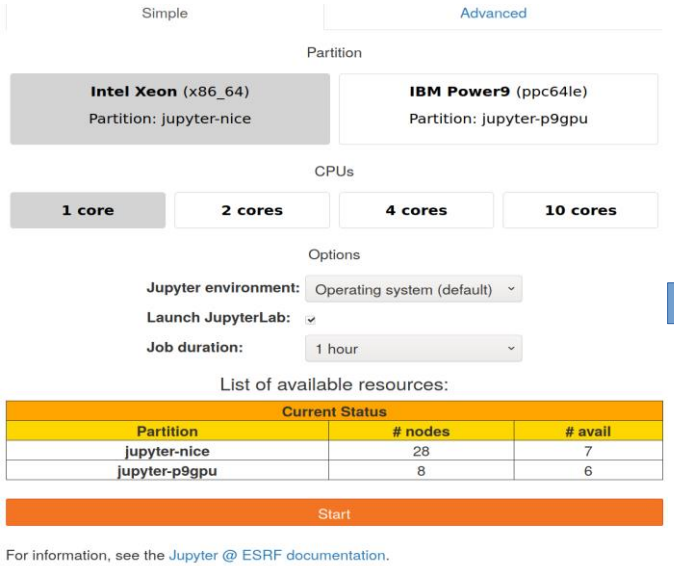
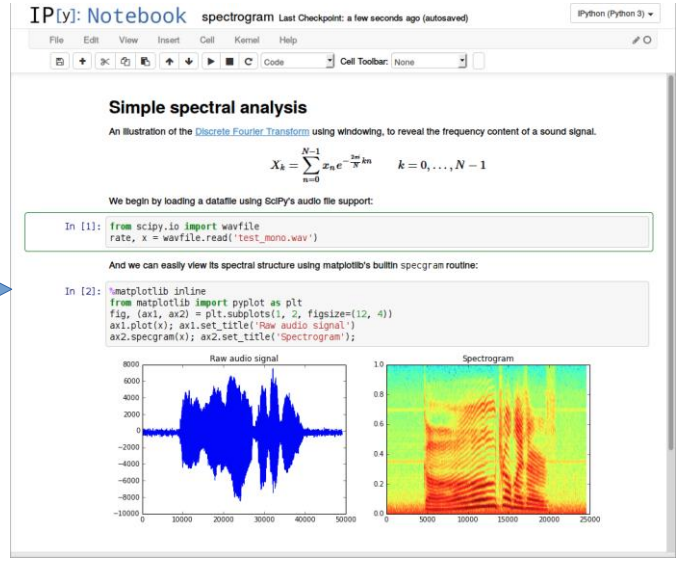
Example Jupyter service @ https://jupyter-slurm.esrf.fr

- Enables users to run Jupyter Notebook on ESRF SLURM cluster





Unique users@ESRF: 156 (monthly average**), 276 (total)** over **4 months**

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Open Science with Jupyter notebooks

- Notebooks n in one document
- If used app
- For exampl
- Notebooks e-usable
- Currently, l vork of others, before they

EOSC could provide training on making reproducible publications for FAIR data

https://youtu.be/vStbMUDI_jU

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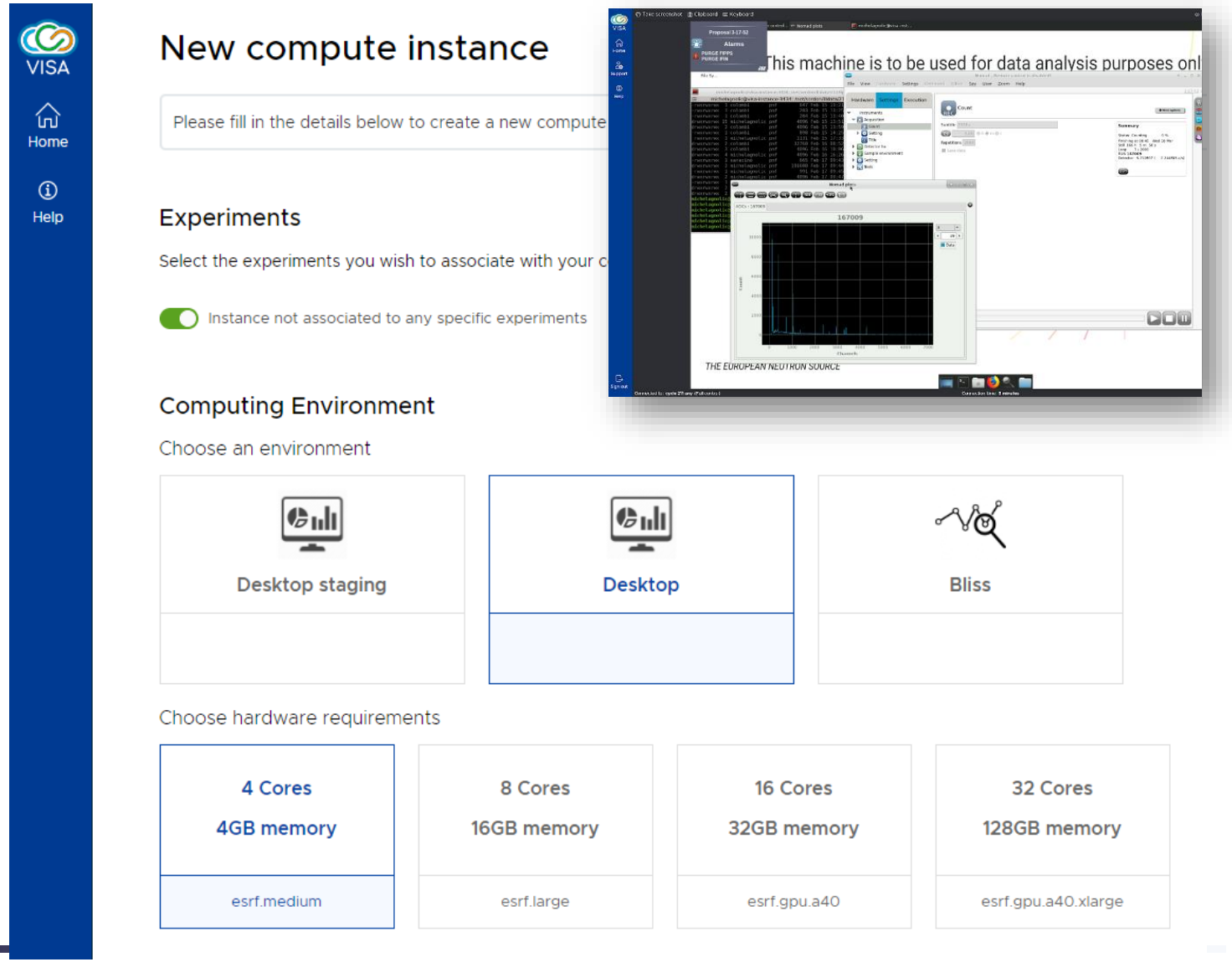
VISA - Remote Data Processing/analyses



- Infrastructure for remote data processing / analysis
- Users dedicated VM
- Access to data
- Access to Provisioning of scientific SW using CVMFS and Containers
- Access to the GPUs, HPC cluster
- Infrastructure based on OpenStack
- Development led by ILL in the scope of the PaNOSC project

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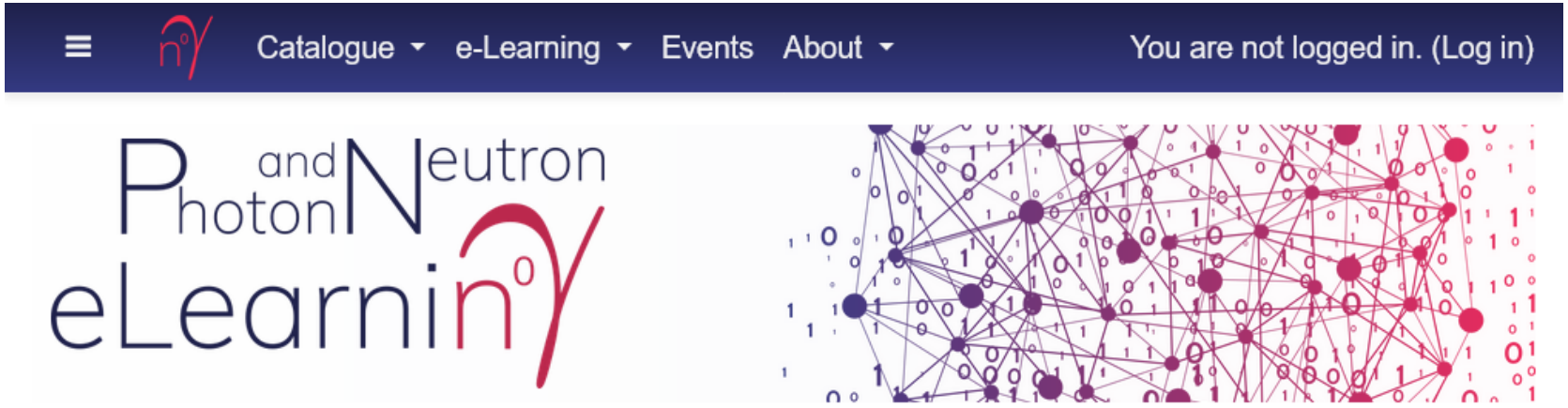
The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641.
The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.

Open Training - courses on Pan-learning.org

Achieving100% Open Educational Resources:

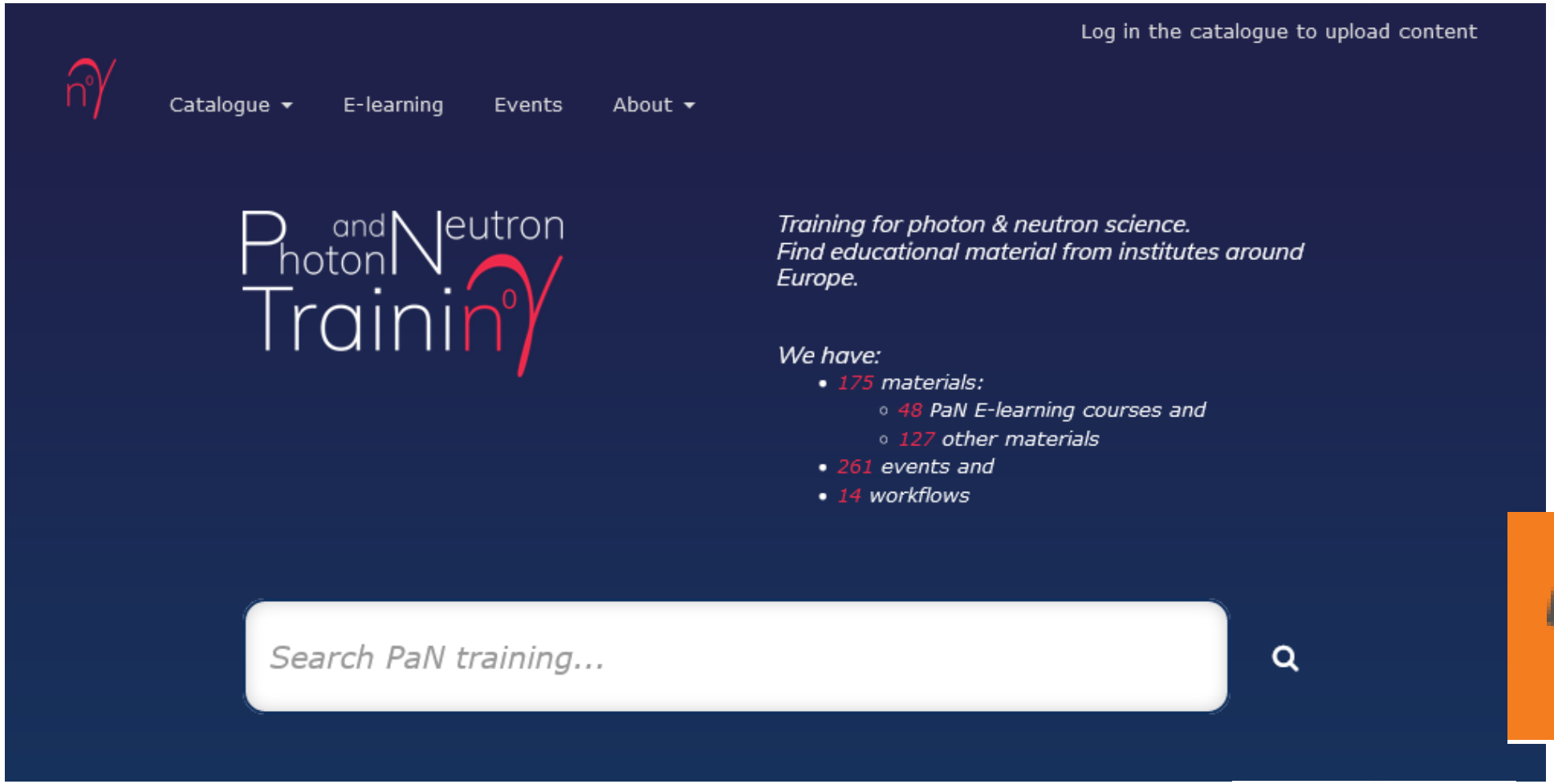
1. *Publish training material on pan-training.org*
2. *Develop learning material on pan-learning.org*



https://e-learning.pan-training.eu/moodle/

PaNOSC and E
and innovation p

Share training material, videos, events, etc. on Pan-training.org



https://pan-training.eu/

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Conclusion

1. Science clusters are providers + consumers of tools and platforms which need to be supported by the EOSC

2. Software tools make a big difference for scientists

3. Science clusters will actively collaborate around tools in the future

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