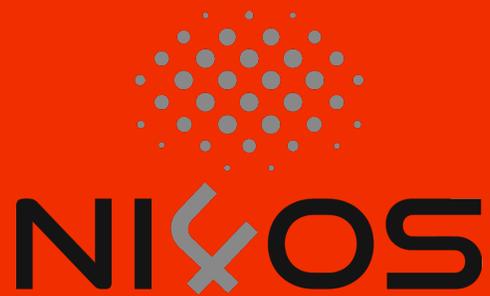


arnes 



National Initiatives for Open Science in Europe

# PaNOSC - Fotonski in nevtronski oblak odprte znanosti

Aljoša Hafner, CERIC-ERIC

Mreža znanja 2020, 25. in 26. november



EVROPSKA UNIJA  
EVROPSKI SKLAD ZA  
REGIONALNI RAZVOJ  
NALOŽBA V VAŠO PRIHODNOST

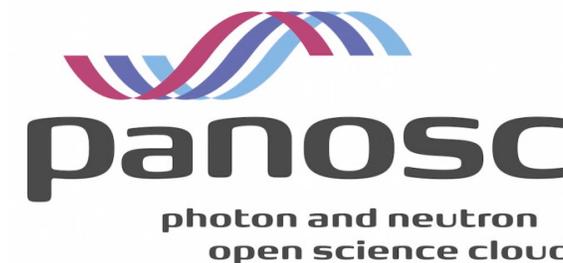


REPUBLIKA SLOVENIJA  
MINISTRSTVO ZA IZOBRAŽEVANJE,  
ZNANOST IN ŠPORT

Naložbo sofinancirata Republika Slovenija in Evropska unija iz Evropskega sklada za regionalni razvoj

## **PaNOSC**

Fotonski in nevtronski oblak odprte znanosti  
Photon and Neutron Open Science Cloud



Aljoša Hafner – CERIC-ERIC – [aljosa.hafner@ceric-eric.eu](mailto:aljosa.hafner@ceric-eric.eu)

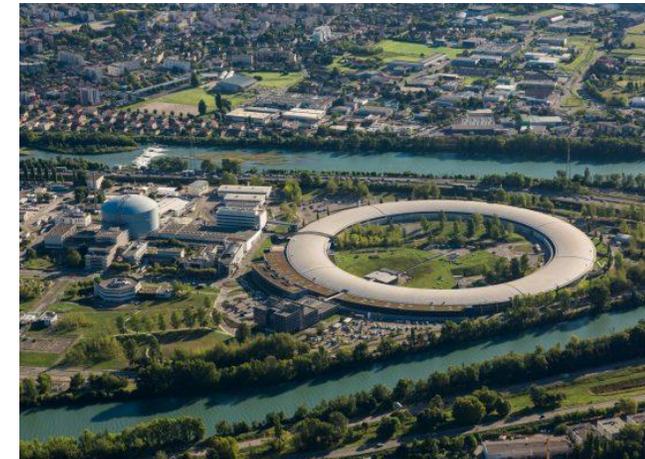
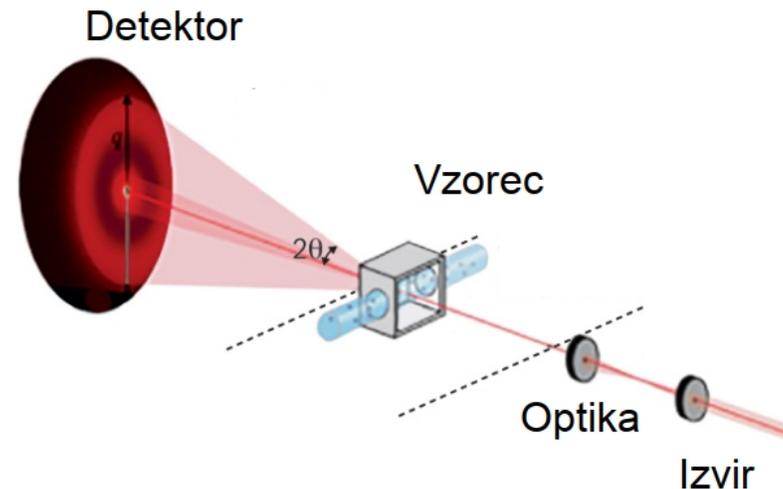
# Zakaj fotonski in nevtronski izvori?

- Izviri rentgenskih žarkov (**fotonov**): sinhrotroni in laserji na proste elektrone
- Izviri **nevtronov**: reaktorji in spalacijski izviri

- Aplikacije (struktura in lastnosti snovi, časovni potek pojavov):

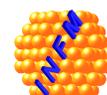
- fizika
- kemija
- biologija
- raziskave materialov
- farmacija
- arheologija
- restavratorstvo
- ...

Slike: (desno zgoraj) Sinhrotron ESRF in reaktor ILL;  
(desno spodaj) sinhrotron Elettra in laser na proste elektrone FERMI;  
(spodaj) splošna shema eksperimentov.



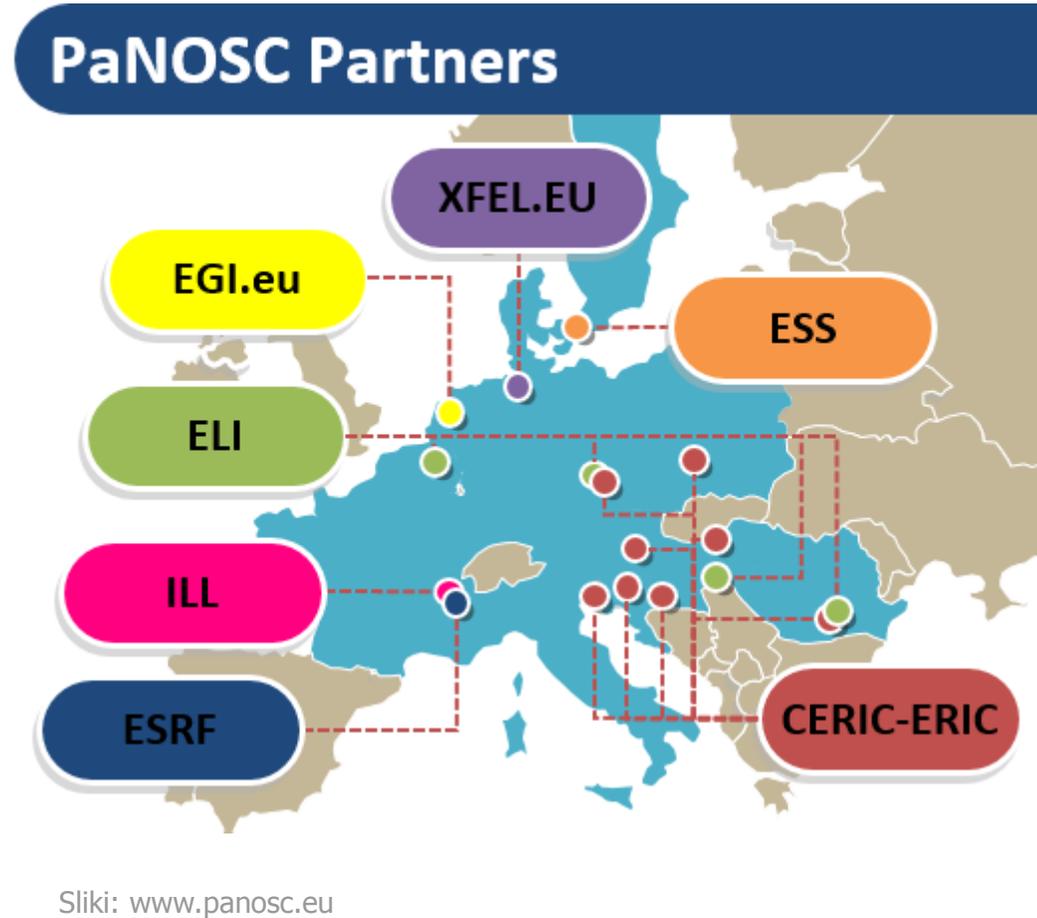
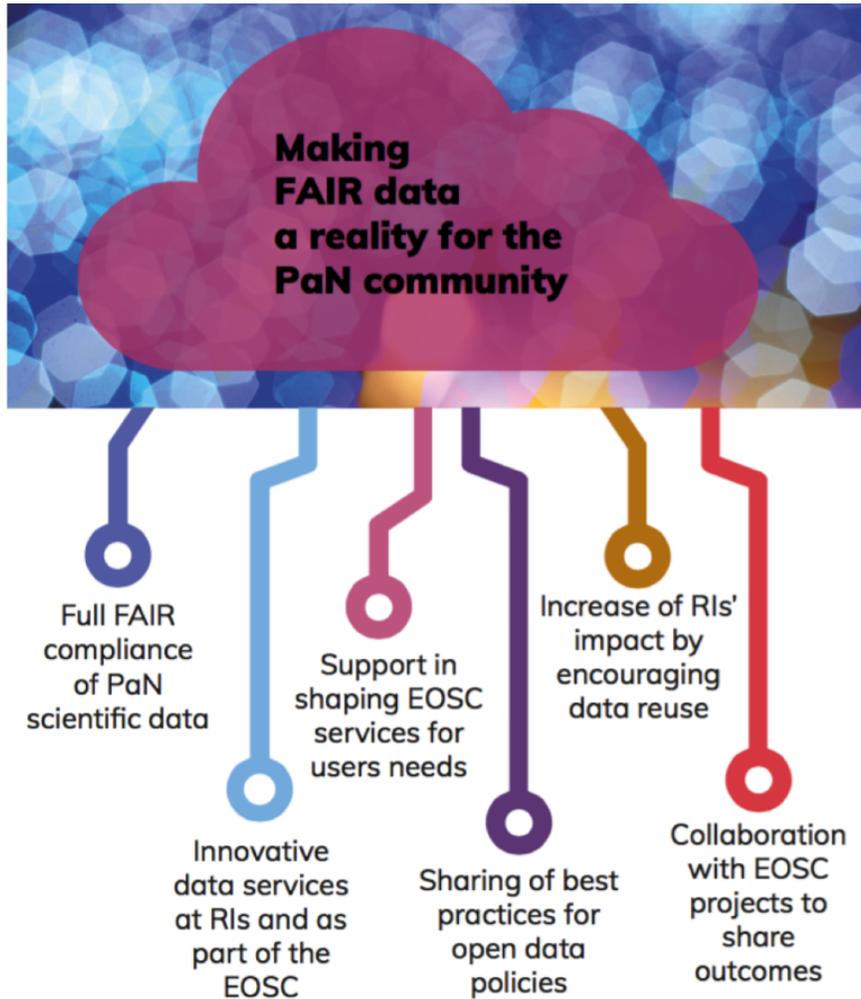
# CERIC-ERIC

- Central European Research Infrastructure Consortium
- Konzorcij 8 inštitutov iz 8 držav
  - *Uporabniku dostopna* infrastruktura (user facility)
- Enotna vstopna točka za prijavo na poskuse
  - Interdisciplinarnost



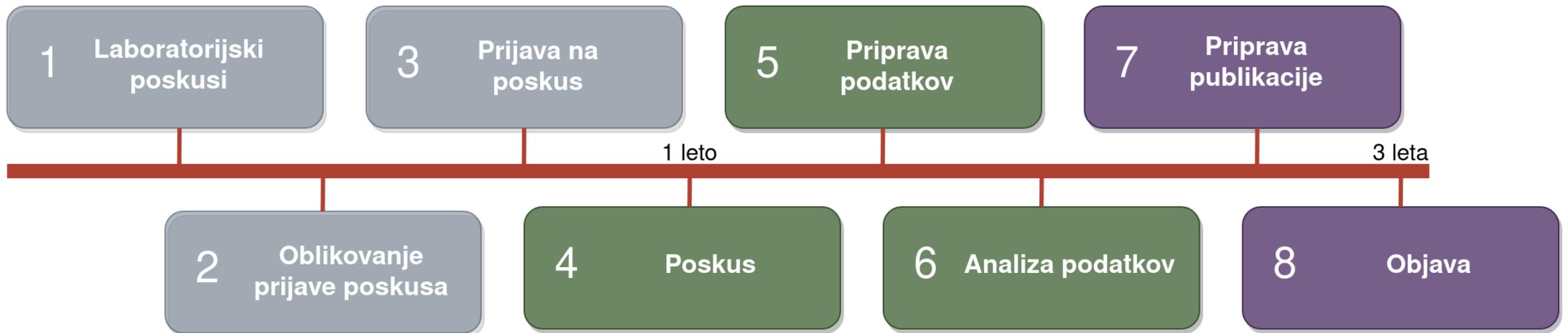
Slike: [www.ceric-eric.eu](http://www.ceric-eric.eu)

# PaNOSC - struktura



# Eksperimentalni proces – stanje (1)

- Tipičen potek poskusa na *uporabniku dostopni* raziskovalni ustanovi (user facility)
- Infrastruktura je prezasedena in *žarkovni čas* (beam time) je omejen
- Povprečni čas od poskusa do objave 2-3 leta

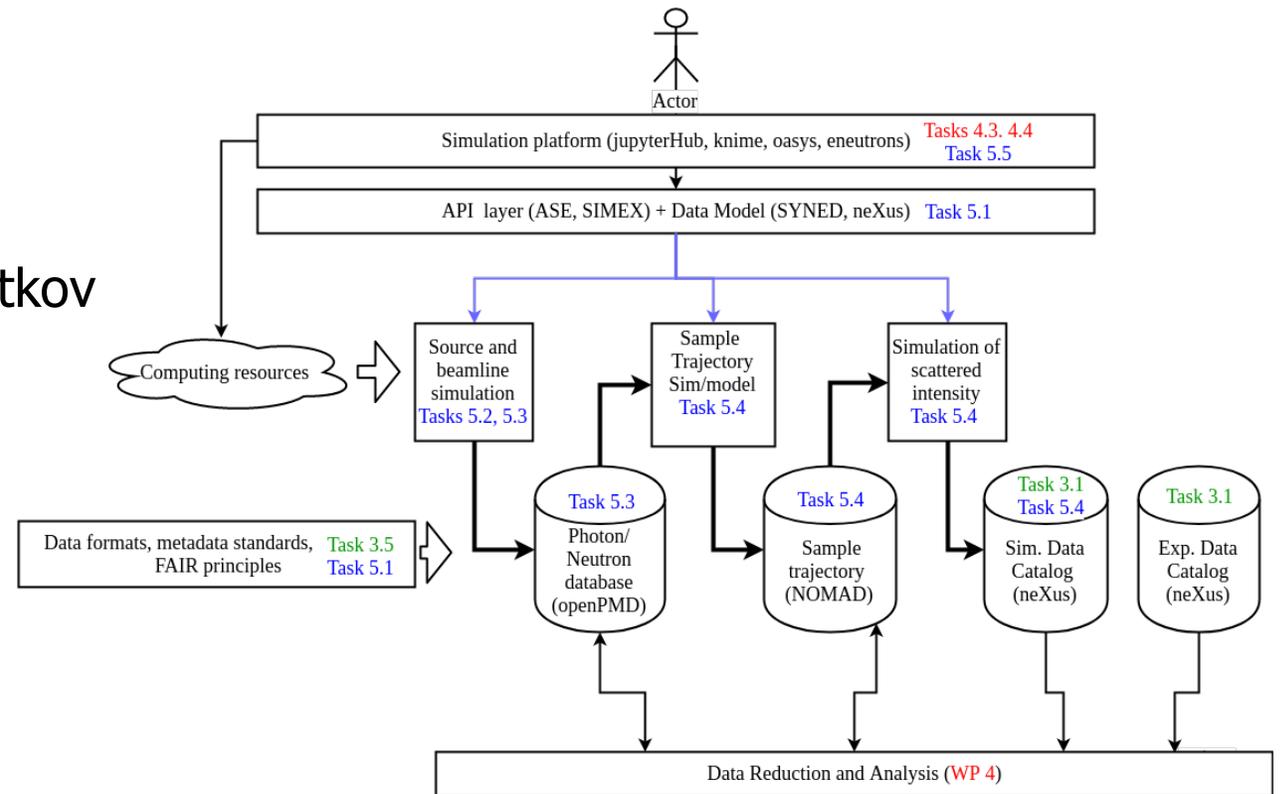


# Eksperimentalni proces – stanje (2)

- Neenoten uporabniški račun
- Orodja za zajem narejena po meri
- Nestandardizirani podatkovni formati in metapodatki
  - Programska orodja za analizo in simulacije
- ▶ **Dolg čas** od poskusa do objave! Veliko poskusov **nikoli** ne obrodi objave!

# Oblačno okolje – PaNOSC (1)

- 8 delovnih sklopov:
  - Administracija
  - Hranjenje in politika hranjenja podatkov
  - Podatkovni katalogi
  - Analiza podatkov
  - Simulacije
  - Integracija v EOSC
  - Trajnost – poslovni model
  - Izobraževanje



Slike: shema PaNOSC aplikacij in storitev okrog simulacij.

# Oblačno okolje – PaNOSC (2)

- Enotna prijavna shema (*user ID*)
- Neposredno shranjevanje zajetih podatkov v oblak
- Podatkovni katalogi in baze
- Delovni proces s podatki v oblaku
  - Računska zmogljivost
  - Sodelovanje
  - Dostopnost

# Oblačno okolje – PaNOSC – Predogled portala

The screenshot displays the PaNOSC portal interface. At the top, there is a search bar and navigation icons. The main content is divided into three columns: Filters, Datasets, and PaNOSC.

**Filters:** A sidebar on the left lists various categories and their counts:

- Data Type:** Simulation (521), Experiment (2560), Derived (423)
- Field:** X-Ray Sources (368), Plasma Physics (49), Ion Acceleration (76), Electron Acceleration (85), Material and Biomolecular Applications (122)
- Technique:** X-ray phase contrast imaging (59), X-ray Diffraction (45), X-ray absorption spectroscopy (85), Coherent Diffractive Imaging (26), Atomic, Molecular and Optical Science (736), Soft X-ray Materials Science (48), Pulsed Radiolysis (29), WW pump-probe (47), X-ray Phase contrast imaging (14), X-ray fluorescence (238), Absorption spectroscopy, WDM@10Hz (45)

**Datasets:** The central area shows three dataset cards:

- Time-resolvent spectroscopy - run 1-52:** Includes a heatmap image, description of RP4-SRS experiments, and metadata (Created: 2019/03/15, Size: 328 MB, Views: 3). Tags include Dataset, X-ray Spectroscopy, Pulsed Radiolysis, and All Tags 8. Action buttons: jupyterlab, launch VM.
- Two-color XUV+NIR femtosecond photoionization of neon in the near-threshold region:** Includes a spectroscopy image, description of RP4-SRS experiments, and metadata (Created: 2019/03/15, Size: 7 GB, Views: 3). Tags include Dataset, X-ray Spectroscopy, XFEL. Action buttons: jupyterlab, launch VM.
- Laser-driven Ion Acceleration from Plastic Target:** Includes a text description of ion acceleration, metadata (Created: 2021/11/03, Size: 214 GB, Views: 7). Tags include Dataset, Ion Acceleration, ELI Beamlines. Action buttons: jupyterlab, launch VM.

**PaNOSC:** The right column features a section titled "The Photon and Neutron Open Science Cloud (PaNOSC)" with a description of the project and a list of objectives:

- Participate in the construction of the EOSC by linking with the e-infrastructures and other ESFRI clusters.
- Make scientific data produced at Europe's major Photon and Neutron sources fully compatible with the FAIR principles.
- Generalise the adoption of open data policies, standard metadata and data stewardship from 15 photon and neutron RIs and physics institutes across Europe
- Provide innovative data services to the users of these facilities locally and the scientific community at large via the European Open Science Cloud (EOSC).
- Increase the impact of RIs by ensuring data from user experiments can be used beyond the initial scope.
- Share the outcomes with the national RIs who are observers in the proposal and the community at large to promote the adoption of FAIR data principles, data stewardship and the EOSC.

A "READ MORE" link is provided at the bottom of this section.

# Oblačno okolje – PaNOSC – Predogled portala

The screenshot displays the PaNOSC cloud portal interface. At the top, there is a navigation bar with a search bar and several active tabs: 'My Home', 'jupyterlab Time-resolvent spectroscopy...', and 'VM Laser-driven Ion Acceleration from...'. The main content area is divided into two columns: 'My Datasets' and 'Dashboard'.

**My Datasets:**

- Time-resolvent spectroscopy - run 1-52:** Created 2019/03/15, Size 328 MB, Views 3. Includes tags: Dataset, X-ray Spectroscopy, Pulsed Radiolysis, All Tags 8. A 'launch VM' button is present.
- Two-color XUV+NIR femtosecond photoionization of neon in the near-threshold region:** Created 2019/03/15, Size 7 GB, Views 3. Includes tags: Dataset, X-ray Spectroscopy, XFEL. A 'launch VM' button is present.
- Laser-driven Ion Acceleration from Plastic Target:** Created 2021/11/03, Size 214 GB, Views 7. Includes tags: Dataset, Ion Acceleration, ELI Beamlines. A 'launch VM' button is present.

**Dashboard:**

- New Messages 1:** A message from Alice Fischer titled 'Analysis of experiment at ESRF'. A 'GO TO MESSAGES' link is provided.
- Resources:**
  - CPU-hours used: 72 / 140. A progress bar shows 72% usage. A 'REQUEST MORE' button is available.
  - GPU-hours used: 15 / 20. A progress bar shows 75% usage. A 'REQUEST MORE' button is available.

# Oblačno okolje – PaNOSC – Predogled portala

My Home / Time-resolv..


jupyterlab Time-resolvent spectros....
VM Laser-driven Ion Acceleration fro...

## Time-resolvent spectroscopy - run 1-52

**Description**

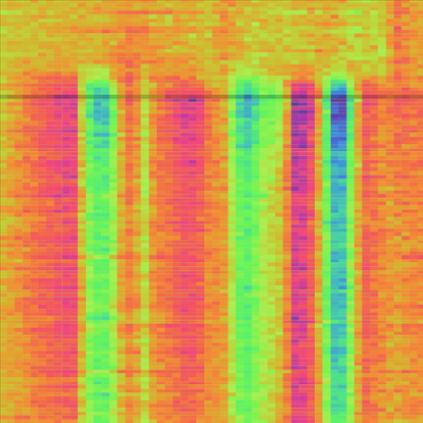
RP4-SRS focuses on time-resolvent spectroscopy experiments in the full range of frequencies from IR to UV. Users can measure samples as varied as solid state crystals, or proteins in their natural environment. Time-resolved spectroscopy is the collection of techniques that are used to examine the dynamic processes of materials and chemicals upon illumination with a pulsed laser. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed diam nonummy nibh euismod tincidunt ut laoreet dolore magna aliquam erat volutpat. Ut wisi enim ad minim veniam, quis nostrud exerci tation ullamcorper suscipit lobortis nisl ut aliquip ex ea commodo consequat.

Title	Time-resolvent spectroscopy - run 1-52
Publisher	ELI Beamlines, Institute of Physics of the Czech Academy of Sciences
Author	Dr. Mark Green
Contact Email	mark.green@eli-beams.eu
Public Access Level	Public
Citation	Mark Green; (2016), Time-resolvent spectroscopy - run 1-52, DOI:110.7283/T5930R7W
Dataset Identifier	<a href="https://doi.org/10.7283/T5930R7W">https://doi.org/10.7283/T5930R7W</a>
Category	Time-resolved spectroscopy
Tags	Dataset, X-ray Spectroscopy, Pulsed Radiolysis, ELI Beamlines

## Dataset

Date Created	2019-03-15 21:58:32
Last Update	2019-05-02 11:23:15
Views	8
Downloads	1
Size	328 MB
Files	26

## Preview Visualization



## Analysis

**Existing Environments**

**Scattering - RUN 5**  
Last Update: 2019-05-02 11:23:15  
Basic jupyterlab OPEN

ADD TO MULTI-DATASET ENVIRONMENT

**jupyterlab Environments**

<p><b>Basic</b></p> <p>1 CPU 16 GB RAM</p> <p style="text-align: center;">CREATE</p>	<p><b>GPU Enabled</b></p> <p>1 CPU 16 GB RAM GPU</p> <p style="text-align: center;">CREATE</p>
<p><b>Cluster</b></p> <p>1 CPU 16 GB RAM Slurm Cluster</p> <p style="text-align: center;">CREATE</p>	<p><b>Custom</b></p> <p>Configure your own Jupyter environment</p> <p style="text-align: center;">SETUP</p>

**VM Remote Desktop Environments**

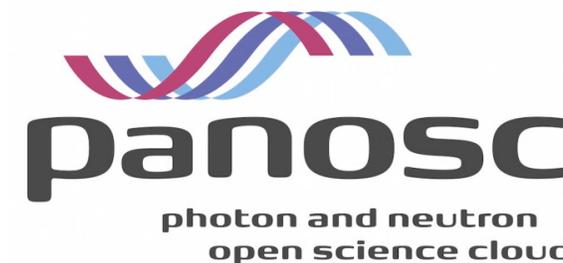
<p><b>Basic</b></p> <p>1 CPU 16 GB RAM</p>	<p><b>GPU Enabled</b></p> <p>1 CPU 16 GB RAM</p>
--	--

# Pogled v prihodnost - Virtualni eksperimenti

- Implementacija **FAIR**
  - Findable: iskalnik po katalogih, metapodatkih in identifikatorju (DOI)
  - Accessible: kratko- in dolgoročna hramba
  - Interoperable: standardni formati podatkov (hdf, Nexus, openPMD) in metapodatkov (ontologija) za uporabo v različnih programih (APIs)
  - Reusable: dovolj metapodatkov za kasnejšo uporabo
- Strojno učenje in umetna inteligenca

## PaNOSC

Fotonski in nevtronski oblak odprte znanosti  
Photon and Neutron Open Science Cloud



Aljoša Hafner – CERIC-ERIC – [aljosa.hafner@ceric-eric.eu](mailto:aljosa.hafner@ceric-eric.eu)