



Introduction and objectives for day 1

**Paul Millar**

WP3 spokesperson

# The background

- Facility policies are shifting towards supporting **open, FAIR data**
  - Allowing secondary/additional use of collected data.
  - Maximising **scientific output** from beam-time.
  - Connection with **FAIR data**: Findable Accessible Interoperable and Reusable.
  - The transition is **on-going**: the work is not finished.
- Machine learning, established as an **important technique** in various fields
  - Often requires **considerable data** for training purposes.
  - Something of a **nascent field** with data from synchrotron and FEL facilities.
  - Curated **reference datasets** are of particular value.



# Why this workshop?

- **Showcase** existing and emerging research areas
  - Learn what other people are doing, or are planning to do
  - Stimulate possible innovation: new applications of existing work.
- Explore **commonalities**
  - Identify possible common areas of work: software, approaches, ...
  - Start to capture common problems: across different ML approaches, across different facilities.
  - Which curated datasets could be used by different communities?
- Identify a possible new **user community**
  - Do you feel you belong to a wider community? If not, would you want to?
  - Is this community something we should support: mailing lists, workshops, ...

# A workshop of two halves

- Day 1
  - Focus is more on **presenting their work**: keynote speakers and community talks.
  - Cataloguing (part of) the research “landscape”, from the perspective of people using data.
- Day 2
  - More focus on **discussion groups**: identifying possible areas for future work and collaboration: the “work” part of a workshop!
  - More details tomorrow from Sophie.

# Objectives for day 1

- Prove a platform to allow you to gain a **broader understanding** of how LEAPS and LENS data is being used for machine learning.
  - Learn of possibly related activity that might be of use in your own research.
- Gain an understanding of some of the **challenges** other people are facing.
  - Perhaps you facing similar issues?
- Provide **background information** for informed discussion during the break-out sessions on day 2.

# Overview of day 1: keynote talks

- “Machine learning in the PaN software landscape and the role of open data” by **Robert McGreevy** (Director of Ada Lovelace Centre)
- “Next-generation materials-data curation and processing methods for machine-learning applications” by **Jacqui Cole** (Head of the Molecular Engineering group at the Cavendish Laboratory, Cambridge)

For details, see [the Indico page](#).

# Overview of day 1: community talks

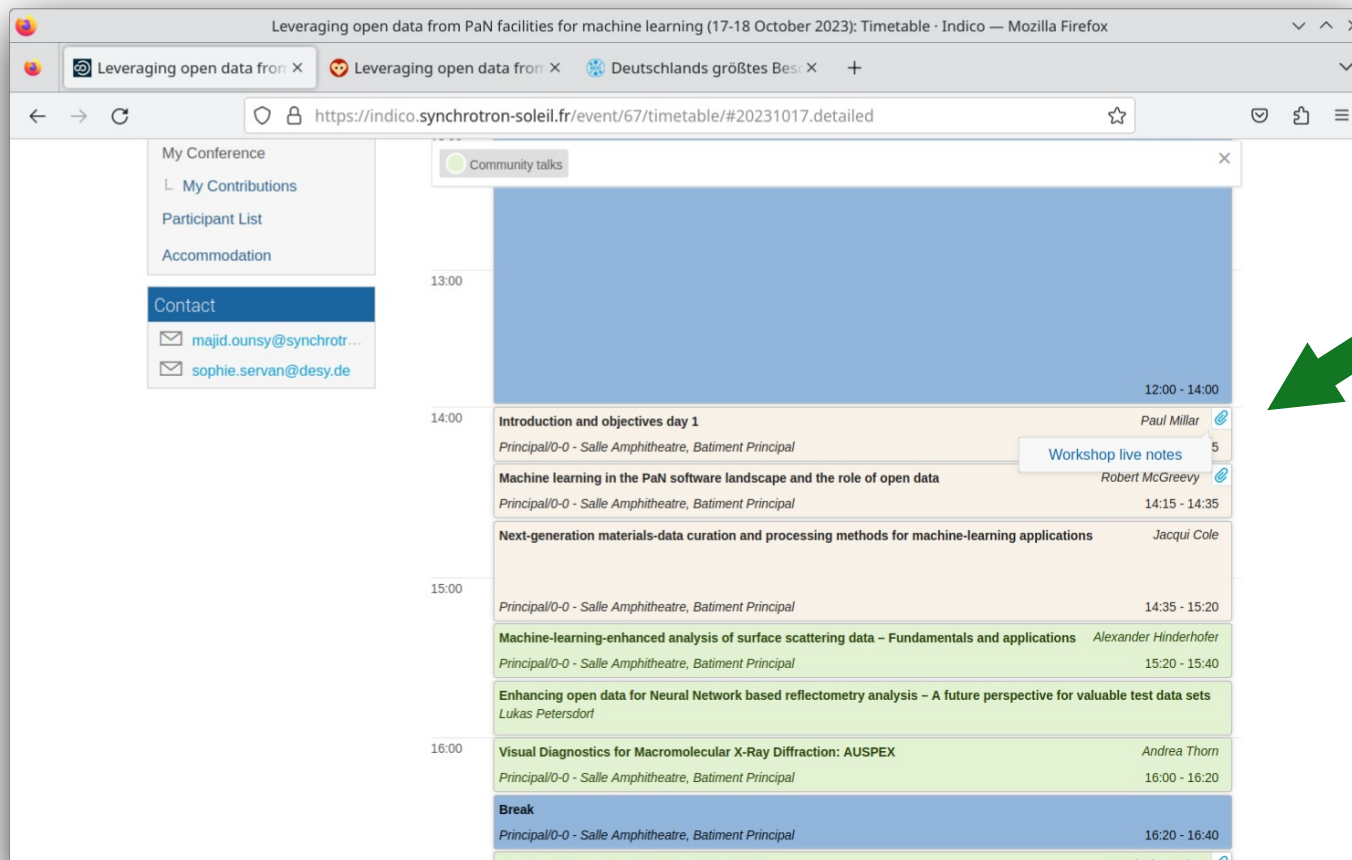
- “Machine-learning-enhanced analysis of surface scattering data – Fundamentals and applications” **Alexander Hinderhofer** (Uni Tübingen).
- “Enhancing open data for Neural Network based reflectometry analysis – A future perspective for valuable test data sets” **Lukas Petersdorf** (Christian-Albrechts-Universität zu Kiel).
- “Visual Diagnostics for Macromolecular X-Ray Diffraction: AUSPEX” **Andrea Thorn** (Universität Hamburg).
- “Microcrystal segmentation for SSX (project)” **Nicolas Soler** (ALBA).
- “Suggestions for human accessibility of photon science dataset” by **Peter Steinbach** (HZDR)

For details, see [the Indico page](#).



# Notes for the workshop

- Live notes are available for everyone to contribute:  
Please feel free to contribute!
- Link on the INDICO page:



The screenshot shows a Mozilla Firefox browser window displaying the Indico event page for "Leveraging open data from PaN facilities for machine learning (17-18 October 2023)". The URL is <https://indico.synchrotron-soleil.fr/event/67/timetable/#20231017.detailed>. The page features a left-hand navigation menu with options like "My Conference", "My Contributions", "Participant List", "Accommodation", and "Contact". The main content is a timetable starting at 13:00. A "Community talks" pop-up is visible at the top. A green arrow points to the "Workshop live notes" link in the 14:00-14:35 slot.

Time	Event Title	Speaker	Location	Duration
13:00				12:00 - 14:00
14:00	Introduction and objectives day 1	Paul Millar	Principal/Q-0 - Salle Amphitheatre, Batiment Principal	14:00 - 14:35
	Machine learning in the PaN software landscape and the role of open data	Robert McGreevy	Principal/Q-0 - Salle Amphitheatre, Batiment Principal	14:15 - 14:35
	Next-generation materials-data curation and processing methods for machine-learning applications	Jacqui Cole	Principal/Q-0 - Salle Amphitheatre, Batiment Principal	14:35 - 15:20
15:00	Machine-learning-enhanced analysis of surface scattering data – Fundamentals and applications	Alexander Hinderhofer	Principal/Q-0 - Salle Amphitheatre, Batiment Principal	15:20 - 15:40
	Enhancing open data for Neural Network based reflectometry analysis – A future perspective for valuable test data sets	Lukas Petersdorf	Principal/Q-0 - Salle Amphitheatre, Batiment Principal	16:00 - 16:20
16:00	Visual Diagnostics for Macromolecular X-Ray Diffraction: AUSPEX	Andrea Thorn	Principal/Q-0 - Salle Amphitheatre, Batiment Principal	16:00 - 16:20
	Break		Principal/Q-0 - Salle Amphitheatre, Batiment Principal	16:20 - 16:40



# Thanks go to...

- Everyone on the programme committee:  
**Vincent Favre-Nicolin**, ESRF (LEAPS), **Andy Götz**, ESRF (LEAPS), **Markus Janousch**, PSI (LEAPS, LENS), **Zdenek Matej**, MAX IV (LEAPS), **Paul Millar**, DESY (LEAPS), **Paolo Mutti**, ILL (LENS), **Shervin Nourbakhsh**, ILL (LENS), **Joaquín Otón**, ALBA (LEAPS), **Majid Ounsy**, SOLEIL (LEAPS), **Wojciech Potrzebowski**, ESS (LENS), **Sophie Servan**, DESY (LEAPS), **Nicolas Soler**, ALBA (LEAPS), **Peter Steinbach**, HZDR (LEAPS), **Jeyan Thiyagalingam**, STFC (LENS)
- The coordinator for this workshop: Sophie Servan.
- Majid and the other local organisers for providing the venue, the Indico page, the hybrid/video-conference connection.

For details, see [the Indico page](#).

**Thanks  
and  
enjoy the workshop!**



**LEAPS**

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