

PAUL SCHERRER INSTITUT



Markus Janousch:: Group Leader :: Paul Scherrer Institut

# Overview of the group “Data Processing Development and Consulting”

AWI Department Meeting (7902); August 17, 2022

## Bi-Monthly Meeting 7902 Host ✎

📅 Wednesday 17 Aug 2022, 09:00 → 10:30 Europe/Zurich

📍 WHGA/001 (Auditorium) (PSI)

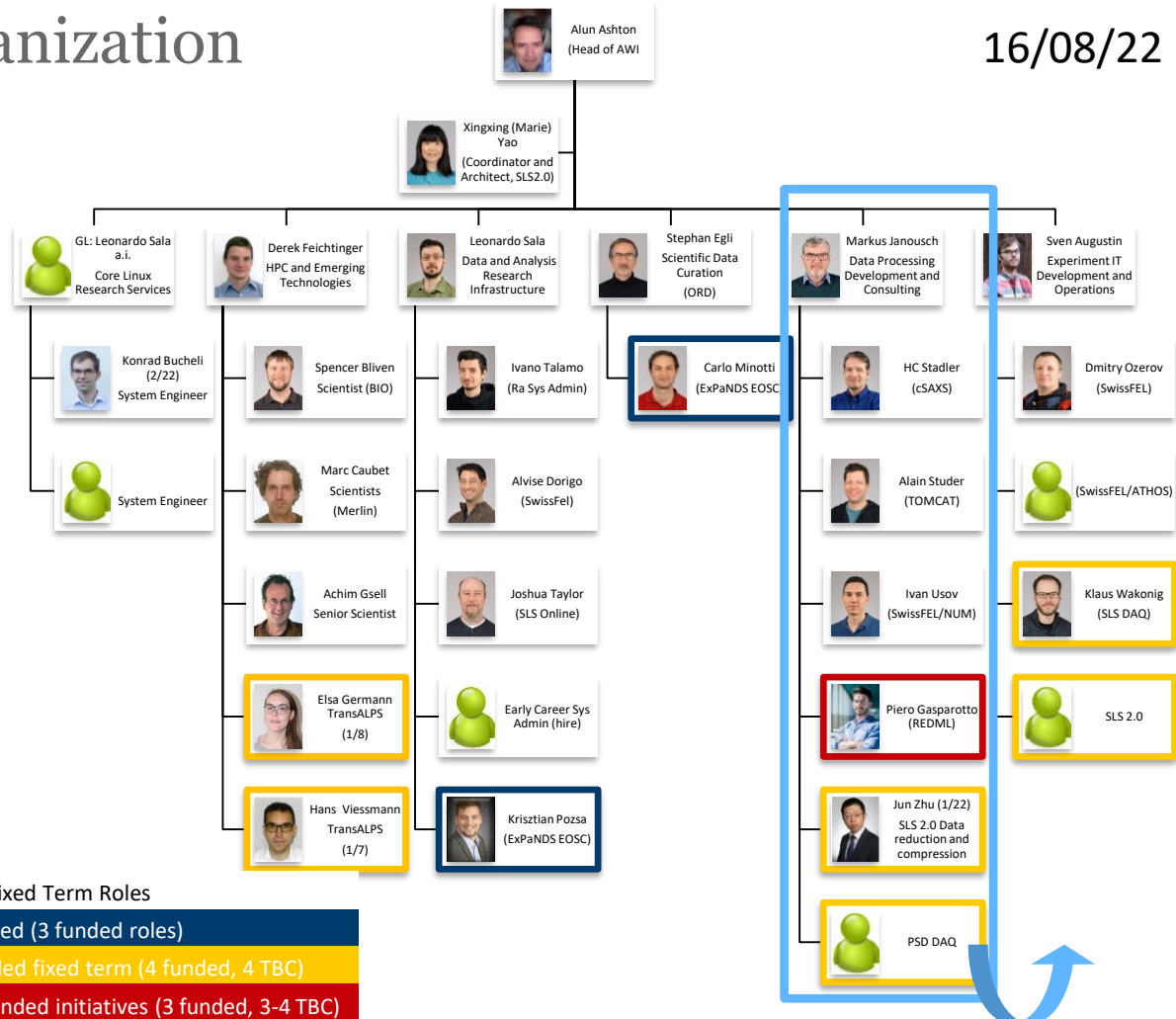
<b>09:00</b>	→ 09:15 <b>AWI General Update</b> Speaker: Alun Ashton (PSI - Paul Scherrer Institut)	🕒 15m ✎
<b>09:15</b>	→ 10:20 <b>7902 Presentations</b> Convener: Markus Janousch (PSI - Paul Scherrer Institut)	✎
<b>09:15</b>	<b>Group Overview</b> Speaker: Markus Janousch (PSI - Paul Scherrer Institut)	🕒 10m ✎
<b>09:25</b>	<b>pyzebra</b> Speaker: Ivan Usov (PSI - Paul Scherrer Institut)	🕒 10m ✎
<b>09:35</b>	<b>The REDML Project</b> Speaker: Piero Gasparotto	🕒 15m ✎
<b>09:50</b>	<b>Protein Crystallography – Spot Finding and Indexing for fast Experiment Feedback</b> Speaker: Hans-Christian Stadler KleeB (PSI - Paul Scherrer Institut)	🕒 10m 📄 Minutes ✎
<b>10:00</b>	<b>TOMCAT data reduction and processing pipelines development</b> Speaker: Jun Zhu (PSI - Paul Scherrer Institut)	🕒 10m ✎
<b>10:10</b>	<b>How Beamline Scientists interact with Reconstruction Software</b> Speaker: Alain Studer (PSI - Paul Scherrer Institut)	🕒 10m ✎
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# Overview

- Organisation
- Main topics and activities
- LEAPS-INNOV

## Data Processing Development and Consulting (7902)



# Topics and Main Activities

- Our central mission is to provide scientists and user communities with expertise in data reduction and processing algorithms in order to meet their experimental and data analysis needs, i.e., to ease the process of answering data-driven particular scientific questions.
- Grants
  - AI4SI, not successful
  - SDSC --> Jun
  - PSI Research grant (Goran Lovric, PI)



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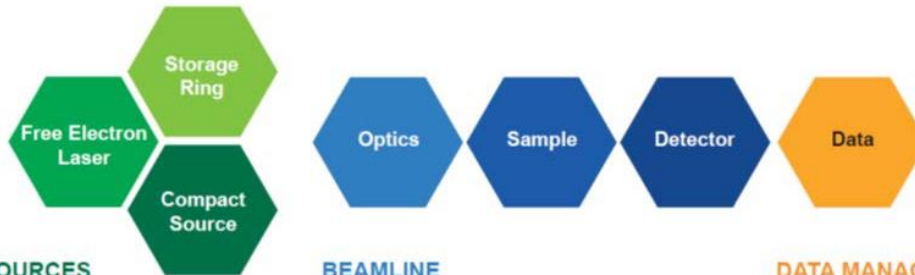
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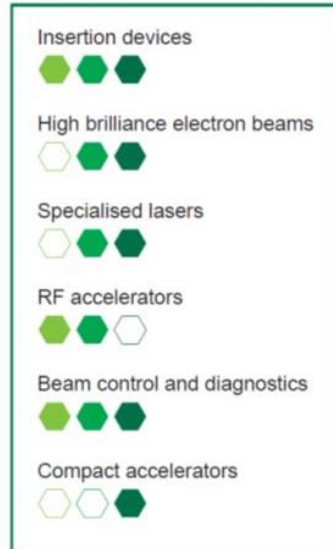
on Radiation and Free  
and constructively ensure  
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# LEAPS Roadmap



## SOURCES



## BEAMLINE

- Mirrors and reflective optics
  - Nanopositioning and optomechanics
  - Diffraction gratings
  - Simulation and modelling
  - At-wavelength metrology and test facilities
  - Crystal monochromators and analysers
  - Multilayer optics
  - Refractive optics
  - Fresnel zone plates
- Higher spatial and time resolution
  - Complex environments
  - Sample through-put and delivery
  - Extreme conditions
- Common technology toolbox
  - High-speed spectroscopy detector
  - Ultra-high frame rate imager
  - High spatial resolution imager
  - Energy-resolving imager
  - XUV to tender X-ray imager

## DATA MANAGEMENT

- Data policy for open science
- High speed data acquisition
- Data analysis and reduction
- Data catalogue
- Cloud services



- Comprised of the 16 LEAPS members plus 6 research and industry laboratories (ENEA, KTI, STFC, nob, RAITH, XRnanotech)
- Funded by the European Horizon 2020 programme with 10 M€.
- Lead by DESY (Elke Plönjes)
- Submitted May 2020, started a year later.
- Organized in 7 work packages



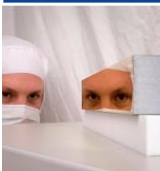
# LEAPS-INNOV Work Packages



**WP 1**  
Project Management  
and Dissemination (DESY)



**WP 2**  
Development of High Throughput X-  
ray Spectroscopy Detector System  
(DIAMOND, SOLEIL)



**WP 3**  
SuperFlat  
(ESRF, SOLEIL)



**WP 4**  
NeXtgrating  
(PSI, HZB)



**WP 5**  
New positioning and scanning  
systems for speed and accuracy (HZB, DIAMOND)



**WP 6**  
LIDs  
(SOLEIL, PSI, ELETTRA)



**WP 7**  
Data Reduction and Compression  
(MAXIV, DESY)



**WP 8**  
Industrial Innovation through Light Source  
(ESRF, DIAMOND, ALBA-CELLS)



**WP 9**  
Innovation by Co-creation towards  
Global Challenges (MAXIV)

## Data Reduction and Compression

- With the ever increasing detector size and frame rates we see a dramatic grow in data rates and volume.
- WP 7 addresses this issue through 4 tasks
- Work package leader Darren Spruce (MAXIV) and David Pennicard (DESY)

1. Collaboration platform for data reduction and compression (MAXIV, DESY)
  - D7.1 Evaluation report on data rates & volumes and assessment of future needs of LEAPS facilities
2. Assessment of future needs and development of metrics for data compression and reduction (Alba, ESRF)
  - D7.2 Report on metrics for data reduction and compression
3. Evaluate and adopt new strategies for data reduction and compression (HZDR)
  - D7.3 Report results on promising data reduction pipelines on datasets provided by LEAPS facilities and release as open-source to the community
4. **Research infrastructure integration with detector suppliers on data (PSI)**
  - **D7.4 Best practices and guidelines for applying data reduction and compression at LEAPS facilities**

- Bring the research laboratories and industry together
- Start a knowledge exchange between research laboratories and industry
- Create a dialogue and the necessary communication flow of technical specifications transmitted in both directions between detector suppliers and participants of WP7
- Define and establish best practices, guidelines, and interfaces
- Propagate them through new developments and products in the community

**Many thanks to my  
colleagues at AWI and  
in particular to my  
group members!**



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