

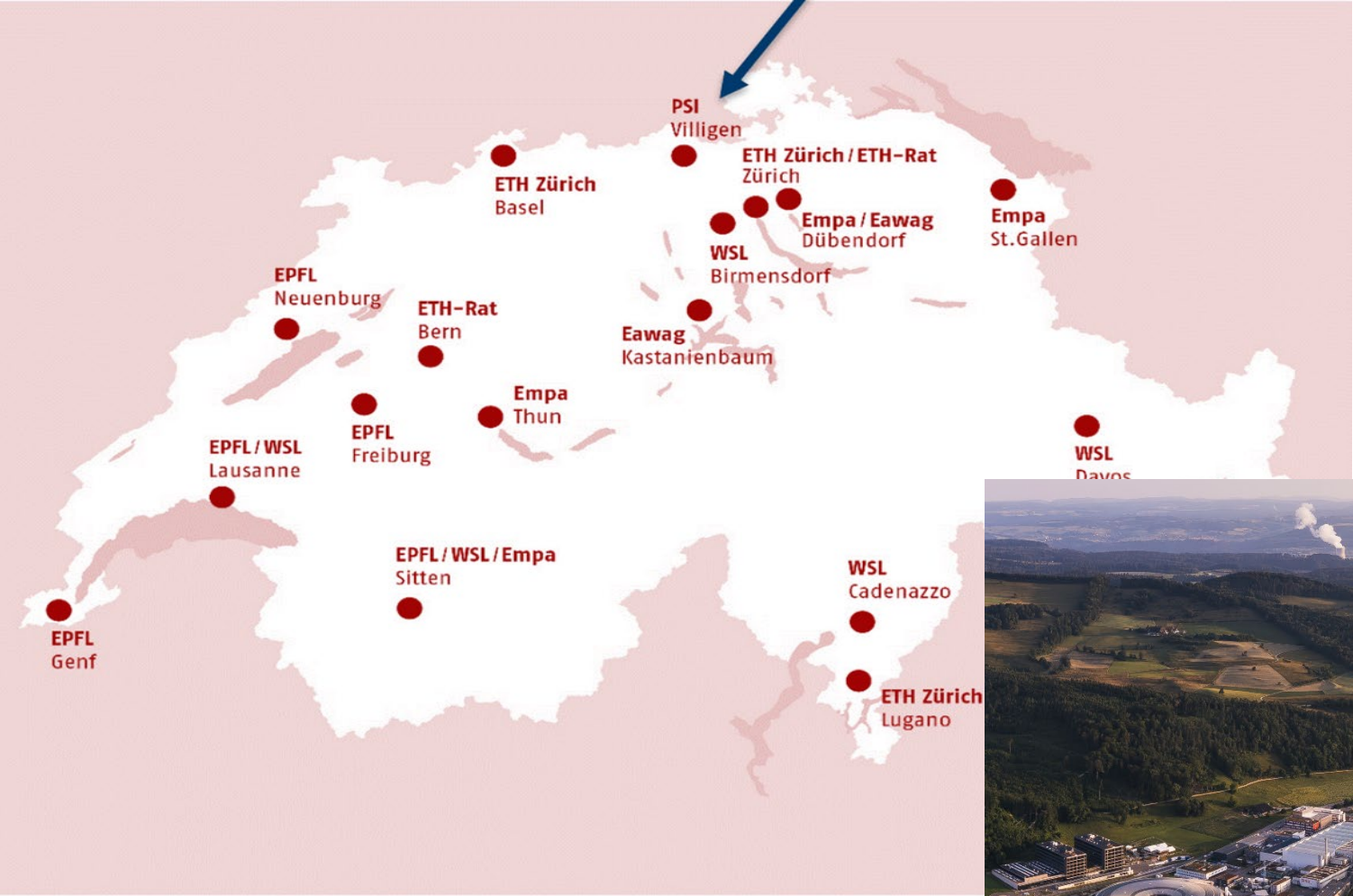
PSI

Center for Scientific Computing,
Theory and Data

General overview

Alun Ashton
17 March 2026

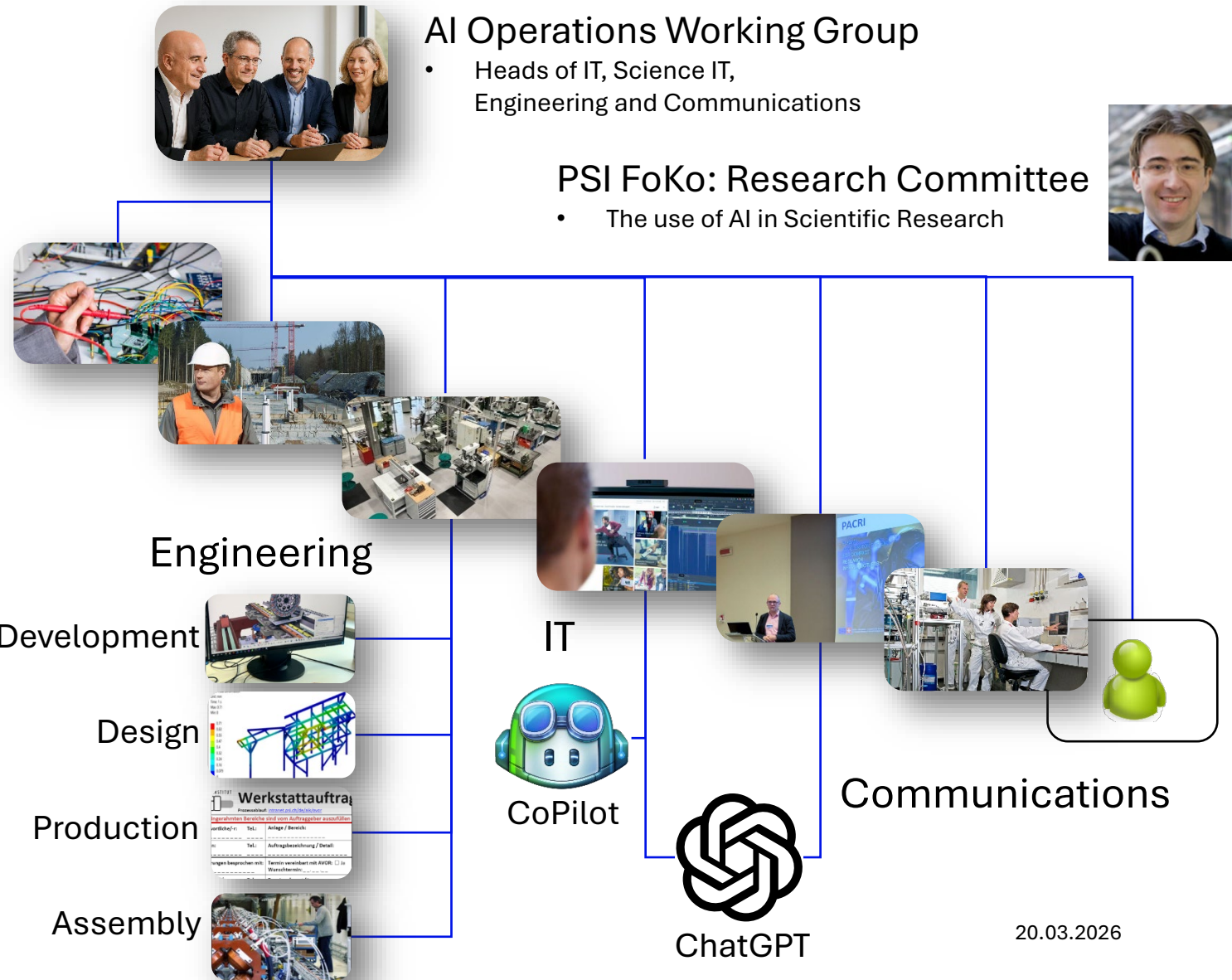
PSI and the ETH-Domain



Center	Primary Focus & Research Areas
Photon Science	Studies atomic-level structures using the Swiss Light Source (SLS) and SwissFEL
Neutron & Muon Sciences	Investigates matter and material properties using the Swiss Spallation Neutron Source SINQ, the Ultra-cold Neutron Source UCN, the Swiss Muon Source S μ S and the facilities for particle physics CHRISP
Energy & Environment	Focuses on sustainable energy, atmospheric chemistry, and climate research
Nuclear Engineering & Sciences	Researches reactor safety, waste management, and nuclear materials.
Life Sciences	Conducts research in structural biology, radiopharmacy, and bioimaging.
Scientific Computing Theory and Data	Dedicated to high-performance computing, computational materials modelling, AI, and data-driven science.
Accelerator Science & Engineering	Operates and develops the institute's large-scale particle accelerator facilities
Corporate Services	Manages IT, finance, communications, infrastructure, and radiation safety.

AI oversight and organisation in PSI operations.

- Established AI Operations Working Group
 - Governance & Compliance
 - Infrastructure & Tooling
 - Adoption & Education
 - Research & Innovation
 - Information & Communication
- First domain pilot projects in engineering, software and communications
- New role for AI Adoption and Governance Coordinator
- Investigations to local hosted LLM as well as commercial solutions



PSI Center for Scientific Computing, Theory and Data

Organisation:



PSI Center for Computing Scientific, Theory and Data

Prof. Dr. Christian Rüegg a.i.
(University of Geneva, ETHZ, EPFL)



Stv. Center-Leitung
Dr. T. Strässle a.i.

Center-Vertretung
Technologietransfer
J. Millard

Center-Personalleitung
S. Mier und S. Minniti

Center-Finanzleitung
M. Engroñat

Simulation and Modelling

Prof. Dr. Laura Grigori (EPFL)

Website →



Theoretical and Computational Physics

Prof. Dr. Andreas Läuchli (EPFL)

Website →



Materials Simulations

Prof. Dr. Nicola Marzari (EPFL)

Website →



Science IT Infrastructure, and Services

Dr. Alun Ashton

Website →



Science IT Infrastructure and Services (AWI)



HIGH PERFORMANCE COMPUTING
Providing advanced computing resources for research



DATA LIFECYCLE SOLUTIONS
Managing and preserving research data



EXPERIMENT SOFTWARE SUPPORT
Developing and maintaining software for data analysis



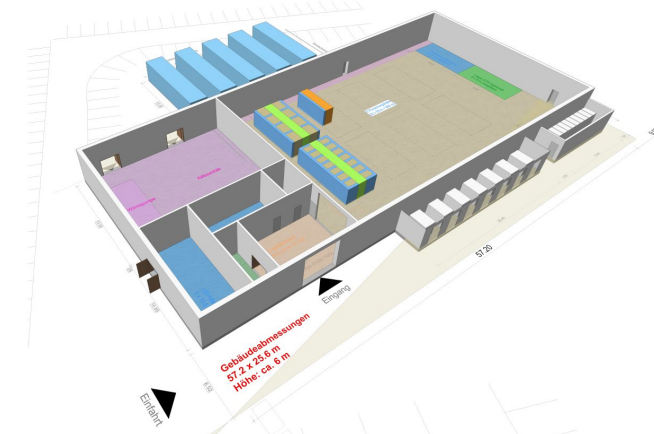
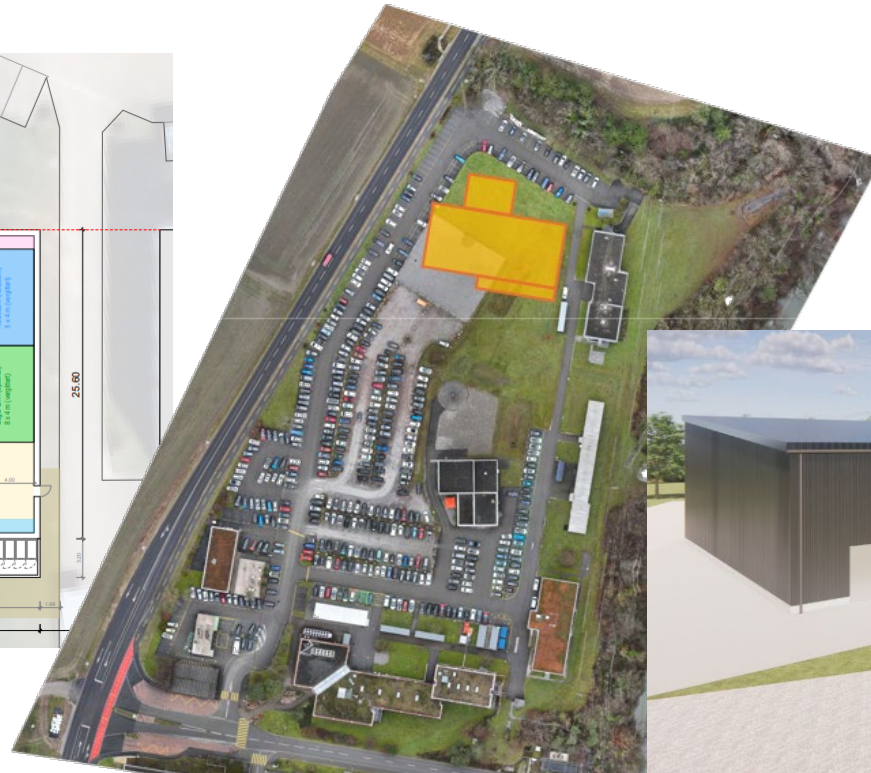
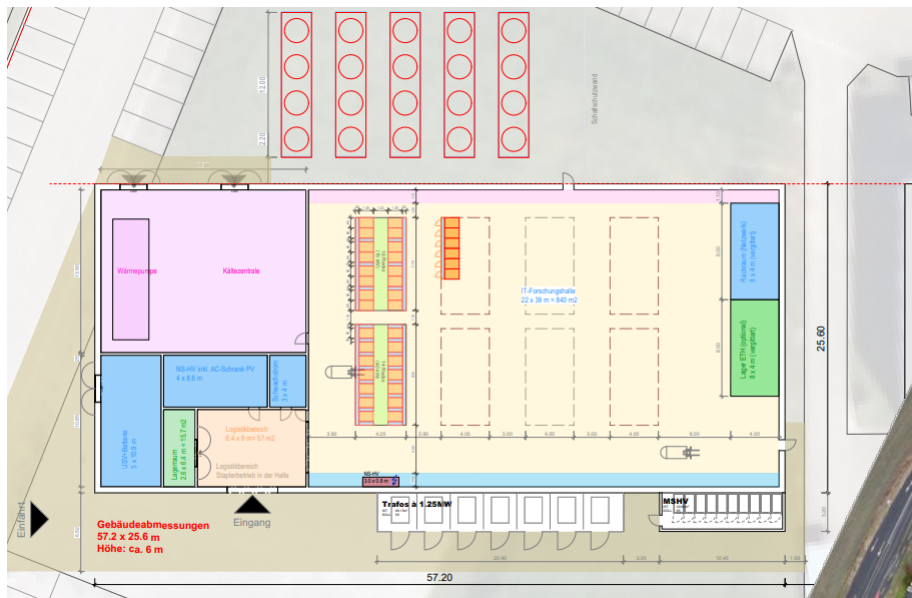
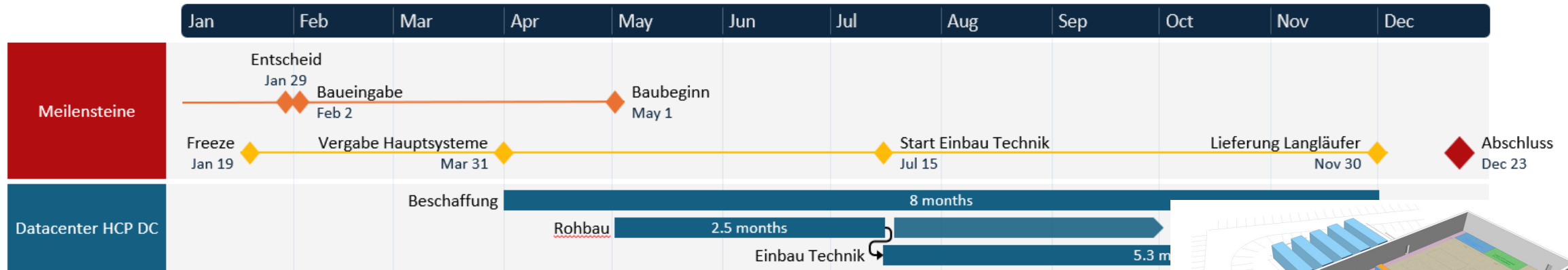
INFRASTRUCTURE SERVICES
Supporting high-throughput scientific experiments



Joint HPC Datacenter ETHZ-PSI



Updated Project Plan and Layout: 1MW 2027, 4MW 2032, 7MW total



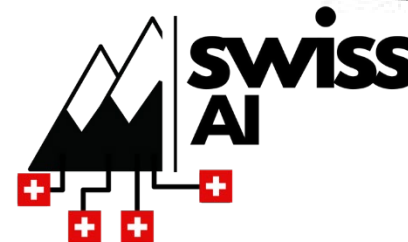
Key ETH Domain Resources



In 2017, a national Data Science initiative from the ETH Board resulted in the creation of a unique joint venture: the Swiss Data Science Center, bringing together the ETH Zürich, the EPFL, and the PSI . The Center’s mission is to accelerate the use of data science and machine learning techniques within academic disciplines of the ETH Domain, the Swiss academic community at large, the public institutions and the industrial sector.

CSCS develops and operates cutting-edge high-performance computing systems as an essential service facility for Swiss researchers. These computing systems are used by scientists for a diverse range of purposes – from high-resolution simulations to the analysis of complex data.

- Center for Scientific Computing, Theory and Data (CSD)
 - Laboratory for Simulation and Modelling (LSM)
 - SDSC Hub at PSI,
 - Dr. Benjamin Bejar Haro



Data Science for Large Scale Infrastructures

Swiss Data Science Center at PSI

Benjamín Béjar Haro
SDSC Hub at PSI
January 27, 2026



Supporting the entire **data science journey** — from collection and management to machine learning, AI, and industrialization — serving **academic labs, hospitals, industry** and **public sector** stakeholders, including cantonal and federal administrations.

From a **Strategic Focus Area** of the ETH Domain to a **National Research Infrastructure** in 2025

Multidisciplinary, agile and impact-driven team of **110+ professionals** across three locations

Applied Research, Innovation, Engineering & Services, Initial and Continuing Education

Health & Biomedical, Climate & Environment, Energy & Sustainability, Large-scale scientific infrastructures

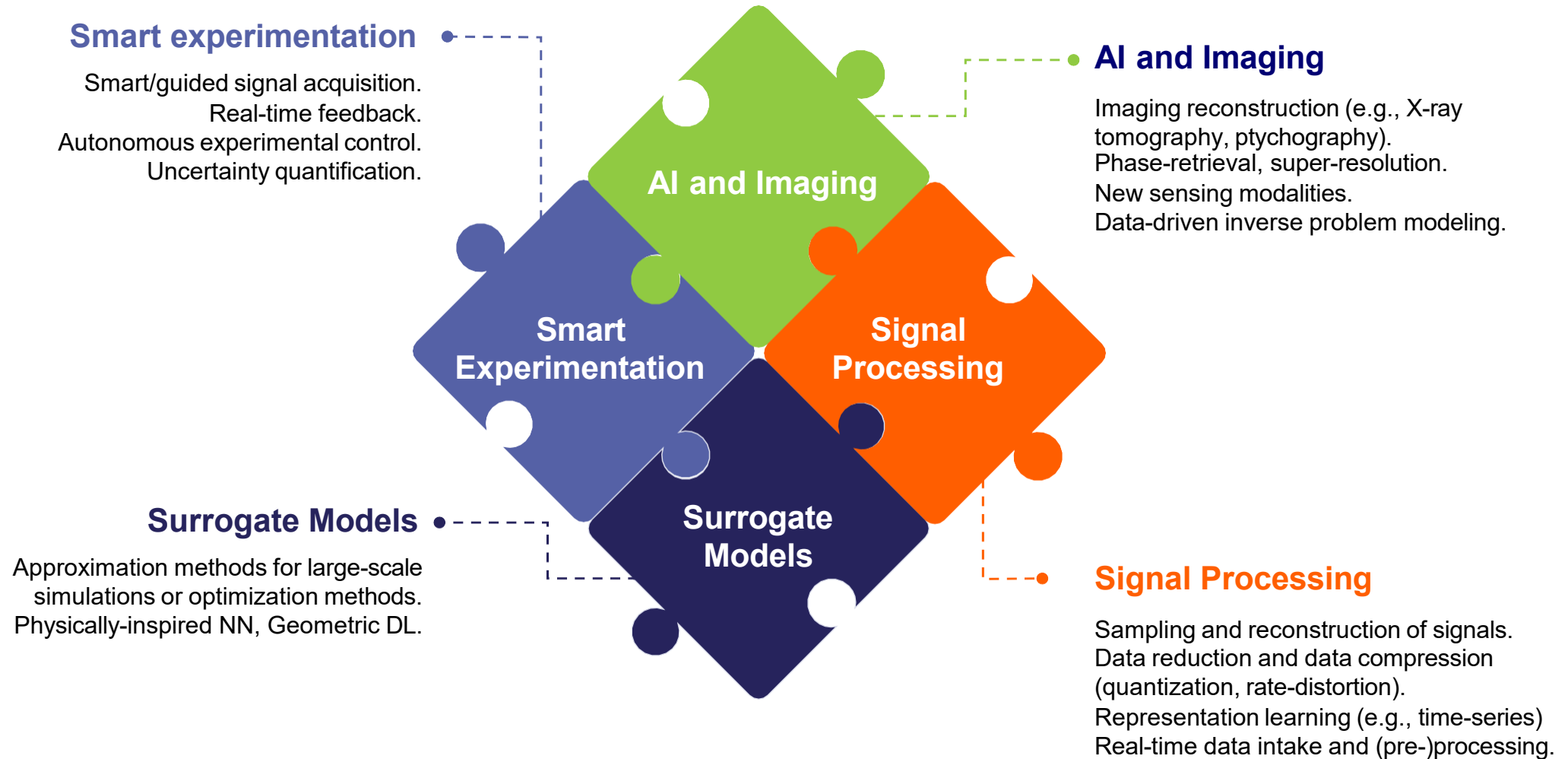


Tailored AI/ML methods for improved operations, exploitation, and data intake of large-scale facilities and specialized instrumentation.



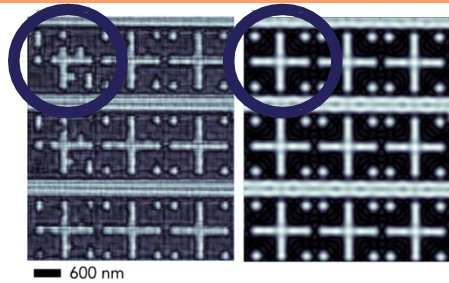
Large Scale Infrastructures at PSI

- **SLS**
- **SwissFEL**
- **SINQ**
- **S μ S**
- **CHRISP**
- **HIPA**
- **ESI**
- **PANDA**



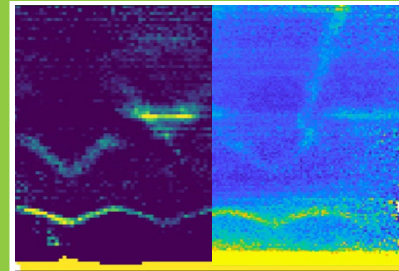
LAMP – Lensless Imaging of Photomasks

- **Ptychographic reconstruction** method with sparse priors.
- **Improved MSE** reconstruction with **fewer measurements**.
- Fully data-driven reconstruction approach using **generative AI** models.
- Accelerated inference.



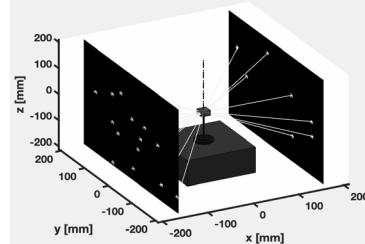
DS4MS – Segmentation of Neutron Scattering Data

- Inverse problem formulation for **background removal** exploiting radial symmetry.
- **Accelerate** tedious manual process of **foreground/background segmentation**.
- Easy to compute metrics to **quantify experiment quality**.



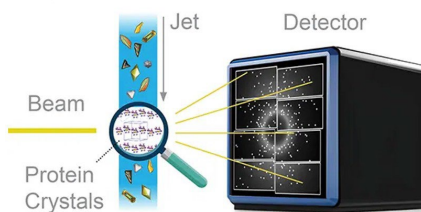
Laue3D – Indexer for Neutron Scattering

- **Polycrystalline indexing** of multi-grain crystals (metal alloys) from neutron scattering data using an inverse problem formulation with **optimal transport**.
- **Scaling to thousands of grains**, speed-up based on parallel implementation.



REDML – Reducing SX Data from SLS

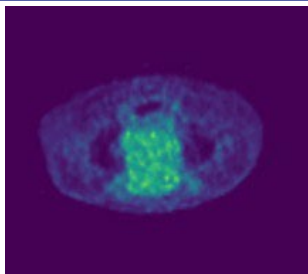
Experiment



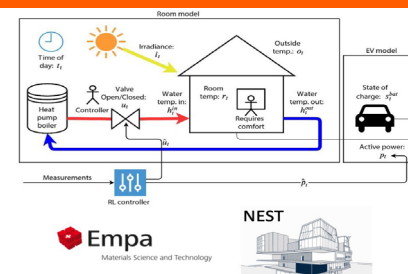
- Developed **very fast and robust indexer** for Serial Crystallography (SX)
- **Operational at SLS and SwissFEL**
- **Tested** in various other facilities in **Europe** (DESY, MAX-IV, ALBA)
- Available in software suites in the community: **CrystFEL** and **DIALS**

DUPLET – Dual tracer PET imaging

- Developed a DL-based method to **predict ratio between two radiotracers**.
- Enabling separation between F-18 and Ga-68 sources, **demonstrated in real clinical scenarios**.
- **Uncertainty quantification** for the tracer ratio prediction, valuable in decision-making for clinicians
- Follow-up submission to build a **dedicated scanner**.



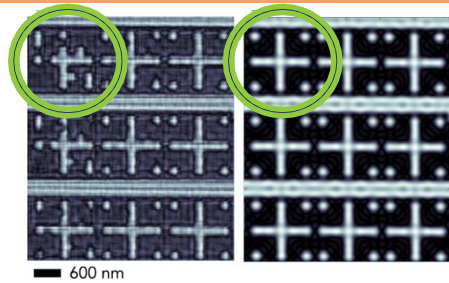
Euthermo – Temperature Control Policy in Buildings



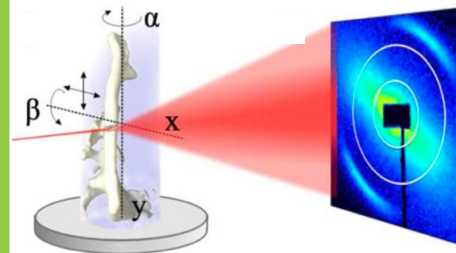
- Data-driven **modeling of building energy consumption** (NEST building at EMPA)
- Modular approach to facilitate **transferability** from one room to another with limited data.

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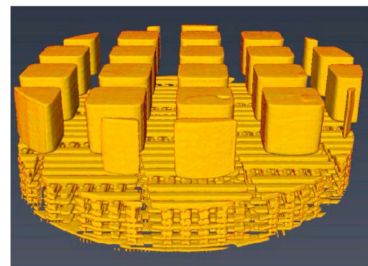
SmartTT – Smart Sampling X-ray Tensor Tomography



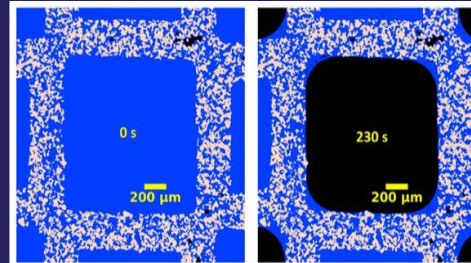
- Inverse problem formulation for **online reconstruction** of 3D scattering density.
- **Reduce acquisition time** by choosing where to measure using data-driven priors
- **Uncertainty quantification**.

CHIP – ML-assisted ptychographic nanotomography

- **Sparse-view** tomographic reconstruction – dose reduction
- **Improved** reconstruction quality
- **Smart scanning** – choose most relevant projections as data is being acquired.



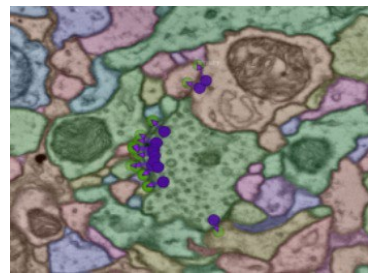
SDATE – Smart Data Acquisition for Tomoscopy



- **Online data reduction** for Tomoscopy experiments
- **Data compression** for reduced storage
- **Data-driven optimization** of data compression parameters

ALBUM – Large-scale Ultrastructural Brain Mapping

- **Neural tissue reconstruction** from **milled volumes** using Transmission Electron Microscopy
- Regularized **inverse problem** with priors
- **Segmentation** of large data volumes of brain tissue with high spatial resolution



MAGNIFY – Energy envelope quantification in buildings



- **Scaling-up energy envelop quantification** for residential buildings incorporating sources of uncertainty
- **Learn representations** for finding similarity between buildings for flexibility envelope approximation

 Large-scale scientific infrastructures

Smart experiments

Smart/guided acquisition.
Real-time feedback.
Experimental design.
Uncertainty quantification.

AI for Imaging

Imaging and image reconstruction (X-ray tomography, ptychography, electron microscopy).
Data-driven inverse problem solving.

Signal Processing

Real-time data intake and pre-processing.
Data reduction and data compression.
Representation learning for time-series.
Sampling and reconstruction of signals.

Surrogate Models

Approximation methods for large-scale simulations or optimization methods.
Physically-inspired NN, Geometric DL.

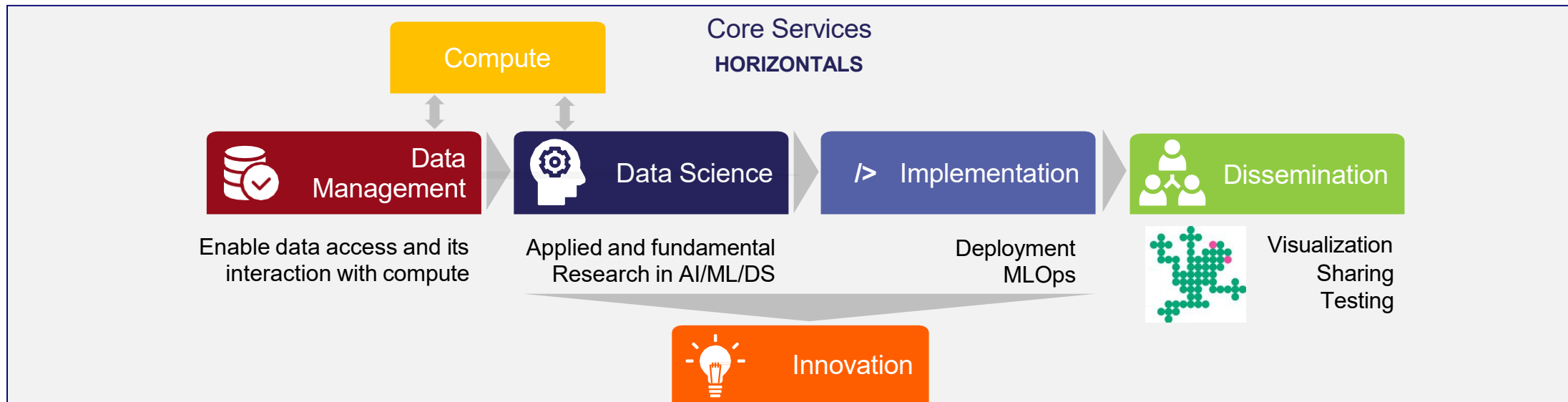
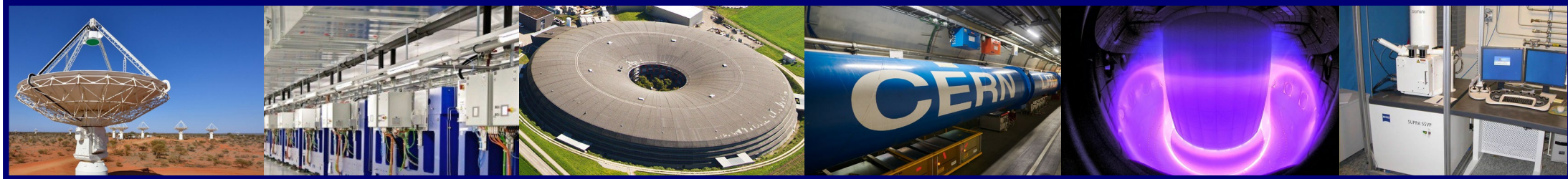
Partners:

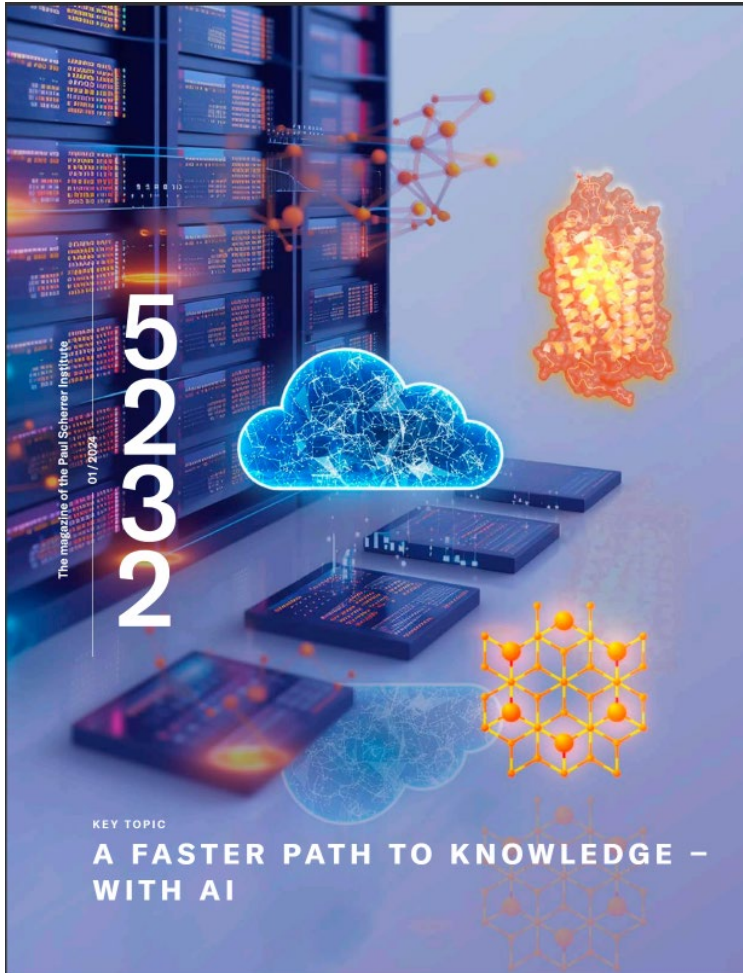
PSI
WSL
Empa
Eawag

CSCS
CERN
ESS
ESRF
SKA

Dedicated Partner office:

Villigen
(PSI)





5232 edition, key topic: a faster path to knowledge – with AI

<https://www.psi.ch/en/news/5232-the-magazine-of-psi>

The PSI Draft Development Plan
2025-2028 status: June 2024

- references to AI/Artificial Intelligence across all themes and centres.



Strategic Planning

Development plan for 2025 – 2028



Thanks to Benjamin and Markus