PAUL SCHERRER INSTITUT

PSI

Leonardo Sala :: DARI Group Leader :: Paul Scherrer Institute

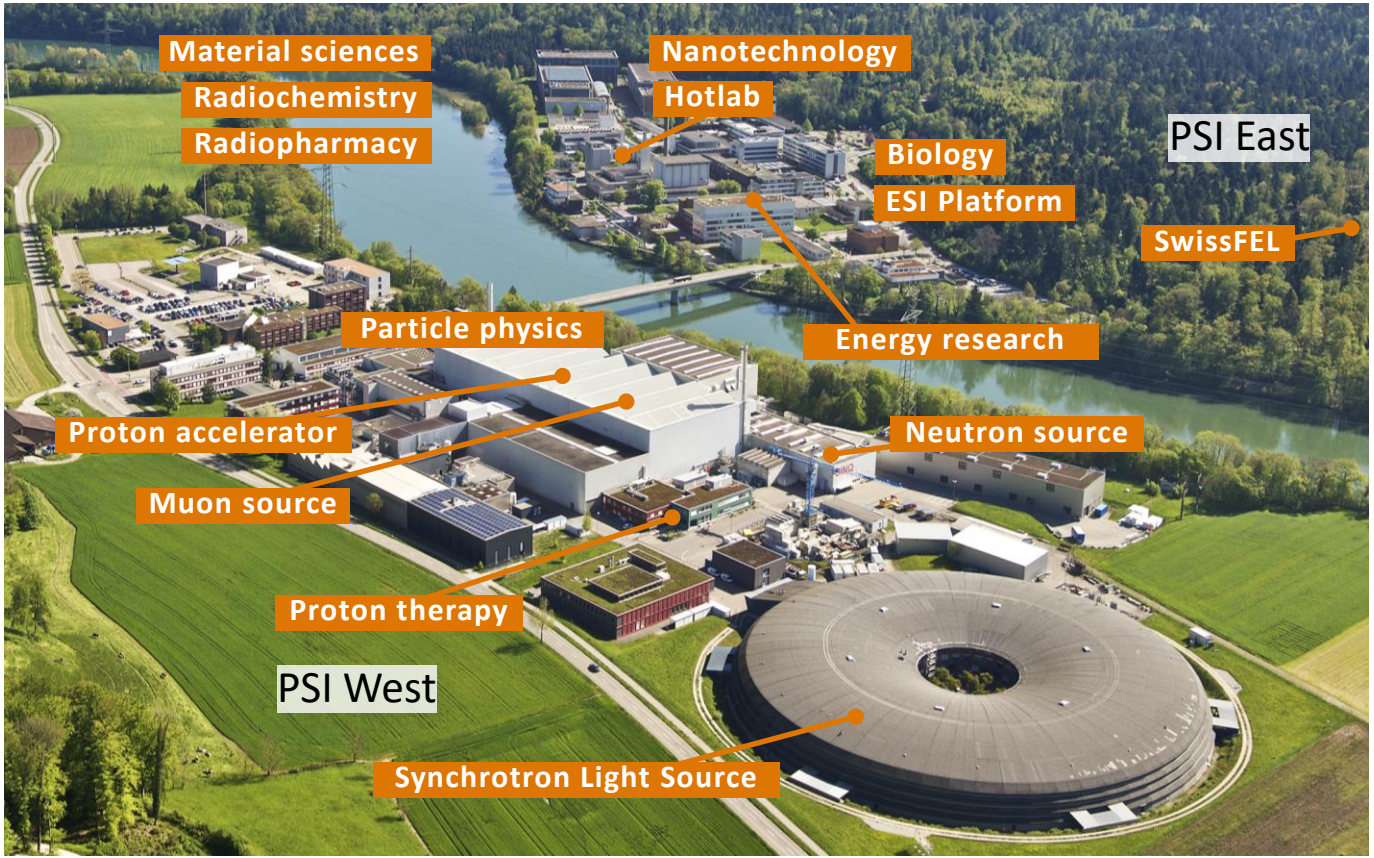
Overview of Data Analysis Infrastructure

FHNW visit – 2024-05-17

Outline

- PSI / AWI overview
- Overview of scope: DARI
- Hardware and architecture
- Services and user support
- Future directions

PSI: Overview



PSI at a glance

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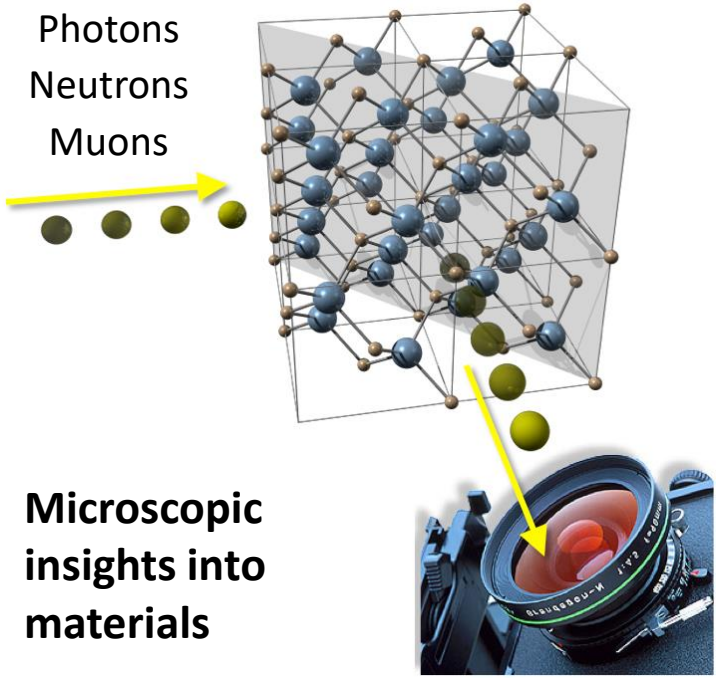
Large Research Facilities at PSI

Research at large facilities

Photons
Neutrons
Muons



Microscopic insights into materials

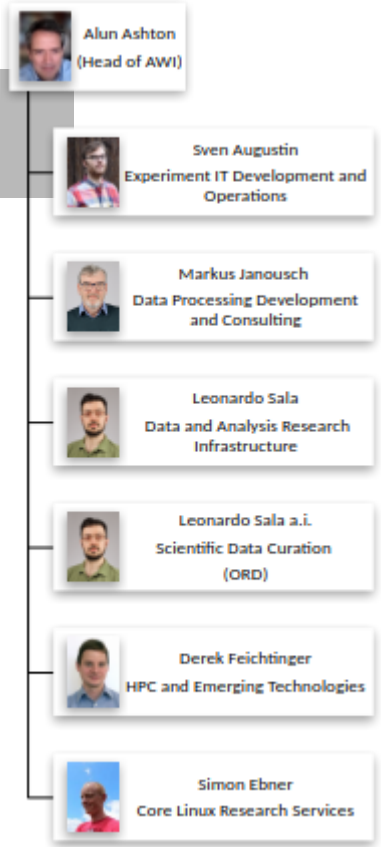
Synchrotron Light Source SLS

Spallation Neutron Source SINQ

Muon Source SµS

Free Electron Laser SwissFEL

Scope: Science IT Infrastructure and Services



- Data Chain (in collaboration with PSD, GFA etc)
  - Deliver and support a range of software and hardware services for the full experimental lifecycle of data and metadata
- Software (based on research demands and prioritization)
  - Deliver and support a range of experiment software or workflows for data compression, reduction and processing.
- Storage (online for SCD, PSD, NES, (NUM) and BIO, archive for PSI)
  - Deliver and support appropriate storage solutions for the experiment/research lifecycle stage
- HPC (for SCD, PSD, NES, (NUM) and BIO, expandable for PSI research)
  - Deliver and support HPC for the experiment/research lifecycle stage
- Coordinator and IT Architect for Controls and Science IT activities for SLS 2.0
  - Communication/Coordination/Community

Scope: DARI

- Data Analysis and Research Infrastructure (DARI) group supports PSI research needs by providing IT infrastructure and services for:
  - Data acquisition
  - Data analysis
  - Interface with Data Management tools
  - Deployment of special services

- Currently our main customer is Photon Science (Synchrotron, Free Electron Laser), with smaller communities from Bio and Nuclear sciences

Architectural overview

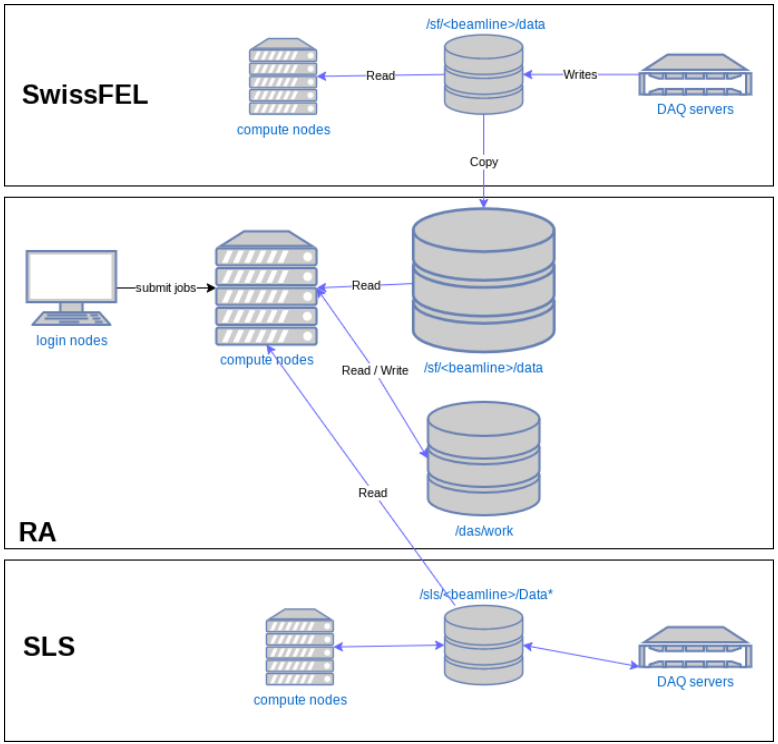
We currently maintain two main clusters:

- SwissFEL online and near-time
- General data analysis cluster (Ra)
- SLS dedicated cluster decommissioned during dark-time

The Ra data analysis cluster has 11 PB, ~3600 cores, 16 GPUs

SwissFEL (and SLS before shutdown) have dedicated online compute nodes.

SwissFEL only have a dedicated short-term buffer storage



Technologies

Storage:

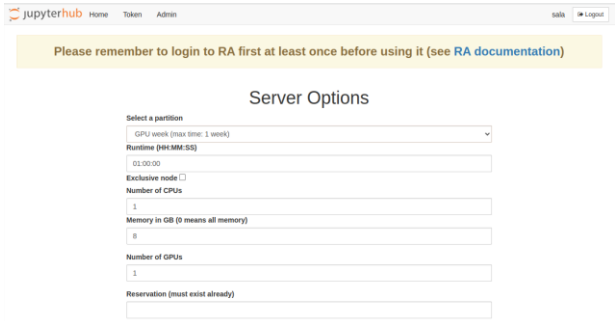
- IBM Storage Scale parallel filesystem
- Lenovo and IBM storage appliances (DSS and ESS series)
- Provide:
  - Native high-performance access
  - CIFS (Linux / Win)
  - NFS (Linux)
  - S3 (in the future)

- **Compute:**
  - Intel and AMD HPE nodes
  - SLURM as job scheduler
  - Jupyterhub for web-based interactive computing

- **Network**
  - 10/25/100/200G Ethernet, based on demand
    - 100/200G maintained internally
  - 100/200G Infiniband as general storage fabric

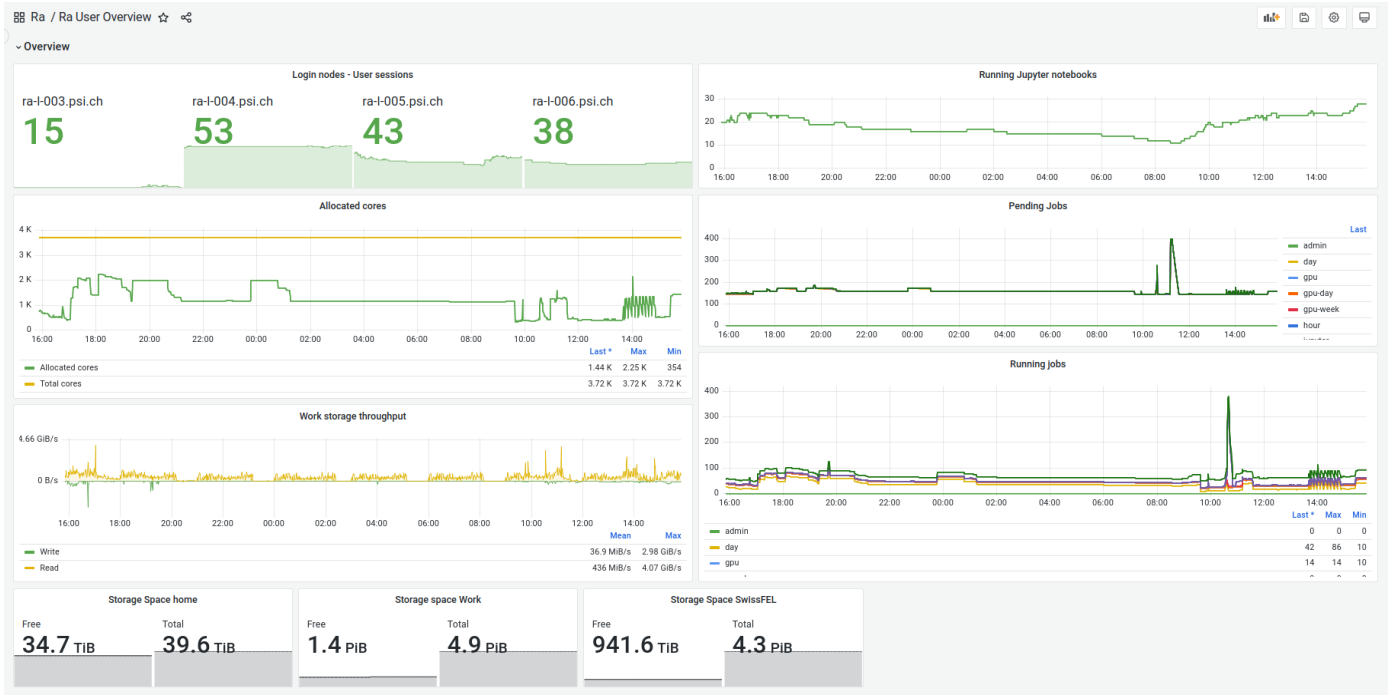
Services

- **Remote access:** ssh, NoMachine (remote graphical desktop)
- **Remote transfer:** rsync, scp, GlobusOnline
- **Storage:**
  - Users home directories
  - Group work areas – 4 T default quota
    - Storage space can be purchased on a yearly basis
    - Temporary quota extensions are supported
  - Experimental data (read-only)
- **Compute:**
  - Fair-share access to various queues (gpu, hour-day-week)
  - Possibility to reserve compute resources during experiments
  - Jupyterhub
- **Software:** various packages managed through pmodules



Services / II

- User support over mailing list, documentation
- Monitoring dashboards



Ongoing improvements

- **Flexible compute resources**
  - Use a single pool of compute nodes and dynamically assign/configure to different usages, e.g. dedicated to an experiment
  - Status: PoC ongoing
- **Self-service API**
  - Enable users to easily request resources (quota, compute)
  - Implement approval logic and limits for requests
  - Enable integration with Digital User Office
  - Status: first release in pre-prod

Wir schaffen Wissen – heute für morgen

Questions?

Future's challenges

- SLS upgrade
  - increased brilliance -> increased photons -> larger data
- New detectors
  - faster, smaller pixel size
  - does not scale with Moore
  - 85 GB/s
- CryoEM
  - long running experiments
  - few PB / year, 1000s GPUs