PAUL SCHERRER INSTITUT

PSI

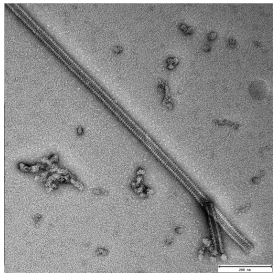
Spencer Bliven :: High Performance Computing & Emerging Technologies :: Paul Scherrer Institute

Open EM Data Network (OpEM)

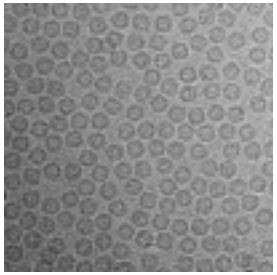
2023-05-02 PSI ORD

Electron Microscopy (EM) Data

Raw Data

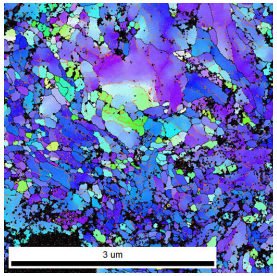


TEM
(Sejwal, PSI)

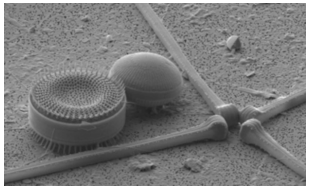


Single particle cryoEM
(EMPIAR-11016, Harder, EPFL)

Typical size:
1-10 TB/dataset
3-4 PB/year for major facilities



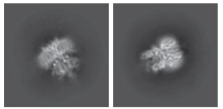
Orientation Maps
(Kunze and Sologubenko, ETHZ)



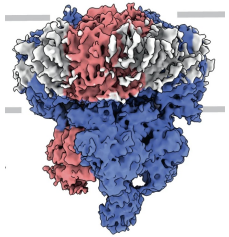
SEM
(Müller, PSI)

Also: Spectrograms, electron tomography, ptychography, 4D STEM, …

Derived Data

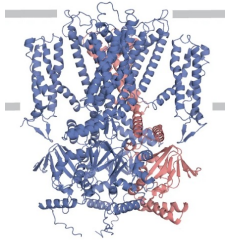


Particles & classes
(Barret, PSI)



Electron Maps (EMDB)

(EMD-12718, Barret, PSI)



Molecular Models (Protein Databank)

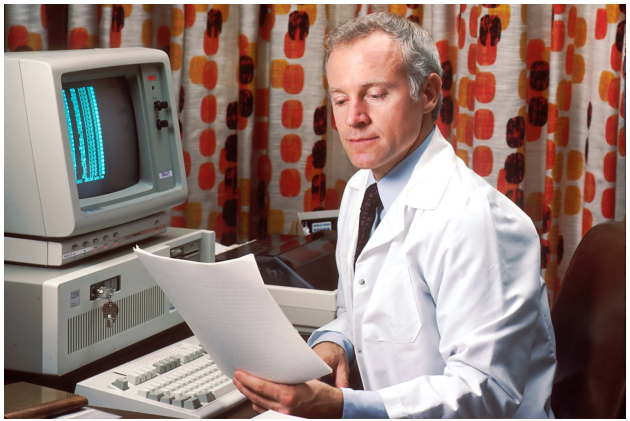
(7o4h, Barret, PSI)

Also: Tomographic reconstructions, segmented models, …

Users

- Data Producers
  - Microscope users
  - EM Facility Scientists
  - Microscope & detector researchers

- Data consumers
  - Data scientists, structural biologists, informaticians
  - Students
  - Training AI/machine learning



Benefits of open data for electron microscopy

- Publishing raw data is essential
  - **Reproducibility.** Check results & apply new methods to old data
  - **Verifiability.** Detect processing mistakes and protect against scientific fraud
  - **Education**. Learn processing techniques by reproducing cutting-edge papers
  - **Method development**. Datasets provide training data for future AI methods
  - **Interdisciplinary**. Images may be relevant for questions beyond the original scope
- Examples from crystallography:
  - PDB redo
  - Phasing old data with molecular replacement (or AlphaFold models)

Open EM Data Network (OpEM)

- How can we improve ORD practices in the electron microscopy (EM) community? → Open EM Data Network
  - ETH ORD M1 Establish application by Henning Stahlberg: 1.5 MCHF
  - swissuniversities by Robbie Loewith: 0.92 MCHF
  - 6.5 new positions
  - ETH: June 2023–Dec 2025 (30 months)
  - Swissuniversities: Jan 2023–Dec 2024 (24 months)

Open EM Data Network (OpEM)

4 ETH Institutes

ETH-RAT

5 Universities

swissuniversities

PAUL SCHERRER INSTITUT

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Mohamed Chami, Timm Maier

Empa

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Marco Cantoni, Alexandra Radenovic, **Henning Stahlberg**

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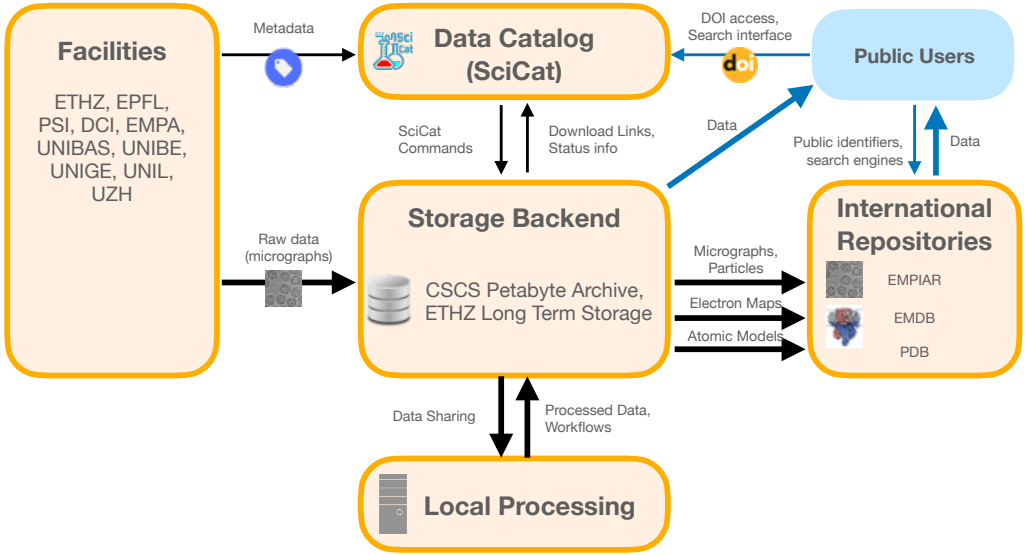
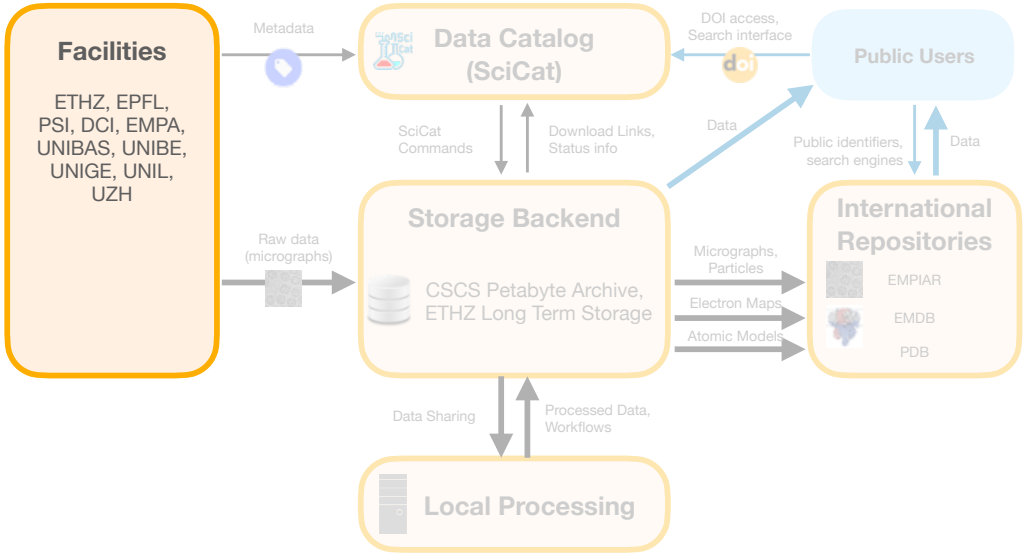
Architecture

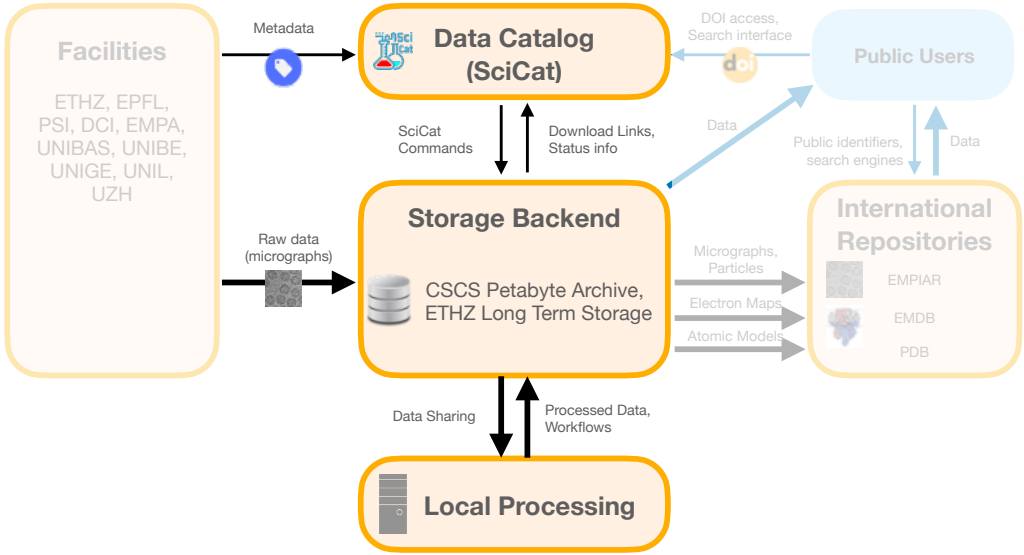


Project Plan



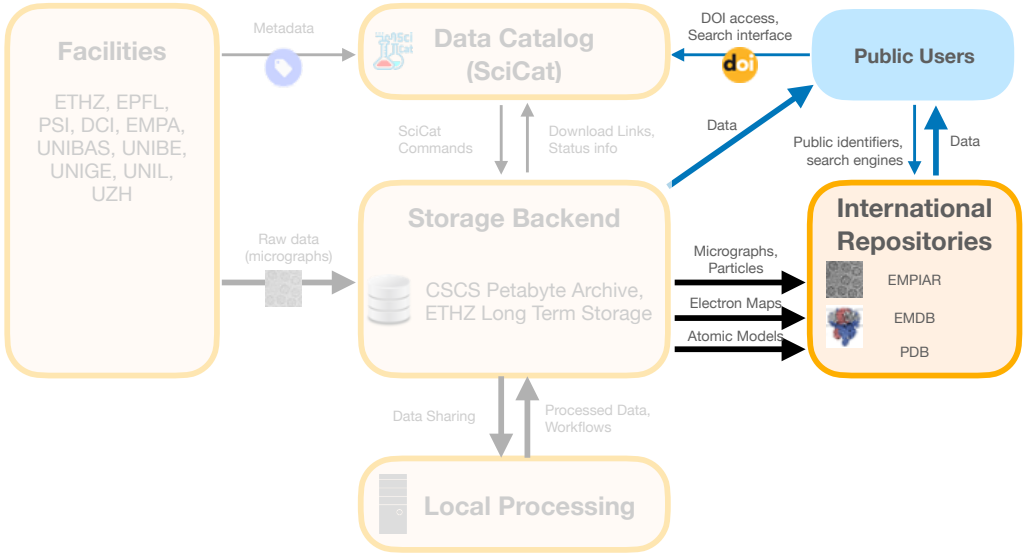
1. Automated collection of metadata during acquisition.
   - Initial focus on single particle cryoEM, but with support for additional domains like material science
   - Coordinate with EU & international standards and initiatives, eg. INSTRUCT-ARIA, 3DEM

Project Plan



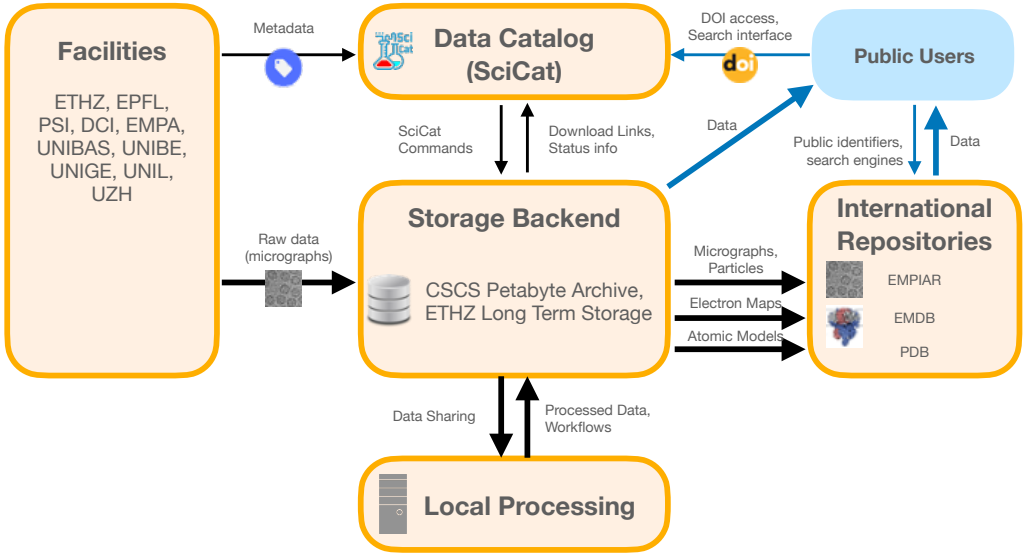
2. Ingestion of metadata from all sites in the Data Catalog
   - PSI will provide data storage for some sites; others adapt existing site-specific storage (e.g. ETHZ LTS)
   - Users deposit derived datasets after processing

Project Plan



3. Seamless deposition in international repositories (EMPIAR/EMDB/PDB)
   - Pre-populate fields from metadata

Project Plan

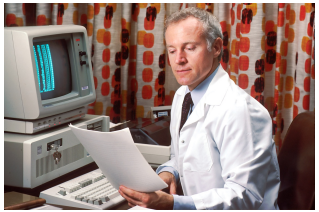


4. Training & outreach
   - Provide user training for researchers, facility managers, and data consumers
   - Find sustainable funding model

For data producers

- Standardized data management at all facilities
- Raw data & metadata are automatically entered in the catalog
- Swiss-wide data transfer with unified authorization (SWITCH AAI)
- Complies with institutional and federal data policies
- Integrates with popular processing software, eg relion, CCPEM-pipeliner, cryoSPARC
- DOI assigned for publication
- Prepares single-particle cryoEM datasets for deposition at EMPIAR+EMDB+PDB

For data consumers



- Findable via OpenAIRE, European Open Science Cloud, Google Dataset search, etc.
- Linked to publications and international repositories
- Searchable via metadata (http://discovery.psi.ch)
- Data retrievable from storage via asynchronous systems
- Scriptable via REST API

Major Tasks

- Now hiring!
- Data Catalog Tasks
  - Federated login outside PSI
  - Permissions model independent of PSI
  - Ingestion from remote sites
  - Support external data storage
- Microscope Facility Tasks
  - Standardize EM scientific metadata
  - Ingestion service for each facility
  - Integrate with institutional storage & services
- Data Publication
  - Collaboration with EBI for EMPIAR/EMDB/PDB deposition
- Train staff & scientists
- Find sustainable funding model

Thanks!

- Henning Stahlberg (EPFL), Robbie Loewith (UNIGE), Gebhard Schertler, Gregor Cicchetti, and other OpEM members
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- Derek Feichtinger & the HPCE Group
- Alun Ashton, Leo Sala, & AWI colleagues
- EM Facility staff