ISPyB & SciCat future plans at MAXIV

Alberto Nardella

Alberto.Nardella@maxiv.lu.se

Summary

- MX metadata problems & tasks to do
- ISPyB & SciCat timelines
- Sample Management
- Teams

MX metadada in SciCat

- **Database problems**
  - Current MongoDB indexes need to be rebuilt.
  - Test if MongoDB can manage the amount of metadata produced at BioMAX and MicroMAX.
  - Investigate if MongoDB can search efficiently the data the user needs.
  - Redesign the schema to fit the new needs (multisweep, multicrystal, reprocessing,...).
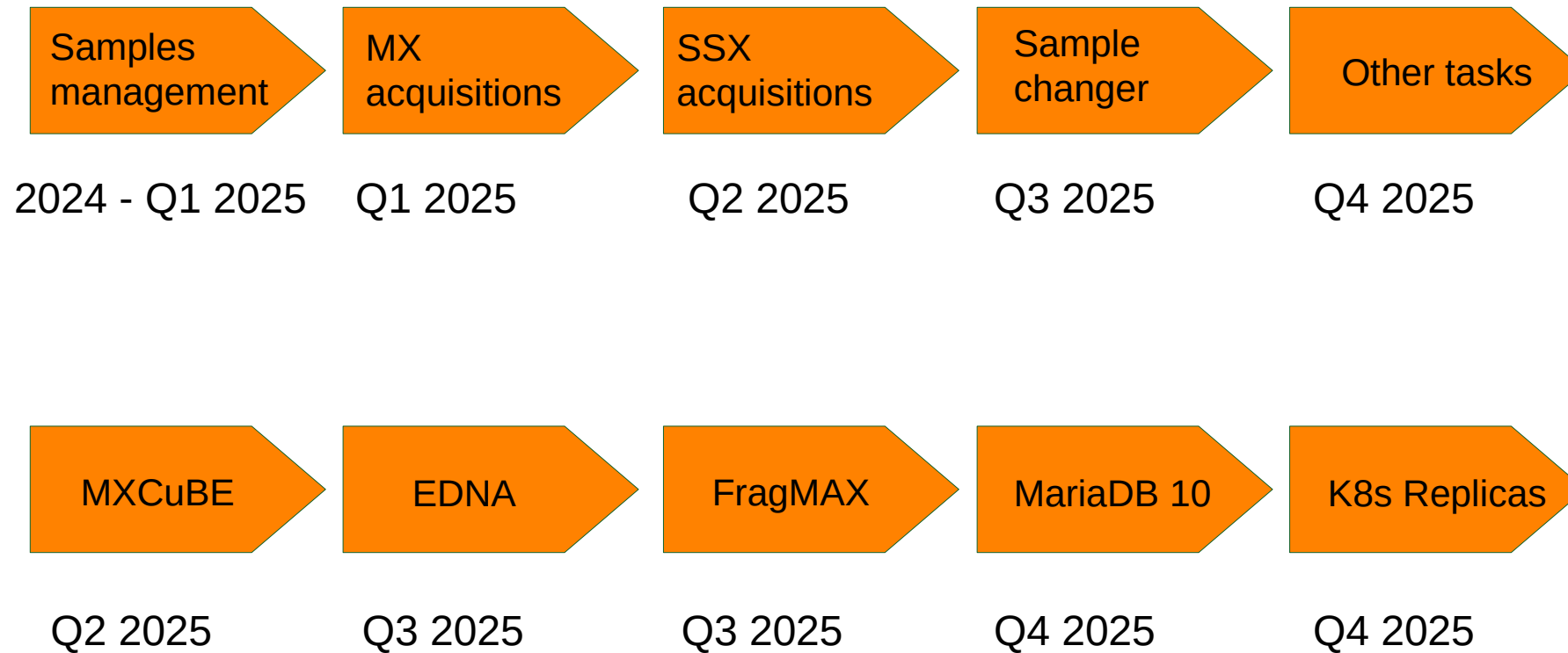
MX metadada in SciCat II

- **Back-end tasks**
  - Improve ingester of MX metadata into SciCat.
  - Develop all the entry-points used by MXCuBE & the pipelines running at BioMAX, MicroMAX and FragMAX.
  - Develop the entry-points used by the front-end to show the data.
  - Develop the entry-points used by third-party applications (e.g., IceBear) to get and push the data.
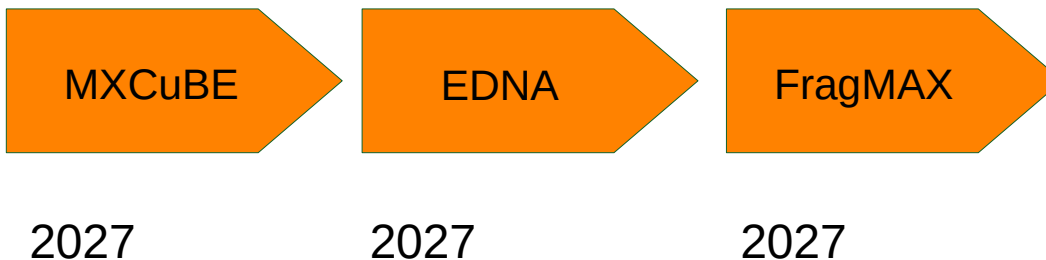
MX metadada in SciCat III

- **Front-end tasks**
  - New widget components to be developed (XRF scan, Energy scan, Generic MX, SSX, Mesh).
  - Improve the layout. It seems like the TopCat I tested more than 15 years ago!
  - Focus on the User experience.

Py-ISPyB timeline

Samples management → MX acquisitions → SSX acquisitions → Sample changer → Other tasks

2024 - Q1 2025   Q1 2025   Q2 2025   Q3 2025   Q4 2025

MXCuBE → EDNA → FragMAX → MariaDB 10 → K8s Replicas

Q2 2025   Q3 2025   Q3 2025   Q4 2025   Q4 2025

SciCat timeline for MX metadata

MongoDB indexes	DB schema redesign	Back-end tasks	Front-end tasks	General layout
2025	2025-2026	2026-2029	2026-2029	2025-2029

MXCuBE	EDNA	FragMAX
2027	2027	2027
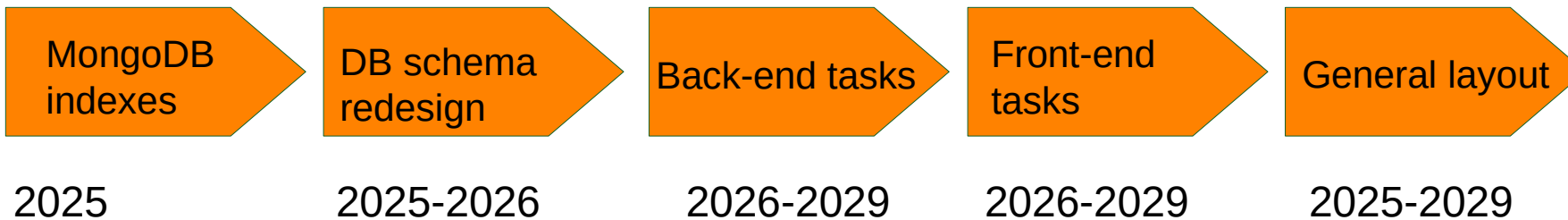
IMPORTANT

- We should consider an extra cost due to the collaboration with other facilities with or without MX metadata.
- We need to reduce the impact in the core of SciCat to avoid to cause problems to other beamlines or facilities.
- +1 or +2 years?

Samples management

- Several beamlines need to manage samples and shipments so created an official request.

- We need to take advantage of the opportunity:

  - Show py-ispyb samples management as a starting point.

- Create a new Samples Management tool or upgrade py-ispyb in order to manage both MX and no MX beamlines samples.

  - It will be part of the SciCat zoo in the future?

ISPyB & SciCat teams at MAXIV

ISPyB *(2014-2023)*

FS

SciCat *(2018-2024)*

FS FS

SciCat + ISPyB *(2027-2030)*

FS FS FS FS FS FE DBA

ISPyB *(2024-2025)*

FS FS DBA

SciCat *(2025-2026)*

FS FS FE DBA

Full **S**tack
Front **E**nd
DB Administrator

Thank you very much