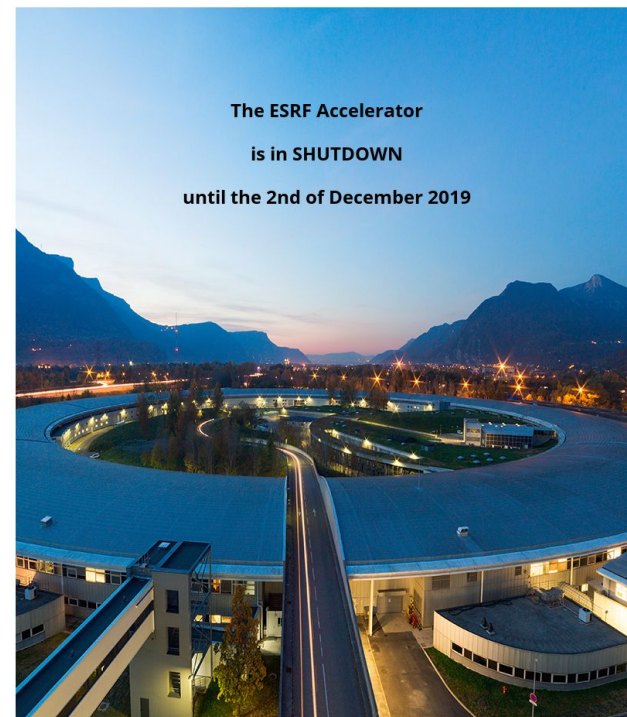


ISPyB Status Report

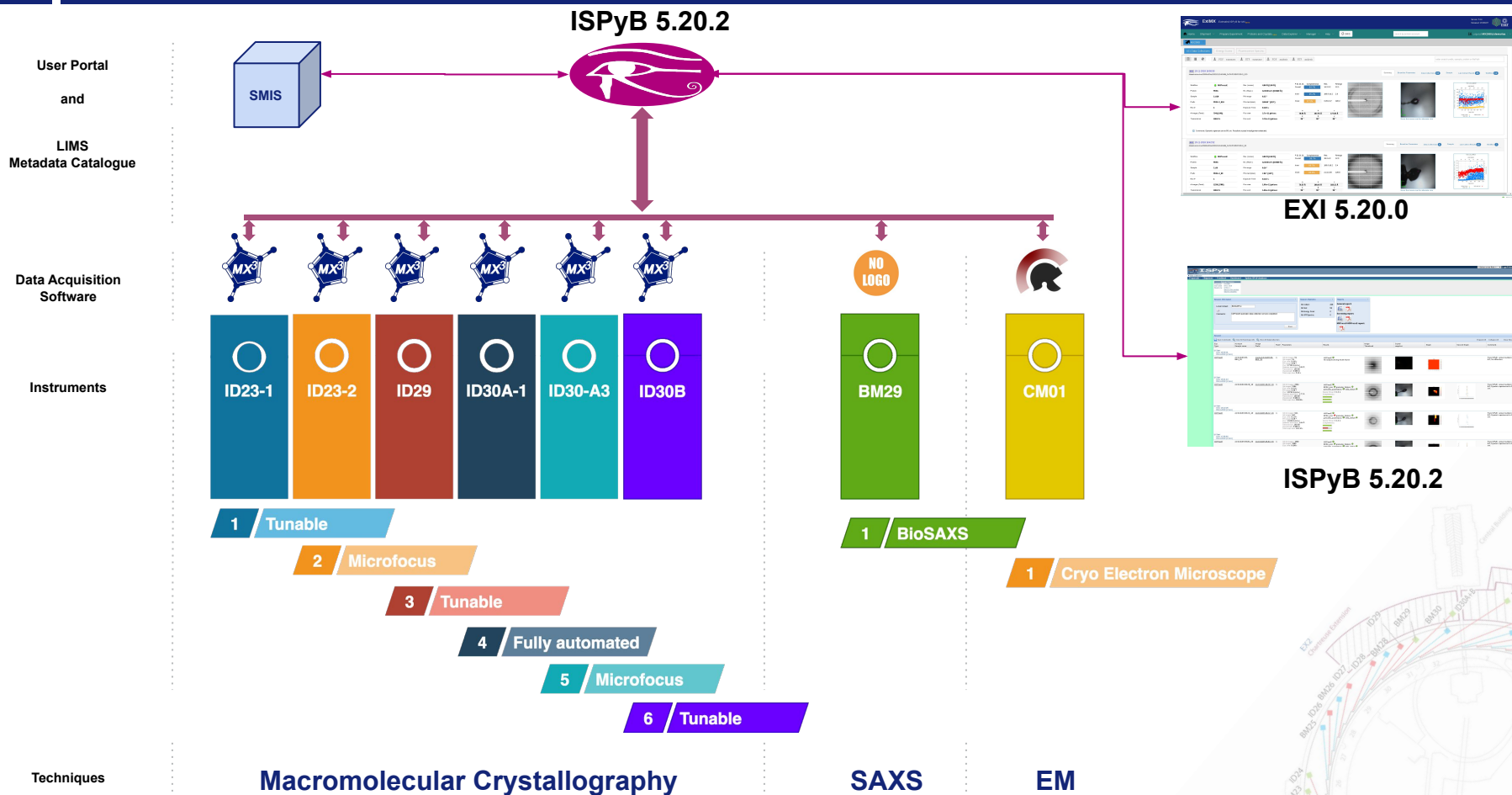
@ESRF

Alex de Maria Antolinos
Software Engineer
Data Manager@Data Analysis Unit
Software Group
ESRF
Berlin 31/10/2019

- Facility
 - In shutdown
 - CM01 is still working in normal basis
 - Users expected by the end of August 2020



Deployments

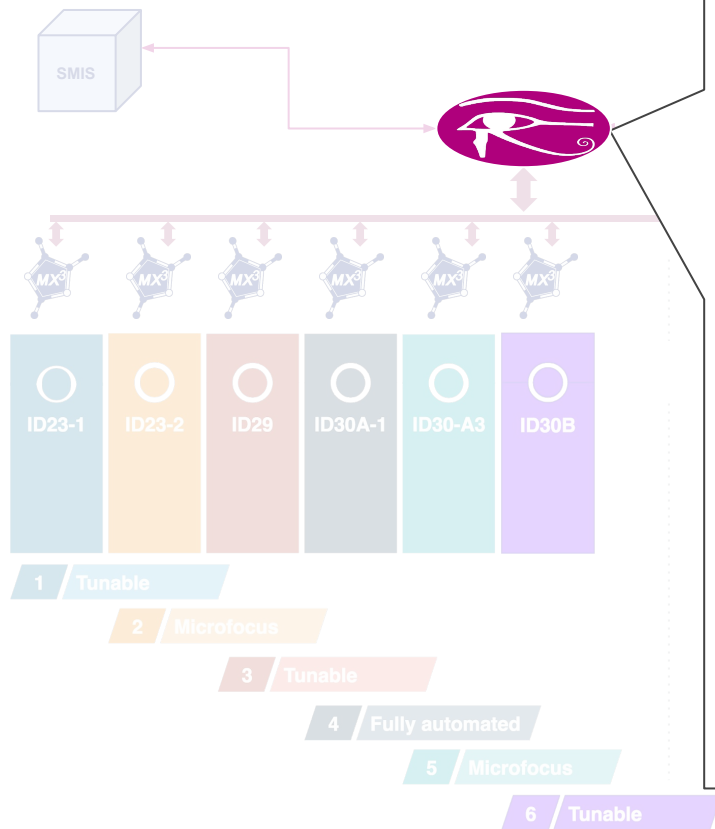


Deployment

User Portal
LIMS
Metadata Catalogue

Instruments

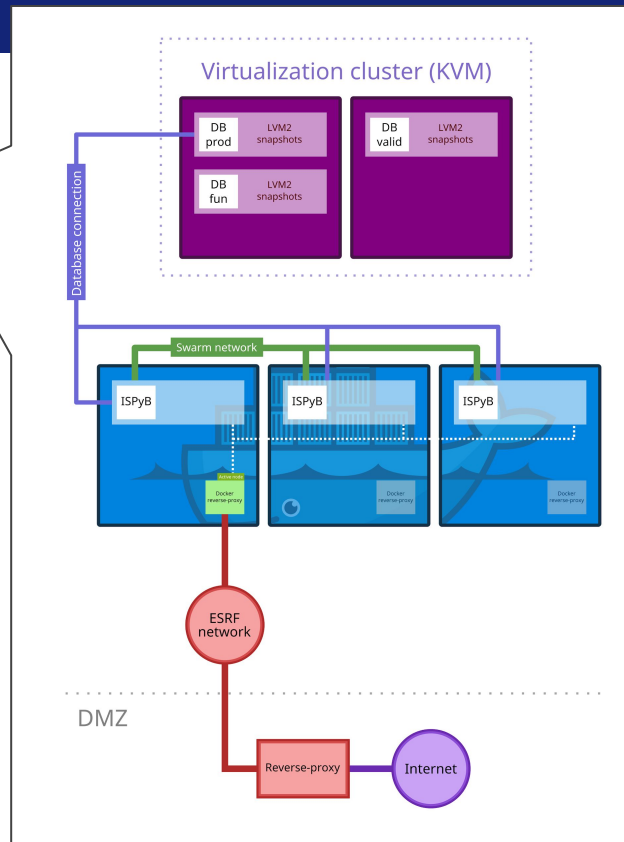
Techniques



Macromolecular Crystallography

SAXS

EM



Developments

- Work in progress
 - JBOSS server
 - Upgrade from v8.2 to v18.0
 - Support for single-sign on
 - Centralized authentication management
 - Offline data analysis
 - Launch jobs from the UI
 - A Mockup is up and running and waiting for real use cases
 - Allows interactive mode
 - Developing a new version of EXI on React
- EXI
 - Molecular replacement
 - Add crystal form to a protein
 - Add multiple PDB/Fasta to a crystal
 - Create a cocktail of ligands for a proposal
- EXI2
 - Migrating EXI to react

Recent events

- Meetings at Soleil (12th-13th September)
 - Data model
 - Participants: Soleil, Alba, Global Phasing and the ESRF
 - Main Topics:
 - Generalization of Sample
 - MX: protein -> crystalForm
 - SAXS: assembly ->macromolecule->Structure
 - Refactor and/or Merge techniques
 - Energy Scan
 - XRF
 - Data Collection
 - Refactor and/or Merge
 - AutoprocProgramAttachment
 - PhasingProgramAttachment
 - Offline data analysis
 - Follow-up
 - Monthly meetings

Thanks!