# MicroMAX – MXCuBE dev.

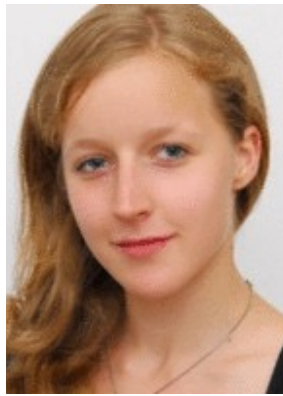Oskar Aurelius, on behalf of MAX IV MX group

# Outline

- **Overview of team**

- The road to MXCuBE at MicroMAX

- **Spinning, running and flowing first experiments**

- The different MXCuBE integration topics compared to BioMAX

- **What comes next?**

# Overview of main contributors to MicroMAX MXCuBE

**Driving the implementation of MXCuBE at MicroMAX**



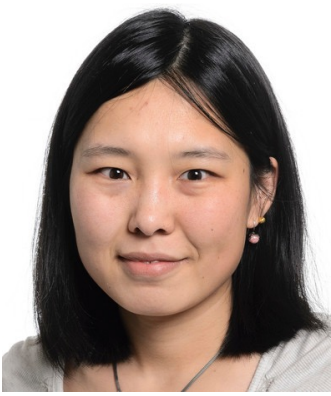Dominika    Elmir    Fabien    Ishkhan    Jie    Meghdad    Mikel

**MX-group**

# The road to MXCuBE at MicroMAX

- **Legacy and divergence**
    - BioMAX MXCuBE3 was forked and not up to speed with main branch

- **Wish to be more involved in contributing and benefitting from the collaboration**
    - Keep up with main branch

- **Invest in new feature sets to cover experiment types that have not been routine at BioMAX**
    - Make SSX and time-resolved experiments more routine

# MXCuBE-Web

# What will MicroMAX actually do [next]?

- Selection from [MAX IV] MX-group review report, end of 2023

| # | Milestone | Timing | Goal |
|---|-----------|--------|------|
| **M1** | Friendly user rotation data collection | 2023 Q4 | First external user experiment: SPINE rotation data collection using MD3 diffractometer |
| **M2** | Routine remote rotation data collection | 2024 Q1 | Remote users operating MicroMAX at fixed-energy and fixed-focus for cryogenic data collection, assisted by the ISARA2, MD3, Cryostream, EIGER2 and data auto-processing |
| **M3** | Fixed-target SSX with SPINE-like sample supports | 2024 Q1 | Collect SSX data from SPINE-like fixed-target mounts, with live image analysis<br>Sample changer assisted and variable temperature [cryogenic and non-cryogenic] |
| **M4** | First injector experiment | 2024 Q2 | Simple injector experiment on MD3 with basic MXCuBE integration<br>User-provided setup if performing pump-probe |
| **M5** | Extended SSX early user program | 2024 Q4 | Open up for sample feasibility checks for users [fixed-target and flow-cell] – proposal-less screening beamtime<br>Collect MLM data for such an experiment and easily switch between the 3 available photon energy bandwidths and variable attenuation |
| **M6 (F)** | High data-rate injector pump-probe experiment | 2025 Q1 | HVE and JUNGFRAU used for chopper pump-probe experiment with nanosecond laser, using pink beam |

MAX IV

# Spinning, running & flowing first experiments

- **Not started using different MXCuBE Web configurations outside of "OSC"**
    - Temporarily been running injector and fixed-target experiments also in "OSC" configuration
    - Will migrate SSX functionality to custom configuration - "Injector", "Fixed-target"

- **Used for first data collection of**
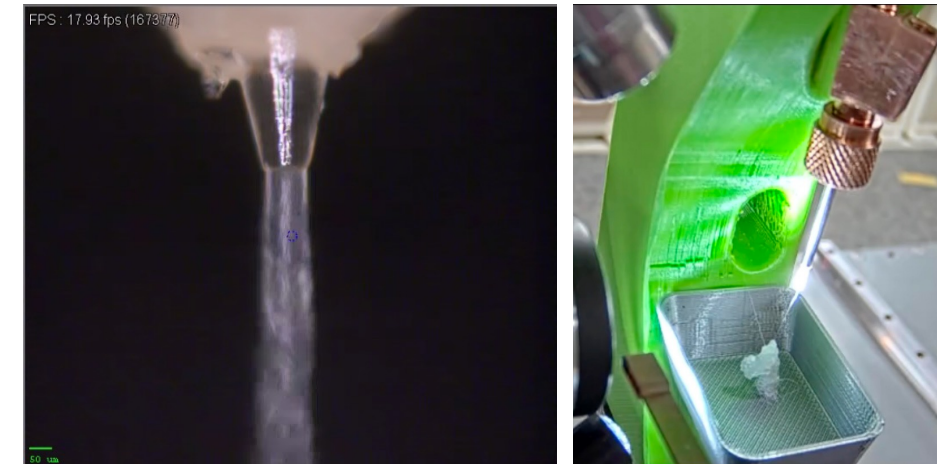    - Rotation data
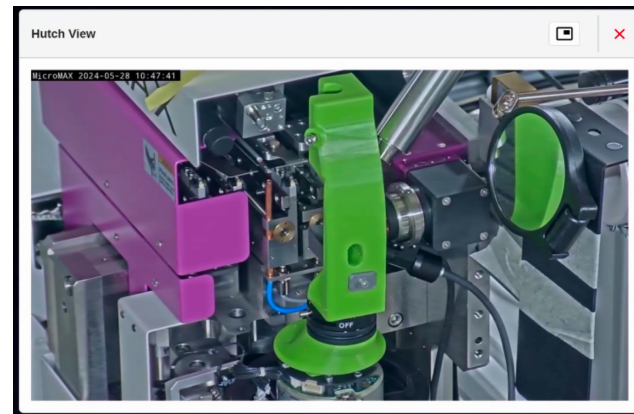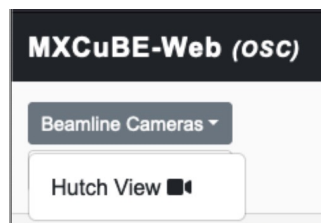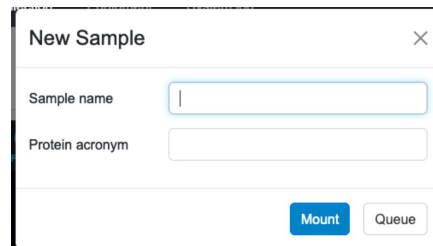    - Fixed-target SSX
    - Injector
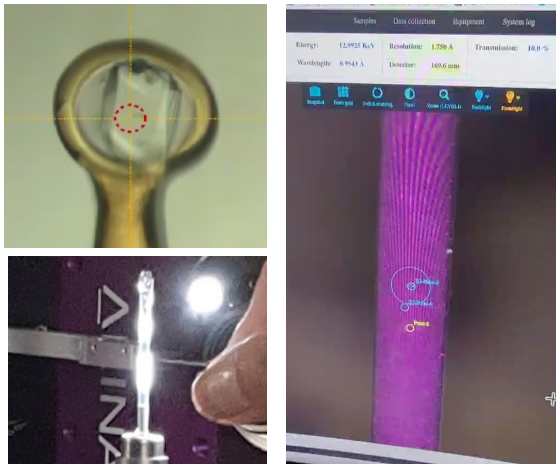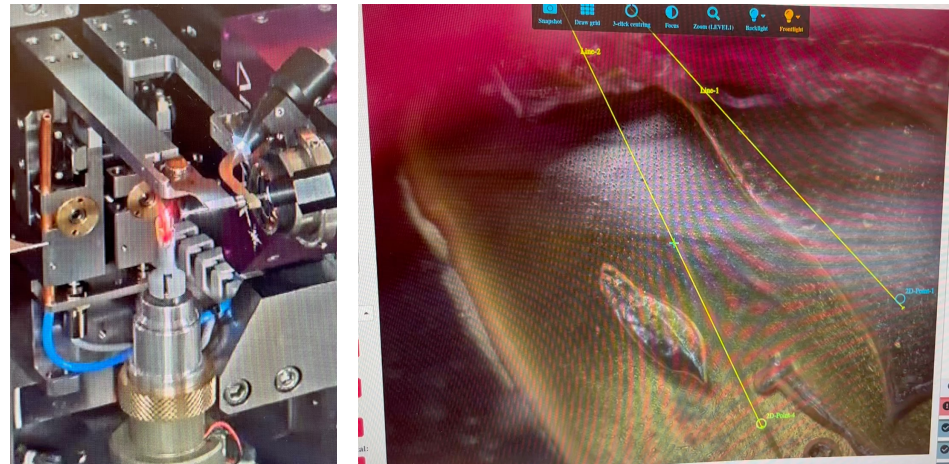
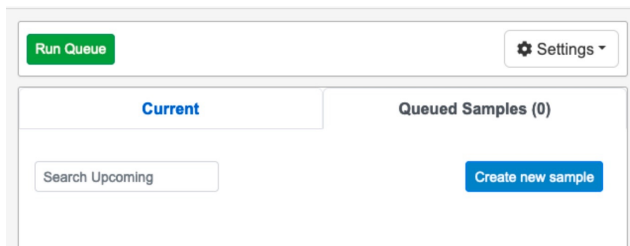**Spinning**                    **Running**                    **Flowing**

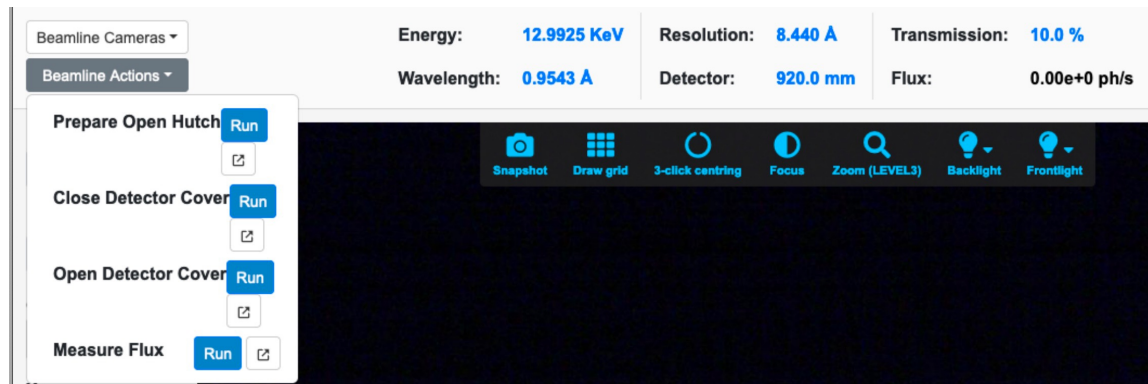# Revisiting old "new features"

- **Hutch cameras**



- **Sample creation**



- **Beamline actions**

# Minor (temporary?) features updates

- **Universal goniometer head for fitting various sample environments**
  - Can use MD3 motion system for positioning

- **Awaiting MD3 software upgrade project with Arinax**
  - To allow custom interlocks and extended functionality
  - Currently identifies itself as a "plate manipulator"

- **Currently limited by interlock mismatches prior to software update**
  - MXCuBE equivalence to MD3 phases
  - MXCuBE individually moves motors and performs checks, instead of standard MD3 phase control



"Empty" goniometer head
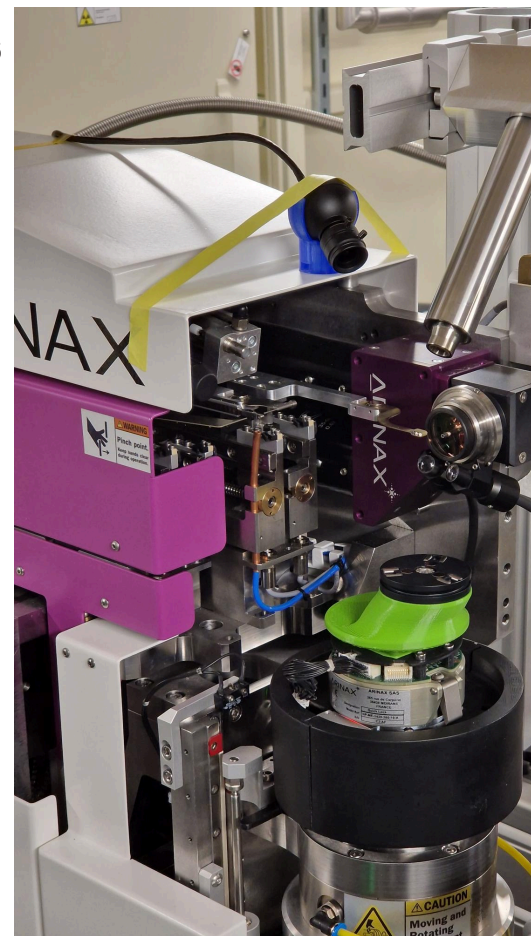


3D-printed HVE-injector holder on kinematic mount
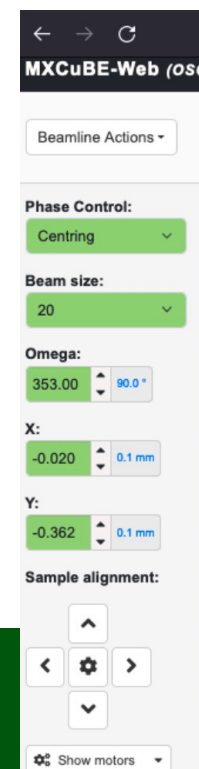
# SSX live data analysis

- **Currently no visualisation or feedback to MXCuBE**

- **Different analysis workflows between EIGER2 and JUNGFRAU**

  - In-house pipeline by Cecilia Casadei, and previously Aleksander Cehovin, for EIGER2 spot-finding [as presented by Jie]

  - Jungfraujoch also includes indexing and cell parameters are parsed from MXCuBE currently

- **CrystFEL input files auto-generated**



Green – peak          Red – indexed solution
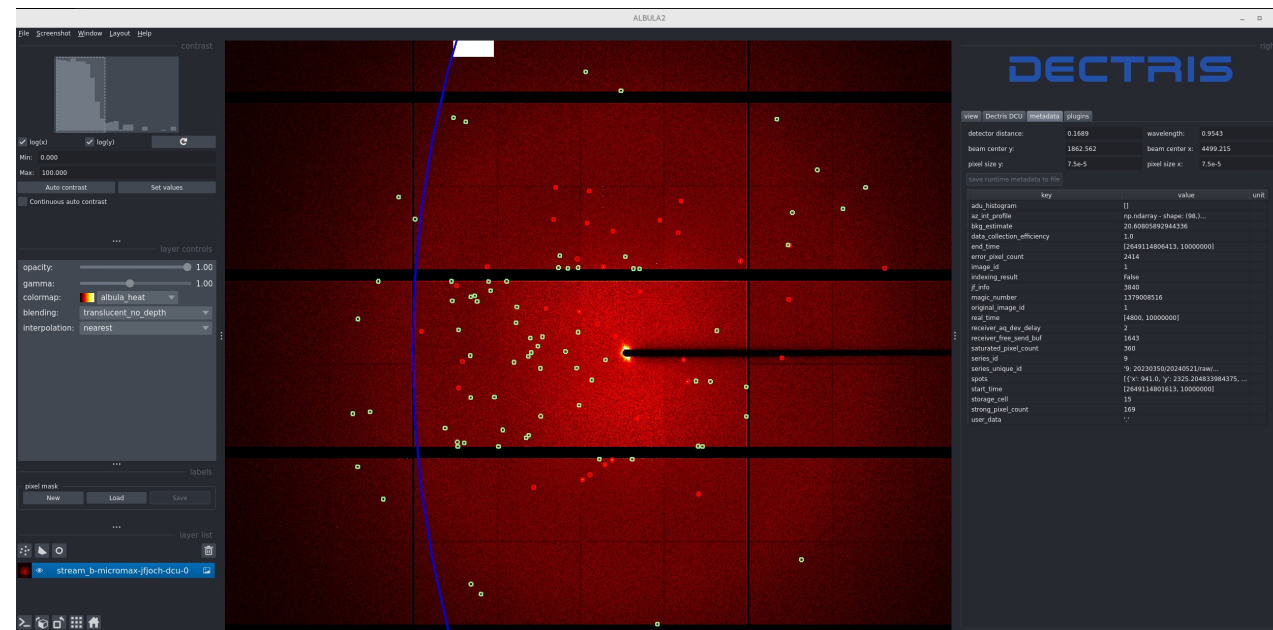
# New complementary features to BioMAX functionality

- **Multi-configuration experiment timing control**

  - PandA-box as a central point for timing control

  - Introduce timing offsets

  - Interfacing both with beamline and user equipment
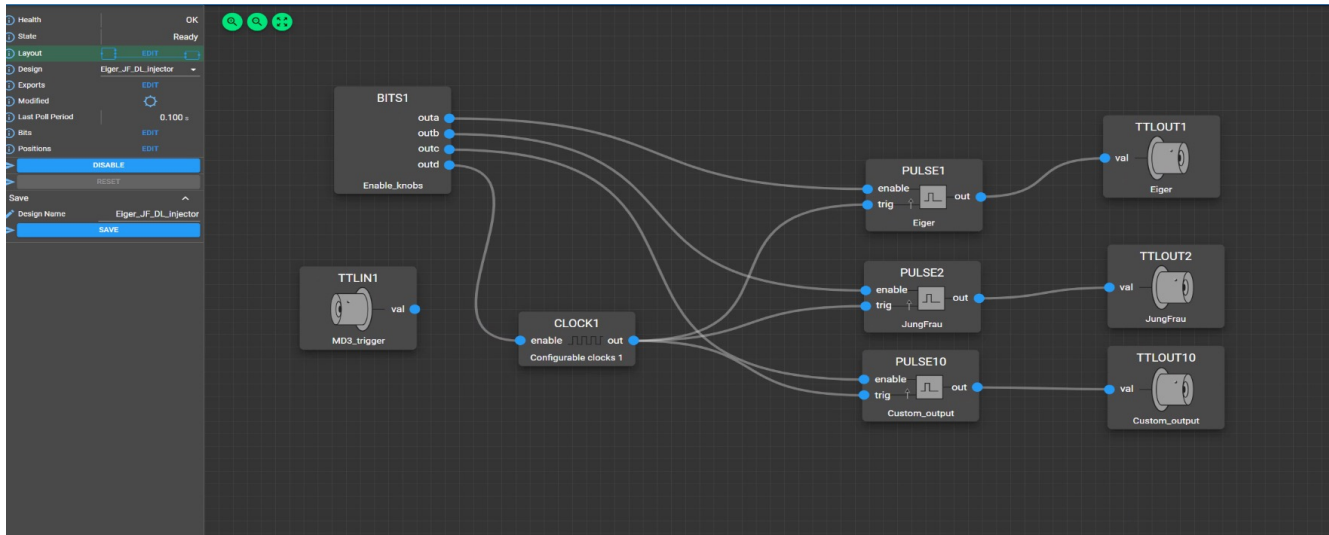
  - *Covered further in later slides*



- **Handling more than 1x diffraction (area) detector**

  - Currently done by two branches of MXCuBE

  - Plan to merge so switch can be done within the same session

  - No technical details for implementation plan yet
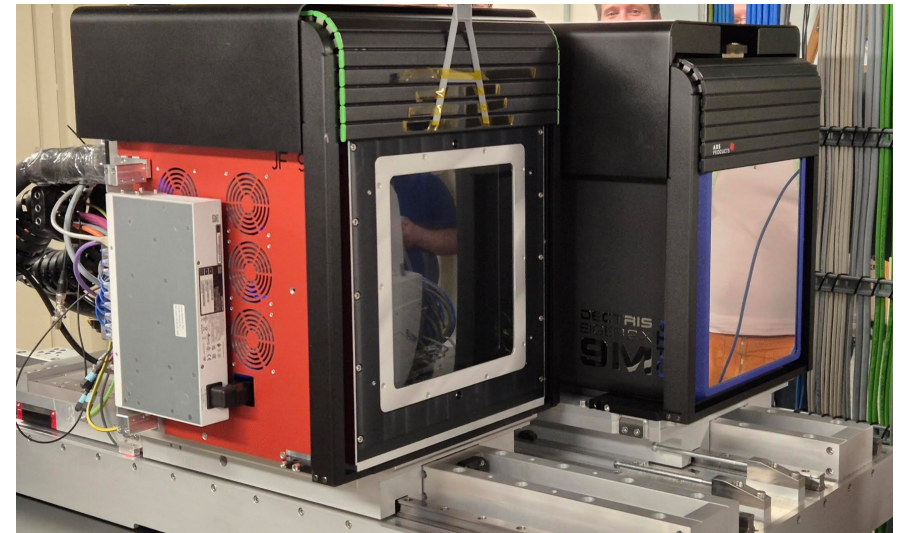
# Timing system
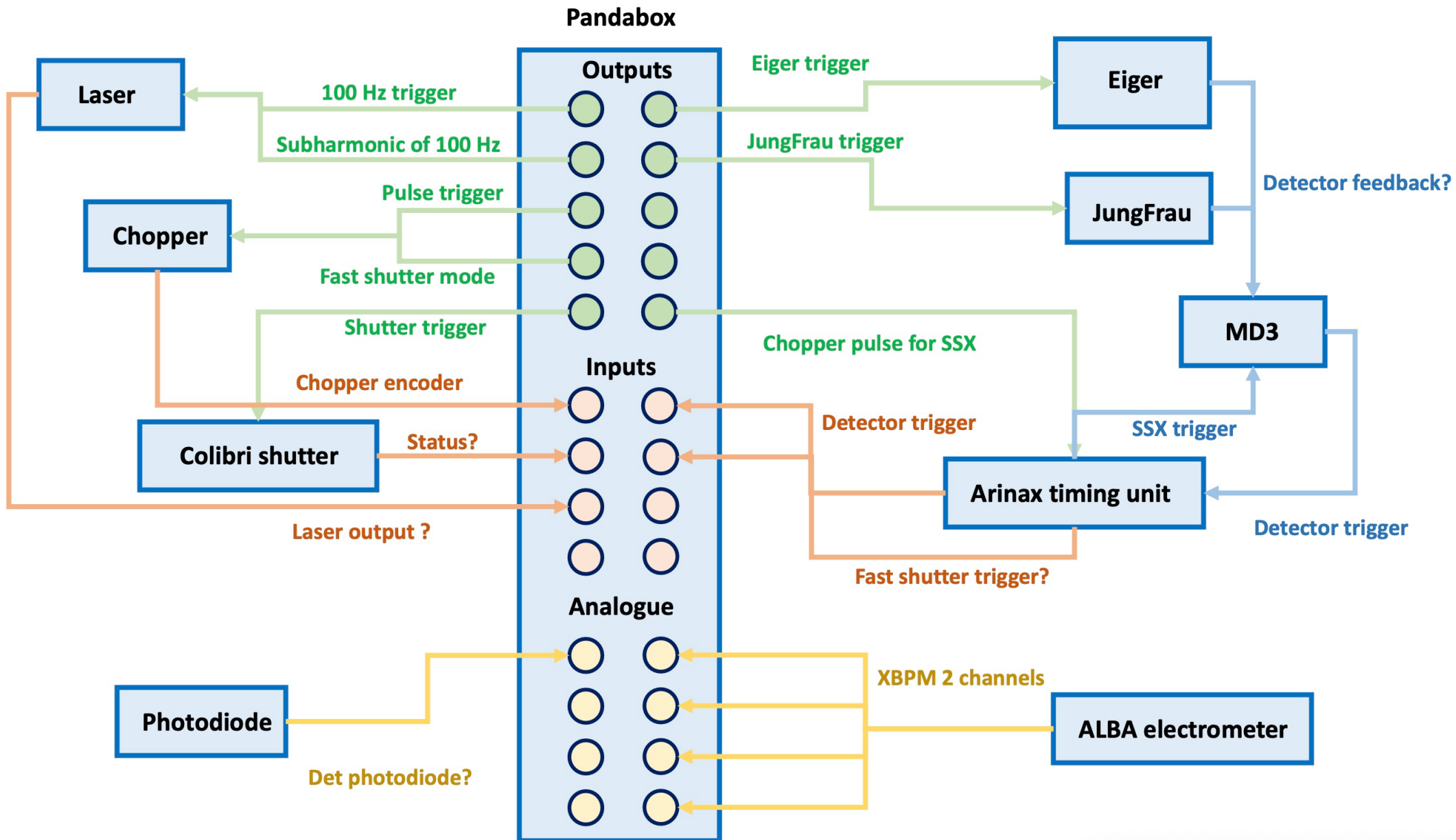
# PandA configuration & Tango interfacing

# MXCuBE-side of timing

# Wrapping up

# Outlook and main conclusions

- **Increase activities towards new features and to participate in the collaboration**
    - Will depend on an investment from the beamline/MX-group -side to produce detailed user stories


- **Move different "packaged" feature sets into separate MXCuBE configurations**
    - "Injector", "fixed-target", … modes


- **Develop timing control and try to learn from experiences on UI work in Qt-MXCuBE at T-REXX**
    - For user friendliness, but also to cover more complex experiment control within MXCuBE


- **Make detector changes trivial within MXCuBE and with minimal (software-related) downtime**
    - Handle reconfigurations of detector parameters, triggering, data analysis, flux estimations, and motor positions


- **Increase presence and interaction with user group to tweak/adjust target functionality**
    - Aided by now being in user operation and performing experiments beyond pure commissioning work

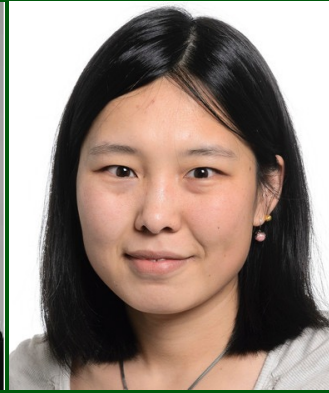# Timely acknowledgement



Dominika     Elmir     Fabien     Ishkhan     Jie     Meghdad     Mikel

MX-group

# Questions?

# HVE run