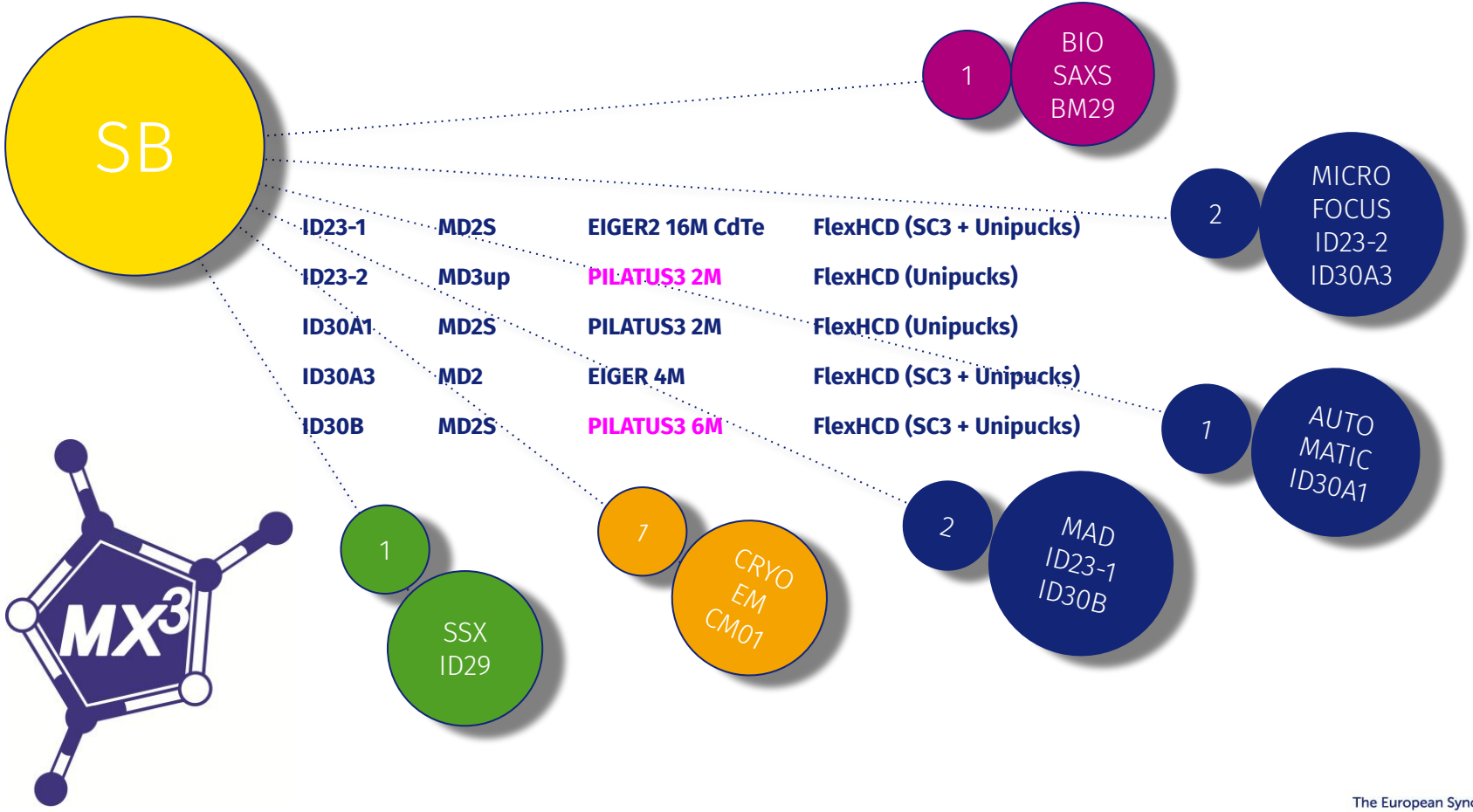
ESRF Status Report

Daniele de Sanctis

On behalf of the rest of the team:
Marcus Oscarsson, Antonia Beteva, Jean Baptiste Florial

With contribution of:
Loic Huder and Axel Bocciarelli (for the Braggy project)


SB
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BM29
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MICRO
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ID30A3
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ID30A1
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ID23-1
ID30B
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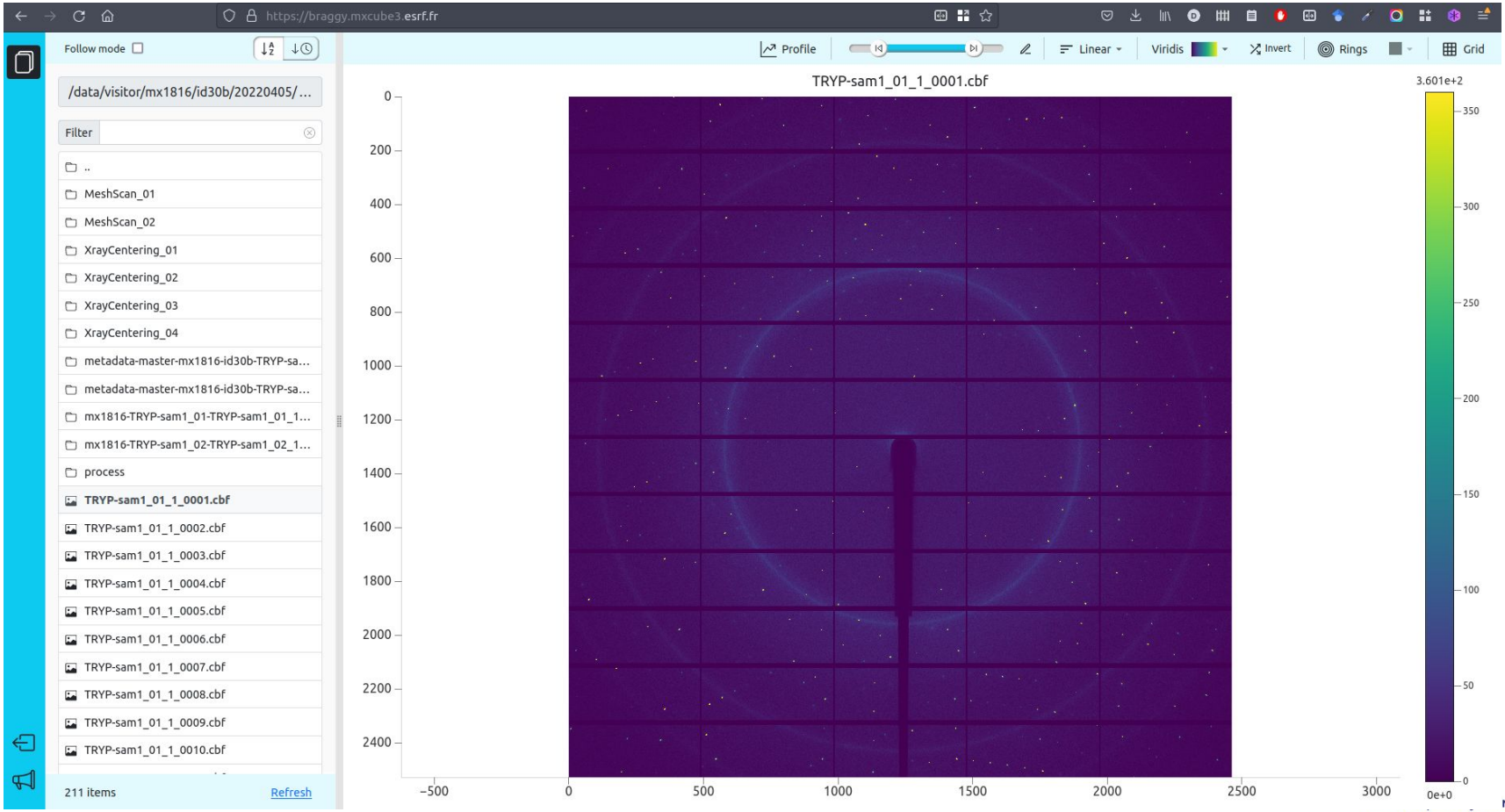
SSX
ID29
ID23-1 MD2S EIGER2 16M CdTe FlexHCD (SC3 + Unipucks)
ID23-2 MD3up PILATUS3 2M FlexHCD (Unipucks)
ID30A1 MD2S PILATUS3 2M FlexHCD (Unipucks)
ID30A3 MD2 EIGER 4M FlexHCD (SC3 + Unipucks)
ID30B MD2S PILATUS3 6M FlexHCD (SC3 + Unipucks)
MX3

LAST SIX MONTHS

- MXCuBE3 on all beamlines
- BSXCuBE3 on BM29
- Hardly any users on beamlines (mainly BM29)
- Most of the effort focused on keeping up with remote operation

- Since last MXCuBE meeting:

    - ID30A1 Crystal Direct Harvester 2 with Cryo and HClab
    - Java Flex software running on linux to control SC on all MX beamlines
    - GPhL workflows in MXCuBE3
    - **Braggy** released for users (braggy.mxcube3.esrf.fr) - new features added
    - mxcubecore 1.0 and MXCuBE-Web 4.0 deployed on ID30A1 and ID29
        - React 14 and Bootstrap 5
    - See Marcus' talk for more!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MeshScan_02
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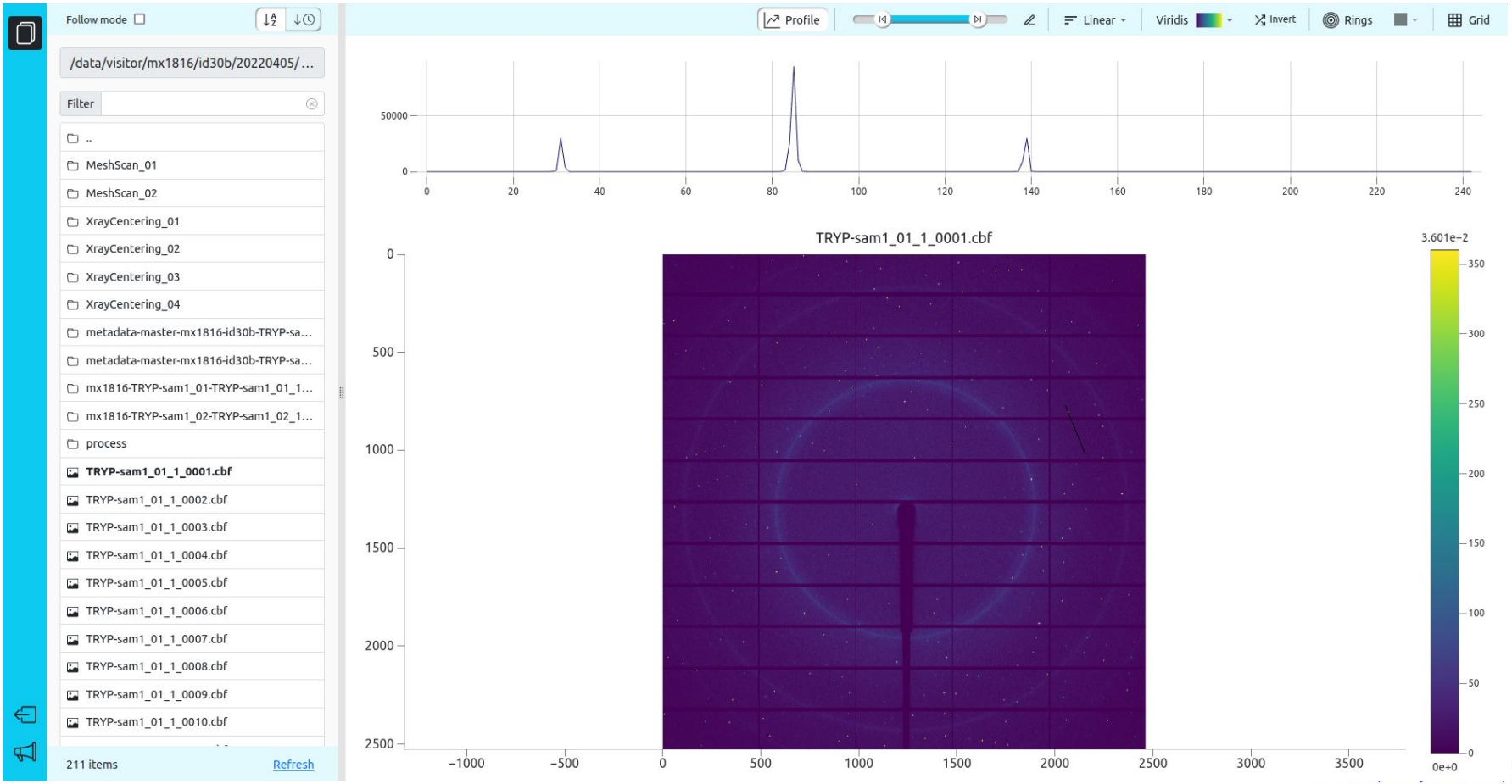
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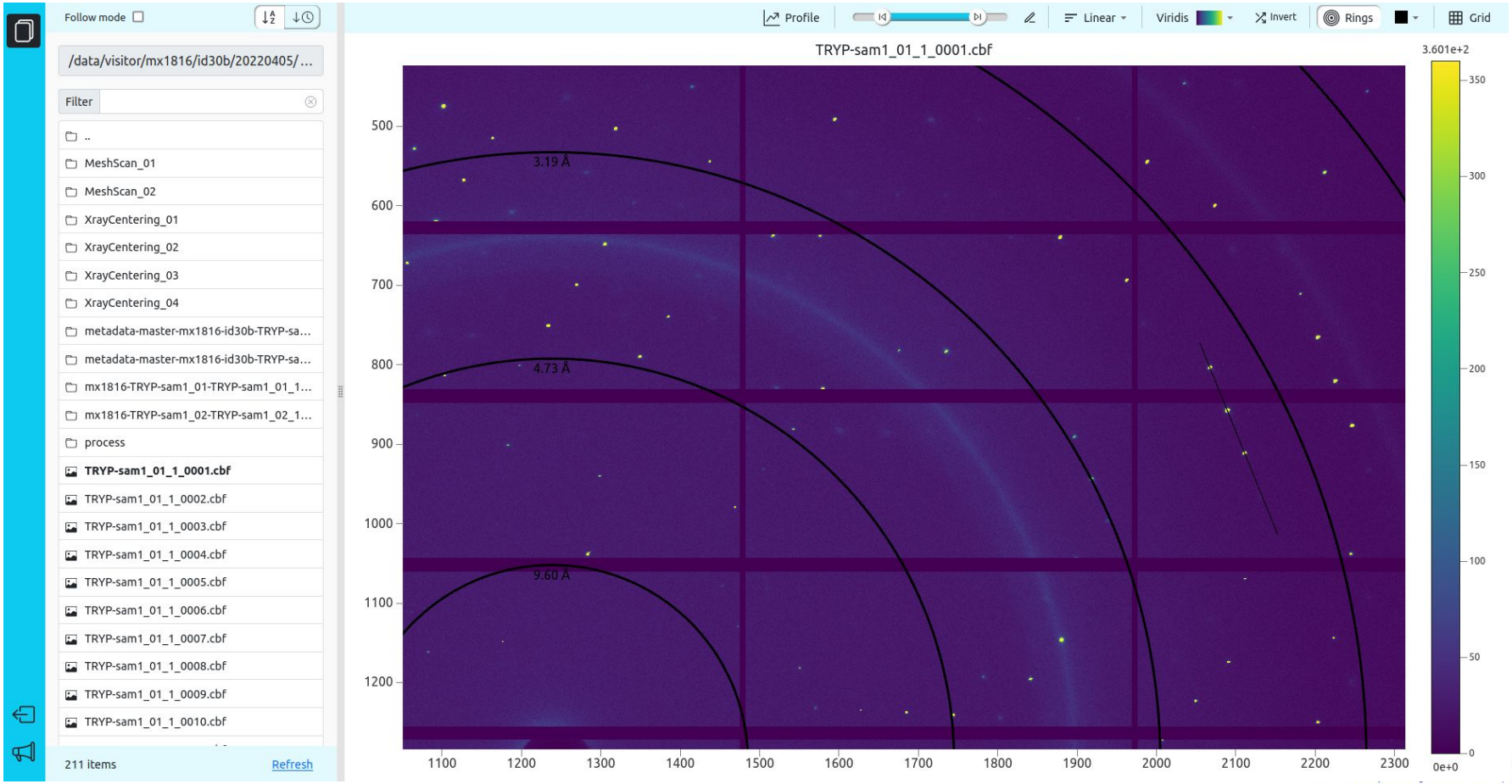
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OLD BUT GOLD

MX2450
The web version of the MXCUBE works really well, and it allows us to easily change between different users, even in remote mode.

MX2451
In general beamline set up and data collection is user friendly and robust.

MX2452
We are particularly pleased with the ease of use of the MxCube3 environment for remote data collection.

MX2462
We are very impressed with the new web-based MXCube, it is a very good environment for data collection.

MX2409
The implementation of the **new MxCube3 went perfectly and it is really pleasant to use**. And the remote access is now really convenient.

MX2415
A huge improvement was the new MXCuBE and EXIMX (ispyb) Interfaces. Overall, as users we believe **beam quality and user interface (for remote data collection) is the best** that we can find in any synchrotron.

WHERE IS MXCUBE3? - OCTOBER 2021

MXCuBE3 provides the **best possible remote** experience and **facilitate complex experiments** by hiding the complexity

- No additional software
- Limited lags
- **Platform independent**
- A smooth user experience: **direct interaction with the sample**, less typing, just clicking
- A **flat learning curve**: only a few minutes are needed to inexperienced users to master it
- (Unfortunately) the pandemic provided the best test bench
- In parallel **mxcubecore** set the basis for **years of fruitful collaboration**

TENTATIVE DISCUSSION AGENDA - OCTOBER 2021

In the near short term:

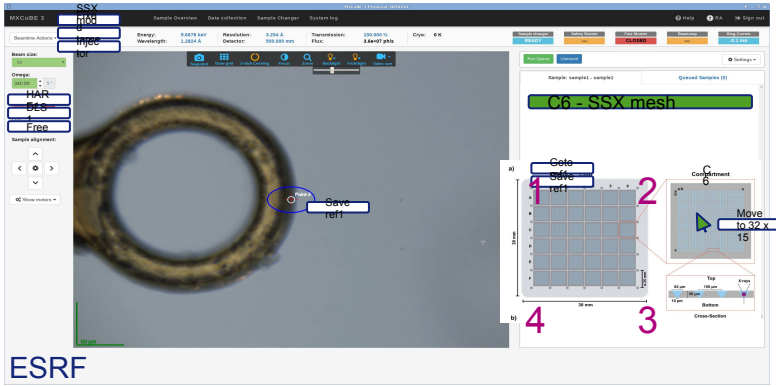
- **Improve results visualisation**, this is strongly intertwined with EXI2 future
- Make mesh (and recently developed 2meshes) results more interactive
- Connect **MXCuBE3 to Braggy** (eventually EXI2 as well)
- **Users are not coming back on site** (if remote works well and if they experiment does not require it

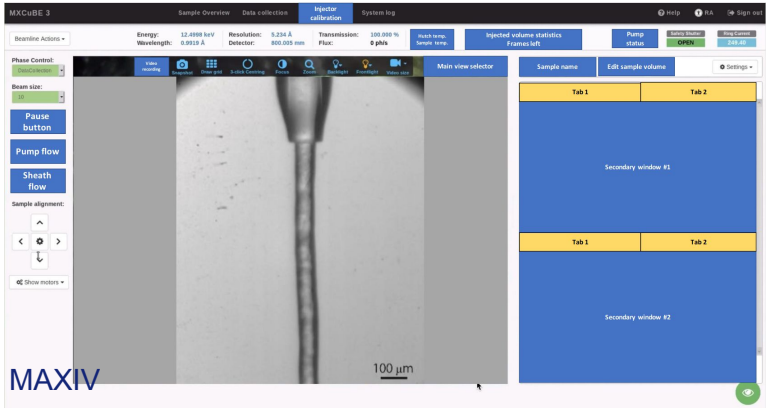
In the short term:

- **Virtualisation of sample representation** (mainly for SSX, but not only)
- **Workflows**: Shall they become part of **MXCuBE3 native features?**
  - Automatic data collections
  - X-ray centring
  - SSX mesh like
- **Braggy** has caught interest from MCE2021 working group, what should be the role within MXCuBE collaboration?
- SSX for ID29 and MicroMAX, some bilateral discussion has started on fixed target and injector data collections methods
  - T-REXX specific development closely linked
  - Prototyping started
  - Opening for general discussion

In the long term:

- What is going to be **MXCuBE in 5-10 years**?
  - **New methods? More automation?** ...?
- Do we need a place for a "**sandbox**"?
- Is there anything we can anticipate in term of technology?

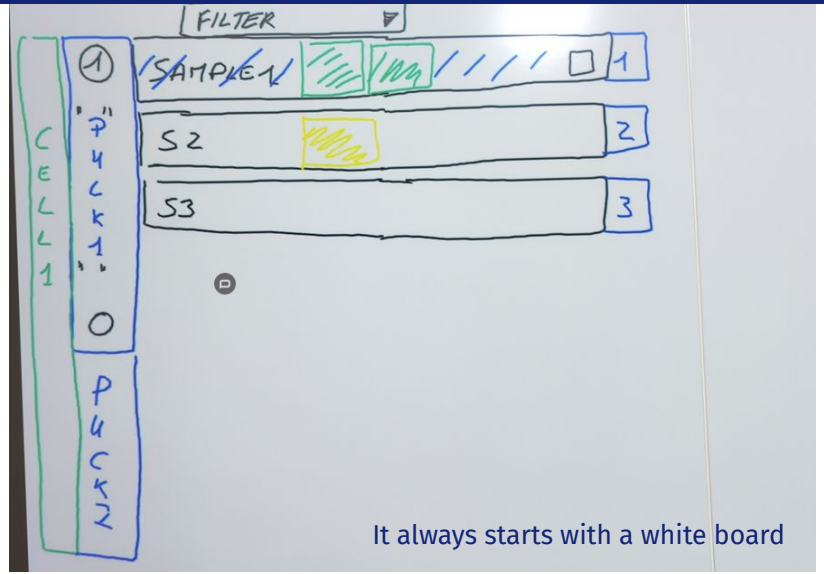




Plan for the next 6 months:

- No additional human resources
  - Is this a common critical point?
- ID29, ID29 and ID29
- Redesign Samples interface - Improve users experience and automatic beamline operation
- New workflow engine
- GPhL workflows

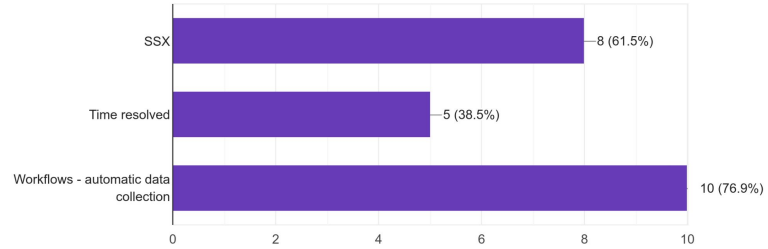
- **Users did not come back on site!**
- Their experiments are getting shorter (and faster)
  - Less samples sent
  - More native data collection? AF2?
- Urgent to make automatic workflows available natively in MXCuBE
- In person meeting at ESRF end 2022 (SSX focused?WFs focused?)



It always starts with a white board

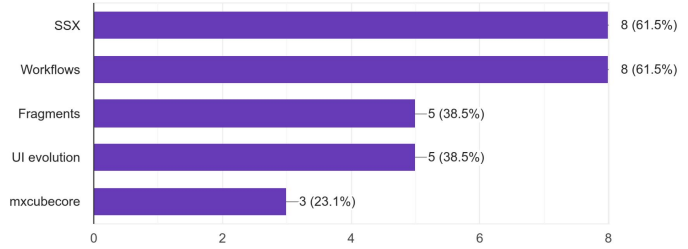
Topics for Scientists and Developers future goals

13 responses



Main topics of the meeting (for the round table discussion)

13 responses



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