

Status report EMBL-HH

Ivars Karpics



Content

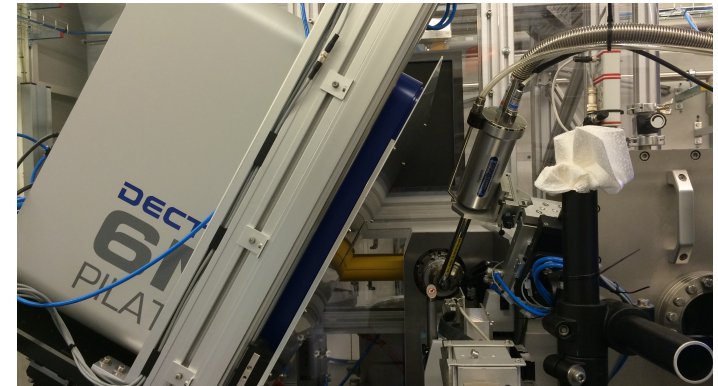
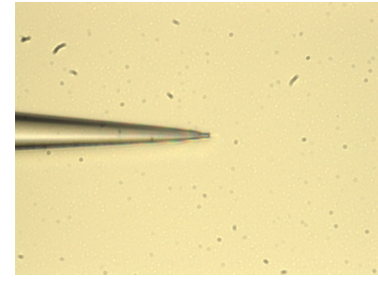
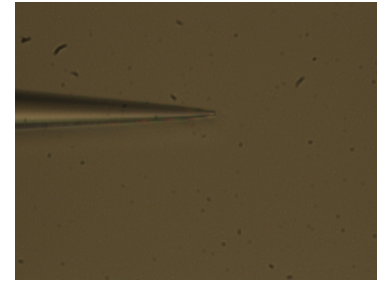
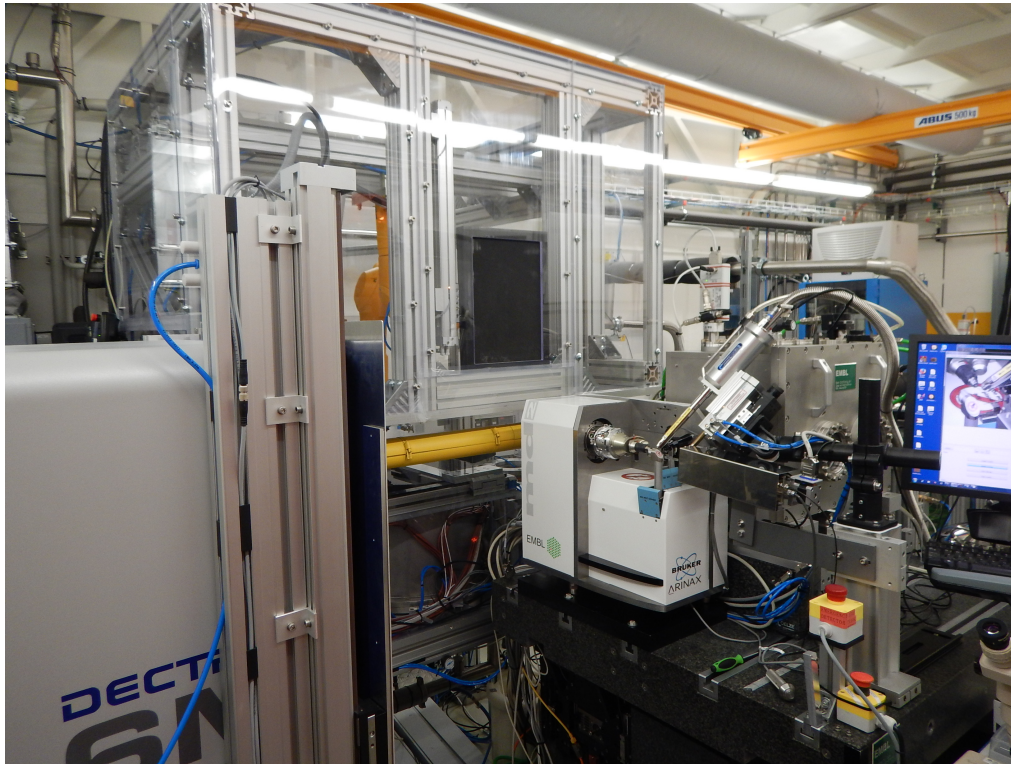
Status report

- MX beamlines at EMBL Hamburg
- Local infrastructure
- From the last meeting
- Last changes
- Integration of Marvin sample changer and plate manipulator

Conclusions

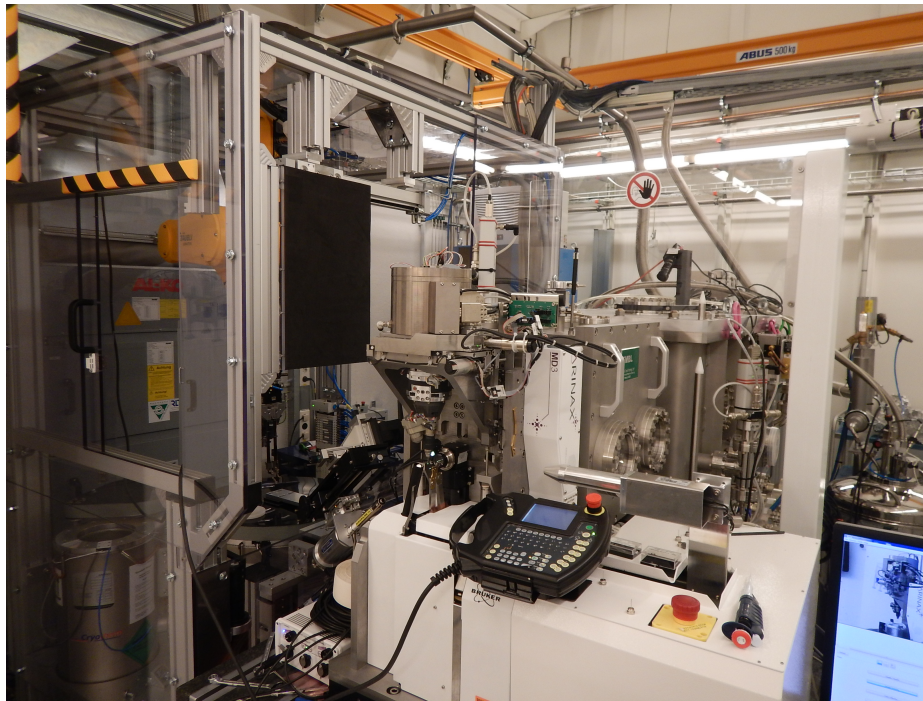
P13 beamline at EMBL Hamburg

- Variable beam size and high flux;
- Tunable energy between 4.5 and 17.5 keV;
- MD2 diffractometer (Refurbished: CPU and software upgrade, new Prosilica camera, backlight installed);
- Pilatus6MF detector (2 θ detector stage tilt);
- EMBL Marvin sample changer (fully operational from MXCuBE).
- Remote access available.

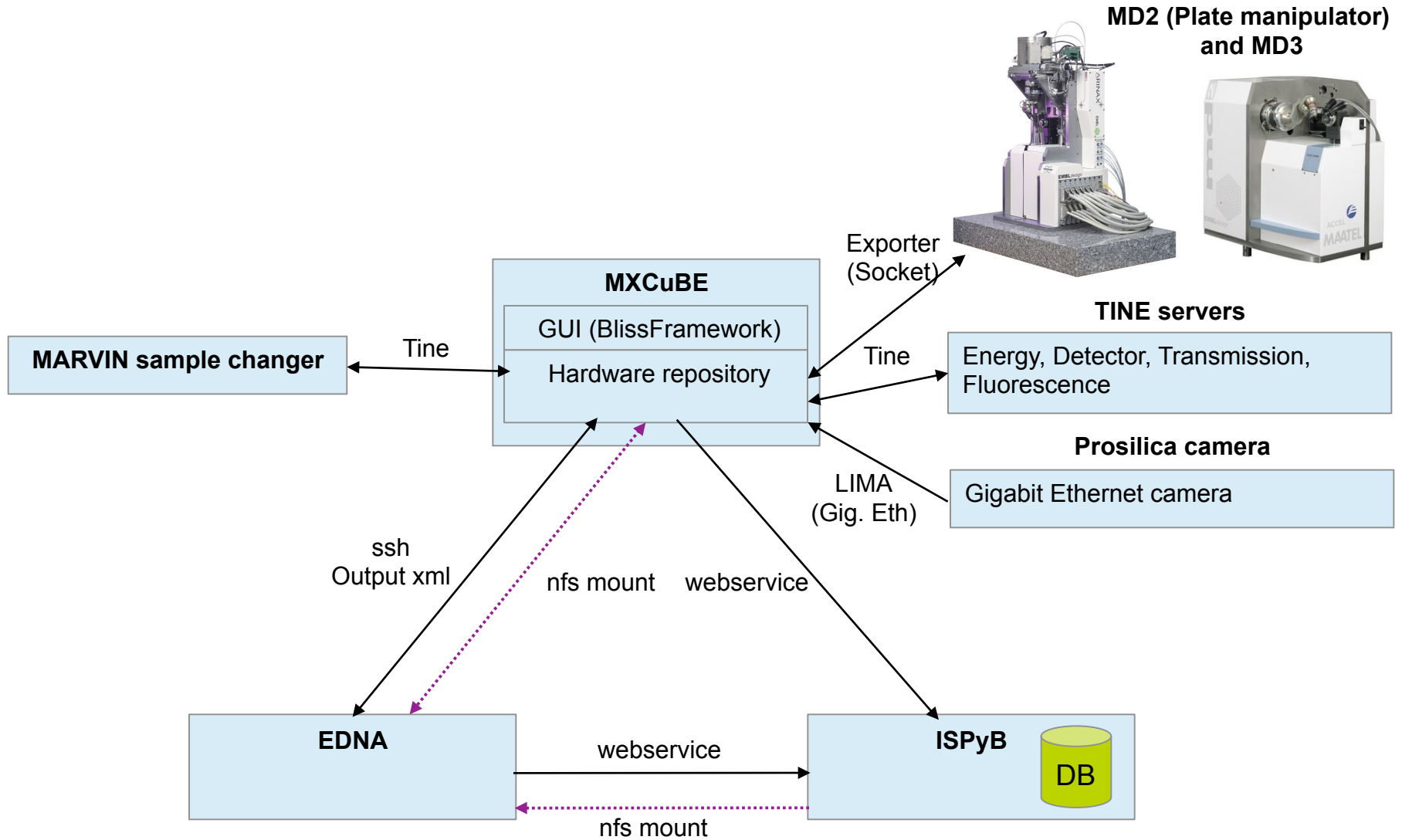


P14 beamline at EMBL Hamburg

- Micro-beam conditions with 5 x 5 micron beam;
- Unfocused, horizontally and double focused modes (5 μ m - 250 (400) μ m);
- Tunable energy between 6 and 20 keV;
- MD3 diffractometer;
- Pilatus6MF detector;
- EMBL Marvin sample changer;
- Compound refractive lenses (ESRF / CINEL) installed. 6 groups, 17 lenses, 63 focal distances. Controlled via Labview and GUI for MXCuBE in development.




Local infrastructure




From the last meeting

1. TODO list from the last meeting in Berlin.
2. Visiting ESRF in July 2015.

Feature list (MXCuBE meeting Berlin 1-2.06.2015) #92

 **IvarsKarpics** opened this issue on 2 Jun · 0 comments




IvarsKarpics commented on 2 Jun Owner

- Mesh drawing tool
- Mesh collection method and analysis
- X-Ray centring
- Integration with EDNA (thumb, char., autoprocessing)
- Generic diffractometer
- Interleave (energy, position, ...): queue handling, collection task, gui. Start with prototype Issue #59
- Workflows (reconsideration). Define Advanced scans task widget
- Autocentring in HutchMenuBrick?
- Temporary disable functionalities due to conflicts, blocks, interlocks

Documentation for developers #94

 **IvarsKarpics** opened this issue on 4 Jun · 0 comments



IvarsKarpics commented on 4 Jun Owner

I added xml configuration for EMBL Hamburg beamlines p13, p14.
See commit: [2ed8b4b](#)

Please feel free to add your site configuration files in a new sub directory (sitename_beamlinename). Also I added some information about configuration files. This documentation is under docs directory.
See commit: [c83e895](#)

See link https://github.com/mxcube/mxcube/blob/master/docs/source/packages/example_files.rst
Marcus did a major work and started this documentation. It is based on sphinx and you have to build it. For example make html will create html pages. I will create a pdf file and add them to git, so all documentation is available in one file.

Configuration example Files

Example configuration files for framework-2 hardware objects. These xml files can also be found in ExampleFiles/HardwareObjects.xml.

Basic configuration file structure

Configuration xml file defines hardware object behaviour. Available configuration methods are described in example:


```
<equipment class="ExampleClassName">
  <!-- Short description -->
  -->
  <!-- Channels -->
  <channel type="exporter" name="chanExporterChannelName">ExporterValueName</channel>
  <channel type="spec" name="chanSpecChannelName">SpecValueName</channel>
  <channel type="tline" name="chanTlineChannelName" tlineName="SpecificTlineName">TlineValueName</channel>
  <channel type="tango" name="chanTangoChannelName" polling="events">ChannelValueName</channel>
  <channel type="taco" name="chanTacoChannelName" taconame="TacoName" polling="3000" compare="False">TacoValueName</channel>
  <!-- Command -->
  <command type="exporter" name="cmdExporterCmdName">ExporterValueName</command>
  <command type="spec" name="cmdSpecCmdName">SpecValueName</command>
  <command type="tline" name="cmdTlineCmdName" tlineName="TlineName">TlineValueName</command>
  <!-- Hardware objects -->
  <object href="/device-role" role="device_role"/>
  <object href="/subdir/device-role-two" role="device_role_two"/>
  <!-- Properties -->
  <propertyNameOne>0</propertyNameOne>
  <propertyNameTwo>1.23</propertyNameTwo>
  <propertyNameThree>true value</propertyNameThree>
  <propertyNameFour>True</propertyNameFour>
  <propertyNameFive>{0, 1, 2, 3}</propertyNameFive>
  <propertyNameSix>{"one": 1, "two": 2}</propertyNameSix>
</equipment>
```

Basic xml file formatting guide lines:

- Xml file starts with class type (**Device**, **Equipment** or **Procedure**) and class name
- Class name should match with hardware object file name and class name defined in this hardware object. If class=ExampleClassName then file ExampleClassName
- It is recommended to organize channels and command alphabetically.
- Channel name should have template **chanExampleName** and initialized as **chan_example_name**
- Command name should have template **cmdExampleName** and initialized as **cmd_example_name**
- Property name should be in camelcase style. For example: propertyExampleName and initialized as self.property_example_name
- It is possible to use boolean, int, float, lists and dictionaries as property names
- Use xmllint filename.xml to verify xml

Abstract classes #99

 **IvarsKarpics** opened this issue on 27 Jul · 0 comments



IvarsKarpics commented on 27 Jul Owner

As each time there is a request to have more abstract classes, I added new ones (see commit [b2e7c4d](#)):

- AbstractDetector,
- AbstractMotor,
- AbstractXRFspectrum.

I also changed AbstractEnergyScan, because from queue just two methods are called. All other methods are not used on all sites. It might be a conflict in this, because method parameters in startEnergyScan differ. This we have to discuss.

I updated also EMBL related hwobj to match these abstract classes (see commit [8fa019f](#))

Any comment and suggestions are welcome!

Last changes

The screenshot displays the mxCuBE software interface with several key components:

- Top Bar:** Menu (Instrumentation, Help), Collect, Log, Test (highlighted with a red box).
- Sample Positioning:** Omega (90.0), Kappa/Phi (-0.50, 0.01), Holder length (-0.881), Focus (0.968).
- Sample Video:** Front light (0.6, 0.1), Back light (1.0, 0.1), Zoom (1), Focus (0.968).
- Central Image:** A large image of a sample, possibly a protein crystal, with a 200 µm and 500 µm scale bar.
- Beam Alignment (Bottom Left, highlighted with a red box):** Beam size (Horizontal: 30 µm, Vertical: 30 µm), Aperture (30 µm), Mode (small), Phase (Centring), Pitch 2nd (0.41), VHM Pitch (2.261), Roll 2nd (0.4533).
- Collection Method (Middle Right):** Acquisition parameters including Oscillation range (0.1000), Exposure time (0.0400), Energy (12.7290 keV), Resolution (0.000 Å), and Transmission (100.000%).
- Data Location (Middle Right):** Folder: /data/Int10736_206/karpics/20151118/RAW_DATA, File name: prefix_1#####.cbf.
- Processing (Middle Right):** N.o. residues: 200, Unit cell parameters (a, b, c, α, β, γ).
- Comments (Bottom Middle):** A text area for user notes.
- Characterisation (Bottom Middle):** Helical Collection, Energy Scan, XRF spectrum, Advanced scan.
- Proposal and Sample List (Right Panel, highlighted with a red box):** Proposal: mxih0001 - Pro, Sample list: 1:1 - testCr-p01..., 1:2 - testCr-p01..., 1:3 - testCr-p01..., 1:4 - testCr-p01..., 2:1 - testCr-p02=01, 2:2 - testCr-p02..., 2:3 - testCr-p02..., 2:4 - testCr-p02..., 3:1, 3:2, 3:3, 3:4, 3:5, 3:6, 3:7, 3:8, 3:9, 3:10, 4:1, 4:2, 4:3, 4:4, 4:5, 4:6, 4:7, 4:8, 4:9, 4:10.
- Information (Top Right):** Machine current (0.0 mA), Machine state text (Wartung), Intensity monitor (177 A), Hutch temperature (23.0 C), Hutch humidity (39.4 %), Storage disc space (Total: 9.7TB, Free: 1.3TB (14%)), Cryojet position (In place), Oxygen level in robot cage (21.64%).
- Energy (Middle Right):** Current (12.7290 keV, 0.97 A), Move to (keV).
- Transmission (Middle Right):** Current (100.00%), Set to (%).
- Resolution (Middle Right):** Current (0.000 Å), Move to (Å).
- Status Indicators (Bottom Right):** Door interlock (Unlocked), Safety shutter (disabled), Fast shutter (disabled), Image tracking (ready), Enable Advx image tracking (checked), Detector status (Ready), Temperature (0.0°), Humidity (0.0%).

MARVIN SC integration

1. Based on the GenericSampleChanger.
2. Up to 16 pucks in the dewar.
3. Mount, dismount and chained mount available from MXCuBE.
4. No barcodes yet, but hopefully soon will be available.
5. Oxygen level and master alarm in MXCuBE.

PlateManipulator

1. Based on the GenericSampleChanger.
2. Possible to define number of columns, rows and drops per cell.
3. Communication via exporter.
4. Connection to CRIMS.
5. PlateManipulatorBrick.

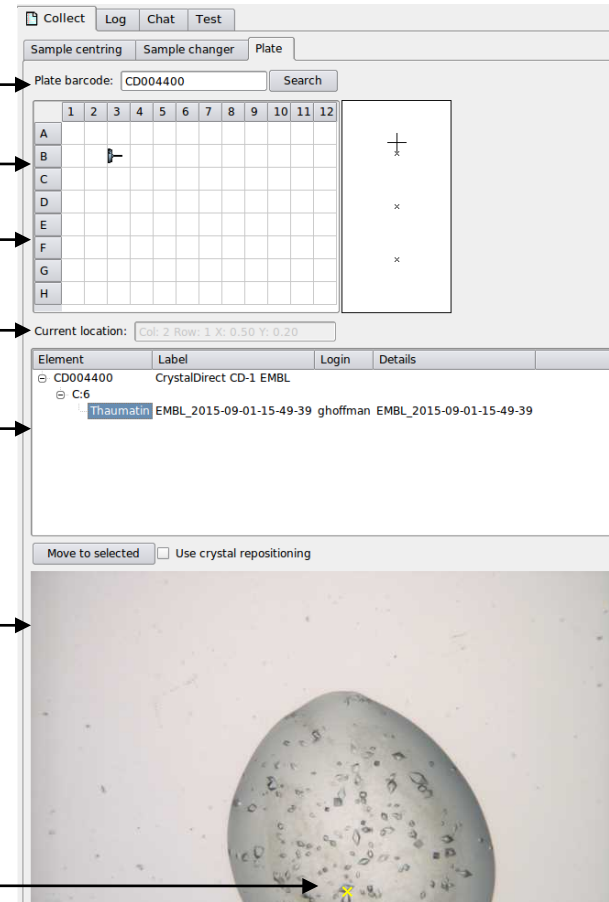
Plate barcode
Navigation table

Navigation in cell
Current location

Crystal tree

Snapshot

Crystal position



Conclusion

1. Full 6/7 operation.
2. New devices installed and commissioned:
 - CRLs at P14;
 - Automatized fluorescence detectors;
 - Marvin sample changer at P14.
3. New plate hardware object and brick.
4. New brick for beamline tests.
5. Successful remote data collection on P13. Remote access will be fully available after the shutdown.

About advanced collection methods and Qt4 in next presentations.

Thank you for your attention