The year 2020 of remote operation at P11

Current and future trends in Macromolecular Crystallography experiments: Focus on Automation, high data rate analysis and User Interfaces

18.03.21

Guillaume Pompidor
Outline

• The P11 beamline at PETRA III

• User Interface

• Remote data collection

• The 2020 year
P11 – High Throughput MX beamline at PETRA III

1) Crystallography experiment

- In user operation since 2013
- Broad energy range: 5.5 - 28 keV
- High-speed sample changer with capacity (23 unipcuks = 364 samples)
- Various focusing options (beamsize from 4 x 9 to 200 x 200 um)
- Pilatus 6M, Eiger2 16M (permanent)
- XRF for experimental phasing (SAD/MAD) and element analysis
- Serial crystallography
2 KB Systems:

- 1st KB system: 2 hor. and 1 vert. deflecting mirrors for generation of a secondary source at 65.5 m

Flexibility in beam size and flux by mirror bending and apertures:

<table>
<thead>
<tr>
<th>Beam size (µm)</th>
<th>Flux (ph/s)</th>
<th>T_xtal (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 x 200</td>
<td>3.1e12</td>
<td>800</td>
</tr>
<tr>
<td>200 x 200</td>
<td>6.45e12</td>
<td>360</td>
</tr>
<tr>
<td>100 x 100</td>
<td>1e13</td>
<td>40</td>
</tr>
<tr>
<td>50 x 50</td>
<td>1e13</td>
<td>10</td>
</tr>
<tr>
<td>20 x 20</td>
<td>1e13</td>
<td>1.6</td>
</tr>
<tr>
<td>4 x 9</td>
<td>1e13</td>
<td>0.17</td>
</tr>
</tbody>
</table>
CrystalControl

- Inhouse-developed Python-based GUI for standard MX applications including SAD/MAD phasing

- Expert mode for beamline support (apertures, rotation axis, beam position...)

DESY.
Sample changer: Puck and sample selection
CrystalView: zoom selection and 3 clicks centering
Data collection: Number of frames, exposure time, angular step
Data collection: Energy, Focus selection, Pinholes, transmission, resolution (det. distance)
CrystalControl

- SAD/MAD phasing
CrystalControl

- ISMO scantool: GUI for fixed-target SSX, data collection with (rotation wedges) and without $\phi$ rotation (still images)

- Heat map overlayed on the sample view
Implementation of remote data collection

• Beamline control by one user only
• Access to needed functionalities only
• Monitoring of user actions
• Possibility to take back the control at any time for the local contacts
• No need of special hardware, software or OS dependencies for the user community
• Authentication against personalized account
• Remote access dependent on valid safety training
Technical Implementation (Spring 2020)

- **FastX**
- Commercial software for Linux remote desktop
- X server from a web browser
- Similar to Maxwell Cluster (computing at DESY)
- Sessions between several users with only one controlling
- Running on a dedicated host
Remote identification via user database: Door

User view

- Selection of ‘remote’, ‘onsite’ or ‘data-access’ during user registration
- Automated e-mail notification once the remote is open
- All participants can log-in at the same time from different locations, one has control over the experiment, can be swapped independently among the users
- Detailed instructions on our public webpage for shipment, remote session and data processing
- Support via zoom
- Successful operation also with users who were never onsite; connection stable and shipments running e.g. to China and India
Remote data collection
Remote data processing on Maxwell Cluster

- Computing cluster for DESY
- Access via scientific account
- Backup (or via Gamma portal)
- Data processing
  - Albula, adxv
  - XDS, imosflm
  - ccp4, Phenix
  - Coot, Chimera
Machine down due to the lock-down!

Gripper repairs
Pandemic vs user operations 2020

Suspended user operations mid-March - April 2020: only Fast-track open

Enhanced remote at P11 since October 2020
Covid-tests since November 2020

Masks & distancing: May-October 2020

IMPORTANT INFORMATION ON COVID-19
FOR WORKERS AND USERS AT P11 BEAMLINE

Dear User/DESY worker,

Due to the current COVID-19 restrictions, the following safety procedures are mandatory for experiments and technical work at P11 Beamline/DESY Campus:

1. The maximum number of participants coming at DESY campus per experiment is 3 persons.
2. The maximum number of participants on site at the beamline (control hutches and experimental hutches) is 2 persons, preferably only 1 if possible.
3. Two persons in a ventilated room can work without masks only if they keep a steady distance of 2 meters.
4. If 2 persons must work in a non-ventilated room for less than 15 minutes at a distance below 2 meters, a simple mouth/nose protection must be worn (so-called surgical mask). Self-sewn masks are also permitted.
5. If 2 persons must work in a non-ventilated room for more than 15 minutes at a distance below 2 meters, FFP2 masks must be worn, and provisionally also FFP3 masks.
6. Gloves should be always used if possible.
7. Please disinfect your hands and any shared equipment (keyboards etc) after use.

In case of doubts, please ask a P11 Team member.

Thank you for your collaboration,

Your P11 Team
User statistics

All shifts

Numbers extracted from shifts actually carried out
Inhouse and commissioning are by P11 staff only
Serial Synchrotron Crystallography with tape-drive 24 shifts, with chips 18 shifts
Some empty days due to repairs and short-notice cancellation
11 shifts given out from INH for ‘friendly users’ i.e. users with no valid proposal => need for rolling access scheme
SARS-CoV2-related research arising from P11
Also outside of the fast-track procedure

37 structures deposited from P11 (Main Protease)

30 from the fast-track screening campaign by Alke Meents
3 through other fast-track projects
2 through priority access
2 through regular proposals

Publications:
“Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved α-ketoamide inhibitor” (Zhang et al., 2020, Science, 368, 409-412)
“Catalytic cleavage of HEAT and subsequent covalent binding of the tetralone moiety by the SARS-CoV-2 main protease” (Günther et al., 2020)
“Repurposing the HCV NS3–4A protease drug boceprevir as COVID-19 therapeutics” (Oerlemans et al., RSC Medicinal Chemistry 2021)
Thank you

Johanna Hakanpää
Sofiane Saouane
Eva Crosas
Spyros Chatziefthymiou
Jan Meyer
Bernhard Kistner
Jakob Urbschat
Jan-Peter Kurz