PAUL SCHERRER INSTITUT

MX Group @ Swiss Light Source

REMOTE OPERATION INSTRUCTIONS FOR USERS

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0.2-0.4	03-06-2020	Incorporation of feedback	DF61
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1 Purpose of this Document

This document describes the procedure for remote operation and provides a step-by-step description for the user. The process is binding, and exceptions to this document have to be agreed upon ahead of time by all sides.

Please make sure you refer to the most recent version of the document. As a rule of thumb, we intend to update it after each shutdown (see SLS schedule).

2 General Information

2.1 Useful Links

User office webpage	https://www.psi.ch/en/useroffice
Digital User Office	https://duo.psi.ch/duo
Remote access instructions	https://www.psi.ch/en/photon-science-data-services/getting-started
Offline computing cluster	https://www.psi.ch/en/photon-science-data-services/offline-computing-facility-for-sls-and-swissfel-data-analysis
Data Acquisition Software	https://www.psi.ch/de/sls/pxiii/data-acquisition
Remote Data Transfer	https://www.psi.ch/en/photon-science-data-services/slsswissfel-data-transfer
TELL sample changer	https://www.psi.ch/en/sls/pxi/sample-changer
TELL spreadsheet validator	https://rp.psi.ch/mx-webapps/spreadsheet/
Dewar shipping	https://www.psi.ch/en/sls/pxi/infrastructuredewars
Members of the MX group	https://www.psi.ch/en/macromolecular-crystallography/people

2.2 Beamlines

The MX group at the SLS is operating three beamlines. For shift assignment and local contact information, please refer to the beamlines calendar.

Beamline	Common name	Type	Calendar
X06SA	PX I / PX 1	Insertion device	https://duo.psi.ch/duo/public_month.php?BEAMLINE=PX
X10SA	PX II / PX 2	Insertion device	https://duo.psi.ch/duo/public_month.php?BEAMLINE=PXII
X06DA	PX III / PX 3	Bending magnet	https://duo.psi.ch/duo/public_month.php?BEAMLINE=PXIII

2.3 Shift schedule

The beamlines are operated in a three-shift scheme, six days a week. Each of the beamlines has a different shift starting time.

Since we need time to check beamline alignment, unload and load samples, the actual measurement time officially starts **one hour after the allocated shift starting time**. Depending on the circumstances, you may be able to start your beamtime earlier, so stay close to your phone.

Usually we try to allocate shifts II & III as a double shift to avoid user switches in the middle of the night. Exceptions have to be agreed upon ahead of time with your beamline scientist.

Since we have routine machine maintenance shifts on Tuesdays, the shift III from Monday to Tuesday ends already at 07:00 on **all three** beamlines.

Please refer to the table below to make sure you have the right times:

Beamline	Shift I	Shift II	Shift III[1]
X06SA	shift time: 09:00 – 17:00 measuring time: 10:00 – 17:00	17:00 – 01:00 18:00 – 01:00	01:00 – 09:00 (02:00 – 09:00)[2]
X10SA	shift time: 10:00 – 18:00 measuring time: 11:00 – 18:00	18:00 – 02:00 19:00 – 02:00	02:00 – 10:00 (03:00 – 10:00)[2]
X06DA	shift time: 09:30 – 17:30 measuring time: 10:30 – 17:30	17:30 – 01:30 18:30 – 01:30	01:30 – 09:30 (02:30 – 09:30)[2]

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[1] Please be aware that the shift III from Mondays to Tuesdays ends already at 07:00 Tuesday morning due to machine maintenance.

[2] Usually we avoid user handover between shifts II and III, but assign double shifts overnight. Exceptions need to be agreed upon with your local contact/beamline scientist.

2.4 Support by the MX Group

The MX group will support you all the way throughout your experiment.

- Before your experiment, we will...

    o ... help you arrange beamtime, shipping of samples, remote connection tests.

    o ... answer any questions related to your upcoming shift and/or experimental challenges

- During the experiment, we will…

    o … setup and check the beamline to ensure perfect operation

    o … load your samples to the sample changer robot (TELL)

    o … help you get started/improve data collection strategy (if arranged ahead of time)

    o … provide you with on-site support to fix issues from 9:00 – 23:00

    o … provide best-effort support at night

    o … unload your samples and prepare them for shipping back

- We will not…

    o … perform experiments for you

    o … backup your data to an external hard disk

3 Before your Beamtime

Your beamline scientist will assist you in booking a suitable beamtime and arranging shipping of your samples to the SLS. Your local contact will help you with the remote connection test, if necessary, and takes care of you during the experiment. To do that, he or she needs all information about what you intend to measure and the sample information ahead of time. If you have any questions, please do not hesitate to contact your local contact or beamline scientist.

3.1 First Time Setup

1. Create a "Digital User Office" (DUO) account at https://duo.psi.ch/duo/, if necessary. If you are the submitting proposer for beamtime proposal, you should already have this. This account is personal (i.e. each natural person needs their own).

2. To access the beamline network from outside of PSI, you need to request an external PSI account (ext-account). This is done via your local contact or beamline scientist in the MX Group. This account is personal (i.e. each natural person needs their own). More information can be found at https://www.psi.ch/en/photon-science-data-services/getting-started.

3. For access to the beamline control console, we use the NoMachine client:

    o Install the NoMachine software on the computer that will be used for remote connection https://www.nomachine.com/download

    o Keep your NoMachine installation updated

    o We strongly recommend that the screen you use have a resolution of at least 3840x2160 (4K) as this is the native resolution of the control computer you connect to

    o Internet connection on the machine should be at fast as possible to ensure stable video transmission

4. Arrange for a test connection with a beamline scientist/local contact

    o Pay special attention to connection speed, quality of video transmission, screen settings (legible text, pixelated or choppy video)

    o Find your local contact person in the beamline calendar (see 2.2) and at: https://www.psi.ch/en/macromolecular-crystallography/people

    o Follow the instructions for the actual connection at https://www.psi.ch/en/photon-science-data-services/remote-interactive-access

5. If you are new at our beamlines or feel you need a refresher, make sure to inform your local contact that you need training. We will arrange for somebody to train you ahead of the beamtime or at the start of you shift. If we are not informed ahead of time, we cannot ensure somebody is available at the start of your shift.

At a Glance

1. Get DUO-account

2. Get ext-account

3. Install NoMachine

4. Arrange Connection Test

5. Arrange Training Session
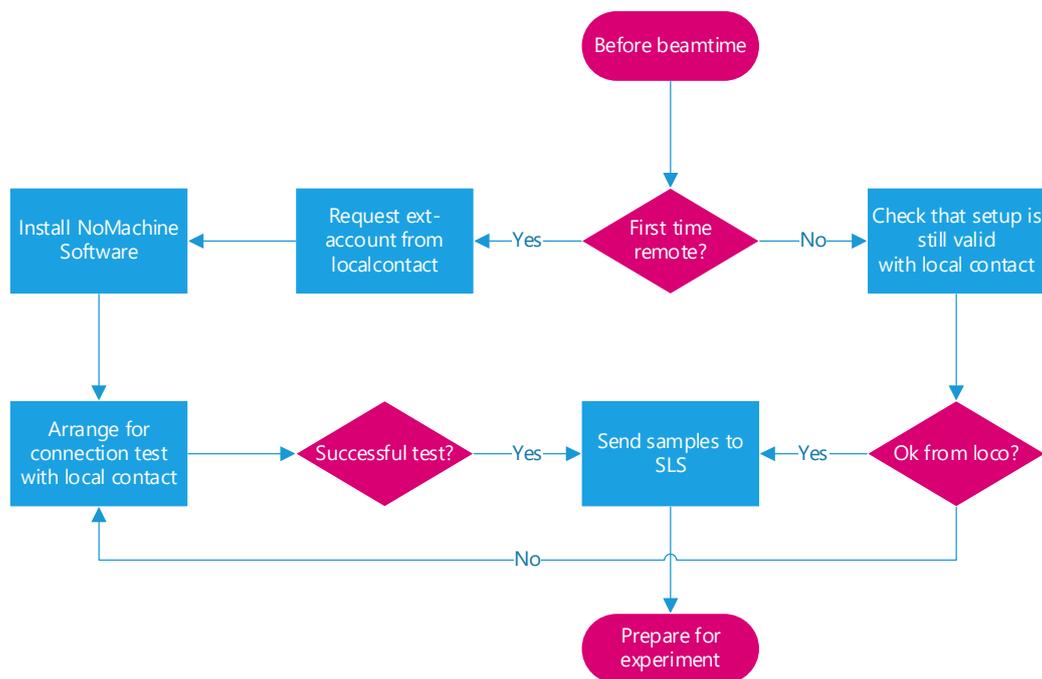
3.2 Regular Procedure

Figure 1: Beamtime preparation for remote users

3.2.1 Coming back?

If you are a returning remote user please make sure you read the most current version of this document. It is available on our website (https://www.psi.ch/en/macromolecular-crystallography). If your last beamtime was more than 4 months ago, please re-arrange for a test connection (see paragraph 4 in Section 3.1 above).

3.2.2 Spreadsheet

To use our automatic sample changer robot (TELL), the use of a spreadsheet containing all sample information is **mandatory**. Please follow the procedure below:

1. Download the XLS template from https://www.psi.ch/en/sls/pxi/sample-changer

2. Name the spreadsheet according to our convention:

        {date as YYYYmmdd}_{beamline}_{shift}_{e-account}.xlsx

                    Example: 20200527_PX2_S2_e10003.xlsx

3. Fill out the spreadsheet according to the instructions you find in the template or in the APPENDIX A.2 below

   o Validate your spreadsheet at https://rp.psi.ch/mx-webapps/spreadsheet/ to find out if there are errors or things that could be improved

   o The spreadsheet **MUST** contain all pucks that are to be measured on a given beamtime, including pucks from dewars that are already at the SLS, e.g. from a previous beamtime.

   o Make sure all dewars are labeled with the **EXACT NAME** as in the spreadsheet. Please add stickers to both the lid and side of the actual dewar, not the shipment box (see Figure 3 below).

At a Glance
1. Download template
2. Name correctly
3. Fill out spreadsheet
4. Validate
5. Send to LoCo

4. Send the spreadsheet to your Local Contact **at least one business day ahead** of the beamtime.

3.2.3 Dewar Shipment

Proper and timely shipping is of utmost importance for a successful remote experiment. To make logistics as stress-free as possible, we ask you to send the samples with plenty of time to spare to accommodate hiccups in shipment. The samples need to **arrive at least a full business day ahead of your beamtime**. This means, for example, that samples for the weekend need to arrive at SLS on Thursday before. Please keep in mind that there is no possibility to accept shipments at PSI outside of business hours (Mon-Thu 7:00-16:00, Fri 7:00-15:00). If there is a Swiss public holiday, the delivery time has to be adjusted accordingly. Late shipment is a major cause of lost or delayed beamtimes.

You can find our detailed logistics information at https://www.psi.ch/en/sls/pxi/infrastructuredewars.

For detailed questions, contact the MX logistics responsible, Sonia Reber (sonia.reber@psi.ch).

1. All Unipucks shipped to SLS for measurement **must** have a 2D Data Matrix engraved on the side of the lid, containing the **exact name** as noted in the spreadsheet.

   o See https://www.psi.ch/en/sls/pxi/sample-changer for details.

   o You can etch the Data Matrix onto your Unipucks free of charge at the PSI – please contact Justyna Wojdyla (justyna.wojdyla@psi.ch) for details.
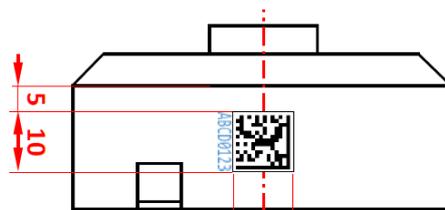
Figure 2: Example of Datamatrix 2D Code on Unipuck lid

2. Make sure the dewars are CLEARLY LABELED (on the side and the lid) with the exact name noted in the spreadsheet.

Figure 3: Locations of dewar name tags

At a Glance
1. Ensure Data Matrix is present
2. Label dewars
3. Verify shipping instructions
4. Pucks will come back as sent

3. Pucks will be loaded as they arrive. We will not check for correct naming, matching names of base and lid, etc. Please double check your pucks are matching the naming of lid, base, and spreadsheet.

4. Pucks will be put back into the original dewar in which they arrived (no reshuffling between dewars).

5. Samples will be shipped back to you earliest one business day after your last shift. If your samples should remain at our site for a follow up experiment, please arrange with the local contact.

3.2.4 Provide Information to your Local Contact

Please make sure that you send your spreadsheet and all additional information needed to your local contact at least one full working day ahead of the beamtime. Please ensure all points below are addressed:

1. **Operators name**. This is the person on your side actually performing the remote experiment.

2. A **phone number** under which the operator is reachable **at all times**.

3. The **e-account** that will be used for data collection.

4. The **ext-account** used for remote connection.

5. Special instructions/comments to the local contact:

   o beam size, energy, etc.

   o dewars to be kept at SLS for the next beamtime

6. If you need assistance at the beginning of the shift, such as:

   o Software introduction

   o Advanced experiment(s)

4   Day of the Experiment

On the day of your experiment, the local contact (LoCo) will first check that the beamline is in a proper state for your measurement. Then the previous users samples are unloaded from the TELL robot, and your samples loaded. When everything is ready, the LoCo will contact you **by phone** and only then you are free to log in and start your experiment. Usually we reserve one hour for this procedure.

Please always contact your local contact by phone only. Emails are not always read in time and are thus not a viable means of communication.

1. Setup:

   o Local Contact ends previous experiment.

   o LoCo unloads samples and checks beamline alignment.

   o LoCo loads your samples according to your info and spreadsheet.

2. Once the setup is performed, the LoCo calls the operator to confirm …

   o … contact phone number

   o … transferred information

   o … working setup

3. Only after successful phone call the remote access is enabled and the operator can log in to the user console:

   `{beamline}-cons-701`, e.g. x06sa-cons-701

At a Glance
1.   LoCo does setup (~1h)
2.   Operator must be on phone
3.   Remote enabled after ok from LoCo only
4.   LoCo provides support via phone

4. During the experiment, the LoCo is reachable by phone (not email) from 09:00 – 23:00. If agreed, also at night on a best effort.

5. Setup remote data transfer
   (https://www.psi.ch/en/photon-science-data-services/slsswissfel-data-transfer)

5   After the Beamtime

Once you are finished with your measurement, please do the following:

1. In TELL GUI, go to **Actions** -> **Load, Remove Pucks**. This will set the robot into dry mode for unloading.

2. Announce your beamtime as finished by selecting "**Conclude beamtime**" in the launcher and follow the steps. If this fails or you forgot, send an email to your local contact. Please refrain from calling if you finish after 23:00.

3. Disconnect from the NoMachine session **without** quitting any software or logging out of the console.

Your samples will be unloaded and prepared for return shipment, unless arranged otherwise with local contact/logistics responsible.

Appendix A.

A.1. Glossary

Beamline Scientist	A Scientist responsible for maintaining and operating one of our MX beamlines. Not necessarily equivalent to the "*Local Contact*"
Beamtime	one or more continuous shifts assigned for proposal
DA+	MX beamline control software
DUO	Digitial User Office
e-account	"experiment account". A Linux account used to log in in the beamline control computer for data collection. This is the account the data is stored in. It is linked to the proposal, i.e. each proposal has its own e-account
Ext-account	"External account". A personal account granted to an individual who is not employed or working at PSI, to use PSI computing facilities, such as computing nodes, remote data transfer rand remote log in
Experiment	see "*Beamtime*"
Local Contact	A member of the MX group supporting you during your beamtime
LoCo	see "*Local Contact*"
MX	Macromolecular Crystallography
Operator	person running the experiment, either on site or remotely
PSI	Paul Scherrer Institut
Shift	8-hour beamtime chunk in beamline calendar
TELL	MX specific automatic sample changer robot

A.2. Spreadsheet instructions

Instructions
==============
Mandatory Columns

DewarName: This name is displayed in the GUI and helps the operator to identify onto which shipping dewar each puck belongs to.

PuckName: This name should correspond to the Data Matrix engraved in the puck, which will be scanned during loading/unloading operations. Only letters [a-z] and digits [0-9] are considered when matching the PuckName with the resulting scanned Data Matrix. The following strings would match a Data Matrix scanned as "PSIMX-100":
   - "PSIMX100"
   - "psimx:100"
   - "PSI:MX-100"
  -"PSIMX100"
    The PuckName is made available in the *sgPuck* macro (see section **On the use of Macros** below).

CrystalName: By default, the text in this column will be transferred to the Prefix field in the DA+GUI. The text is also made available as the macro *sgPrefix* in the DA+GUI.

Valid characters: a-z 0-9 minus period plus underscore

PositionInPuck: An integer number indicating the position within the puck. For Unipucks this number must be within 1-16. Available in the *sgPosition* macro.

Optional but Highly Recommended

Optional means that the content of the cells may be omitted but the
column itself must be present.

Priority: This should be an integer number. The operator will see this number in the TELL-GUI. This number may be used to sort the samples within the TELL-GUI. This number is made available as the macro "sgPriority".

Comments: This text is available to the operator. This text may be used to sort the samples within the TELL-GUI.

Directory: by default the text in this column will be transferred to the Folder field in the DA+GUI. The text is also made available as the macro "sgFolder" in the DA+GUI. Macros may be used in this field to compose folder locations using other macros corresponding to fields from the spreadsheet or dynamic macros corresponding to parameters from the DA+GUI.

ON THE USE OF MACROS
====================
Spreadsheet Macros
----
sgPrefix: text in the column CrystalName

sgFolder: text in the column Directory

sgPuck: text in the column PuckName

sgPriority: text in the column Priority

sgPosition: text in the column PositionInPuck

Dynamic Macros
----
date: the current date as YYYYMMDD; the date will not change after midnight unless the DA+GUI is restarted

run: the run number

beamline: the official beamline name: X06SA, X10SA, or X06DA

prefix: the contents of the GUI field "Prefix"; may differ from the macro sgPrefix

dtz: the detector to sample distance rounded to the mm.

dty: the detector height offset rounded to the mm.

ev: the beam energy in electron volts, rounded.

method: either the string "screen" or "dataset" depending on the experiment

phi: the phi angle, rounded.

chi: the chi angle, rounded.