

PAUL SCHERRER INSTITUT



Kate Smith :: MX Data Software Developer :: Paul Scherrer Institute

Automated Data Collection at the Swiss Light Source using the Smart Digital User Software Suite

2022-03-01 SLS User Meeting – Demonstration

Demonstration - start of automation

The image displays a computer interface for the TELL Sample Changer GUI. The main window title is "NoMachine - PSI" and the application title is "TELL Sample Changer GUI". The interface includes a menu bar (File, Actions, Options, Sorting, Unattended, Help) and a central area with the text "TELL Sample Changer GUI" and "Please [import a spreadsheet](#) to continue..".

On the left, there is a sidebar with a red apple logo and a "Samples" section. The "Samples" section shows "File:" and "Number of Pucks: 0". Below this is a table with columns "Dewar", "Puck", and "Location", which is currently empty. A yellow button labeled "nothing to unmount" is visible below the table.

At the bottom of the sidebar, there is a "Mounted Sample" section with a "Log messages" tab. The "Mounted Sample" section includes fields for "Name", "Comments", "Priority", "Required Res. (Å)", "Spacegroup", "Cell Parameters", and "Heavy atoms". A red button labeled "update comment" is located at the bottom of this section.

At the bottom of the GUI, there is a status bar with the following text: "power:powered state:ready task:none position:cold mode:remote speed:100% magnet:50.0k detection:suppressed crystal:100.0k escape:SampleChange mounted sample:nothing mounted".

On the right side of the image, there are two XRD data plots. The top plot shows a series of diffraction peaks with blue arcs indicating the fit. The peaks are labeled with their corresponding 2θ values: 1.7Å, 2.1Å, 2.7Å, 3.9Å, and 7.7Å. The bottom plot is a dark image, possibly a close-up of a sample or a different view of the same data.

- Non-obligatory parameters are optional
 - All necessary params have defaults
- Parameters are forwarded to:
 - DA+ GUI in manual mode
 - Adp in manual and automated modes
- For automated run we recommend providing the data collection parameters

	PXI/PXII		PXIII	
2D grid scan	Exposure (sec)	0.02	Exposure (sec)	0.1
	Transmission (%)	100	Transmission (%)	100
	Detector distance (mm)	300	Detector distance (mm)	300
	Maximum grid size	4000	Maximum grid size	4000
Line scan	Exposure (sec)	0.05	Exposure	0.1
	Transmission (%)	100	Transmission	100
	Detector distance (mm)	300	Detector distance (mm)	300
	Maximum grid size	4000	Maximum grid size	4000
Data collection	Exposure (sec)	0.01	Exposure (sec)	0.1
	Oscillation (°)	0.2	Oscillation (°)	0.2
	Transmission (%)	60	Transmission (%)	100
	Total range (°)	220	Total range (°)	220
	Detector distance (mm)	200	Detector distance (mm)	200

V6.0									
Sample Information									
DewarName	PuckName	PuckType	PuckLocationInDewar	CrystalName	PositionInPuck	Priority	Comments	PinBarcode	Directory
X06DA CF	E-04	Unipuck	MX 2	lyso_1	1	1	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_2	2	2	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_3	3	3	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_4	4	4	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_5	5	5	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_6	6	6	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_7	7	7	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_8	8	8	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_9	9	9	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_10	10	10	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_11	11	11	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_12	12	12	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_13	13	13	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_14	14	14	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_15	15	15	test crystal		{date}/{prefix}
X06DA CF	E-04	Unipuck	MX 2	lyso_16	16	16	test crystal		{date}/{prefix}

Compulsory

Recommended

Spreadsheet format V6

Protein Name [str]	Data Collection						Automation
	Oscillation [deg]	Exposure [s]	Total Range [deg]	Transmission [%]	Target Resolution [Å]	Aperture [int]	Data Collection Type [str]
lysozyme	0.2	0.01	220	60	1	2	standard
lysozyme	0.2	0.01	220	60	1.5	2	standard
lysozyme	0.2	0.01	220	60	2	2	standard
lysozyme	0.2	0.01	220	60	1	2	standard
lysozyme	0.2	0.01	220	60	1.5	2	standard
lysozyme	0.2	0.01	220	60	2	2	standard
lysozyme	0.2	0.01	220	60	1	2	standard
lysozyme	0.2	0.01	220	60	1.5	2	standard
lysozyme	0.2	0.01	220	60	2	2	standard
lysozyme	0.2	0.01	220	60	1	2	standard
lysozyme	0.2	0.01	220	60	1.5	2	standard
lysozyme	0.2	0.01	220	60	2	2	standard
lysozyme	0.2	0.01	220	60	1	2	standard
lysozyme	0.2	0.01	220	60	1.5	2	standard
lysozyme	0.2	0.01	220	60	2	2	standard
lysozyme	0.2	0.01	220	60	1	2	standard

PXII specific



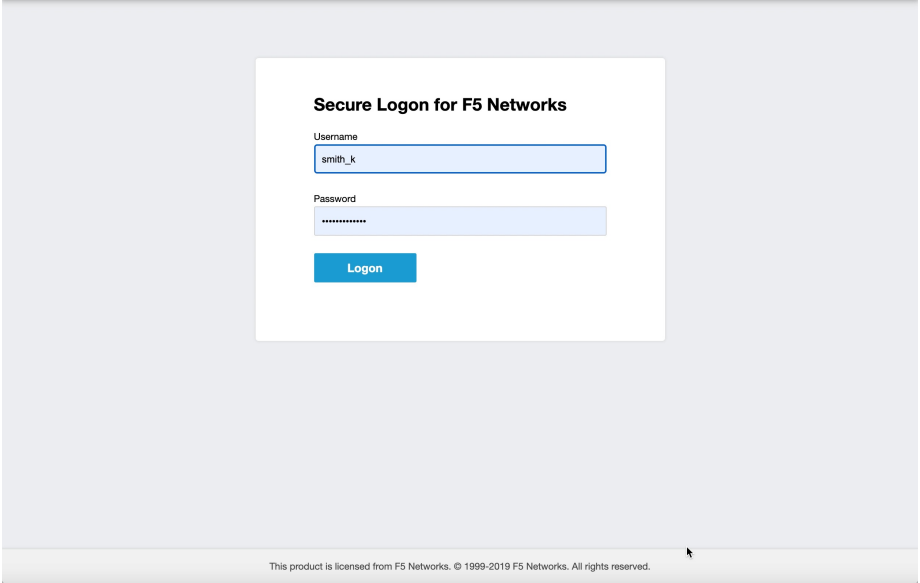
Data Processing										
Processing Pipeline [str]	Space Group Number [1x int]	Cell Parameters [6x real number]	Res Cut Key [str]	Res Cut Value [float]	PDB Model [str]	Autoproc Full [bool]	Autoproc Extra Params [str]	No Ano [bool]	Trusted High [float!]	FFCS campaign [bool]
gopy			is	1.5	6jzi			True		
autoproc			is	1.5	6jzi			True		
xia2dials			is	1.5				True		
gopy			cchalf	40				False		
autoproc			cchalf	40		True		False		
xia2dials			cchalf	40				False		
gopy	89	78 78 37 90 90 90								
autoproc	89	78 78 37 90 90 90								
xia2dials	89	78 78 37 90 90 90								
gopy										
autoproc						TRUE				
xia2dials										
gopy	89									
autoproc	89									
xia2dials	89								0.9	True
gopy									0.9	True

NOTE: adp uses spacegroup and cell parameters. If you do not know the correct values leave these blank.

model for molecular replacement

-parameter value
parameter=value
e.g. -M LowResOrTricky

- Security upgrade (AIT)
 - <https://rp.psi.ch>
- Data model which improves:
 - Spreadsheet validator
 - TELL GUI
 - DA+ GUI
 - DA+ server
 - Adp



The screenshot shows a web-based login interface for F5 Networks. At the top center, there is a red F5 logo. Below it, the title "Secure Logon for F5 Networks" is displayed. The form contains two input fields: "Username" with the value "smith_k" and "Password" with masked characters. A blue "Logon" button is positioned below the password field. At the bottom of the page, a small copyright notice reads: "This product is licensed from F5 Networks. © 1999-2019 F5 Networks. All rights reserved."

Demonstration - end of automation

Applications | ALBUA | X105A Expert Launcher | [DA+ Server: received... | AXIS V9914 View - Moc... | Live view - AXIS F31 N... | TELL1 Sample Changer... | QPAD.x86_64 | Terminal - e14965@x1... | 17:17 | justyna.wojdyla@psi.ch

TELL1 - Sample Changer GUI

Filter [filter expression]

Legend: running success skipped failed unknown

Safety	Mount	ALC	Diff. Center	DAO Dewar	Loc.	Puck ID	Sample #	Prefix	Folder	Priority	# mounts	Comments
7					D5	E-04	7	lyso_7	(date)/(prefix)	7	0	test crystal
8					D5	E-04	8	lyso_8	(date)/(prefix)	8	0	test crystal
9					D5	E-04	9	lyso_9	(date)/(prefix)	9	0	test crystal
10					D5	E-04	10	lyso_10	(date)/(prefix)	10	0	test crystal
11					D5	E-04	11	lyso_11	(date)/(prefix)	11	0	test crystal
12					D5	E-04	12	lyso_12	(date)/(prefix)	12	0	test crystal
13					D5	E-04	13	lyso_13	(date)/(prefix)	13	0	test crystal
14					D5	E-04	14	lyso_14	(date)/(prefix)	14	0	test crystal
15					D5	E-04	15	lyso_15	(date)/(prefix)	15	0	test crystal
16					D5	E-04	16	lyso_16	(date)/(prefix)	16	0	test crystal

Mounted Sample | Log messages

Name lyso_15 | Comments test crystal

Priority 15

Required Res. (Å)

Spacegroup

Cell Parameters

Heavy atoms

MIPause

Abort & Cancel

update comment

SOU Master SOU State: active power:powered state:Ready task:None position:PCoId mode:remote speed:100% magnet:50.0mA detection:suppressed cryojet: 100.0 K escape:SampleAlignment mounted sample:DS-15

axis-acc6ced20742

<https://www.psi.ch/en/sls/pxi/mx-software-documentation>

PXI

Status

User Information ⤴

Operation Schedule

Beamline infrastructure

MX Software Documentation

Remote Operation

Dewar shipping

Sample Changer

Data Transfer Service

Data Acquisition

Data Processing and Analysis

MX Software Documentation

The current software documentation is available in our shared [SWITCHdrive folder](#) 🔗.

Here you will find the following files:

Topic	Filename
General guide to MX Software	MX_software_documentation
Automated data collection (SDU) Overview	SDU_brochure
Instructions for automated data collections (SDU)	SDU_User_Instructions
Latest TELL spreadsheet	V(x)_TELLSamplesSpreadsheetTemplate
TELL spreadsheet instructions	TELL_Sample_Spreadsheet_User_Instructions

SDU User Instructions

Authors of this document: Kate Smith & Justyna A Wojdyla
Swiss Light Source, Paul Scherrer Institut, 5232 Villigen-PSI, Switzerland

Version: v2.1
28.02.2022

Validity of this document:
28.02.2022 to 30.04.2022

Table of contents

SDU Capabilities	2
Before experiment	3
Scheduling	3
Beamtime type	3
How best to use beamtime	3
Spreadsheet	4
Format and how to prepare it	4
Validation	4
Additional SDU run info	4
During experiment	5
How to start SDU	5
How to leave SDU mode	6
After experiment	6
Where to find	6
SDU Report explained	6
Appendix 1 Selection of the best spot	8
Appendix 2 SDU default parameters	9

Many thanks go to

- Justyna Wojdyla
- Zac Panepucci
- Kuba Kaminski
- MX Group
- Controls
- AIT
- Partners
- SLS User Community

