ENHANCING THE MxCuBE USER INTERFACE BY A FINITE STATE MACHINE (FSM) MODEL

Ivars Karpics, Gleb Bourenkov, Thomas Schneider, European Molecular Biology Laboratory (EMBL) Hamburg Unit also at DESY, Notkestrasse 85, 22607, Hamburg, Germany

Abstract

The acquisition of X-ray diffraction data from macromolecular crystals is a major activity at many synchrotrons and requires user interfaces that provide robust and easyto-use control of the experimental setup. Building on the modular design of the MxCuBE beamline user interface, we have implemented a finite state machine model that allows to describe and monitor the interaction of the user with the beamline in a typical experiment. Using a finite state machine, the path of user interaction can be rationalized and error conditions and recovery procedures can be systematically dealt with.

INTRODUCTION

EMBL Hamburg operates two beamlines, P13 and P14, for macromolecular X-ray crystallography (MX) on the PETRA III synchrotron at DESY (Hamburg, Germany). On both beamlines, MxCuBE [1] is used as the user interface. While in MX, a large fraction of data collections are considered as 'measurements' and are often conducted by nonexperts, still many data collections can be considered as 'experiments' in which a fine control of data collection parameters is required to obtain usable data. Both aspects require the user interface to be robust and easy-to-use for measurements while providing flexibility and deeper control for experiments. To make the control of the beamlines more robust and intuitive from the user perspective, we have embarked on describing the interaction of the user with the beamline as a finite state machine (FSM). An FSM is a mathematical model of a closed or open loop discrete-event system with defined states [2]. FSM-graphs are widely used to define, analyse and control the functioning of system. Applications include software engineering and experimental control systems. For example, state graphs are used in Large Hadron Collider experiments at CERN [3, 4] and in data acquisition system at the European X-ray free-electron laser: Karabo SCADA framework [5]. For the case of controlling an experiment/measurement on an MX beamline, the modularity and clean separation between low-level hardware access and the graphical interface within MxCuBE allows implementing an FSM model into the main experimental cycle. Important features of using an FSM are the ability to have an overview of all relevant beamline components, to keep track of user actions, and to guide users and/or beamline staff in case of failure or alarm.

USE CASE

A highly-simplified typical user interaction with a macromolecular crystallography (MX) beamline for the collection of diffraction data includes mounting the sample onto a sample positioning device (goniometer), centering of the sample with respect to the X-ray beam, setting of the data collection parameters, triggering of the data collection, execution of the data collection which consists of rotating the sample in the X-ray beam, and finally unmounting of the sample. The MxCuBE graphical user interface (GUI) for MX beamlines contains numerous widgets to control the settings of the beamline hardware including X-ray energy, beam attenuation factors, size and shape of the X-ray beam, distance between the sample and X-ray detector, and others (Fig. 1). To facilitate sample centering, the user interface offers a life view of the sample and various means to position and orient the sample. The data collection parameters are set by entering numerical values for controlling sample rotation speeds, exposure times etc. The many different ways of collecting data on a given crystals and the interdependencies between different - often technically high-end and thus not ultimately stable - components of the beamline result in a highly complex system for which stable operation is not trivial to achieve. An important factor in this context is also the fact that many users of MX beamlines are inexperienced posing high requirements in terms of making the operation robust and supporting recovery from errors.

FINITE STATE MACHINE

In the case of FSM, a system can be in exactly one finite state. It can move to another state in response to defined external inputs (stimuli). An FSM is defined as a set of states and transitions, an initial state, and conditions for transitions. For a typical user interaction with the experimental GUI during an MX data collection, it is possible to indicate several common steps (transitions in the FSM graph):

- 1. Sample mounting on the sample positioning device (goniometer).
- 2. Sample centring.
- 3. Entry and validation of data collection parameters.
- 4. Execution of data collection.
- 5. Sample dismounting.
- 6. Returning to step 1.

TUPHA187

C The 9400 C # 14 a C Cone Press 0.00 C C C C C C C C C C C C C C C C C	Design numbers Application Design number Application Design number Design number D	Institution of the series of t	Soutien Mucht merosetus and hundyn 23.12.4045 Fair 9.512.4045 Pair 9.512.4045 Pair 9.512.4045 Pair 19.512.505
Proce: 0.00 C (0) (0) (0) (0) (0) (0) (0) (0) (0) (0)	Academic Metanomic Academic Constraints and a constraint	Sample charger Bree Schedult Sample charger Bree Schedult Sample charger Bree Schedult Centrum Manual chart Fear Bree Schedult Image: Schedult Bree Schedult	Ruch Interpolation and bunking Par Par Bit 2016-100 ph/s Bit 9 for consistors (100 - 100 beam Cryopic In place In place Sampler Charger Tradic 120 COS Prever 1304 (1004) Scorage disc space Filed - 1304 (1004) Filed - 1304 (1004) Fi
Proce 0.00 C C C C C C C C C C C C C C C C C	Declarins Sarti, 244 Octo, conger frame 1 Monitor of may T Monitor, conger frame 1 Construction Construction 2 2 Construction Construction 0 2 Construction Construction 0 0 Construction Construction 0 0 Construction Construction 0 0 Construction Construction Construction 0 Construction Construction Construction Construction	Mode Samplic charger Show 52-ditulity Samplic Image: Samplic charger Image: Samplic charger Conting Massi 23 click Image: Samplic charger Filter Image: Samplic charger Image: Sampl	Flax Flax: 1.002+00 pNG B 1910 tenoresolat 000 potent initiation MigBace Sangle changer Deve level in range Rom016: 526 Flax: 1.002+00 Press: 128C08 Press: 128C0
Control Contro	Decidencial: 234 Dict. ang part hang. El Instal moje. I Bald accuses Instal moje. I Bald accuses Decidencial and the second secon	Sanjie Centing File: F	© 50 transmissier, 100 k 100 been Cytoject in jakoe Sample changer Dewor levelin range Randisk ize oos Tetaki 128 oos Pres: 128.668 (100%) Storage dis: sako Tetaki 1378 Pres: 4378 (35%) Energy
	Number of image: Total oncessage: 0 Total mage: 1 Defaust: Total mage: Total mage: 0 1 Defaust: Total mage: Totage (shr) 101 Defaust: Total Total Totage (shr) 12.7 Mage: Mage: Mage: Mage: Totage (shr) 12.7 Mage: Magee: <td>Centring Matsuid Sciol. Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter</td> <td>In place Sample changer Dewor level in caspe Ramdick Size Total: 128.0GB (100%) Storage disc space Total: 13.0TB Pres: 4.9TB (38%) Exercy</td>	Centring Matsuid Sciol. Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter Filter	In place Sample changer Dewor level in caspe Ramdick Size Total: 128.0GB (100%) Storage disc space Total: 13.0TB Pres: 4.9TB (38%) Exercy
Size Line Crid Crid Foco Foco Escapato Kapo algo	Trist maps 1 Detector mode 164 state Doport En (%) 0.81 Detector mode 164 v Doport En (%) 2.0 Pik 9.0 <td>Pitter No filter v +- Pick 1 - - +- Pick 3 - - +- Pick 3 - - +- Pick 3 - - *- Pick 4 - -</td> <td>Sample Changer Devor level in range Ramdick Size Total: 128.005 Free: 128.005 (100%) Storage dis: space Total: 13.018 Free: 4.918 (35%) Ecency</td>	Pitter No filter v +- Pick 1 - - +- Pick 3 - - +- Pick 3 - - +- Pick 3 - - *- Pick 4 - -	Sample Changer Devor level in range Ramdick Size Total: 128.005 Free: 128.005 (100%) Storage dis: space Total: 13.018 Free: 4.918 (35%) Ecency
Line Crief O Separation Kazosa Jopo Kazosa Jopo	Doposition Dot Detector mode Tuff w V Gapaix 2:00 Hit Mod Freego (w/s) Tuff w Freego (w/s) Freego (w/s) <td< td=""><td>Image: Second Second</td><td>Parndisk size Total: 128.008 Pree: 128.008 Storage dis: space Total: 13.018 Pree: 4.918 (35%)</td></td<>	Image: Second	Parndisk size Total: 128.008 Pree: 128.008 Storage dis: space Total: 13.018 Pree: 4.918 (35%)
Line Grid Grid Sargabaci Kapopa align Kapopa align	Logic 220 Mit 30 trangg (kir/): 12.7 MAD Mit menulation (kir): 0.315 Mit Mit Strutterlies Strutterlies Mit Mit	Pock1 Pock2 Pock3 Pock3 Pock4 Pock5 Pock5 Pock6	Free: 128.6G8 (100%) Storage dis space Total: 13.0TB Free: 4.9TB (35%) Exercts
Crid O Focus Separator Kapoga aligon	thergy (keV): 12.7 MAD (k): ✓ Resolution (A): 7.604 Treenmission (N): 20.315 ✓ Shutterless	Puck 3 Puck 4 Puck 5 Puck 6	Total: 13.0TB Free: 4.9TB (35%)
O Focus Snapshot Kappa align	Penolution (A): 7.684 Transmission (Na): 50.315	 Prock 4 Prock 5 Prock 6 	Free 4.910 (30%)
Focus B Snapshot Kappa align Value align	Transmission (%): 50.315	Puck S Puck 6	hI#COV
Snapshot Kappa align	🗹 Shutterless	Parto	Cummb (12 7003 htt)
Shiphtor Rappa align		- 61	Wavelength: 0.9763 Å
Kappa align	Datalocation	62	Status
The second	Folder	63	Setto: kuV v
Falact all	/dataint/p14/10736_205/karpics/20170928/RAW_DATA	65	Transmission
Setace at		0.0 📖 -	Ourrent: 50.32 %
× Charal	Browse	- 67	Settor
B	Fle name: mil/0021 1 mmm ch/	62	Providelan
Auto	Prafix mehr0021	6:10	7.684 Å
	Dus number 1	Prock 7	Ourrent: 1200.00 mm
	Part instants i	Process	Set to: A
	Processing	> Puck 10	Beamstop distance
	N.o. residues: 200 Space group: v	Prock 11	Current: 28.00 mm
40*		Prock 12 Prock 13	Set to:
	a: 0 ß: 0 y: 0	> Puck 14	
	 Run processing after collection 	> Puck 15	
	Run parallel processing	- Puck 17	
			Dogristerlock
			Unlocked
			🖉 Unlock
			Safety shutter
			disabled
and the second			Close Close
			Fast shutter
			disabled
			Open Close
			Image tracking
	Characterisation		ready
red point or start a new centring	Helical Collection	C Dictive history sizes	 Enable Adxv image tracking
Phase	Energy Scan	1 B	Detector status
Transfer 🗸 🗸	XRF Spectrum	Collect Queue Pause	Frame rate : 0 Hz
	Advanced		Temperature : 30.3*
	Sa Add to direos		Humidity :2.8%
[2017-09-28 13:02:22] Samp [2017-09-28 13:02:22] Samp	ple changer: SystemStatus:Status:Idle Systemample-EndCloseLid/StartMoveDe ale changer: Last conveand - 28/09/2012 12/3867 12/3102/1044	wToMD3 mple detection	
(2017-09-28 13:02:23) Data	collection is enabled		
[2017/09/28 13:02:23] - Safe	ety shutter is closed (Open the safety shutter to enable collections)		
2017-09-28 13:02:25 Data	o proposac mannova i - reac crystals i collect is disabled		
(2017-09-28 13:02:26) - Safe	ety snutter is closed (Open the sarety shutter to enable collections)		
		Na andre de la seu se andre de l	NA profes of and a second seco

Figure 1: Graphical user interface MxCuBE as seen at EMBL beamline P14. In the left half, a life view of the sample is displayed. The sample view is surrounded (clockwise from above) by controls for sample orientation and microscope settings, controls for sample centering procedures, and widgets for controlling the size and shape of the X-ray beam (which need to be modified to match the size of the sample). In the right half, the left section offers several tabs that allow the definition of parameters of relevance to various data collection procedures, the middle section controls the loading and unloading of samples and the assembly of sequences of data collection procedures, while the right section allows to monitor (and partly control) general properties of the synchrotron, the experimental environment etc. At the bottom of the screen logging information is displayed.



Figure 2: State graph of a user interaction during a macromolecular crystallography data collection. Circles represent FSM discrete states. Normal states are shown in white, while states painted in red are error states and require actions to return system to a normal state. Blue arrows point to *Sample mounted* state and are executed automatically, red arrows indicate the request from a user to unmount a sample. FSM graph includes also *Beam alignment* state where several xray beam alignment procedures are allowed.

Based on these transitions, a state graph was created (Fig. 2). The graph originates from the Start node. If there is a sample mounted on the goniometer, then the state is changed to the Sample mounted state, otherwise to the Sample not mounted state. From the Sample not mounted state it is possible to reach the Sample mounted state via Sam*ple mounting* state (an attempt to mount a sample). In case the of successful mounting, the system reaches the Sample mounted state while for a failed mounting procedure it resorts to the Sample not mounted state. The next state, Sample centered, is reached from Sample mounted state via three different transitions aka positioning methods (manual, automatic optical, or xray based centering). To reach the state in which data are actually collected - Collection running - the system has to go through several preparatory stages. These include reaching a set of Valid input parameters, arriving in a set of Accepted conditions, and leaving the Confirmation window displayed state with a positive confirmation. To ensure a closed loop system most of the states have transitions to the Sample mounted state.

IMPLEMENTATION IN THE GRAPHICAL USER INTERFACE MXCUBE

Both P13 and P14 use MxCuBE with Qt4 graphics [6, 7] as an experimental graphical user interface. MxCuBE is written in Python and is logically divided into a hardware access and a graphical representation layer. The hardware access level is called 'Hardware Repository' and contains a set of configurable hardware objects. The modularity of the Hardware Repository allows sharing data across and between hardware objects and creating complex so called 'procedures' to perform scans, data collections, beam centering and other complex processes. We have implemented the FSM in MxCuBE as a hardware object that can connect to all hardware objects relevant to performing measurements or experiments. The implementation of the FSM-graph is defined via an yaml-file describing graph nodes, transitions and conditions. Transitions are triggered upon request when the conditions as evaluated by individual hardware objects are fulfilled. For example, the *sample_is_loaded* condition (Fig. 2) is broadcasted by the goniometer hardware object. For debugging purposes a window with information about the state of the FSM is available. It contains a table displaying all available states, conditions and a history of states assumed by the system (Fig. 3).

CONCLUSION AND PERSPECTIVES

We have presented an idealized Finite State Machine model for the interaction of a beamline user with a beamline to collect diffraction data from a crystal. While analyzing the current implementation of the process in the MxCuBE graphical user interface running on the MX beamlines at EMBL-Hamburg, we realized the high complexity of the real-world interaction between a user of a beamline. When restricting the FSM-model to the steps relating to a simple measurement on a single sample, the resulting description is helpful for the





Figure 3: Window for monitoring the FSM described in (Fig. 2) as implemented in MxCuBE. In the matrix in the upper part of window, each column corresponds to a state and each row of the matrix relates to a condition that needs to be fulfilled for a transition between two states to be executed. For each condition, the corresponding state is indicated by a green tick-mark (true) or a red cross (false). At the bottom, a state history is displayed. In this example, the sample was mounted and successfully centered: the FSM has progressed through Sample not mounted, Sample mounting, Sample mounted into the Sample centered state. According to the FSM graph, the system can now progress to Valid input parameters or to Invalid input parameters. As the condition Data path valid is not fulfilled system is in the error state Invalid input parameters (column 8 painted in red). To progress towards the Data collection state, the system has to go through the Valid input parameters state which can be achieved by entering correct data collection path.

user of the beamline, the beamline scientist supporting the beamline user, and for the developers of the beamline control interface. For the (inexperienced) beamline user, being informed about the current state/current transition is useful especially in situations in which the beamline is seemingly idle or blocked, e.g. during a technical wait period when a sample is robotically mounted. The clean information about error state and - when possible - suggested recovery procedures make the beamline user more autonomous and reduces the need for the beamline scientist to recover the beamline. Error situations unrecoverable by the beamline user can also be recognized and an automatic notification can be sent to the beamline scientist to address the problem. For the developer, the state history provides an important tool for debugging. Gathering statistics about the behaviour of beamline components as seen via the states assumed and transitions take can be used to build a knowledge base for pin-pointing fault-causing beamline components. During the design and implementation of the FSM, a number of

16th Int. Conf. on Accelerator and Large Experimental Control Systems ISBN: 978-3-95450-193-9

and DOI. conceptual challenges surfaced. In particular, the possibility publisher. of accessing many beamline functionalities from the same interface-section at the same time will need be reassessed. A hierarchical approach could be envisioned in which actions that can be triggered by the beamline are cleanly grouped so work. that only a subset of functionalities - that is less complex to he maintain in a consistent way - is accessible, while the other of functionalities are blocked. Blocked functionalities can be itle easily indicated by 'greying-out' the respective parts of the GUI. While the description of an entire beamline as an FSM author(s). may be conceptually of interest, the involved effort may be prohibitive. Nevertheless, describing subsystems as FSMs, such as done here for the interaction of the user with the to the beamline for a standard diffraction data measurement, can be useful both for achieving a better understanding of the Content from this work may be used under the terms of the CC BY 3.0 licence (© 2017). Any distribution of this work must maintain attribution t needs and for optimizing procedures in terms of efficiency and robustness.

REFERENCES

- [1] J. Gabadinho et al., "MxCuBE: a synchrotron beamline control environment customized for macromolecular crystallography experiments", Journal of synchrotron radiation. vol. 17, pt. 5, pp. 700-707, 2010.
- [2] D. Harel, "Statecharts: a visual formalism for complex systems", Science of Computer Programming, vol 8, iss 3, pp. 231-274, 1987.
- 3] F. Calheiros, P. Golonka, and F. Varela, "Automating The Configuration Of The Control Systems Of The Lhc Experiments", in Proc. of ICALEPCS2007, Knoxville, USA, October 2007, paper RPPA04, pp. 529-531.

- [4] G. De Cataldo, A. Augustinus, M. Boccioli, P. Chochula, and L. Stig Jirdén, "Finite State Machines for Integration and Control in ALICE", in Proc. of ICALEPCS2007, Knoxville, USA, October 2007, paper RPPB21, pp. 650-652.
- [5] B. C. Heisen et al., "Karabo: An Integrated Software Framework Combining Control, Data Management, And Scientific Computing Tasks", in Proc. of ICALEPCS2013, San Francisco, USA, October 2013, paper FRCOAAB02, pp. 1465-1468.
- [6] I. Karpics, G. Bourenkov, M. Nikolova, and T. R. Schneider, "Graphical user interface and experiment control software at the MX beamlines at EMBL Hamburg" in Proc. of NOBUGS (New Opportunities for Better User Group Software), NOBUGS2016, Copenhage, Denmark, October 2016, paper 10.17199/NOBUGS2016.91, pp. 53-58.
- [7] M. Cianci et al., "P13, the EMBL macromolecular crystallography beamline at the low-emittance PETRA III ring for highand low-energy phasing with variable beam focusing", Journal of synchrotron radiation, vol. 24, no. 1, pp. 323-332, 2017.