

MxCuBE2





2 I Title of Presentation I Date of Presentation I Author

- Evaluate and collect of MASSIF samples
- Fully exploit µbeam capabilities
- Describe and perform (automagically) more complex experiments
- A control software shared on different MX beamlines at different SR sources
 - Different hardware same GUI
 - Easy to install and maintain



CONVENTO DO CRISTO, TOMAR, PORTUGAL



Romanesque, Gothic, Manueline and Renaissance architectural styles

all together

as MxCuBE v1



•After ESRF long shutdown (May 2012)

- Abstraction level introduced
- Roots for new version

Design of new GUI

- New functionalities
- New concept
- April 2013 third mxCuBE workshop
 - Agreements on common and specific needs
- September 2013 deployment
- •February 2014 release of v2.0.9



•Which sample(s)?

•Where? (Which position(s)?)

•What? (Which task(s)?)

		mxCuBE (mx-1539)		+ -
e Instrumentation Help				Expert m
Collect In YPE construm	() System DEard	back OChat		Machine current
conect ARP spectrum	() System Preed	back Uchat		193.8 mA
4		Sample centring Data collection		7/8 multibunch
User: mx-1539 Group:	Set 🔏 Logout	Sample position	Collection method	0.6
Sample list	New Association		Discrete	Flux: 3.65e+11
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E 4.9	۲	Light 13 . T V rocus: 0.0 . 2 0.01 . Prone light 0.0 . 200m: 3 .	Oscillation overlap: 0.0 Number of images: 1230	Prote to a state of a
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C Characterisation - 1			Part in the second s	
□ ref #4 10 1	Dorw		Data location	
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a D Diffinition plan - 1	2747	Ou k realign	Purity Dr. 2	
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D 85 2 w1 1				- Conc
TO De Sin	Centring !		Anomalous Space group:	
5:4		Aperture diameter: 30 •	Characterise	Current users
5.5			Helical	
0 5.6			Energy Scan	X Selecting gives control
	1 (212)		Advanced	X Allow timeout control
2 4	1			
Second	C. Baller		Add to queue	Ask for control
Contract Constant	Pause			My name: David
14-01-31 22:42:34) Preparing mini	diff for sample centrin			
14-01-31 22:42:34] Ready	the second s			
+ 01-31-22:42:341 Centring in pro	gress. Please save th	suggested centring or m-center		
a la	2.3	xCuBE (mx-1539) G Terminal		ריבחיבב
and the buseness		CONN.		

SC - Queue

Sample - Position



Tasks - Data Collection

Which? Where? What?

Combinations are infinite. For example:

- •Collect a MAD with energy scan at N different positions
- •Collect the same Data collection (or characterisation, or ...) over N samples
- •Collect the same Data collection over N positions on one sample
- •Any parameter (including centered position) can still be edited before collection

•_____





DETAILS - DATA COLLECTION

ample centring	Data collection							
Data location Folder: /data/vis File name: R5_2_w1 Prefix: R5_2	sitor/mx1539/id29/2014 1_1_####.cbf	0131/RAW_DAT/ Run nun	A /AS	wse Centred position				
Acquisition Acquisition Signature First image: Transmission (%): Exposure time: X Shutterless Processing X Process and analy Anomalous Unit cell: a: 0 b: 0 α: 0 β: 0	63.0 Oscillation r 1 Number of i 42.62 Resolution (0.037 Vise data yse data N.o. residu Space grou C: 0 Y: 0	range: 0.1 images: 1230 (Å): 2.23	Oscillation overlap: Number of passes: Energy (KeV):	0.0 1 12.4 MAD i	P:- ▼			
			Diff	actic	on plai	n details	View Rest	



DETAILS - CHARACTERIZATION

ample centring Cha	racterisation	×
Reference images Acquisition parameters Data location Folder: /data/id14eh File name: ref-opid144_	4/inhouse/opid144/20131030/RAW_DATA/	Centred position
Prefix: opid144 Acquisition Oscillation start: 0.0 First image: 1 Transmission (%): 100 Exposure time: 0.5	Run number: 1 Oscillation range: 1.0 Oscillation overlap: -89.0 Number of images: 4 Number of passes: 1 0.0 Resolution (Å): 2.302 Energy (KeV): 1	
Characterisation type Routine-DC © Use min dose O Use min time SAD Radiation damage	Dose limit MGy:	Optimization parameters Aimed I/o at highest resolution: 3.0 Strategy complexity: Single subwedge • Aimed completeness: 0.99 Use permitted rotation range: • • • Maximum resolution: • • • • • • Aimed multiplicity: • • • • • • Calculate low resolution pass strategy • • • • • •
Radiation damage model pÅ ² /MGy: 1 y 1/MGy: 0.06 Sensetivity: 1.0	Crystal Space group: • Vertical crystal dimension (mm): Min: 0.1 Max: 0.1 • at min: 0.0 • at max: 90	Characterization details
		View Results

ESRF

Tuesday, February 4, 14

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DETAILS - CHARACTERIZATION RESULTS

× Sample centring Characterisation **Characterization details** Aimed Forced Anomalous Aimed Aimed I/sigma Aimed space group data multiplicity completeness at highest res. resolution (Å) (results) False 4.00 0.99 3.00 1.00 Collection plan strategy (RADDOSE log file , BEST log file) Best has detected that the sample can diffract to 1.73 Å! The current strategy is calculated to 2.06 Å. In order to calculate a strategy to 1.73 Å move the detector to collect 1.73 Å data and re-launch the EDNA characterisation. Resolution limit is set by the initial image resolution Wedge Subwedge Start (7) Width (*) No images Exp time (s) Max res (Å) Rel trans (%) Distance (mm) 48.00 1.45 86 0.10 49.63 1 1 2.06 302.23 -----1.0 Indexing summary: Selected spacegroup: P3, forced space group: Refined unit cell parameters (Å/degrees) a (Å) b (Å) c (Å) alpha (") beta (") gamma (*) 54.745 54.745 107.776 90.000 90.000 120.000 ref-opid144_1_0003.img ref-opid144_1_0004.img Indexing log file ref-opid144_1_0002.img ref-opid144_1_0001.img Integration log file 1 Integration log file 2 Integration log file 3 Integration log file 4 Image quality indicators File Tot integr signal Spot total In-Res Total Good Bragg Ice Rings Meth 1 Res Meth 2 Res Max unit cell ref-opid144_1_0001.img 444.0 593418 398 297 207 9 2.70 3.44 ref-opid144_1_0002.img 13704880 964 885 528 10 2.10 2.09 205.2 1 10 4 4 4 0000 1011100 1.111 3.00 22.2.2

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ESR

View parameter





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SIMPLER AND ROBUST

C3D



mxCuBE



Processing server







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SIMPLER AND ROBUST









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BETTER AND EASIER INTEGRATION WITH ISPYB

Sample location	3	Image Prefix	Run No	Experiment Type	Protein Acronym	∎.	Start Time	# images	Experiment Parameters (Expand)	Status	Space Group	Completeness	Res
1:2 - TRYP-sample2 1:3 - TRYP-sample3 1:4 - TRYP-sample4				All ‡	All 🛟								
- 1:5 FAE-sample5 1:6 FAE-sample6	<u>4_w1</u>		1	OSC		03-02- 12:0	-2014 8:50	2000	٩	••••	P 1 21 1		100. 2.23 100.
∏ i ∐ 1:7 - FAE-sample7	ref-4		1	Characterization		03-02- 12:0	2014 5:55	2	٩	••••	P2		-
	<u>3_w1</u>		1	OSC		03-02- 12:0	2014 0:05	2000	۲	••••			
Sample list	ref-3		1	Characterization		03-02- 11:56	2014 8:56	2	٩	••••	P2		
Campie list	<u>1_w1</u>		2	osc		03-02- 11:50	-2014 0:36	2350	۲	••••	P 1 21 1		47.6 1.83 47.6
	ref-1		2	Characterization		03-02- 11:4	-2014 7:42	2	٥	••••	P2		
Data are labeled by type OSC, Characterization, Helical, Mesh etc, and corresponding			osc		03-02- 11:3	2014 9:04	2000	٩	••••	P 1 21 1		100. 2.32 100.	
			Characterization		03-02- 11:3	2014 5:25	2	٩	••••	P2			
results and parame	ed Characterization		03-02- 11:30	-2014 0:27	2	٩	••••						
	ref-34	00	1	Characterization		03-02- 11:2	2014 5:01	2	0	••••	P3		
see Stephanie's tall	ref-06	48	1	Characterization		03-02- 11:20	-2014 0:36	2	0	••••			

SCIENTIFIC ABSTRACTION LAYER



Open to external descriptors: build more complex data collection

Possible to interactively fill the queue with different tasks, analyse results and expand, without limit to imagination

see Olof's talk









WHERE WE ARE GOING?

New tools for meshes and sample interaction Use beamsize as mesh unit Overlay results of mesh

Abstract diffractometer descriptor

Expand Data Collection Model Other axes DC (kappa...) Beamsize descriptor

.....

Adapt interface to *RoboDiff* and *NewDewar* Generic SC Plate screening

Redesign Data collection group concept Tag data collections???





WHERE DO YOU WANT US TO GO?





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MxCuBE is a big project that runs with small resources

It is shared among different institutions, BESSY, EMBL, GLOBAL PHASING, MAXLAB, SOLEIL



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Marcus Oskarsson (SB - BCU) Matias Guijarro (BCU) Antonia Beteva (BCU) Stephanie Monaco (SB-BDO) Marjolaine Bodin (SB) Thomas Boeglin (SB - DAU) Matthew Bowler (EMBL) Sandor Brockhauser (EMBL) Alejandro De Maria Antolinos (SB) Solange Delageniere (SMIS) David Flot (SB) Etienne Francois (BCU) Alexandre Gobbo (EMBL) Elspeth Gordon (SB - BDO) Jerome Kieffer (DAU) Christoph Mueller Dieckmann (SB) Max Nanao (EMBL) Staffan Ohlsson (BCU) Sasha Popov (SB) Olof Svensson (DAU) David von Stetten (SB)

Automation Task Force





Tuesday, February 4, 14

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