

ID23-EH2 Refurbishment

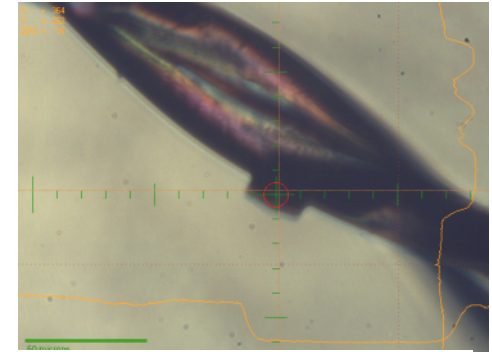
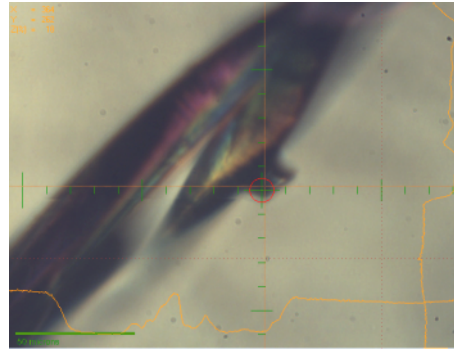
Max Nanao



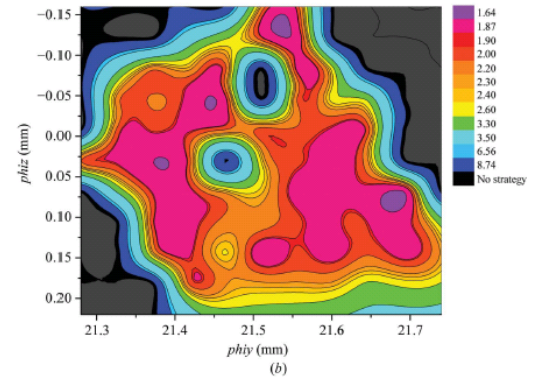
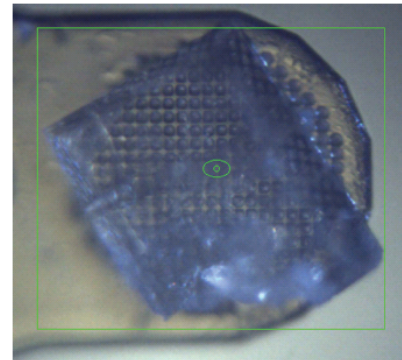
| The European Synchrotron

USE CASES FOR SMALL BEAMS IN MX

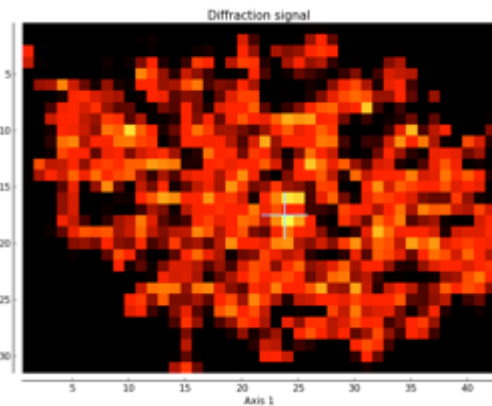
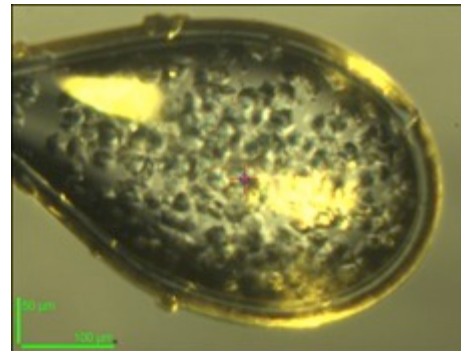
Smaller crystals



Diffractive mapping



Serial crystallography



Add new beam size ($\sim 2 \times 2 \mu\text{m}^2$, $> 2 \text{E} 12 \text{ ph/s}$) (x5 ESRFII, $\sim 25\%$ reduction in size)

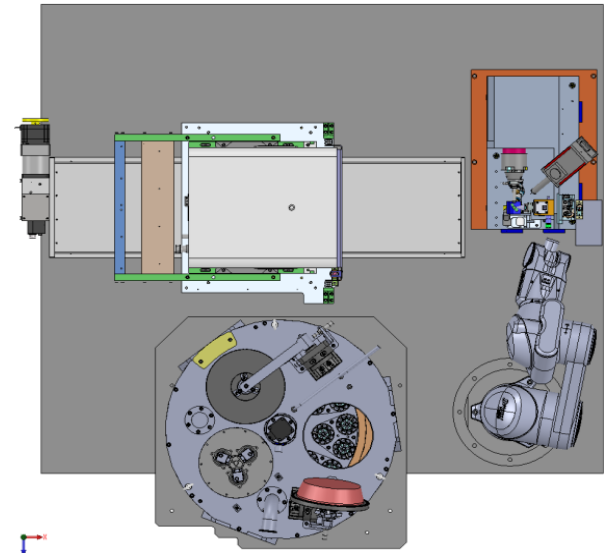
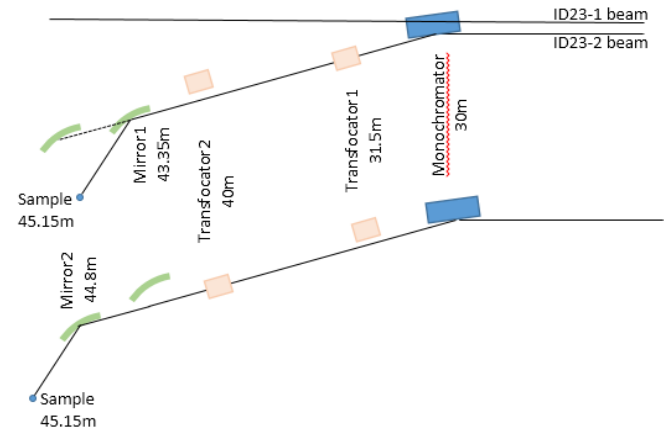
Switchable between beam sizes in ~ 15 minutes

Hutch Ante chamber, improved temperature stability ($\pm 1 \text{ C} \rightarrow \pm 0.5 \text{ C}$)

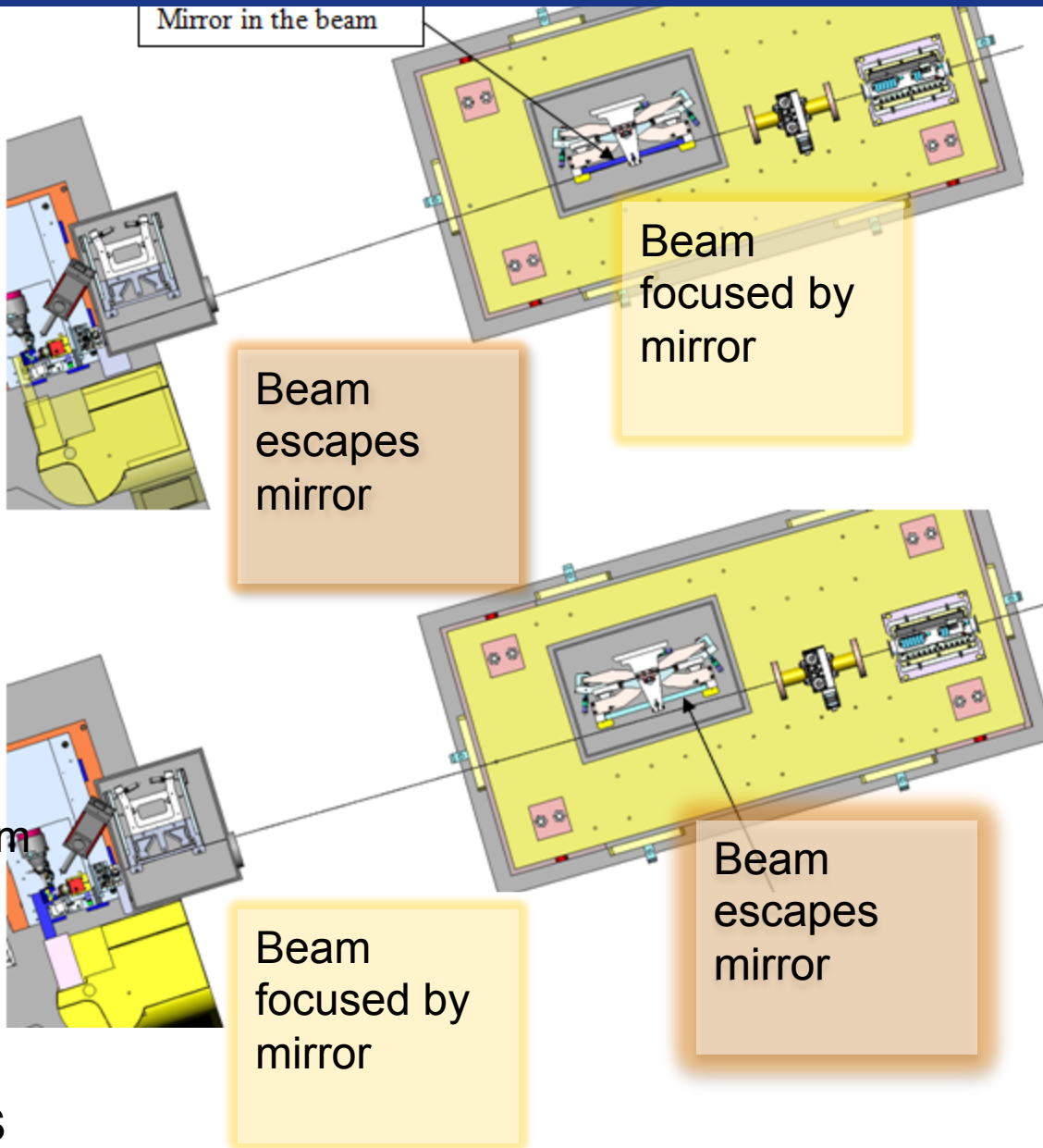
New sample environment

High capacity dewar, FLEX SC

New diffractometer



BEAM SIZE SWITCHING



OPTICS

Add new beam size ($\sim 2 \times 2 \mu\text{m}^2$, $> 2 \times 10^{12}$ ph/s) (x5 ESRFII, $\sim 25\%$ reduction in size)

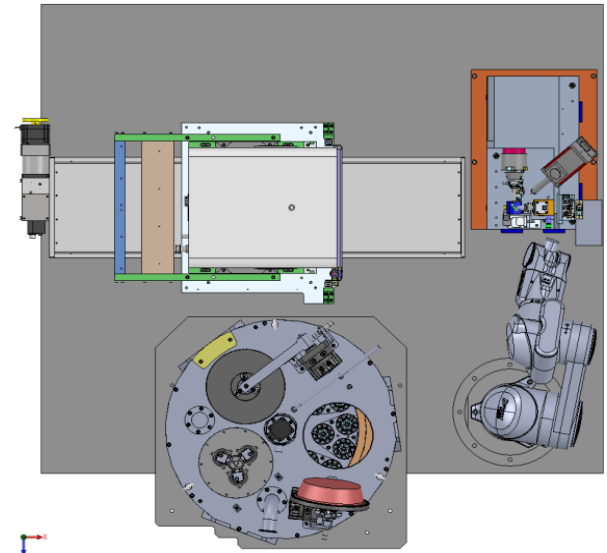
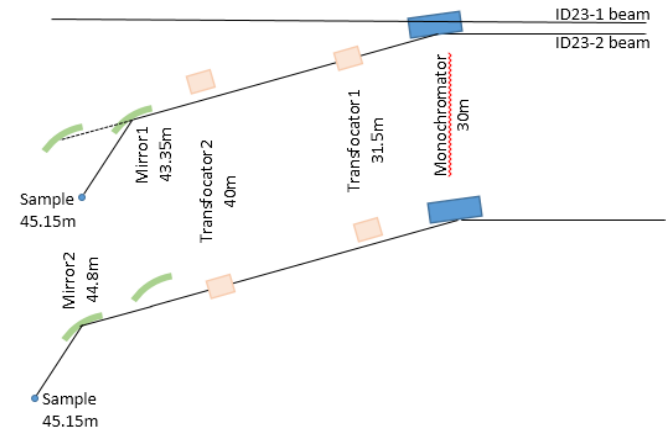
Switchable between beam sizes in ~ 15 minutes

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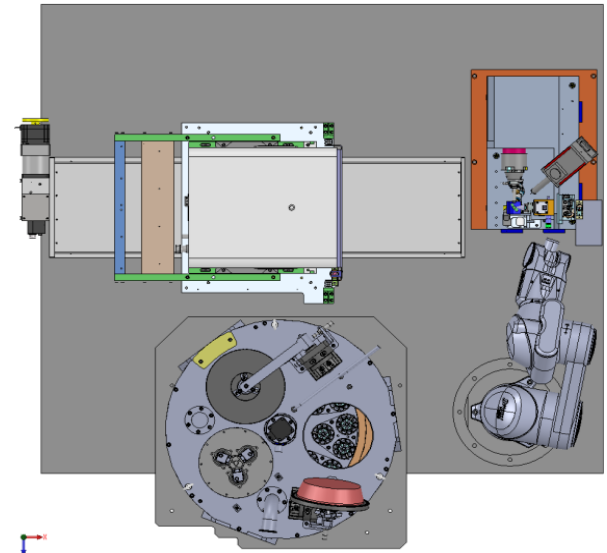
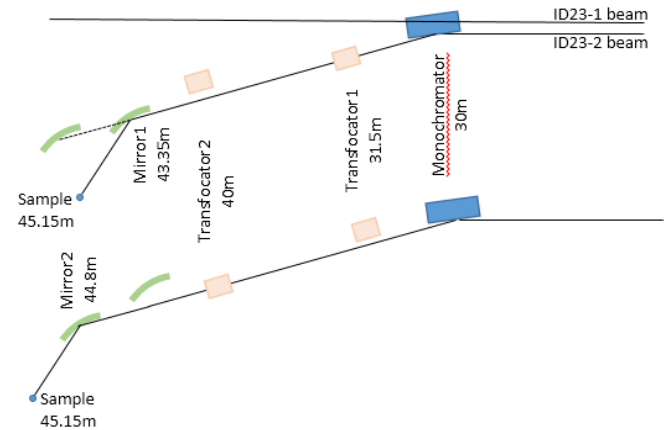
Switchable between beam sizes in ~ 15 minutes

Hutch Ante chamber, improved temperature stability ($\pm 1 \text{ C} \rightarrow \pm 0.5 \text{ C}$)

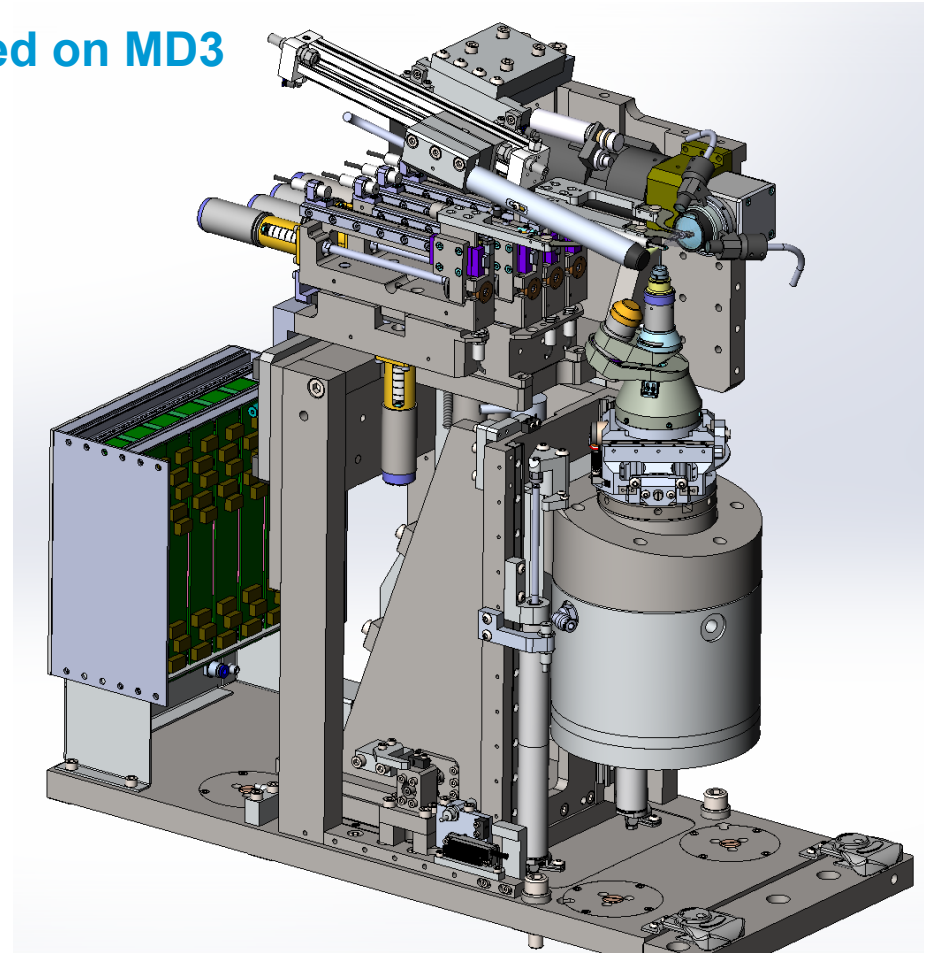
New sample environment

High capacity dewar, FLEX SC

New diffractometer



- Co-developed by EMBL and Arinax based on MD3
- FLEX SC compatility (UNIPUCK only)
- Plate gripper
- Large vertical throw
- Small footprint

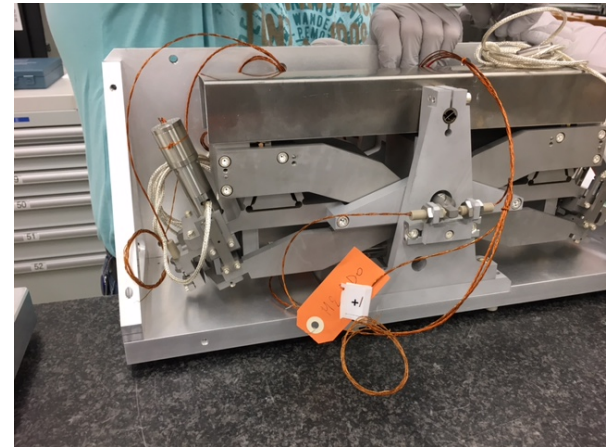


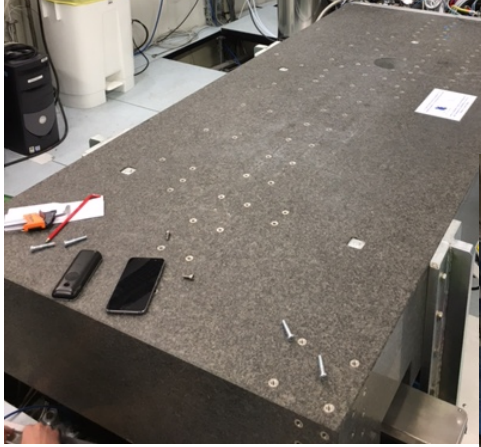
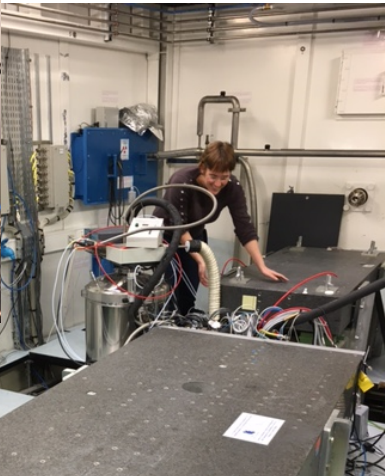
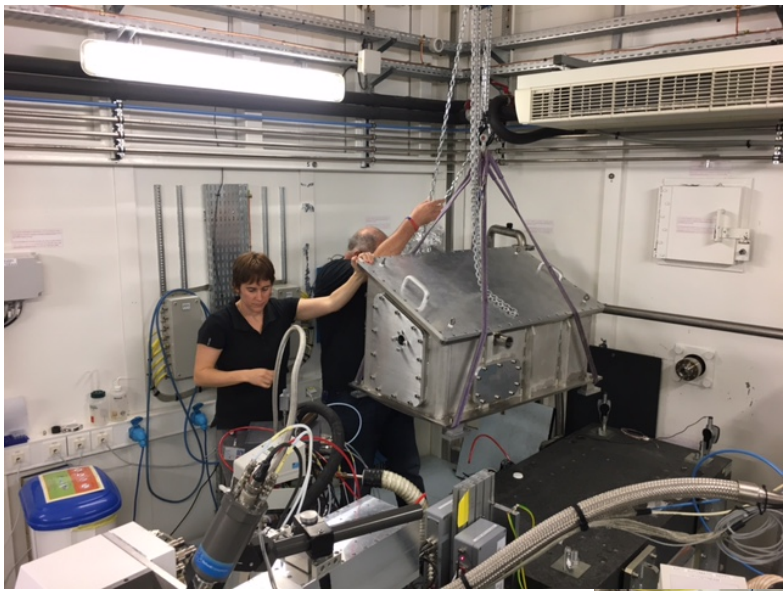
Old end station removed

New tables in

New mirrors in, commissioning soon

Transfocators+lenses mid February







2 beam sizes:

2x2 μm^2

5x8 μm^2

Mesh scans will be significantly faster

UNIPUCKS ONLY

8 cells (one puck position reserved)

3 pucks per cell

16 samples per puck = 368 samples

Non diffractometer motors: new control hardware (ICEPAP)

No more SPEC -> BLISS

New pipelines added

Better ISPyB integration of automatic SAD phasing

Higher performance– more nodes, improved queuing system

Current configuration:

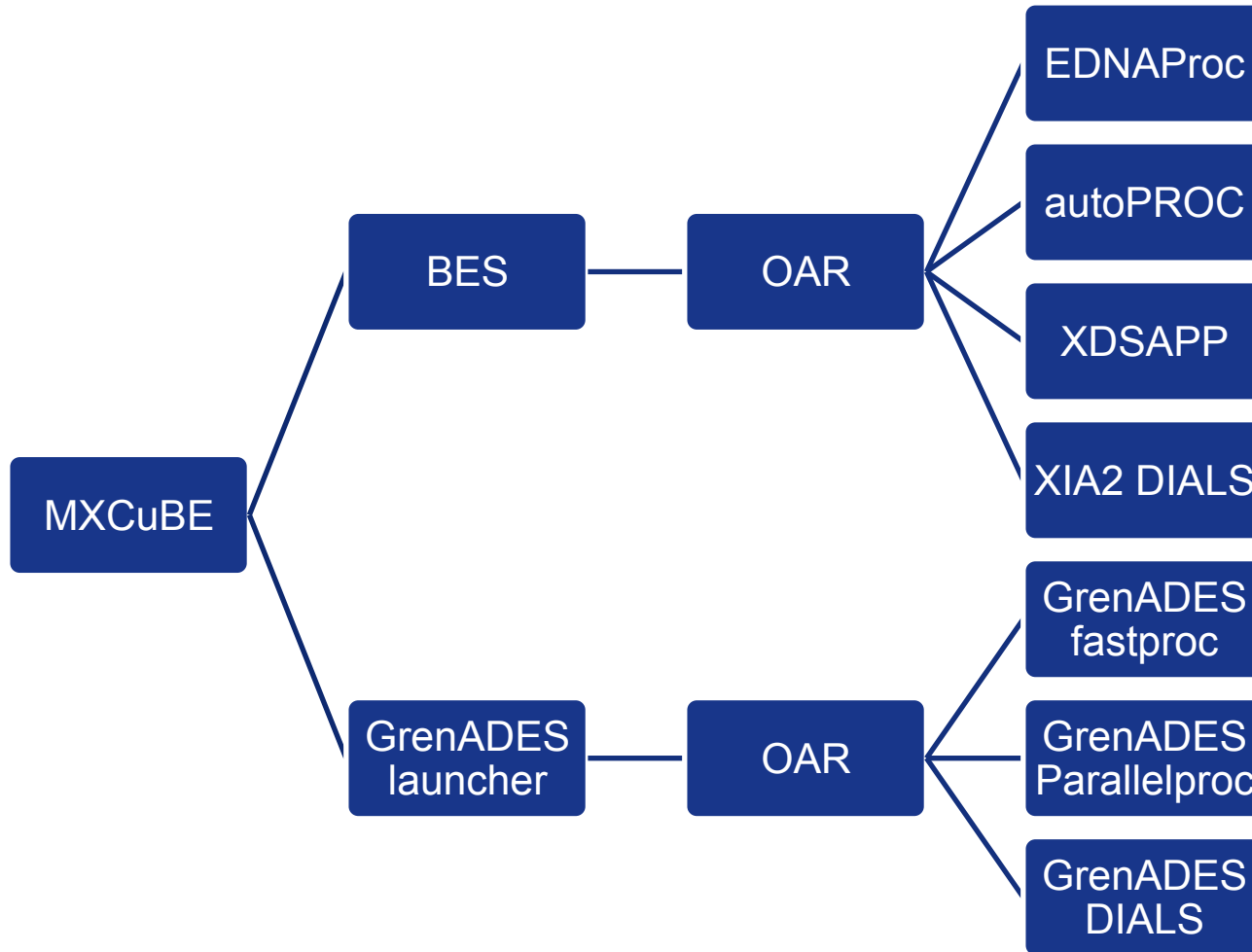
OAR queuing/scheduling *with a separate scheduler*

29 hosts

3-3.6 Ghz AMD

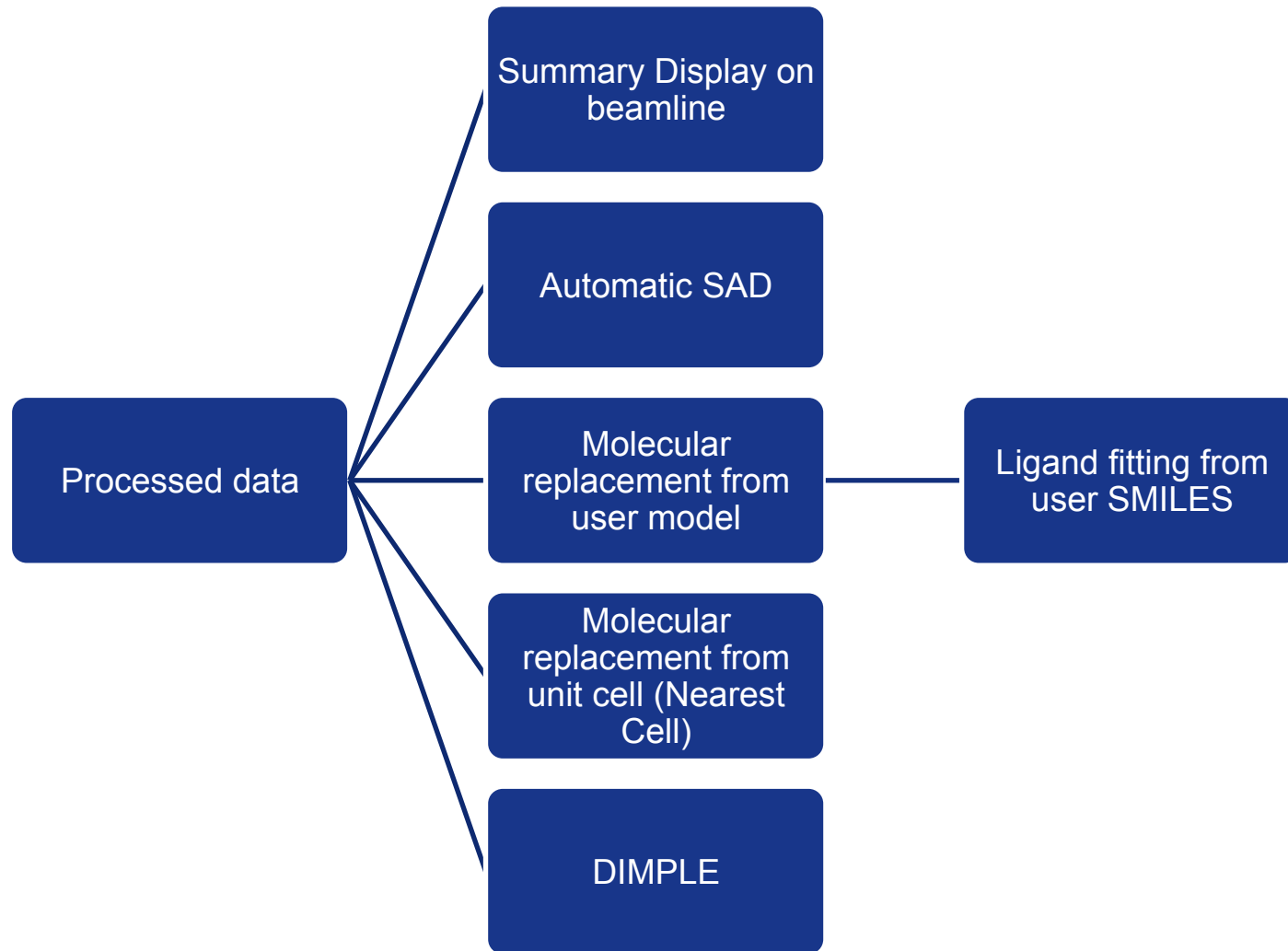
564 “cores”

GPFS



OAR=Queuing system
BES=Beamline Expert System

POST PROCESSING TASKS



NOTIFICATION THAT PHASING WAS SUCCESSFUL

ExiMX Extended ISPyB for MX₂ESX

Version: 9.9.8 Released: 2016/12/22 ESRF

Home | Shipment | Proteins and Crystals | Prepare Experiment | Data Explorer | Offline Data Analysis | Help

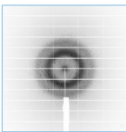
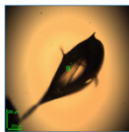
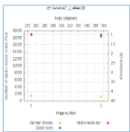
search by protein acronym

Log out | anano

Run #1 Characterisation Dec 12, 2016 10:04:47 PM

Summary | Beamline Parameters | Data Collection 1 | Sample | Results | Workflow 1

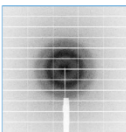
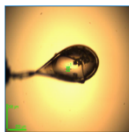
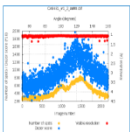
Workflow	Characterisation	Type	Characterization	Monoc	Movicity	0.2	
Protein		Res. (open)	1.16 Å (0.98 Å)	Monoc	Space Group	P2	
Sample		Wavelength	0.973 Å	Plan. Res.	1.16 Å	Exp. Time	0.02 s
Prefix		Omega range	1°	Images	1300	Total rotation	0.1°
Images	2	Omega start (stat)	450° (180°)	Transmission	5.496		
Transmission	100	Exposure Time	0.05 s	cell A	cell B	cell C	
Flux start	2.46e+12 ph/sec	Flux end	2.43e+12 ph/sec	42.84	41.5	32.93	
				Alpha	Beta	Gamma	
				99	104.52	90	

Run #2 OSC Dec 12, 2016 9:59:29 PM

Summary | Beamline Parameters | Data Collection 1 | Sample | Results 10 | Workflow | Phasing 37

Workflow		Type	OSC	P 1 2 1	Completeness	Res.	Rmerge
Protein		Res. (open)	1.18 Å (0.98 Å)	Initial	74%	4.9	2.1
Sample		Wavelength	0.973 Å	Overall	45%	1.1	30.0
Prefix		Omega range	0.05°	Overall	60%	1.1	2.7
Images	2100	Omega start (stat)	160° (160°)	cell A	cell B	cell C	
Transmission	4.9048	Exposure Time	0.02 s	42.2	41.2	72	
Flux start	1.48e+11 ph/sec	Flux end	1.54e+11 ph/sec	Alpha	Beta	Gamma	
				99	104.3	90	



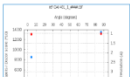




Automatic SAD appears to have worked with the space group P1211

Run #1 Characterisation Dec 12, 2016 9:57:01 PM

Summary | Beamline Parameters | Data Collection 1 | Sample | Results | Workflow 1

Workflow	Characterisation	Type	Characterization	Monoc	Movicity	0.15	
Protein		Res. (open)	1.19 Å (1 Å)	Monoc	Space Group	P2	
Sample		Wavelength	0.973 Å	Plan. Res.	1.16 Å	Exp. Time	0.02 s
Prefix		Omega range	1°	Images	2180	Total rotation	0.05°

COMPLETE VIEW OF ALL PHASING TRIALS

ExiMX Extended ISPyB for MX_{data}

Home | Shipment | Proteins and Crystals | Prepare Experiment | Data Explorer | Offline Data Analysis | Help

search by protein acronym

Logout MX1841@jnanao

Version: 0.5.8
Released: 20161202

ESRF

Transmission: 100
Exposure Time: 0.05 s
Flux start: 2.43e+12 ph/sec
Flux end: 2.43e+12 ph/sec

cell A	cell B	cell C
42.54	41.5	72.83
Alpha	Beta	Gamma
90	104.52	90

Run #3 Dec 12, 2016 9:59:29 PM

Summary | Beamline Parameters | Data Collections (1) | Sample | Results (18) | Workflow | Phasing (32)

Phasing	PREPARE	SUBSTRUCTURE	PHASING	MODEL	Download	Program	Method	Resolution	Solvent	Chain Count	Residues Count	Average Fragment Length	CC of partial model	Electron Density	PDB
P1211	✓	✓	✓	✓	📄	shelx	SAD	2.71-80.0	0.37	10	220	23	38.04	📄	🔍
						shelx	SAD	2.71-80.0	0.37	9	198	22	34.35	📄	🔍
						shelx	SAD	2.71-80.0	0.62	8	198	25	33.22	📄	🔍
						shelx	SAD	2.71-80.0	0.42	11	198	18	32.82	📄	🔍
						shelx	SAD	2.71-80.0	0.42	14	208	15	31.52	📄	🔍
						shelx	SAD	2.71-80.0	0.47	9	208	23	30.42	📄	🔍
						shelx	SAD	2.71-80.0	0.47	10	183	18	29.3	📄	🔍
						shelx	SAD	2.71-80.0	0.52	12	198	13	28.25	📄	🔍
P121	✓	✓	✓	✗	📄	shelx	SAD	2.71-80.0	0.62				6.88	📄	🔍
						shelx	SAD	2.71-80.0	0.67				6.81	📄	🔍
						shelx	SAD	2.71-80.0	0.42				6.54	📄	🔍
						shelx	SAD	2.71-80.0	0.47				6.48	📄	🔍
						shelx	SAD	2.71-80.0	0.47				4.75	📄	🔍
						shelx	SAD	2.71-80.0	0.42				4.48	📄	🔍
						shelx	SAD	2.71-80.0	0.37				4.44	📄	🔍
						shelx	SAD	2.71-80.0	0.67				4.08	📄	🔍

PNG snapshot of PDB

Interactive density viewer (UglyMol)

PNG CARTOON OF SHELXE MODEL

The screenshot displays the ExiMX web interface. At the top, there is a navigation menu with options: Home, Shipment, Proteins and Crystals, Prepare Experiment, Data Explorer, Online Data Analysis, and Help. Below the menu, there is a 'New Tab' button and a table of experiment parameters:

Transmission	100	Exposure Time	0.05 s	cell A
Flux start	2.40e+12 ph/sec	Flux end	2.43e+12 ph/sec	42.54 Alpha 60

Below the parameters, there is a section for 'Run #1 2016 Dec 12, 2016 9:59:29 PM'. A table shows the progress of various steps:

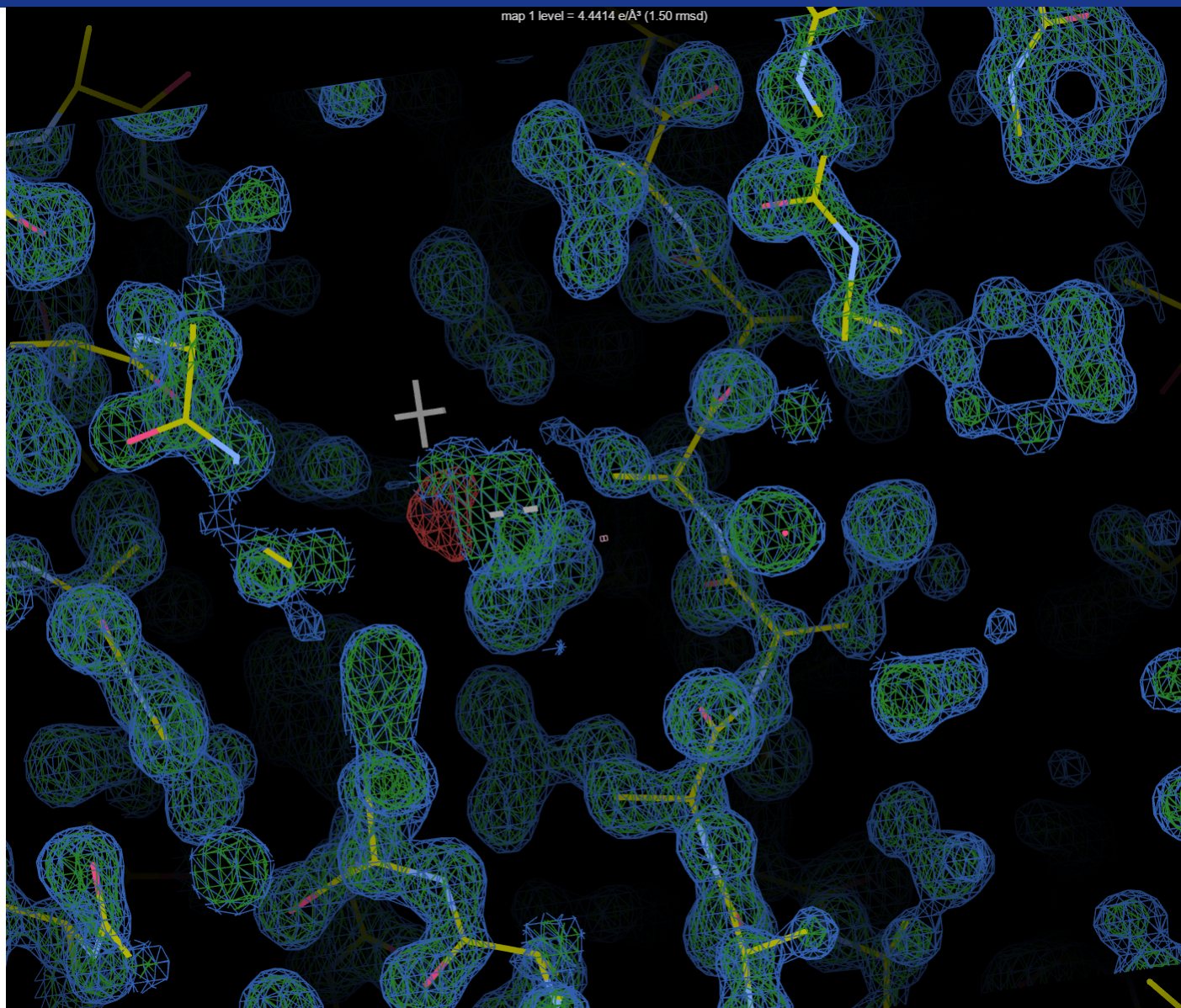
Phasing	PREPARE	SUBSTRUCTURE	PHASING	MODEL	Download	Progress
P1211	✓	✓	✓	✓	Ⓜ	phasing

A modal window titled 'MODELBUILDING : P1211 image 1 of 8' is open, showing a 3D protein model in a green cartoon representation. The model is a complex, multi-domain protein structure. Below the model, there is a table with columns for 'SAD', '2.71 - 50.0', '0.42', '14', and '208'. The table contains 10 rows of data, with the last row having a red 'x' icon in the 'MODEL' column.

SAD	2.71 - 50.0	0.42	14	208
phasing	2.71 - 50.0	0.47	9	208
phasing	2.71 - 50.0	0.47	10	183
phasing	2.71 - 50.0	0.82	12	158
phasing	2.71 - 50.0	0.82		
phasing	2.71 - 50.0	0.87		
phasing	2.71 - 50.0	0.43		
phasing	2.71 - 50.0	0.47		
phasing	2.71 - 50.0	0.47		
phasing	2.71 - 50.0	0.42		
phasing	2.71 - 50.0	0.37		
phasing	2.71 - 50.0	0.87		

At the bottom of the interface, there is a section for 'Run #1 Characterization 2016 Dec 12, 2016 9:57:01 PM' with 'Summary' and 'Beamline Parameters' links.

INTERACTIVE ELECTRON DENSITY

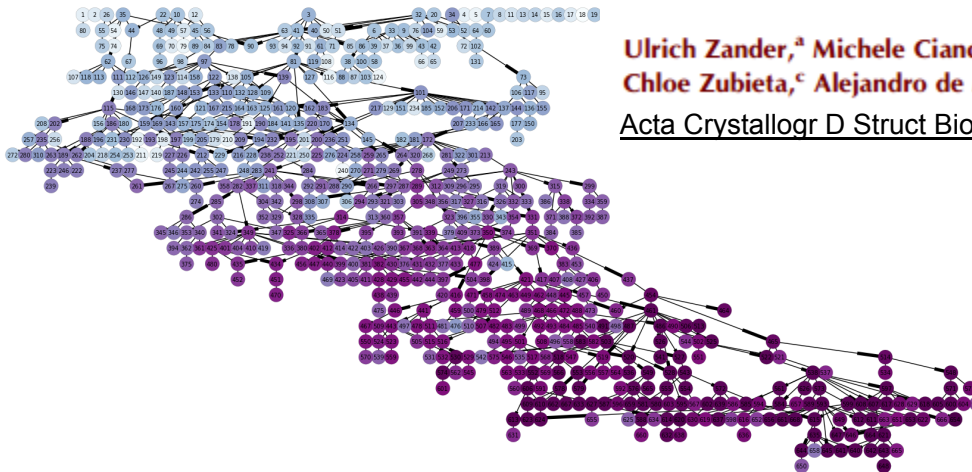


- +Molecular Replacement results into database and in EXI
- +More information from user (MXCubE, EXI) on sample – sequence, anom scatterer
- +Automatic merging of SSX data
 - +HCA
 - +Genetic Algorithm

Merging of synchrotron serial crystallographic data by a genetic algorithm

Ulrich Zander,^a Michele Cianci,^b Nicolas Foos,^a Catarina S. Silva,^c Luca Mazzei,^d Chloe Zubieta,^c Alejandro de Maria^a and Max H. Nanao^{a,c*}

Acta Crystallogr D Struct Biol. 2016 Sep;72(Pt 9):1026-35.



PEOPLE

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Florent Cipriani
Franck Felisaz
Ulrich Zander
Hugo Caserotto
Handling Group
Vacuum Group
Pascal Theveneau
David Flot
Amparo Vivo
Christian Morawe
Fabien Dobias
Francois Torrecillas
Bob Baker
Alexis Van der Kleij



Mario Lentini
October shutdown