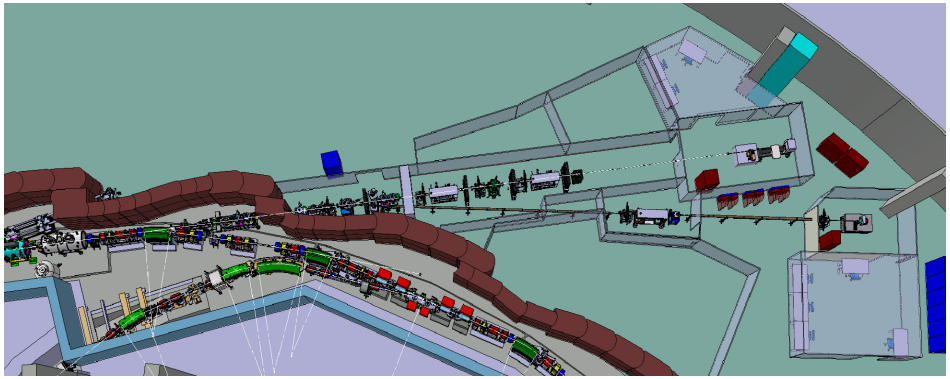
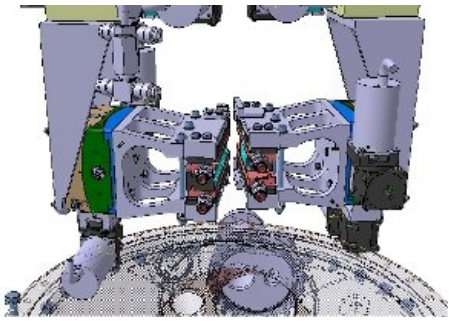
Joint Meeting
Trieste 2018

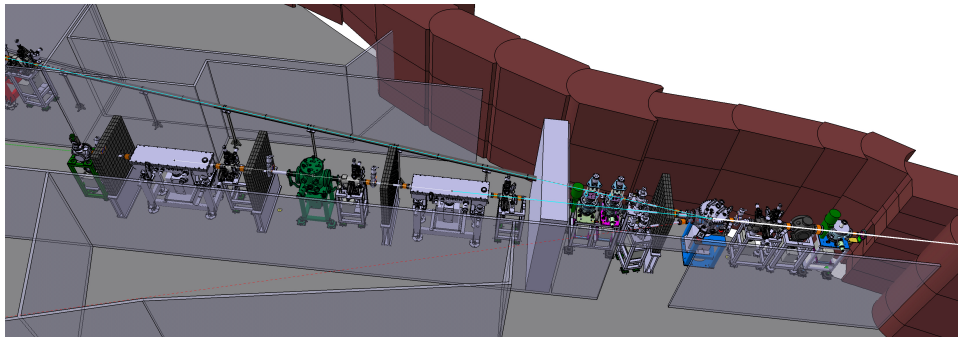
ISPyB

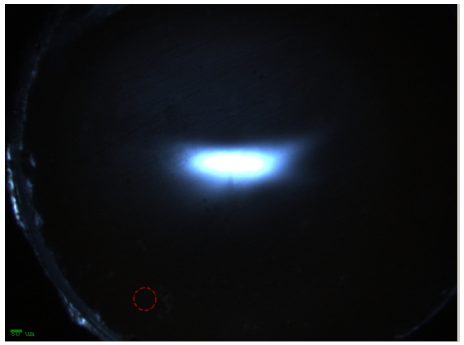
MXCuBE status at Elettra (XRD2 beamline)

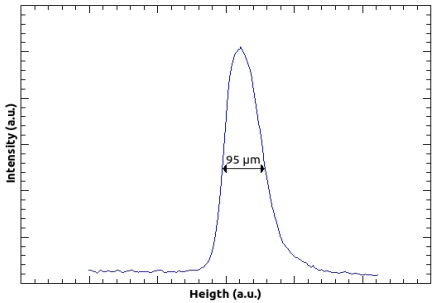
MXCuBE Status Report - XRD2

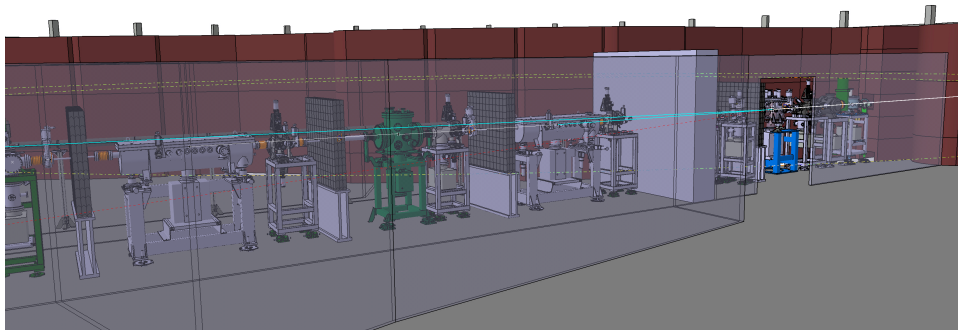










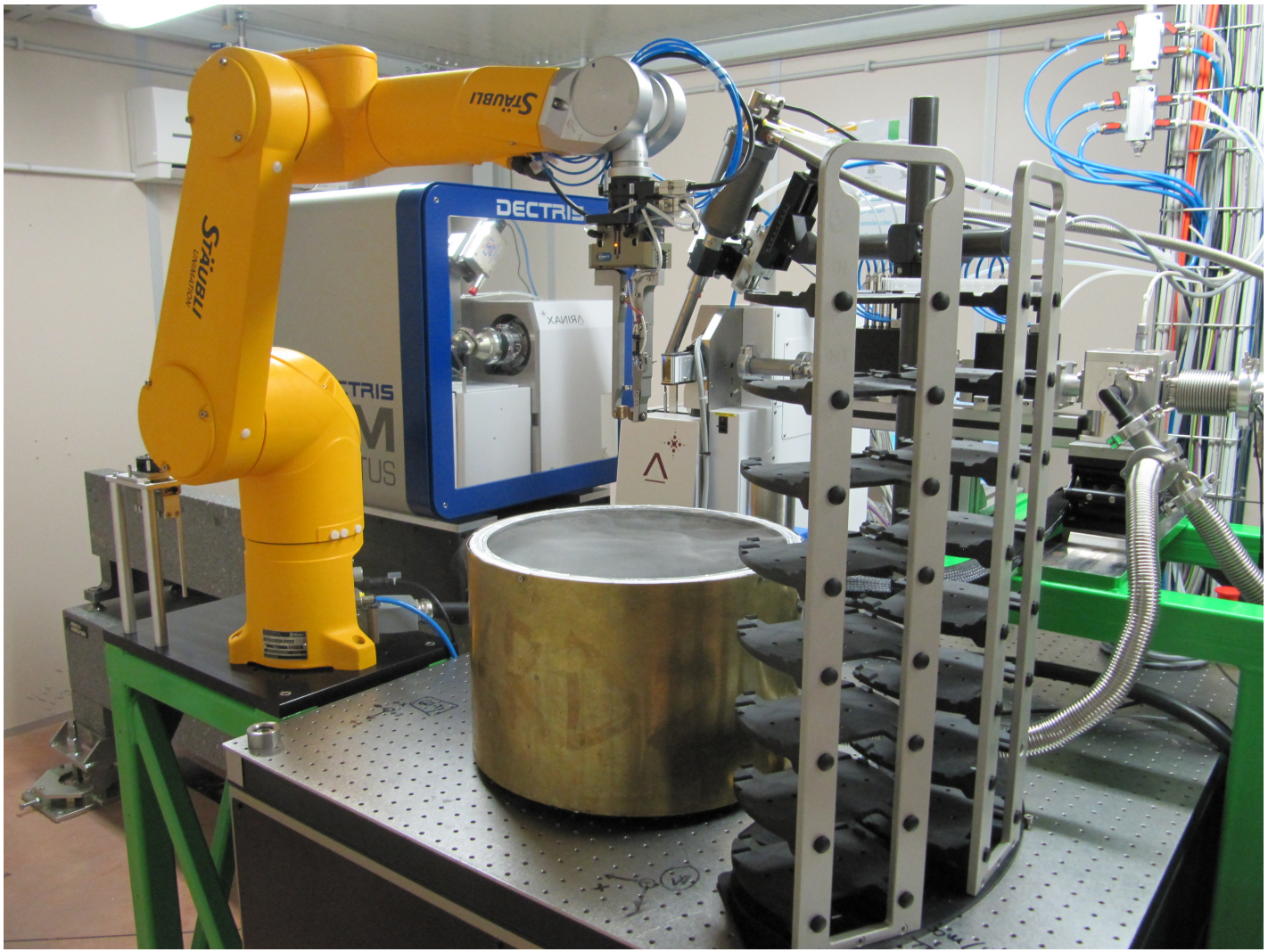


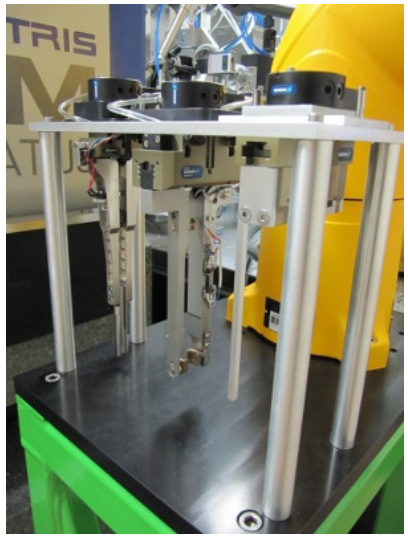
MEASURED flux (@13keV) = 2.2x10^{13} ph/sec (3x10^{13})

Mono bandpass (@13keV) < 4eV

Spectrum from 7.5 keV to > 30 keV

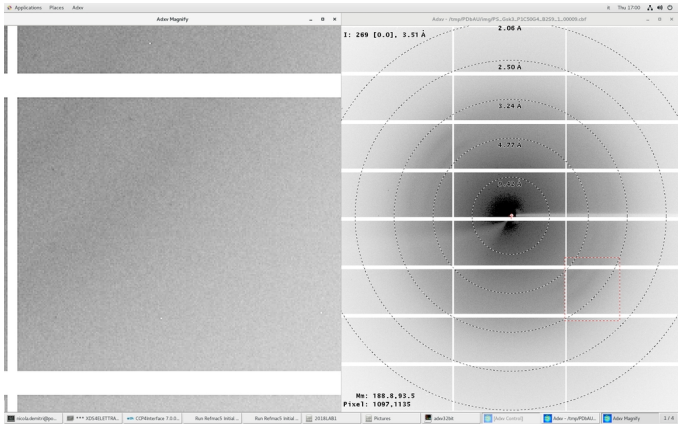
MXCuBE Status Report – Exp. Setup

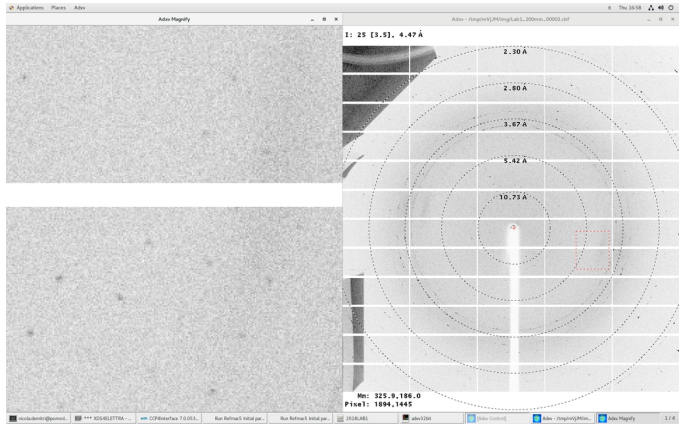


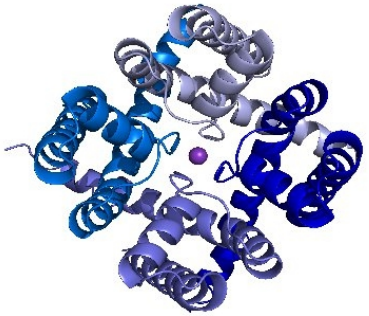


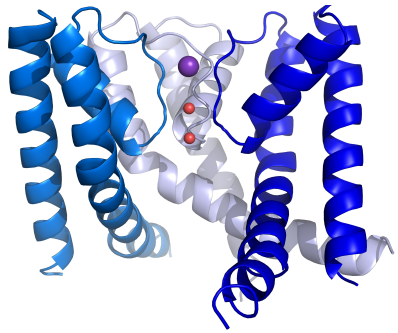
MXCuBE Status Report – BL valitation

Initial test using a real-life, poorly diffracting crystal (80x50x10 micron^3)- GSK-3.









SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION	NUMBER OF REFLECTIONS			COMPLETENESS	R-FACTOR	R-FACTOR COMPARED	I/SIGMA	R-ɪɪ
9.72	2994	2277	2338	97.4%	5.2%	5.4%	1434	9.09
6.95	4674	3695	4126	89.6%	8.4%	8.0%	1958	5.33
5.69	5604	4487	5260	85.3%	21.7%	20.2%	2234	2.23
4.94	7258	5604	6154	91.1%	19.9%	19.7%	3308	2.36
4.42	8609	6605	7090	93.2%	14.4%	14.8%	4008	2.96
4.04	9382	7226	7766	93.0%	19.5%	19.5%	4312	2.23
3.74	8998	7208	8336	86.5%	35.4%	34.0%	3580	1.26
3.50	9591	7731	9084	85.1%	51.1%	49.9%	3720	0.96
3.30	10942	8519	9670	88.1%	62.6%	68.9%	4846	0.62
total	68052	53352	59824	89.2%	20.1%	20.2%	29400	2.27

7.4%	98.8*	23*	0.909	317				
1.9%	98.4*	12	0.974	367				
30.7%	88.2*	14	0.853	378				
28.2%	88.6*	13	0.846	563				
20.4%	94.1*	7	0.793	659				
27.6%	91.2*	2	0.772	659				
50.1%	78.2*	8	0.805	465				
72.3%	70.8*	8	0.741	448				
88.6%	51.9*	-1	0.654	643				
28.4%	94.6*	9	0.801	4499				

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION	NUMBER OF REFLECTIONS			COMPLETENESS	R-FACTOR	R-FACTOR COMPARED	I/SIGMA	R-ɪɪ
8.86	4701	2888	3158	91.5%	3.8%	4.0%	3626	15.06
6.32	8978	5220	5502	94.9%	6.6%	6.5%	7516	9.06
5.18	11583	6591	6964	94.6%	11.7%	12.2%	9984	5.88
4.49	13972	8047	8408	95.7%	10.7%	11.2%	11850	6.17
4.02	16029	9018	9538	94.5%	14.9%	15.7%	14022	4.78
3.67	14131	8265	10510	78.6%	18.3%	17.2%	11732	2.52
3.40	16249	9354	11346	82.4%	25.3%	23.5%	13790	1.91
3.18	19637	10997	12144	90.6%	86.1%	92.7%	17280	0.85
3.00	21692	12303	13128	93.7%	137.8%	160.8%	18778	0.52
total	126972	72683	80698	90.1%	17.1%	17.7%	108578	3.81

5.4%	99.5*	-15	0.665	811				
9.3%	99.2*	-3	0.771	1714				
16.5%	97.0*	0	0.747	2323				
15.2%	97.6*	-1	0.729	2763				
21.1%	96.5*	-6	0.687	3276				
25.9%	99.8*	6	0.681	2395				
35.8%	99.1*	11*	0.640	2861				
121.8%	87.7*	-2	0.612	3939				
194.9%	51.3*	-3	0.578	4393				
24.2%	99.5*	0	0.665	24475				

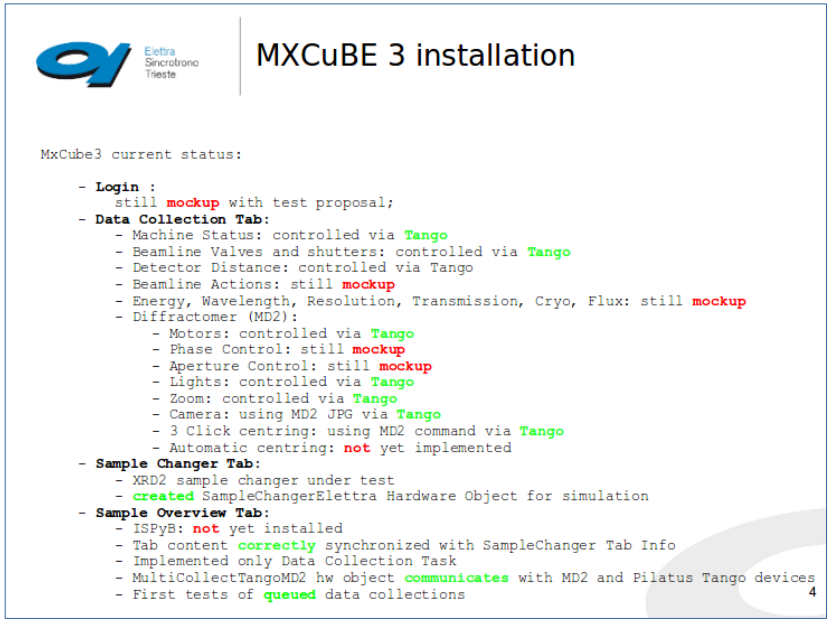
Bacterial CNG-mimicking chimera channel

Cell parameters: 181.32, 135.26, 67.50 – 90, 87.9, 90 (C2) Resolution:47.79-3.2 (3.37-3.2) Rsym or Rmerge: 0.15 (0.35)
I over sigma 4 (3.4) Refinement Rw/Rfree 0.30/0.35 **Deposited in Protein Data Bank: 6FIZ**

Glycogen synthase kinase 3 (GSK-3) phosphorylates more than 100 different substrates and is involved in a great number of cellular pathways. It has a role in glycogen metabolism and is now getting notorious for being considered as target for Alzheimer disease.
Cyclic Nucleotide Gated (CNG) channels are nonselective cation channels playing a key role in visual and olfactory transduction

MXCuBE Status Report – MXCuBE 3

- ✓ MXCuBE 3 installed (*minimal* configuration), **in use** with our initial, friendly users
- ✓ Login with user/proposals credentials (linked to VUO)
- ✓ MD2-SC coordination, 3 click centering, *simple* data collections, few “actions” implemented
- ✓ Data collected download-able *via* VUO



MXCuBE Status Report – working on ..

- ✓ Sample changer OK for SPINE pucks, under test for UNIPUCK, under development for crystallization PLATES and Test-Samples
- ✓ Set-Up of disk space and computing power: sw installed in *local* Pilatus PPU and in a computer cluster:

  Cluster of 16 servers, 252 cores @ 3GHz and 128 GB RAM each (2TB total), Tesla supercomputing machines with nVidia K80 boards (total of almost 5000 CUDA cores) with 480 GB/sec bandwidth.

- ✓ ISPyB/EXI missing: we are working on files describing the dewars content (users are supposed to upload them together with dewars tracking number now) – VUO integration
- ✓ No remote access yet.

MXCuBE Status Report – Next

- ✓ System debug in order to offer a minimal but robust beamline
  (deadline: the onset of ESRF upgrade program)

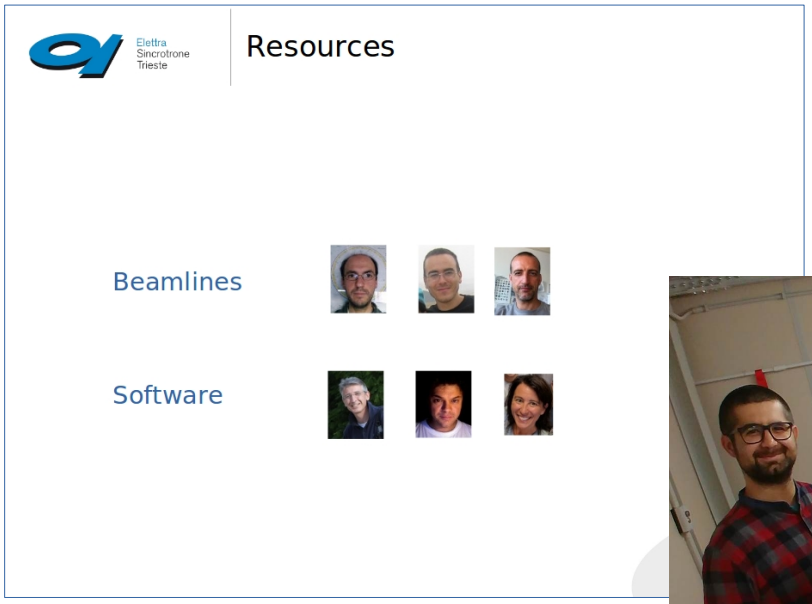
- ✓ XRD1 MX users are invited to collect data at XRD2.
  A common XRD1 and XRD2 call, based on a monthly evaluation and continuous submission already running

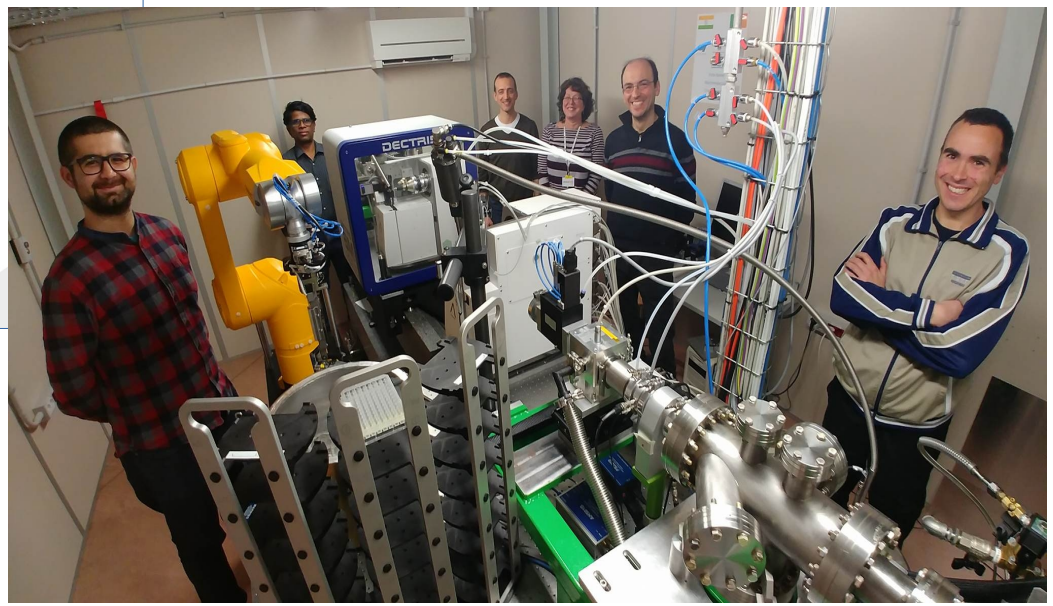
- ✓ Link MXCuBE with ISPyB/EXI

- ✓ …

Elettra Sincrotrone Trieste

Resources





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