MASSIF-3: Latest News

David von Stetten

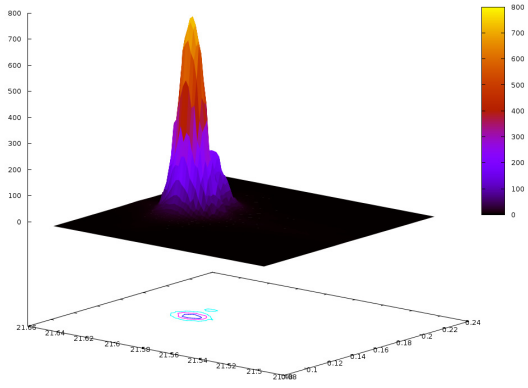
BAG meeting

8th February 2016

ESRF

MASSIF-3 (a.k.a. ID30A-3)

- available to users since December 2014
- MASSIF-3 is *not* fully automatic
- fixed energy: 12.8 keV
- beam size: 15 µm (CRLs + multi-layer mirror)
- flux: 1.3×10^{13} ph/s



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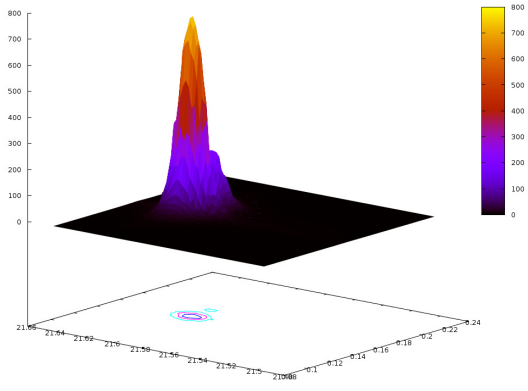

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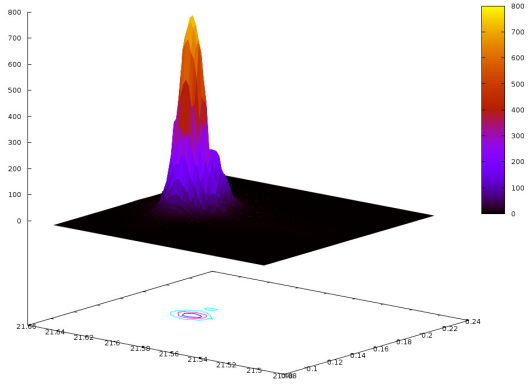
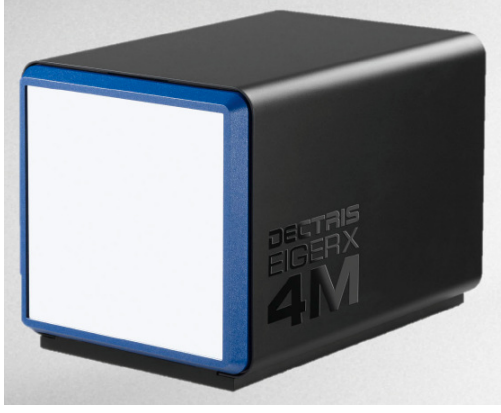


- latest version of MxCuBE (v2.1)
- MD2 minidiffractometer
- SC3 sample changer
- Eiger 4M detector
- maximum resolution: 1.4 Å



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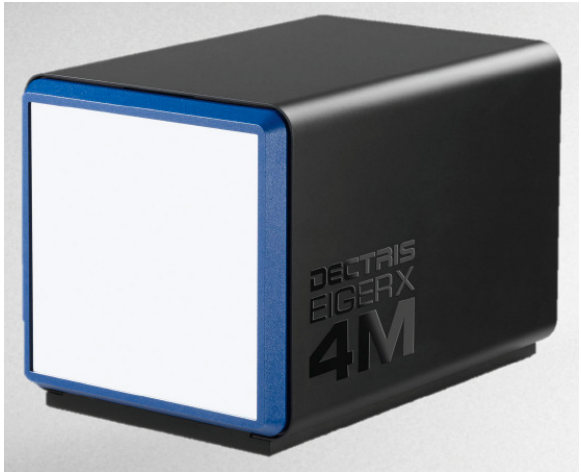
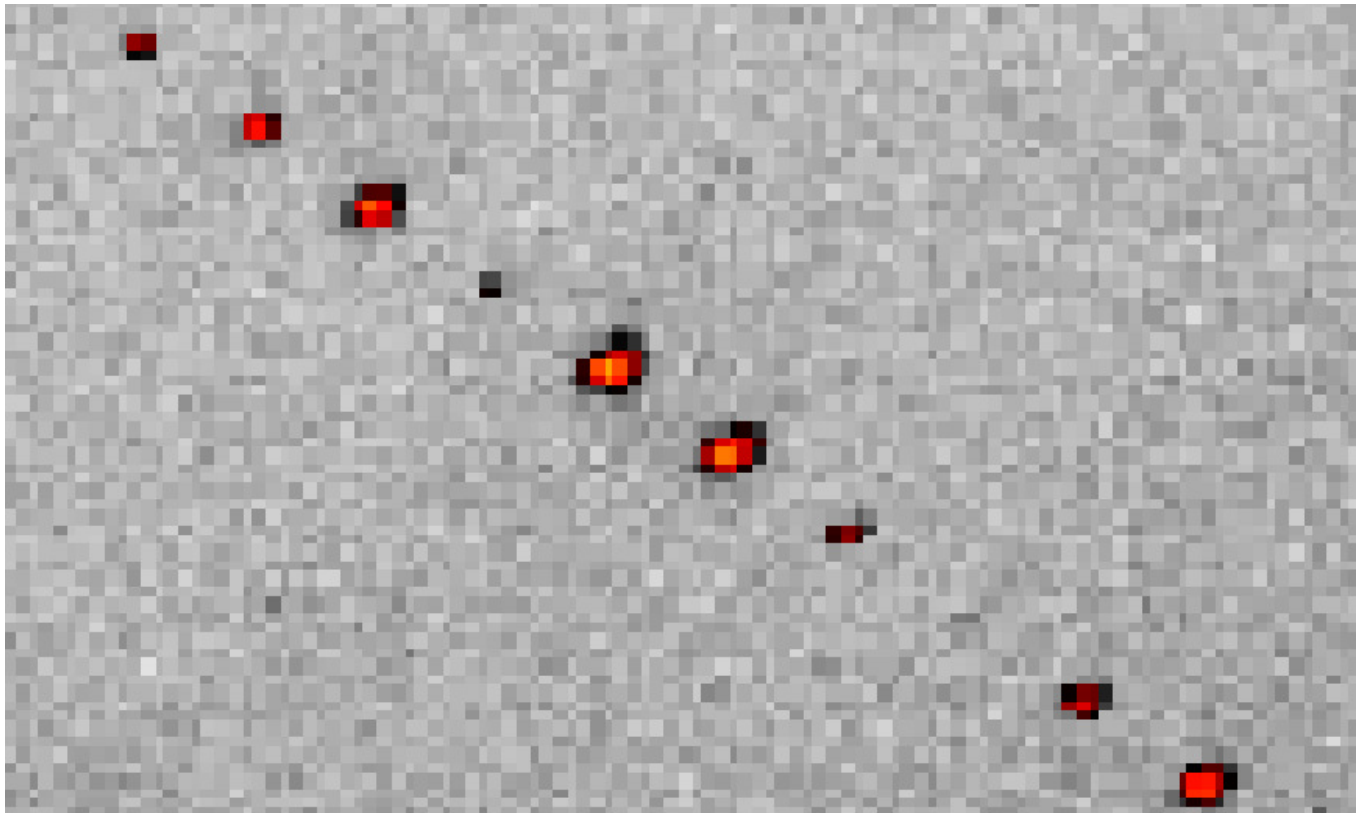
New detector: Eiger 4M

- available to users since last Friday
- up to 750 frames/sec
- small pixels (75×75 µm)





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New detector: Eiger 4M

Data collection with up to 750 frames/sec:

Image Prefix	Run No	# images	Exp. Param.	Status	Space Group	Completenes	Resolution	Rsymm *Inner* *Outer* *Overall*	Unit_cell *a, b, c* *alpha, beta, gamma*
thaumatin1_750Hz_w1	3	1300			P 41 21 2		45.78 - 5.23 1.4 - 1.35 45.78 - 1.35	3.5 81.3 10.5	57.76, 57.76, 150.16 90.00, 90.00, 90.00
thaumatin1_500Hz_w1	2	1300			P 41 21 2		45.77 - 5.23 1.4 - 1.35 45.77 - 1.35	3.5 82.1 10.4	57.75, 57.75, 150.12 90.00, 90.00, 90.00
thaumatin1_100Hz_w1	1	1300			P 41 21 2		45.76 - 5.23 1.4 - 1.35 45.76 - 1.35	3.5 79.1 10.4	57.73, 57.73, 150.07 90.00, 90.00, 90.00

Limited by the maximum speed of the omega axis ($\approx 100°/s$)

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New data format: HDF5

Containers instead of individual image files (100 images per file):

```
-rw-r--r-- 1 opid30 jsbg  87M Feb 4 11:45 insulin_w1_5_1_master.h5
-rw-r--r-- 1 opid30 jsbg 304M Feb 4 11:45 insulin_w1_5_1_data_000001.h5
-rw-r--r-- 1 opid30 jsbg 313M Feb 4 11:45 insulin_w1_5_1_data_000002.h5
-rw-r--r-- 1 opid30 jsbg 328M Feb 4 11:45 insulin_w1_5_1_data_000003.h5
-rw-r--r-- 1 opid30 jsbg 350M Feb 4 11:45 insulin_w1_5_1_data_000004.h5
-rw-r--r-- 1 opid30 jsbg 367M Feb 4 11:45 insulin_w1_5_1_data_000005.h5
```

New data format: HDF5

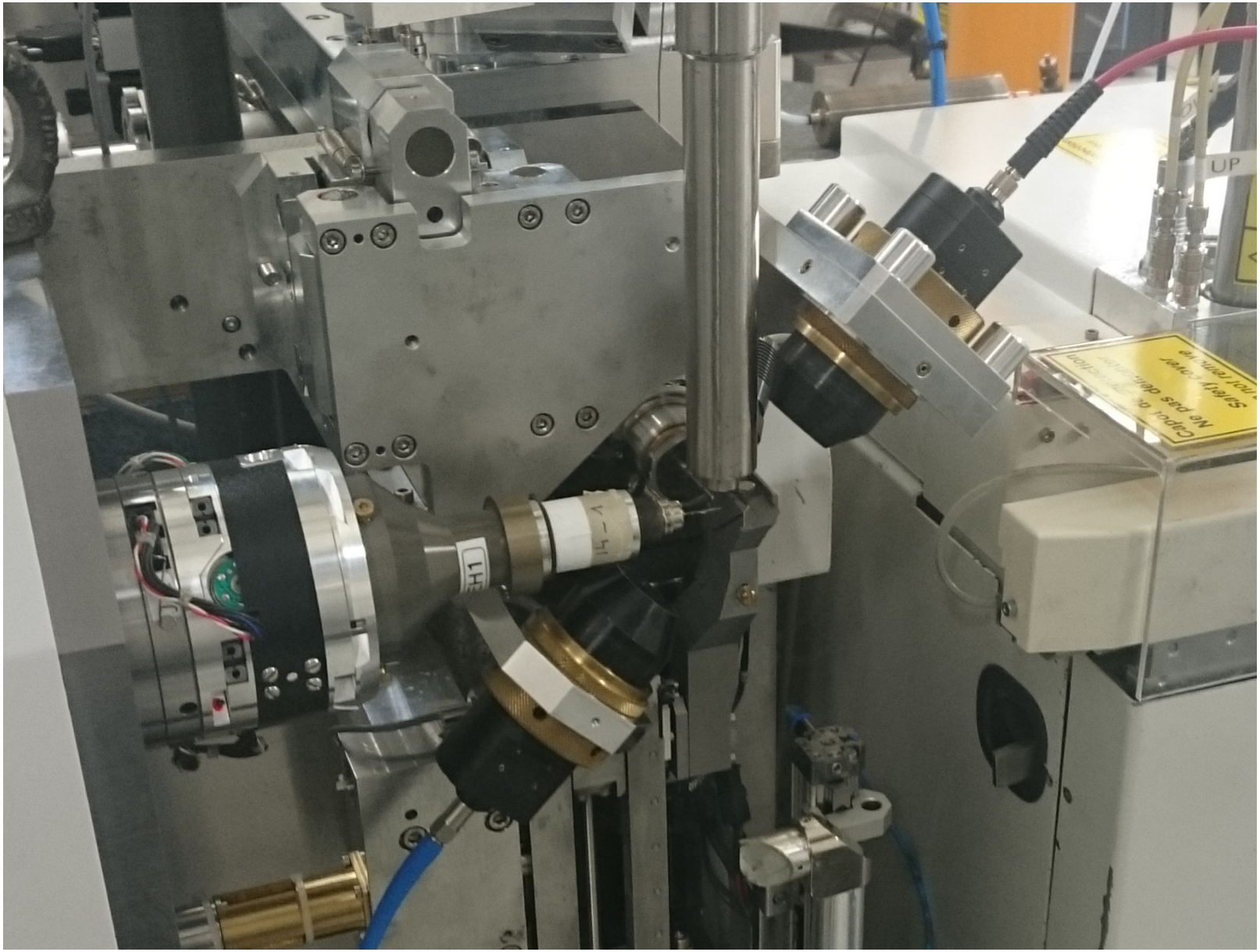
Containers instead of individual image files (100 images per file):

```
-rw-r--r-- 1 opid30 jsbg  87M Feb 4 11:45 insulin_w1_5_1_master.h5
-rw-r--r-- 1 opid30 jsbg 304M Feb 4 11:45 insulin_w1_5_1_data_000001.h5
-rw-r--r-- 1 opid30 jsbg 313M Feb 4 11:45 insulin_w1_5_1_data_000002.h5
-rw-r--r-- 1 opid30 jsbg 328M Feb 4 11:45 insulin_w1_5_1_data_000003.h5
-rw-r--r-- 1 opid30 jsbg 350M Feb 4 11:45 insulin_w1_5_1_data_000004.h5
-rw-r--r-- 1 opid30 jsbg 367M Feb 4 11:45 insulin_w1_5_1_data_000005.h5
```

Viewing and processing:

- EDNA characterisation and data collection working
- ESRF autoprocessing working; some workflows not tested yet
- for viewing: adxv and albula can read hdf5 files
- XDS can read hdf5 files if the `H5ToXds` tool is installed:
  `NAME_TEMPLATE_OF_DATA_FRAMES= insulin_w1_5_1_??????.h5 ! HDF5`
- other software: your mileage may vary...

Online optical spectroscopy



Online optical spectroscopy

Microspec permanently installed on MASSIF-3:

- compatible with sample changer and cryostream
- online microspec allows:
  - UV/vis absorption
  - fluorescence
  - actinic light
- integration into workflows ongoing

[von Stetten *et al.*, *Acta Cryst.* *D***71**, 15–26 (2015)]

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Astrophysics (20 min exposure)

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Acknowledgements

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