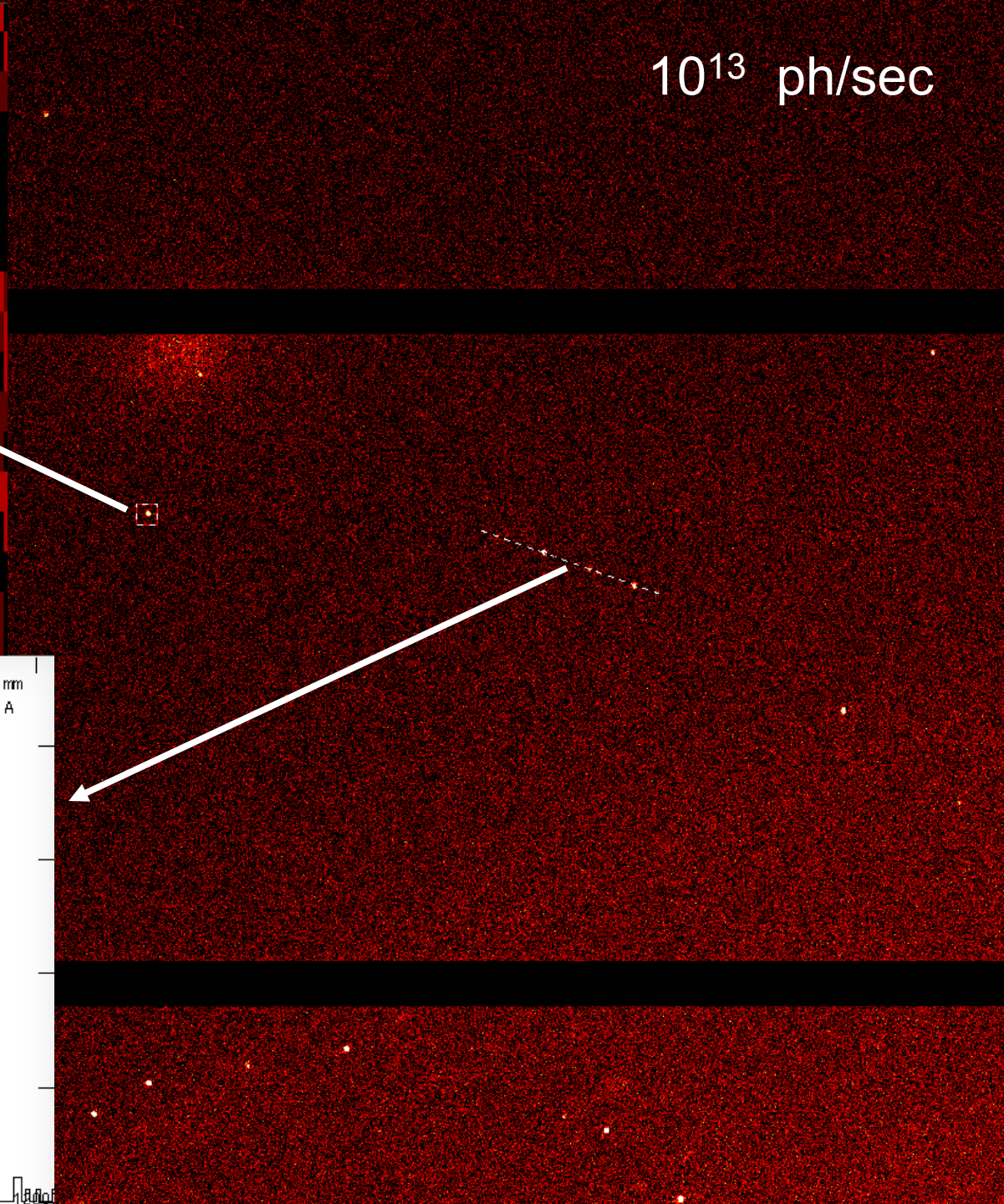
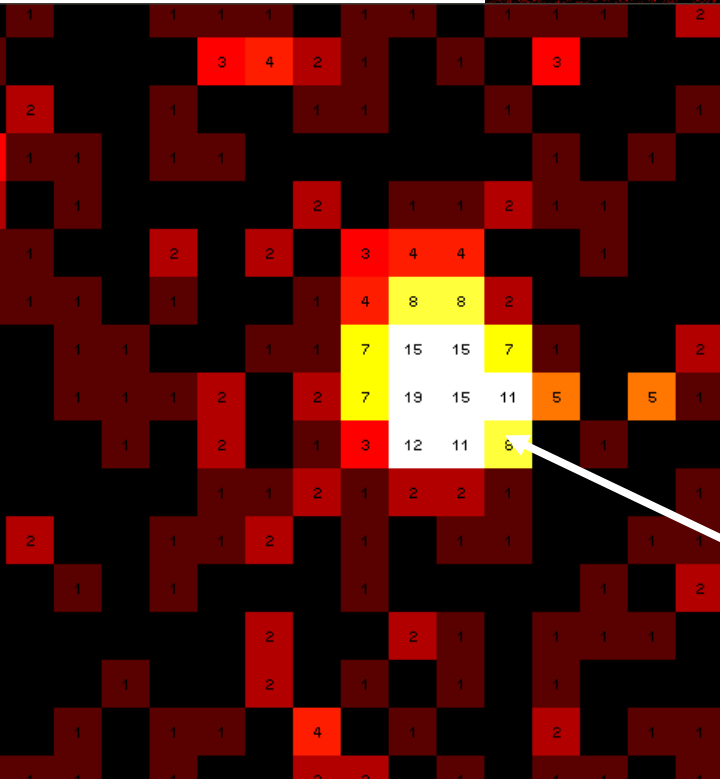


# MxCuBE for time-resolved SSX at T-REXX

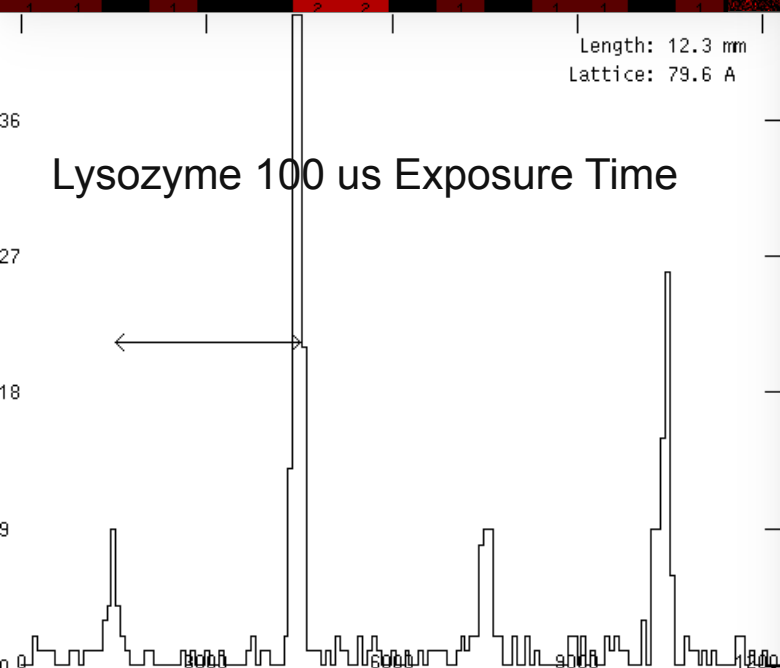
[gleb.bourenkov@embl-hamburg.de](mailto:gleb.bourenkov@embl-hamburg.de)

$10^{13}$  ph/sec



Length: 12.3 mm  
Lattice: 79.6 Å

Lysozyme 100 us Exposure Time



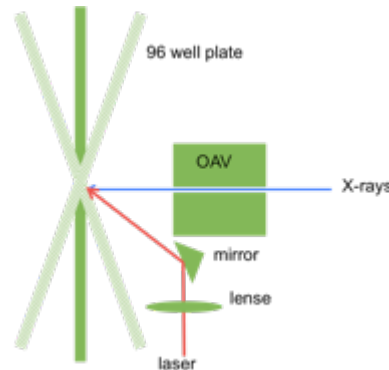
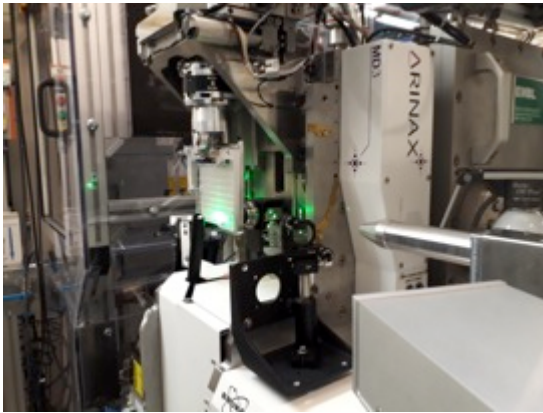
**Exposure time = 7.6  $\mu$ s**  
**40 PETRAIII bunches**

**Count rate limit:**  
**18 events/pixel**

3.07 Å

5.97 Å

# Time-resolved SSX by serial helical scans

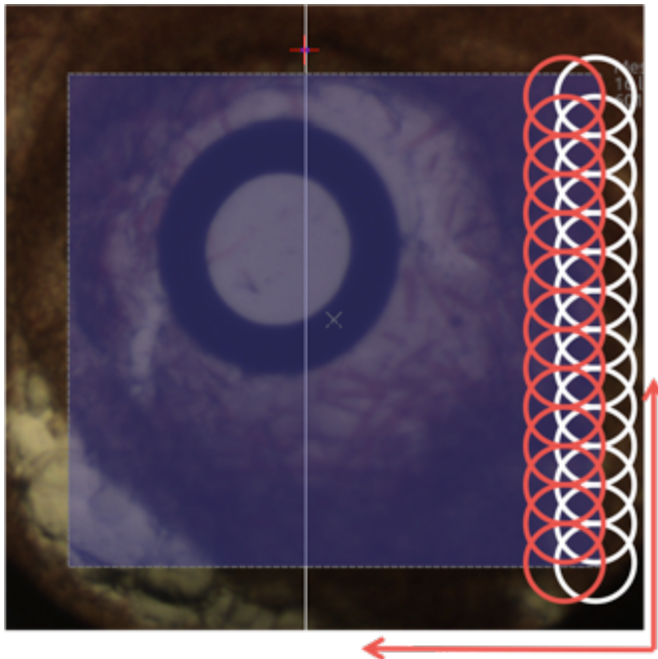


Laser-flashes delivered at the sample in 96-well plate at a sub-harmonic of the detector framing frequency

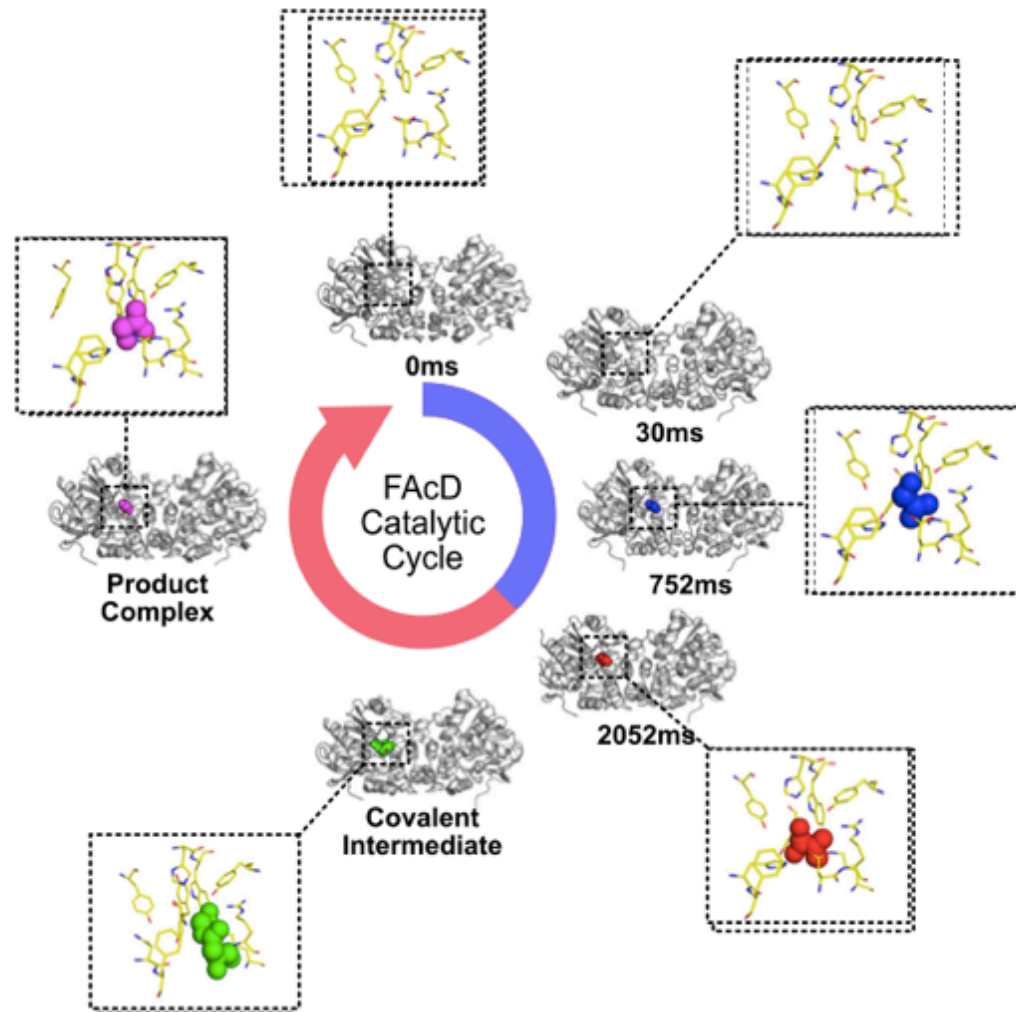
- Laser beam  $\varnothing$  50  $\mu\text{m}$
- Exposure time 1.3 ms / frame
- Ver. translation 1  $\mu\text{m}/\text{frame}$
- Laser flash at every 30<sup>th</sup> frame
- Hor. translation 30  $\mu\text{m}$  / line

**== 30 time points x 1.3 ms**

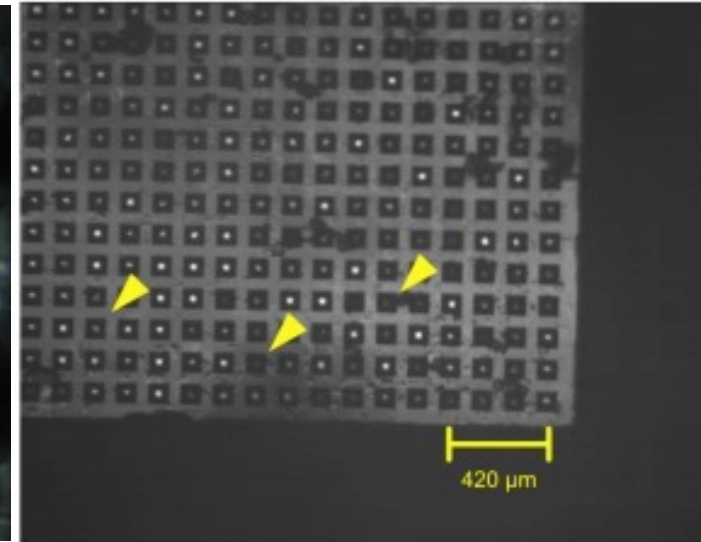
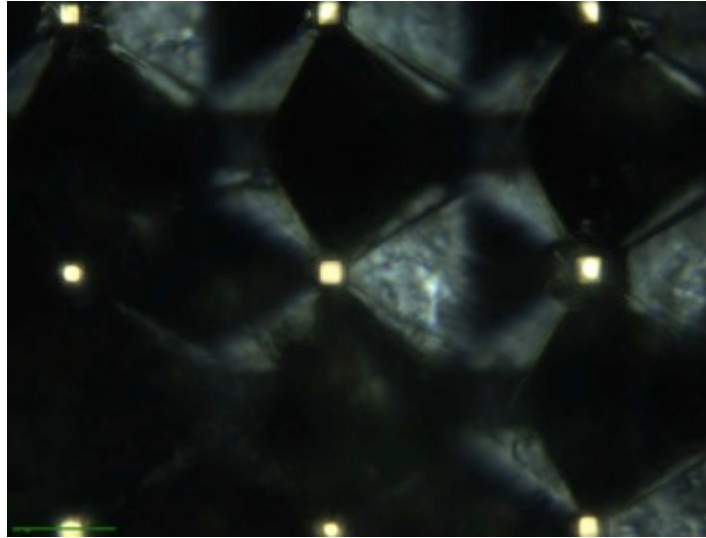
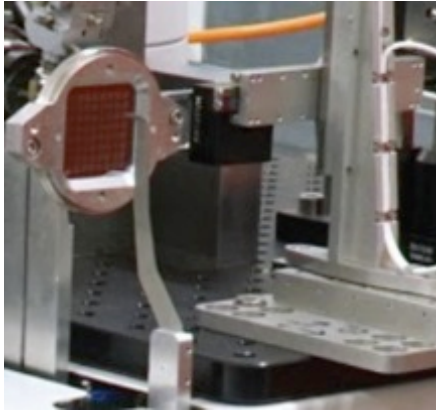
**10<sup>6</sup> frames in 3 hours wall clock  
~30% hit rate**



# Time series: *linear vs logarithmic*



# Si chips for sample delivery

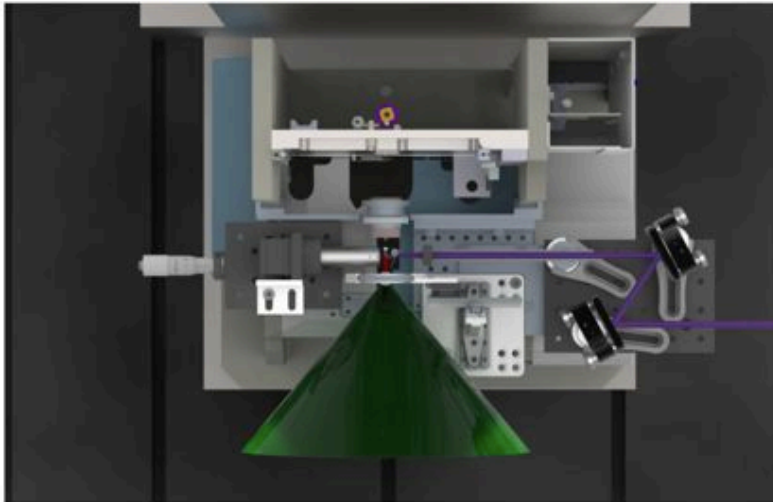
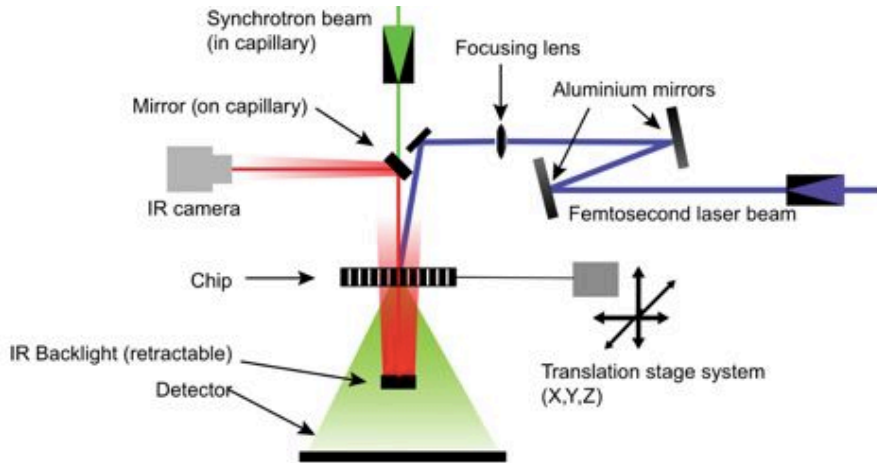


Zarrine-Asfar et al. (2012) Acta Cryst. D  
Sherrell et al. (2015) J Synch. Rad.

- 20000-25000 compartments
- 120-150 μm pitch
- 25 Hz re-positioning

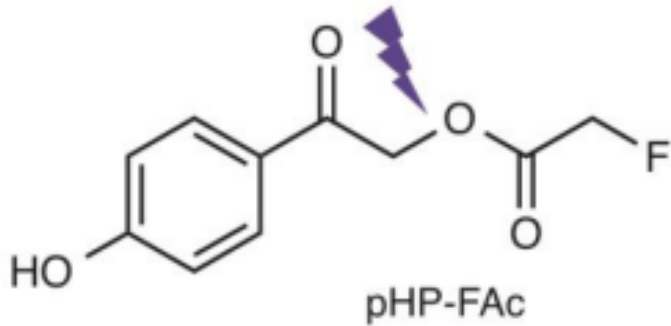
Eike Schulz, Pedram Mehrabi, Rike  
Müller-Werkmeister, Dwayne Miller,  
MPISDM Hamburg

# Un-caging experiments at P14.EH1

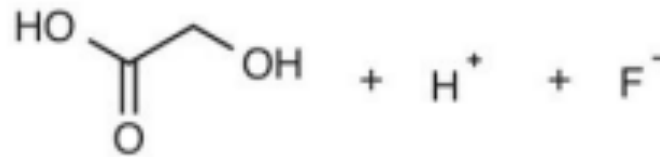
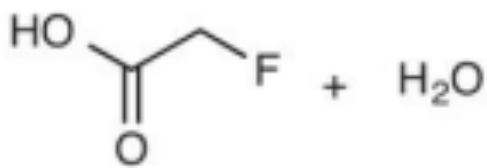


Eike Schulz, Pedram Mehrabi, Rike  
Müller-Werkmeister, Dwayne Miller,  
MPISDM Hamburg

# Fluoroacetate dehalogenase substrate un-caging



Pump: 340 nm 45 nJ / 100x100  $\mu\text{m}^2$   
4-15 ms X-ray exposures  
20000 frames x 4 time delays in 1 hour  
>3.5K diffraction images per time delay  
Resolution 1.8 Å

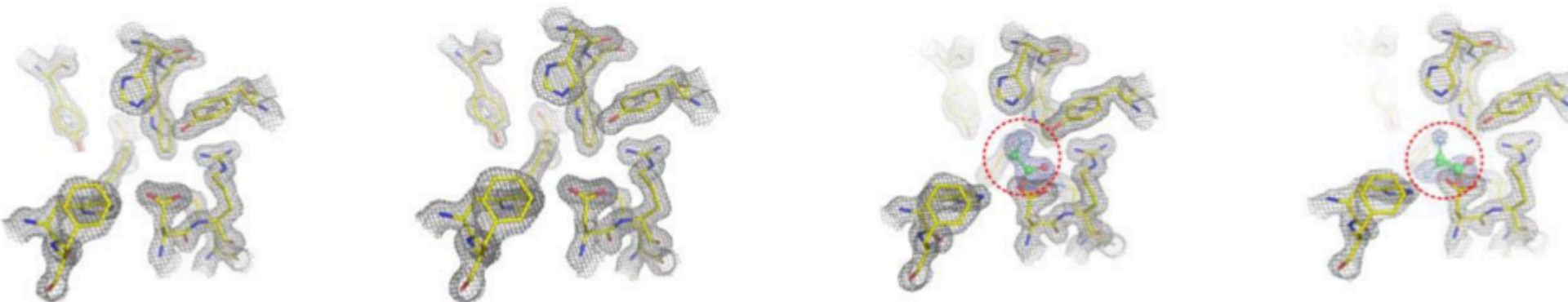


0MS

30MS

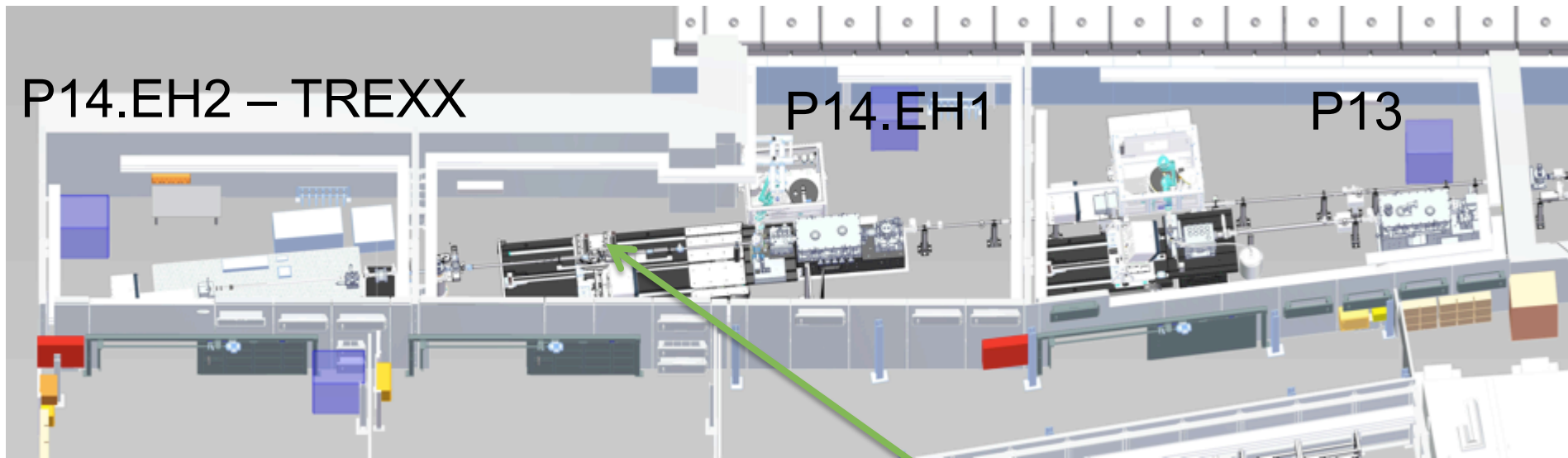
752MS

2052MS





# Dedicated P14 end station for time-resolved MX

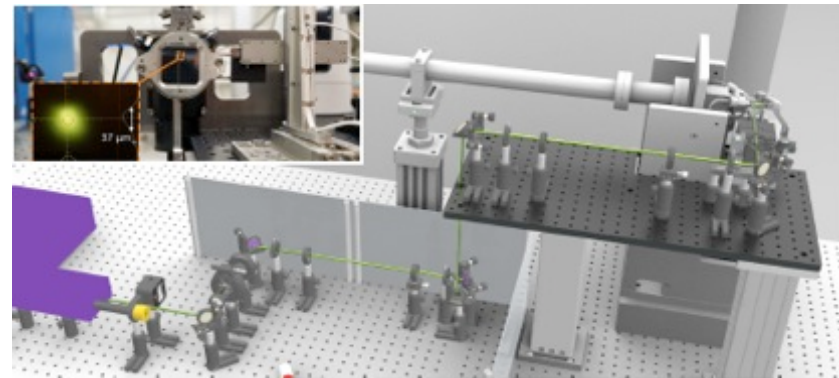
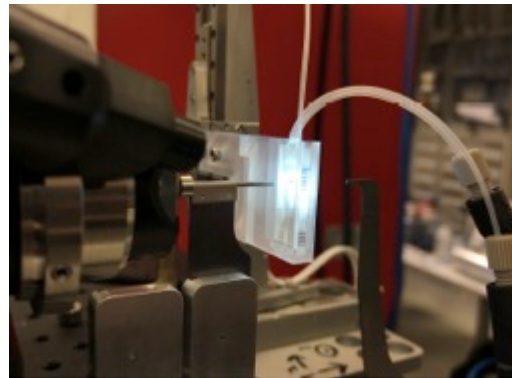
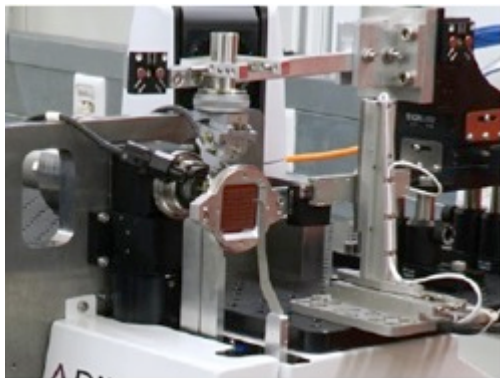
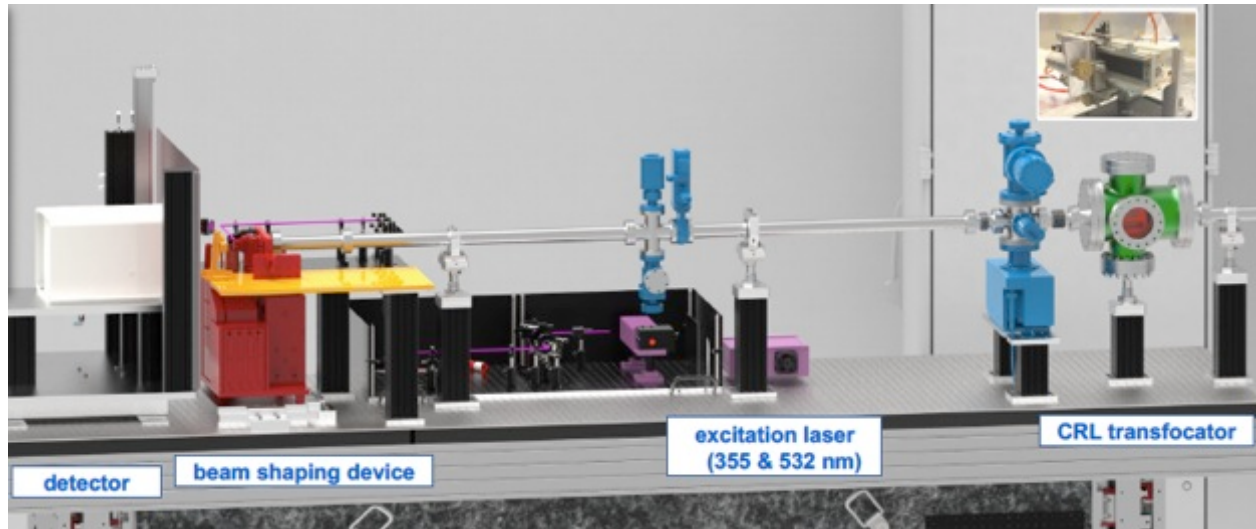


- In operation since 10/2018
- EH1/EH2 switch in 1 hour
- 66 shifts scheduled for 2019
- 1-day allocations



beam transport

# TREXX Instrumentation



# MXCuBE @ TREXX : data acquisition

The screenshot displays the MXCuBE data acquisition software interface. The main window shows a diffraction pattern with a central spot and surrounding rings, overlaid with a green grid. The interface is divided into several panels:

- Top Left:** "Collect" and "Log" buttons, "Sample centring" section, and "Front light" and "Back light" indicators.
- Top Center:** "Zoom" control and "catalase\_chip1\_532nm\_1" title.
- Top Right:** "ISPyB proposal" section with "mai0026 - Proposal" and "Group" dropdown, and "Sample tree" showing "manually-mounted" and "catalase\_chip1\_532nm\_1".
- Middle Left:** "Acquisition" parameters: Number of triggers: 25600, Images per trigger: 20, Number of images: 512000, Exposure time (s): 0.0014, Energy (keV): 12.6799, Resolution (Å): 1.844, Transmission (%): 100.
- Middle Center:** "Data location" section with "Folder:" and "File name:" fields.
- Middle Right:** "Machine current" section showing "86.3 mA" and "Machine state" as "Setup-Experiment".
- Bottom Left:** "Beam size" section with "Horizontal" and "Vertical" values (15.0 μm), "Aperture" and "CRL eh1" settings, and "Beam positioning" controls.
- Bottom Center:** "Heat map" section showing a grid of data points.
- Bottom Right:** "Queue history" section with a "Stop" button and a "Collection" status indicator.
- Bottom Center (Log):** A log window showing the following messages:

```
[2018-10-29 17:35:14] Collection: Preparing to collect
[2018-10-29 17:35:14] Collection: Starting data collection in LIMS
[2018-10-29 17:35:17] Collection: Creating directories for raw images and processing files
[2018-10-29 17:35:17] Collection: Getting sample info from parameters
[2018-10-29 17:35:17] Collection: Storing sample info in LIMS
[2018-10-29 17:35:17] Collection: Moving to centred position
[2018-10-29 17:35:17] Collection: Taking 1 sample image(s)
[2018-10-29 17:35:17] Collection: Setting transmission to 100.00
[2018-10-29 17:35:17] Collection: Setting energy to 12.6799
[2018-10-29 17:35:17] Collection: Setting resolution to 1.844
[2018-10-29 17:35:17] Collection: Updating data collection in LIMS...
[2018-10-29 17:35:17] Collection: Data collection in LIMS updated
[2018-10-29 17:35:18] Detection: Data change in progress.
Please wait...
[2018-10-29 17:35:40] Collection: started
```

# MXCuBE at TREXX : chip centering in IR light (Arinax OAV)

The screenshot displays the MXCuBE control software interface. The main window shows a grid of sample positions with a live camera view of the sample. The interface includes several control panels and status indicators.

**Top Panel:** Collect Log, Sample centring, Front light: 0.20, Back light: 2.00, Zoom 2.

**Sample: manually-mounted**

**ISPyB proposal:** mxhr0026 - Proposal, Group: Set

**Sample tree:** Mode: Manually mounted, Sample: Sample, Centring: Manual 3-click, Filter: manually-mounted

**Machine current:** 89.9 mA

**Machine state:** Machine state: Battery-Experiments, 6.08 GeV, 40 Bunches

**Front End:** Front End: Opened, Hutch temperature and humidity: 23.6 C, 22.8 %

**Disk space:** Total: 226.9 GB, Free: 203.0 GB (89%)

**Energy:** Current: 12.6799 keV, Wavelength: 0.9778 Å

**Status:** Stopped, Failed, Collection c, Collection c

**Transmission:** Current: 100.00 %, Set to: Resolution: 1.844 Å, Current: 120.00 mm, Set to: Beamstop distance: 6.00 mm, Set to:

**Door interlock:** Locked (unlock enabled), Unlock, Safety shutter: out, Open, Close, Fast shutter: Closed, Open, Close

**Image tracking:** ready, Enable Advx image tracking

**Detector status:** Ready, Frame rate: 313 Hz, Temperature: 26.1°, Humidity: 2.3%

**Beam positioning:** Horizontal: 11.0 µm, Aperture: 3.5µ, CRL eh1: Manual, Set, Vertical: 11.0 µm, PARK, Out

**Phase:** Centring

**Heat map:** A plot showing the distribution of data points, with a result of Resolution: Image: R, value #.

**Log:** [2018-10-29 20:14:40] Collection: Moving to centred position  
[2018-10-29 20:14:40] Collection: Taking 1 sample snapshot(s)  
[2018-10-29 20:14:40] Collection: Setting transmission to 100.00  
[2018-10-29 20:14:40] Collection: Setting energy to 12.6799  
[2018-10-29 20:14:40] Collection: Setting resolution to 1.844  
[2018-10-29 20:14:40] Collection: Updating data collection in LIMS...  
[2018-10-29 20:14:40] Collection: Data collection in LIMS updated  
[2018-10-29 20:14:44] Diffractometer: Current phase changed to DataCollection  
[2018-10-29 20:14:46] Collection: started  
[2018-10-29 20:41:59] Processing: Done  
[2018-10-29 20:42:27] Collection: Finished  
[2018-10-29 20:59:04] Data collect is disabled  
[2018-10-29 20:59:04] - Safety shutter is closed (Open the safety shutter to enable collections)  
[2018-10-29 20:59:34] Diffractometer: Setting Transfer phase. Please wait...  
[2018-10-29 20:59:34] Diffractometer: Current phase changed to Transfer  
[2018-10-29 21:01:37] Diffractometer: Current phase changed to Centring

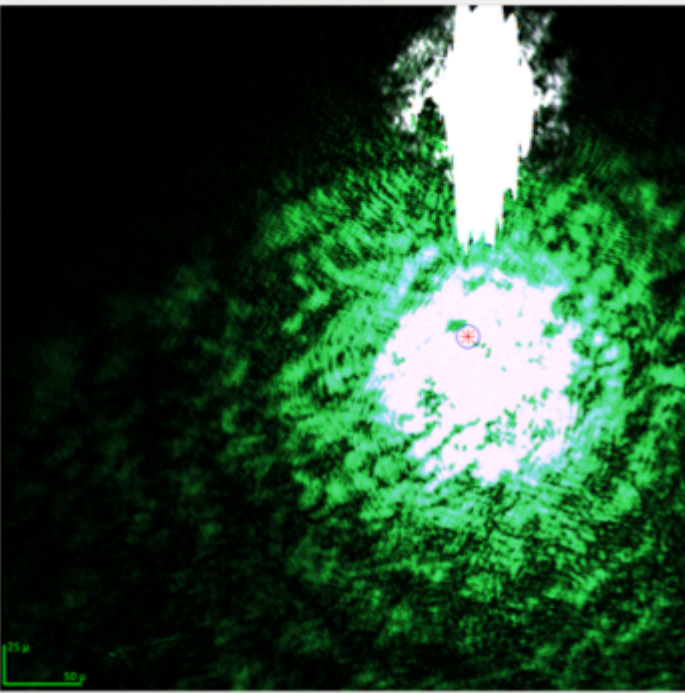
Currently not connected to the chip scanner motors

# MXCuBE @ TREXX : data acquisition

Up to 1024000 frames in 35 min  
on average 494 fps  
sustainable

Collect Sample

Front light: 0.26 Back light: 0.06



X: 1198 Y: 1003


Beam size: Horizontal: 15.0 µm Vertical: 15.0 µm

Aperture: CRL eh1

Manual Set Out

Beam positioning: Horizontal: 0.003 Vertical: 0.003

Heat map



Result: Resolution: Image: K, value: R

bonstetten@PE2 State: Queue running Diffractionmeter: Ready Sample changer: Last collect: -

### catalase\_chip1\_532nm\_1

#### Still

##### Acquisition

Number of triggers: 25600 Images per trigger: 20

Number of images: 512000

Exposure time (s): 0.0014 Detector mode: 0

Energy (keV): 12.6799

Resolution (Å): 1.844

Transmission (%): 100

##### Data location

Folder:

/mnt/beegfs/PE2/2018/11264\_206/dvonstetten/20181029/RAW\_DATA

/catalase\_chip1\_532nm

File name: catalase\_chip1\_532nm\_1\_#####.cbf.gz Browse

Prefix: lase\_chip1\_532nm

Run number: 1

✖ Compress data

##### Processing

N.o. residues: 200 Space group:

##### Unit cell:

a: 0 b: 0 c: 0

α: 0 β: 0 γ: 0

✖ Run processing after collection

✖ Run Dozor

Machine current: 86.3 mA

Machine state: Behind-of-experiments 6.08 GeV, 40 Bunches

Front End: Opened

Hutch temperature and humidity: 23.5 C, 29.8 %

Disk space: Total: 228.9GB Free: 203.0GB (89%)

Energy: Current: 12.6799 keV Wavelength: 0.9778 Å

Status: Set to: kV ... Center beam after energy change

Transmission: Current: 100.00 % Set to:

Detector distance: Current: 1.844 Å Set to: 120.00 mm Beamstop distance: Current: 6.00 mm Set to:

Door interlock: Locked (unlock disabled) Unlock

Safety shutter: In Open Close

Fast shutter: Opened Open Close

Image tracking: tracking Enable Advn image tracking

Detector status: Exposing

Frame rate: 311 Hz

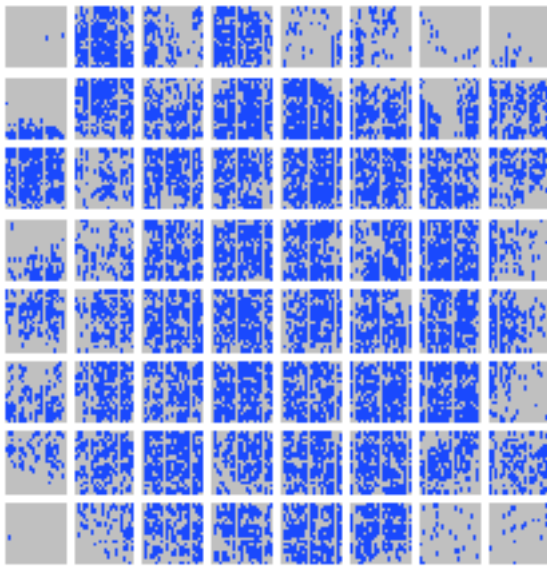
Temperature: 26.1°

Humidity: 3.3%

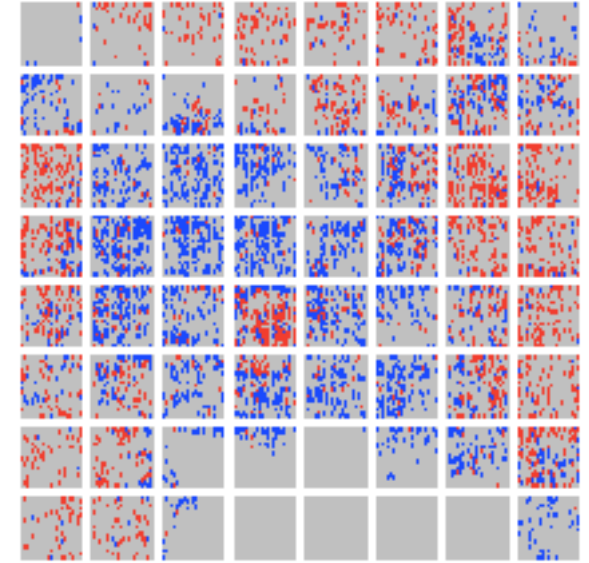
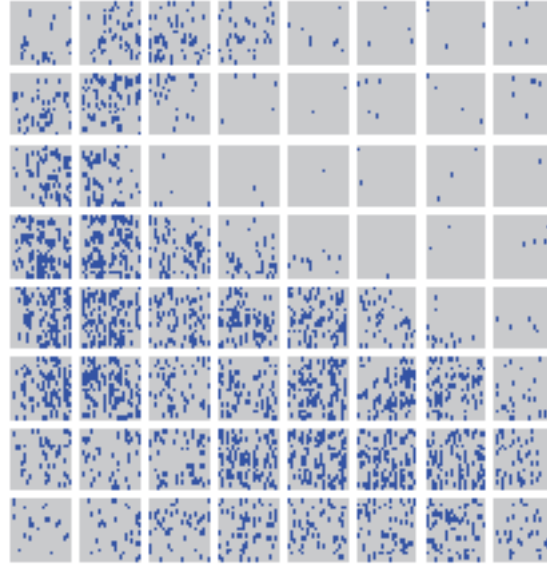
Please wait... [2018-10-29 17:35:40] Collection started

File system: EDNA ISPyB

# Hit maps



DOZOR  
real time  
chip coverage



CRYSTFEL  
post processing  
different unit cells

## On going

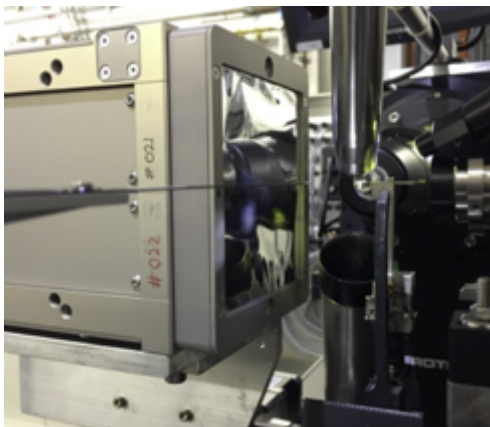
- Chip scanner device server
- Scan trajectory and triggers definition in MXCuBE
- On line auto-processing with
  - EDNA CRYSTFEL plugin
  - EDNA nXDS plugin

# Future



Ionized air glow ,  $4 \times 10^{14}$  photon/second  $\Delta E/E=1.5\%$   
with Double SiW multilayer @ P12/PETRAIII  
S. Fiedler, EMBL-Hamburg Instrumentation group

- 100 fold increase in flux with broad energy bandwidth optics
- 150 ps single-bunch exposures will become feasible

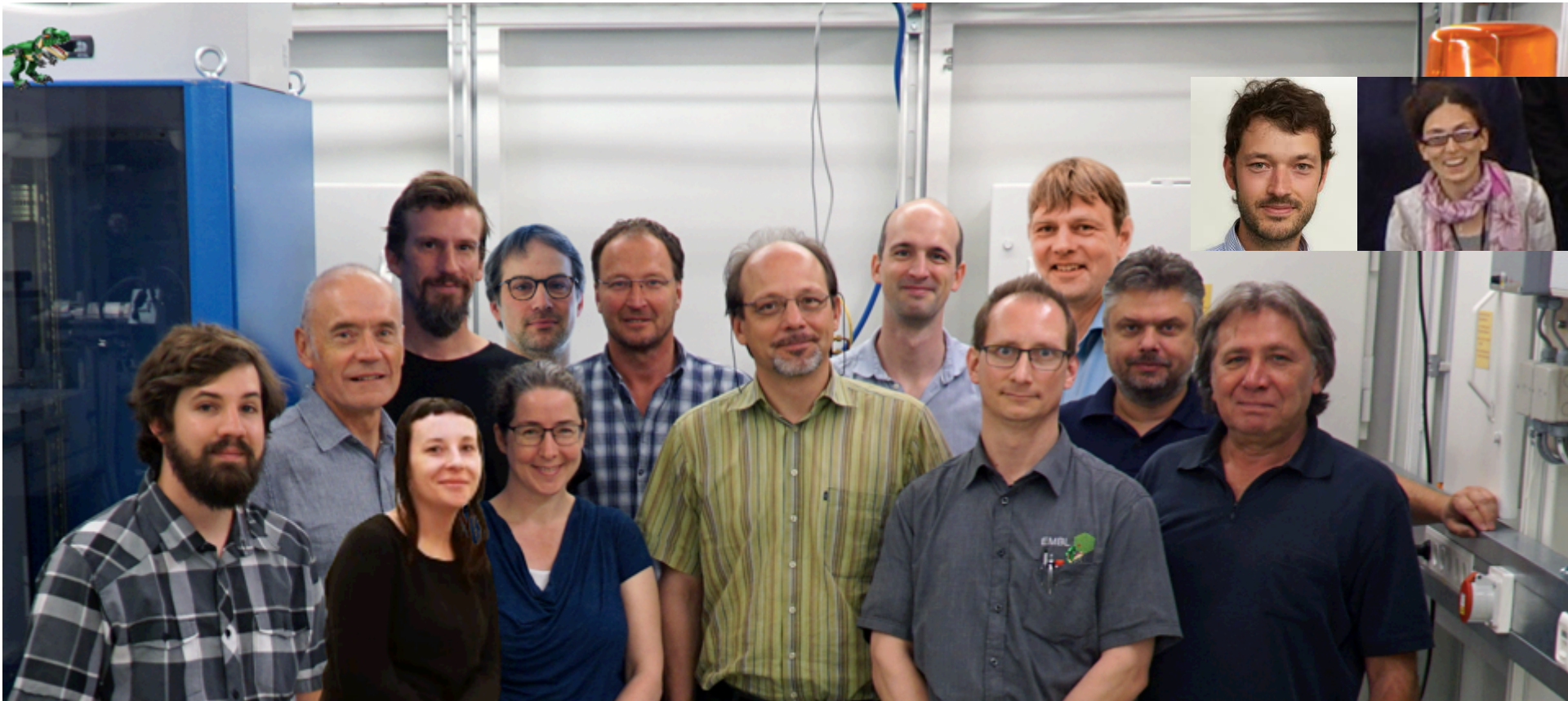


JUNGFRAU Detector at SLS

- Integrating pixel-array detectors



# Acknowledgements



**Michael Agthe<sup>1</sup>, David von Stetten<sup>2</sup>, Gleb Bourenkov<sup>2</sup>, Maxim Polikarpov<sup>2</sup>, Sam Horrell<sup>1</sup>, Briony A. Yorke<sup>1</sup>, Godfrey S. Beddard<sup>3</sup>, Marina Nikolova<sup>2</sup>, Ivars Karpics<sup>2</sup>, Thomas Gehrman<sup>2</sup>, Jochen Meyer<sup>2</sup>, Uwe Ristau<sup>2</sup>, Stefan Fiedler<sup>2</sup>, Diana C.F. Monteiro<sup>1</sup>, Martin Trebbin<sup>4</sup>, Pedram Mehrabi<sup>5</sup>, Eike-Christian Schulz<sup>5</sup>, Friedjof Tellkamp<sup>5</sup>, Dwayne R. Miller<sup>5,6</sup>, Nils Huse<sup>1</sup>, Arwen R. Pearson<sup>1</sup>, and Thomas R. Schneider<sup>2</sup>**

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<sup>4</sup> University at Buffalo, Buffalo (USA); <sup>5</sup> Max Planck Institute for Structure and Dynamics of Matter, Hamburg (Germany); <sup>6</sup> University of Toronto, Toronto, (Canada)