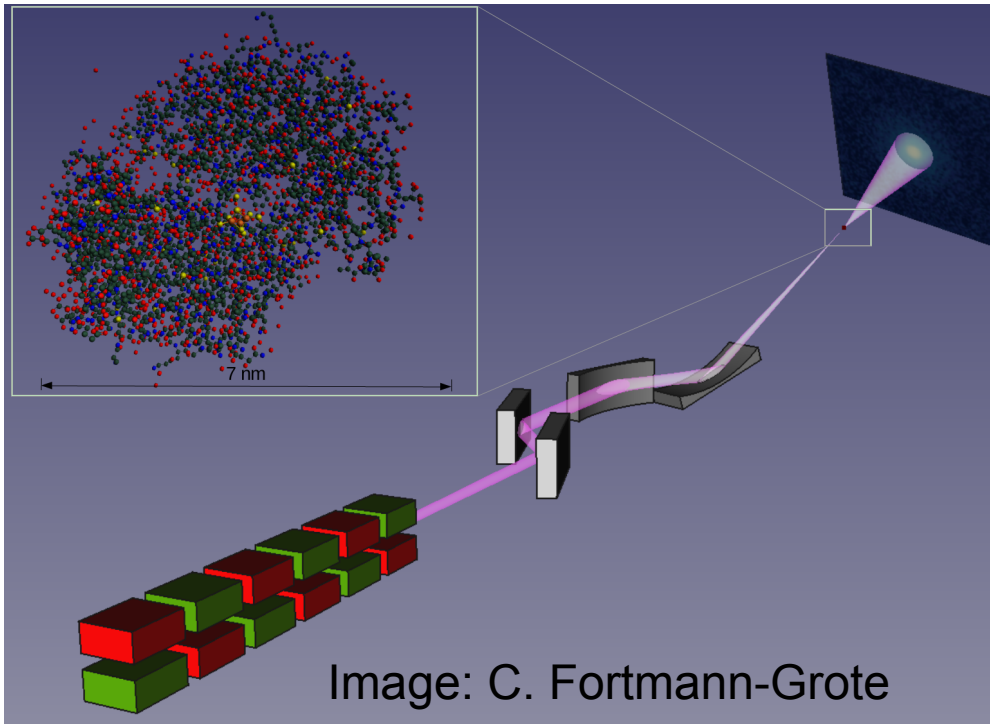


# The SPB/SFX Instrument: Installation, commissioning and some highlights from first user experiments

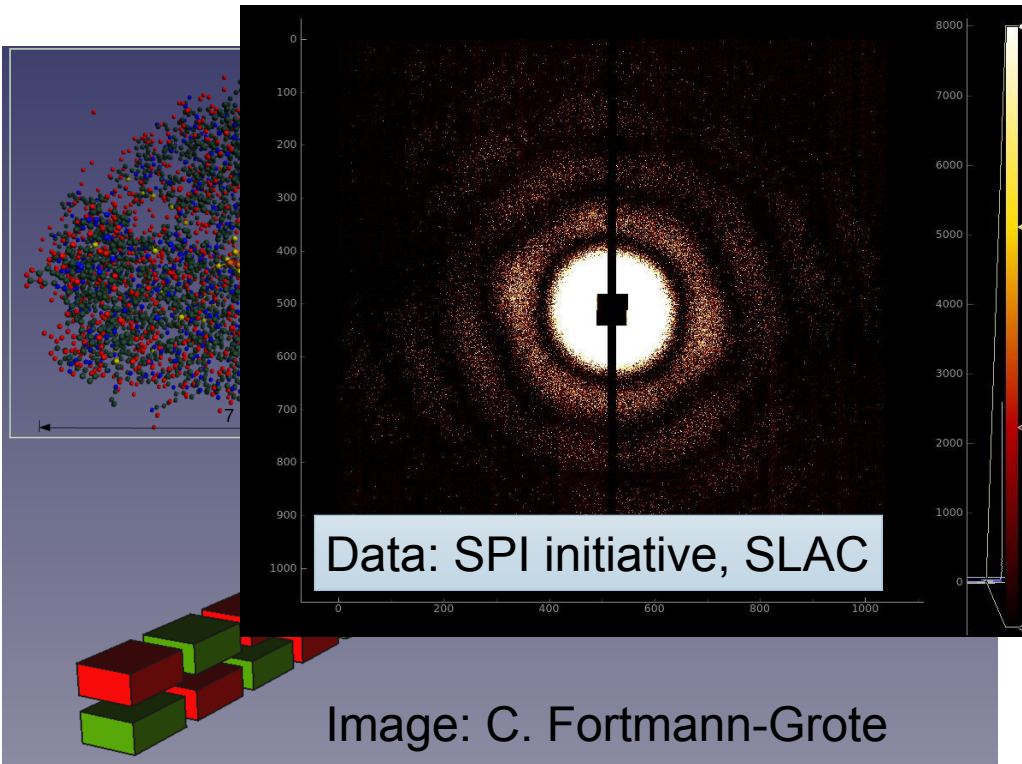
Adrian Mancuso  
Leading Scientist  
SPB/SFX Instrument  
European XFEL



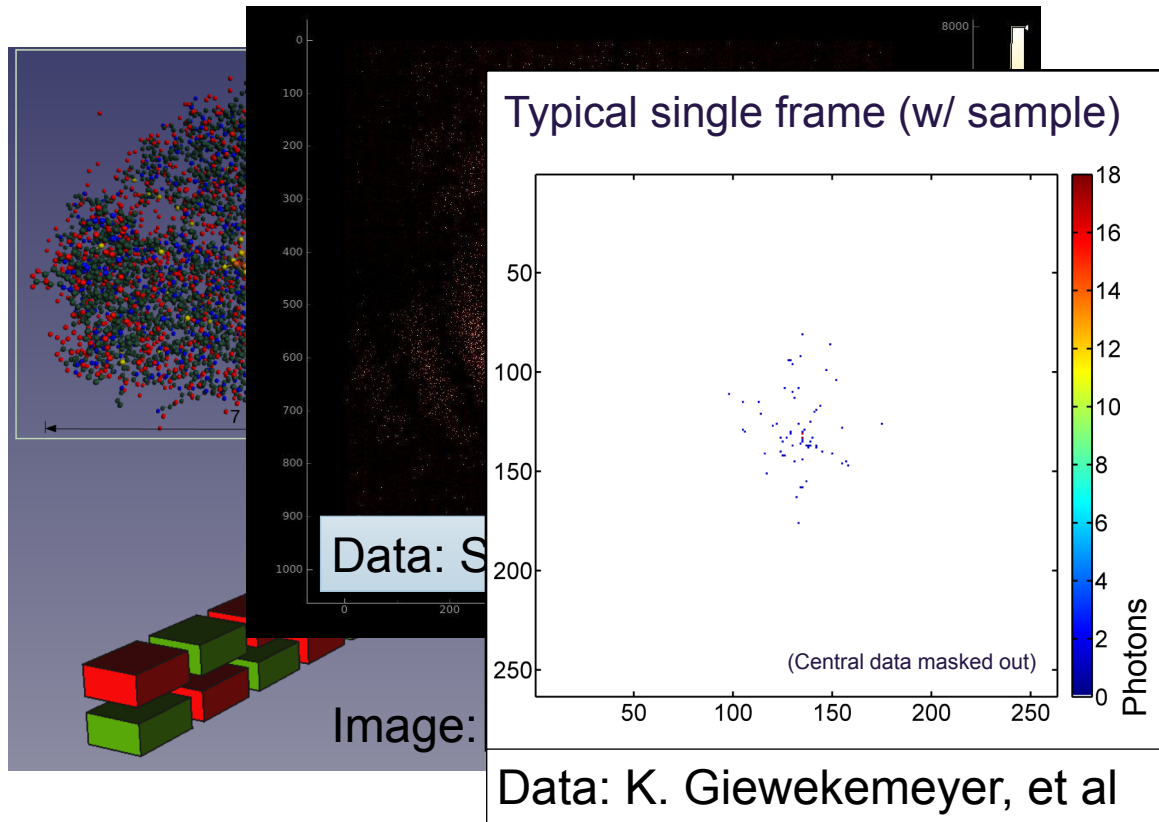
## Reminder: The scope of the SPB/SFX Instrument



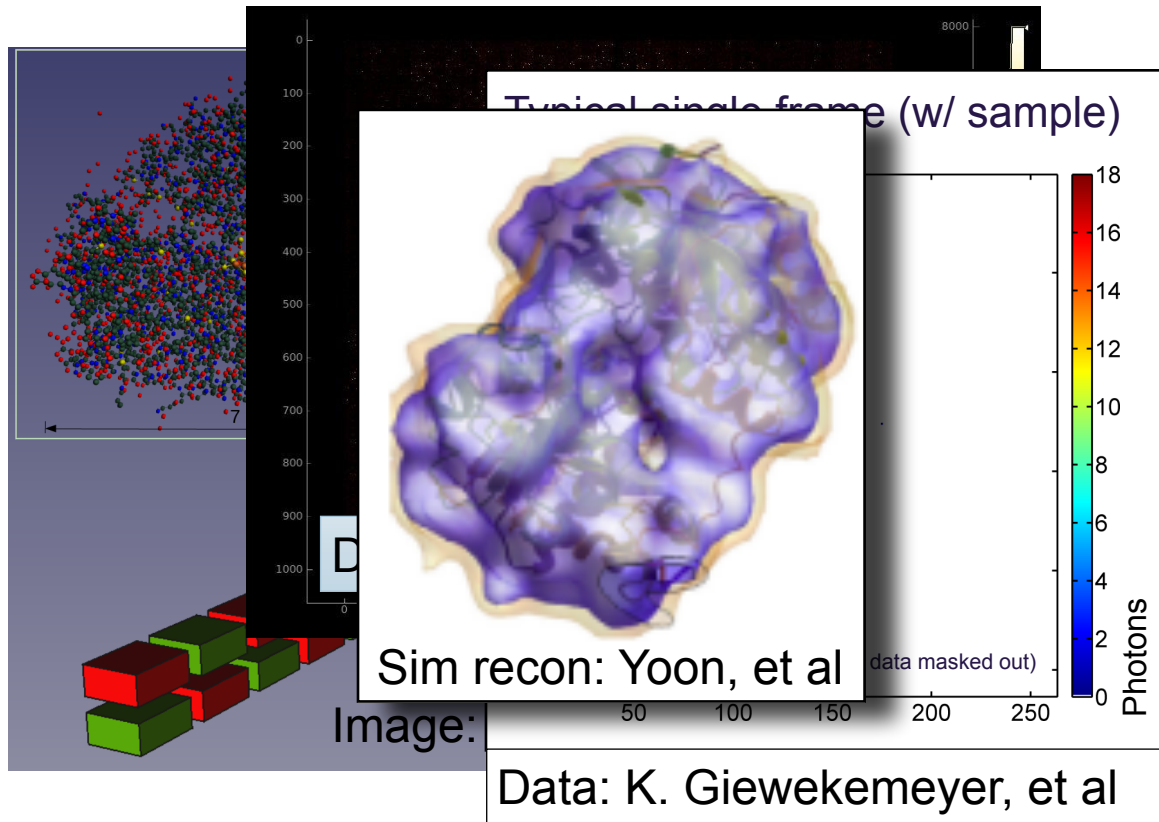
## Reminder: The scope of the SPB/SFX Instrument



# Reminder: The scope of the SPB/SFX Instrument



# Reminder: The scope of the SPB/SFX Instrument



# Reminder: The scope of the SPB/SFX Instrument

Typical single frame (w/ sa

Sim recon: Yoon, et al

Image: data masked ou

Data: K. Giewekemeyer, et al

LCP injector

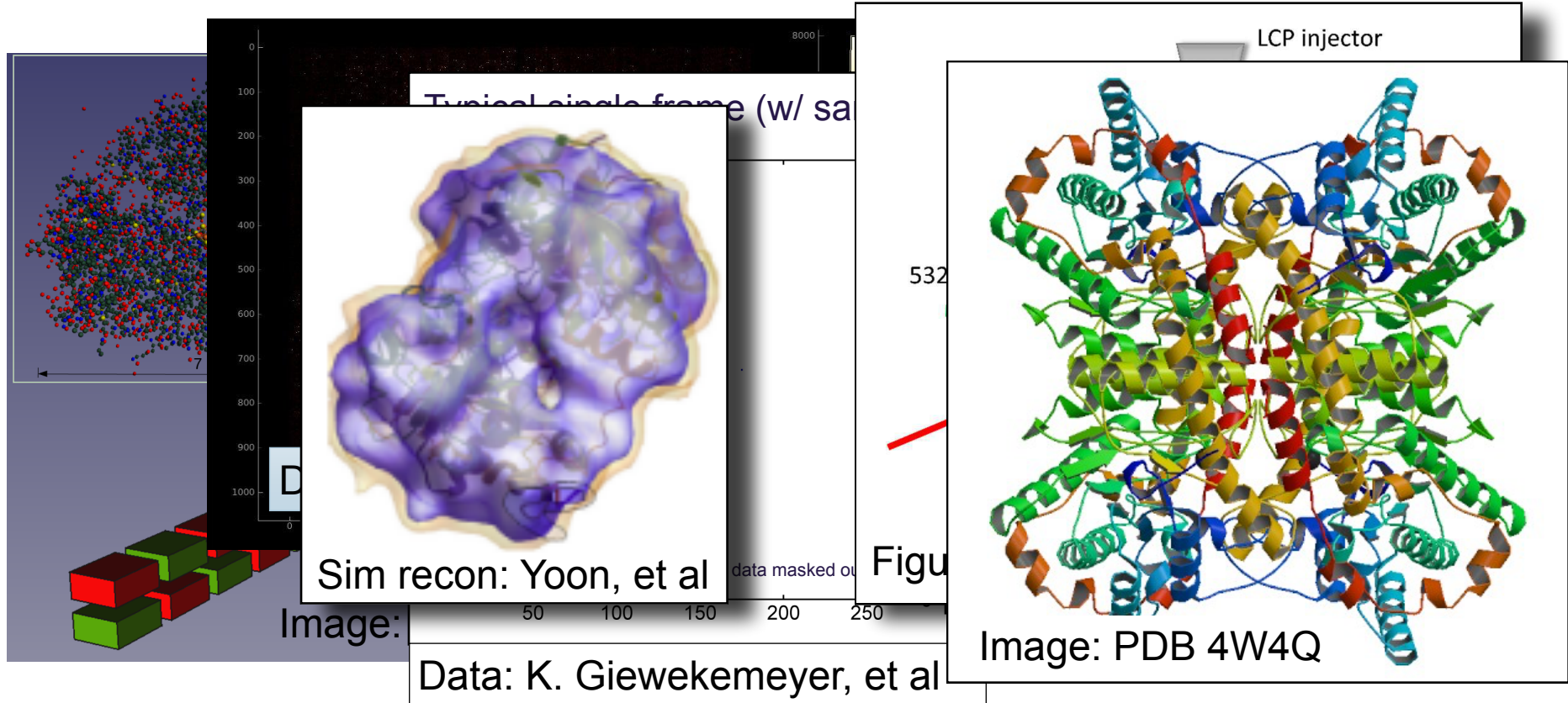
bR crystals

532 nm Pump Laser

XFEL

Figure: Nango, et al, Science, 2016

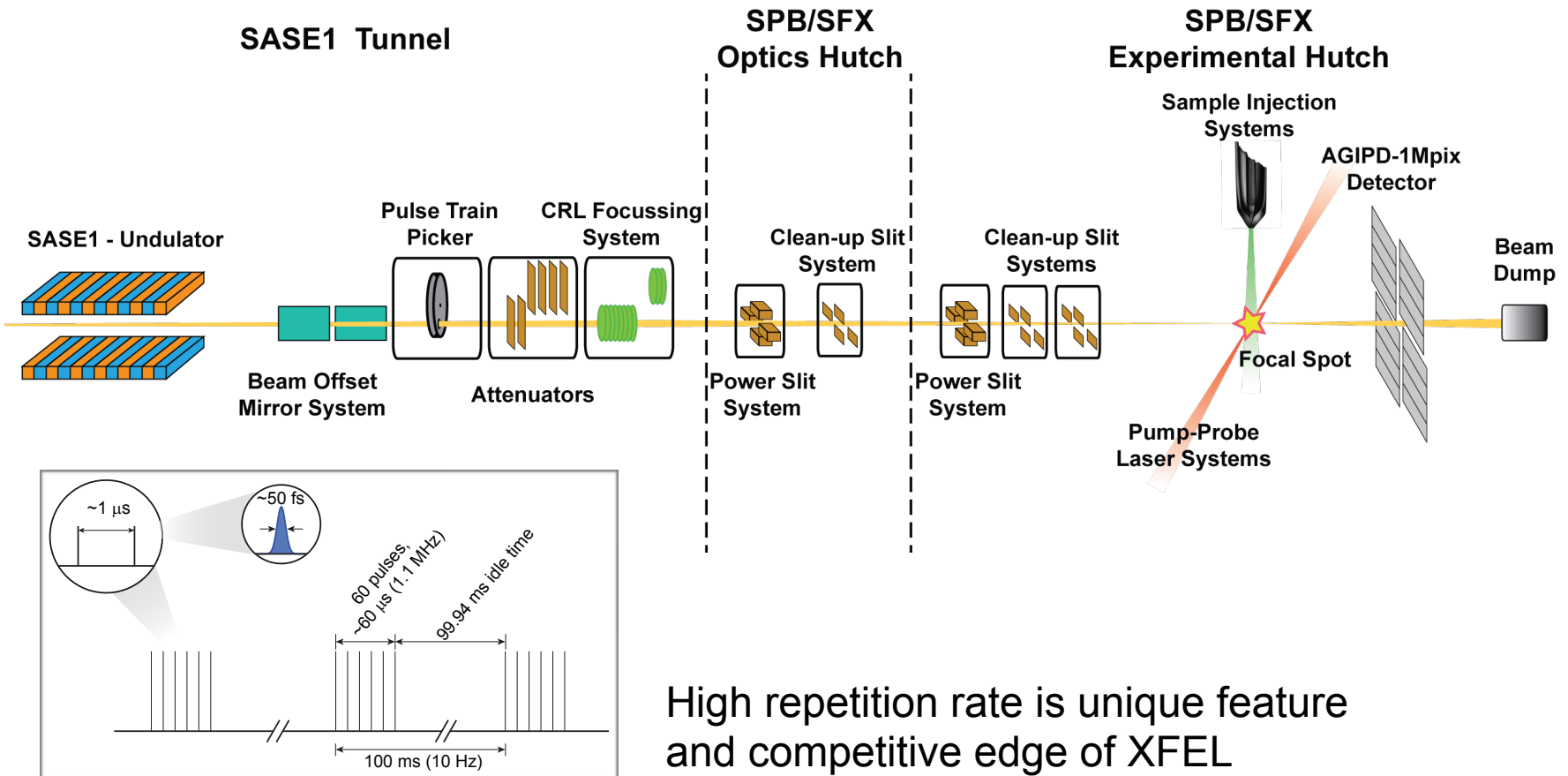
# Reminder: The scope of the SPB/SFX Instrument



Everything forward scattering—predominantly **Serial Crystallography** and **single particle imaging** of biological samples and including time resolved experiments

# Schematic of the “Day one” SPB/SFX Instrument

3-16 keV



High repetition rate is unique feature and competitive edge of XFEL



## The SPB/SFX instrument *before*

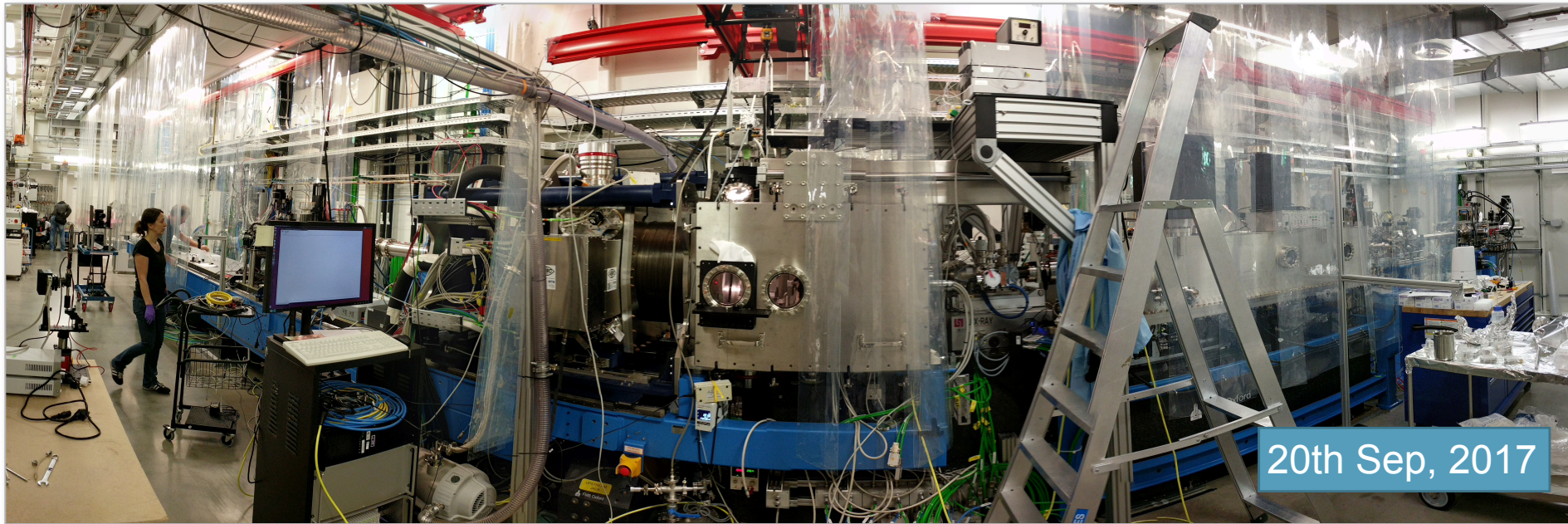


17th October 2016

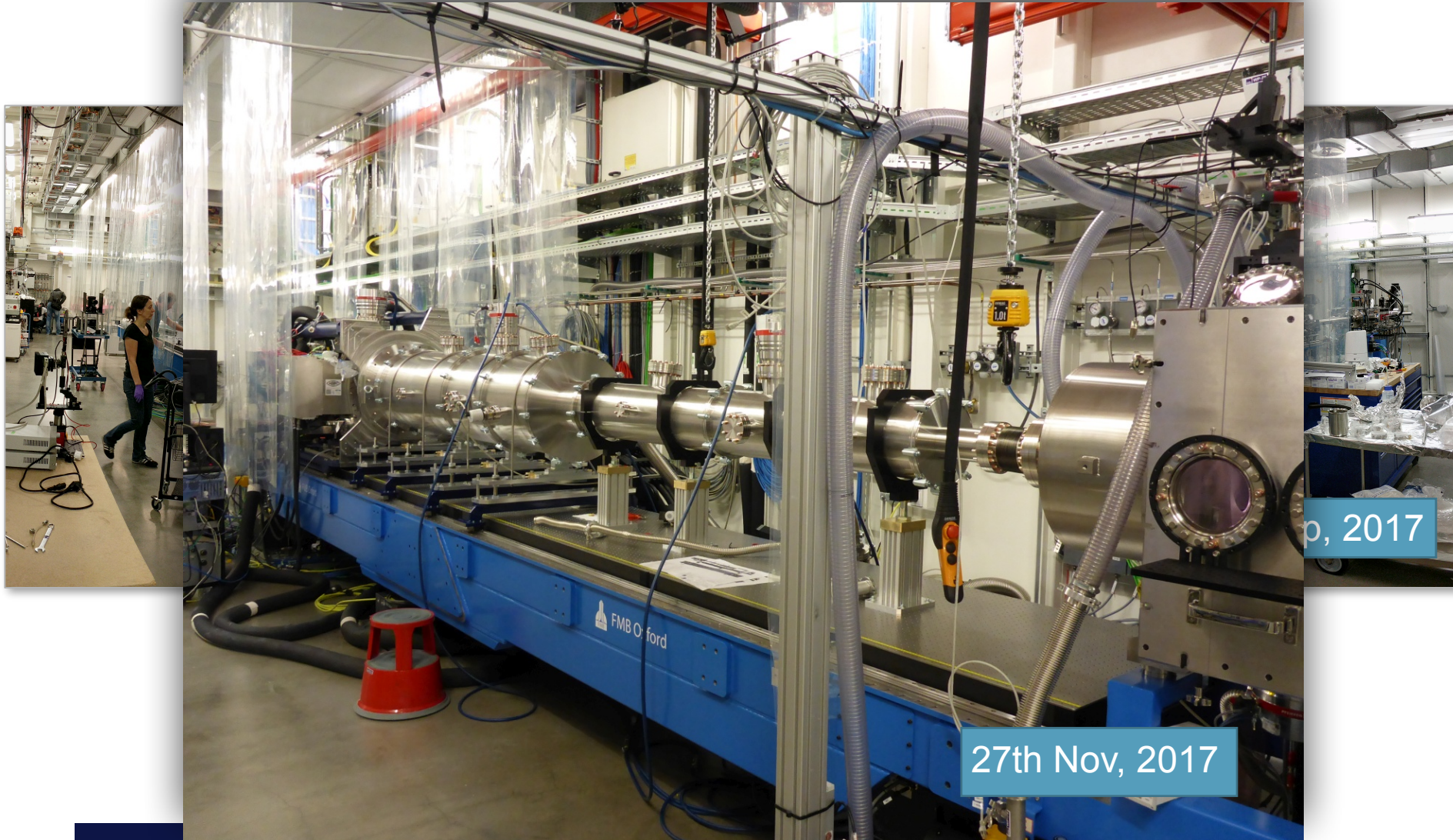


17th October 2016

## ..and after



## ..and after



27th Nov, 2017

p, 2017

## How did we get there? How did we get to data and results?

- 24.02.17 — Delivery of mirror chambers and supports (first “big” component to be installed)
- 31.03.17 — Mirror mechanics installed
- 10.04.17 — Sample chamber and Component Support Structure (CSS) installed
  - Not yet internals of sample environment
- 15.05.17 — Experiment hutch cabling completed
- 28.05.17 — Experimental hall flooded (a Sunday!)
- 31.06.17 — Cable flood damage (corrosion) repairs completed
- 20.06.17 — Commissioning setup (sample chamber internal) installed
- 23.06.17 — First beam in hutches
- 24.06.17 — First coherent diffraction (edges, slits), 29.06.17 (Far-field aperture diffraction) 30.06.17 (Fresnel diffraction)
- 13.08.17 — AGIPD delivered, 19.08.17 — AGIPD first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — AGIPD used in first user experiment at SPB/SFX!
- 22.08.17 — Liquid Jet sample delivery system installed
- 14.09.17 — Liquid Jet sample delivery system used with beam
- 16.09.17 (night) — First Serial Crystallography data on AGIPD from lysozyme
- 17.11.17 — First analysed results communicated to entire first experiment collaboration by lead investigator Anton Barty

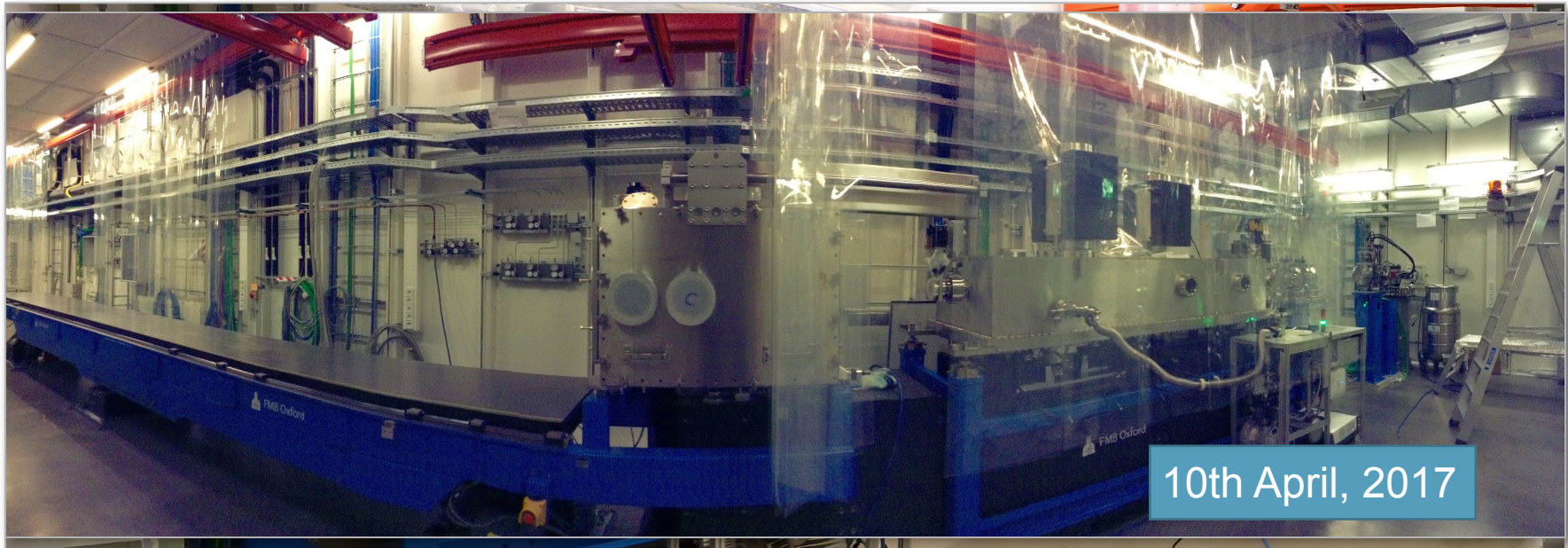
## Mirror chambers, sample chamber and support structure installed...



...even before the hutch infrastructure was completed!

- First “big” components installed
- Essential part of the SPB/SFX vacuum system (remember the instrument’s in vacuum and windowless)

## Mirror chambers, sample chamber and support structure installed...



...even before the hutch infrastructure was completed!

- First “big” components installed
- Essential part of the SPB/SFX vacuum system (remember the instrument’s in vacuum and windowless)

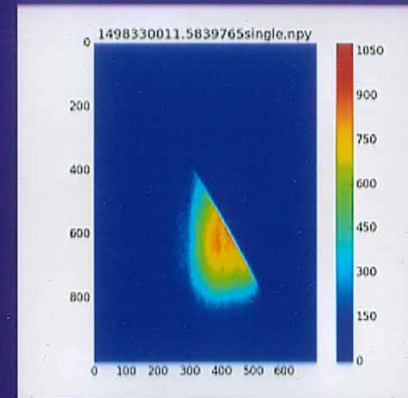
# First Beam in the hall

## Coherent diffraction from early commissioning



Commemorating first beam in the European XFEL Experiment Hall.

23rd June, 2017

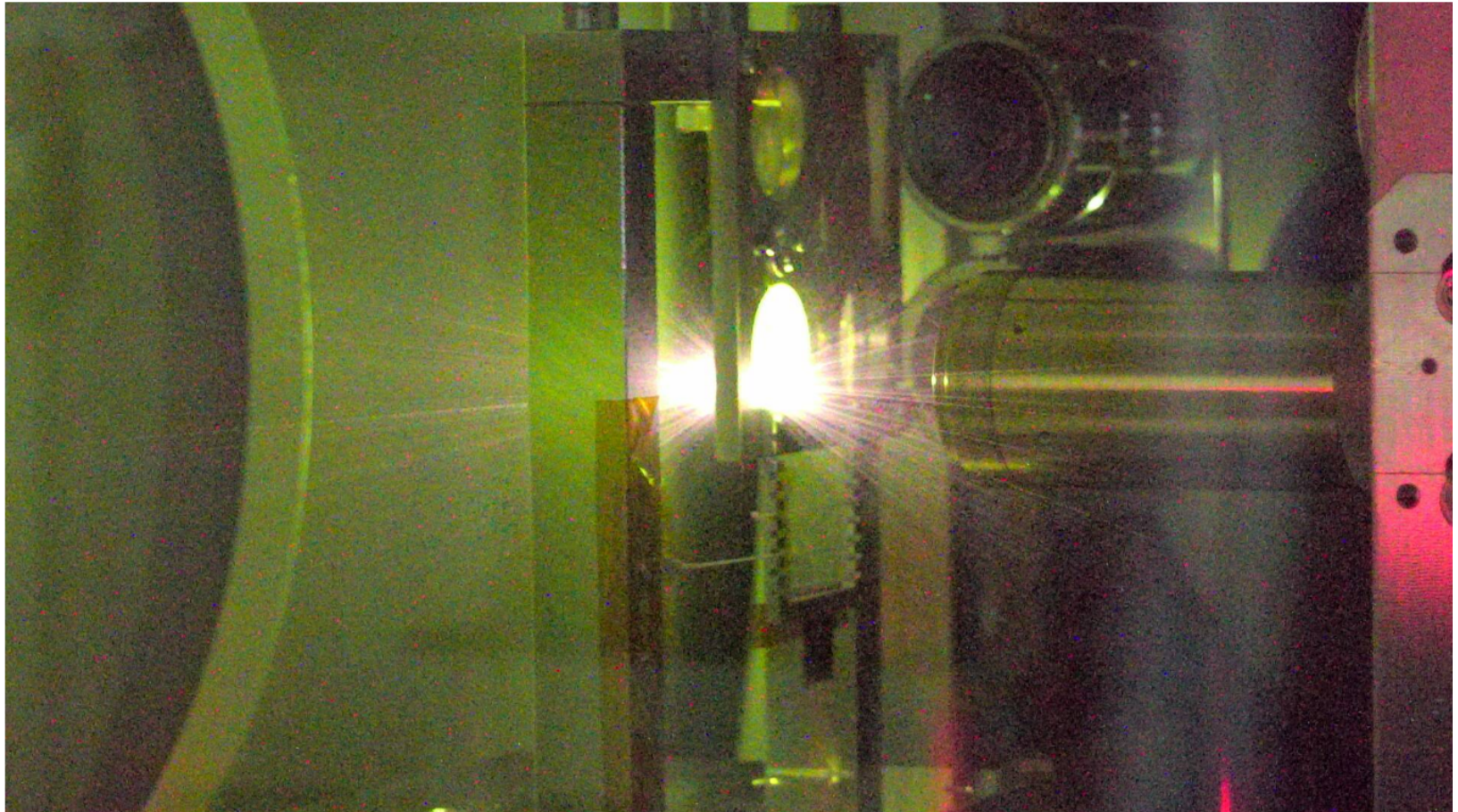


SPB/SFX Control Room



# First Beam in the hall

## Coherent diffraction from early commissioning



Video

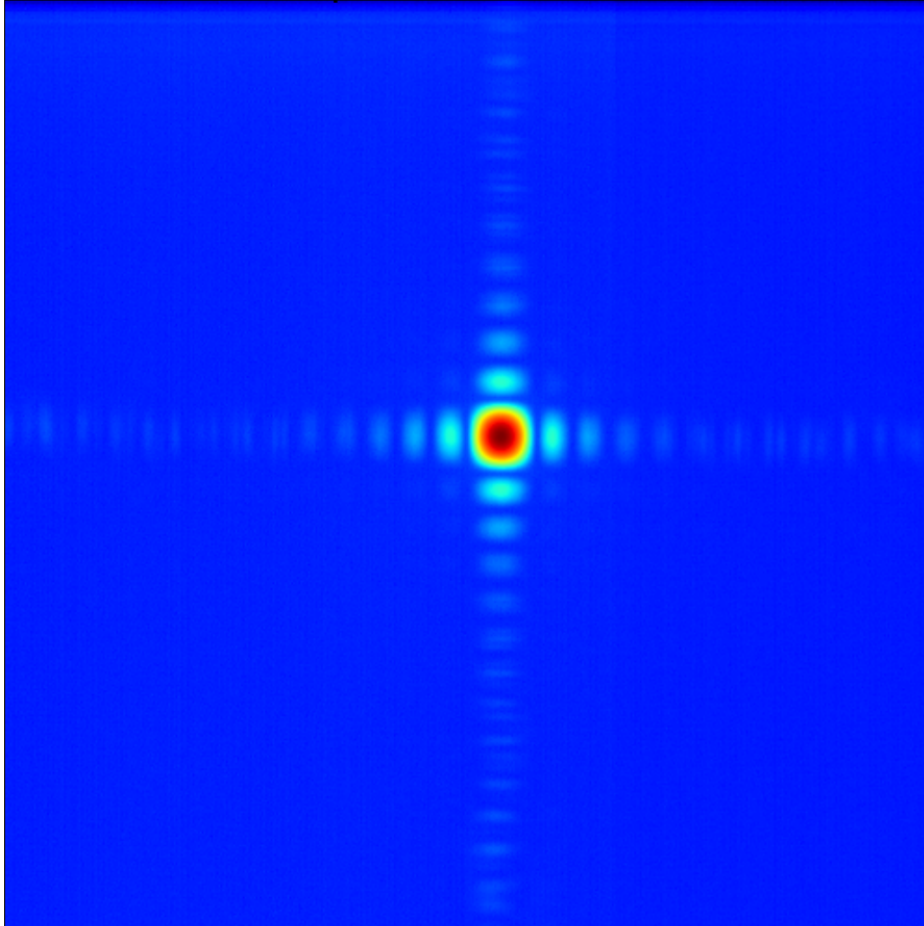
PTZ



# First Beam in the hall

## Coherent diffraction from early commissioning

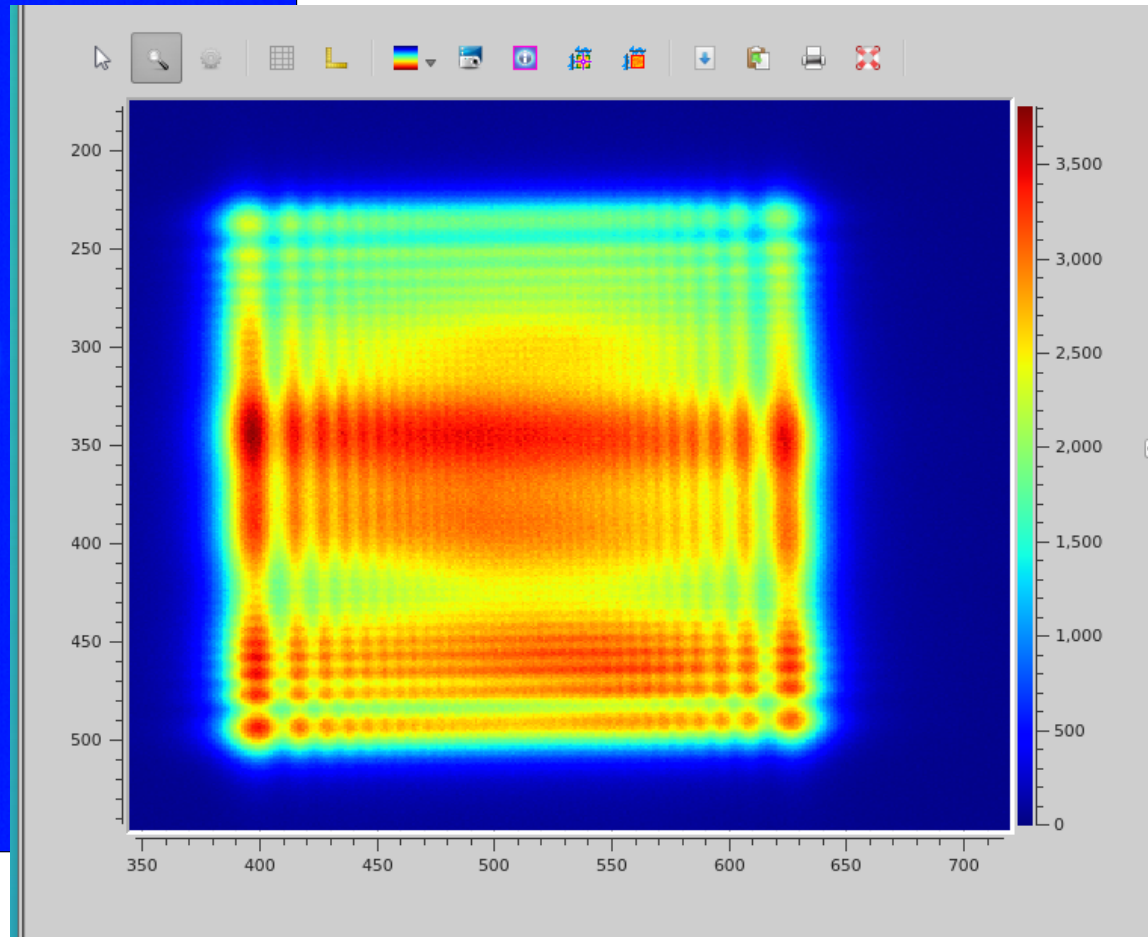
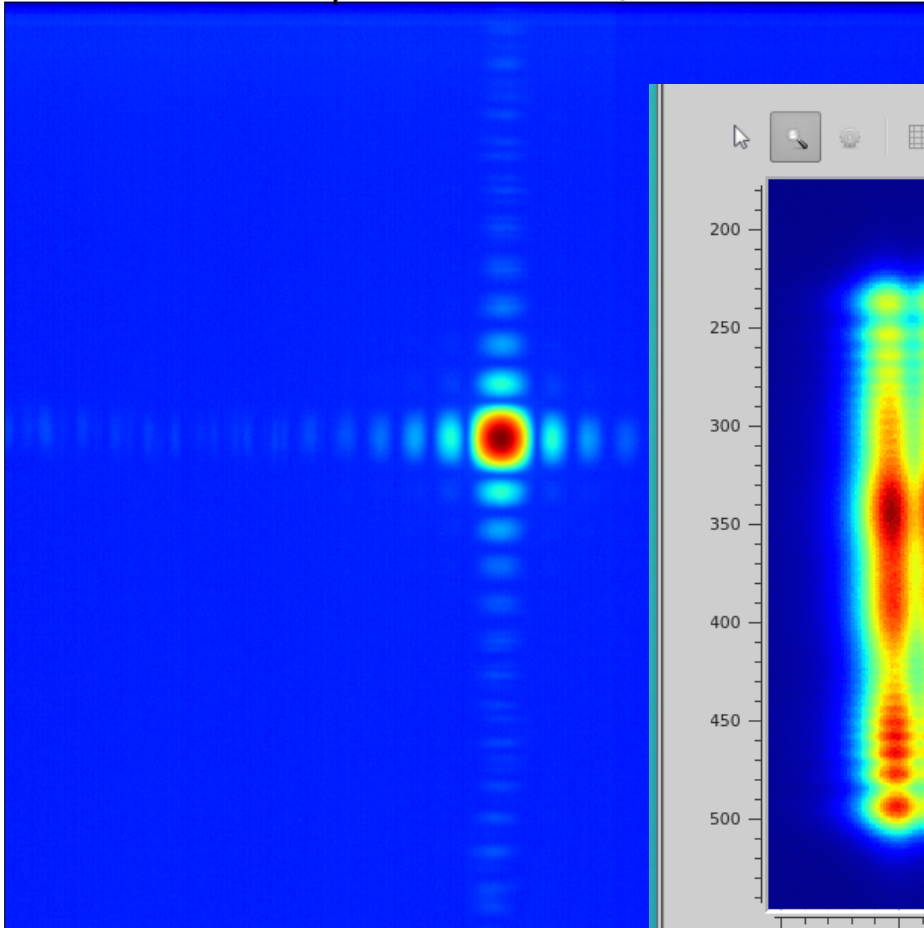
First diffraction pattern at SPB/SFX 29.6.2017



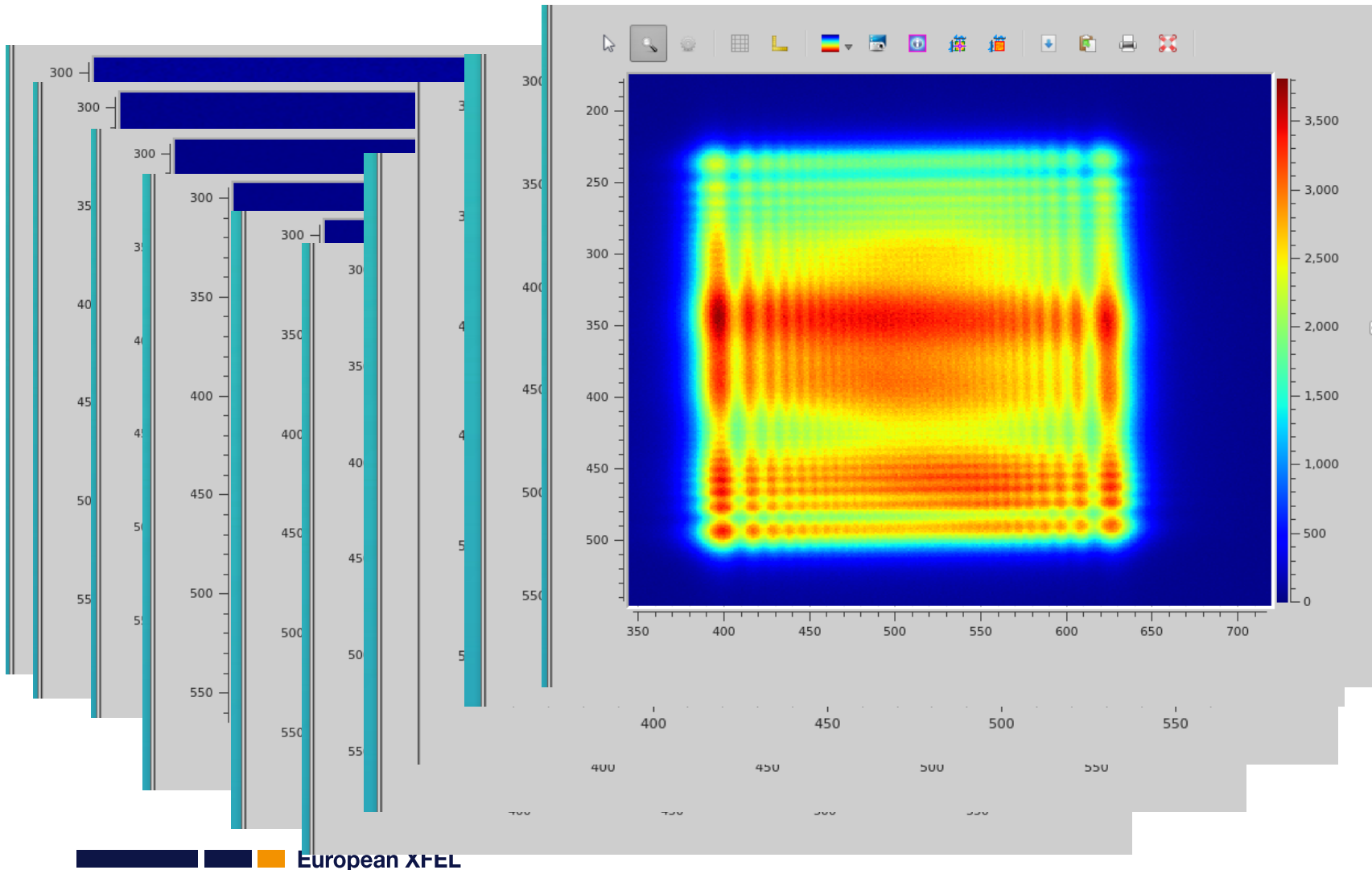
# First Beam in the hall

## Coherent diffraction from early commissioning

First diffraction pattern at SPB/SFX 29.6.2017



# A coherent walk through Fresnel number...



## Installation of AGIPD at SPB/SFX

# 14.08 at 1:00p.m.: ...welcome to XHQ



13.08.17 — AGIPD delivered, 19.08.17 — AGIPD first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — used in first user experiment at SPB/SFX!

European XFEL

## Installation of AGIPD at SPB/SFX



First dark data at SPB/SFX 19.08.17



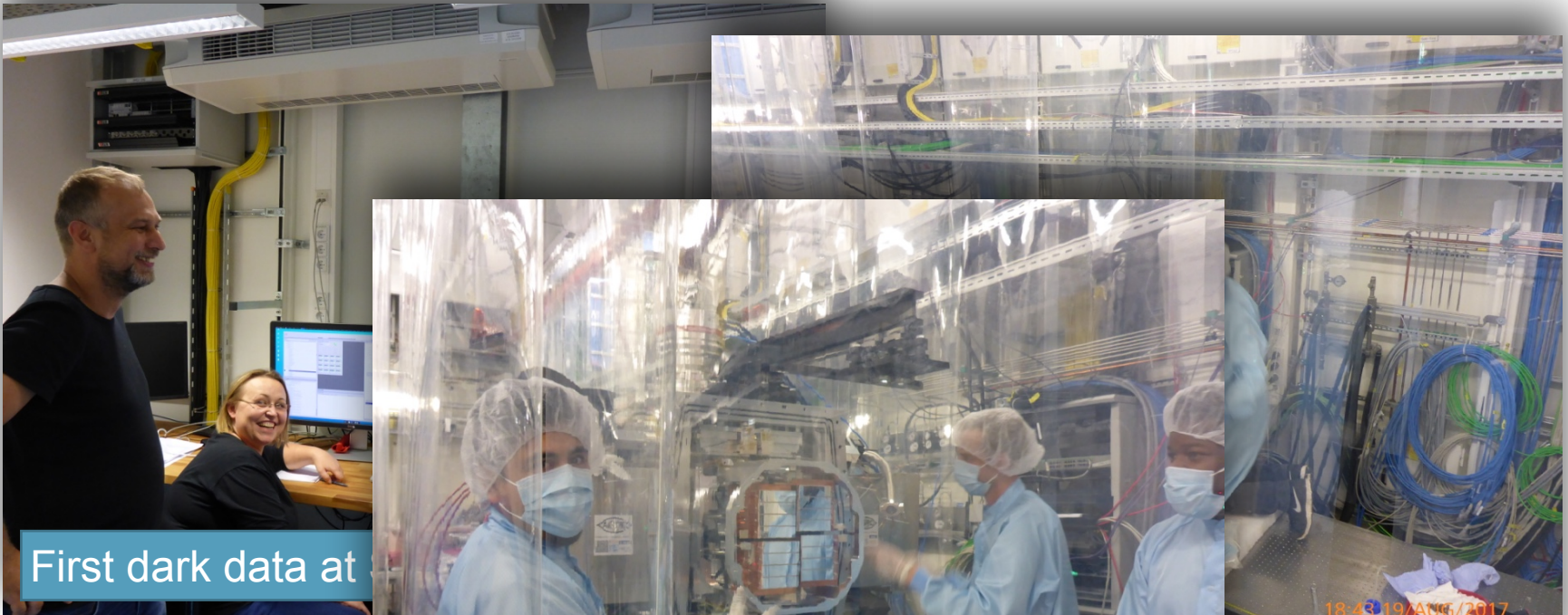
Removal of "cap"

18:43 19/AUG/2017

13.08.17 — AGIPD delivered, 19.08.17 — AGIPD first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — used in first user experiment at SPB/SFX!

European XFEL

## Installation of AGIPD at SPB/SFX



First dark data at

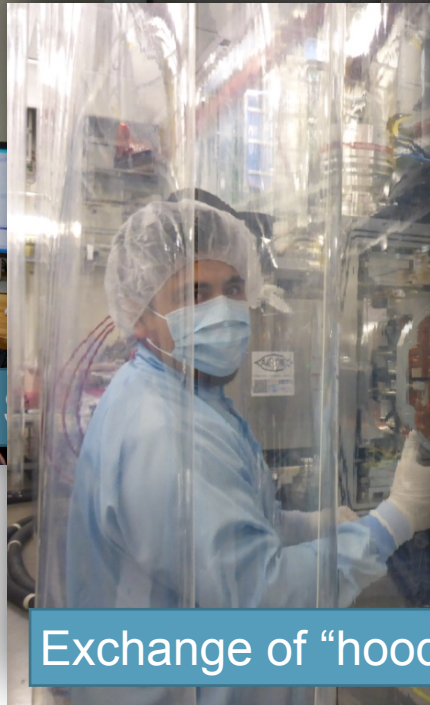
Exchange of "hood"

13.08.17 — AGIPD delivered, 19.08.17 — AGIPD first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — used in first user experiment at SPB/SFX!

## Installation of AGIPD at SPB/SFX



First dark data at



Exchange of "hood"



Installation of "cage"

20:49 19/AUG/2017

18:57 19/AUG/2017

13.08.17 — AGIPD delivered, 19.08.17 — AGIPD first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — used in first user experiment at SPB/SFX!





Completed "cage" with L. Lopez, C. Takem and P. Schütt  
9:30pm, Saturday 19th August 2017

13.08.17 — AGIPD delivered, 19.08.17 — AGIPD first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — used in first user experiment at SPB/SFX!

European XFEL

European XFEL

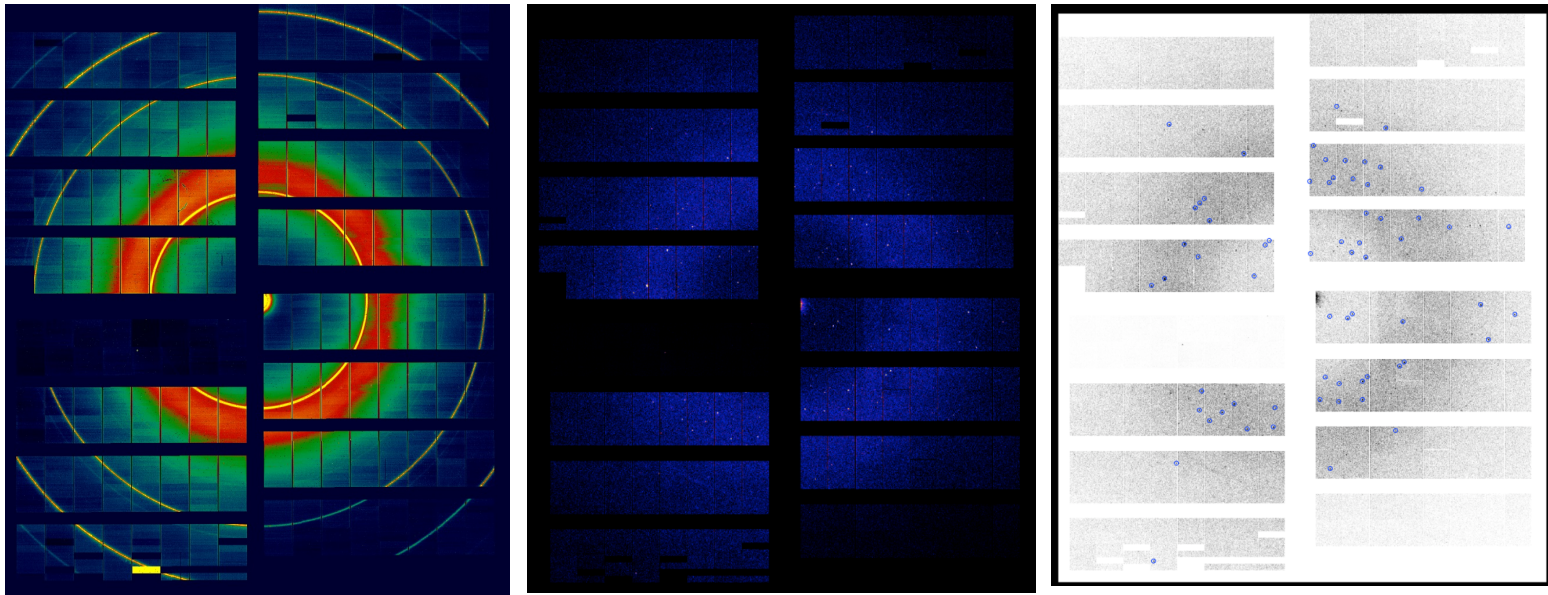
Live demonstration experiment on the occasion of the European XFEL inauguration, including AGIPD data. SPB/SFX Scientific Instrument September 1st, 2017

... and P. Schütt

13.08.17 — AGIPD commissioning first darks at SPB/SFX, 28.08.17 — AGIPD first X-ray data at SPB/SFX, 14.09.17 — used in first user experiment

European XFEL

## First data from AGIPD at SPB/SFX



### The experiment:

- Powder diffraction from LiTi (left)
- Liquid jet with crystals (centre)
- Automatic indexing (right)
- Frame rate 4.5 MHz
- 30 pulses @ 1.1MHz/train
- E=8keV

On behalf of the AGIPD consortium, DESY-CXI & XFEL

#### AGIPD consortium

A. Allahgholi<sup>1</sup>, J. Becker<sup>1</sup>, A. Delfs<sup>1</sup>, R. Dinapoli<sup>2</sup>, P. Göttlicher<sup>1</sup>, H. Graafsma<sup>1,5</sup>, D. Greiffenberg<sup>2</sup>, H. Hirsemann<sup>1</sup>, S. Jack<sup>1</sup>, R. Klanner<sup>3</sup>, A. Klyuev<sup>1</sup>, H. Krueger<sup>4</sup>, M. Kuhn<sup>1</sup>, S. Lange<sup>1</sup>, T. Laurus<sup>1</sup>, A. Marras<sup>1</sup>, D. Mezza<sup>2</sup>, A. Mozzanica<sup>2</sup>, J. Poehlsen<sup>1</sup>, S. Rah<sup>6</sup>, B. Schmitt<sup>2</sup>, J. Schwandt<sup>3</sup>, I. Sheviakov<sup>1</sup>, X. Shi<sup>2</sup>, S. Smoljanin<sup>2</sup>, U. Trunk<sup>1</sup>, Q. Xia<sup>1</sup>, J. Zhang<sup>1</sup>, M. Zimmer<sup>1</sup>

1 – Deutsches Elektronen-Synchrotron, 2 – Paul Scherrer Institute, 3 – Universität Hamburg, 4 – Universität Bonn, 5 – Mid Sweden University, 6 – Pohang Accelerator Laboratory.

#### XFEL Detector group

Steffen Hauf, Alexander Kaukher, Astrid Münnich, Jolanta Sztuk-Dambietz

# And then—just like that—we're doing experiments with 100+ users



First user group (experiment 2012) was an open collaboration with 100+ participants  
Lead investigator: Anton Barty

# And then—just like that—we're doing experiments with 100+ users



First user group (experiment 2012) was an open collaboration with 100+ participants  
Lead investigator: Anton Barty

# And then—just like that—we're doing experiments with 100+ users

## SPB/SFX Instrument Scientists

Adrian Mancuso  
Richard Bean  
Klaus Giewekemeyer  
Marjan Hadian  
Yoonhee Kim  
Romain Letrun  
Marc Messerschmidt  
Grant Mills  
Adam Round  
Tokushi Sato  
Marcin Sikorski  
Stephan Stern  
Patrik Vagovic  
Britta Weinhausen

## XFEL Detector

Steffen Hauf  
Alexander Kaukher  
Astrid Münnich  
Jolanta Sztuk-Dambietz

## AGIPD

Heinz Graafsma  
Aschkan Allahgholi  
Dominic Greiffenberg  
Alexander Klyuev  
Manuela Kuhn  
Torsten Laurus  
Davide Mezza  
Jennifer Poehlsen  
Ulrich Trunk

## Samples

Dominik Oberthuer  
Carolin Seuring  
Imrich Barak  
Sadia Bari  
Christian Betzel  
Matthew Coleman  
Chelsie Conrad  
Connie Darmanin  
XY Fang  
Petra Fromme  
Raimund Fromme  
S. Holmes  
Inari Kursula  
김경현  
Kerstin Mühlig  
Anna Munke  
Allen Orville  
Arwen Pearson  
Markus Perbandt  
Lars Redecke  
Mia Rudolph  
Iosifina Sarrou  
Marius Schmidt  
Robin Schubert  
Jonas Sellberg  
Megan Shelby  
Jason Stagno  
Yun-Xing Wang

## Jets & Diagnostics

Max Wiedorn  
Saša Bajt  
Jakob Andreasson  
Salah Awel  
Miriam Barthelmess  
Anja Burkhardt  
Francisco Cruz-Mazo  
Bruce Doak  
Yang Du  
Holger Fleckenstein  
Matthias Frank  
Alfonso Gañán Calvo  
Lars Gumprecht  
Janos Hajdu  
Michael Heymann  
Daniel Horke  
Mark Hunter  
Siegfried Imlau  
Juraj Knoska  
Jochen Küpper  
Julia Maracke  
Alke Meents  
Diana Monteiro  
Xavier Lourdu  
Tatiana Safenreiter  
Ilme Schlichting  
Robert Shoeman  
Ray Sierra  
John Spence  
Claudiu Stan  
Martin Trebbin  
Uwe Weierstall

## Analysis

Anton Barty  
Steve Aplin  
Andrew Aquila  
Kartik Ayyer  
Wolfgang Brehm  
Aaron Brewster  
Henry Chapman  
Florian Flachsenberg  
Yaroslav Gevorkov  
Helen Ginn  
Rick Kirian  
Filipe Maia  
Valerio Mariani  
Andrew Morgan  
Keith Nugent  
Peter Schwander  
Marvin Seibert  
Natasha Stander  
Pablo Villanueva-Perez  
Thomas White  
Oleksandr Yefanov  
Nadia Zatsepin

## XFEL Sample Environment

Johan Bielecki  
Katerina Dörner  
Rita Graceffa  
Joachim Schulz

## XFEL Information Technology and Data

Krzysztof Wrona  
Djelloul Boukhelef  
Illia Derevianko  
Jorge Elizondo  
Kimon Filippakopoulos  
Manfred Knaack  
Siriya Kujala  
Luis Maia  
Maurizio Manetti  
Bartosz Poljancewicz  
Gianpietro Previtali  
Nasser Al-Qudami  
Eduard Stoica  
Janusz Szuba

## XFEL Controls and Software

Sandor Brockhauser  
Andreas Beckmann  
Valerii Bondar  
Cyril Danilevski  
Wajid Ehsan  
Sergey Esenov  
Hans Fangohr  
Gero Flucke  
Gabriele Giovanetti  
Dennis Goeries  
Burkhard Heisen  
David Hickin  
Anna Klimovskaia  
Leonce Mekinda  
Thomas Michalet

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 Raimund Fromme  
 S. Holmes  
 Inari Kursula  
 김경현  
 Kerstin Mühlig  
 Anna Munke  
 Allen Orville  
 Arwen Pearson  
 Markus Perbandt  
 Lars Redecke  
 Mia Rudolph  
 Iosifina Sarrou  
 Marius Schmidt  
 Robin Schubert  
 Jonas Sellberg  
 Megan Shelby  
 Jason Stagno  
 Yun-Xing Wang

Sarah Awer  
 Miriam Barthelmeß  
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 Daniel Horke  
 Mark Hunter  
 Siegfried Imlau  
 Juraj Knoska  
 Jochen Küpper  
 Julia Maracke  
 Alke Meents  
 Diana Monteiro  
 Xavier Lourdu  
 Tatiana Safenreiter  
 Ilme Schlichting  
 Robert Shoeman  
 Ray Sierra  
 John Spence  
 Claudiu Stan  
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 Uwe Weierstall

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 Thomas Michelat  
 Andrea Parenti  
 Hugo Santos  
 Alessandro Silenzi  
 Martin Teichmann  
 Kerstin Weger  
 Chen Xu  
 Chris Youngman  
 John Wiggins

**XFEL Sample Environment**

Johan Bielecki  
 Katerina Dörner  
 Rita Graceffa  
 Joachim Schulz

First user group (experiment 2012) was an open collaboration with 100+ participants  
 Lead investigator: Anton Barty

# Experiment 2012: Collaborative 100+ participants

## Lead investigator: Anton Barty

<unpublished data>

xfel2012: Anton Barty, Valerio Mariani, Andrew Morgan, Tom White (CFEL), Helen Ginn (Oxford), Filipe Maia (Uppsala) and others

FS-DS detector group: Manuela Kuhn, Thorsten Laurus, Aschkan Allagholi

XFEL detector group: Steffen Hauf



# The data collected at SPB/SFX can be used to solve for structure

<unpublished data>

# First XFEL2012 results compare well to previous SFX structures

In short, **the instrument works**  
and we can do serial crystallography  
at SPB/SFX!

<unpublished data>

Slide: Anton Barty

Dominik Oberthur: Structure refinement  
17 Nov 2017

## **Metrics show resolution independent of pulse number in the train**

For the parameters of the early user experiments (15  $\mu\text{m}$  focal spot, 1.1 MHz repetition rate), **the train can be usefully exploited for serial crystallography**

<unpublished data>

## Pump-probe serial crystallography: experiment #2066

Collected > 54 000 frames of time-resolved serial crystallography data

<unpublished data>

## **Diffraction data from single viruses: SPB/SFX #2013**

Viruses injected with aerosol jet and diffraction data recorded

<unpublished data>

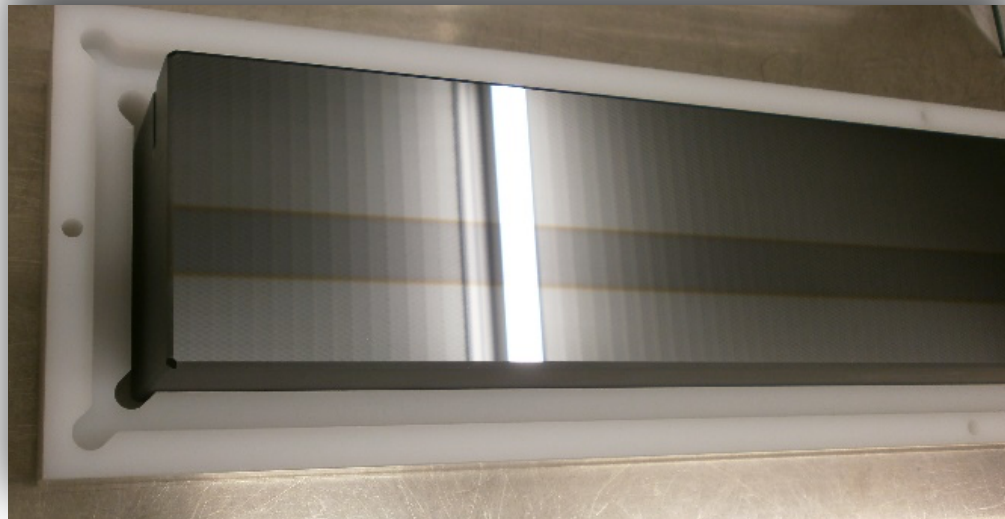
## Not everything went to plan: Expected vs delivered parameters

	Planned parameters (Dec 2016 / Jan 2017)	Delivered beam parameters
Photon Energy	8.86 keV	~ 9.3 keV
Repetition rate	1.1 MHz	1.1 MHz
# of pulses per train	60	30
Focal spot size	3 $\mu\text{m}$	15 $\mu\text{m}$
Pulse energy	~300 $\mu\text{J}$	300–1000 $\mu\text{J}$

Focal spot size large than expected due to CRLs  
(chromaticity, perhaps additional effects)

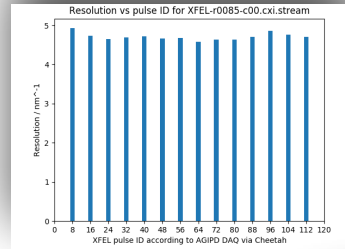
## What's next?

### Mirrors for higher transmission and smaller spot sizes



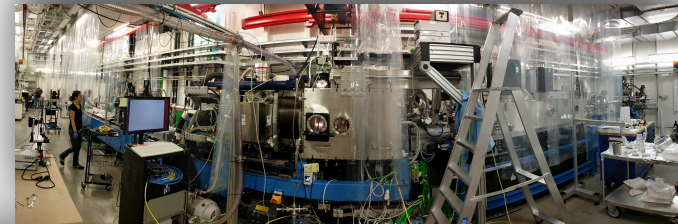
- First mirrors presently coated and to be installed next week. Scheduled for operation in run 3 (end 2018).
- To the best anyone can ascertain, the mirrors meet the 2 nm P-V height error specification
- Should provide vastly superior optical properties compared to the CRLs, particularly in transmission, aperture and spot size as well as benefits due to achromaticity
- Downstream interaction region (SFX contribution) to be in-part installed in 2018 too for early 2019 delivery (in atmosphere system)

## Headline Conclusions

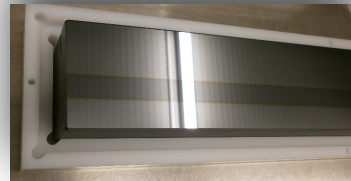


For the parameters used (1.1 MHz rep rate, 15  $\mu\text{m}$  spot)  
**the European XFEL rep rate can be successfully exploited**  
 for both serial crystallography and SPI

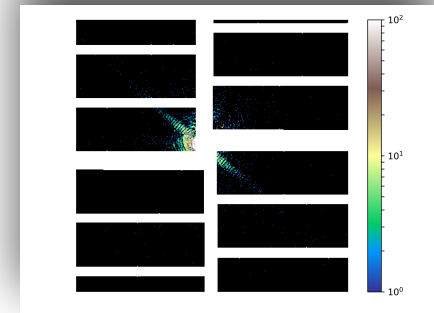
**Day one instrument works—first structure determined!**  
 Publishable results generated!



Mirrors are coming for better focal spot sizes

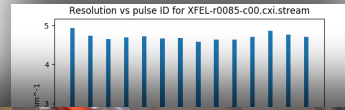


Call for run 3 (inc. use of mirrors) will open in (approx.) March this year.  
 A detailed description of instrument capabilities will be available then.



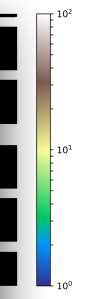
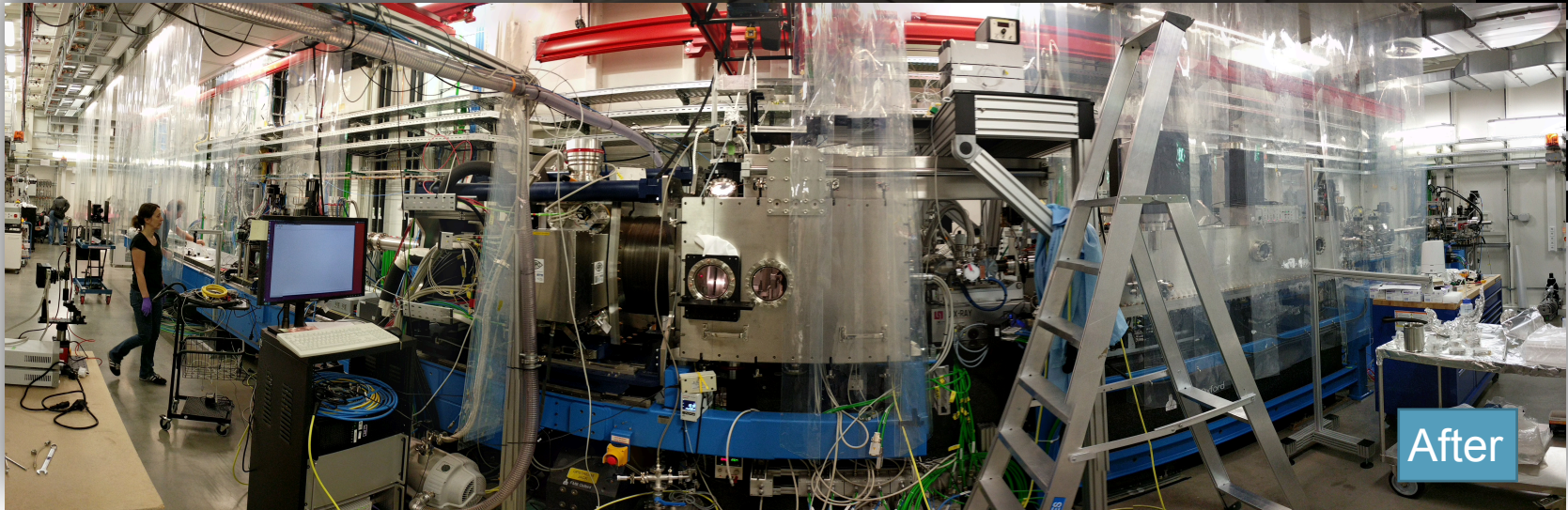
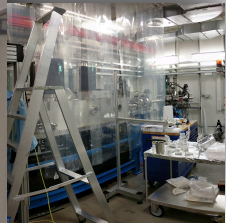
Still plenty of work to be done at the instrument, however already we can use SPB/SFX for  
 serial crystallographic structure determination and first single particle imaging projects!





# Headline Conclusions

- For the parameters used (1.1 M) **the European XFEL rep rate can** for both serial crystallography and
- Day one instrument works—f** Publishable results generated!
- Mirrors are coming for better fo



# Acknowledgments: People—the most important components

Zunaira Ansari  
 Richard Bean  
 Johan Bielecki (sample env.)  
 Thomas Dietze  
 Carsten Fortmann-Grote  
 (EUCALL project)  
 Klaus Giewekemeyer  
 Henry Kirkwood  
 Yoonhee Kim  
 Grant Mills  
 Luis Lopez Morillo  
 Bradley Manning  
 Masoud Mehrjoo (student)  
 Marc Messerschmidt  
 Nadja Reimers  
 Adam Round  
 Tokushi Sato  
 Philipp Schütte  
 Marcin Sikorski  
 Andrew Stawniczy  
 Stephan Stern  
 Prasad Thute  
 (Sample environment)  
 Britta Weinhausen  
 Patrik Vagovic



A. P. Mancuso, A. Aquila, G. Borchers, K. Giewekemeyer & N. Reimers, Technical Design Report: Scientific Instrument SPB, 2013. [dx.doi.org/10.3204/XFEL.EU/TR-2013-004](https://dx.doi.org/10.3204/XFEL.EU/TR-2013-004)

Many thanks to the **SFX Executive Board** for very constructive collaboration and support. Particular thanks to **all European XFEL groups supporting** (too many to mention), the AGIPD consortium, the accelerator team and many more.



## Acknowledgments: Even more people!

Sample environment team (internal and external)

### CFEL

Lars Gumprecht  
Tatiana Safenreiter

### Max Planck Institute for Medical Research

Bruce Doak  
Robert Shoeman

### Sample Environment XFEL

Johan Bielecki  
Katerina Dörner  
Rita Graceffa  
Matthäus Kitel  
Kristina Lorenzen  
Dennis Ropers  
Prasad Thute  
Joachim Schulz

AGIPD Consortium and European XFEL detector group

### AGIPD consortium

A. Allahgholi<sup>1</sup>, J. Becker<sup>1</sup>, A. Delfs<sup>1</sup>, R. Dinapoli<sup>2</sup>, P. Göttlicher<sup>1</sup>, H. Graafsma<sup>1,5</sup>, D. Greiffenberg<sup>2</sup>, H. Hirsemann<sup>1</sup>, S. Jack<sup>1</sup>, R. Klanner<sup>3</sup>, A. Klyuev<sup>1</sup>, H. Krueger<sup>4</sup>, M. Kuhn<sup>1</sup>, S. Lange<sup>1</sup>, T. Laurus<sup>1</sup>, A. Marras<sup>1</sup>, D. Mezza<sup>2</sup>, A. Mozzanica<sup>2</sup>, J. Poehlsen<sup>1</sup>, S. Rah<sup>6</sup>, B. Schmitt<sup>2</sup>, J. Schwandt<sup>3</sup>, I. Sheviakov<sup>1</sup>, X. Shi<sup>2</sup>, S. Smoljanin<sup>2</sup>, U. Trunk<sup>1</sup>, Q. Xia<sup>1</sup>, J. Zhang<sup>1</sup>, M. Zimmer<sup>1</sup>

1 – Deutsches Elektronen-Synchrotron, 2 – Paul Scherrer Institute, 3 – Universität Hamburg, 4 – Universität Bonn, 5 – Mid Sweden University, 6 – Pohang Accelerator Laboratory.

### XFEL Detector group

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