Welcome to the 2018 European XFEL Users Meeting

Robert Feidenhans'l
Management Board
Managing Director, Chairman of the Management Board

Schenefeld/Bahrenfeld, 24 January 2018

Wednesday, 24 January 2018: Plenary Sessions			
8:30–10:00	**Registration**		
10:00–10:20	**Opening Session**		
10:00	Welcome	R. Feidenhans'l	European XFEL
10:10	Opening address from the Council Chair	M. M. Nielsen	DTU
10:20–12:50	**Project Update Session**	*Chair: M. M. Nielsen (DTU)*	
10:20	General status of the project	R. Feidenhans'l	European XFEL
10:50	Electron accelerator – commissioning experience and plans	H. Weise	DESY
11:20	Photon beamlines commissioning	J. Grünert	European XFEL
11:50	SASE3 instruments – status and plans	S. Molodtsov	European XFEL
12:20	SASE2 instruments – status and plans	A. Madsen	European XFEL
12:50–14:00	**Lunch Break**		
14:00–17:40	**Science Session: Early User Experiments and Hard X-ray FELs Science Highlights**	*Chair: Nina Rohringer (CFEL-DESY)*	
14:00	FXE: instrument and commissioning progress + highlights	Ch. Bressler	European XFEL
14:20	SPB/SFX: instrument and commissioning progress + highlights	A. Mancuso	European XFEL
14:40	Revealing the nanoscale structure of viruses with XFEL pulses	R. Kurta	European XFEL
15:10	Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions	D. Kraus	HZDR, Dresden
15:40-16:10	**Coffee Break**		
16:10	Femtosecond response of polyatomic molecules to ultra-intense hard X-rays	B. Erk	DESY, Hamburg
16:40	Drop-on-demand sample delivery for studying biocatalysts in action at X-ray free-electron lasers	F. D. Fuller	LBNL, Berkeley
17:10	Light-induced ultrafast structural reorganizations in the hybrid perovskites	A. Lindenberg	Stanford Univ. and PULSE
18:30	**European XFEL Dinner Reception (DESY Canteen)**		

General status of the project

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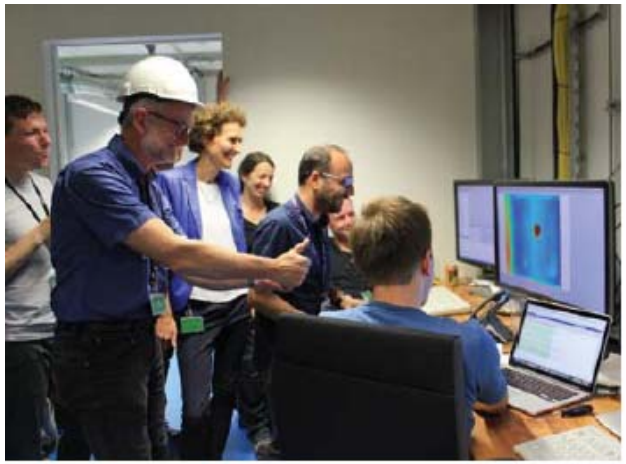
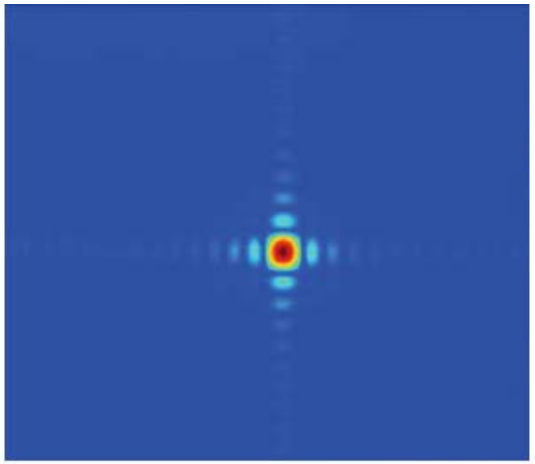
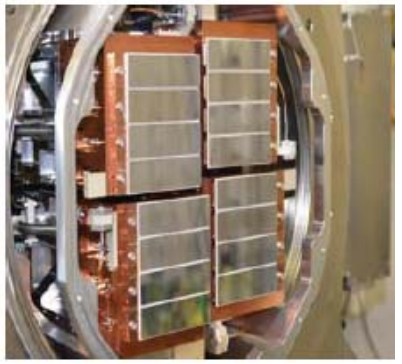
It has been a fantastic Year!



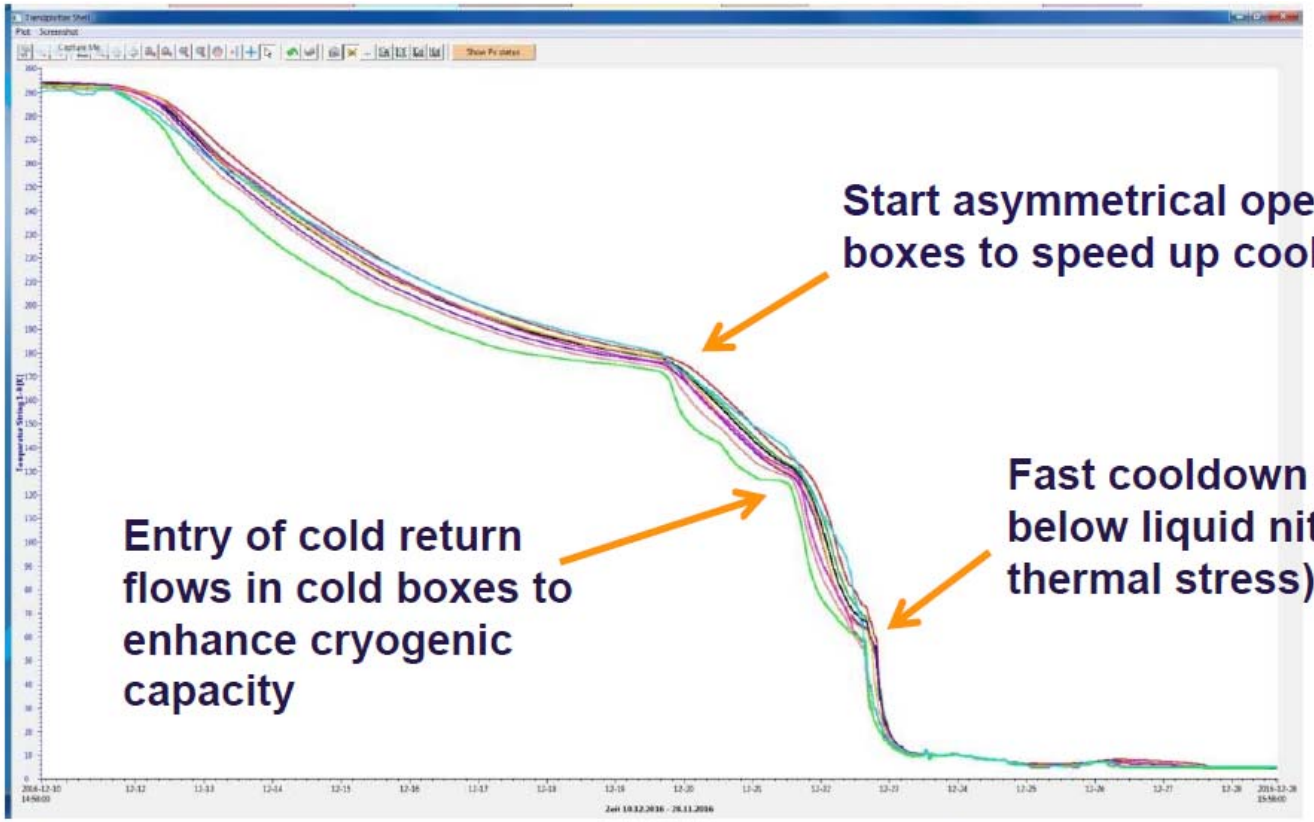


The European XFEL Users' Meeting is an annual opportunity to strengthen the interaction between the European XFEL and the scientific user community. The scope of this meeting includes:

- Progress and current status of the European XFEL
- Instrument design developments & advances
- Early Userexperiments and selected science applications
- Current developments in the field of XFEL facilities



10.12.2016: Start of Accelerator Commissioning First Cooldown of XFEL Linac (300K to 4K)



Start asymmetrical operation of two cold boxes to speed up cooldown

Fast cooldown at temperatures below liquid nitrogen (no more thermal stress)

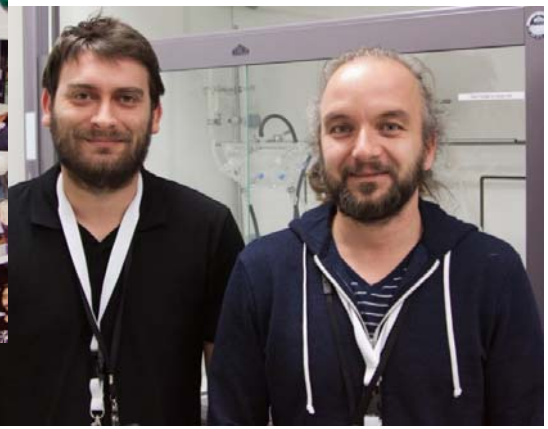
Entry of cold return flows in cold boxes to enhance cryogenic capacity

10.12.2016

24.12.2016

No Cold Leaks

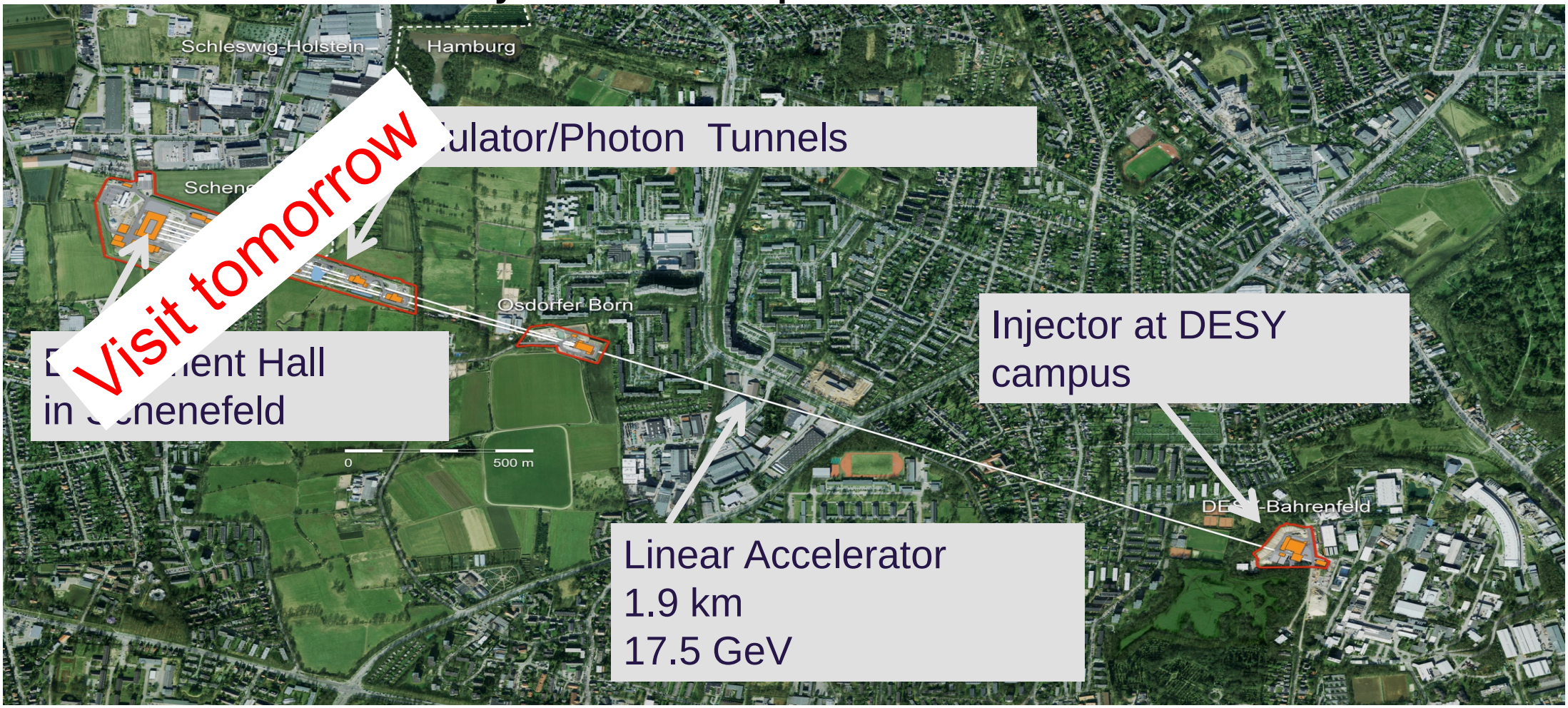
Users at European XFEL!



About the European XFEL

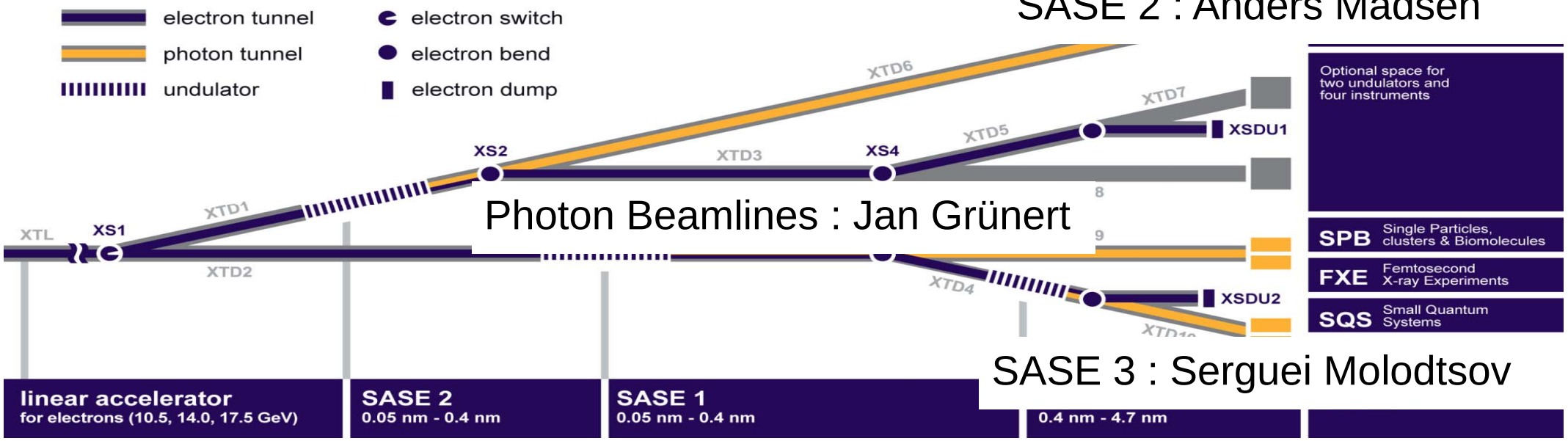
- Start 2009
- Task : Construction and running of the X-ray Laser Facility
- Germany (Bund, Hamburg (65 M€) und Schleswig-Holstein (25M€)) 58%, Russia 27 %, others 1–3%
- DESY operates the accelerator
- Staff XFEL about 350, Staff @ DESY about 250
- Start of operation 1. July 2017
  - 1,22 Mrd. € (2005 prices)
  - 600 Mio € in cash, 600 Mio € in-kind
  - Yearly running costs 117,6 Mio € (2018)

General layout of the European XFEL



Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24 (Hard XR)	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 – 3 (Soft XR)	4.6 – 0.4

SASE 2 : Anders Madsen



Photon Beamlines : Jan Grünert

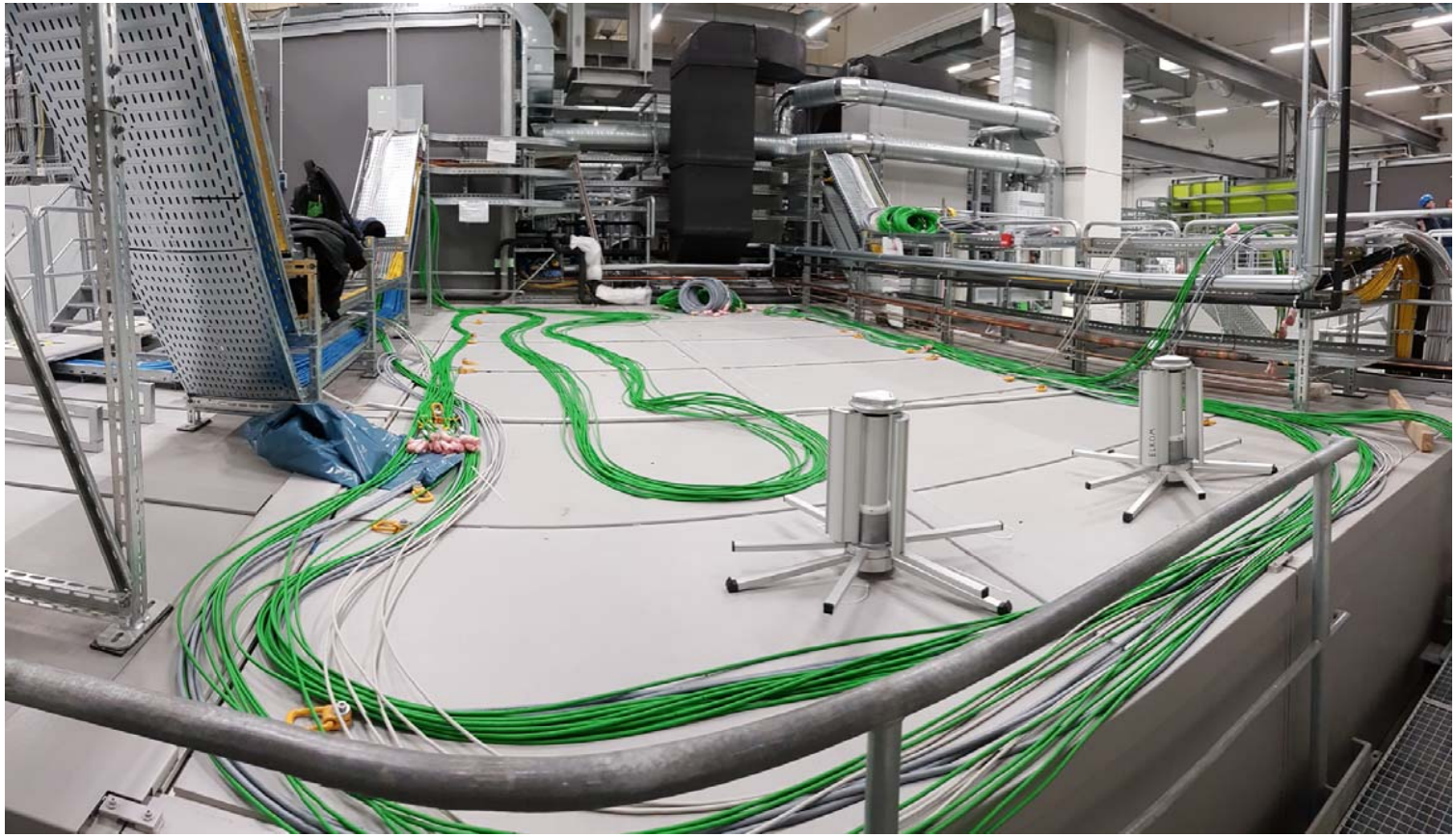
SASE 3 : Serguei Molodtsov

European XFEL

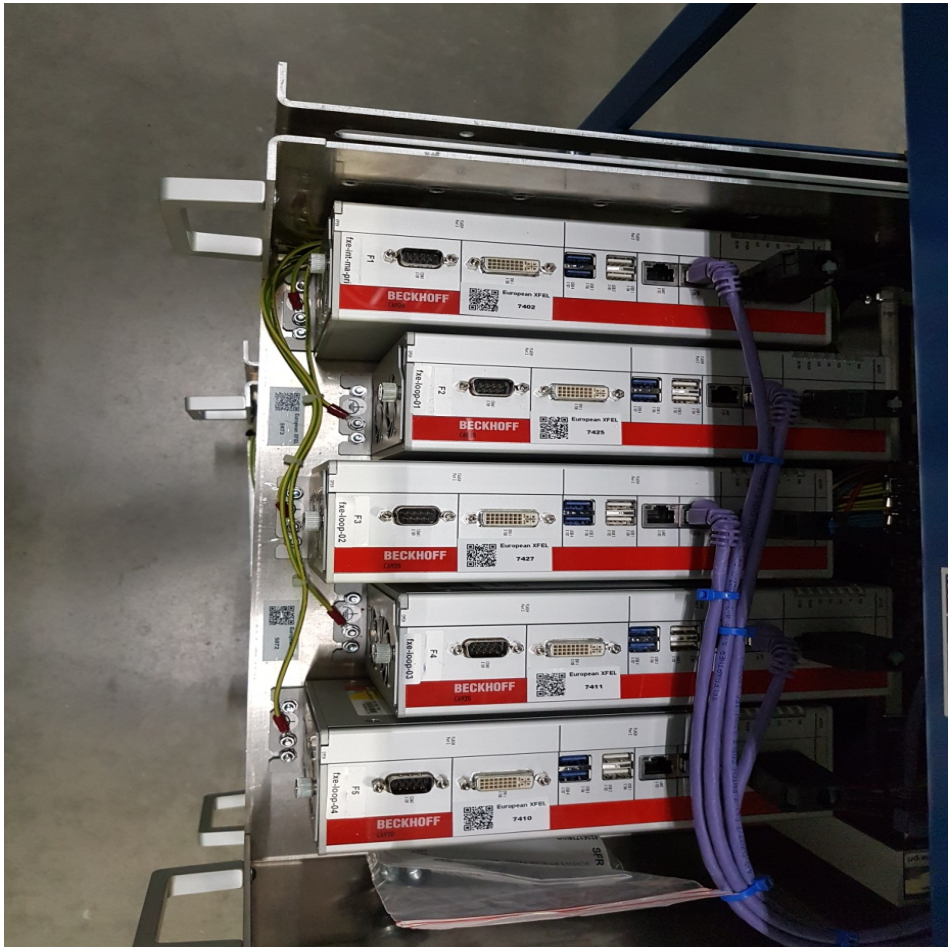
Orange color: X-ray optics & Beam Transport

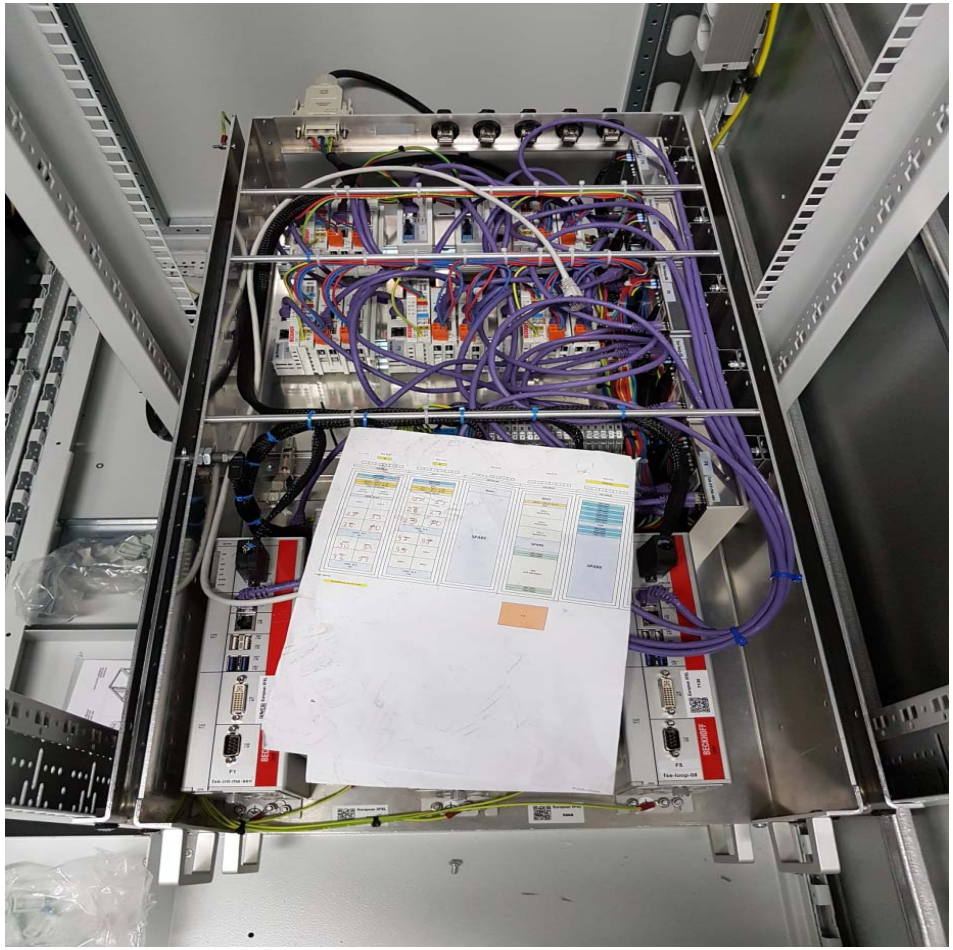
10.1.: First instrument cables have arrived for FXE…

10.1.: … and are being pulled.



10.1.: Beckhoff CPUs being installed.



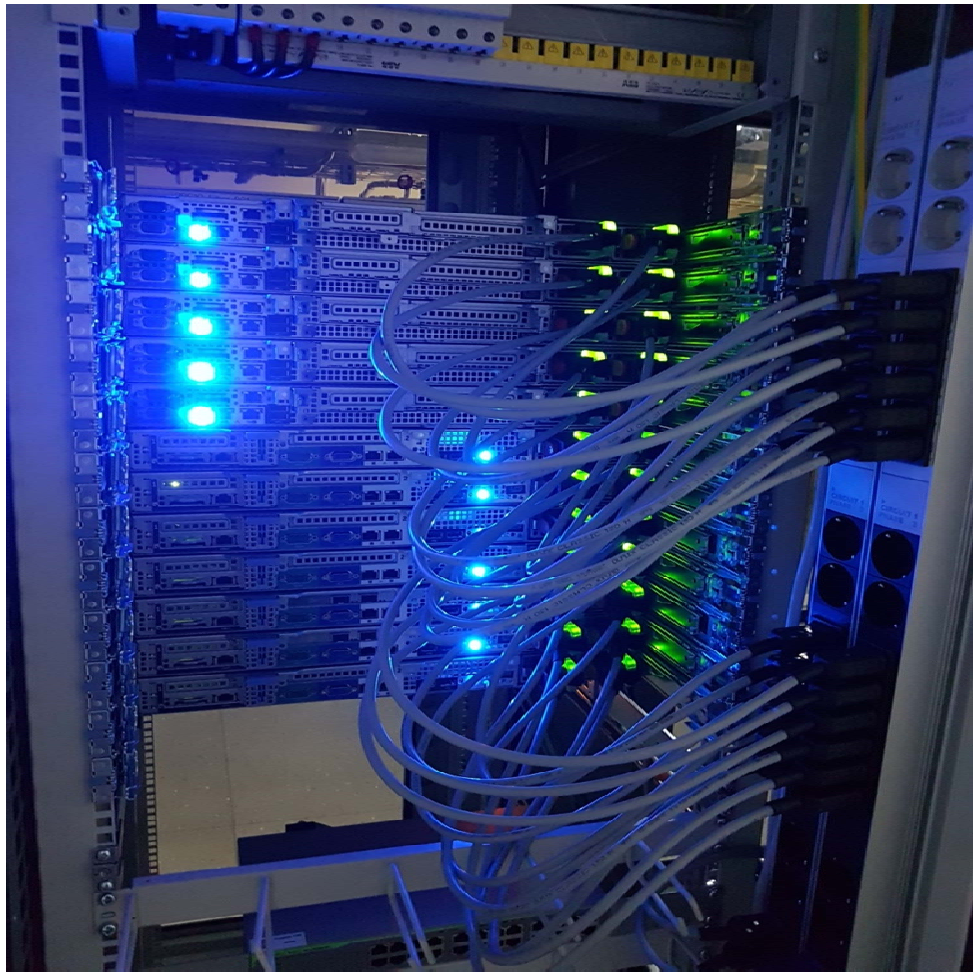


25.1.: First intrument cables have arrived for SPB optics… and been put into place.

20.1.: XFEL Biolabs

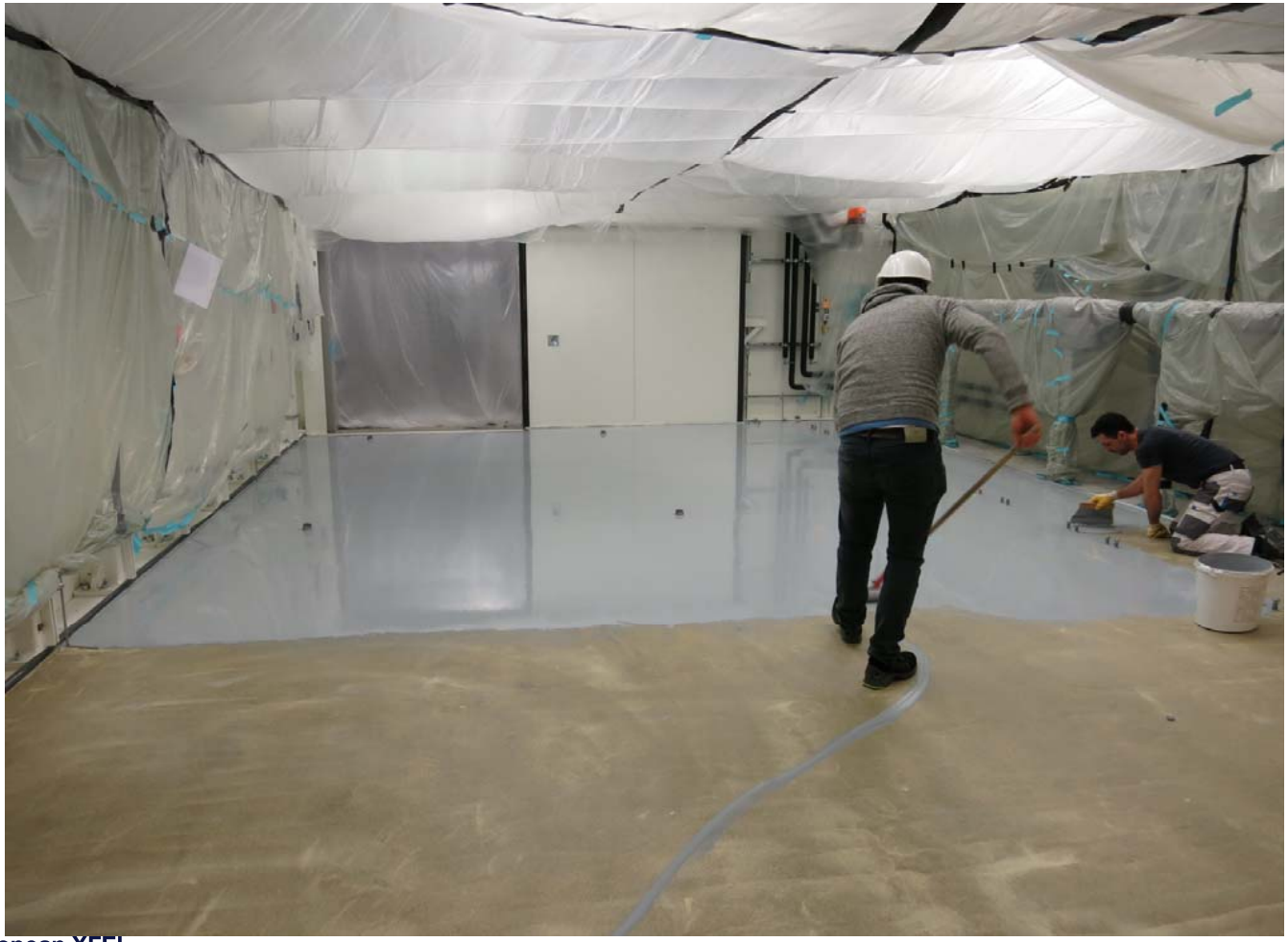
8.2.: SPB-Experiment D.09 with curtains, first cables being pulled.

07.2.: Karabo Servers installed in the rackrooms



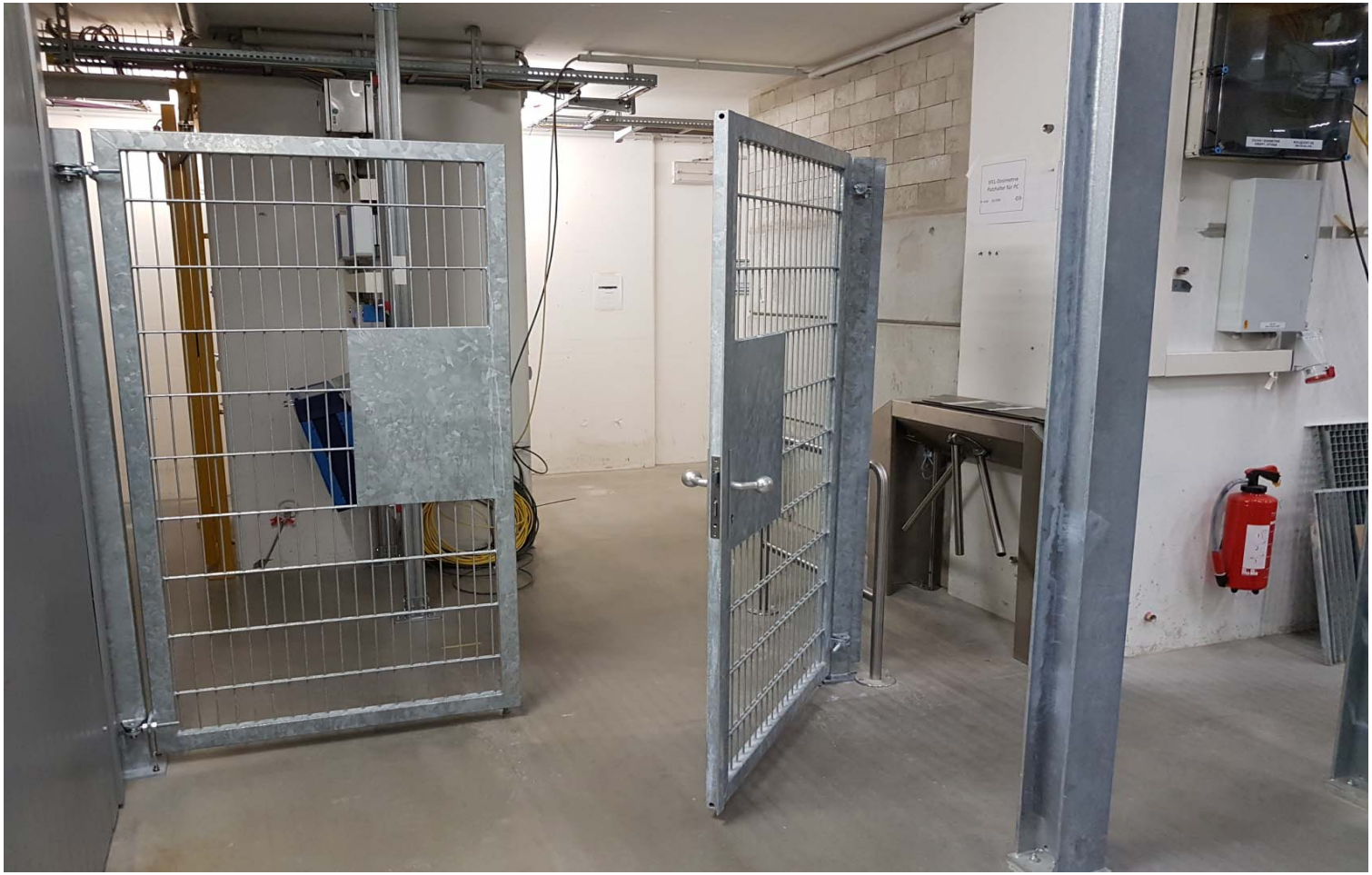
9.2.: Interlock installations have started in D.09

08.03. SASE1: FXE-floor improvement Top layer



16.03. FXE: First Beckhoff modules pushed in place and connected

Entire hall: Turnstiles / Interlock installation ongoing for XTDs

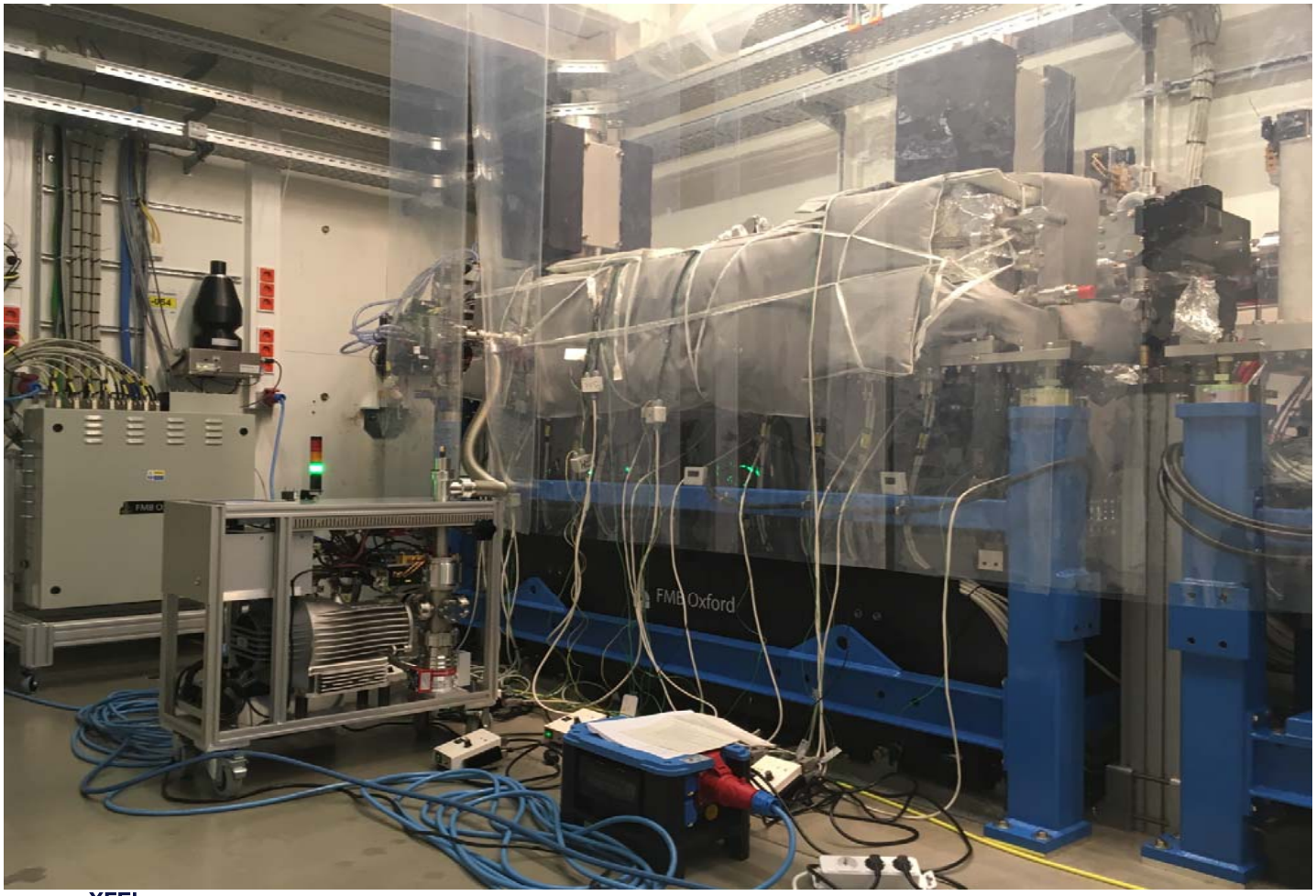


4.4.: Component Support Structure being installed in SPB/SFX

4.4.: Status of radiation interlock installation: End of XTD9

6.4.: First crates in SPB-optics racks

20.4.: Bake out in SPB Optics hutch D.02 Courtesy R. Bean



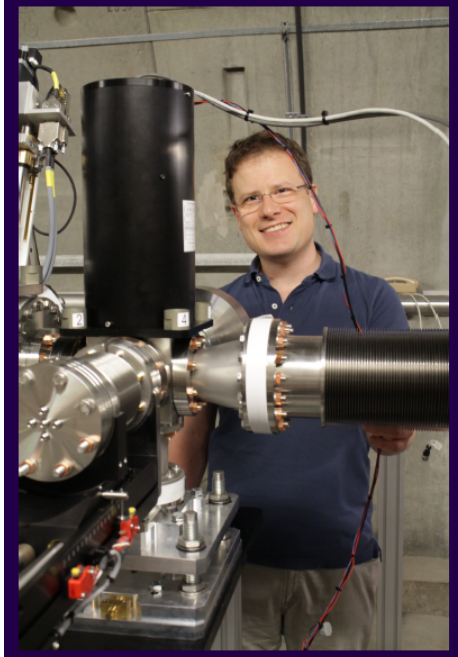
4.5.: First lasing event with the press @ BKR

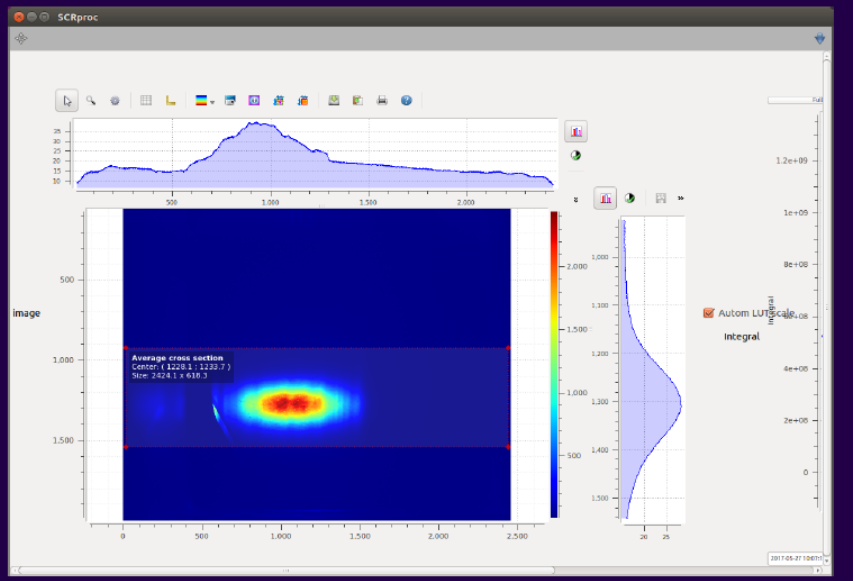
17.5.: Managing Director @ FXE

Lasing at 2 Å on May 24 and beam at the end of tunnel May 27

European XFEL

Commemorating European XFEL's first X-ray beam at the end of the tunnel.





Klaus Giewekemeyer, SPB/SFX Instrument

28.5.: Sunday morning - water in the XHEXP1…

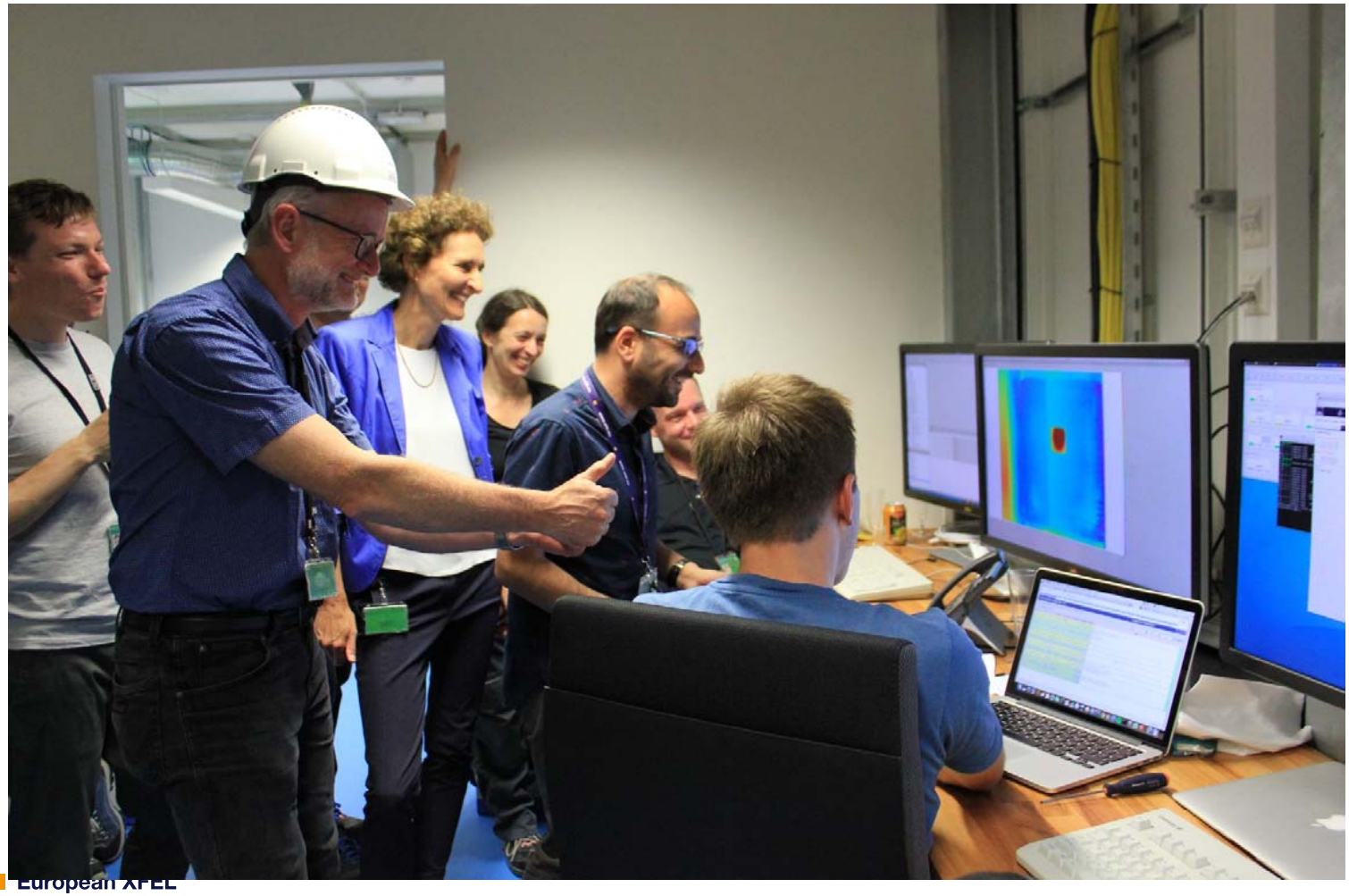
28.5.: … and in the XTDs.

28.5.: „All hands on deck!“ – by Sunday evening, the situation was contained.



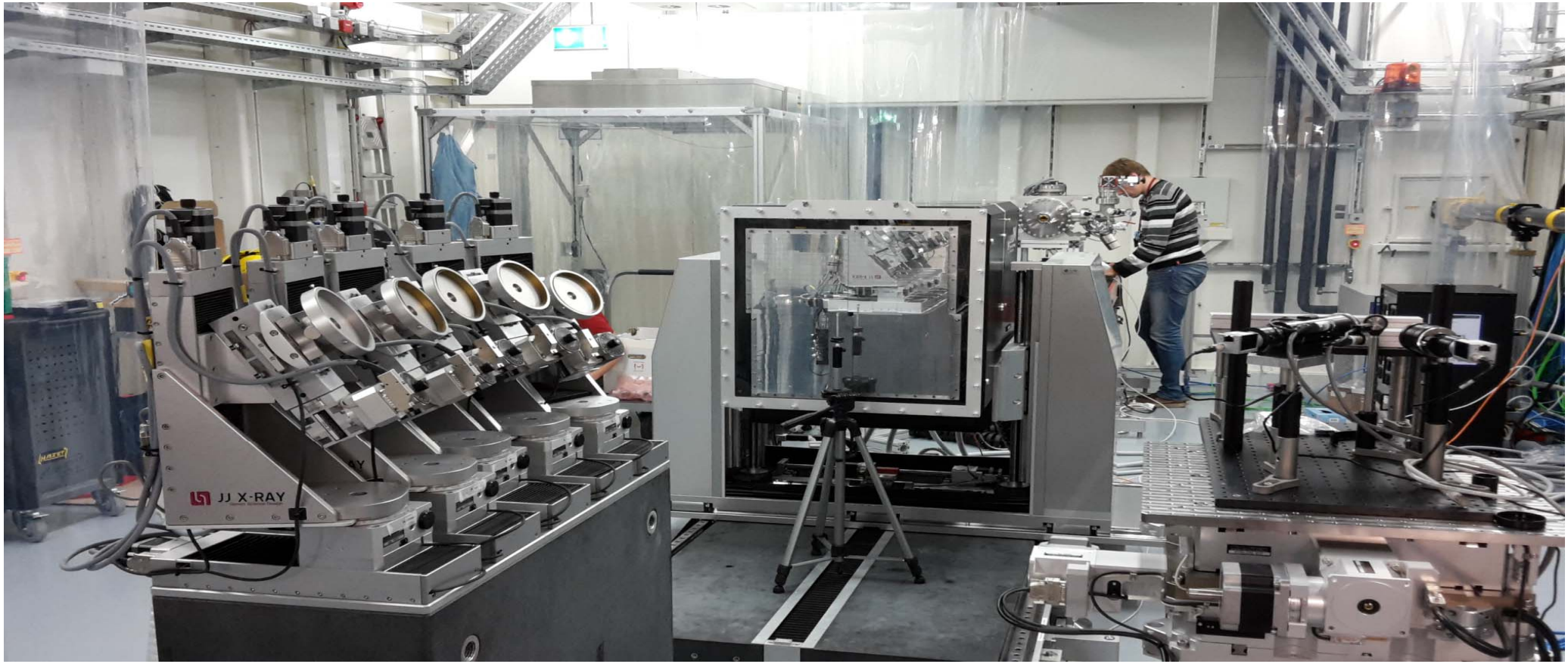
7.6.: FXE instrument hutch is getting filled…

23.6.: First beam @ SPB/SFX



23.6.: First X-ray beam @ FXE

18.7.: LPD @ FXE



24.8.: Tangerine-Laser in FXE, has been synchronized by now with light from injector

1.9.: SASE1 instruments ready for the start of user operation

1.9.: Freeway between SASE1 and SASE3

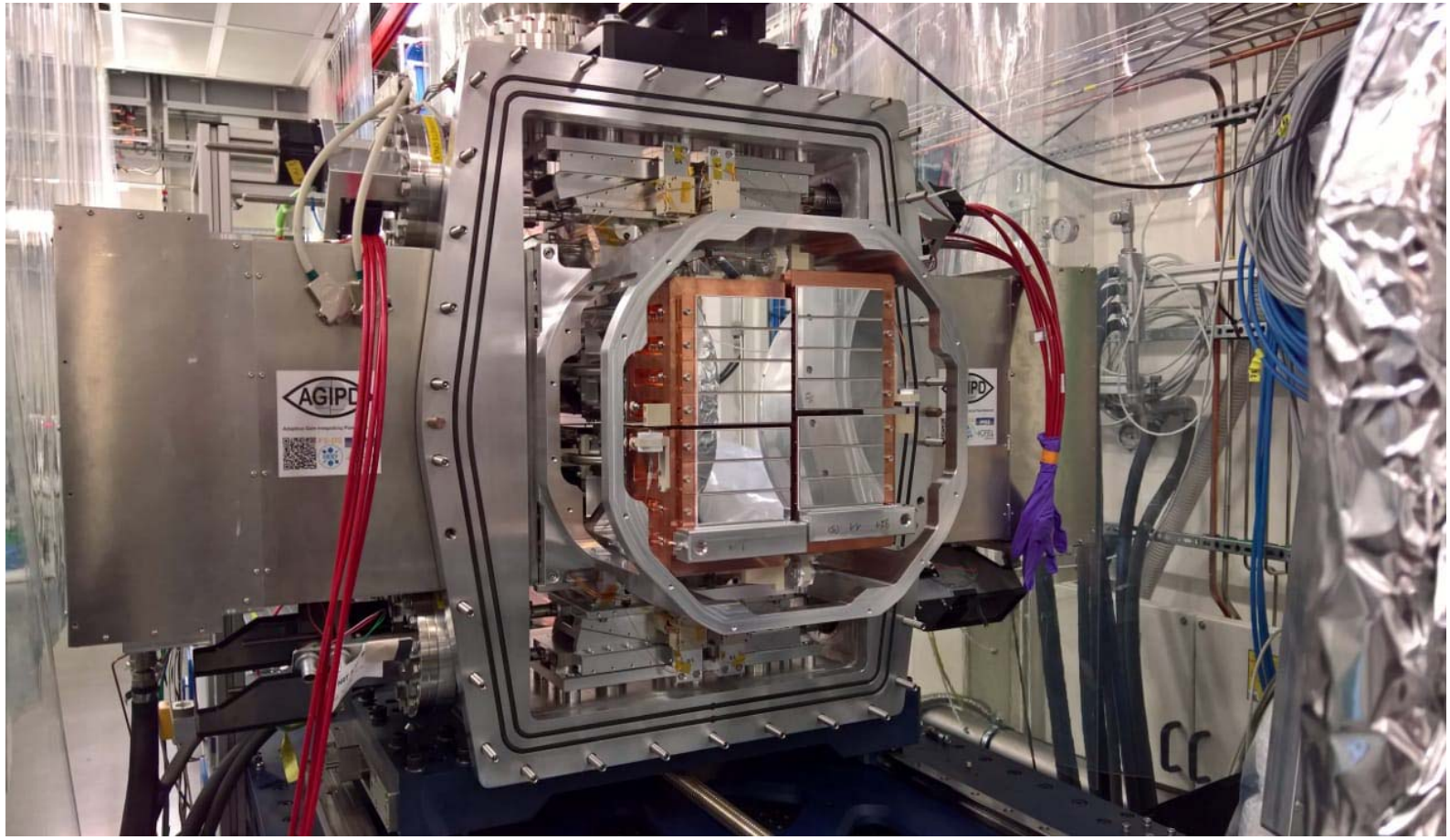
1.9.: Start of user operation

1.9.:

1.9.: FXE instrument ready for user operation

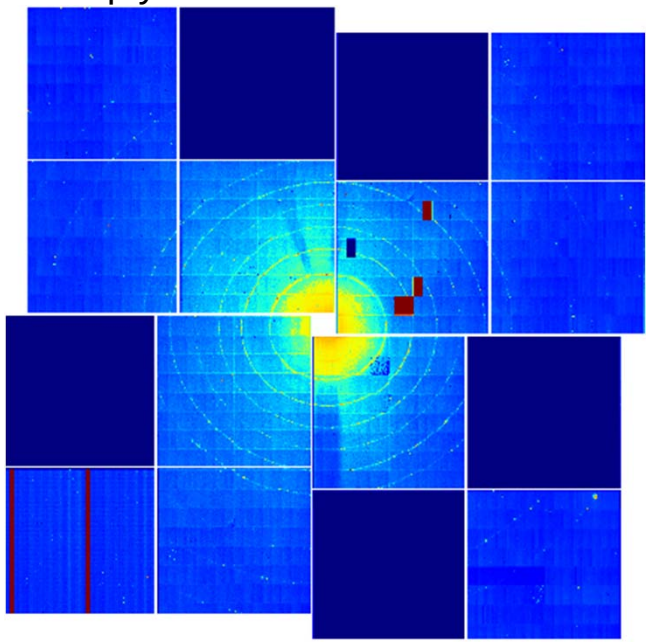
14.11.: FXE experimental setup

11.12.: Working on the AGIPD @ SPB

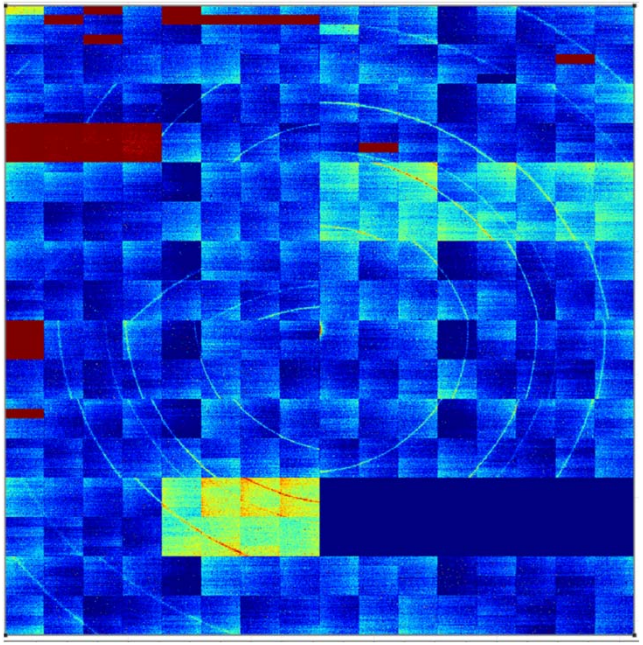


LPD tests at FXE, 12-13.08

LaB_6 calibration powder, ~140 mm to detector
LPD single shot image; per train 2 images filled,
30 are empty as should



AGIPD Sep 1.

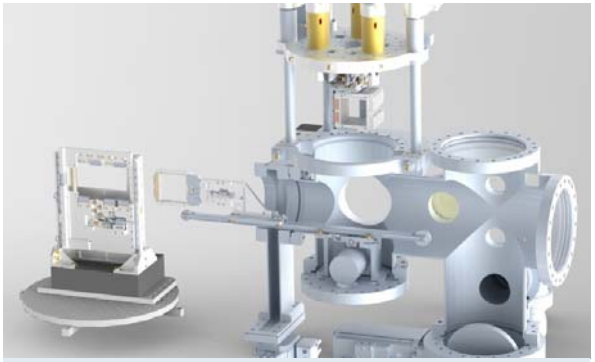


Both detectors worked and took data in user mode!

Highlights from the Sample Environment group

SPB/SFX liquid jet sample environment

Aerosol injector:
an in-kind contribution from Uppsala University



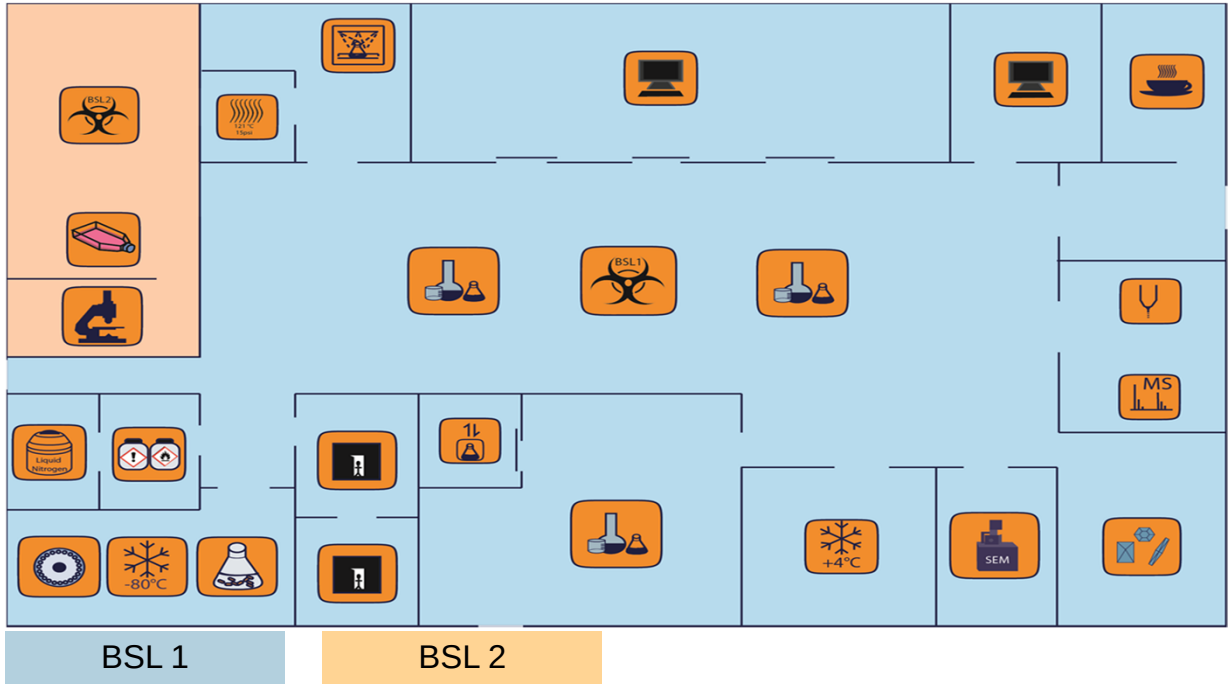
Fast solid sample scanner with load-lock sample changer for SCS.
Versions for MID and HED in preparation

Compact pulsed magnet for MID and SCS:
15 Tesla 0.6 ms pulse length sample at 4.2 – 300 Kelvin

Confocal microscope and scanning electron microscope (SEM) for sample characterization

Courtesy Joachim Schulz

Biological User Laboratories: Everything from growing cells to sample injection

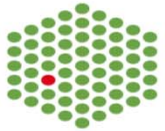


XBI Team

Huijong Han, Jana Makroczyova, Yasmin Gül, Robin Schubert, Ekaterina Round, Kristina Lorenzen

The XBI User Consortium:

ASU EMBL



UKE HAMBURG

UNIVERSITY OF OULU

UPPSALA UNIVERSITET

European XFEL

Courtesy Kristina Lorenzen

First Users

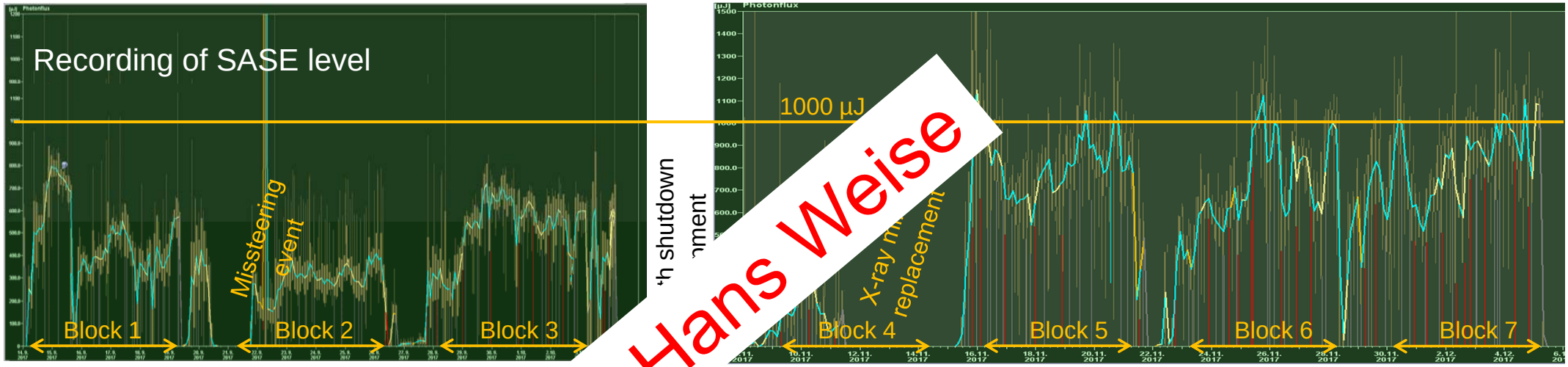
- 5-15 Users per SPB Beamtime (about 40 in total)
- Very positive feedback
- Usage:
  - Handling of cells
  - Dark room
  - Cold room
  - Anaerobic Box
  - Centrifugation
  - Cryogenic storage
  - Sample analysis
  - Microscopy
  - Growing crystals
  - Characterization
  - Preparation for injection

Courtesy Kristina Lorenzen

14.9.: First SPB/SFX user group

18.9.: First FXE user group

Accelerator performance in first user runs

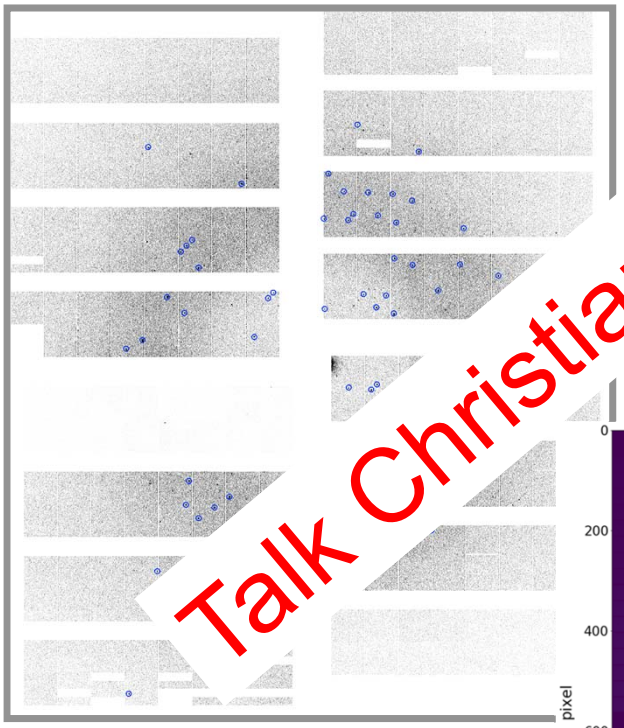


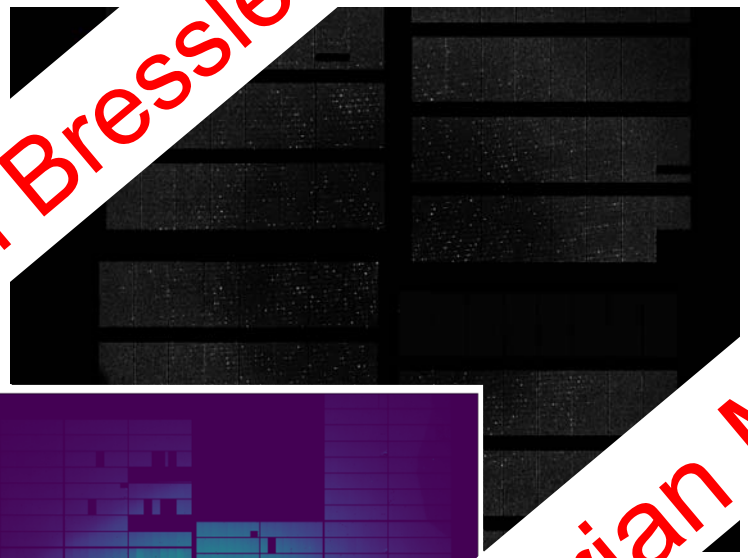
Talk Hans Weise

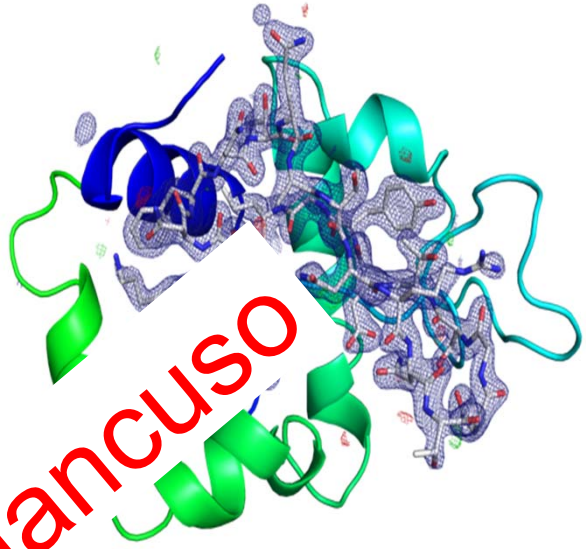
- 7 user blocks, 5 days each, ... ys in between for set-up & tunin
- 14 GeV, 1-30 bunches, 9.2-9.3 ...V
- Availability (= SASE delivery above threshold) between 10% (Block 4) and 97% (Block 6&7)
- Prominent error sources: X-ray mirror, operation & controls, trips (frequent but speedy recovery), magnets

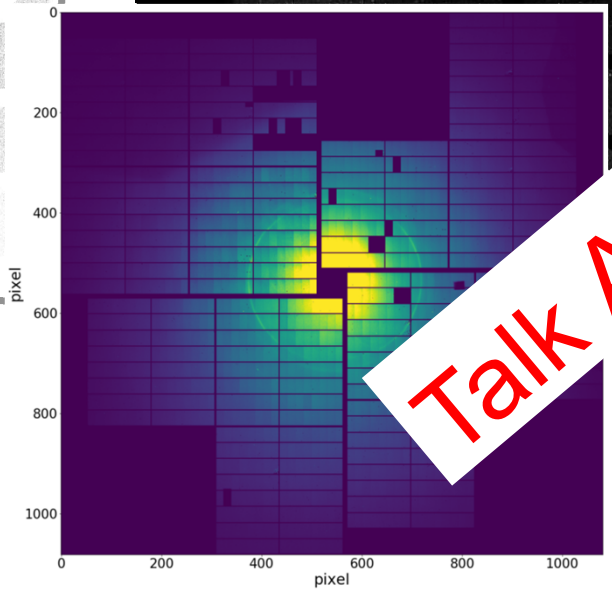
Courtesy Winni Decking

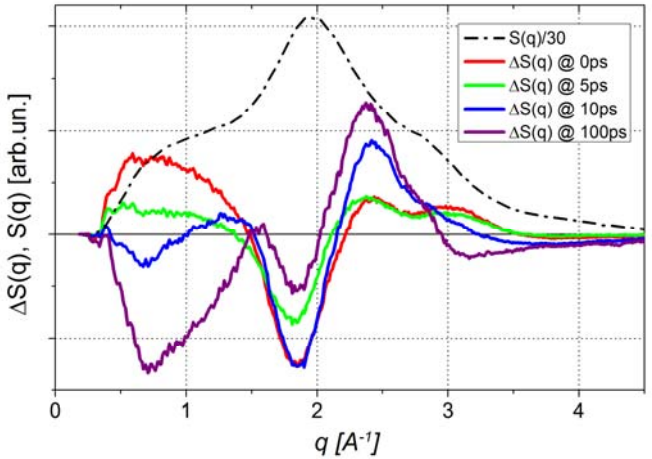
Data was taken









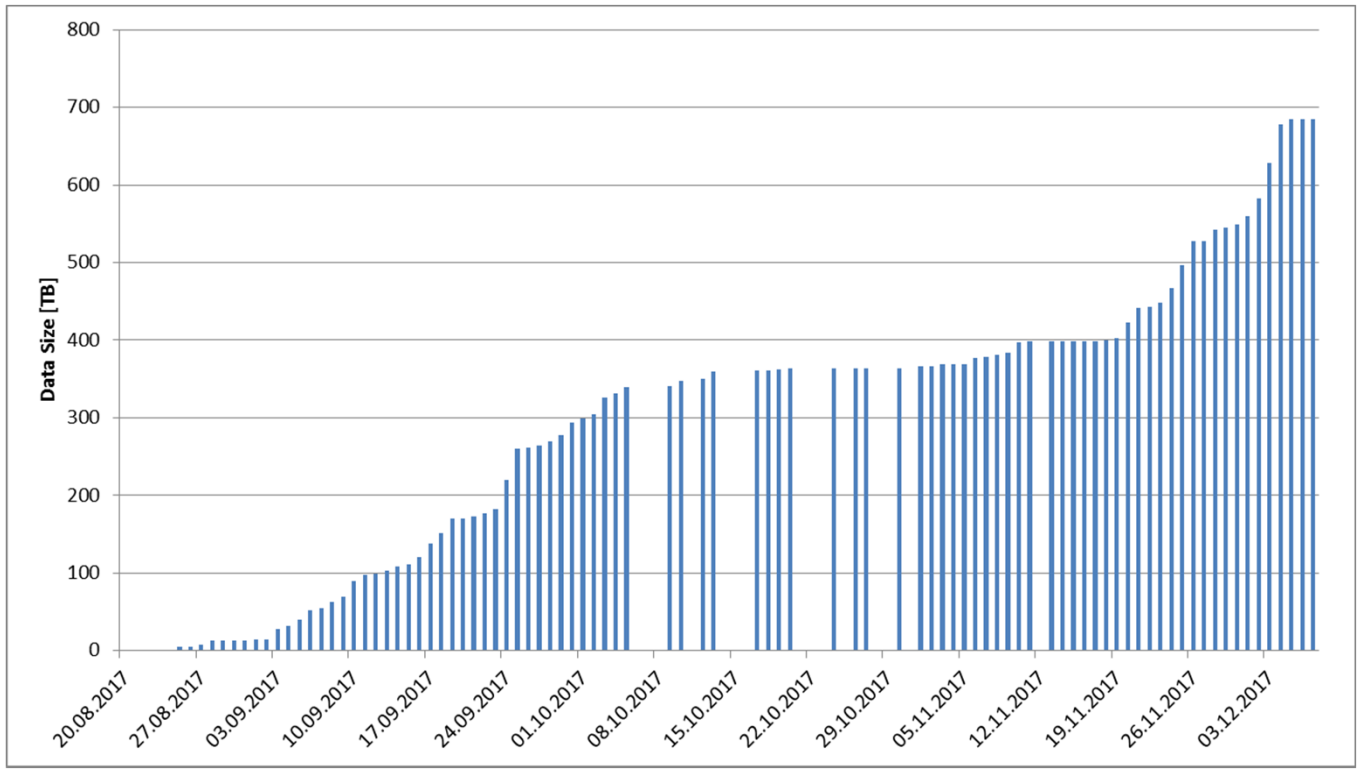


Talk Christian Bressler

Talk Adrian Mancuso

All generated data

- Includes User Experiments and Commissioning Activities
- FXE, SPB/SFX instruments and SASE1 tunnel



Courtesy Krzysztof Wrona

User Beam Team – Outcome and first Experiences.

Mail to first users : User assisted commissioning

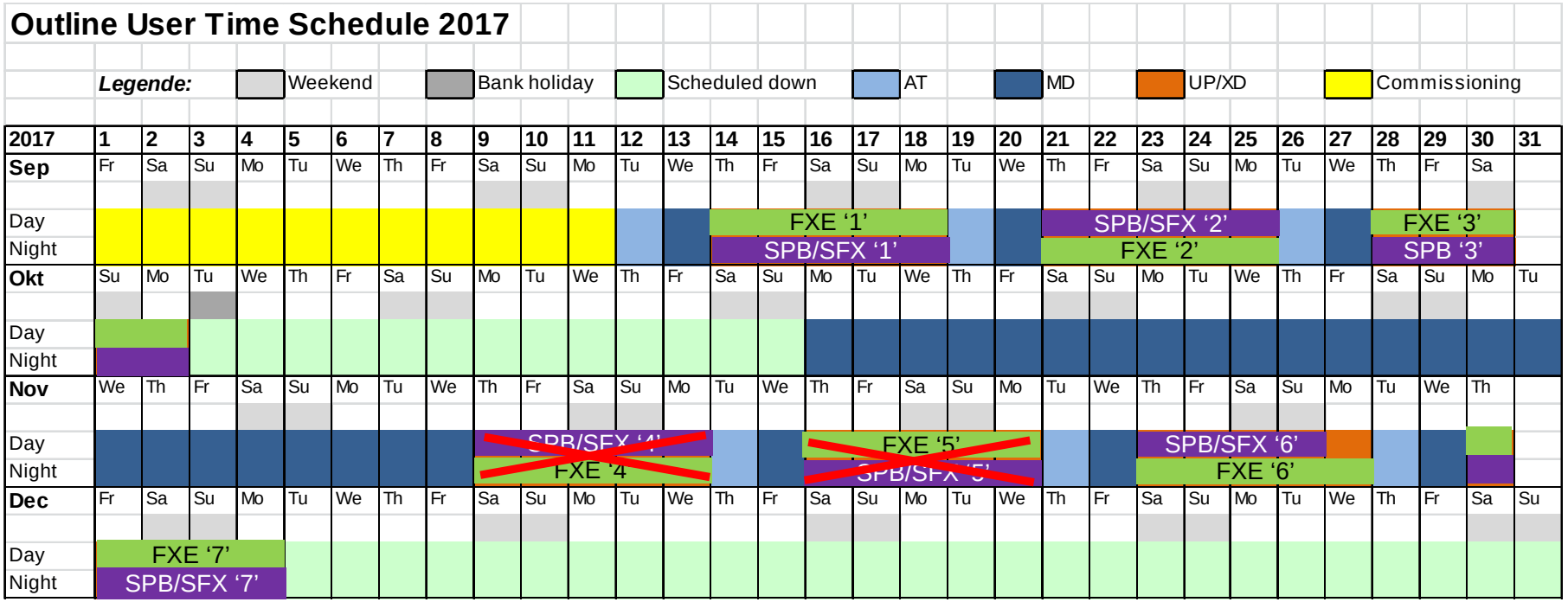
- The instruments and supporting teams have made great progress in recent weeks and months as we approach the first users arriving for measurements at the European XFEL. X-ray beam delivery, photon diagnostics and x-ray optics, and also instrument key systems, such as sample delivery, detectors and controls and DAQ have been setup and were used successfully during first tests and measurements during the instrument commissioning time. Nevertheless, certain subsystems and, in particular, the overall level of integration, stability, and familiarity with our instrumentation does not yet meet the standards we expected to offer to users for the Early User Experiments at the European XFEL. As such, we have decided to take two important actions.

- The first action is that we need to change the focus of your upcoming beamtime. We want to use this rather in the spirit of Users Assisted Commissioning time, which will allow to do first complete experiments. This means that you will still be part of the very first measurements at the European XFEL, however, some of the focus needs to be shifted to ensure that we make good progress on advancing the state of our facility—particularly on the data and controls front—while working towards collecting valuable scientific data with you over the duration of the beamtime. In practice, this means that some of the first shifts of the September beamtime should be expected to be used with development work, though the goal will still be to measure good data for at least a subset of the time awarded.

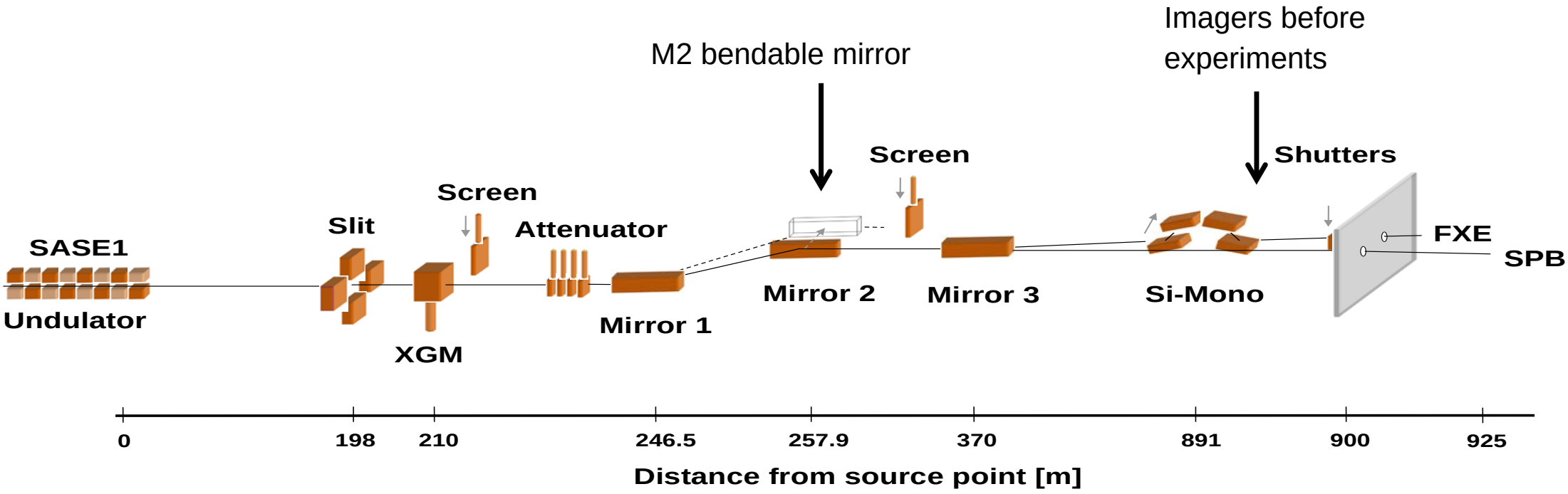
- The second action is that we reserved user beamtime for you in March 2018 that shall compensate for the fact that your experiments may not achieve the original goals possible with a fully commissioned instrument. We will after the end of the coming September beamtime together with you evaluate what was achieved and what not and, if necessary and wanted, will be able to allocate time in the early spring next year to compensate for lost time.

1st allocation period 2017 – assignment to EUE experiments

- 2 slots of 3 and 4 wks each; schedule 12-hr shifts at both instruments
- ~840 hrs
- Incl. tuning



Failure of M2-Bender: SASE1 photon beamline layout

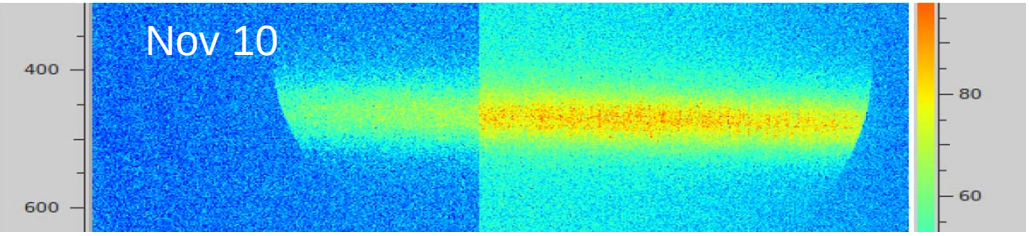


Failure of M2-bender system during User-Run on Nov. 10, 2017

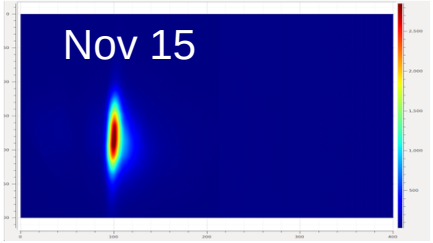
Chronology:

- **Friday, Nov 10, 23:00:** FXE has problems to achieve collimated beam with M2-bender in XTD2 Tunnel . Instead, a very wide diverging beam is observed. Attempts to fix the problem remotely by moving the bender motor fail. Beam is not usable for FXE experiment.
- **Saturday, Nov 11, 9:00**: SPB confirmed that the beam is also not usable for them. 5 experts from X-ray Optics group and Vaccum [illegible] haining user beam time for this
- **Sunday, Nov 12:** The M2-bender is exchanged and vacuum system closed. Start of pump down.
- **Monday, Nov. 13:** Final leak test is successful. XTD2 tunnel is closed Monday afternoon.
- **Wednesday Nov. 15:** New bender aligned during machine startup time

Fantastic and dedicated work by the XFEL team



Beam on imager in front of experiments before and after exchange of M2-bender (same scale)



Accepted proposals published on xfel.eu

User assisted commissioning

No.	Title	Main Proposer	Instrument
2012	Serial Femtosecond Crystallography at MHz repetition rates	A. Barty	SPB/SFX
2013	Internal Structure of the Melbournevirus by Flash X-ray Imaging	F. Maia	SPB/SFX
2016	Tracking ultrafast ligand exchange reactions using combined femtosecond X-ray solution scattering and emission spectroscopy	W. Gawelda	FXE
2017	Collaborative early experiments in time-resolved SFX: i) mix and inject methods	A. Orville	SPB/SFX
2026	Investigating the charge transfer excited state dynamics in mixed-ligand Cu(I) complexes using time-resolved X-ray diffuse scattering	K. Kubicek	FXE
2038	Structural dynamics induced by and studied with XFEL pulses	I. Schlichting	SPB/SFX
2042	Droplet on Demand to Massively Reduce Sample Amount for Time Resolved Serial Femtosecond Crystallography with XFELs	A. Ros	SPB/SFX
2045	Investigation of electronic, structural and solvation dynamics following the metal-to-ligand charge transfer in halogen containing Cu diimine complexes	L. X. Chen	FXE
2046	XFEL pump - optical probe study of ultrafast energy dissipation in semiconductors	T. Sato	SPB/SFX
2050	Unraveling the electronic and structural origin of intramolecular cooperativity in polynuclear transition metal complexes by combined femtosecond X-ray emission spectroscopy and X-ray solution scattering	S. Canton	FXE
2052	Singlet excited state of Cu-based material for Organic Light Emitting Diodes probed with pump-probe X-ray scattering and emission	G. Smolentsev	FXE
2066	Time resolved fs crystallography of electron transfer reactions and the water splitting process in Photosynthesis	P. Fromme	SPB/SFX
2072	Structural dynamics in the binding of messenger molecules to heme proteins	D. Kinschel	FXE
2073	Atomic-scale rearrangements after photon absorption in the hybrid perovskites	A. Lindenberg	FXE

Some Users Statistics

Beamtime Allocation Period	201701 (Sep-Dec 2017)	201801 (Aug-Oct 2018)
Proposals submitted	63	61
Total proposers	505	440
User shifts requested	275	341
Proposals for FXE	37	42
Proposals for SPB/SFX	26	19
Users in Sep-Dec		
Users visits Schenefeld	463	
Remote access users	41	
Individual users	341	

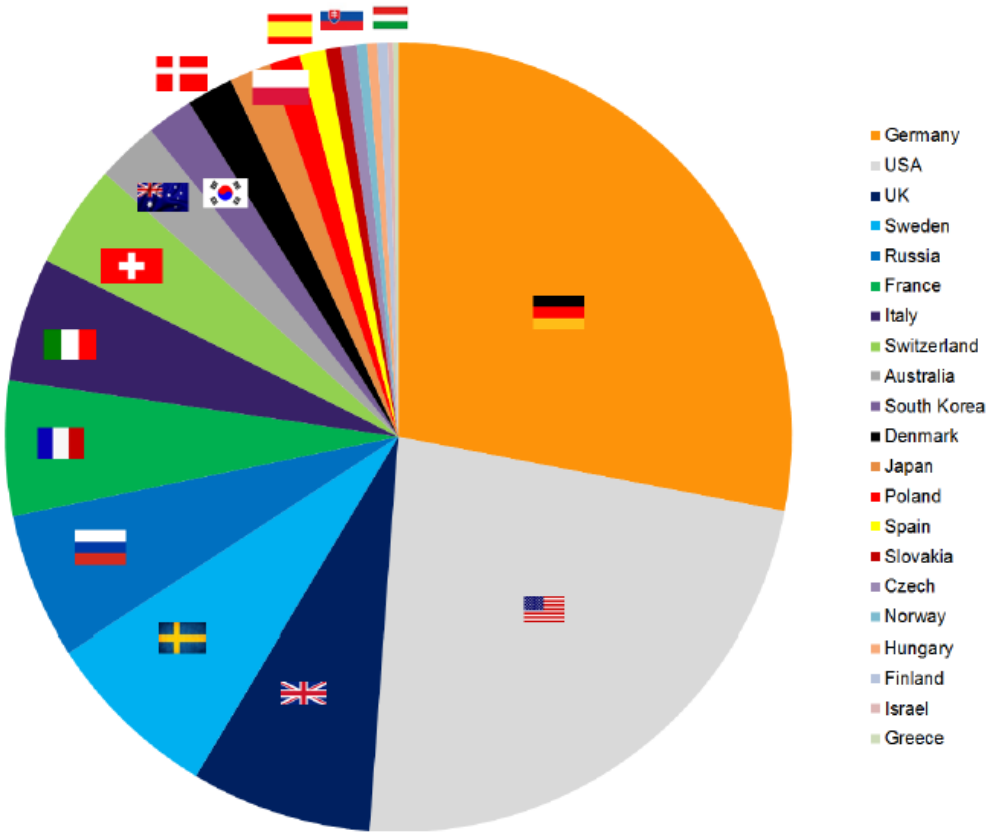


Figure 11: Number of co-proposers per country (except European XFEL)

European XFEL

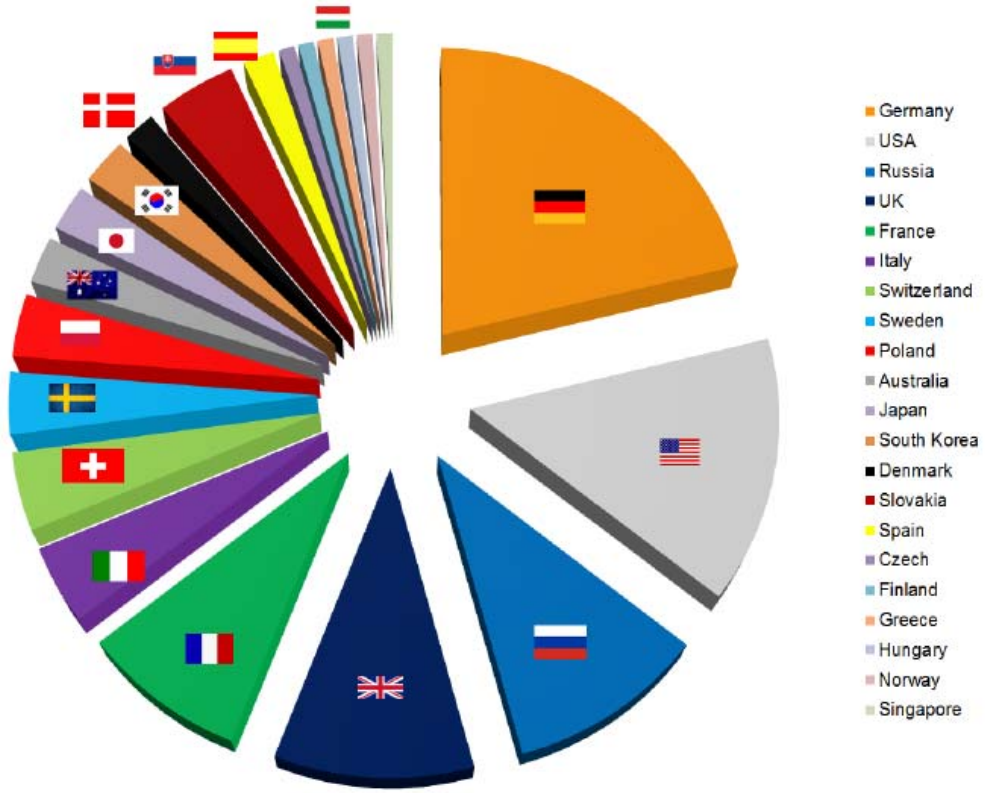


Figure 12: Institutions on proposals per country (excluding international institutions)

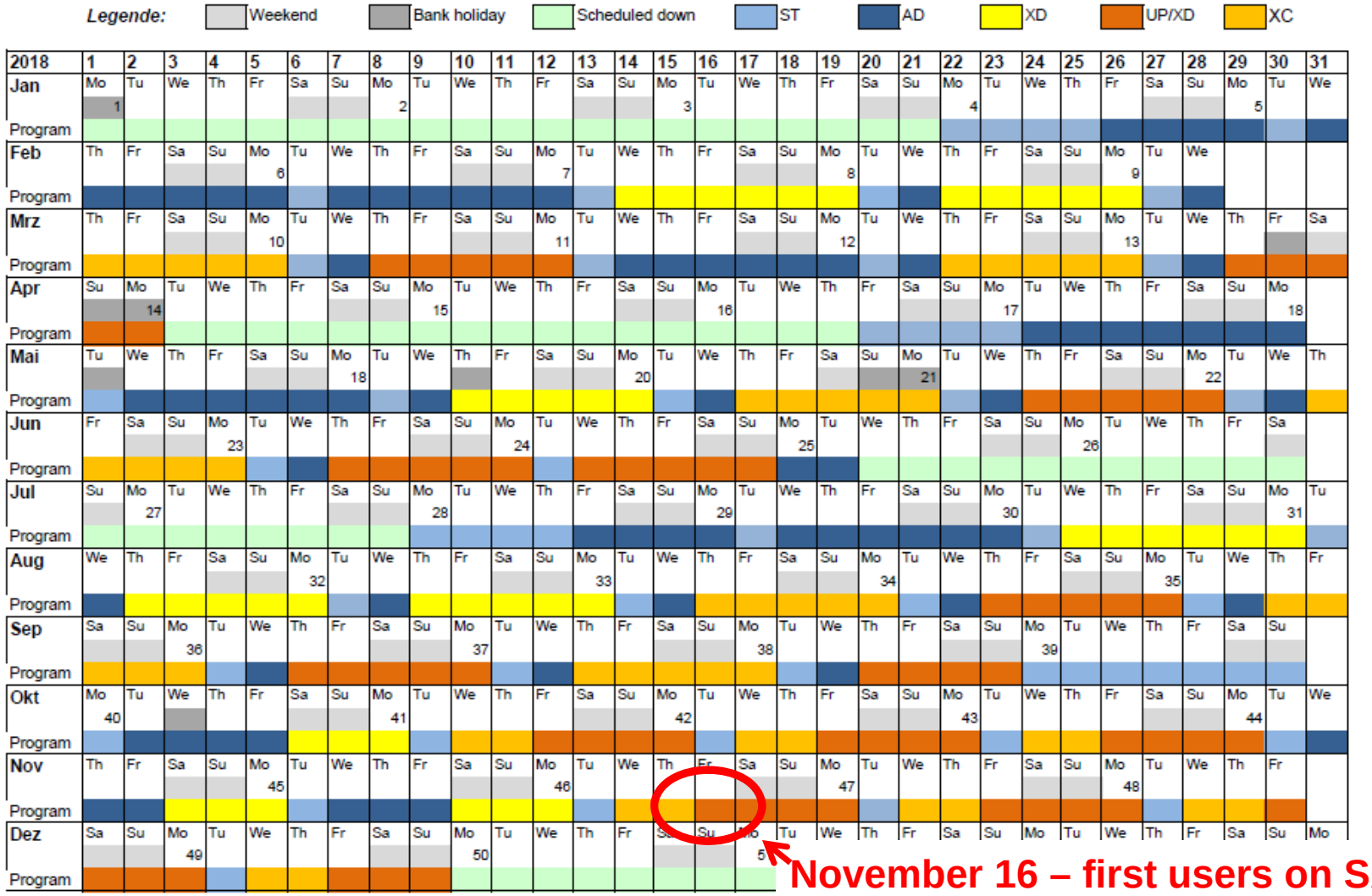
Experience from first users experiments

- Extremely motivated and dedicated staff and users
- Strong prioritisation on SASE 1 was necessary
- Shift work and on call duty (OCD) was negociated with Works Council
- Access to bio-laboratories worked well
- Satefy approval worked well
- Handling of Users by User Office worked well
- Operational meetings with users
- Debriefing meetings and written feedback from users
- Stability issues with Karabo, only basic functionalities installed
- Pump-probe laser not used for experiments in 2017, ready for end of March 2018

Plans for 2018

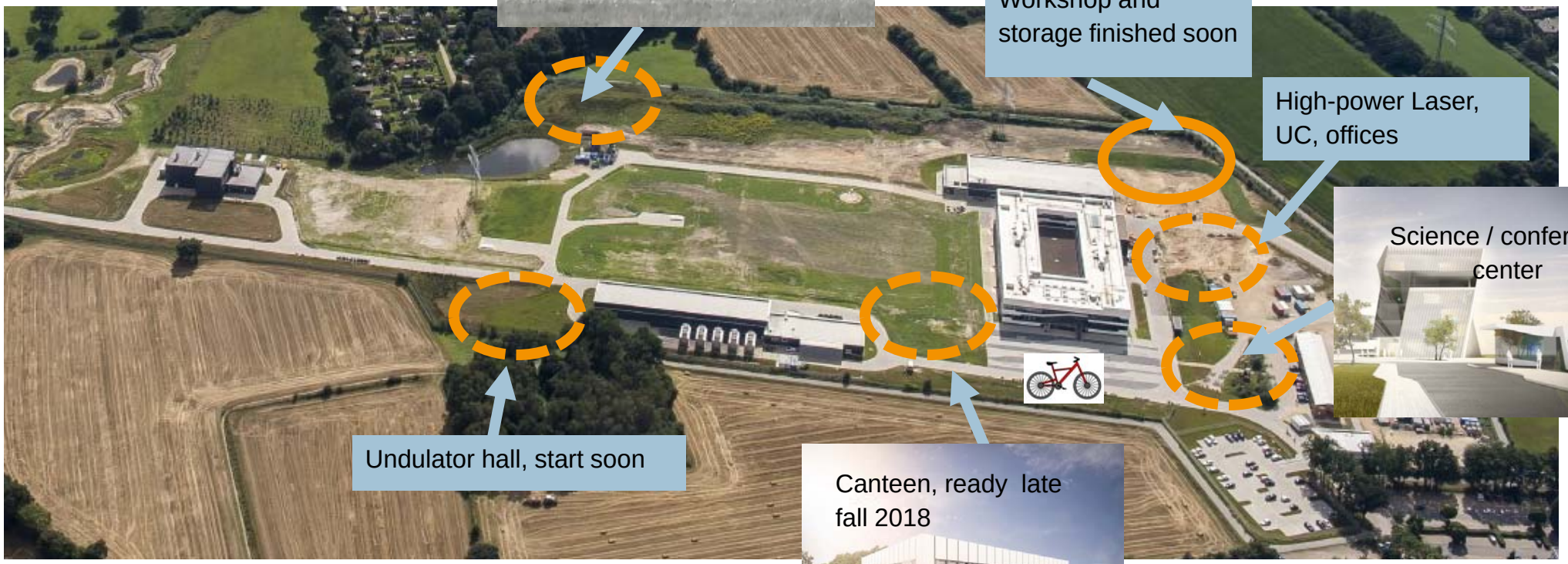
- SASE1:
  - Continuous improvement of understanding lasing performance
  - Enhance flexibility and stability
- SASE2:
  - Commission electron beam path (February)
  - First lasing (May)
  - Commission photon systems (May-June)
  - First Users Early 2019
- SASE3:
  - First lasing (Feb)
  - First Users 16. November
- Commission photon systems (distributed over year, influences SASE1 operation) Bunch number
  - 27000 bunches/second in XTL by end of the year
  - 6000 bunches/second in routine operation into north & south branch by end of the year
  - 3000 bunches/second lasing in SASE1 by mid of the year

- Reallocation
  1st proposal round
  (March-June)
- 2nd proposal round
  (Aug-Oct)
- 3nd proposal round
  including SASE 3
  and SASE 2 (2019)
  (Nov - ?)



November 16 – first users on SASE 3

Campus development



NEW : European XFEL Users Organisation

To be formally established at Users Meeting 2019

- Set the framework for a dialog between users and Management
- Representation at SAC meetings
- Direct contact to Management

- User Support and users friendliness
- Transport, accommodation, food, ….
- Input to Program for coming Users Meeting
- Help to New Users Group
- Diversity of scientific fields and groups

- Rules of Procedures must be defined
- Group of 3-5 persons needed to get started.

Thank you for your attention

SCIENCE FELs
Stockholm 2018

25-27 June
Alba Nova University Center
Stockholm, Sweden

FEL Science and Applications award

Conference chairs
Prof. Mats Larsson and
Prof. Sverker Werin

Scientific chairs
Prof. Anders Nilsson and
Doc. Per Johnsson

http://indico.maxiv.lu.se/e/science-at-fels-2018