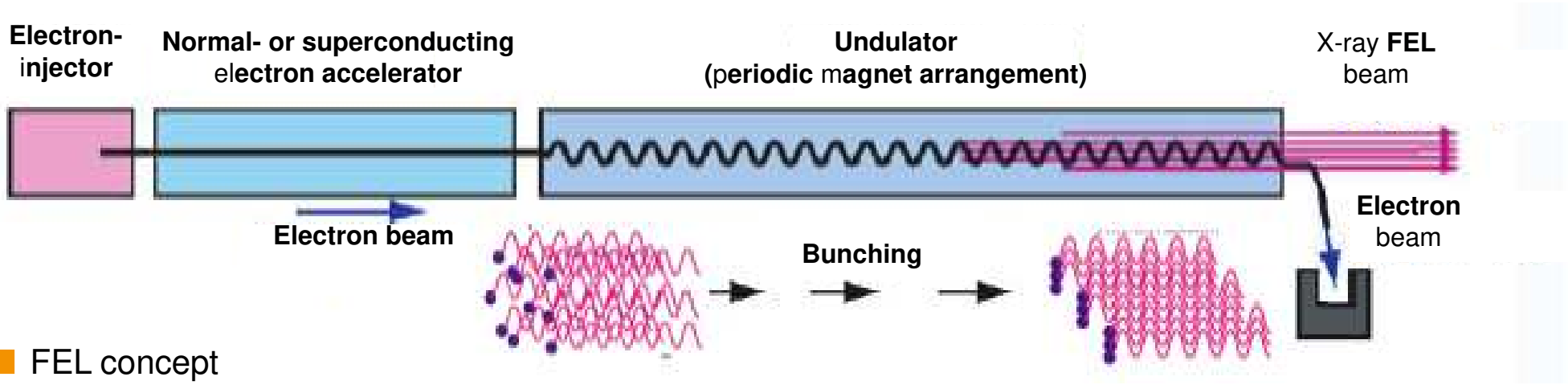
Scientific Applications Using High Repetition Rate Hard X-ray FELs

Thomas Tschentscher (European XFEL)

19th Int. Conference on RF Superconductivity,
Dresden, July 1 – 5, 2019

thomas.tschentscher@xfel.eu

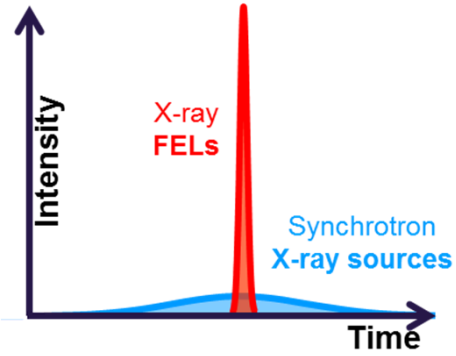
X-ray Free-Electron Laser (X-ray FEL)

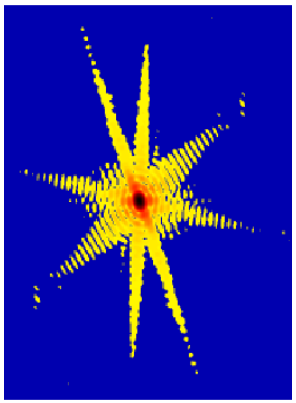


- FEL concept
  - J.M.J. Madey, J. Appl. Phys. 42, 1906(1971)
- SASE FEL radiation
  - **High Gain Single Pass regime:** A.M. Kondratenko, E.L. Saldin, Part. Accel. 10, 207 (1980)
  - **Collective instability and self-organization**: R. Bonifacio, C. Pellegrini, L.M. Narducci, Opt. Communications 50, 373 (1984)

- Properties of SASE x-ray FEL radiation
  - **Ultrashort duration (fs – 200 fs)**
  - **Very high pulse energies (0.1 – 1 mJ)**
    ► 10^{12} (10^{13}) photons at 0.1 (1) nm
  - **Full transverse coherence (<10 keV)**
  - **Limited longitudinal coherence**
  - **Single pass generation / fluctuations**

New opportunities offered by X-ray FELs





Ultrashort pulses

1 – 100 fs

Coherence

Fully transverse

Partially temporal

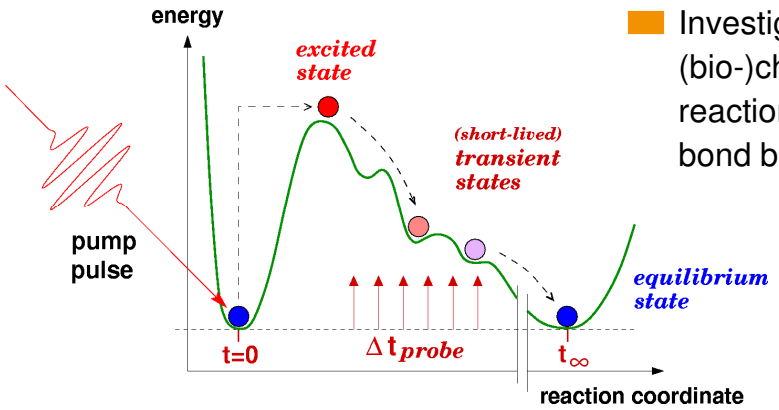
Intensity/power

up to few mJ

up to >10^{20} W/cm^2

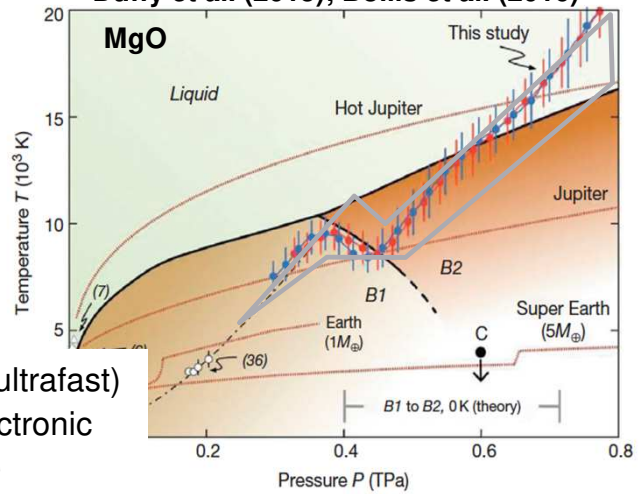
- Structural dynamics
  - **Measurement of atomic and electron dynamics with high spatial [0.1 nm] and temporal [10 fs] res.**
  - **physics, materials sciences, chemistry, life science**
- Imaging at the nanoscale
  - **Imaging experiments on confined and extended objects with atomic to mesoscale resolution [0.1–1000 nm]**
  - **physics, materials sciences, chemistry, life science**
- Non-linear x-ray science
  - **Start using non-linear techniques to obtain hidden information (off-diagonal elements in reaction matrices)**
  - **physics, chemistry**

Science problems addressed by X-ray FELs

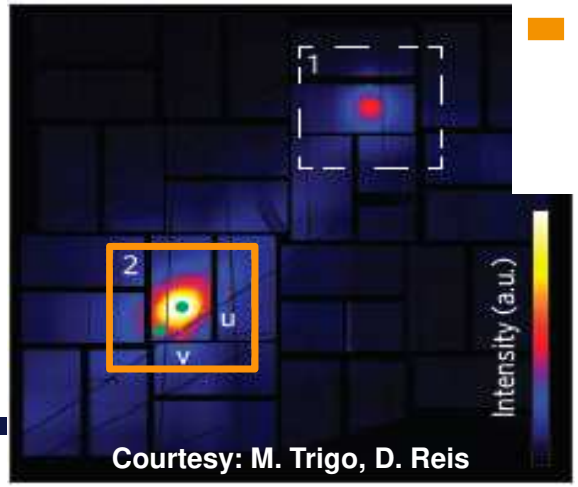


- Investigation of (ultrafast) (bio-)chemical processes: reactions, phase transitions, bond breaking & forming

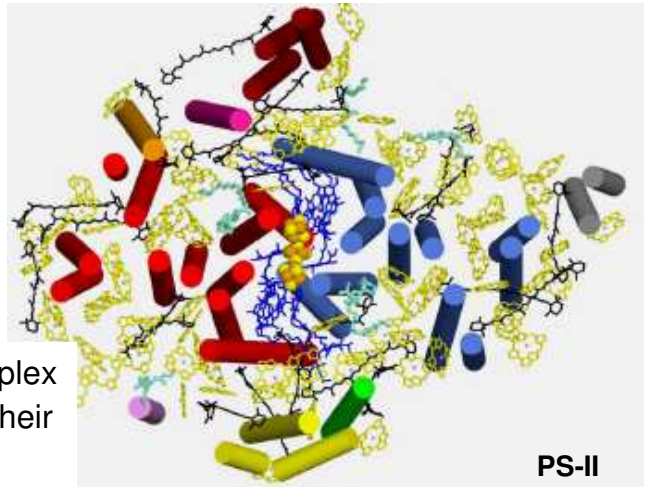
Duffy et al. (2015); Bollis et al. (2016)



- Investigation of (ultrafast) structural and electronic transitions: phase transitions, new states

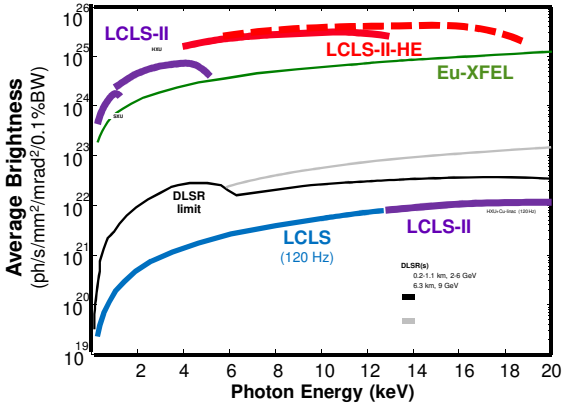


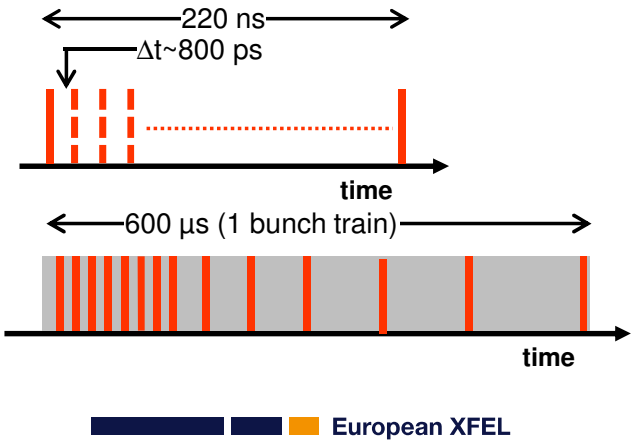
- Investigation of systems ‚in function': excited states,non-reversible processes



- Investigation of complex (bio-)structures and their temporal evolution

New opportunities offered by high repetition rate X-ray FELs





European XFEL

High average flux

10^{15} – 10^{18} phts/s

Sub-ns to ms pulse separation

Direct probing of non-ergodic systems

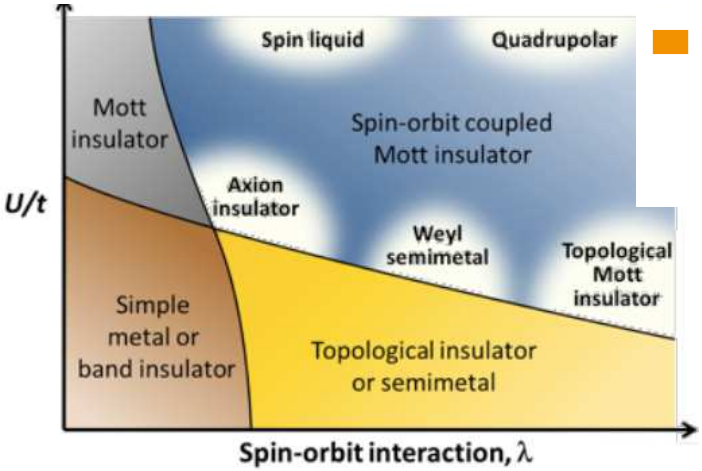
Beam delivery

High stability due to feedbacks

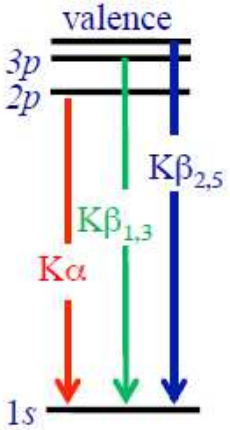
Parallel operation of several instruments

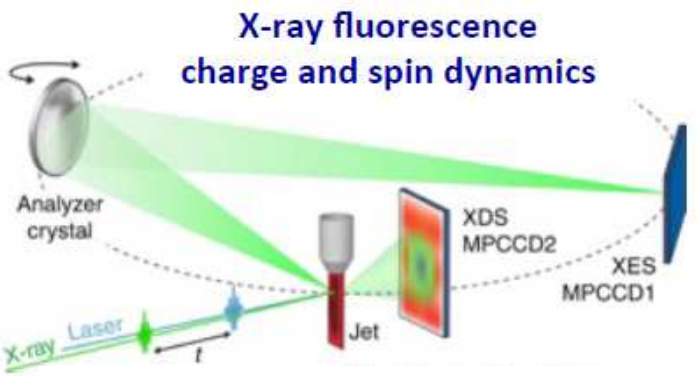
- Processes with very low signal yield
  - **Very dilute systems; high resolution spectroscopy; Non-linear x-ray science**
  - **Physics, chemistry**
- Processes needing high repetition rates
  - **Single particle imaging; Parameter studies for chem. compounds; Coincidence experiments; Photo-emission; Photo-correlation**
  - **Biology, chemistry, physics**
- Image non-repetitive processes
  - **Materials science**
- More experiments & dedicated instruments
  - **All science domains**

Science problems benefitting of high repetition rates

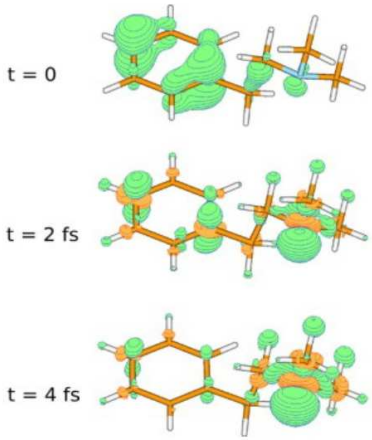


- High resolution spectroscopy reveals electronic & structural dynamics of complex materials (from LCLS-II)



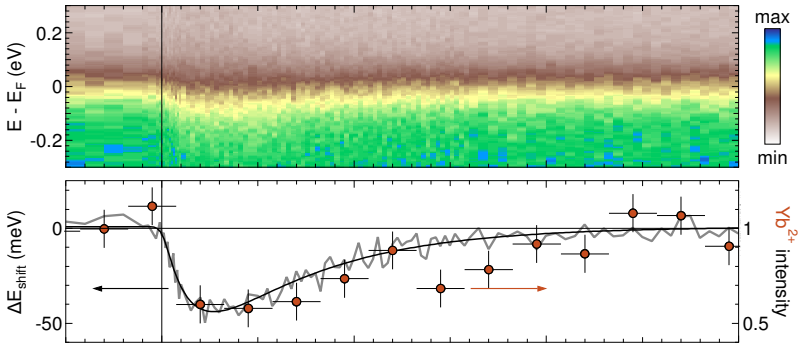


- Combination of scattering and spectroscopy reveals coupling of charge migration, chemical bonding & structure (from LCLS-II)



- High finesse experiments will reveal how charges migrates over molecules and bonds (from LCLS-II)

- Reveal materials dynamics using fs – high rep rate photo-electron spectroscopy

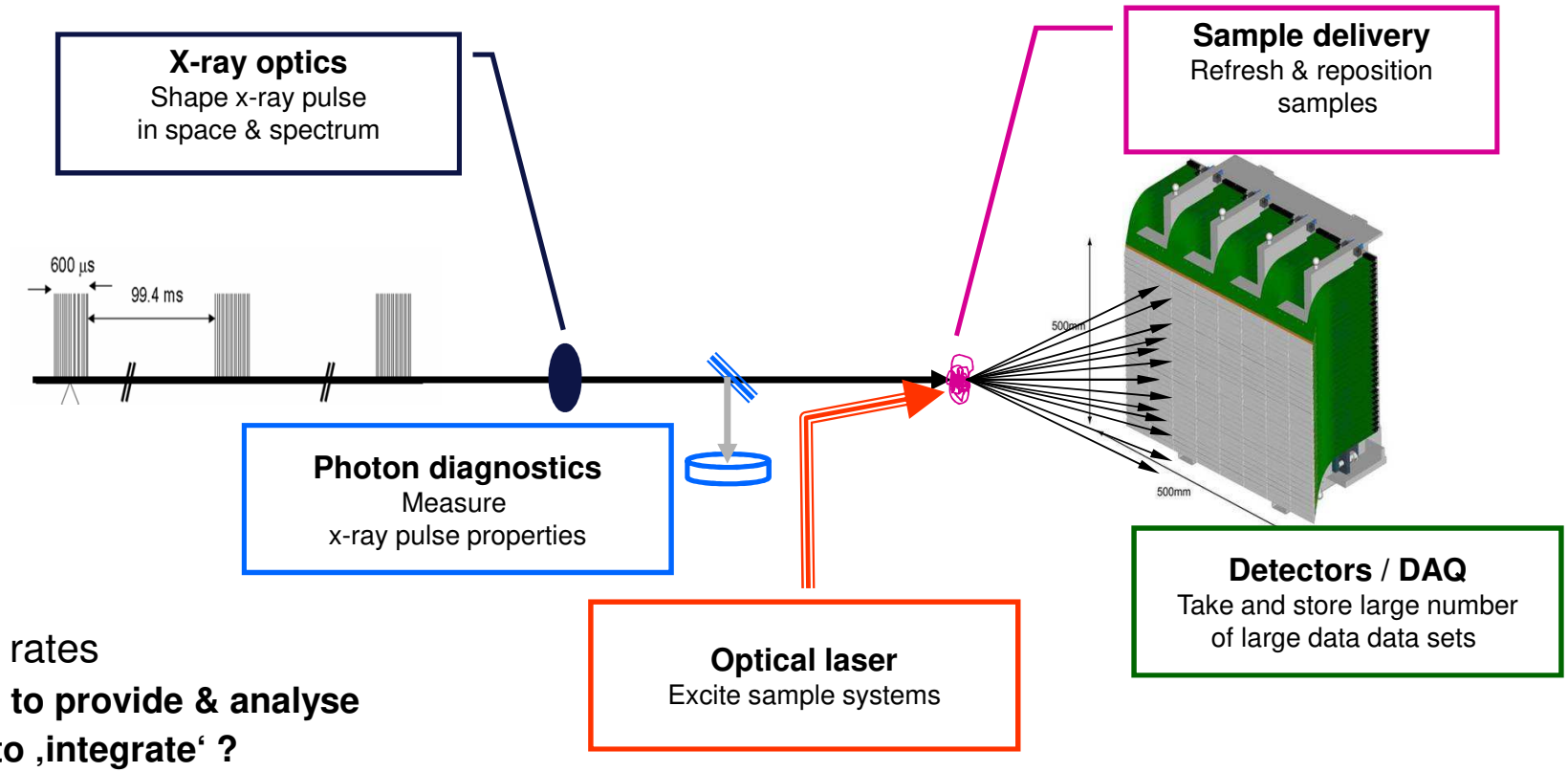


Side aspects of use of high repetition rates

- Scientifically
  - **Consider power limitations to beam transport and samples (1 mJ @ 100 kHz == 100 W !)**
  - **Not only x-ray power, but also pump source matter**
  - **Decay times or ion flight times can be very long → use rather 100 kHz than 1 MHz**
  - **Burst mode corresponds to cycling of high – low – high excitation states (no thermal equilibrium)**

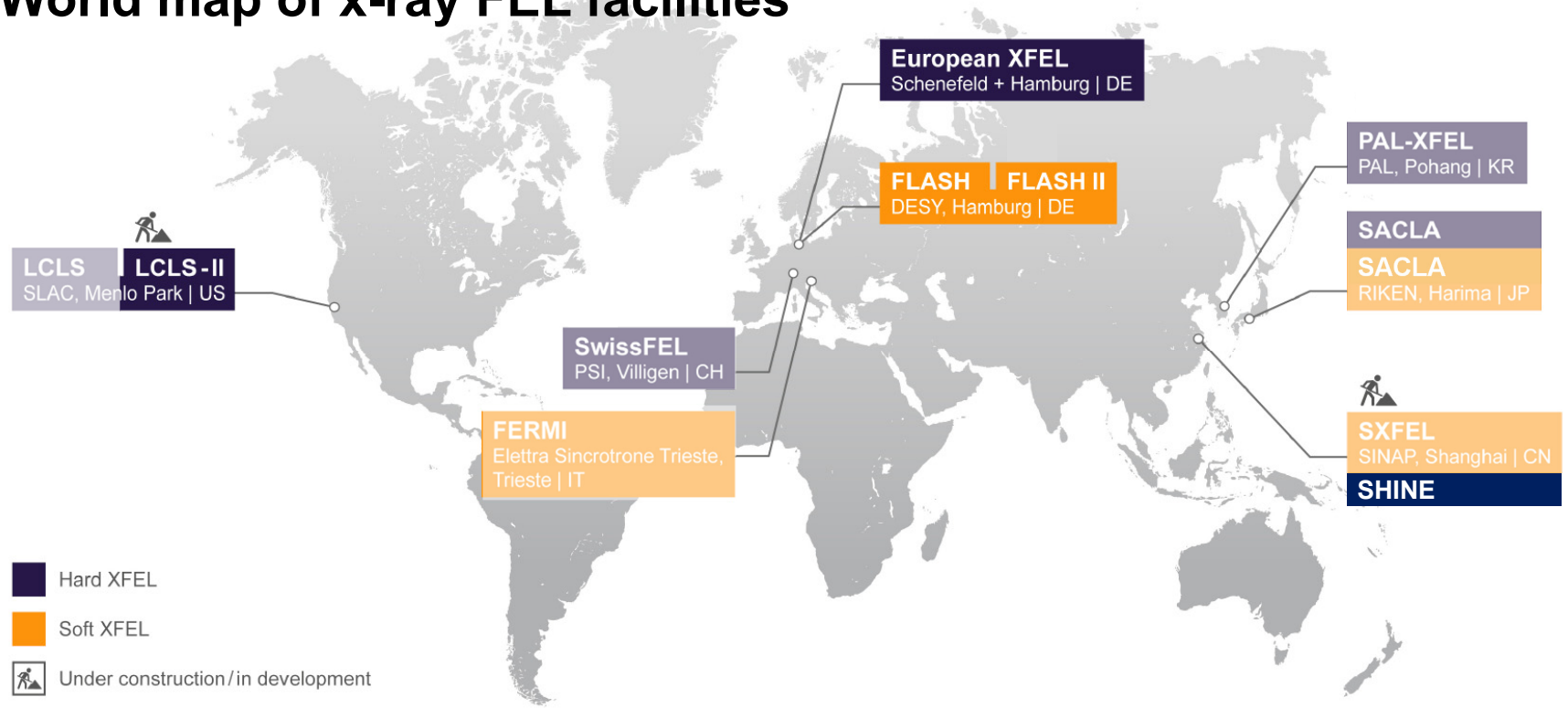
- Technically
  - **If fluctuations are critical to monitor → need diagnostics and detectors operating at high rate, too.**
  - **Pump sources (e.g. optical lasers) need to operate at high rate, too.**
  - **Power requirements/limitations for electronics and lasers**

Single shot experiments



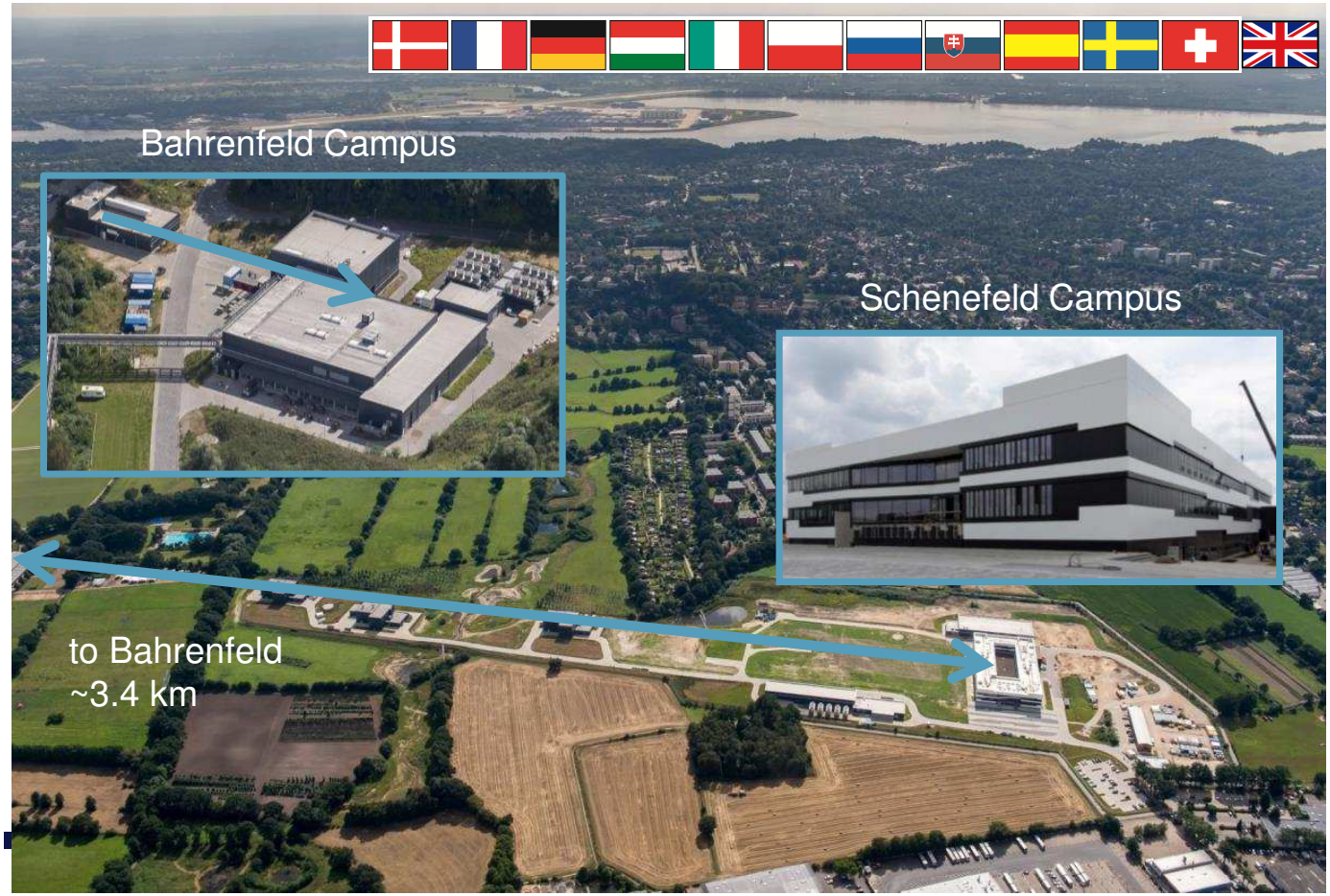
- High repetition rates
  - **Large effort to provide & analyse**
  - **Possibility to ‚integrate' ?**

World map of x-ray FEL facilities



European Strategy Forum on Research Infrastructures ESFRI

The European XFEL



- International user facility for FEL research
- Multi-disciplinary science community
- Using soft & hard X-ray FEL radiation.

Construction 2009 – 2017
Experiments starting 2017

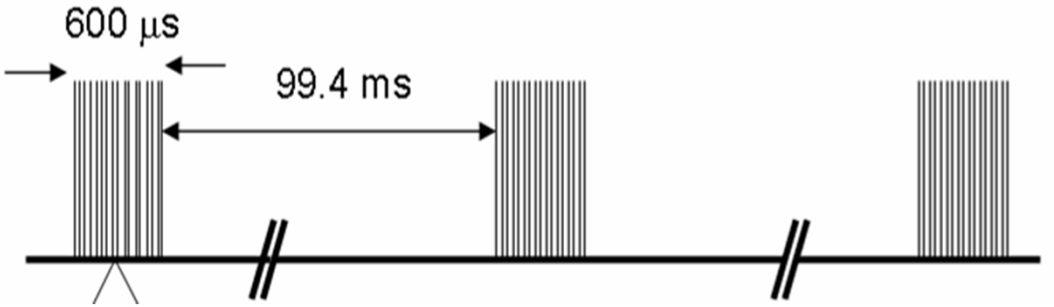
Super-conducting accelerator

- Worlds first long sc accelerator, 20 GeV, ~1000 m acc. length, 800 Nb cavities, 100 cryo-modules

Burst mode operation of European XFEL

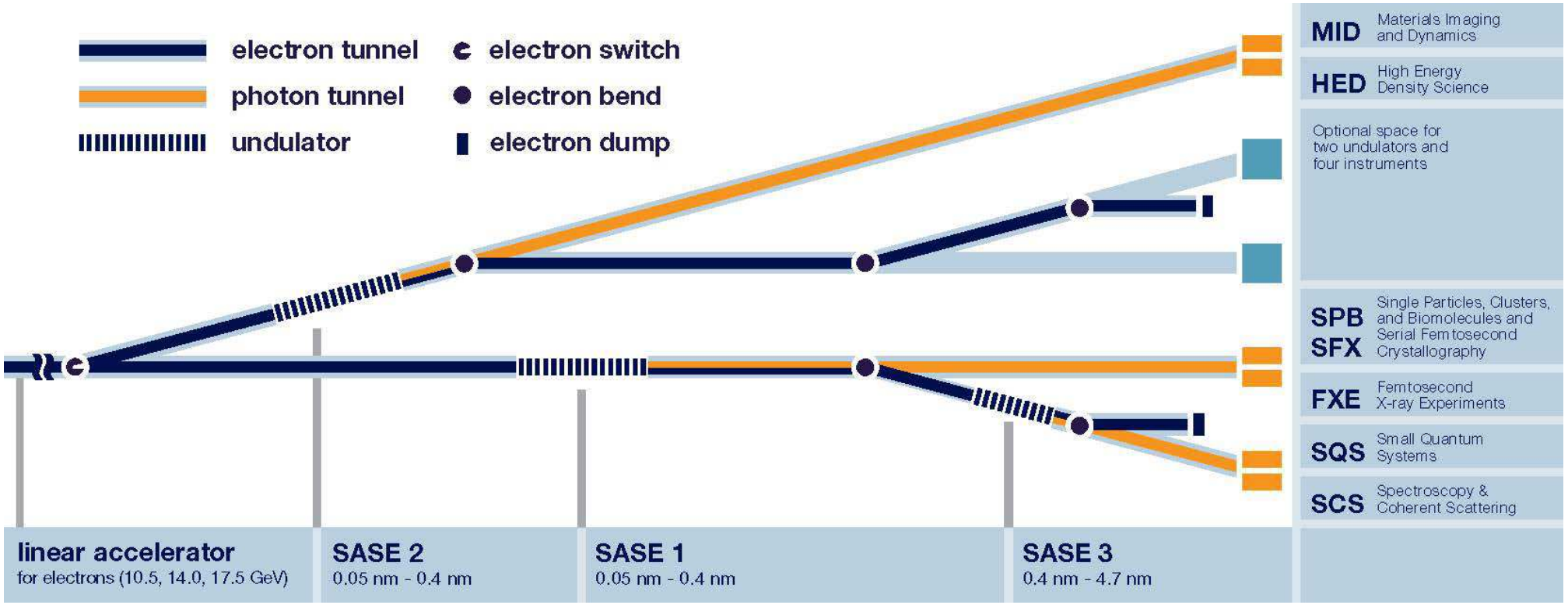
- Combination of high peak and average brilliance
  - **High peak brilliance for FEL only applications**
  - **High average brilliance to in addition enable very low cross-section experiments**
  - **Highly flexible time and beam distribution scheme**
    - ► Parallel operation of several beam lines & FELs
    - ► Dedicated pulse delivery to FELs/users
  - **Feedback → time and space stabilization**

- Background
  - **Pulsed RF system to optimize accelerated charge vs. requirements to RF & cryo power**
  - **Normal cond. injector for low-emittance e^--beams**
  - **Technology decisions 2002 - 2006**

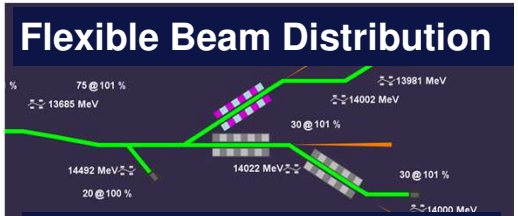


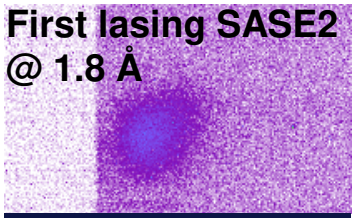
Train parameters	Value
RF fill factor	~0.0015
Repetition rate	10 Hz
In-train pulse rate	100 – 4500 kHz
Pulse separation	10 – 0.22 µs
Pulse number	1 - 2700

Beam distribution & instruments

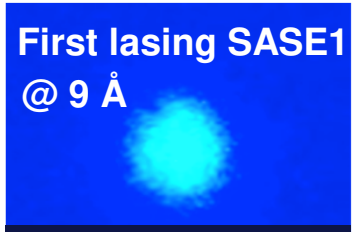


Commissioning Milestones 2017-2018

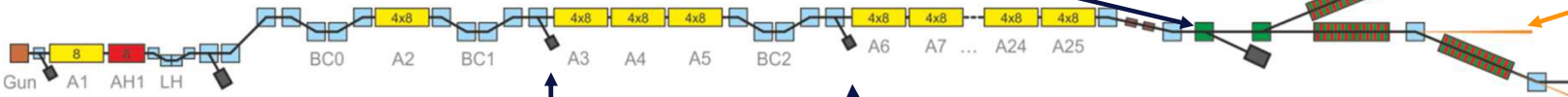




March 13, 2018



April 27, 2017



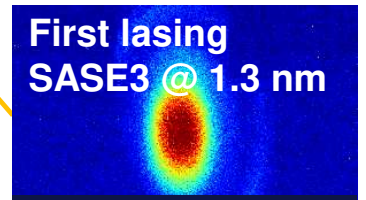
Jan 13, 2017

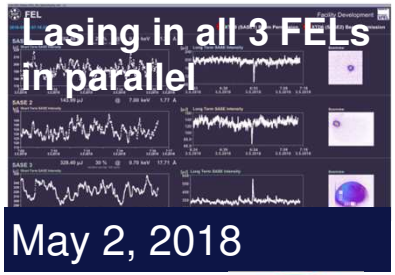
Jan 15, 2017: 130 MeV
Jan 19, 2017: 600 MeV

Feb 2, 2017: 600 MeV
Feb 22, 2017: 2.5 GeV

Feb 25, 2017: 2.5 GeV
April 8, 2017: 12 GeV
Oct 23, 2017: 14.9 GeV
July 12, 2018: 17.6 GeV

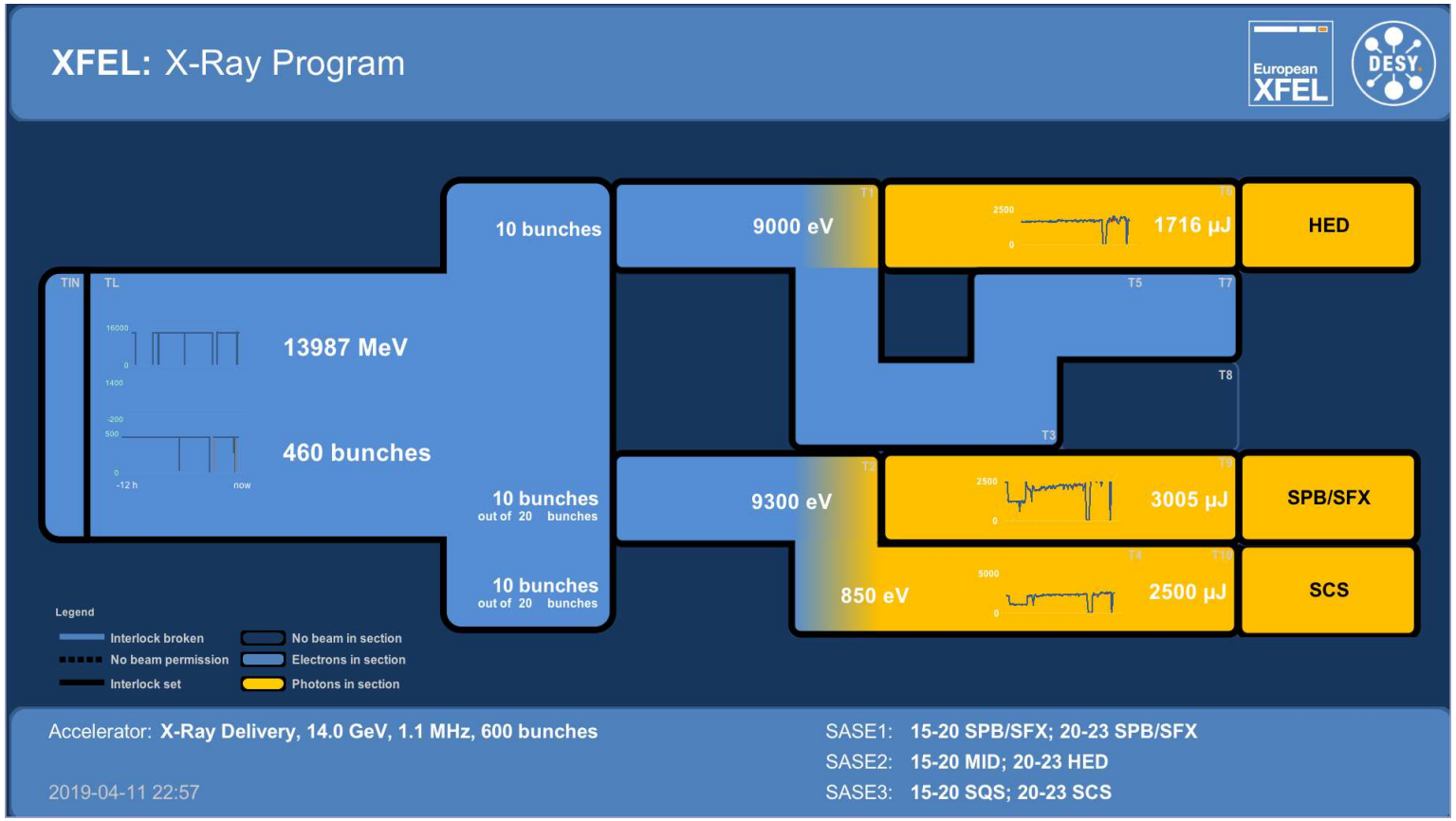
Nov 2, 2018: 2699 bunches/RF pulse

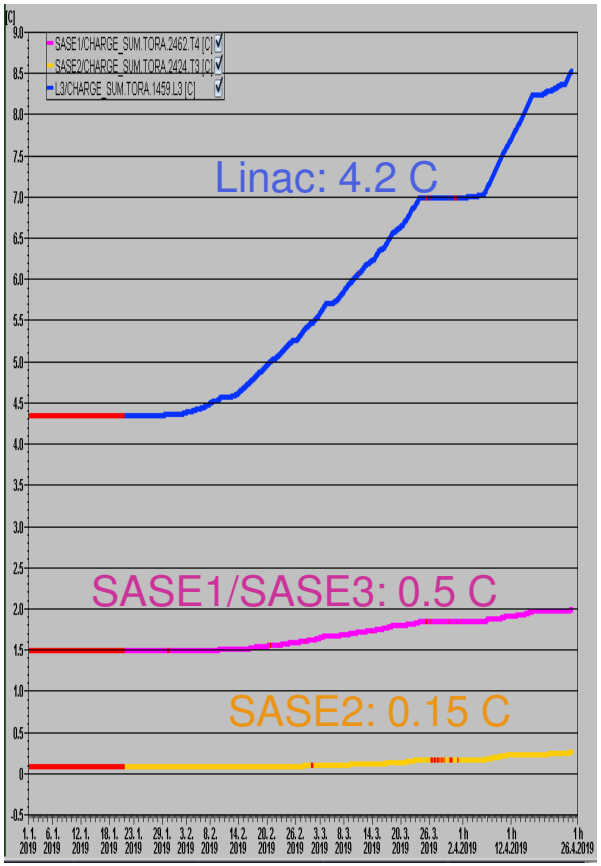




Slide by W. Decking (DESY)

Parallel operation of 3 FELs

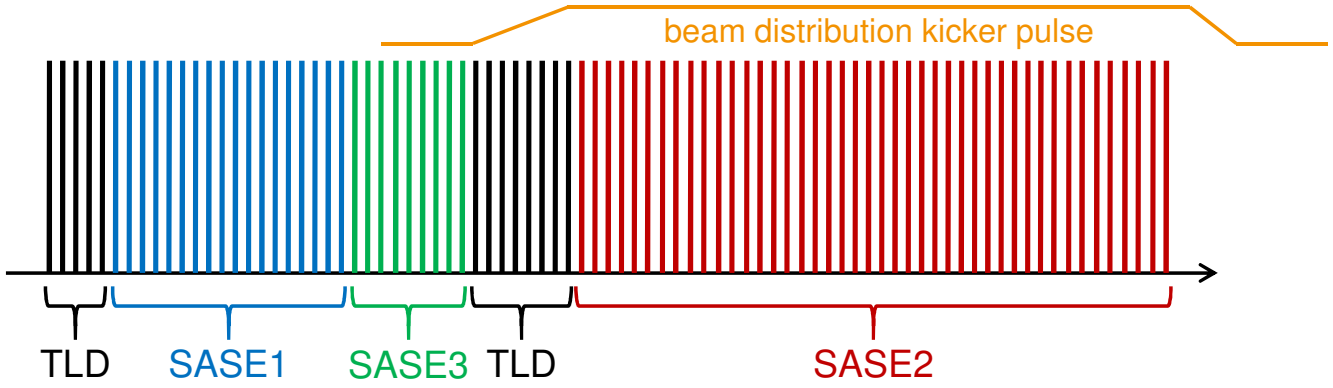


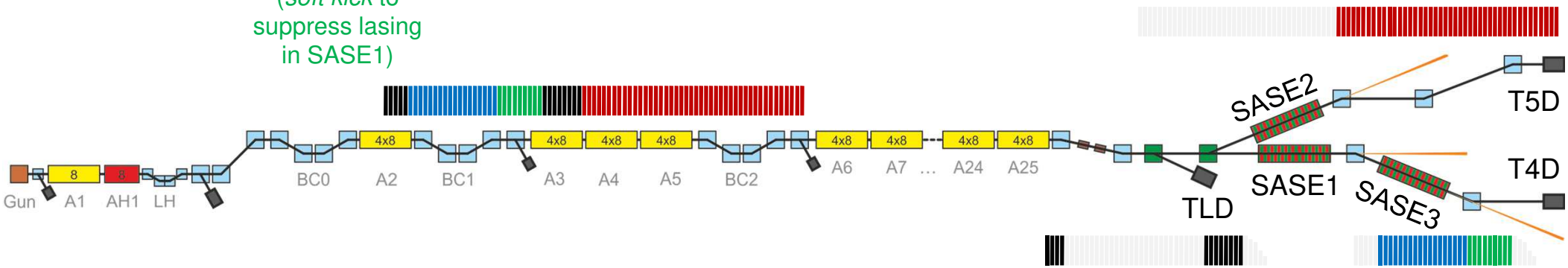


European XFEL

Jan → Apr 2019

A Typical Bunch Pattern for User Operation





Slide by L. Fröhlich (DESY)

First science examples from European XFEL

- Chemical dynamics
  - **Use high repetition rates to sample low cross-section x-ray emission from ‚real' liquids**
  - **Learn at the same time about electronic & structural dynamics following photo-excitation**

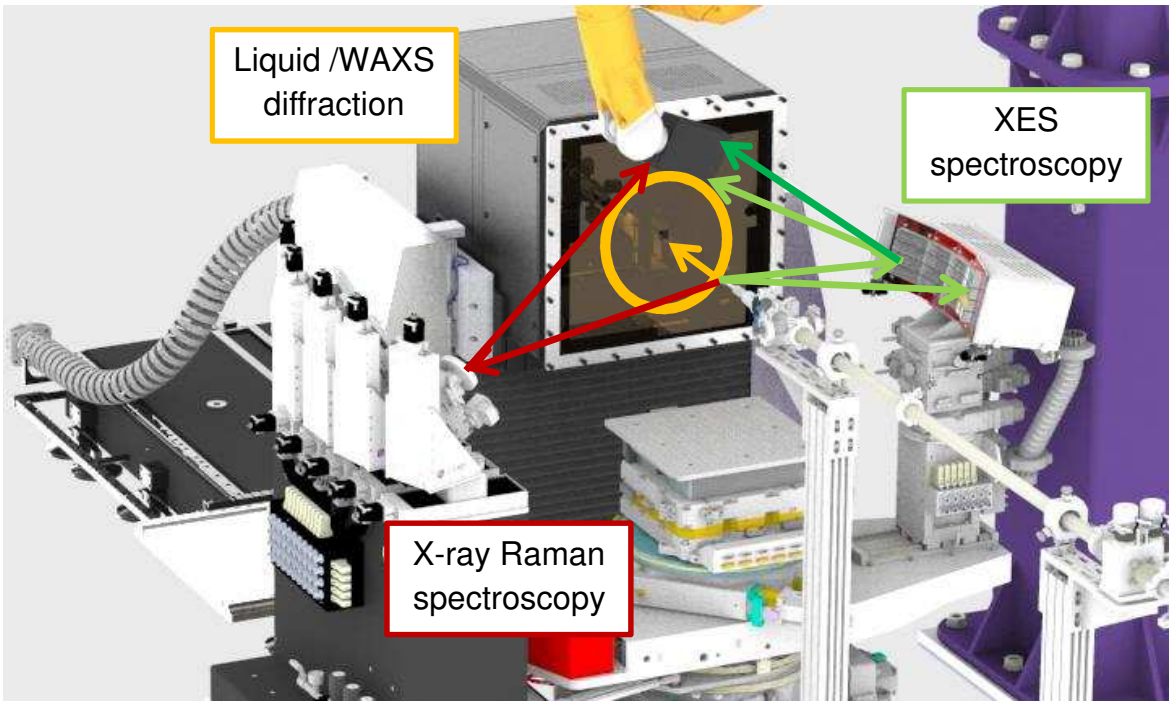
- Structural biology
  - **Take molecular movies from bio-molecules in action – a high resolution structure for every time point**
  - **Learn about structural dynamical of bio-molecules**
  - **2 examples for fs – ns and ns – ms time-scale dynamics**

  - **Sample single particle structures (Au-nanoparticles, virus particles)**

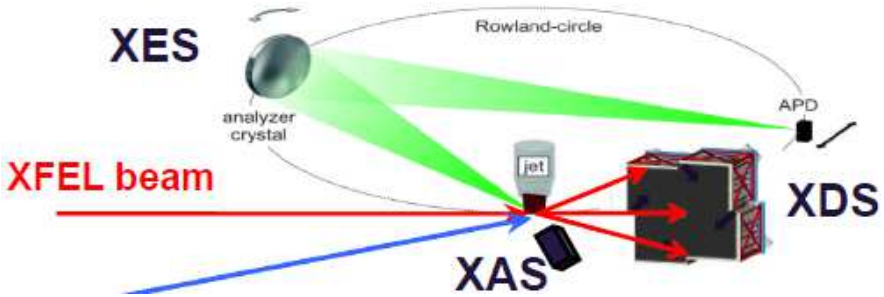
- Materials science
  - **Image real-time processes using sequence of x-ray pulses**

Chemical dynamics: combining diffraction & spectroscopy

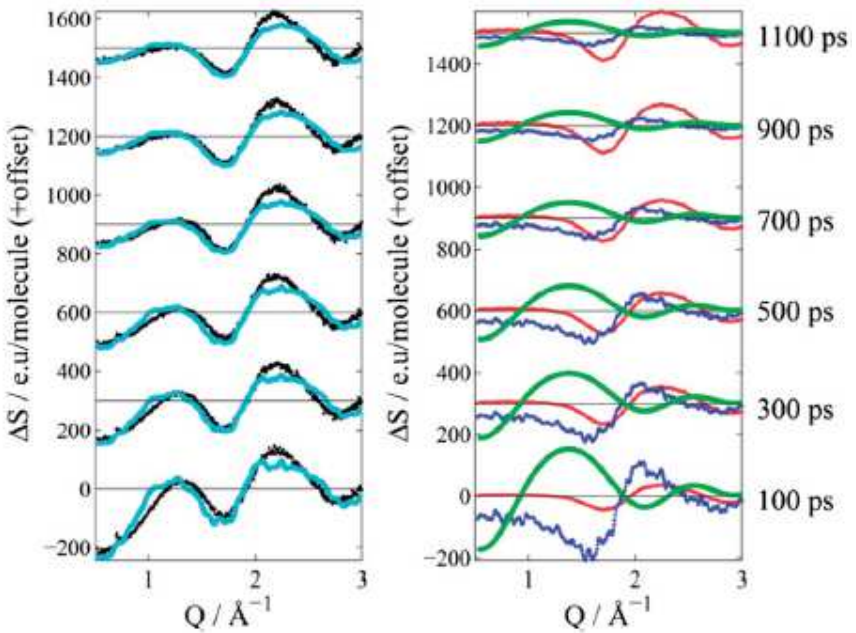
- Investigate atomic and electronic structure simultaneously

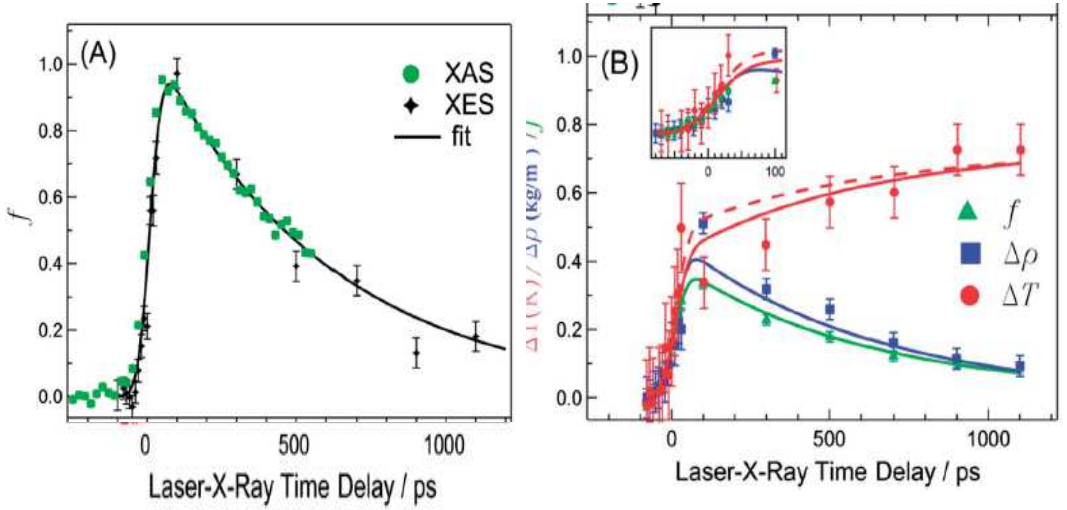


Combining diffraction & spectroscopy



- Take a complete look at solvation (dynamics)
- Use structural parameters to fix conditions in dynamic reaction

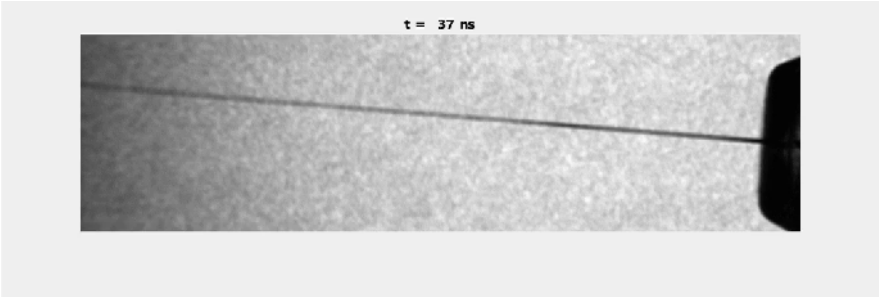




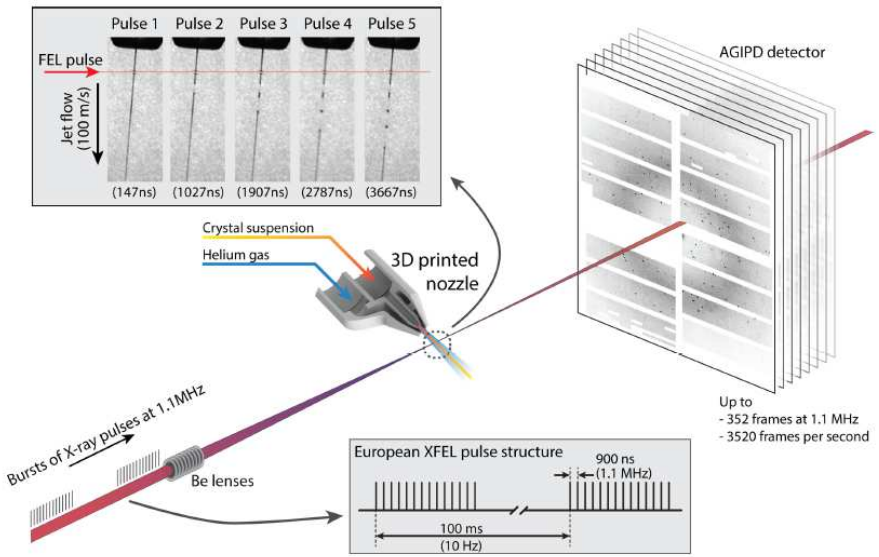
C. Bressler et al., Faraday Discuss. 171, (2014)

Structural biology – at MHz x-ray delivery ?

- Proof of serial femtosecond crystallography at MHz repetition rates
- Proposals #2012 (PI A. Barty) and #2038 (PI I. Schlichting)
- Use of high speed (~100 m/s) liquid jets



9.3 keV, ~580 µJ XFEL pulses, ~15 µm FWHM focus, 1.1 MHz rep. rate

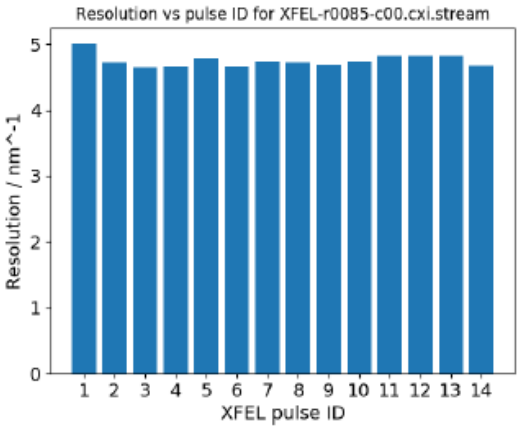


- Reduced sample consumption (very fine jet)

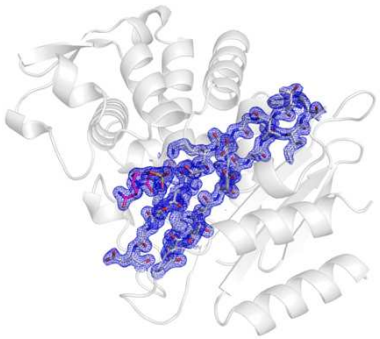
All figures: M. Wiedorn, …, A. Barty, Nat. Comm. 9:4025 (2018)

MHz serial femtosecond crystallography

- Both experiments were highly successful
- Obtaining high quality structures
- Establishing data exchange and data analysis chain

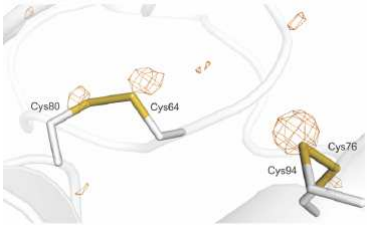


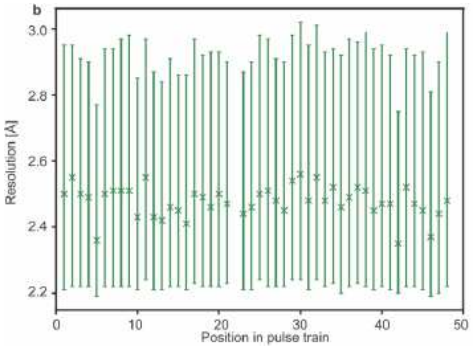
ß-lactamase
(1.7 Å res.)



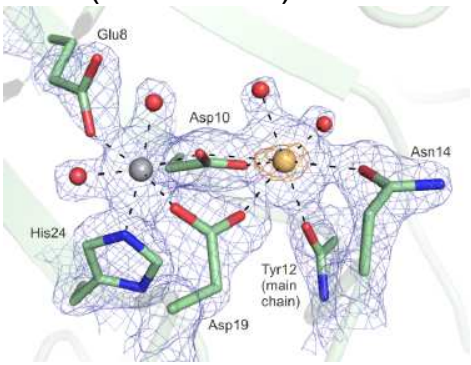
M. Wiedorn, …, A. Barty,
Nat. Comm. 9:4025 (2018)

Lysozyme
(2.2 Å res.)





Concavalin A
(2.1 Å res.)



M. Grünbein, …, I. Schlichting,
Nat. Comm. 9:3478 (2018)

Acknowledgements-I: The XFEL Accelerator Consortium

Acknowledgements-II: The European XFEL staff

Acknowledgements-III: Additional contributions

- SFX & XBI User Consortia (enabling SPB/SFX experiments)
- HIBEF User Consortium (contributing to HED instrument)

First experiments at European XFEL science instruments


SPB/SFX, Sep 2017


FXE, Sep 2017


SCS, Dec 2018


SQS, Dec 2018


MID, Mar 2019


HED, May 2019

Summary

- European XFEL started successfully its operation phase
- First papers have been published and several more are under preparation
- All science instruments are in operation
- High repetition rate x-ray delivery has been utilized and its exploitation is continously developed

Thank you for your attention