European XFEL

Enlightening Science

Antonio Bonucci

Industrial Liaison Office

In-Kind Contribution Supply Chain Manager

Outline

- General information about European XFEL
- How it works: the main parts
- The Industrial Liaison Office: new approach for innovation
- Program for next years
  - Beamline layout & experiment stations: the finalization of the construction
  - Cutting edge technology: data management, detectors, laser, sample environment,
- Call for tender: basic indications and references.

European XFEL—a leading new research facility

Schenefeld research campus on 14 August 2017

- The European XFEL is a new research facility that uses high-intensity X-ray light to study the structure of matter.
  - User facility with more than 350 employees (+250 from DESY)
  - Location: Hamburg and Schenefeld, Germany
  - September 2017 start of user operation

About European XFEL

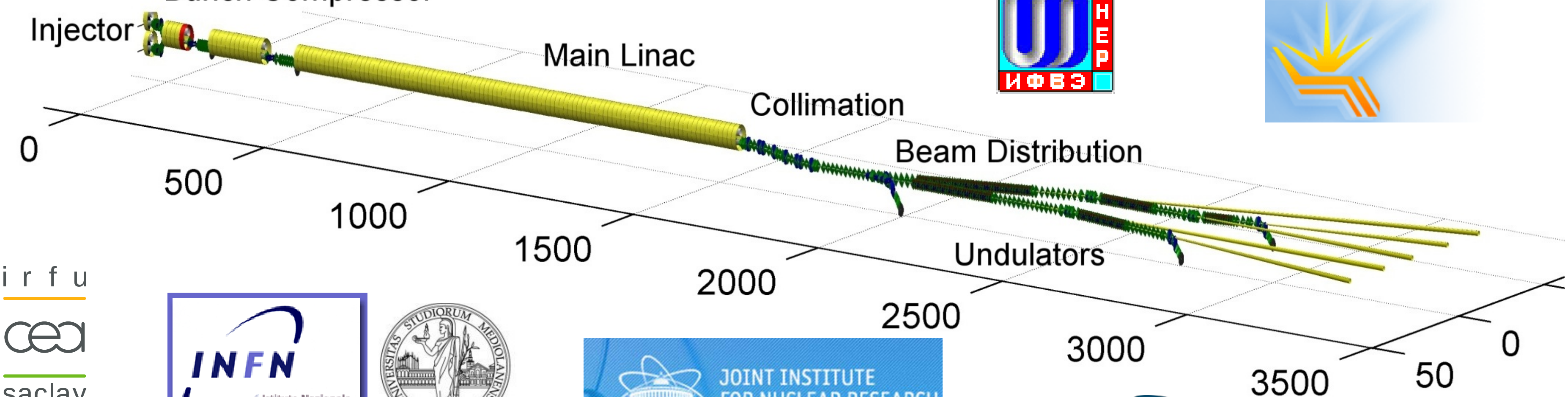
- Organized as a non-profit corporation in 2009 with the mission of design, construction, operation, and development of the free-electron laser
- Supported by 12 partner countries
- Germany (federal government, city-state of Hamburg, and state of Schleswig-Holstein) covers 57% of the costs; Russia contributes 26%; each of the other international shareholders 1–3%
- Total budget for construction (including commissioning)
  - 1.25 billion € at 2005 prices, about 117 M€ operating budget
  - 600 M€ contributed in cash, over 550 M€ as in-kind contributions (mainly manufacture of parts for the facility)

DESY and European XFEL—strong partners

- DESY is European XFEL‘s largest shareholder
- Facility concept developed at DESY
  - FLASH user facility, opened to users in 2005
- DESY and European XFEL collaborate on construction, commissioning, and operation of X-ray free-electron laser
  - DESY built the European XFEL accelerator alongside international partners and is responsible for the technical operation of the accelerator

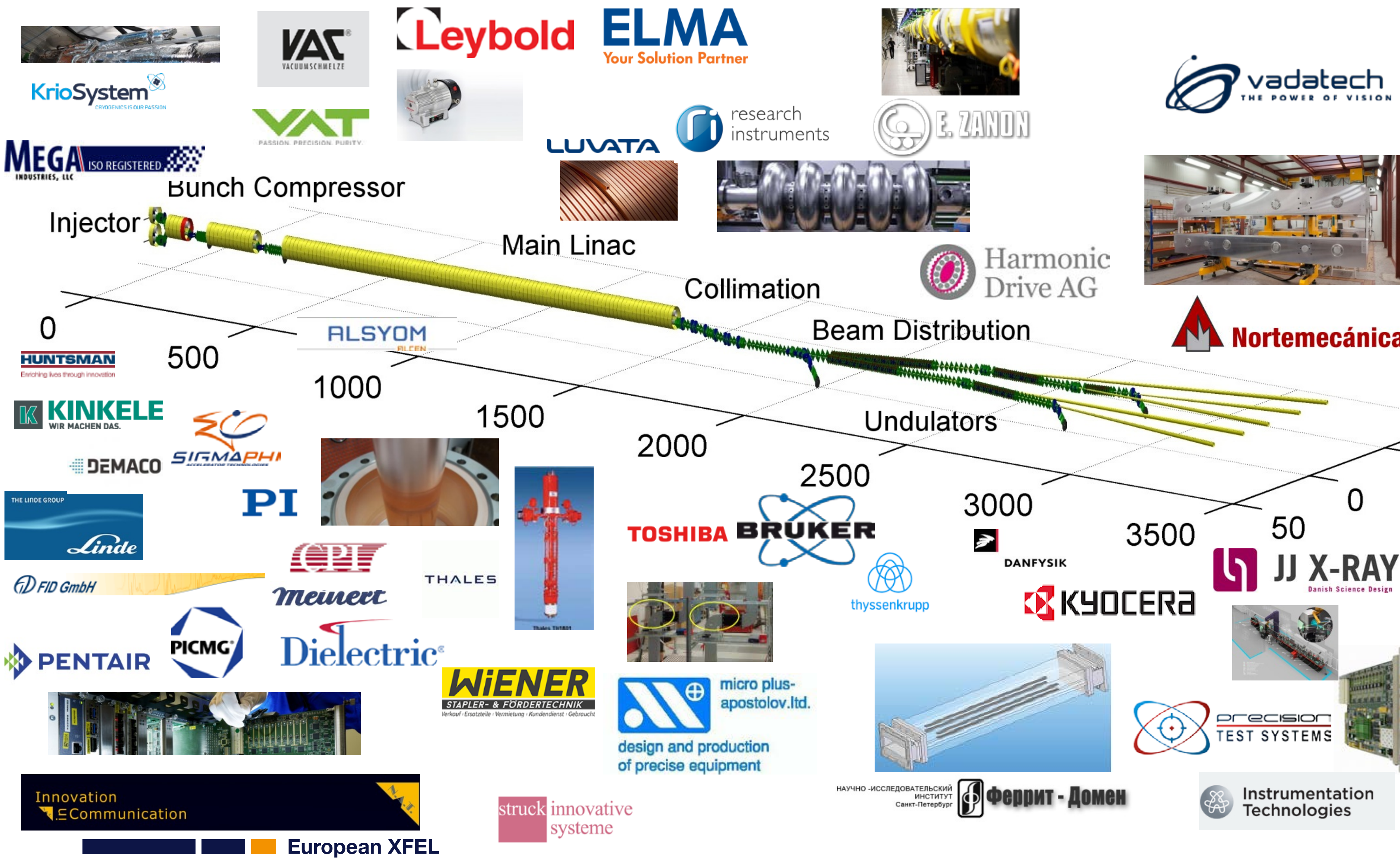
Institutes contributing in-kind to the construction

DESY
KTH VETENSKAP OCH KONST
Stockholm University
FYSIKUM
UPPSALA UNIVERSITET
IHEP ИФВЭ

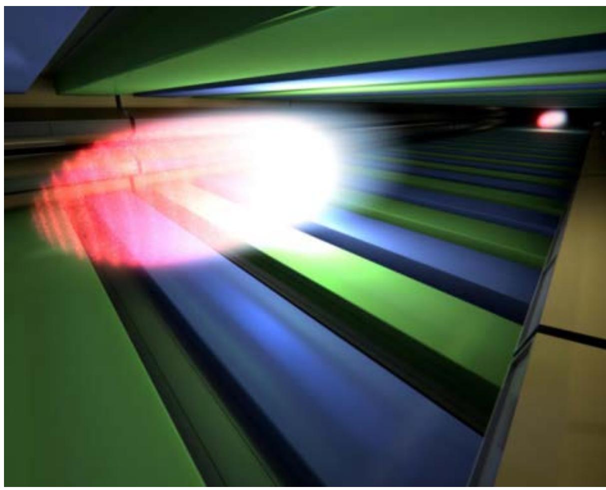


irfu cea saclay
INFN Istituto Nazionale di Fisica Nucleare
UNIVERSITAS STUDIORUM MEDIOLANENSIS
JOINT INSTITUTE FOR NUCLEAR RESEARCH
PAUL SCHERRER INSTITUT PSI
cnrs In2p3
ncbj
Wrocław University of Technology
MINISTERIO DE EDUCACIÓN Y CIENCIA
Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas
UNIVERSIDAD POLITECNICA MADRID
DTU Technical University of Denmark

Companies contributing in-kind to the construction



What can the European XFEL do?

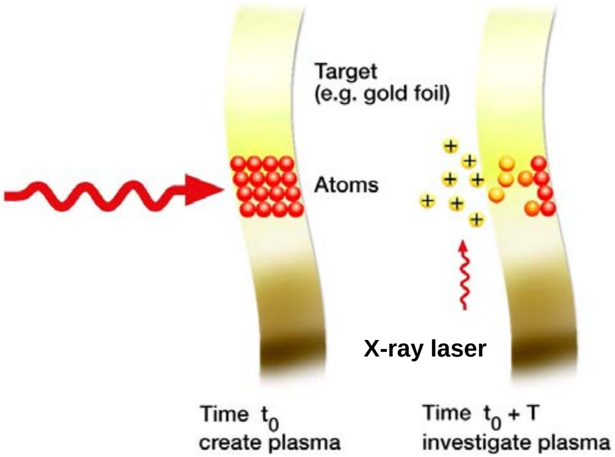


X-ray light
See samples at atomic resolution

Ultrashort flashes
Film (bio-)chemical reactions

Intense X-ray pulses
Study single molecules or tiny crystals

…and under extreme conditions

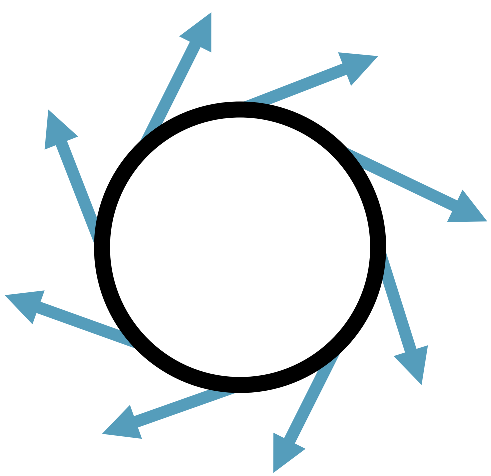


- Can generate high-energy plasmas at high pressures and densities for analysis with X-ray laser
- Plasmas with properties similar to the cores of large planets, such as Jupiter

Using X-rays to explore matter

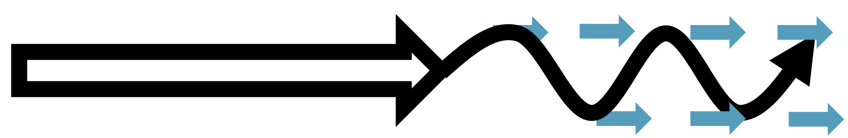
Synchrotrons

- Electrons traveling in a wide circular path, emitting light as they change directions
- Light is UV or X-ray, but not coherent



Free-Electron Lasers

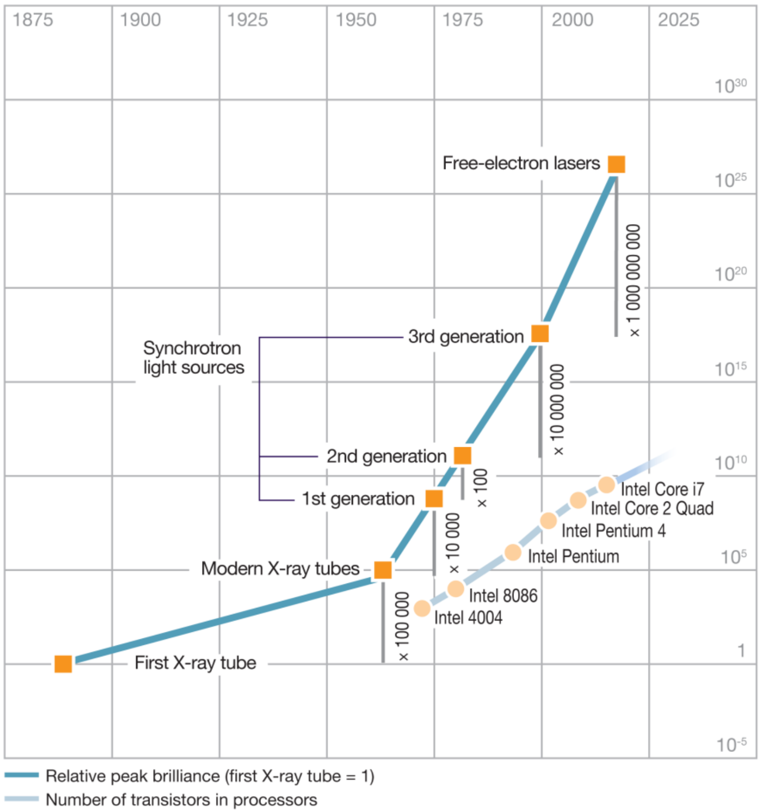
- Electrons accelerated in a straight line and manipulated to generate light
- Light is coherent and intensely bright in very short pulses, showing objects in even more detail and revealing processes



X-ray free-electron lasers worldwide

The European XFEL will put Europe in the lead among industrialized nations in a highly competitive scientific and technical environment.

Free-electron lasers worldwide in comparison



- The peak brilliance of X-ray free-electron lasers exceeds that of the most modern synchrotron radiation sources by several orders of magnitude
- The European XFEL will be capable of generating more pulses per second and more intense X-rays than any other X-ray free-electron laser in the world.

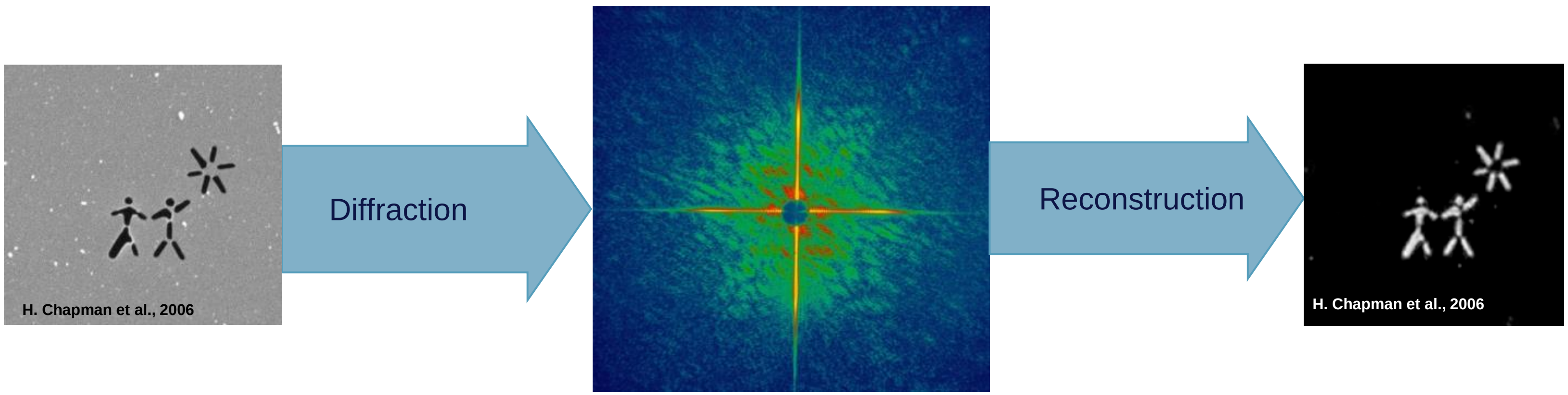
X-ray free-electron lasers worldwide

Project	LCLS (USA)	LCLS-II CuRF	LCLS-II SCRF	SACLA (Japan)	SwissFEL (CH)	PAL-XFEL (S. Korea)	FERMI (Italy)	European XFEL
Max. electron energy (GeV)	14.3	15	4.5	8.5	5.8	10	1.55	17.5
Wavelength range (nm)	0.1–4.6	0.05–1.23	0.25–6	0.06–0.3	0.1–7	0.06–10	4-100	0.05–4.7
Photons/pulse	~10^{12}	2 x 10^{13}	3 x10^{13} (soft Xrays)	2 x 10^{11}	~5 x 10^{11}	10^{11}–10^{13}	10^{11} -10^{14}	~10^{12}
Peak brilliance	2 x 10^{33}	2 x 10^{33}	1 x 10^{32}	1 x 10^{33}	1 x 10^{33}	1.3 x 10^{33}	10^{30} -10^{32}	5 x 10^{33}
Pulses/second	120	120	10^{6}	60	100	60	10-50	**27 000**
Date of first beam	**2009**	**2020**	**2020**	**2011**	**2016**	**2016**	**2010**	**2017**

Data of Fermi were kindly shared by Dr. Peloi by personal communication.

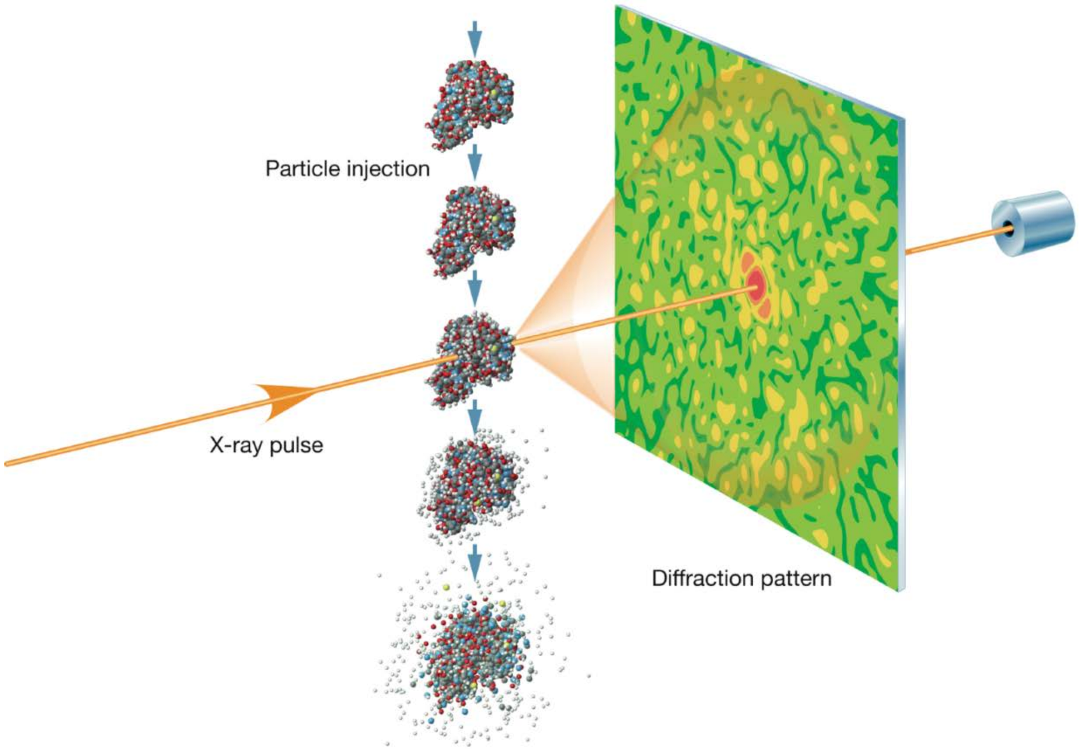
Making pictures without a camera lens

- Crystallography method developed by Laue and Bragg, 1912–1914
- Similar method used in X-ray FELs



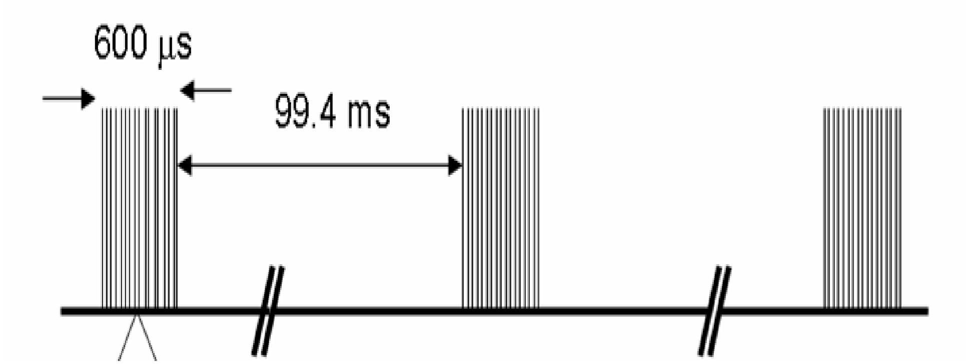
- X-rays scatter (diffract) off objects (1, microscopic shapes cut from metal)
- Detectors record the scattered X-rays (2, diffraction pattern)
- Original shapes reconstructed in high detail from detector data (3, reconstructed image)

Making pictures without a camera lens



- Samples injected as liquids into vacuum chamber
- X-ray pulse hits sample and diffracts onto detector
- Sample is destroyed, but diffraction pattern is recorded beforehand

More flashes = faster experiments



- The European XFEL can produce 27 000 X-ray laser flashes per second
- Experiments formerly worked with max 120 flashes per second
- Bunch trains: 4.5 MHz total repetition rate
- Means more detector data at a faster frame rate—faster experiments than before

Opportunities: biology, medicine, pharmacology

- Molecular movies reveal biochemical processes
  - Causes of protein misfolding → treatments for Alzheimer’s, BSE, etc.
  - Understanding enzymatic action in greater detail → better medicines, fewer side effects
  - Viewing mechanisms of infection

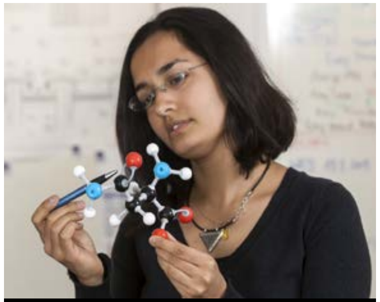
- High intensity X-rays show structures in greater detail
  - Searching for weaknesses in viral and bacterial outer coats

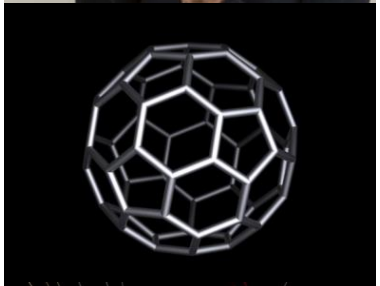


Opportunities: ultra fast phenomena

- Atomic-level imaging can uncover action of catalysts
  - Better catalytic converters lessen impact of emissions
  - Less toxic production processes

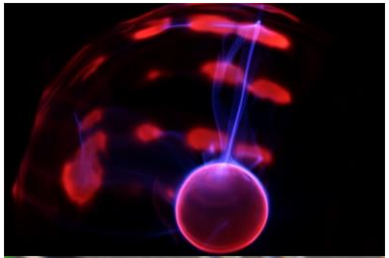
- Studying structure and properties of materials as never before
  - How properties (e.g. durability, conductivity, magnetism) manifest
  - Reducing atoms needed to store digital information → ultrahigh-capacity hard drives

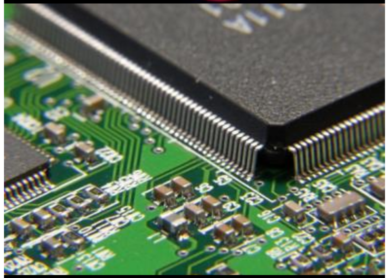




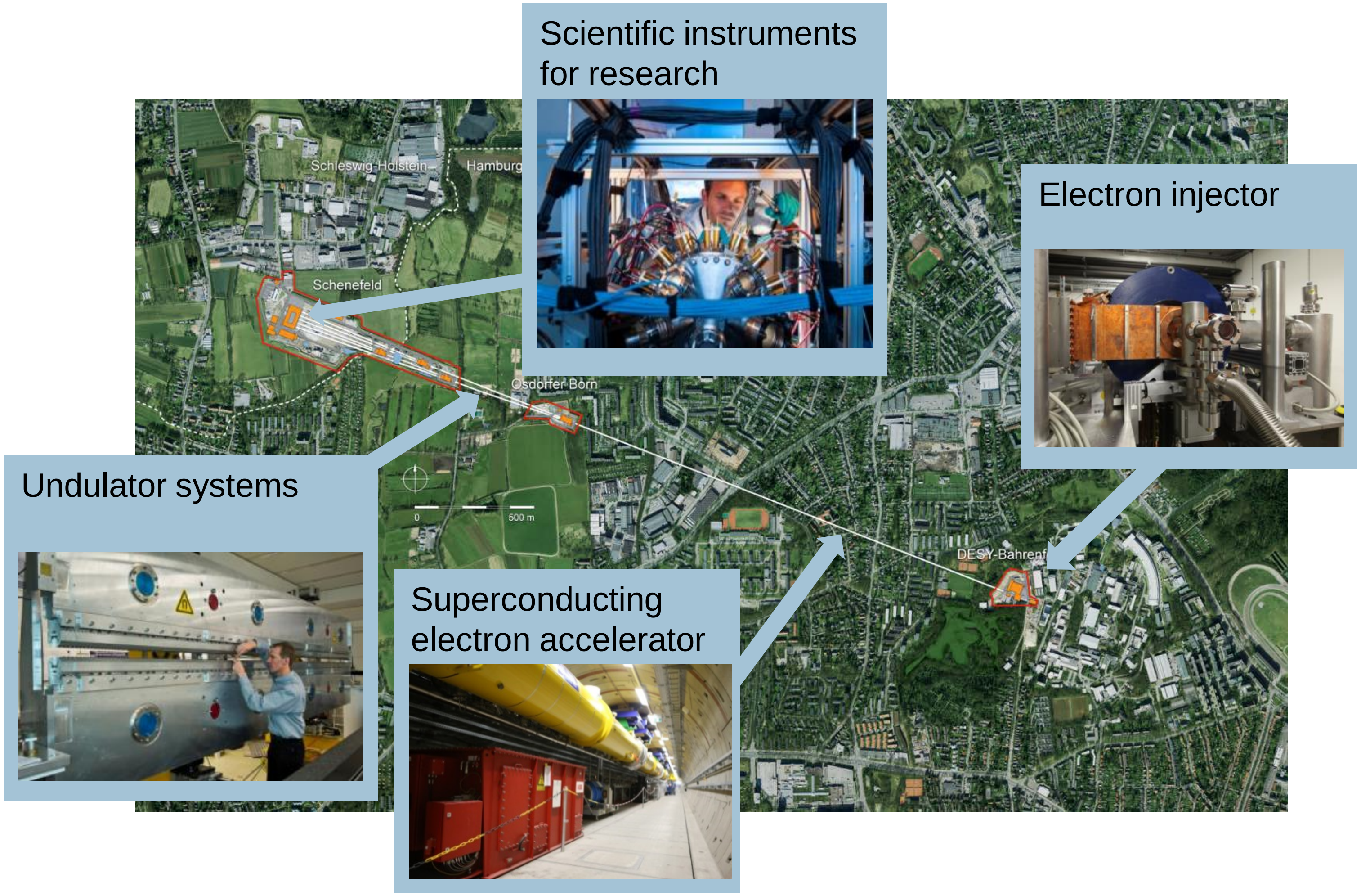
Opportunities: physics and astrophysics

- New details of physical processes
  - New understanding of states of matter and their transitions
  - Next-generation processors
- Quantum world in action
  - Better linking physical phenomena to atomic and subatomic activity
- Extreme states of matter
  - Studying conditions inside gas giants without ever leaving Earth

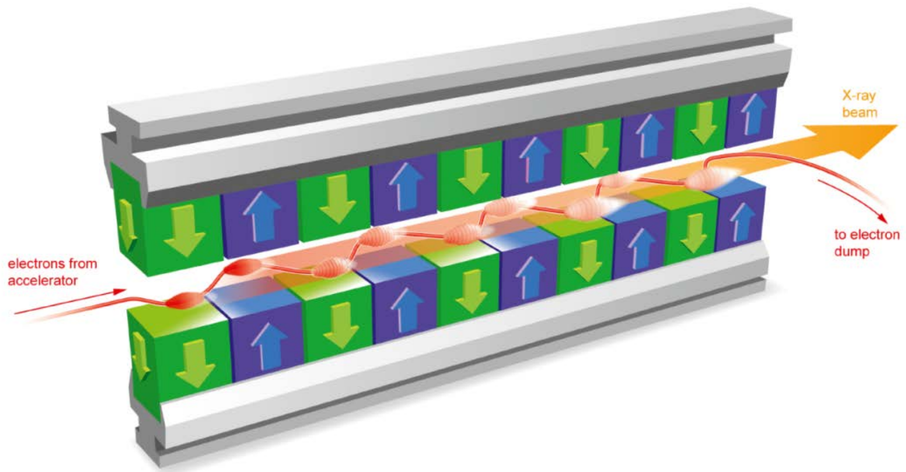




How it works: a closer look at the facility



SASE undulators: inducing electrons to emit X-ray light



- Alternating magnetic fields cause electrons to take “slalom” course
- Electrons release X-rays with each turn
- SASE process builds intense, laser-like flashes

ILO

In order to implement the targets of the vision, three main ways have been identified:

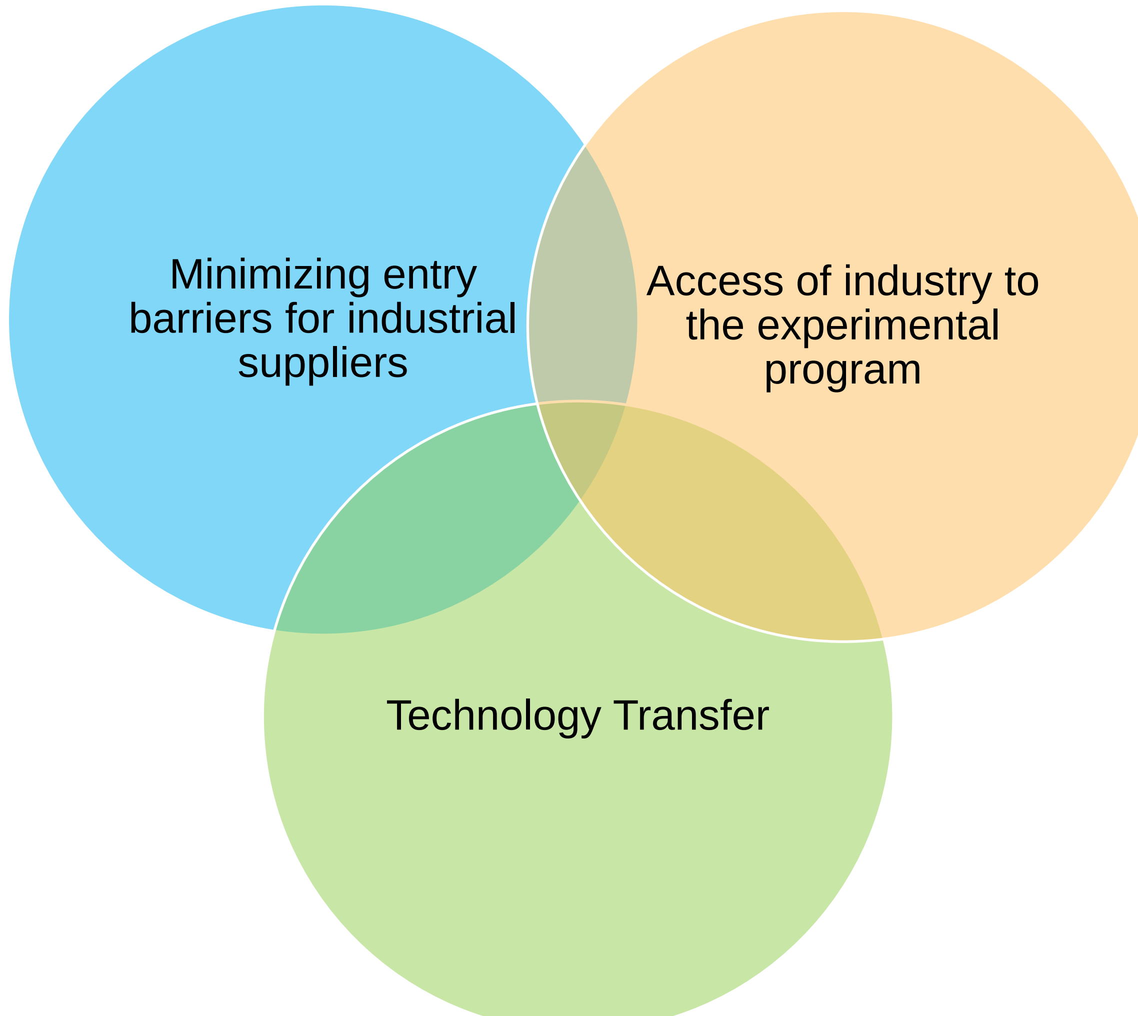
- Access of industry to the experimental program, to the lab facilities and knowledge
- Minimizing entry barriers for industrial suppliers increasing the competition in the tender procedures in particular for cutting-edge components and challenging specifications
- Technology Transfer

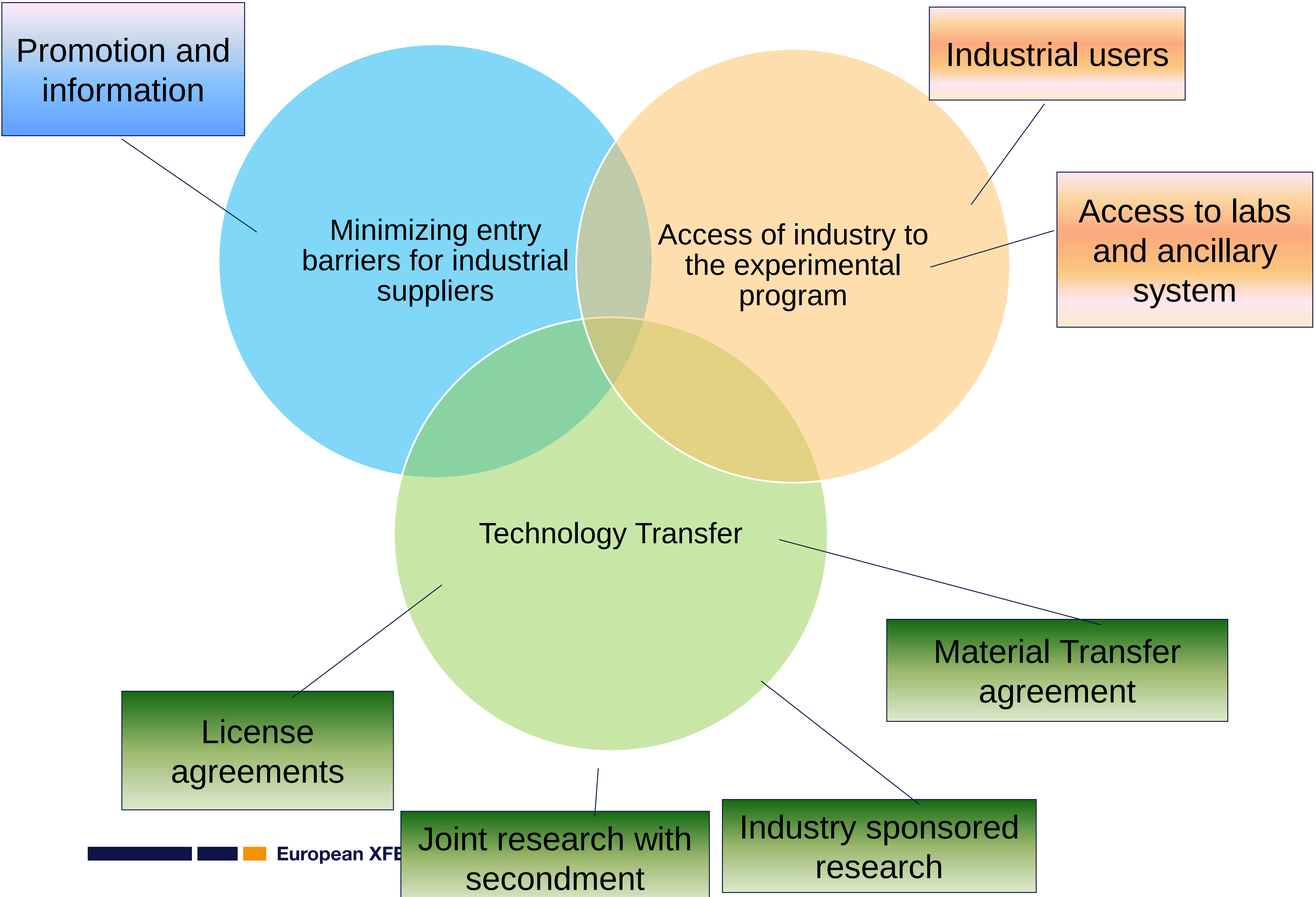
and

- Measuring, monitoring, reporting the impact

Industrial Liaison Office
Impact in industrial innovation context

Antonio Bonucci
Rebecca Jones-Krüger




Promotion and information
Minimizing entry barriers for industrial suppliers
Industrial users
Access of industry to the experimental program
Access to labs and ancillary system
Technology Transfer
Material Transfer agreement
License agreements
Joint research with secondment
Industry sponsored research

Technology Transfer: Open Science/Innovation Model example of the construction phase

The main goal of the technology transfer is to maximize the impact of our internal development in the innovation context

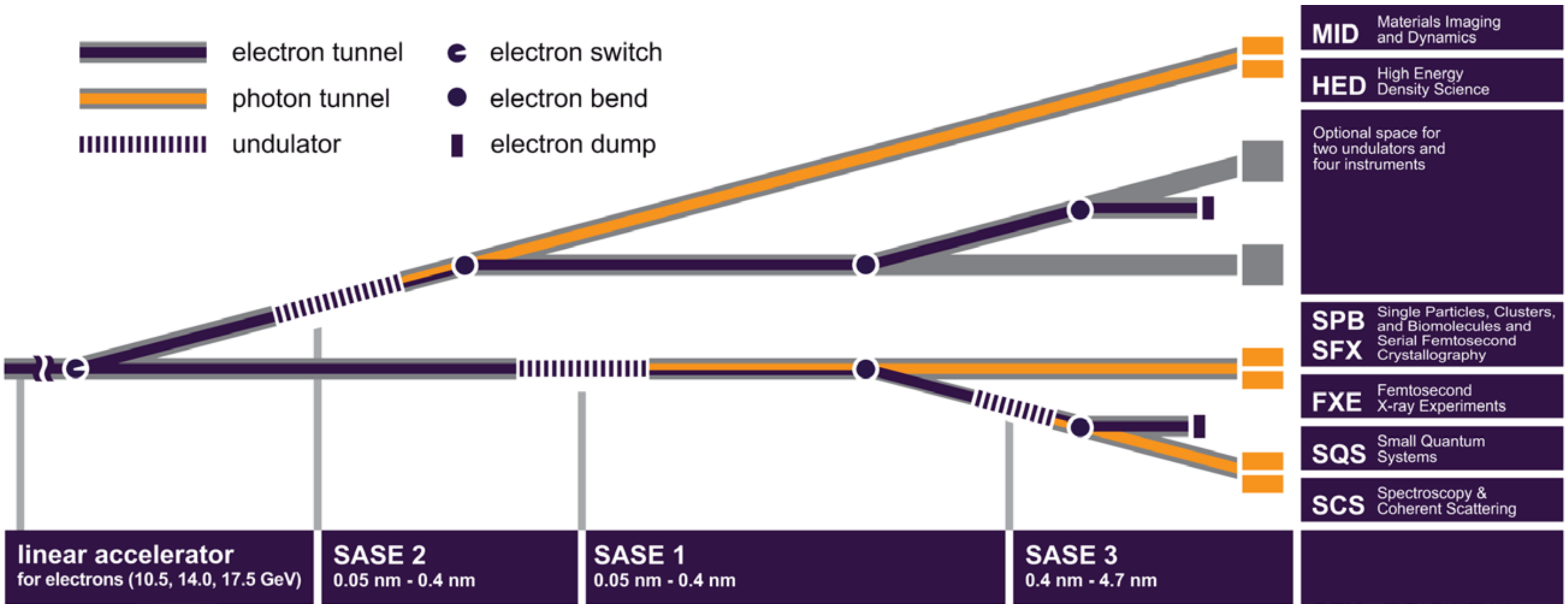
During the construction, we had already such a impact, that we can summarize at the following levels:

- **Specification:** if we provided only challenging specification to be achieved
- **Conceptual design:** If we has provided the conceptual design, including results of simulation for the main parameter or dimension
- **Technical Drawings:** if we have provided the 3d model/ general drawings, but the details were improved by the industry
- **Detailed Drawings:** if we have provided the detail drawings, but the industry has improved them and did fabrication drawings, oriented to the production
- **Production:** If we have provided everything and has taken advantage from the expertise of mass production of the industry

Program for next years

- The annual budget for the operation for next years is estimated about 117 Mio.€
- The investment on capital assets for next 5 years will be about 100-120 Mio. €: IT (data management and advanced electronics) and detectors and diagnostic will be the main areas. Sample environment, X-ray Optics, Optical laser are also relevant.
- All together the XFEL has 5 Tunnels (called SASE). XFEL started its first user operations on the 2nd of September 2017 with the first tunnel, called SASE 1, SASE 2 & 3 are in operation. SASE 4 & 5 is still to be completed in a future project.
- The campus is developing with:
  - a campus restaurant (canteen) has been recently inaugurated ,
  - a guesthouse is planned and construction will start soon,
  - 2 more construction projects are waiting to be finalized:
    - ► the High-BEF building
    - ► the visitors centre.

Beamline layout & experiment stations



Scientific instruments—Hard X-ray

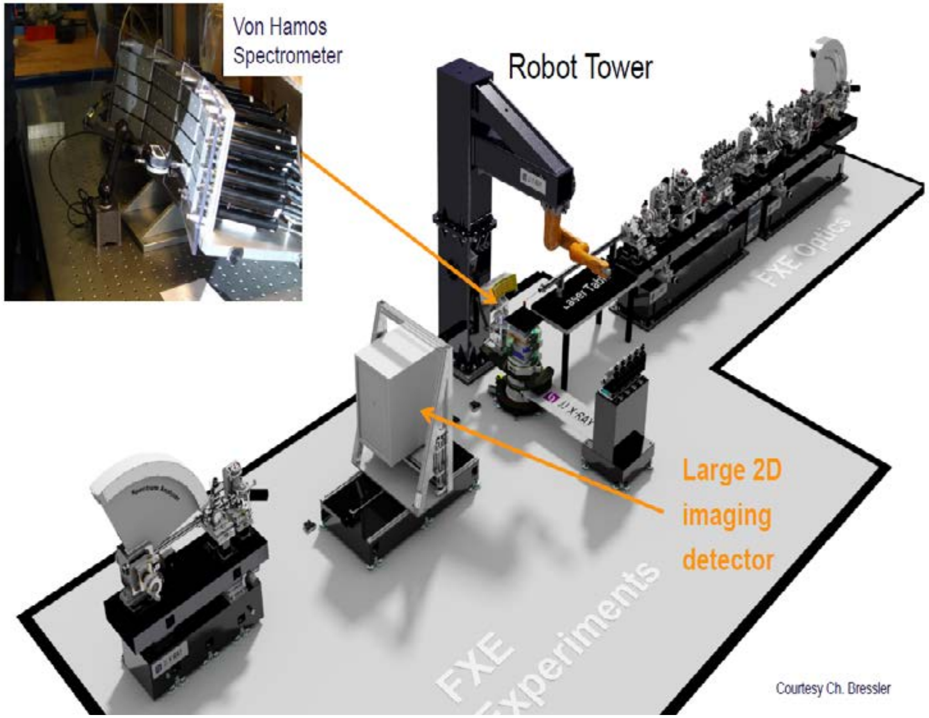
- SPB/SFX
  - Will determine the structure of single particles, such as atomic clusters, viruses, and biomolecules
- MID
  - Will be able to image and analyze nano-sized devices and materials used in engineering
- FXE
  - Will investigate chemical reactions at the atomic scale at short time scales—molecular movies
- HED
  - Will look into some of the most extreme states of matter in the universe, such as the conditions at the centre of planets

Scientific instruments—Soft X-ray

- SQS
  - Will examine the quantum mechanical properties of atoms and molecules
- SCS
  - Will determine the structure and properties of large, complex molecules and nano-sized structures

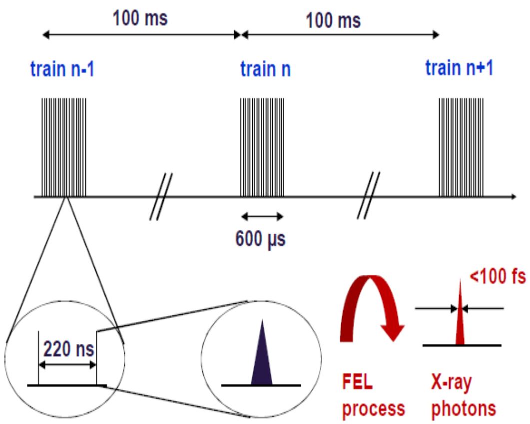
Data Management Challenges

- Aggregate and record large volumes of data during experiments
- Provide deep insight into the data during experiment
- Organize and manage data in a coherent way
- Enable users to analyze experiment data when back at home institute



DAQ Challenges

- Readout rate driven by bunch structure
  - 10 Hz train of pulses
  - 4.5 MHz pulses in train
- Data volume driven by detector type

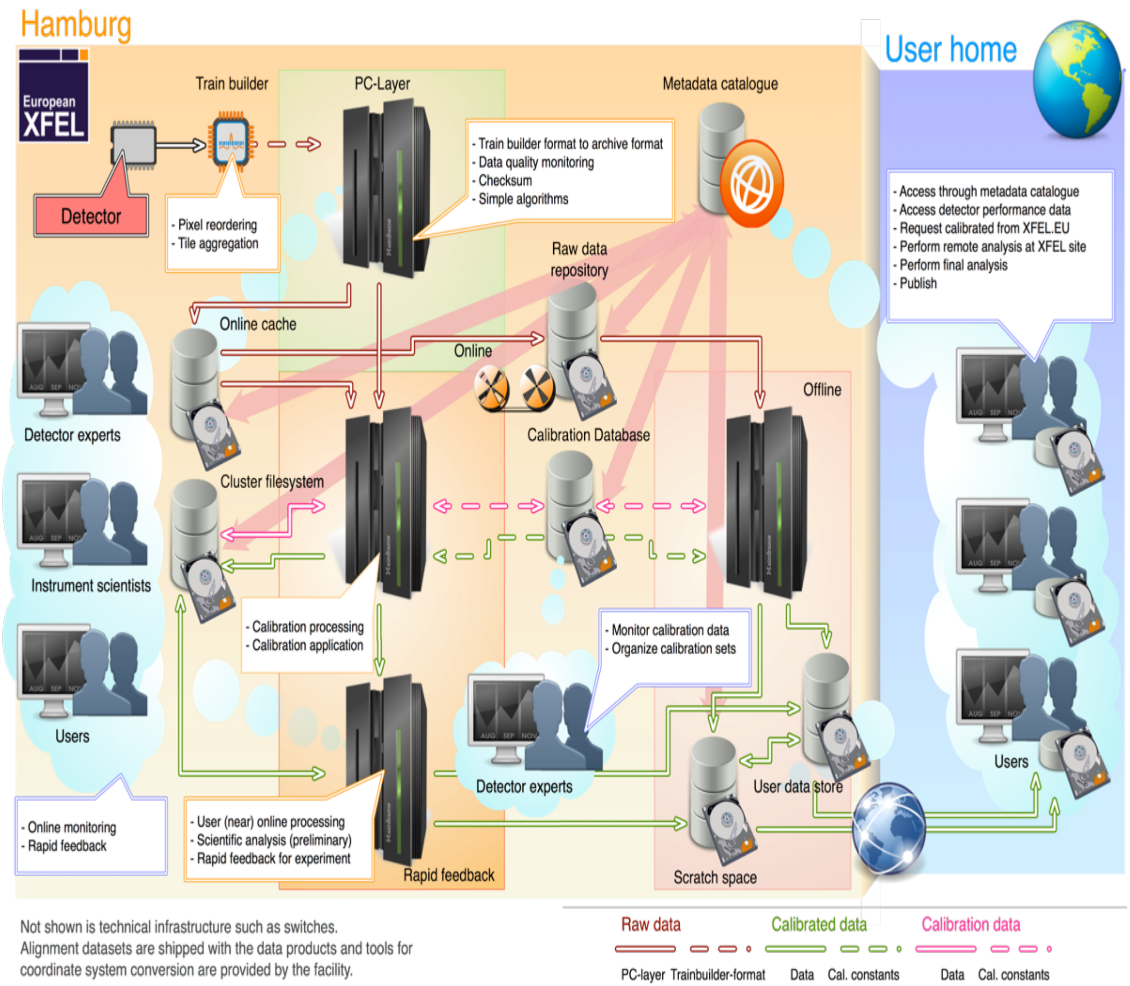


Detector type	Sampling	Data/pulse	Data/train	Data/sec
1 channel digitizer	5 GS/s	~2 kB	~6 MB	~60 MB
1 Mpxl 2D camera	4.5 MHz	~2 MB	~1 GB	~10 GB
4 Mpxl 2D camera	4.5 MHz	~8 MB	~3 GB	~30 GB*

e.g. LPD detector at FXE instrument

* Limited by AGIPD detector internal pipeline depth (352 img/sec), hence factor 3 compare to LPD 1MPx

Data Management Big Picture



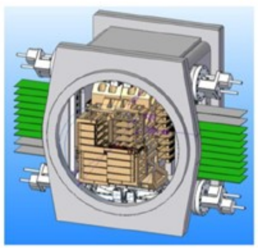
- Shown on the picture
  - Actors
  - Data flow
  - Storage resources
  - Computing resources
  - Processes

Detectors

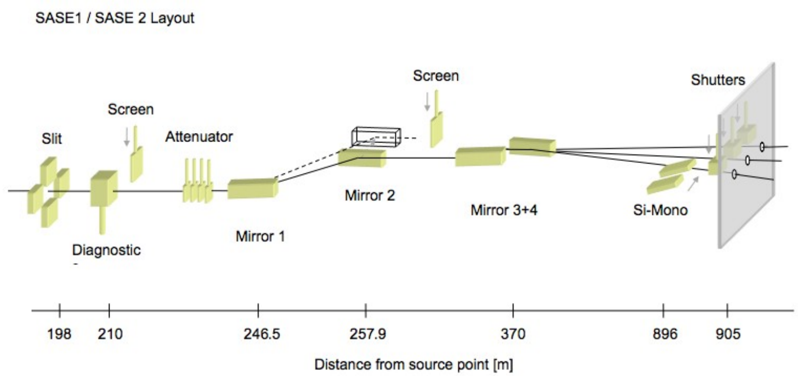
Optical systems, diagnostics, P&P Lasers, detectors, DAQ, sample delivery, etc., were designed and are being built to exploit the high repetition rate at best.

Mainly for coherent diffraction imaging and X-ray photon correlation spectroscopy, dynamic range from 1 photon to 10^4

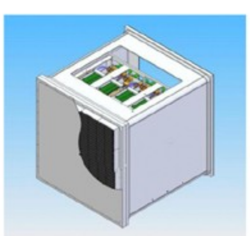
AGIPD Adaptive Gain Integrating Pixel Detector (AGIPD)



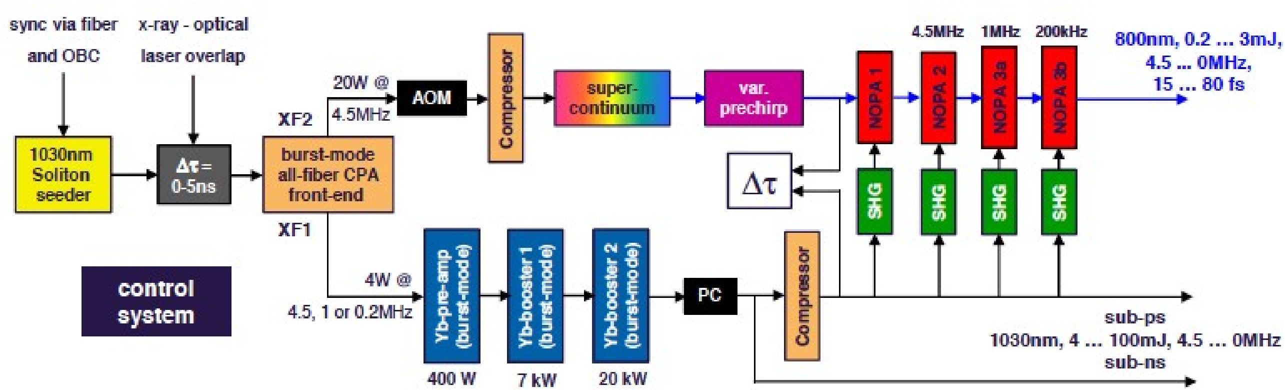
Energy range
3 - 13 keV (25keV)
Dynamic range
10^4@12 keV
Single Photon Sens.
Storage Cells ≈ 360
Pixel Size 200 x 200 µm^2



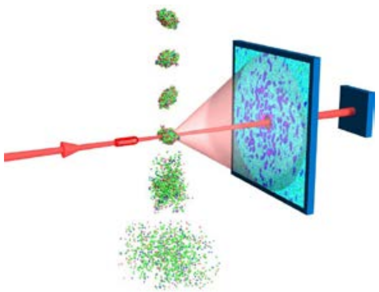
Large Pixel Detector (LPD)

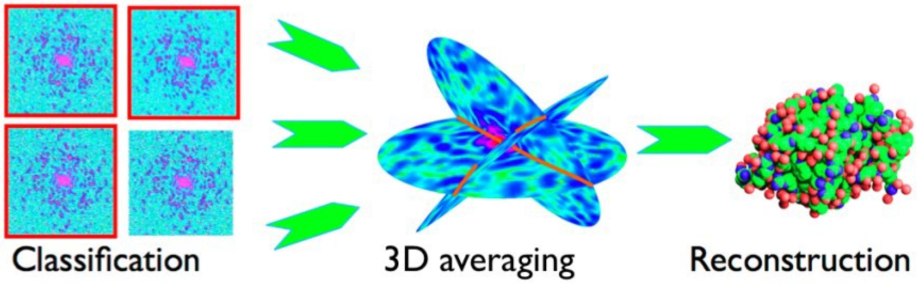


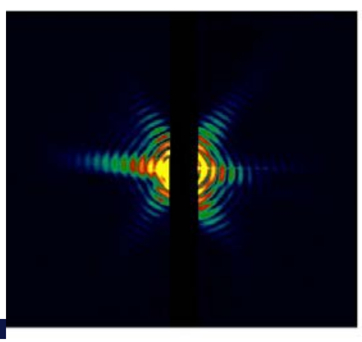
Energy range
5 (1) - 20 keV (25 keV)
Dynamic range
10^5@12 keV
Single Photon Sens.
Storage Cells ≈ 512
Pixel Size 500 x 500 µm^2

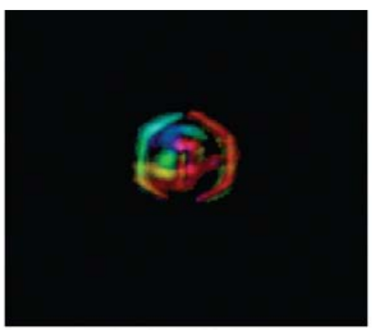


In-kind contribution SE01 for WP79
Sample Injection Technology









Reconstruction by Anton Barty
Relaxed Averaged Alternating Reflection

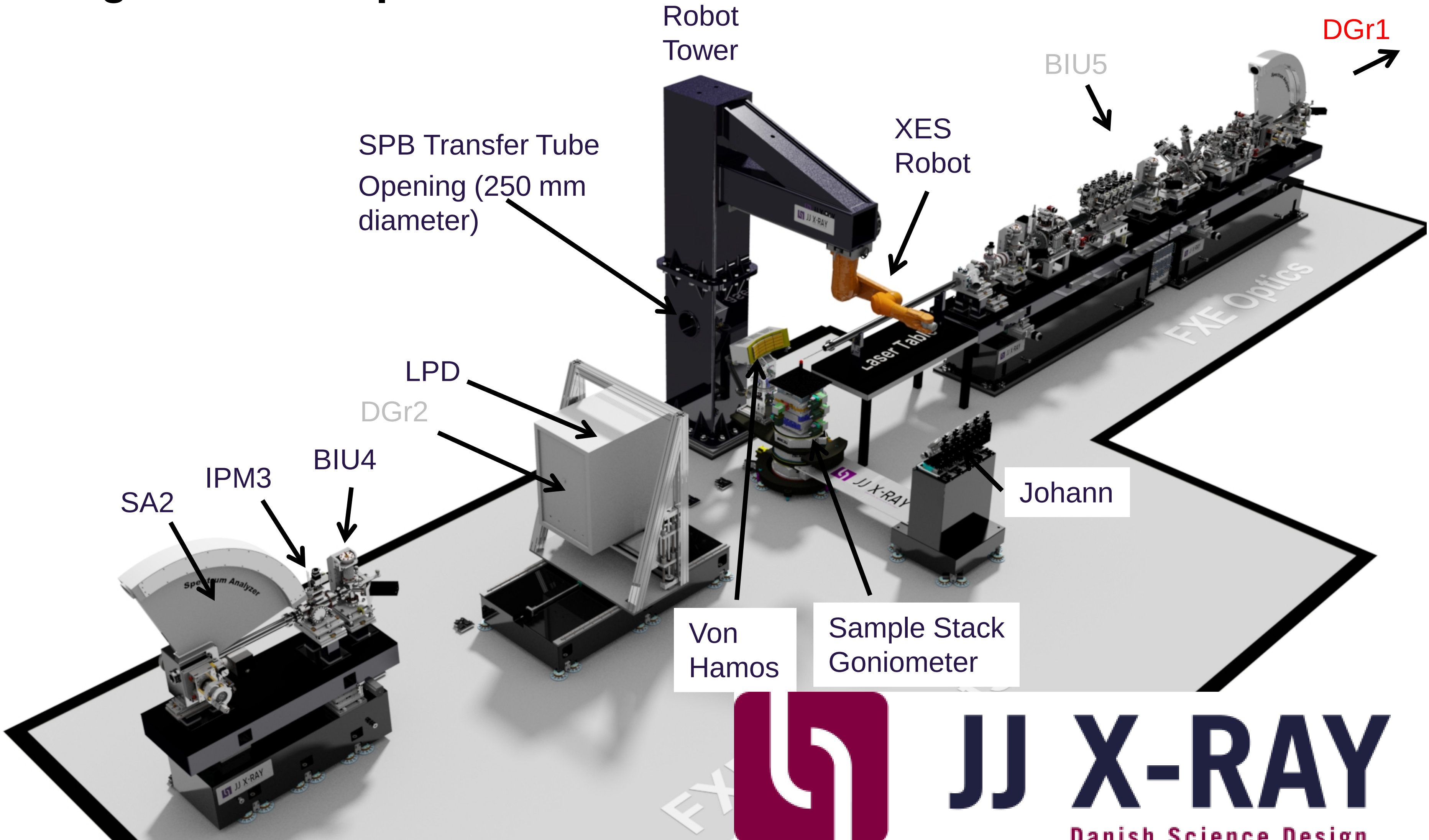
Operation:

1. Many single particle images
2. Classify for orientation
3. Average each class
4. Combine to 3D image
5. Reconstruct

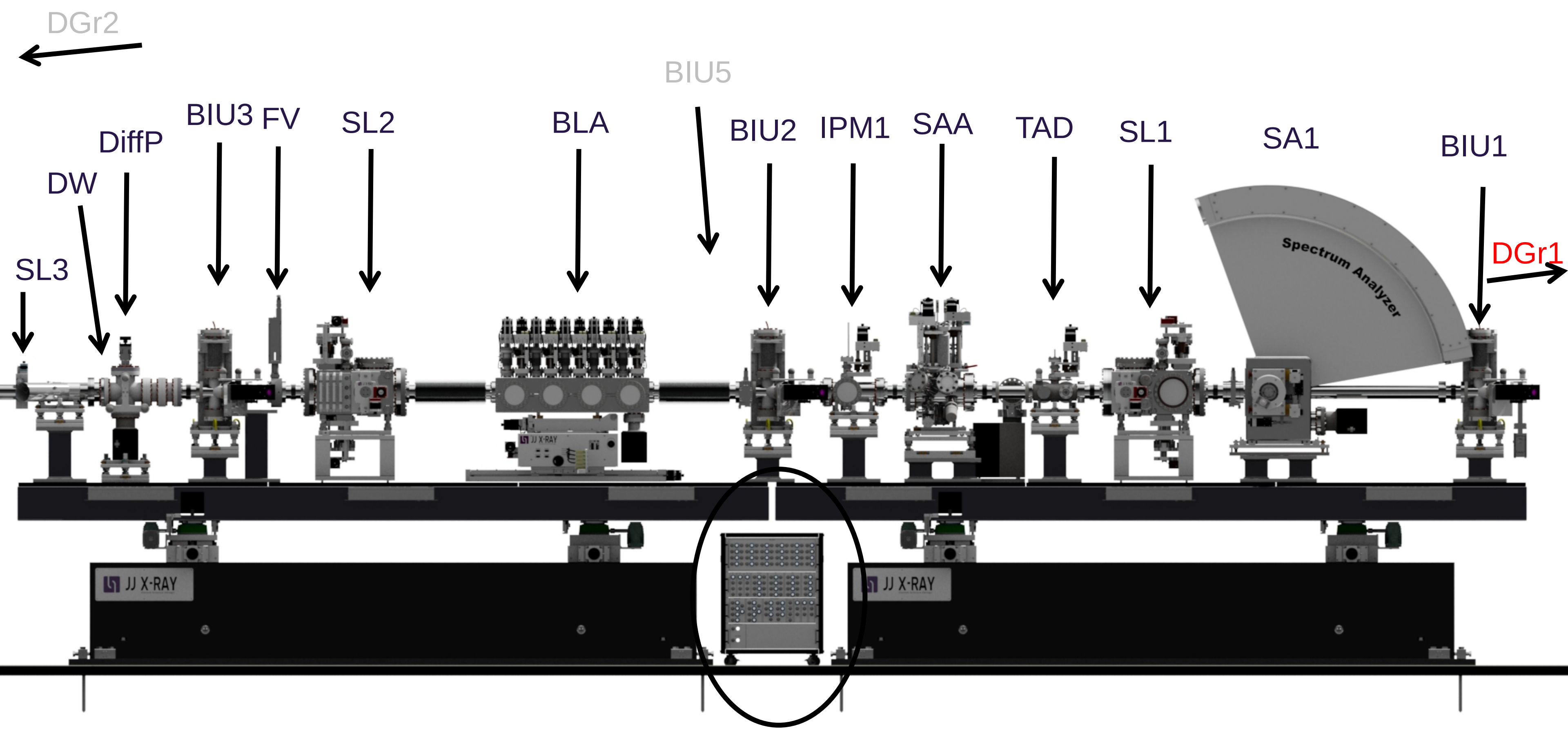
In-kind contribution DK01 for WP81
High-Tech components for FXE Instrument

List of deliverables
Solid Attenuator Assembly, water cooled, UHV
I0 Monitor (integrated incident intensity), water-cooled, UHV
Spectrum Analyzer, water-cooled, UHV
Beam Imaging unit, UHV
Be Transfocator Assembly, water cooled UHV
DW, diamond window, water cooled
Motorized granite support for accommodating DCM offset
Sample Mounting Stage
Von Hamos spectrometer
Johann Scanning Spectrometer, incl. crystals
Time Arrival Detector and Laser Port (TAD/LP)
Primary and secondary beam slits (SL1, SL2)
Long translation and support for large detector

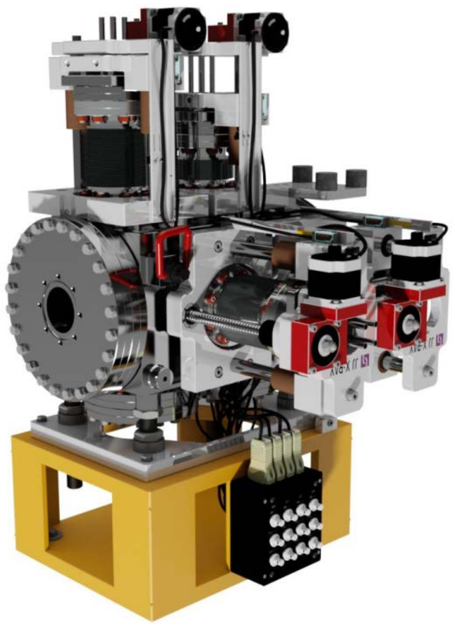
In-kind contribution DK01 for WP81
High-Tech components for FXE Instrument



JJ X-RAY
Danish Science Design

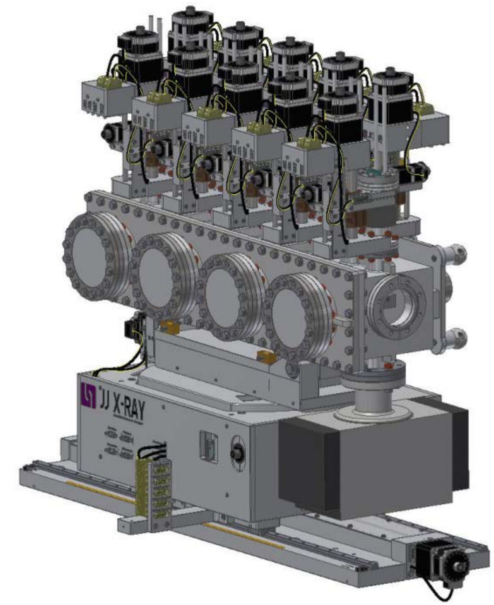


- Patch Panel with Lemo Connectors



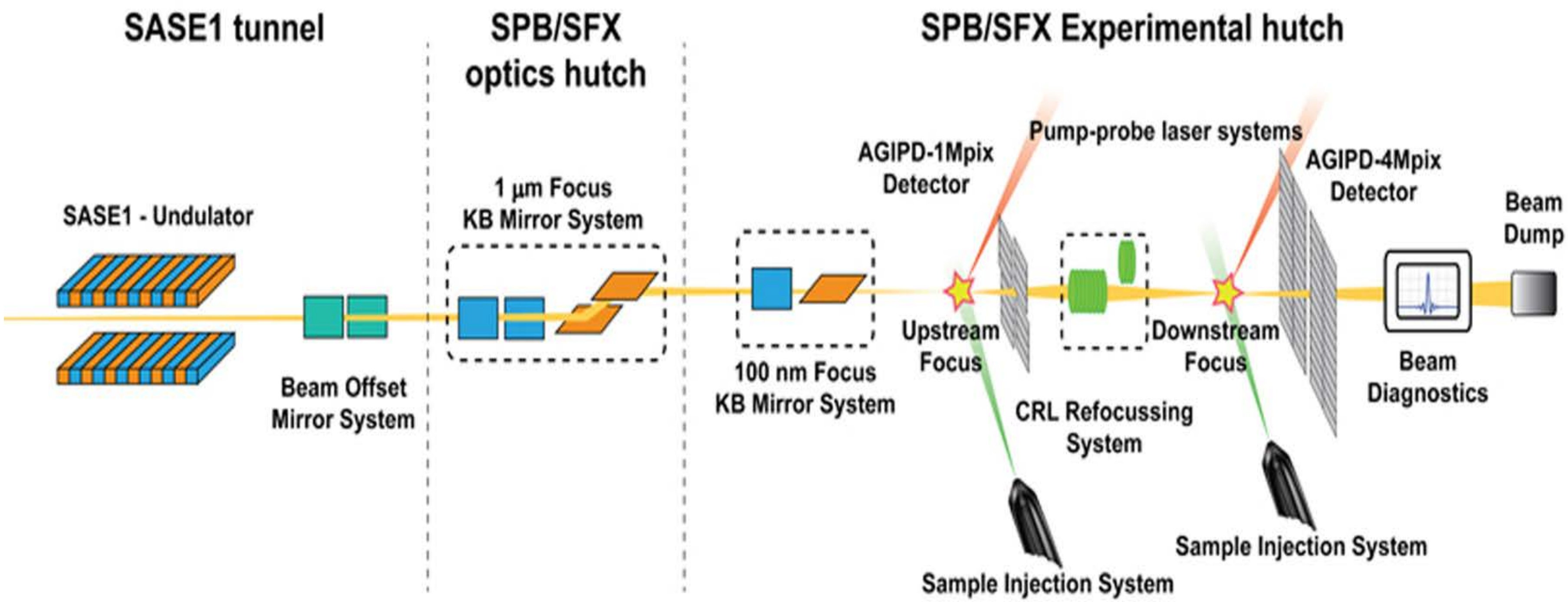
Compact Slit system

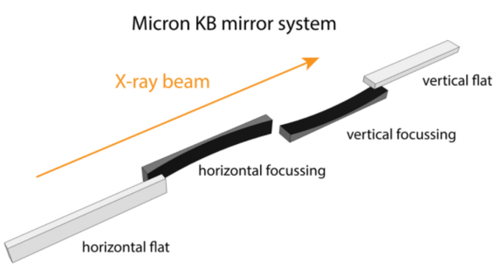
Compact Solid Attenuator

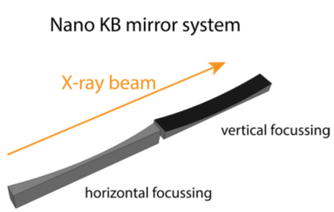


Beryllium
Compound
Refractive
Lens System

JJ X-RAY
Danish Science Design

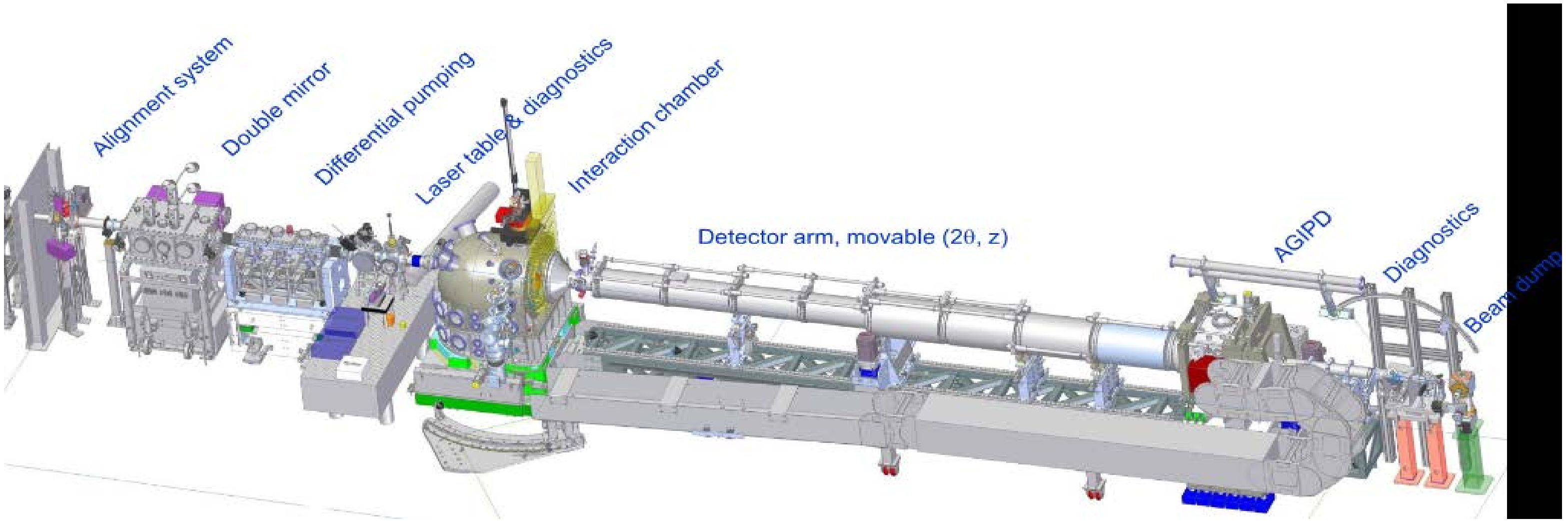






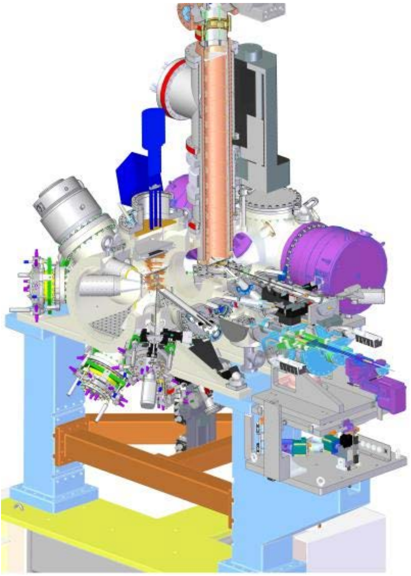
The SPB/SFX instrument is equipped with two KB mirror systems for focusing the X-ray beam into a common focal plane in the upstream interaction region, creating focal sizes of approximately 1 µm and 100 nm (as a function of photon energy, with larger sizes at lower photon energy). Two different coatings for both mirror systems ensure good transmission over the entire primary photon energy of 3–16 keV.

MID instrument



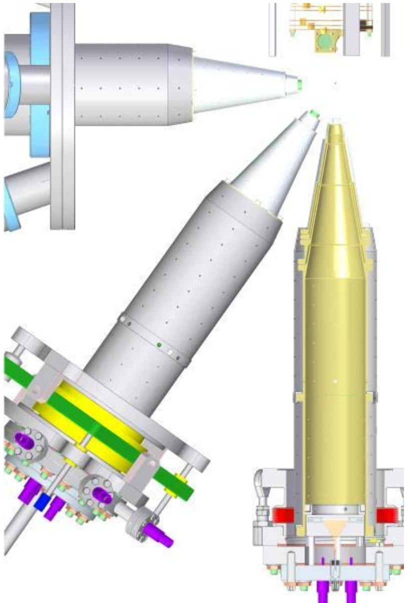
- Different X-ray energies and pulse patterns are possible, adjusted to the experimental requirements.
- energy tunable in a range from 5 to 25 keV
- pink SASE bandwith about 10^{-3}
  - two additional monochromators available Si-111, $\Delta E/E = 1.4 \times 10^{-4}$; Si-220, $\Delta E/E = 5.9 \times 10^{-5}$
- Self-seeding will be implemented first at MID/SASE2
- pulse energy ~0.5 mJ = $3\ 10^{11}$ photons/pulse at 10 keV
- pulse duration <100fs
- 10 pulse trains/s
- Intra-bunch up to 4.5 MHz
  - i.e. Δt = 220 ns spacing between single pulses
  - Integers $n\Delta t$ possible (n=4 tested)
  - 1, 30, 120, ..., 2700 pulses/train

AQS end station in SQS



The Atomic-like Quantum Systems (AQS) experimental station is tailored to study fundamental quantum systems, i.e. free atoms or small molecules. The vacuum chamber hosts different spectrometers for detection of charged particles, and, later, also of fluorescence photons. All in-vacuum components are selected to reach a background pressure (without load of the target gas) in the order of 10^{-10} mbar.
Two interaction regions spaced by 35 cm allow for different spectrometers to be mounted simultaneously. In the final operation mode rapid changes from one setup to the other can be realized in this way without venting or moving the chamber.

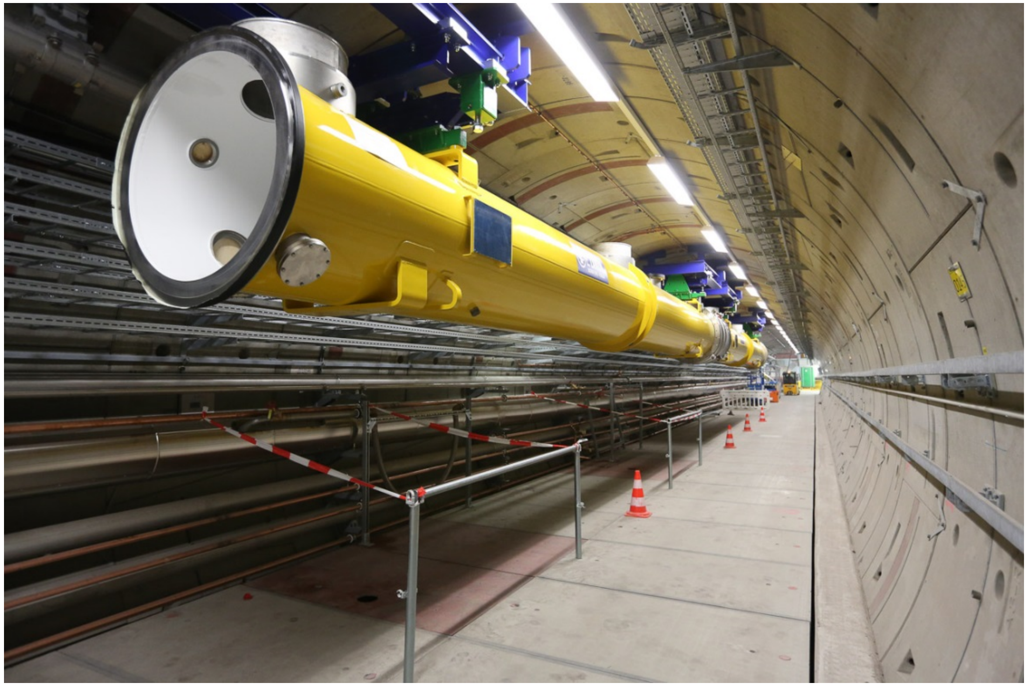
Electron time-of-flight spectrometers

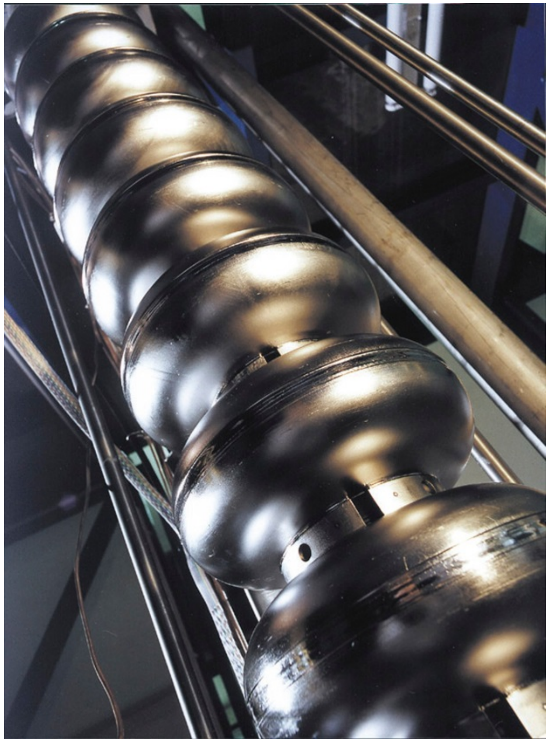


At the upstream position, three identical Electron Time-Of-Flight (eTOF) spectrometers are mounted in the dipole plane (perpendicular to the beam propagation axis). In combination with a fast digitizer, they record high-resolution electron spectra at the full 4.5 MHz repetition rate. Three further eTOFS will be installed later in the backward hemisphere for measurements of non-dipole effects.
The eTOFs can also be used for ion detection when switching the polarity of the applied voltages. All etofs can be operated simultaneously or in coincidence with the VMI spectrometer, enabled by fast switching of the high voltages on the VMI.

Three example of Technology Transfer during the construction

- Ettore Zanon S.p.A.: Collaboration with INFN-Activities for the Project XFEL Superconducting cavities and cryostats

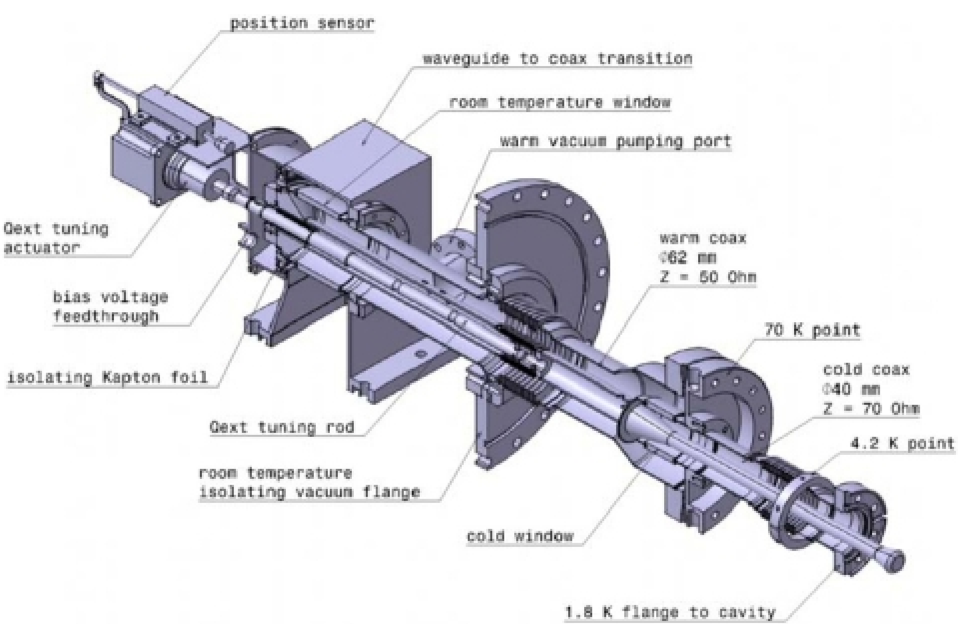




Three example of Technology Transfer during the construction

The future Industrial Liaison office is collecting the huge quantity of cases of TT. It is worth to Highlight:

- RI Research Instruments GmbH: Superconducting Cavities (similar to the experience of Zanon. RI produced the remaining ones). Power Couplers assembly and treatm



In-kind contribution SE05 for WP28
Timing & synchr. System + configuration mngmt

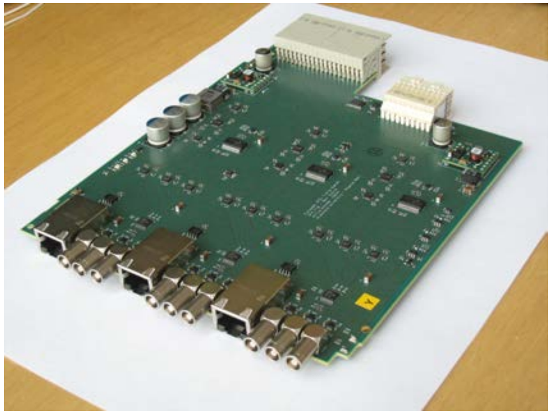
Tasks:

Timing and synchronization system:

Design and production of two prototype versions, tests and validation of the prototypes,

Preparation and supervision of the production of the final system, and installation and commissioning at European XFEL Company.

Configuration and authentication and access management system:



MTCA.4 is a new standard form the PICMG to extend the applications of the existing µTCA crate system

Technology transfer case:

The design (XFEL_Timing_AMC_rev0.2.2, XFEL_Timing_RTM_Trg1, XFEL_Timing_RTM_Trg2) has been transferred to N.A.T. for commercialization. Information can be found at http://tesla.desy.de/doocs/doocs.html

ESS in Lund has shown interest in using such technology to drive and control their superconducting RF system.

Accelerator Module Test Facility (AMTF)

Call for tender

- As the European XFEL biggest shareholder is the Federal Republic of Germany represented via BMBF and DESY, the XFEL is obliged to use the German National and the European Public tender rules, laws and regulations:
  - All calls for tender above the threshold for European wide tenders (> 221k € for goods and service and > 5,548 k € for construction) are announced on the TED website (Tenders Electronic Daily)
  - All tenders considered a national tender (below the value of 221 k€) are announced on a National/Federal website called “Bundesanzeiger”.

- All performed tenders are also announced on the European XFEL website.

  https://www.xfel.eu/organization/procurement/calls_for_tender/index_eng.html

- Some call for tenders related to the Accelerator, which is located on the DESY (Deutsches Elektronen Synchroton) campus, are administrated by DESY procurement, as agreed within the operations agreement between DESY and European XFEL GmbH

Call for tender

- The European XFEL GmbH is a public-equivalent body and is therefore subject to special legal regulations concerning the award of contracts and placement of purchase orders. This includes, for example:
  - the VOB ("Verdingungsordnung für Bauleistungen“, regulations for civil construction contracts),
  - the VOF (“Verdingungsordnung für freiberufliche Leistungen“, regulations for freelance and professional services contracts)
  - the VOL (“Vergabe- und Vertragsordnung für Leistungen“, regulations on contract awards for public supplies and services),

  https://www.xfel.eu/organization/procurement/legal_and_regulatory_information/index_eng.html

- The award of contracts and placement of purchase orders fall under the responsibility of the Procurement Group

Call for tender

- Due to the fact that we are a goverment-funded organization, we are not allowed to accept other terms and conditions than these. Please read them carefully and include them as part of your public tender documentation.

https://www.xfel.eu/sites/sites_custom/site_xfel/content/e35152/e46557/e47200/e47202/xfel_file47204/XFELGeneralConditionsofPurchase26.8.2010_eng.pdf

- **Acceptance**

Even if acceptance is not prescribed by law or by the applicable VOB/VOL, formal acceptance testing of all items produced or services rendered specifically for the Principal must be carried out and documented by a written acceptance test report. [...] Acceptance shall be formally stated following flawless trial run if trial operation has been agreed to under contract. Such acceptance shall be no charge, including of any ancillary costs, either by way of repair, exchange of the faulty part or replacement delivery, at the Principal's discretion.[…]

party.

Call for tender

- **Proprietary rights, licences**
  - The Agent accepts liability for ensuring that the delivered items are unencumbered by rights of third parties in Germany or in the intended destination country, and in particular that no third party patents, licences, or other proprietary rights are infringed by the supply and use of the contracted items. In the event of infringement of industrial property rights, the Agent shall be obliged to compensate the Principal for any resulting loss and shall indemnify the Principal against any such claims by third parties.
  - […] The Agent grants the Principal free, non-exclusive, irrevocable licence to all industrial property rights, applications for such rights and inventions arising from performance of this contract in Germany or abroad. The Agent further grants the Principal irrevocable, free, nonexclusive right of use of all know-how and all innovations and improvements arising from performance of this contract. The Principal shall be entitled to transfer to its shareholders' licences and rights of use […]. This shall also apply beyond the duration of the contract.

Thank you for your time