The Materials Imaging and Dynamics station

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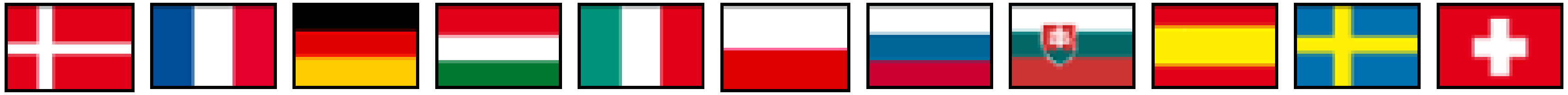


+

soon….

Early science at the Materials Imaging and Dynamics (MID) instrument

8:30	**Welcome**	S. Molodtsov	European XFEL
8:45	Introduction to MID	A. Madsen	European XFEL
9:30	Microscopic cryogenic liquid jets as novel tool to study non-equilibrium phase transition at European XFEL	A. Schottelius	University of Frankfurt
10:00	High-Purity X-ray Polarimetry - A Unique Method at MID	K.S. Schulze	University of Jena
10:30	Hard X-ray split-delay line for the MID station	S. Eisebitt	MBI Berlin
11:00	**Coffee**		
11:20	Equilibrium dynamics of deeply supercooled water probed by ultrafast X-ray Speckle Visibility	F. Perakis	Stockholm University
11:50	X-ray diffuse scattering as a probe of anharmonic phonon-phonon coupling in solids	M. Trigo	Stanford University
12:20	Studies of IR laser induced periodic plasma in colloidal crystals probed by XFEL radiation	S. Lazarev	DESY Hamburg
12:50	**Summary & Wrap-up** (G. Grübel, DESY)		
13:00- 14:00	**Lunch**		
14:00 -18:30	**Proposal discussions and facility tour**		
18:30	**Buffet dinner**		

After lunch: proposal discussions and facility tour

2:00 pm (meeting point: XFEL reception)

- Discussion about early science proposals: DYNAMICS (E1.041)

  (presentations by C. Gutt, F. Lehmkuehler,… everyone, whiteboard,…)

- Discussion about early science proposals: IMAGING (E1.096)

  (presentations by R. Kurta, C. Kim,… everyone, whiteboard,…)

- Experimental hall visit (?)

~3:30 pm - Coffee and plenary session with reports from discussions (E1.041)

~4:30 pm (meeting point: XFEL reception)

- Experimental hall visit. Posters with more details about MID

  (guides: J. Hallmann and A. Zozulya)

6:30 pm - Buffet dinner in foyer

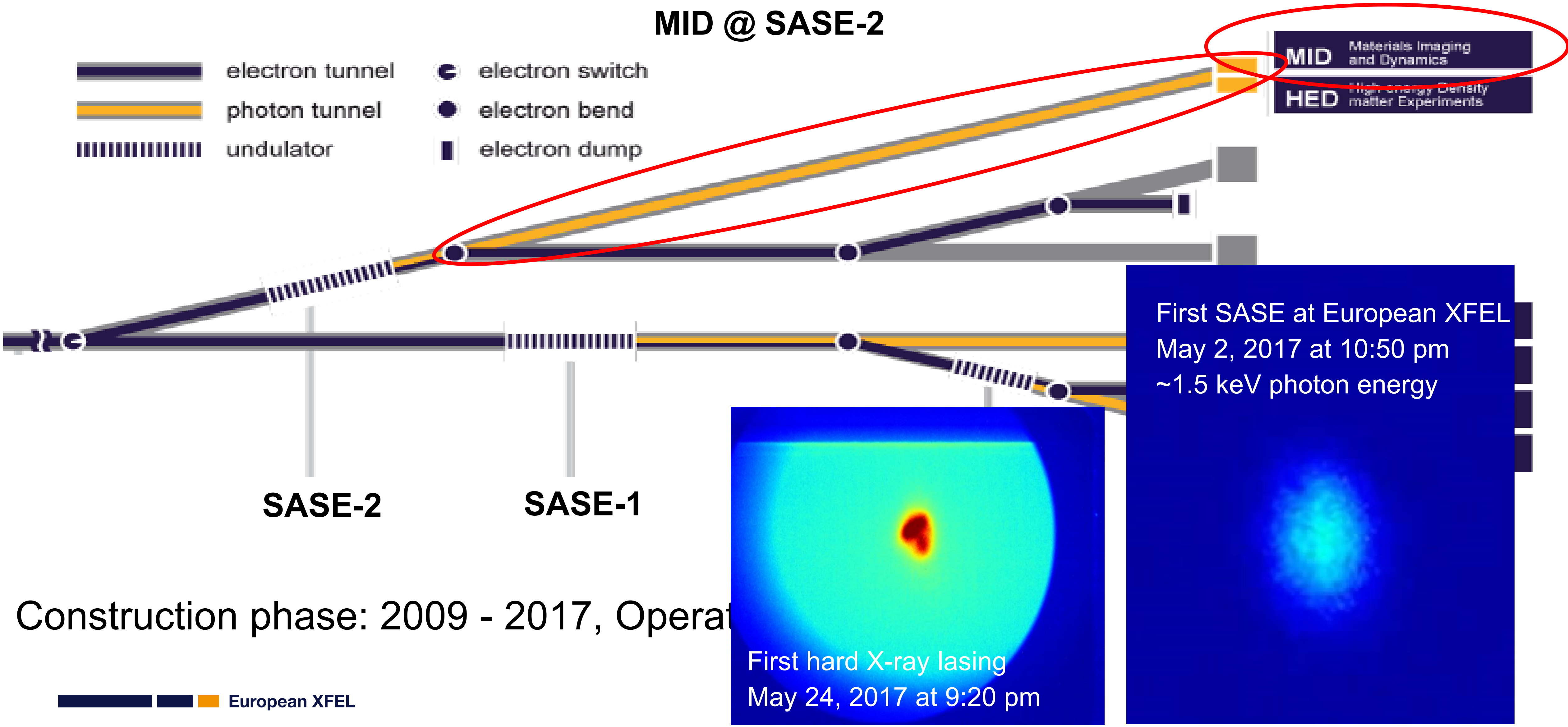
https://www.xfel.eu/facility/instruments/mid/index_eng.html

MID@XFEL.EU

Gabriele Ansaldi
Alexander Bartmann
Ulrike Boesenberg
Jörg Hallmann
Chan Kim
Iker Lobato
Wei Lu
Anders Madsen
Johannes Möller
Mario Reiser
Andreas Schmidt
Markus Scholz
Roman Shayduk
Konstantin Sukharnikov*
Alexey Zozulya

* missing on photo

Facility outline



Construction phase: 2009 - 2017, Operat

Six phase-1 stations

~3 – 25 keV

Hard X-rays

SPB: Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules

- Structure determination of single particles: protein crystallography, biomolecules, cells

MID: Materials Imaging & Dynamics

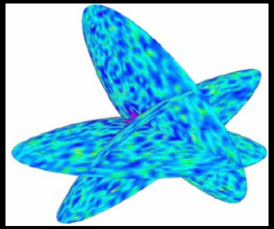
- Structure determination of materials and dynamics at the nanoscale.

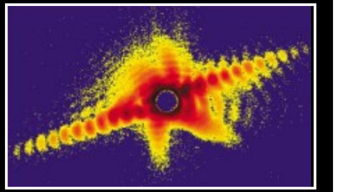
FXE: Femtosecond X-ray Experiments

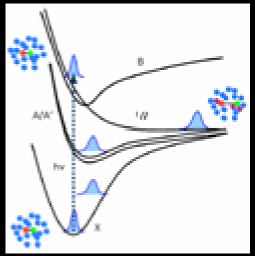
- Time-resolved investigations of the dynamics of chemical reactions

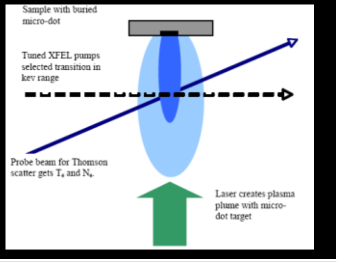
HED: High Energy Density Matter

- Investigation of matter under extreme conditions, e.g. probing dense plasmas









~0.3 – 3 keV

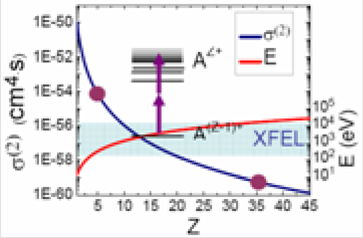
Soft X-rays

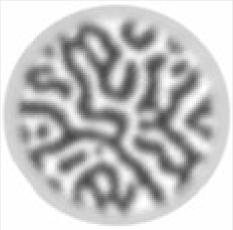
SQS: Small Quantum Systems

Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena

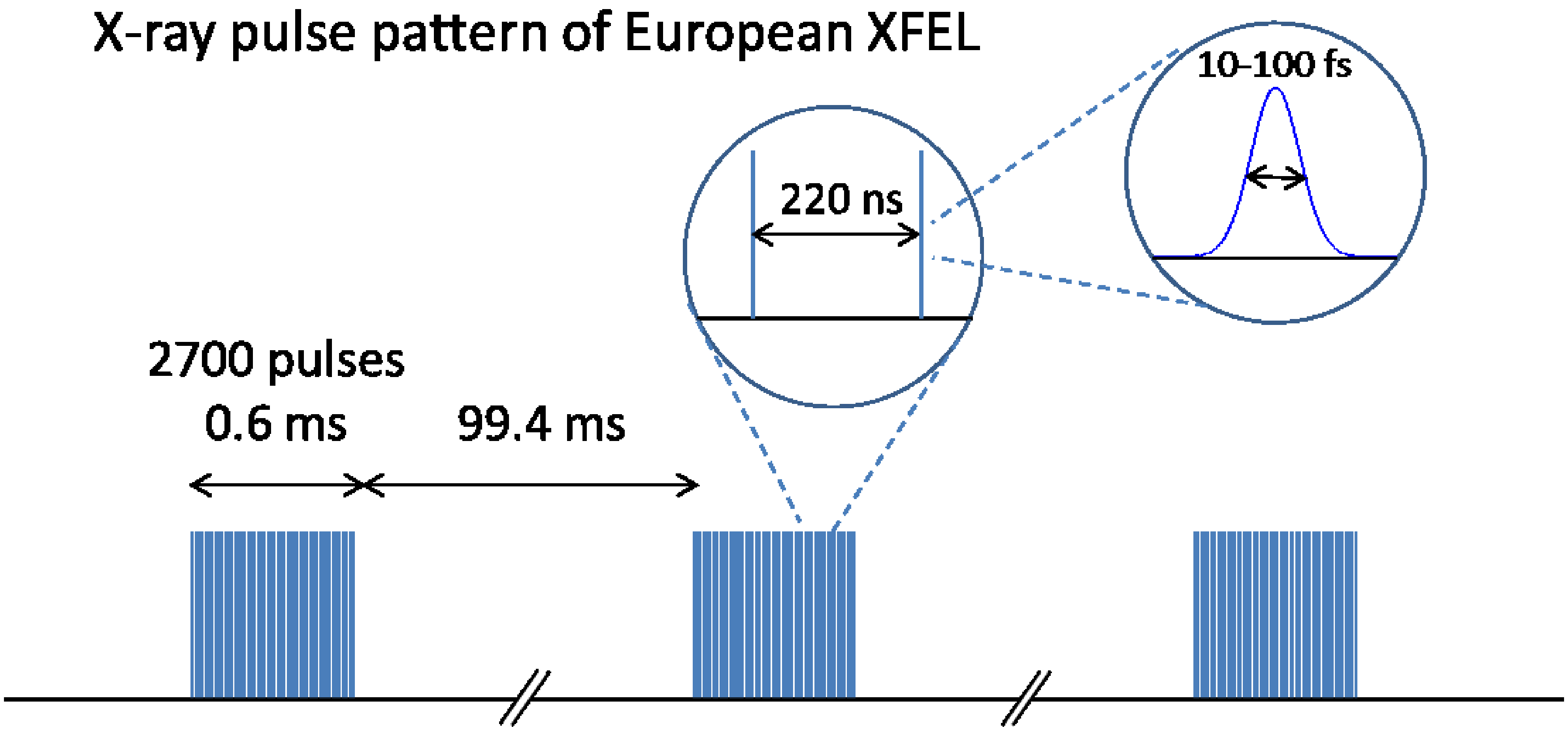
SCS: Soft x-ray Coherent Scattering/Spectroscopy

Electronic and real structure, dynamics of nano-systems and of non-reproducible biological objects





Time structure of European XFEL



MID specifications

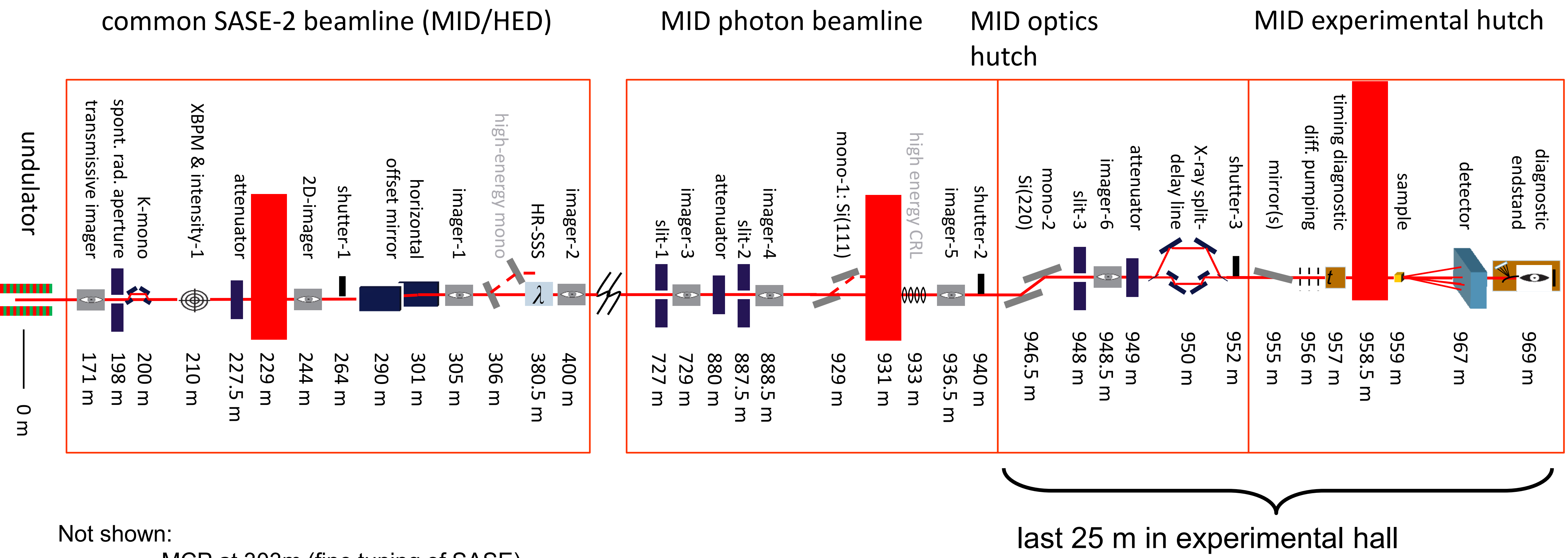
- 5-25 (9?) keV X-rays, focusing with CRLs: down to few µm, nano-focusing option
- synchronized optical fs laser (not available for EUE)
- pink SASE (bw ~10^{-3}), Si(111) or Si(220) mono
- SASE-2 is the undulator where self-seeding will be implemented first (not available for EUE)
- Up to 4.5 MHz i.e. Δt = 220 ns spacing. Integers n·Δt possible (n=4 tested).
  1, 30, 120,… pulses/train tested so far. 10 trains/s
- 0 - 800 ps spacing using split-delay line (SDL) (not available for EUE)
- pulse energy ~0.5 mJ = 3×10^{11} photons/pulse at 10 keV. Pulse duration <100 fs
- window-less setup (differential pump) or sample in air/He (diamond window)
- 2d detectors (AGIPD, ePix, Jungfrau), attenuators, slits, diagnostics,…
- pulse resolved energy dispersive spectrometer
- liquid jet, cryostat, B-field, fast sample scanner, hexapods, goniometer,…

SASE-2 undulator

- SASE-2 undulator >95% installed (35 x 5 m segments) NdFeB magnets, period 40 mm
- Jan 2018: Mechanical comm.
- Installation of dose monitors and air coil correctors
- Ready for beam: March 2018
- 1st lasing attempt: April 2018?

The SASE-2 undulator located behind protection panels for better AC control
View from segment 27 and downstream (credit: J. Pflueger and XFEL undulator group)

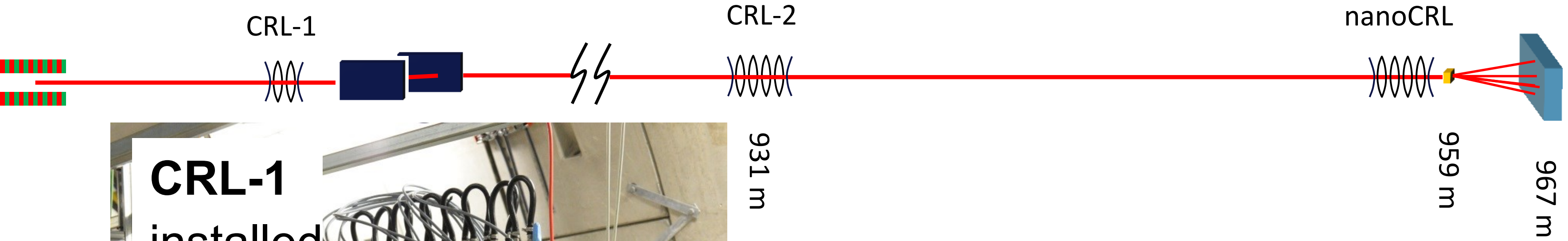
MID beamline overview



Not shown:
- MCP at 303m (fine tuning of SASE)
- Distribution mirror(s) at 390m and 395m (MID on central branch)
- Beam loss monitors, PES

Tunnel responsibles: Optics group, Vacuum group, Photon diagnostics group, MID and HED

MID focusing



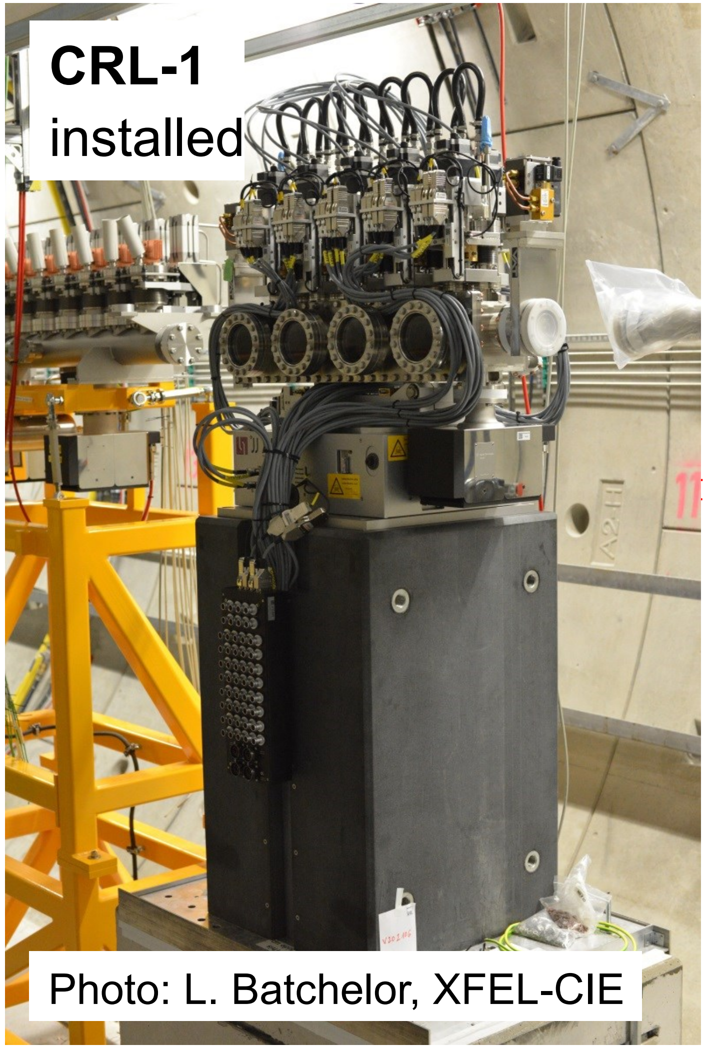


Photo: L. Batchelor, XFEL-CIE

CRL-1 collimation

simple CRL-1 focusing

combined CRL-1&2 focusing

focusing via intermediate focus

collimate, then focus

brute CRL-2 focusing

Beam size on sample ~ 2-1000 μm

Eff. >80% for most schemes and energies

Nanofocusing option

Energy	Beam size (FWHM)
5 keV	187 nm
8 keV	117 nm
12 keV	78 nm
16 keV	58 nm
25 keV	37 nm

Calculation for f = 300 mm

Efficiency ~50% with prefocusing

~10 nm focus for f = 50 mm at 12 keV

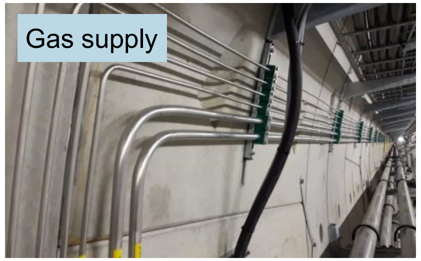
MID tunnel components

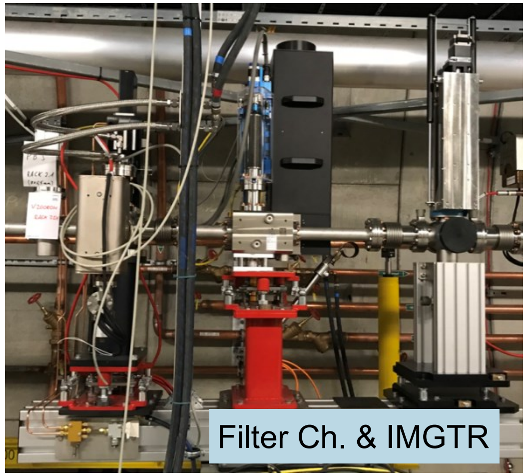
- All components are delivered and installed
- Survey of components 60% completed (XTD1 complete, XTD6 ongoing)
- Establishing of complete vacuum system is ongoing (currently about 10% under vacuum)
- All electronic racks are installed on connected, local cabling ongoing (40% complete).
- All safety relevant components (shutters&shieldings) were approved by TÜV.
- Optics: Beam transport mirrors were received and characterized in Metrology lab. Coating is ongoing (B4C +Pt). Optics will be mounted, as soon as overall system (vacuum, controls) allow save operation.
- Major challenges are electronics installations, cabeling, and software development and debugging (Beckhoff and Karabo).
- First lasing, start of commissioning with beam in tunnel in May

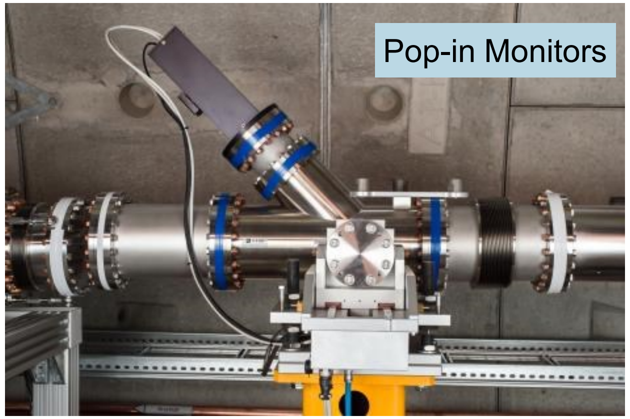
Slide from Harald Sinn
XFEL optics group

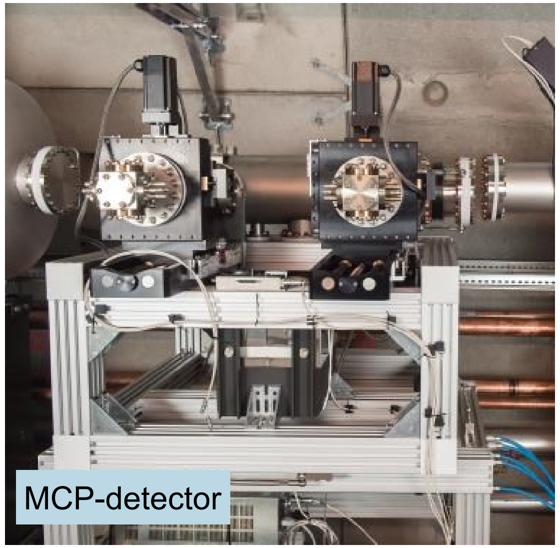
Tunnel diagnostics

- all SASE2 diagnostics vacuum systems are in the tunnel



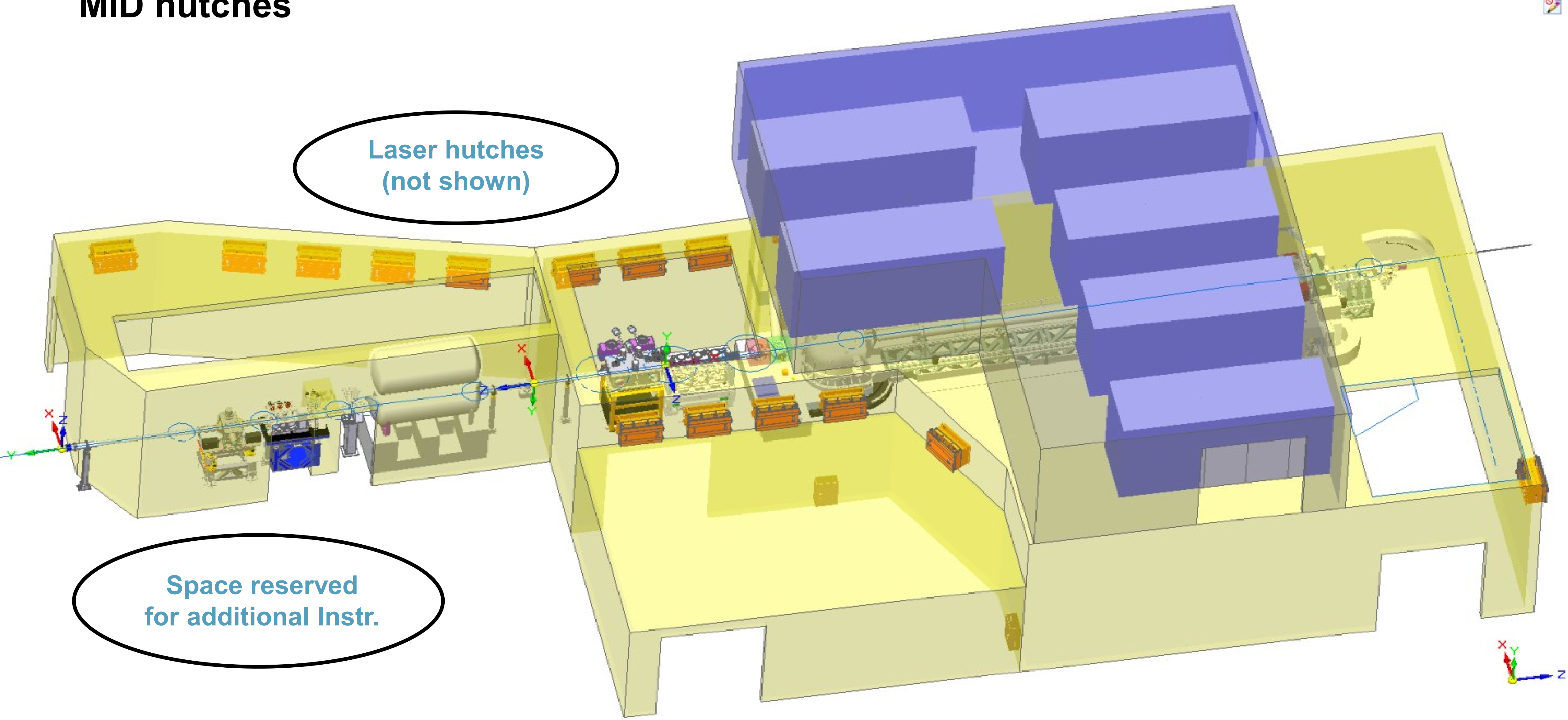




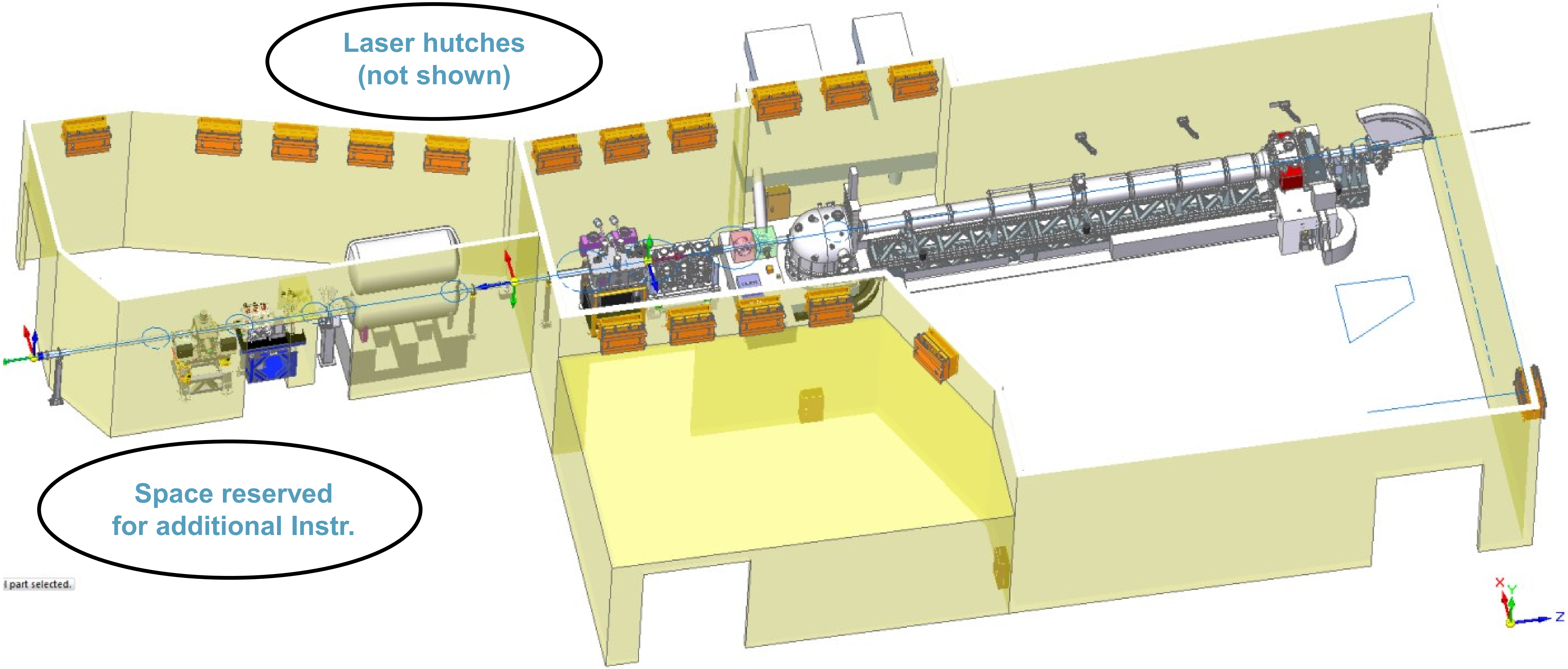


Courtesy of Jan Grünert and the photon diagnostics group

MID hutches


Laser hutches
(not shown)
Space reserved
for additional Instr.

MID hutches


Laser hutches
(not shown)
Space reserved
for additional Instr.
1 part selected.
X
Y
Z

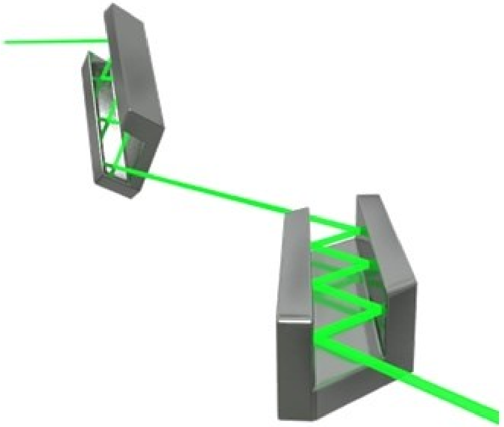
Optics hutch

- Alignment system
- Slit, imager, attenuator
  (JJ X-ray, XFEL coordinator: L. Batchelor)
- Monochromator Si(220)
  (XFEL optics group)

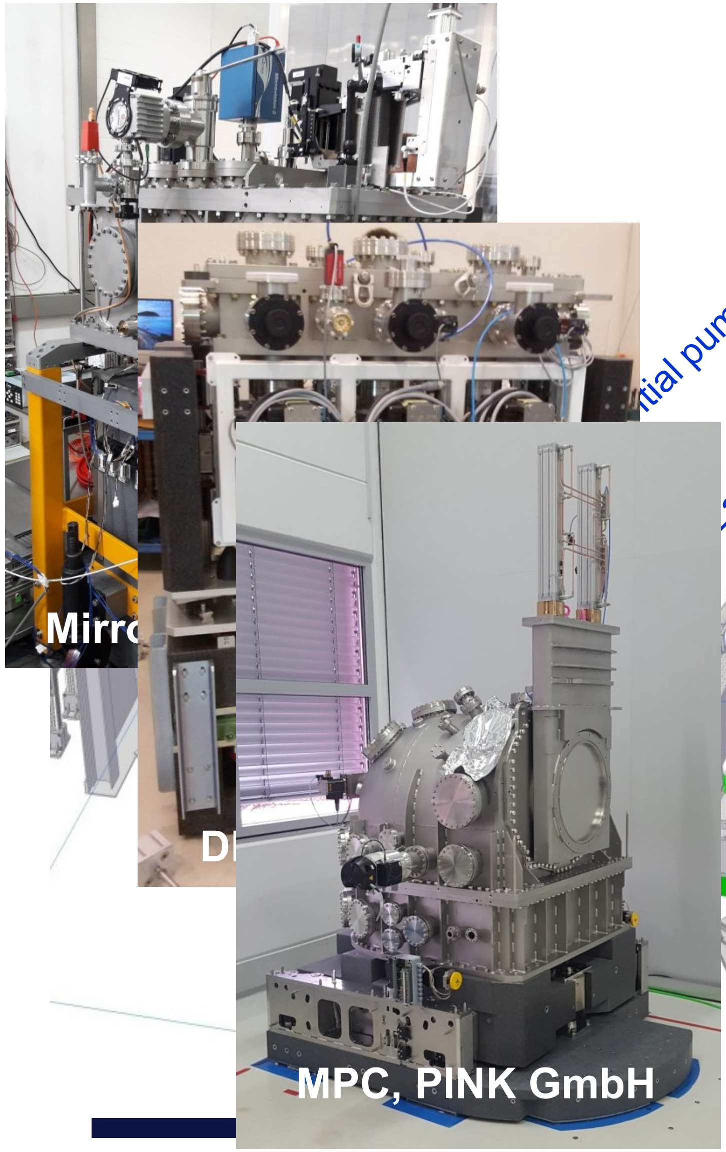
- Split-Delay Line (S. Eisebitt - W. Lu presentation)

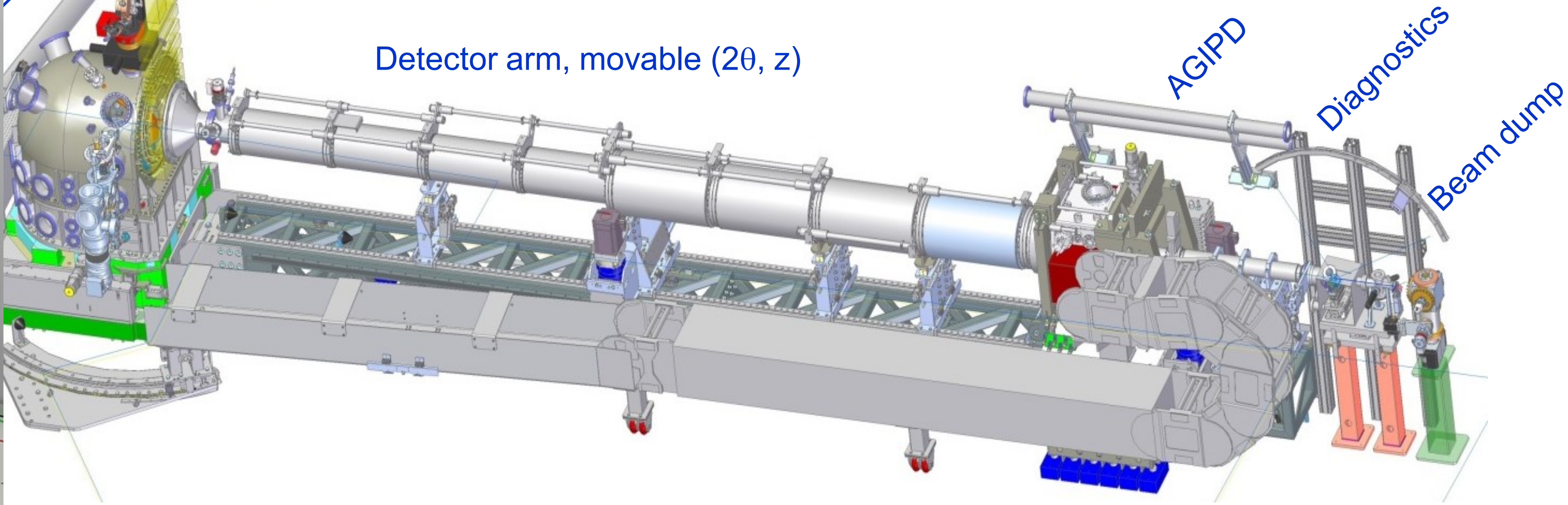
Split-Delay Line prototype tested in MID lab

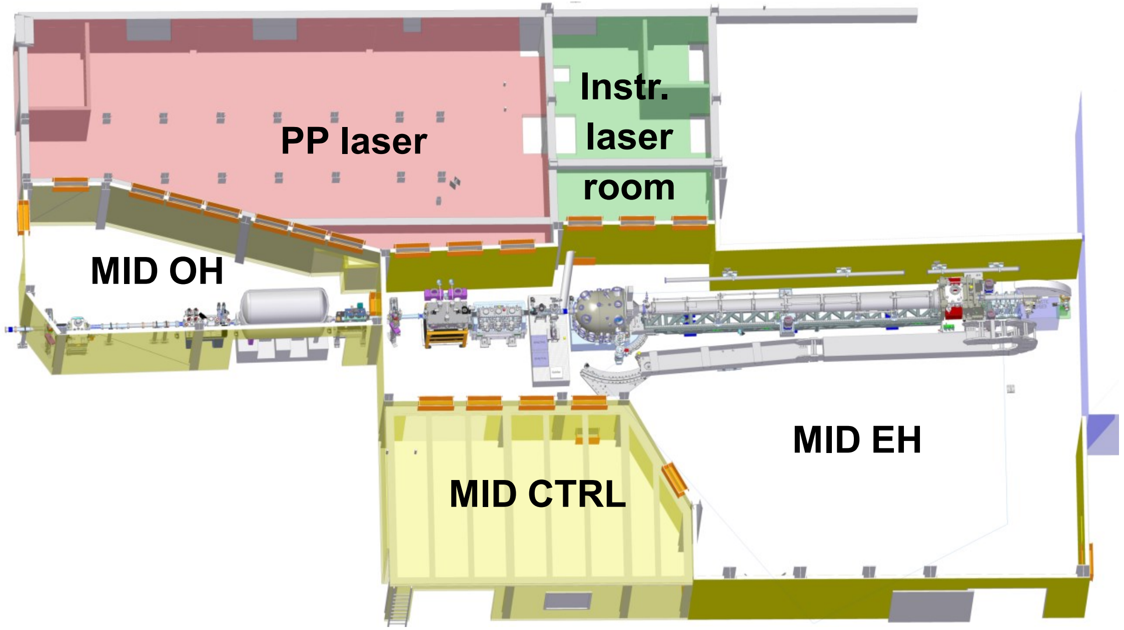
- Polarizer-polarimeter (K. S. Schulze presentation)



Experimental hutch





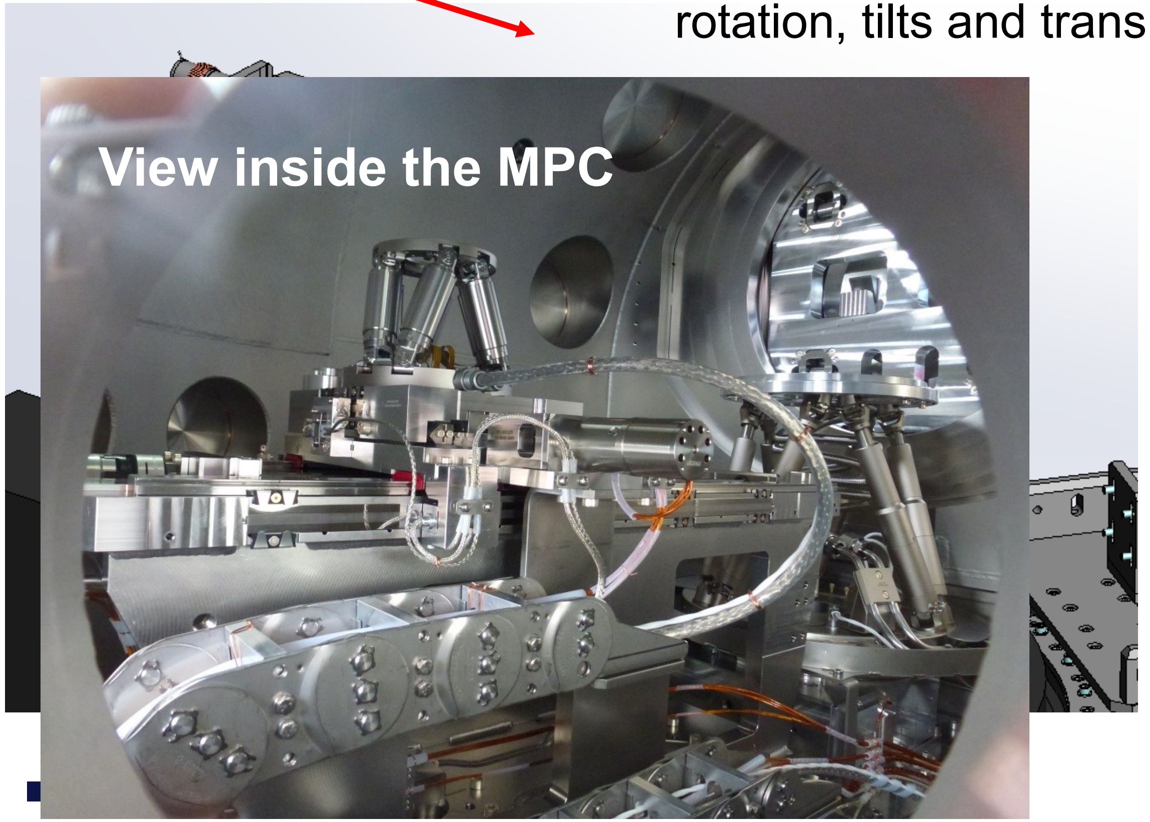


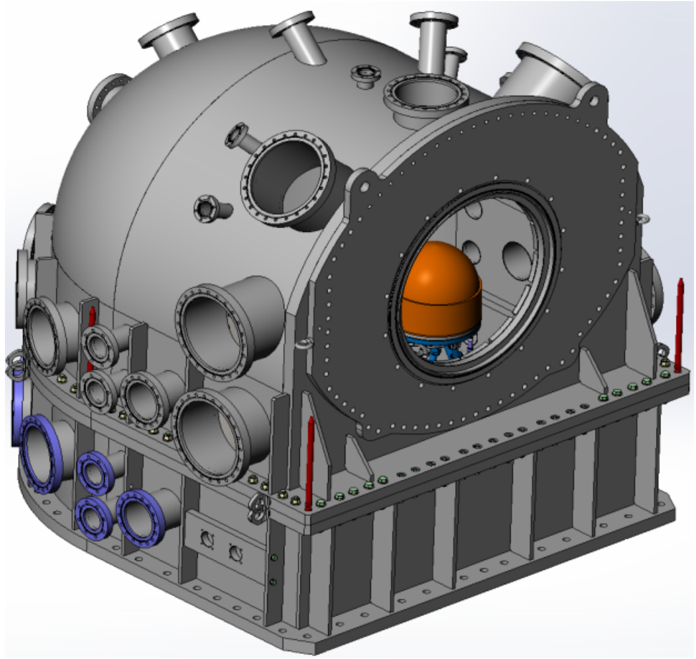
Experimental chamber (MPC: Multi Purpose Chamber)

1st stage (hexapod on linear stage)
carries e.g. nanoCRL

beam

2nd stage (hexapod + Huber stack)
rotation, tilts and translations

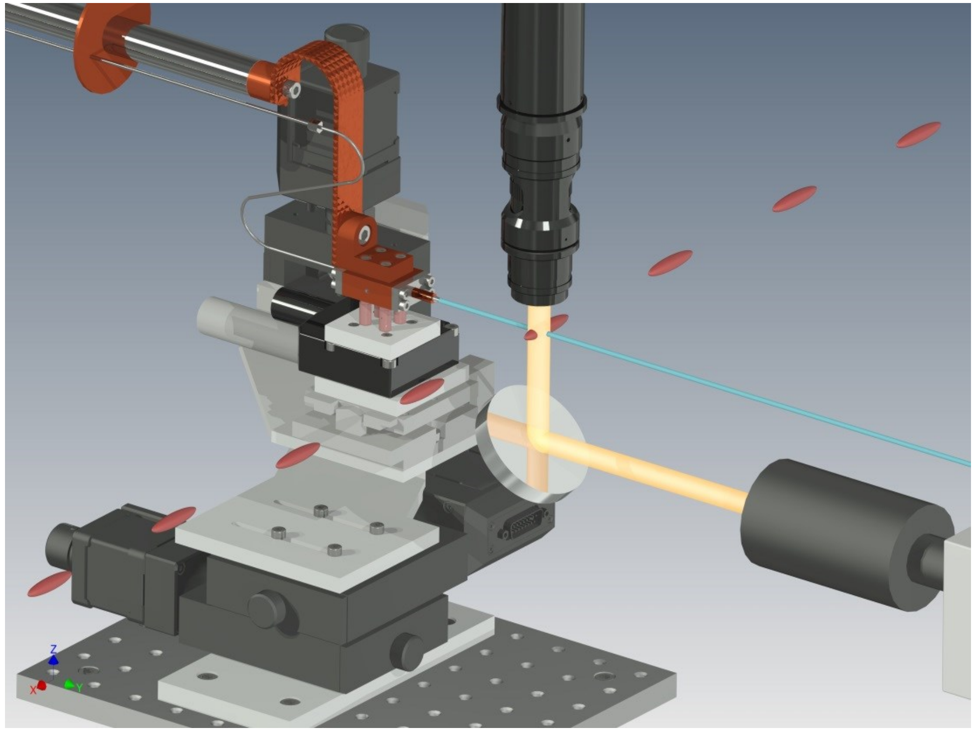




MPC operates under vacuum, windowless config.
Possibility to work without lid (in air or He bag)

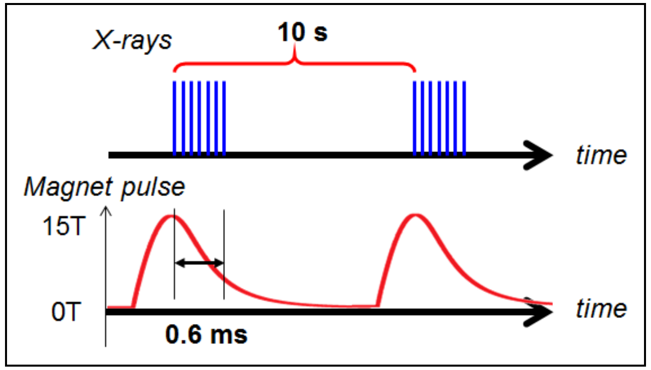
Sample environment (posters in Exp. Hall):
- 10 Hz solid sample scanner (C. Deiter, XFEL)
- Pulsed B field (Up to ~15T, 1 ms pulse)
- Liquid jet
- ….

Sample environment

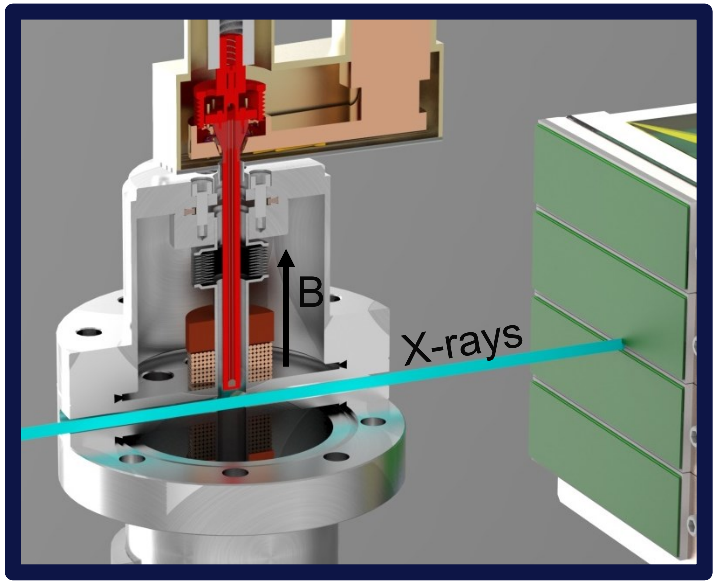


Cryo-jet (presentation by A. Schottelius)

Pulse timing

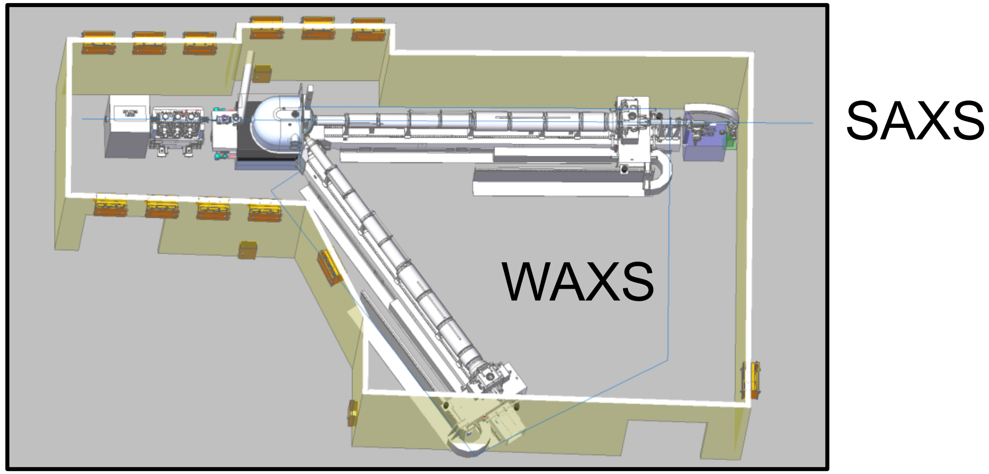


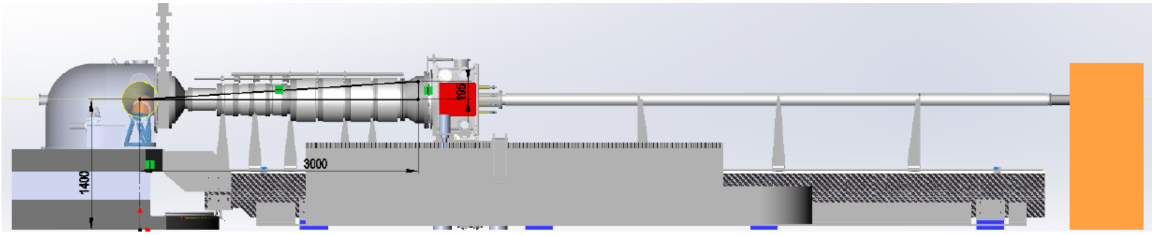
Coil cryostat

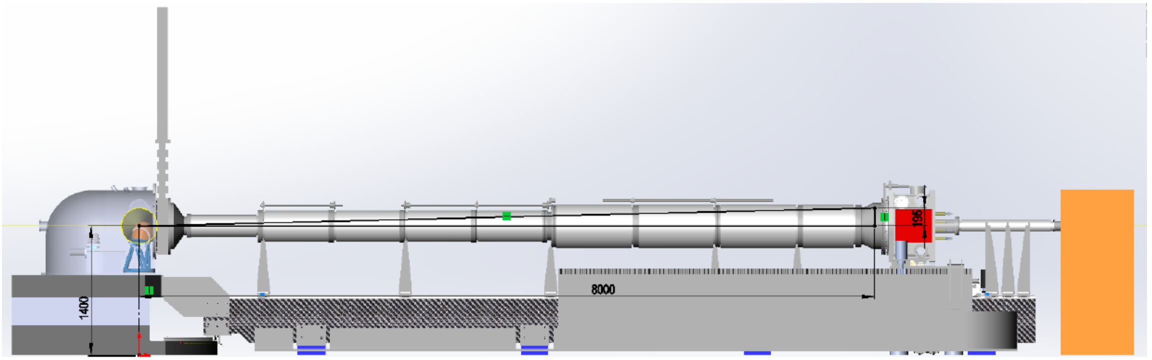


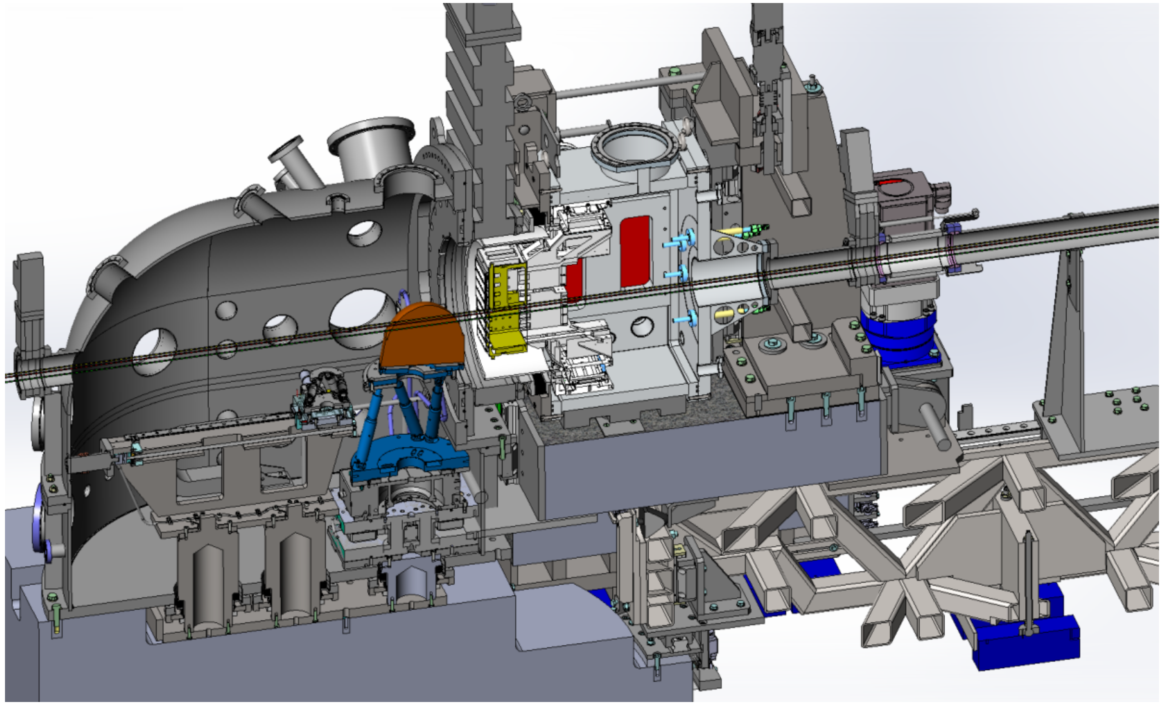
James Moore
XFEL sample env. group

Scattering geometry







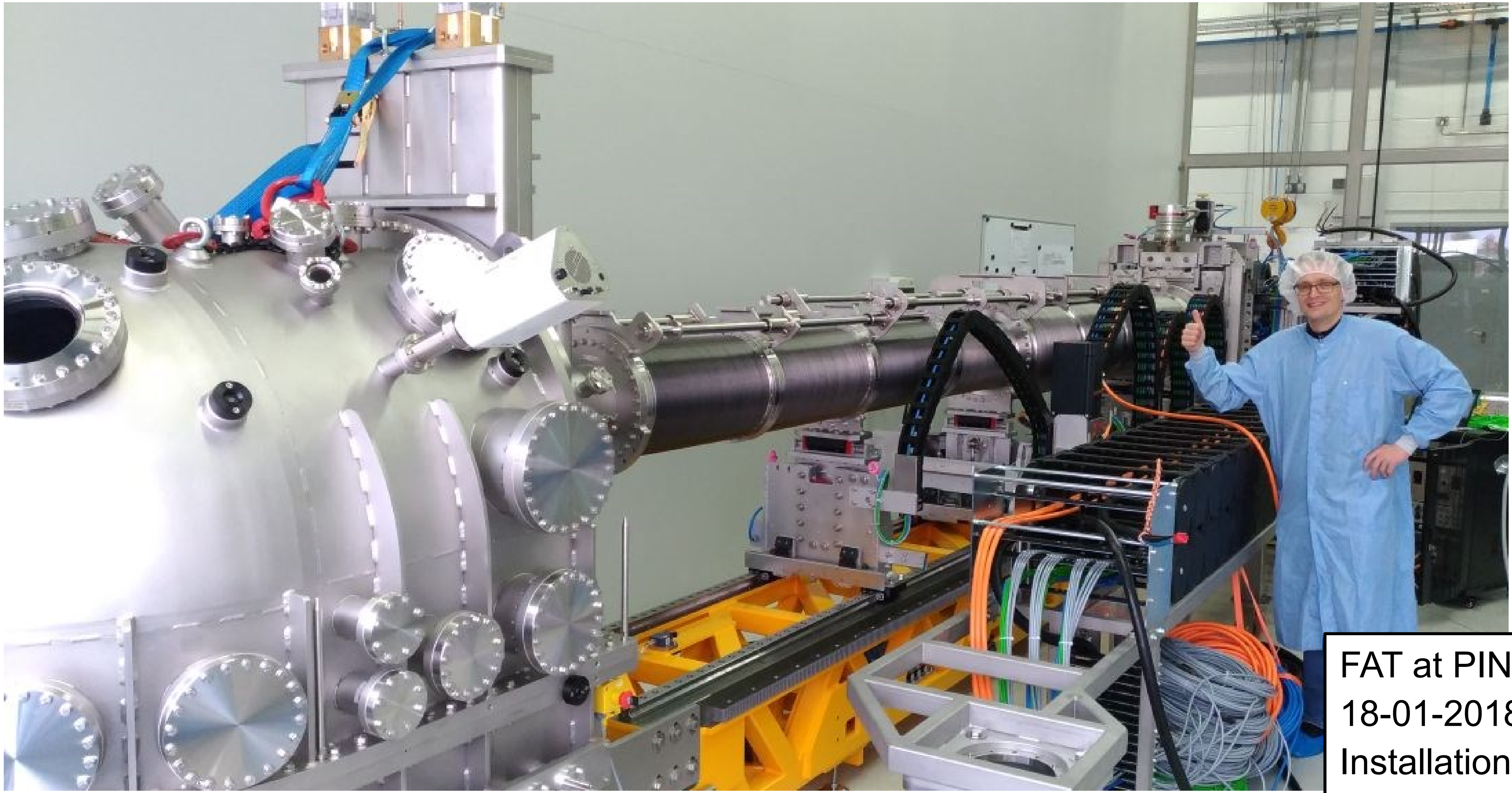


Detector ~20 cm from sample (large field of view config) or between ~3 – 8 m (SAXS – WAXS)

2θ up to ~55°

AGIPD detector size: ~ 20 x 20 cm, 200 μm pixels

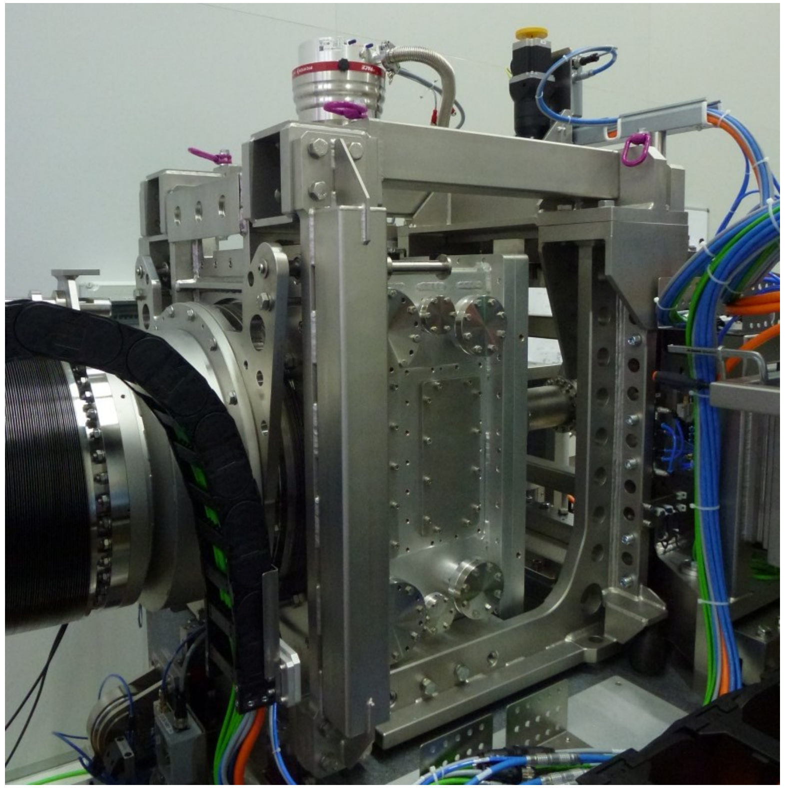
The X-ray scattering and imaging setup



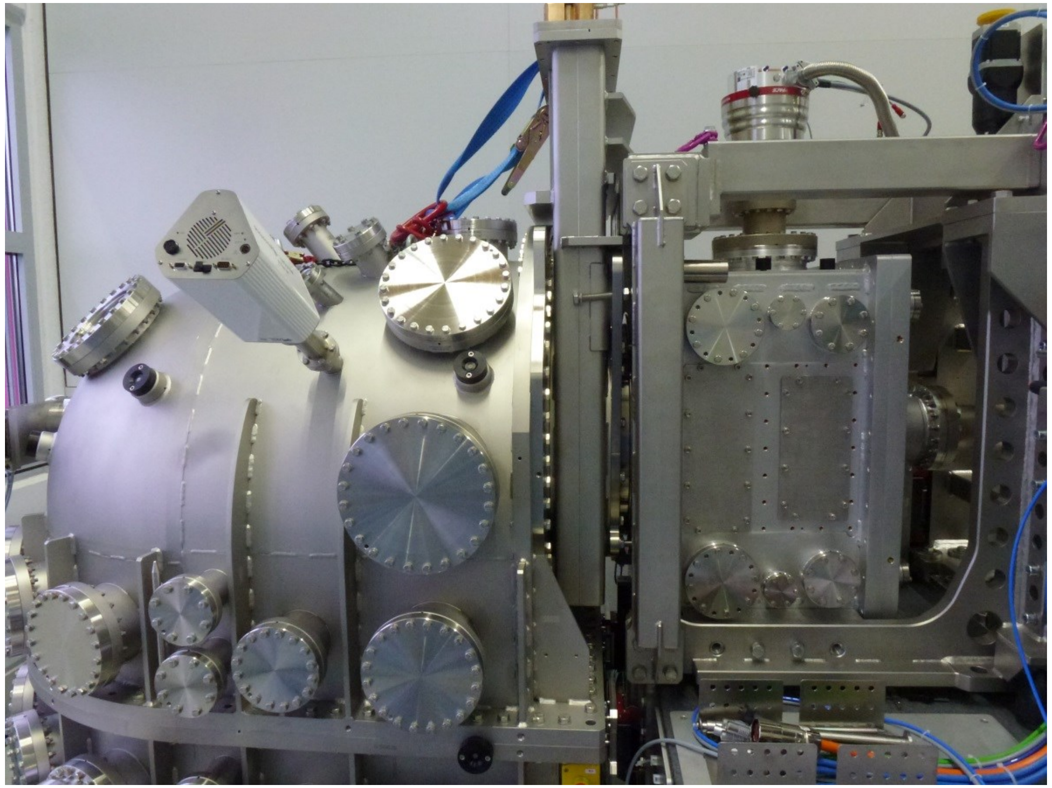
FAT at PINK GmbH
18-01-2018
Installation at MID:
Feb – Mar

Mechanical integration of 2D detector

AGIPD 8 m from sample



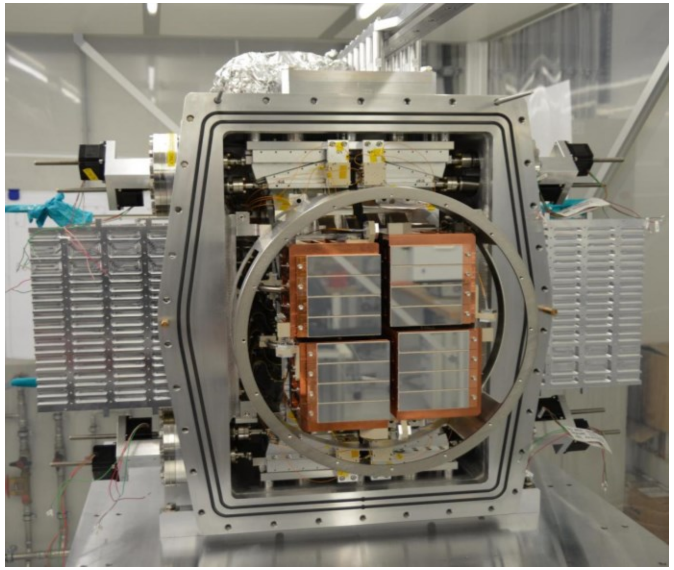
AGIPD ~20 cm from sample



- Use of AGIPD “dummy” to test mechanics and motion

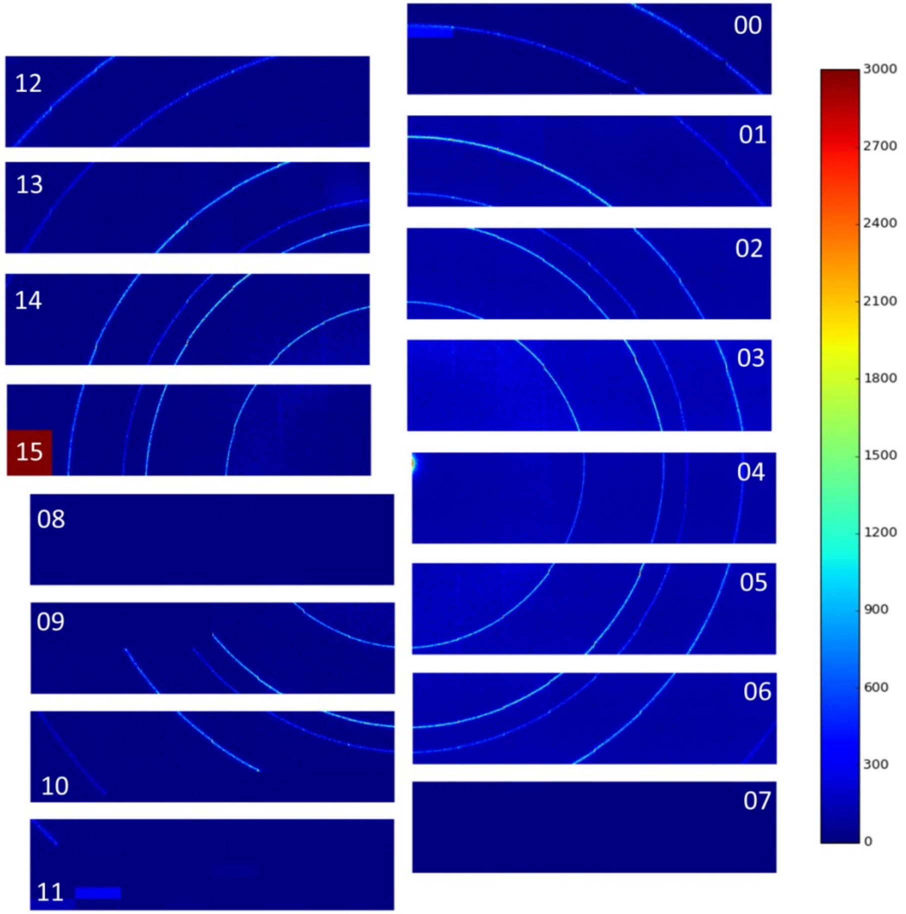
AGIPD detector

MID's AGIPD in the lab (DESY FS-DS)



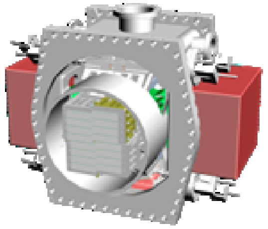
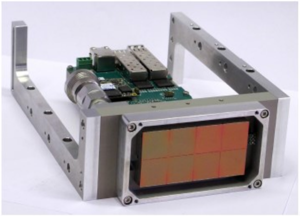
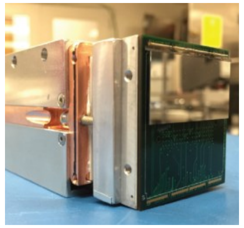
AGIPD for MID (similar to SPB's AGIPD)
- ~1M pixels, 200 μm pixel size
- MHz rep rate
- Aim: available for 1st user experiments at MID
- AGIPD patch panel: A. Liebetrau

Al_2O_3 power rings (AGIPD calibration SPB)



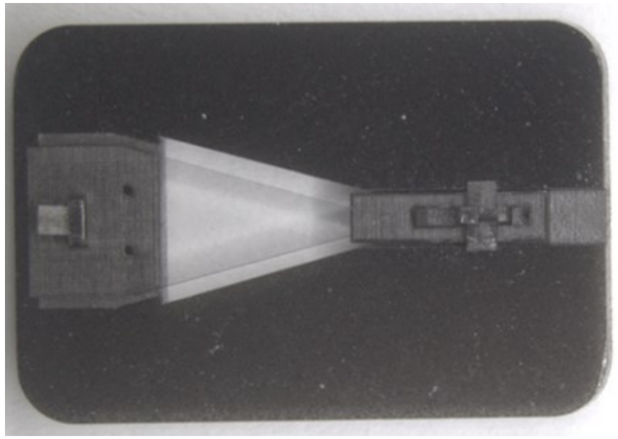
AGIPD coordinator H. Graafsma (DESY)
Slide adapted from Aschkan Allahgholi

Other detectors for MID

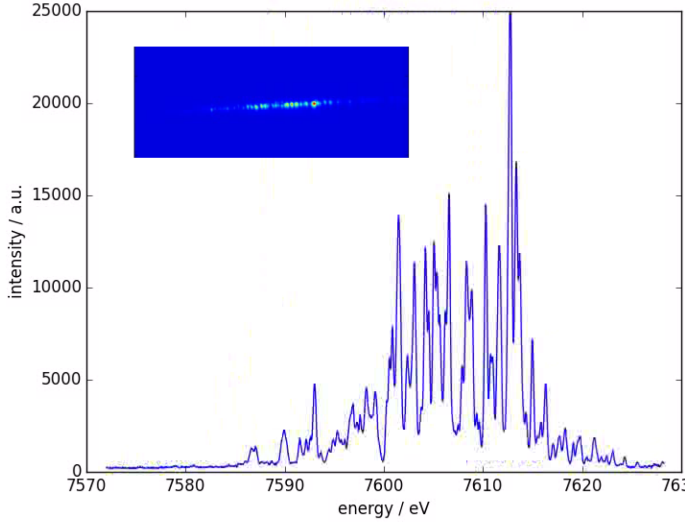
	AGIPD 1M	JUNGFRAU 1M	ePix 100 1M	GOTTHARD (-II)
				
Energy range (keV)	3-25	3-25	3-20	3-25
Dynamic range	10^4 ph/px/pulse @12 keV	10^4 ph/px/pulse @12 keV	100 ph/px @8 keV	10^4 ph/px/pulse @12 keV
Pixel size	200 × 200 μm^2	75 × 75 μm^2	50 × 50 μm^2	50 (25) μm
Noise	~1000eV	~200eV (HG)	<200eV	<750eV
Repetition rate	4.5 MHz	Currently 200kHz	120Hz	800kHz (4.5 MHz)
Number of storage cells	352	16	-	(Compact storage for full pulse train)
In-vacuum	Yes	Yes	Yes	No
(#mod) Array size	(4) 110×110mm² /mod	(2)40×80mm² /mod	(2)35×38mm² /mod.	(1) ~6×64mm² 1280 (2560) pxl

Beam diagnostics at instrument

- Towards spectral analysis at MHz rate



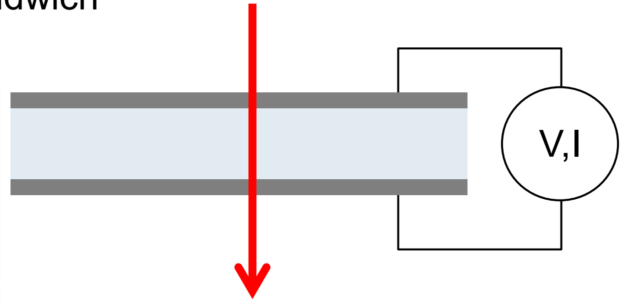
Diamond crystal bender
C*(220)

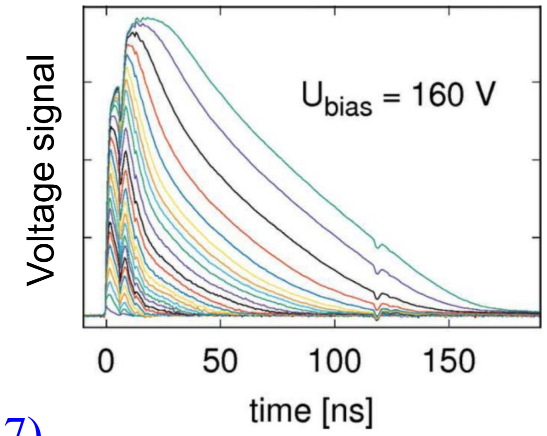


Pulse resolved spectra
recorded at LCLS (120 Hz)

- Non-invasive, MHz rate characterization of intensity and position

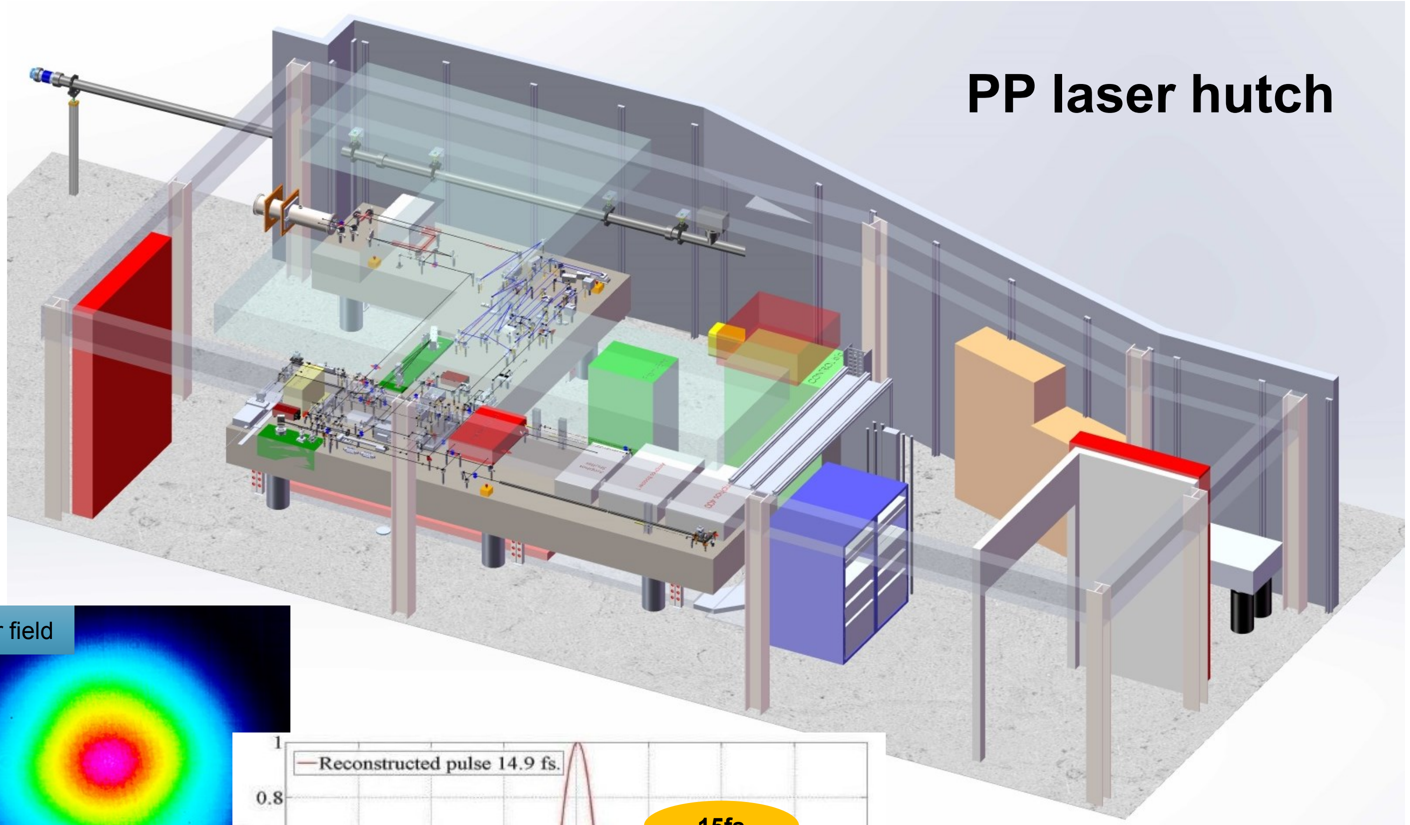
Diamond ionization chamber
Be-C-Be sandwich





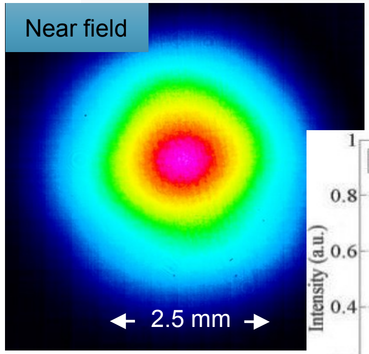
U. Boesenberg *et al.*, Optics Express **25**, 2852 (2017)
T. Roth *et al.*, J. Synchrotron Rad. **25**, 177 (2018)

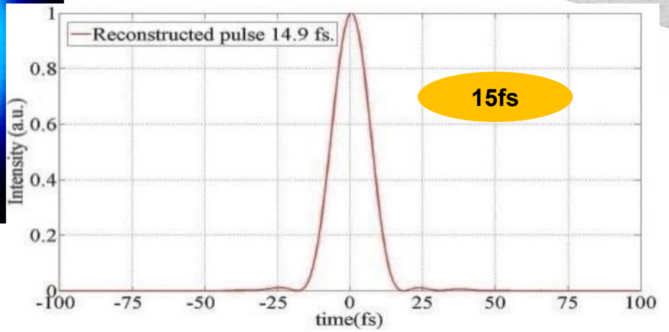
Pump-probe fs laser



Concept: fs-pumped NOPA stages
Down to ~ 15 fs pulse duration
Advanced cross-correlation scheme (low jitter)

Same pulse structure ("burst mode") as the X-rays



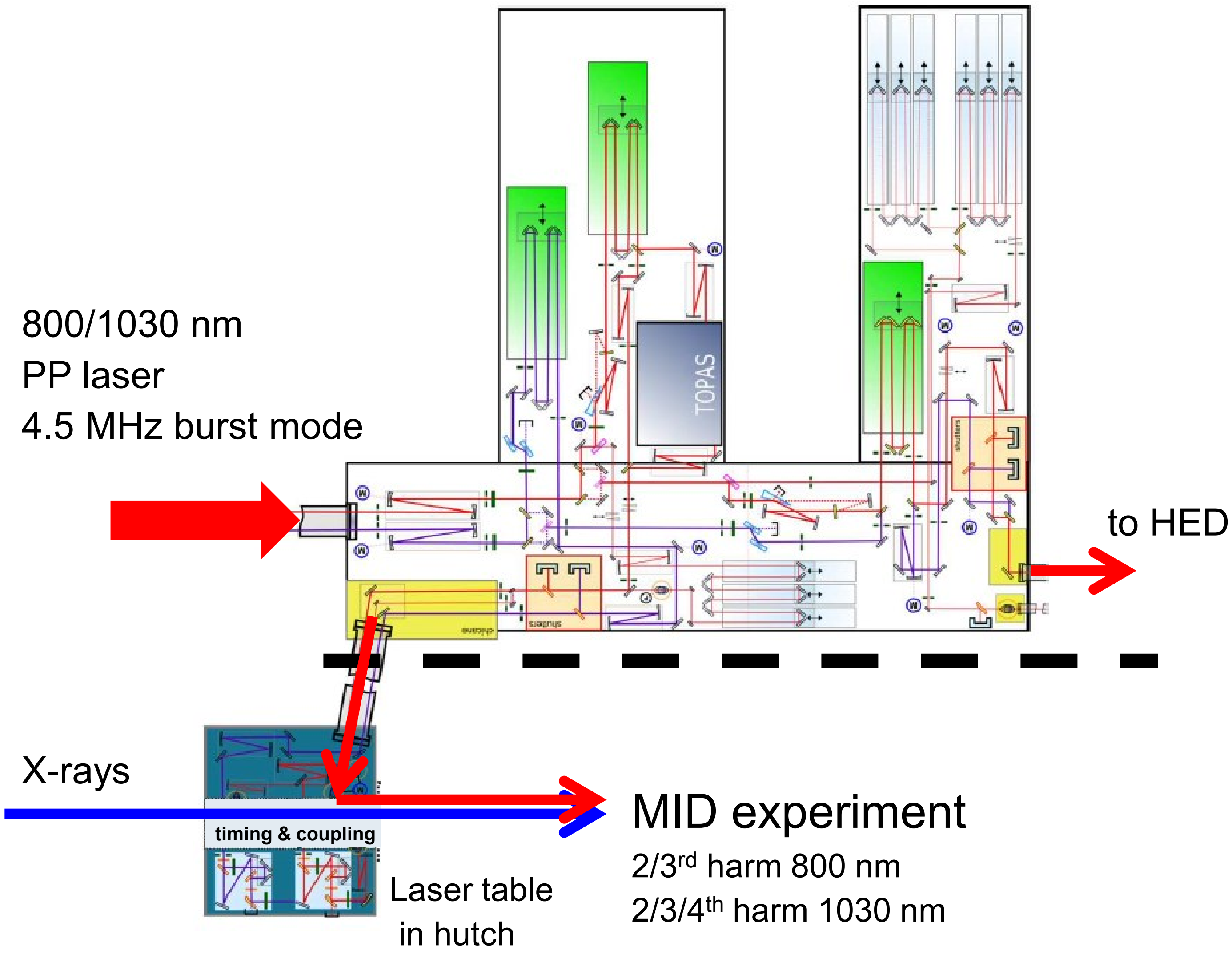


1030 nm **800 nm**

Set point	Rep-rate (MHz)	NOPA
1	4.5	I + II
2	1.13	I + II
3	0.188	I + II + III
4	0.1	I + II + III

Slide from Max Lederer
XFEL Optical Laser Group

Instrument laser hutch



- SASE-2 laser system installation will being in April 2018 (tables and infrastructure first
- SASE-2 laser hutch follows same schedule
- Beam delivered to users not before June 2019
- Still challenges with parallel installation of PP laser at SASE-2 and SASE-3
- Laser definitely not available for first batch of user experiments at SASE-2
- THz generation under study (lower rep rate)

Installation progress and plans

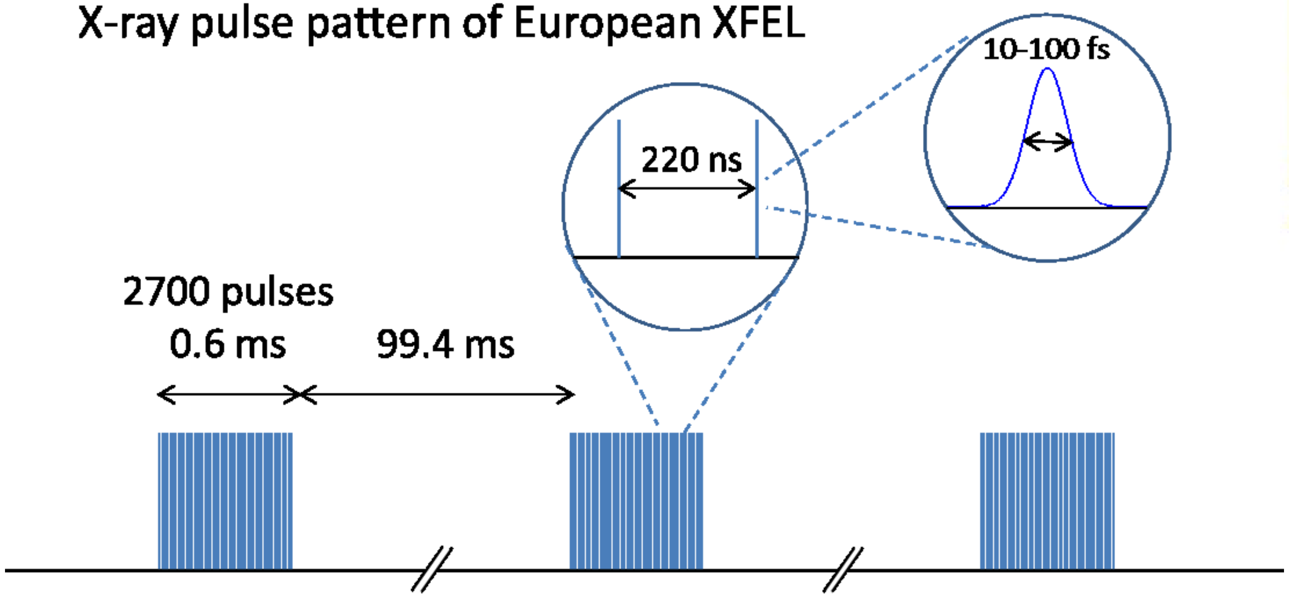
- Slits, monochromators, attenuators, CRL transfocators, shutters, DPS, mirrors arrived
- All parts to build vacuum beamline are in house
- MPC + detector arm and support to be installed in Feb-Mar 2018
- AGIPD detector to arrive this spring
- Cabling in progress; infrastructure and utilities under installation.
- Electronics installation in progress. All infrastructure for instrument only ready in June
- First lasing April, commissioning beam transport May, instrument commissioning Aug

…

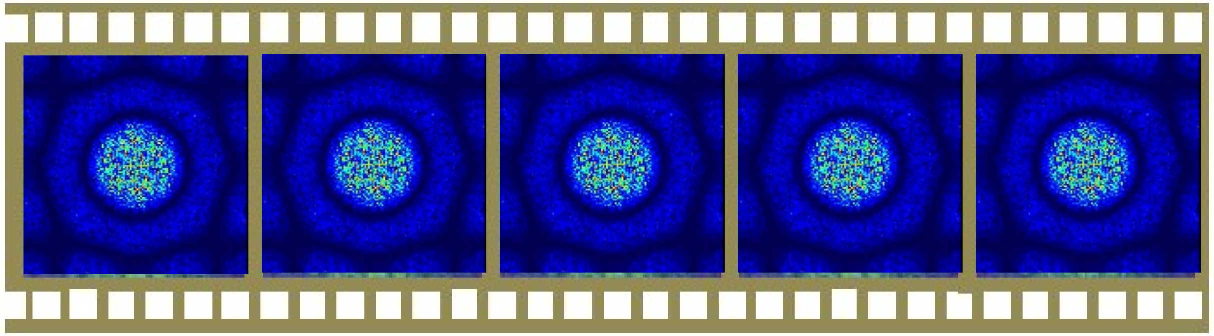
- Jan 2019 is a realistic estimate of first EUE
- fs PP laser, SDL, self-seeding,… not available for first EUE

Early science possibilities. Dynamics

X-ray pulse pattern of European XFEL



Sequential XPCS, must be non-destructive



$$g^{(2)}(t) = \frac{\langle I(\tau)I(\tau+t)\rangle}{\langle I\rangle^2}$$
$$= \beta \mid f(Q,t) \mid^2 +1$$

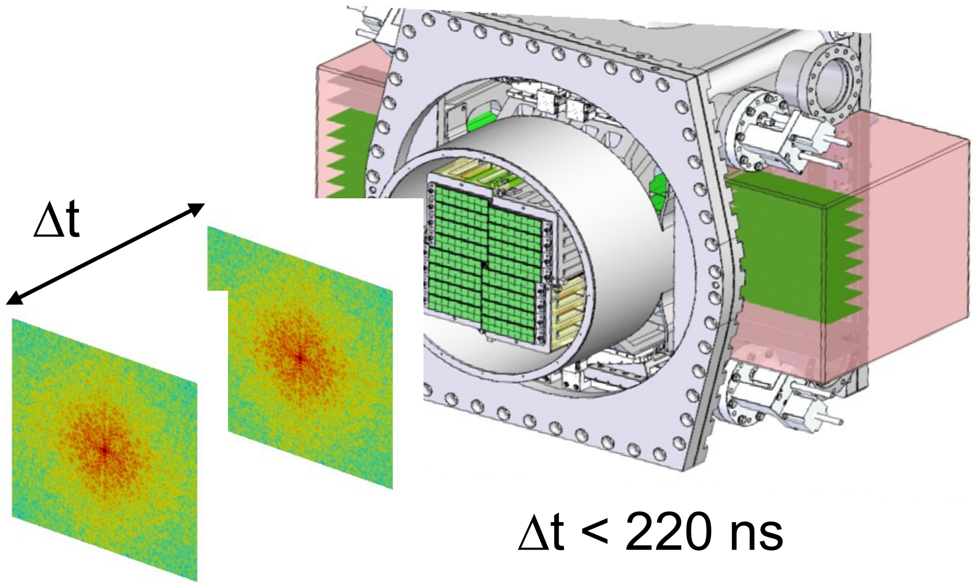
Autocorrelation at MHz rep rate…

Early science possibilities. Dynamics

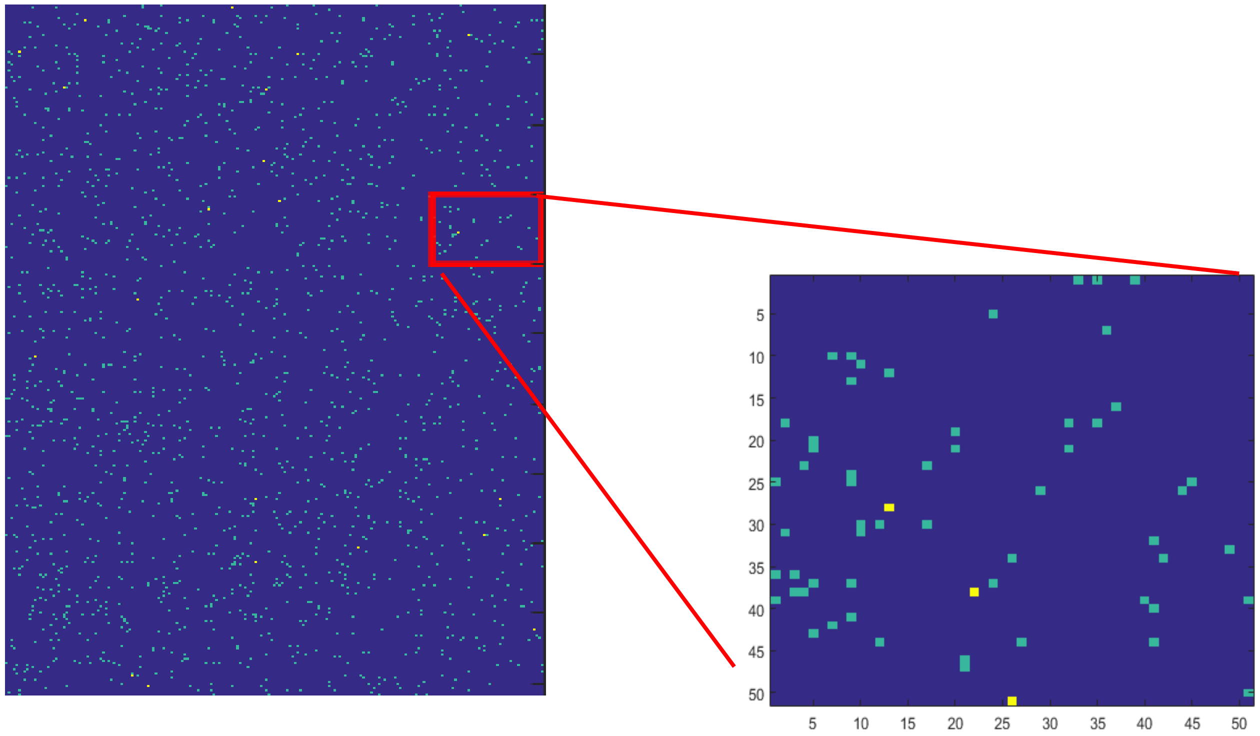
Speckle Visibility Spectroscopy

by: variation of pulse length

or by summing two pulses (SDL, or machine)



summed image



Contrast can be determined from the probability of 2-photon events P(2):

$$\beta = \frac{2P(2)}{\langle k \rangle^2} - 1$$

XSVS can be with a new sample for every pulse pair

Early science possibilities. Imaging

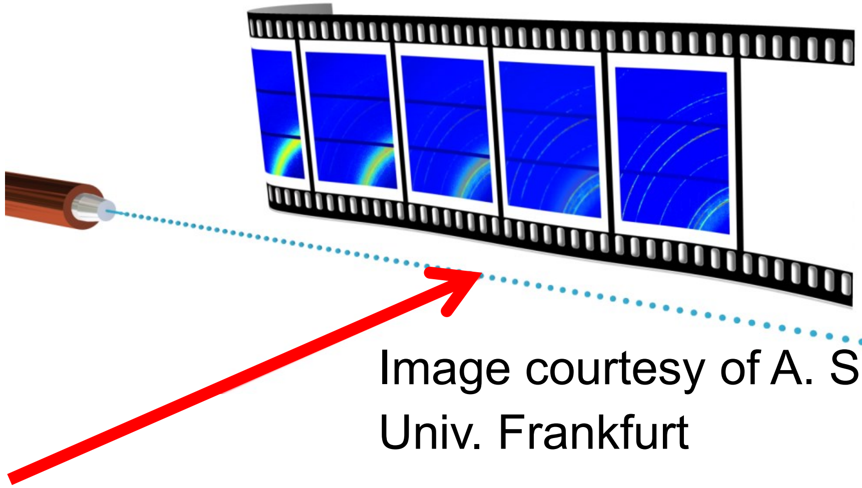
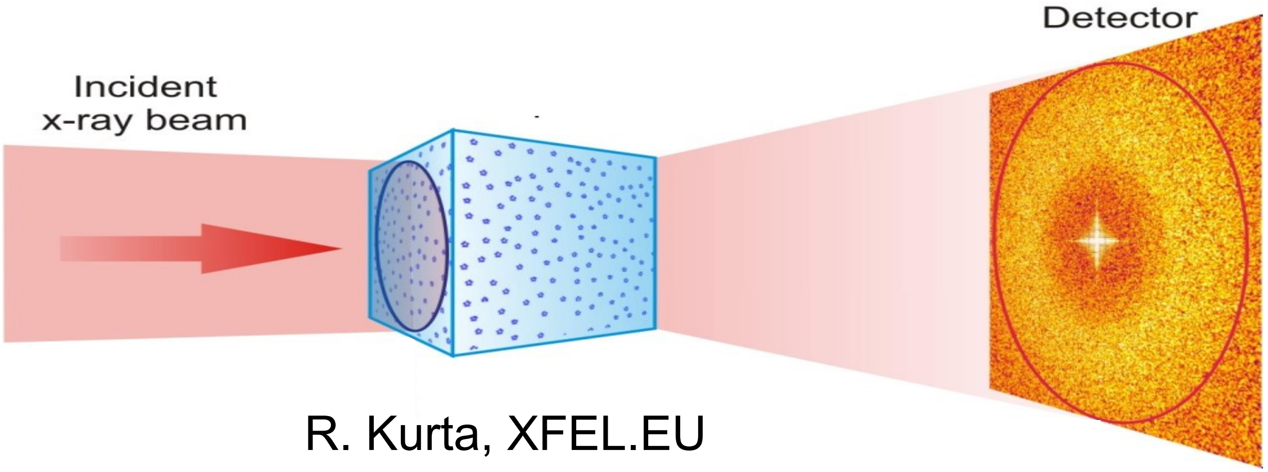
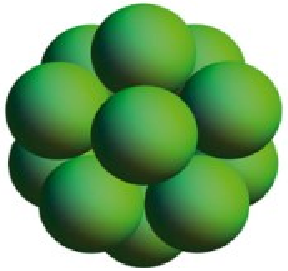


Image courtesy of A. Schottelius, Univ. Frankfurt

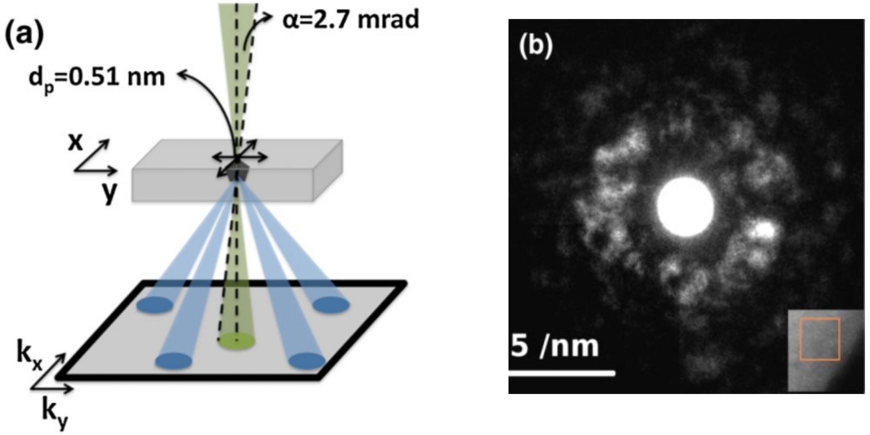


R. Kurta, XFEL.EU

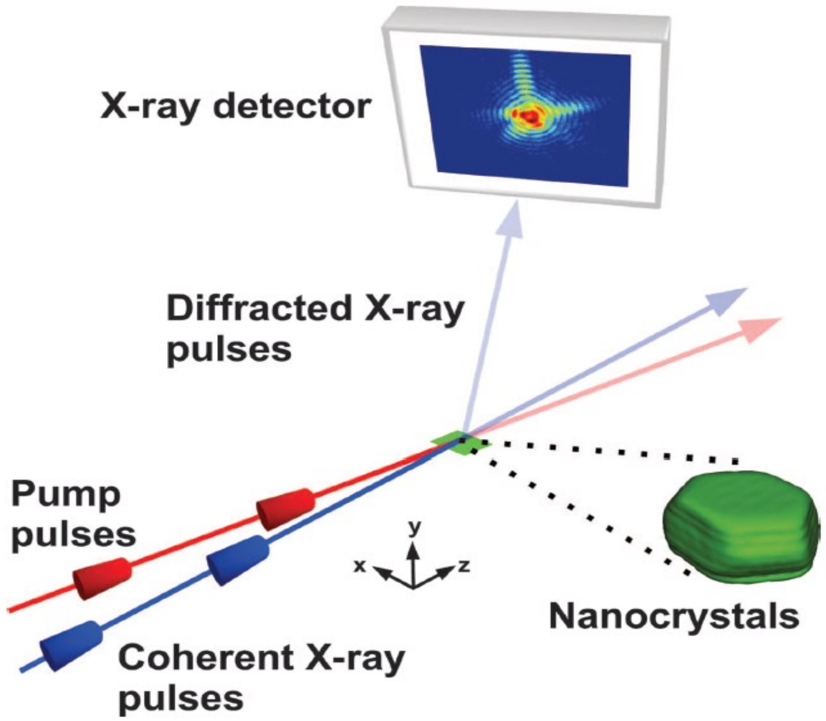


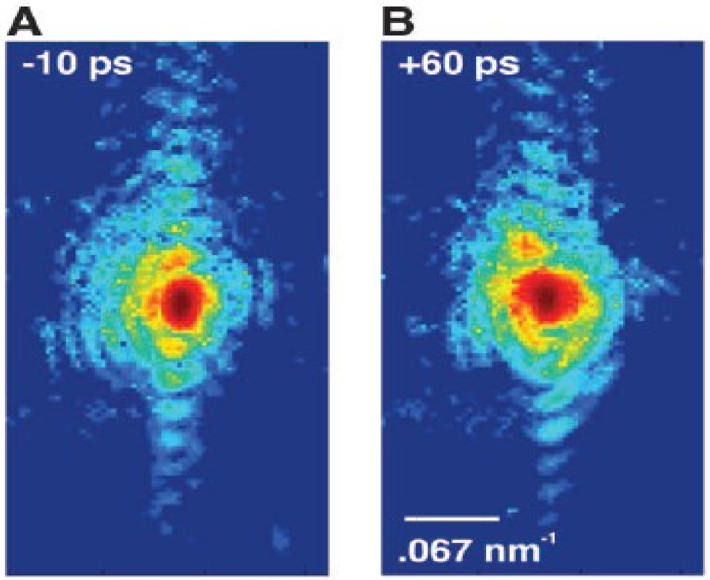
Unique combination:
Nano-beam, small scattering volume, high photon flux ph/s/μm^2

Angular correlation studies by electron diffraction
Lui *et al*, PRL **110**, 205505 (2013)



Early science possibilities. Imaging





Measuring phonons in Au nanocrystals by PP CDI at LCLS

J. Clark et al., Science **341**, 56 (2013)

ns too slow for phonons but OK for certain phase transitions, critical dynamics, surface dynamics,…

Pump-probe CDI or speckle imaging

fs PP-laser will only become available in 2019

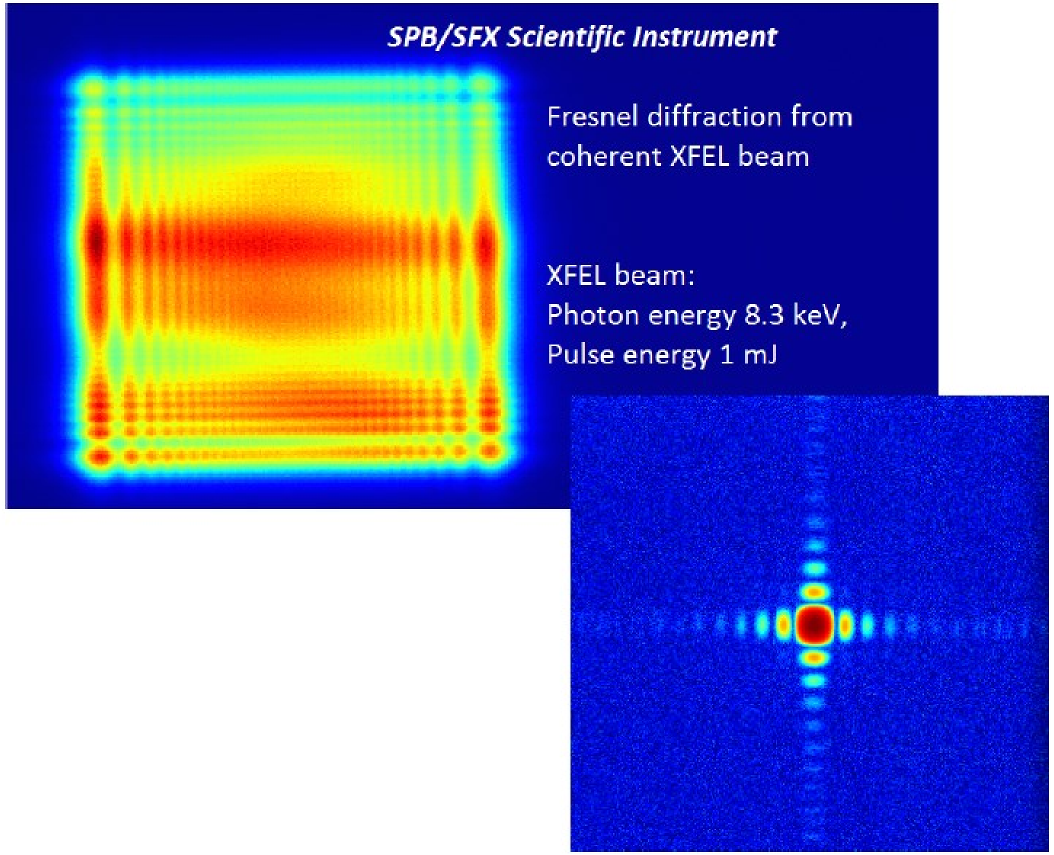
If users argue for a ns/ps laser at day 1 (science case?) we could possibly provide one (specs?)

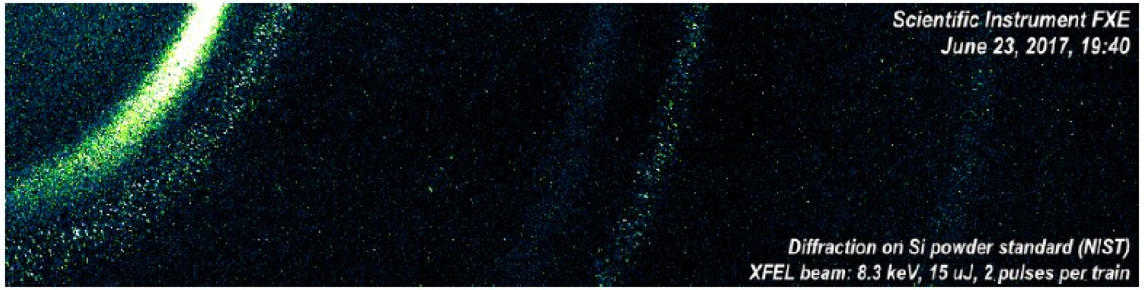
User Access

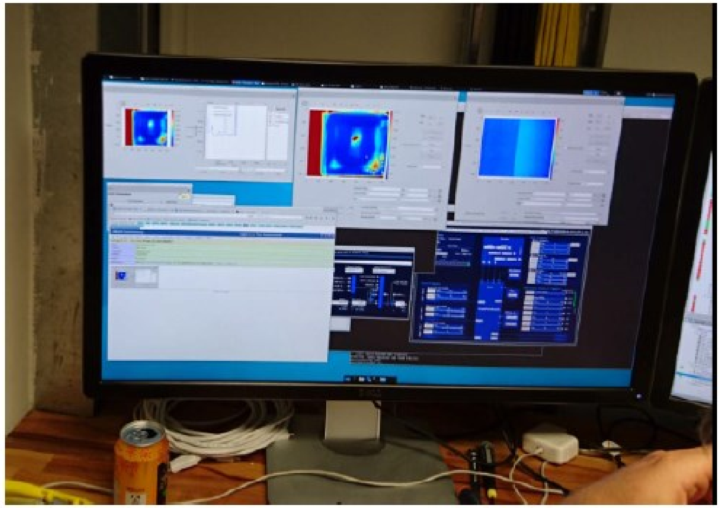
- Beamtime proposals via User Portal to the European XFEL (UPEX): **https://in.xfel.eu/upex**
- 2 calls/year, regularly from 2019
- Information for users: **https://www.xfel.eu/users** ; ask staff about instrument details
- One PRP per instrument. Guidelines: scientific merit, novelty, XFEL need, feasibility, safety,…
- Decisions communicated about 3 months after call deadline
- Travel and accommodation covered for up to 6 persons/proposals (member countries)
- XFEL travel office can help organizing the trip
- Construction of canteen and guesthouse on the way (end 2018 - 2019)
- 3rd call opens soon, deadline end of March
- EUE could start Jan 2019 at MID

1st experiments at SASE-1, June 23 2018

- Requested by Council to show ability to start operation → Council decision to formally start Operation







Karabo control system
XFEL CAS group

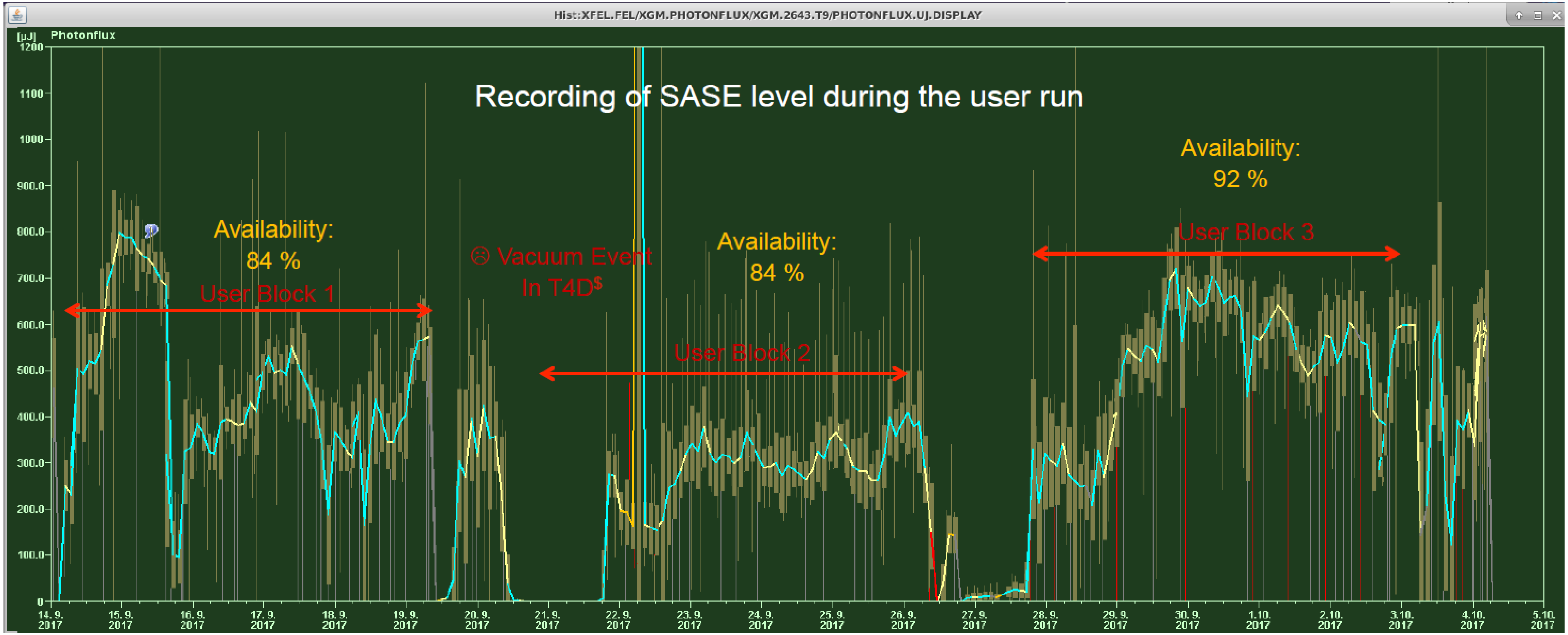
Experience from 1st experiments at SASE-1

Accelerator – Achieved e-beam parameters

Quantity	Target	Achieved
electron energy	14 GeV	14 GeV
macro pulse repetition rate	10 Hz	10 Hz
RF pulse length (flat top)	600 µs	600 µs
Bunches per second	1- 600	1-3000
bunch repetition frequency within pulse	1.13 Mhz	1.13, 4.5 MHz
bunch charge	0.5 nC	0.1, 0.5 nC
electron bunch length after compression (FWHM)	90 fs	90 fs
Slice emittance	1 mm mrad	0.6 mm mrad$
beam power	5 kW	18 kW

Courtesy: W. Decking and T. Tschentscher

Experience from 1st experiments at SASE-1

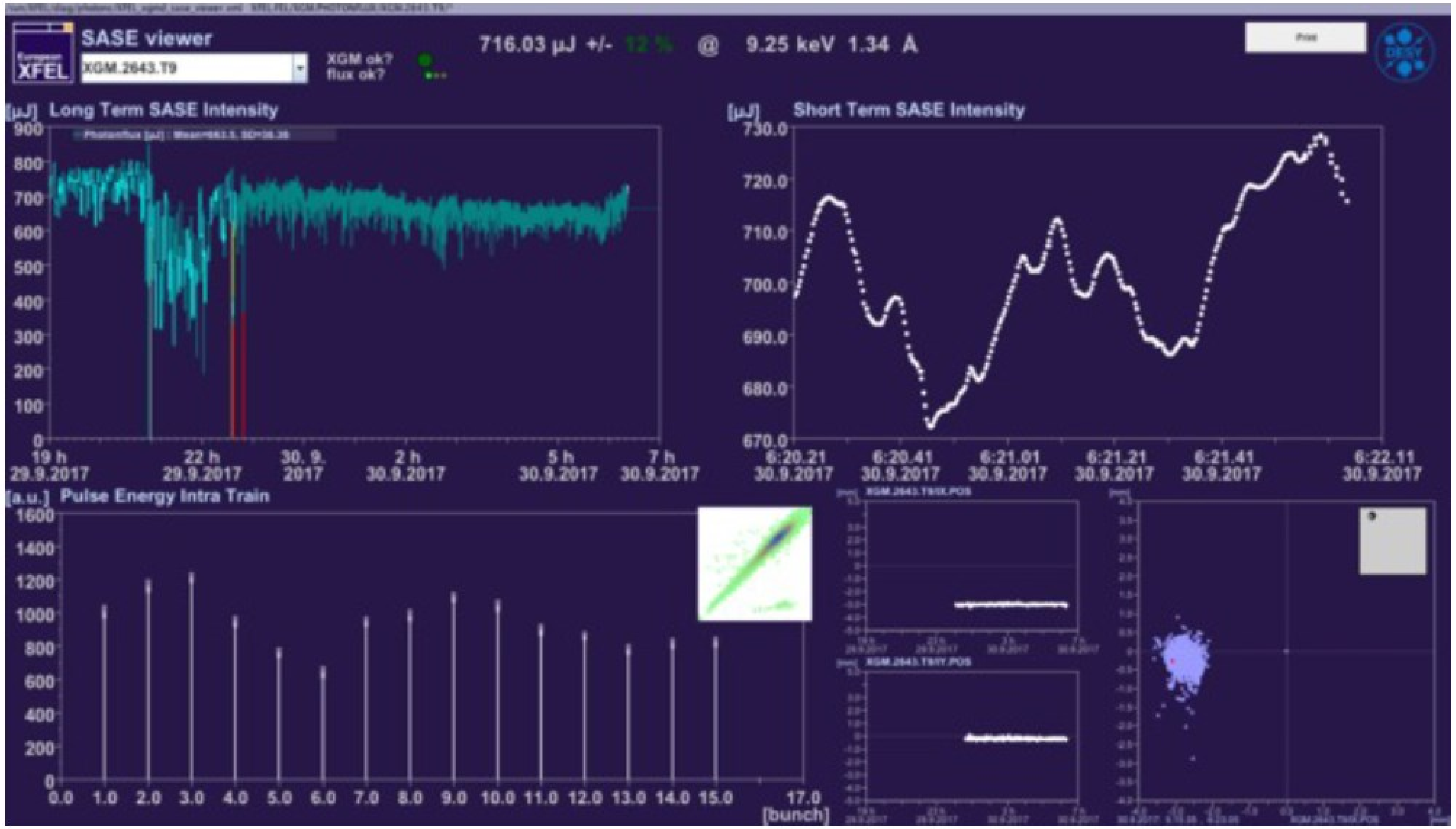


Start of user experiments: 14 Sept. 2017. Many periods >24h without interruptions is SASE beam delivery

Courtesy: W. Decking and T. Tschentscher

Experience from 1st experiments at SASE-1

Good User Day (30.09.)



- 3 Weeks of User time, 2 Experiments
  - 5 days user time/week
  - 2 days repair & tuning
  - Experiments changing every 12 hours
- 14 GeV, 500 pC, 1 to 30 bunches
- Photon energies: 9.2 – 9.3 keV
- fine tuning: Gap & number of bunches on user demand

- We were missing:
  - close control of photon wavelength
  - Possibility to look for correlation between electron and photon signals.

Courtesy: W. Decking and T. Tschentscher

3rd call for proposals

Parameter	Unit	1st Call	2nd Call	3rd Call	Regular
Photon energy (range)	keV	~ 9	~ 9 (7 – 14)	~ 9 keV	0.26 to >20
Pulse number		1 – 60 (30)	1 – 60 (300)	1 - 300	1 – 2500
Intra-train rep.-rate	MHz	1.1	1.1	1.1/4.5	0.1/1.1/4.5
Pulse energy (at source)	µJ	~ 500	~ 500	~ 500	depends
Bandwidth	%	0.14*	0.2	~ 0.2	~0.1 - .8
Pointing stability	µrad	~ 2	2	< 2	0.2
Focus size	µm	2 – 3*	5 - 15	0.1 – 20 µm	0.2 – 100
Instruments		SPB/SFX, FXE	SPB/SFX, FXE	MID	all

- Allocation period: Nov 2018 – June 2019 (tentative)
- Parameters for EUE at MID (3rd call) defined by the commissioning and progress in understanding of the SASE-2 undulator (1st lasing attempt in April 2018?)
- Steady progress of linac towards 17.5 GeV, 4.5 MHz, and 2700 pulses/train

Courtesy: W. Decking and T. Tschentscher

"Community proposals"

- Term emerged after 1st call: 3 sfx/spi proposals submitted for SPB had ~100 proposers
- All "community proposals" went through in 1st application round → 100% score
- Compare to overall success rate of 15-20%

- Can/will the MID community team up in community proposals like the biologists did ?
- Advantages: everybody in from beginning, 100% acceptance and success rate (at SPB), beneficial for MID team to manage conflicts of interest and bridge EUE with commissioning
- Challenge: different way of working together than for SR experiments
- Open process, self-organization could start at this workshop…

Questions ?