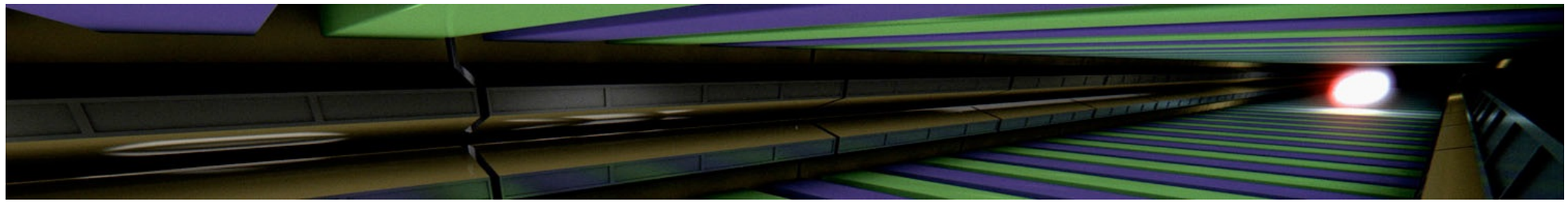
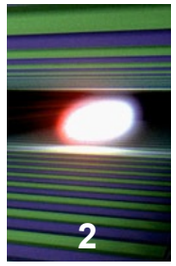


The Single Particles, Clusters and Biomolecules (SPB) Instrument of the European XFEL

Adrian Mancuso

European XFEL

Outline



- The SPB science cases
- The key goals of the instrument
- Overview & layout
- Mirror optics
- Sample delivery
- Detection
- Ancillary instrumentation
- Conclusions

European XFEL

Outline

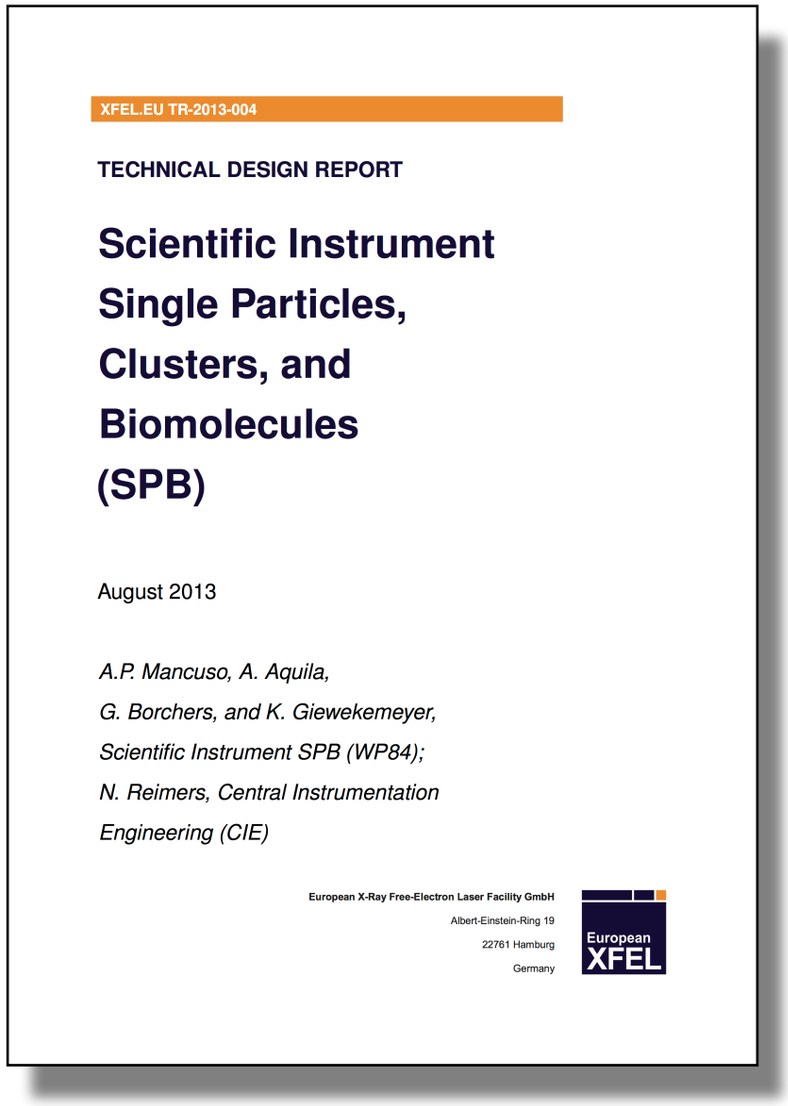
- The SPB science cases
- The key goals of the instrument
- Overview & layout
- Mirror optics
- Sample delivery
- Detection
- Ancillary instrumentation
- Conclusions

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

European XFEL

Outline

- The SPB science cases
- The key goals of the instrument
- Overview & layout
- Mirror optics
- Sample delivery
- Detection
- Ancillary instrumentation
- Conclusions


XFEL.EU TR-2013-004

TECHNICAL DESIGN REPORT

Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB)

August 2013

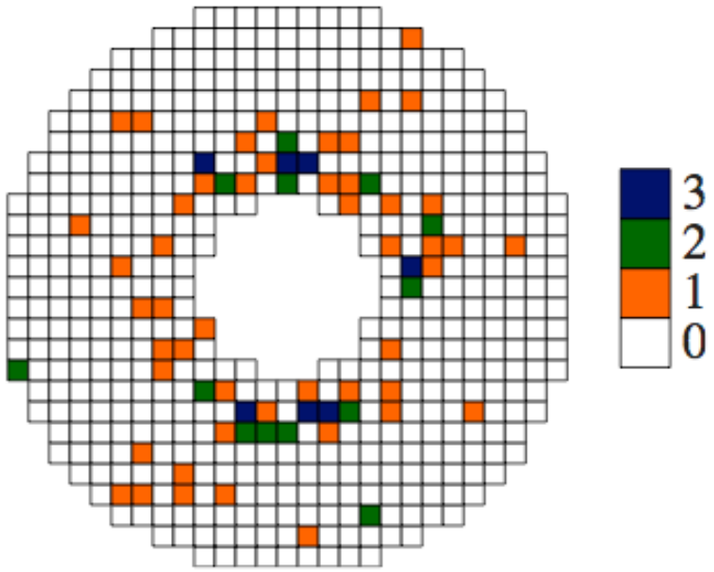
A.P. Mancuso, A. Aquila, G. Borchers, and K. Giewekemeyer, Scientific Instrument SPB (WP84); N. Reimers, Central Instrumentation Engineering (CIE)

European X-Ray Free-Electron Laser Facility GmbH
Albert-Einstein-Ring 19
22761 Hamburg
Germany

European XFEL

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

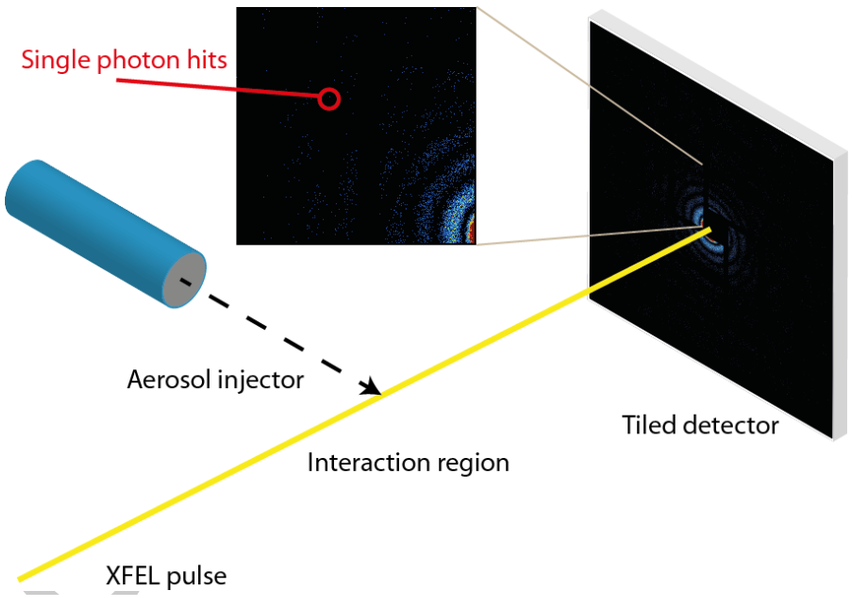
Reminder:
The 3 Canonical SPB-type Experiments



- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

A B C

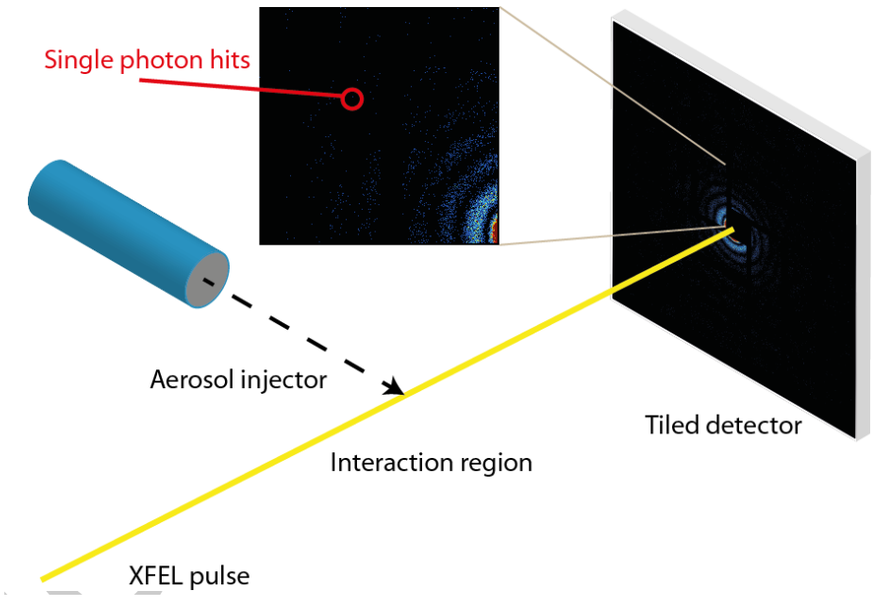
Reminder:
The 3 Canonical SPB-type Experiments



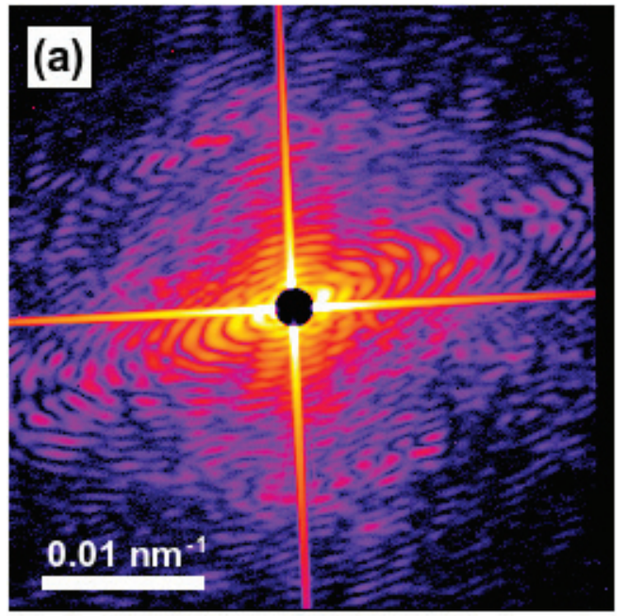
- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

A B C

Reminder:
The 3 Canonical SPB-type Experiments



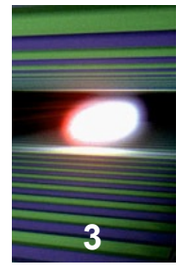
- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

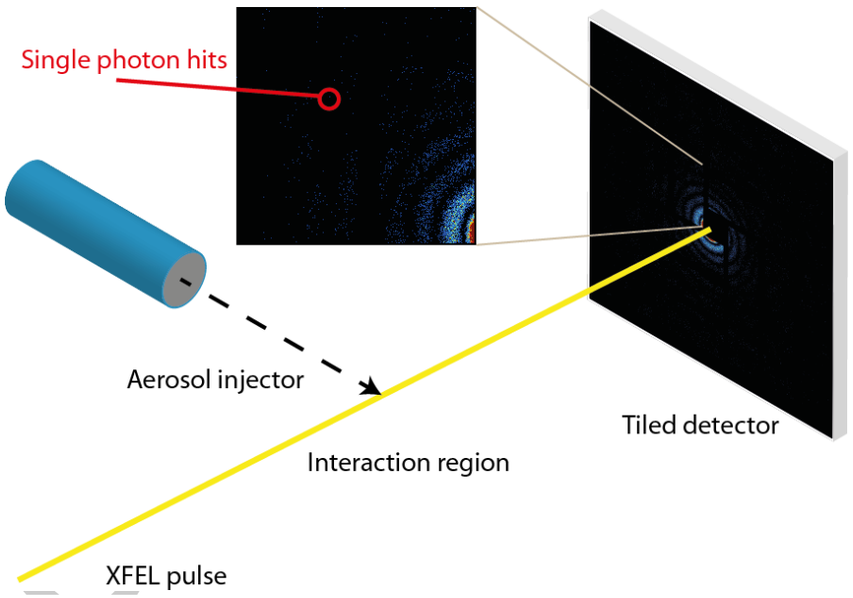


- A. P. Mancuso et al, New J. Phys. (2010)

A B C

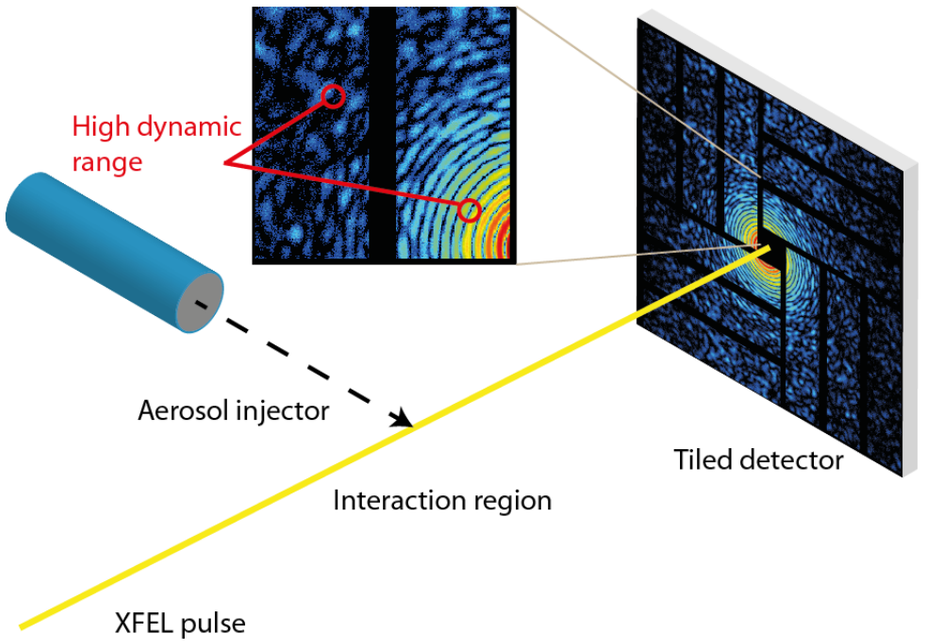
Reminder:
The 3 Canonical SPB-type Experiments





- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

A

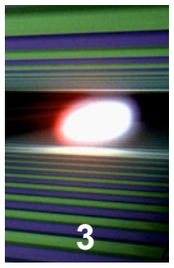


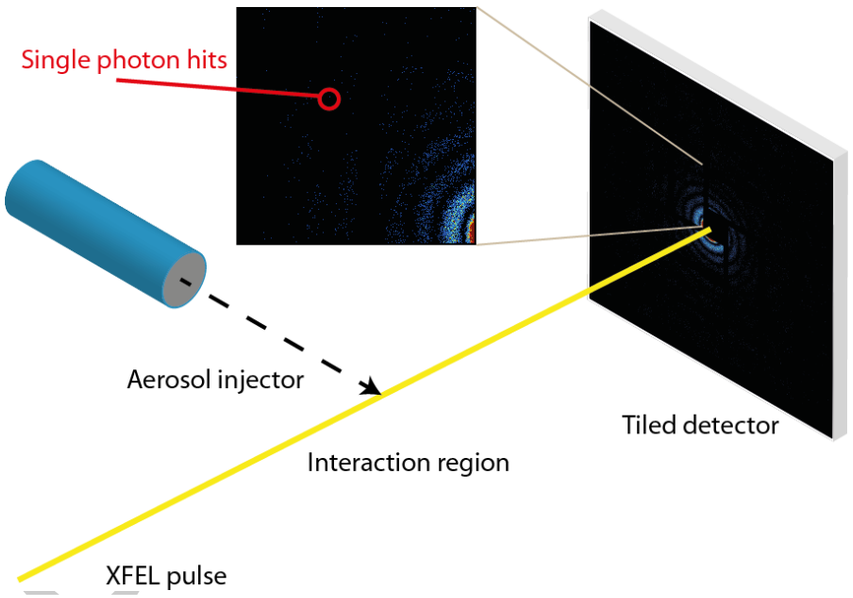
- A. P. Mancuso et al, New J. Phys. (2010)

C

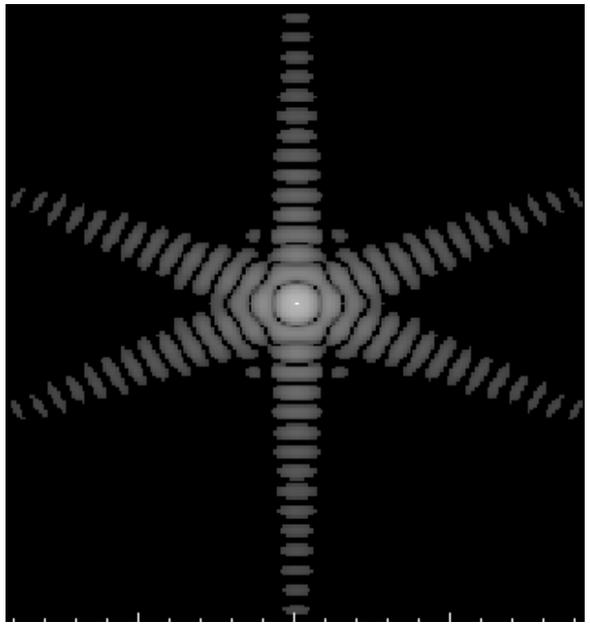
B

Reminder:
The 3 Canonical SPB-type Experiments

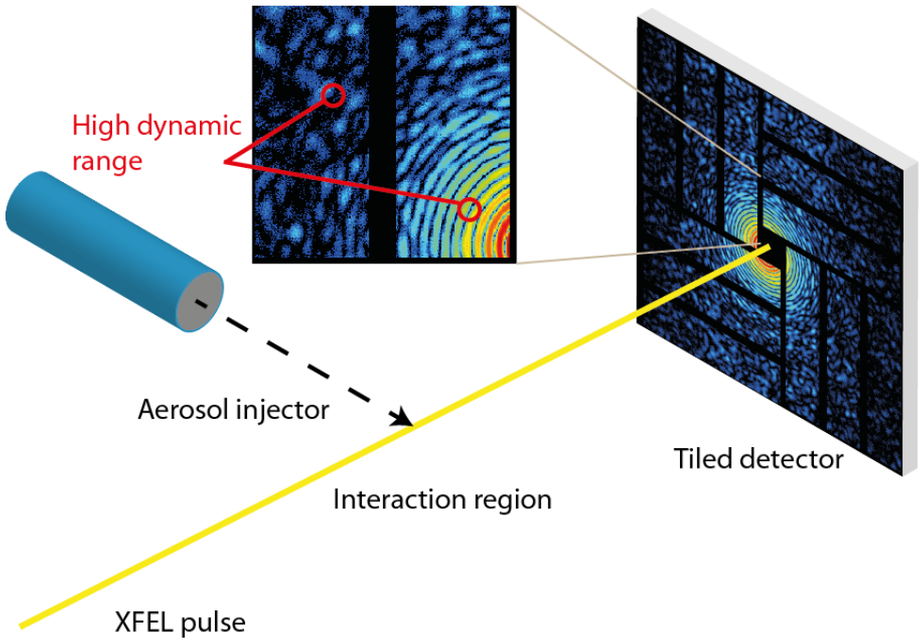




- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)



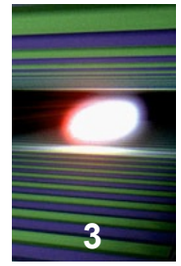
- Simulated diffraction pattern around a Bragg peak produced from an icosahedral nanocrystal

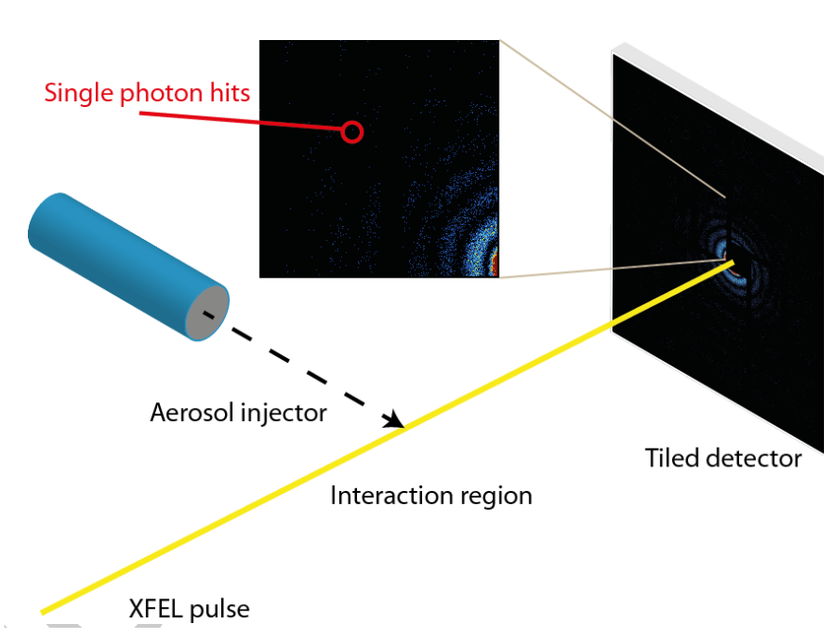


- A. P. Mancuso et al, New J. Phys. (2010)

A B C

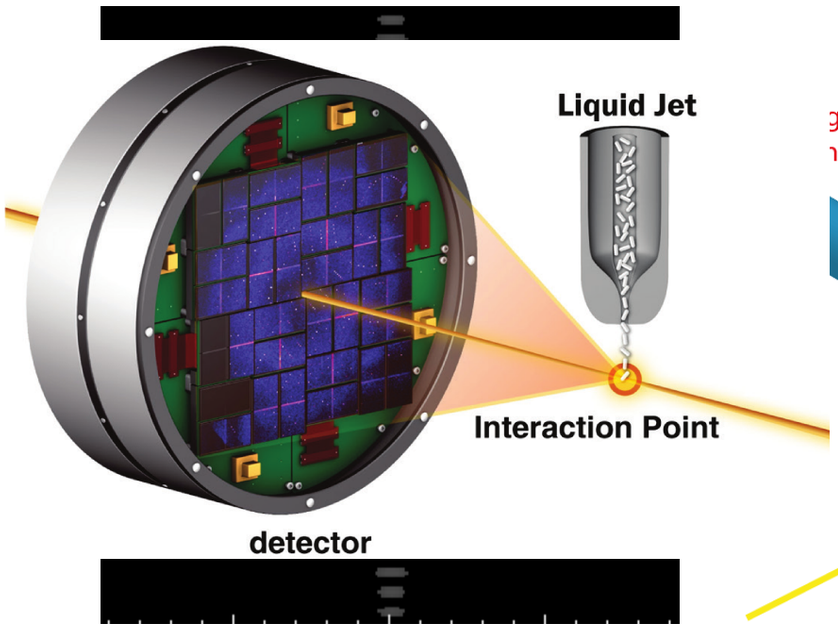
Reminder:
The 3 Canonical SPB-type Experiments





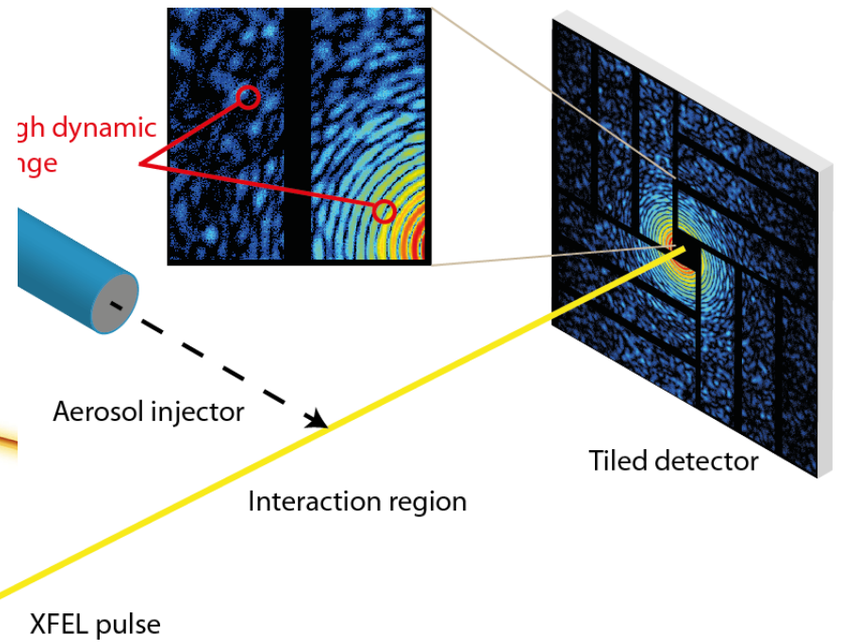
- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

A



- Simulated diffraction pattern around a Bragg peak produced from an icosahedral nanocrystal

B

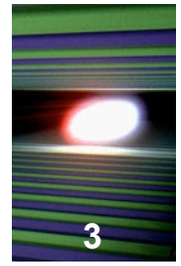


- A. P. Mancuso et al, New J. Phys. (2010)

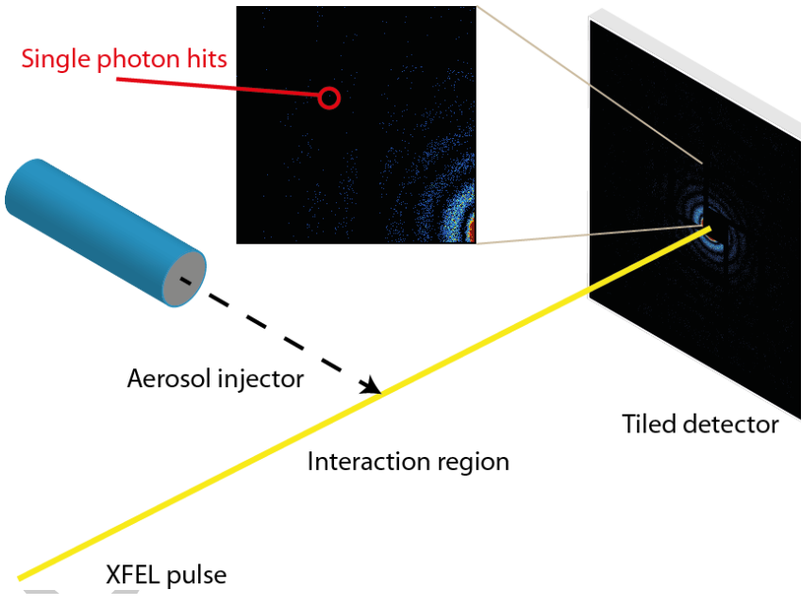
C

Image from Boutet, et al, Science, 2013.

Reminder: The 3 Canonical SPB-type Experiments

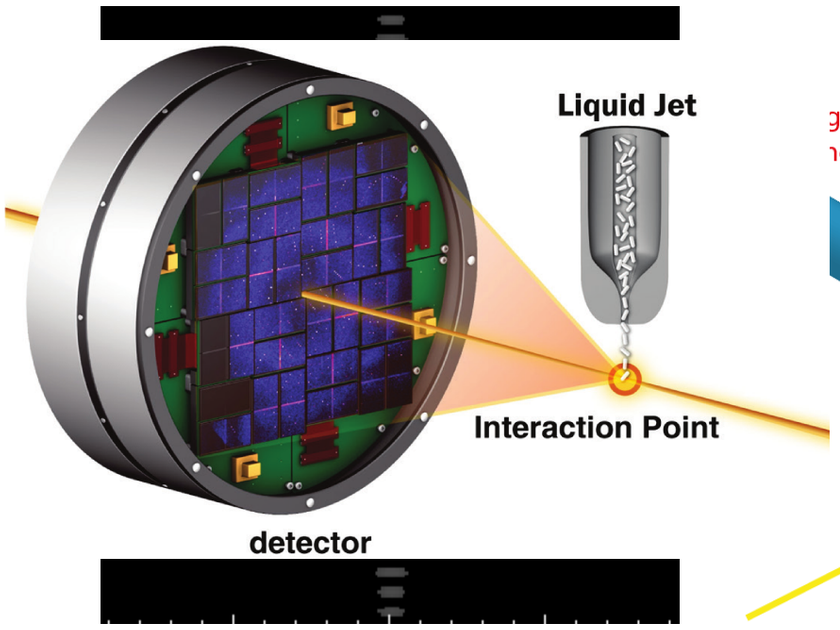


Weakly scattering



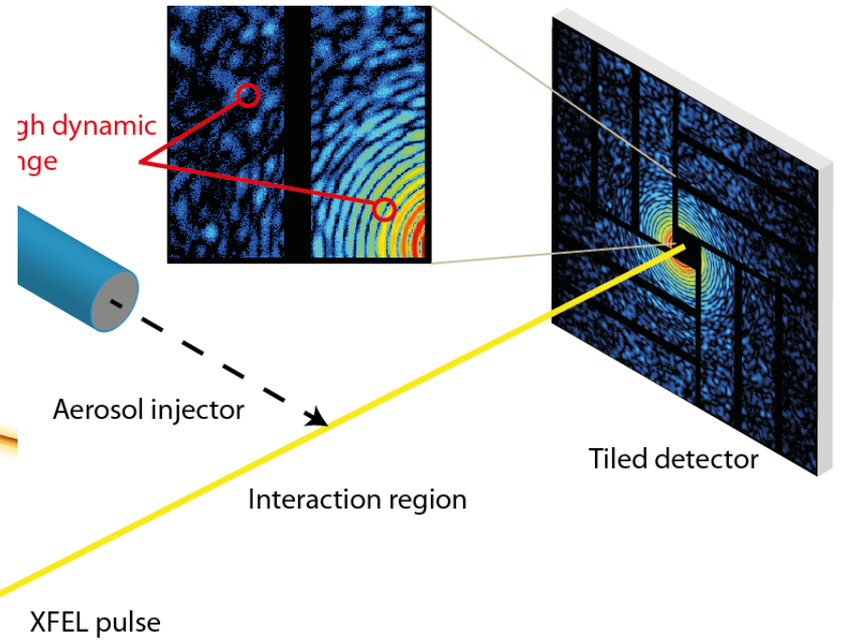
- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

Nanocrystal



- Simulated diffraction pattern around a Bragg peak produced from an icosahedral nanocrystal

Not so weakly scattering



- A. P. Mancuso et al, New J. Phys. (2010)

Image from Boutet, et al, Science, 2013.

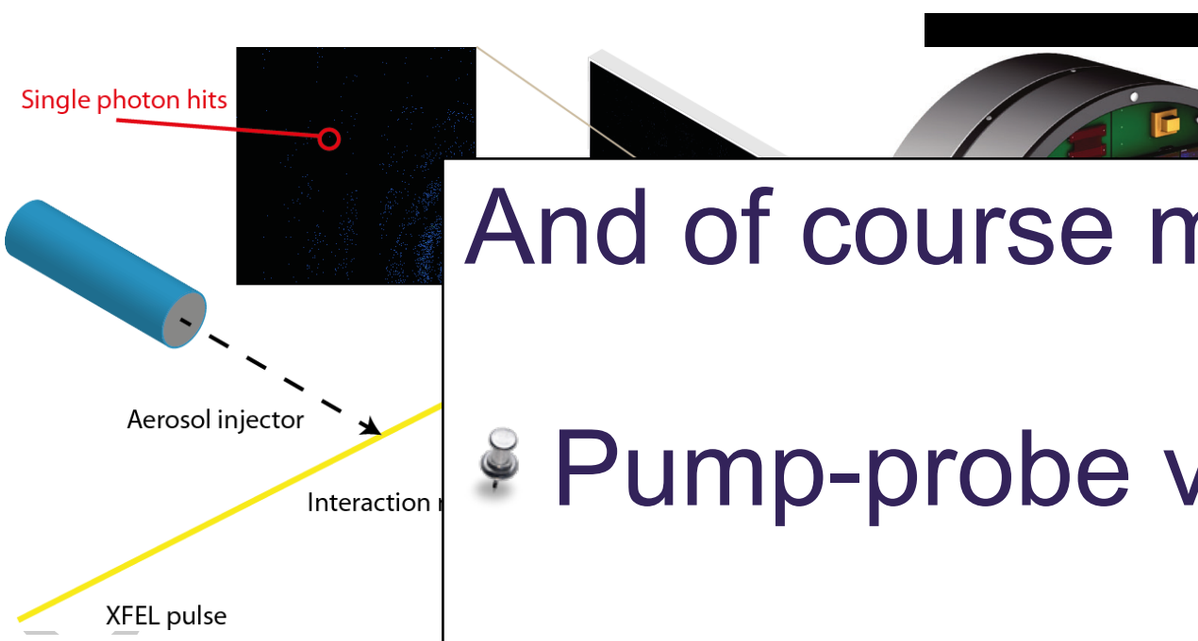
A B C

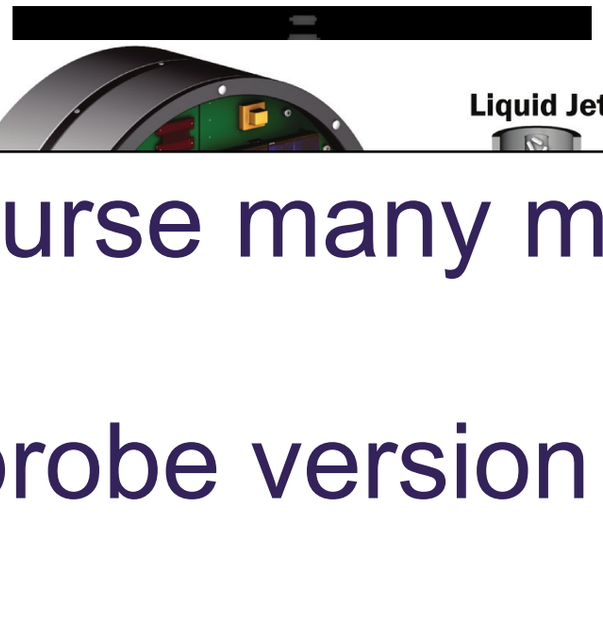
Reminder: The 3 Canonical SPB-type Experiments

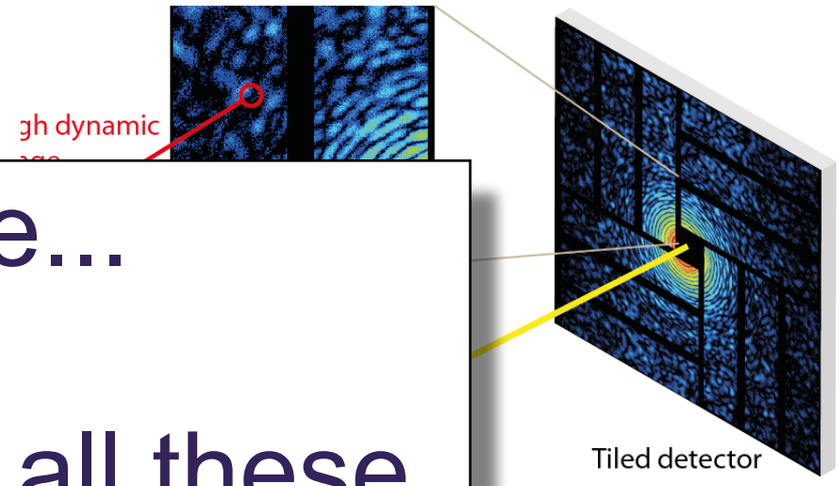
Weakly scattering

Nanocrystal

Not so weakly scattering







And of course many more...

- Pump-probe version of all these

- N. Loh and … Phys. Rev. E, **80**, 026705 (2009)

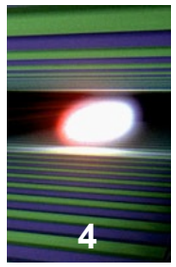
… et al, New J. Phys. (2010)

Bragg peak produced from an icosahedral nanocrystal

Image from Boutet, et al, Science, 2013.

A B C

Reminder: Requirements, Goals and Constraints

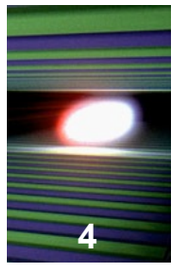


[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints



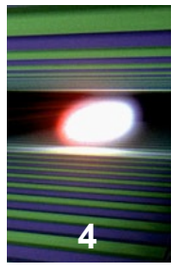
- (R) 3–16 keV, forward scattering instrument

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints



- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints

- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints

- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints

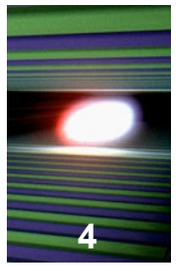
- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints



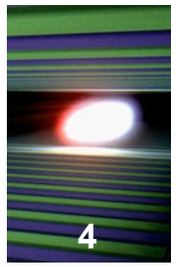
- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)
- (G) Highest quality wavefront

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints



- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)
- (G) Highest quality wavefront
- (G) Full train rate compatible

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints

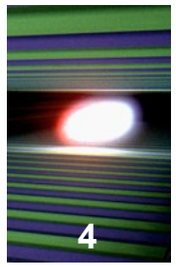
- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)
- (G) Highest quality wavefront
- (G) Full train rate compatible
- (C) Pulse durations < 10 fs – 100 fs

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints



- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)
- (G) Highest quality wavefront
- (G) Full train rate compatible
- (C) Pulse durations < 10 fs – 100 fs
- (C) Highly spatially coherent beam

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints

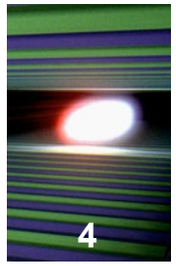
- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)
- (G) Highest quality wavefront
- (G) Full train rate compatible
- (C) Pulse durations < 10 fs – 100 fs
- (C) Highly spatially coherent beam
- (C) 930 m to source (large beam at exp. hall)

[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

Reminder: Requirements, Goals and Constraints



- (R) 3–16 keV, forward scattering instrument
- (R) Micron-scale and 100 nm scale focal spots
- (R) Natural bandwidth (< 0.3%)
- (R) High dynamic range, single photon sensitivity and large number of pixels in detector(s)
- (G) Highest pulse energies delivered to sample (maximise transmission)
- (G) Highest quality wavefront
- (G) Full train rate compatible
- (C) Pulse durations < 10 fs – 100 fs
- (C) Highly spatially coherent beam
- (C) 930 m to source (large beam at exp. hall)

	Electron energy: 17.5 GeV									
Photon energy [keV]	2.76		4.96		8.27		12.4		15.5	
FWHM pulse length [fs]	–	–	–	–	1.68	107	1.68	107	1.68	107
FWHM bandwidth [%]	–	–	–	–	0.21	0.14	0.18	0.12	0.16	0.10
Bunch charge [nC]	–	–	–	–	0.02	1.00	0.02	1.00	0.02	1.00
RMS electron energy jitter [MeV]	–	–	–	–	4.10	2.00	4.10	2.00	4.10	2.00
Expected FWHM wavelength jitter[a] [%]	–	–	–	–	0.11	0.05	0.11	0.05	0.11	0.05
Photons per pulse [10^{12}]	–	–	–	–	0.06	2.29	0.032	0.91	0.02	0.58
Pulse energy [mJ]	–	–	–	–	8.09e-2	3.04	6.35e-2	1.80	5.36e-2	1.43
Peak power [GW]	–	–	–	–	48.1	28.4	37.8	16.8	31.9	13.3
Source size [µm]	–	–	–	–	28.6	43.0	27.3	42.7	26.5	46.5
Source divergence [µrad]	–	–	–	–	2.83	1.91	2.00	1.35	1.65	1.07
Coherence degree	–	–	–	–	0.96	0.941	0.96	0.82	0.96	0.71

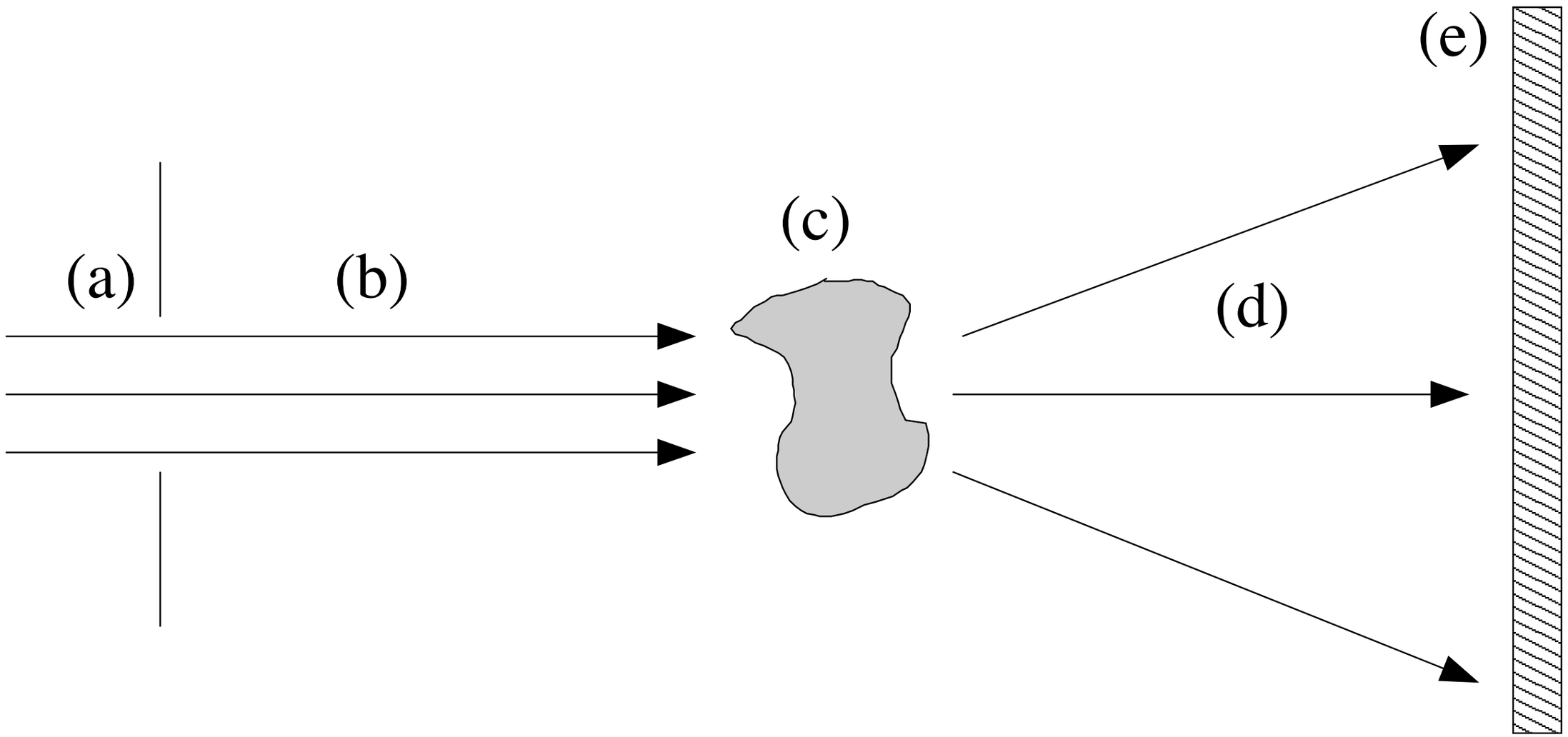
[1] A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. dx.doi.org/10.3204/XFEL.EU/TR-2011-007

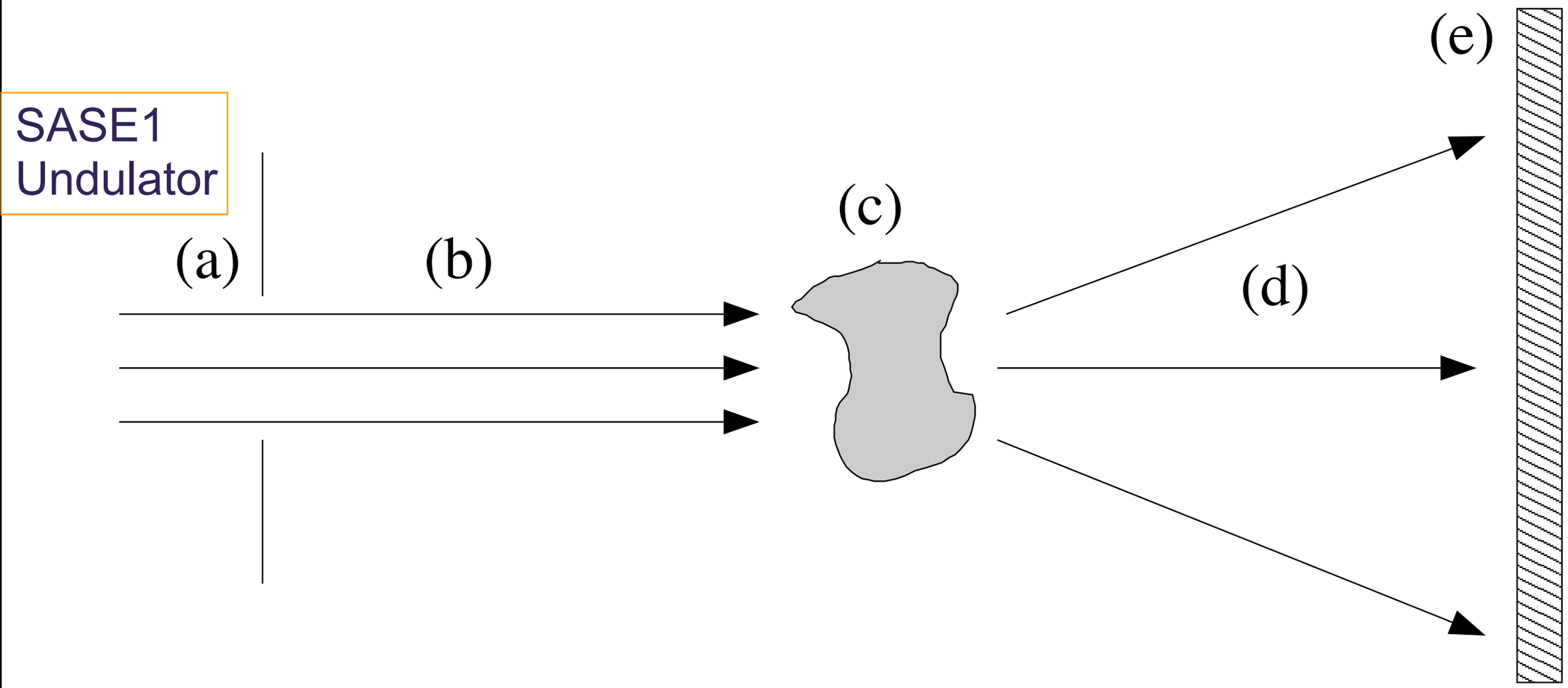
[3] A. P. Mancuso, et al, Technical Design Report: Scientific Instrument SPB, 2013. dx.doi.org/10.3204/XFEL.EU/TR-2013-004

[4] E. A. Schneidmiller and M. V. Yurkov, “Photon beam properties at the European XFEL (Dec 2010 revision).”

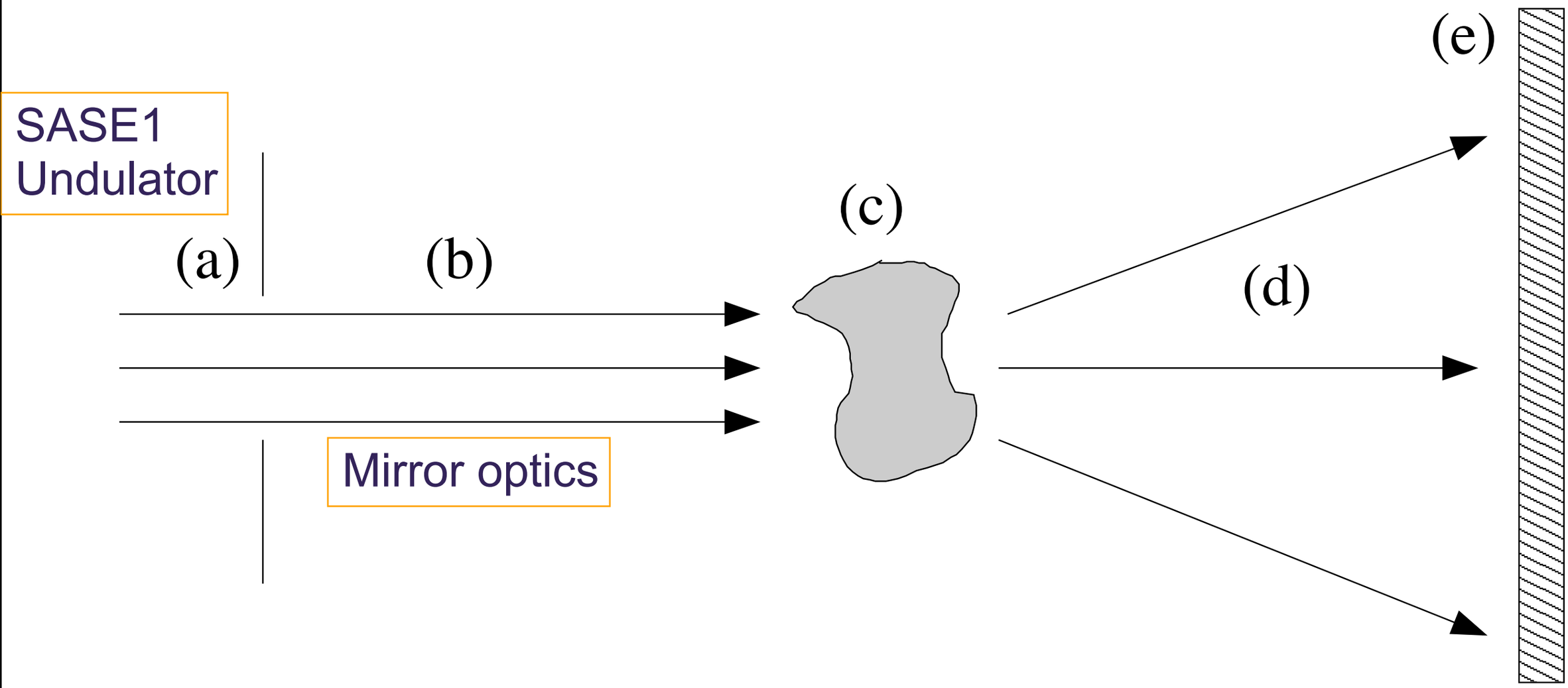
The big picture features of SPB: Forward scattering for all



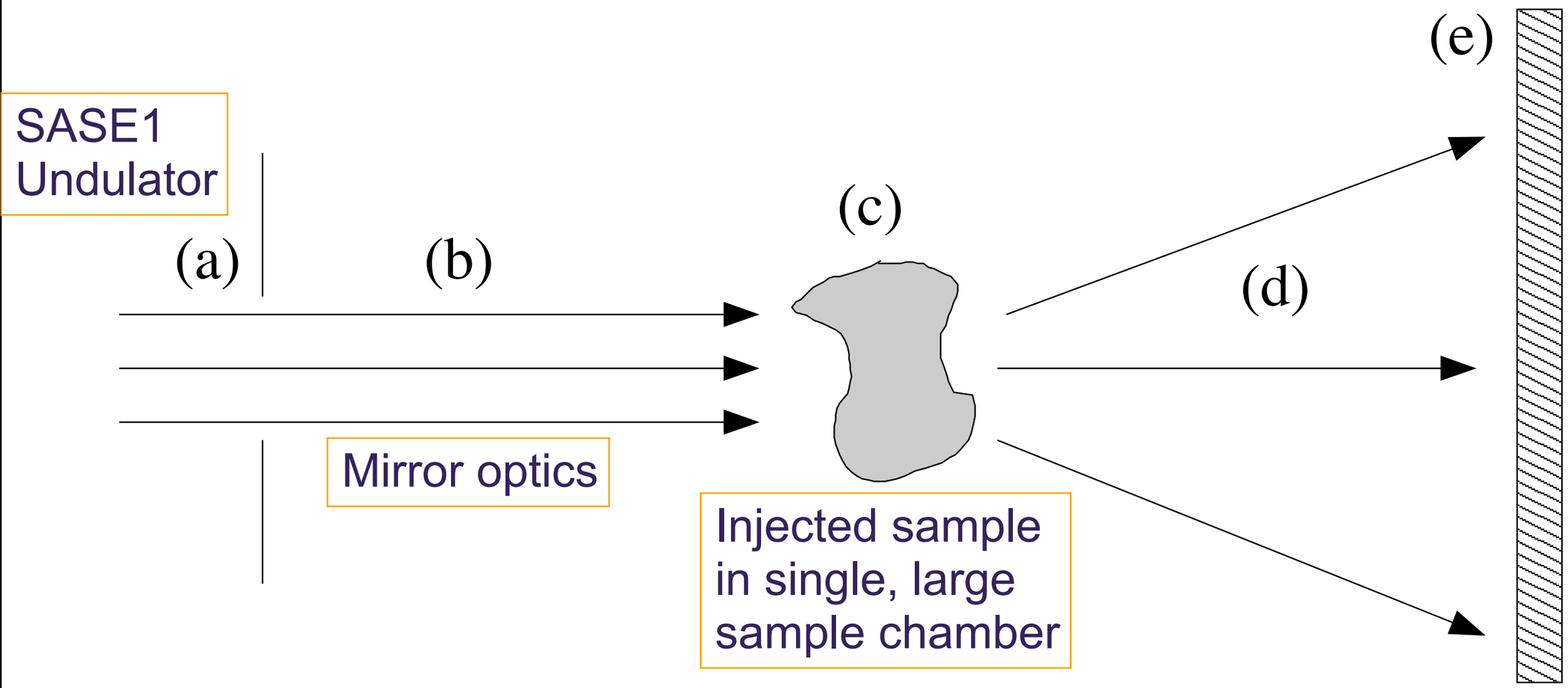
The big picture features of SPB: Forward scattering for all



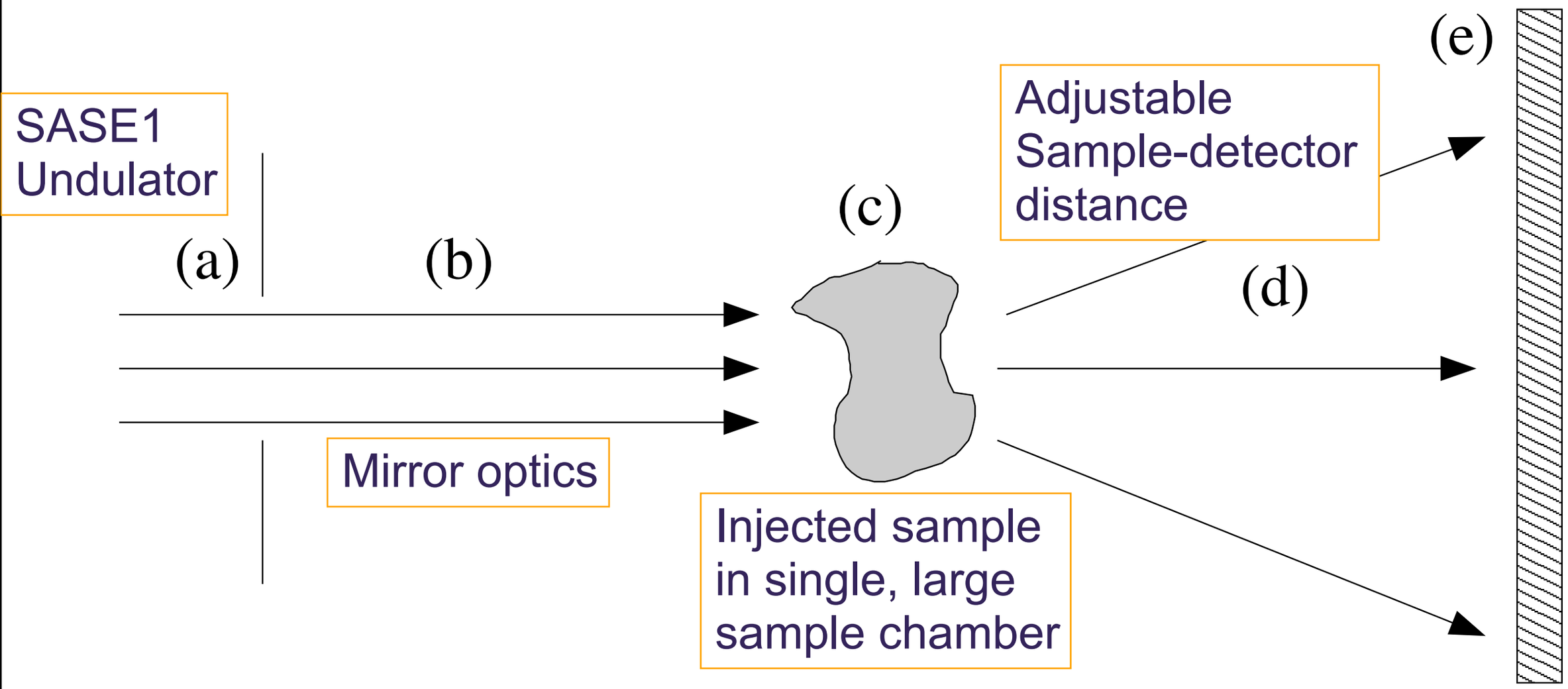
The big picture features of SPB: Forward scattering for all



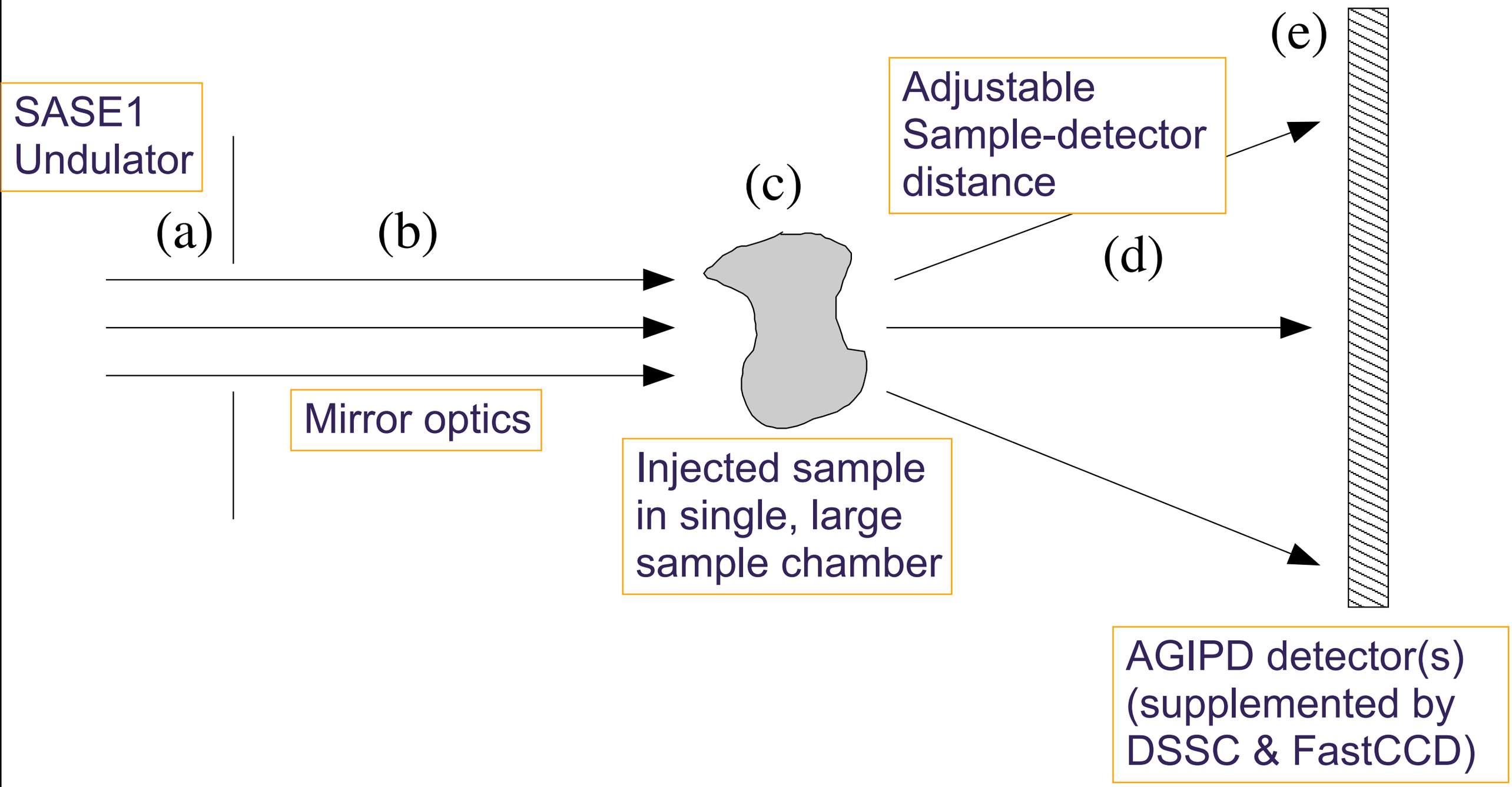
The big picture features of SPB: Forward scattering for all



The big picture features of SPB: Forward scattering for all

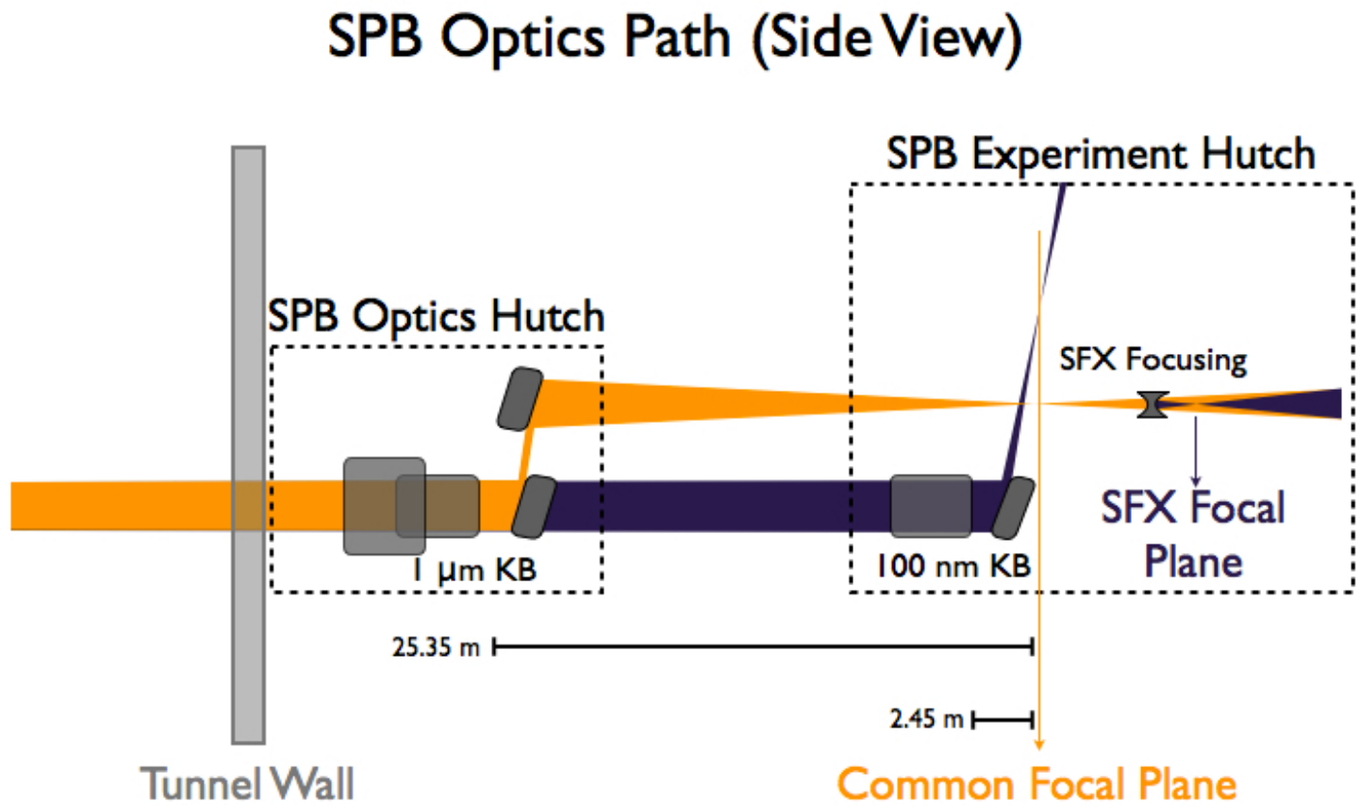


The big picture features of SPB: Forward scattering for all



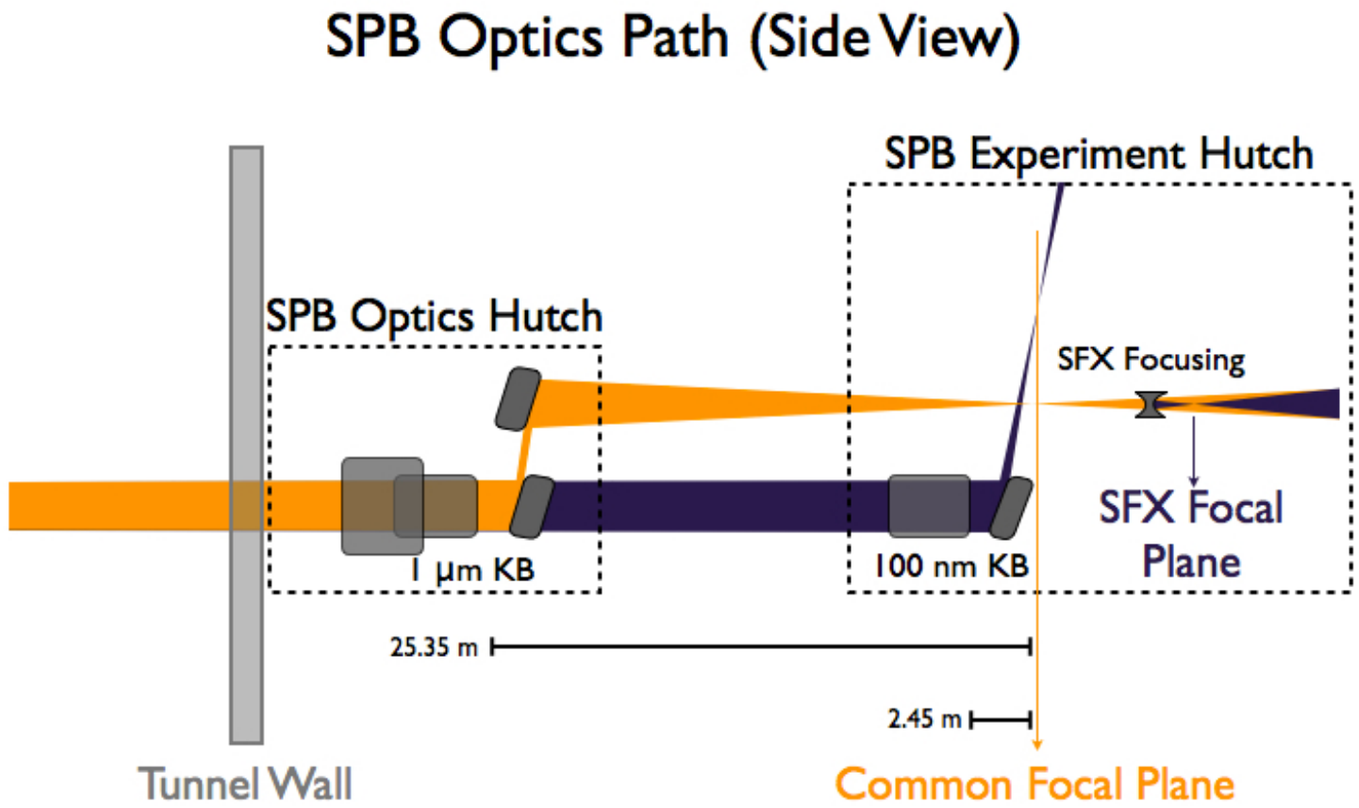
European XFEL

Global view of the optical layout



European XFEL

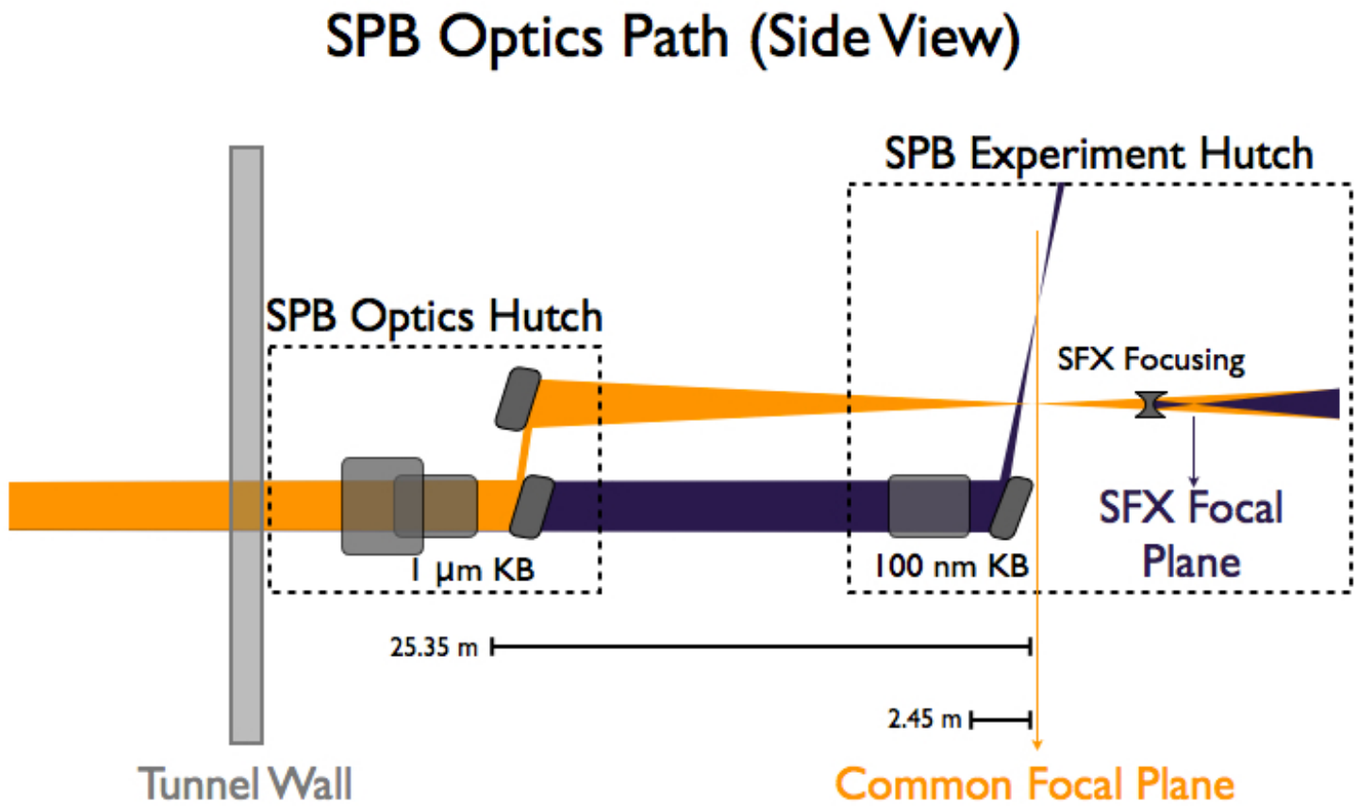
Global view of the optical layout



- Both optics span the entire energy range with no gaps

European XFEL

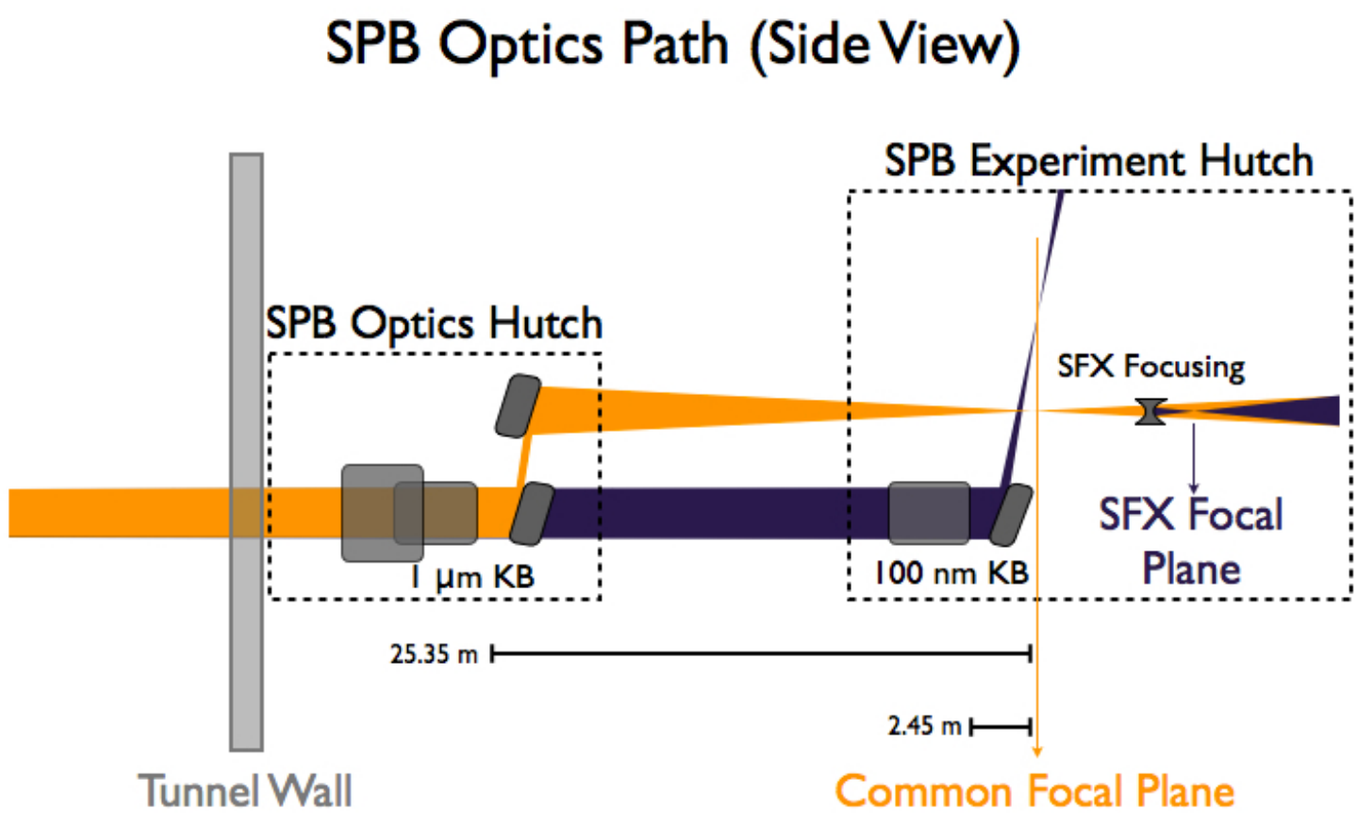
Global view of the optical layout



- Both optics span the entire energy range with no gaps
- Mirror coatings tested and expected to survive XFEL beam @ 4mrad

European XFEL

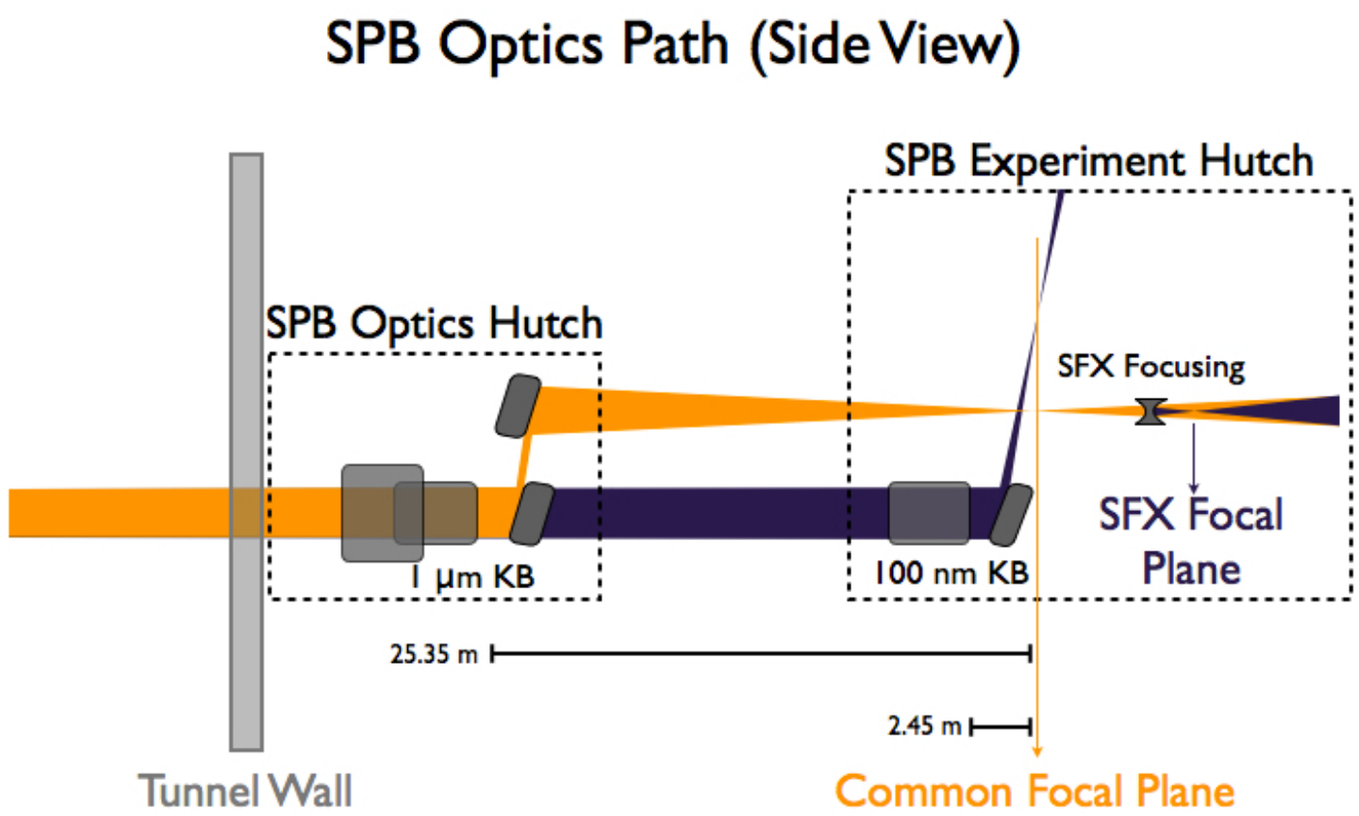
Global view of the optical layout



- Both optics span the entire energy range with no gaps
- Mirror coatings tested and expected to survive XFEL beam @ 4mrad
- Can leave 100 nm mirrors coarsely aligned while using the micron scale optics

European XFEL

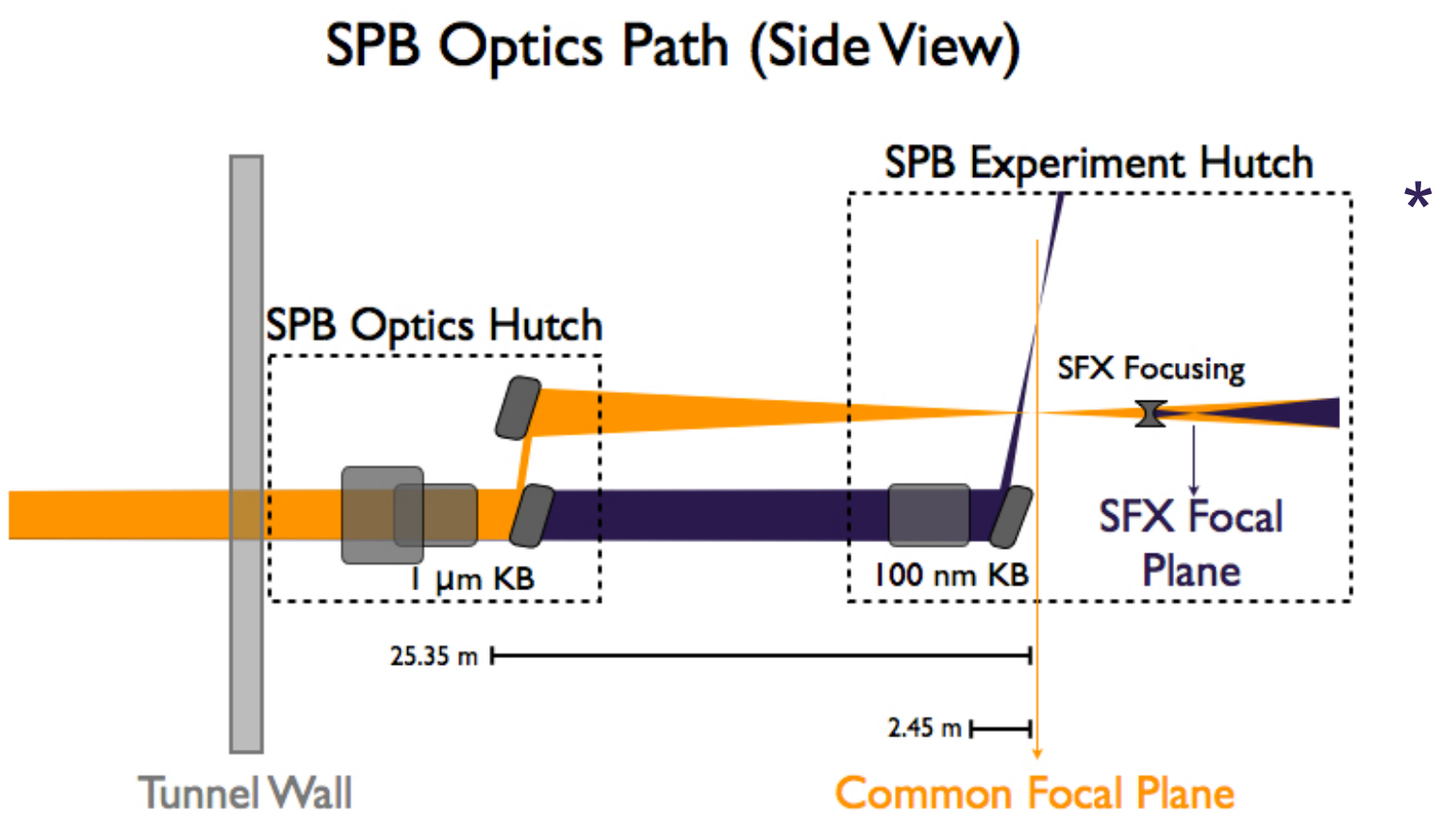
Global view of the optical layout



- Both optics span the entire energy range with no gaps
- Mirror coatings tested and expected to survive XFEL beam @ 4mrad
- Can leave 100 nm mirrors coarsely aligned while using the micron scale optics
- 2nd interaction region in hutch for additional parasitic experiments (SFX consortium, Chapman et al)

European XFEL

Global view of the optical layout

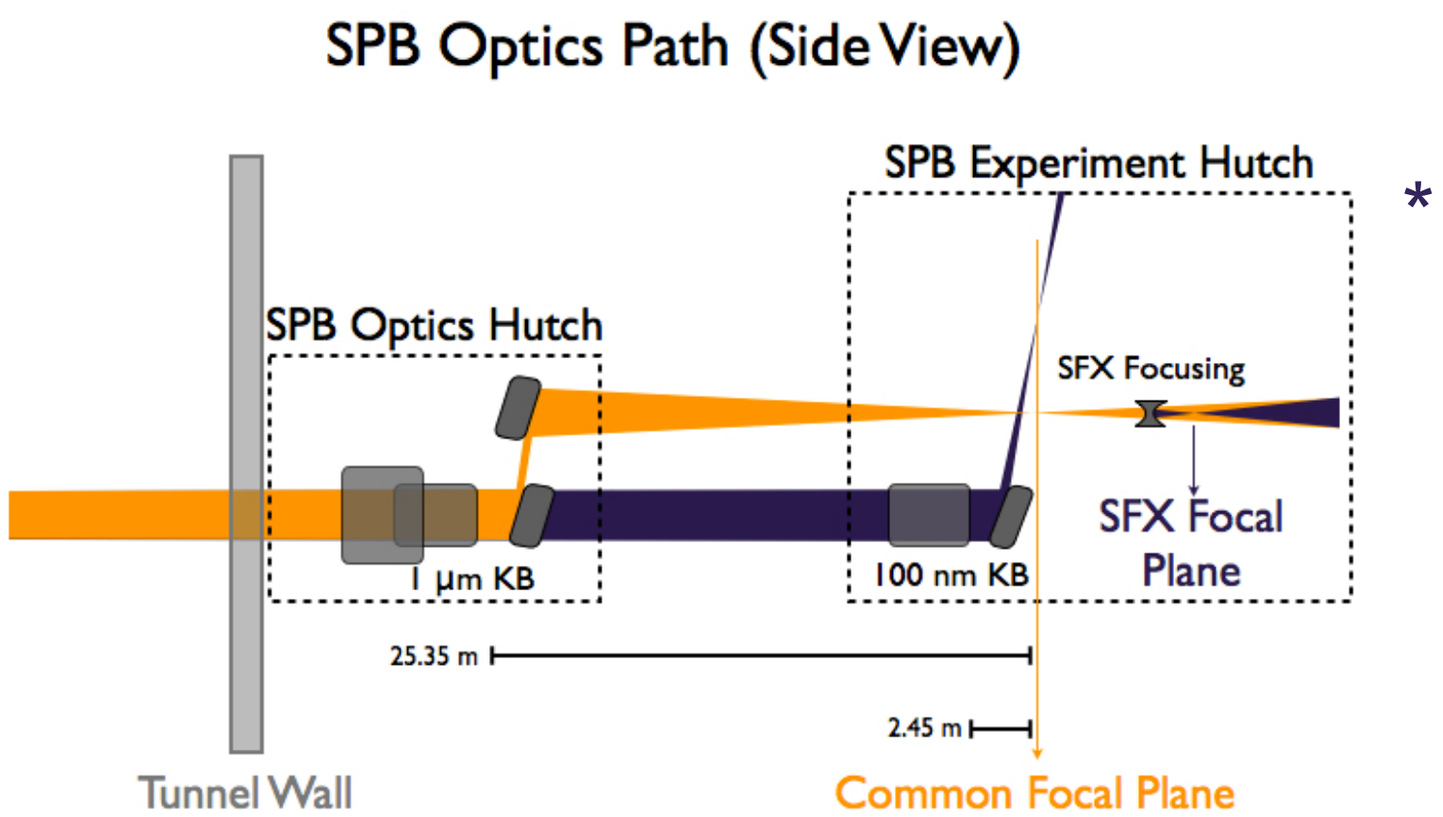


*

- Both optics span the entire energy range with no gaps
- Mirror coatings tested and expected to survive XFEL beam @ 4mrad
- Can leave 100 nm mirrors coarsely aligned while using the micron scale optics
- 2nd interaction region in hutch for additional parasitic experiments (SFX consortium, Chapman et al)

European XFEL

Global view of the optical layout



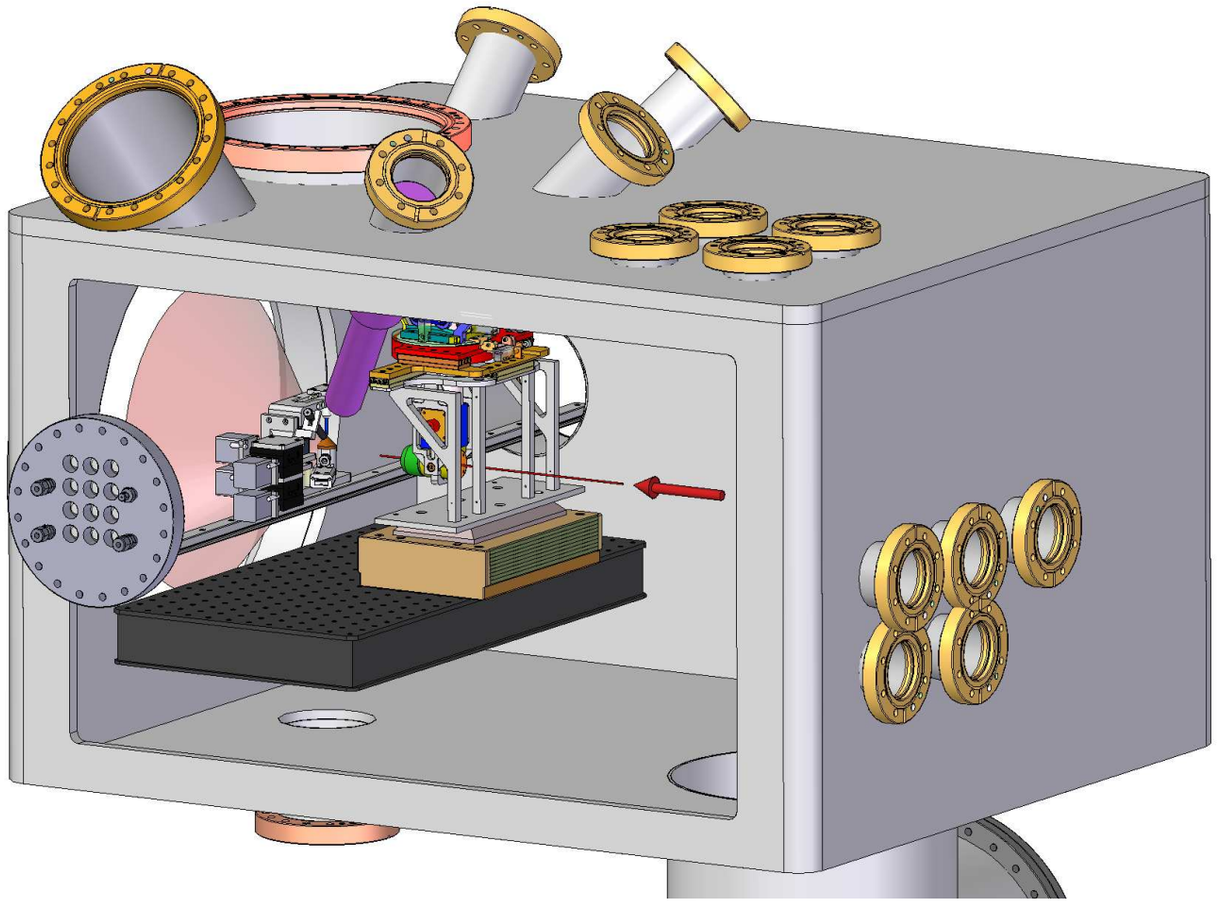
*

- Both optics span the entire energy range with no gaps
- Mirror coatings tested and expected to survive XFEL beam @ 4mrad
- Can leave 100 nm mirrors coarsely aligned while using the micron scale optics
- 2nd interaction region in hutch for additional parasitic experiments (SFX consortium, Chapman et al)

* For more info than you'll ever need about these optics, speak with Andrew Aquila

European XFEL

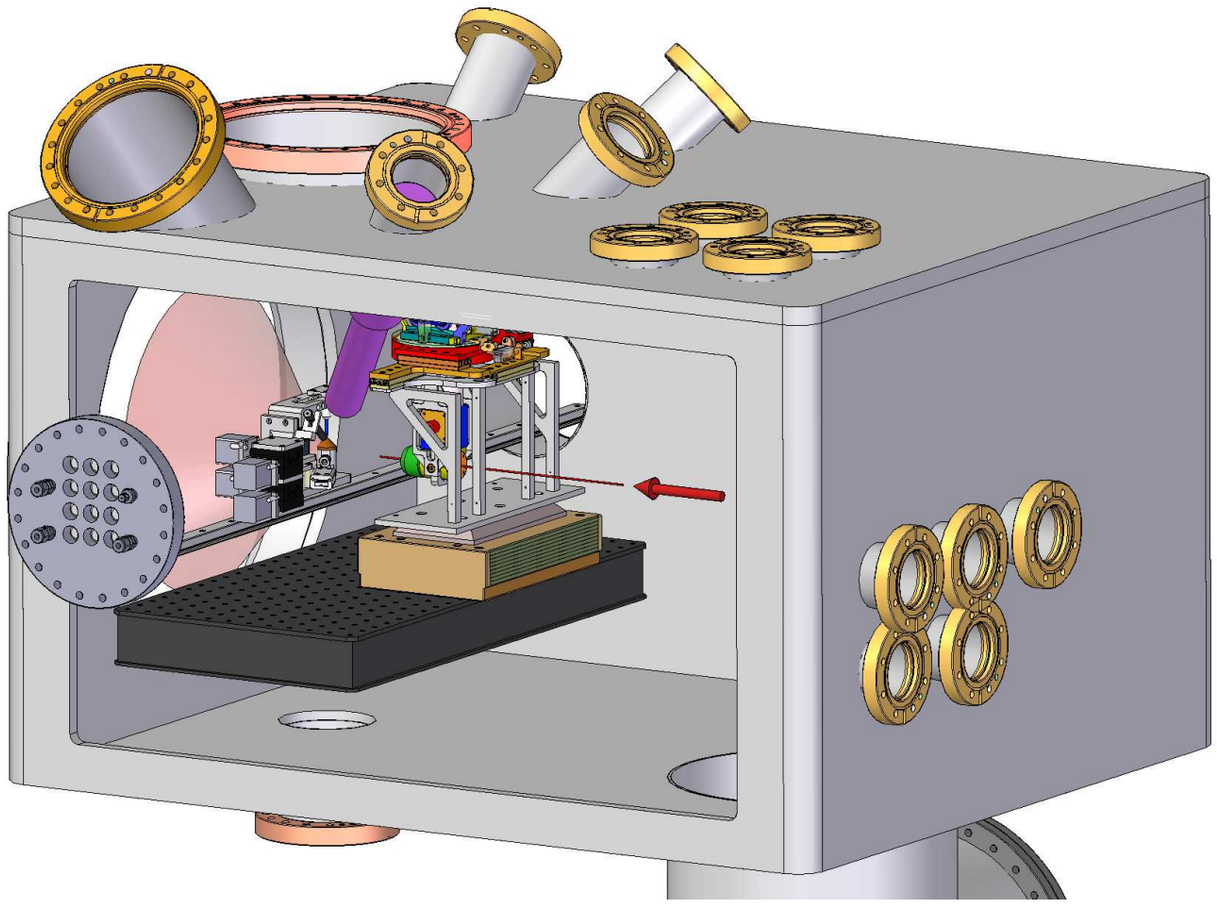
Sample delivery systems and chamber



European XFEL

Sample delivery systems and chamber

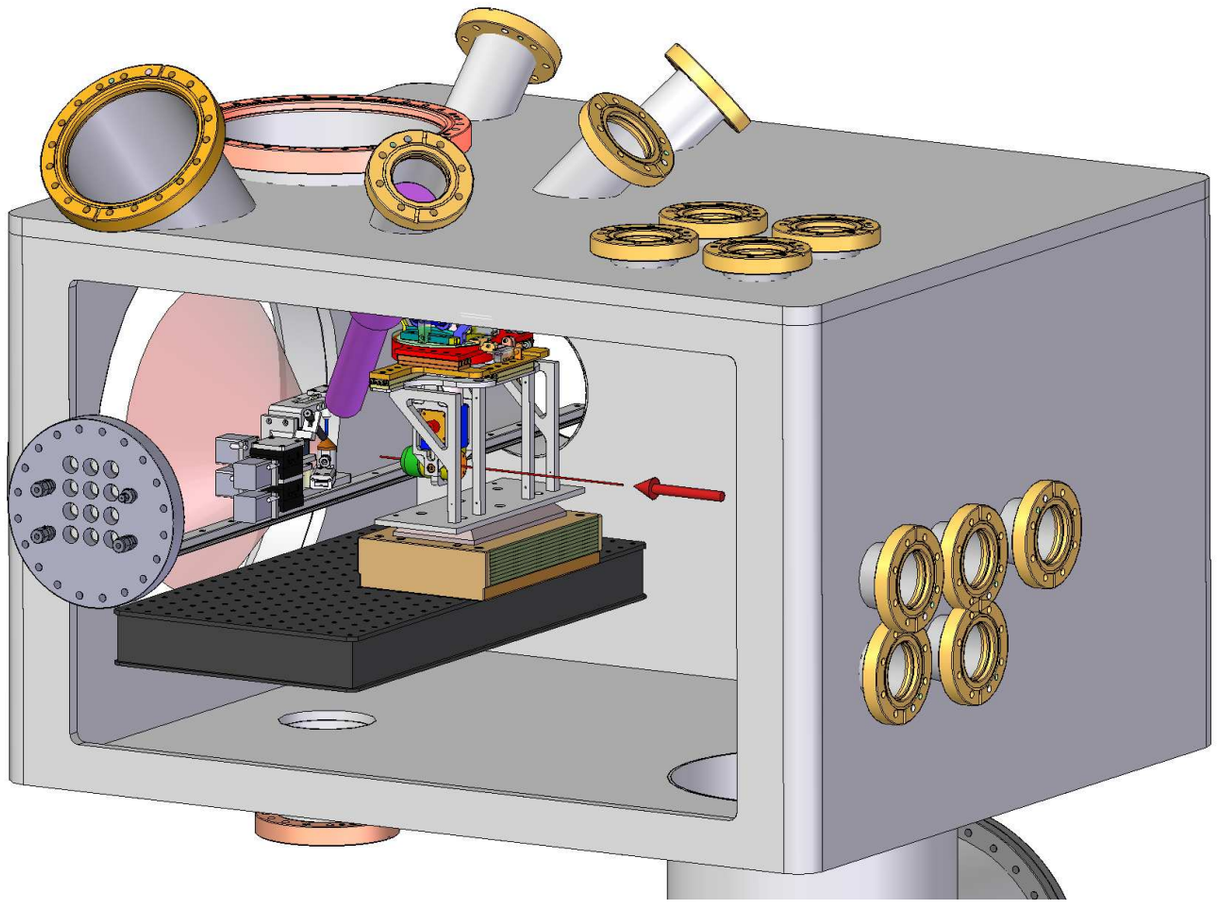
- Injected sample systems
  - liquid jet injection (primary crystal delivery system)
    - ➔Rayleigh jets (⌀ > 5 µm)
    - ➔Gas nozzle jets (⌀ < 2 µm)
  - aerosol injection
    - ➔Uppsala model



European XFEL

Sample delivery systems and chamber

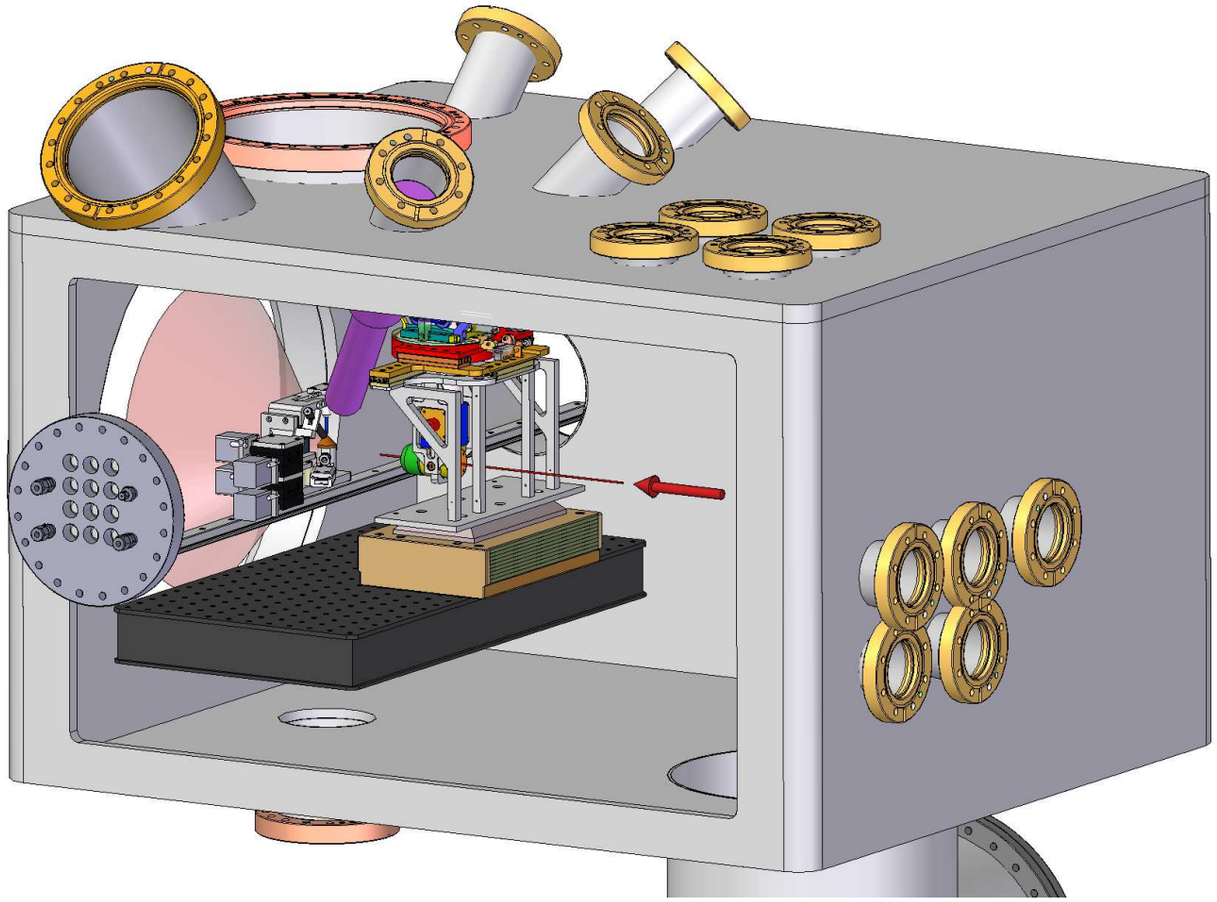
- Injected sample systems
  - liquid jet injection (primary crystal delivery system)
    - ➔Rayleigh jets (⌀ > 5 µm)
    - ➔Gas nozzle jets (⌀ < 2 µm)
  - aerosol injection
    - ➔Uppsala model
- Sample stages for fixed targets
  - various commercial solutions available



European XFEL

Sample delivery systems and chamber

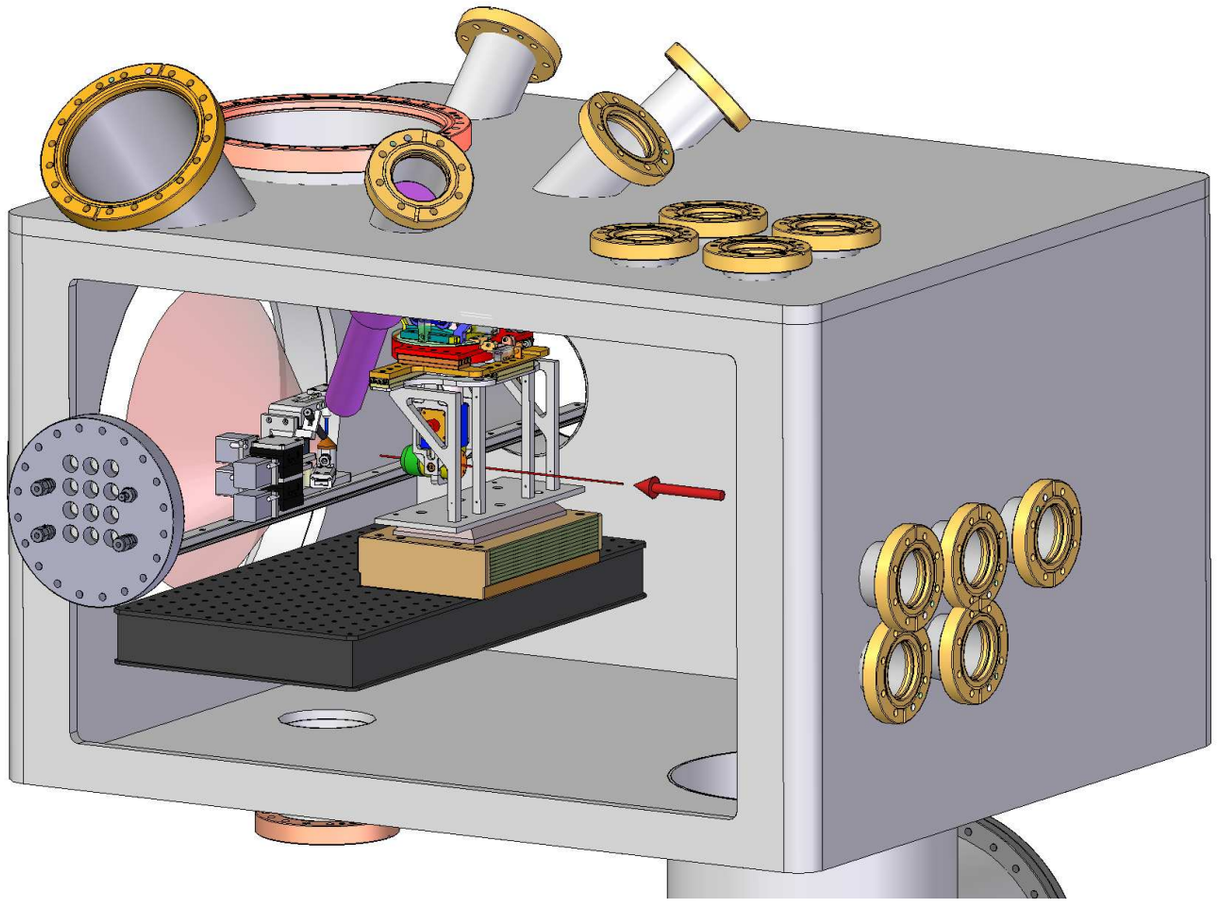
- Injected sample systems
  - liquid jet injection (primary crystal delivery system)
    - ➔Rayleigh jets (⌀ > 5 µm)
    - ➔Gas nozzle jets (⌀ < 2 µm)
  - aerosol injection
    - ➔Uppsala model
- Sample stages for fixed targets
  - various commercial solutions available
- Optional (possible) extras
  - ion injection (mass spectrometry)



European XFEL

Sample delivery systems and chamber

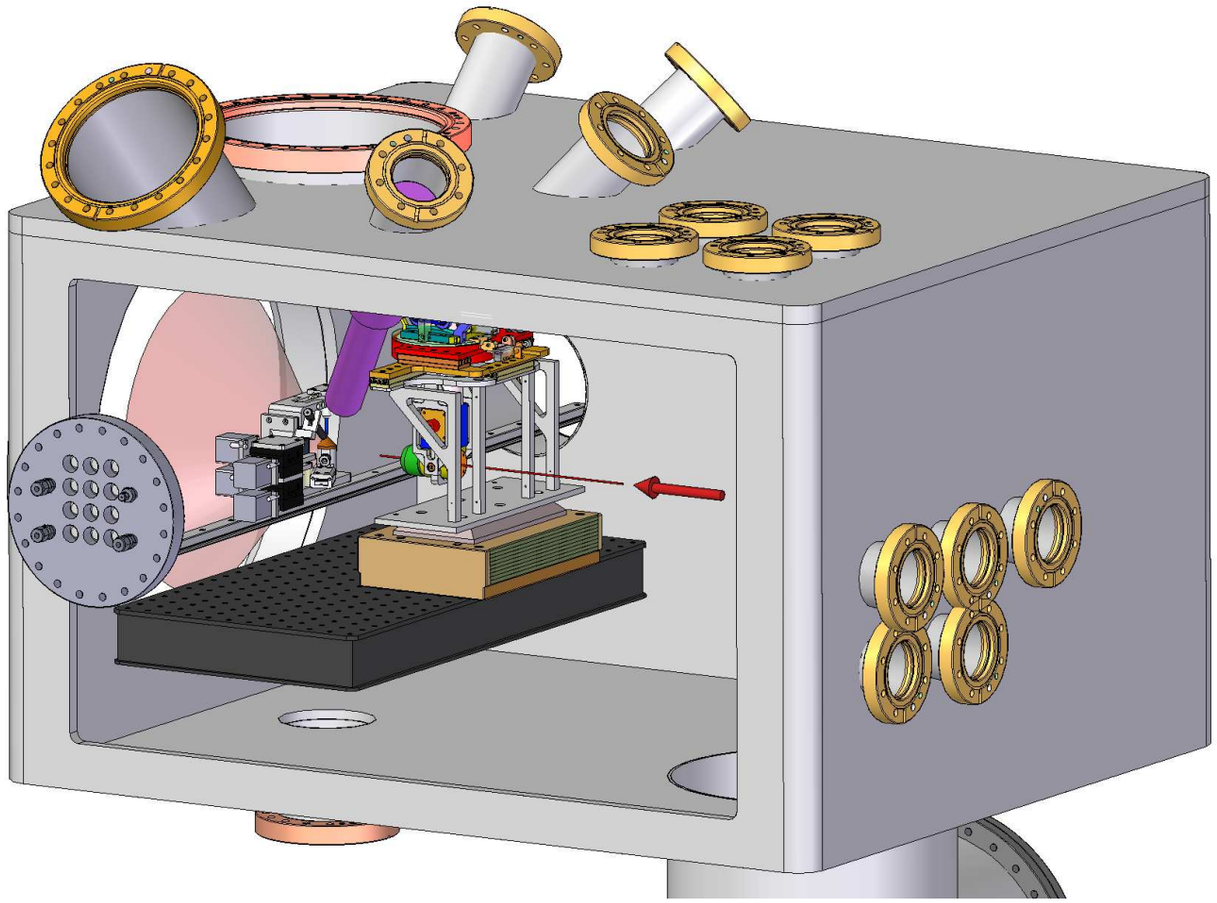
- Injected sample systems
  - liquid jet injection (primary crystal delivery system)
    - ➔Rayleigh jets (⌀ > 5 µm)
    - ➔Gas nozzle jets (⌀ < 2 µm)
  - aerosol injection
    - ➔Uppsala model
- Sample stages for fixed targets
  - various commercial solutions available
- Optional (possible) extras
  - ion injection (mass spectrometry)
- Single, large chamber design
  - inc. breadboard for rapid changes



European XFEL

Sample delivery systems and chamber

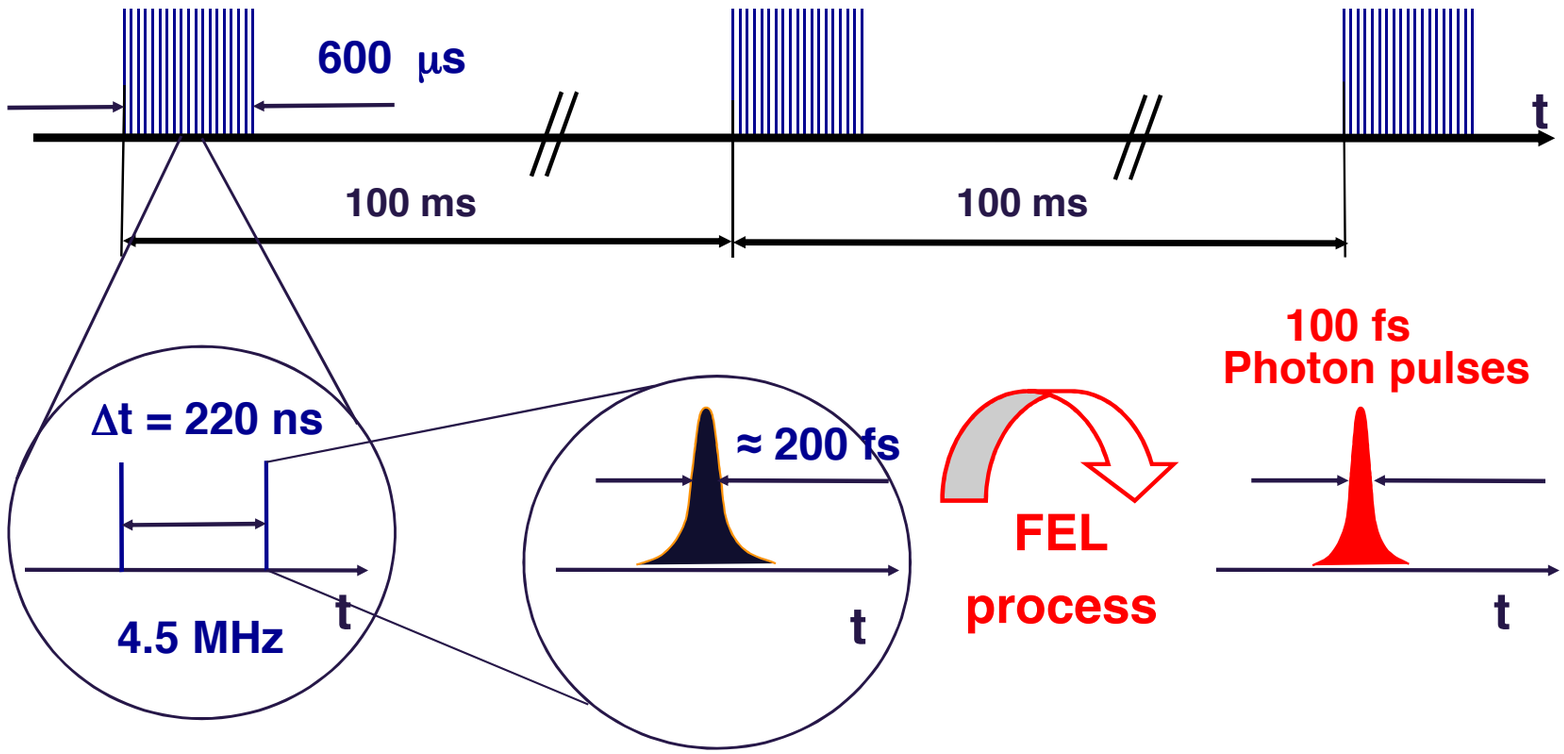
- Injected sample systems
  - liquid jet injection (primary crystal delivery system)
    - ➔Rayleigh jets (⌀ > 5 µm)
    - ➔Gas nozzle jets (⌀ < 2 µm)
  - aerosol injection
    - ➔Uppsala model
- Sample stages for fixed targets
  - various commercial solutions available
- Optional (possible) extras
  - ion injection (mass spectrometry)
- Single, large chamber design
  - inc. breadboard for rapid changes



Sample environment group of J. Schulz (WP-79) responsible for general sample delivery for all instruments

A source and instrumentation for better sample consumption

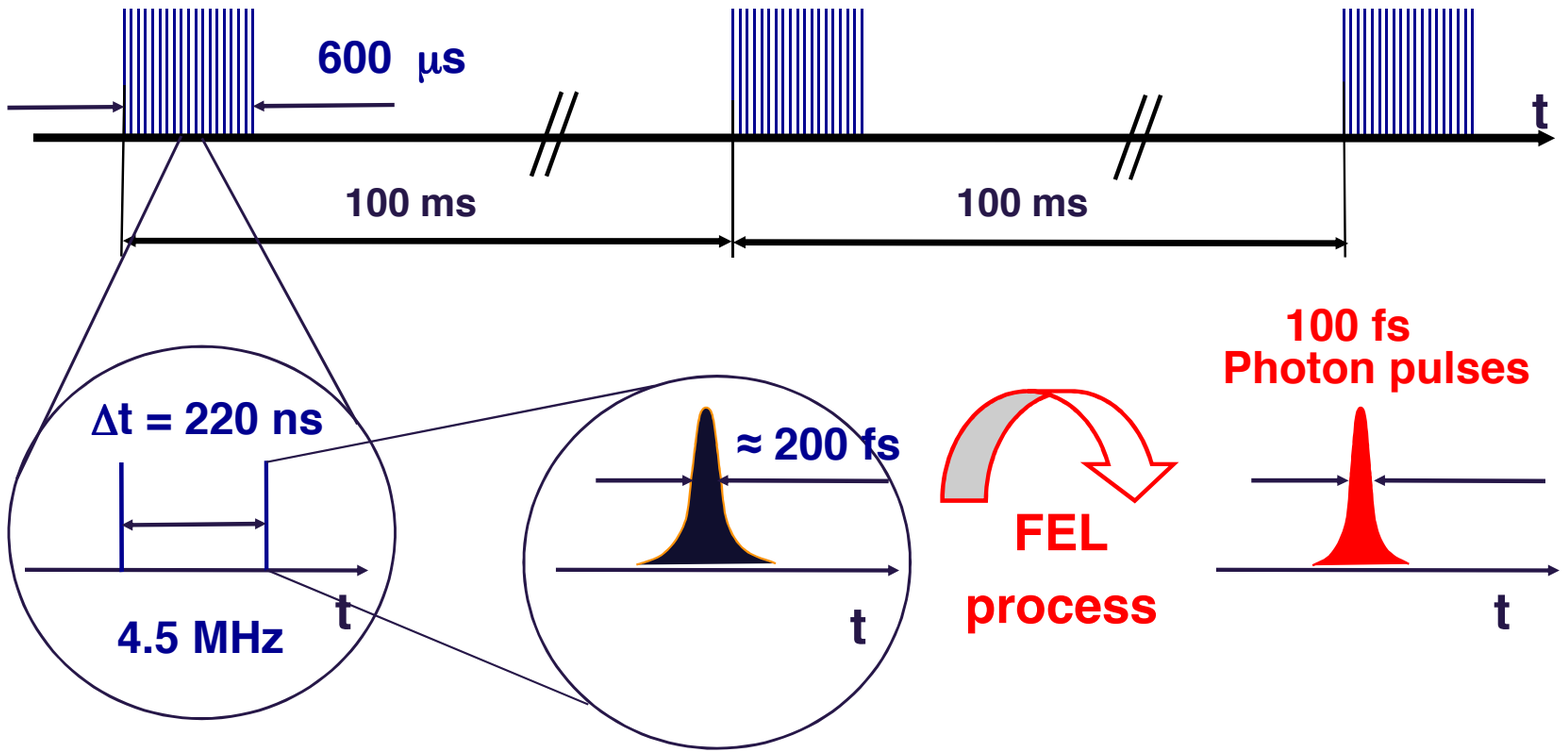
10Hz electron bunch trains
(with up to 2700 bunches à 0.1…1 nC)



A source and instrumentation for better sample consumption

- Repetition rate
  - SACLA - 20 Hz
  - LCLS - 120 Hz
  - European XFEL - effectively 3500 Hz (given by detector limit- 27 kHz beam limit)

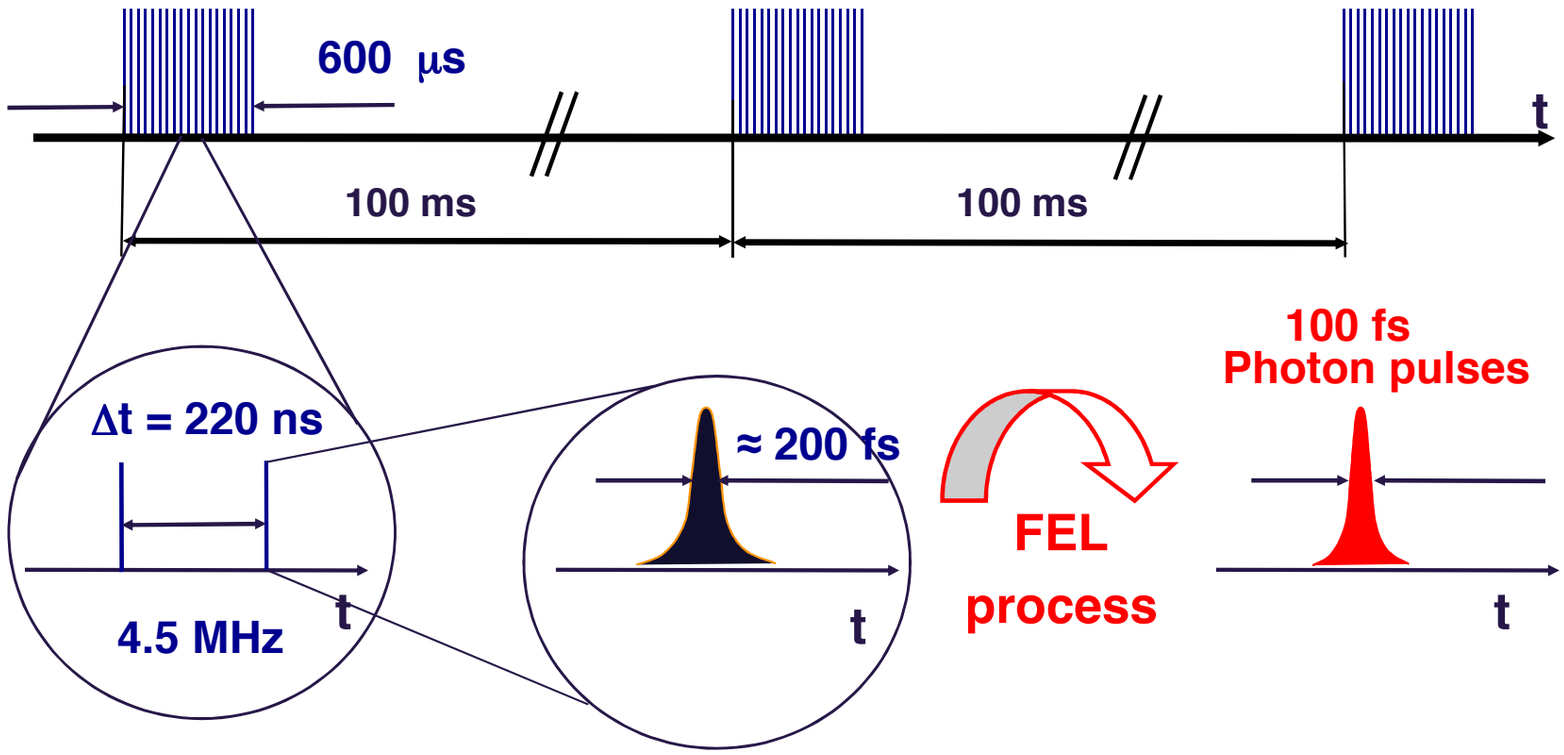
10Hz electron bunch trains
(with up to 2700 bunches à 0.1…1 nC)



A source and instrumentation for better sample consumption

- Repetition rate
  - SACLA - 20 Hz
  - LCLS - 120 Hz
  - European XFEL - effectively 3500 Hz (given by detector limit- 27 kHz beam limit)

10Hz electron bunch trains
(with up to 2700 bunches à 0.1…1 nC)

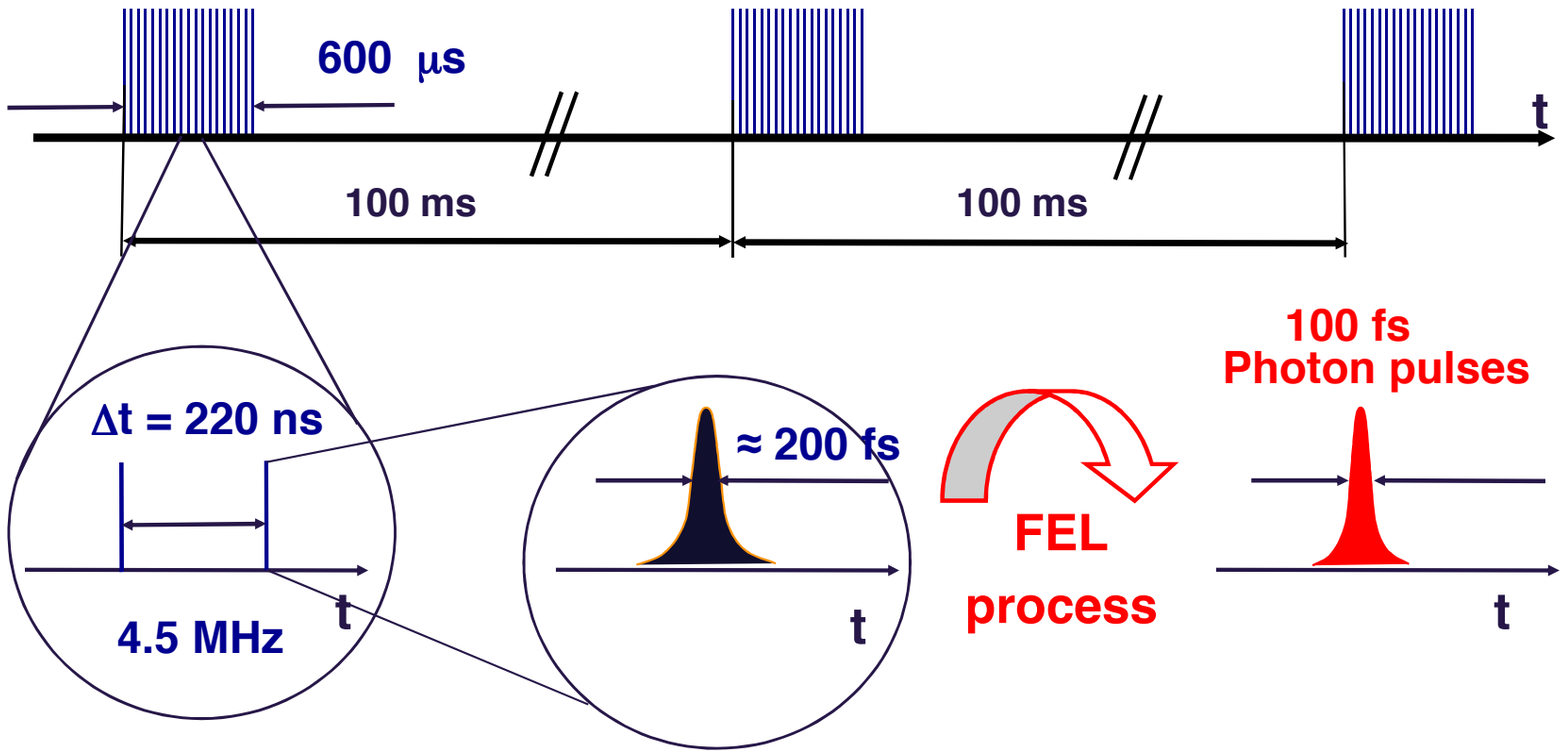


A source and instrumentation for better sample consumption

- Repetition rate
  - SACLA - 20 Hz
  - LCLS - 120 Hz
  - European XFEL - effectively 3500 Hz (given by detector limit- 27 kHz beam limit)

10Hz electron bunch trains
(with up to 2700 bunches à 0.1…1 nC)

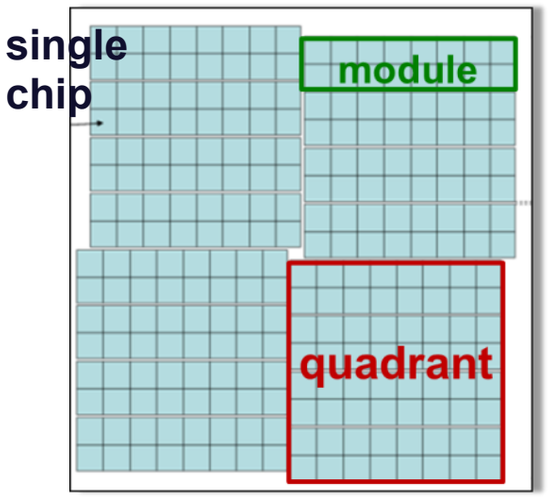
- ⇒ ≳200× data for the same sample consumption!
  - very useful for rare or valuable sample



European XFEL

Adaptive Gain Integrating Pixel Detector

High repetition rate (4.5 MHz) 1MPix imaging detector

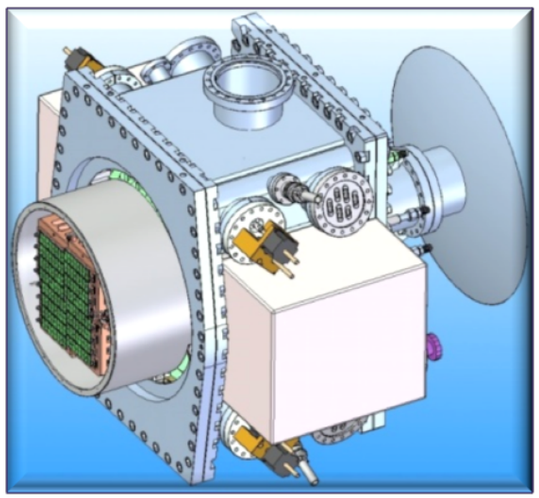


64x64 pixels/chip

2x8 chips/module

modules/quadrant

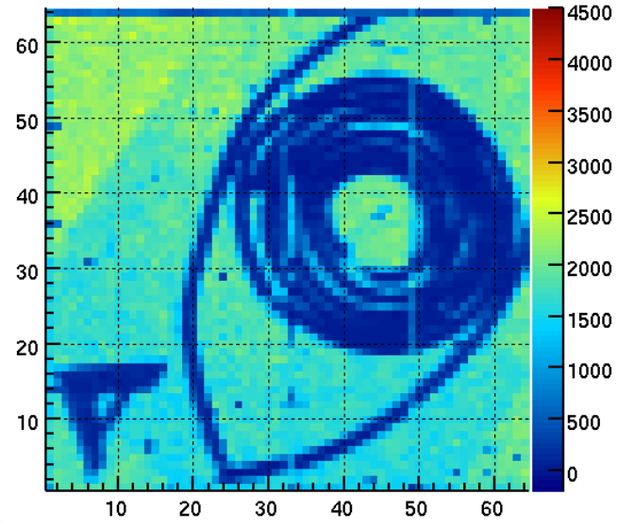
4 quadrants/detector



Parameter	AGIPD
Energy Range	3-16 keV
Dynamic Range	10^4 ph @12 keV
Single Photon Sens	Yes → Noise ~350e- rms
Storage cells/pixel	352 (analog)
Pixel size	200x200 μm^2 (squared)
Variable hole	Yes→ four independently movable quadrants
Veto capability	Yes

Status

- The full scale chip **AGIPD1.0** exists
  - Fist test results show no major problems → very encouraging
  - Measured parameters within the specification
- **Mechanics** design for 1MPix detector in advanced state
  - Initial tests of movement system successful
- **Integration** of the detector in the XFEL beamlines in progress



Slide: J. Sztuk-Dambietz, XFEL
Image: AGIPD consortium

European XFEL

Detection geometry requirements

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, “Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument”, European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

- Key points:

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, “Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument”, European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

- Key points:
  - Sample to detector distance

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, “Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument”, European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

Detection geometry requirements

- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, “Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument”, European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, “Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument”, European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

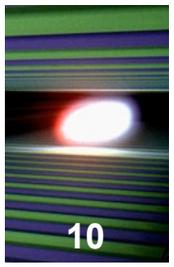
Detection geometry requirements

- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

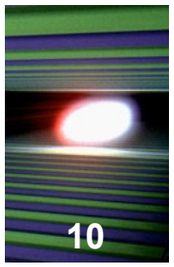


- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications
  - Imaging requires 2nd plane

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

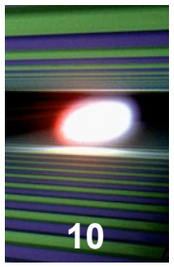


- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications
  - Imaging requires 2nd plane
  - Mechanical integration

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements



- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications
  - Imaging requires 2nd plane
  - Mechanical integration
    - ➔Tricky

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

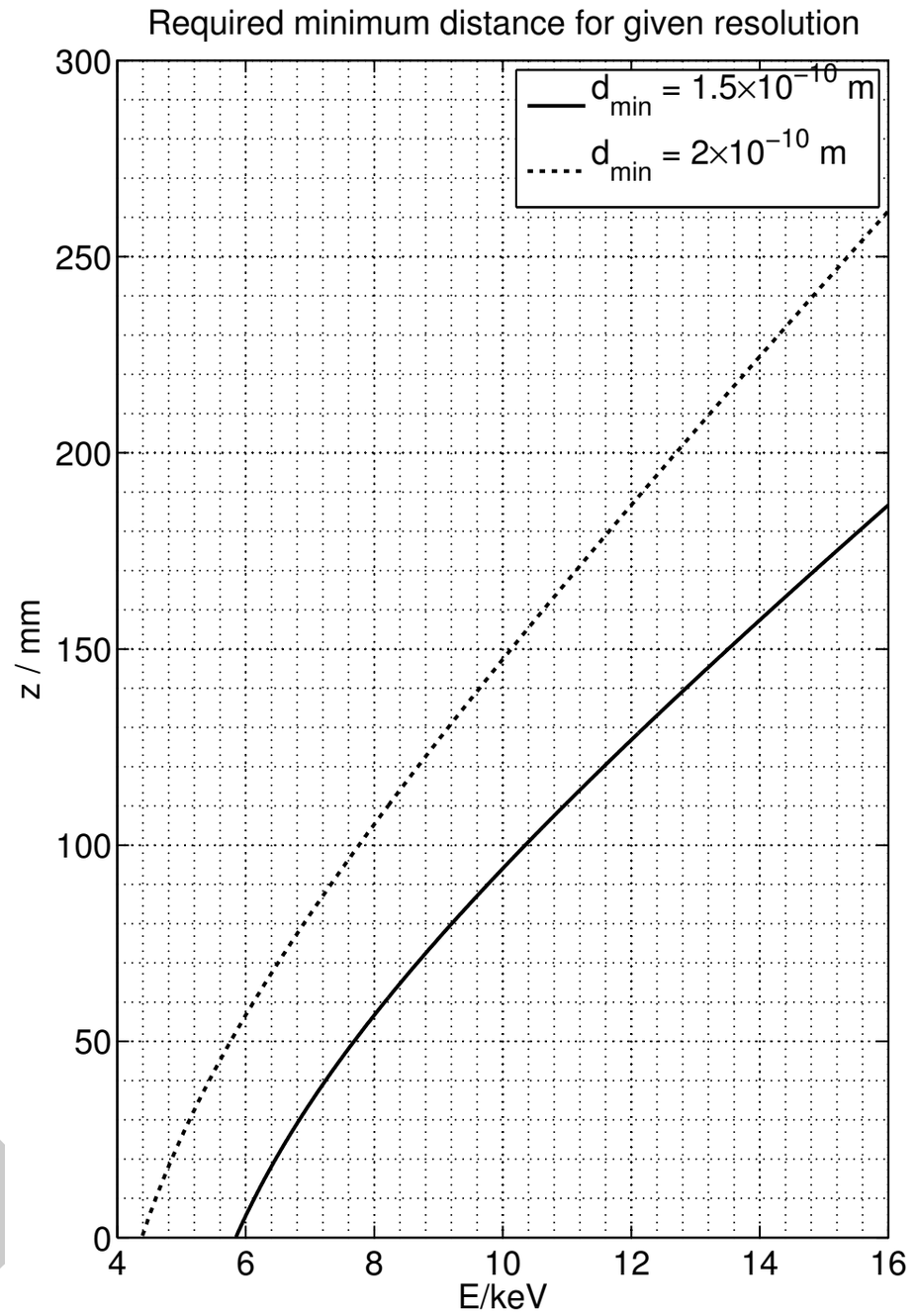
- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications
  - Imaging requires 2nd plane
  - Mechanical integration
    - ➔Tricky
    - ➔Must satisfy points above

See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications
  - Imaging requires 2nd plane
  - Mechanical integration
    - ➔Tricky
    - ➔Must satisfy points above

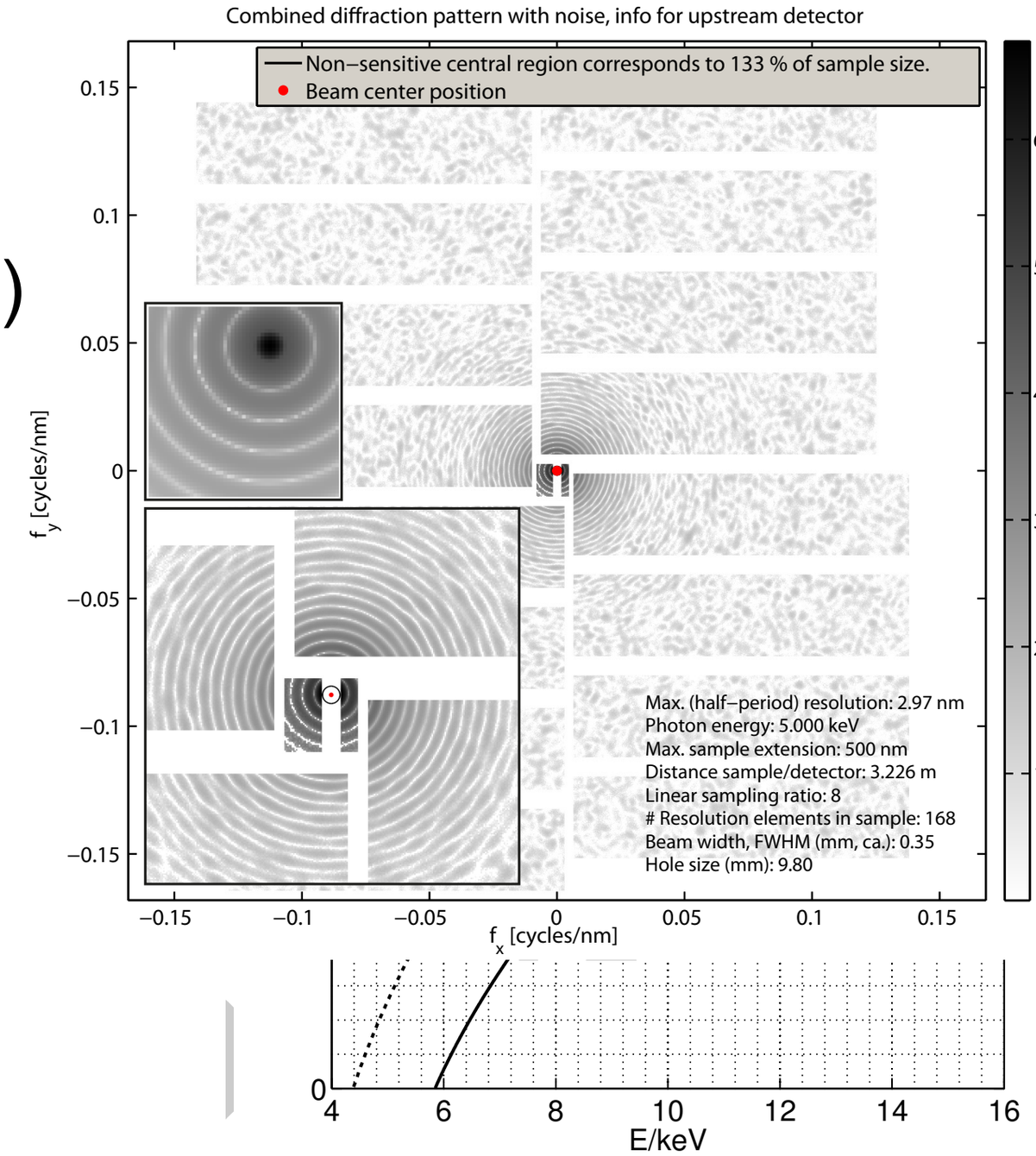


See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

Detection geometry requirements

- Key points:
  - Sample to detector distance
    - ➔Close for nanocryst (~13 cm)
    - ➔Far for imaging (~12 m)
  - Detector's Central hole size
    - ➔Must vary for different applications
  - Imaging requires 2nd plane
  - Mechanical integration
    - ➔Tricky
    - ➔Must satisfy points above



See: K. Giewekemeyer, M. Turcato, A. P. Mancuso, "Detector Geometries for Coherent X-Ray Diffractive Imaging at the SPB Instrument", European XFEL Technical Report, XFEL.EU Technical Report (2013) doi:10.3204/XFEL.EU/TR-2013-007.

European XFEL

AGIPD Mechanical integration

European XFEL

AGIPD Mechanical integration

- “Correct” mechanical integration essential to support science cases

European XFEL

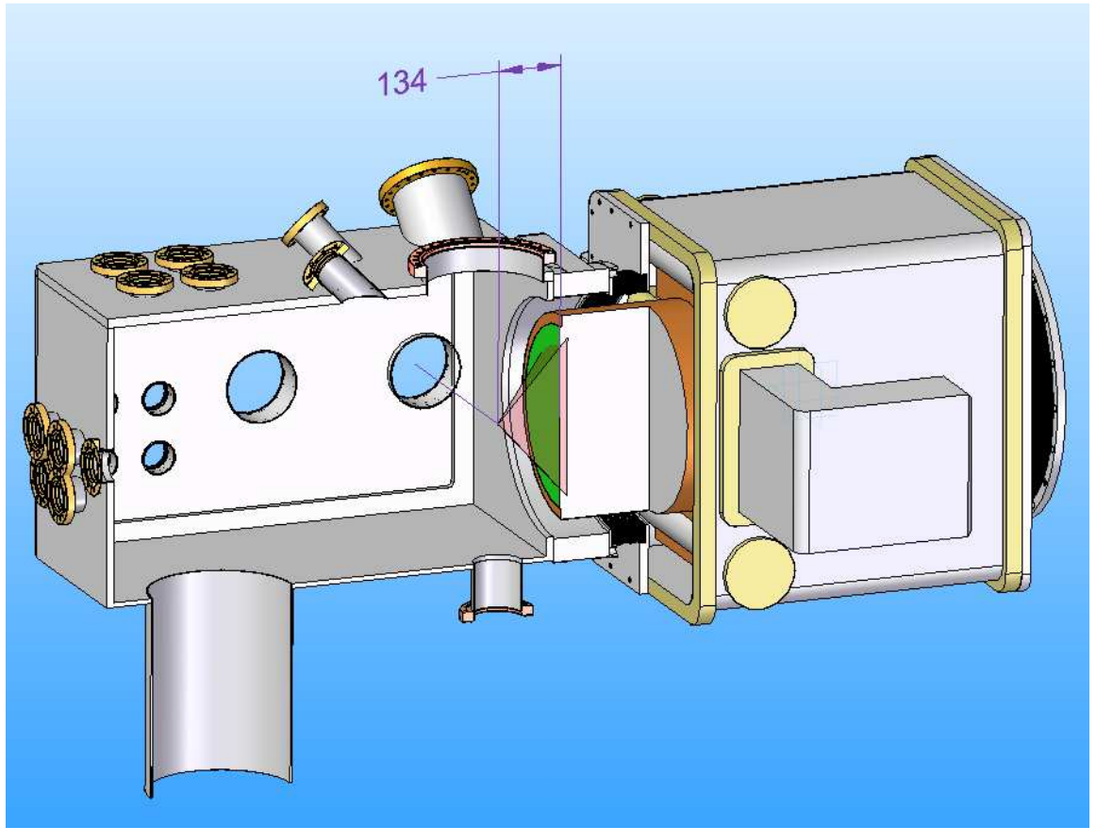
AGIPD Mechanical integration

- “Correct” mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm

European XFEL

AGIPD Mechanical integration

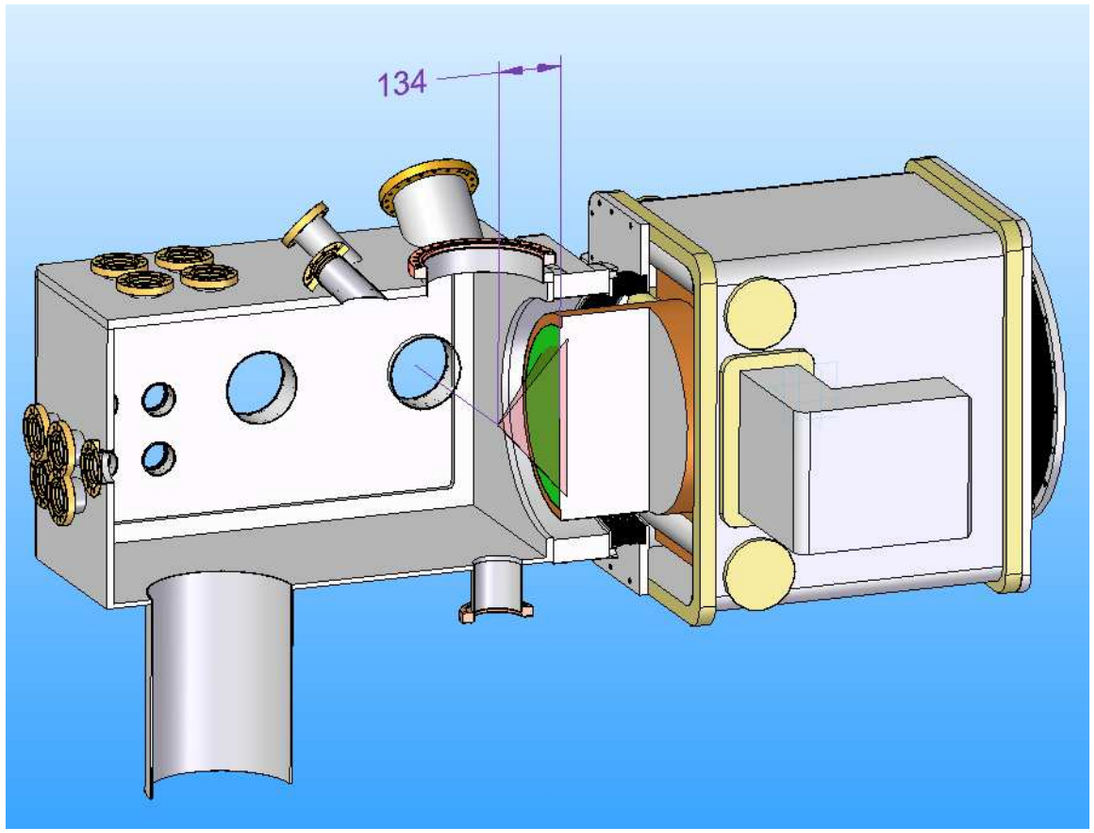
- “Correct” mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm



European XFEL

AGIPD Mechanical integration

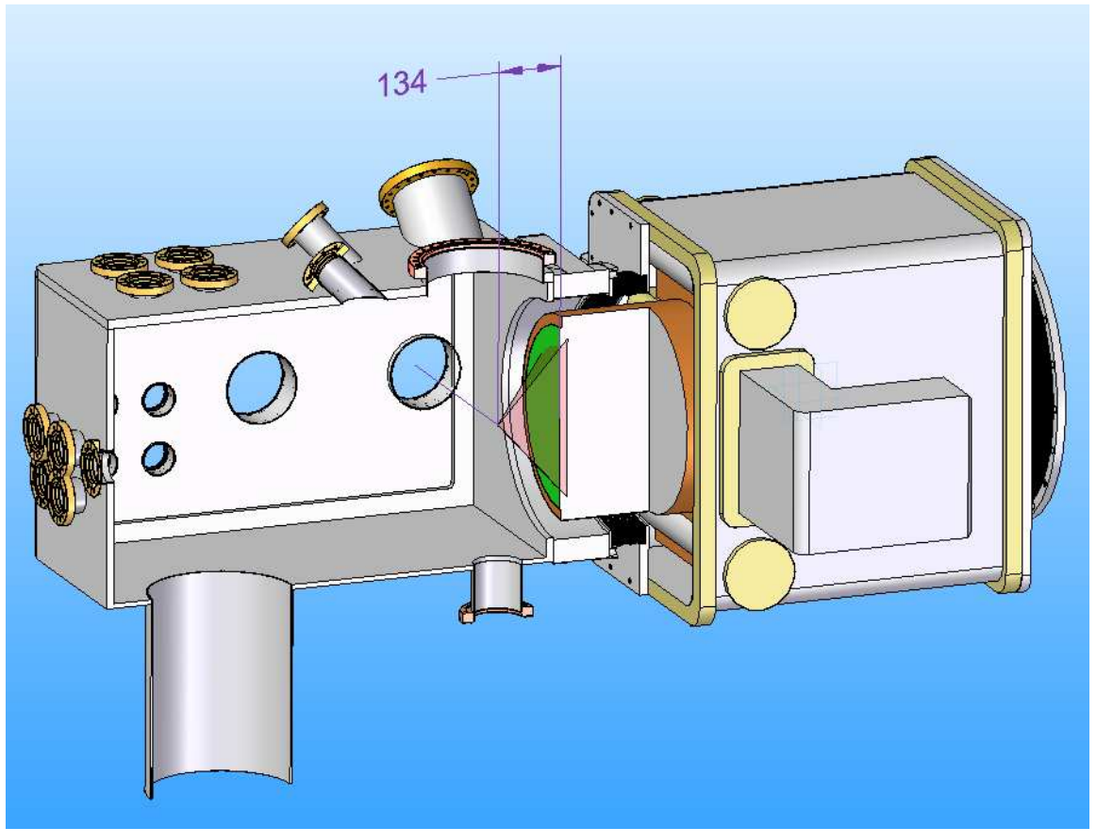
- “Correct” mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly



European XFEL

AGIPD Mechanical integration

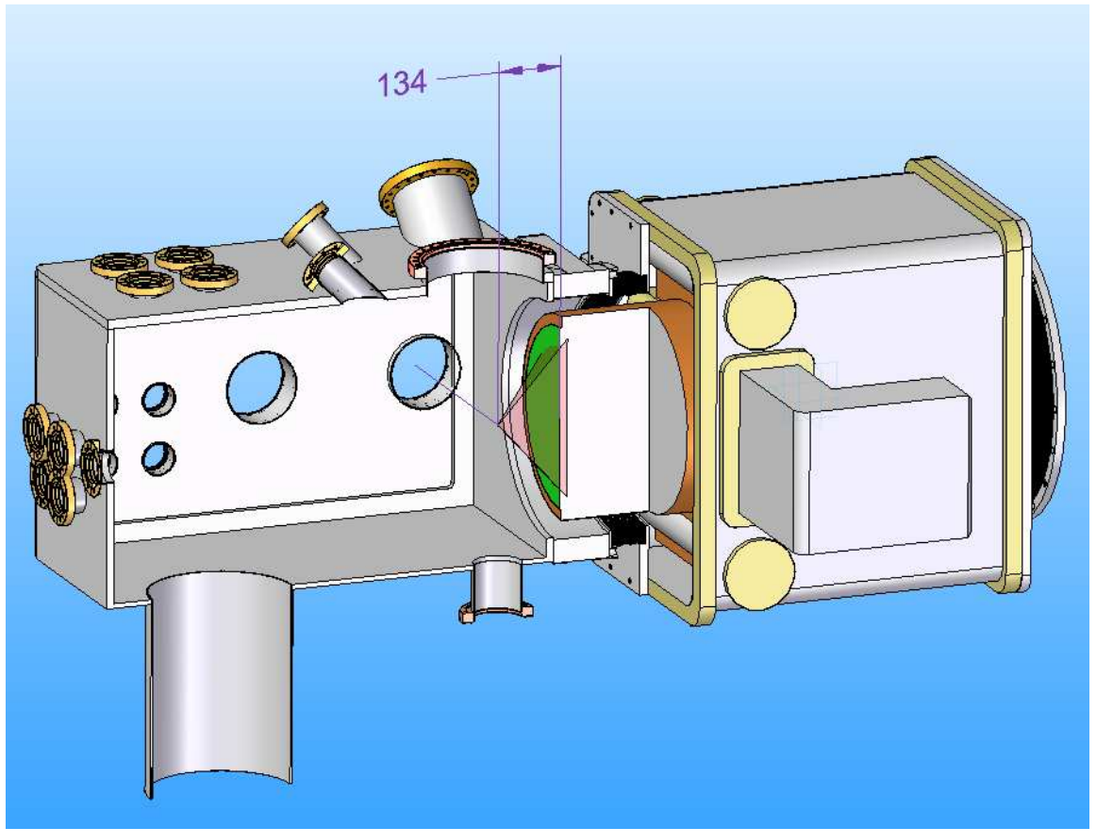
- “Correct” mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly
- Requires:



European XFEL

AGIPD Mechanical integration

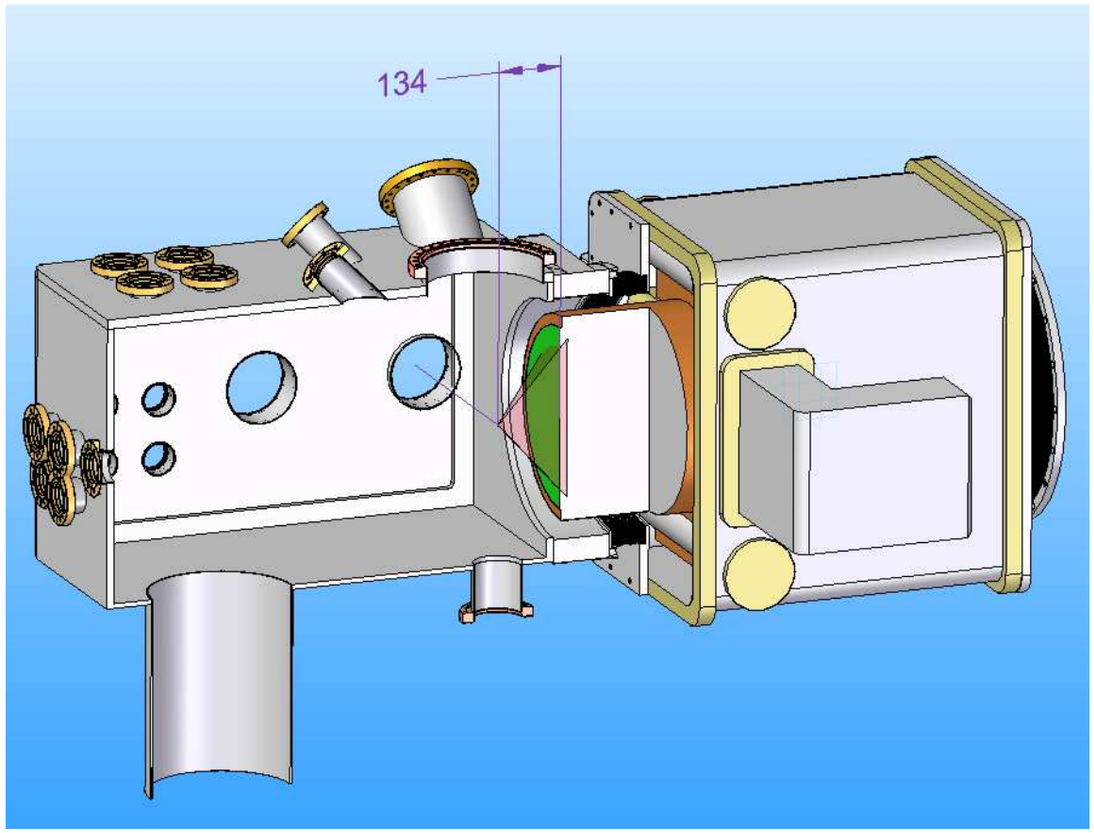
- “Correct” mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly
- Requires:
  - sample chamber compromises



European XFEL

AGIPD Mechanical integration

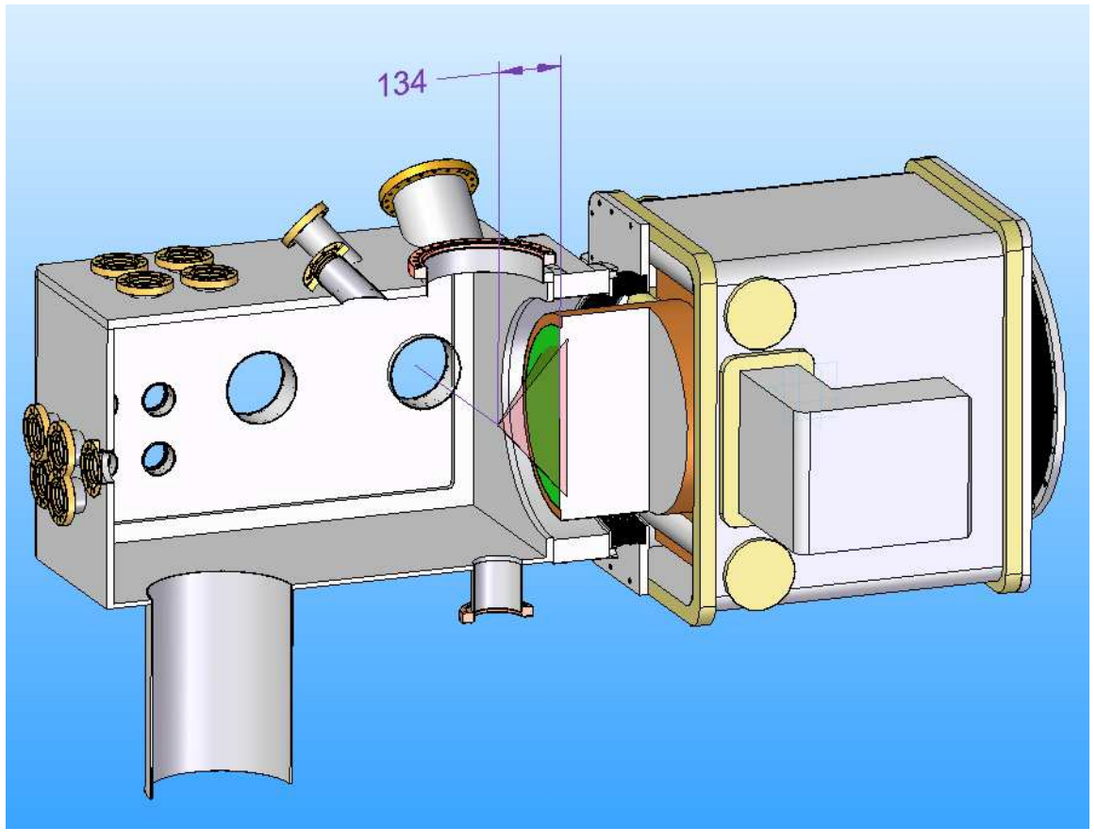
- "Correct" mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly
- Requires:
  - sample chamber compromises
  - custom bellows



European XFEL

AGIPD Mechanical integration

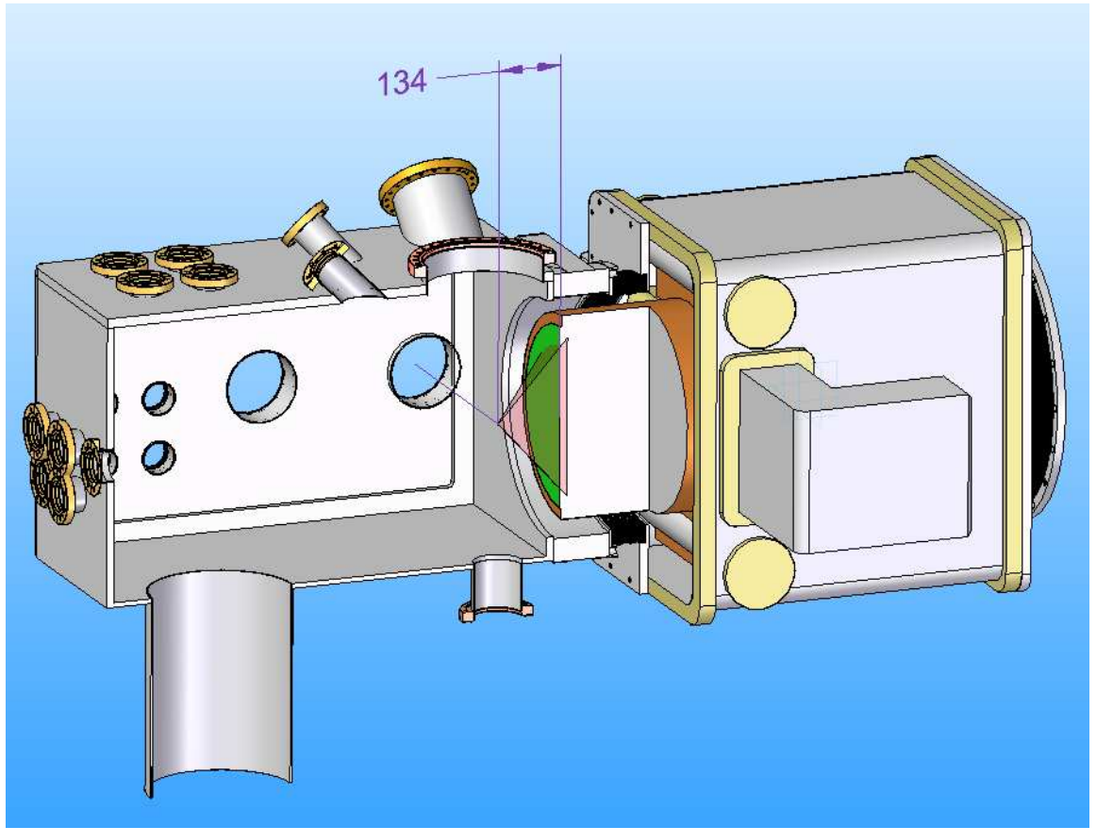
- "Correct" mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly
- Requires:
  - sample chamber compromises
  - custom bellows
  - 500 mm gate valve welded in sample chamber wall

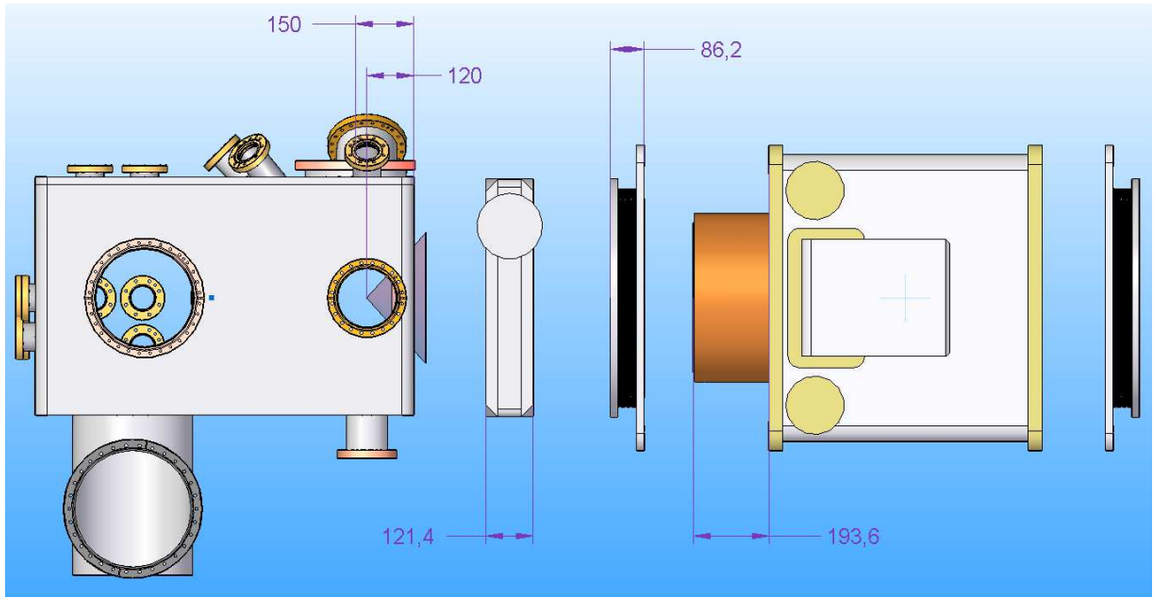


European XFEL

AGIPD Mechanical integration

- “Correct” mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly
- Requires:
  - sample chamber compromises
  - custom bellows
  - 500 mm gate valve welded in sample chamber wall

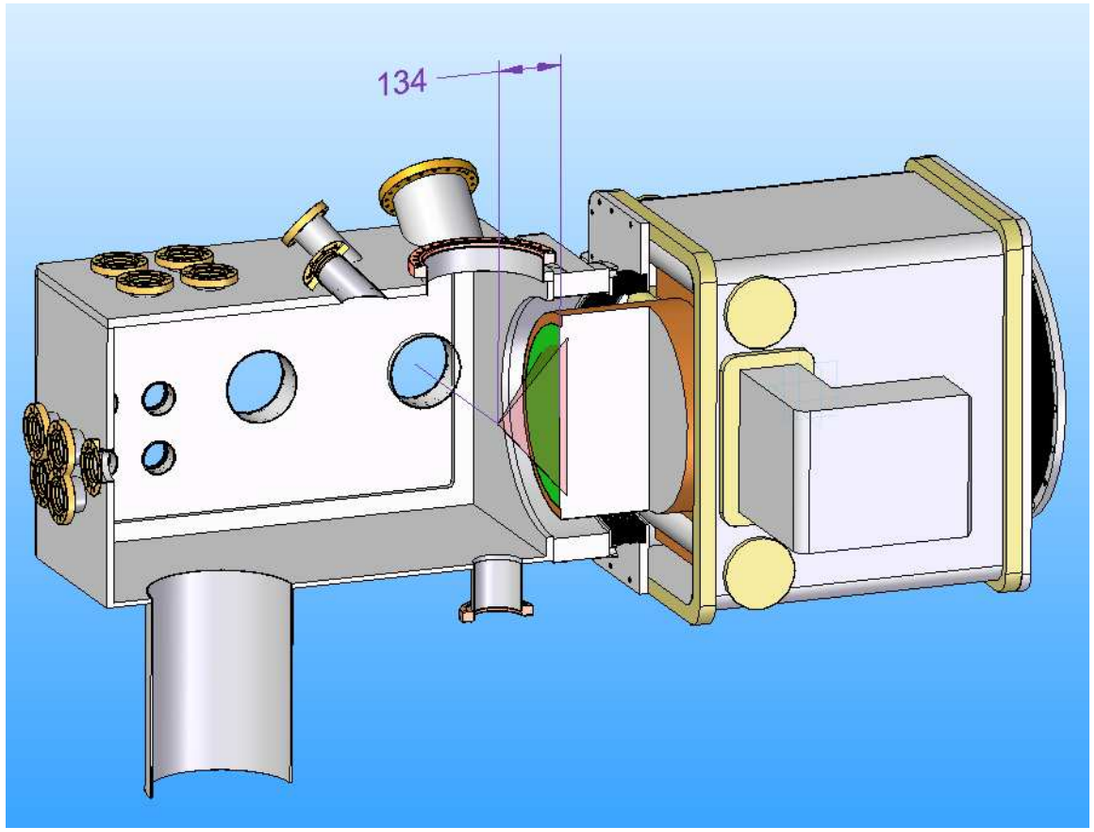


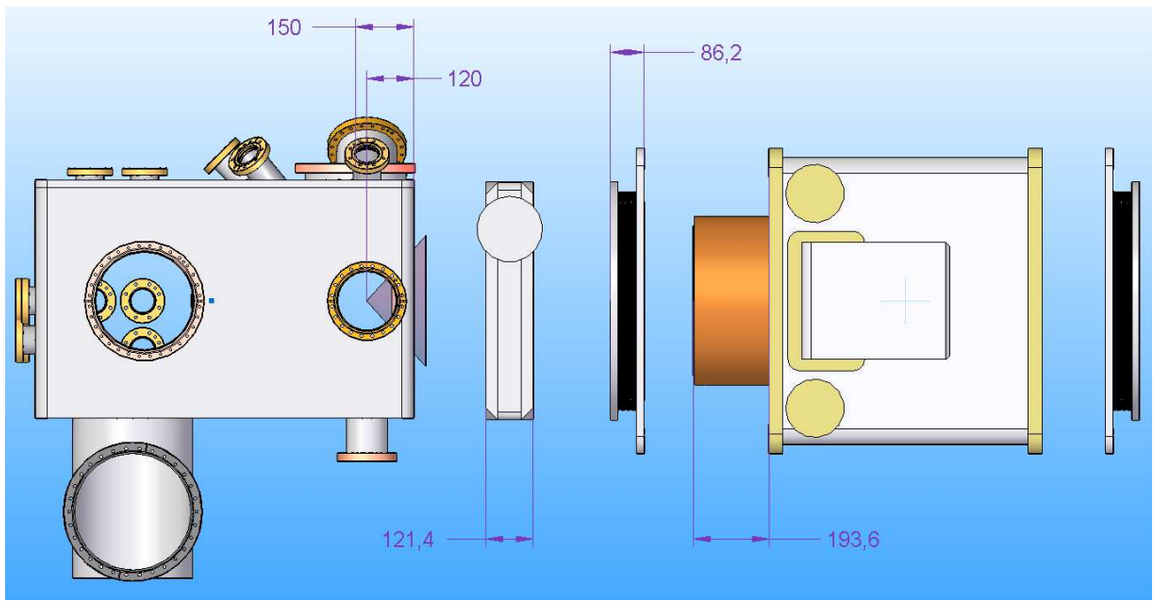


European XFEL

AGIPD Mechanical integration

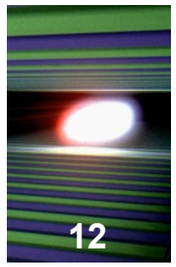
- "Correct" mechanical integration essential to support science cases
- Min. sample-detector distance now 134 mm
  - Unlikely to improve significantly
- Requires:
  - sample chamber compromises
  - custom bellows
  - 500 mm gate valve welded in sample chamber wall
- Min. distance gives 2Å geometrical resolution @ 8.8 keV





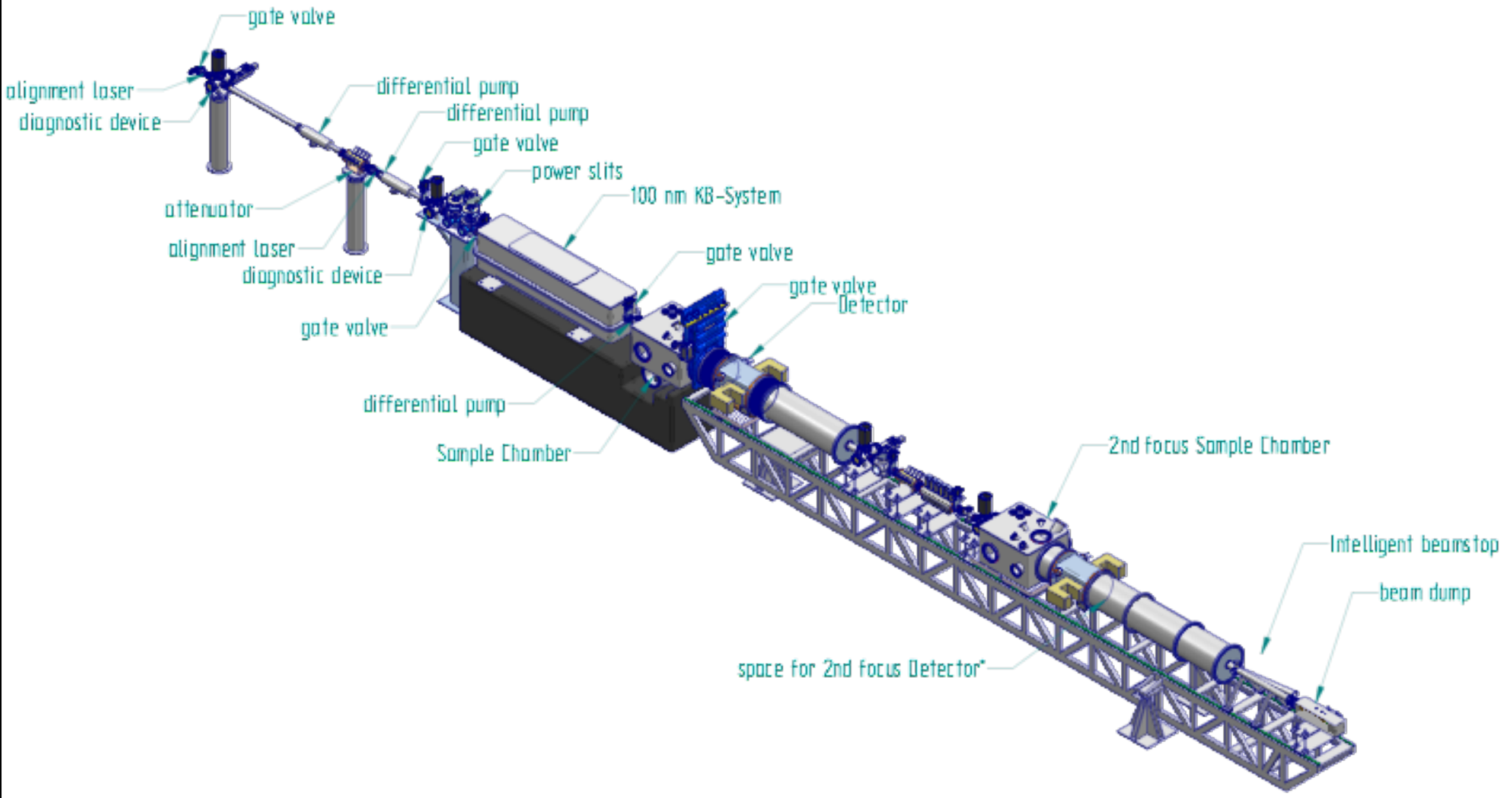
European XFEL

SPB Experiment hutch



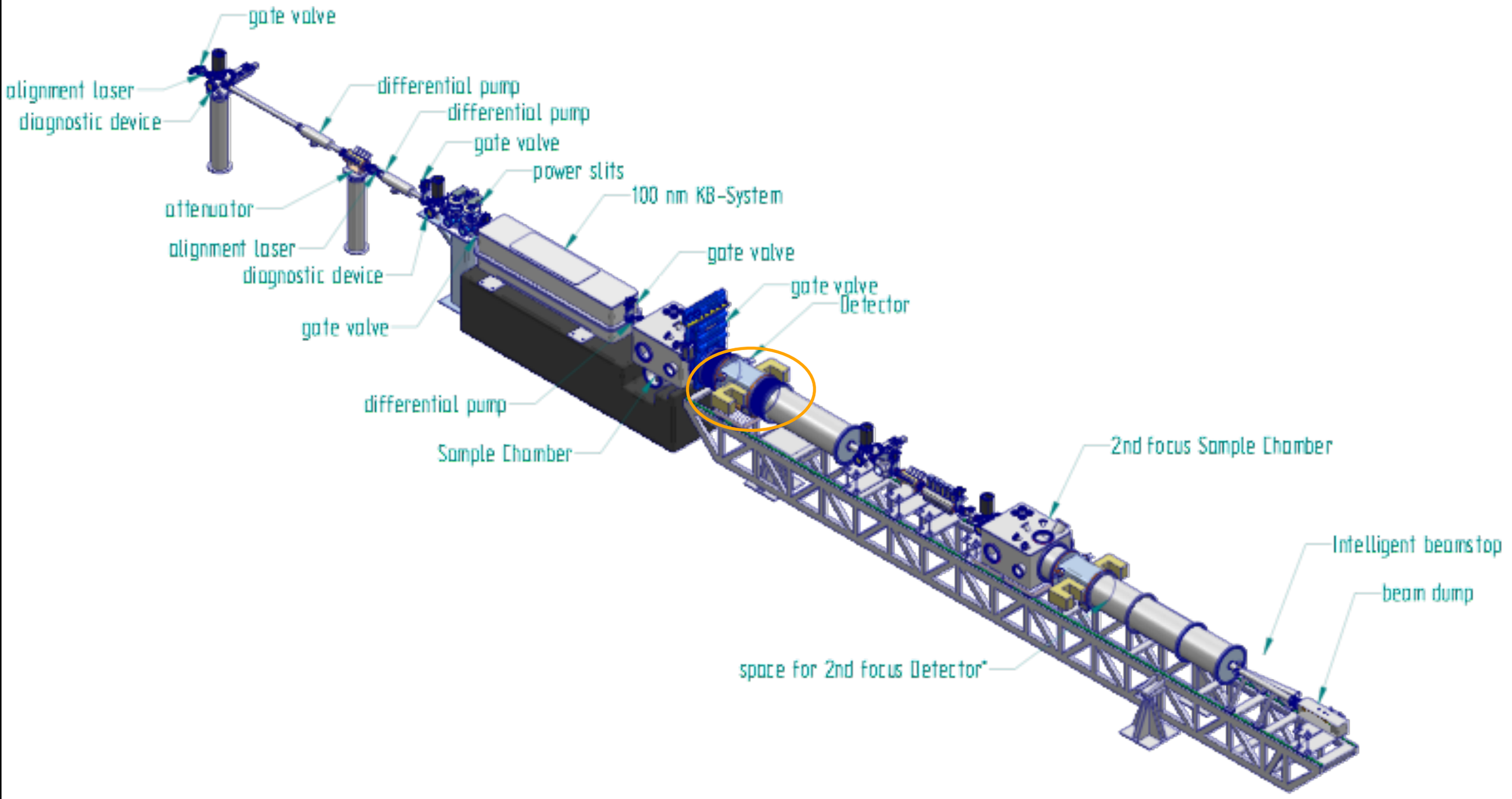
European XFEL

SPB Experiment hutch



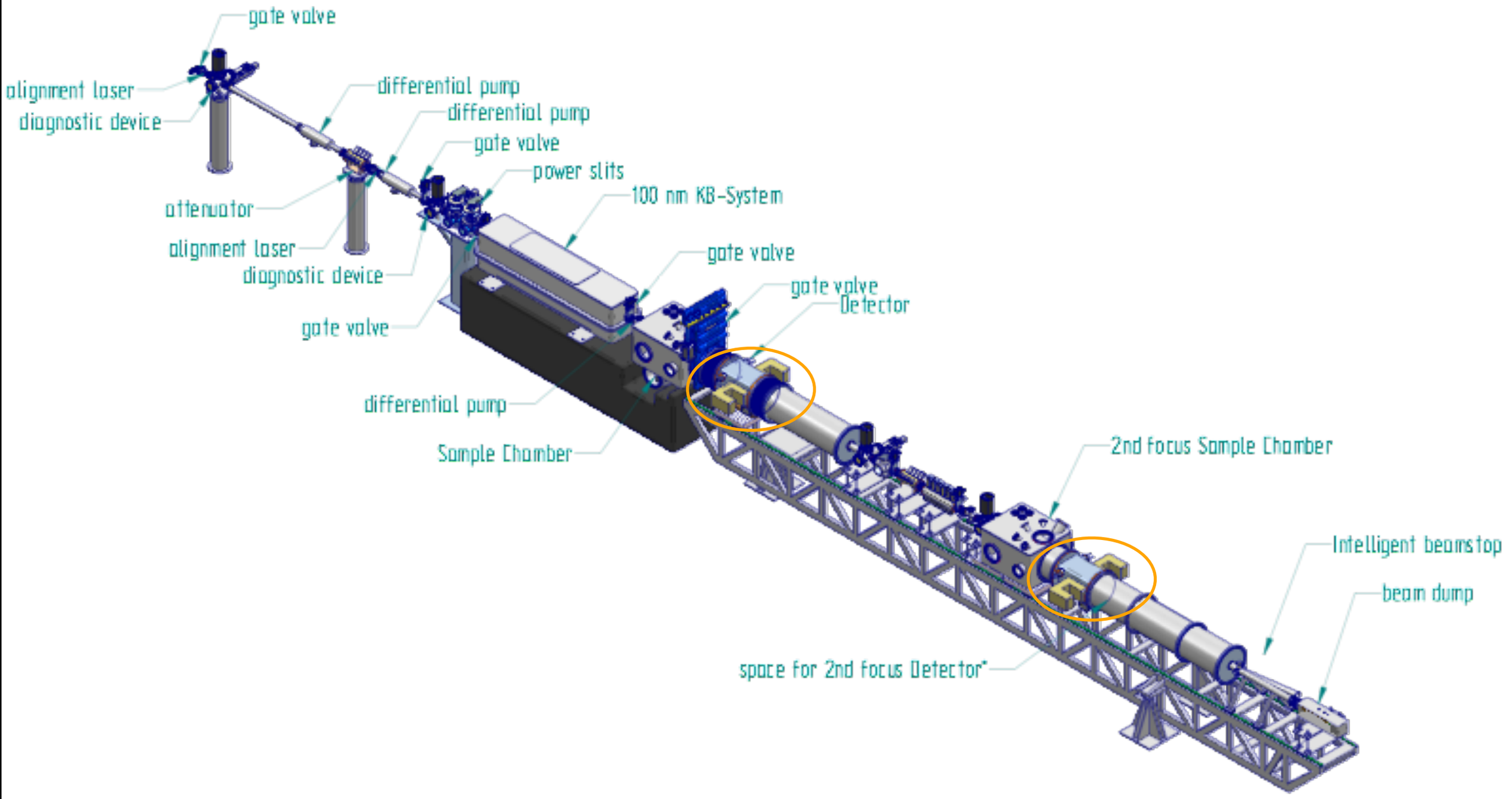
European XFEL

SPB Experiment hutch



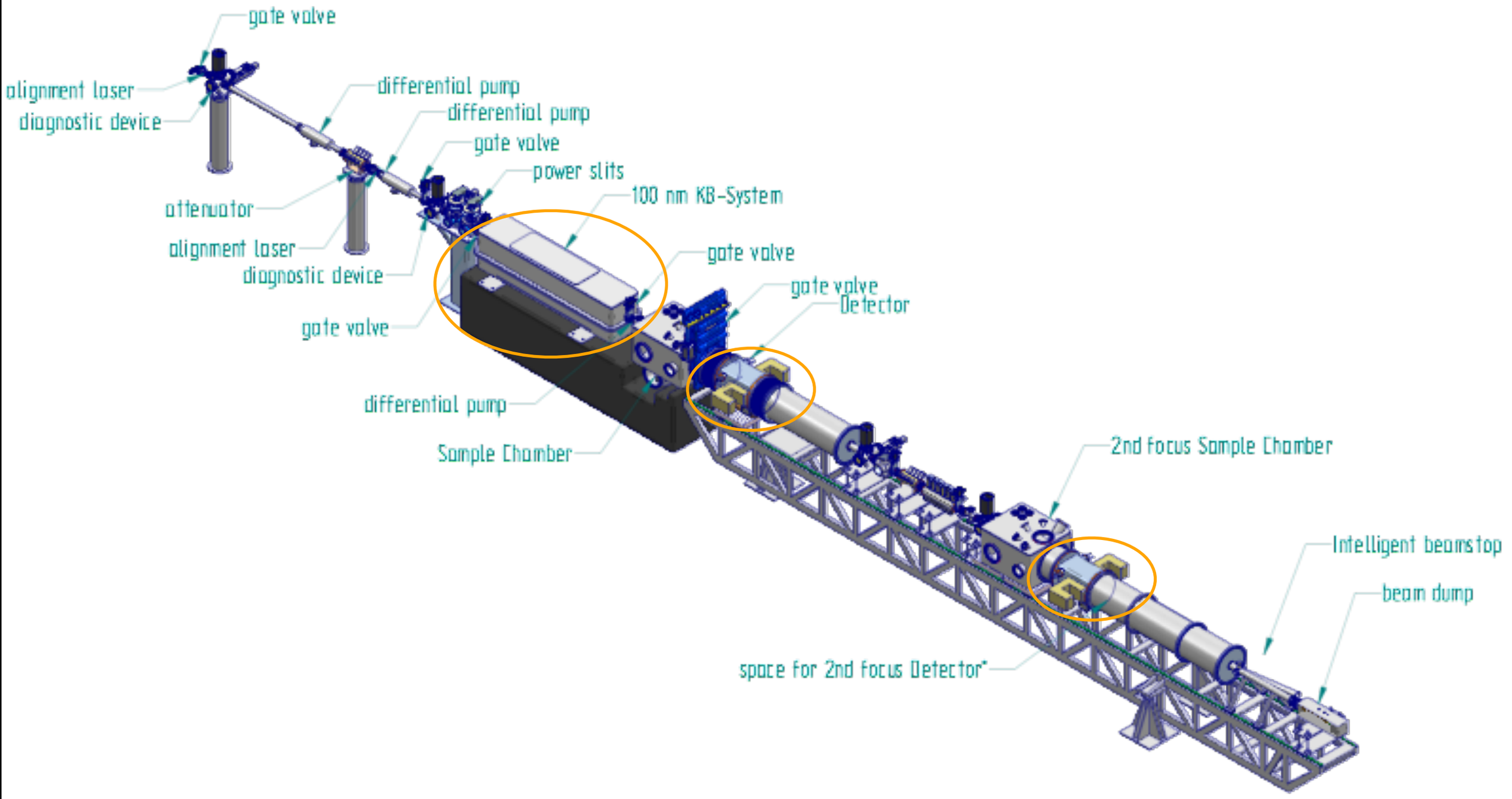
European XFEL

SPB Experiment hutch



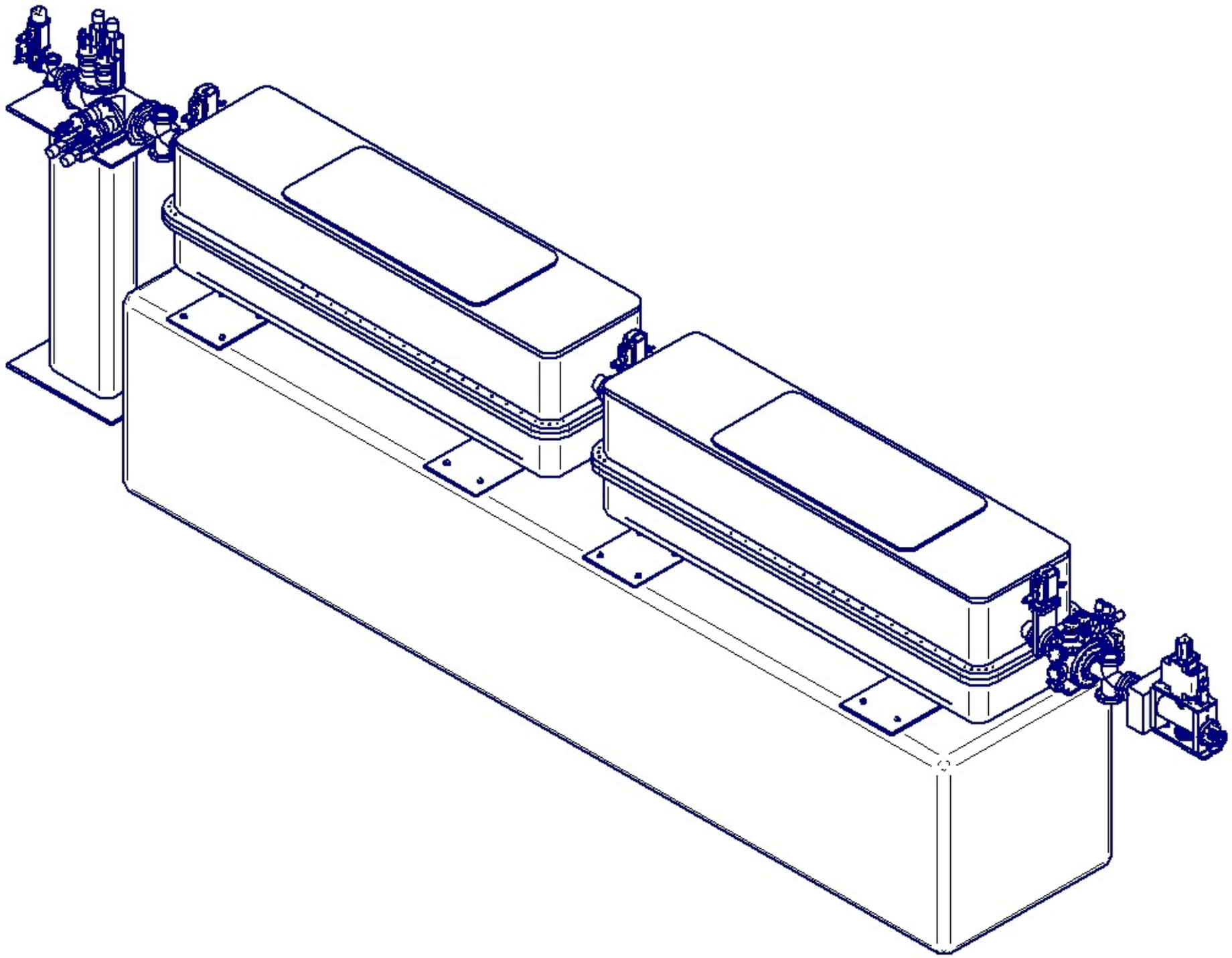
European XFEL

SPB Experiment hutch



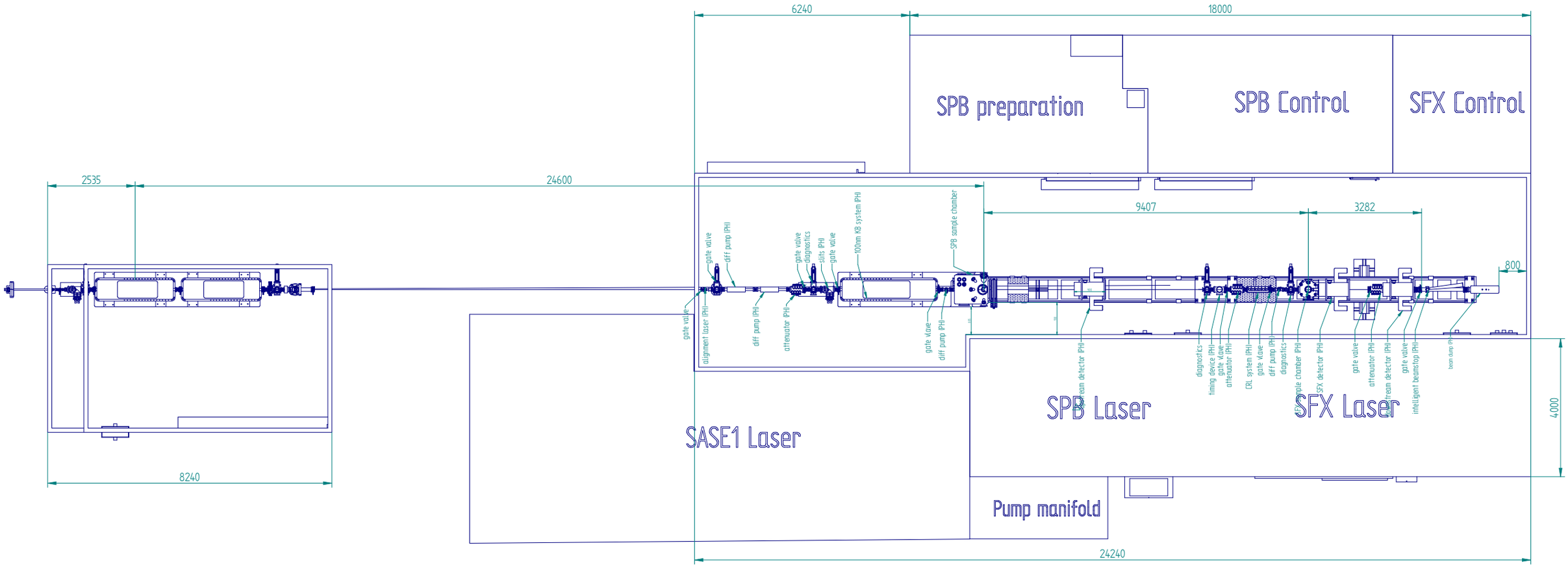
European XFEL

SPB Optics hutch



European XFEL

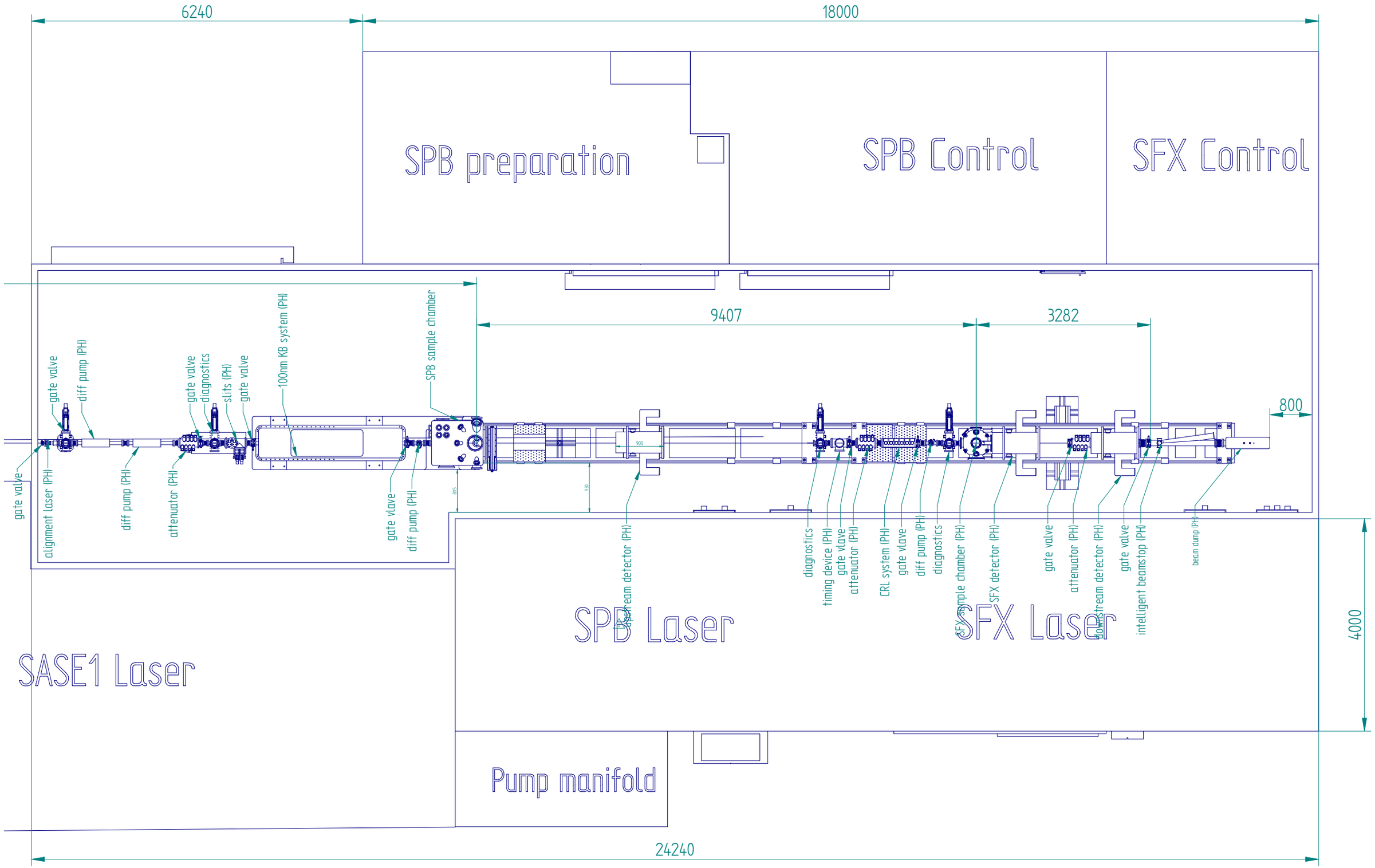
Additional SPB relevant spaces



Additional SPB relevant spaces

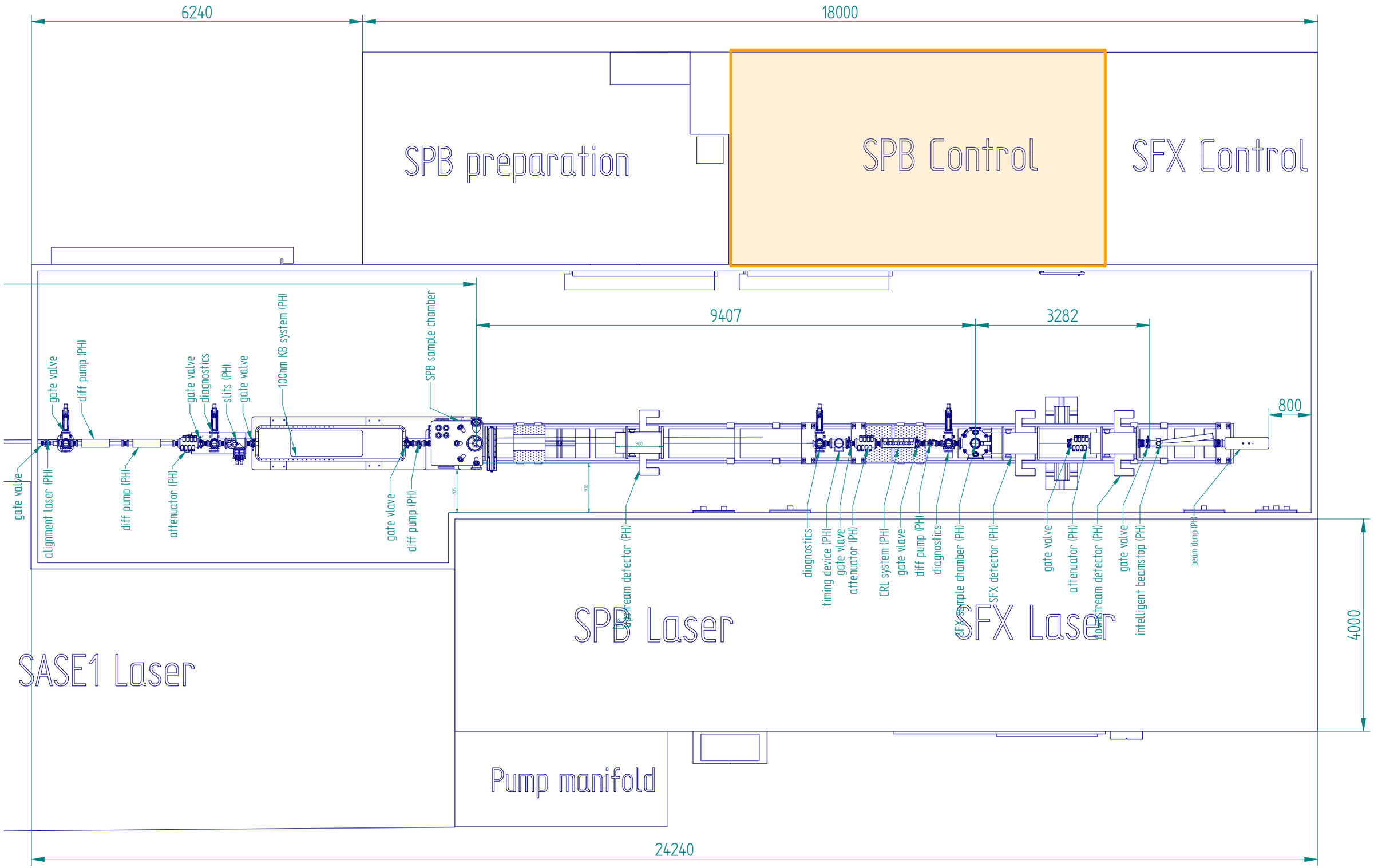
European XFEL

Additional SPB relevant spaces



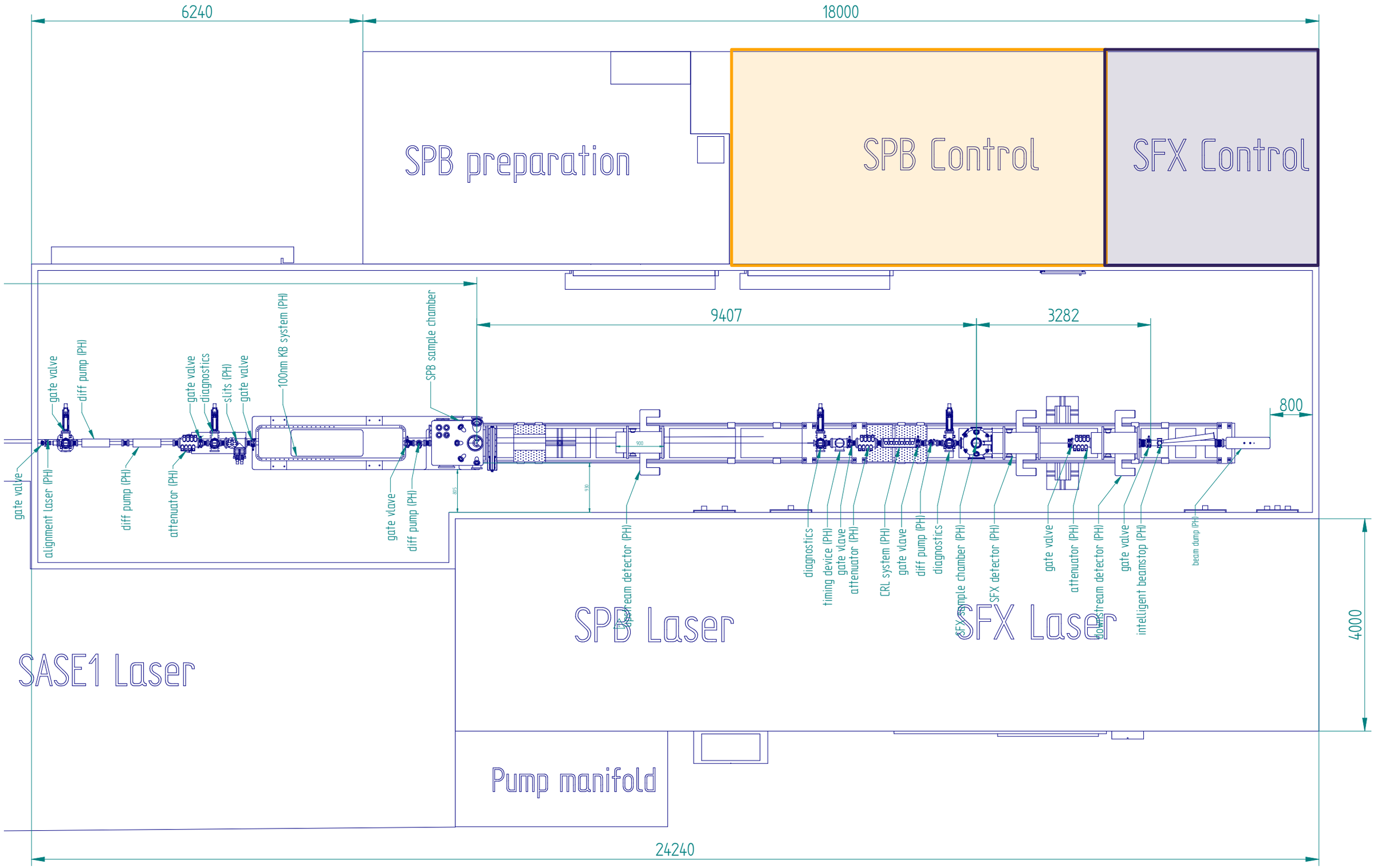
European XFEL

Additional SPB relevant spaces



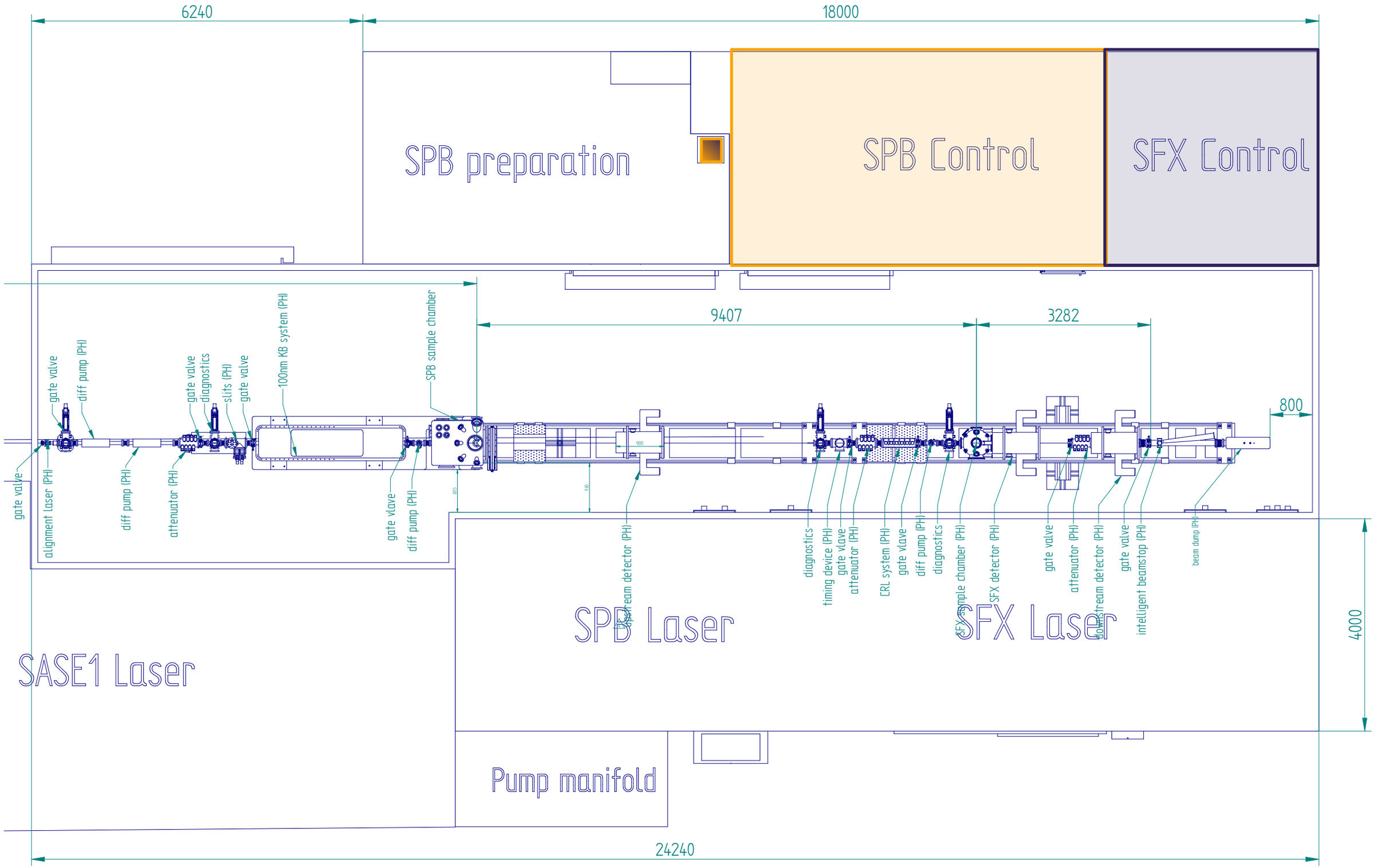
European XFEL

Additional SPB relevant spaces



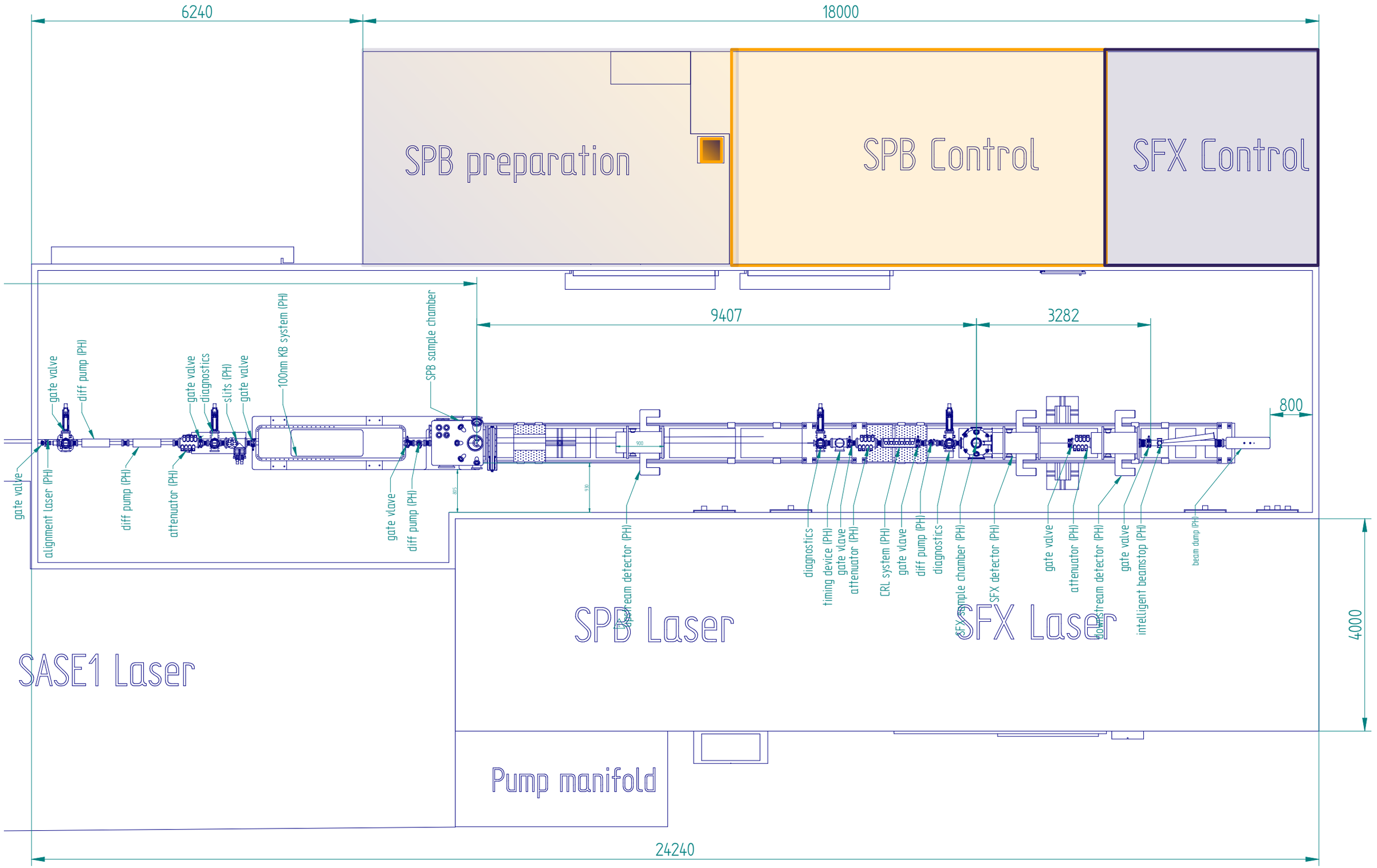
European XFEL

Additional SPB relevant spaces



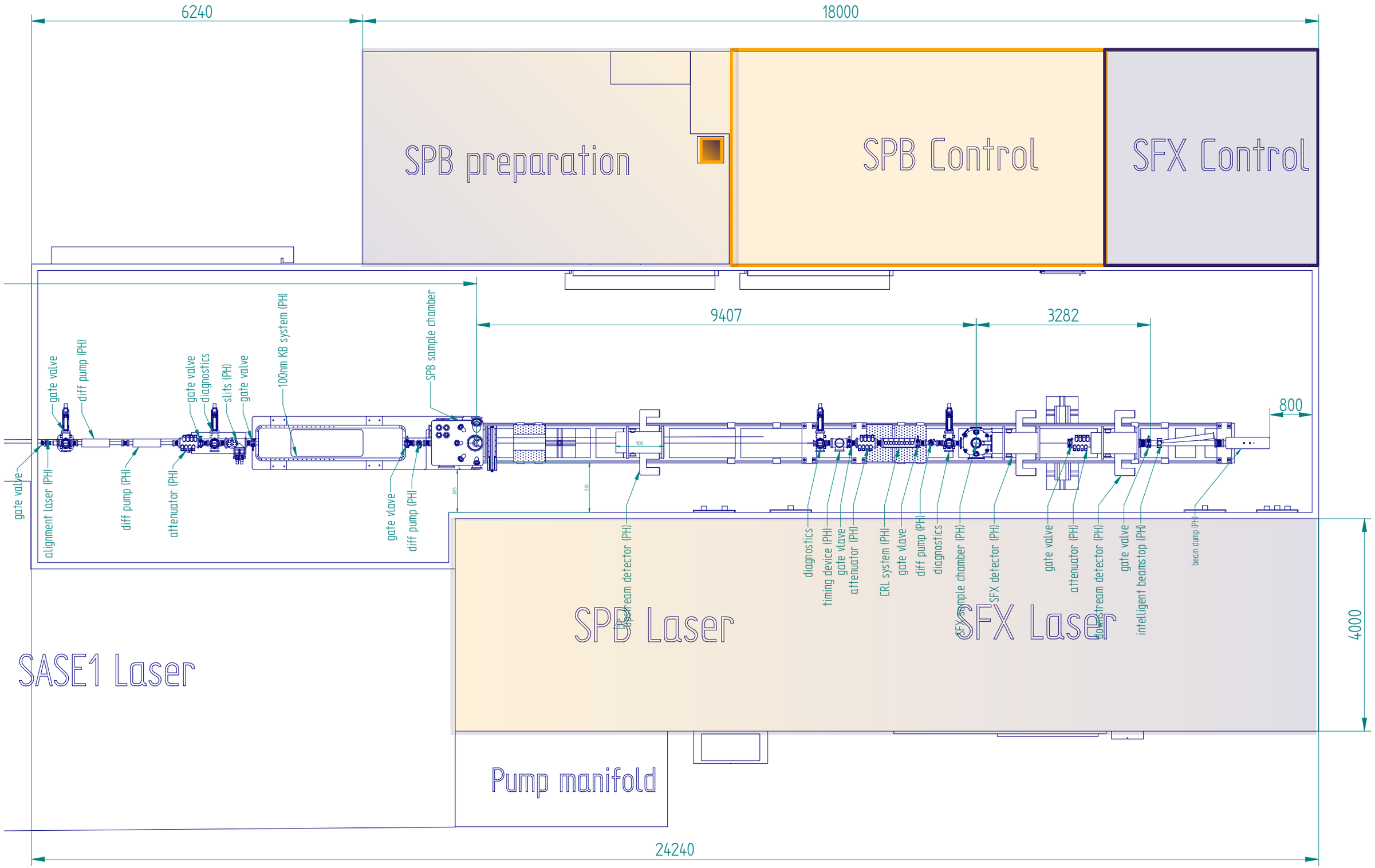
European XFEL

Additional SPB relevant spaces



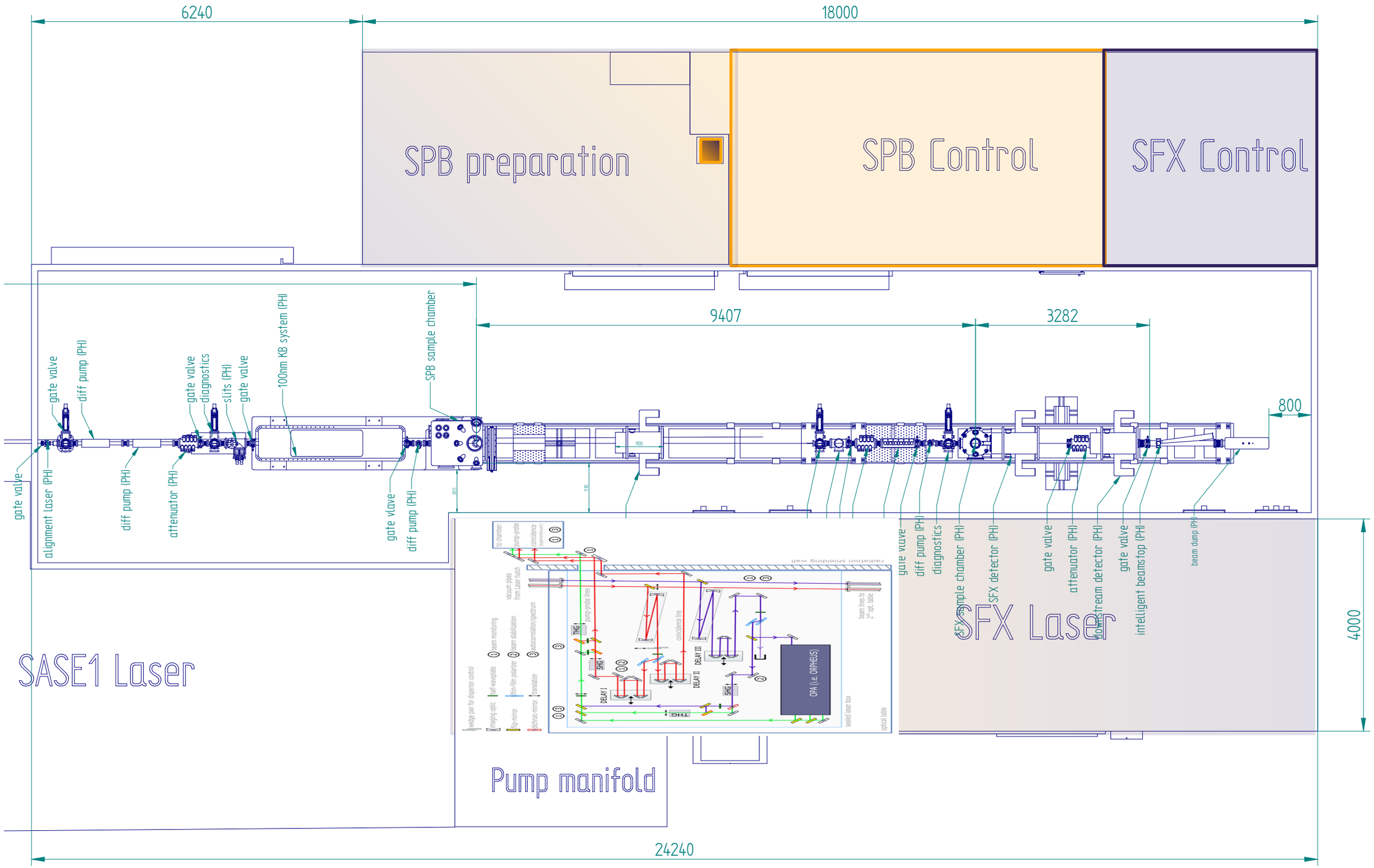
European XFEL

Additional SPB relevant spaces



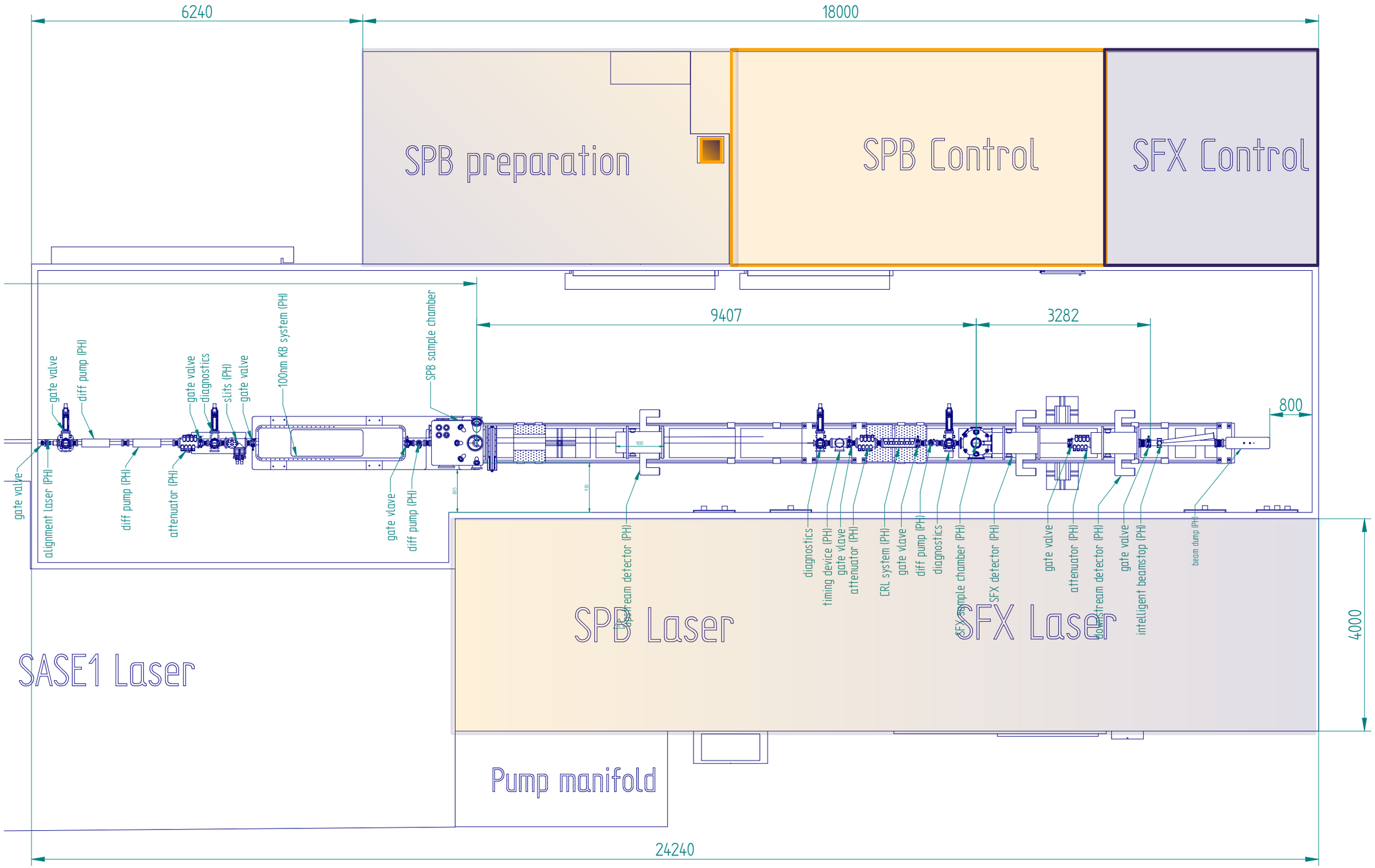
European XFEL

Additional SPB relevant spaces



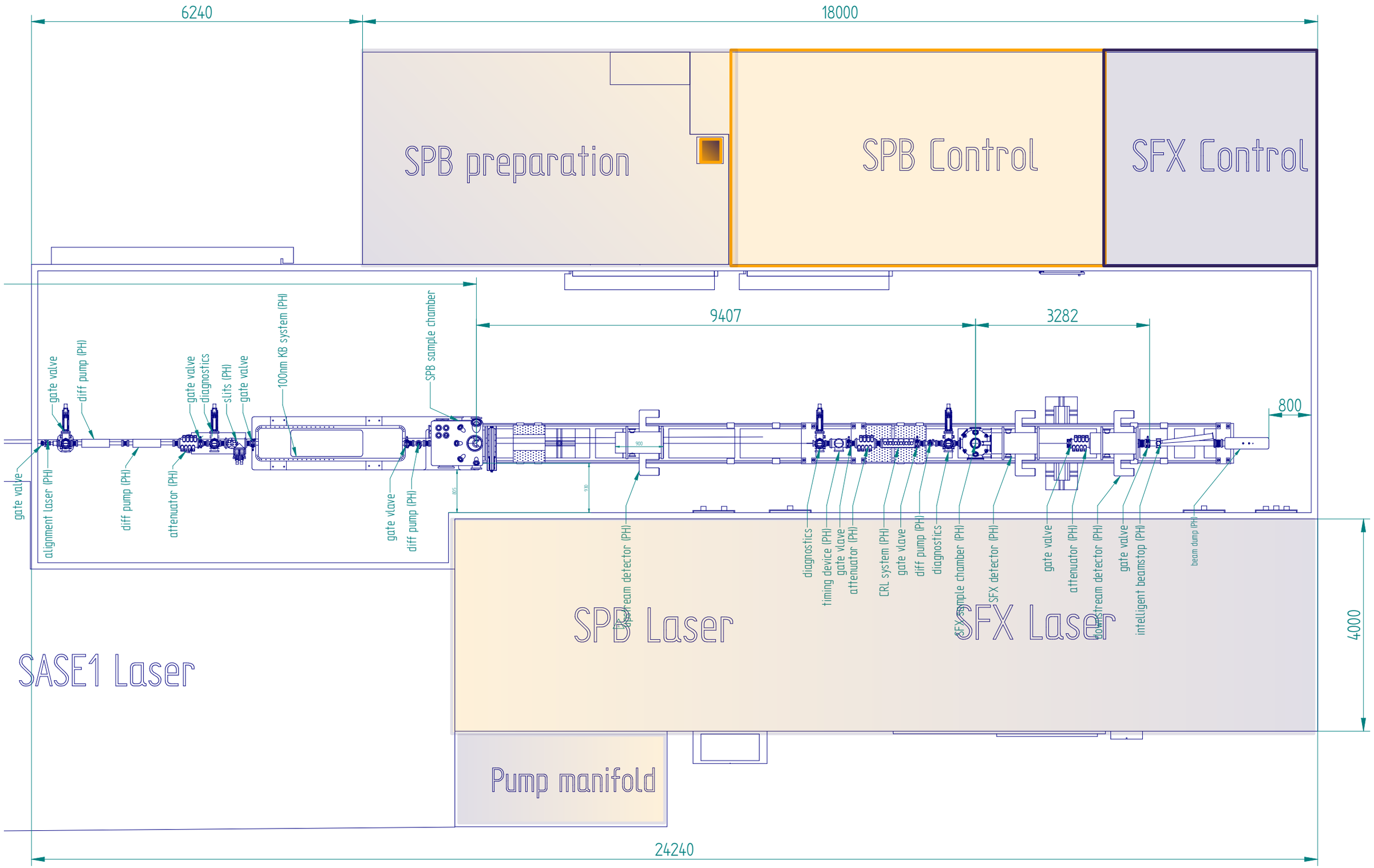
European XFEL

Additional SPB relevant spaces



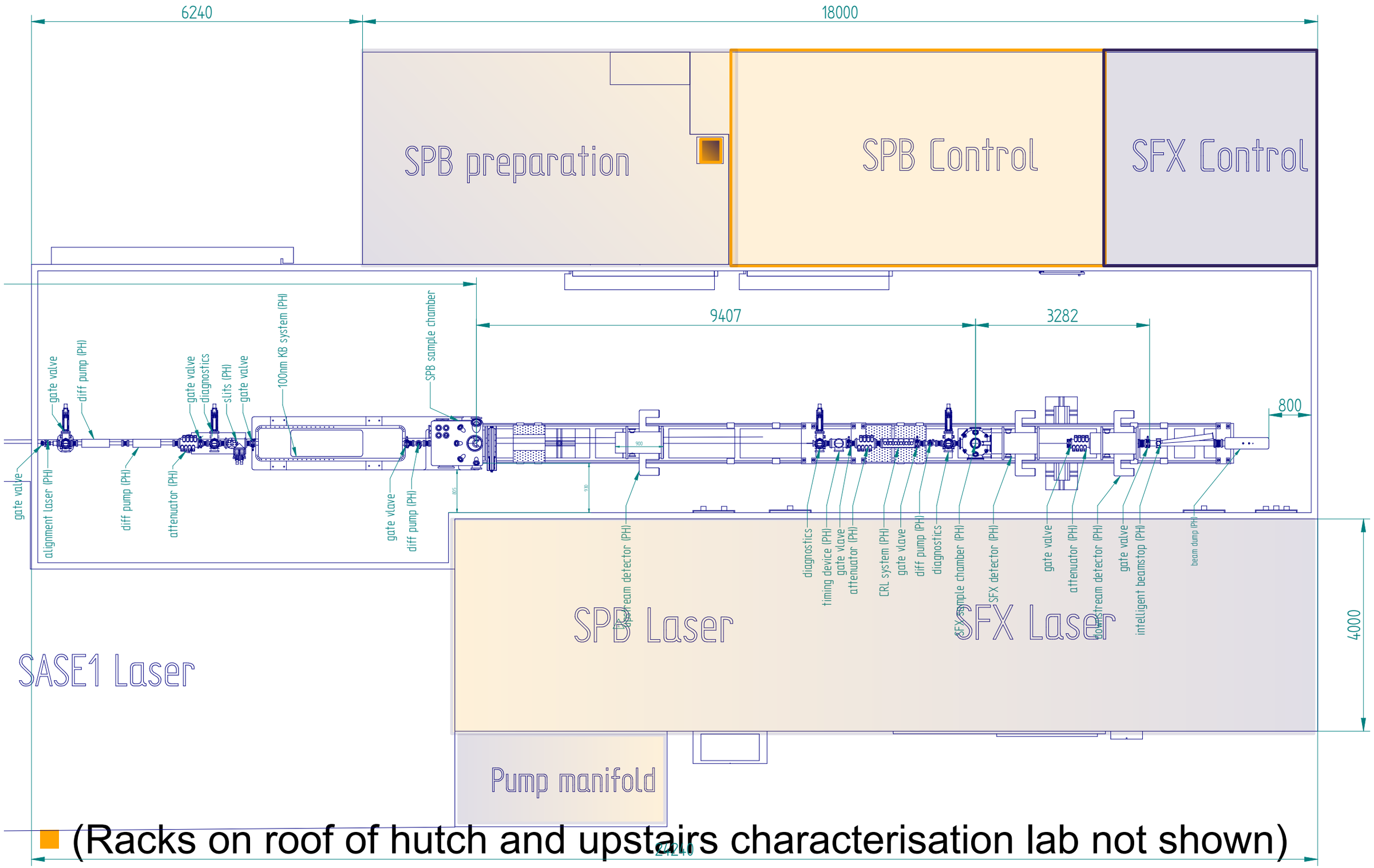
European XFEL

Additional SPB relevant spaces



European XFEL

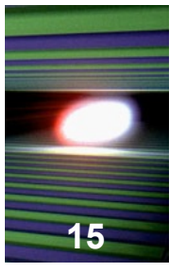
Additional SPB relevant spaces



- (Racks on roof of hutch and upstairs characterisation lab not shown)

European XFEL

Conclusions and recap I



Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles

European XFEL

Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection

European XFEL

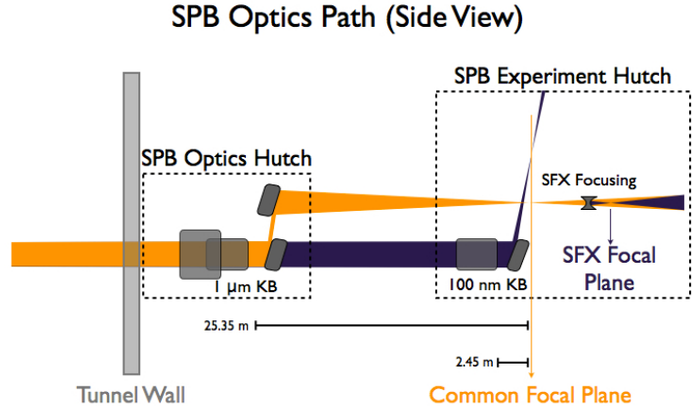
Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection

European XFEL

Conclusions and recap I

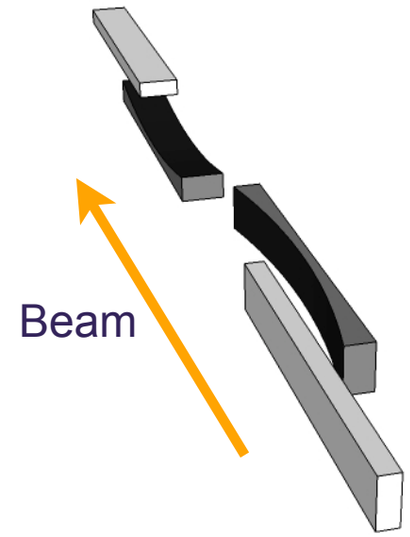
- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection



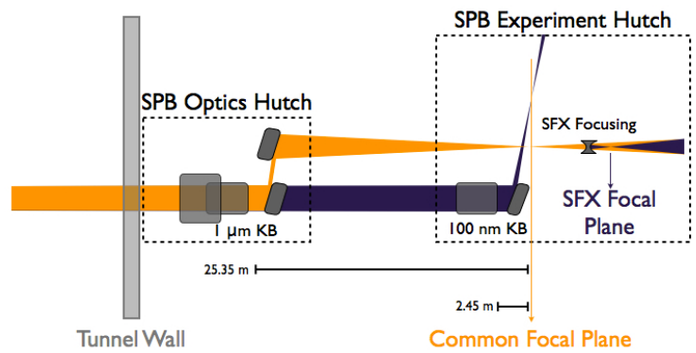
European XFEL

Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection

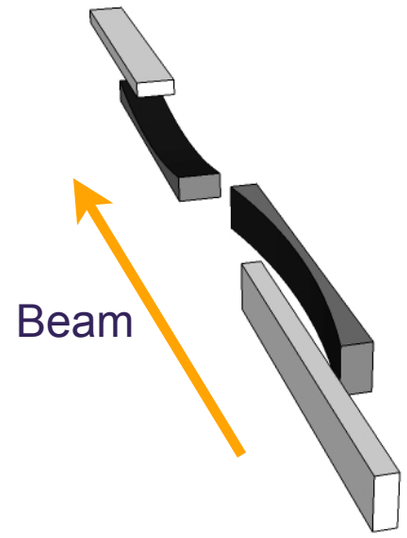


SPB Optics Path (Side View)

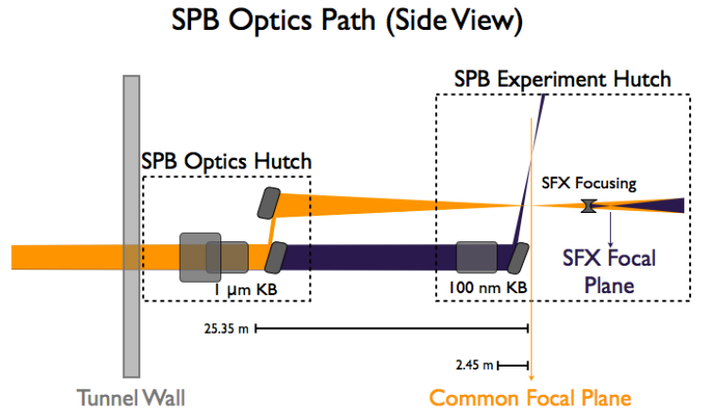


Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection

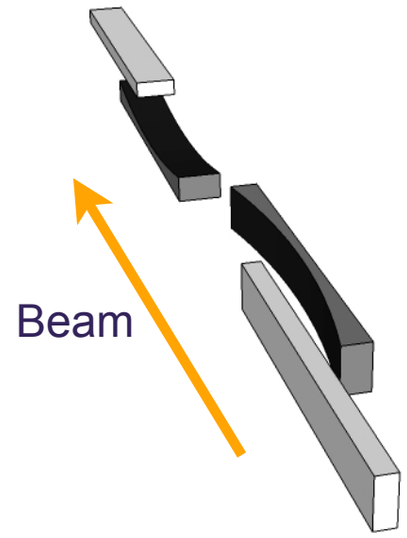


- Key component: Mirror optics
  - needs large aperture
  - challenging, inc. coating

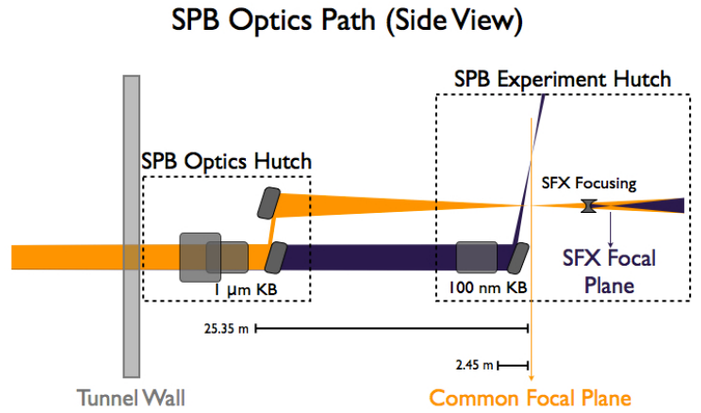


Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection

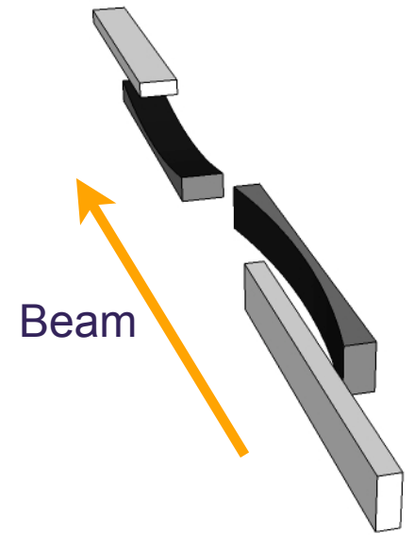


- Key component: Mirror optics
  - needs large aperture
  - challenging, inc. coating

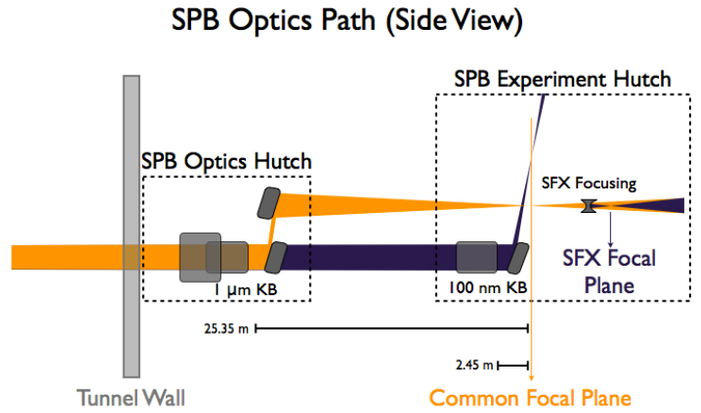


Conclusions and recap I

- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection



- Key component: Mirror optics
  - needs large aperture
  - challenging, inc. coating

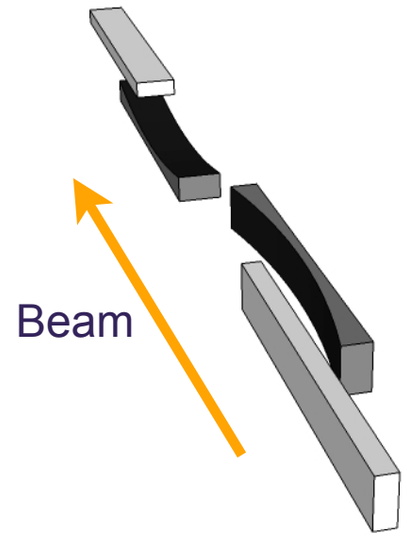


- Sample delivery
  - key methods tested and in use today
  - novel methods also actively pursued

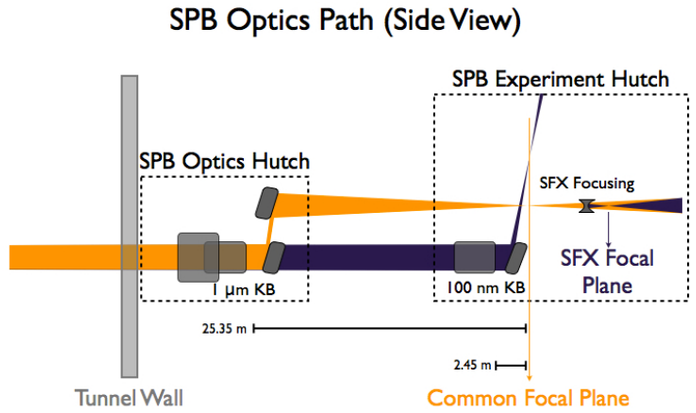
European XFEL

Conclusions and recap I

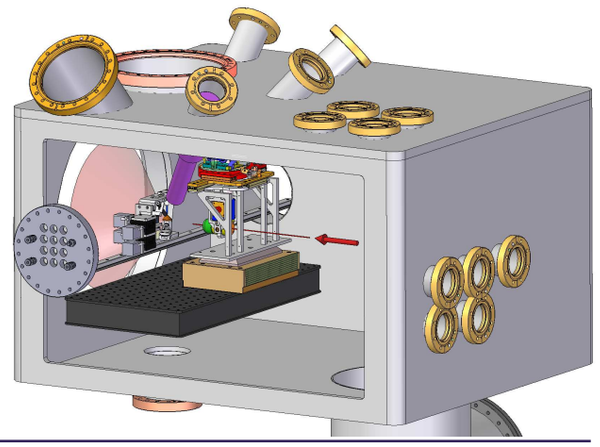
- SPB@XFEL potentially allows us to understand the structure of previously unseen crystalline and non-crystalline particles
- Instrument design includes optics, sample delivery and detection



- Key component: Mirror optics
  - needs large aperture
  - challenging, inc. coating



- Sample delivery
  - key methods tested and in use today
  - novel methods also actively pursued



Conclusions and recap II

Conclusions and recap II

- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions

Conclusions and recap II

- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions
- From 3–16 keV, SPB caters for:
  - Single particle imaging of < 100 nm particles
  - Single particle imaging of < 1μm particles
  - Nanocrystallography

Conclusions and recap II

- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions
- From 3–16 keV, SPB caters for:
  - Single particle imaging of < 100 nm particles
  - Single particle imaging of < 1μm particles
  - Nanocrystallography

Conclusions and recap II

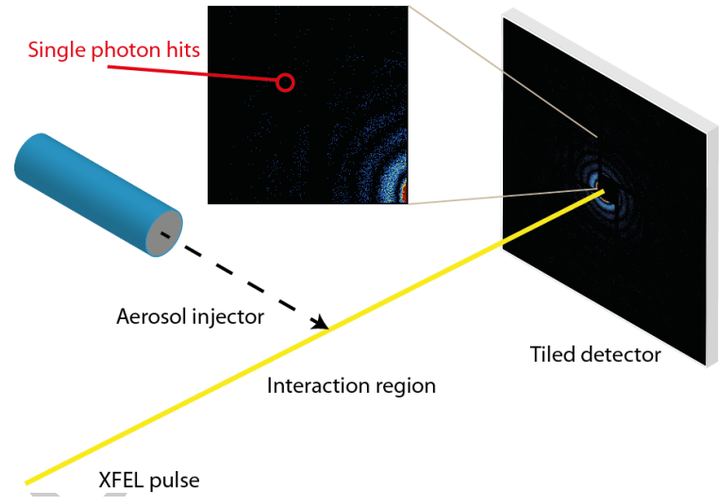
- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions
- From 3–16 keV, SPB caters for:
  - Single particle imaging of < 100 nm particles
  - Single particle imaging of < 1μm particles
  - Nanocrystallography

- **Meets specifications as asked by science cases**

European XFEL

Conclusions and recap II

- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions
- From 3–16 keV, SPB caters for:
  - Single particle imaging of < 100 nm particles
  - Single particle imaging of < 1μm particles
  - Nanocrystallography

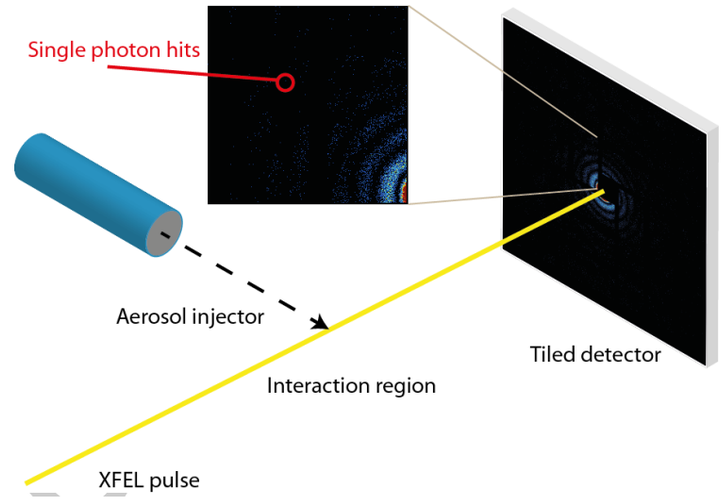


- **Meets specifications as asked by science cases**

European XFEL

Conclusions and recap II

- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions
- From 3–16 keV, SPB caters for:
  - Single particle imaging of < 100 nm particles
  - Single particle imaging of < 1μm particles
  - Nanocrystallography



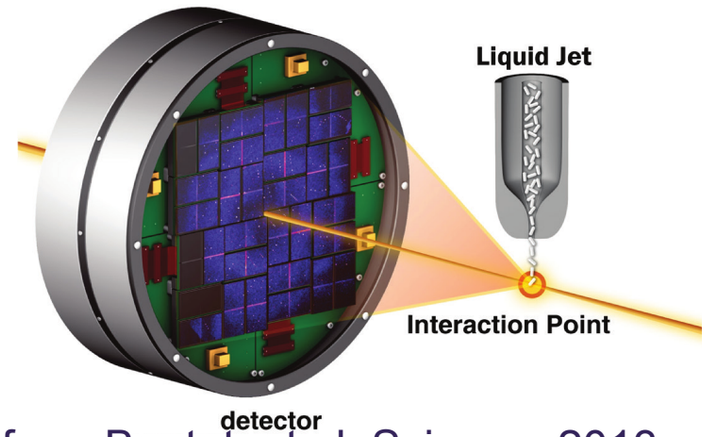


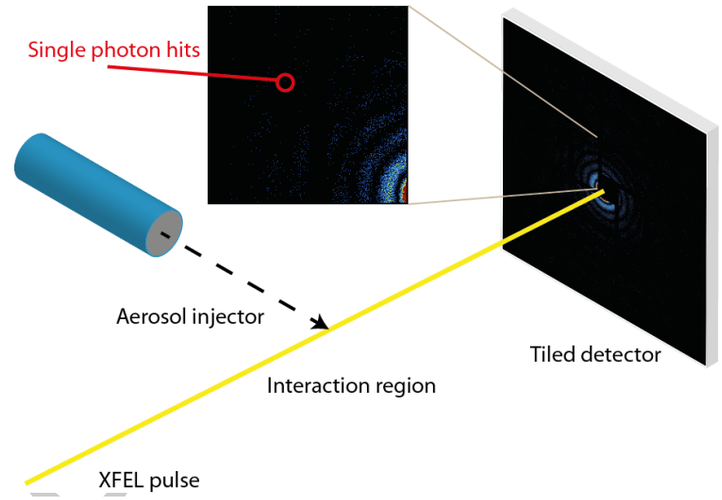
Image from Boutet, et al, Science, 2013.

- **Meets specifications as asked by science cases**

European XFEL

Conclusions and recap II

- AGIPD detector primary, day-one detector
  - Mechanical integration requires
    - ➔close (~13 cm) and far (~12 m) positions
- From 3–16 keV, SPB caters for:
  - Single particle imaging of < 100 nm particles
  - Single particle imaging of < 1μm particles
  - Nanocrystallography
- **Meets specifications as asked by science cases**



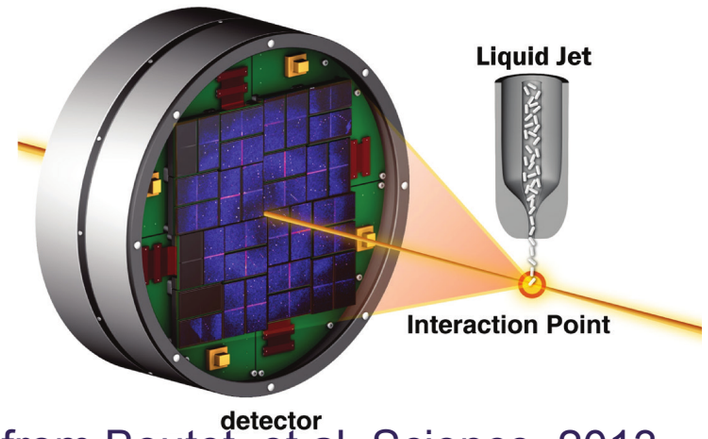
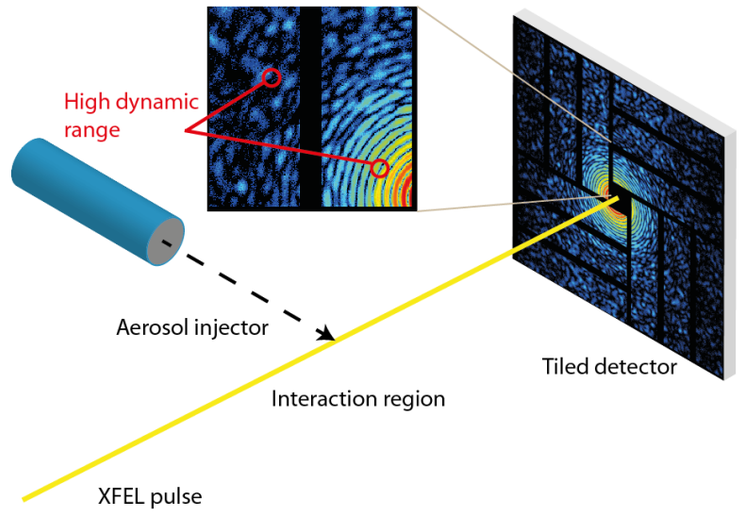
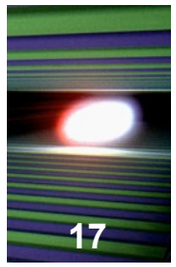


Image from Boutet, et al, Science, 2013.



European XFEL

Acknowledgments



Harald Sinn, of the X-ray beam transport group of the European XFEL.

Yamauchi-sensei of Osaka University, Ueda-san of JTEC corporation and Riccardo Signorato of Bruker Corporation. Frank Siewert of Helmholtz Zentrum Berlin, Cameron Kewish of Soleil Synchrotron, France. Regina Souffli LLNL.

Eric Gullikson of Lawrence Berkeley National Lab for useful discussions on slope errors and scatter.

Liubov Samoylova, Oleg Chubar and Alexey Buzmakov are thanked for their efforts in delivering and assistance with SRW code for propagation of wavefields.

Jan Grünert and team, including Cigdem Ozkan, Jens Buck and Wolfgang Freund. Ryan Coffee of the LCLS.

Joachim Schulz, Sadia Bari and Charlotte Uetrecht.

Markus Kuster and supported by Jola Sztuk-Dambietz, Monica Turcato, Andreas Koch and Steffen Hauf.

The AGIPD consortium, led by Heinz Graafsma with the assistance of Julian Becker, Helmut Hirsemann.

The DSSC consortium, led by Matteo Porro is similarly thanked for their efforts developing the DSSC and communicating those developments with us. Georg Weidenspointer is particularly thanked for valuable discussions.

Chris Youngman, Nicola Coppola, Krzysztof Wrona, Burkhard Heisen. Chun Hong Yoon

Haiou Zhang, Raùl Villanueva and Martin Dommach are thanked for their advice on vacuum technology.

Holger Fleckenstein and Lars Gumprecht of CFEL, DESY. Wolfgang Tscheu and the CIE group of the European XFEL.

Our user consortia partners, in particular, Henry Chapman as the spokesperson for the SFX consortium, Victor Lamzin as spokesperson for the XBI consortium and Anton Barty for the dataXpress consortium.CXI instrument of the LCLS, particularly Sebastien Boutet and Garth Williams.

Valuable feedback on this text was provided by Thomas Tschentscher of the European XFEL and as well as Massimo Altarelli, Andreas Schwarz, and Serguei Molodtsov, all members of the European XFEL Management Board. Michael Meyer, Anders Madsen, Christian Bressler, and Andreas Scherz, are all leading scientists at the European XFEL. They and their groups are also thanked for their continued feedback and valuable discussions.

Leo Chavas, Meng Liang, Patrik Vagovic, Stephan Stern, Steffen Raabe, Hamidreza Dadgostar, Sunil Ananthaneni and Henry Chapman form the SFX team which will design and deliver the SFX apparatus to be included in the SPB instrument hutch.

Finally, the SPB ART (Ilme Schlichting, Garth Williams, Sebastien Boutet, Dan DePonte, Victor Lamzin, Anton Barty, Franz Pfeiffer, David Stuart), and the Scientific Advisory Committee of the European XFEL have contributed review comments and insights at each stage of design of the SPB instrument. Their diligent work in providing advice and feedback–often at short notice and in considerable detail–is thoroughly appreciated and highly valued. The instrument will be better because of their generosity in providing scientific input, critical feedback, and specialist knowledge.

European XFEL

SPB Contributors

- SPB
  - Andrew Aquila
  - Klaus Giewekemeyer
  - Gannon Borchers
  - Nadja Reimers (Central Instruments Engineering)

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

European XFEL

SPB Contributors

- SPB
  - Andrew Aquila
  - Klaus Giewekemeyer
  - Gannon Borchers
  - Nadja Reimers (Central Instruments Engineering)

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

European XFEL

SPB Contributors

- SPB
  - Andrew Aquila
  - Klaus Giewekemeyer
  - Gannon Borchers
  - Nadja Reimers (Central Instruments Engineering)

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

European XFEL

SPB Contributors

- SPB
  - Andrew Aquila
  - Klaus Giewekemeyer
  - Gannon Borchers
  - Nadja Reimers (Central Instruments Engineering)

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

European XFEL

SPB Contributors

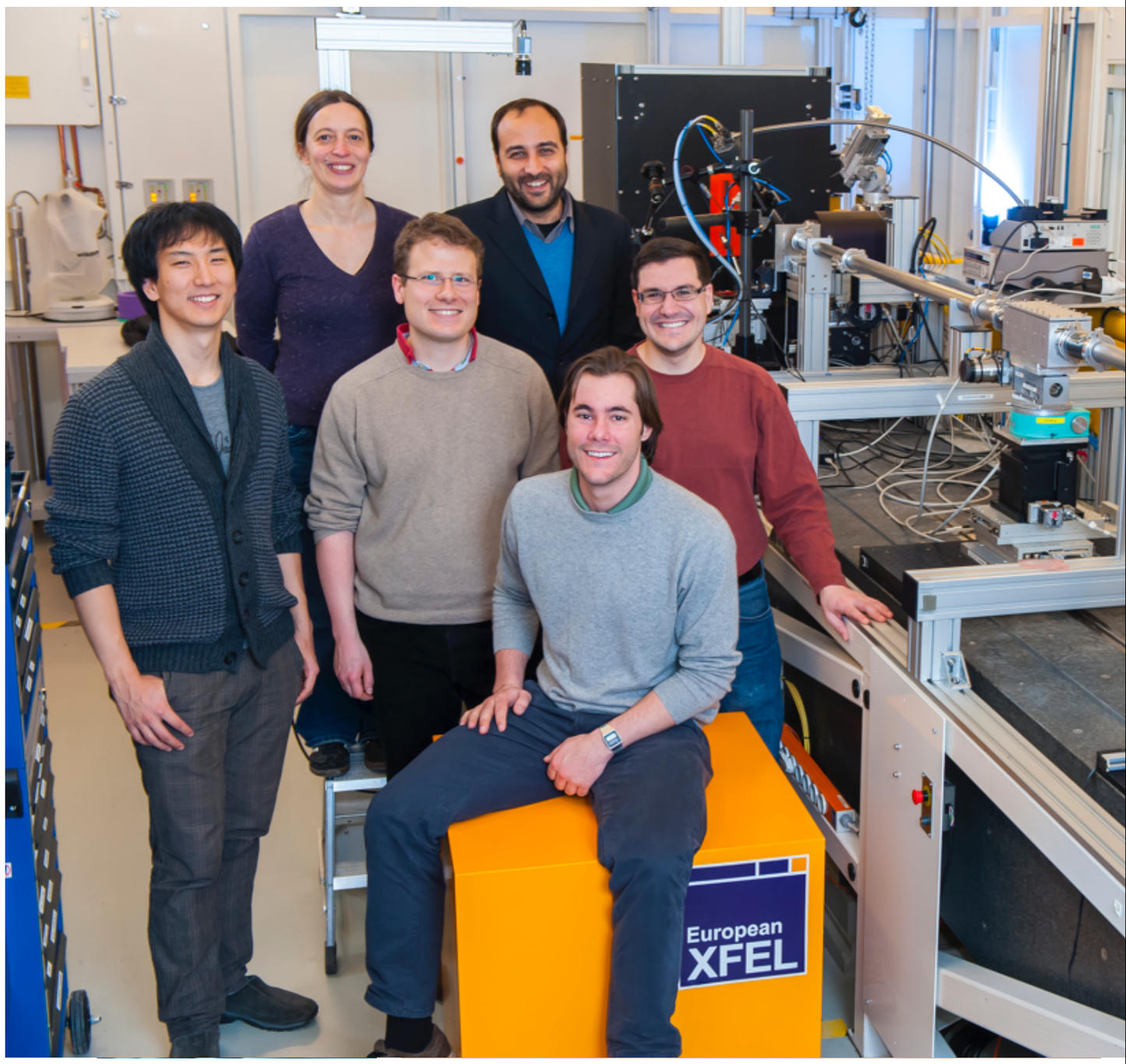
- SPB
  - Andrew Aquila
  - Klaus Giewekemeyer
  - Gannon Borchers
  - Nadja Reimers (Central Instruments Engineering)

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

European XFEL

SPB Contributors

- SPB
  - Andrew Aquila
  - Klaus Giewekemeyer
  - Gannon Borchers
  - Nadja Reimers (Central Instruments Engineering)



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