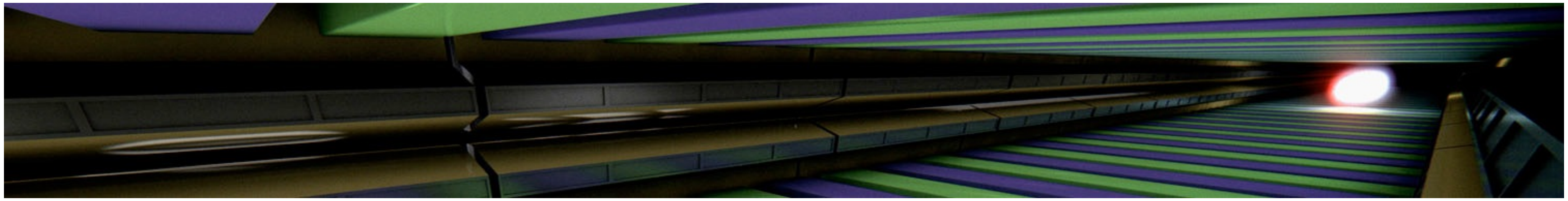


Installation & first experiments at SPB/SFX

Adrian Mancuso

Overview

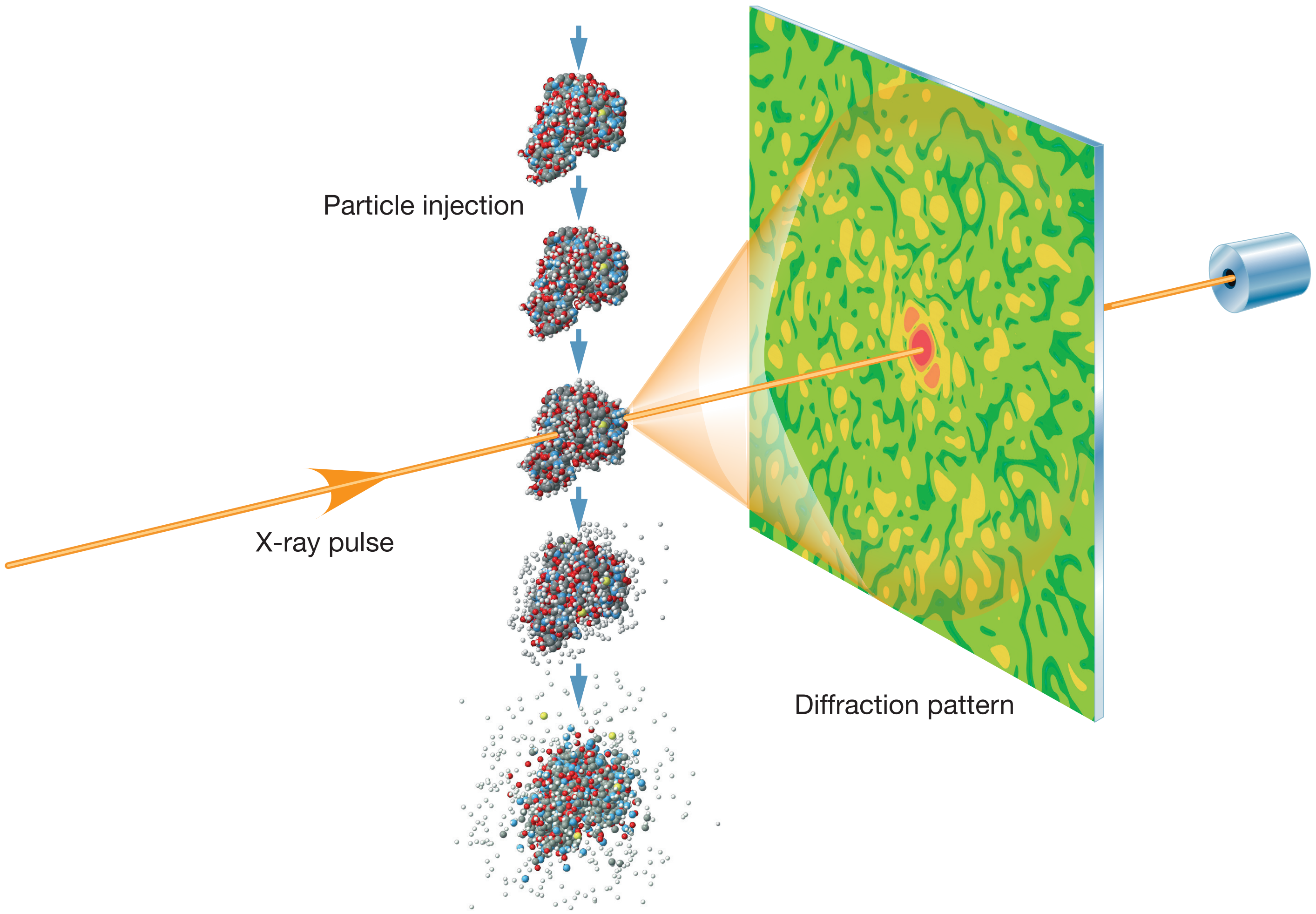
- Reminder: SPB/SFX science
- Reminder: The SPB/SFX instrument
- Day one beam parameters
- Sketch of first possible experiments
- Requirements to instrumentation to perform these experiments
- Conclusions

Reminder: SPB/SFX Science

Reminder: SPB/SFX Science

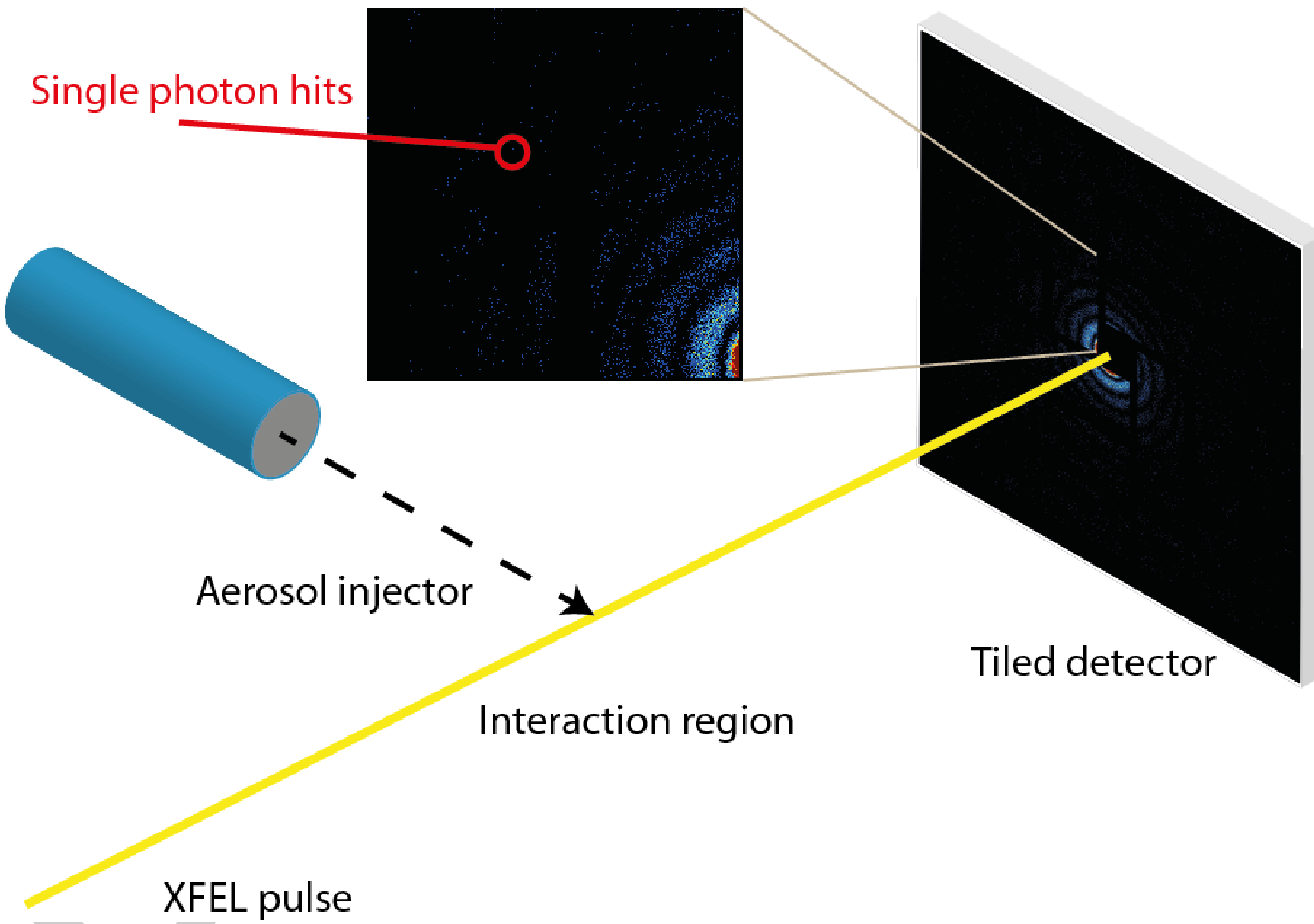
Imaging of “big” and “small”
non-crystalline samples

Reminder: SPB/SFX Science



Imaging of “big” and “small” non-crystalline samples

Reminder: SPB/SFX Science



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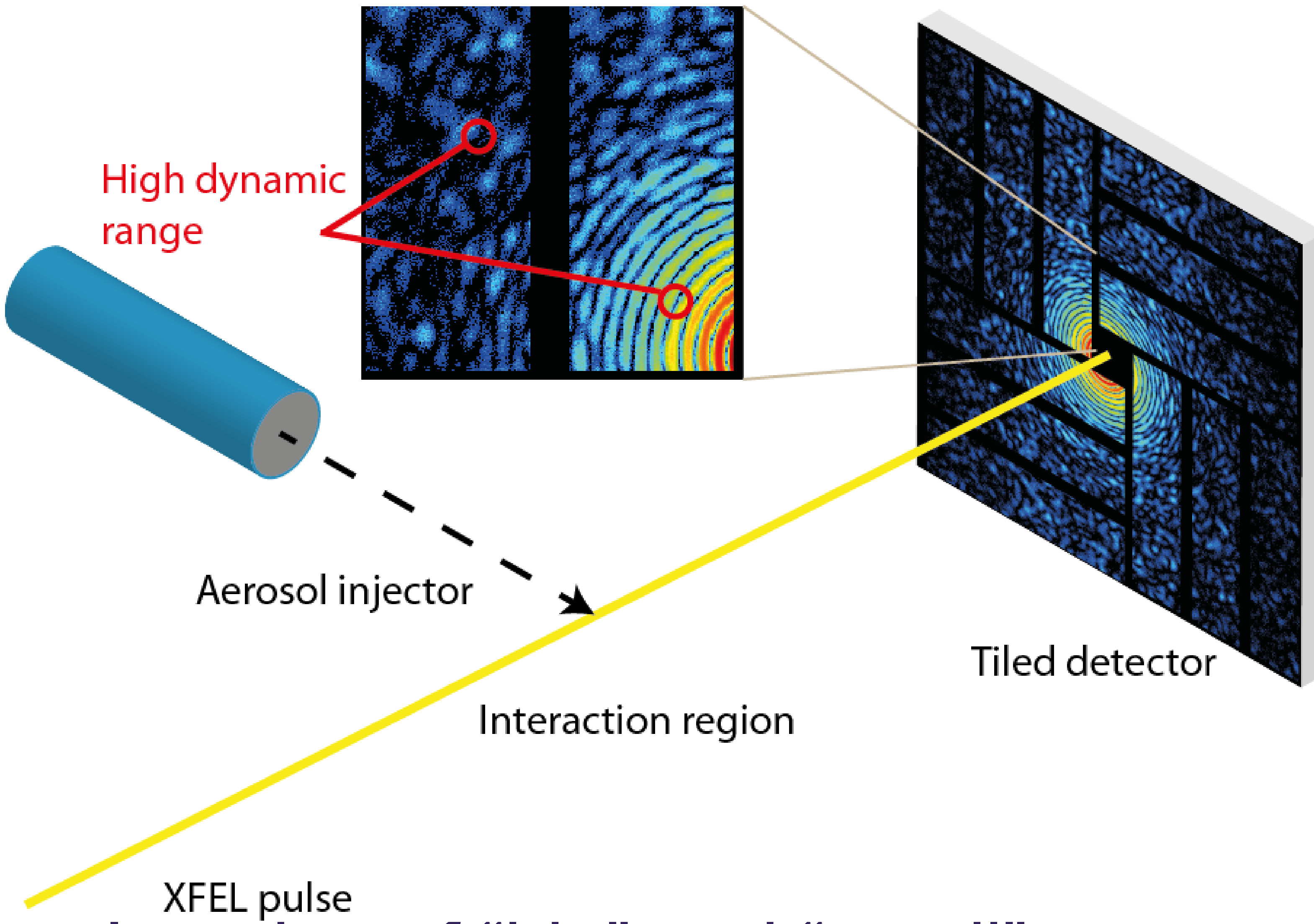

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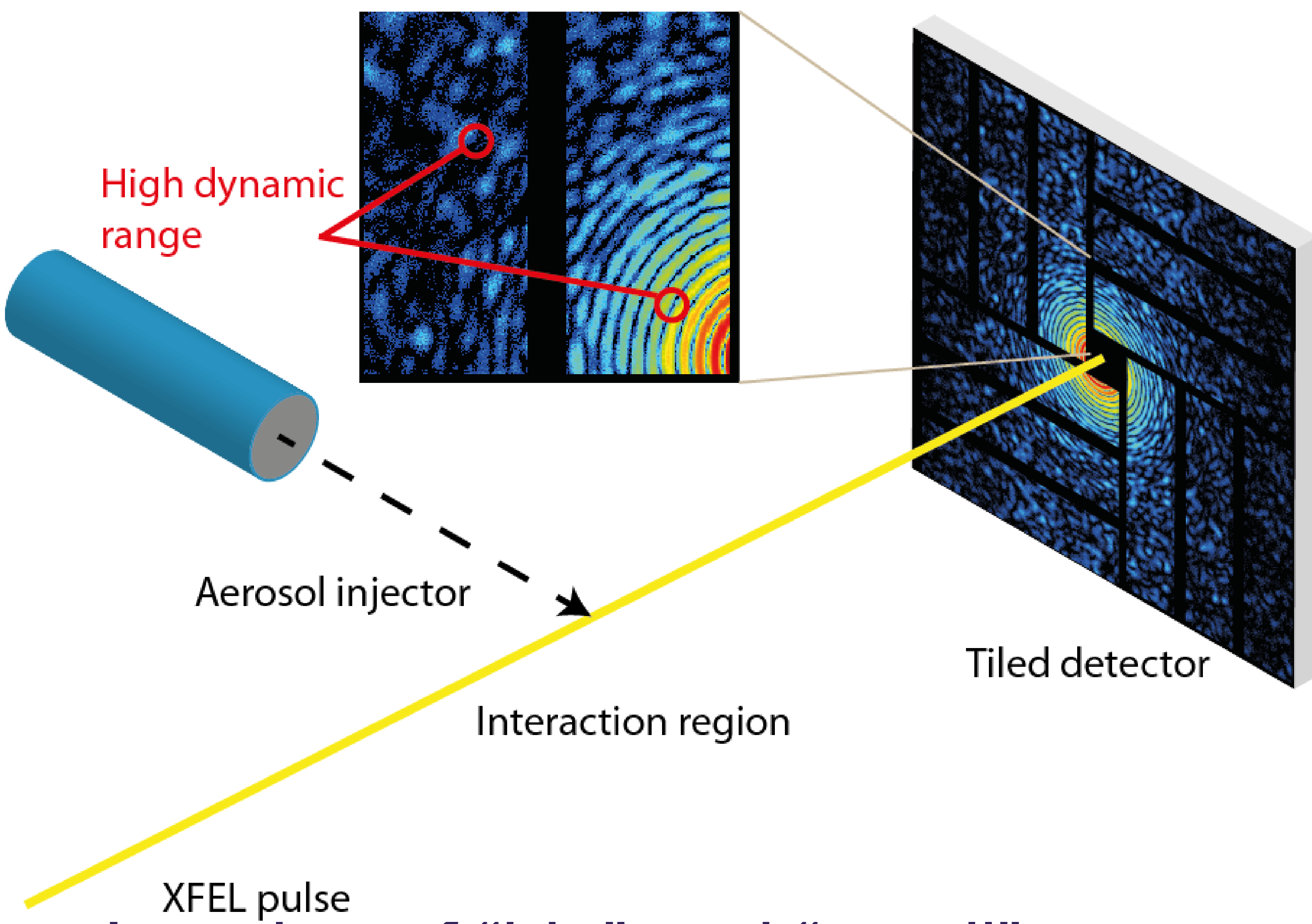
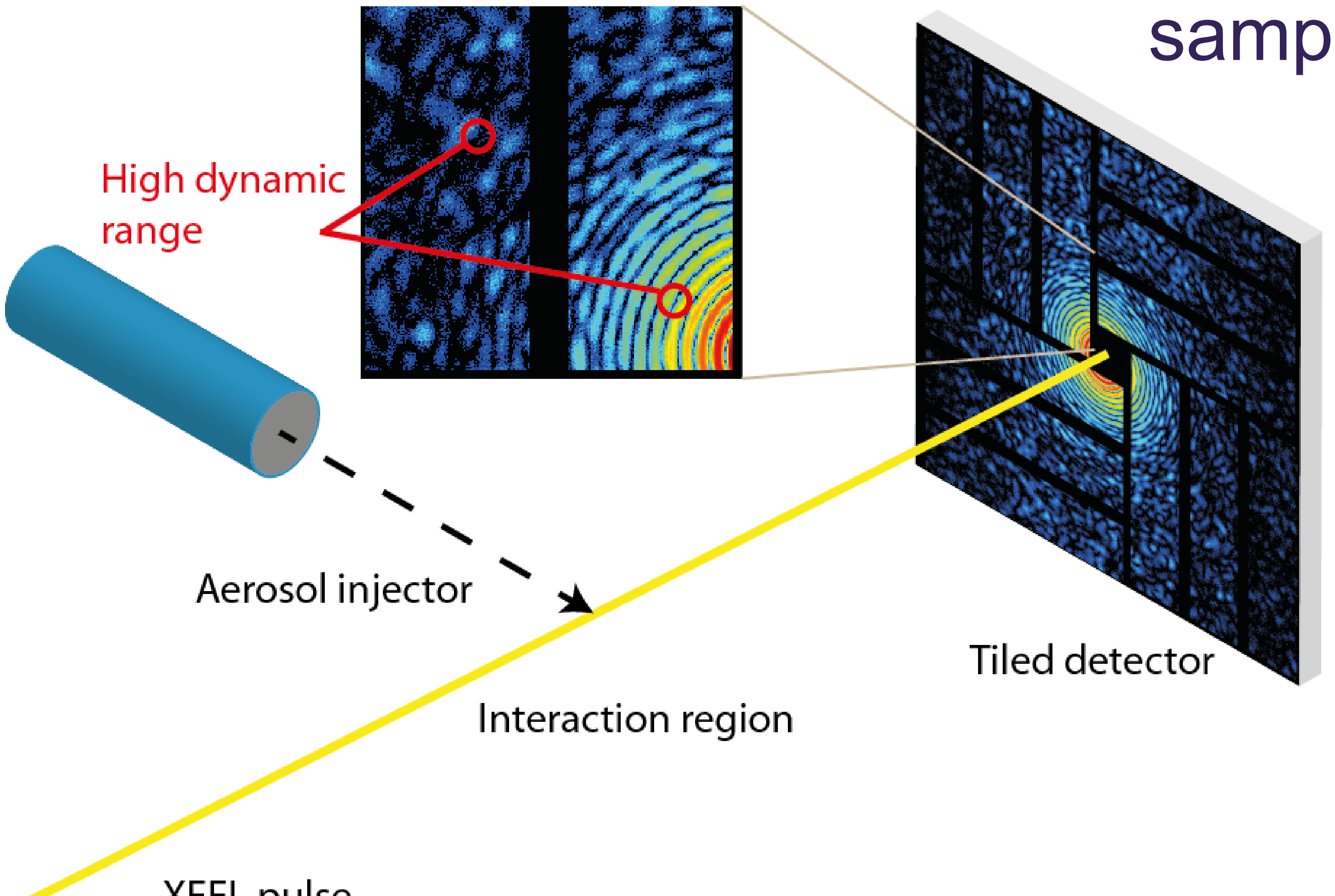


Imaging of “big” and “small” non-crystalline samples $\lim_{N \to \infty} = \text{SAXS}$

Reminder: SPB/SFX Science

Crystallography of “small”, “radiation sensitive” or “dynamic” samples



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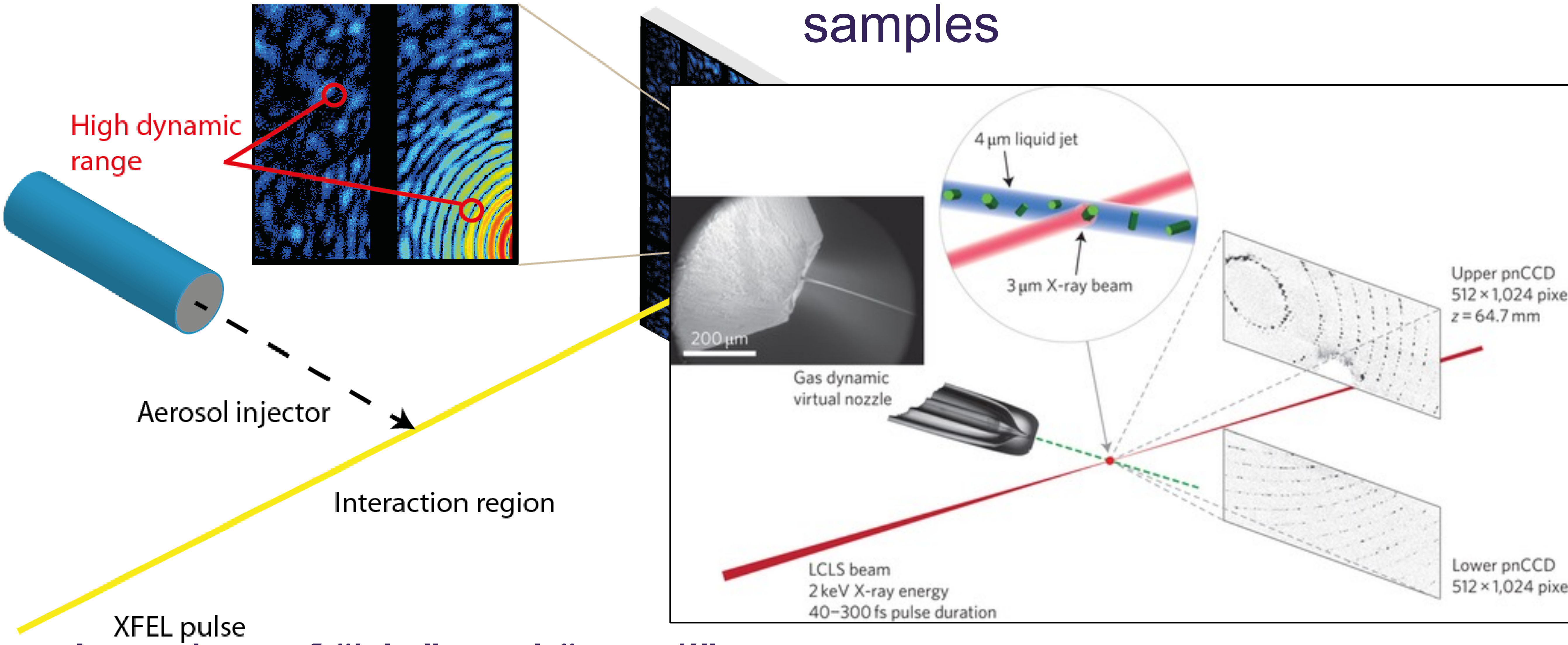
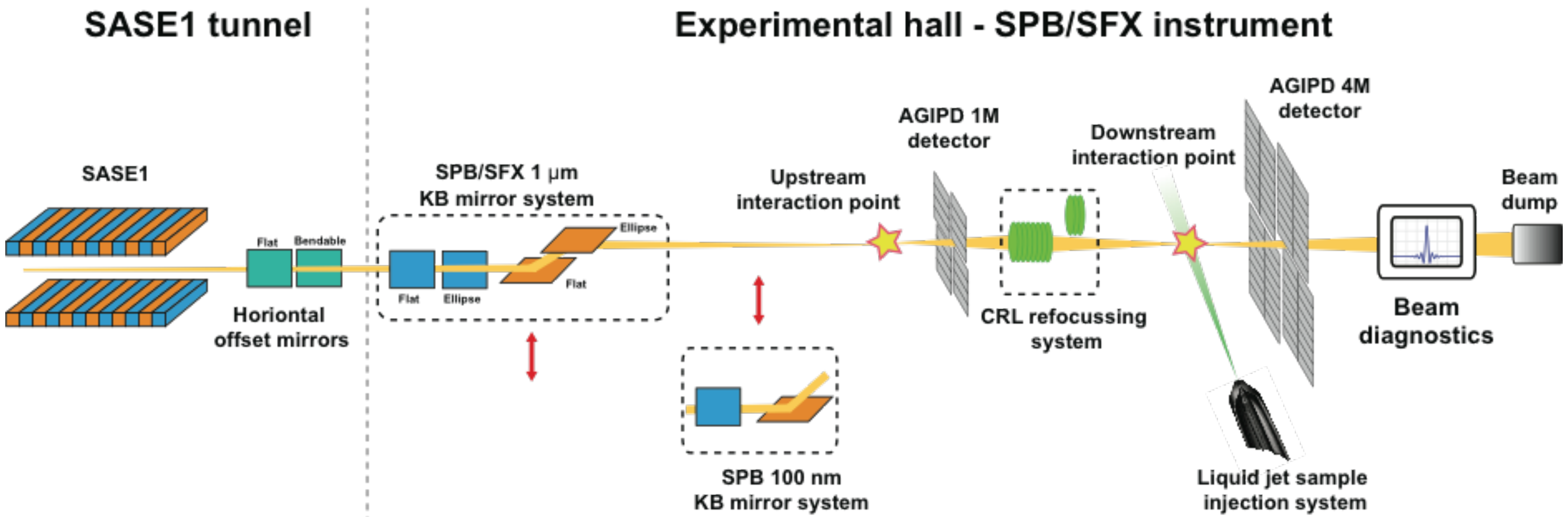


Imaging of “big” and “small” non-crystalline samples $\lim_{N \to \infty}$ = SAXS

Image from: Barty, et al, Nature Photonics 6, 35–40 (2012)

Reminder SPB/SFX instrument



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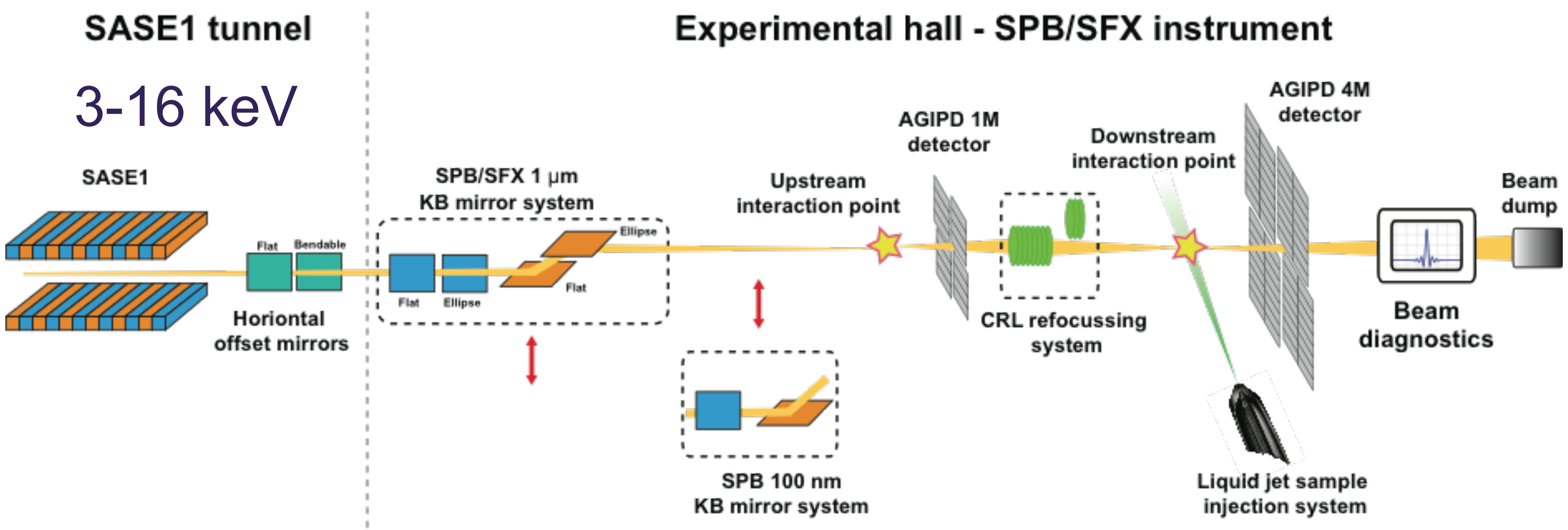

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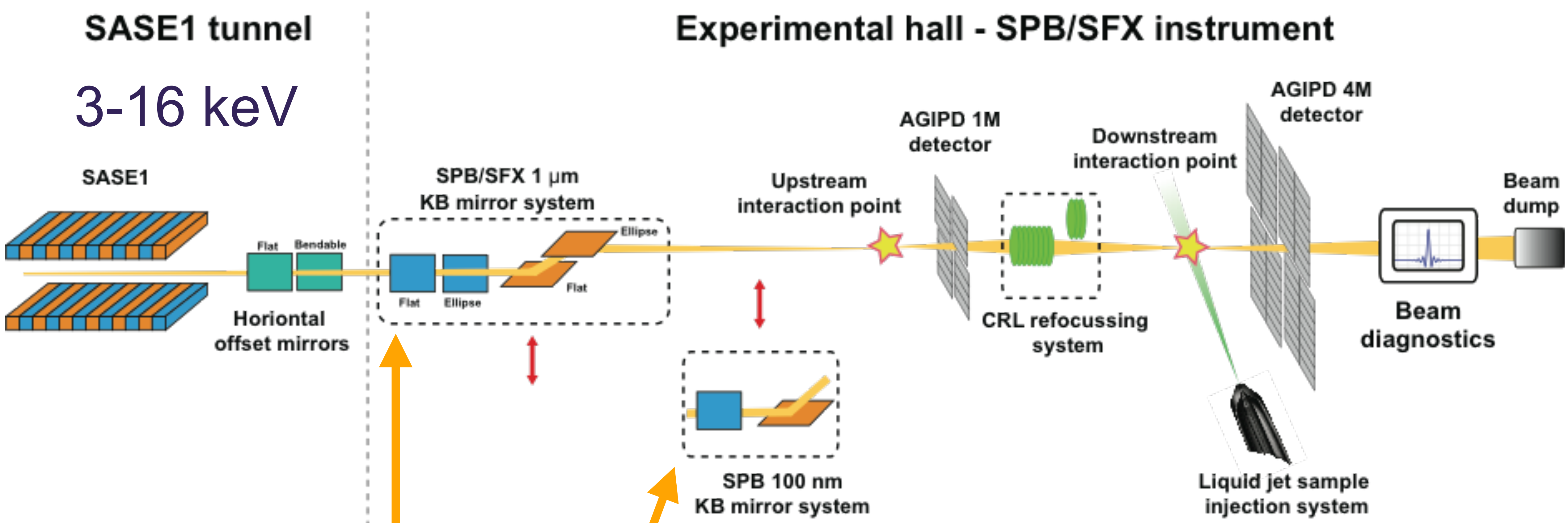
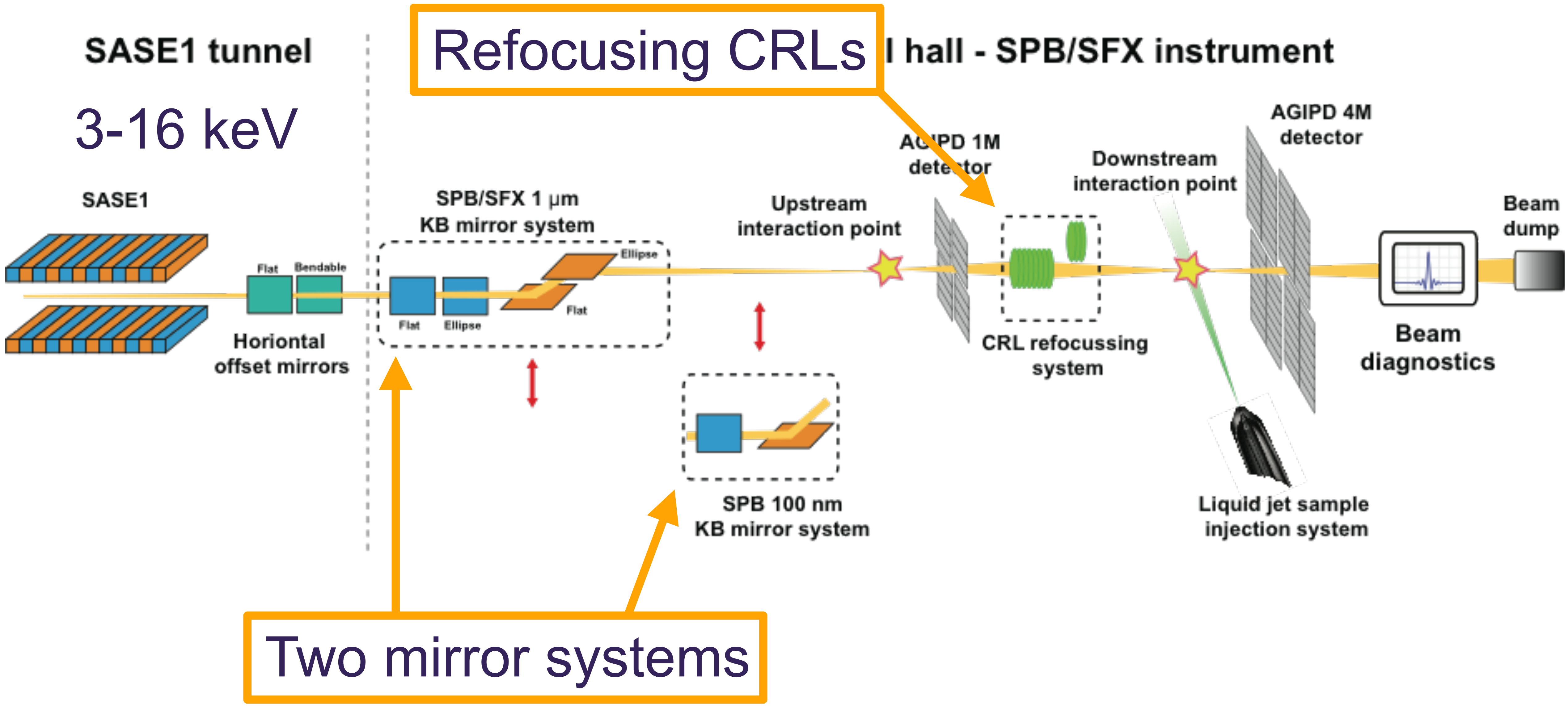


Two mirror systems

Reminder SPB/SFX instrument



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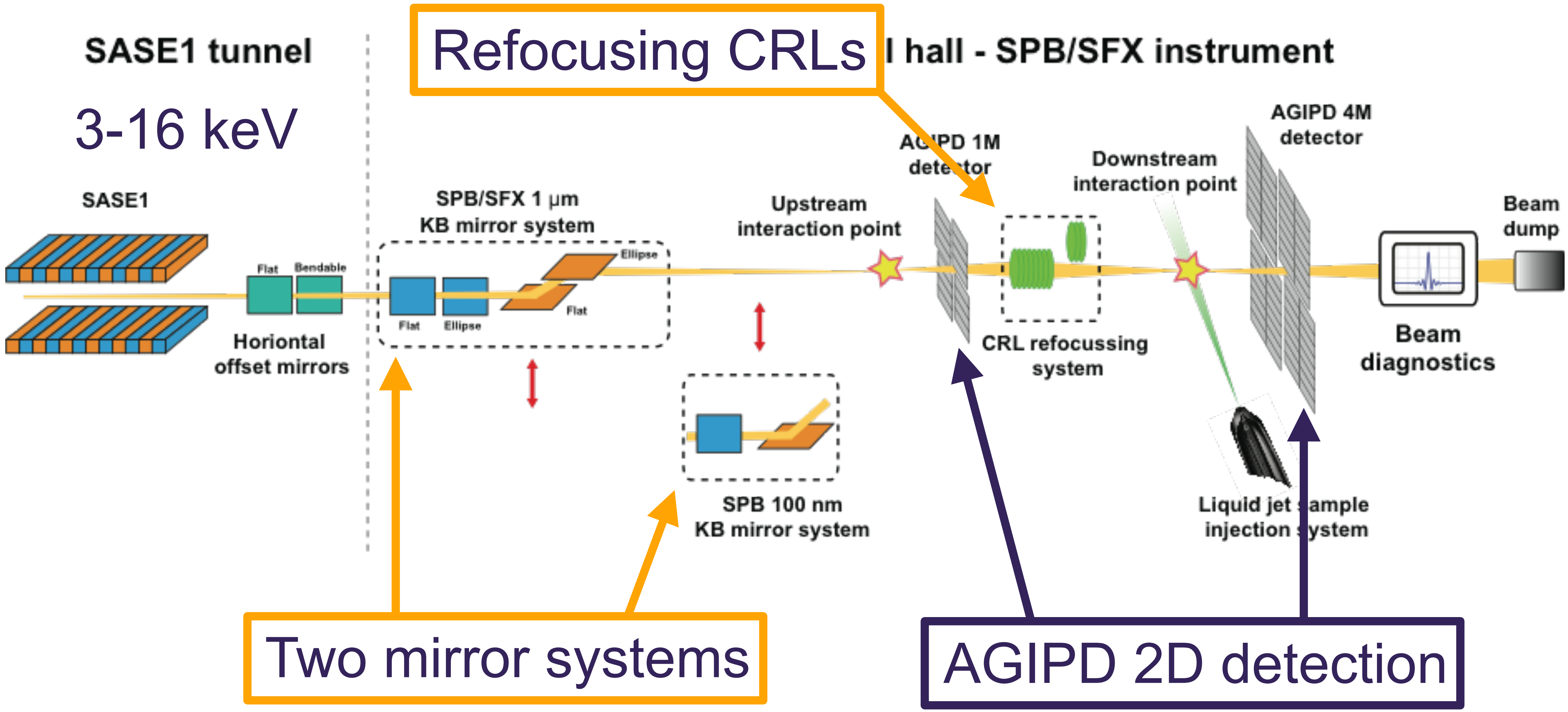
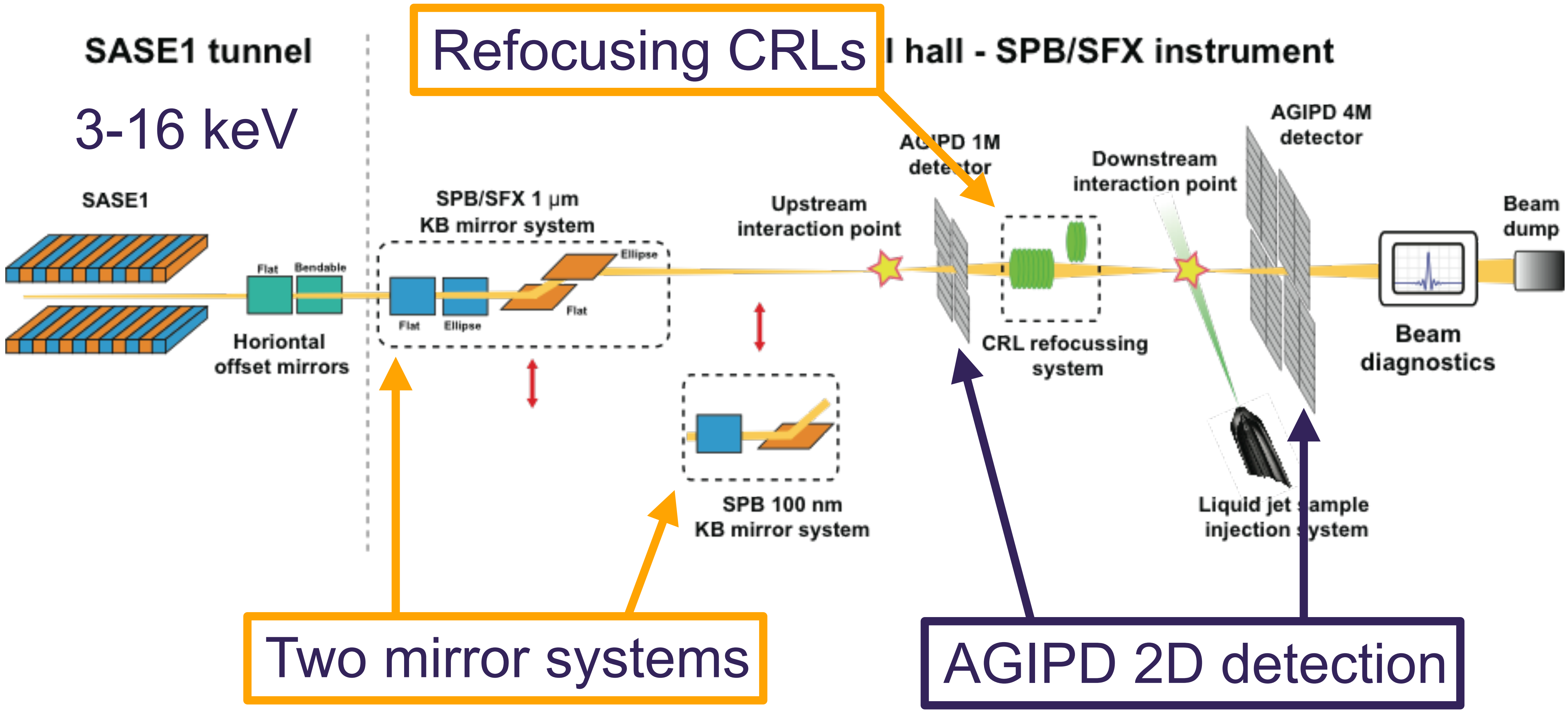


European XFEL

Reminder SPB/SFX 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

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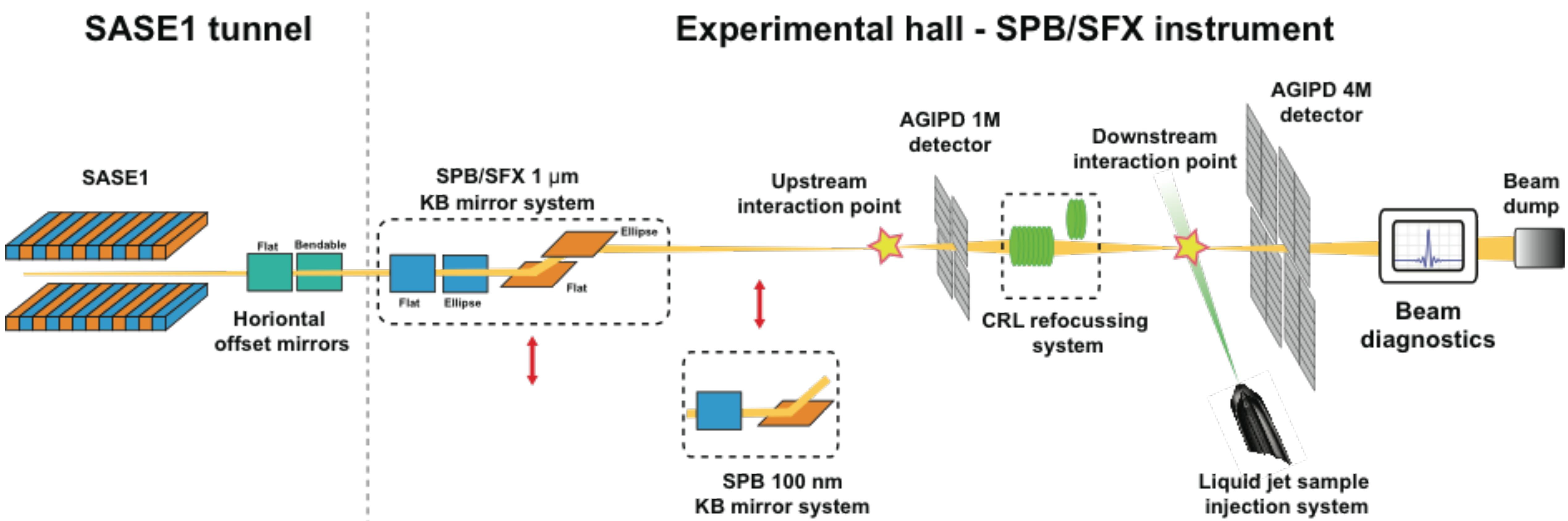

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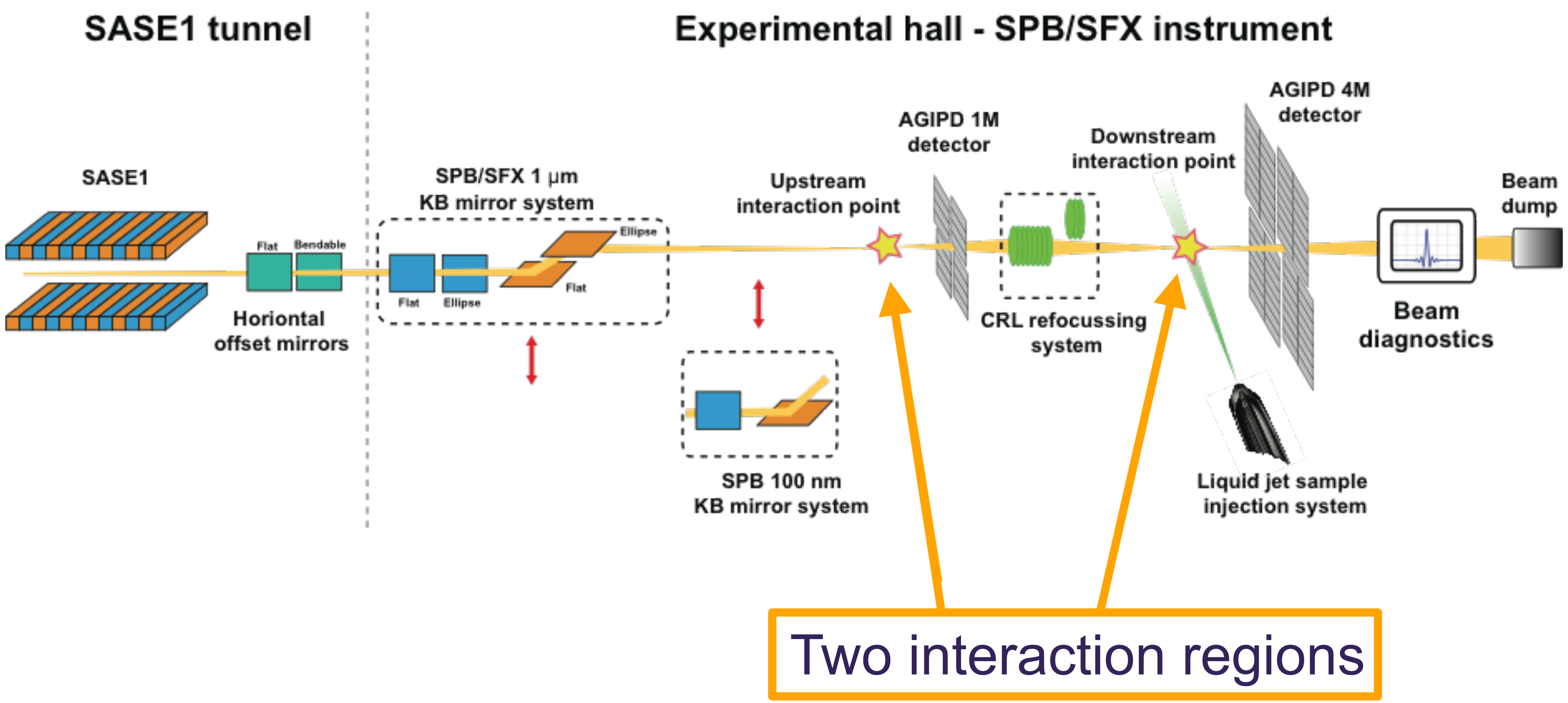

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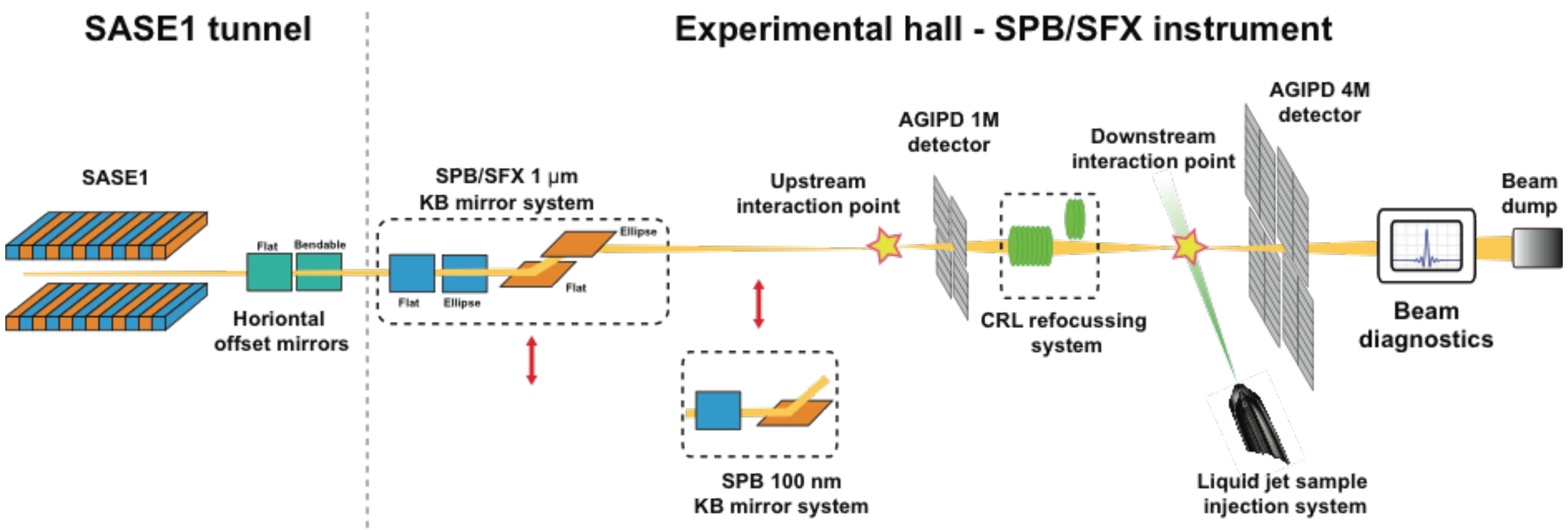

European XFEL

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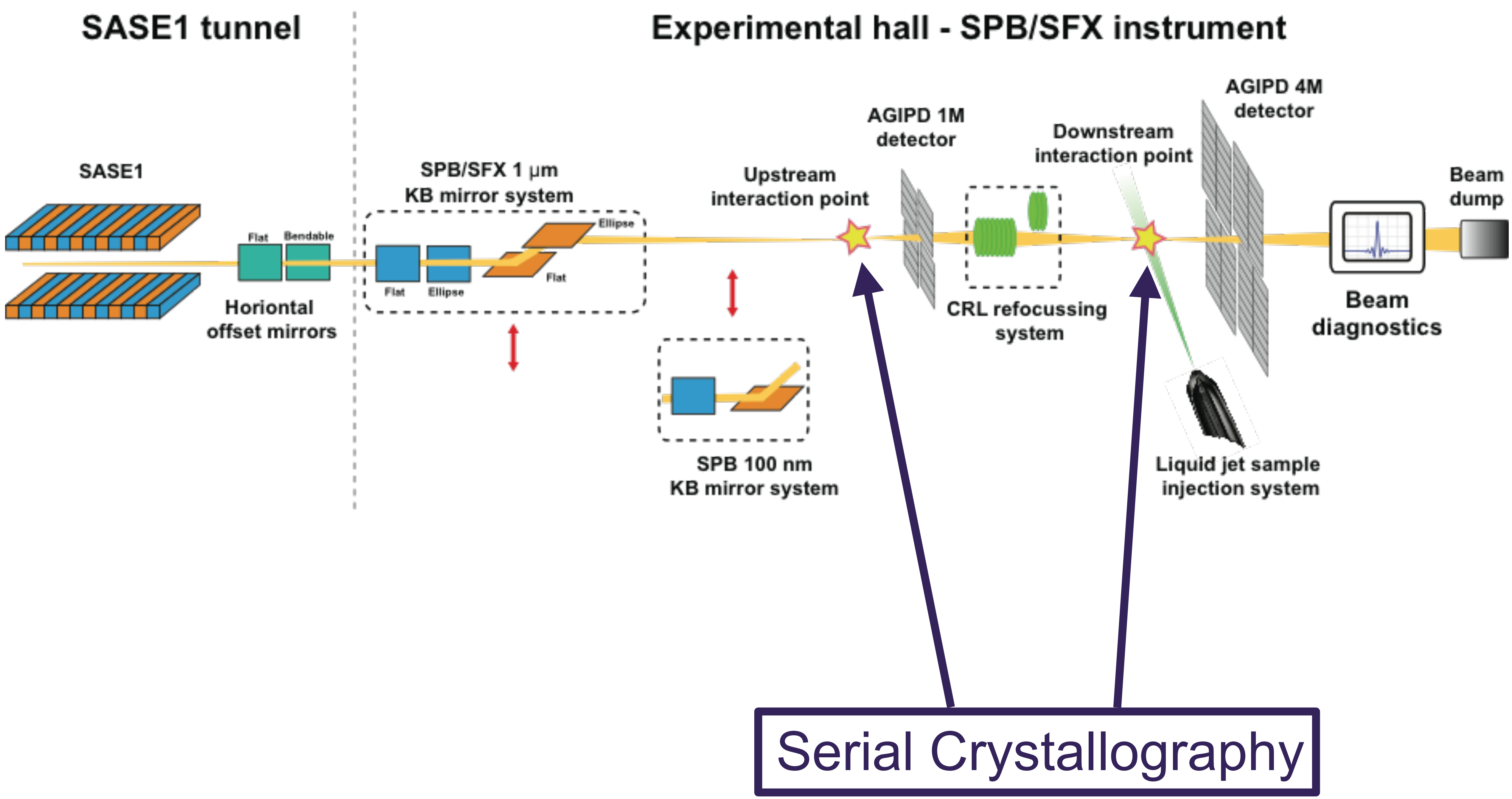

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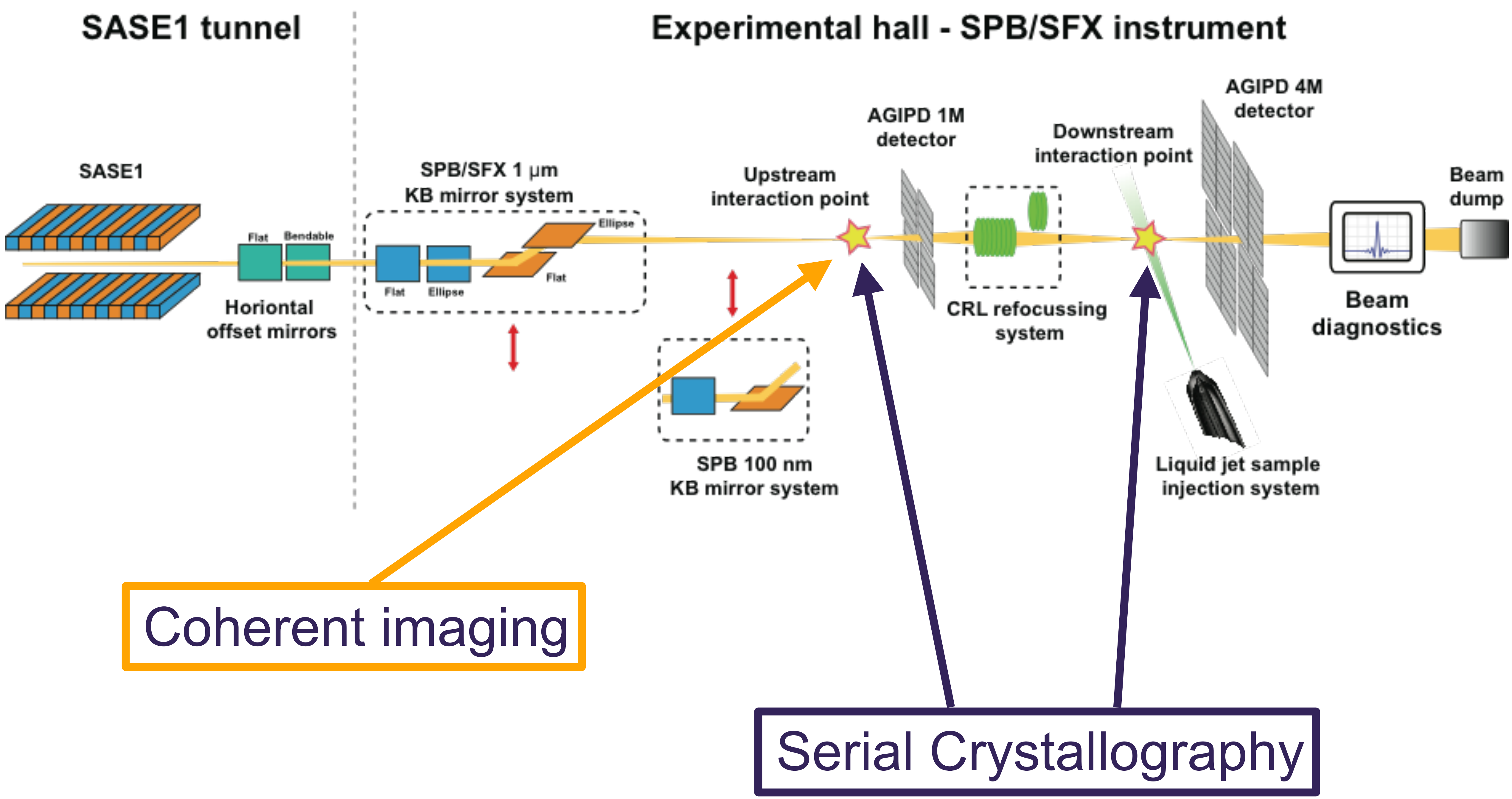

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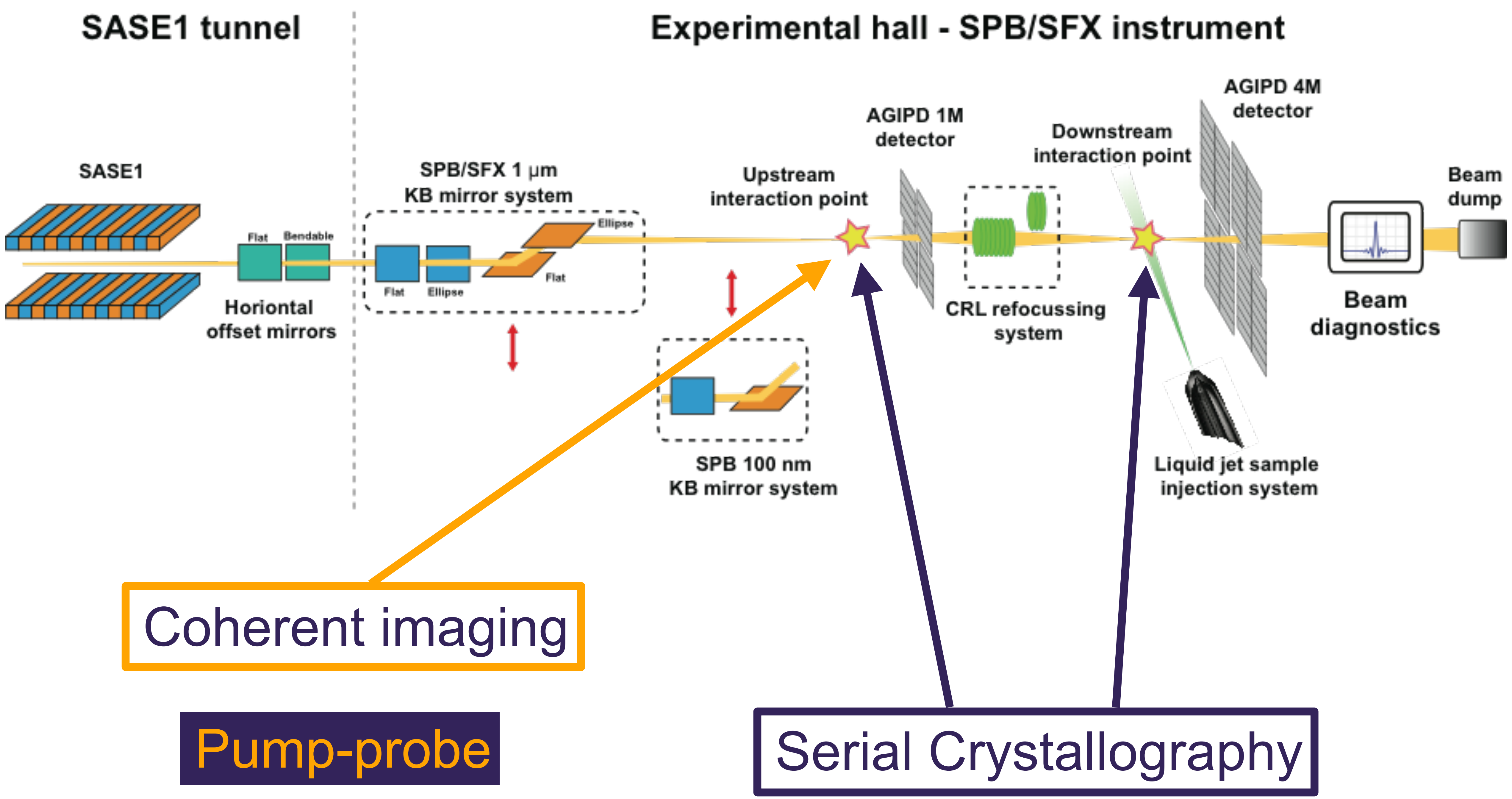

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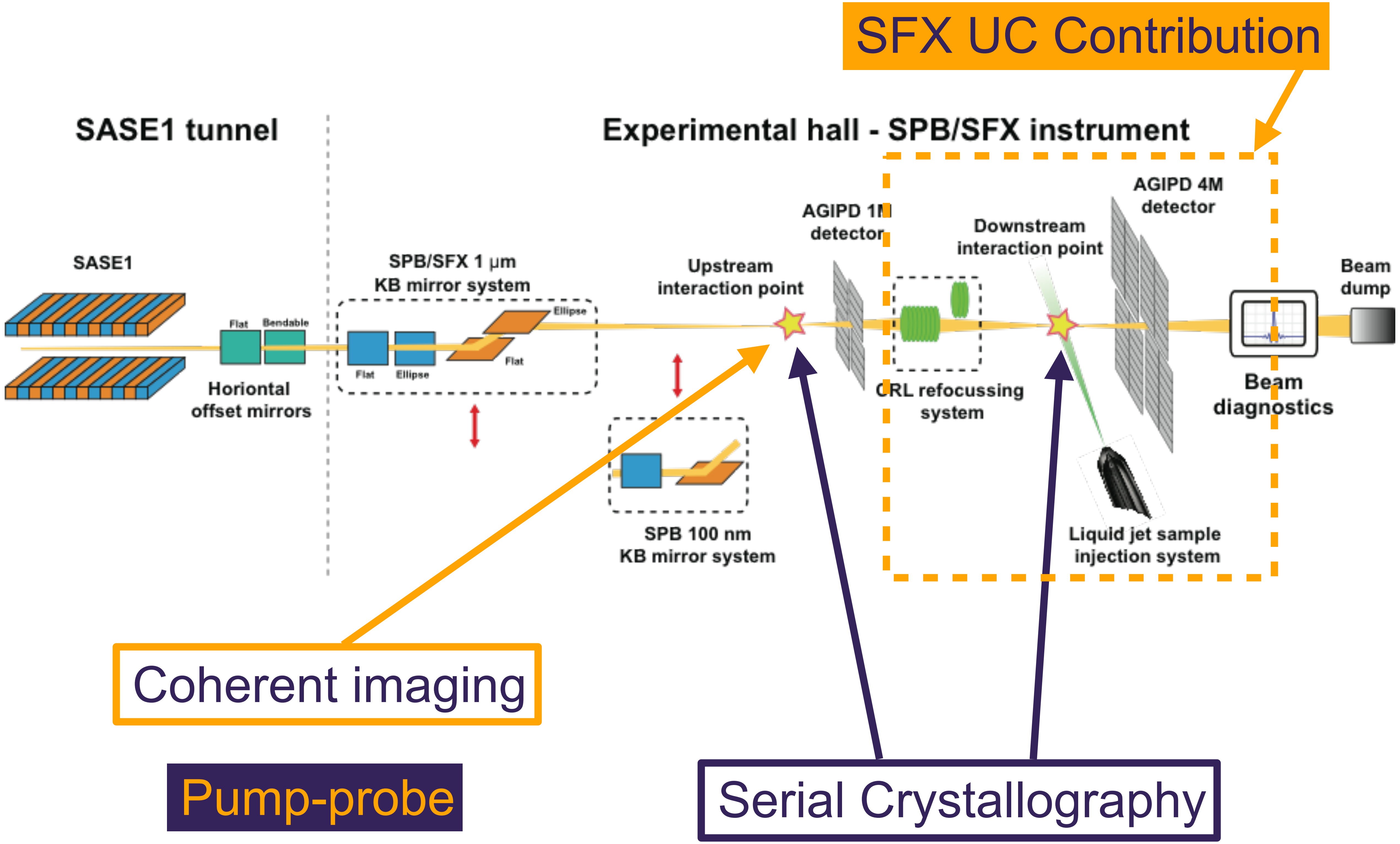
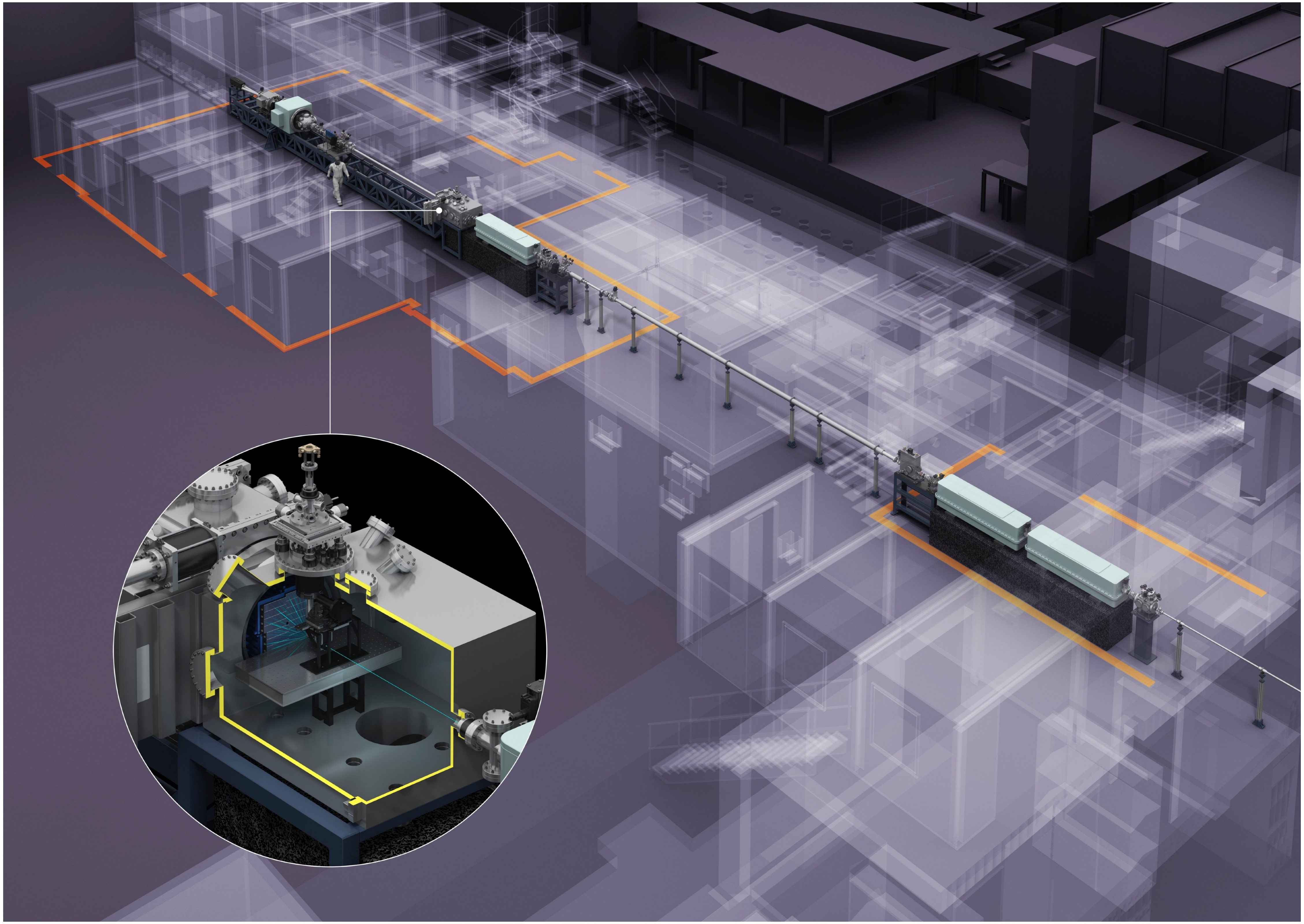


Bird’s eye view of instrumentation



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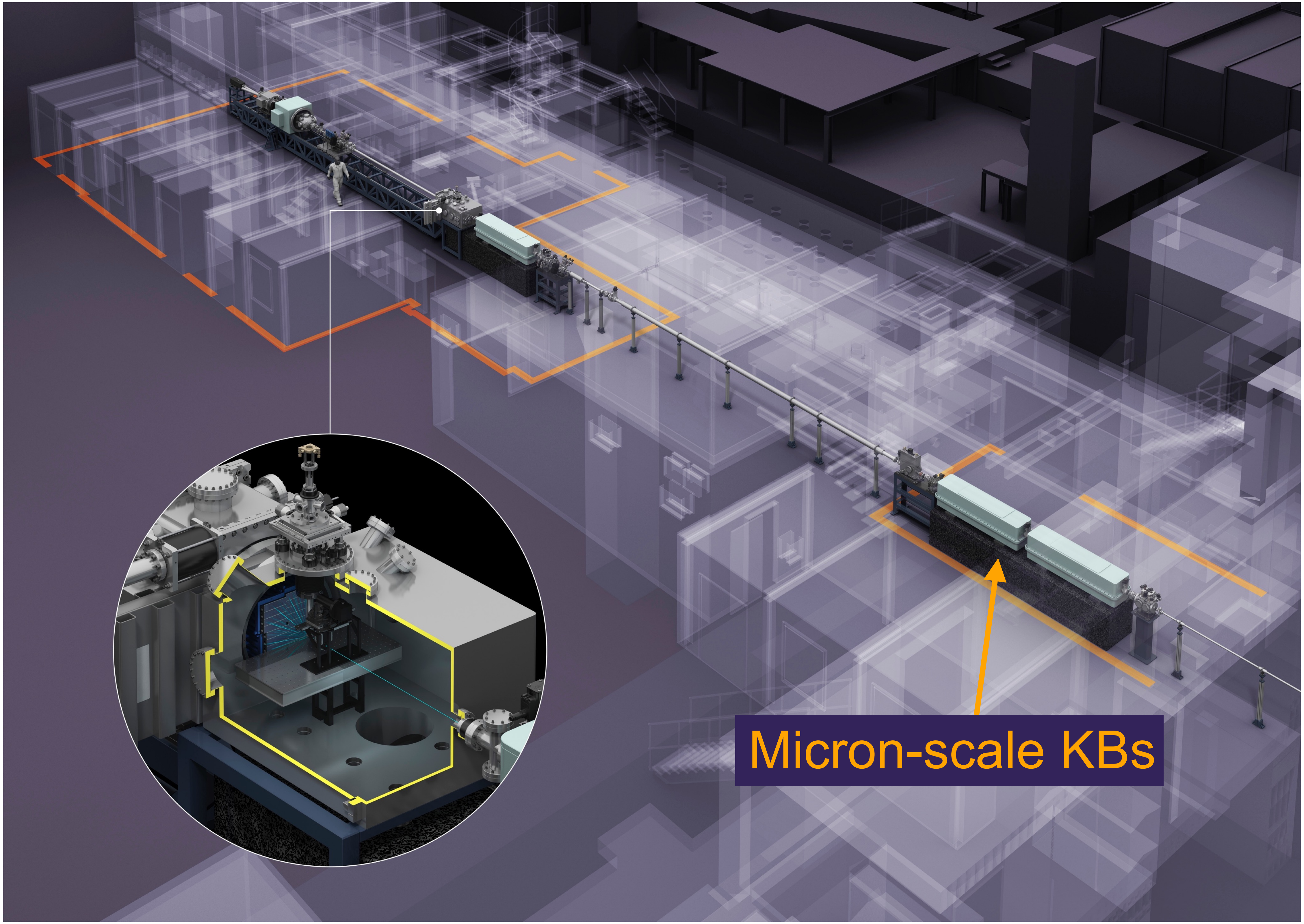

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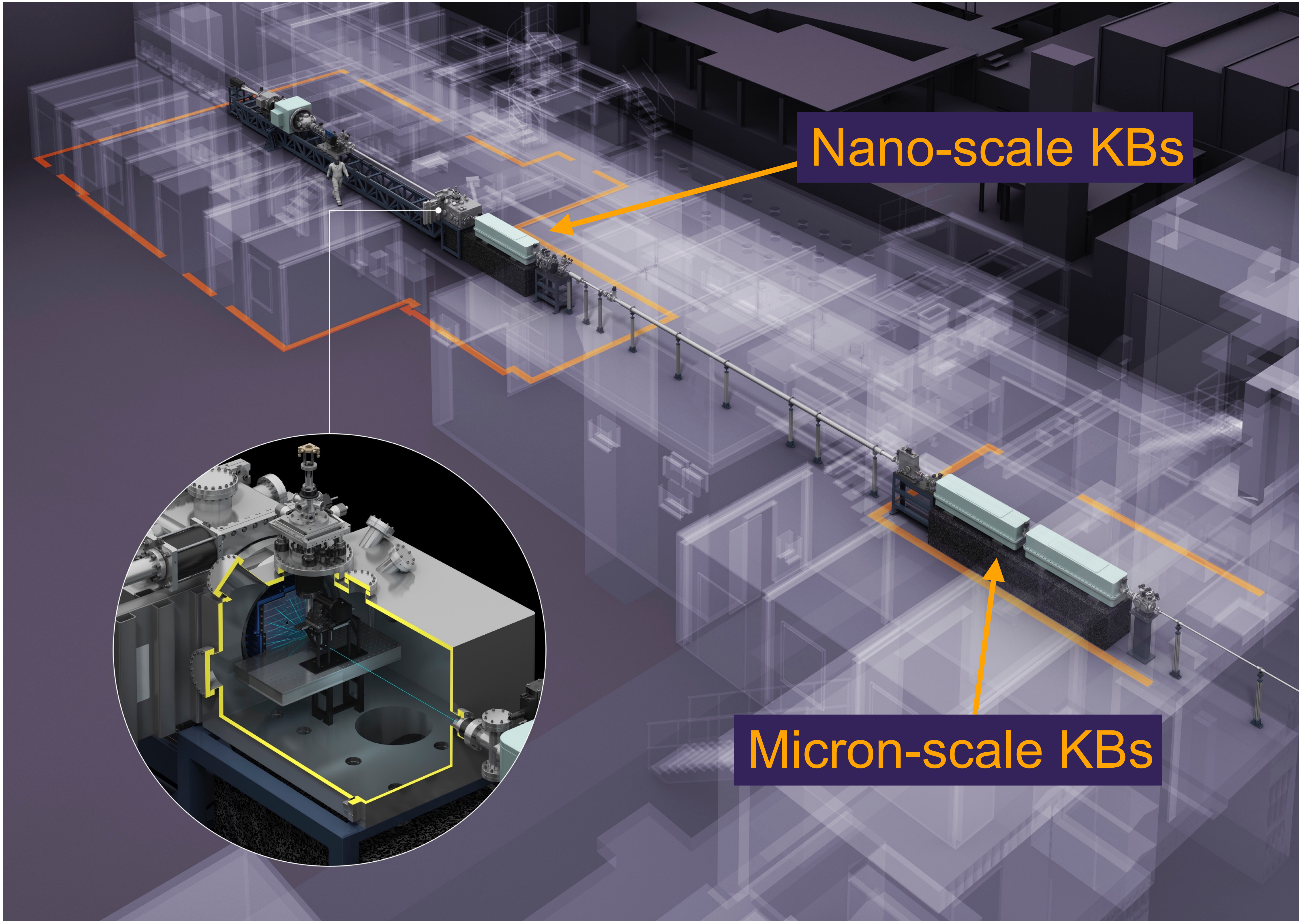

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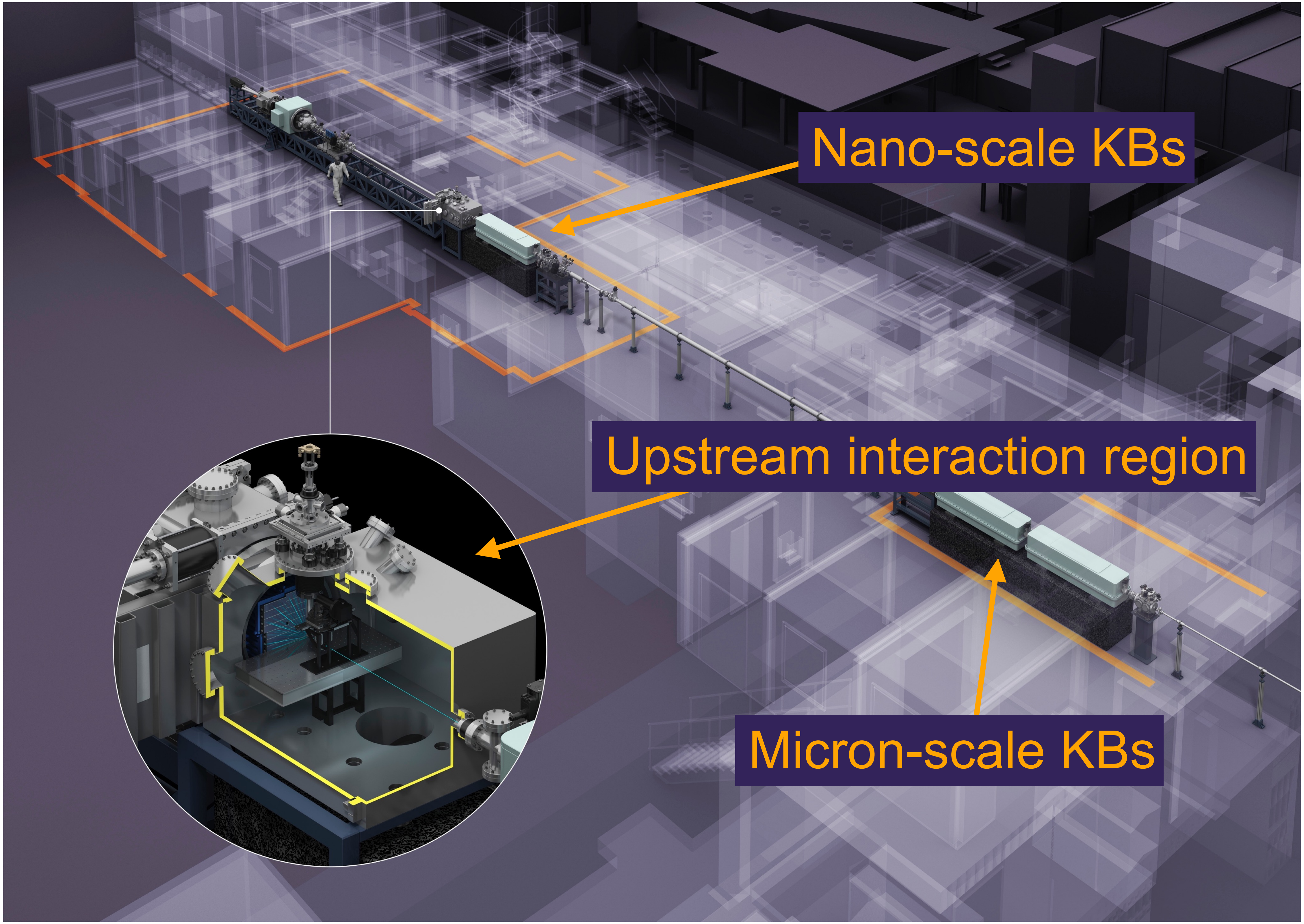

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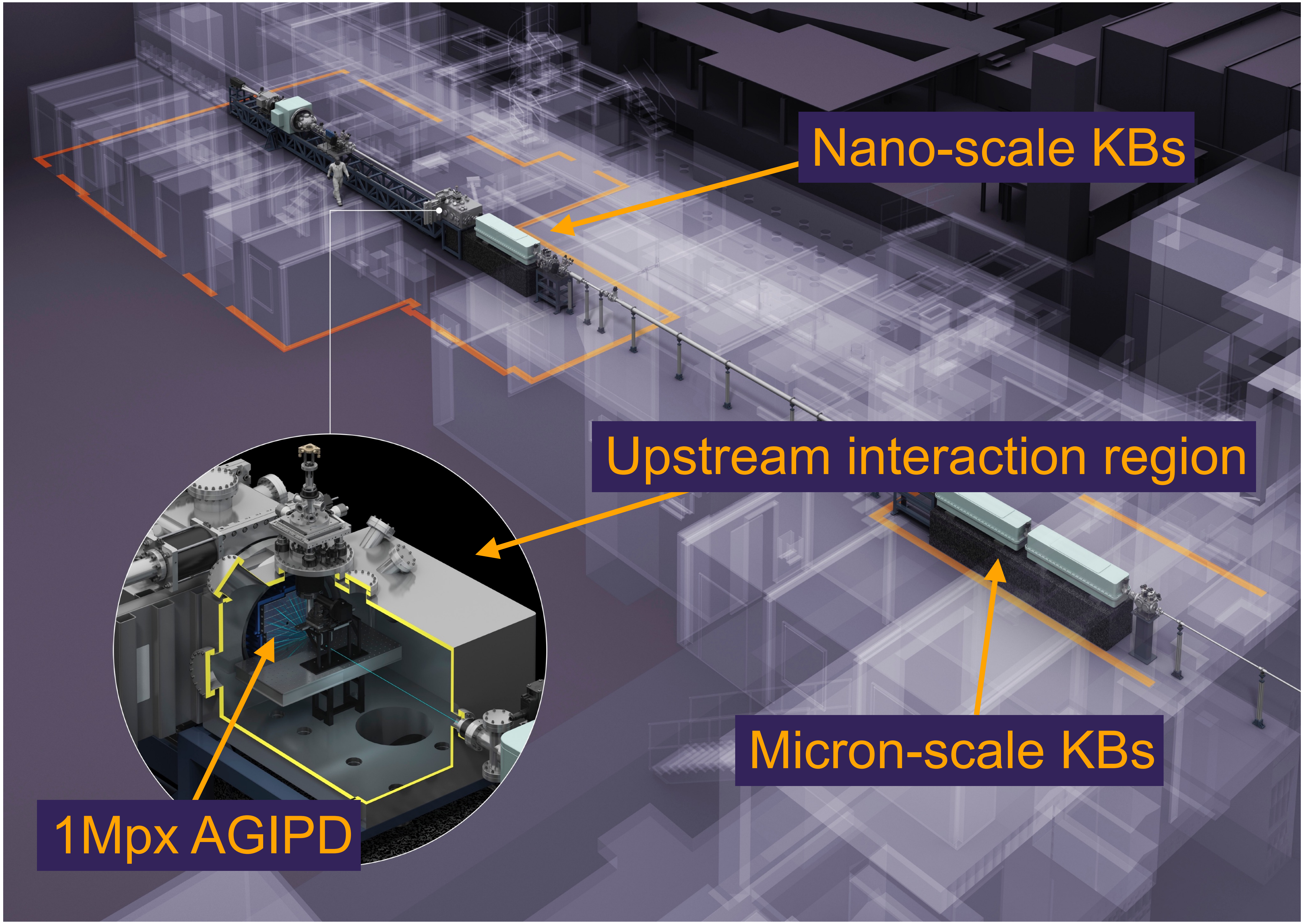

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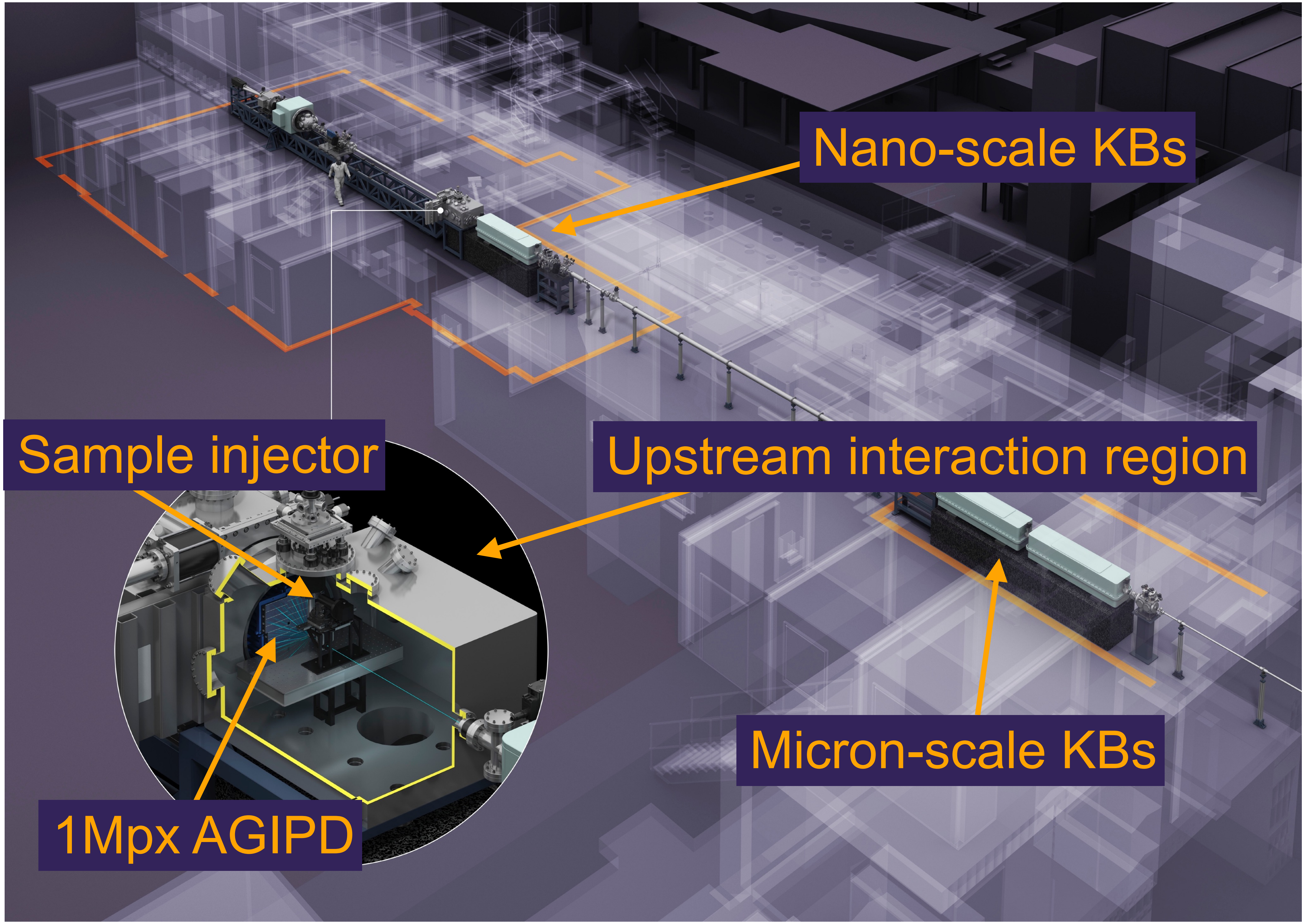

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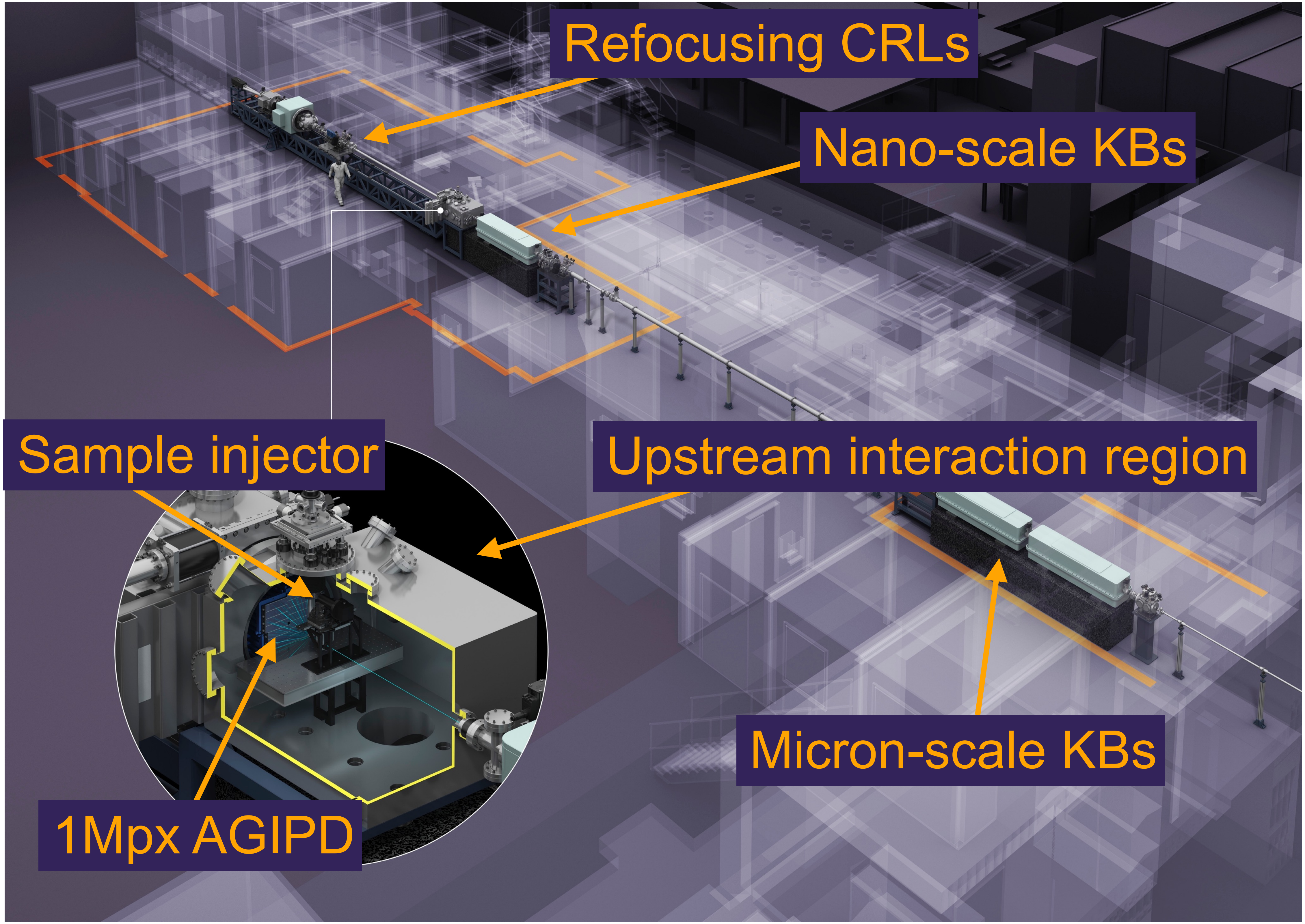

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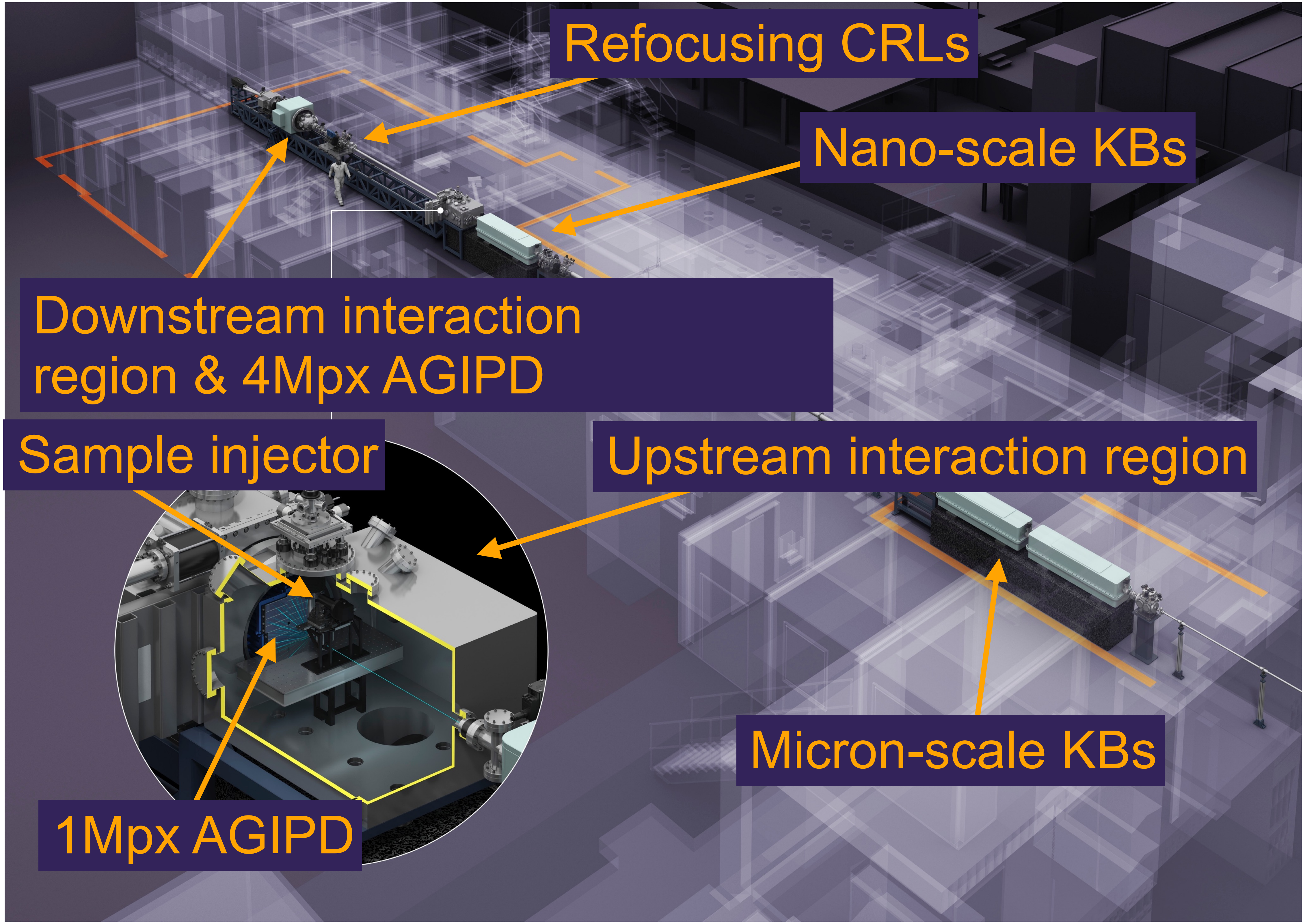

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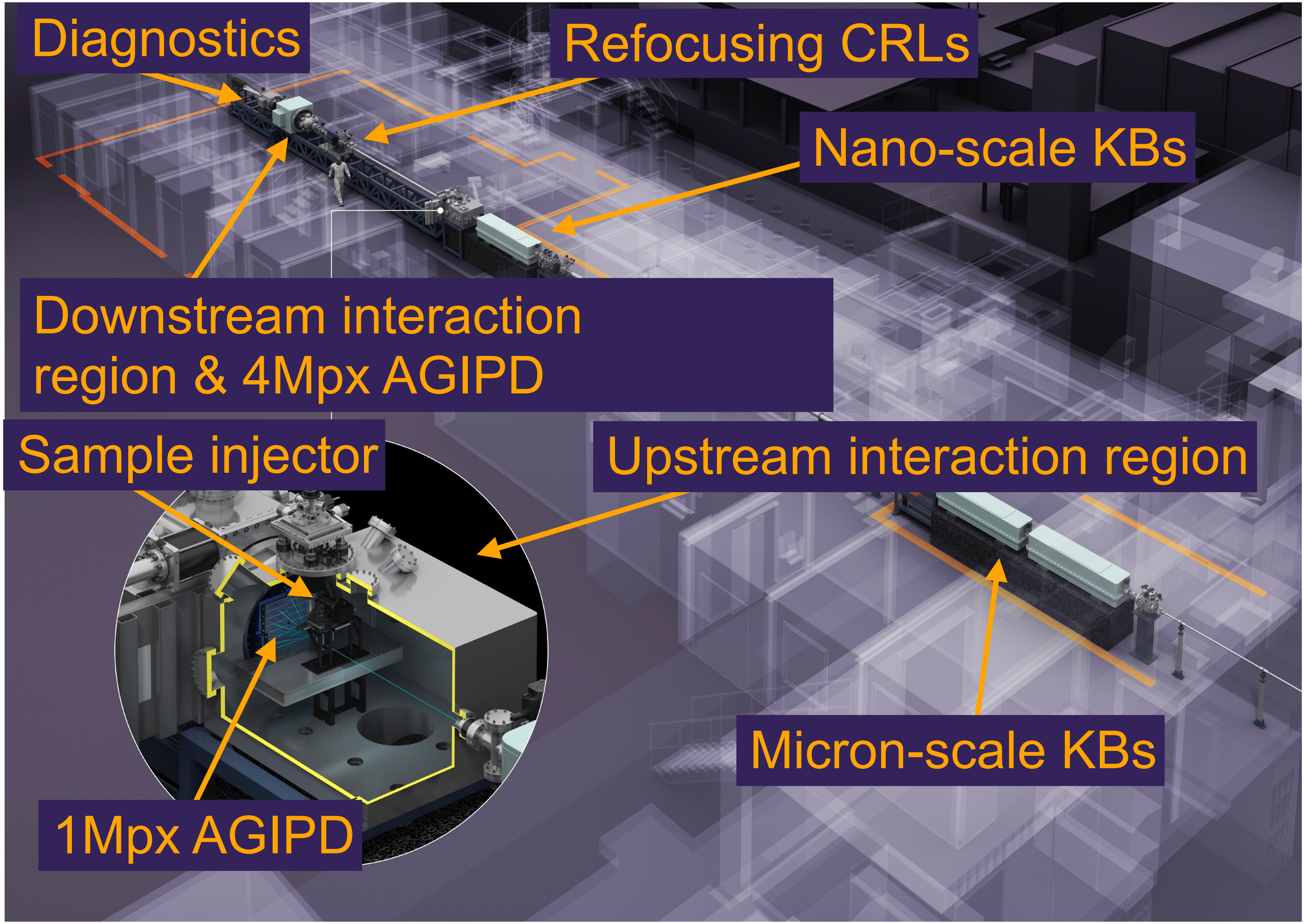

Example: Serial crystallography

Image courtesy A. Aquila, LCLS, SLAC

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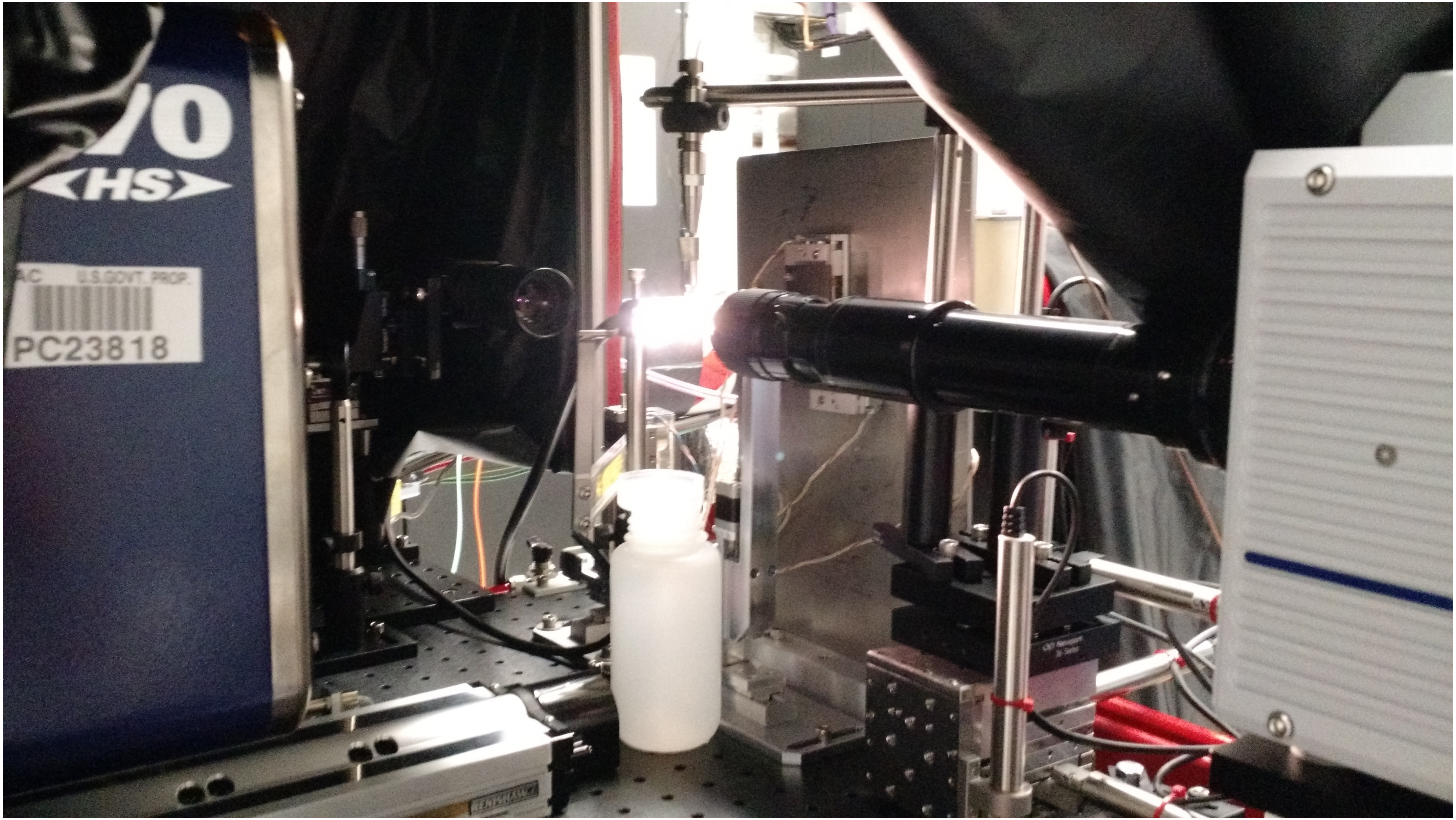

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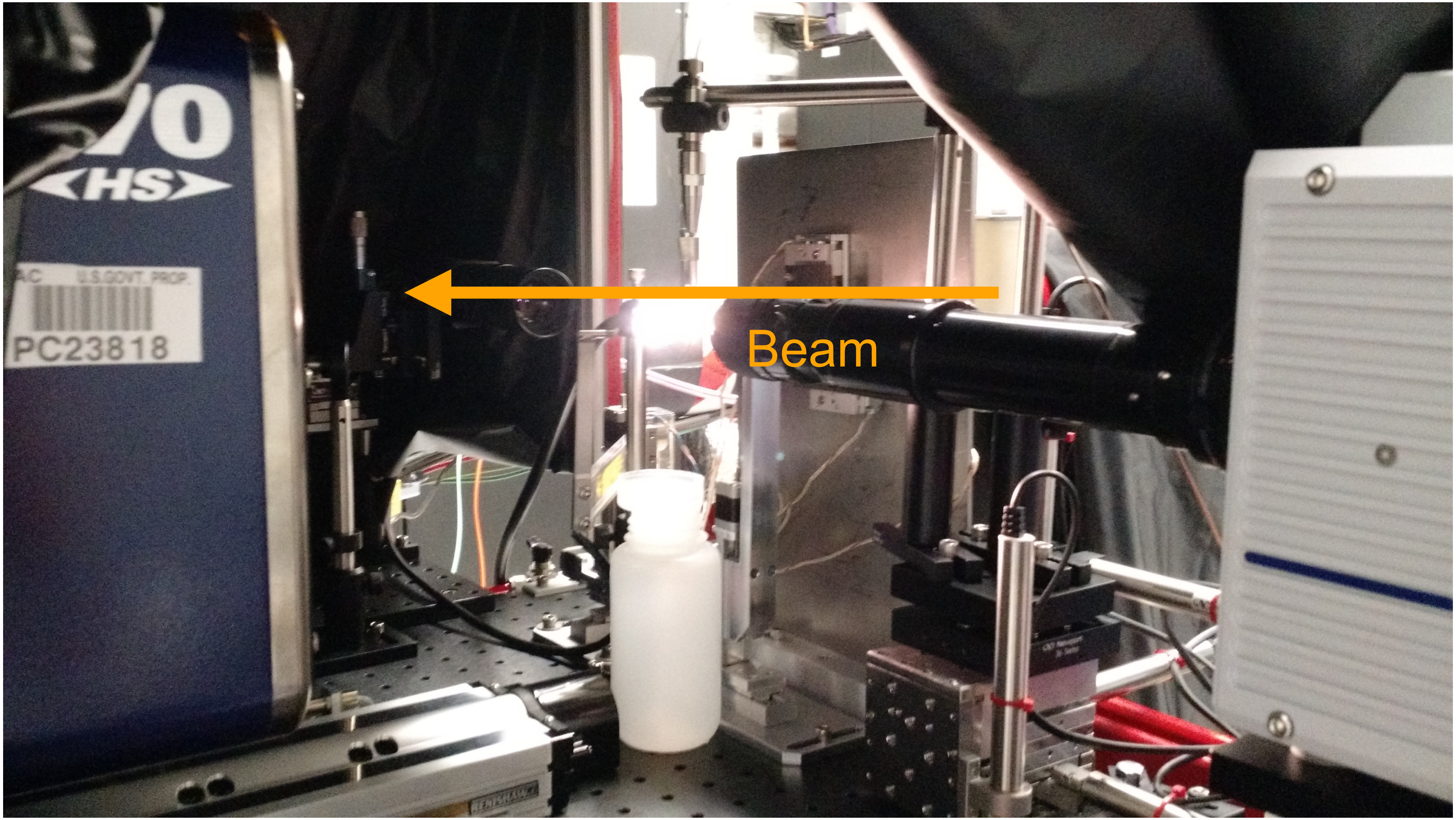

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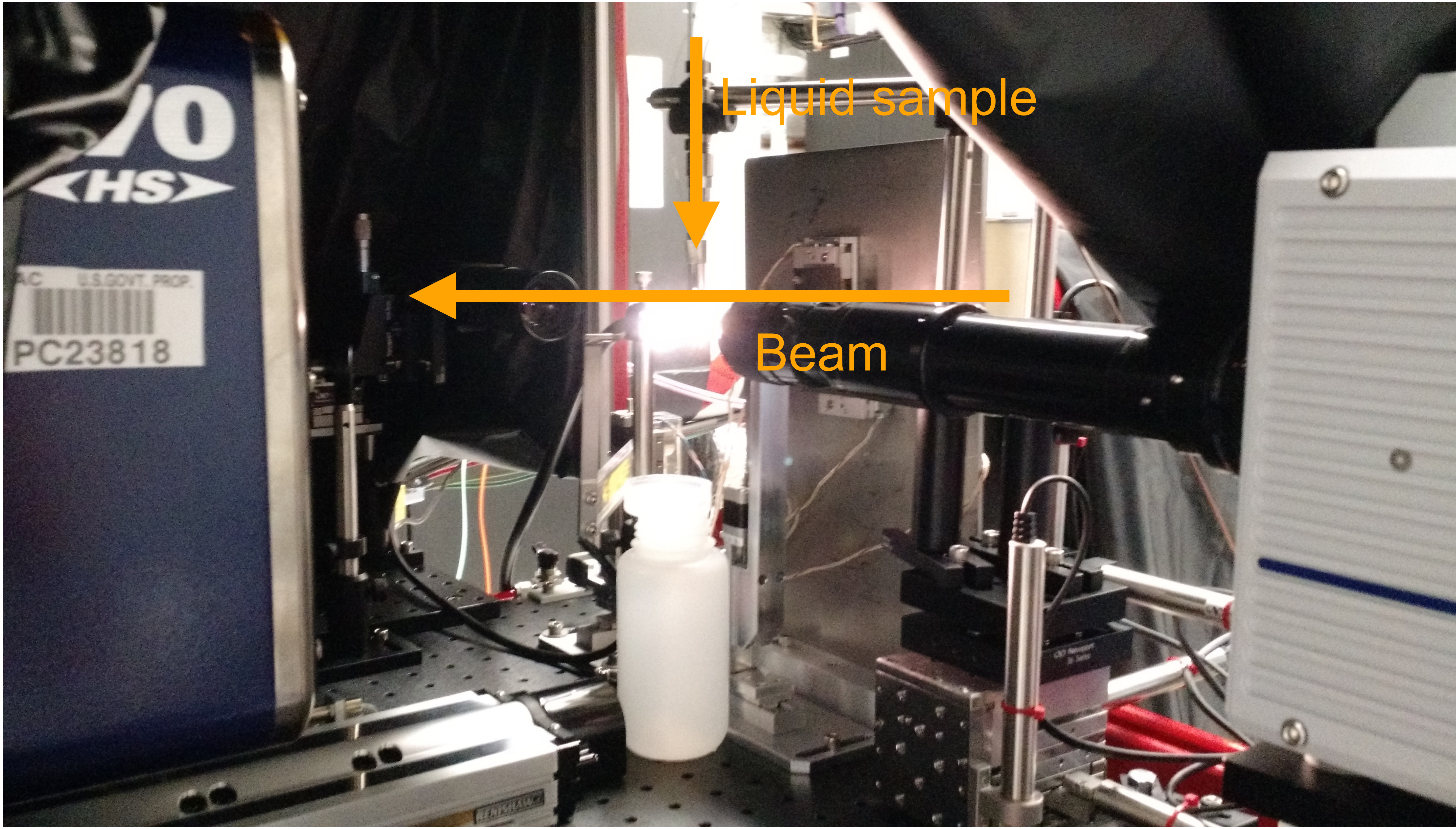
European XFEL

Example: Serial crystallography



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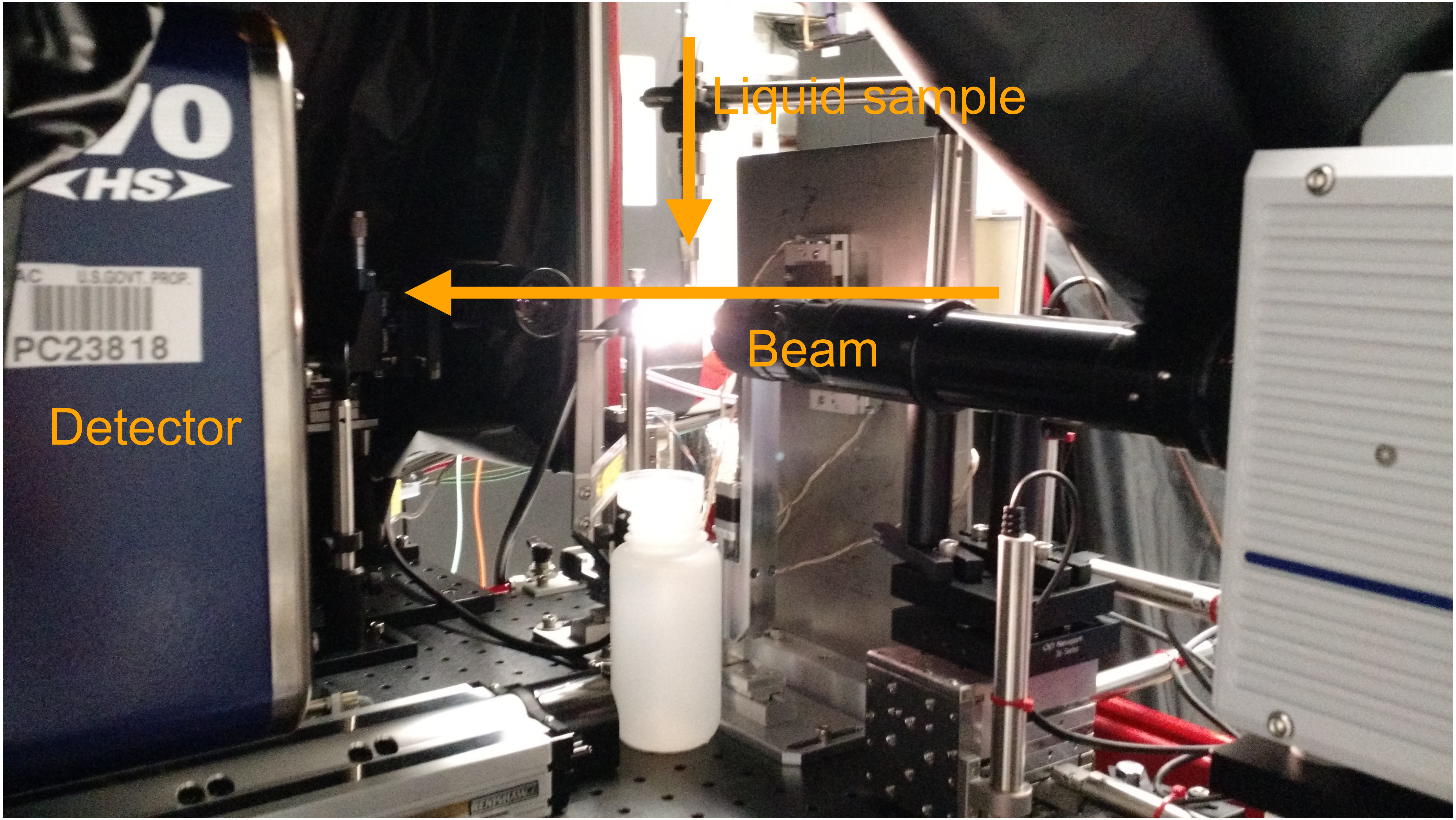

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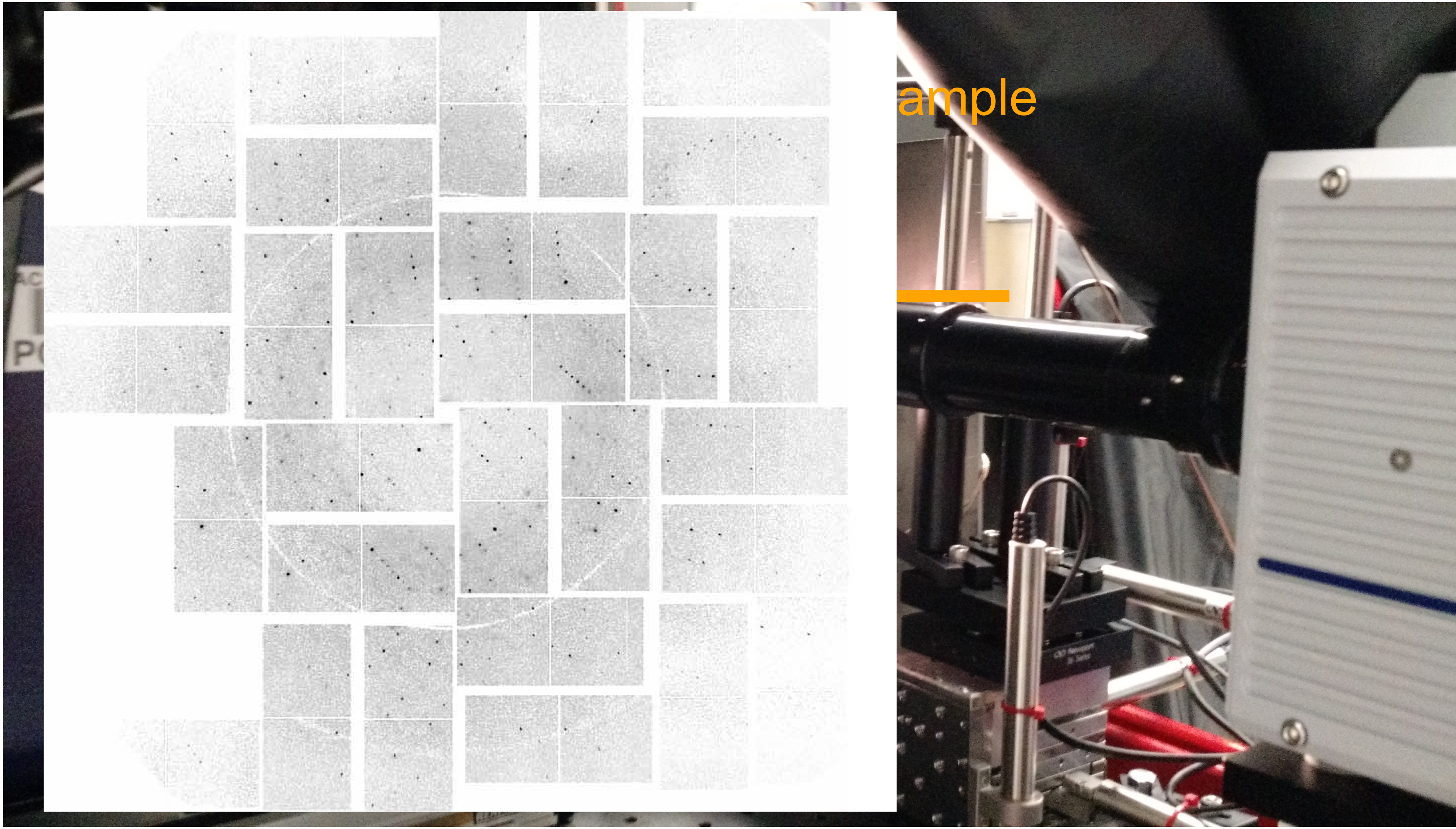

Data: A. Barty, et al, J. Appl. Cryst. 2014

Image courtesy A. Aquila, LCLS, SLAC

Day one parameters for hard X-ray beamlines

Electron energy	17.5 GeV
Photon energy	8.4 keV
Repetition rate	100 kHz
Max. number pulses per train	60
Undulator K-value	3.9
Undulator Gap	10 mm
Pulse energy	2 mJ (slightly oversaturated)
Divergence	2.2 urad
Pulse duration	43 fs
Saturation length	58 m

H. Sinn, European XFEL

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Suitable for serial crystallography and more

H. Sinn, European XFEL

First experiments

- Common requirements for day one experiments (non exhaustive list)

General requirements to do any of the planned Day-1 experiments

- um size beam
- cleanup apertures
- beam attenuator
- 2D detector
- gain calibration for detector
- detector debris shield (in practice)

additional requirements for some of the experiments

- fixed target stage (all non jet)
- rotation stage (2D crystals only)
- efficient catcher (jet experiments)
- differential pumping (jet experiments)
- windowed gate valve? (jet experiments)
- post attenuator (SPI maybe)
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KB focussing optics

Preliminary granite support and vacuum tank designs

- Optics supported on granite plinths
- Vacuum tanks and controls / pumping infrastructure supported independently on stainless steel super-structure

FMB-Oxford competition sensitive, non-distributable

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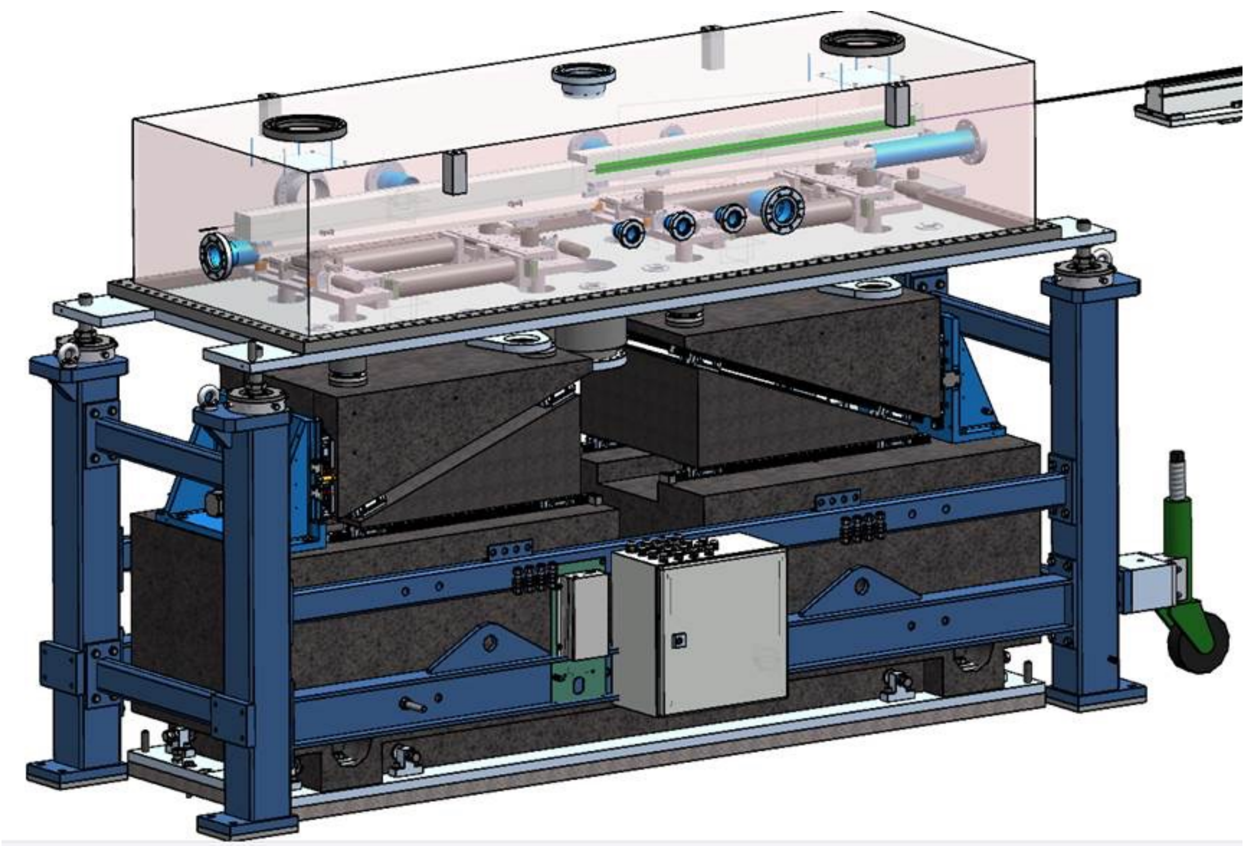

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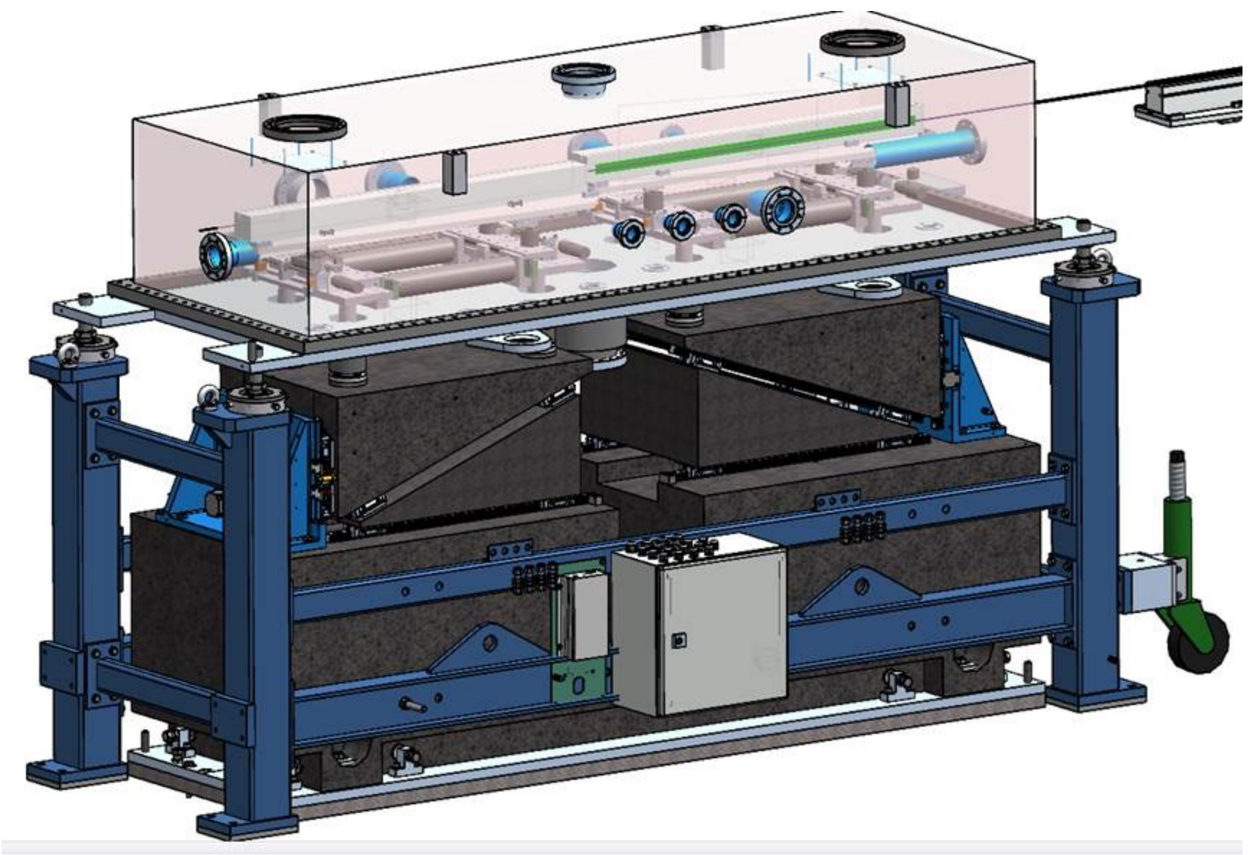

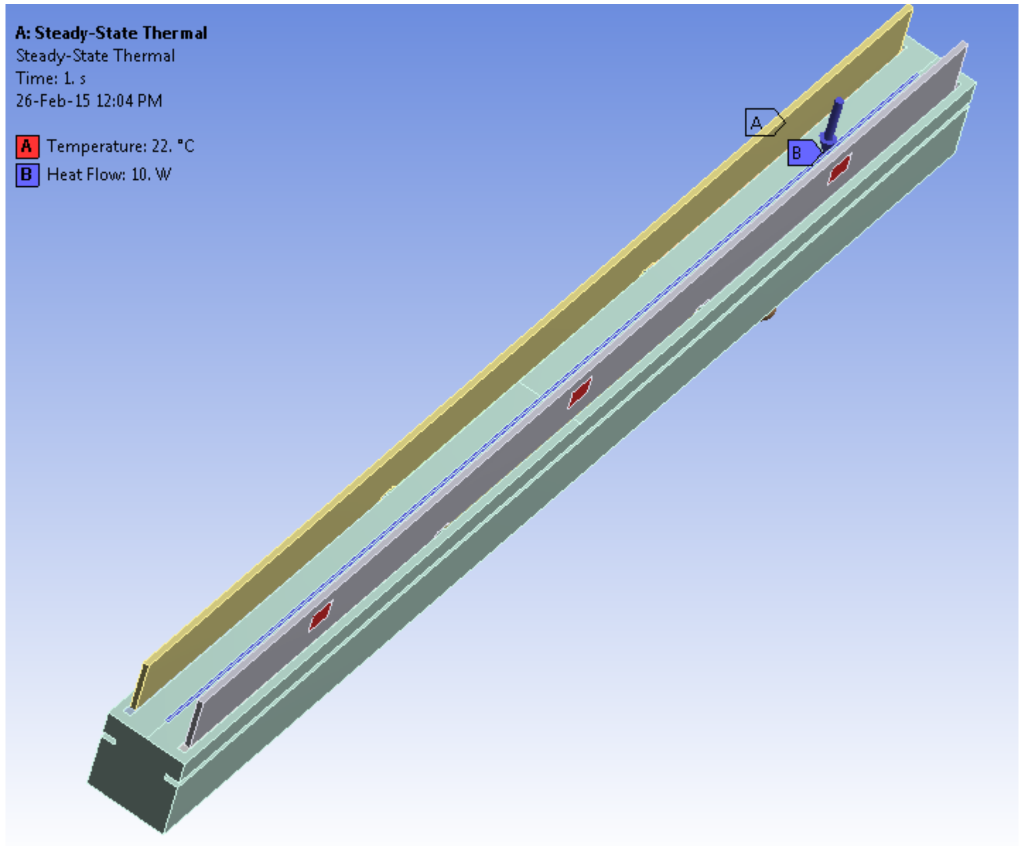

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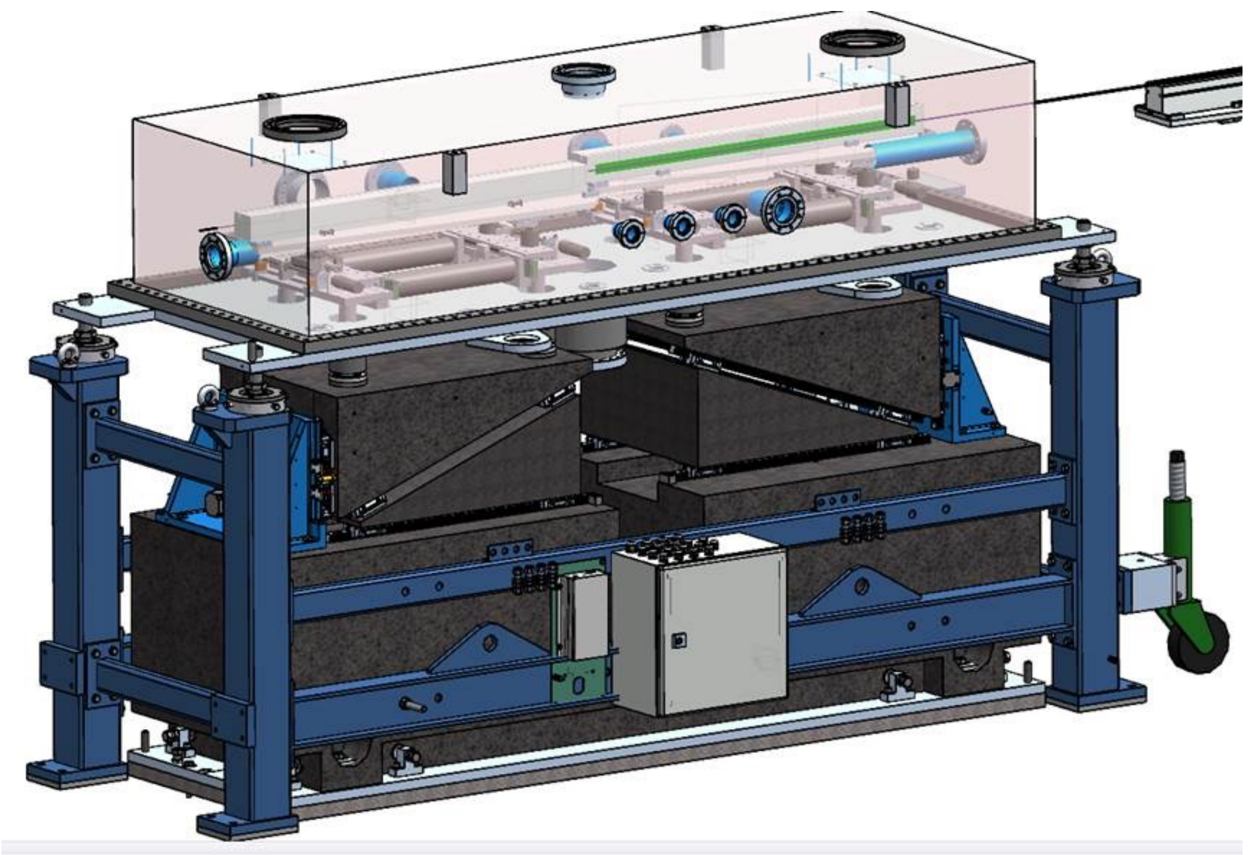

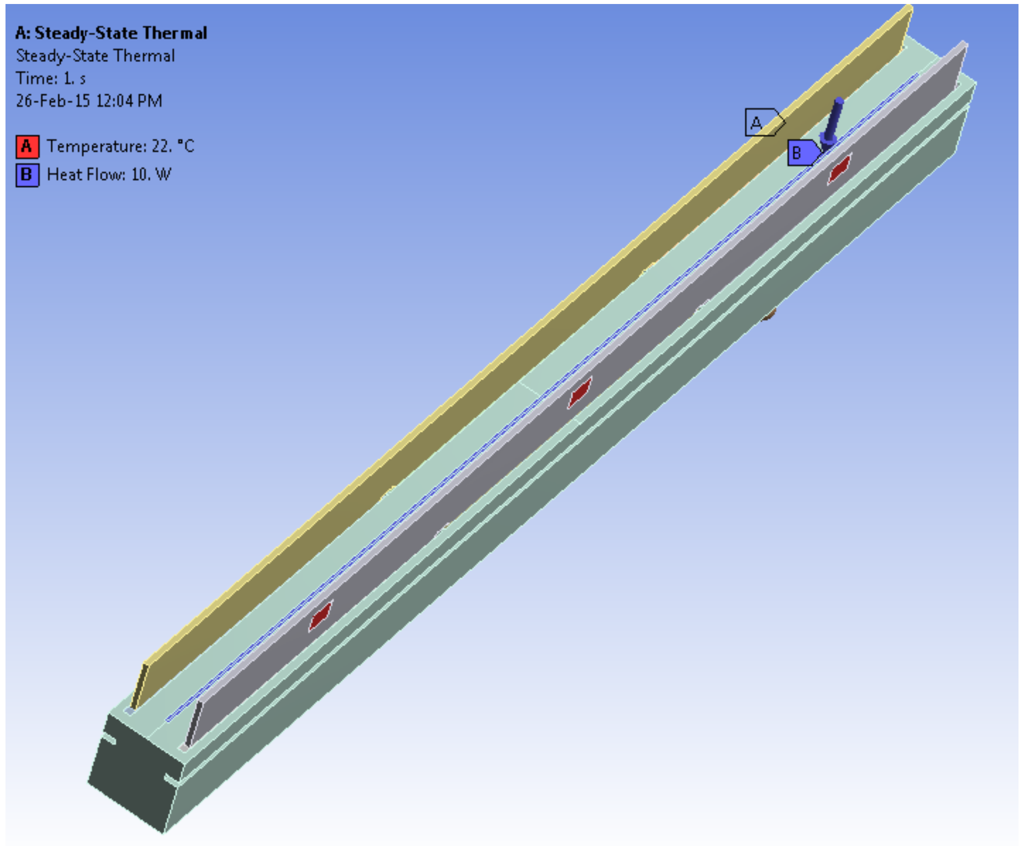

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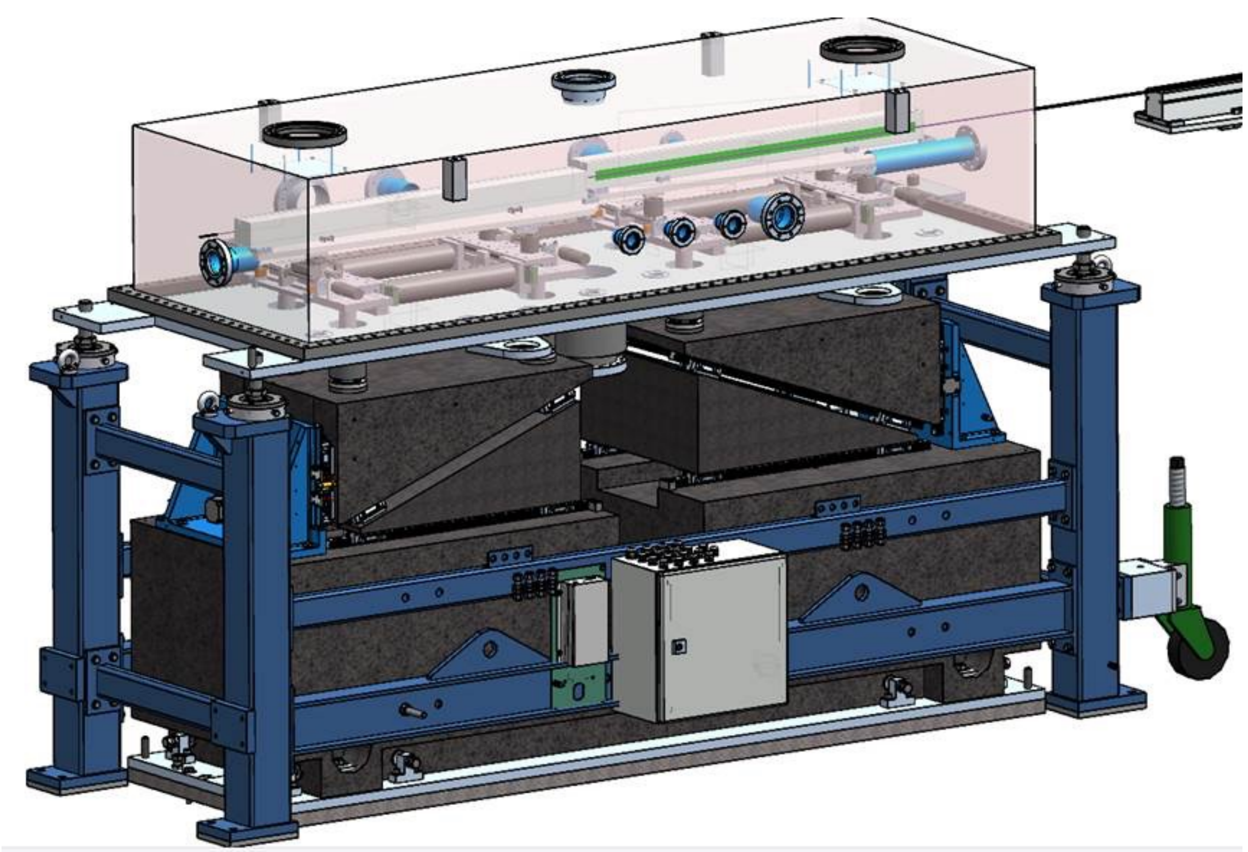
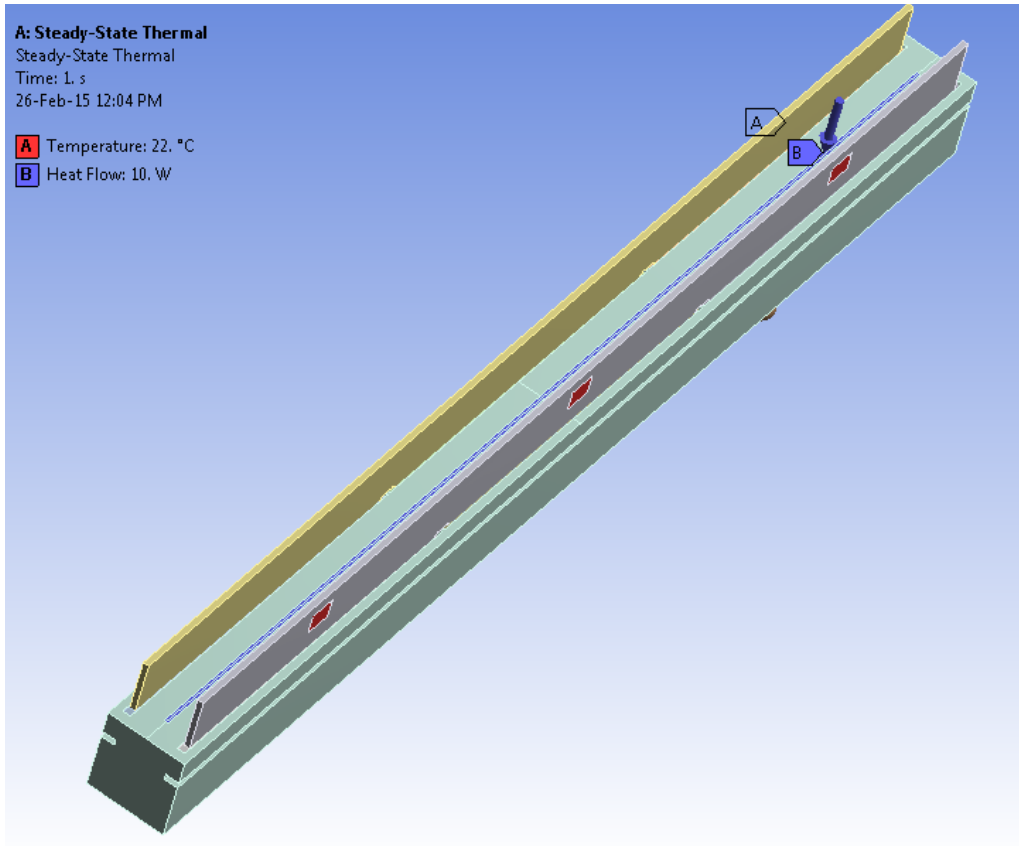


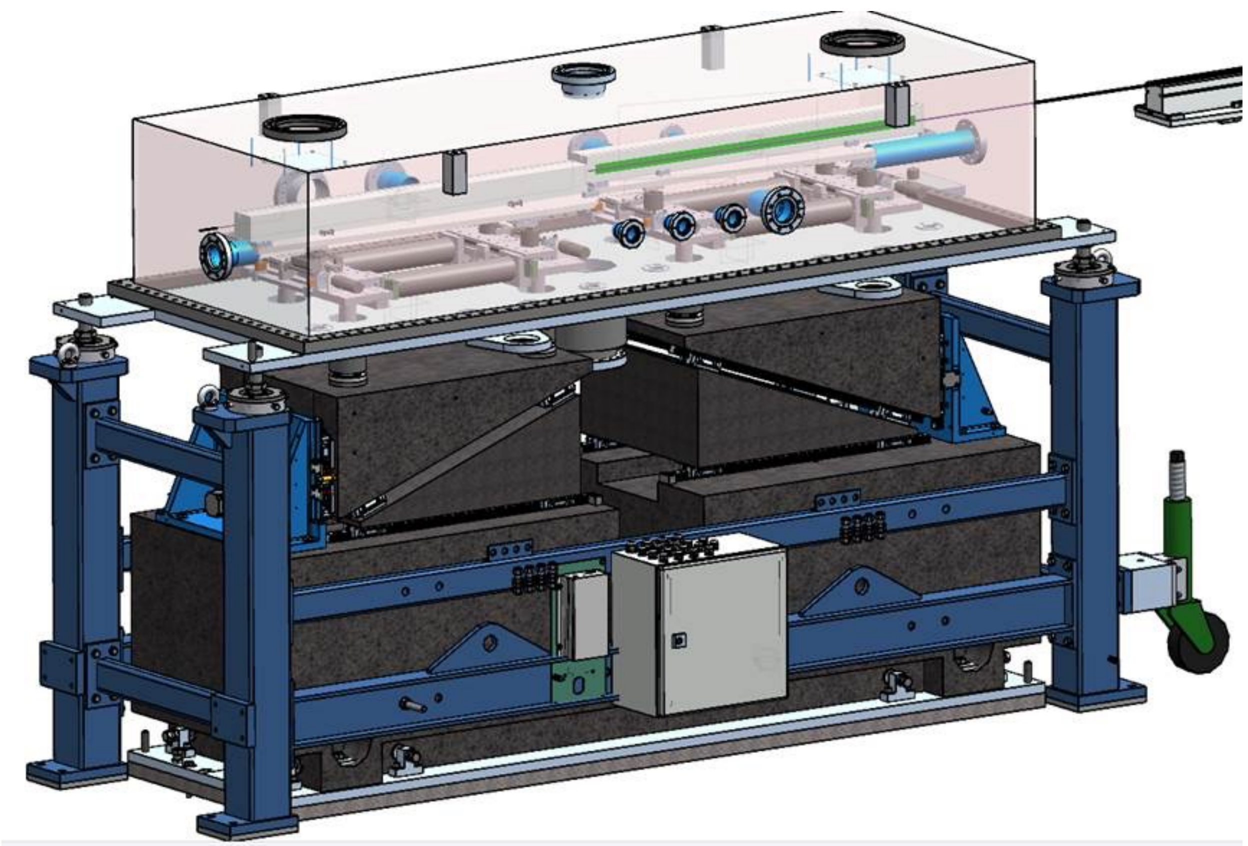


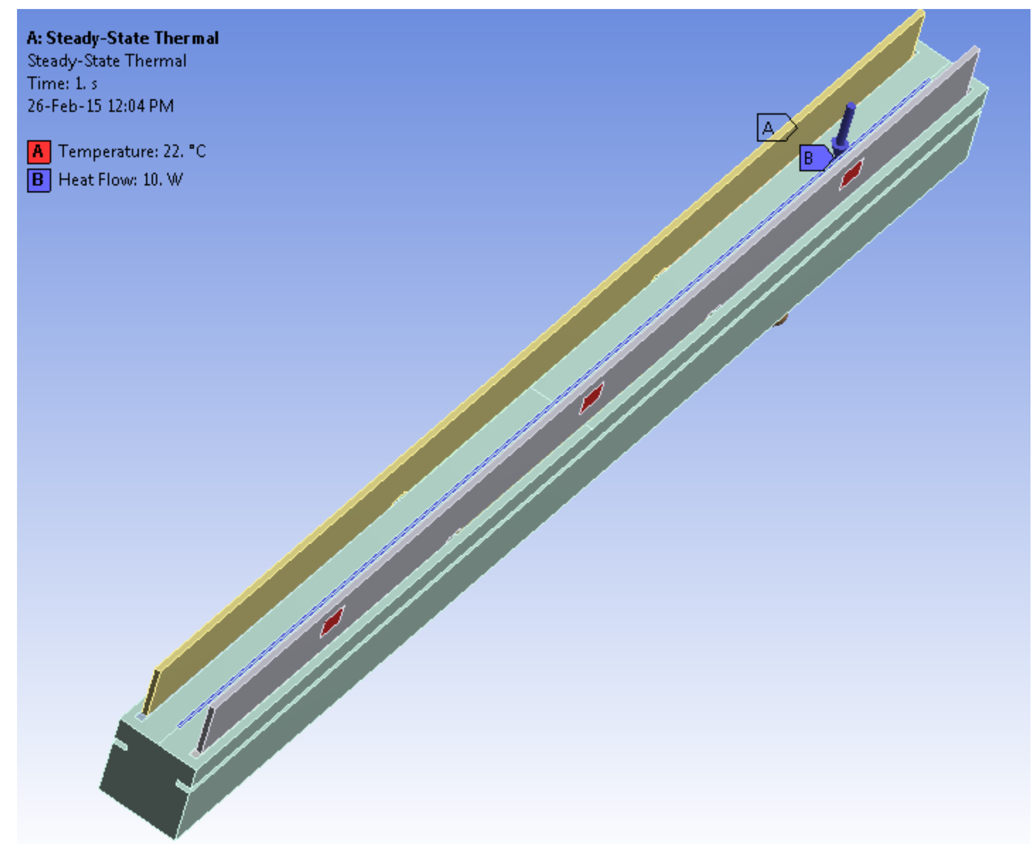
FMB-Oxford competition sensitive, non-distributable

European XFEL

KB focussing optics

- Optics have long lead times (polishing bottlenecks at JTEC)
- Substrate / cooling design optimised by FEA and reviewed at FMB-Oxford PDR meeting to minimise thermal deformations





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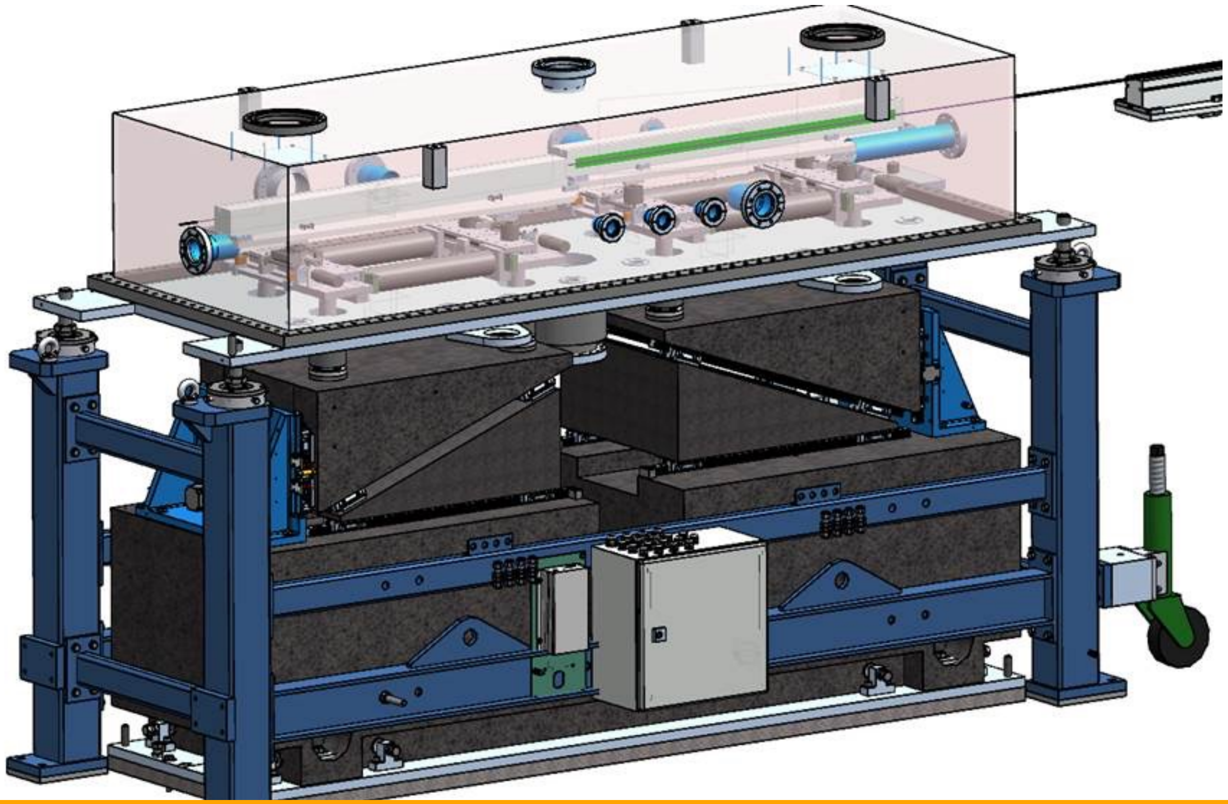
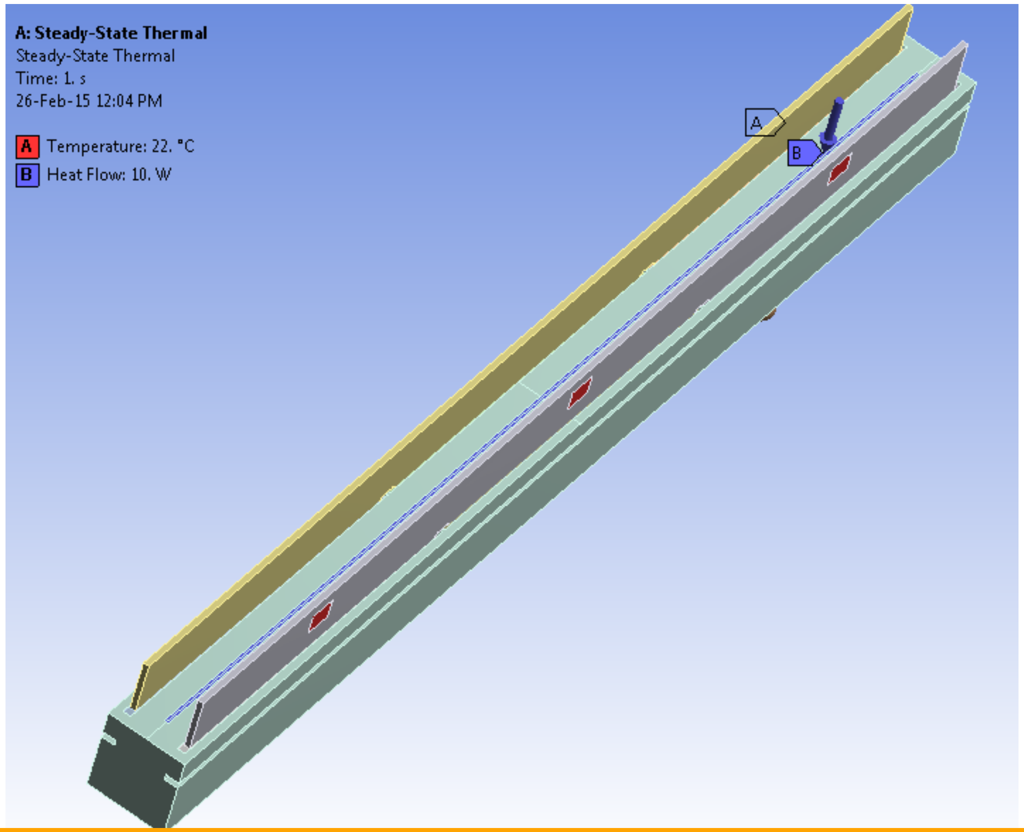
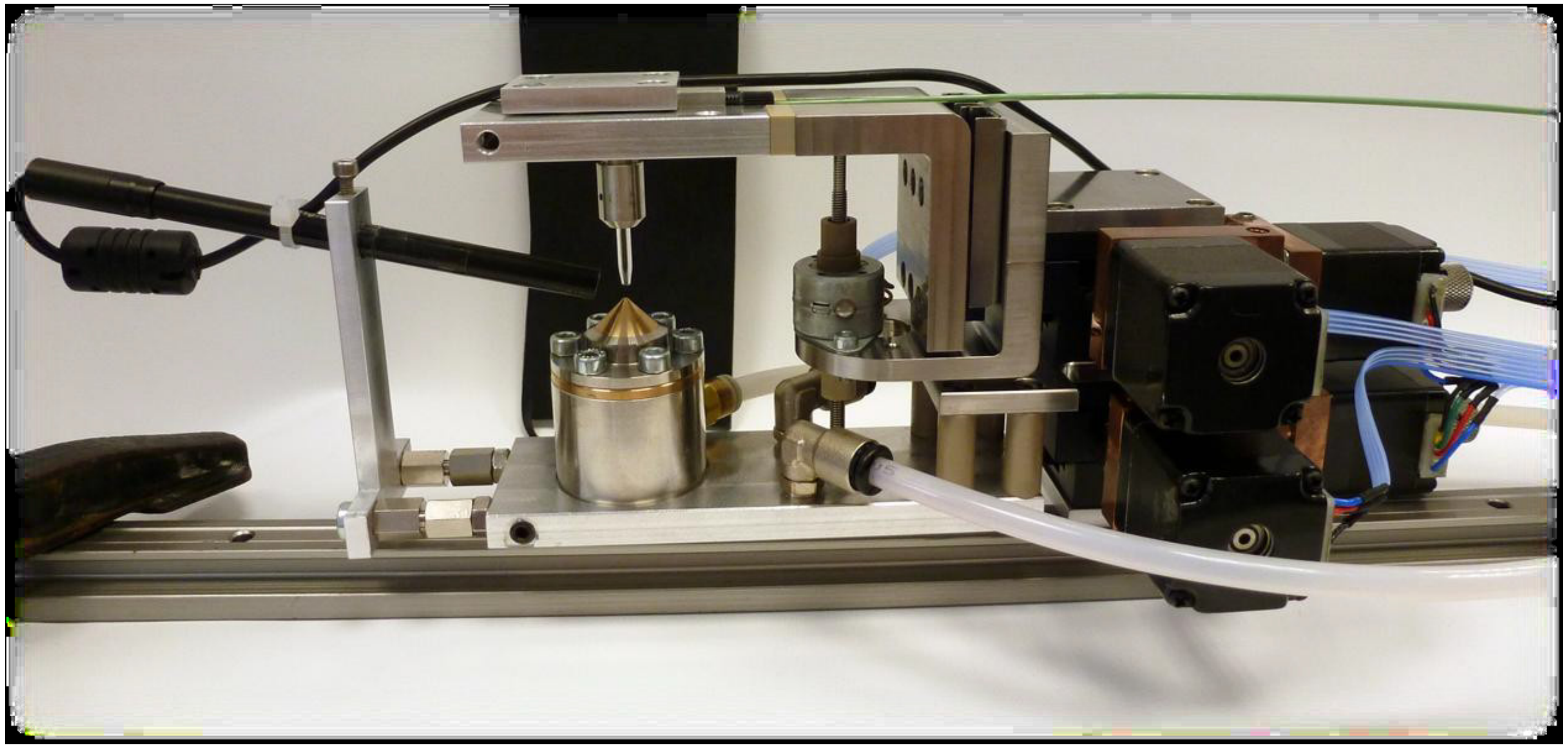




Possible delay hedged by alternative focusing system which supports crystallography

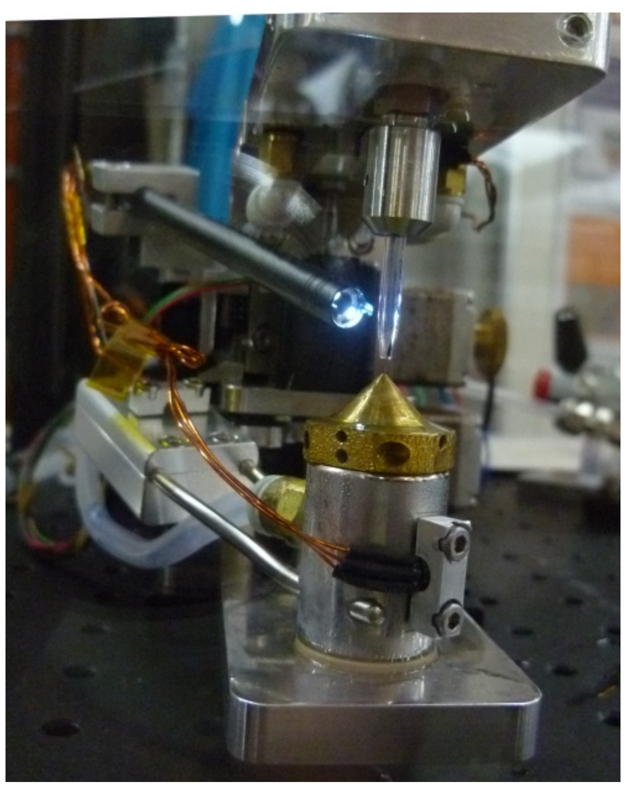
FMB-Oxford competition sensitive, non-distributable

Sample delivery systems: Compact and versatile liquid jet



Specifications

- Modular design
- Independent adjustment of nozzle and catcher
- Large opening angles for detectors
- Precise positioning

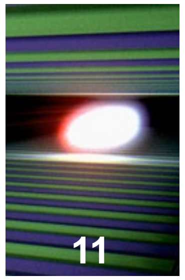


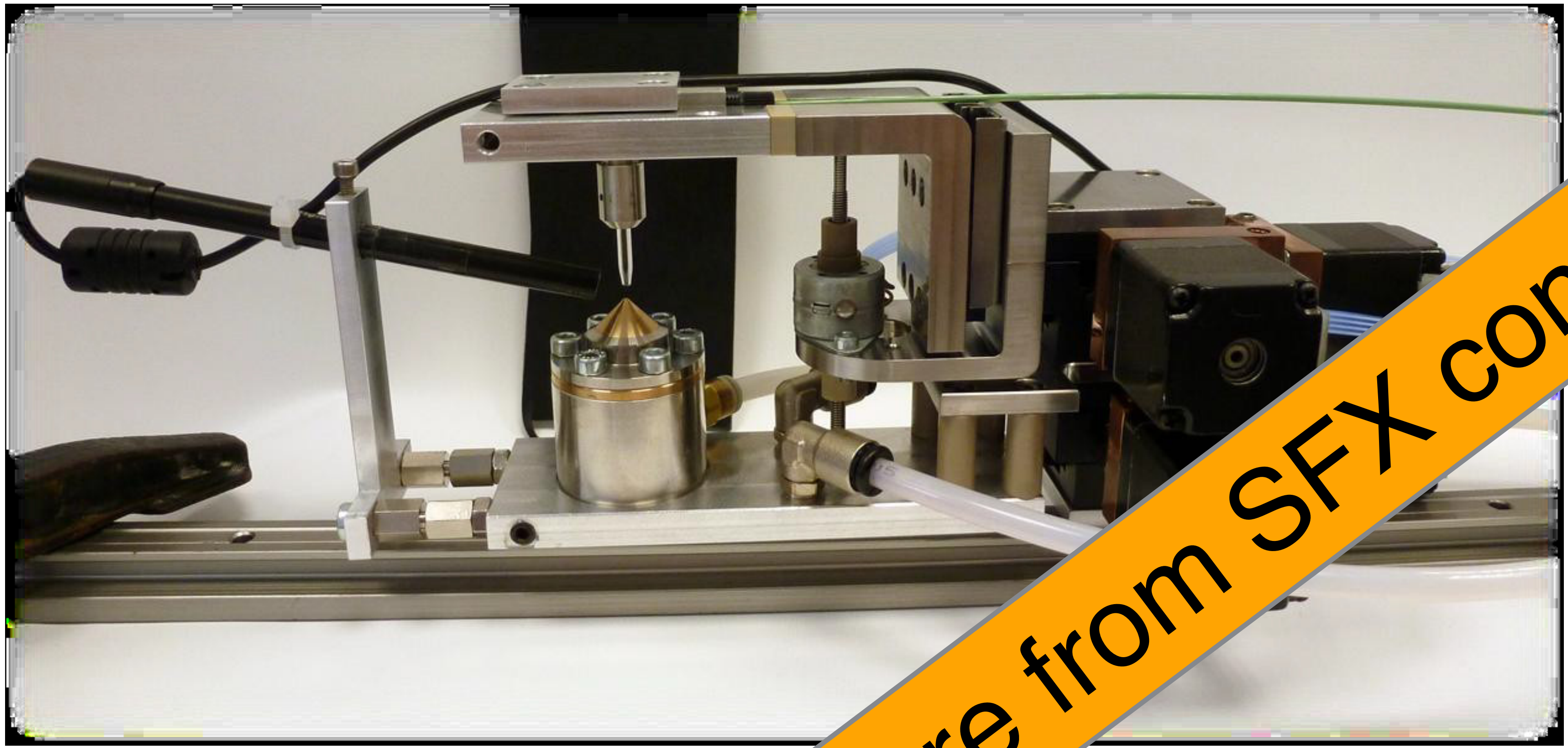
Ongoing development

Recovering catcher for sample recycling
Integration of gas dynamic nozzles for sub-µm jets
Detector protection
Differential pumping and vacuum system

Slide courtesy J. Schulz, Sample environment group, European XFEL

Sample delivery systems: Compact and versatile liquid jet





and many more from SFX consortium

Sp cations

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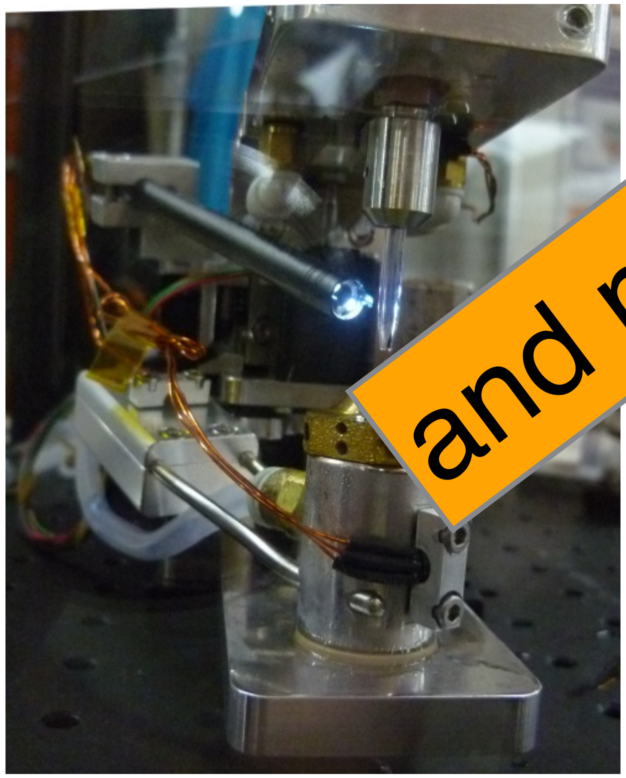
- Precise positioning



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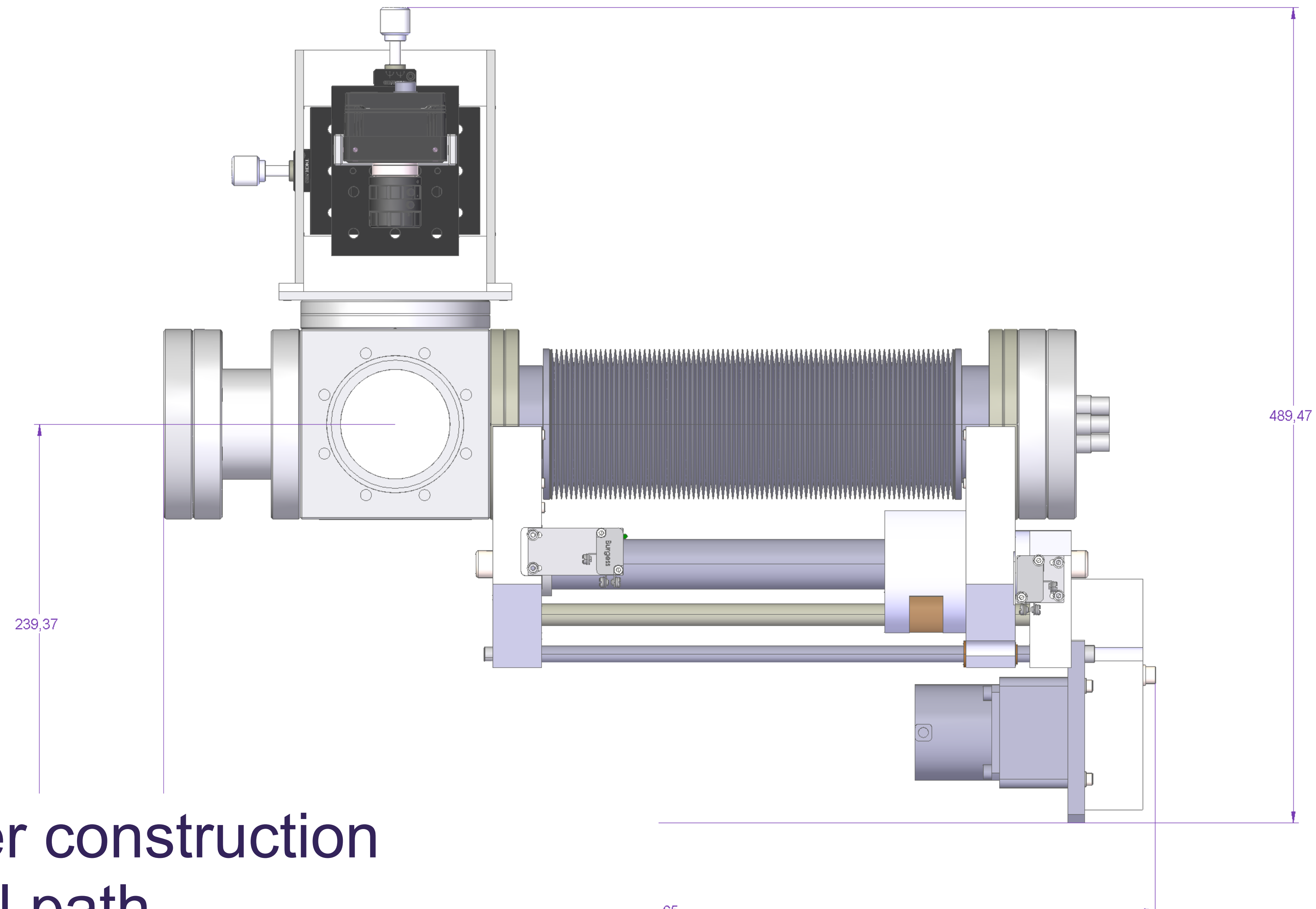
Slide courtesy J. Schulz, Sample environment group, European XFEL

Alignment diagnostics

Alignment diagnostics

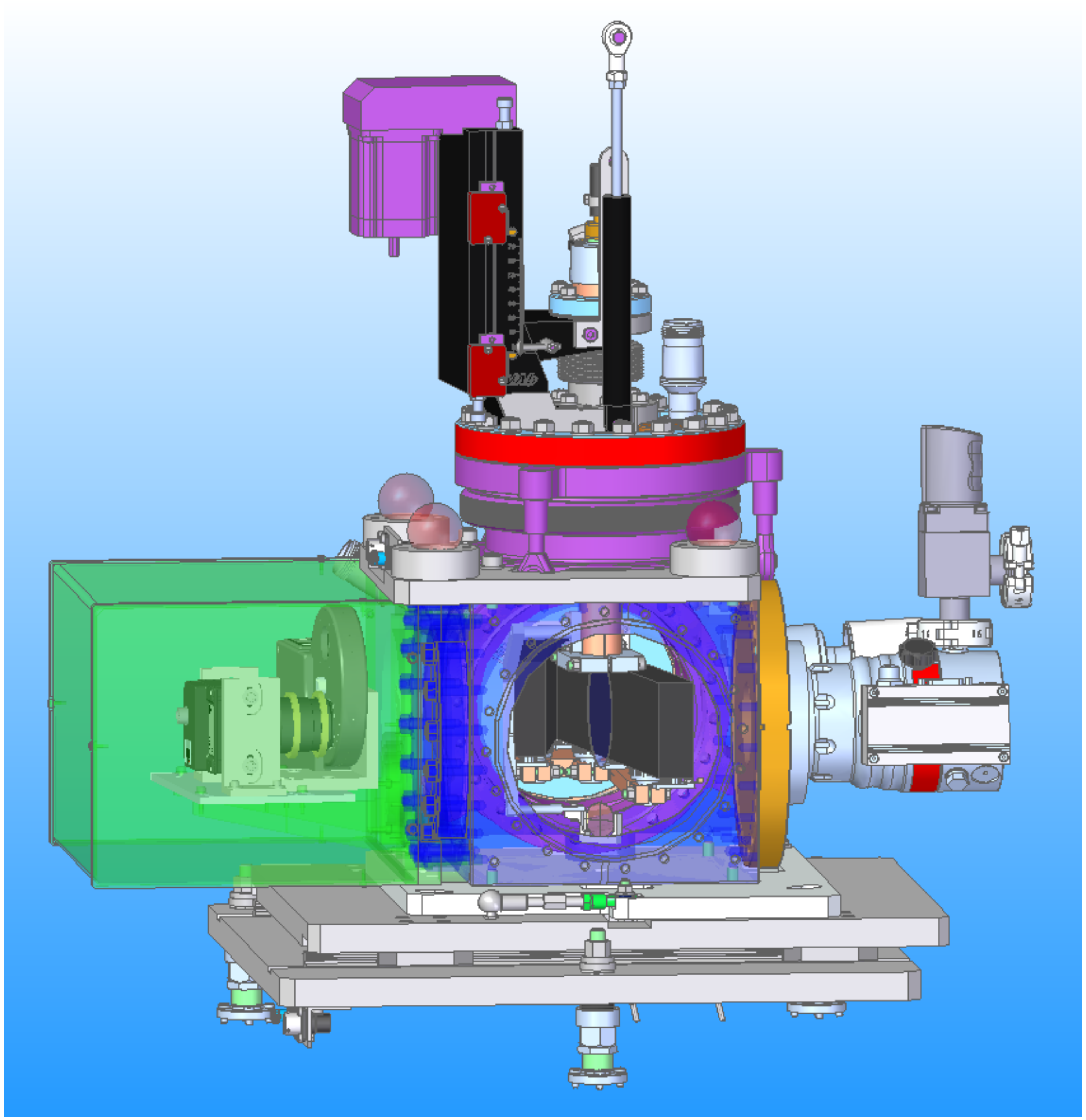


- Prototype under construction
- Far from critical path
- Uses Ce:YAG screens in removable cartridge

G. Borchers & O. Kelsey

Instrument beam stop

Instrument beam stop



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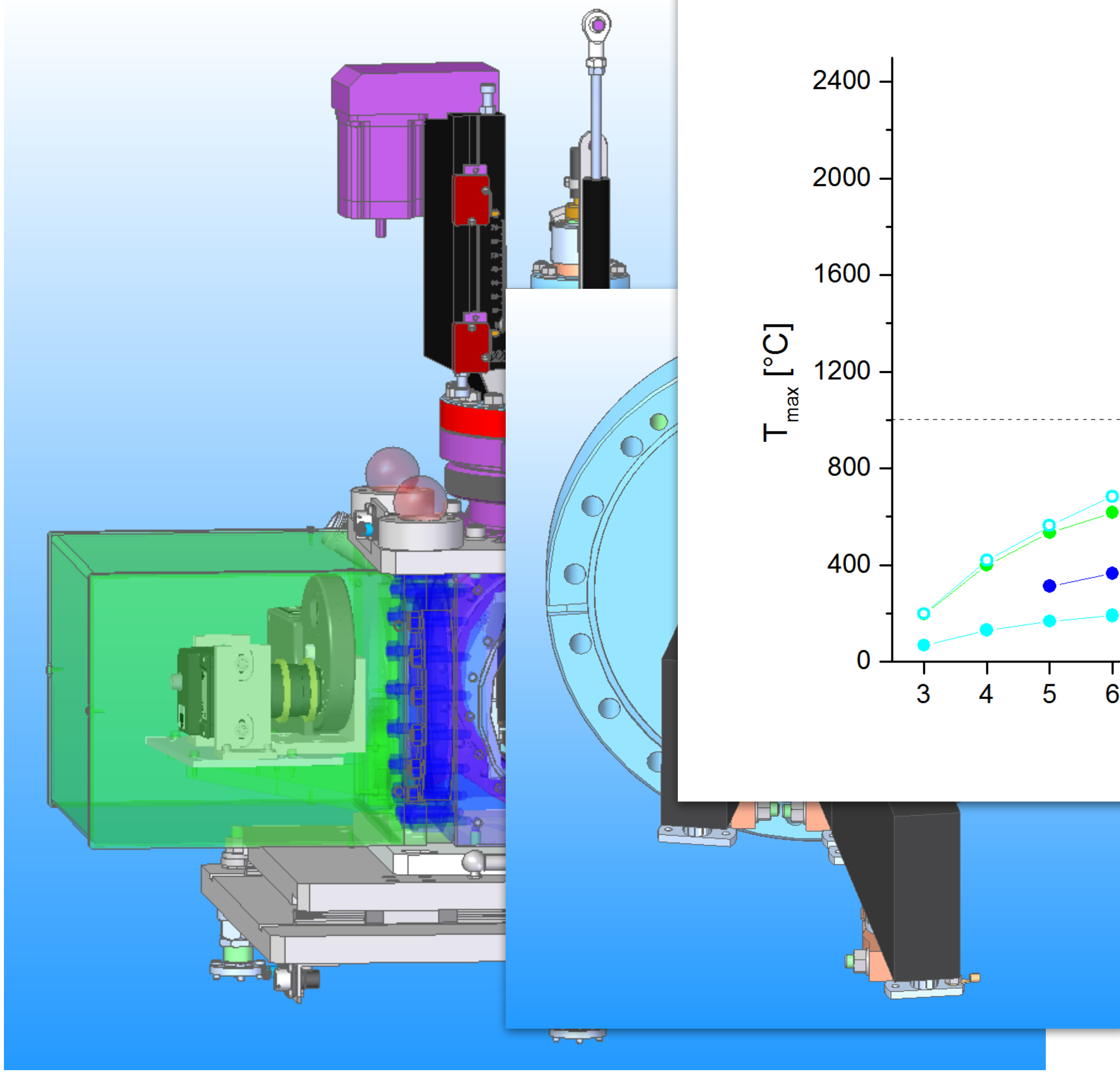
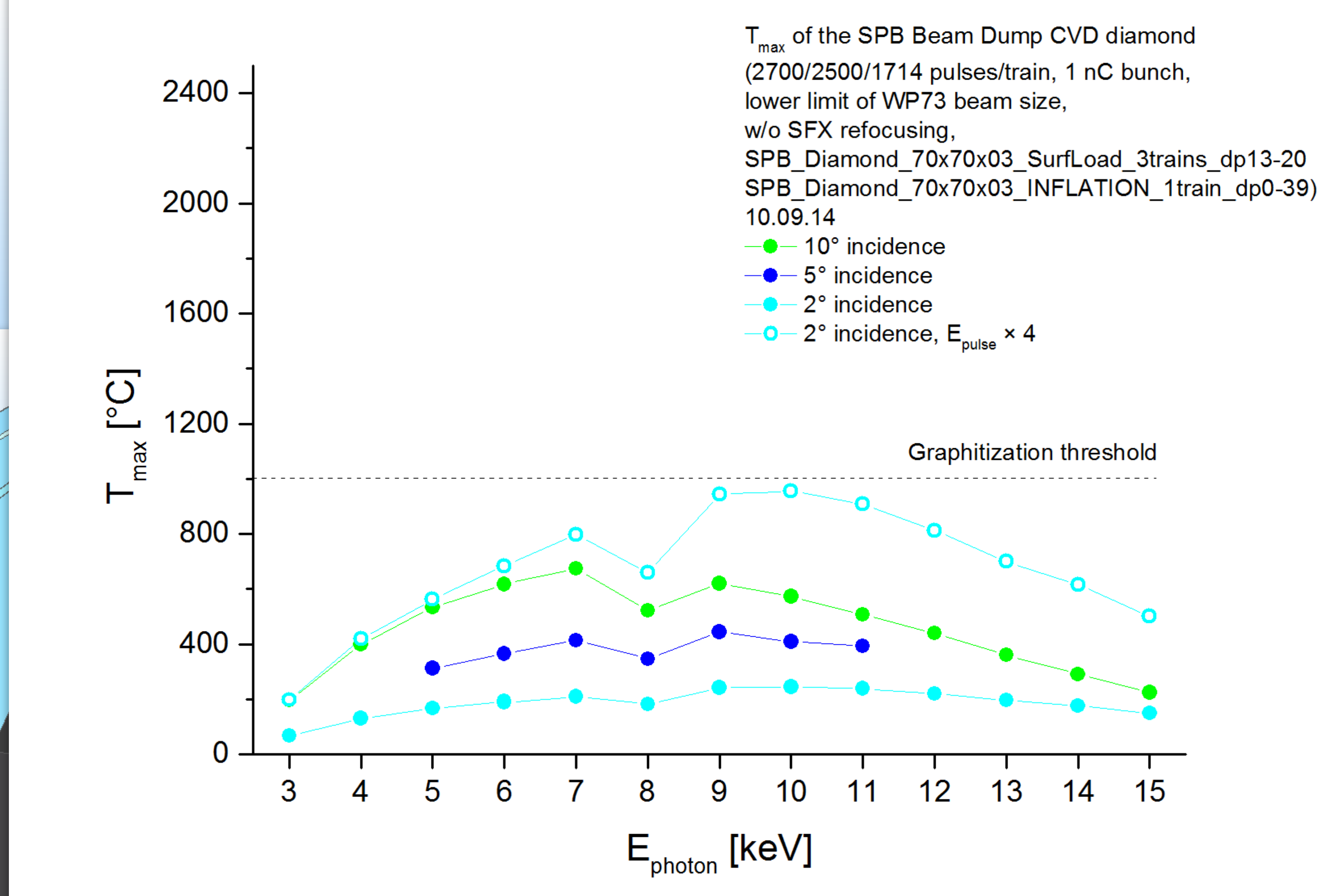
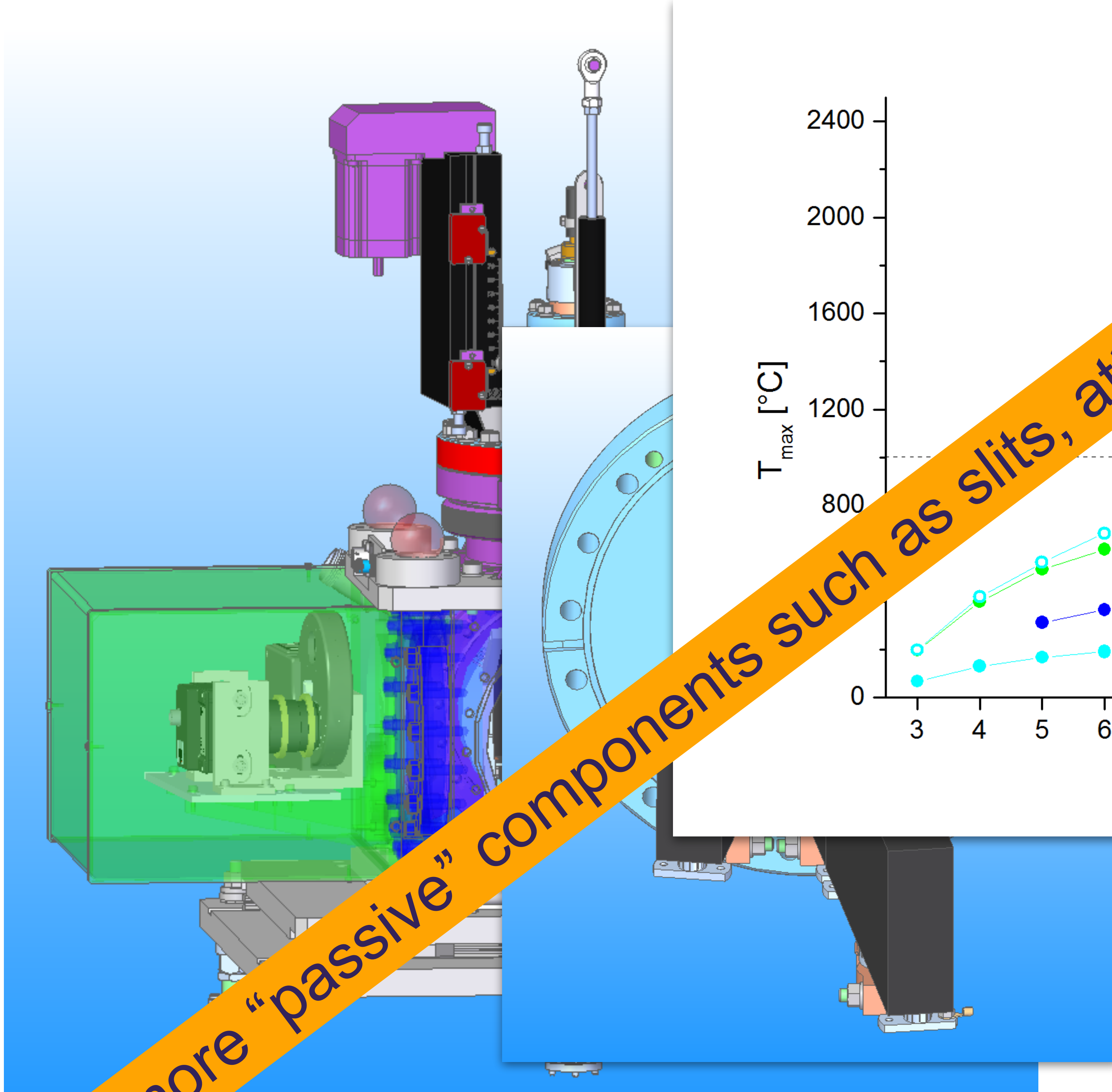
Instrument beam stop

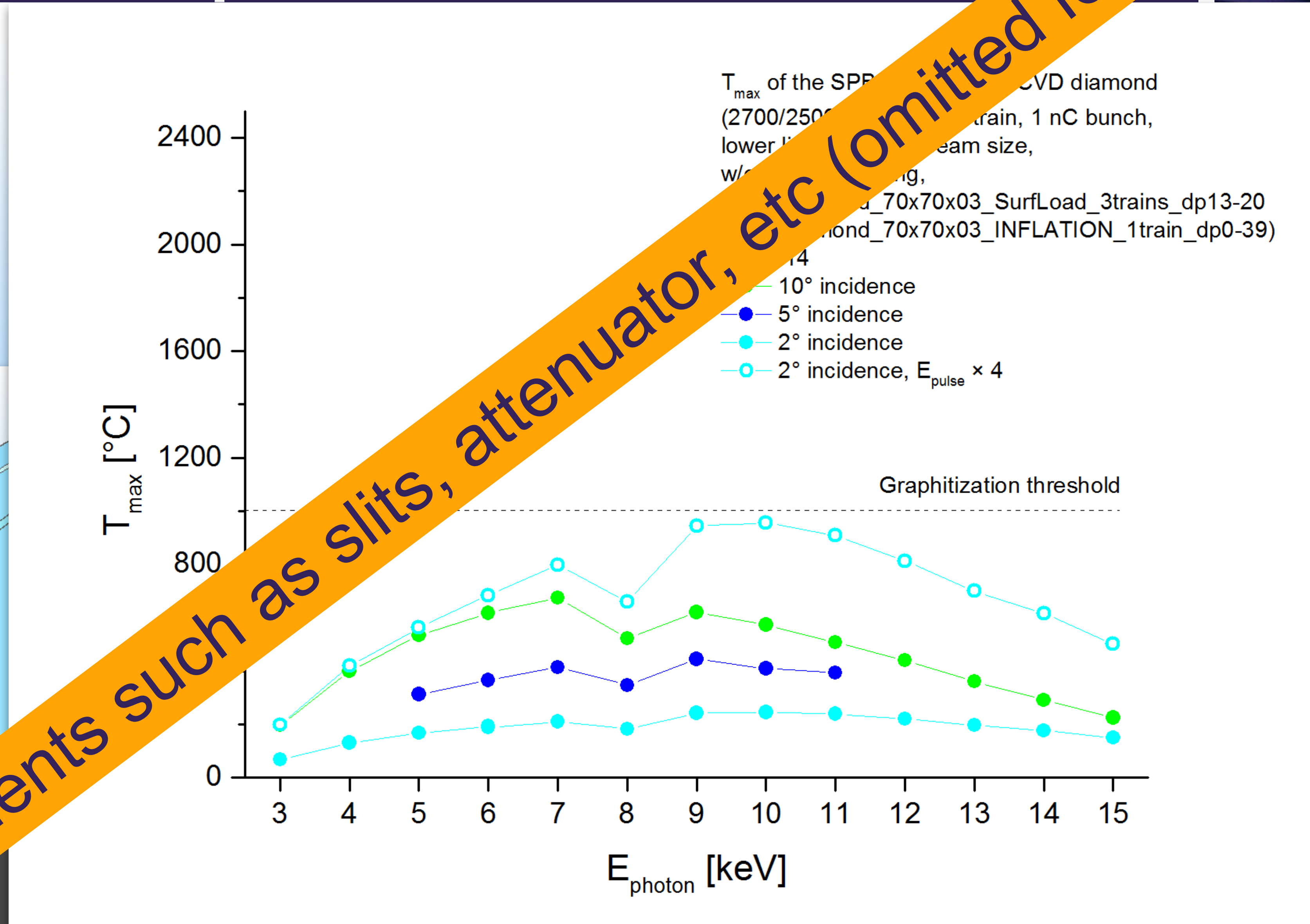




V. Lyamayev, CIE

Instrument beam stop





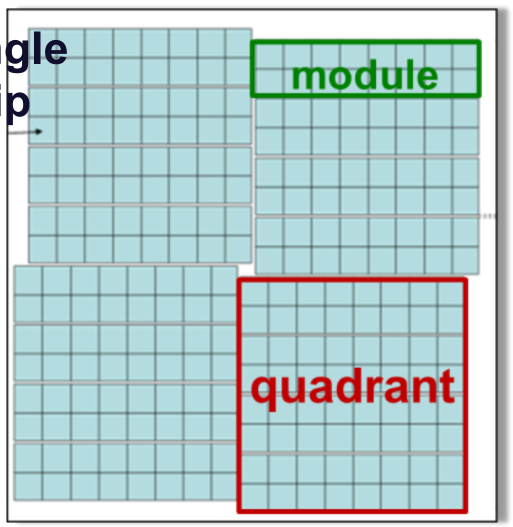
V. Lyamayev, CIE

And more “passive” components such as slits, attenuator, etc (omitted for brevity)

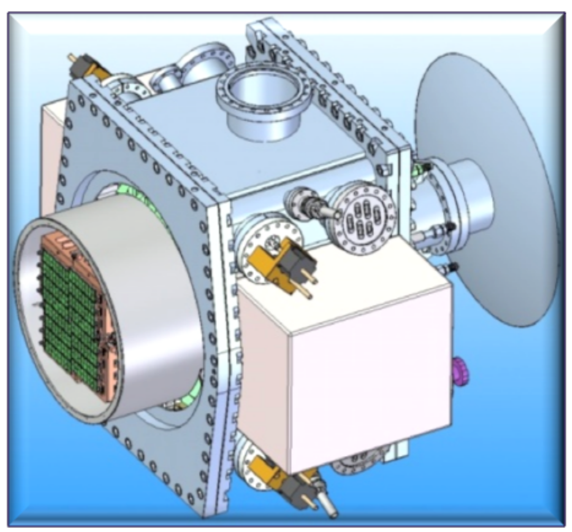
European XFEL

Adaptive Gain Integrating Pixel Detector

High repetition rate (4.5 MHz) 1MPix imaging detector



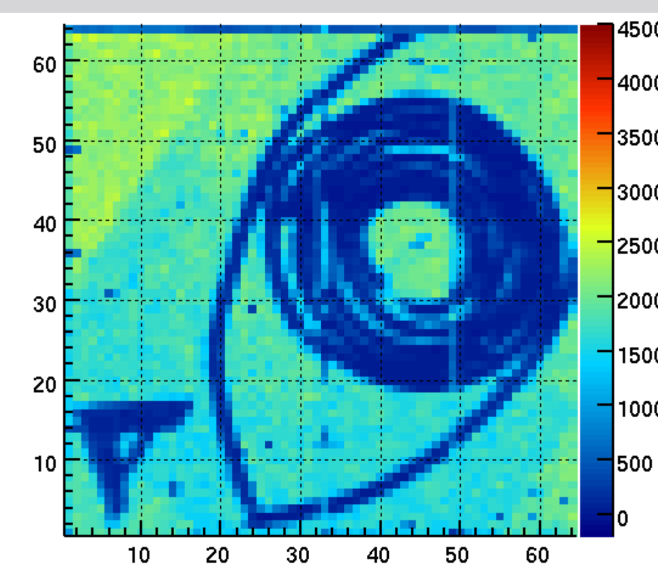
64x64 pixels/chip
2x8 chips/module
modules/quadrant
4 quadrants/detector



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



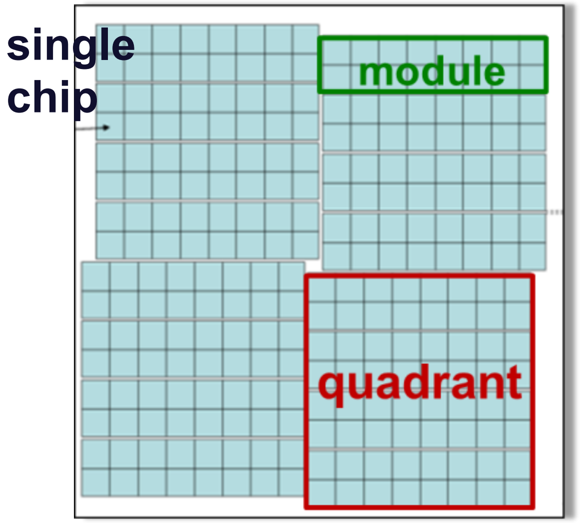
Slide: J. Sztuk-Dambietz, XFEL
Image: AGIPD consortium

European XFEL

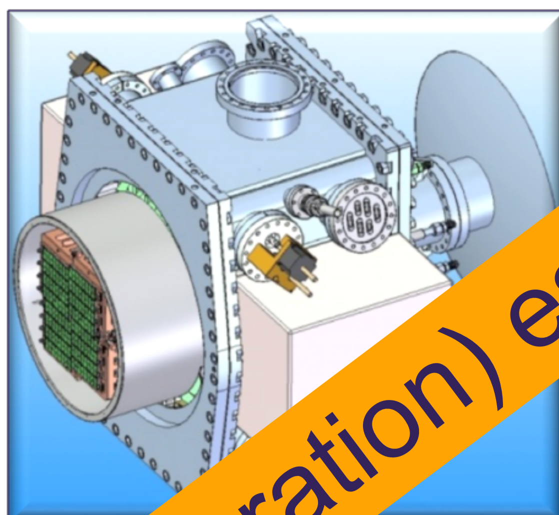
Adaptive Gain Integrating Pixel Detector

Linearity (gain calibration) essential for day one experiments

High repetition rate (4.5 MHz) 1MPix imaging detector



64x64 pixels/chip
2x8 chips/module
modules/quadrant
4 quadrants/detector



Parameter	A
Energy Range	3-16 keV
Dynamic Ra	10^4 ph @12 keV
Single P sens	Yes → Noise ~350e- rms
St ells/pixel	352 (analog)
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Variable hole	Yes→ four independently movable quadrants
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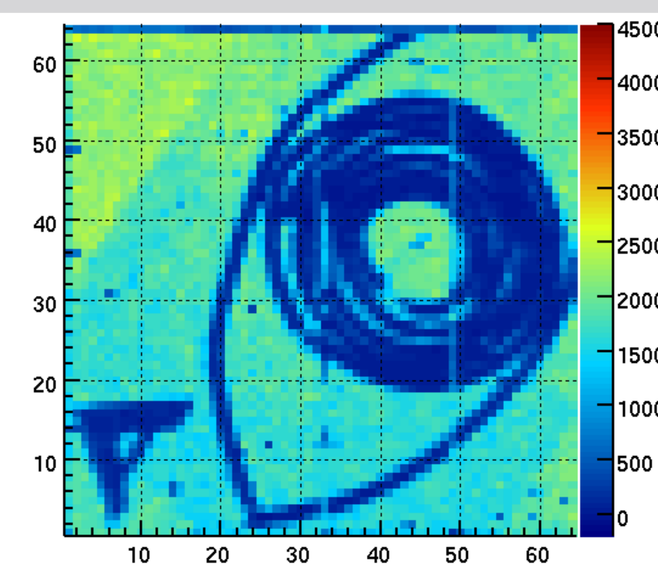


Slide: J. Sztuk-Dambietz, XFEL
Image: AGIPD consortium

Controls, Analysis, Metadata

- Karabo controls must exist in time for commissioning without beam

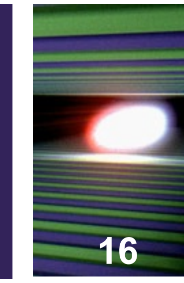
- Some analysis code (e.g. CrystFEL for serial crystallography analysis) must be available to interpret measurements
  - inc. basic online analysis functions
  - inc. simple scripting analysis tools

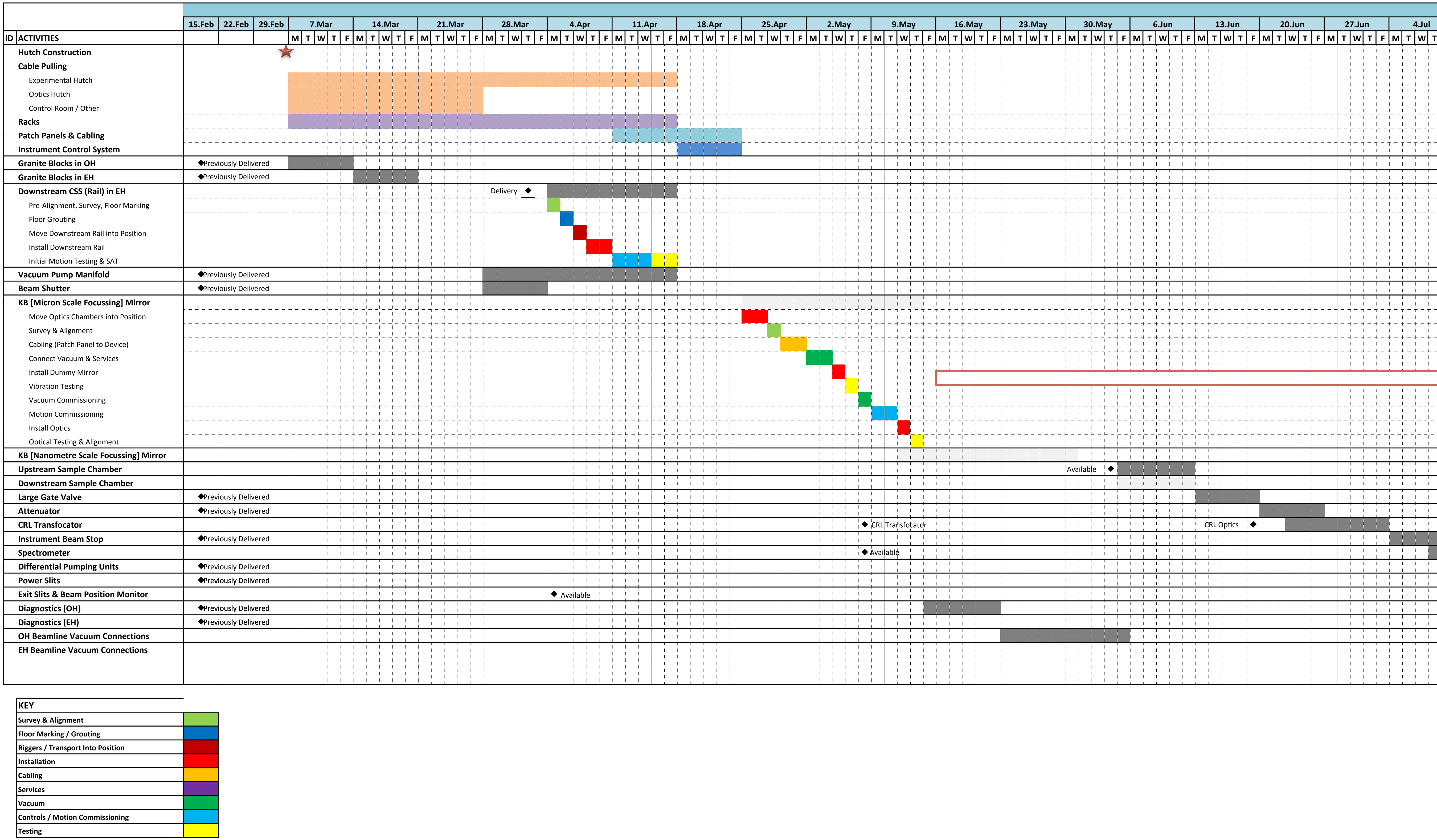
- Metadata related to data (frames) such as pulse energy, I_0 and the diagnostic info must be accessible for analysis
  - Statistical analysis of serial crystallographic data increasingly valuable (correlation analysis, etc)

Cartoon of installation plan

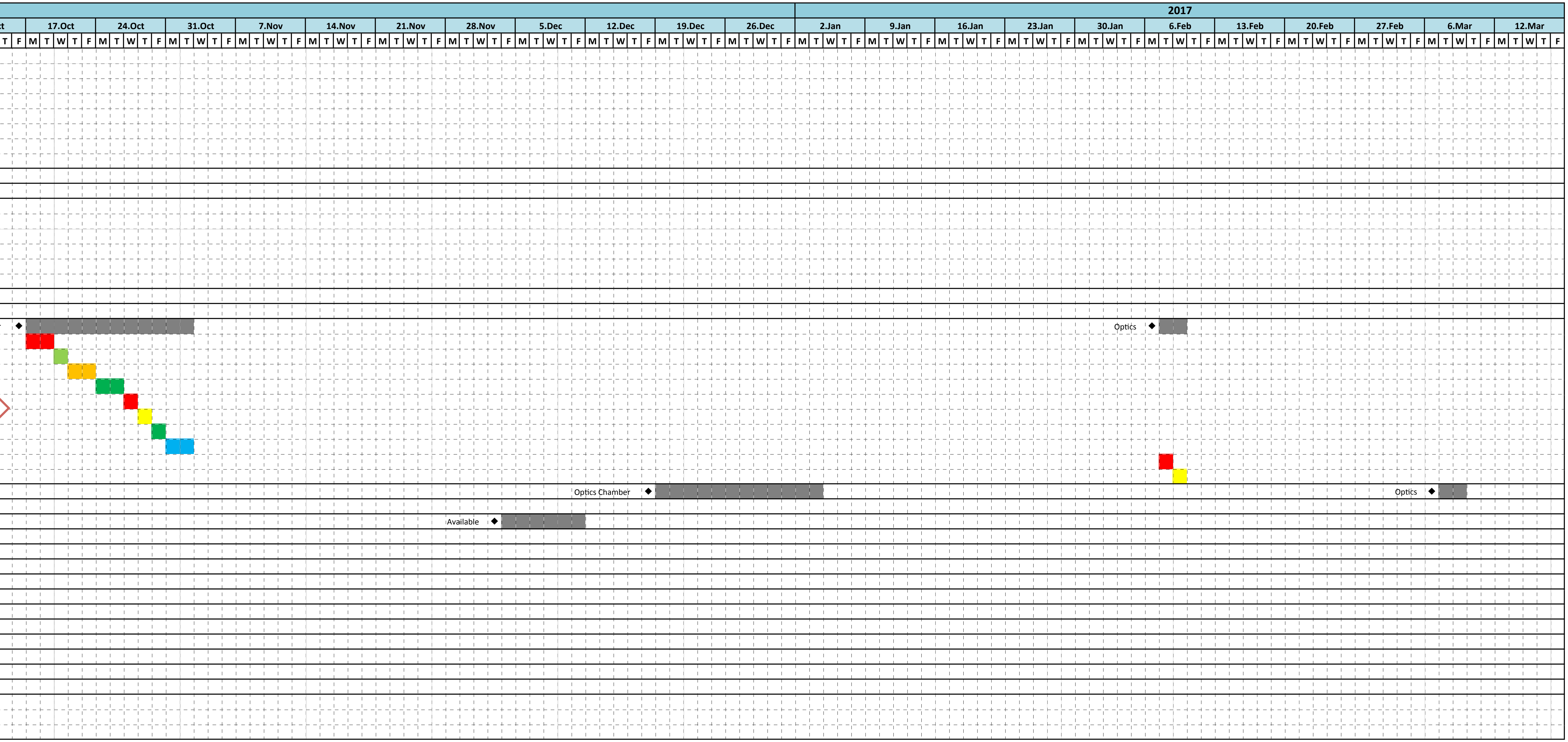
Installation & first experiments SPB/SFX

Cartoon of installation plan





Cartoon of installation plan



Aggressive installation requires ~6 months from “ready” hutches to seeing first beam

Ridiculously optimistic route to fast “1st measurements”

- Approximately focus optics
  - Using diagnostics screens, mirrors (or lenses)
  - Characterise beam size & coherence
  - 6 shifts
- Align sample delivery system
  - Using in-chamber diagnostic microscopes
  - Test with known sample
  - 2 shifts
- Confirm and refine detector geometry
  - Using “easy” nanocrystal sample
  - 2 shifts
- Taking data on a first sample
  - Requiring implemented serial crystallography analysis software
  - 5 shifts

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Total = 1+ weeks

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Compare with LCLS ≈ 6 weeks/instr.

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These states ≠ commissioned

Acknowledgments

- SPB/SFX
  - Andrew Aquila (until Oct ’14)
  - Richard Bean (from Oct ’14)
  - Gannon Borchers
  - Klaus Giewekemeyer
  - Masoud Mehrjoo
  - Marc Messerschmidt (Sci computing)
  - Nadja Reimers (Central Instruments Engineering)
  - Stephan Stern
  - Tokushi Sato
  - Steffen Raabe
  - Chun Hong Yoon

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

Australian Government Australian Research Council
Ministry of Education, Science, Research and Sport of the Slovak Republic
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DESY
European XFEL