



# The SPB/SFX Instrument: An update

Adrian Mancuso

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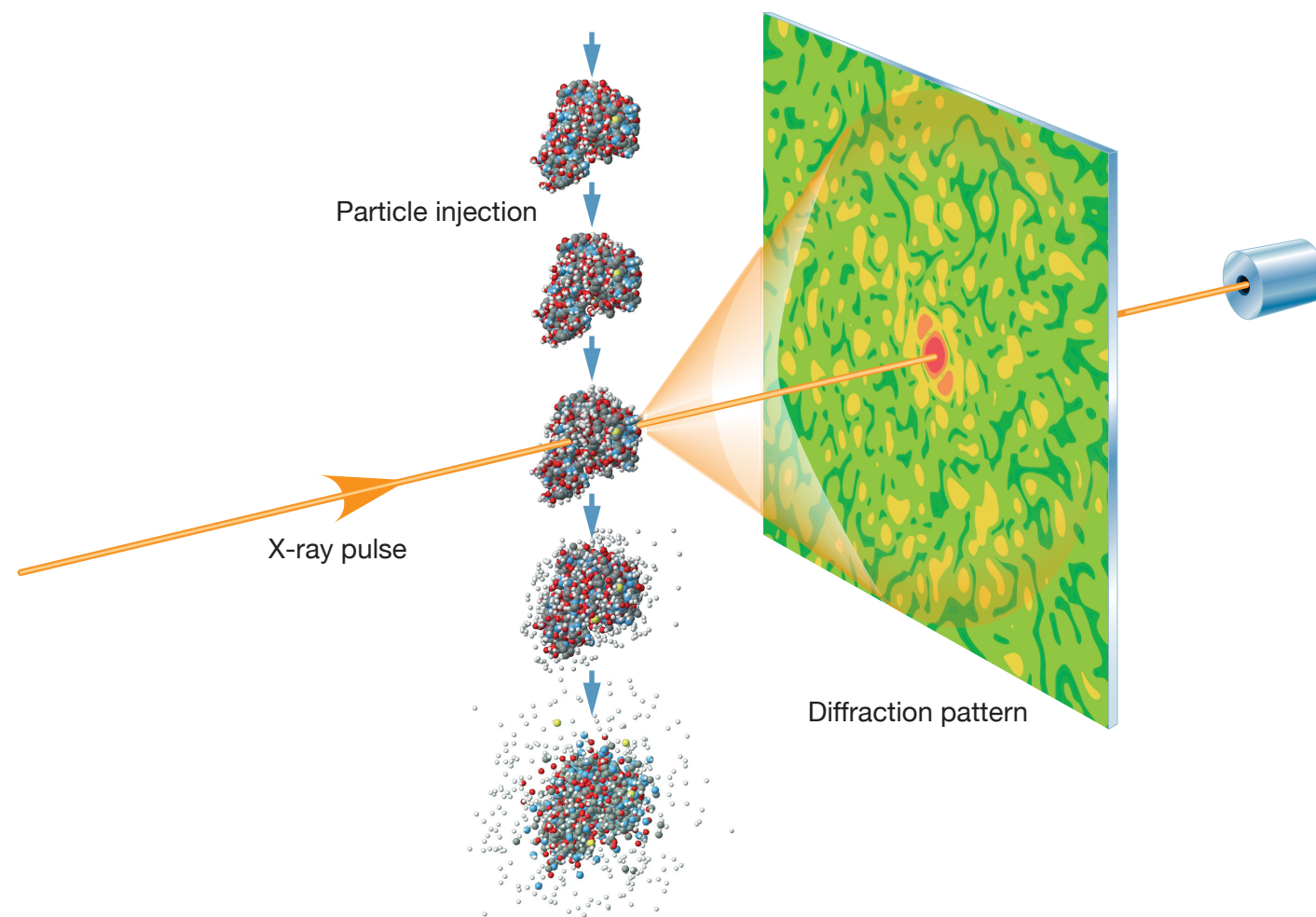
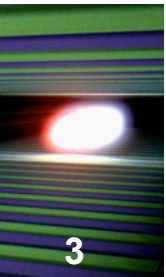


# The Single Particles, Clusters and Biomolecules and Serial Femtosecond Crystallography Instrument

Adrian Mancuso

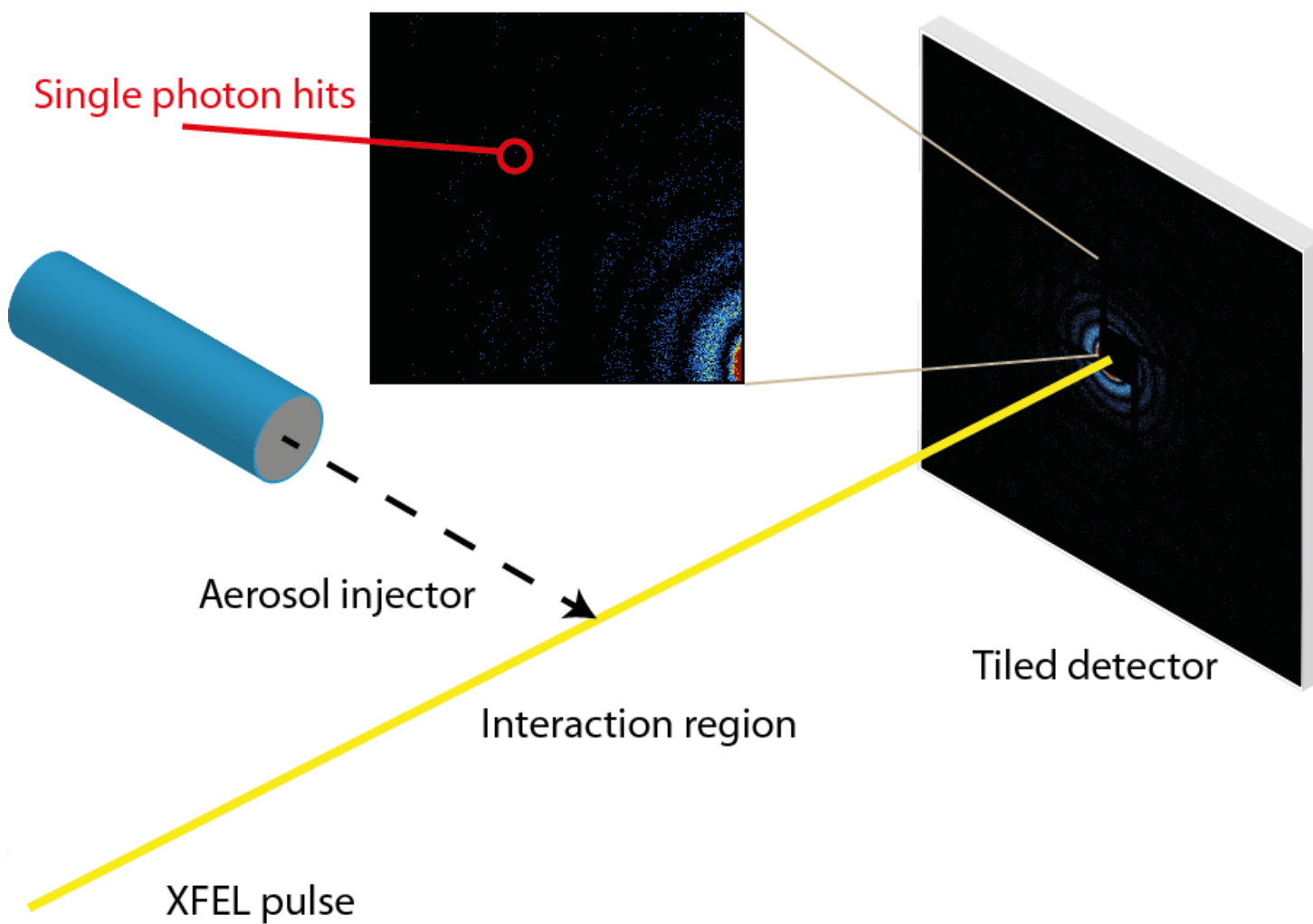
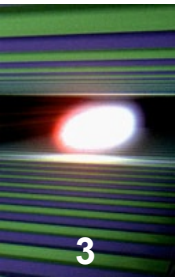
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# Reminder: SPB/SFX Science



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

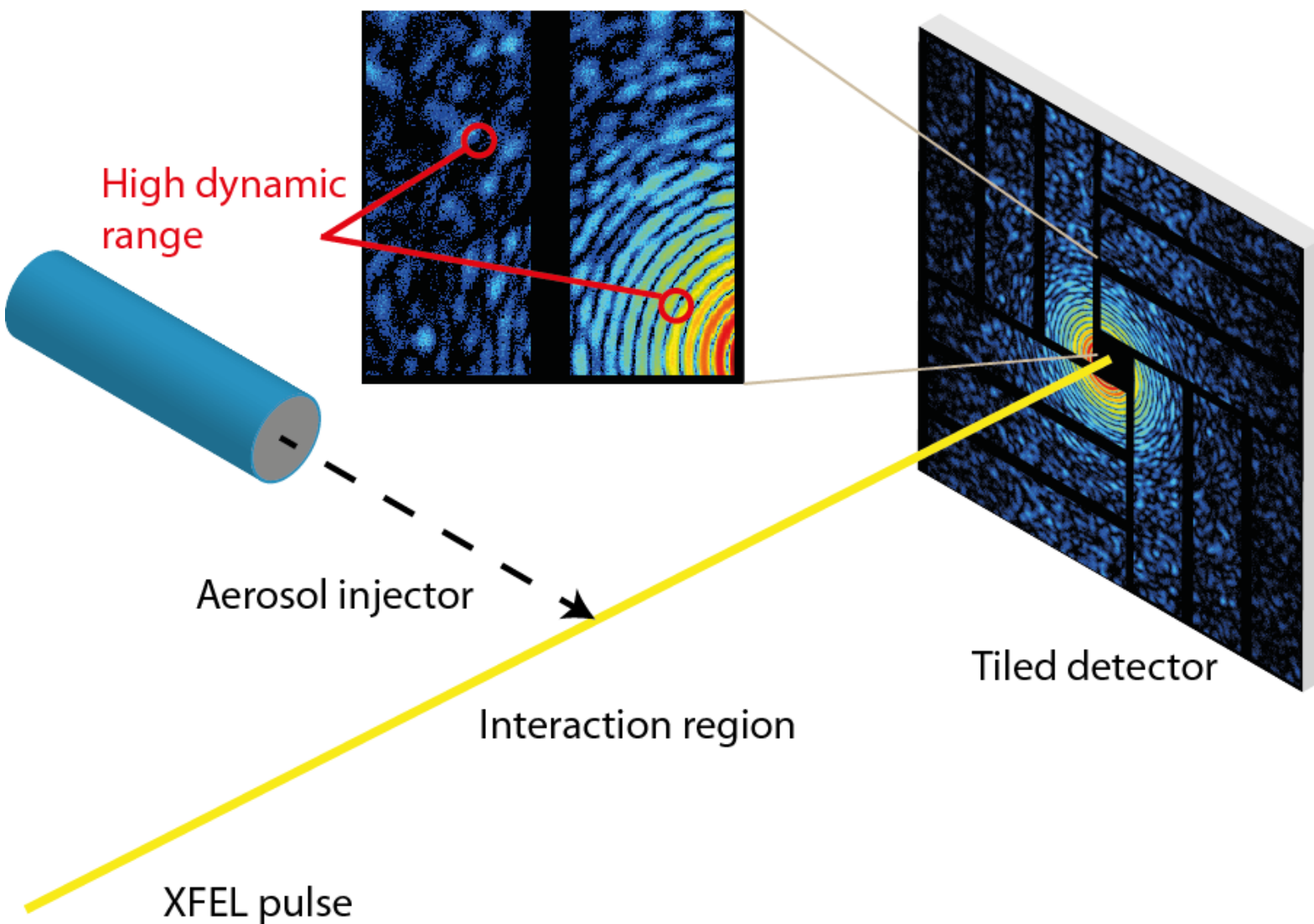
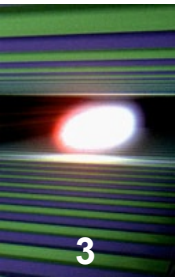
# Reminder: SPB/SFX Science



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

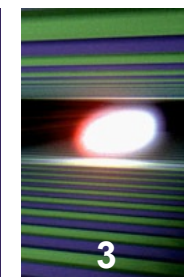


# Reminder: SPB/SFX Science

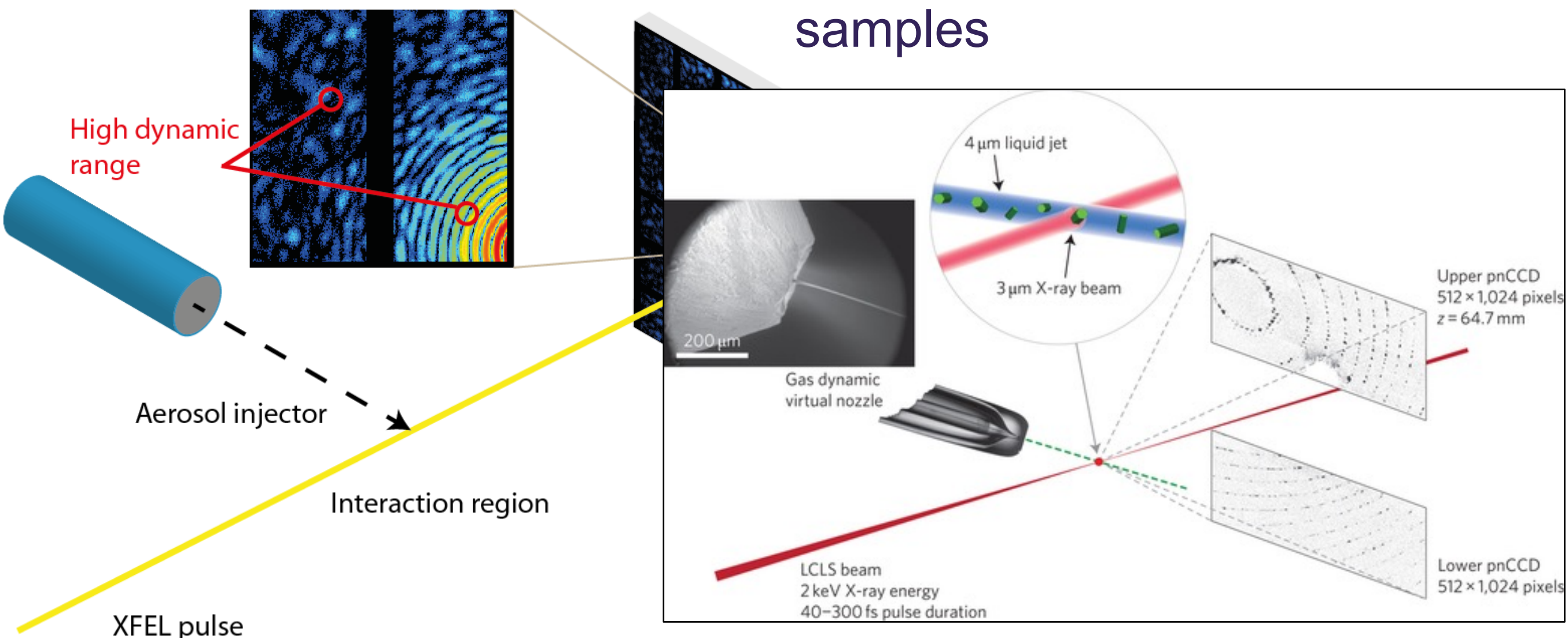


Imaging of “big” and “small”  
non-crystalline samples

# Reminder: SPB/SFX Science



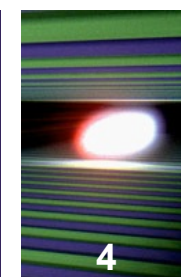
## Crystallography of “small”, “radiation sensitive” or “dynamic” samples



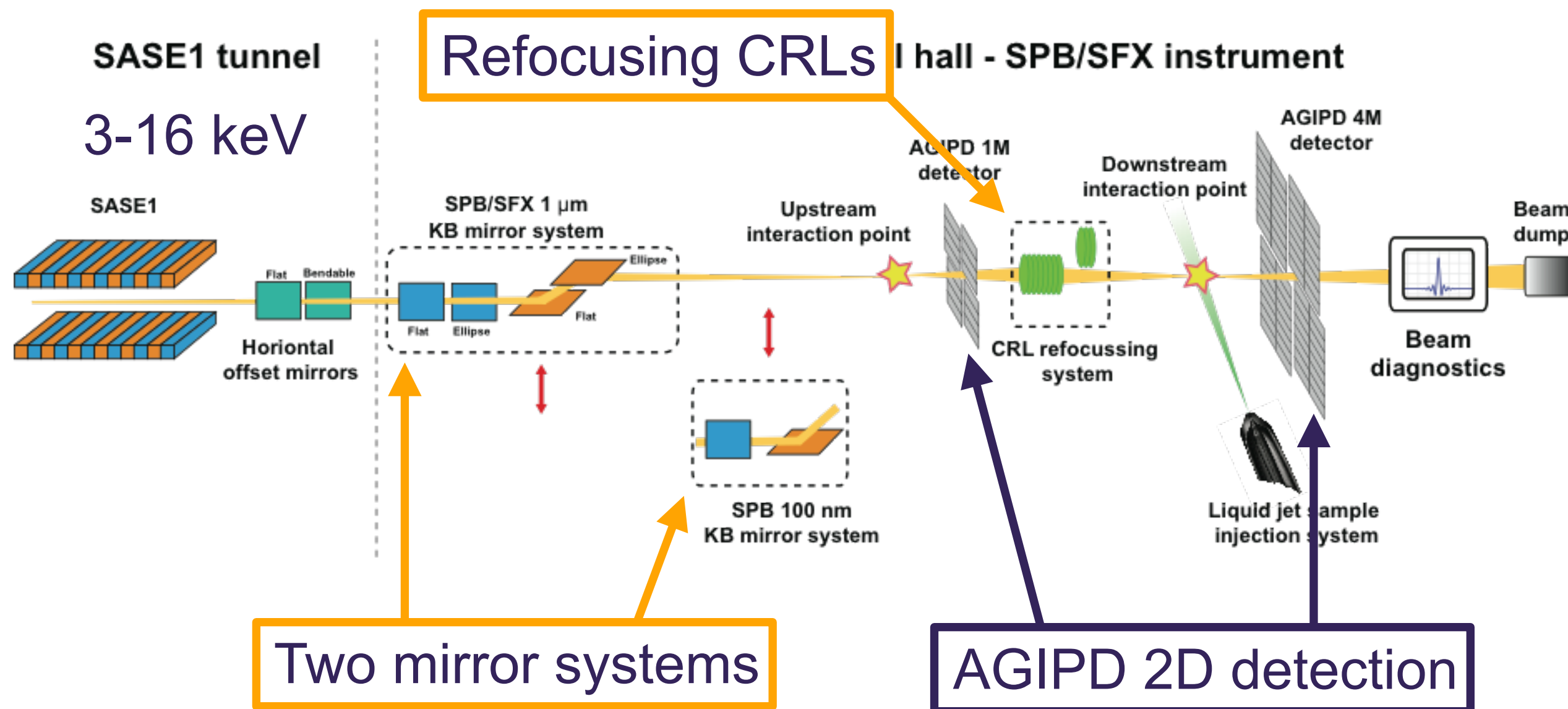
Imaging of “big” and “small” non-crystalline samples

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

# Overview SPB/SFX instrument



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[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).

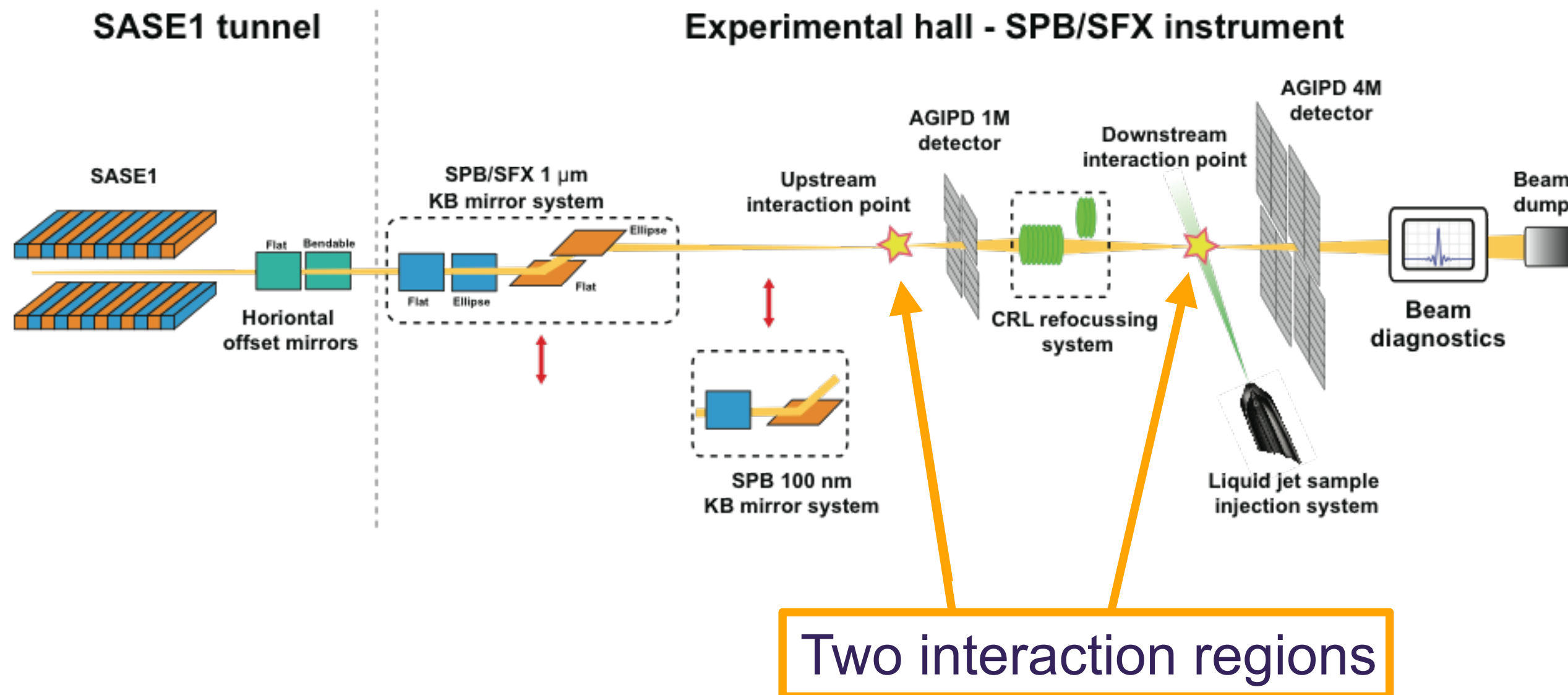
[2] A. P. Mancuso, Conceptual Design Report: Scientific Instrument SPB, 2011. [dx.doi.org/10.3204/XFEL.EU/TR-2011-007](https://dx.doi.org/10.3204/XFEL.EU/TR-2011-007)

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

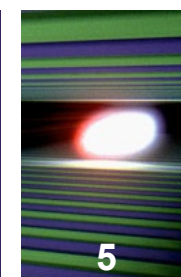


# Overview SPB/SFX instrument

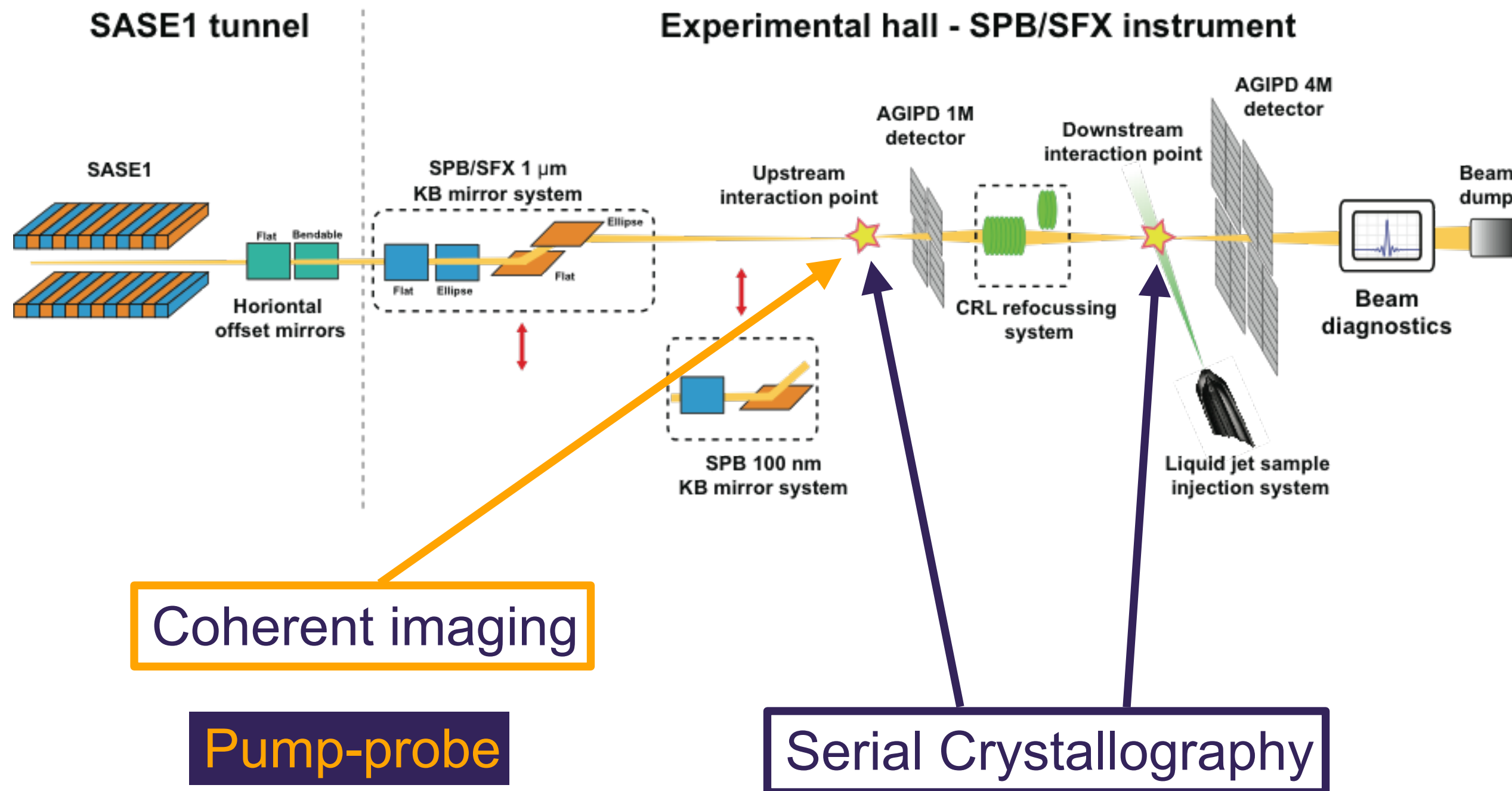
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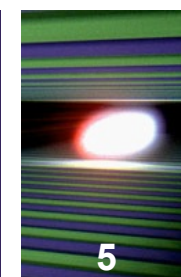
# Overview SPB/SFX instrument



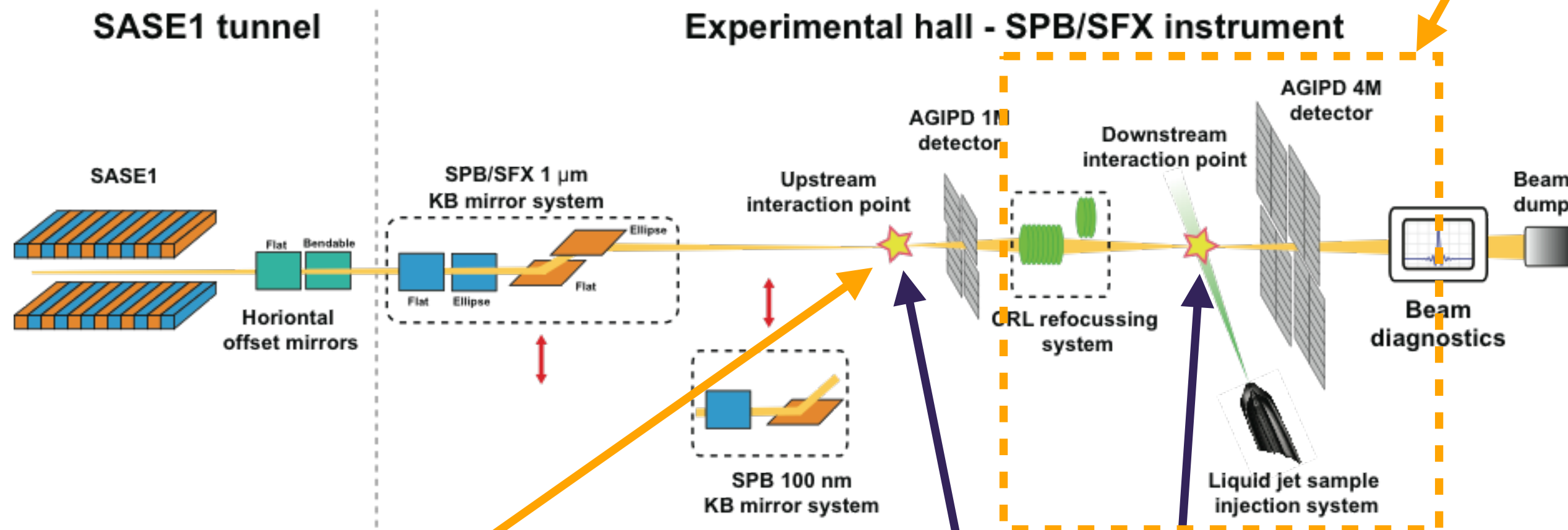
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# Overview SPB/SFX instrument



## SFX UC Contribution



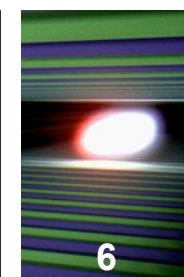
Coherent imaging

Pump-probe

Serial Crystallography



# The SPB/SFX instrument at a glance



XFEL.EU TR-2013-004

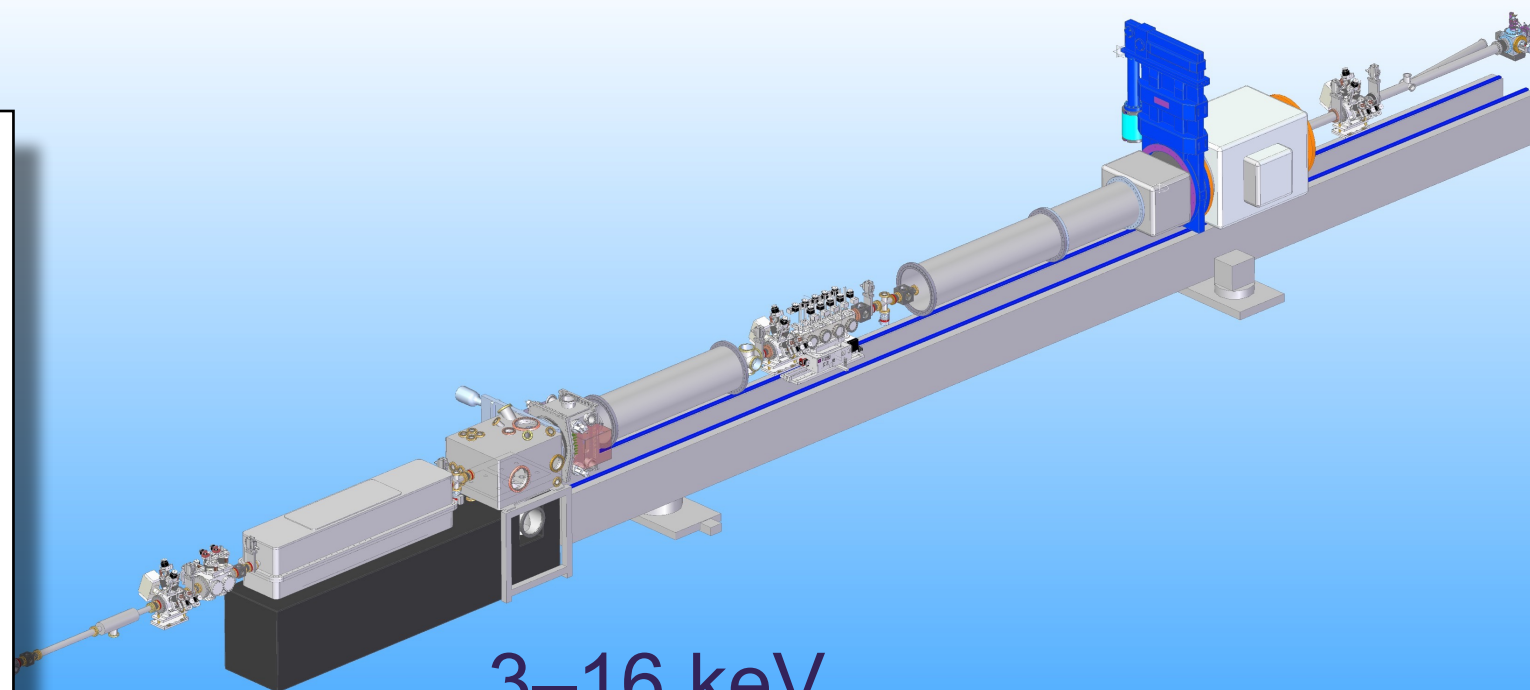
## TECHNICAL DESIGN REPORT

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

August 2013

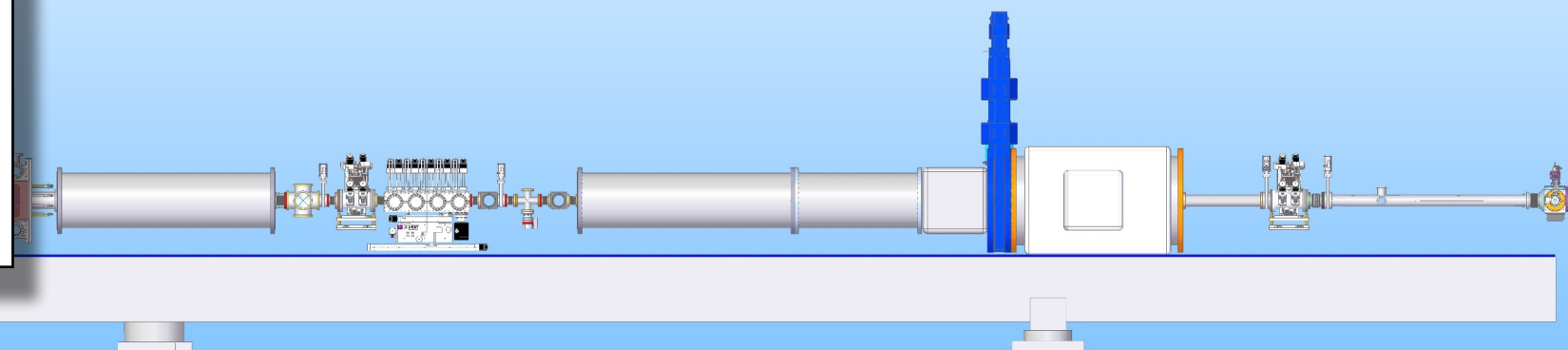
*A.P. Mancuso, A. Aquila,  
G. Borchers, and K. Giewekemeyer,  
Scientific Instrument SPB (WP84);  
N. Reimers, Central Instrumentation  
Engineering (CIE)*

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



3–16 keV

1  $\mu\text{m}$  and 100 nm scale focal spots  
2 $\times$  interaction regions



A. P. Mancuso, et al, Technical Design Report: Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB)  
<http://dx.doi.org/10.3204/XFEL.EU/TR-2013-004>

# The SPB/SFX instrument at a glance

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XFEL.EU TR-2013-004

## TECHNICAL DESIGN REPORT

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

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A.P. Mancuso, A. Aquila,  
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N. Reimers, Central Instrumentation  
Engineering (CIE)

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



SFX ODR 2014

## OVERVIEW DESIGN REPORT

### The Serial Femtosecond Crystallography (SFX) Apparatus Overview Design Report (ODR)

April 15, 2014

SPB/SFX Team, Center for Free  
Electron Laser Science, DESY,  
and European XFEL GmbH



**wellcome**trust

Australian Government  
Australian Research Council



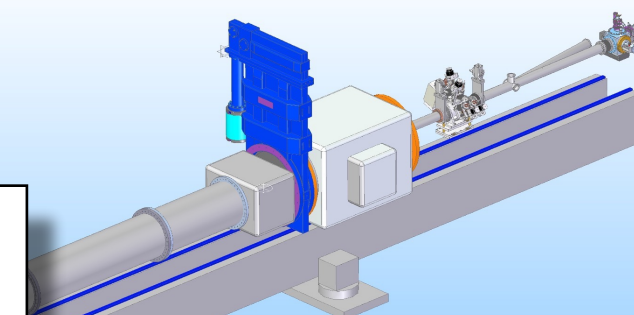
Universität Hamburg  
DER FORSCHUNG | DER LEHRE | DER BILDUNG



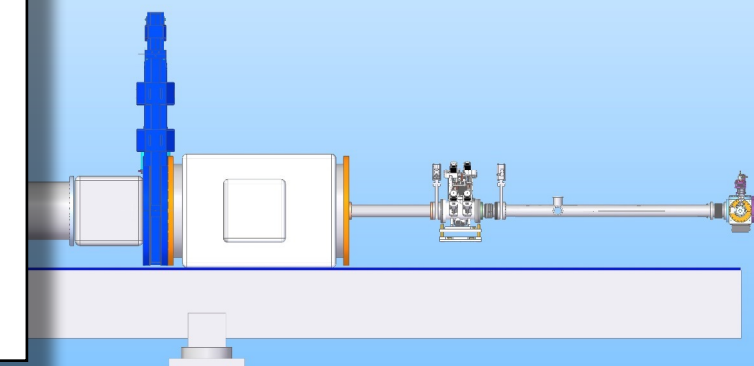
PAUL SCHERRER INSTITUT



Ministry of Education,  
Science, Research and Sport  
of the Slovak Republic

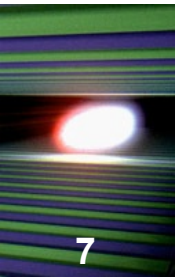


100 nm scale focal spots  
in regions



A. P. Mancuso, et al, Technical Design Report: Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB)  
<http://dx.doi.org/10.3204/XFEL.EU/TR-2013-004>

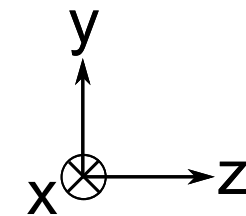
# Optical considerations



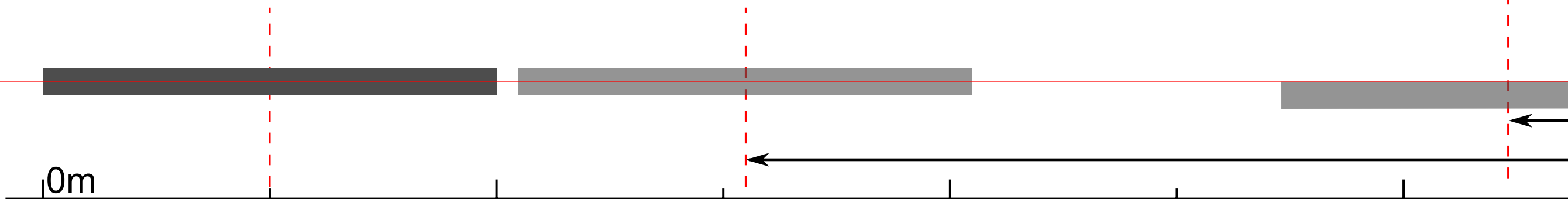
## SPB/SFX Optical Layout

MHP, 4mrad

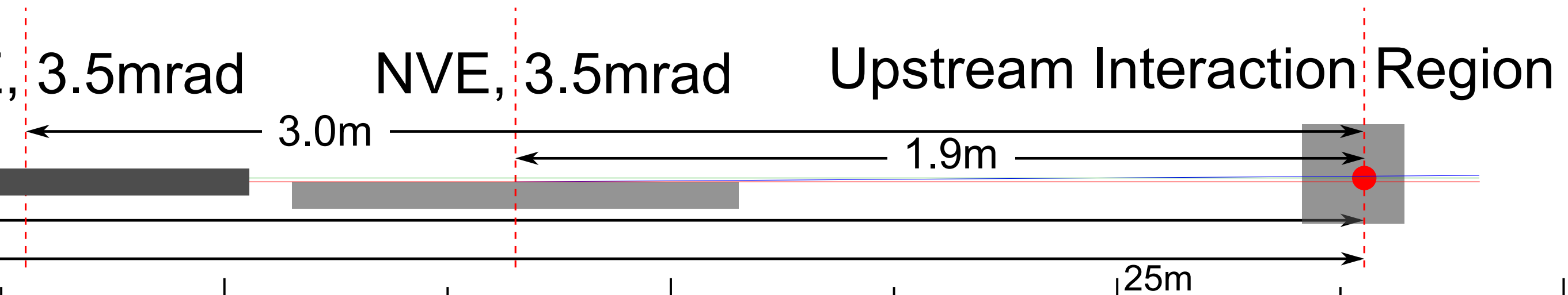
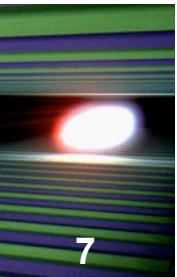
MHE, 4mrad



MVE, 4mrad

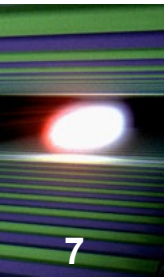


# Optical considerations





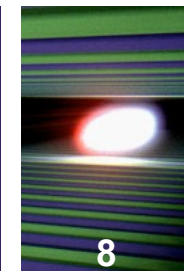
# Optical considerations



**Short conclusion:**  
Our mirror optics are expected to survive as designed

**A. Aquila, et al, submitted**

# Mirrors and mechanics (with commercial partners)



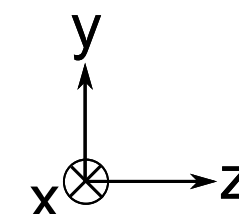
## ■ Key issues:

- Mirror stability (vibrational)
- Alignment procedure and spot characterisation

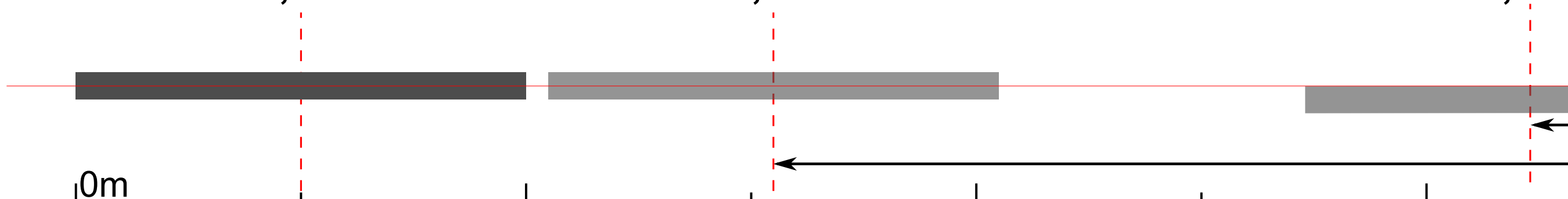
## SPB/SFX Optical Layout

MHP, 4mrad

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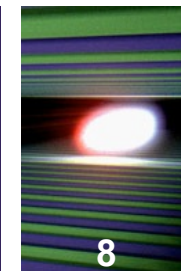


MVE, 4mrad



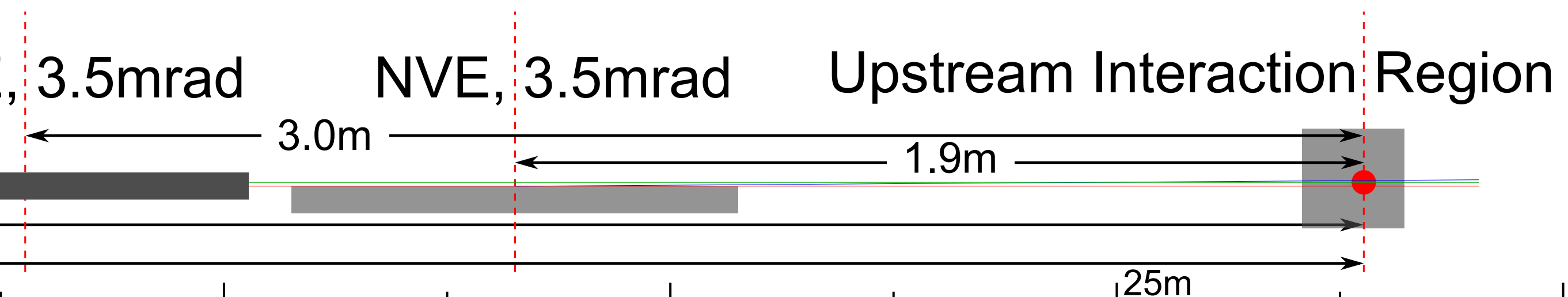


# Mirrors and mechanics (with commercial partners)

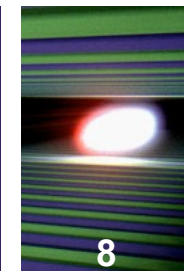


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# Mirrors and mechanics (with commercial partners)



## ■ Key issues:

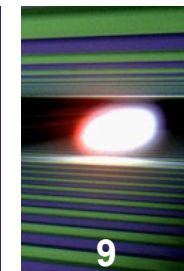
- Mirror stability (vibrational)
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## ■ Key progress:

- Continuous vibrational monitoring of experimental hall
  - Allows identification of vibrational noise sources
- Development of wavefront measurement techniques
  - Aids focal spot characterisation
- Vendor Finite Element Analysis of static and thermal



# Key progress 2014 – SFX Integration: Optics, sample delivery and detector



## ■ Optics

- CRL refocusing optics at advanced stage of design
- Design optimised for continuous photon energy coverage

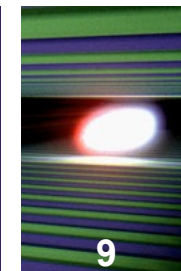
## ■ Sample delivery

- SFX sample delivery work package led by J. Schulz, XFEL
- Both sample environments will accommodate a number of sample delivery methods (allowing all to capitalise on the SFX UC's sample delivery expertise)

## ■ Detector: AGIPD 4Mpx

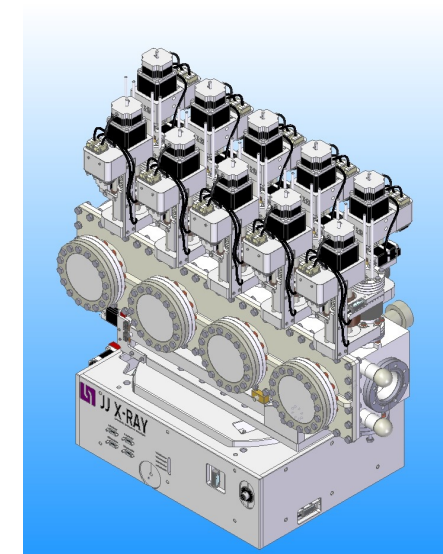
- Integration goals defined (sampling, resolution, etc)
- First steps to mechanical integration begun

# Key progress 2014 – SFX Integration: Optics, sample delivery and detector

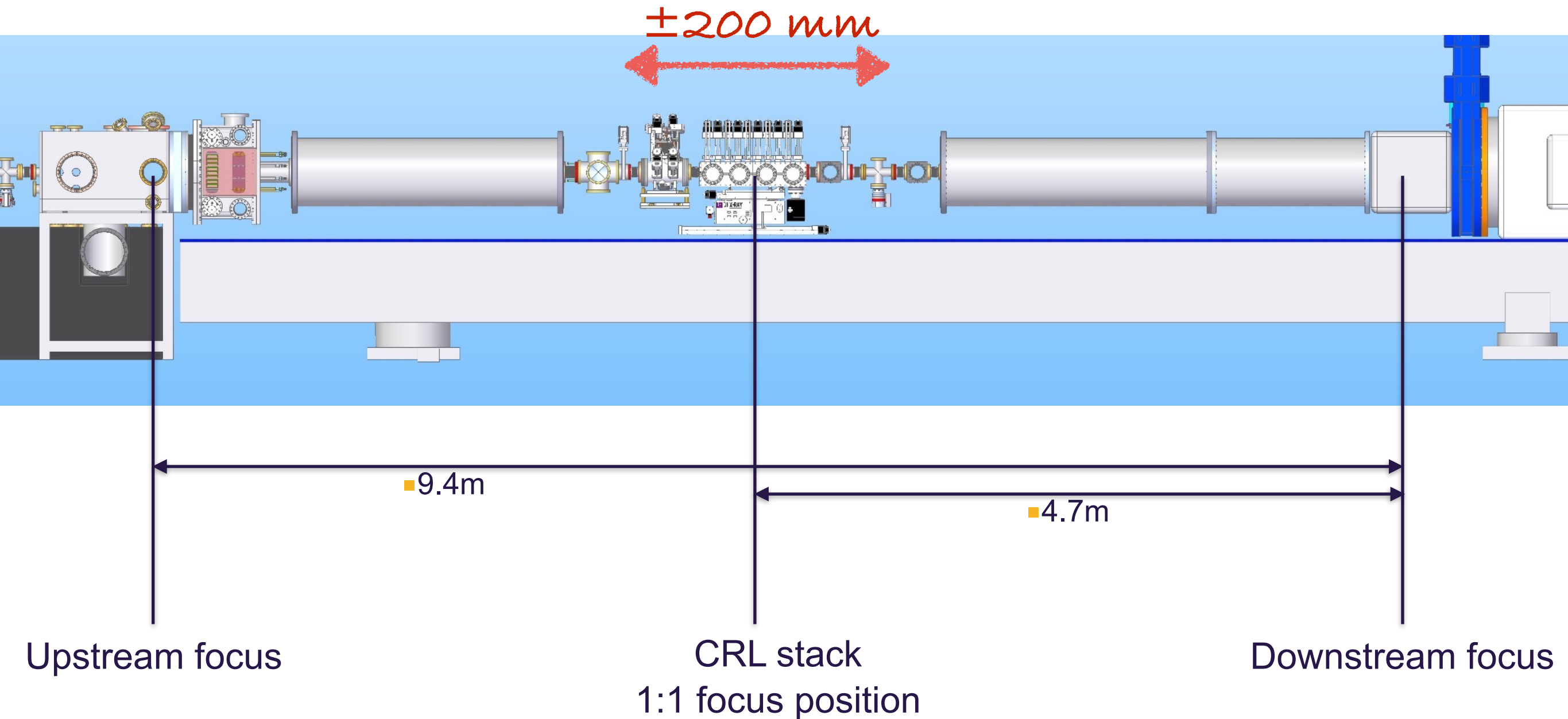
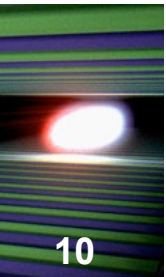


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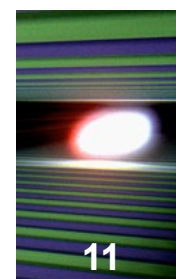


# Compound Refractive Lens Refocusing System

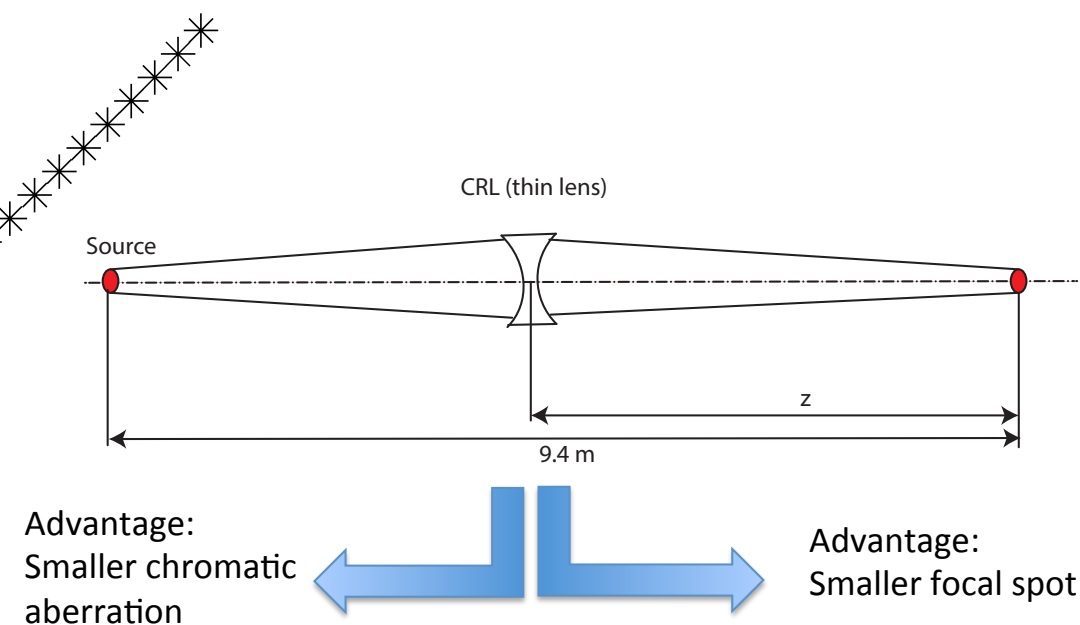
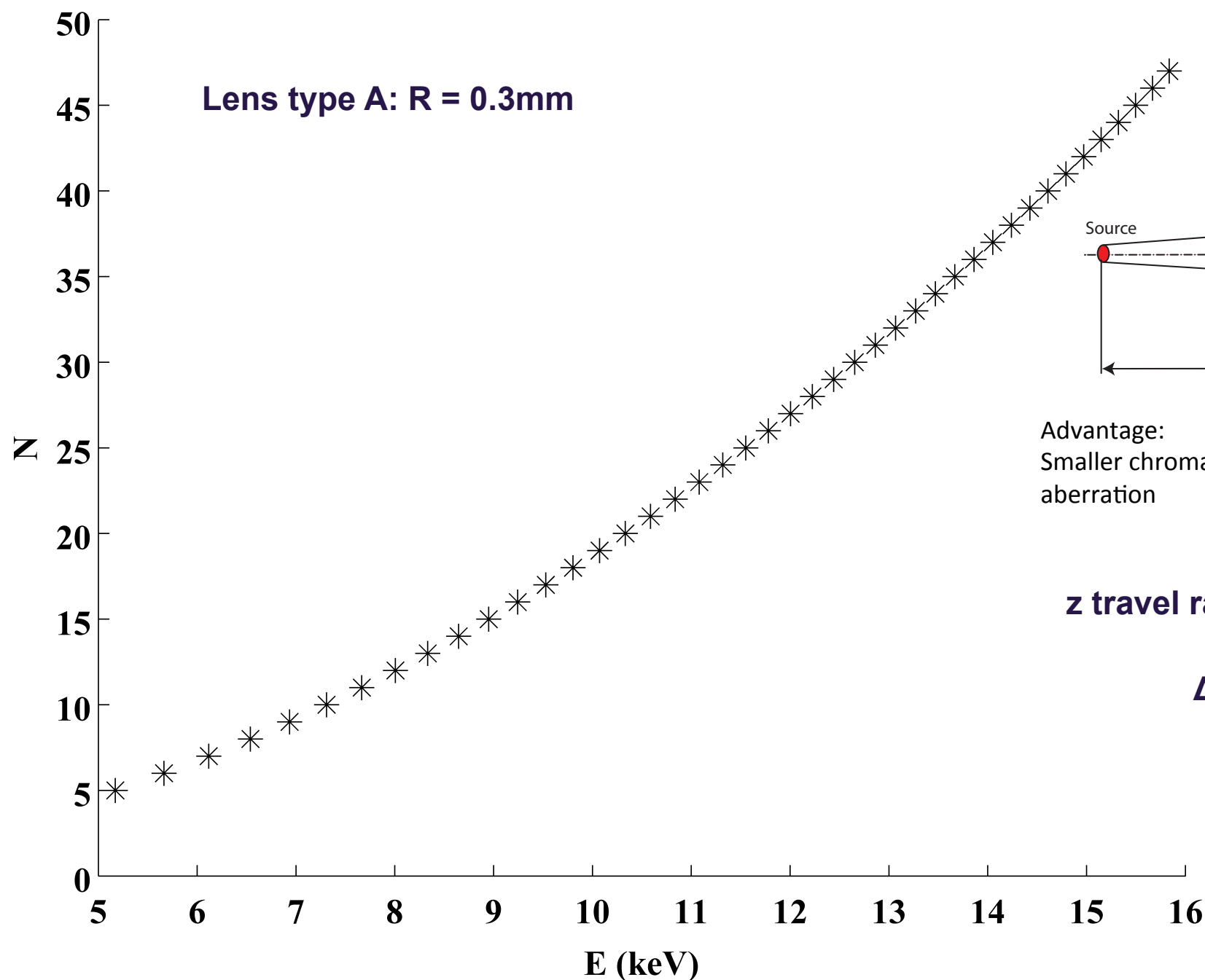


- Travel range limited to 400mm (without manual repositioning)

# Optimisation of CRL stack

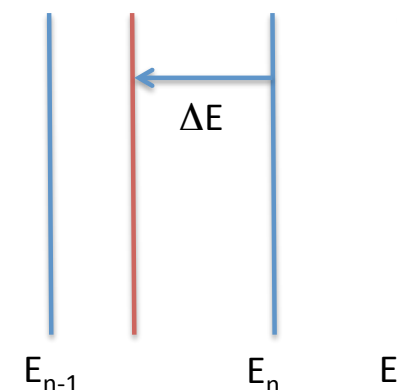


## Number of lenses vs photon energy, 1:1 geometry



**z travel range  $\Delta z = 400$  mm**

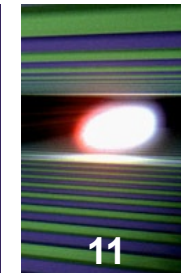
**$\Delta E$  ?**



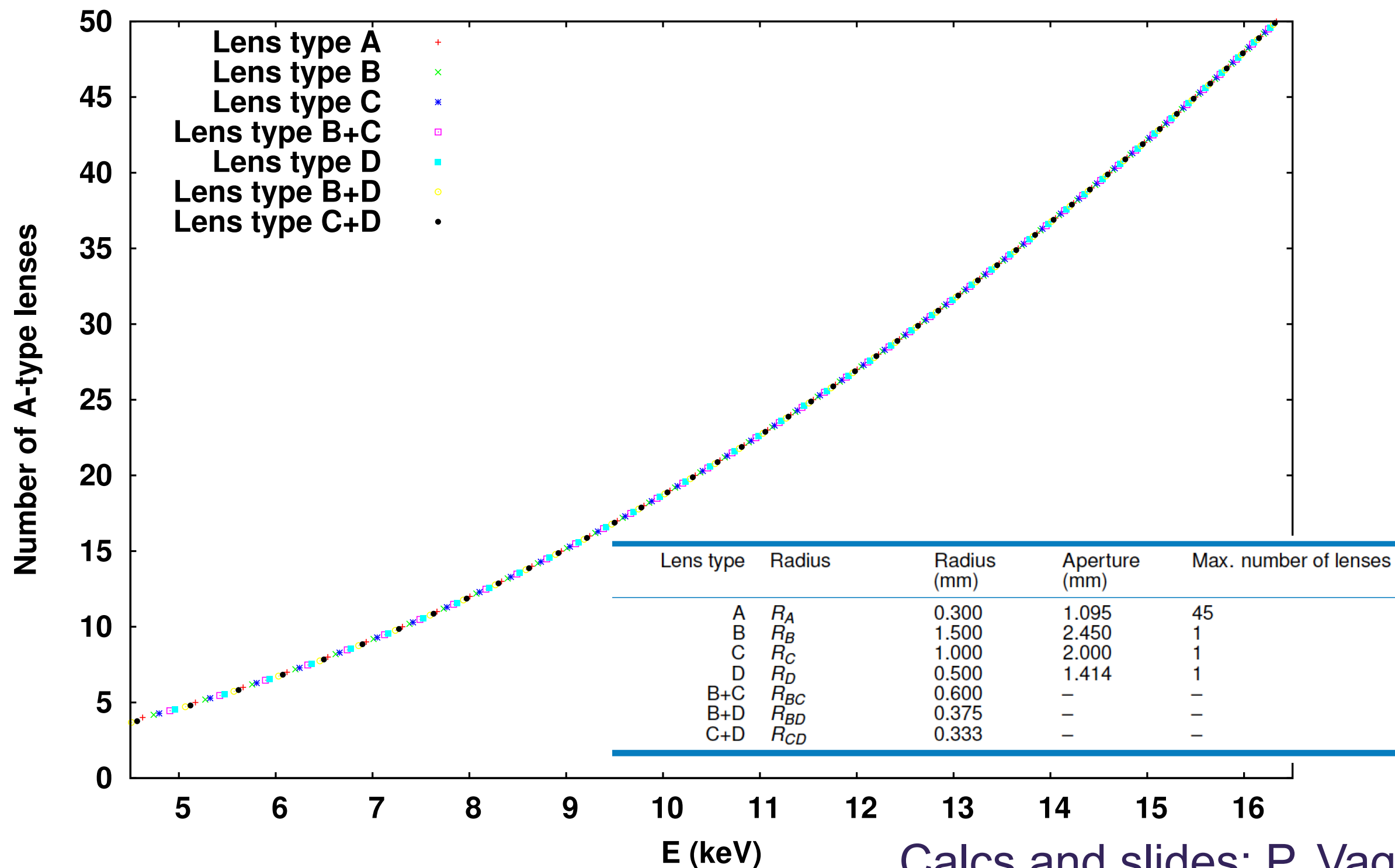
**Calcs and slides: P. Vagovič**



## Optimisation of CRL stack

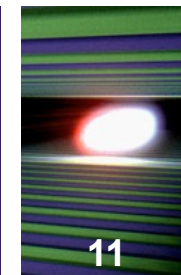


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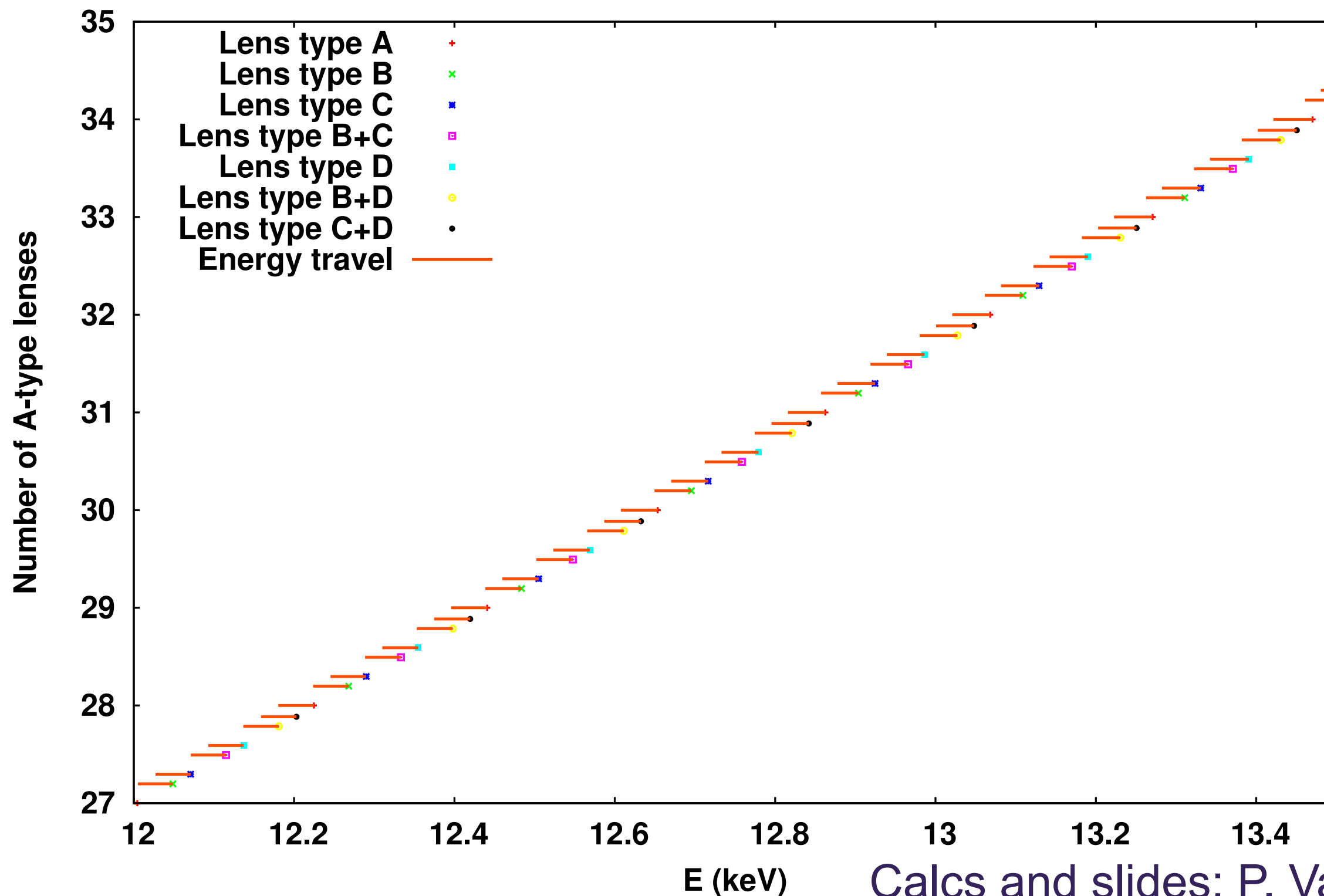
Energy points at  $z=4.7\text{m}$  with mixed A,B,C,D lenses

Calcs and slides: P. Vagovič

# Optimisation of CRL stack

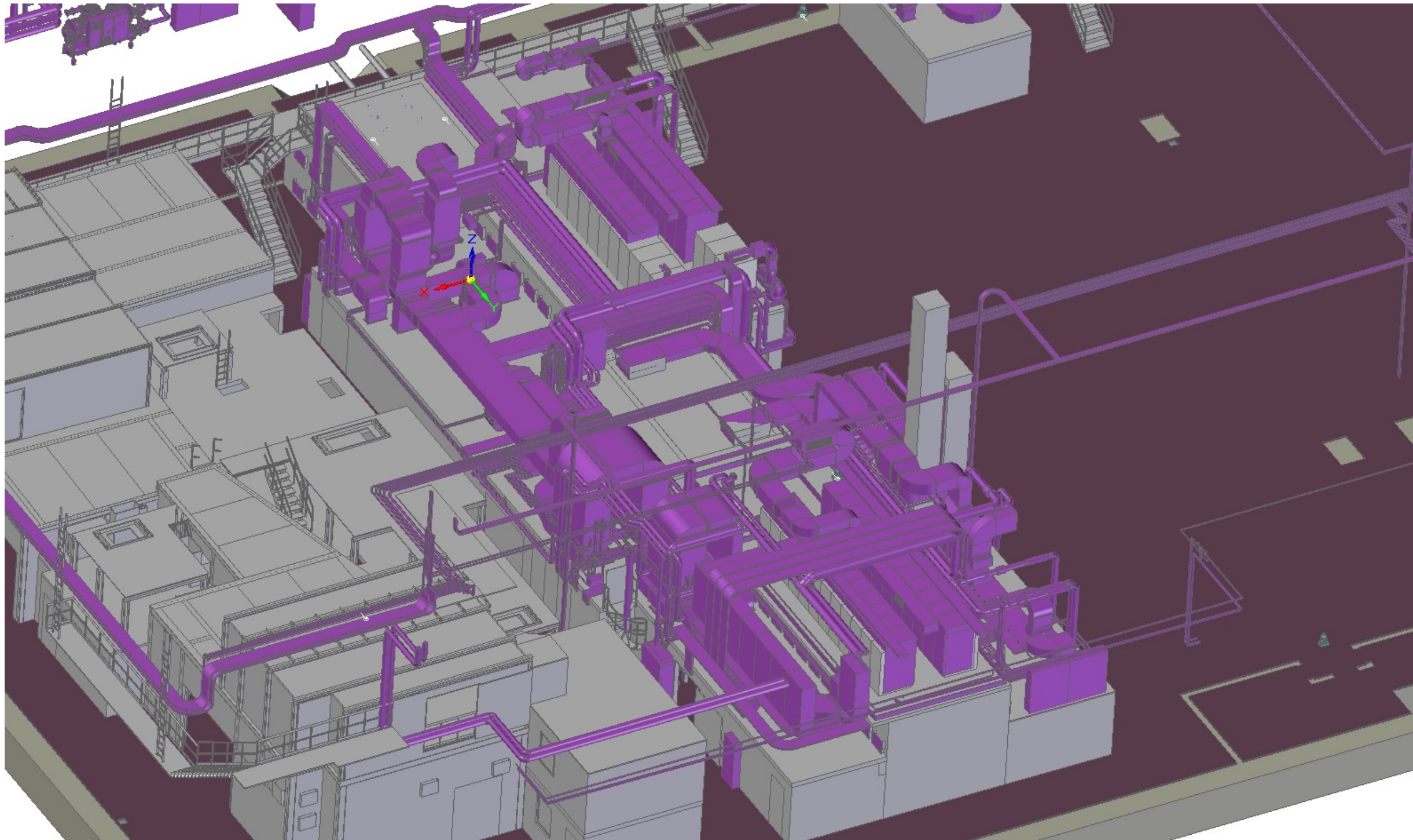
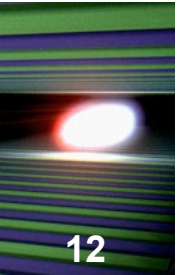


Energy points and travel range at  $z=4.7\text{m}$  with mixed A,B,C,D lenses



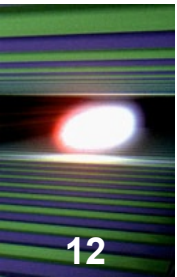
Calcs and slides: P. Vagovič

# Boring but important: Hutch and infrastructure

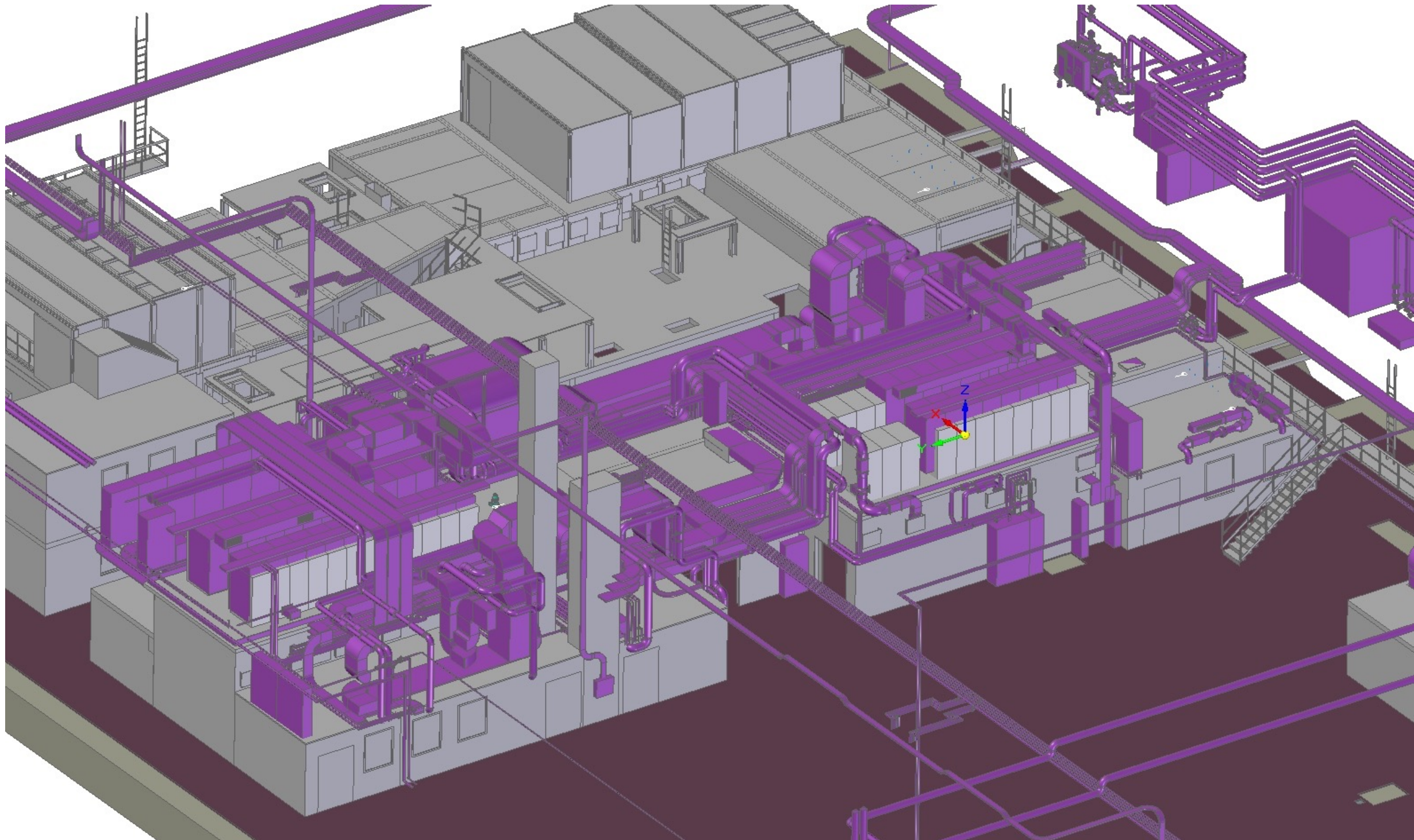




# Boring but important: Hutch and infrastructure



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and a whole lot more...



# Summary of the summary!

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- From 3–16 keV, SPB/SFX caters for:
  - Single particle imaging of  $< 100$  nm particles
  - Single particle imaging of  $< 1\mu\text{m}$  particles
  - Serial crystallography of small, sensitive or dynamic systems
- SFX UC contributed apparatus now incorporated at the conceptual level
  - CRL refocusing optics at advanced state of design
  - AGIPD 4Mpx integration goals defined
  - Sample delivery options – accommodate multiple efforts from the different UC partners
- Much progress on all instrumentation systems (and even more on the boring systems too!)

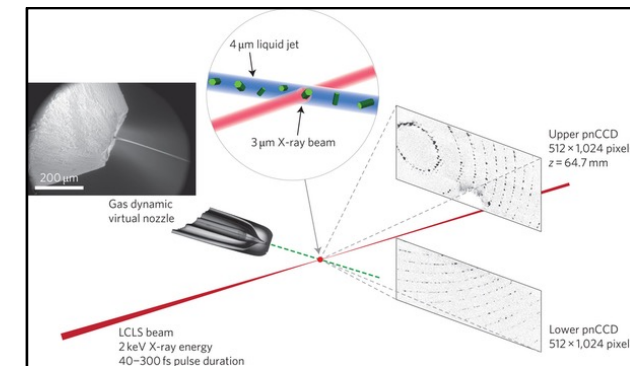
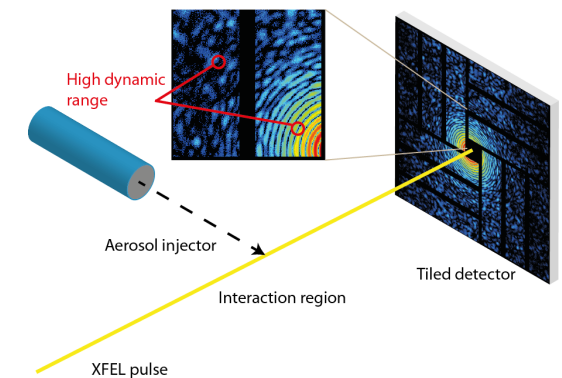
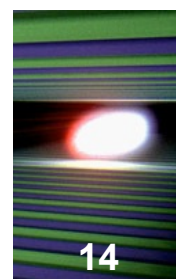


Image from: Barty, et al, Nature Photonics 6, 35–40 (2012)



# Do you want to know more?



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## There's much more to know:

- See on Friday:
  - Poster #2 – S. Stern, et al, SFX UC contributions
  - Poster #121 – R. Bean, et al, SPB/SFX Instrument

- Or anytime this week:
  - Talk to any of the team—at the posters, dinner, lunch, etc

## Or join the team: we're (soon) hiring!

- Scientists, engineers, and more...
- For more details contact: [adrian.mancuso@xfel.eu](mailto:adrian.mancuso@xfel.eu)



# SPB/SFX Instrument team

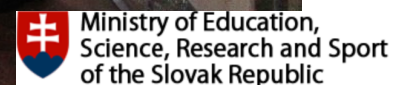
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## ■ SPB/SFX

- Richard Bean
- Gannon Borchers
- Klaus Giewekemeyer
- Masoud Mehrjoo
- Marc Messerschmidt  
(Sci computing)
- Nadja Reimers  
(Central Instruments  
Engineering)
- Stephan Stern
- Tokushi Sato
- Steffen Raabe
- Chun Hong Yoon
- Andrew Aquila  
(now at SLAC)



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](https://doi.org/10.3204/XFEL.EU/TR-2013-004)



Many thanks to Steve Readman for exceptional assistance with the project plan

