Production and Characterization of Hard X-rays Beyond 25 keV

Pushing forward technical frontiers at the European XFEL

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FLS 2023, Lucerne, Switzerland, August 28th 2023

European XFEL

DESY.

HELMHOLTZ

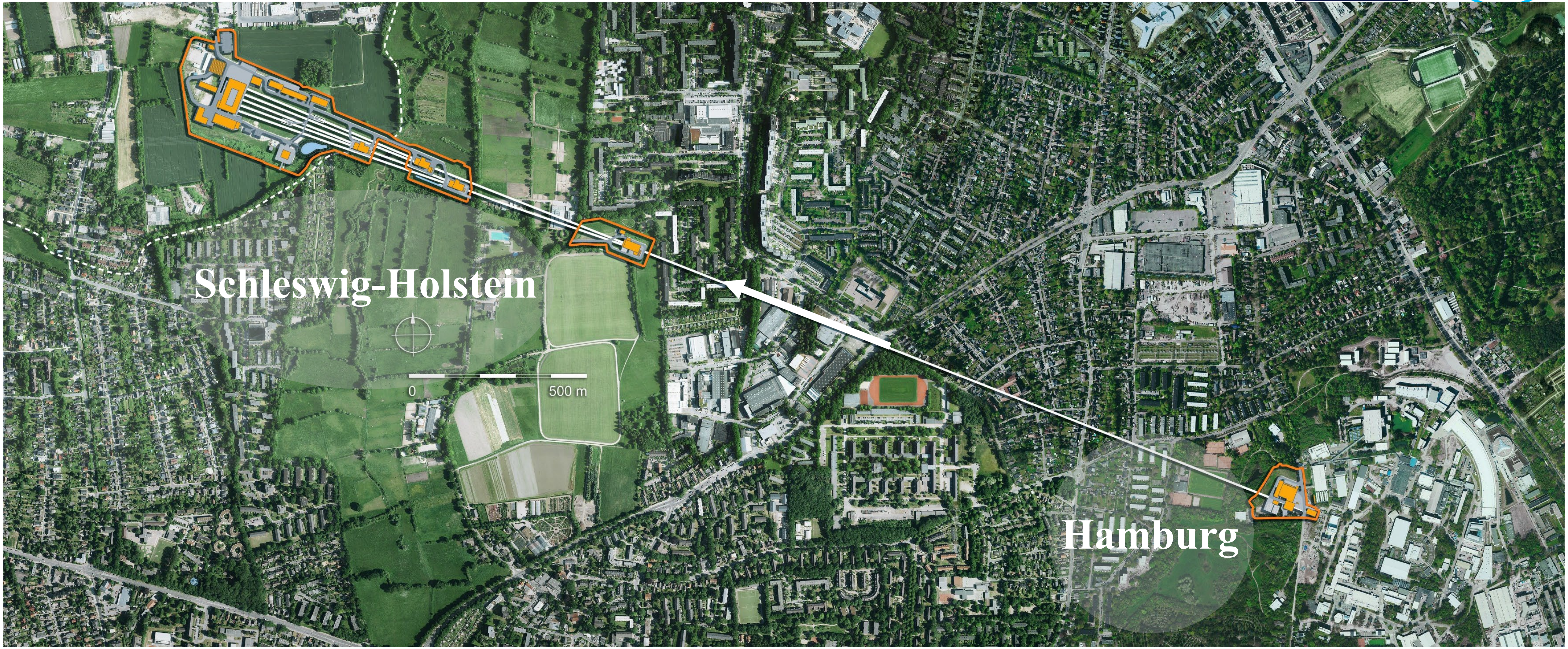
Outline

- ❑ Introduction
- ❑ Simulations
- ❑ First experiments
- ❑ Parallel R&D activities
- ❑ Summary

Introduction

European XFEL

W. Decking et al., Nature Photonics 14, 391–397 (2020)



Three SASE undulators

- Serving **7** experimental stations
- Two **175 m** Hard X-Ray beamlines **"SASE 1"** & **"SASE 2"**
- One soft X-Ray beamline **"SASE 3"**

Superconducting linac

- **10 Hz** burst mode with **600 µs** RF-pulses
- Up to **27000** pulses per second
- Up to **17.5 GeV** electron energy
- Flexible beam parameters & beam distribution

European XFEL surpassed the design photon energy by a factor of two

First light signal at 25 keV in 2020

News and Events > News

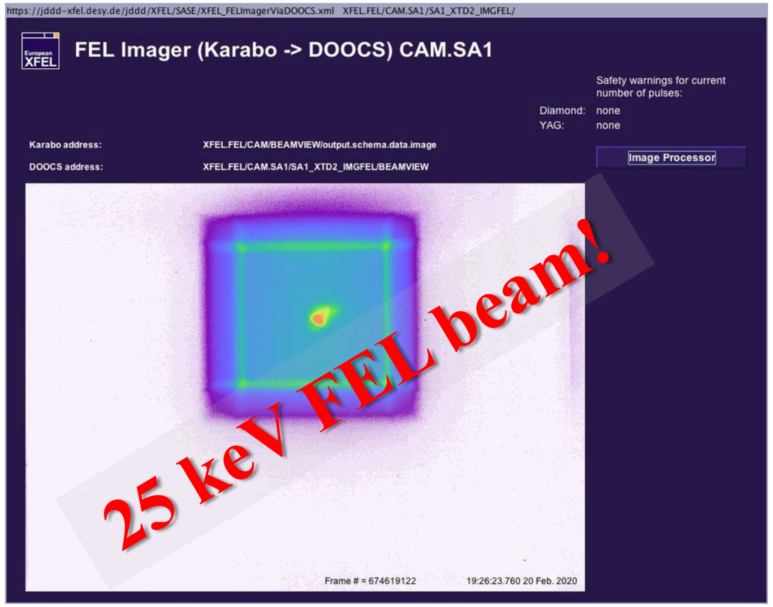
← Back

2020/04/08

European XFEL reaches world record photon energies

X-RAY LASER MAKES BIG STEP TOWARDS EXPERIMENTS AT VERY HIGH PHOTON ENERGIES

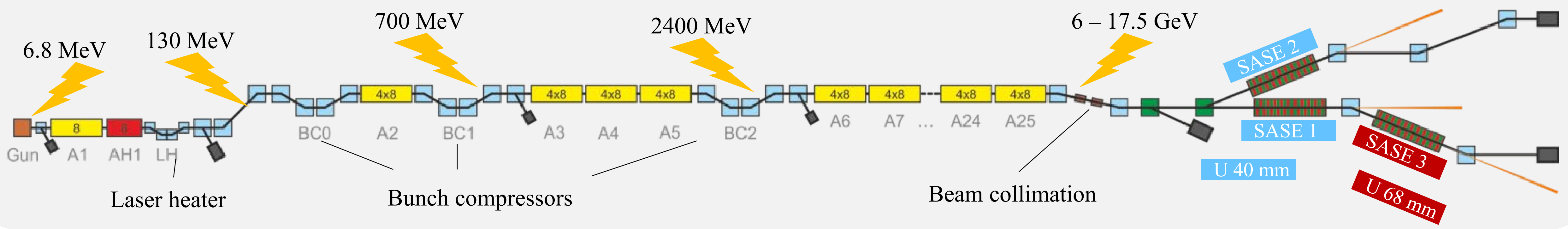
The availability of femtosecond pulses of hard X-rays at light source facilities such as European XFEL, opens up unprecedented scientific opportunities to probe matter and materials at the atomic scale at ultra-short timescales. With its unique capability to generate intense X-ray pulses at energies of 25 keV and beyond, the European XFEL is the only X-ray free-electron laser worldwide to enable the possibility to delve into unchartered worlds and study complex phenomena like never before.

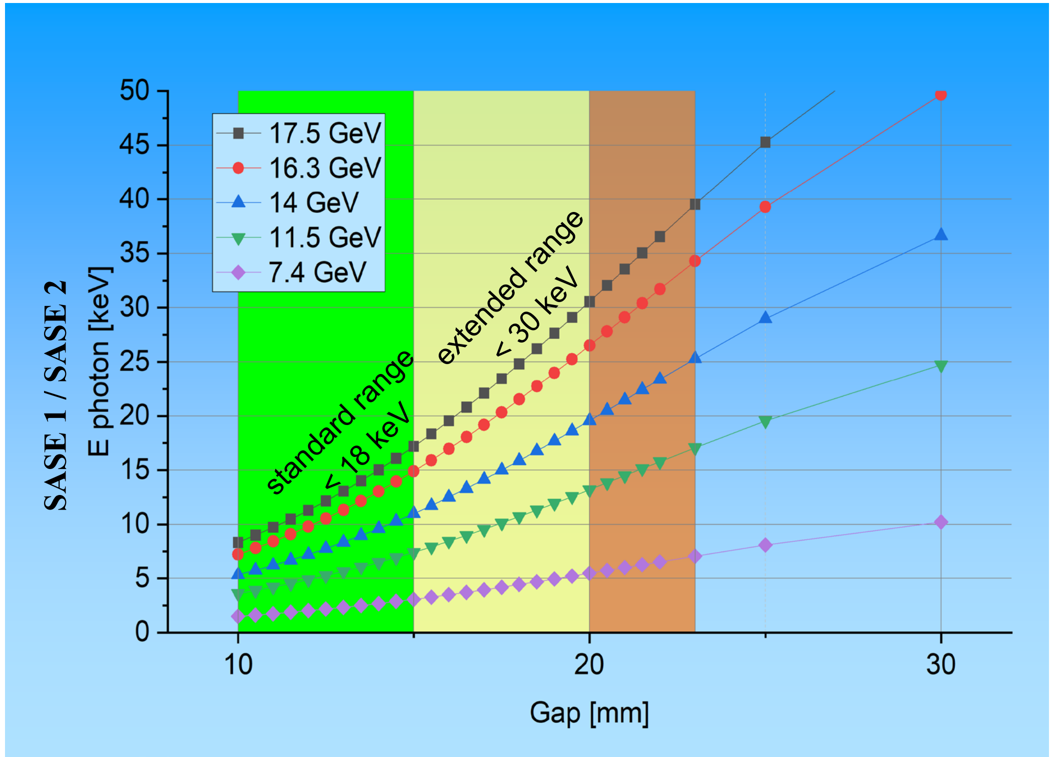


→ **Demonstrating unique capabilities of the facility in combining a high energy linac and long flexible undulators**

no dedicated SASE tuning; pulse energy on the level of tens of microjoules

Facility layout



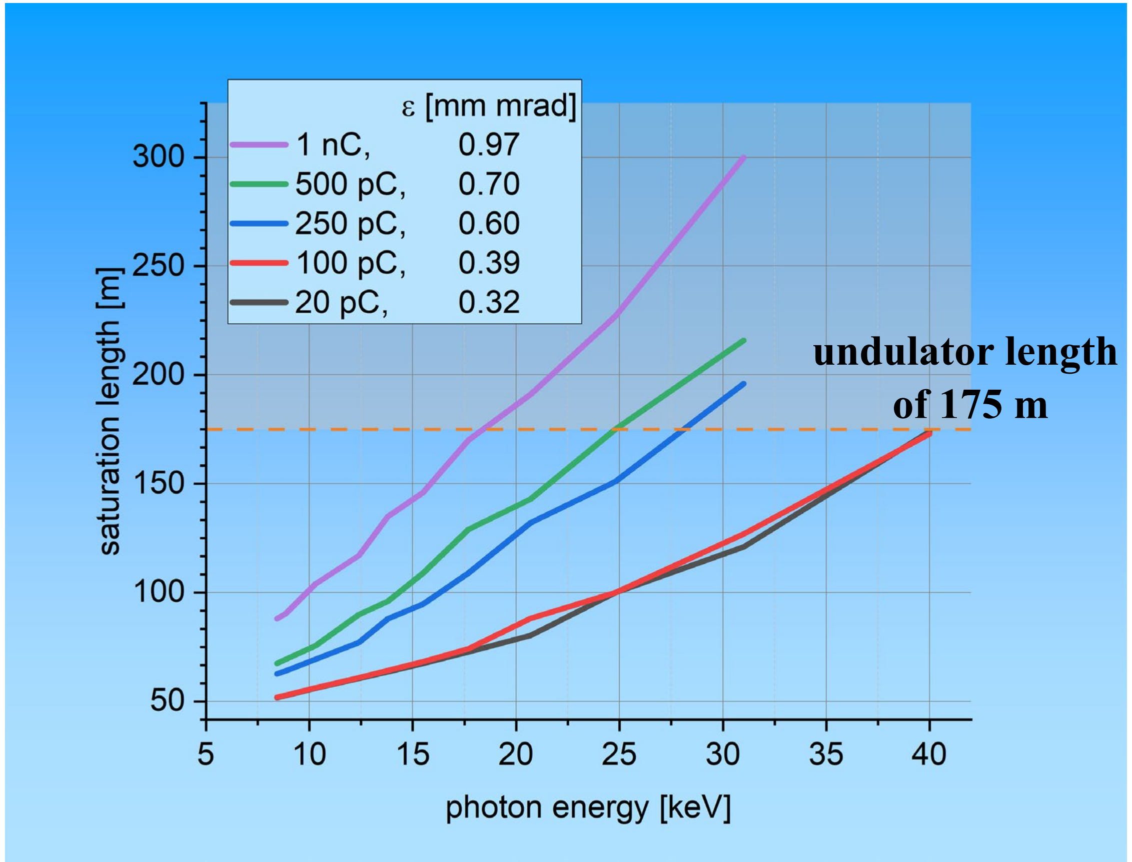


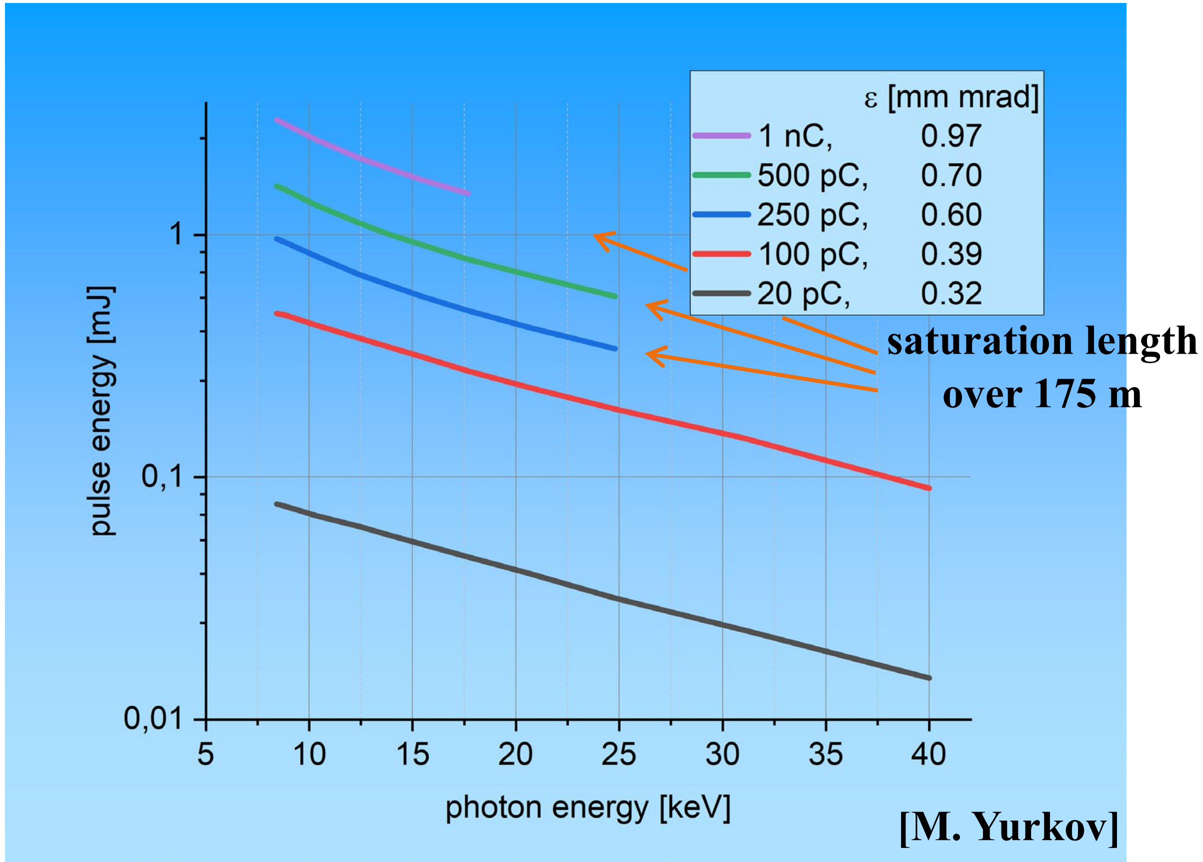
- **Photon energy range**

  (vs. electron energies vs. undulator gaps)
- **Routine operation covers up to 20 keV**
  - ❑ undulator gap < 15 mm, K > 2.5
  - ❑ straightforward SASE setup with shorter gain lengths and higher intensities

Facility capability

In combining a high energy linac and long flexible undulators

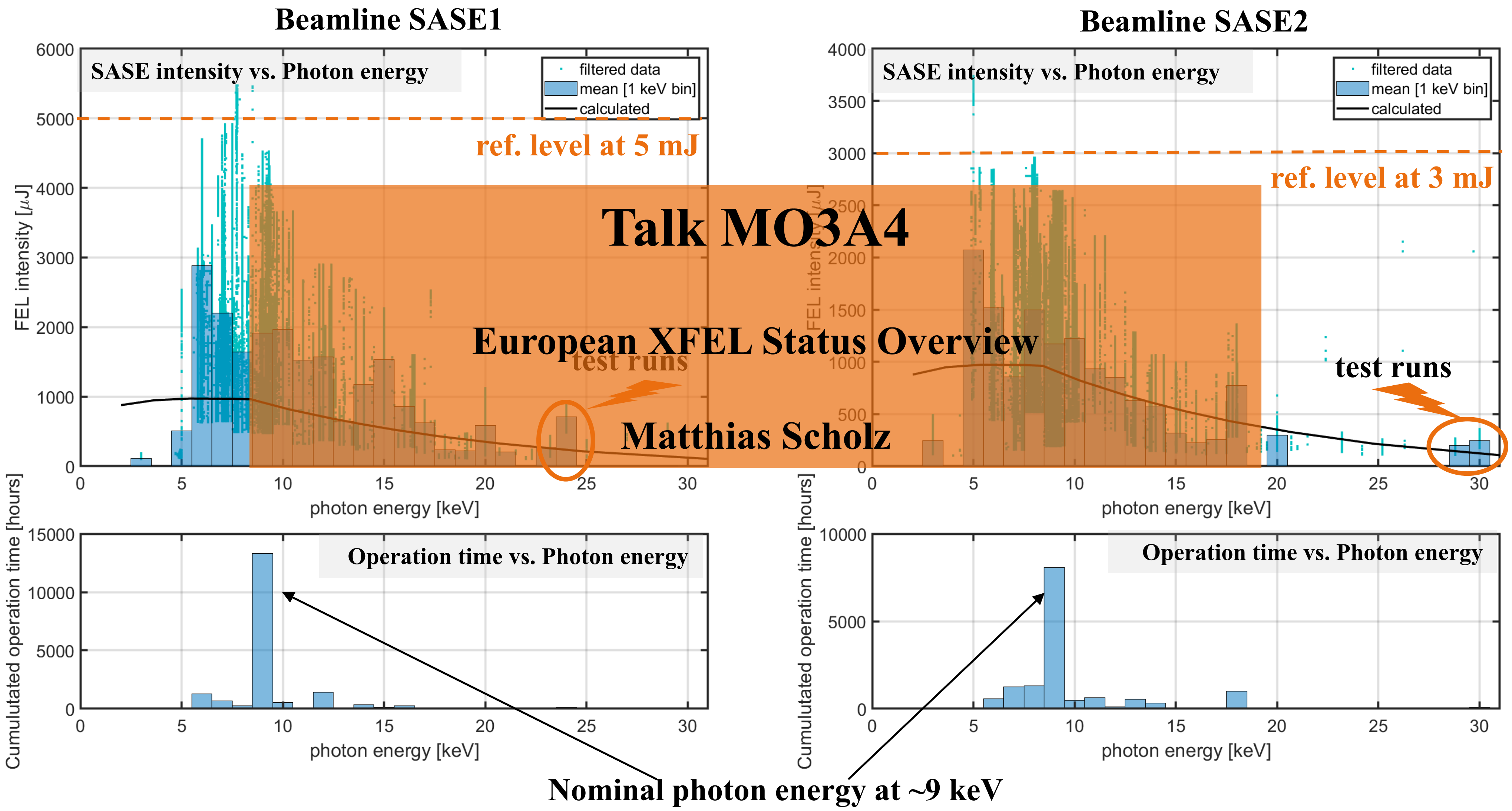




- ❑ Electron beam energy **17.5 GeV**
- ❑ Calculations with FAST until point of saturation using a bunch with **moderate emittance and energy spread**
- ❑ With post saturation taper significantly higher pulse energies can be reached

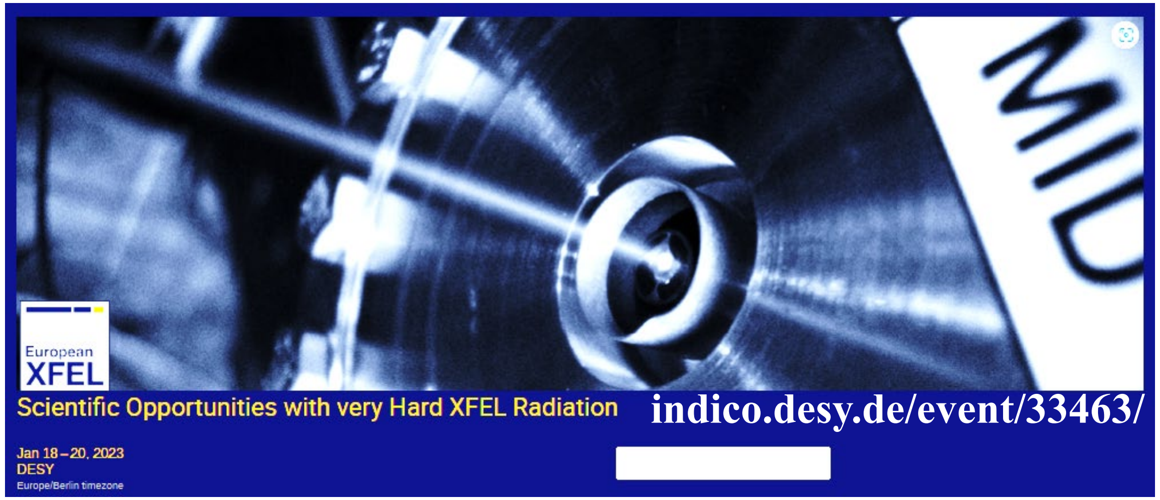
FEL performance at two hard X-ray beamlines

User-Requested photon energies & intensities reached during the last years



Scientific opportunities with very hard XFEL radiation

Advanced user-experiments driving facility developments



Workshop at the EuXFEL, January 2023:

Scientific Opportunities with very Hard XFEL Radiation

Workshop Sessions

- Applied Materials and Industrial Applications
- Structural Dynamics in Disordered Materials
- Enabling Techniques and Instrumentation for New Scientific Avenues
- Dynamics of Functional Materials
- High Pressure, Planetary Science and Geology, Electron Dynamics, Warm Dense Matter, Relativistic Laser Plasma, Strong Field Science

Advantages of using very hard X-rays

Users' Vision

- **high Q-range coverage**: larger momentum transfer at moderate scattering angles (> 40 keV)
- **high penetration**: larger penetration depth for bulk sensitivity
- **access to K-edge spectroscopy of high-Z materials**: enabling tracking of chemical dynamics for high-Z materials and for high-Z materials under extreme (hot, high pressure) conditions.

Experiments may benefit more from FEL characteristics compared to storage ring sources:

- ❑ large coherence: better contrast, phase measurements
- ❑ short pulses (~fs): single shot imaging, freezing of dynamic processes (dynamic laser compression, ultra cold liquids, …)
- ❑ variable pump-probe delay from few fs to ms
- ❑ higher brightness – small bandwidth

Intermediate Summary

- **Producing X-rays at 25+ keV** in the fundamental is **difficult** (beyond routine operation at the EuXFEL)
- **Delivering such X-rays** with decent intensities to the users is **challenging**
- **Scientific opportunities** towards using harder X-rays **calling for** FEL **facility developments**
- Dedicated **R&D activities** thus **strongly motivated**

Simulations

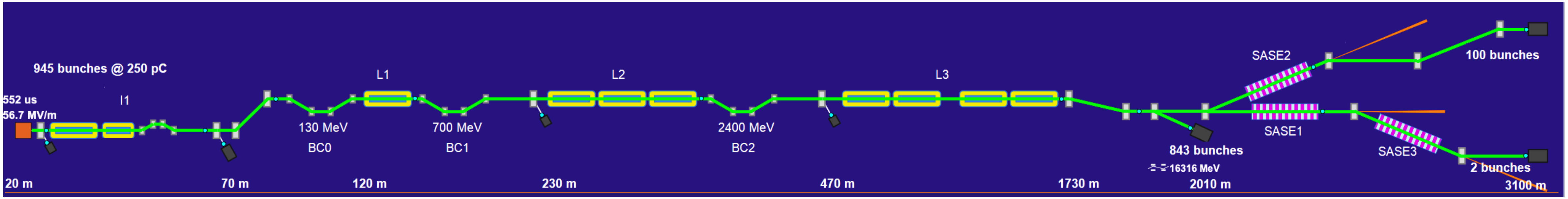
Working point at 250 pC

Using parameters very-close-to those of the EuXFEL

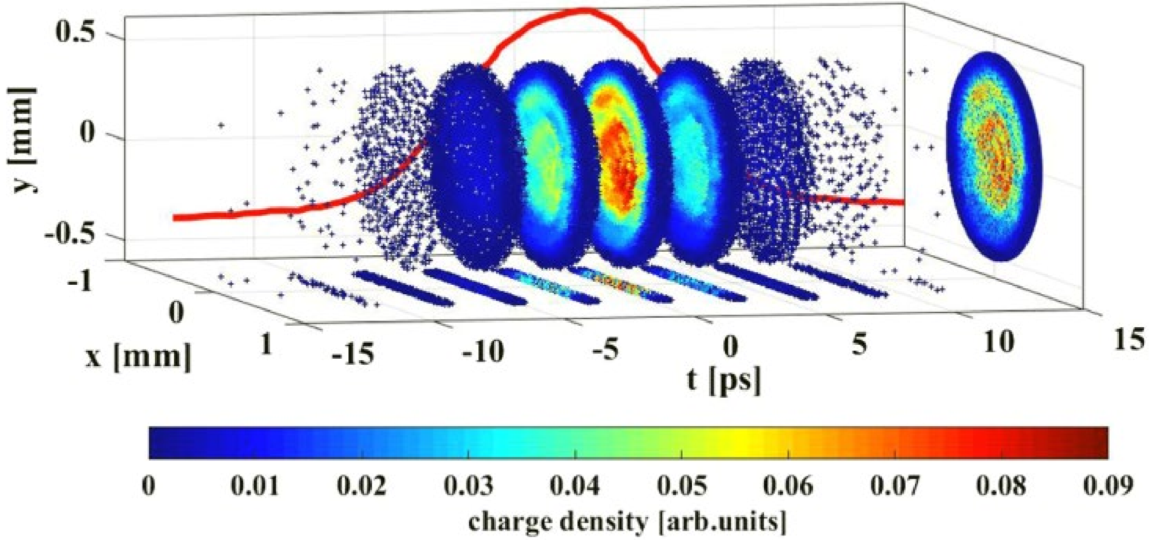
Exploring FEL performance by beam physics simulations

Electron bunch generation at cathode via photoemission modeling

Overall simulation layout



3D modeling of an electron bunch produced at photocathode



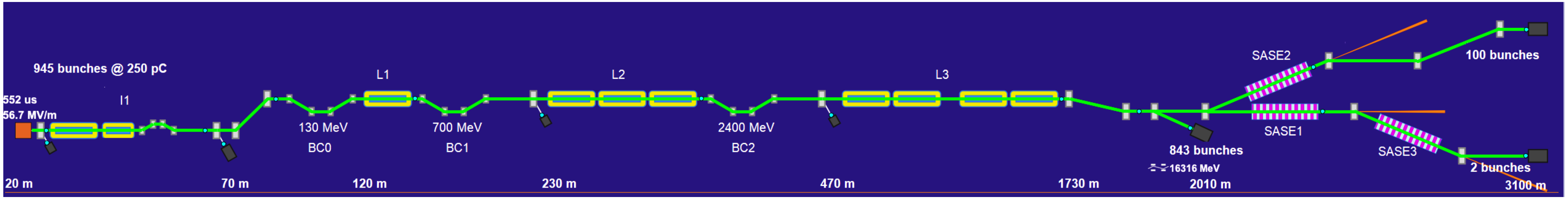
- ❑ more realistic **3D electron bunch generation at the cathode** based on photoemission modeling
- ❑ **using measured cathode** quantum-efficiency **(QE) map** & **measured** transverse and temporal **distributions of the** drive **laser** pulse

PRAB 23, 044201 (2020)

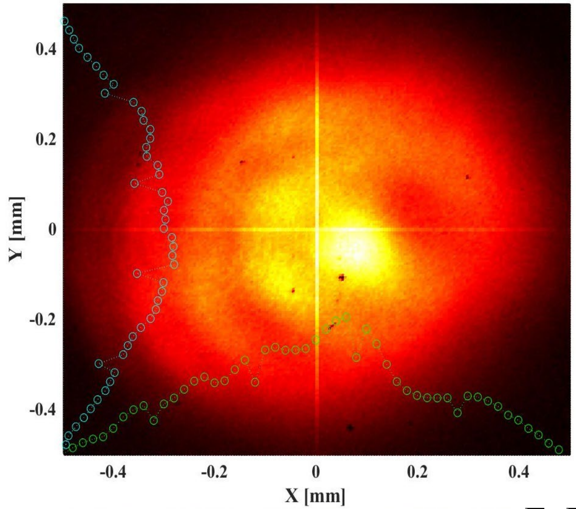
Exploring FEL performance by beam physics simulations

Bunch quality delivered by the injector using ASTRA & KRACK[3]

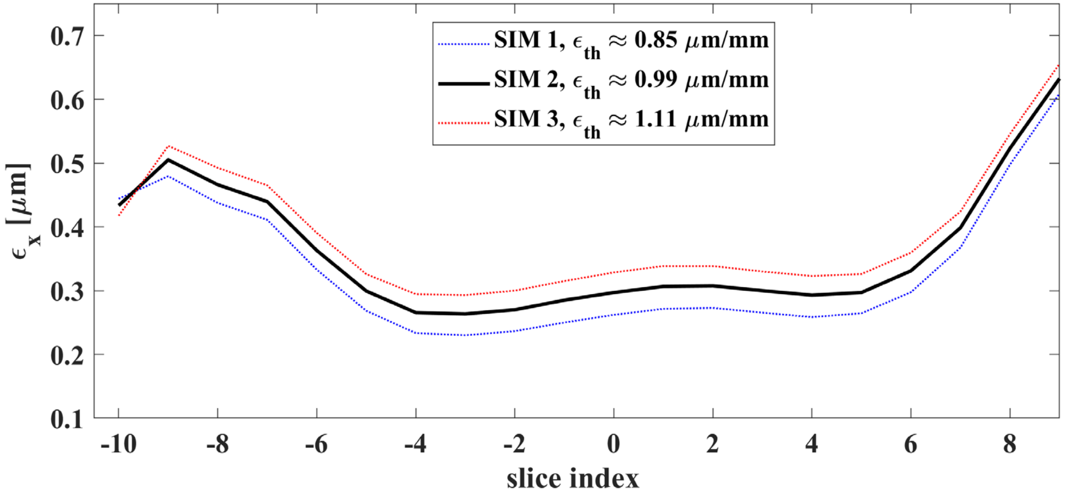
Overall simulation layout



Measured transverse laser profile
as used in the simulations



~0.3 µm overall emittance (central slice) **at injector exit**
for a measured thermal emittance of about 0.99 µm/mm

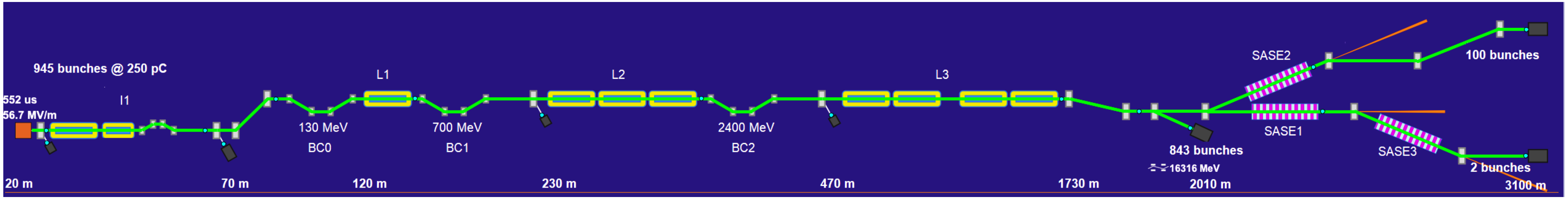


E. Prat et al. PRL 123, 234801 (2019)   P.W. Huang et al. PRAB 23, 043401 (2020)

Exploring FEL performance by beam physics simulations

Electron bunch tracking through the linac including collective effects in OCELOT

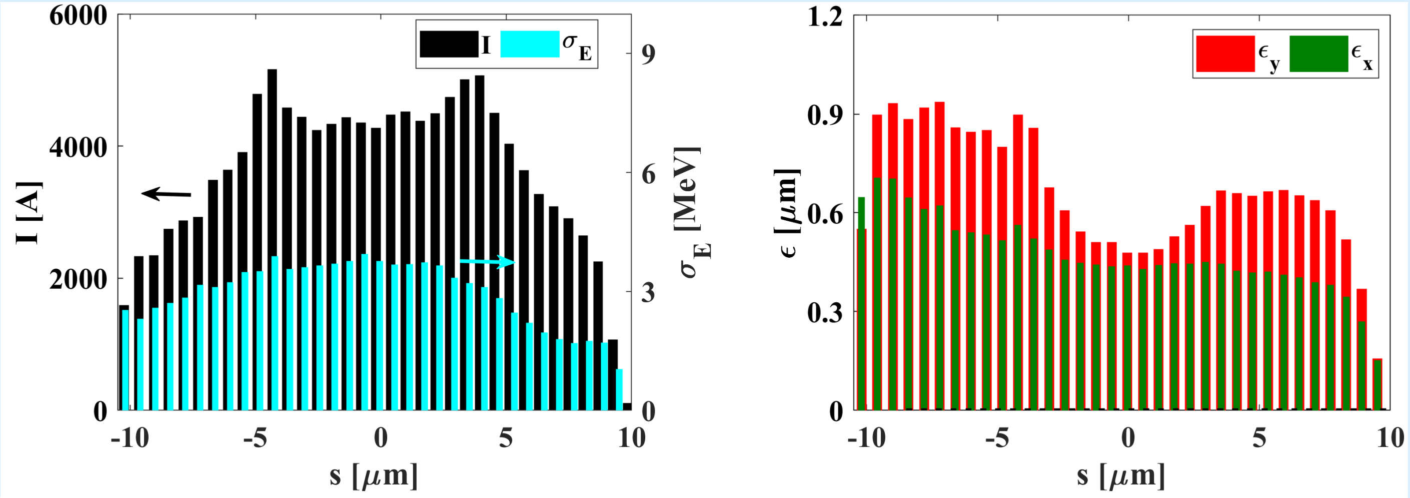
Overall simulation layout



Parameter	Value	Unit
Bunch charge	250	pC
Bunch shaping aperture	1.0	mm
Cathode laser pulse shape	Gauss	n/a
Cathode laser pulse length	3.0	ps
Cathode accelerating gradient	56.7	MV/m
Beam energy at BC0	130	MeV
Beam energy at BC1	700	MeV
Beam energy at BC2	2400	MeV
Beam energy downstream L3	16300	MeV
R56 at BC0	-50	mm
R56 at BC1	-50	mm
R56 at BC2	-30	mm
Undulator period[4]	4	cm
Undulator length	175	m

Bunch quality in front of undulators

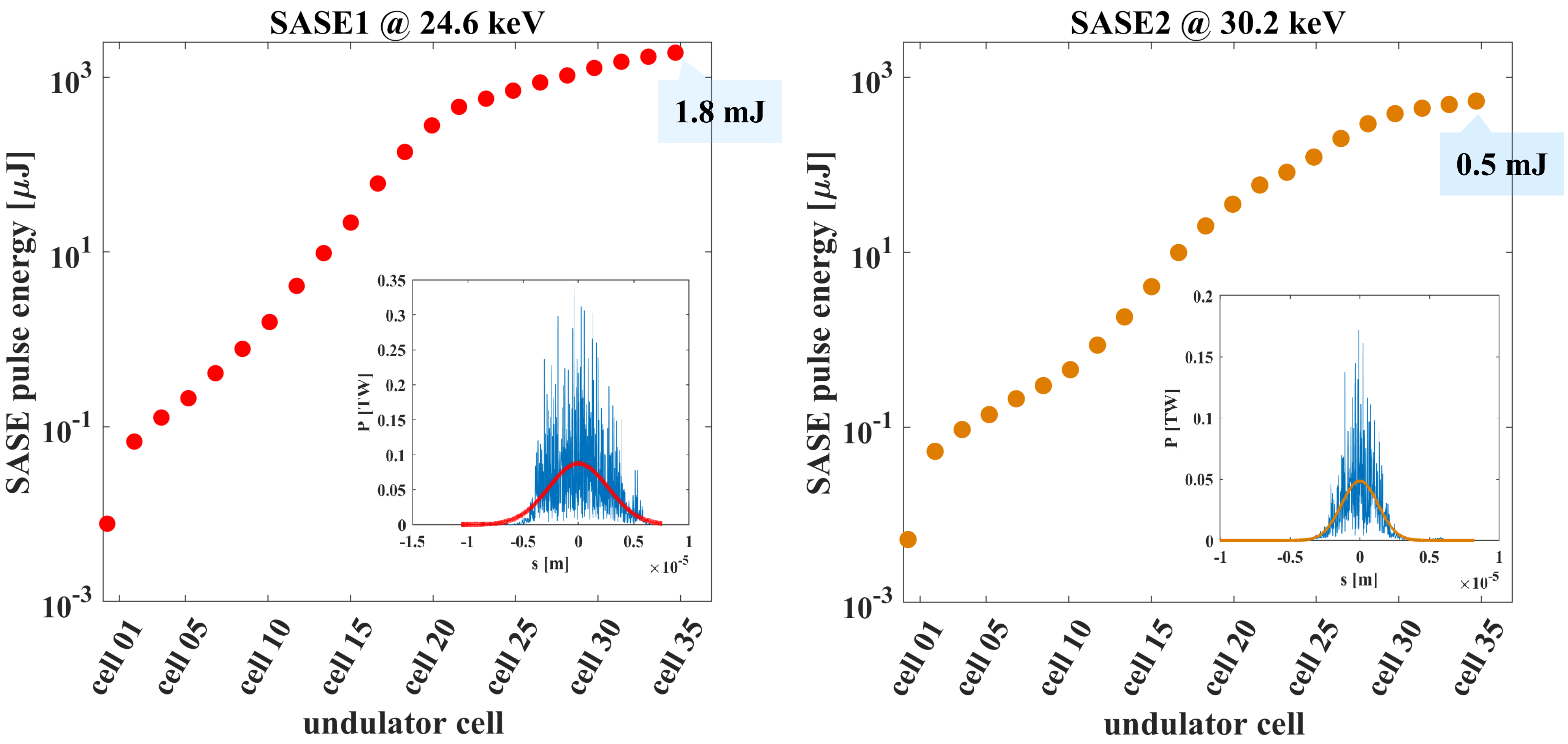
~4.5 kA peak current **~3.5 MeV** energy spread **~0.6 µm** emittance



3D space-charge, wake fields & CSR effects included in the simulation, as in PRAB 22, 024401 (2019)

Optimized SASE performance at 24 keV & 30 keV

Genesis simulations for SASE1 at 24 keV & SASE2 at 30 keV



Simulated SASE intensities at 24.58 keV (left) and 30.24 keV (right) for beamlines SASE1 and SASE2.
Linear & quadratic tapers optimized; No alignment error considered.

Working point at 100 pC

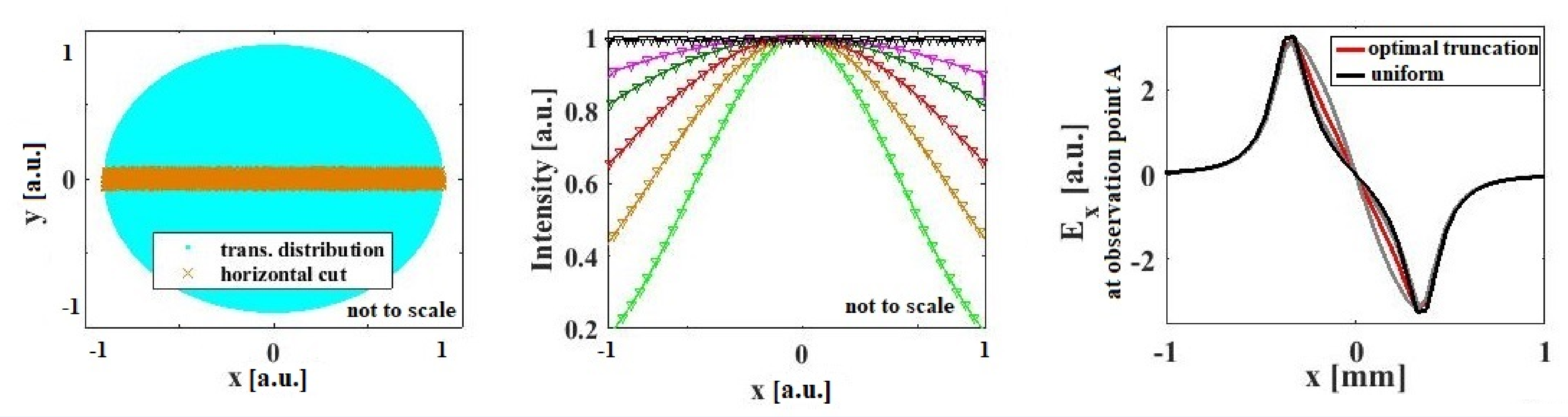
Emittance optimization via transverse laser pulse shaping at photocathode

Improving SASE performance by injector emittance optimization

Simulation Study: using an optimized transverse cathode drive laser pulse shape

- **Reducing space-charge contribution to overall emittance** via linearizing transverse space-charge force at cathode
- Similar ideas **verified,** for example, in M. Groß et al. TUPTS012, IPAC'19 & F. Zhou et al. PRAB 15, 090701 (2012)
- **Optimization** by searching for an optimal intensity ratio between center & edge of a truncated gaussian distribution

Optimization of a transverse Gaussian cathode drive laser distribution by adjusting the truncation ratio



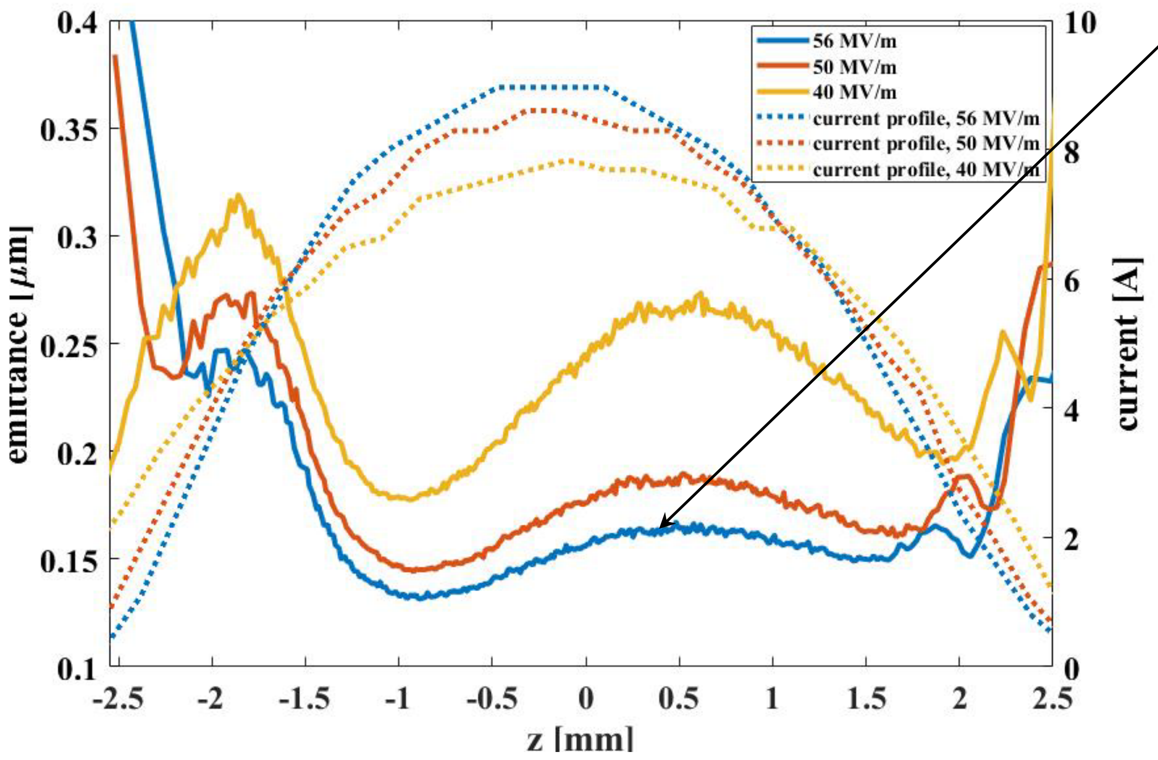
→ an optimal ratio of about 0.65 found and used in further simulations

→ still to be implemented in the cathode laser system

Improving SASE performance by injector emittance optimization

Simulation Study: optimized bunch quality in the injector

Accelerating gradients of 40, 50, 56 MV/m at cathode considered for 100 pC

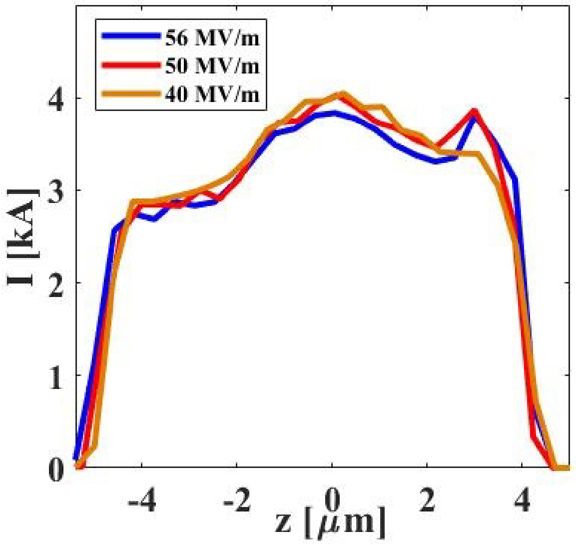


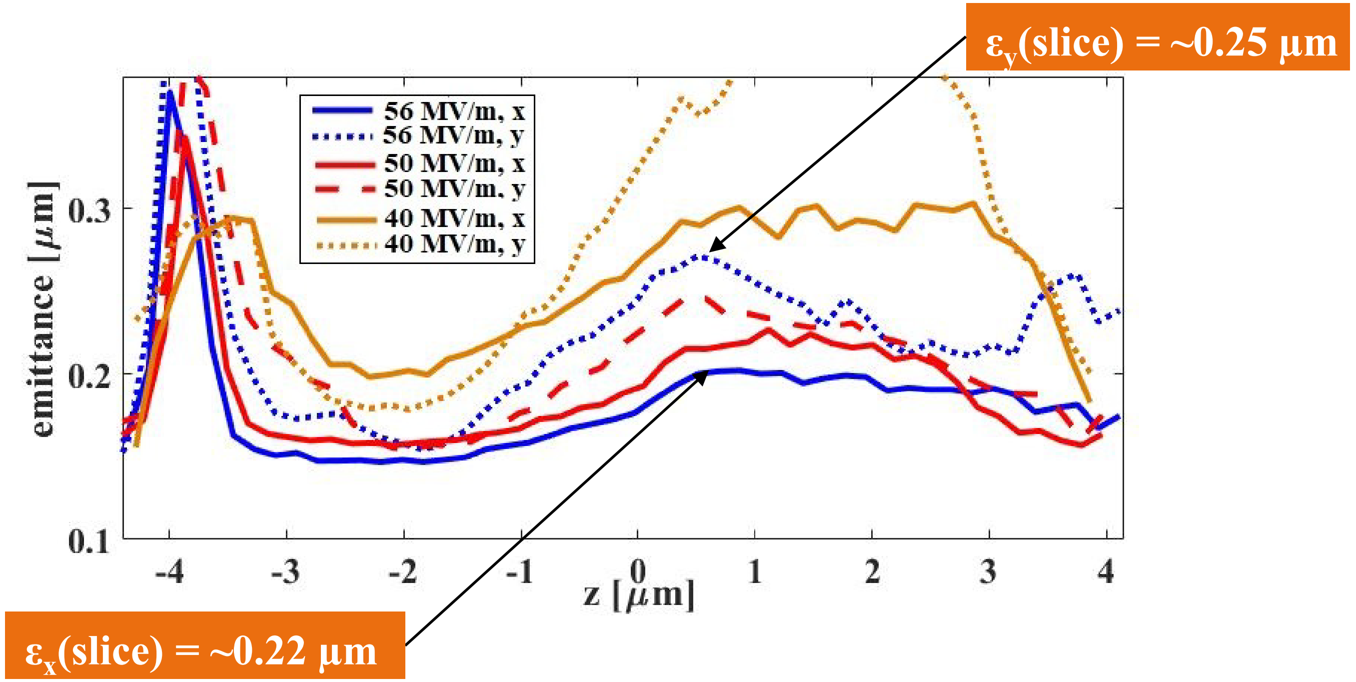
ε(slice) = ~0.16 μm at 56 MV/m

→ with optimized transverse cathode laser shapes significantly reduced emittances can be achieved

Improving SASE performance by injector emittance optimization

Simulation Study: tracking the bunch through the whole linac with collective effects on

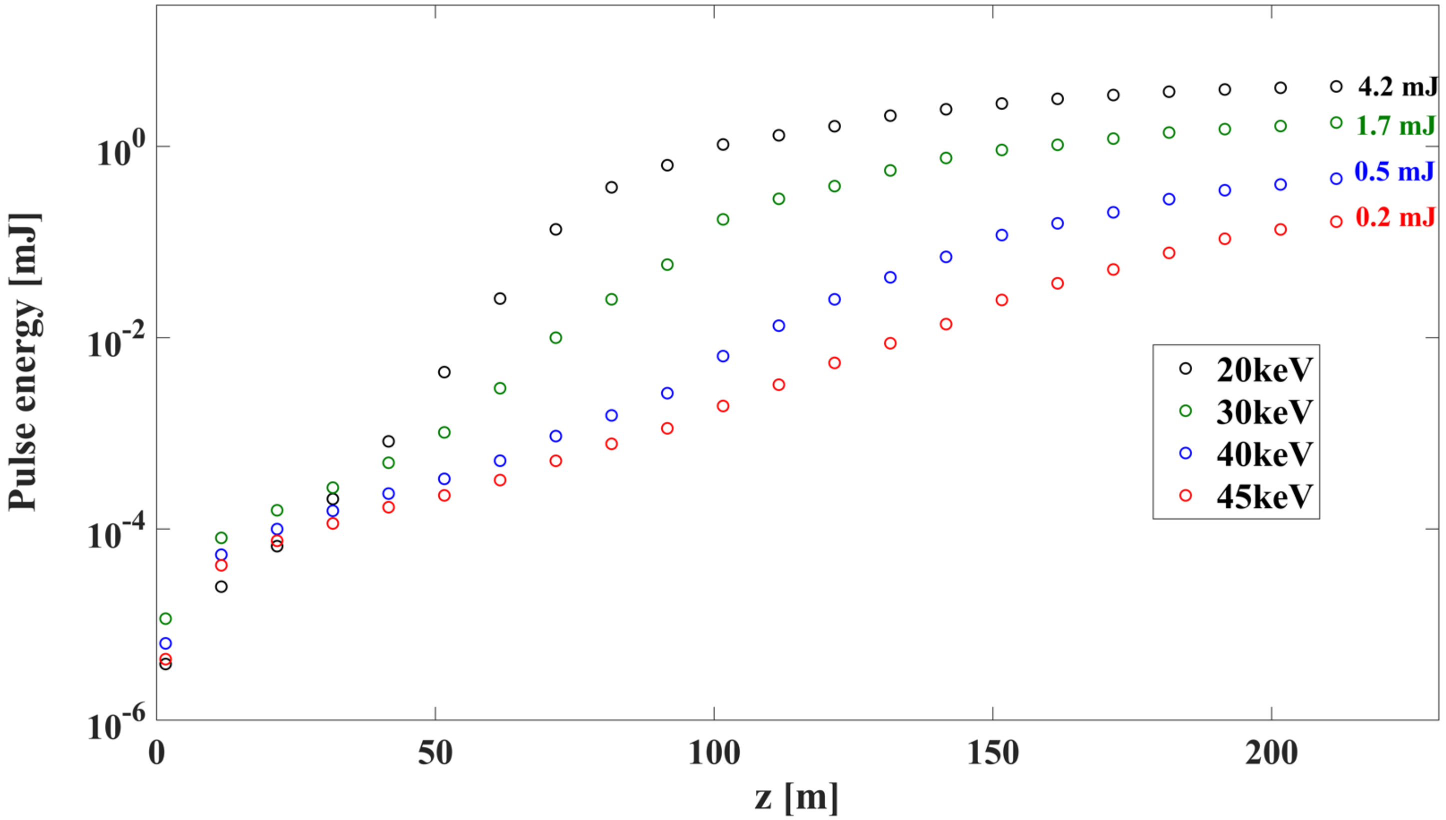




Improving SASE performance by injector emittance optimization

Simulation Study: optimized SASE performance via further emittance optimization in the injector

Simulated intensities assuming a low emittance beam with medium energy spread and perfectly aligned undulator sections



Photon energy	Wave length	Power / pulse
20 keV	0.62 Å	4.2 mJ
30 keV	0.41 Å	1.7 mJ
40 keV	0.31 Å	0.5 mJ
45 keV	0.28 Å	0.2 mJ

Electron energy	17.5 GeV
Bunch charge	100 pC
Emittance	0.25 µm
Cathode gradient	56 MV/m
Energy spread	2.5 MeV
35 cells with 5 m undulators	

Intermediate Summary: Simulations

- Nominal case at 250 pC suggests **mJ-level lasing at 24 keV** and **half mJ-level lasing at 30 keV**
- Study case at 100 pC takes advantage of **emittance optimization via transverse laser pulse shaping**, boosting the lasing performance at 30 keV up to 1.7 mJ and 0.2 mJ at 45 keV

Experiments

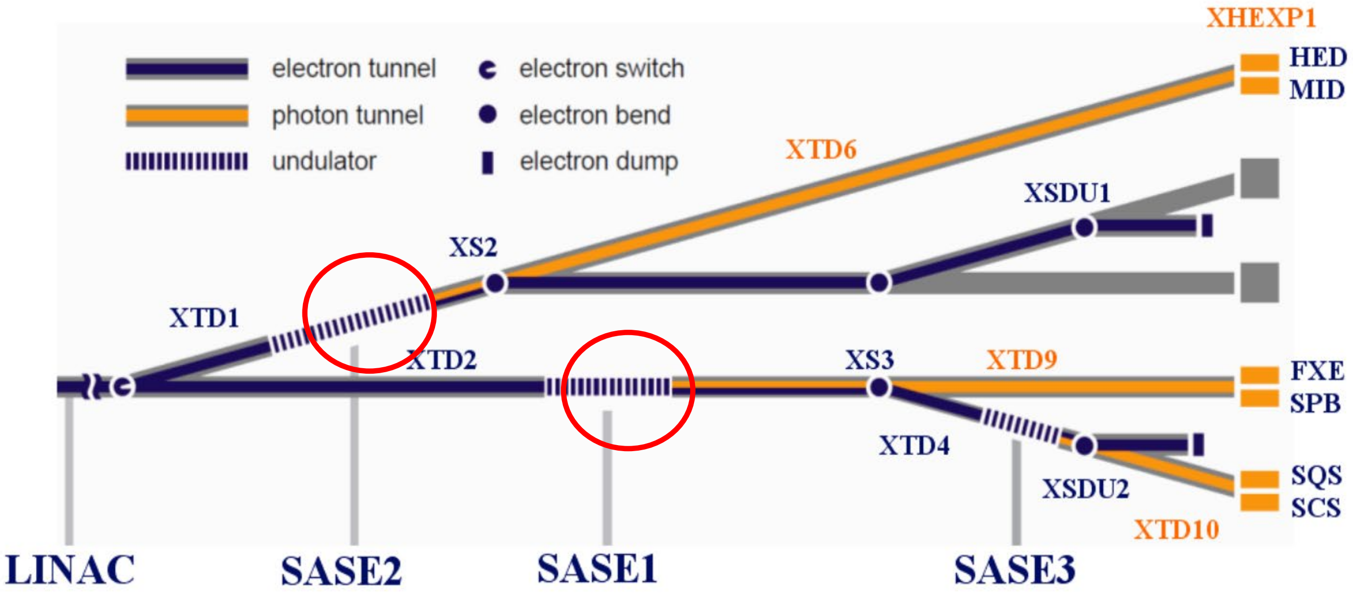
Two experimental attempts so far in the past

1st Attempt (Oct.19th – 21st 2021)

- ❑ SASE1 planned at 24 keV & SASE2 at 30 keV

2nd Attempt (Nov. 23rd – 26th 2022)

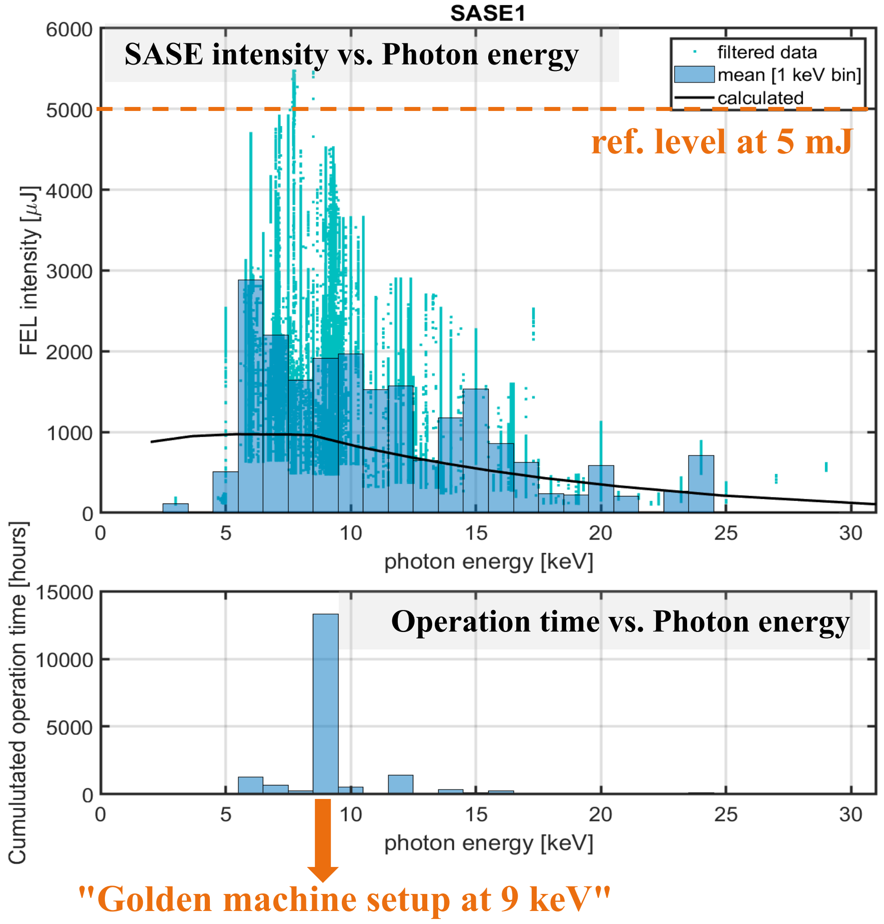
- ❑ SASE2 planned at 30 keV



Choice of planned photon energies determined by transport capability of the photon beamlines

First Experimental Attempt (Oct. 19th – 21st 2021)

Dedicated for SASE1 at 24 keV & SASE2 at 30 keV



Strategy of SASE tuning

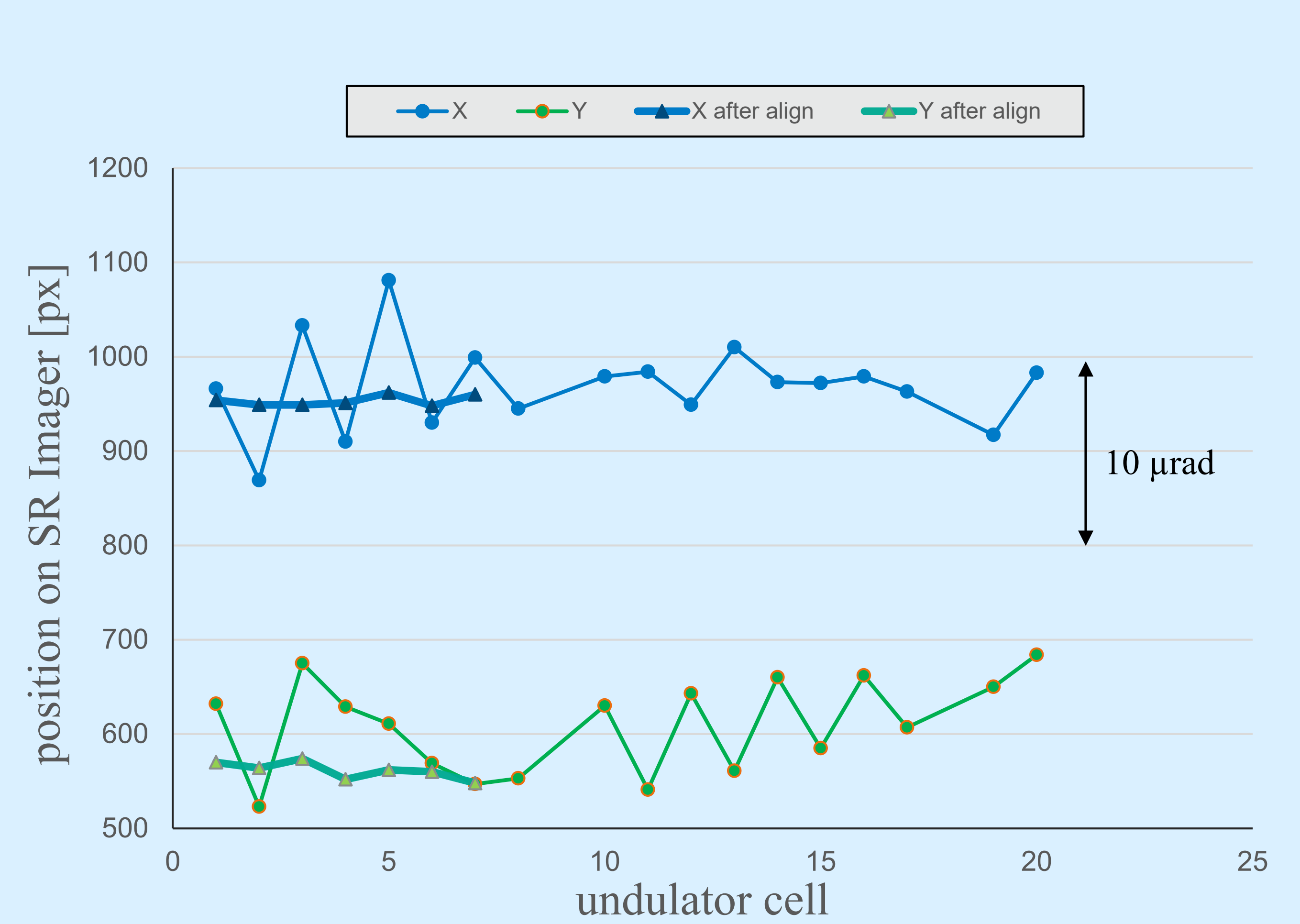
- ❑ Starting from a **statistically golden machine setup at 9 keV**
  - ✓ **beam based alignment**[1] of quadrupoles in the undulators
  - ✓ **emittance optimization** in the injector[2]
  - ✓ **dispersion correction**[3]
- ❑ Increasing photon energy stepwise while keeping reasonable signals for tuning
- ❑ Online optimization of
  - ✓ **trajectory** with correctors (few μm level)
  - ✓ **phase** between undulators with phase shifters
  - ✓ **pointing** of individual undulators using the "K-Mono"
  - ✓ linear and quadratic **tapers** of the undulators

1. M. Scholz et al. THP002, FEL'19 2. S. Meykopff and B. Beutner, THPHA116, ICALEPCS'17 3. N. G. Ghazaryan et al. JPCS 874 012084 2017

First Experimental Attempt (Oct. 19^{th} – 21^{st} 2021)

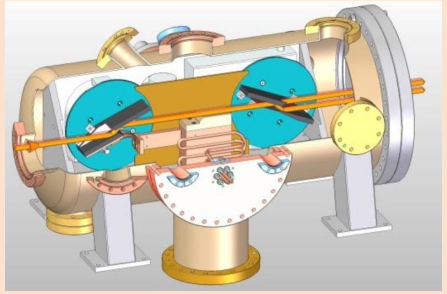
Pointing of undulators with K-Mono

SASE2 pointing measured with K-Mono Si333 on SR-imager



W. Freund et al. J. Synchrotron Rad. (2019). 26, 1037–1044

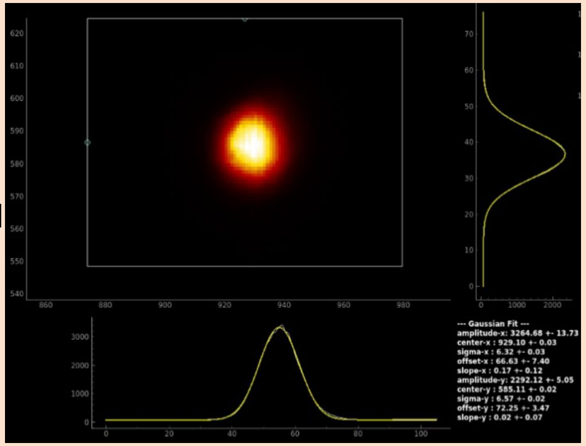
- **K-Mono:** monochromator to analyze the pointing and wavelength of the spontaneous radiation from a single undulator



- K-Mono shows the **pointing of individual undulators** and gives an absolute **energy calibration**

Exemplary image from the K-Mono after SASE2 measured energy: **30.57 keV**

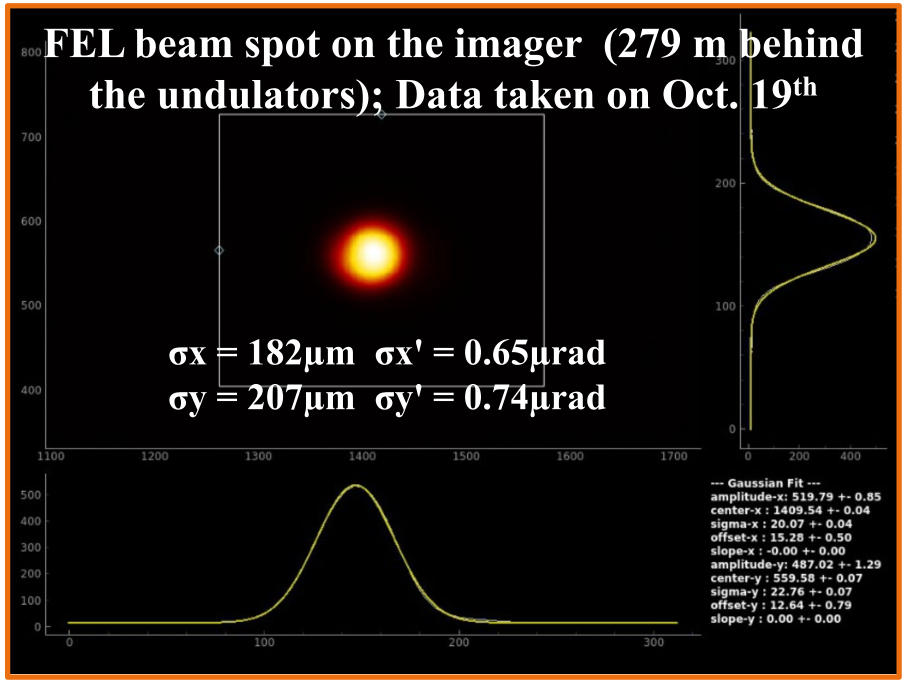
Si(333)



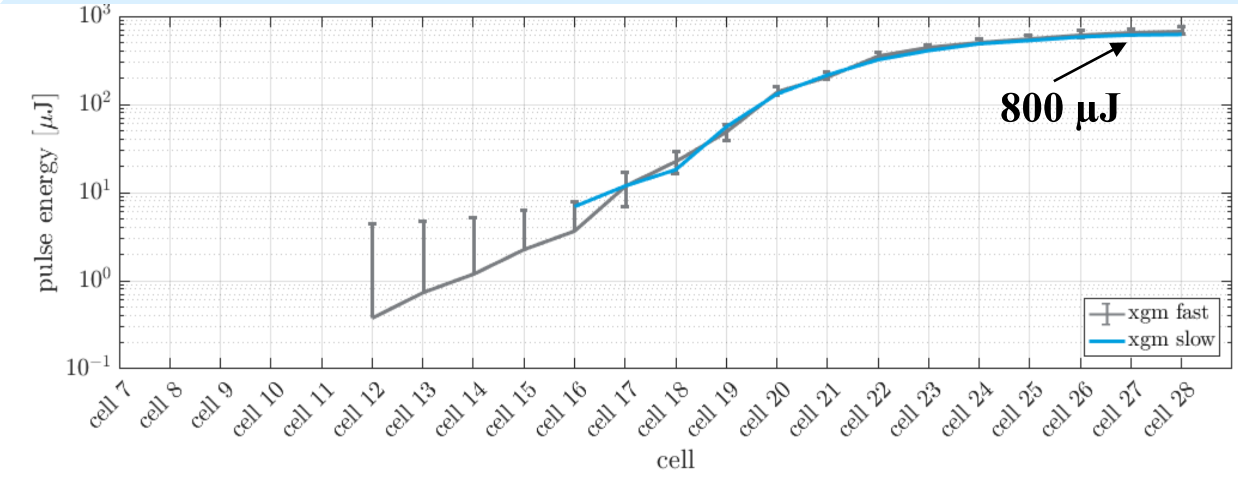
First Experimental Attempt (Oct. 19th – 21st 2021)

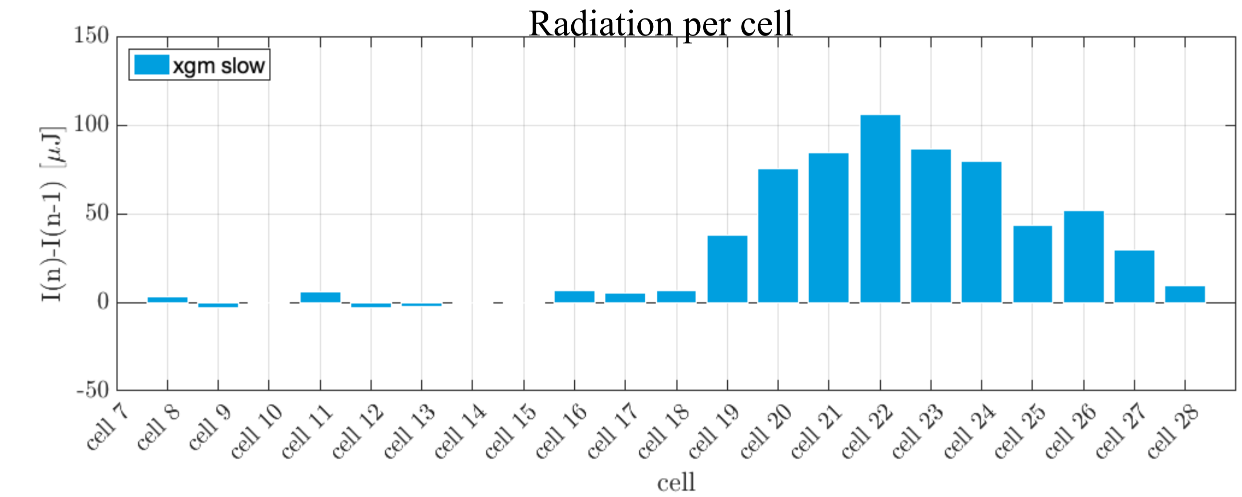
X-ray at 24 keV generated & briefly characterized at SASE1

- Difficult to get last 7-9 cells contributing
  - → K-Mono based adjustment in the pointing of individual undulators helped getting another 2-3 cells contributed
- Measured SASE intensity at **24 keV ~800 µJ**



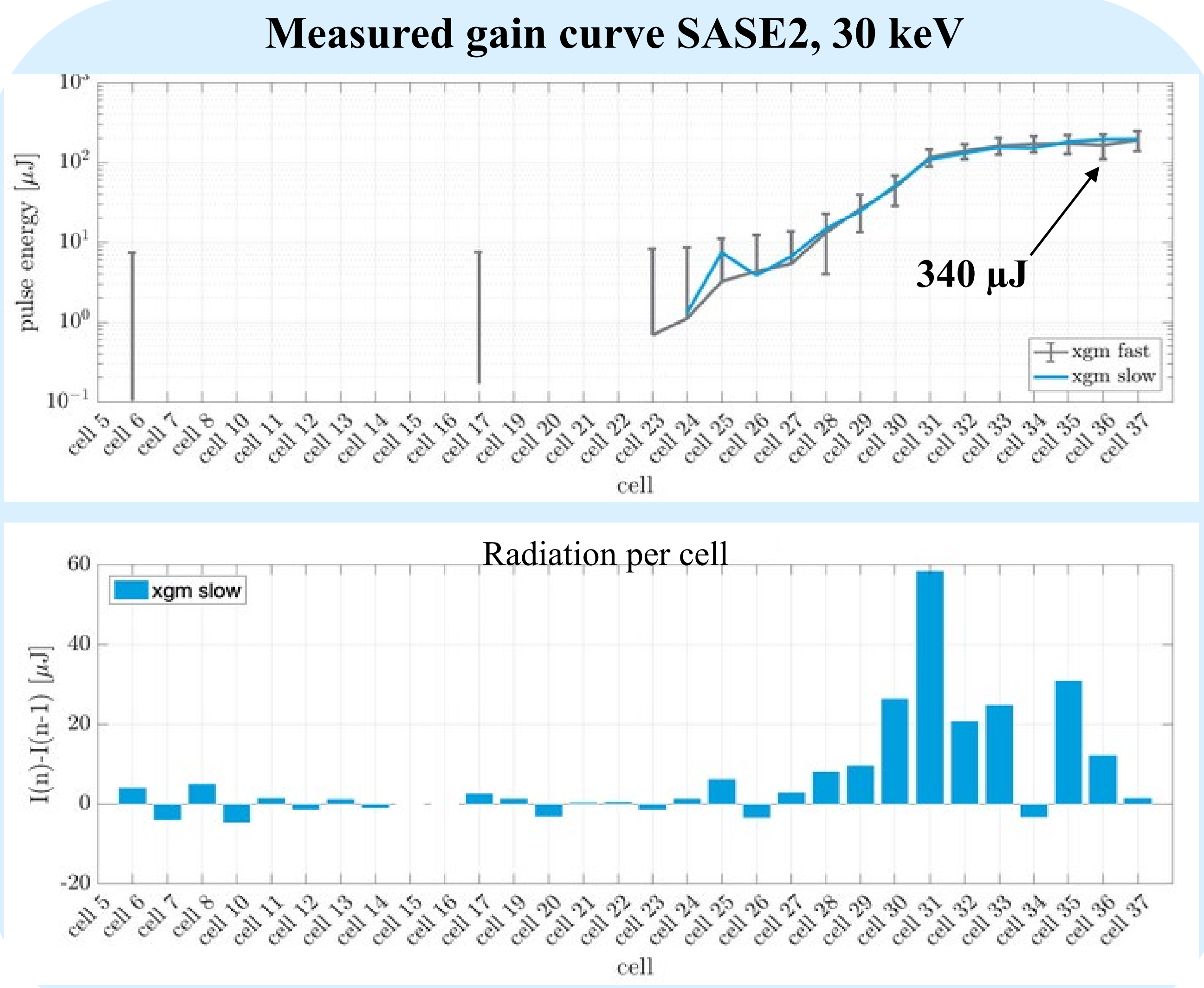
Measured gain curve SASE1, 24 keV



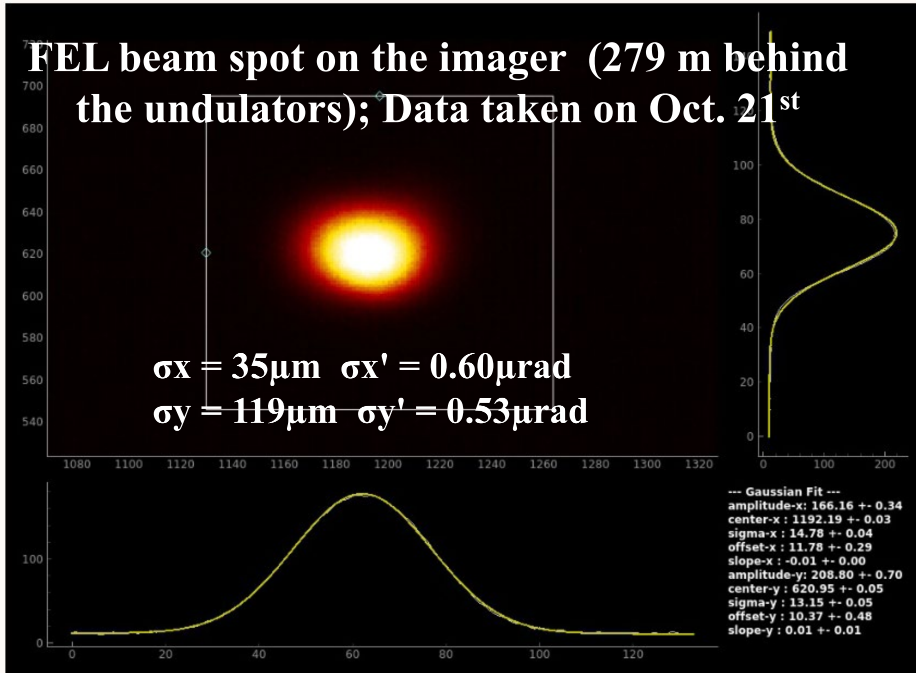


First Experimental Attempt (Oct. 19th – 21st 2021)

X-ray at 30 keV generated & briefly characterized at SASE2



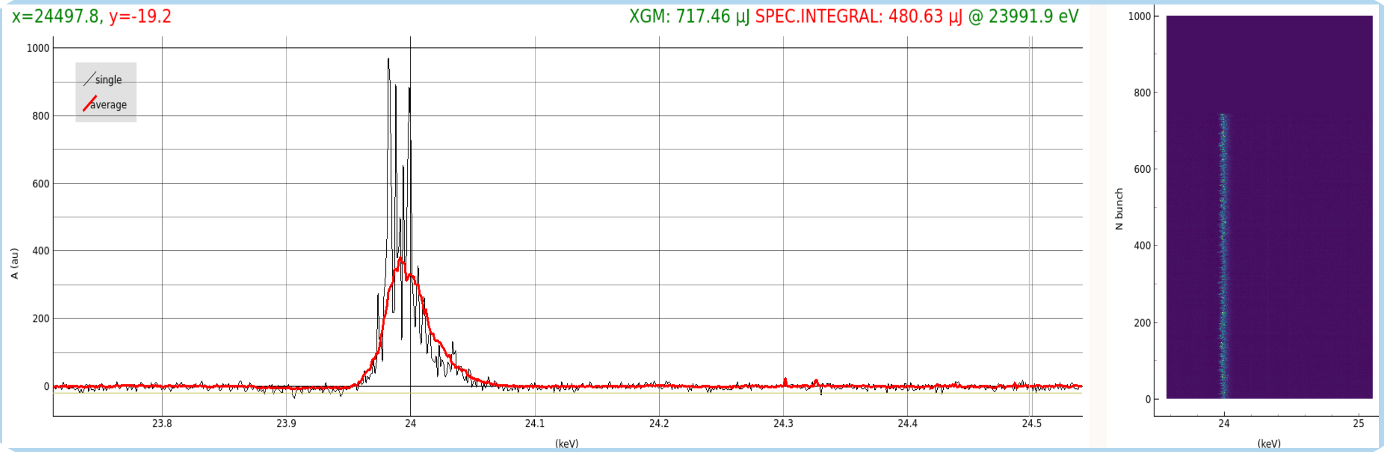
- K-Mono based undulator alignment plus residual air coil optimization helped boosting the intensity, finally to **~340 μJ at 30 keV** after tuning



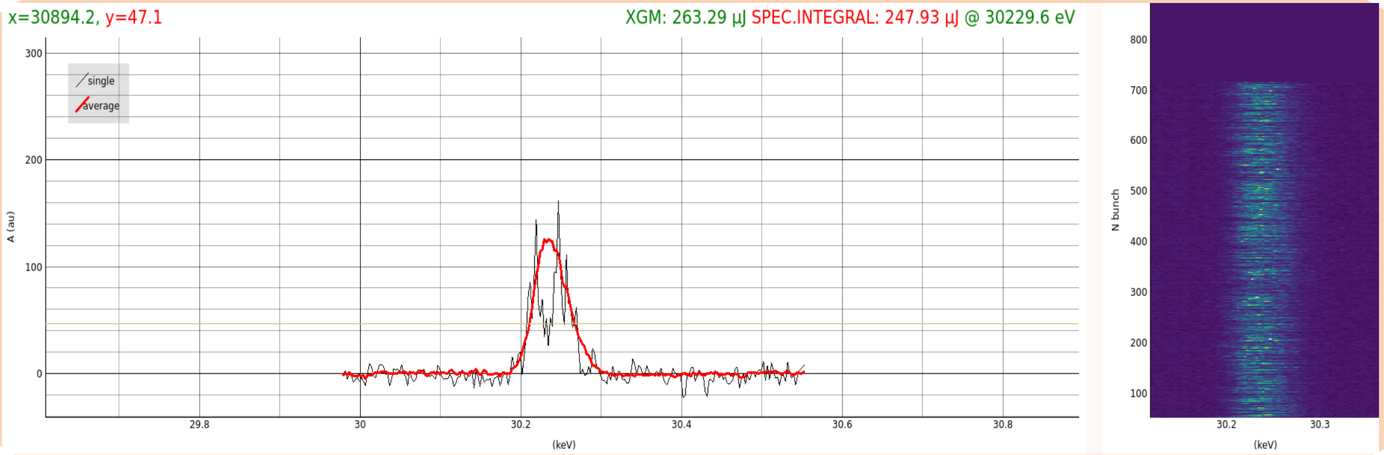
First Experimental Attempt (Oct. 19th – 21st 2021)

Spectrum measurements

Measured photon energy at SASE1 → 24. 58 keV

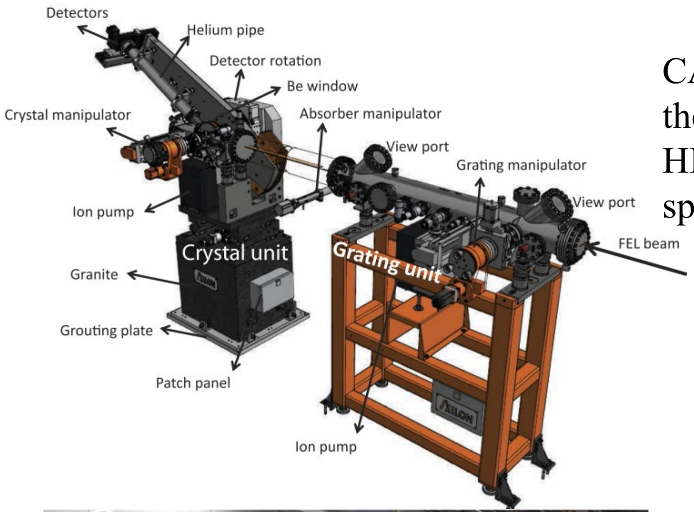


Measured photon energy at SASE2 → 30.24 keV



Hard x-ray single-shot spectrometer

N. Kujala et al. 2020 RSI 91 (2020)



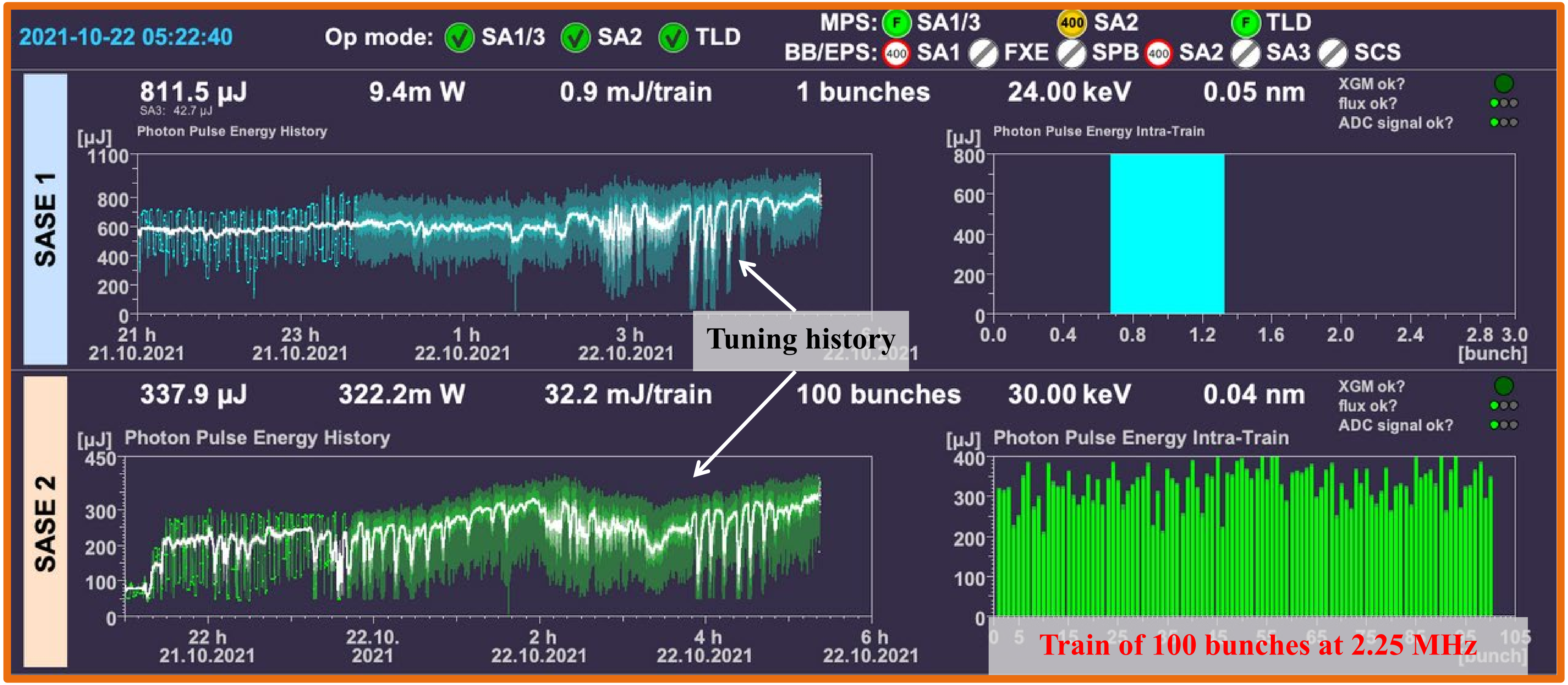
CAD model of the SASE1 HIREX spectrometer

Photograph of the HIREX spectrometer in the tunnel

First Experimental Attempt (Oct. 19th – 21st 2021)

0.3 mJ X-rays at 30 keV generated & characterized

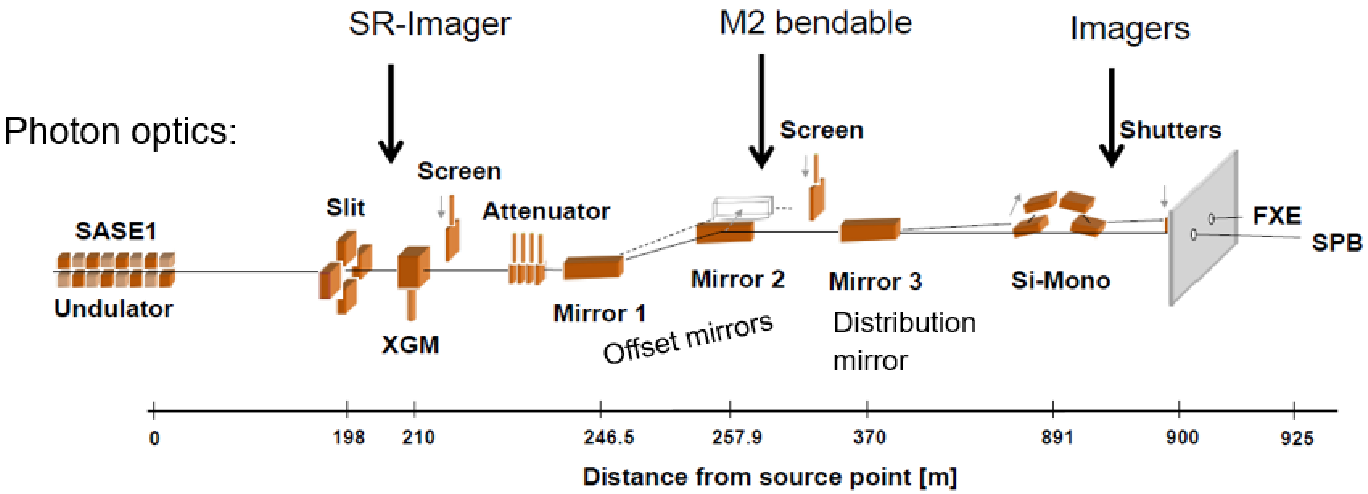
First experiments delivered hard X-rays of 0.8 mJ and 0.3 mJ at photon energies of 24 keV & 30 keV for beamlines SASE 1 and 2, respectively, using an electron energy of 16.3 GeV



First Experimental Attempt (Oct. 19th – 21st 2021)

X-rays of 24 keV at SASE1 delivered to the user station

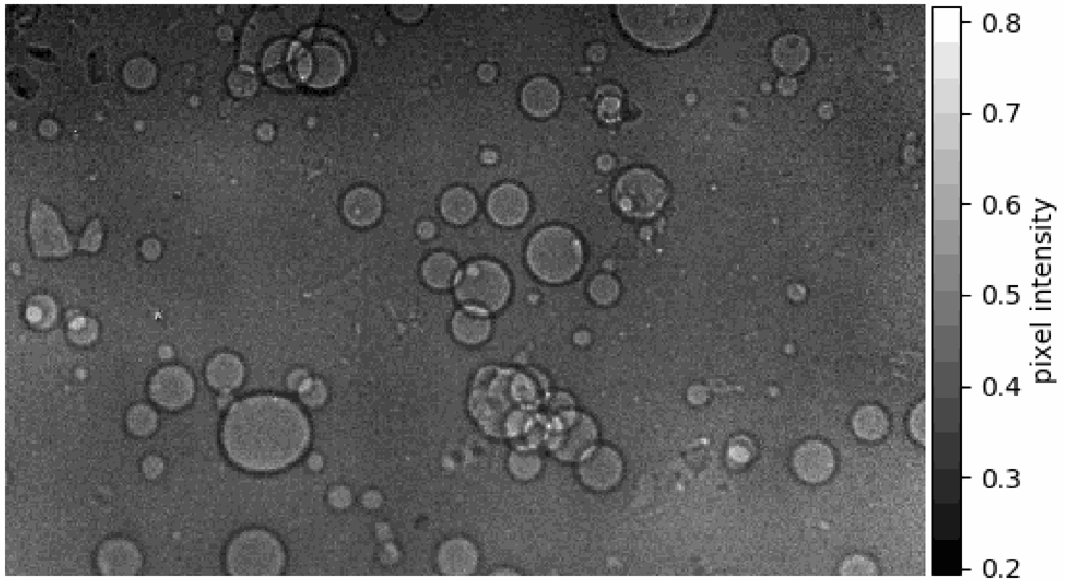
- **Photon beamline transport capability** limiting the delivery of 30 keV X-rays to the experiment hutch at SASE2
- **24 keV** hard X-rays at beamline SASE1 **successfully transported** to the user station for microscopy



SASE1 photon beamline

- ❑ Distance from source point **>900 m**
- ❑ Photons guided over 2-3 mirrors
- ❑ Incident angles **> 1.3 mrad**
- ❑ Limit at SA1: ~24 keV

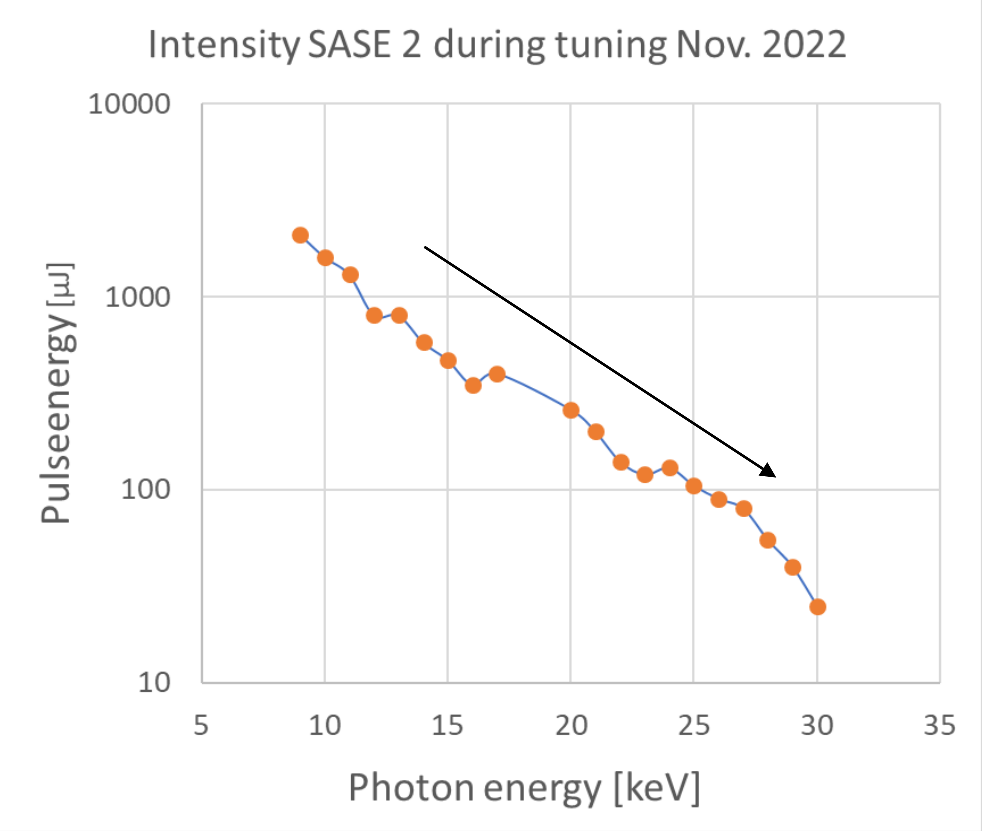
Early foaming in Al in slow motion recorded at SPB EuXFEL, P. Vagovic



Courtesy of Meik Noak and Francisco Garcia-Moreno, TU Berlin

Second Experimental Attempt (Nov. 23rd – 26th 2022)

Dedicated photon beam transport study for SASE2 at 30 keV

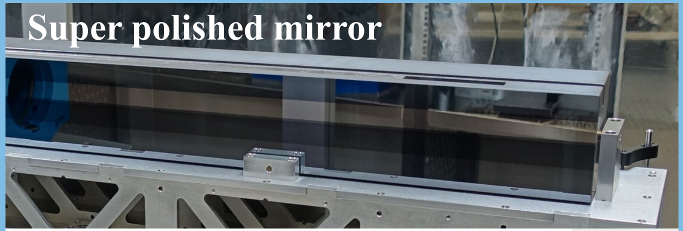


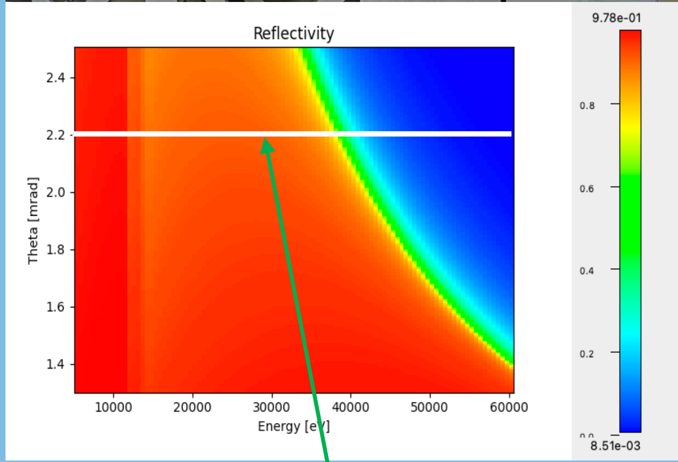
- **SASE tuning aiming to reach 30 keV** with some intensity for photon beam transport
- Electron energy set at 16.5 GeV
- **20-40 µJ at 30 keV left** by increasing the photon energy set-point stepwise, then giving the beamline to alignment studies

Second Experimental Attempt (Nov. 23rd – 26th 2022)

Successful transmission of 30 keV at SASE2 to user stations

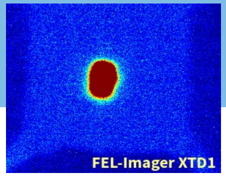
- Great efforts of the EuXFEL optics group on the beamline alignment [M. Vannoni et.al.]
- Experiments done with a transmission of
  - ❑ **About 60% at 27 keV**
  - ❑ **About 40% at 30 keV**

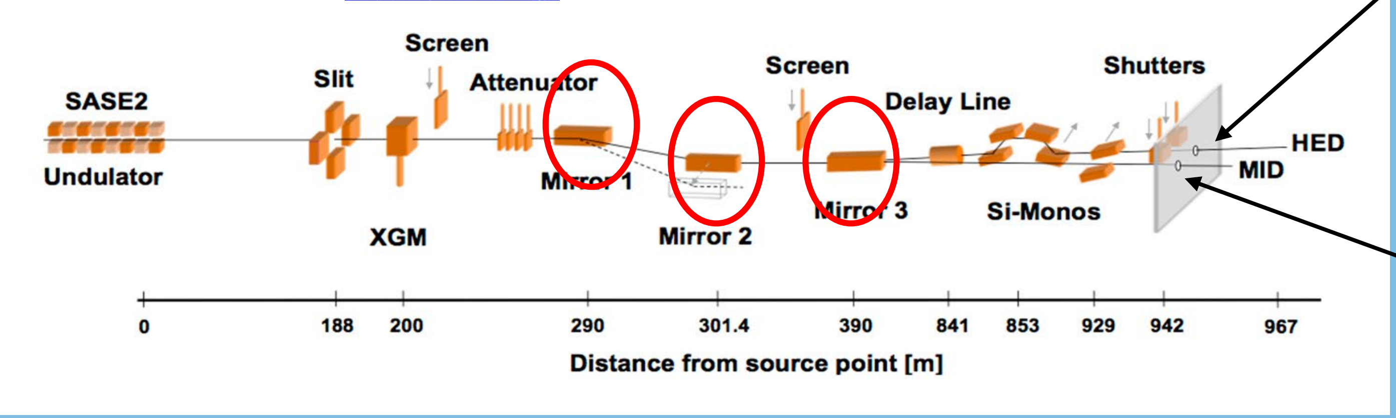


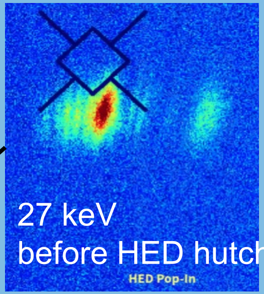


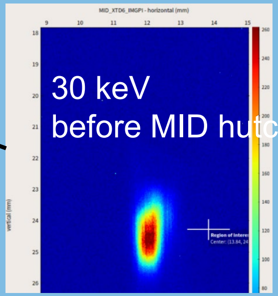
90% reflectivity at 2.2 mrad and 30 keV, mirror coated with platinum

SASE2 photon beamline





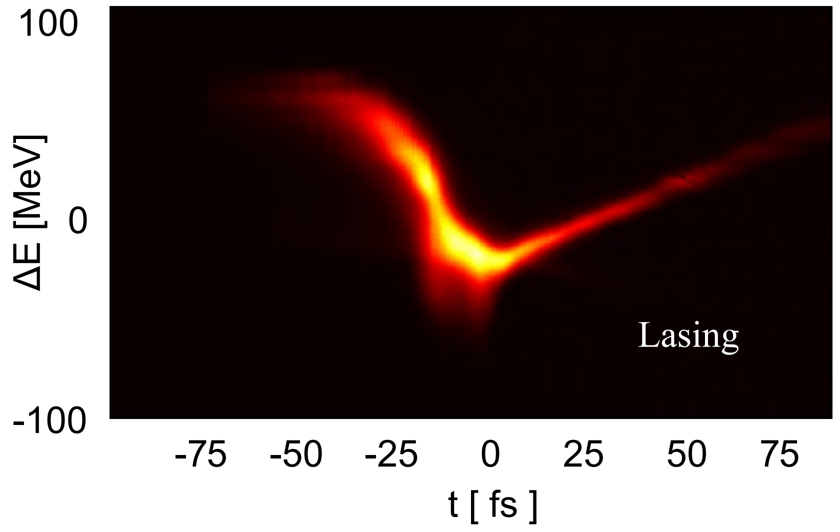


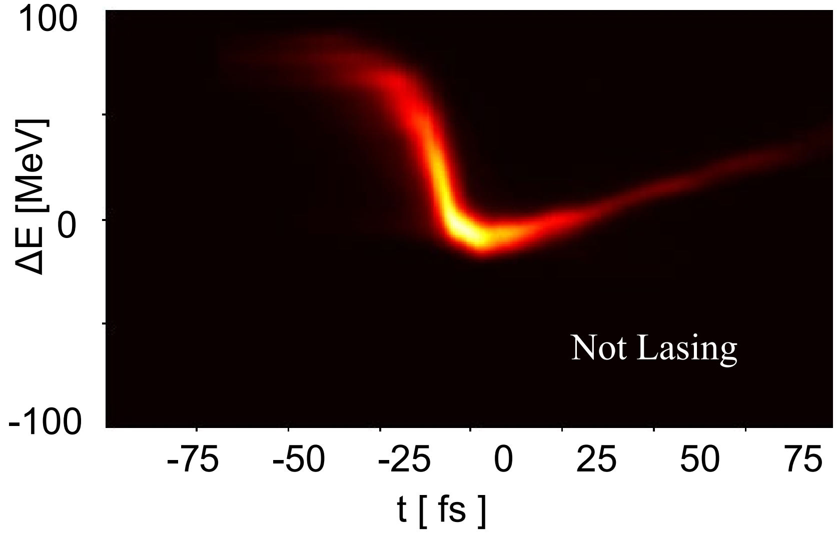


Newly available diagnostics during the 2nd experiment for longitudinal phase space (LPS) measurements

Corrugated structure at the European XFEL

S. Tomin et al, MOPOPT020, IPAC'22





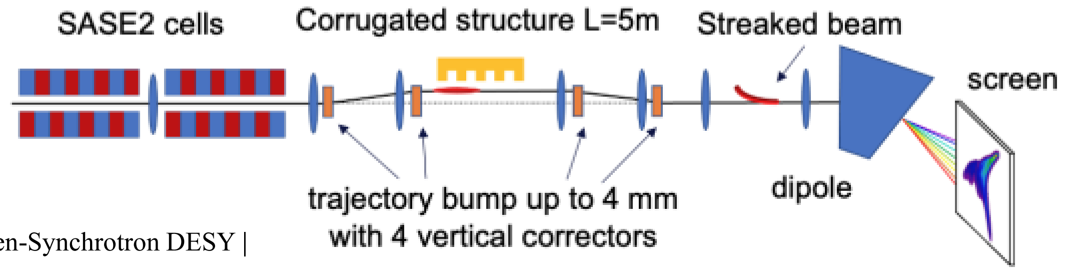
- One-sided corrugated wakefield structure installed after SASE2 beamline for LPS diagnostics
- Planned LPS studies for next 30 keV run in 2023

Poster WE4P07

Longitudinal Phase Space Diagnostics with Corrugated Structure at the European XFEL

Philipp Dijkstal

Diagnostic beam line for LPS measurement after SASE2



Intermediate Summary: Experiments

Experiments so far have demonstrated:

- ❑ **0.8 mJ at 24 keV** (SASE1) & **0.3 mJ at 30 keV** (SASE2) with **16.3 GeV** beam energy
- ❑ SASE2 operated at **30 keV**: flat intensity pulse train of **100 bunches at 2.25 MHz**
- ❑ **first testing user experiments** at 24 keV at SASE1
- ❑ successful **30 keV photon beam** at SASE2 **transported** to experiment hutches

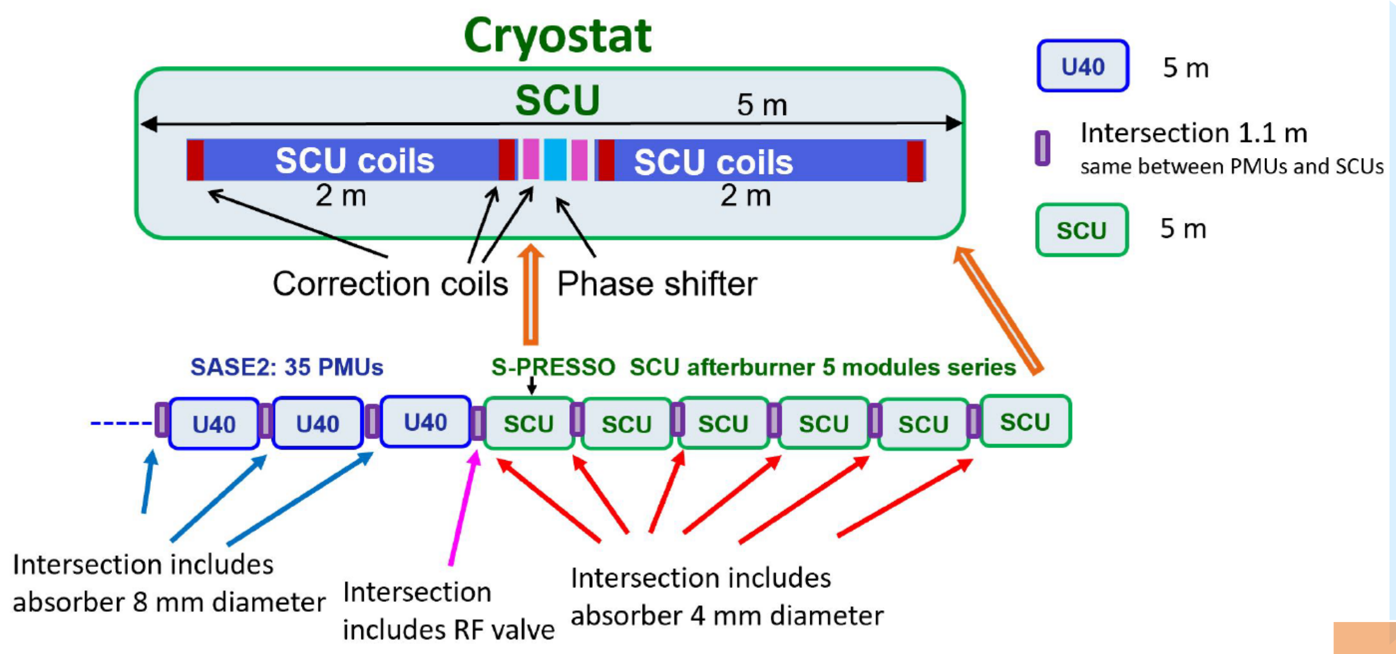
Parallel R&D activities

towards even higher photon energies

The super-conducting after burner

Expected for end of 2024 at the European XFEL

S. Casalbuoni et al, Front. Phys. 11:1204073 (2023)



PMU: permanent magnet undulators **SCU**: superconducting undulators

S-PRESSO, the prototype of the super conducting undulators has been ordered and is expected for end of 2024.

Main parameter	PMU	SCU
Period	40 mm	18 mm
Peak field	1.12 T	1.82 T
K max.	3.93	3.06
Vacuum chamber	8 x 40 mm	5 x 10 mm
Magnetic length	5 m	4 m

Talk TH1D1

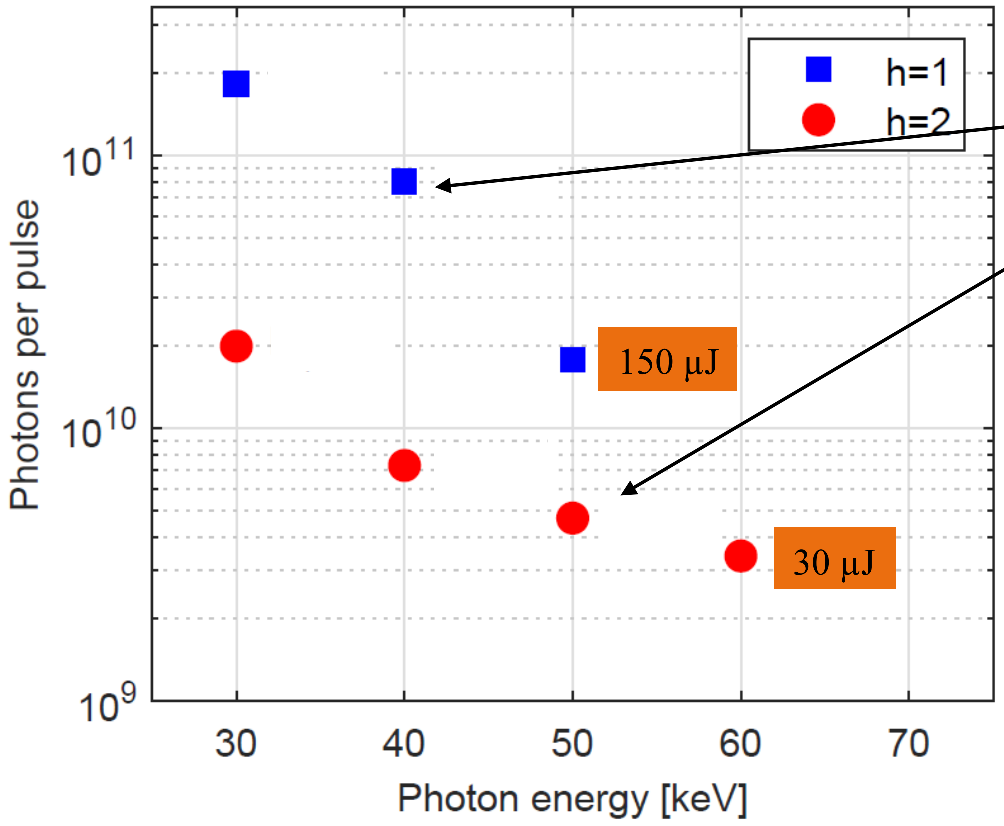
Application of Superconducting Undulator Technology for Hard X-ray Production at European XFEL

Johann Baader

Scenarios to work with the afterburner using the fundamental & 2^{nd} harmonic

Simulations with 24 m SCUs after the SASE2 undulators

C. Lechner et al 2022 JPCS 2380 012009



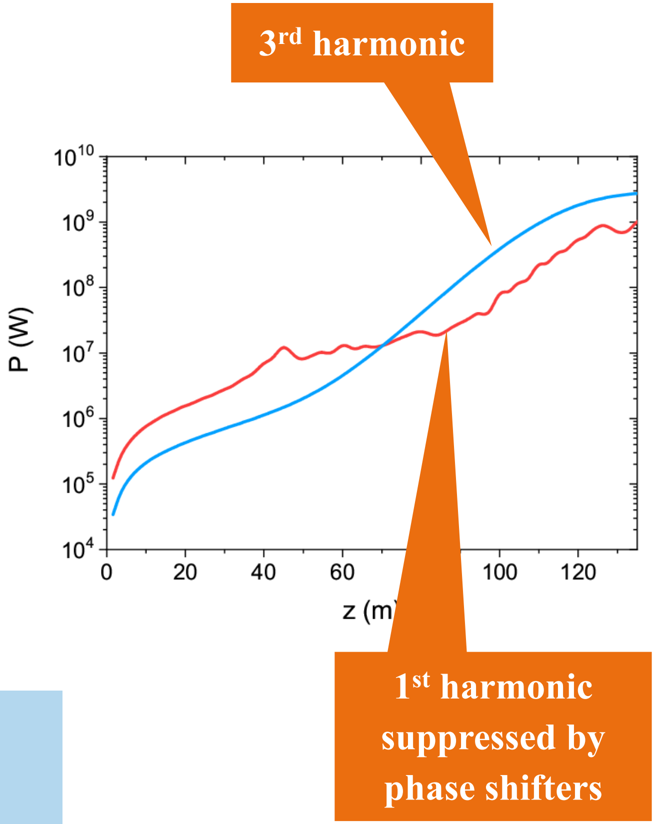
Setup for lasing at wavelength λ	Effect	Gain
All undulators set to λ	Additional undulators with larger K	Higher intensity
PMUs set to 2 λ SCUs set to λ	Nonlinear harmonic generation – 2^{nd} harmonic	Extended energy range

Electron beam parameters for the simulation	
Energy	16.5 GeV
Norm. emittance	0.4 mm mrad
Initial Energy spread	3 MeV
Peak current	5 kA
Bunch charge	150 pC
bunch length	30 fs

Lasing on the 3rd harmonic

Demonstrated at SASE3 & being studied for SASE2

- **Harmonic lasing** on the odd harmonics of the fundamental wavelength develops independently of the fundamental
- The **fundamental lasing has to be disrupted** to keep the energy spread low and let the harmonic saturate
- To preserve the beam quality for the SCUs the development of the first harmonic radiation has to be suppressed by two methods:
  - ➢ Insertion of filters for the fundamental wavelength
  - ➢ Setting the phase shifters between the undulators to $2\pi/3$, $4\pi/3$ to get destructive interference for the fundamental



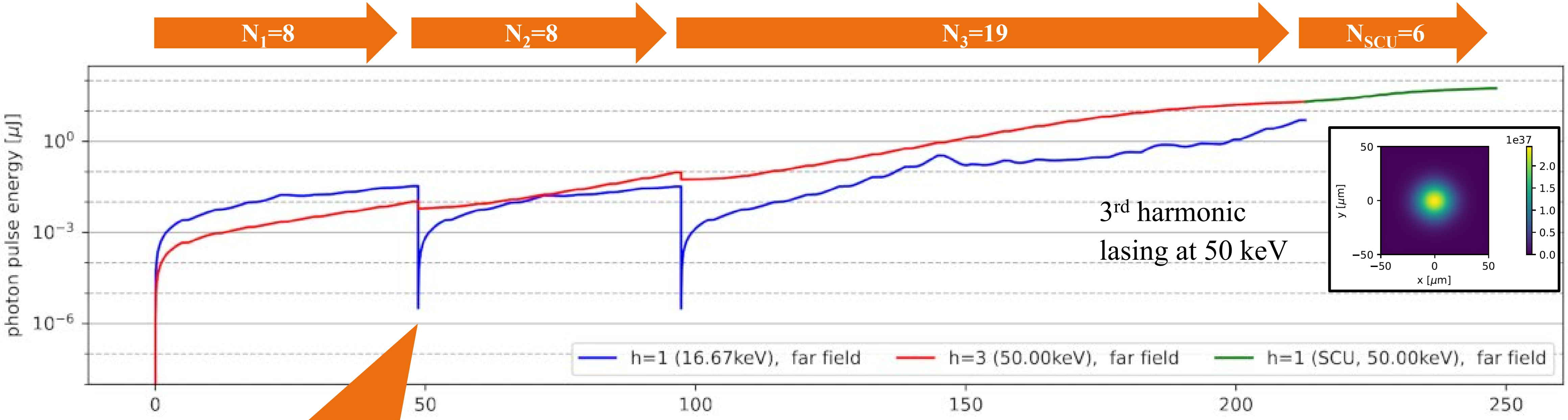
This scheme has been demonstrated at the soft X-Ray beamline SASE3 at 4.5 keV (2.75 Å) using the 3rd harmonic of 1.5 keV and 5th harmonic of 0.9 keV in 2019/2020 using the phase shifters to suppress the fundamental and last 6 cells set to the fundamental.

E. A. Schneidmiller and M. V. Yurkov, PRAB 15, 080702 (2012)   E. Schneidmiller PRAB 24, 030701 (2021)

Simulation Study

3rd harmonic lasing at 50 keV

Recent simulations show the evolution of the photon pulse energy in SASE2 at the **fundamental wavelength (blue)** and at the **third harmonic (red)**, respectively, and in the **SCUs (green)** tuned to the third harmonic of SASE2.



Disruption of the fundamental by a Si filter using the self seeding chicanes in SASE2

Poster WE4P01

Numerical Simulation Studies of Superconducting Afterburner Operation for European XFEL

Christoph Lechner

Summary

- **Scientific opportunities** with very hard X-rays calling for FEL **facility developments**

- **A progressive step made at the EuXFEL** towards user experiments at very high photon energies

  → systematical simulation studies carried out

  → dedicated experimental photon beamline studies performed

  → 0.3 mJ @ 30.24 keV experimentally demonstrated & transported

  → 0.8 mJ @ 24.58 keV delivered for first user experiments

- **Promising advanced schemes** towards harder X-rays (50+ keV)

  → super-conducting afterburner, fundamental & 2^{nd} harmonic

  → harmonic lasing, 3^{rd} & 5^{th} harmonics

- Next high photon energy **study planned for Oct. 2023**

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from DESY &**

**M. Vannoni, S. Casalbuoni, W. Freund, T. Maltezopoulos, N. Kujala,
J. Gruenert, A. Koch, H. Sinn, C. Lecher, P. Vagovic, J.W. Yan, A. Mancuso,
U. Boesenberg, R. Bean from the European XFEL**