Elettra
Sincrotrone
Trieste

Optical performances and challenges within Elettra 2.0

Luca Rebuffi
Elettra-Sincrotrone Trieste (ITA)

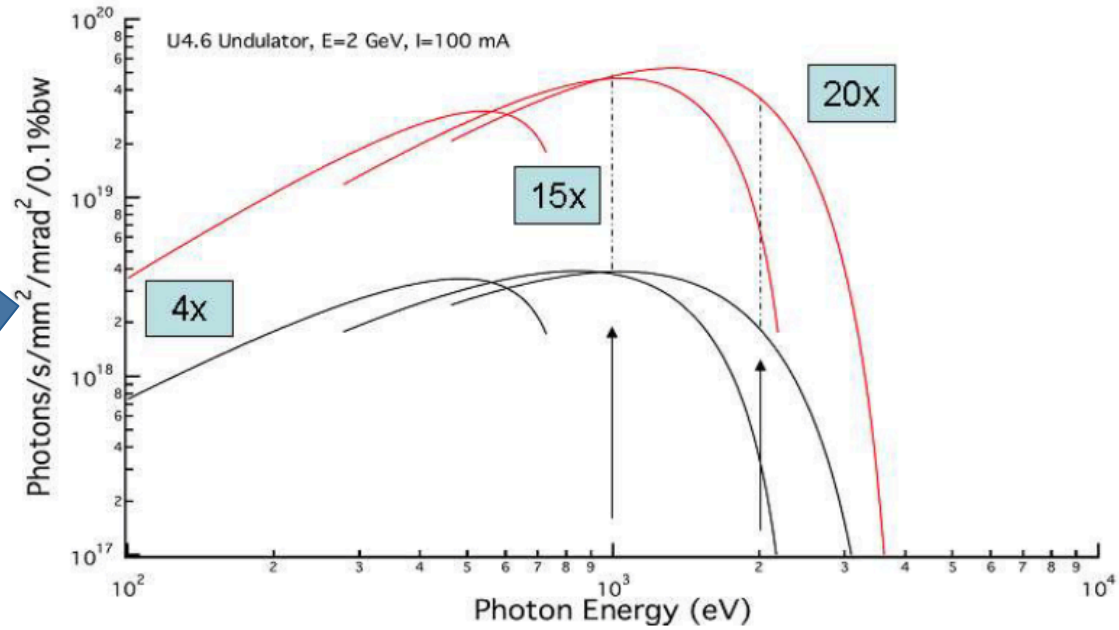
Elettra
Sincrotrone
Trieste

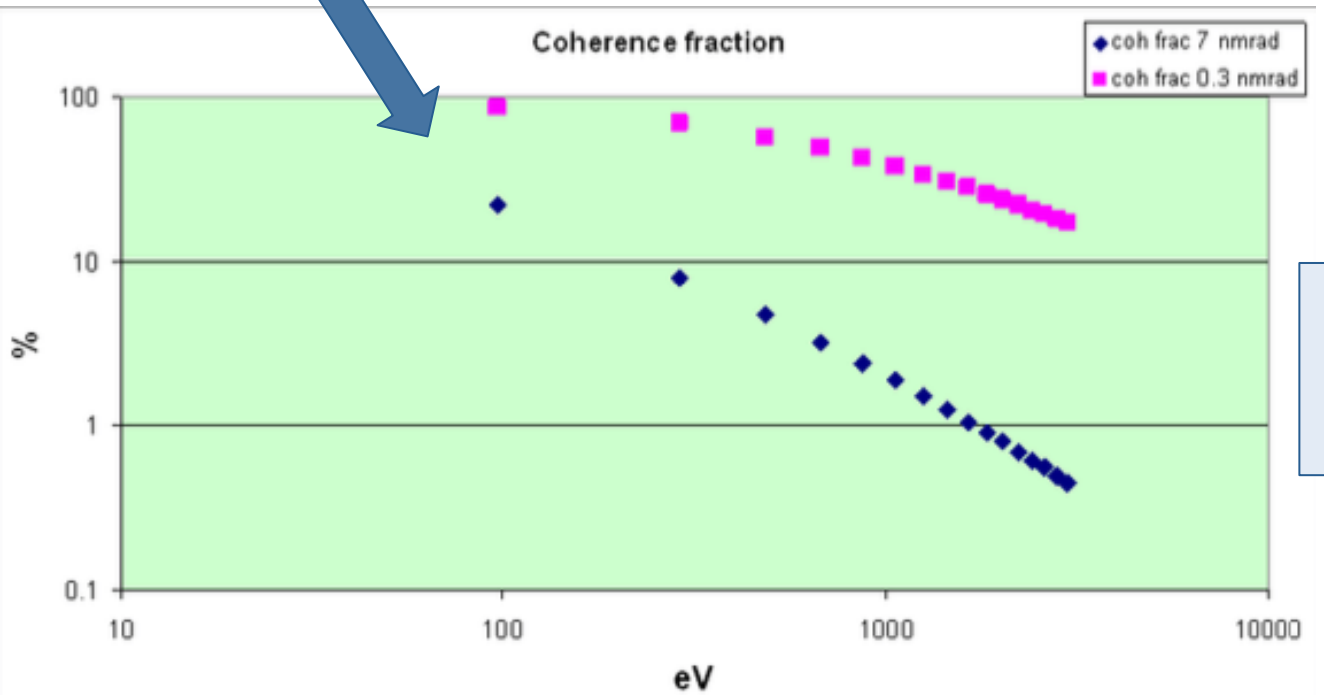
1. Introduction

INTRODUCTION

ELETTRA 2.0 SOURCES:

- INCREASED BRILLIANCE
- INCREASED COHERENCE



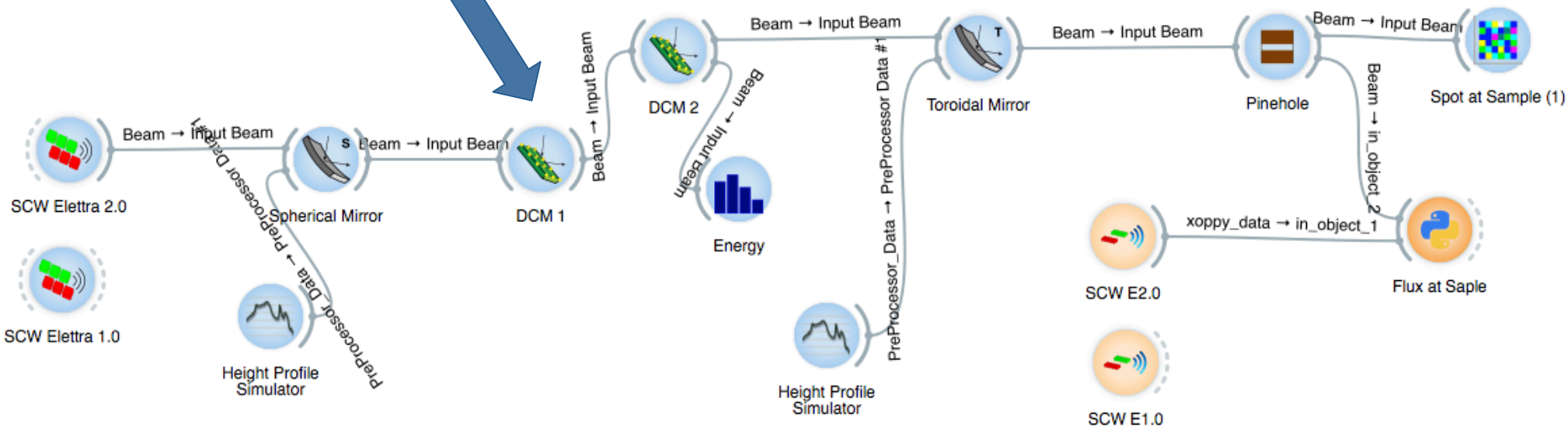


A
CHALLENGE
FOR OPTICAL CALCULATIONS

INTRODUCTION

SIMULATION TOOLS:

- SHADOW (RAY-TRACING)
- XOP/SRW (FLUX/POWER DENSITY)



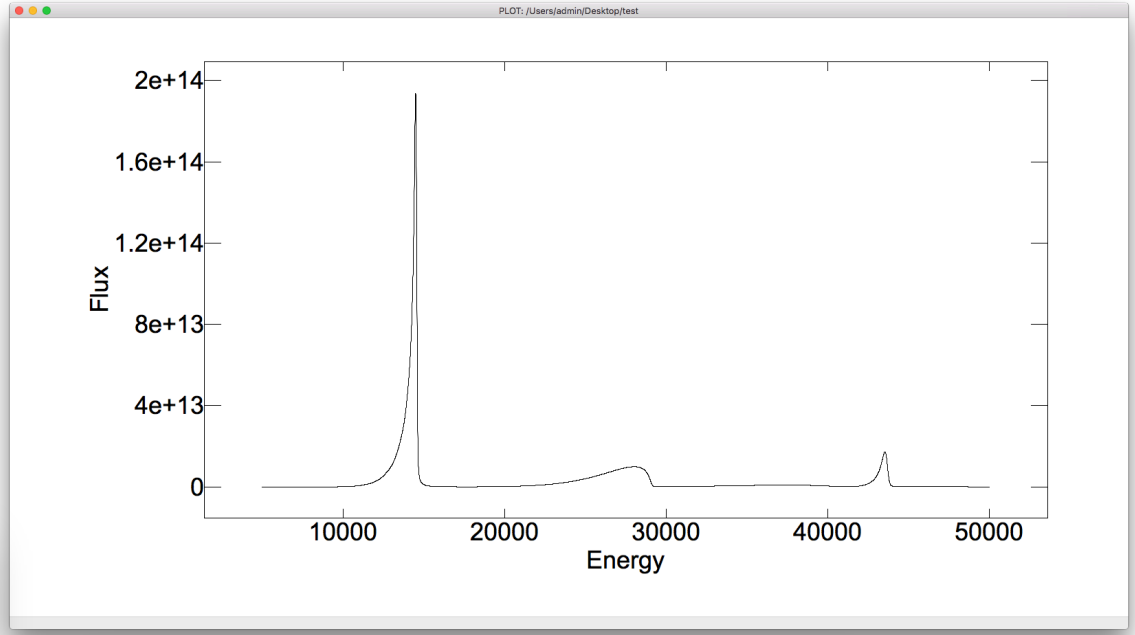
Luca Rebuffi, Manuel Sanchez del Rio, "OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for x-ray virtual experiments", Proc. SPIE 10388, Advances in Computational Methods for X-Ray Optics IV, 103880S (23 August 2017); doi: 10.1117/12.2274263

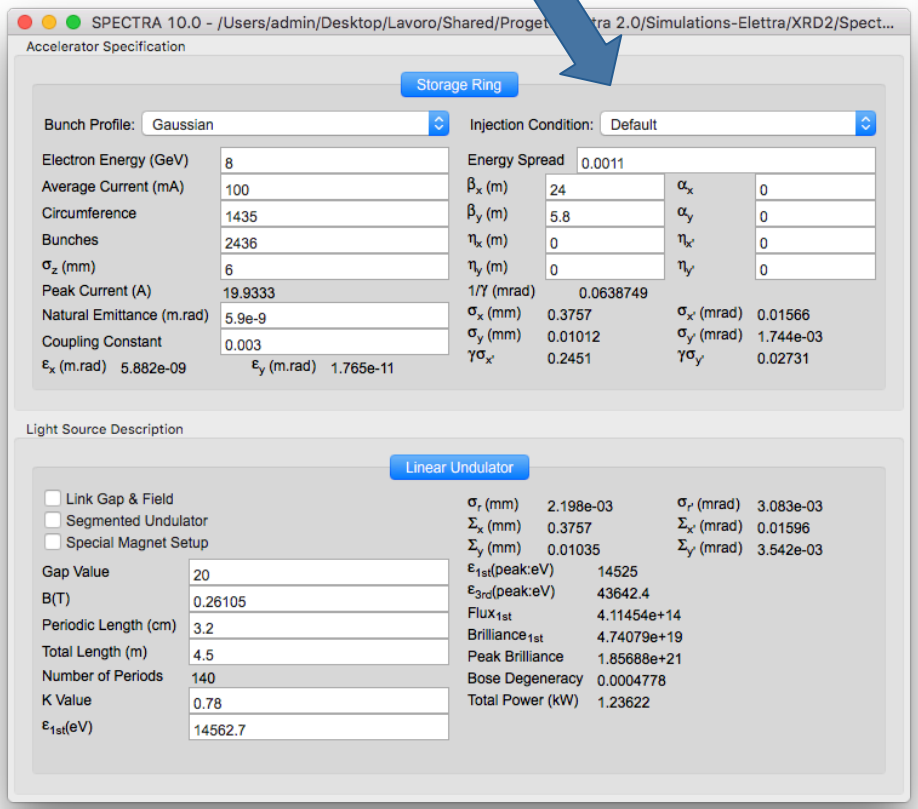
Rebuffi L. and Sánchez del Río M., "ShadowOui: A new visual environment for X-ray optics and synchrotron beamline simulations", J. Synchrotron Rad. 23 (2016), pp. 1357–1367. doi: 10.1107/S1600577516013837

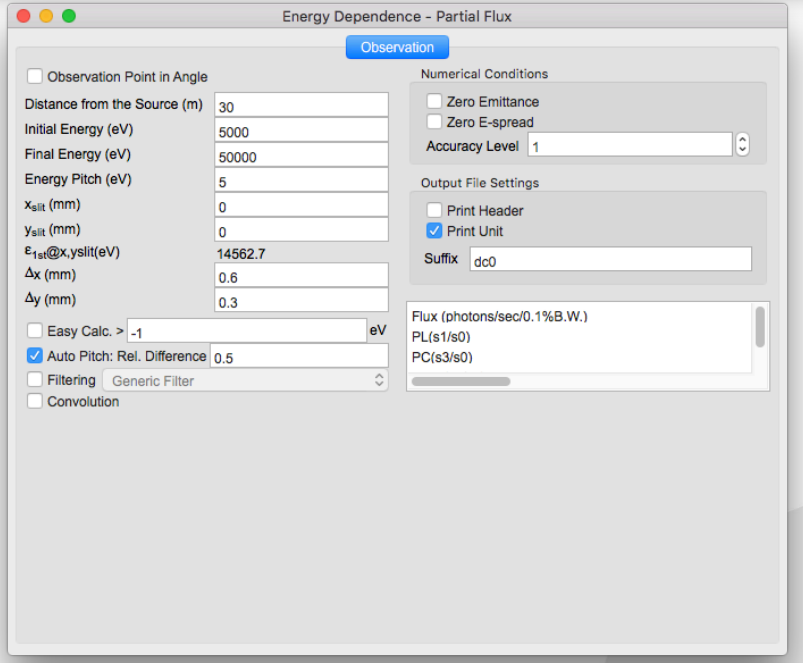
INTRODUCTION

SIMULATION TOOLS:

- SPECTRA (SOURCES ANALYSIS)



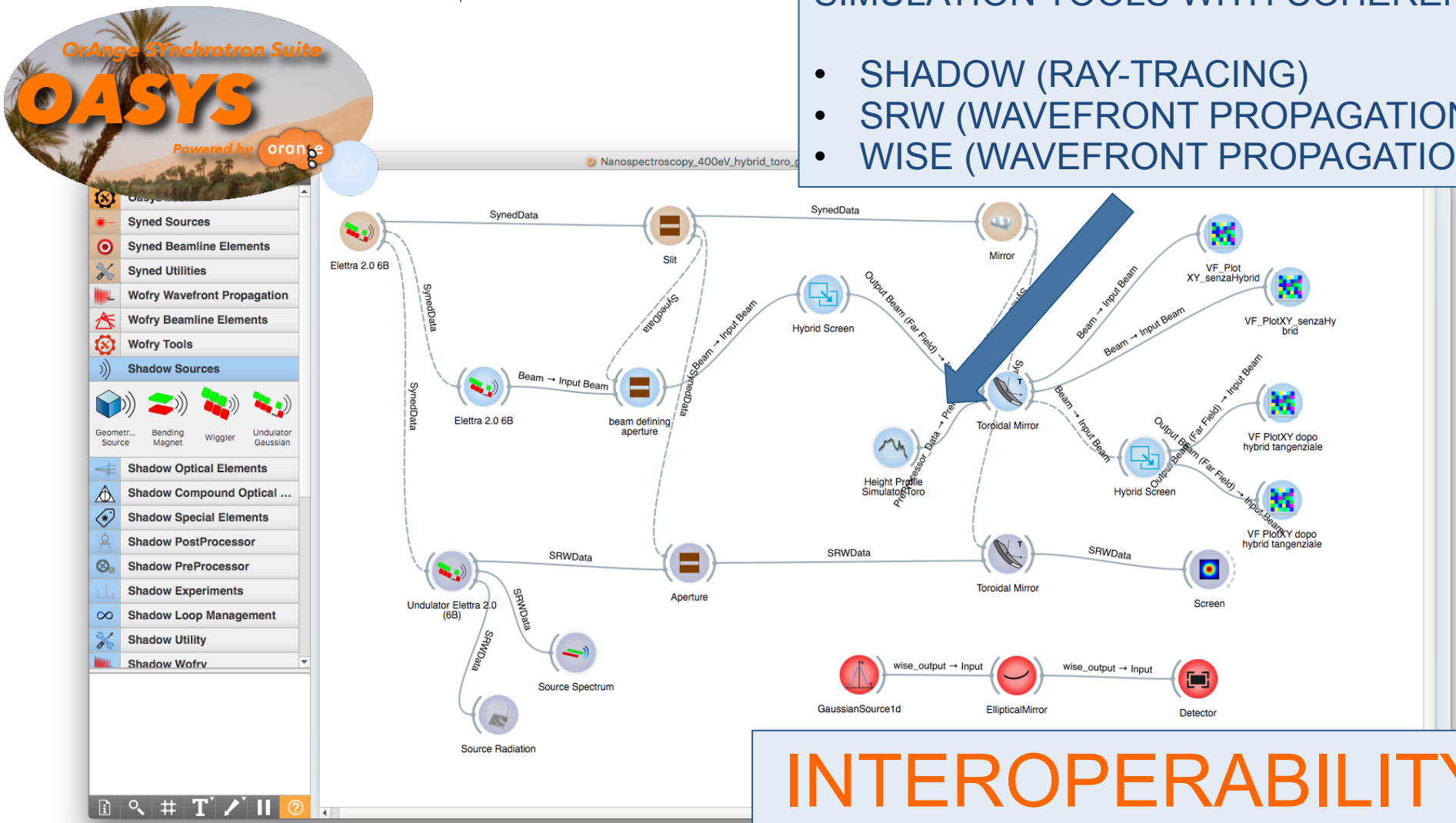




INTRODUCTION

SIMULATION TOOLS WITH COHERENCE:

- SHADOW (RAY-TRACING)
- SRW (WAVEFRONT PROPAGATION)
- WISE (WAVEFRONT PROPAGATION)



INTEROPERABILITY!!!!

Luca Rebuffi, Manuel Sanchez del Rio, "Interoperability and complementarity of simulation tools for beamline design in the OASYS environment", Proc. SPIE 10388, Advances in Computational Methods for X-Ray Optics IV, 1038808 (23 August 2017); doi: 10.1117/12.2274232

Elettra
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Trieste

2. Hard X-ray Beamlines

Elettra Sincrotrone Trieste

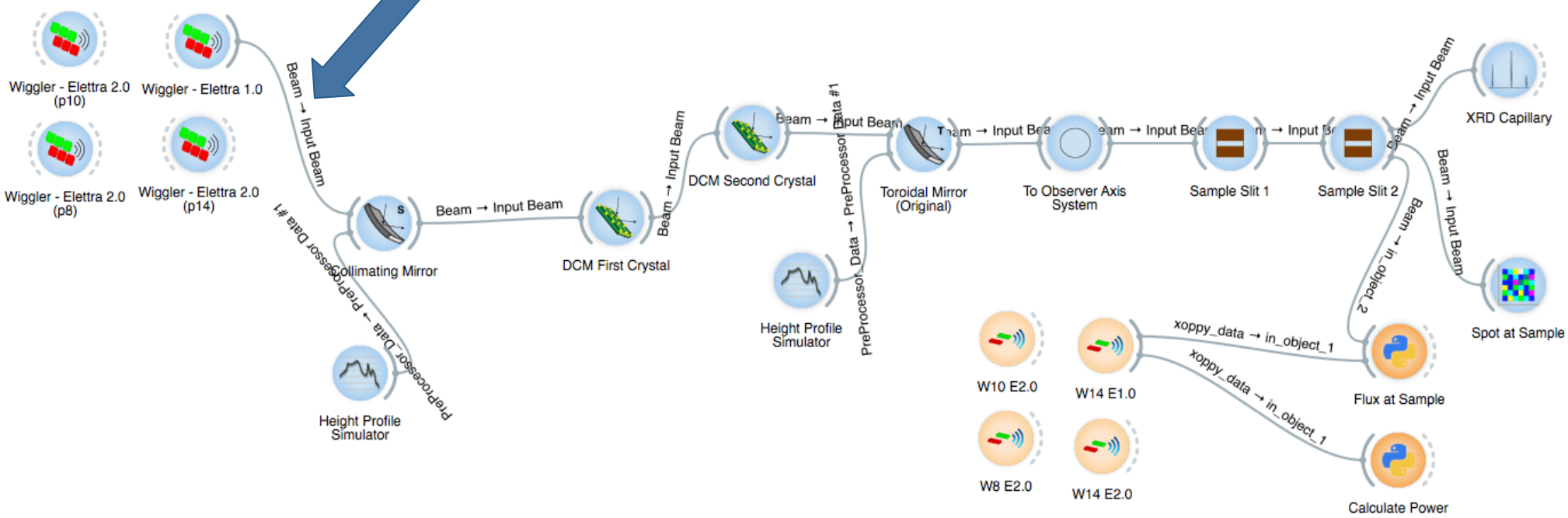
XRD1

XRD1 @ ELETTRA

WIGGLER SOURCE (W14):

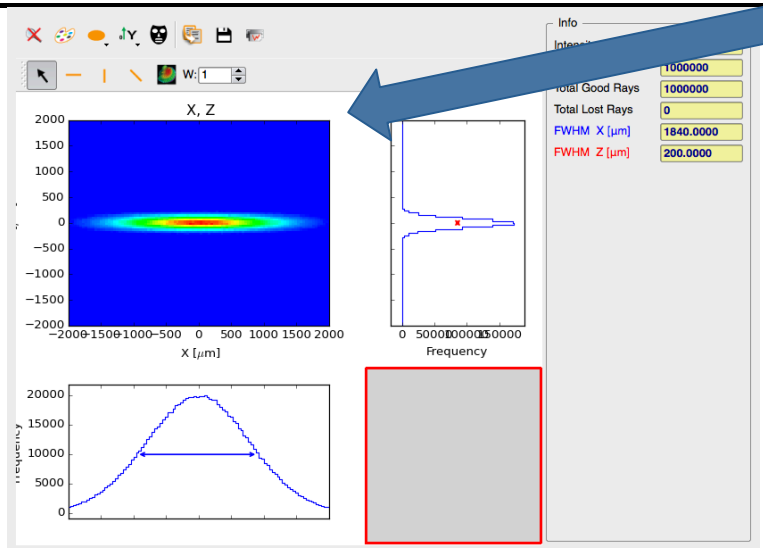
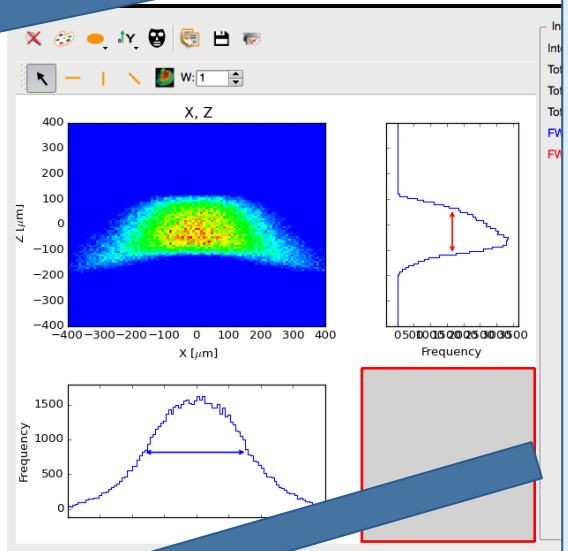
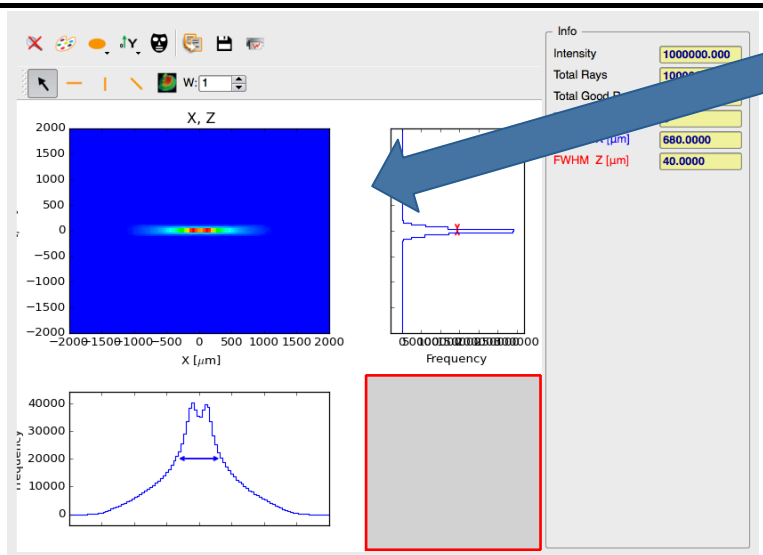
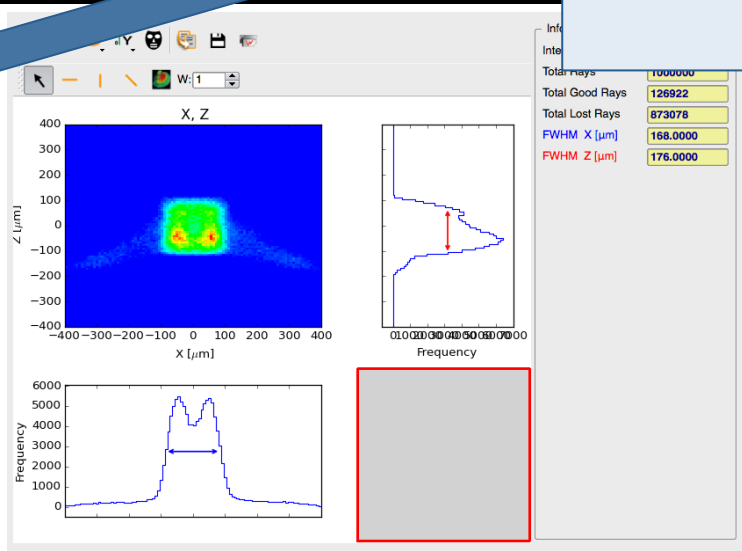
- B = 2.0 T
- Period = 0.14 m
- N Periods = 29
- K = 21.0

PROTEIN CRYSTALLOGRAPHY



Elettra Sincrotrone Trieste

XRD1

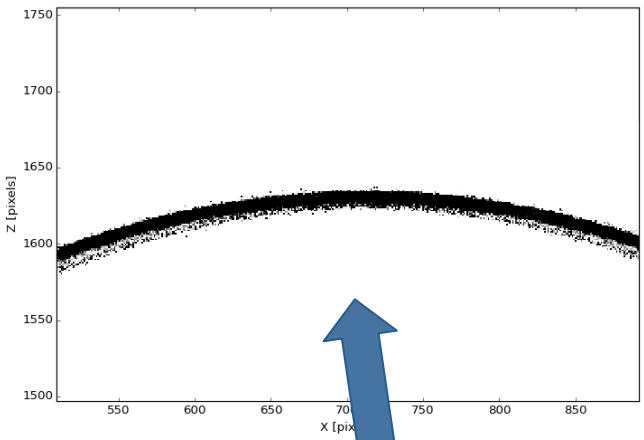
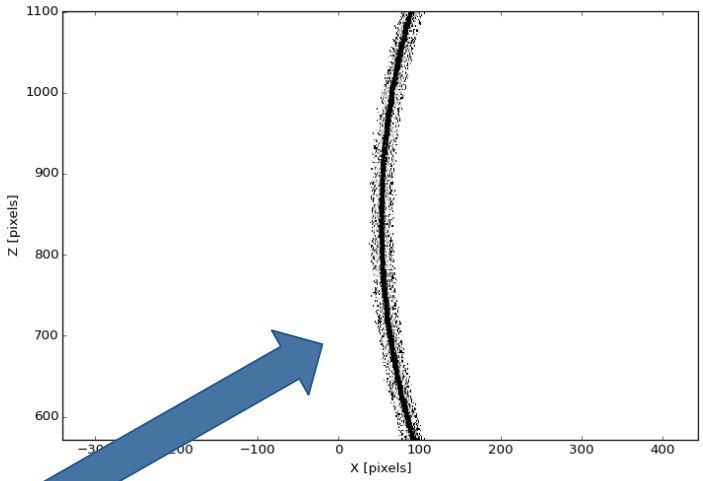
	Effective Source Size	Beam size at the sam
Elettra 1.0 W14		
Elettra 2.0 W14		

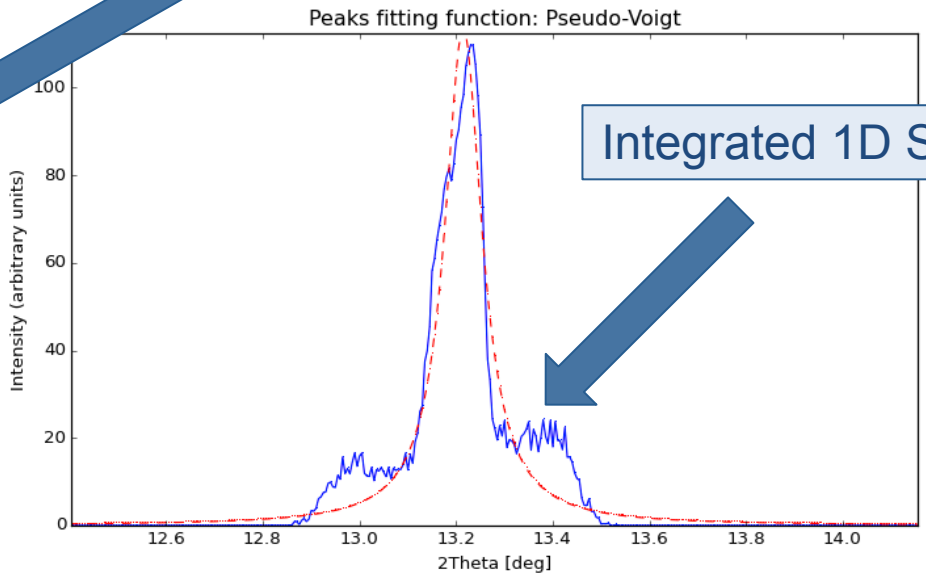
The Wiggler W14 source, having a strong magnetic field in the wiggler, combined with a small emittance of the electron beam, generates a source profile where the two parallel cones of light are resolved with a distance between the two peaks of ~300 µm. XRD1 optical layout propagate this irregular shape generates up to the sample position.

Elettra Sincrotrone Trieste

XRD1

Effect on the INSTRUMENTAL PROFILE: Simulated LaB6 Diffraction Signal at 13 KeV (Ray-Tracing)

Diffraction Ring: upper area	Diffraction Ring: left area
	



Integrated 1D Signal

The diffraction pattern has a different shape along a horizontal plane passing through the center of the pattern respect to the one it has in the corresponding vertical plane

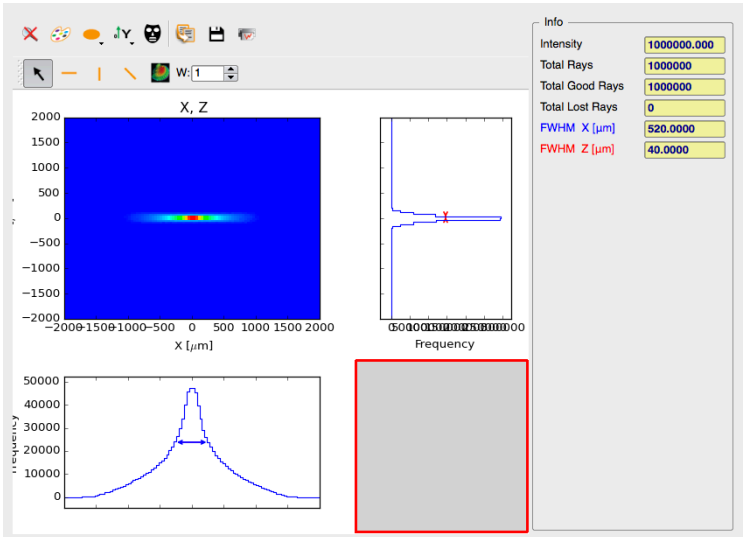
Rebuffi L., Sanchez del Rio M., Busetto E. and Scardi P., “Understanding the instrumental profile of synchrotron radiation X-ray powder diffraction beamlines”, J. Synchrotron Rad. 24 (2017), pp. 622–635. doi: 10.1107/S1600577517005434

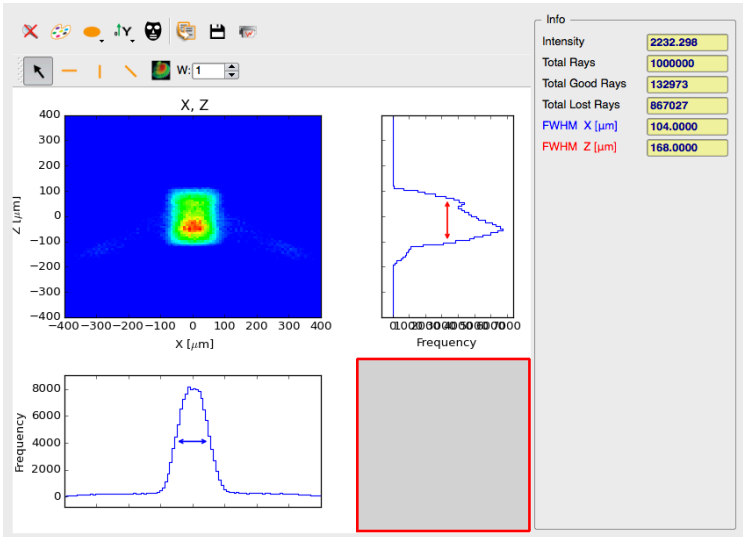
Elettra Sincrotrone Trieste

XRD1

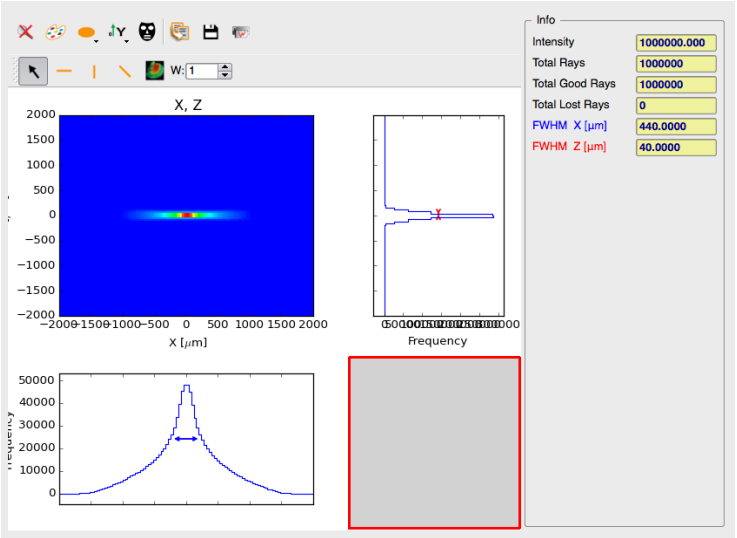
Different solutions with a shorter period (10 and 8 cm) has been studied

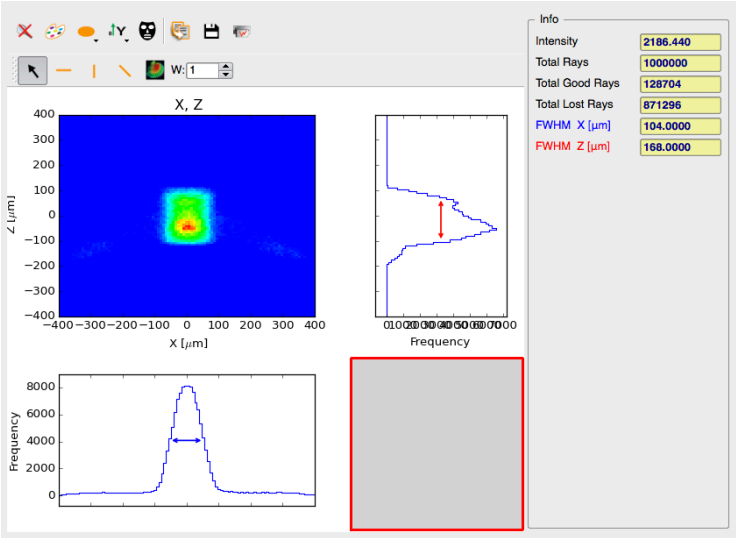
Elettra 2.0 W10





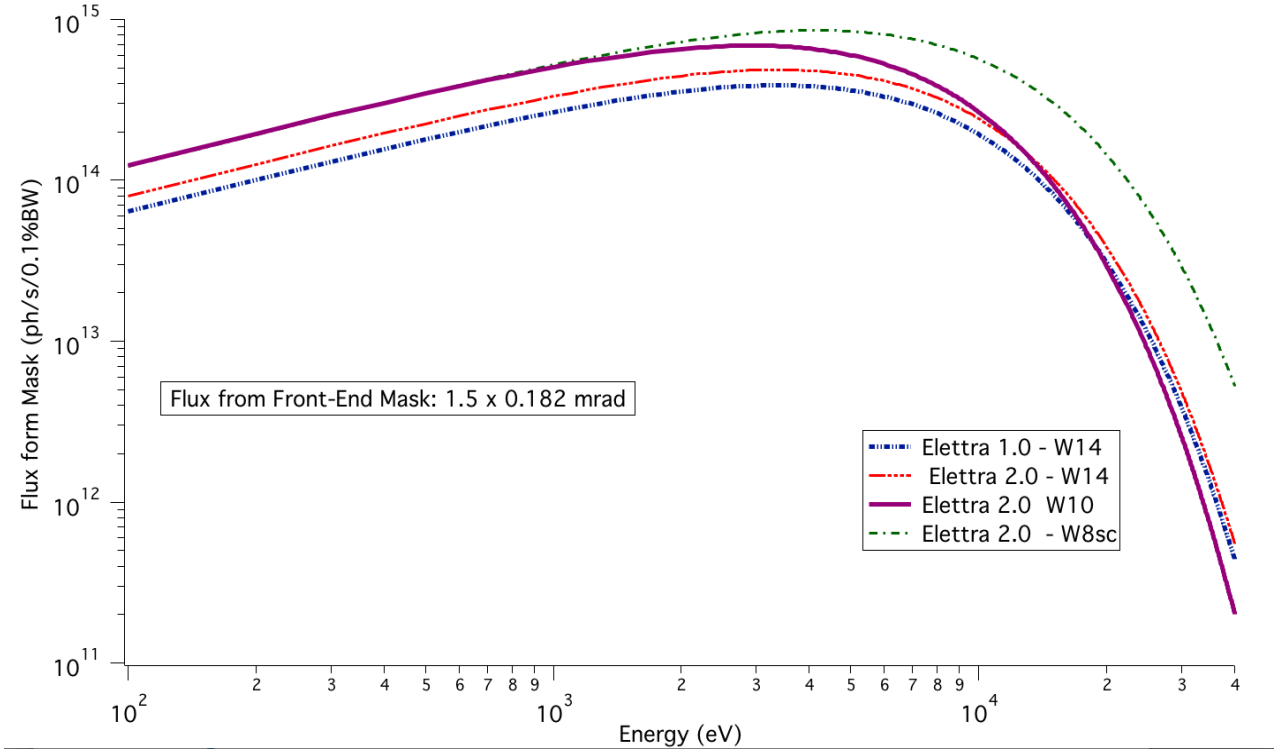
Elettra 2.0 W8sc





Elettra Sincrotrone Trieste

XRD1



FLUX FROM MASK
1.5 x 0.182 mrad

(XOPPY)

	Period (cm)	*Nr. Periods*	*B (T)*	*K*	*Total Power (W)*
Elettra 1.0 (W14)	14.0	29	1.6	21.0	654
Elettra 2.0 (W14)	14.0	29	1.6	21.0	818
Elettra 2.0 (W10)	10.0	41	1.4	13.08	1003
Elettra 2.0 (W8sc)	8.0	51	2.0	14.94	1785

Flux at Sample at 13 KeV
(XOPPY + SHADOWOUI)

	Flux at sample (ph/s)
Elettra 1.0 (W14)	1.09e+12
Elettra 2.0 (W14)	2.32e+12
Elettra 2.0 (W10)	2.49e+12
Elettra 2.0 (W8sc)	6.67e+12

COULD BE CRITICAL!!!

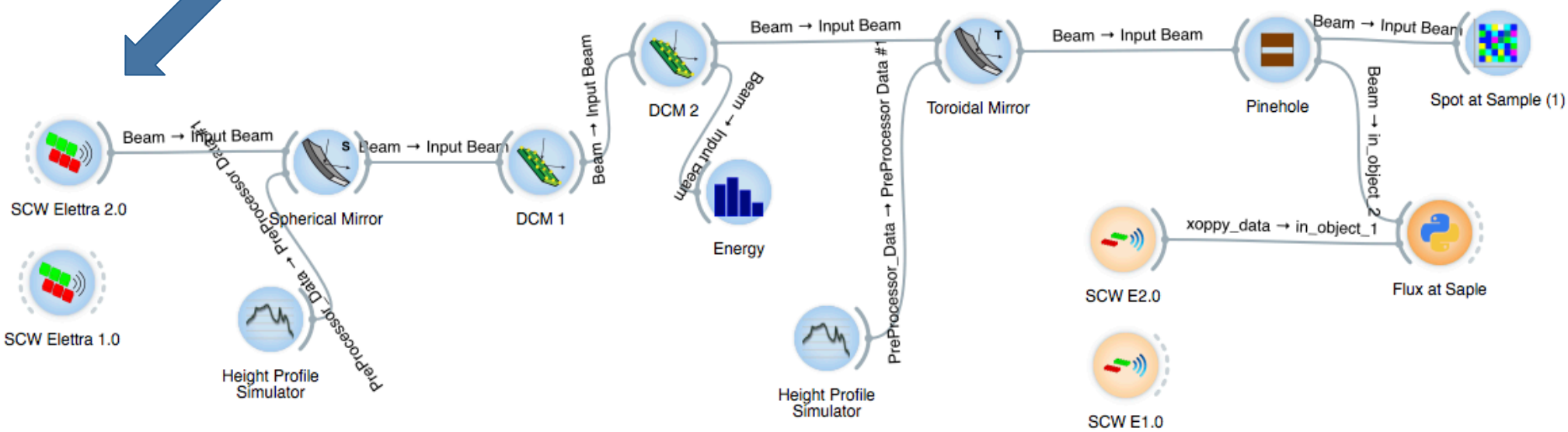
XRD2

XRD2 @ ELETTRA

SUPER-CONDUCTING WIGGLER SOURCE:

- B = 3.5 T
- Period = 0.064 m
- N Periods = 24.5
- K = 20.92

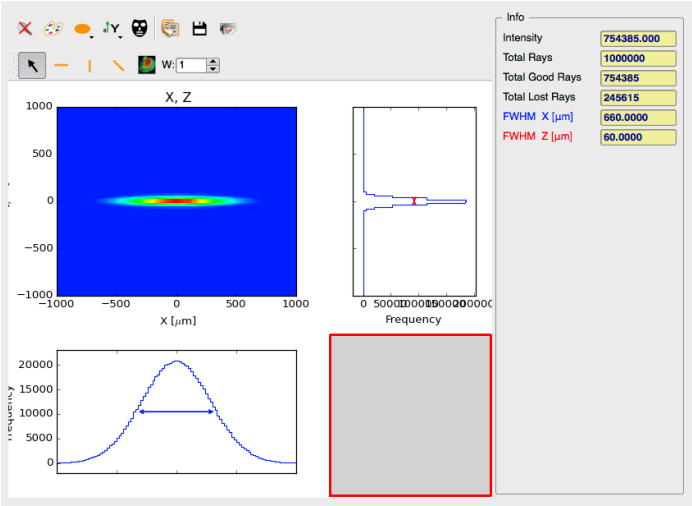
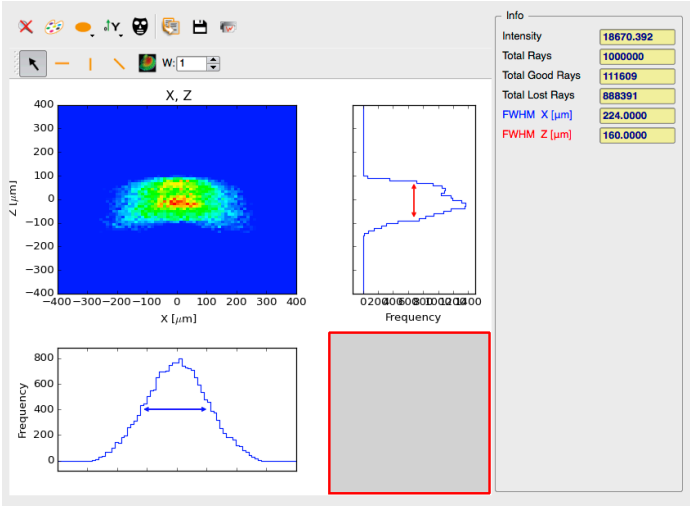
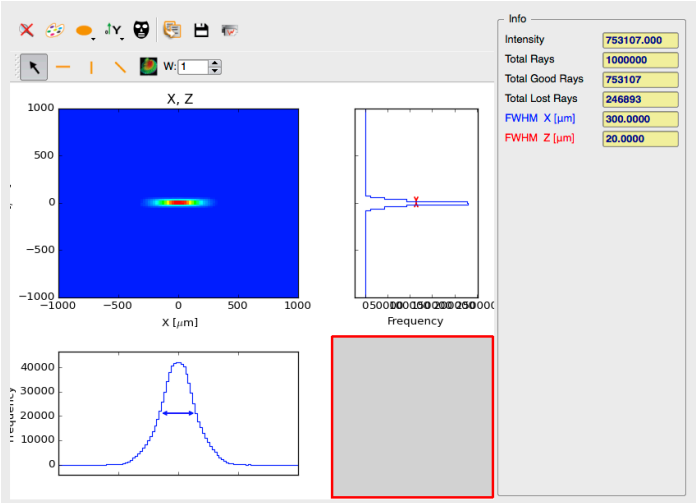
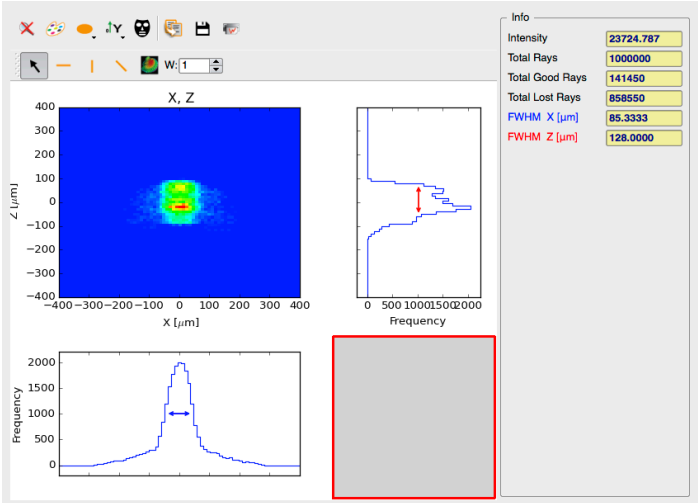
PROTEIN CRYSTALLOGRAPHY



Elettra Sincrotrone Trieste

XRD2

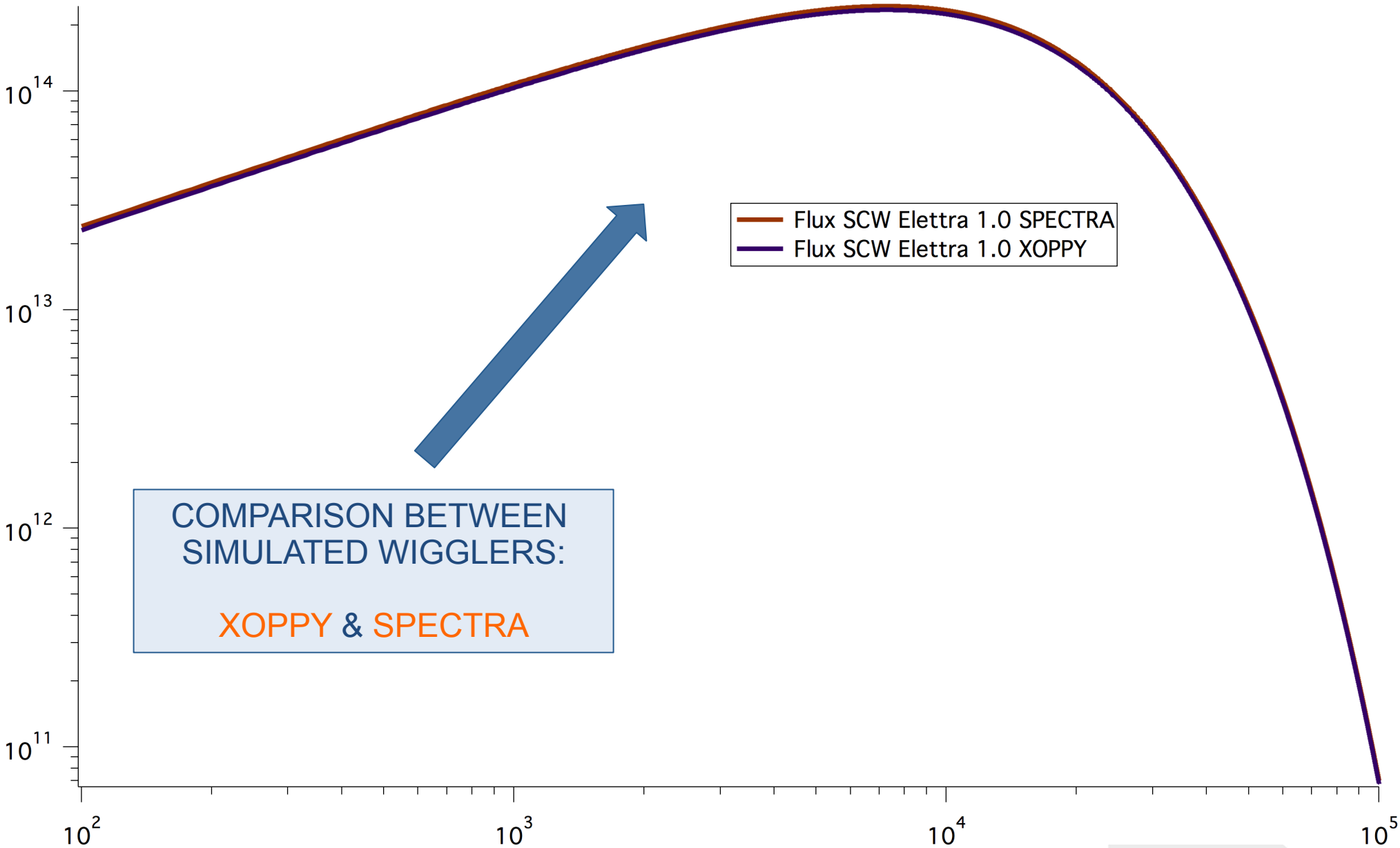
SCW source doesn't show any issue in terms of shape, when running in Elettra 2.0

	Effective Source Size	Beam size at the sample
Elettra 1.0 SCW		
Elettra 2.0 SCW		

Elettra Sincrotrone Trieste

XRD2

BENCHMARK!



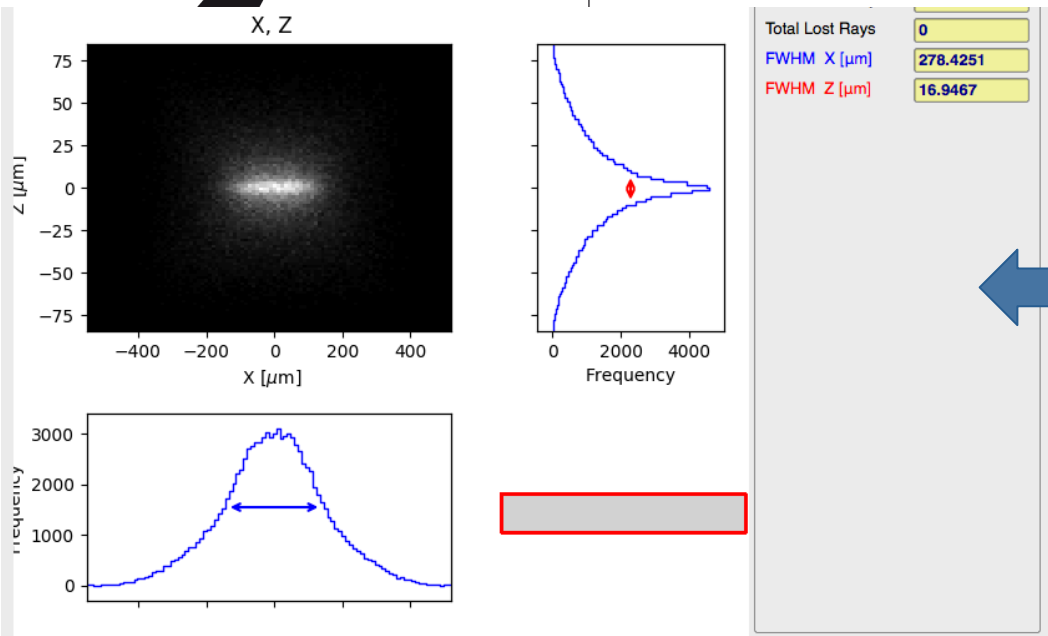
COMPARISON BETWEEN SIMULATED WIGGLERS:

XOPPY & SPECTRA

Elettra Sincrotrone Trieste

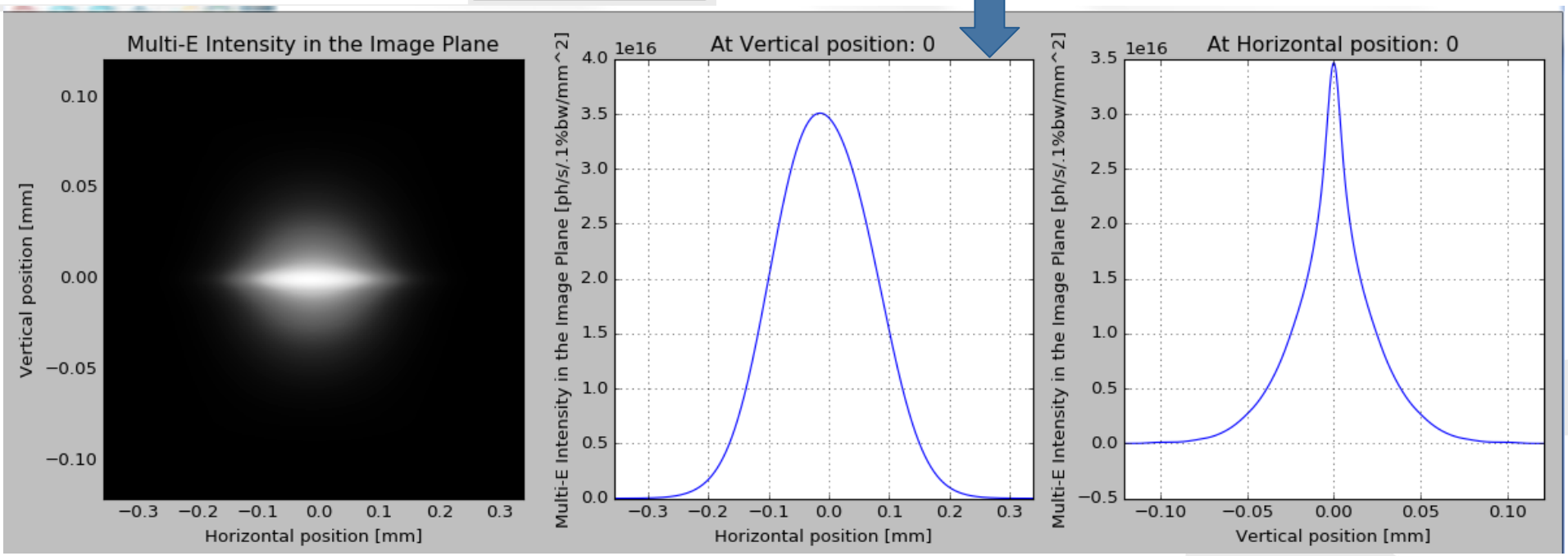
XRD2

BENCHMARK!



COMPARISON BETWEEN SIMULATED WIGGLERS:

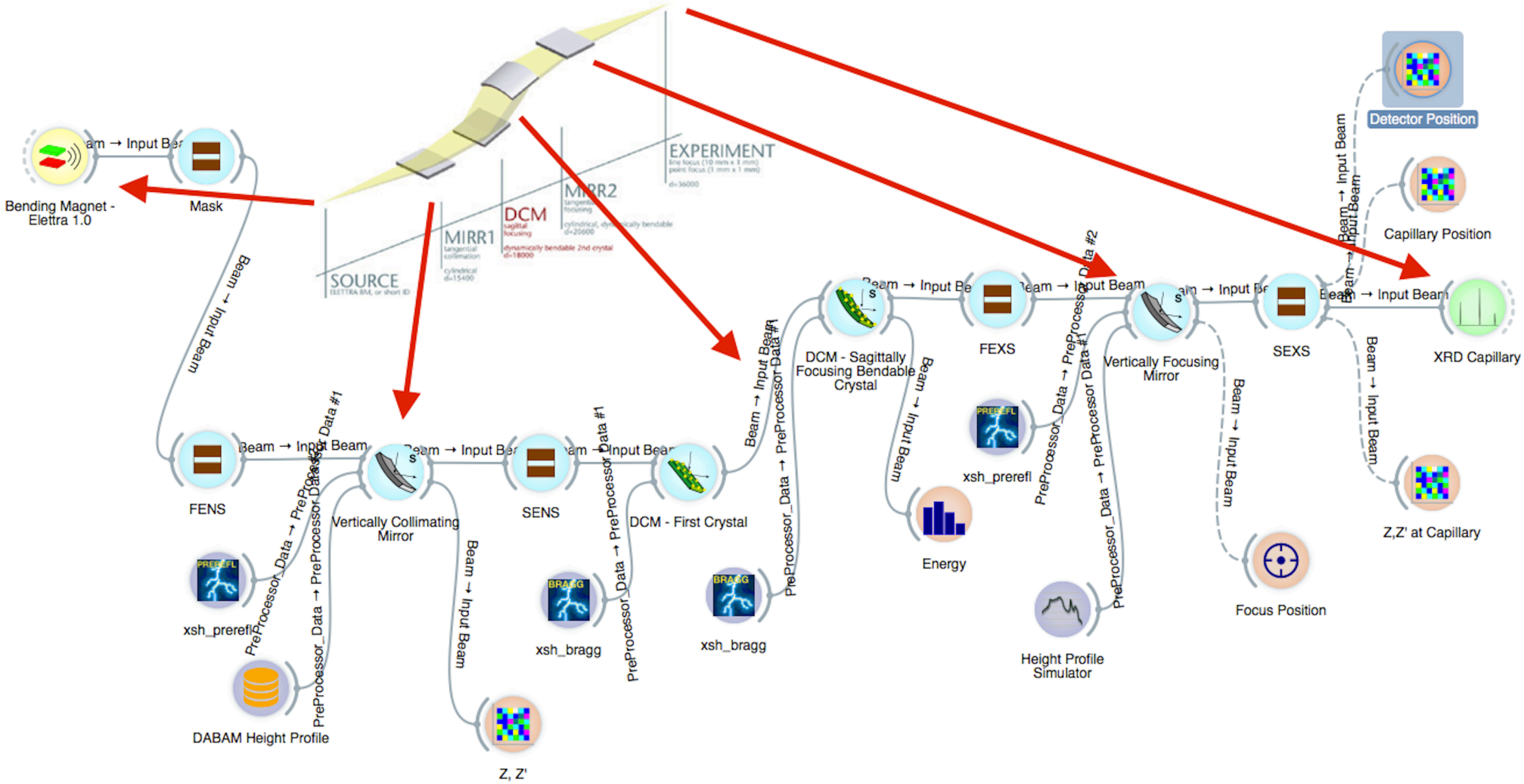
SHADOWOUI
&
SRW (Courtesy of O. Chubar)



Elettra Sincrotrone Trieste

MCX

POWDER DIFFRACTION

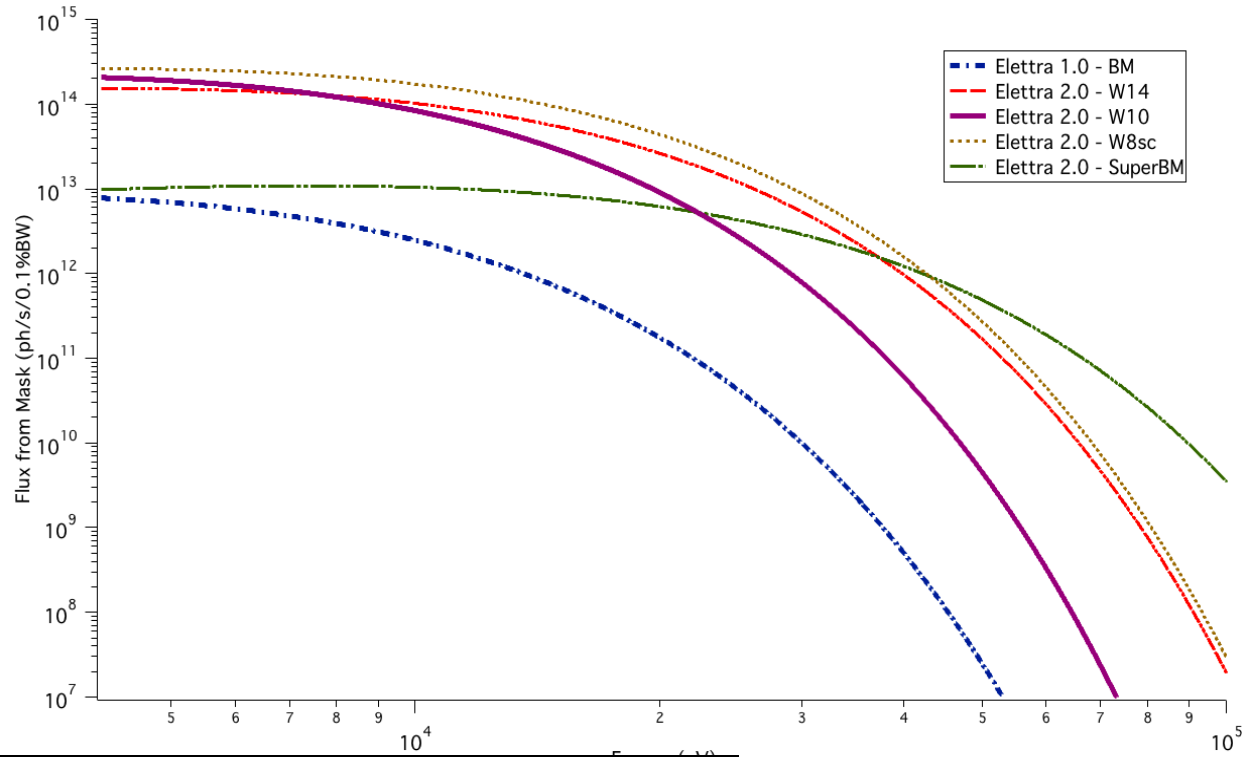


Elettra Sincrotrone Trieste

MCX

FLUX FROM MASK
2.0 x 0.18 mrad

(XOPPY)

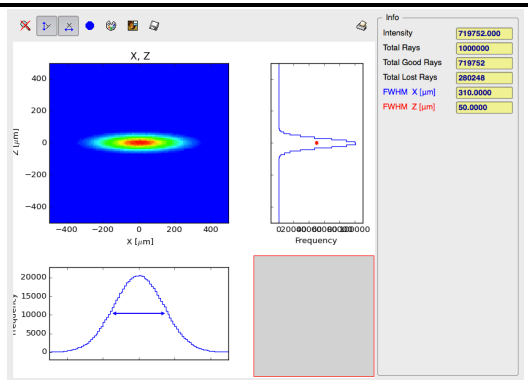
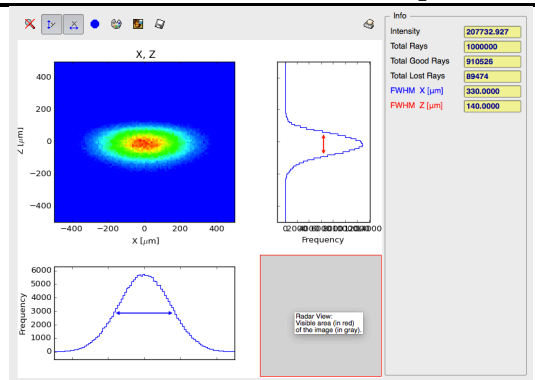
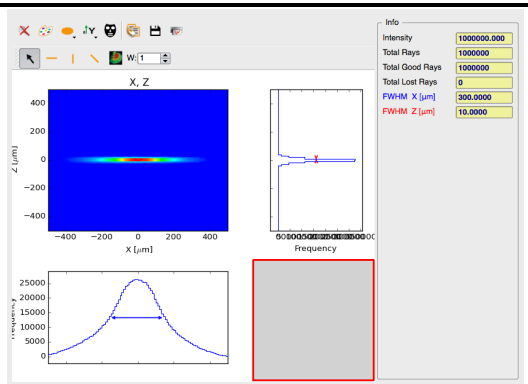
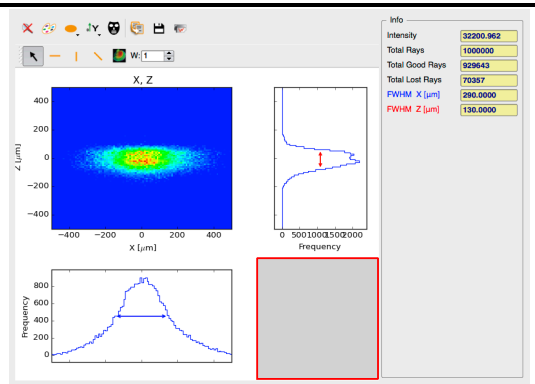
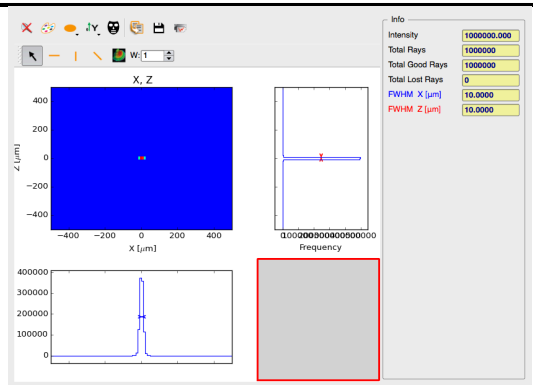
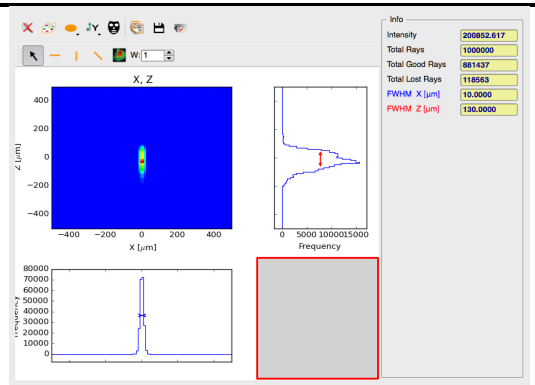


	Period (cm)	*Nr. Periods*	*B (T)*	*K*	*Total Power (W)*
Elettra 1.0 (BM)			1.2		11
Elettra 2.0 (miniW14)	14.0	7	2.0	26.15	319
Elettra 2.0 (miniW10)	10.0	10	1.4	13.08	315
Elettra 2.0 (miniW8sc)	8.0	12	2.0	14.94	543
Elettra 2.0 (superBM)			3.5		40

Flux at Sample
(XOPPY
+
SHADOWOUI)

	Flux at sample (ph/s)		
Energy (keV)	*15*	*27*	*30*
Elettra 1.0 (BM)	1.93e+11	3.11e+09	1.27e+09
Elettra 2.0 (miniW14)	1.49e+13	1.11e+12	6.58e+11
Elettra 2.0 (miniW10)	8.09e+12	2.16e+11	1.01e+11
Elettra 2.0 (miniW8sc)	2.50e+13	1.82e+12	1.09e+12
Elettra 2.0 (superBM)	2.26e+12	4.55e+11	3.50e+11

MCX

	Effective Source Size	Beam size at the sample
Elettra 1.0 BM		
Elettra 2.0 miniW10		
Elettra 2.0 superBM		

OPTICAL PERFORMANCES:

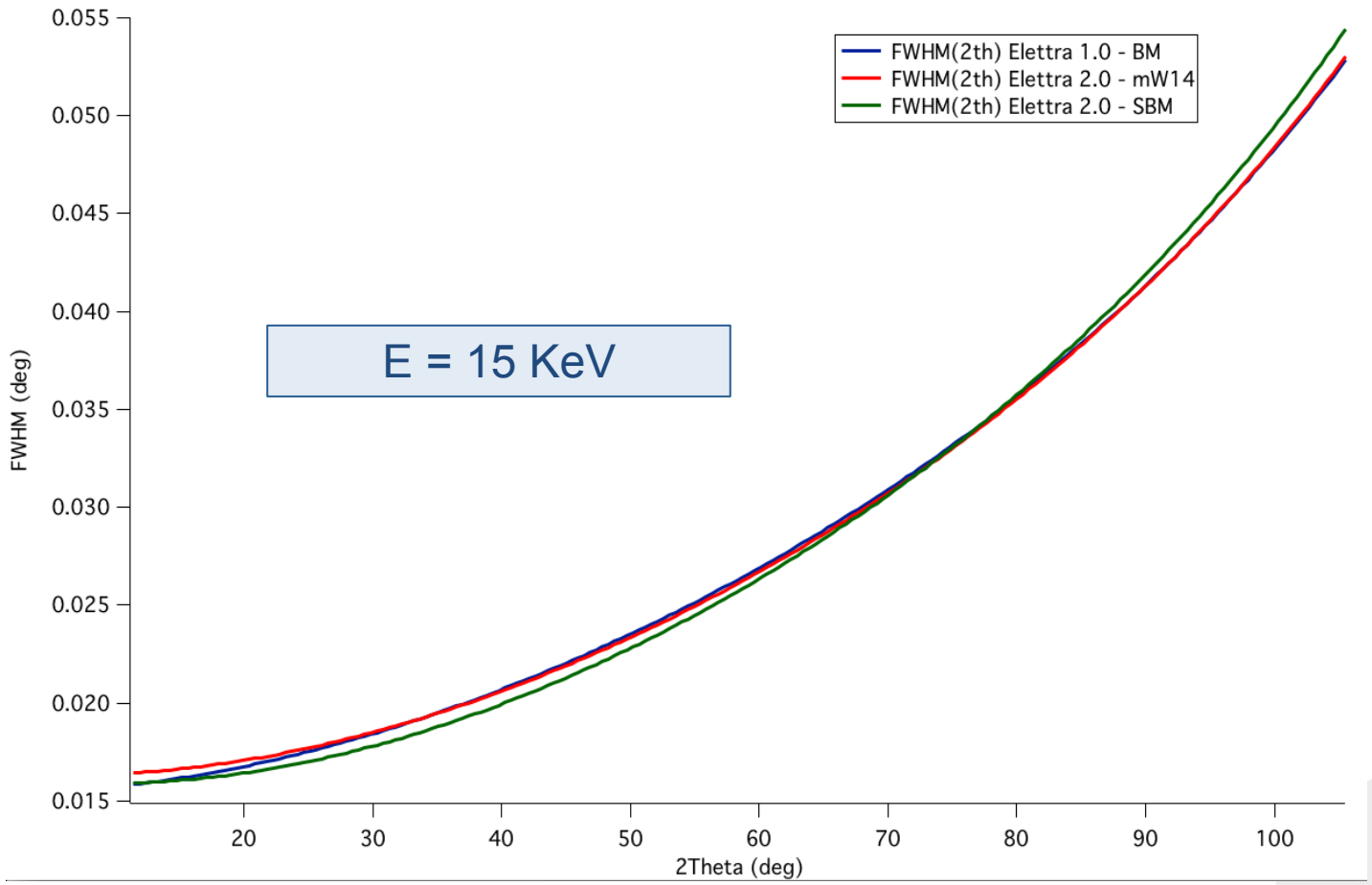
(SHADOWOUI)

THE ELETTRA 2.0 SOURCES AFFECT THE HORIZONTAL DIRECTION

MCX

MCX INTEGRATES SIGNAL IN THE HORIZONTAL DIRECTION:

NO EFFECTS ON THE INSTRUMENTAL PROFILE FUNCTION



Elettra Sincrotrone Trieste

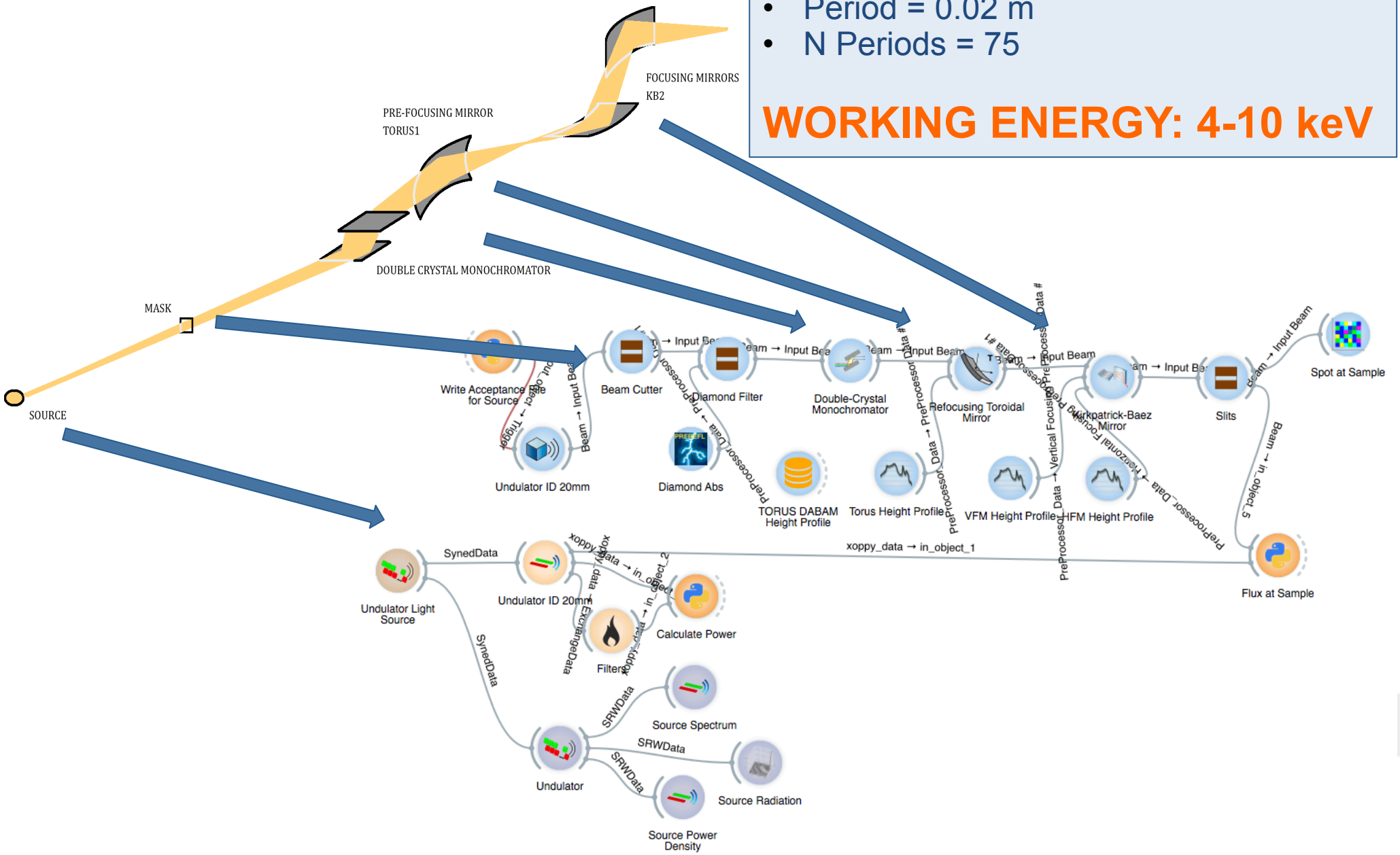
µXRD (NEW)

µXRD @ ELETTRA 2.0

IN-VACUUM UNDULATOR SOURCE:

- K = 1.5 (gap = 6 mm)
- Period = 0.02 m
- N Periods = 75

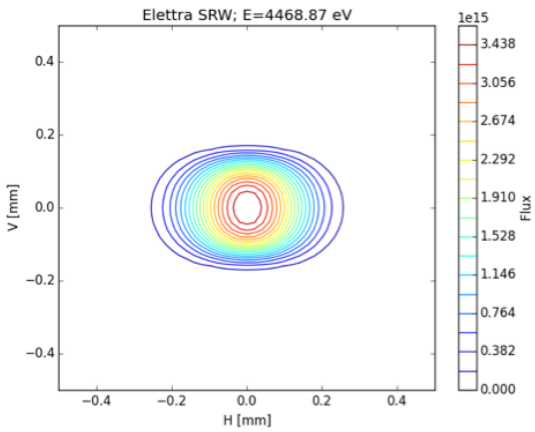
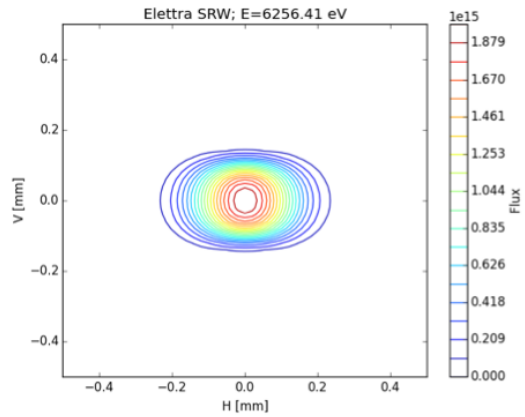
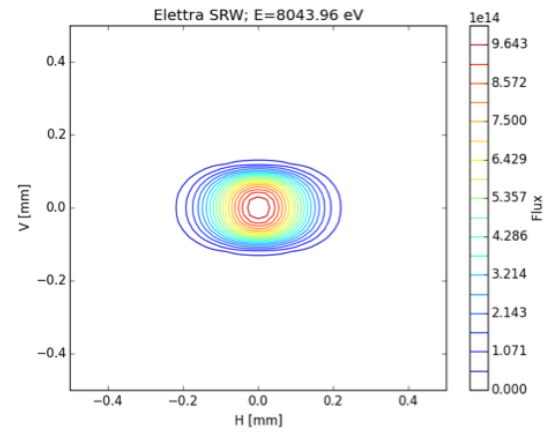
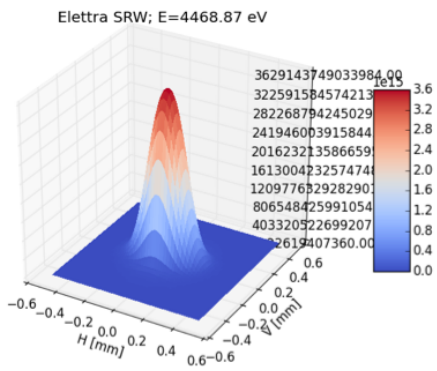
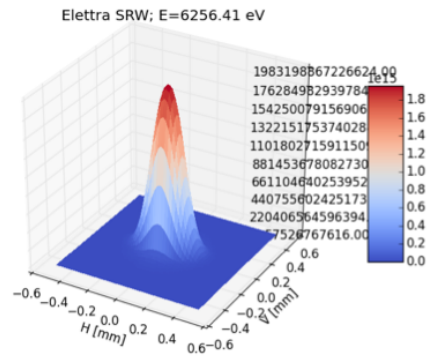
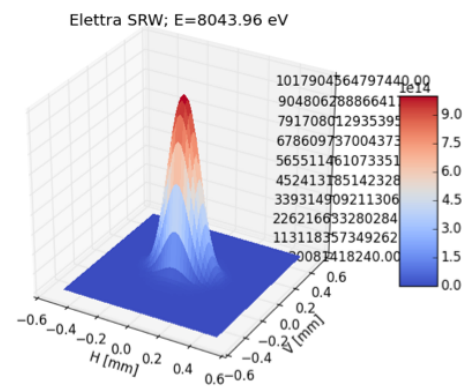
WORKING ENERGY: 4-10 keV



µXRD (NEW)

SOURCE DESIGN (SRW):

FRONT END MASK 0.1 x 0.1 mrad

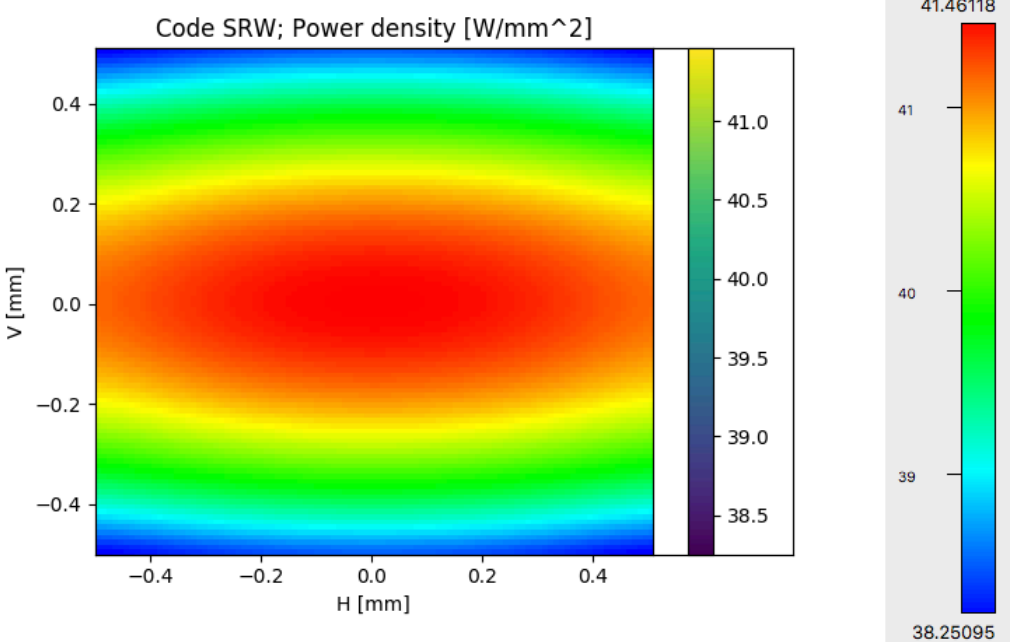
5th Harmonic (4469 eV)	7th Harmonic (6256 eV)	9th Harmonic (8044 eV)
		
		

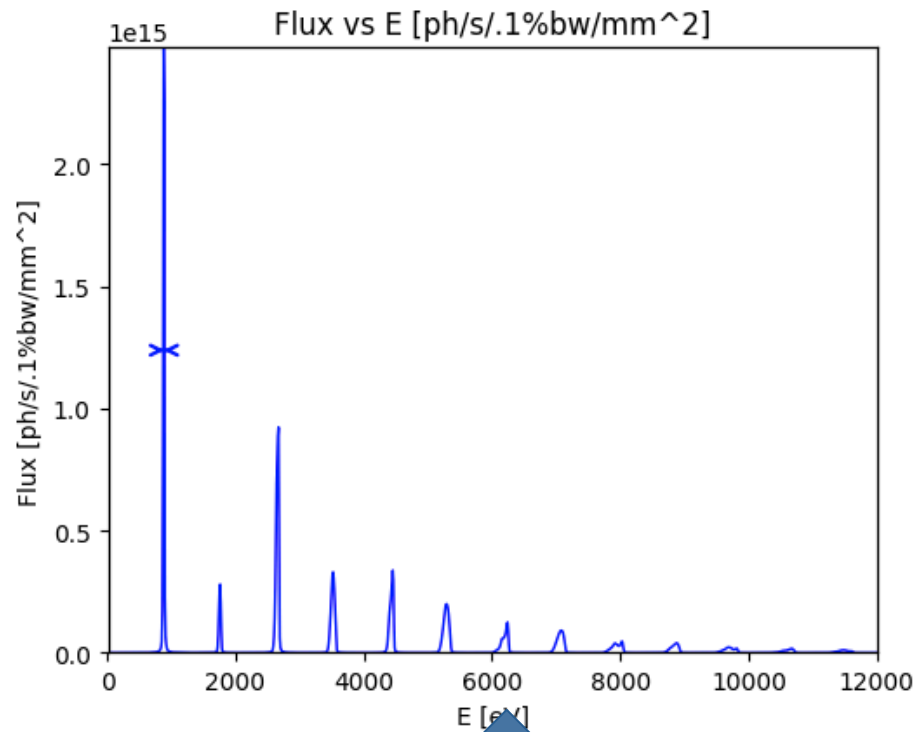
μXRD (NEW)

SOURCE DESIGN (SRW):

FRONT END MASK 0.1 x 0.1 mrad

TOTAL POWER: 41 W



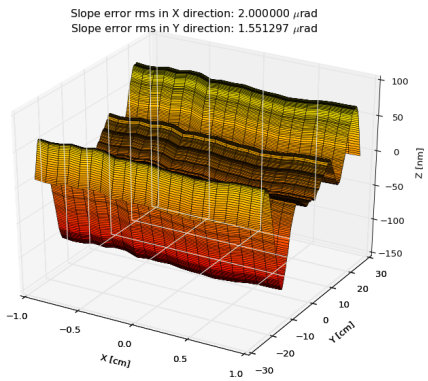
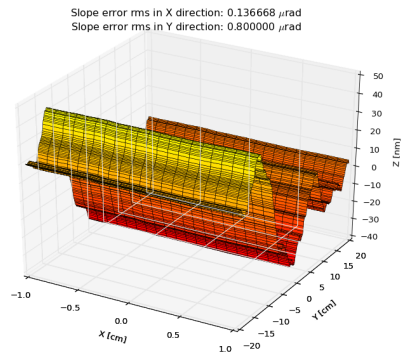
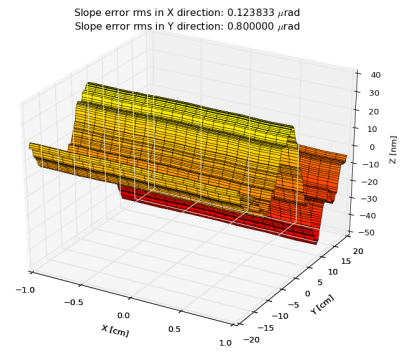


SIMULATION ENERGY:

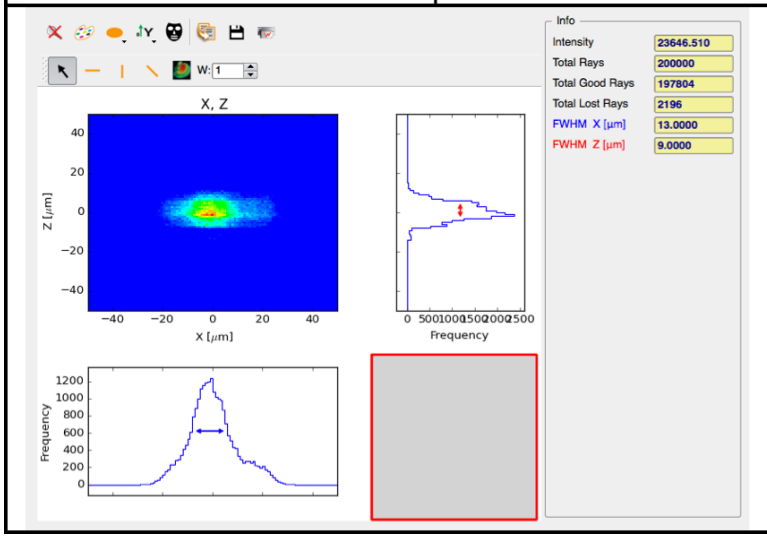
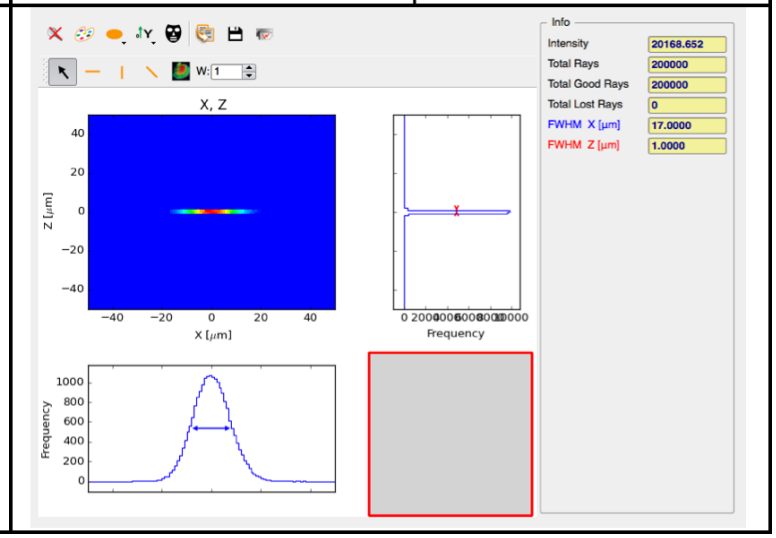
6256.41 eV (7th harmonic)

µXRD (NEW)

OPTICAL LAYOUT (SHADOWOUI)

TORUS1	KB2 Horizontally Focusing Mirror	KB2 Vertically Focusing Mirror
		

REALISTIC OPTICS WITH SIMULATED HEIGHT ERROR PROFILES

Realistic Optics	Ideal Optics
	

SPOT AT SAMPLE:

~ 15 x 10 µm

FLUX AT SAMPLE:

~ 8.0e+12 ph/s

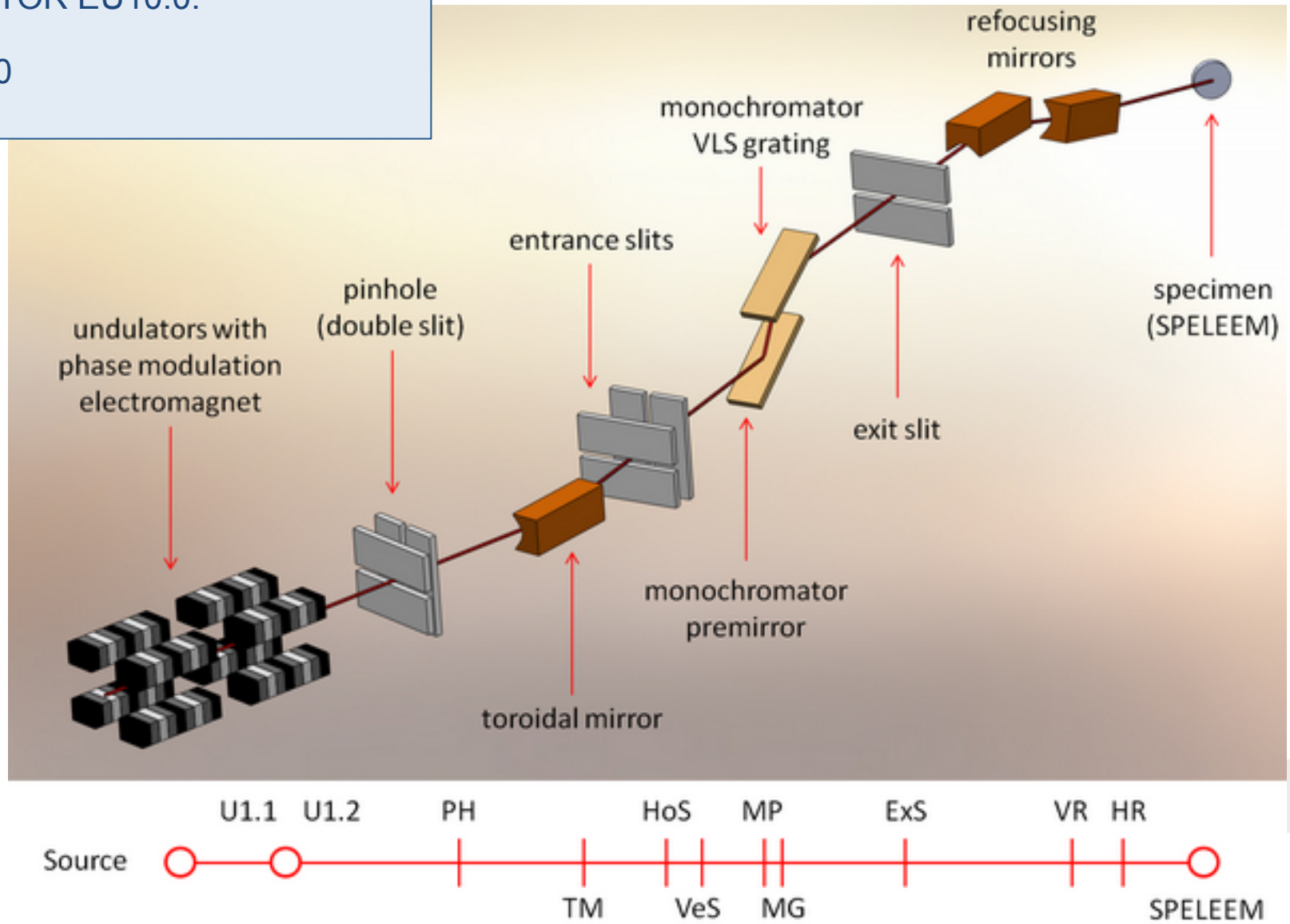
Elettra
Sincrotrone
Trieste

2. Soft X-ray Beamlines

Nanospectroscopy

XPEEM & LEEM

ELLIPTICAL UNDULATOR EU10.0:
- Period = 10 cm
- N Periods = 20 + 20
- Kmax=9.55



Electron beam

Present Elettra (2GeV) vs Elettra 2.0 4-BA and Elettra 2.0 6-BA

E-beam emittance reduction:

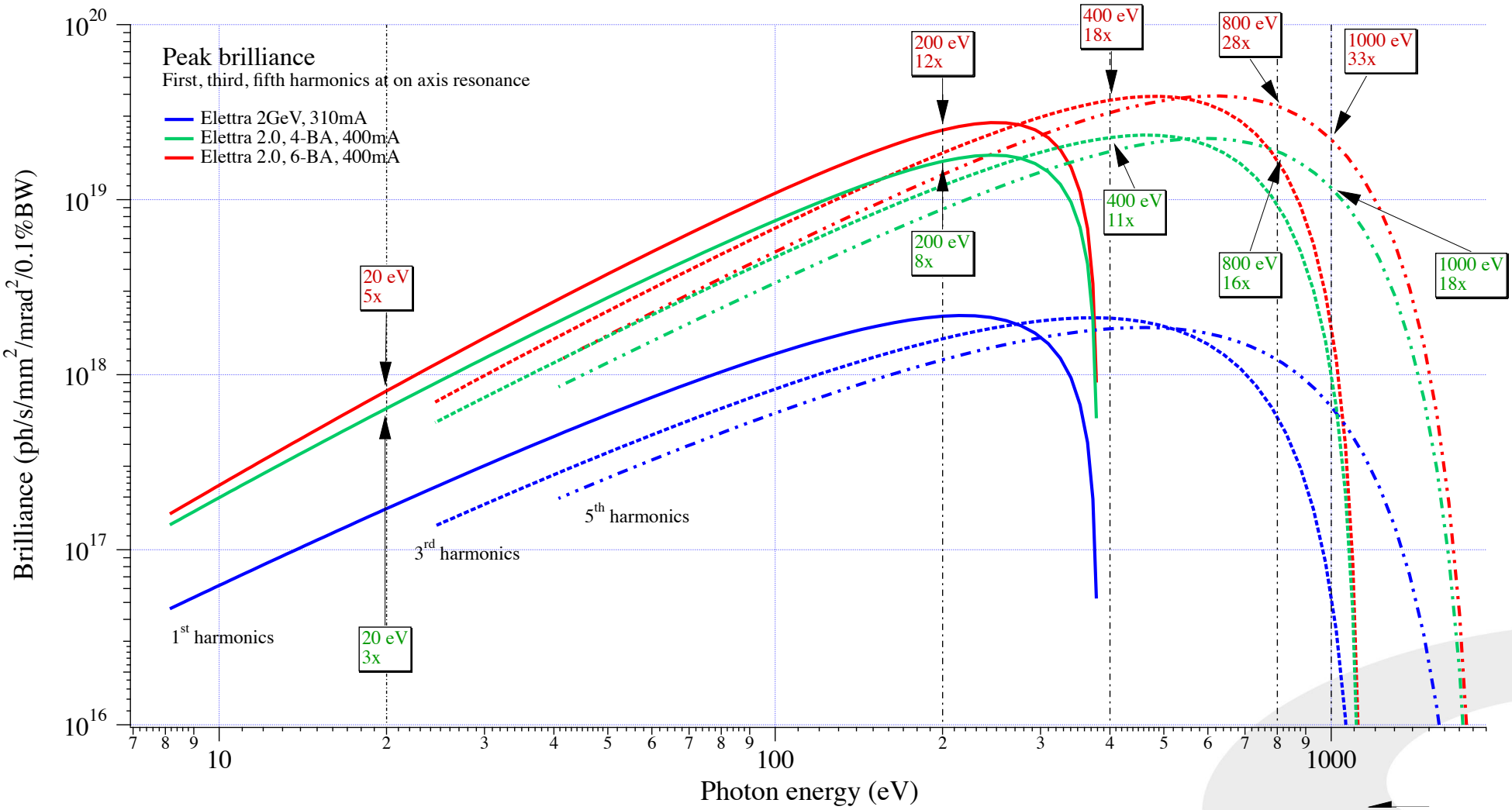
	Present	Upgrade 4-BA	Upgrade 6-BA
ε (nm rad)	7	0.73	0.25

Smaller electron source size and divergence
(center of the long straight section):

	Present	Upgrade 4-BA	Upgrade 6-BA
σ_x (μm)	253	81	55
σ_z (μm)	18	5	3
σ'_x (μrad)	29	9	5
σ'_z (μrad)	5	2	1

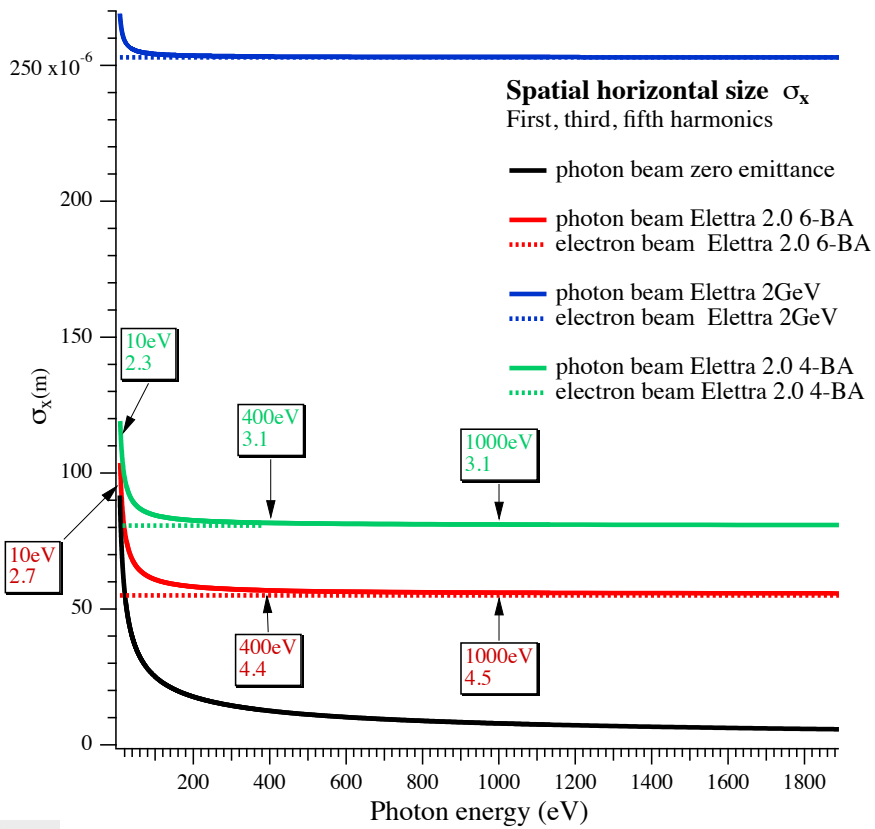
Brilliance - EU10.0 (Horizontal polarization) (SPECTRA)

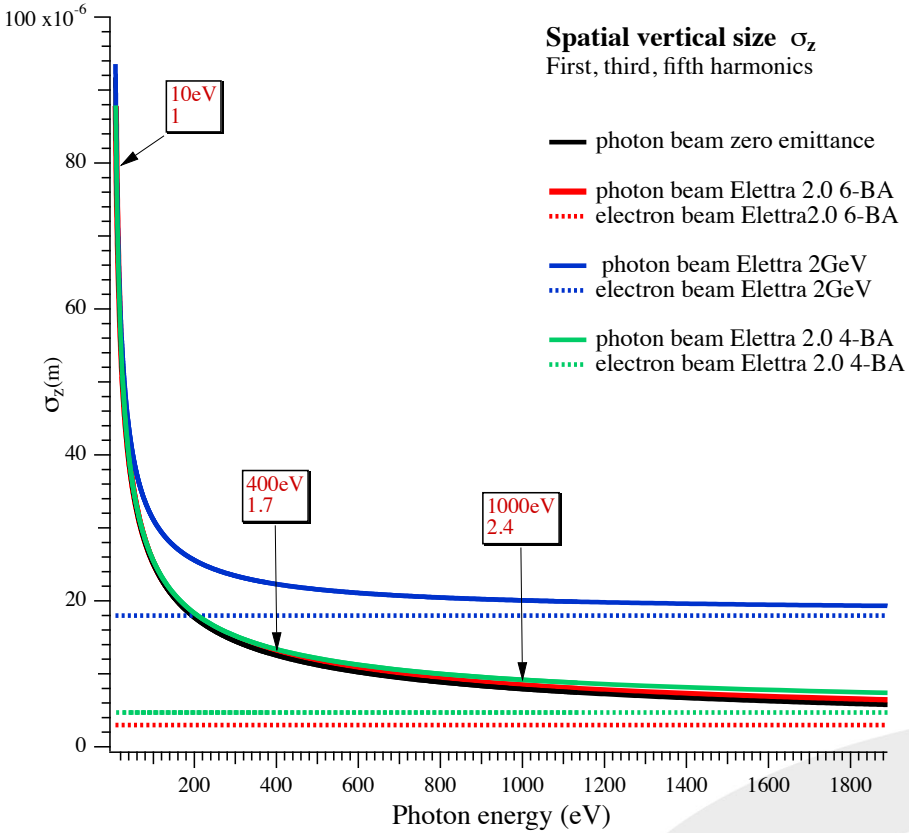
Present Elettra (2GeV) vs Elettra 2.0 4-BA and Elettra 2.0 6-BA



Photon source spatial size - EU10.0 (Horizontal polarization)

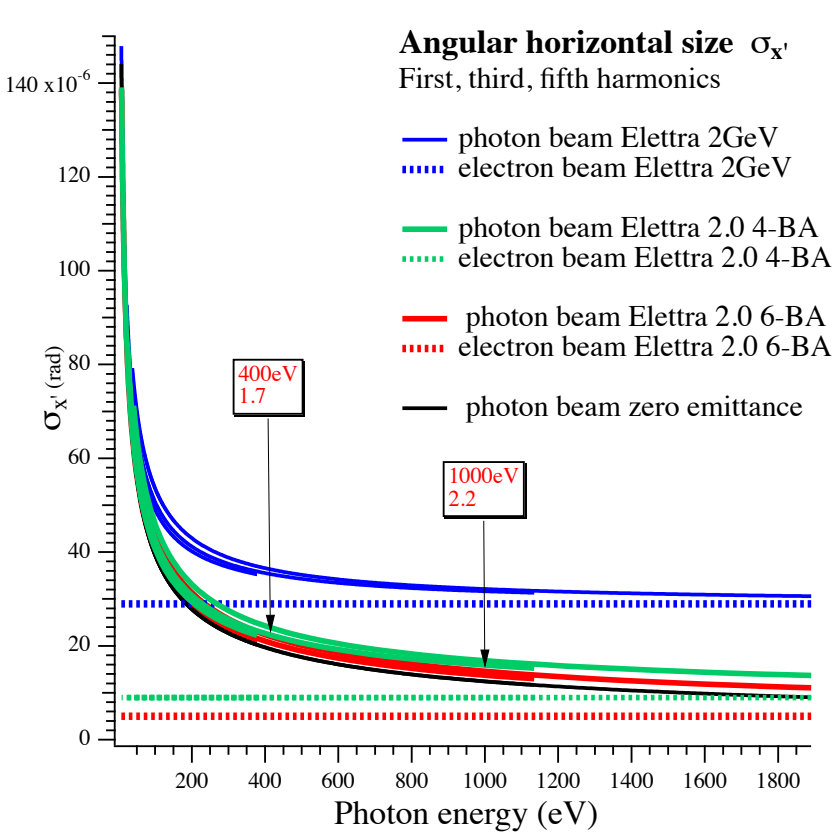
Present Elettra (2GeV) vs Elettra 2.0 4-BA and Elettra 2.0 6-BA

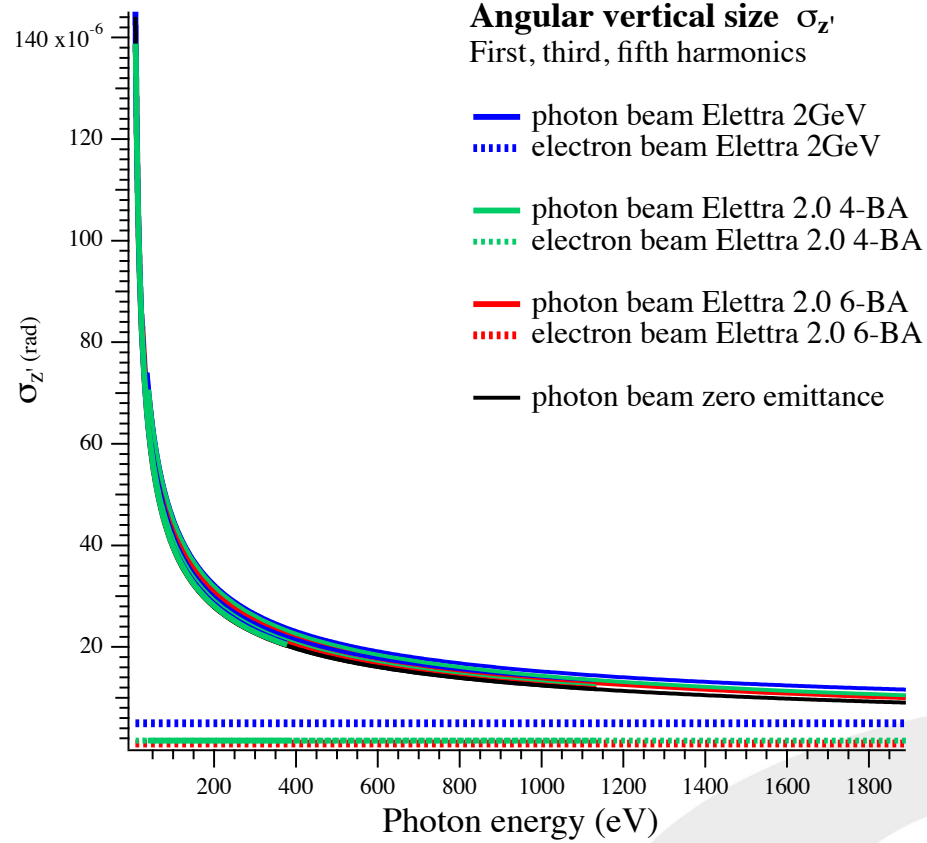




Photon source angular size - EU10.0 (Horizontal polarization)

Present Elettra (2GeV) vs Elettra 2.0 4-BA and Elettra 2.0 6-BA





Case study: photon source 400eV - EU10.0 (Horizontal polar.)

	'natural' undulator emission
σ_r (μm)	12
σ'_r (μrad)	20

(*)reduction factors

	Present	Upgrade 4-BA	Upgrade 6-BA
Σ_x (μm)	253	82 (3.1)(*)	57 (4.4)
Σ_z (μm)	22	13 (1.7)	13 (1.7)
Σ'_x (μrad)	35	23 (1.6)	21 (1.7)
Σ'_z (μrad)	21	21 (1)	21 (1)

In horizontal plane:
- Reduced source size (**3.1**; **4.4**)
- Reduced divergence (**1.6**; **1.7**)

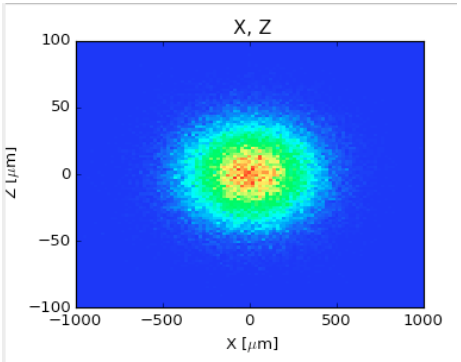
In vertical plane:
- Reduced source size (**1.7**; **1.7**)
- Almost unchanged divergence

Nanospectroscopy

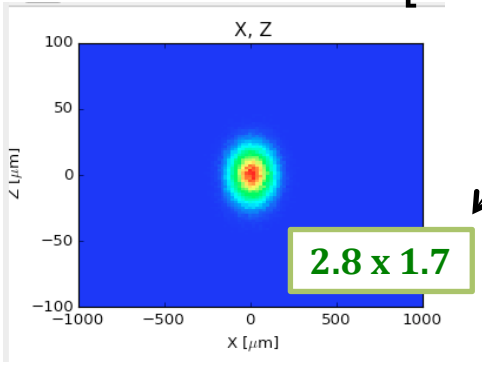
Raytracing at 400 eV (SHADOWOUI)

Present Elettra | **Elettra 2.0 4-BA** | **Elettra 2.0 6-BA**

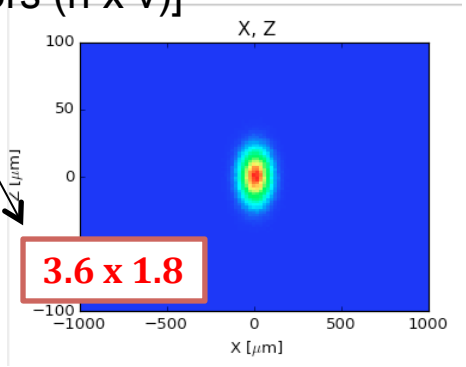
Effective source at 400eV [reduction factors (h x v)]



479 μm * 50 μm FWHM

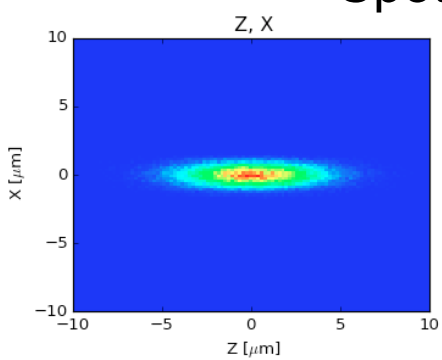


171 μm * 30 μm FWHM

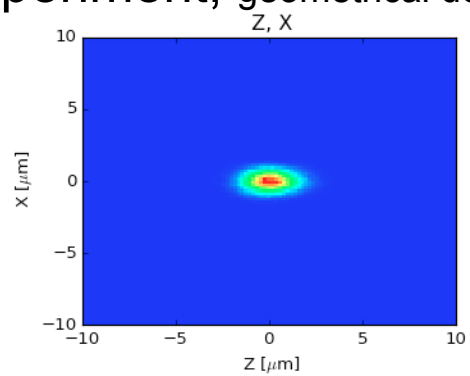


132 μm * 28 μm FWHM

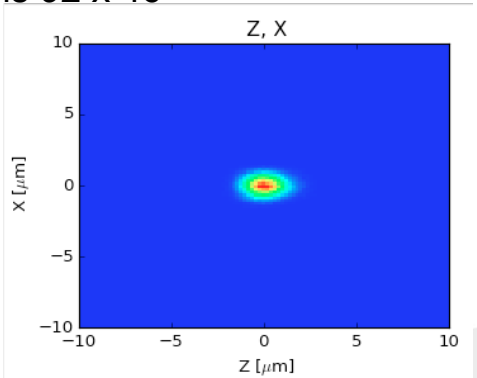
Spot at the experiment, geometrical demagnifications 92 x 46



5.7 μm * 1.3 μm FWHM



2.2 μm * 1.2 μm FWHM



1.7 μm * 1.2 μm FWHM

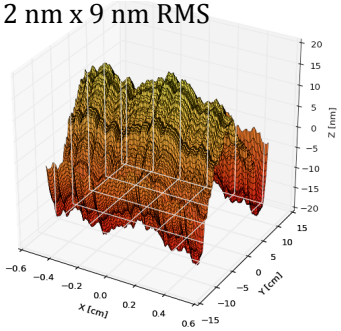
Present beamline but optical elements with enhanced surface quality requirements!

With "reasonable" optics, source properties are carried out at the experiment!!!!!

Raytracing at 400 eV (SHADOWOUI)

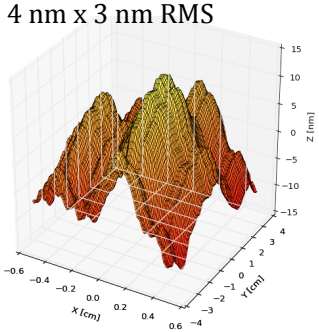
Simulated optical profiles with shape errors obtained reducing measured profiles:

Toroidal mirror
5.7 μrad x 0.7 μrad RMS
2 nm x 9 nm RMS



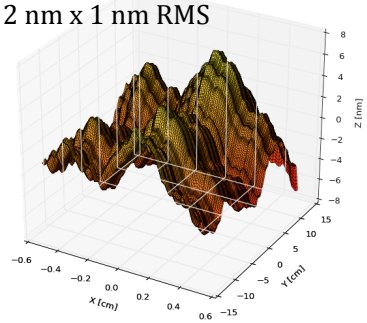
100 mm x 10 mm

VLS grating
6 μrad x 0.5 μrad RMS
4 nm x 3 nm RMS



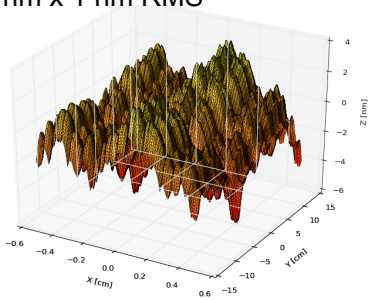
80 mm x 10 mm

VRM plane elliptical bendable mirror
2.6 μrad x 0.1 μrad RMS
2 nm x 1 nm RMS



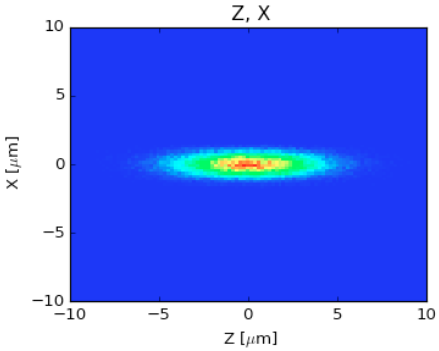
300 mm x 10 mm

HRM plane elliptical bendable mirror
3.7 μrad x 0.1 μrad RMS
1 nm x 1 nm RMS



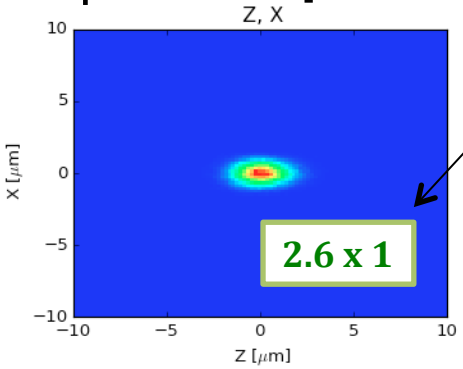
300 mm x 10 mm

Spot at the experiment [reduction factors (h x v)]



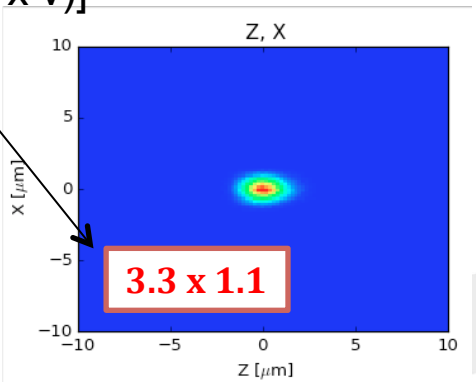
5.7 μm * 1.3 μm FWHM

Present Elettra



2.2 μm * 1.2 μm FWHM

Elettra 2.0 4-BA

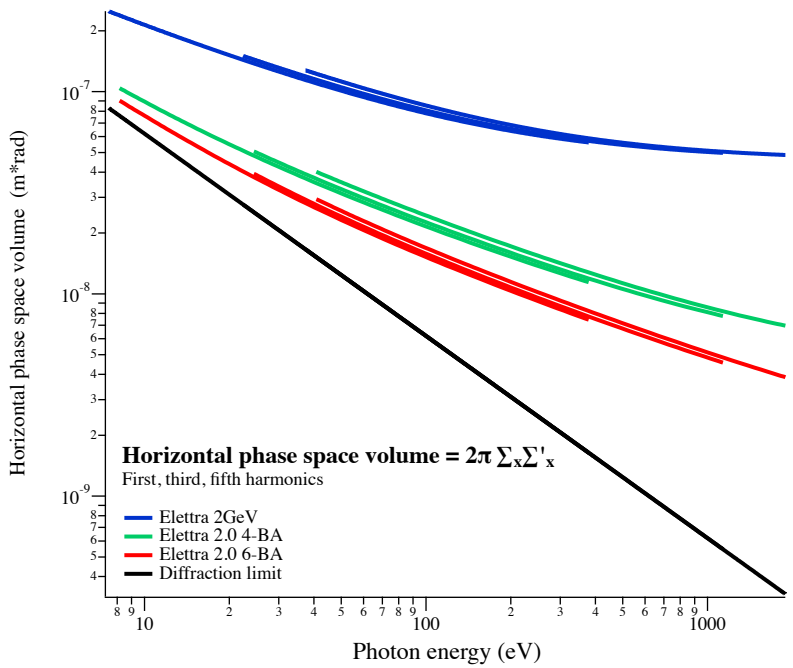


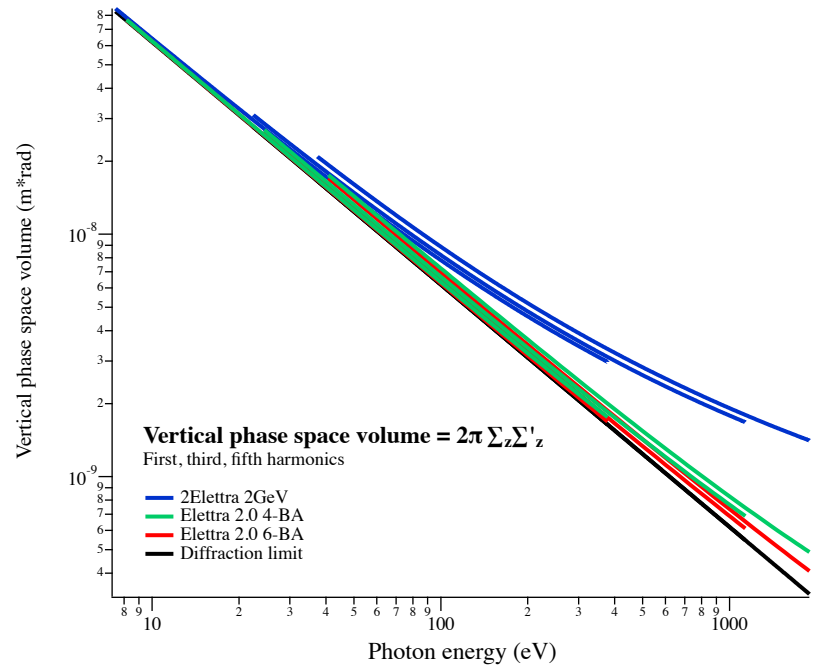
1.7 μm * 1.2 μm FWHM

Elettra 2.0 6-BA

Phase space volume - EU10.0 (Horizontal polarization)

Present Elettra (2GeV) vs **Elettra 2.0 4-BA** and **Elettra 2.0 6-BA**

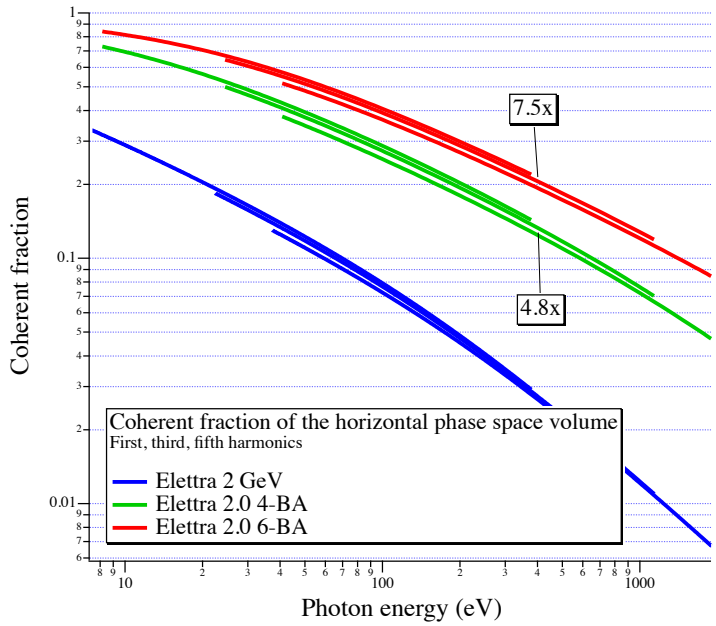


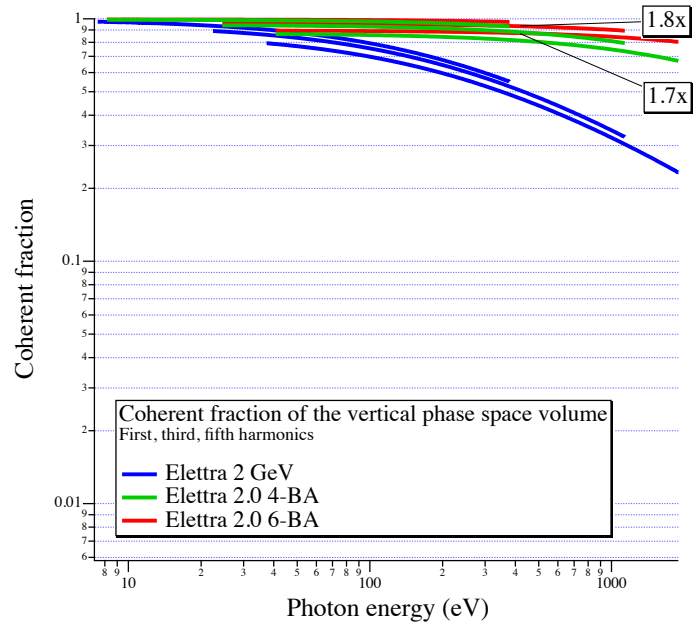


Elettra 2.0 4-BA and 6-BA: in vertical plane almost diffraction limited up to 1 keV

Coherent fraction - EU10.0 (Horizontal polarization)

Present Elettra (2GeV) vs Elettra 2.0 4-BA and Elettra 2.0 6-BA



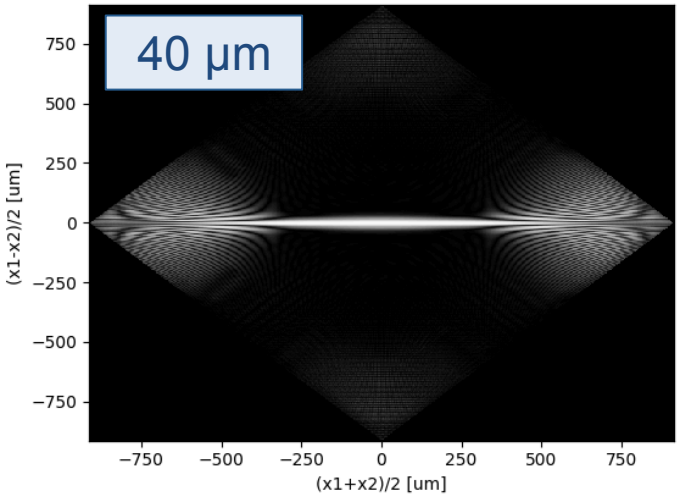


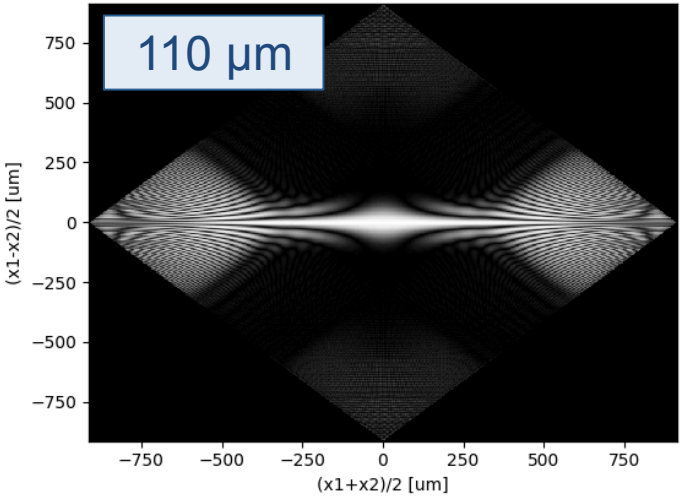
Elettra 2.0 4-BA and 6-BA: in vertical plane almost diffraction limited up to 1 keV

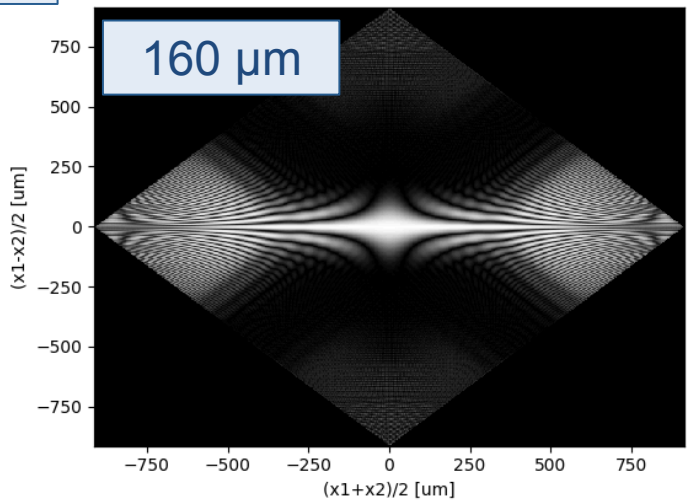
CALCULATION OF COHERENCE LENGTH WITH SRW – MULTI-ELECTRON (TORUS POSITION)

Present Elettra (2GeV) | **Elettra 2.0 4-BA** | **Elettra 2.0 6-BA**

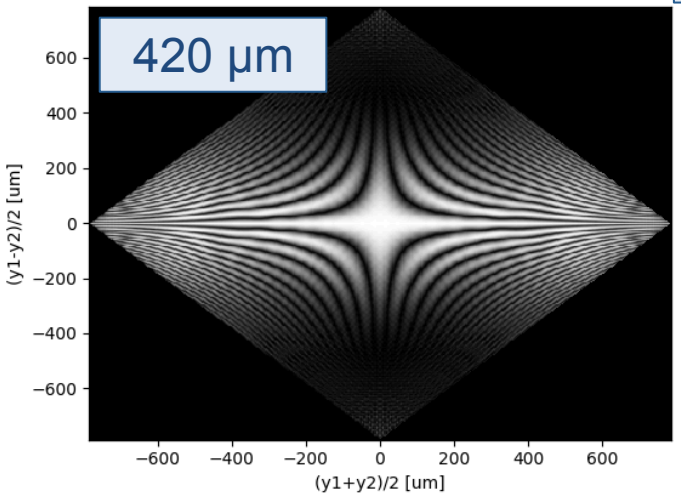
HORIZONTAL DIRECTION

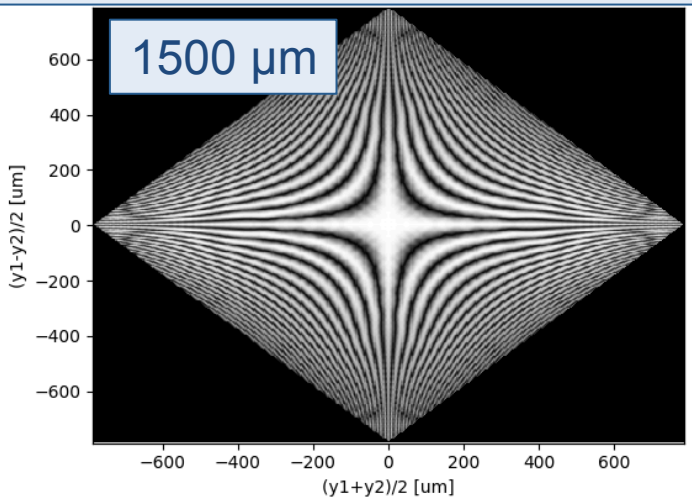


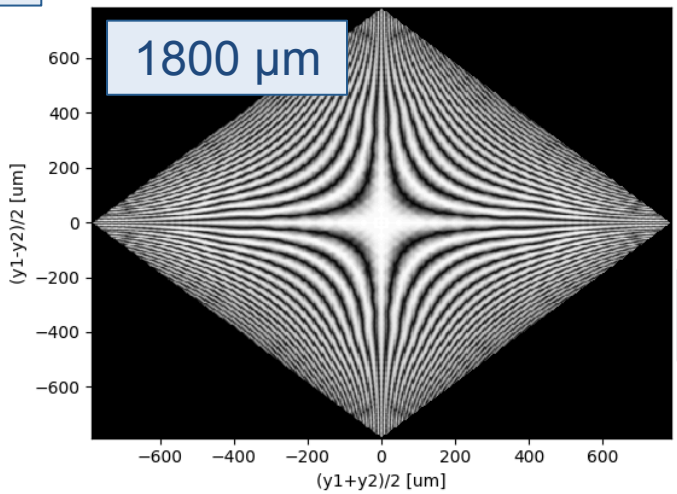




VERTICAL DIRECTION







Nanospectroscopy

INCREASED DEGREE OF COHERENCE

NEED FOR **WAVE OPTICS CALCULATIONS**

ACCURATE CALCULATIONS WITH FULL AND PARTIAL COHERENCE RADIATION :

SRW MULTI-ELECTRON (+ COMSYL)

ACCURATE CALCULATIONS OF SCATTERING OF COHERENT LIGHT FROM MIRRORS + HEIGHT ERROR PROFILES + μ-ROUGHNESS:

WISE

SRW:
2D HEIGHT ERROR PROFILE FOR TORUSES NOT YET IMPLEMENTED

COMSYL:
TO BE RELEASED SOON

WISE:
WISE 2.0 (MULTI-REFLECTION) TO BE RELEASED SOON

Elettra Sincrotrone Trieste

Nanospectroscopy WORK IN PROGRESS

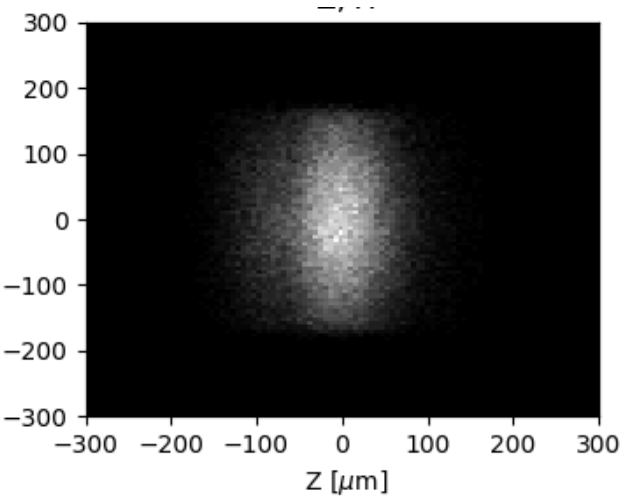
BENCHMARK!

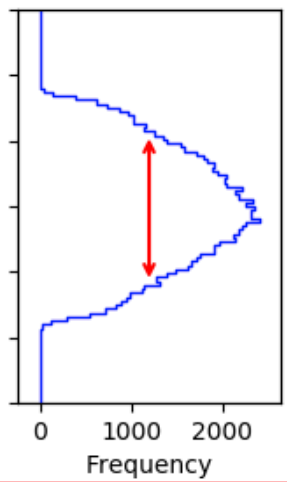
WORK IN PROGRESS

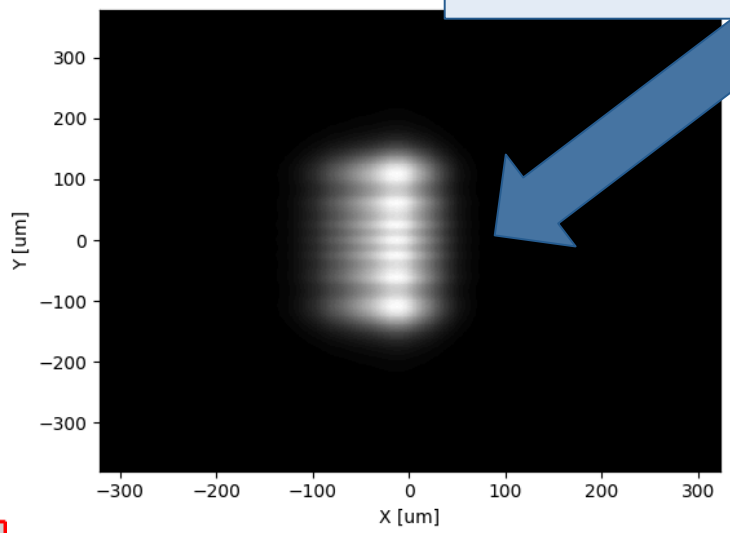
INTENSITY AT TORUS HORIZONTAL FOCUS
SHADOWOUI & SRW – MULTI-ELECTRON

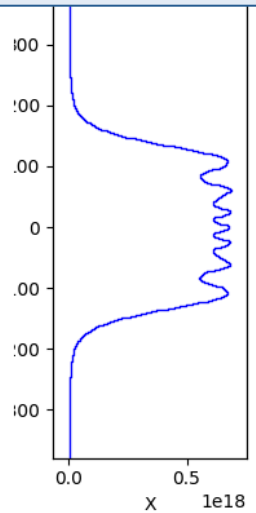
Present Elettra (2GeV)

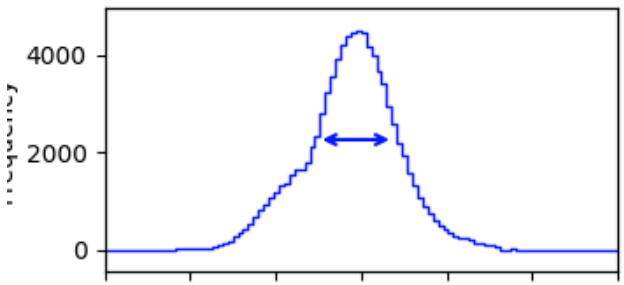
DIFFRACTION FROM FRONT END MASK EFFECTS

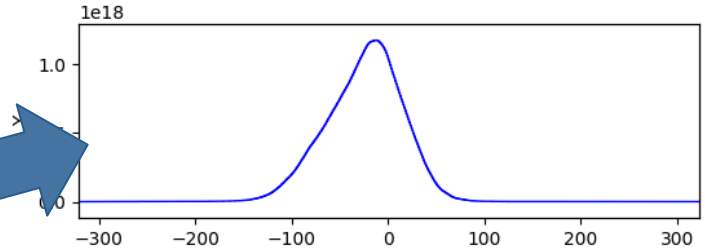












SRW WITH 1D ERROR PROFILE!!!!!

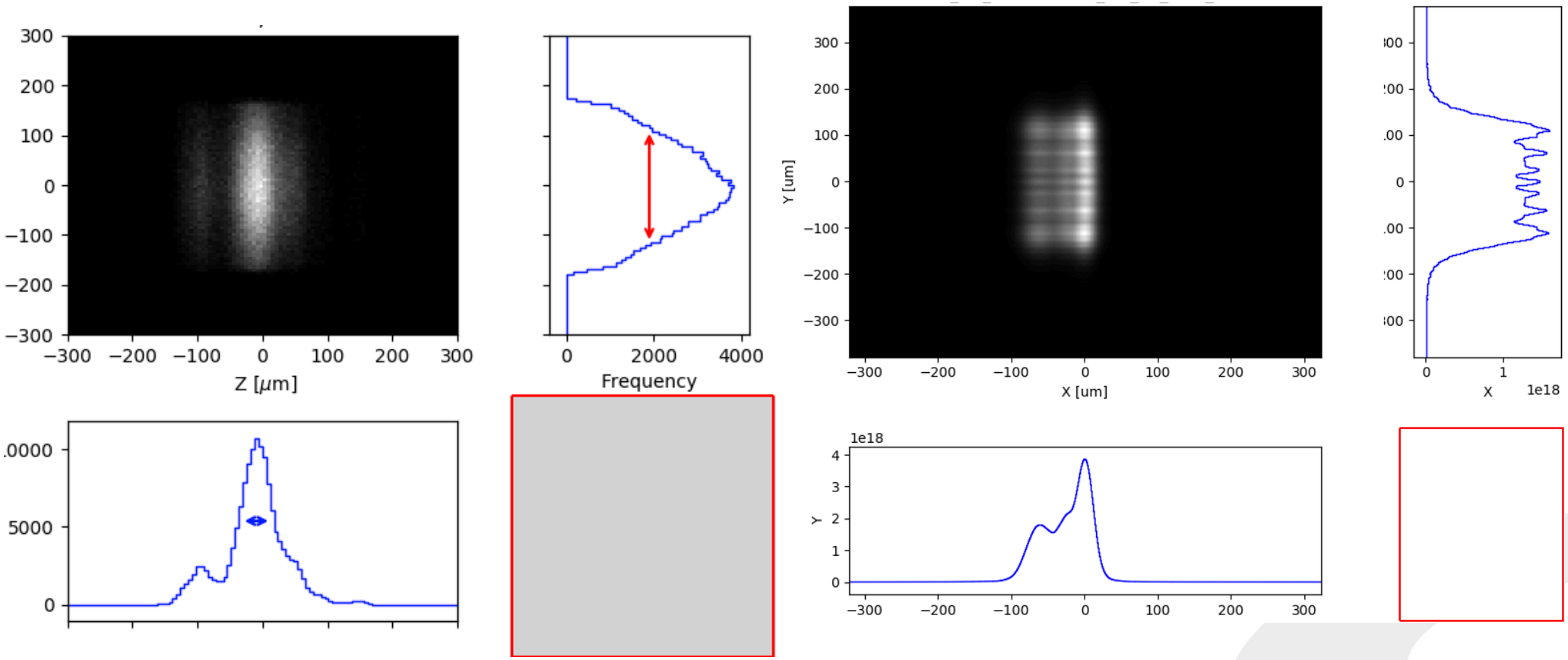
Elettra Sincrotrone Trieste

Nanospectroscopy WORK IN PROGRESS

BENCHMARK!

INTENSITY AT TORUS HORIZONTAL FOCUS
SHADOWOUI & SRW – MULTI-ELECTRON

Elettra 2.0 4-BA



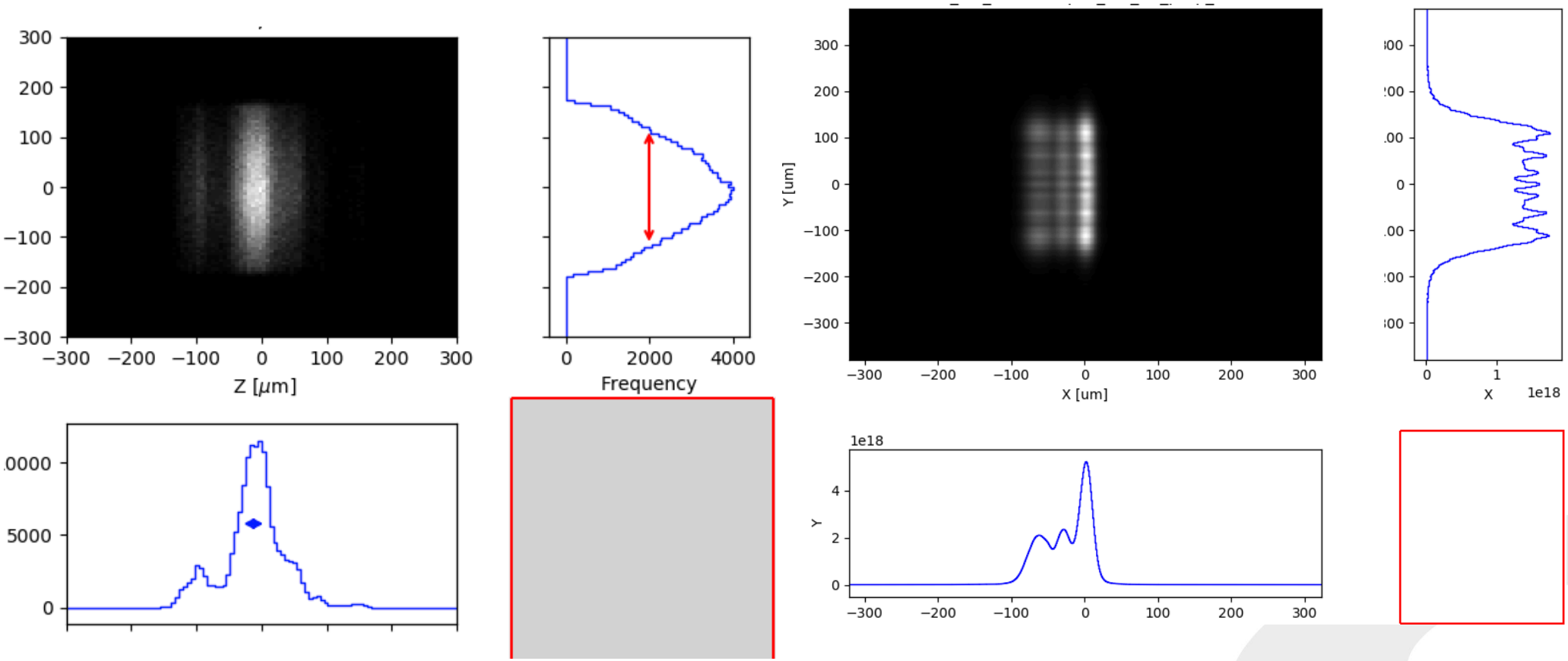
Elettra Sincrotrone Trieste

Nanospectroscopy WORK IN PROGRESS

BENCHMARK!

INTENSITY AT TORUS HORIZONTAL FOCUS
SHADOWOUI & SRW – MULTI-ELECTRON

Elettra 2.0 6-BA



Elettra Sincrotrone Trieste

Nanospectroscopy
WORK IN PROGRESS

WISE – progress bar

Github repository https://github.com/lucarebuffi/wiselib

OASYS download at https://www.elettra.trieste.it/oasys.htm

Coded in Python 3.0

Involved people: L. Raimondi, M. Manfredda, L. Rebuffi (Elettra), M.Sanchez Del Rio (ESRF)
In collaboration with D. Spiga (OAB)

Propagator engine
Huygens Integral

multi reflection

Propagator Engine
FFT-based (WPA)

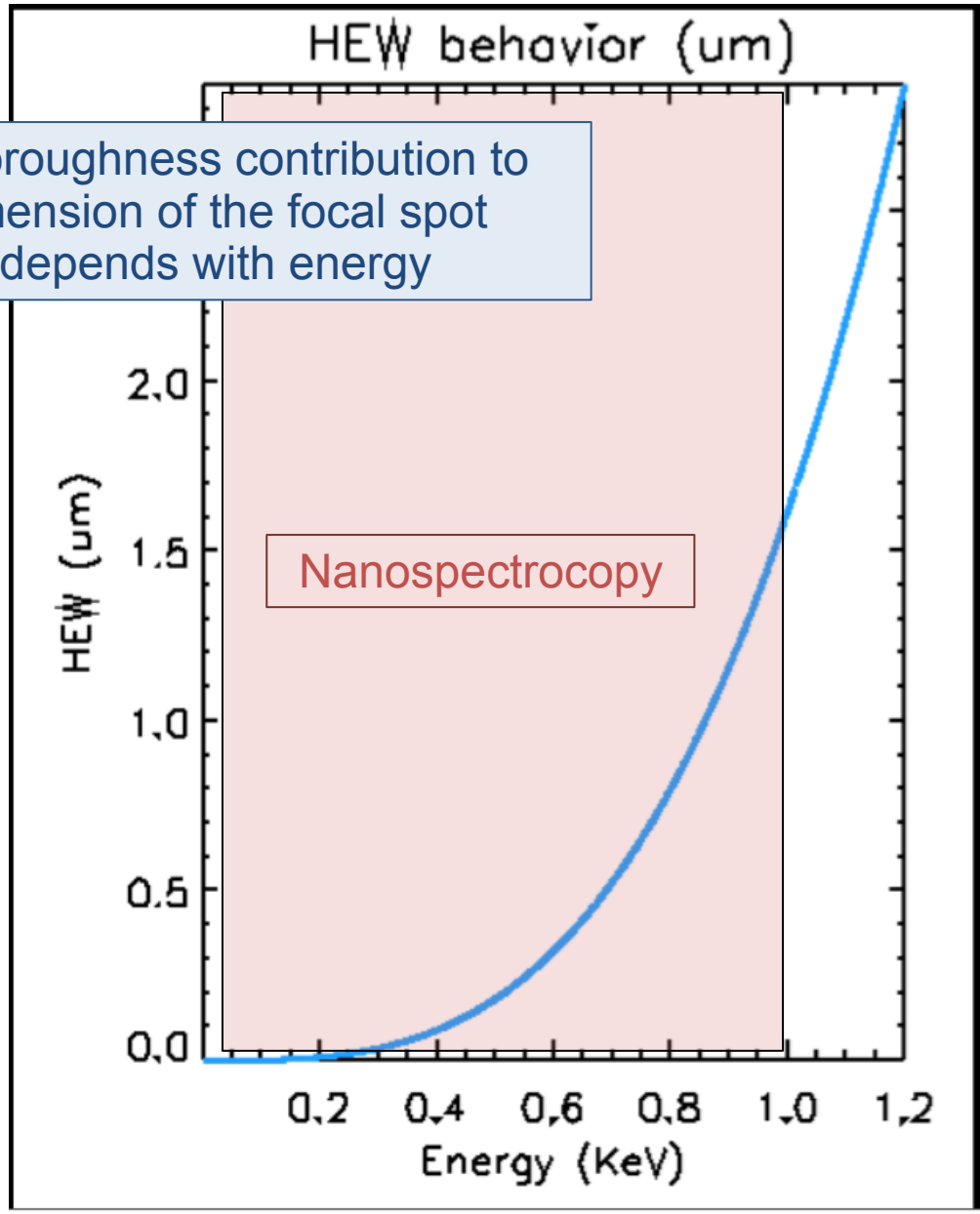
Done	Ongoing (December)	Planned
Figure Error	Numerical source	Average over Fig errors
Microroughness (statistical)	Utilities script (OASYS)	Optimized Python kernel
Best Focus search	Cross-talk with Shadow	
Gaussian source		
Multi-threading		

Nanospectroscopy
WORK IN PROGRESS

HEW = Half-Energy width twice the median value of the Point Spread Function

PSF = the angular integral of the focused X-ray intensity around the center of the focal spot

Microroughness contribution to dimension of the focal spot depends with energy



As the profile shows a distribution of heights, it is possible to have a non-zero constructive interference in other directions than the ideal one: the consequence is the scattering of the beam and the reduction of reflectivity in the ideal direction.

Scattering first order analysis[3]

PSD power law: $PSD(f) \sim K_n f^{-n}$

HEW Spot size formula:

$$H(\lambda) \sim \left(\frac{K_n}{n-1}\right)^{\frac{1}{n-1}} \left(\frac{\sin\theta_i}{\lambda}\right)^{\frac{3-n}{n-1}}$$

(3) D. Spiga, A&A 468, 775 (2007)

Elettra Sincrotrone Trieste

ACKNOWLEDGEMENTS

- Analysis of EU10.0 source of Nanospectroscopy beamline, ray-tracing calculations and slides made by Dr. Anna Bianco (Elettra-Sincrotrone Trieste)

- SRW simulations of Nanospectroscopy beamline optimized with the help and supervision of Dr. Oleg Chubar (Brookhaven National Laboratories)

- WISE slides: courtesy of Dr. Lorenzo Raimondi (Elettra-Sincrotrone Trieste)

Elettra
Sincrotrone
Trieste

Thank you!

Elettra
Sincrotrone
Trieste

www.elettra.eu