

X-ray photon transport simulators comparison: which will win?

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Motivation

- Upgrades to storage ring(s)
- OASYS development*
- Beamline scientists wanting to “tinker”:
 - Which tool do I use for..??
 - How can I evaluate mirror’s quality?

* L. Rebuffi, M. Sanchez del Rio Proc. SPIE 10388, 103880S (2017).

Outline

- ✓ Briefly on simulators
- ✓ "Experimental" conditions
- ✓ Tour around the results
- ✓ Key lessons learned

Briefly on simulators



L. Rebuffi, M. Sanchez del Rio Proc. SPIE 10388, 103880S (2017).

SHADOW

F. Cerrina, SPIE 503 (1984) 68,
Lai B., Cerrina F., Nucl. Instrum. Methods Phys. Res. A, 246 (1986), pp. 337-341,
L. Rebuffi, M. Sanchez del Rio, J. Synchrotron Rad. 23 (2016).

SRW

Chubar, O. and Elleaume, P., Proceedings of the European Particle Accelerator Conference (EPAC 98), 1177–1179 (1998).

Hybrid

X. Shi, et al., J. Synchrotron Rad. **21**, 669 (2014), X. Shi, et al., Proc. SPIE 9209, 920911 (2014).

WISEr

L. Raimondi, et al, Nucl. Instrum. and Meth A 710, 131-138 (2013),
M. Manfreda, L. Raimondi, D. Cocco; J. Synchr. Rad. 29, 1344-1353 (2022).

"Experimental" conditions

Summary of “experiments”

- ✓ 3 Energies
- ✓ Gaussian source, PM/KB beamline (reflectivity assumed ideal).
- ✓ 4 simulation tools (SHADOW, SHADOW+Hybrid, SRW, WISEr)
- ✓ 4 figure error, namely:
 - *Ideal mirrors’s surface (i.e. no figure error, no roughness)*
 - *Decent mirrors figure error ($1\mu\text{rad}$ rms slope error)*
 - *Good mirrors figure error ($0.3\mu\text{rad}$ rms sloper error)*
 - *State-of-the-art mirrors figure error ($0.1\mu\text{rad}$ rms slope error)*
- ✓ **Chosen figure of merit: spot sizes @ final screen**

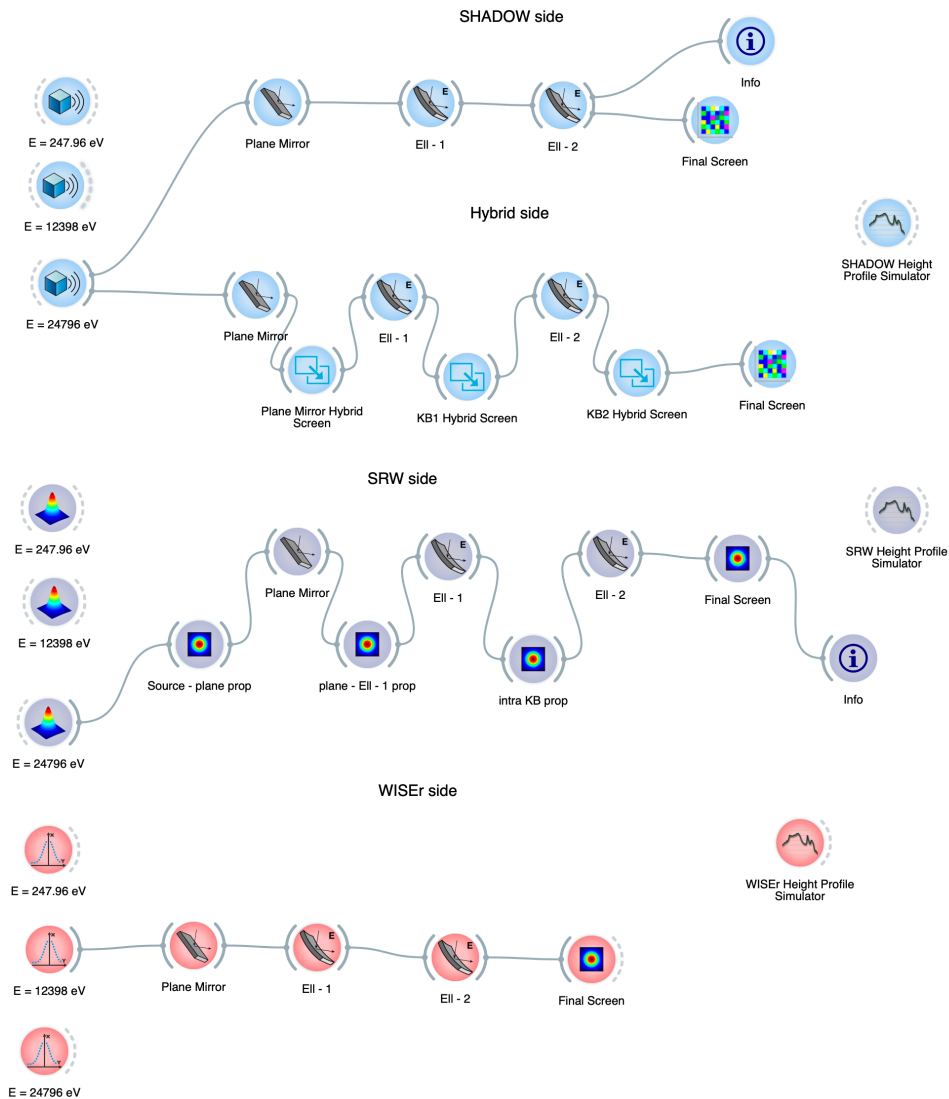
Geometry and energy

Divergence semi-cone $\Delta = 10 \mu\text{rad}$

	Distance (m)	Incidence (mrad)	Size (mm)	Facing
Plane mirror	60	3	800 x 40	Up
Elliptical 1	80	3	800 x 40	Down
Elliptical 2	80.8	3	800 x 40	Right
Image	81.6			
Wavelength (nm)	Energy (keV)	Source waist (μm)	Source sigma (μm)	
5	0.24796	159.155	5.000	
0.1	12.398	3.183	1.592	
0.05	24.796	1.592	0.796	

Gaussian source: $\omega_0 = \frac{\lambda}{\pi * \Delta}$

Source size = $\frac{\omega_0}{2}$



Beamline Info

Info Sys Plot (Side View) Sys Plot (Top View) OE Info Source Info **Distances Summary**

***** SUMMARY OF DISTANCES *****

** DISTANCES FOR ALL O.E. [m] **

OE	TYPE	p[m]	q[m]	src-oe	src-screen
1	MIRROR	60.0000	0.0000	60.0000	60.0000
2	MIRROR	20.0000	0.0000	80.0000	80.0000
3	MIRROR	0.8000	0.8000	80.8000	81.6000

***** FOCUSING ELEMENTS *****

OE	SHAPE	p_foc	q_foc	1/M
2	ELLIPSE	80.00	1.60	50.00
3	ELLIPSE	80.80	0.80	101.00

Sum of Alphas [deg]: 90.000000
Sum of Alphas Mod 180 [deg]: 90.000000
Sum of Alphas Mod 360 [deg]: 90.000000

Total deflection angle H = 0.006000 rad = 0.344 deg
Total deflection angle V = 0.012000 rad = 0.688 deg

***** GAUSSIAN SOURCE *****

Photon Energy: 24796.0000 eV
Acceptance Slit aperture (h x v): 0.001000 x 0.001000 m
Acceptance Slit points (h x v): 500 x 500
Acceptance Slit distance: 10.0000 m

***** SUMMARY OF DISTANCES *****

** DISTANCES FOR ALL O.E. [m] **

OE#	TYPE	p [m]	q [m]	src-oe	src-screen
1	Screen	50.0000	0.0000	60.0000	60.0000
2	PlaneMirror	0.0000	0.0000	60.0000	60.0000
3	Screen	10.0000	10.0000	70.0000	80.0000
4	EllipticalMirror	0.0000	0.0000	80.0000	80.0000
5	Screen	0.8000	0.0000	80.8000	80.8000
6	EllipticalMirror	0.0000	0.0000	80.8000	80.8000
7	Screen	0.8000	0.0000	81.6000	81.6000

***** ELLIPTICAL ELEMENTS *****

OE#	p(ell)	q(ell)	p+q(ell)	M
4	80.0000	1.6000	81.6000	50.0000
6	80.8000	0.8000	81.6000	101.0000

Some more sims parameters

SRW source (i.e. @ 12398 eV)

Light Source Setting

Wavefront Setting

Gaussian Source Parameters

Beam center at waist x [m]

0.0

Beam center at waist y [m]

0.0

Beam center at waist z [m]

0.0

Average angle at waist x [rad]

0.0

Average angle at waist y [rad]

0.0

Energy per pulse [J]

0.001

Repetition rate [Hz]

1

Polarization

Linear Horizontal

σ_x at waist [m]

1.592e-06

σ_y at waist [m]

1.592e-06

Pulse duration [s]

1e-06

Transverse Gauss-Hermite mode order x

0

Transverse Gauss-Hermite mode order y

0

Light Source Setting

Wavefront Setting

Propagation

Wavefront Parameters

Photon Energy [eV]

12398.0

H Slit Gap [m]

0.001

V Slit Gap [m]

0.001

H Slit Points

500

V Slit Points

500

Propagation Distance [m]

10.0

Intensity Units

phot/s/0.1%bw/mm²

Precision Parameters

Sampling factor for adjusting n_x/n_y
(effective if > 0)

0.0

Hybrid screen example

Run HYBRID

Basic Setting

Advanced Setting

Calculation Parameters

Diffraction by Simple Aperture

Diffraction by Mirror or Grating Size

Diffraction by Mirror Size + Figure Errors

Diffraction by Grating Size + Figure Errors

Diffraction by Lens/C.R.L./Transf.Size

Diffraction by Lens/C.R.L./Transf.Size + Thickness Errors

Number of bins for I(Tangential) histogram

50

Number of diffraction peaks

20

Number of points for FFT

100000

Run HYBRID

Basic Setting

Advanced Setting

Calculation Parameters

Diffraction Plane

Tangential

Calculation

Diffraction by Mirror Size + Figure Errors

Numerical Control Parameters

Number of bins for I(Sagittal) histogram

50

Number of bins for I(Tangential) histogram

50

Number of diffraction peaks

20

Number of points for FFT

100000

Optional file output

Files to write out

None

only far field calcs!

SHADOW sources: 1Mrays

Mirror figure error generation

$$z(x) = \sum_{f_1=f_{\min}}^{f_{\max}} f^{-\beta} \sin(2\pi f x + \varphi_r) \quad f_{\min} = \frac{1}{L} \quad f_{\max} = \frac{1}{2x_s}$$

Sanchez del Rio, M., et al, J. Synchrotron Rad. 23, 665-678.

Slope error (μrad, tang)	step (mm, tang)	MC seed (tang), PM/EI1/EI2	Slope Error (μrad, sag)	step (mm, sag)	MC seed (sag), PM/EI1/EI2	Beta
1.0	0.01	548/549/550	2.0	1.5	2548/2549/2550	2.7
0.3	0.01	2198/2199/2200	0.6	1.5	1523/1524/1525	2.5
0.1	0.01	41005/41006/41007	0.2	1.5	1152/1153/1154	2.2

Input Parameters Output Use of the Widget

Length Width

Calculation Parameters

Kind of Profile Fractal

Dimensions [m] 0.8

Step [m] 1e-05

Monte Carlo initial seed 55849

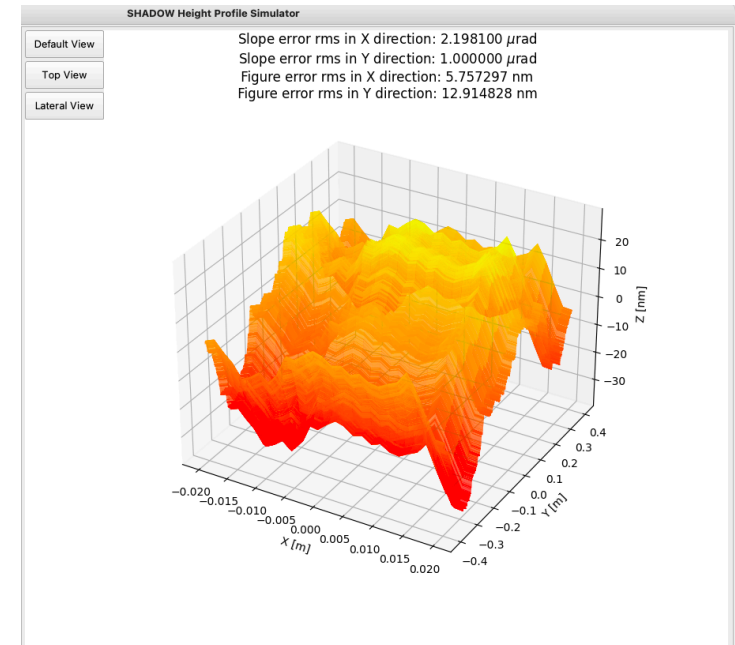
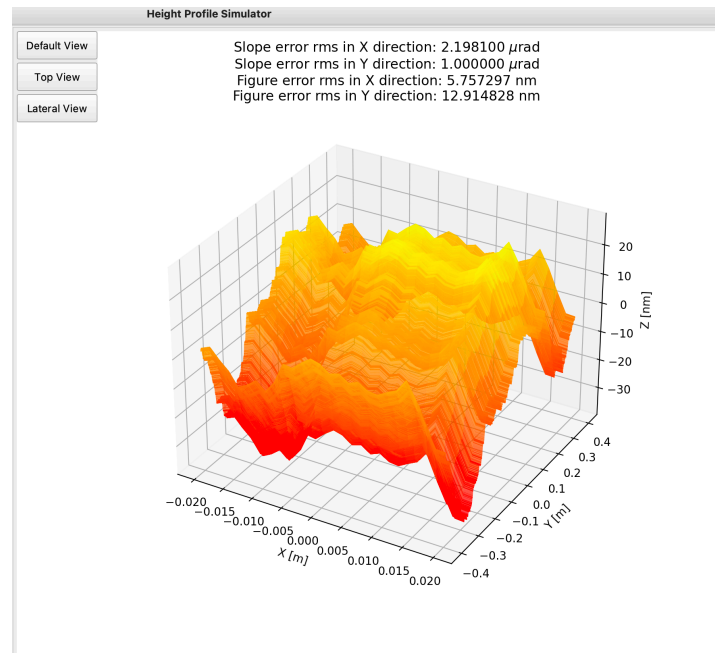
Beta Value 2.2

Normalization to Slope Error (μrad)

Rms Value 0.1

Outputs

Output File Name SRW_PM_Ourad1.dat



All encompassing, unintelligible results table

Ideal mirrors, spot size @ final screen

	Shadow		Hybrid		SRW		WISer	
	FWHM X [μm]	FWHM Y [μm]	FWHM X [μm]	FWHM Y [μm]	FWHM X [μm]	FWHM Y [μm]	FWHM X [μm]	FWHM Y [μm]
E = 247.96 eV	1.5	3.4	1.8	4.1	1.8	3.8	2.04	4.2
E = 12.398 keV	0.03	0.07	0.03	0.08	0.04	0.08	0.04	0.08
E = 24.796 keV	0.015	0.035	0.019	0.042	0.02	0.04	0.02	0.04

“Real” mirrors, spot size @ final screen

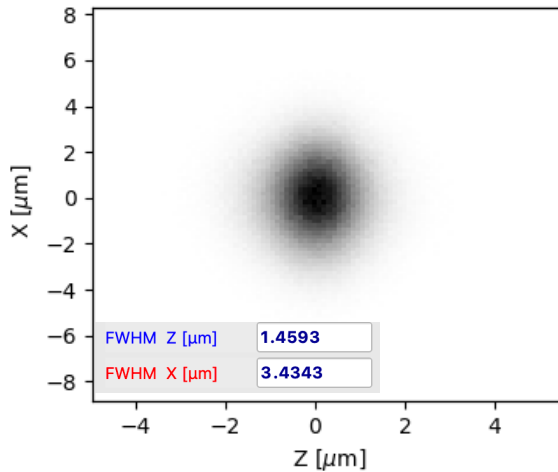
		Shadow		Hybrid		SRW		WISer	
		FWHM X [μm]	FWHM Y [μm]	FWHM X [μm]	FWHM Y [μm]	FWHM X [μm]	FWHM Y [μm]	FWHM X [μm]	FWHM Y [μm]
1 μrad	E = 247.96 eV	3.4	9.5	2.1	4.8	2	4	2.1	4.2
	E = 12.398 keV	3.0	8.5	0.4	1.5	0.4	0.8		
	E = 24.796 keV	3	8.6	0.06	0.92	0.2	0.5		
0.3 μrad	E = 247.96 eV	1.7	4.2	1.8	4.2	1.9	3.8	2.2	4.7
	E = 12.398 keV	0.9	2.7	0.04	0.2	0.04	0.08		
	E = 24.796 keV	0.9	2.8	0.02	0.2	0.04	0.4		
0.1 μrad	E = 247.96 eV	1.5	3.5	1.8	4.2	1.93	3.8	2.1	4.4
	E = 12.398 keV	0.3	0.9	0.04	0.09	0.04	0.08	0.02	0.04
	E = 24.796 keV	0.3	0.9	0.02	0.05	0.02	0.04	0.02	0.04

Some interesting results

247.96 eV, ideal mirrors

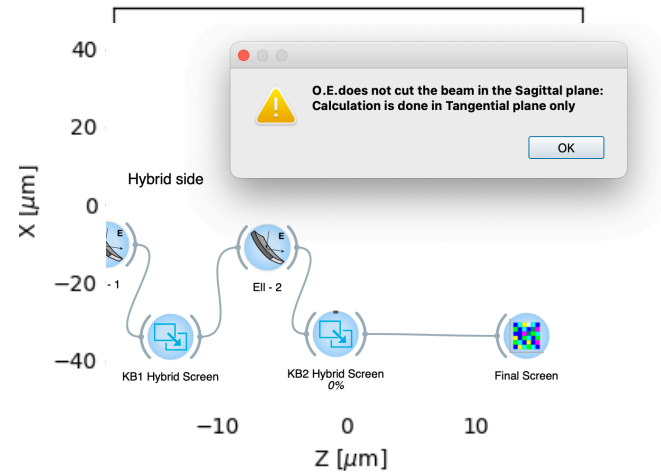
Shadow

Z, X



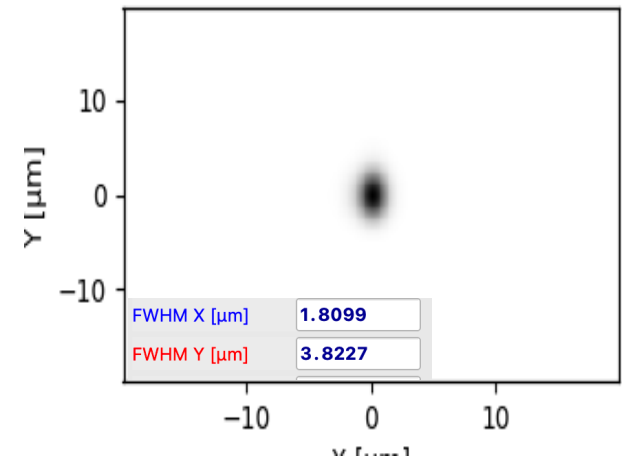
Hybrid

Z, X

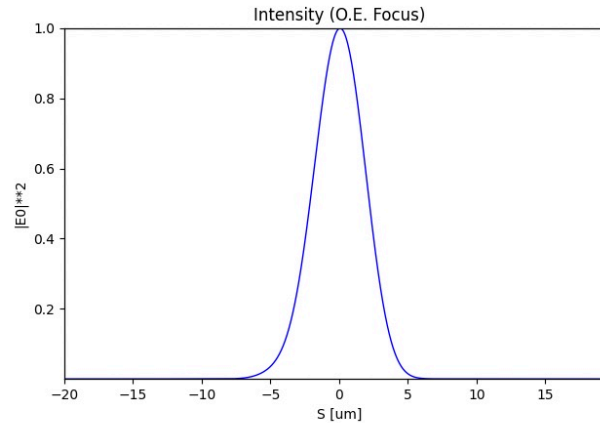
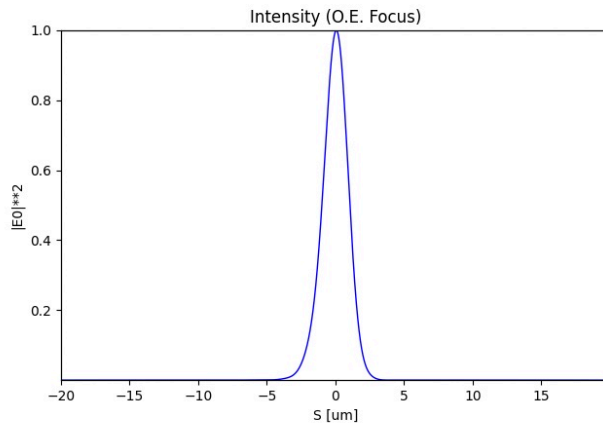


SRW

Intensity SE [ph/s/.1%bw/mm²]

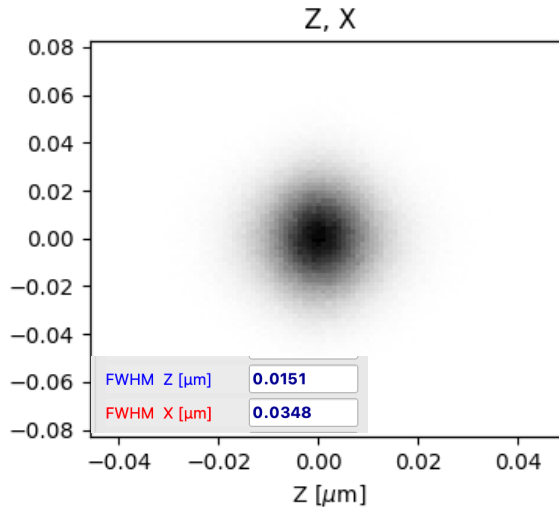


WISEr

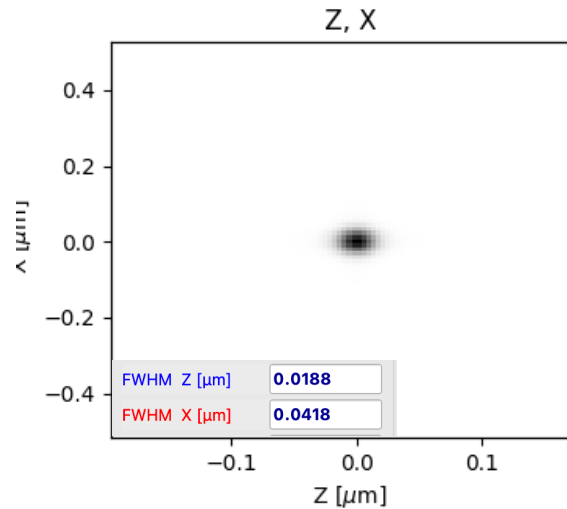


24.796 KeV, ideal mirrors

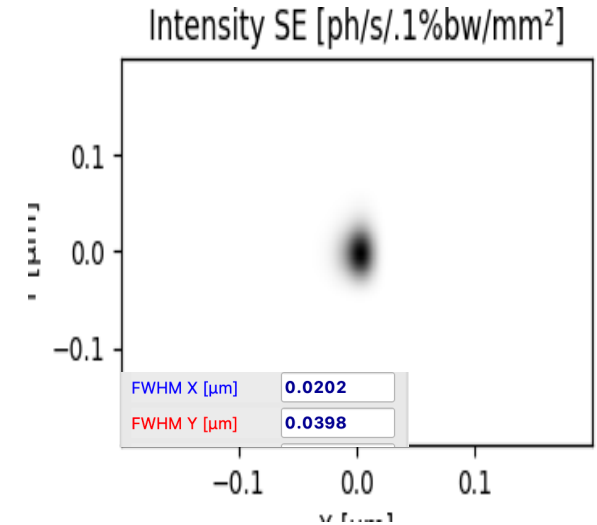
Shadow



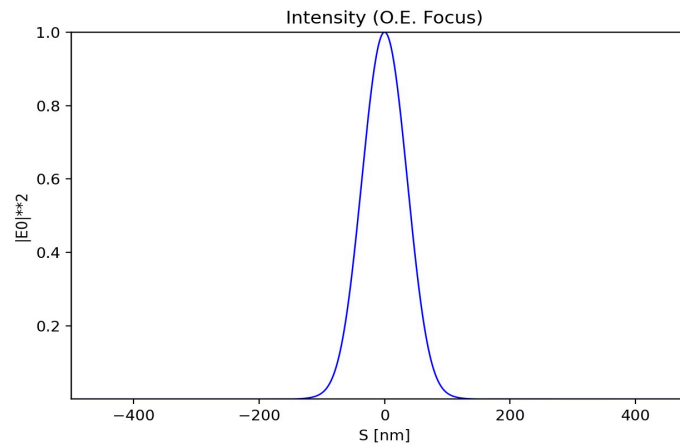
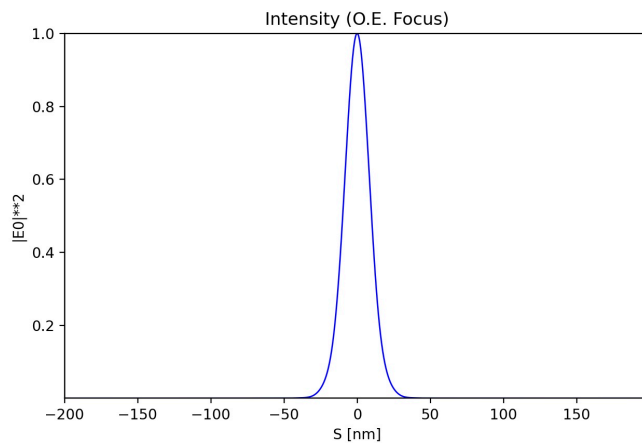
Hybrid



SRW



WISEr

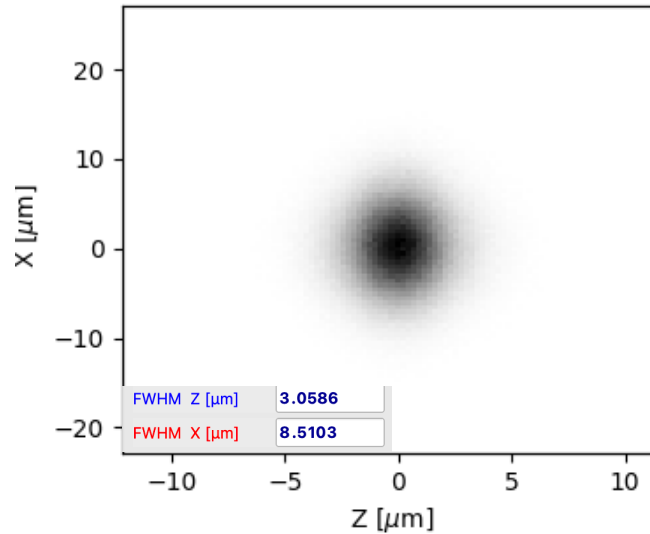


FWHM = 0.02 X 0.040

12.398 KeV, 1 μ rad slope error

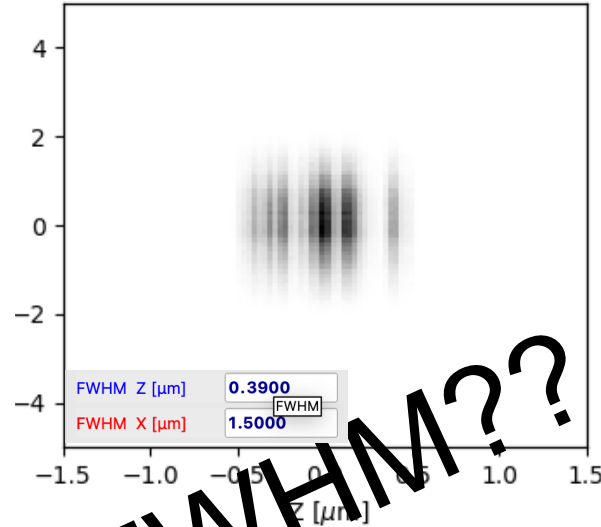
Shadow

Z, X



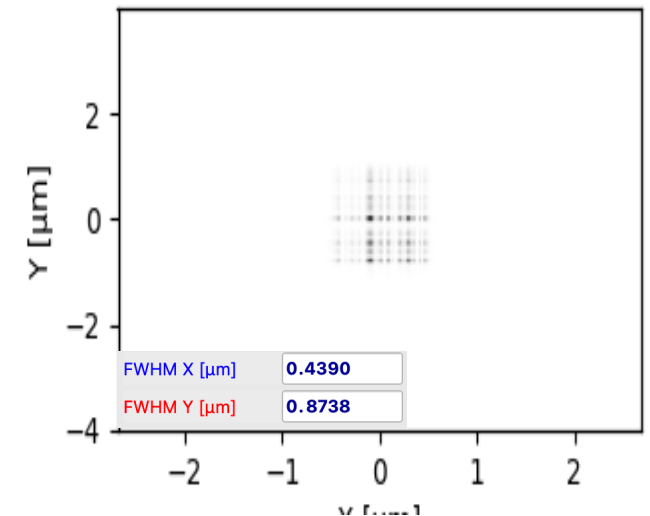
Hybrid

Z, X

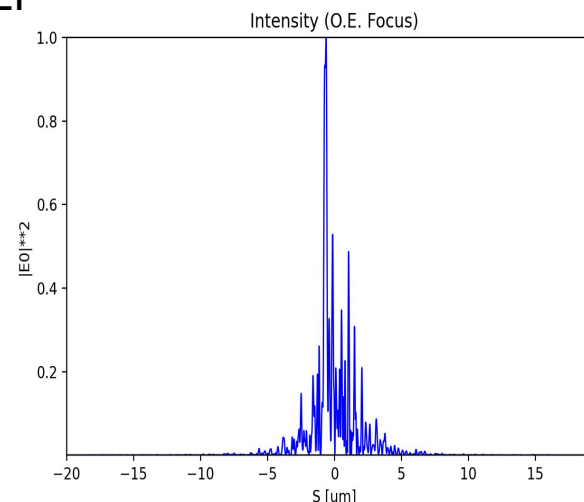
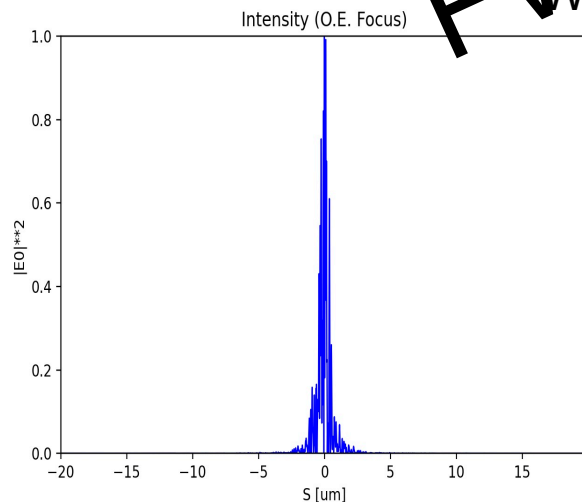


SRW

Intensity SE [ph/s/.1%bw/mm²]

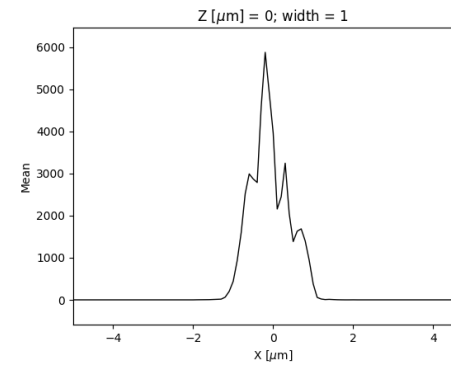
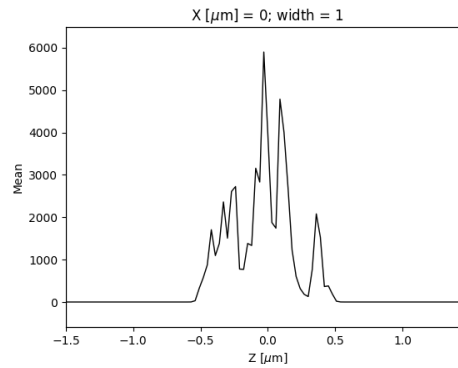


FWHM???

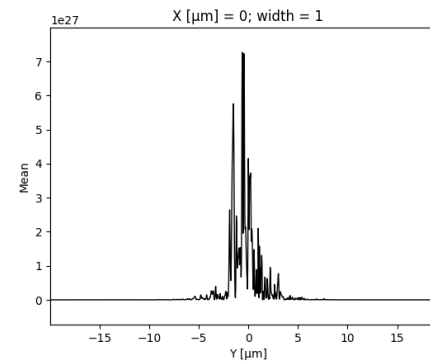
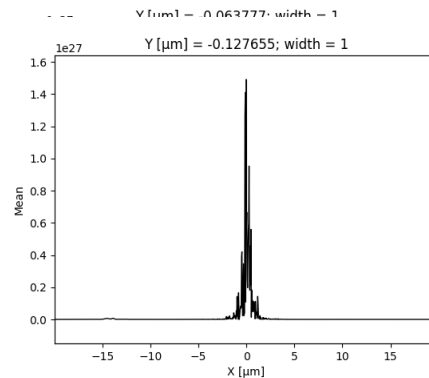


12.398 KeV, 1 μ rad slope error

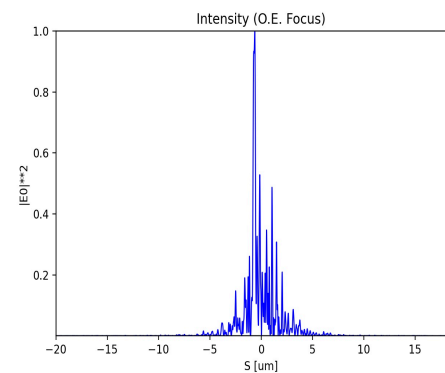
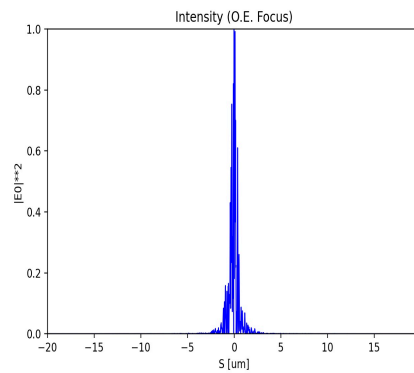
Hybrid



SRW



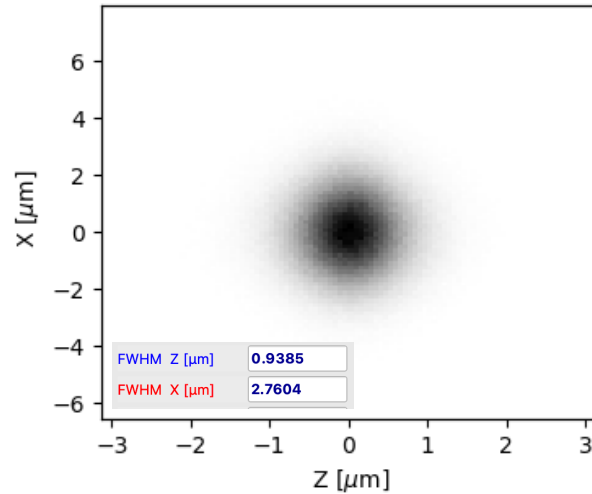
WISEr



12.398 keV, 0.3 μ rad slope error

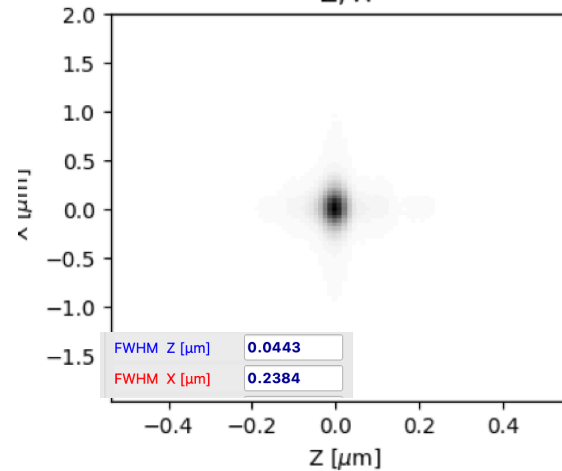
Shadow

Z, X



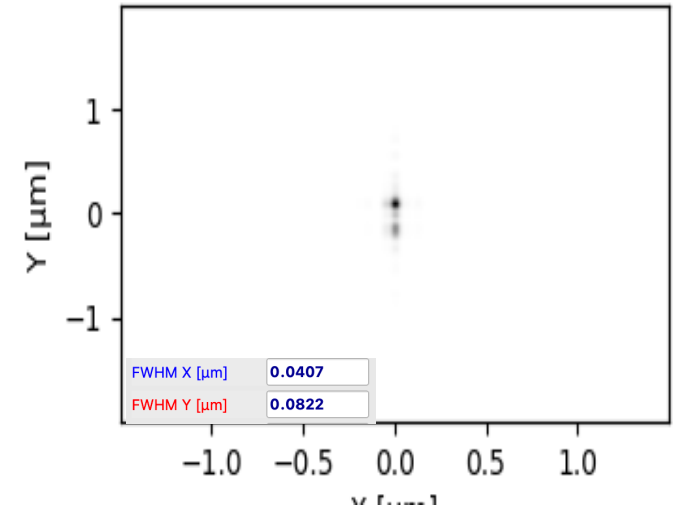
Hybrid

Z, X

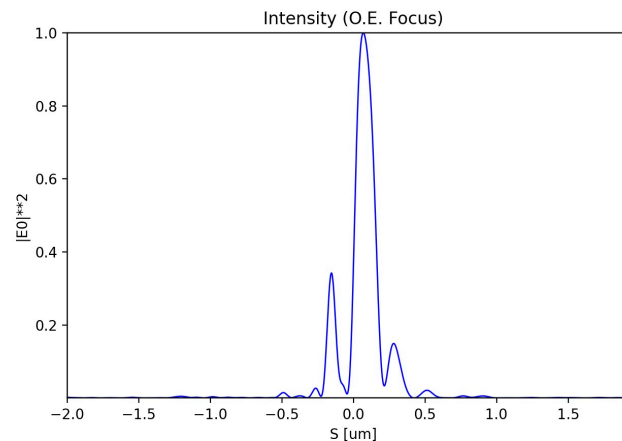
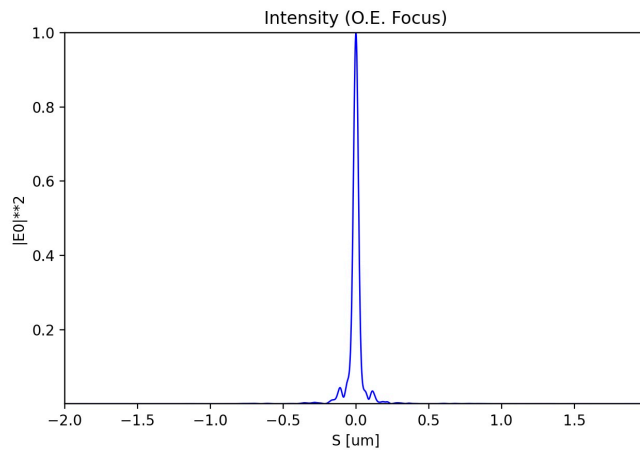


SRW

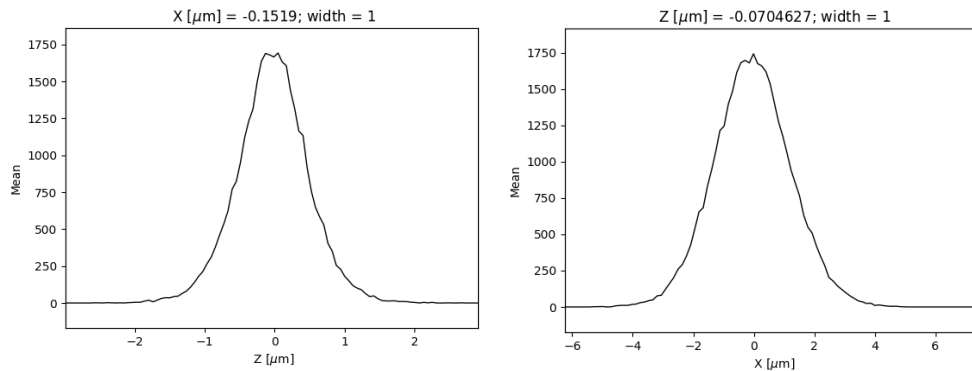
Intensity SE [ph/s/.1%bw/mm²]



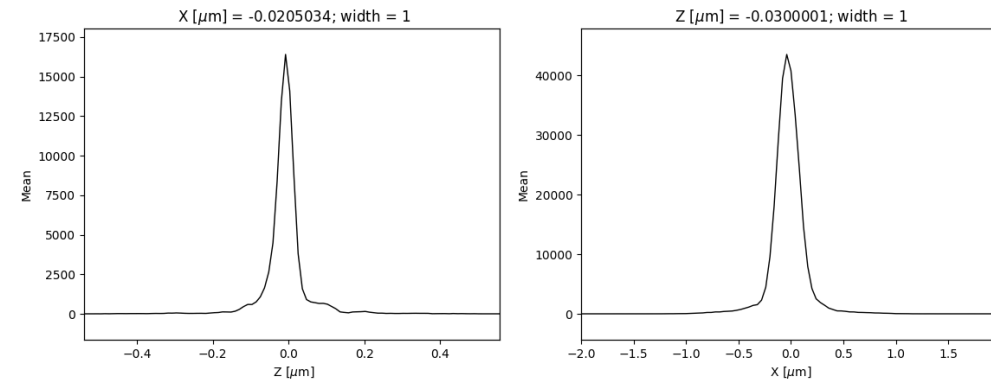
WISer



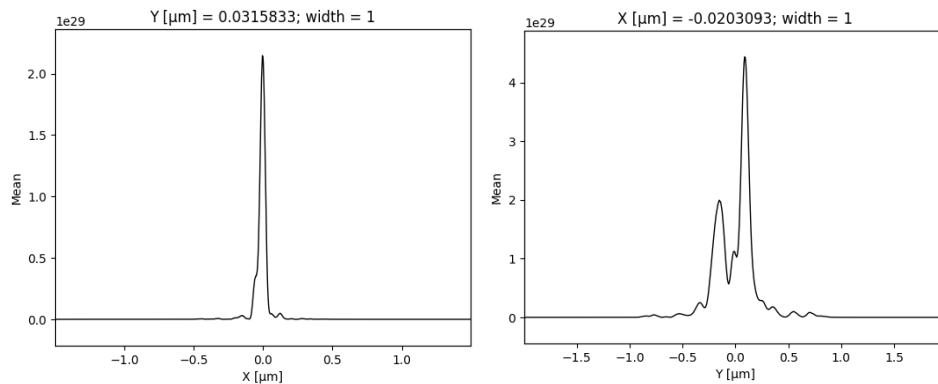
SHADOW



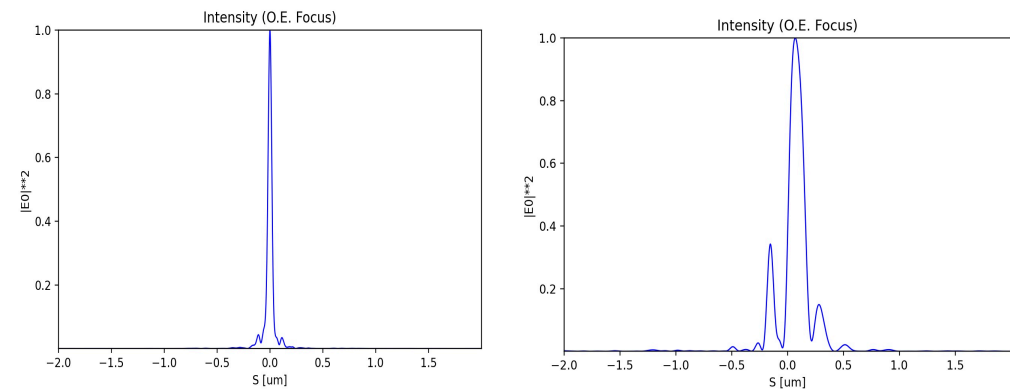
Hybrid



SRW



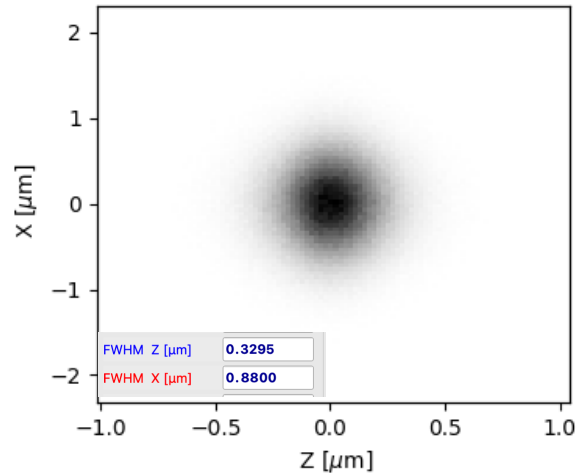
WISER



24.796 keV, 0.1 μ rad slope error

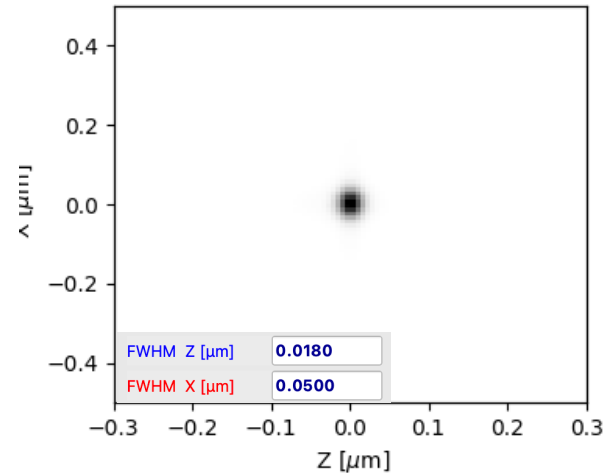
Shadow

Z, X



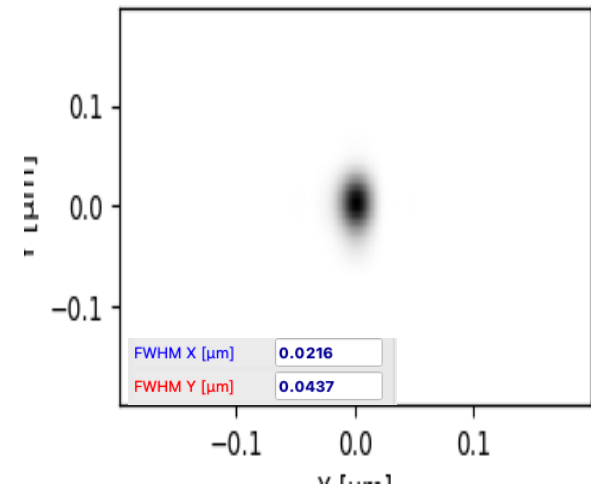
Hybrid

Z, X

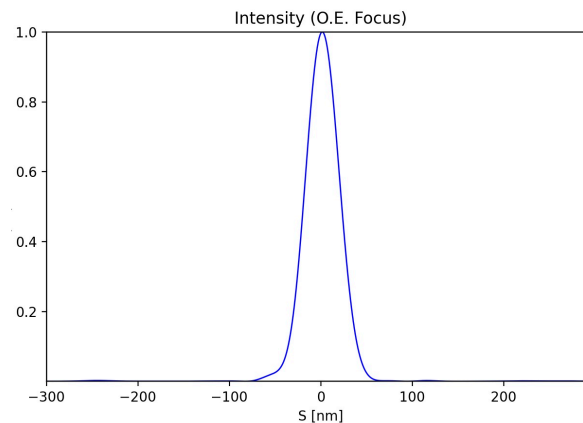
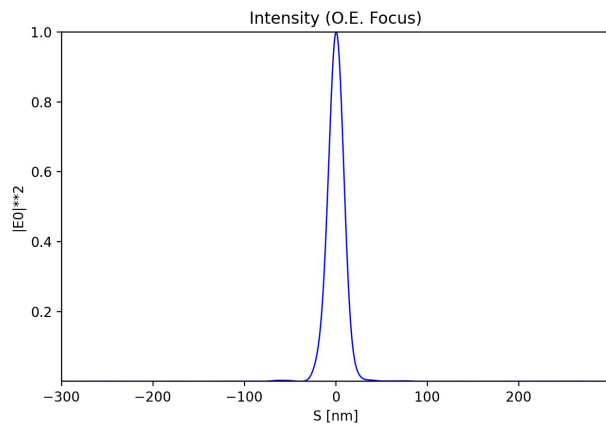


SRW

Intensity SE [ph/s/.1%bw/mm²]



WISer



$$\text{FWHM} = 0.02 \times 0.042$$

So, which one wins?

Everyone's a winner!

Within Oasys:

SHADOW: beamline geometry, mirror sizing, crystal diffraction setups, ML setups... and a million more things

Hybrid: pupil diffraction, mirror quality assessment

SRW: pupil diffraction, mirror quality assessment, wavefront quality, partial coherence analysis

WISEr: mirror quality assessment, scattering contributions

Thank you!

