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Trieste

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

M. Altissimo and L. Raimondi

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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).

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Outline

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

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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. Manfredda, L. Raimondi, D. Cocco; J. Synchr. Rad. 29, 1344-1353 (2022).

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"Experimental" conditions

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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 (1µrad rms slope error)*
  - *Good mirrors figure error (0.3 µrad rms sloper error)*
  - *State-of-the-art mirrors figure error (0.1µrad rms slope error)*
- ✓ **Chosen figure of merit: spot sizes @ final screen**

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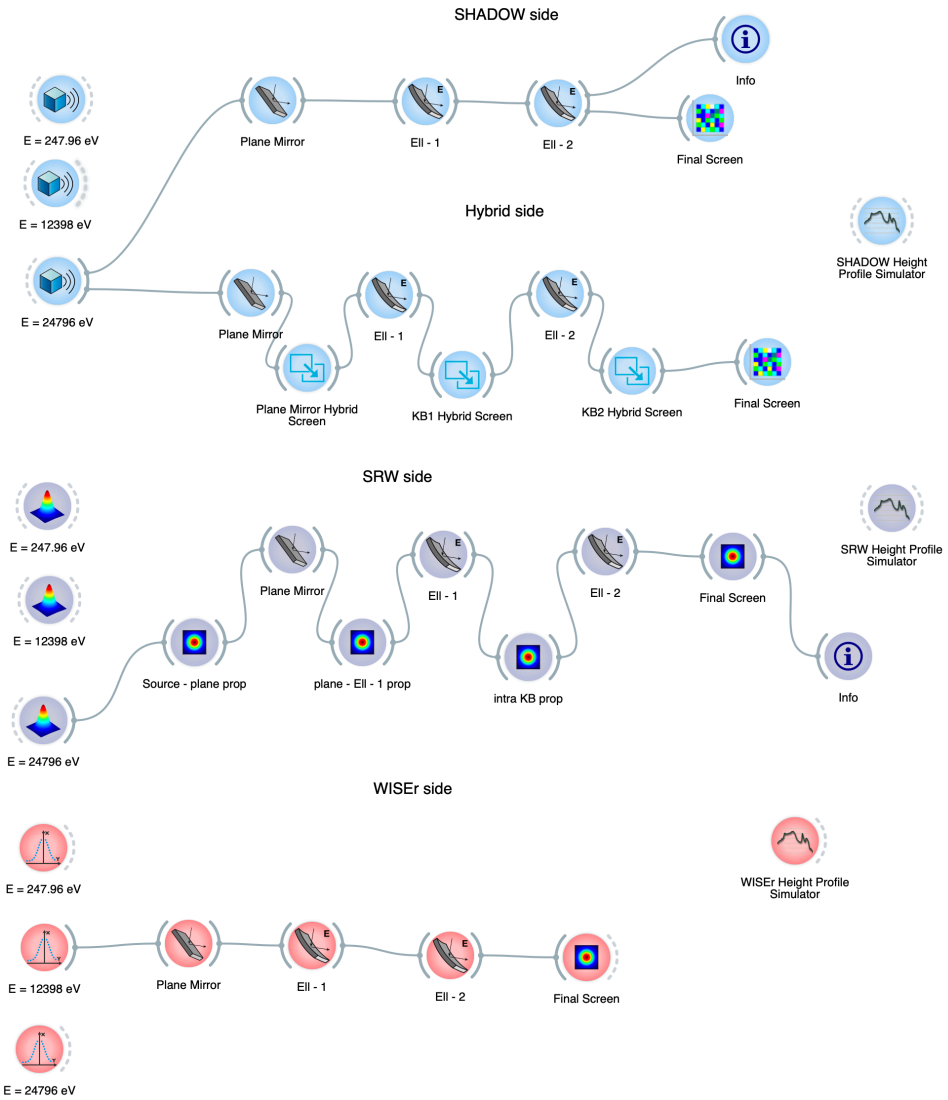
Geometry and energy

Divergence semi-cone Δ = 10 μrad

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

Oasys Canvas



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
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```
********    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

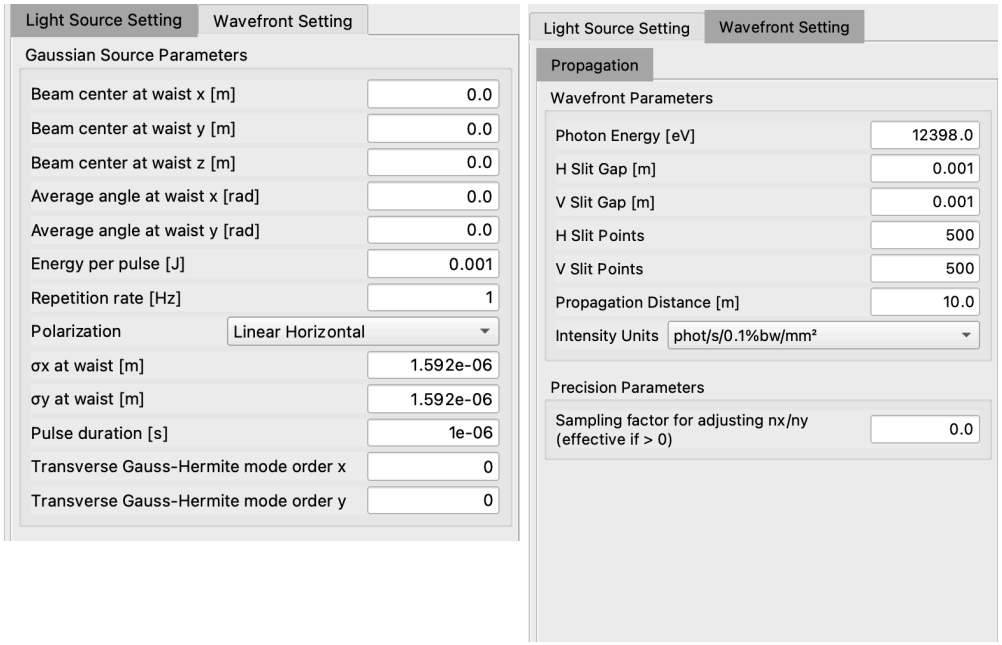
********  SUMMARY OF DISTANCES ********
 ** DISTANCES FOR ALL O.E. [m] **

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

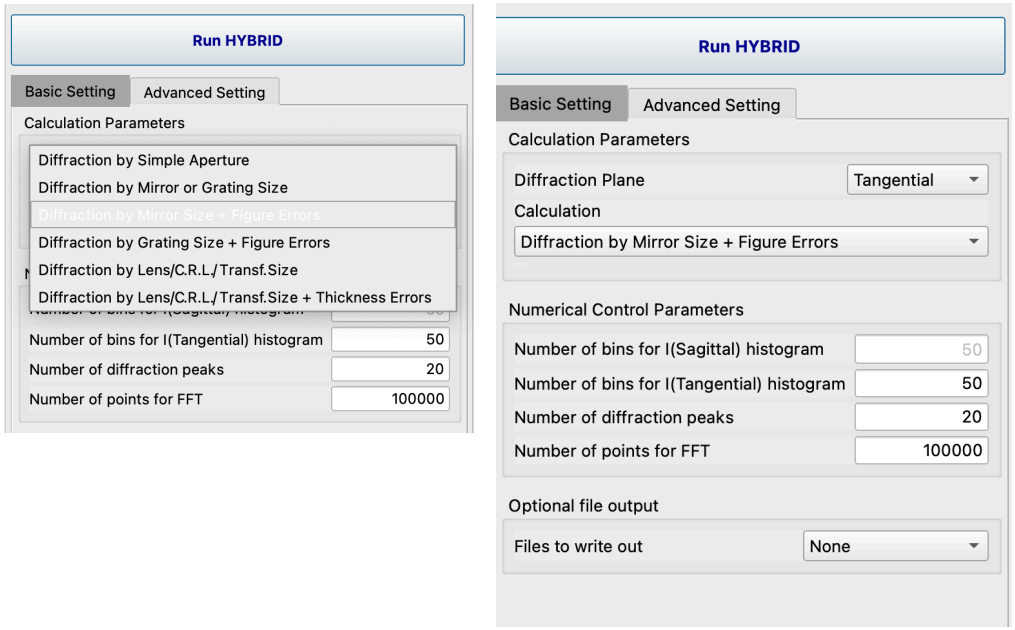

********  ELLIPTICAL ELEMENTS  ********
OE#   p(ell)   q(ell) p+q(ell) M
-------------------------------------------------------------------
  4  80.0000   1.6000  81.6000  50.0000
  6  80.8000   0.8000  81.6000 101.0000
```

Some more sims parameters

SRW source (i.e. @ 12398 eV)



Hybrid screen example



only far field calcs!

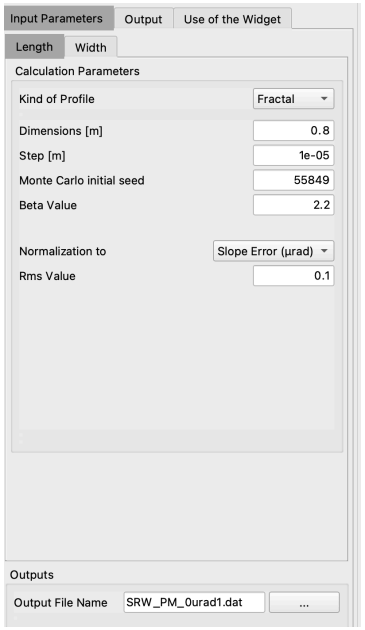
SHADOW sources: 1Mrays

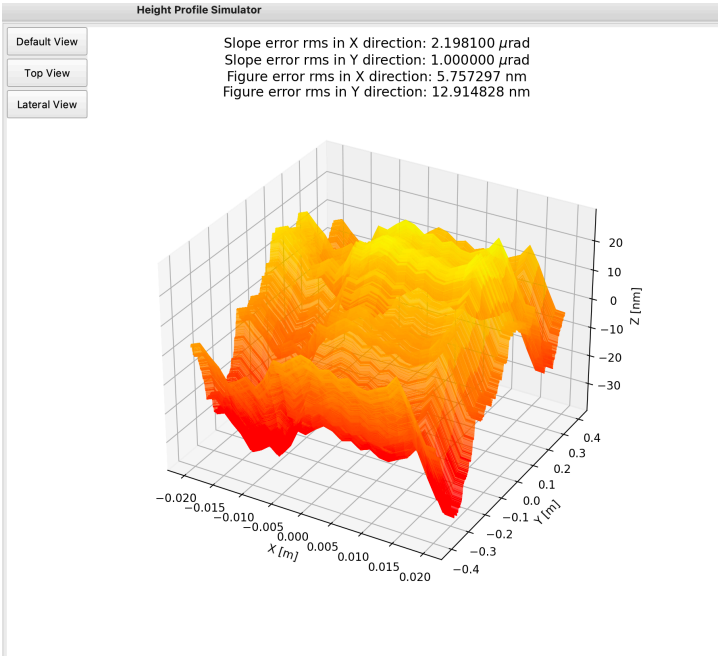
Mirror figure error generation

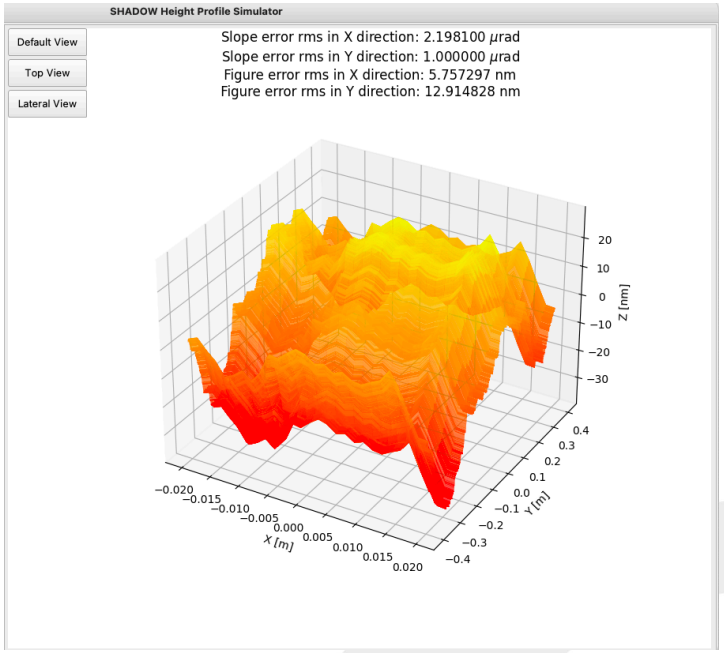
$$z(x) = \sum_{f_1 = f_{min}}^{f_{max}} f^{-\beta} \sin(2\pi f x + \varphi_r) \qquad f_{min} = \frac{1}{L} \qquad f_{max} = \frac{1}{2x_s}$$

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

Slope error (μrad, tang)	step (mm, tang)	MC seed (tang), PM/Ell1/Ell2	Slope Error (μrad, sag)	step (mm, sag)	MC seed (sag), PM/ Ell1/Ell2	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







All encompassing, unintellegible 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]
1μrad	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		
0.1μrad	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

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Some interesting results

247.96 eV, ideal mirrors

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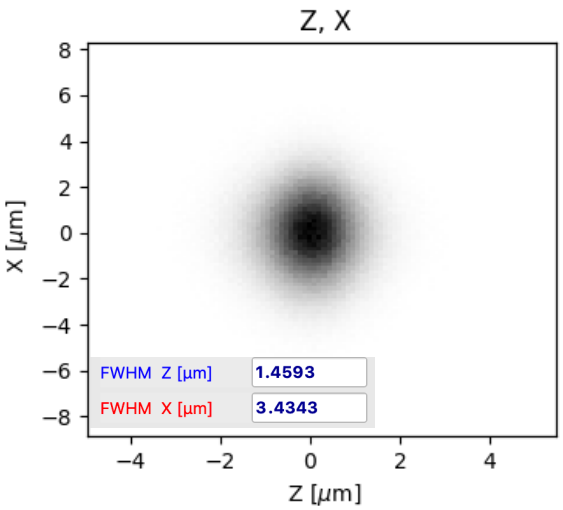
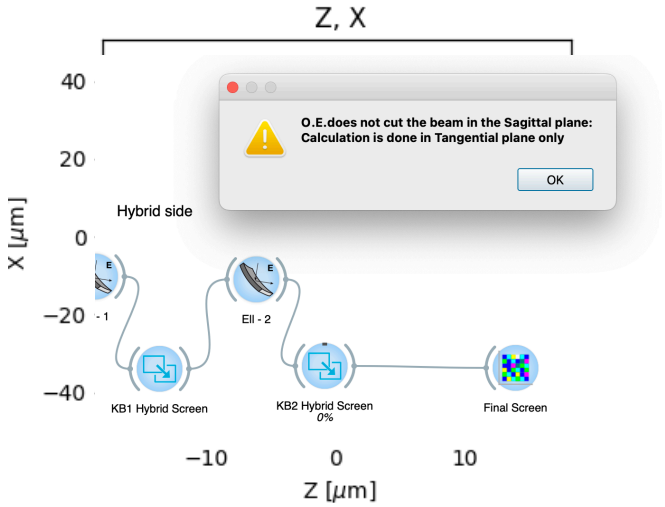
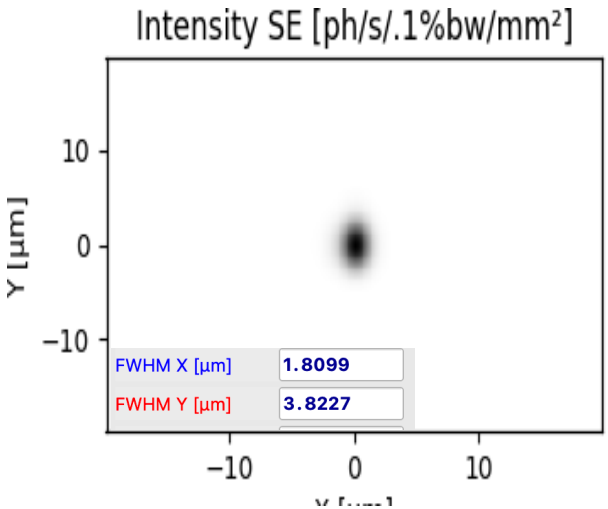
Shadow



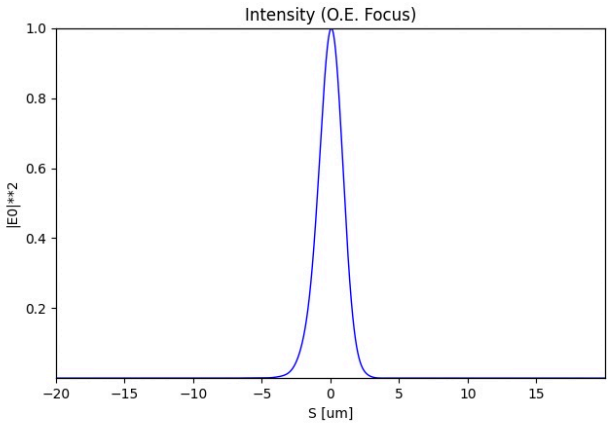
Hybrid

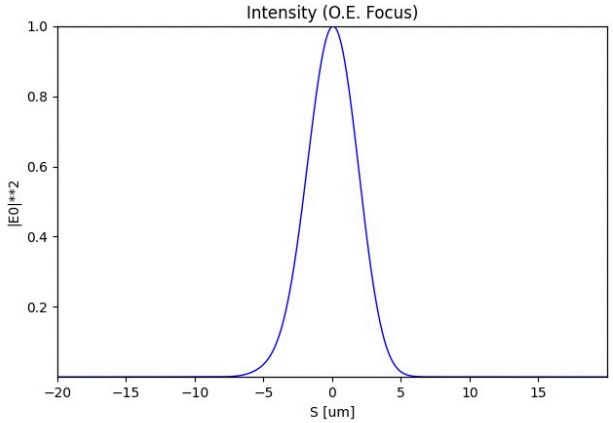


SRW



WISEr

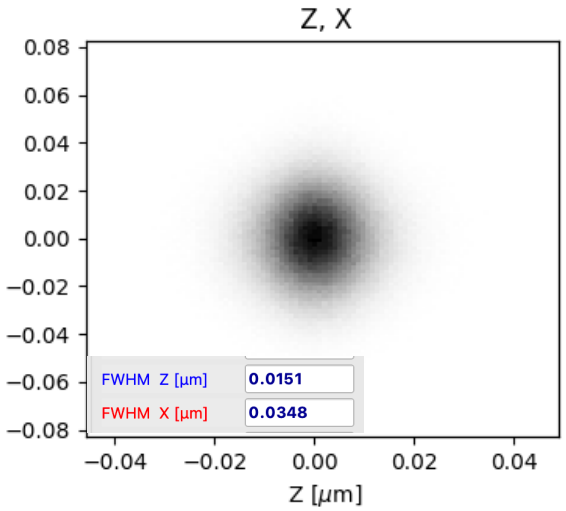




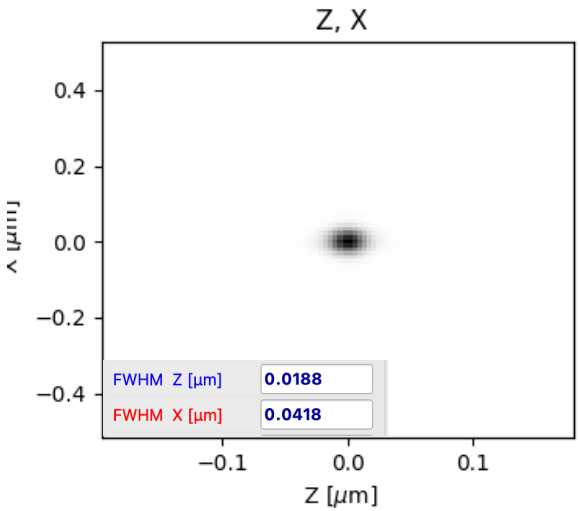
FWHM = 2.03 x 4.18

24.796 KeV, ideal mirrors

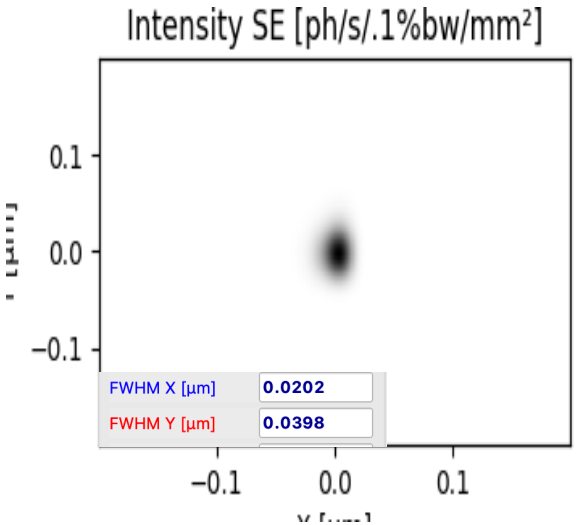
Shadow



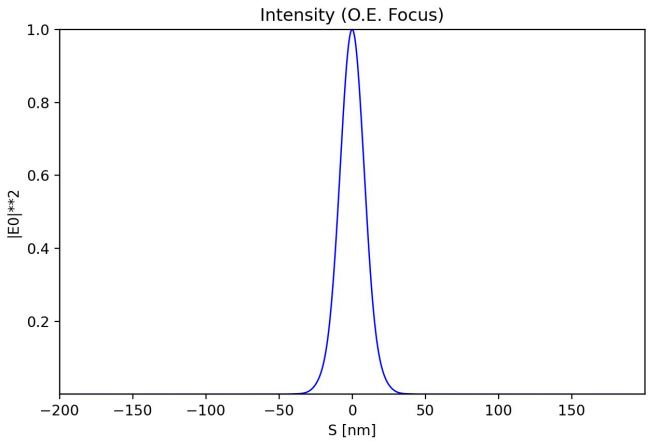
Hybrid

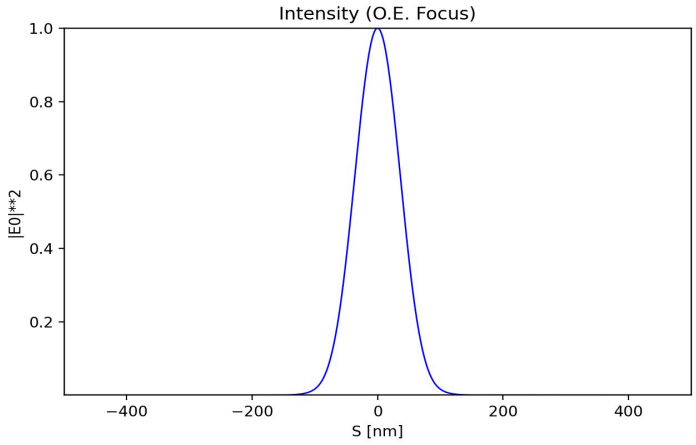


SRW



WISEr

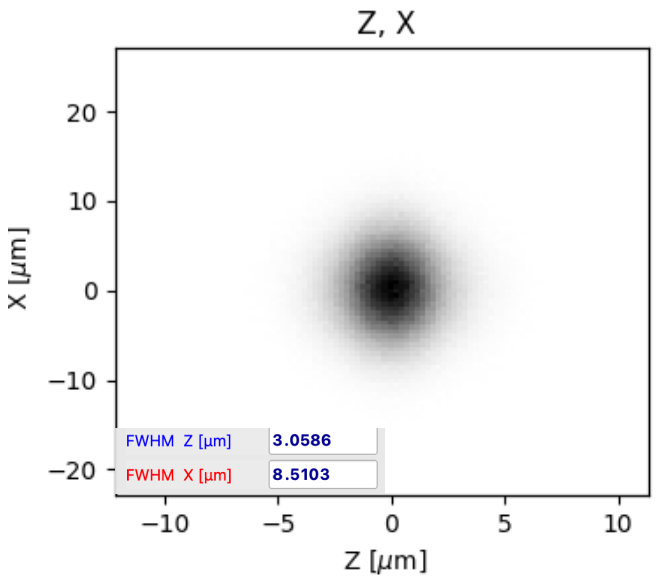




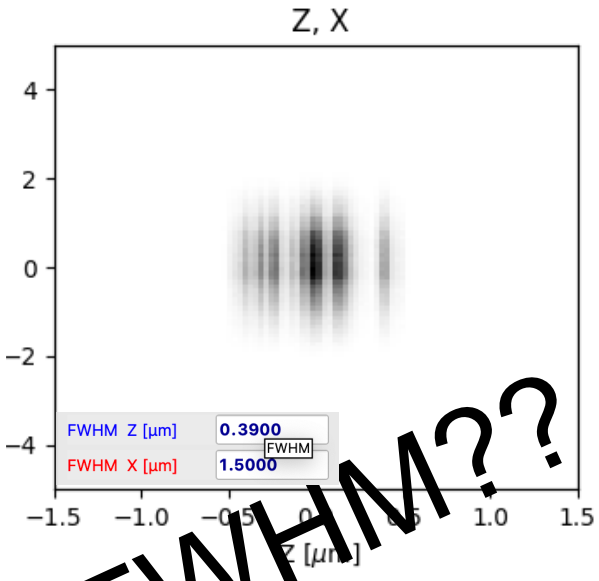
FWHM = 0.02 X 0.040

12.398 KeV, 1 µrad slope error

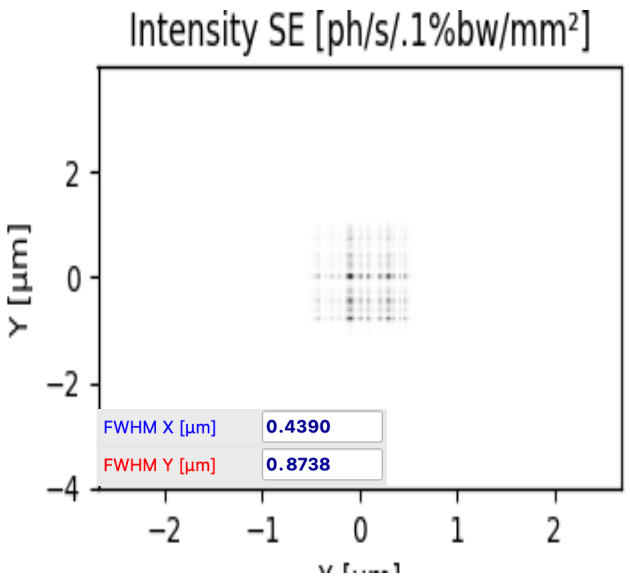
Shadow



Hybrid

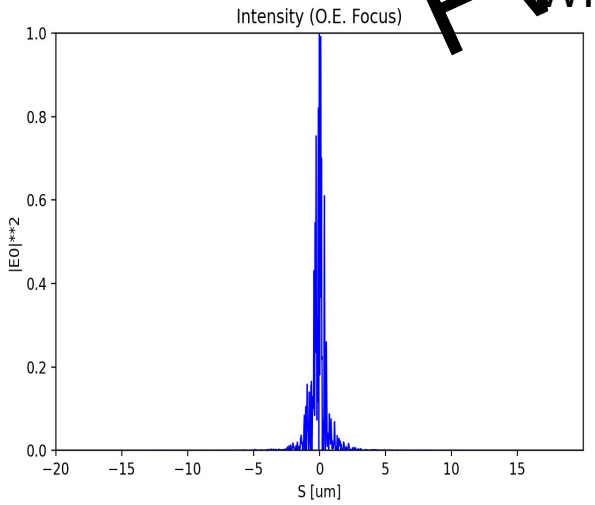


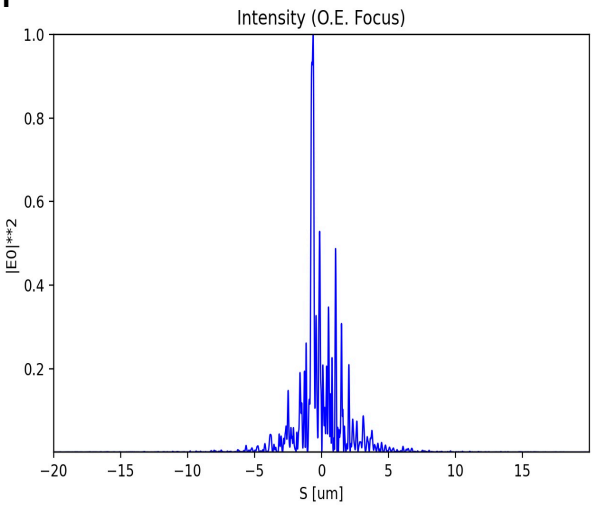
SRW



FWHM??

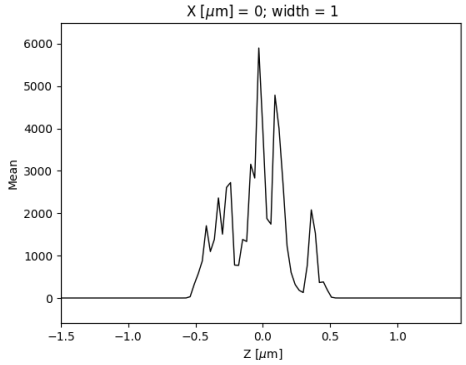
WISEr

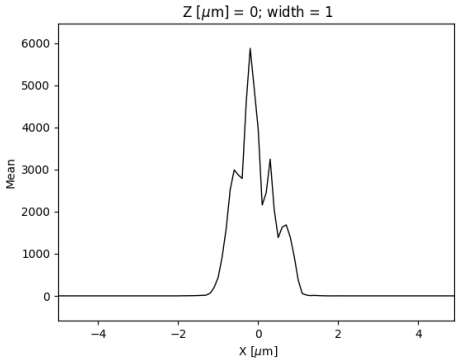




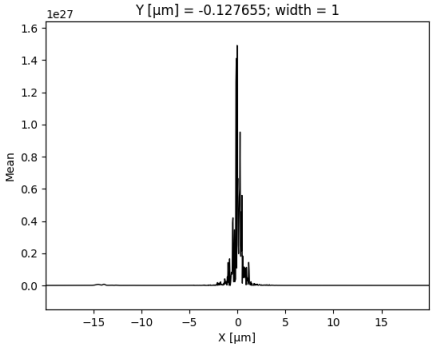
12.398 KeV, 1 µrad slope error

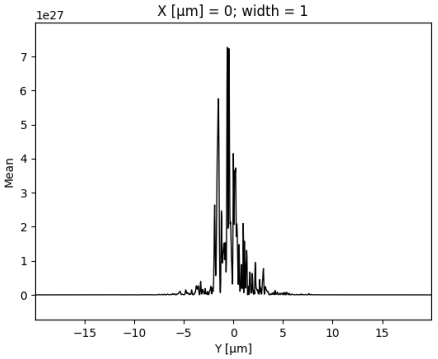
Hybrid



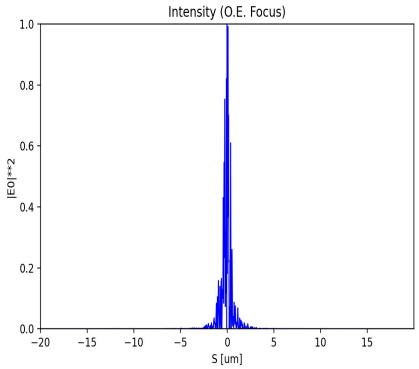


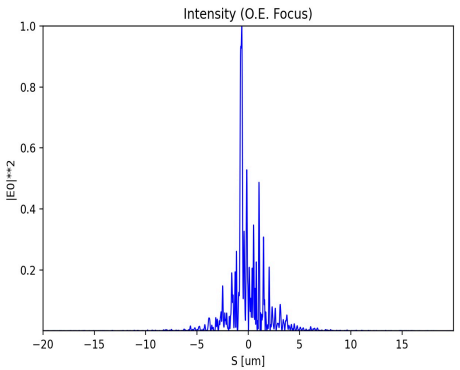
SRW





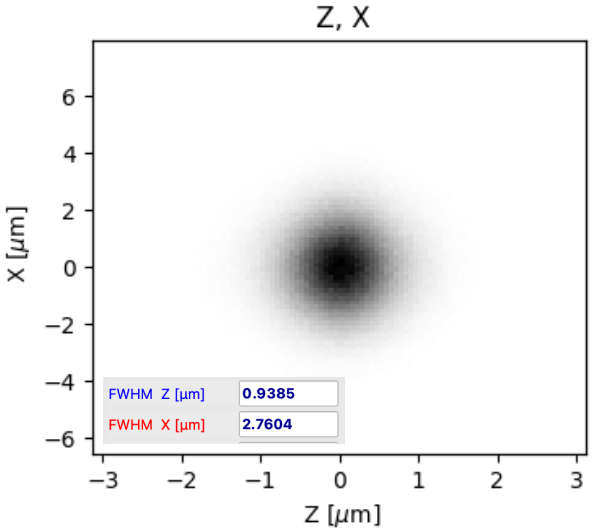
WISEr



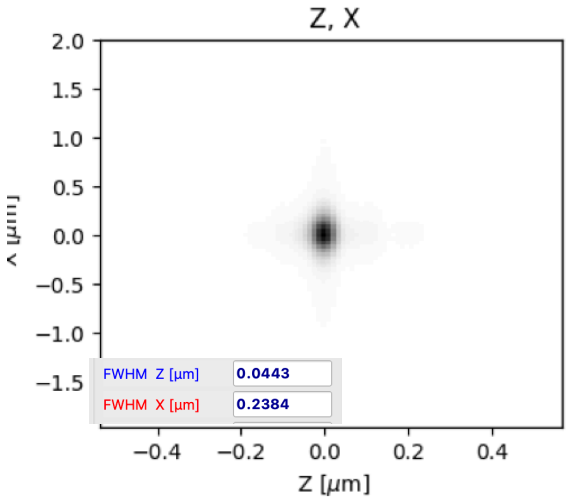


12.398 keV, 0.3 µrad slope error

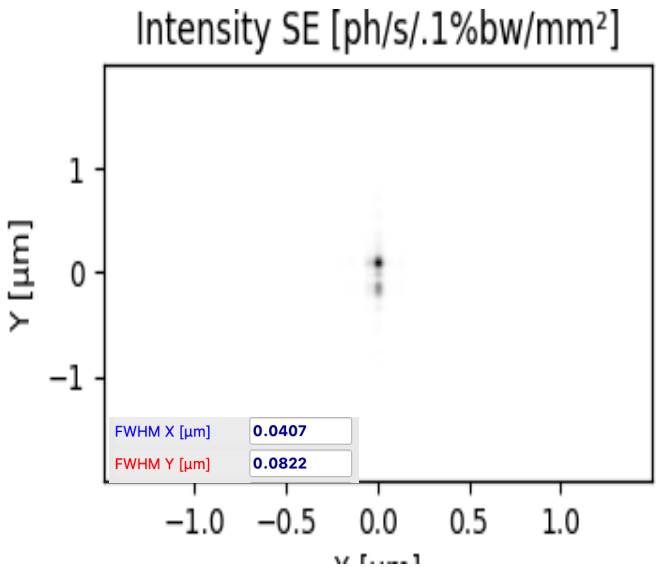
Shadow



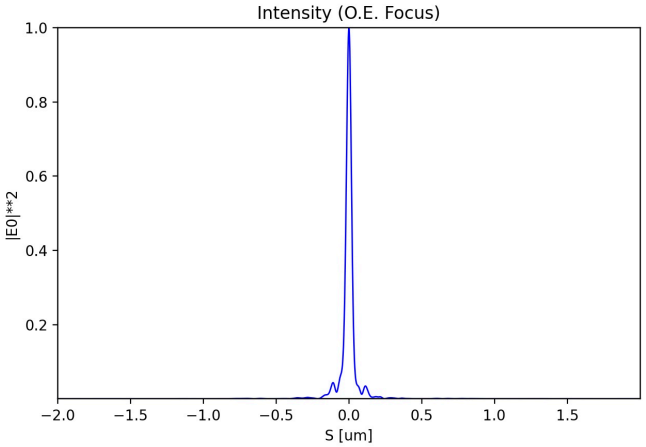
Hybrid

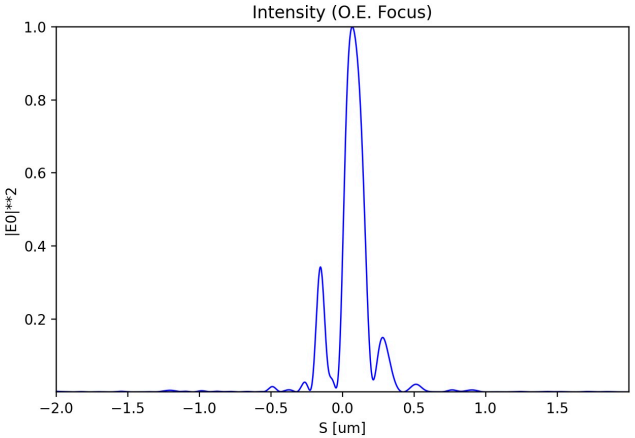


SRW



WISEr





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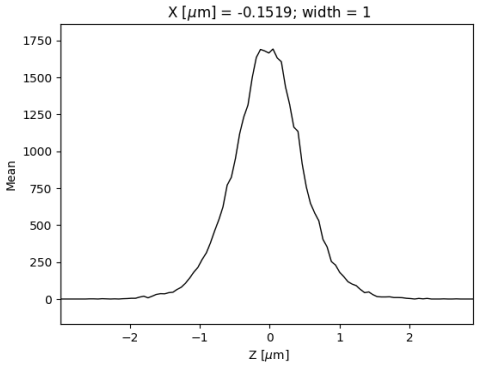
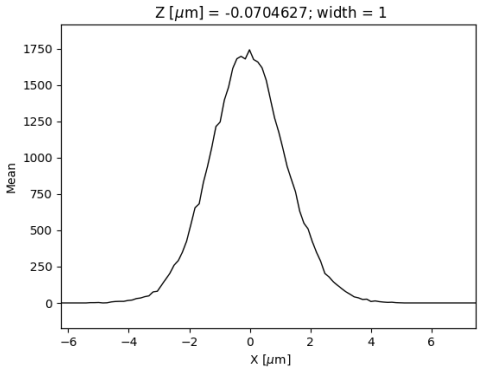
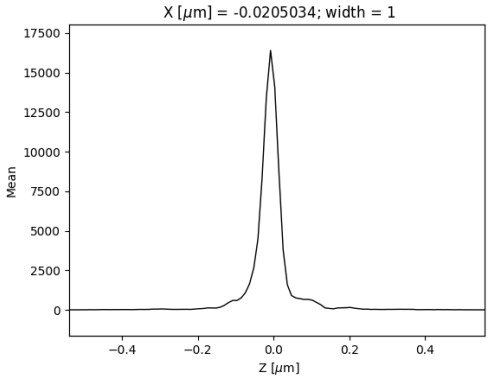
12.398 keV, 0.3 µrad slope error

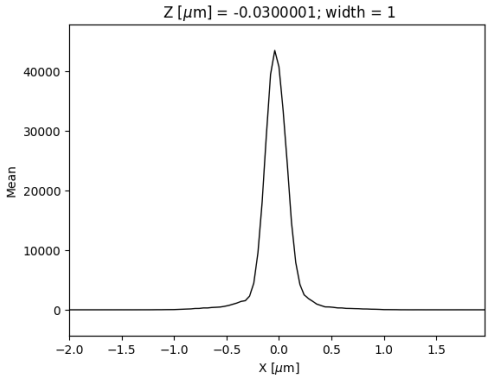
SHADOW



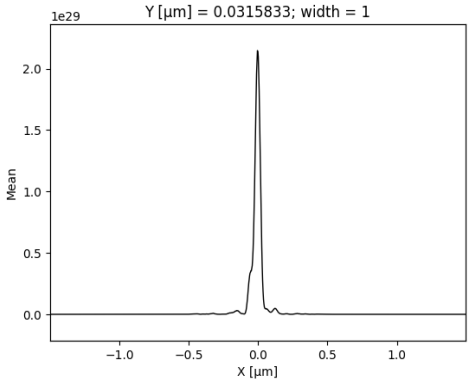


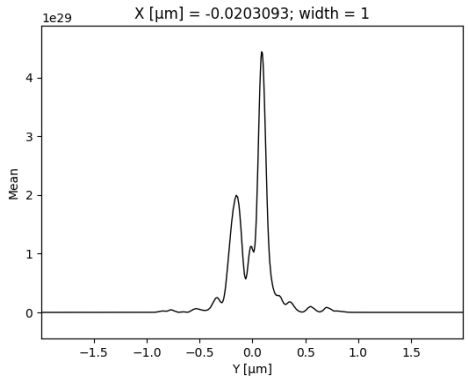
Hybrid



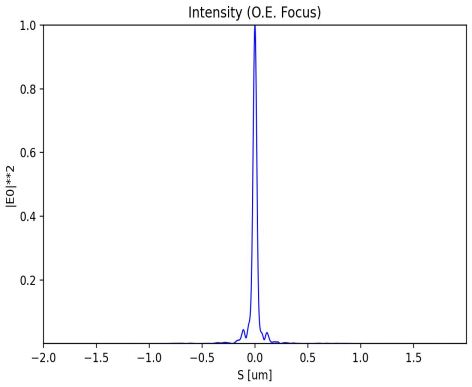


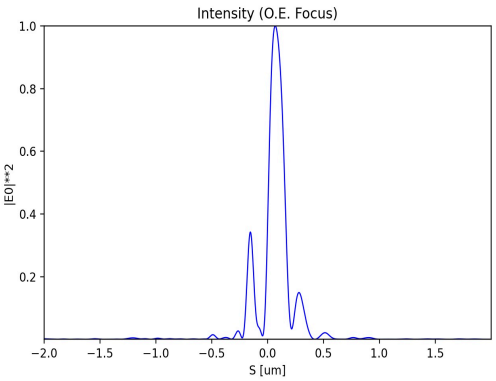
SRW





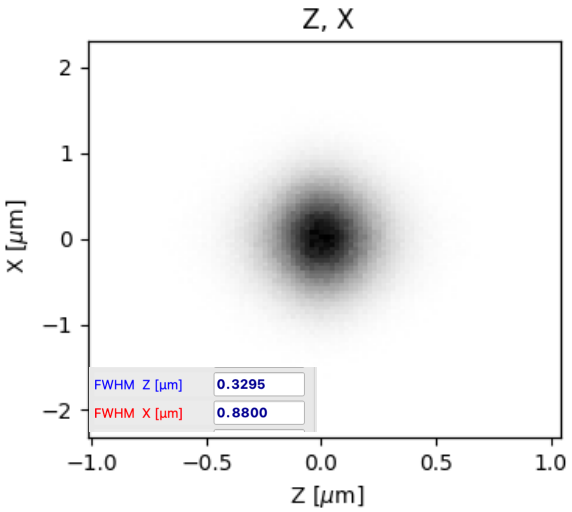
WISEr



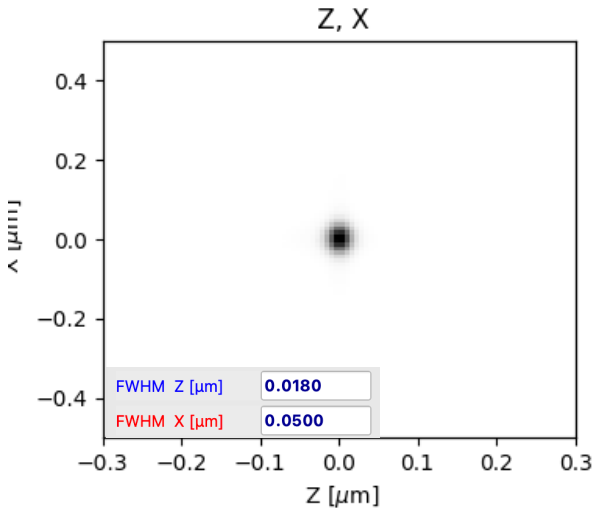


24.796 keV, 0.1 µrad slope error

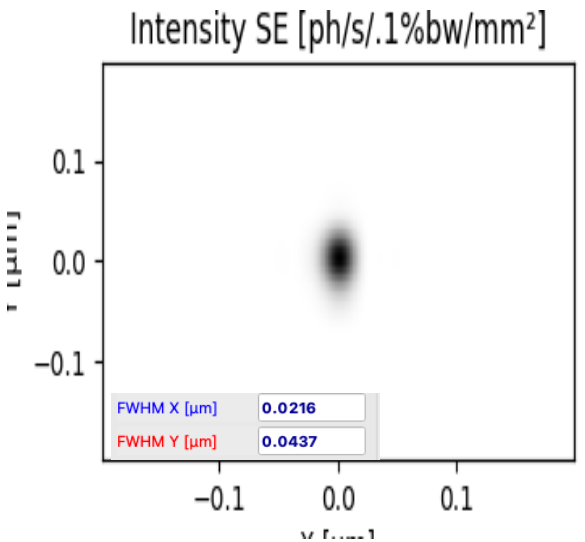
Shadow



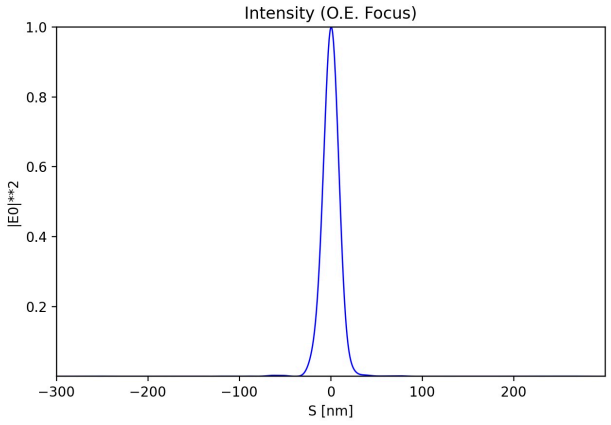
Hybrid

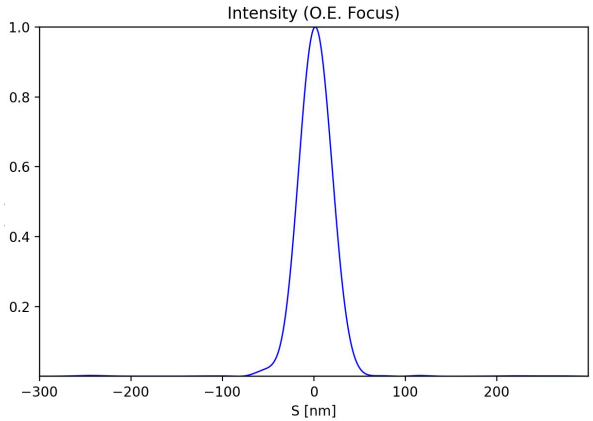


SRW



WISEr





FWHM = 0.02 X 0.042

Elettra
Sincrotrone
Trieste

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

Elettra
Sincrotrone
Trieste

Thank you!

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Trieste

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