X-ray Optics Simulation and Beamline Design Using a Hybrid Method

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Advanced Photon Source Upgrade Project

4th Diffraction Limited Storage Ring (DLSR) Workshop

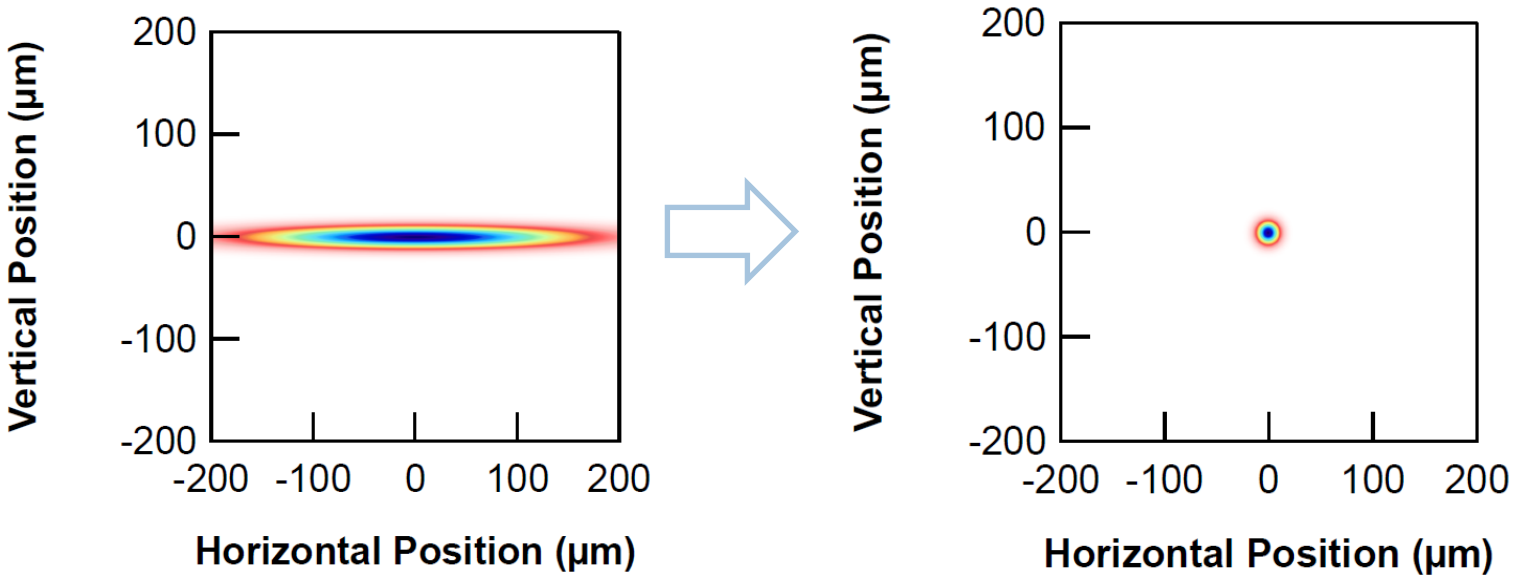
Nov. 19-21, 2014

Outline

- Motivation
- Hybrid method (HM) combining ray-tracing and wavefront propagation
  - Single optics: near-field
  - Multiple optics: far-field
  - SHADOWVUI implementation
- Beamline design using HM
  - Partial coherence, benchmark against SRW
  - Impacts of the MBA upgrade
- Summary

Motivation

- New light sources and upgrades with higher brightness, smaller emittance and partial or full coherence



- New experimental techniques: nano-scale imaging, diffraction, spectroscopy, ultrafast experiments, coherent diffraction imaging.

Optical system design and optimization

Motivation

- Geometrical ray tracing, e.g., SHADOW
  - Total intensity, beam size, mirror figure errors, reflectivity
  - Fast, robust, parameter optimization
  - No diffraction
- Wavefront propagation
  - Fourier optics, e.g., SRW
  - Stationary phase, e.g., PHASE
  - Diffraction effects
  - Partial coherent source: multi-electron simulation
  - Very slow, result cannot be carried over
- Fast simulation tool for beamline design and optimization
  - Diffraction effects when beam is clipped
  - Simulate mirror figure errors as wave optics
  - Partial coherent source

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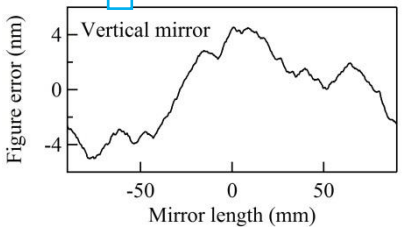
Hybrid method (HM): Single optics

Wavefront Propagation

$$E_{1e}(z_{1e}) = [I_{1e}]^{1/2} \times \exp\left[-ik\left(\frac{z_{1e}^2}{2f_z}\right)\right] \times \exp\{-i2k\Delta h(z_{1e})\, sin[\theta_1(z_{1e})]\}$$

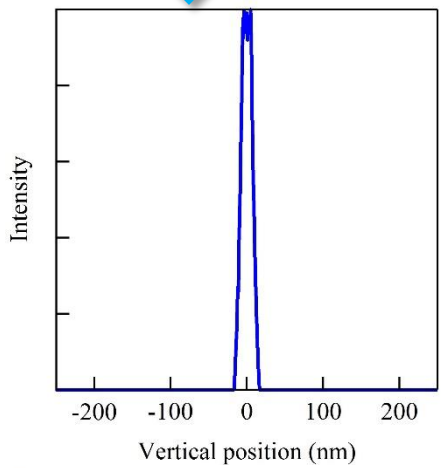
Ideal lens with focal length of f_z



Exit pupil

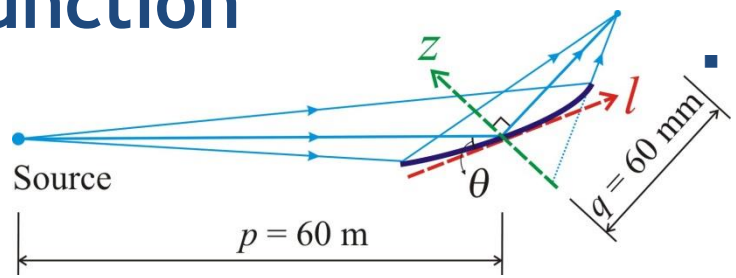
Ray tracing

Ideal optics



Exit pupil function

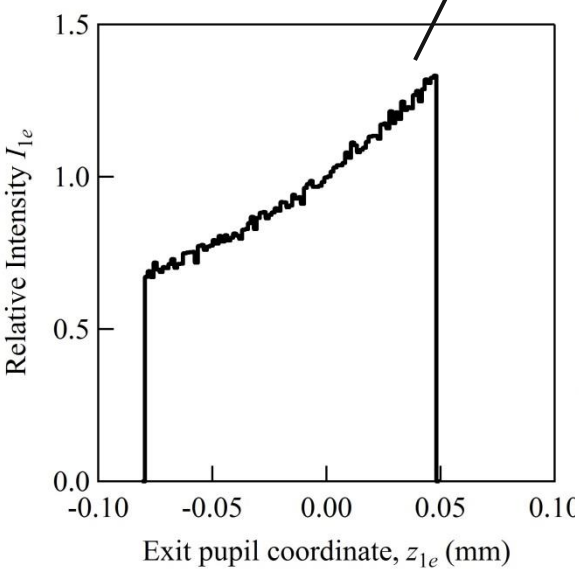
- Point source
  E = 15 keV

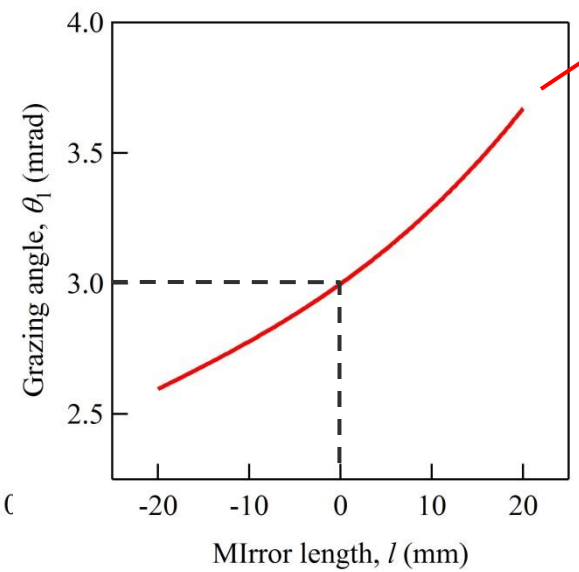


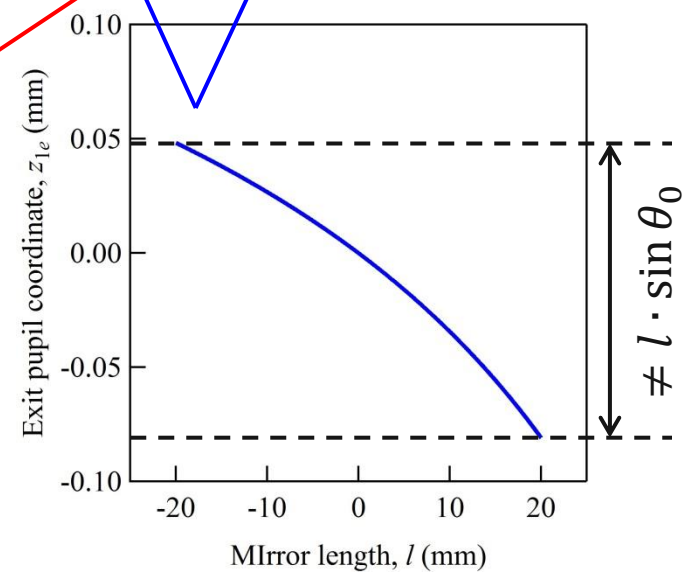
- Elliptical cylinder mirror
  Mirror length L = 40 mm
  Grazing angle at center: θ = 3 mrad
  Demagnification: 1000:1

Pupil function

$$E_{1e}(z_{1e}) = [I_{1e}]^{1/2} \times \exp\left[-ik\left(\frac{z_{1e}^2}{2f_z}\right)\right] \times \exp\{-i2k\Delta h(z_{1e})\, sin[\theta_1(z_{1e})]\}$$







- Intensity scaling
- Grazing angle correction
- Coordinate transformation

Hybrid method (HM): Single optics

Wavefront Propagation

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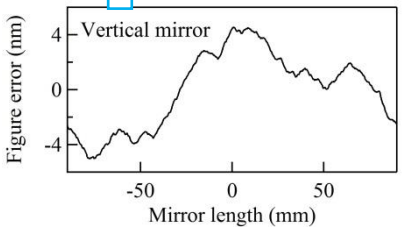
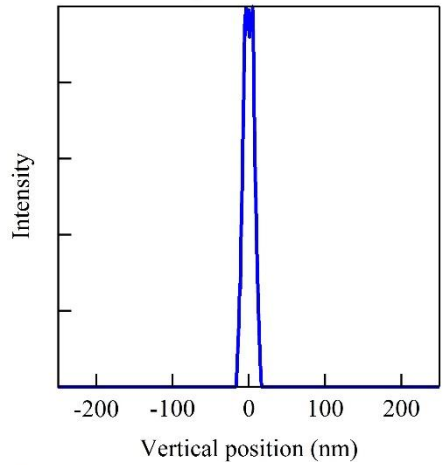


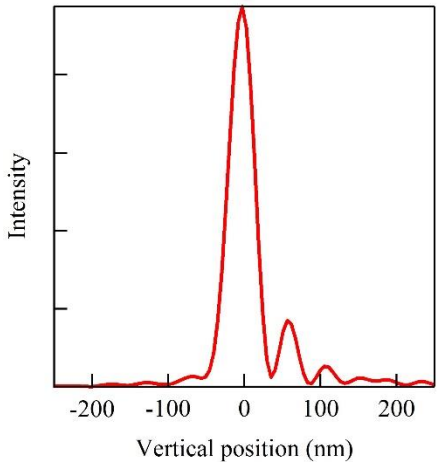
Exit pupil

Ray tracing

$$E_{1e}(z_{1e}) \rightarrow \boxed{\text{FFT}} \xrightarrow{\mathcal{F}(v_{1e})} \boxed{\times \exp[-i\pi\lambda D v_{1e}^2]} \xrightarrow{\mathcal{F}'(v_2)} \boxed{\text{Inverse FFT}} \rightarrow E_2(z_2)$$

Ideal optics





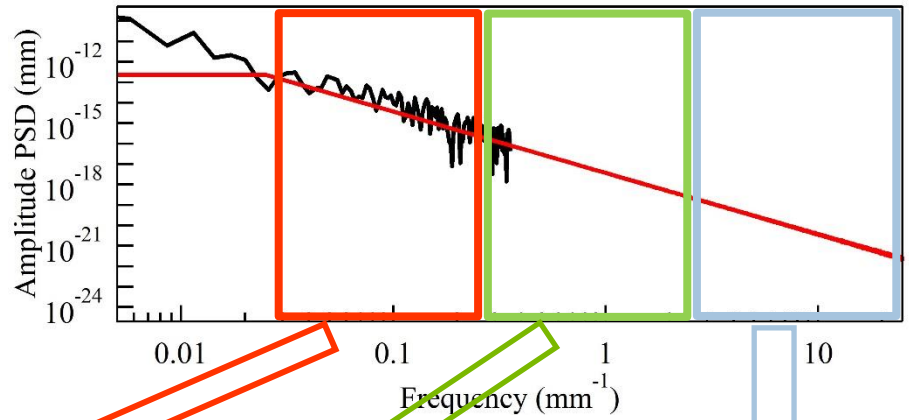
- Kirchhoff tangent plane
- Paraxial approximation

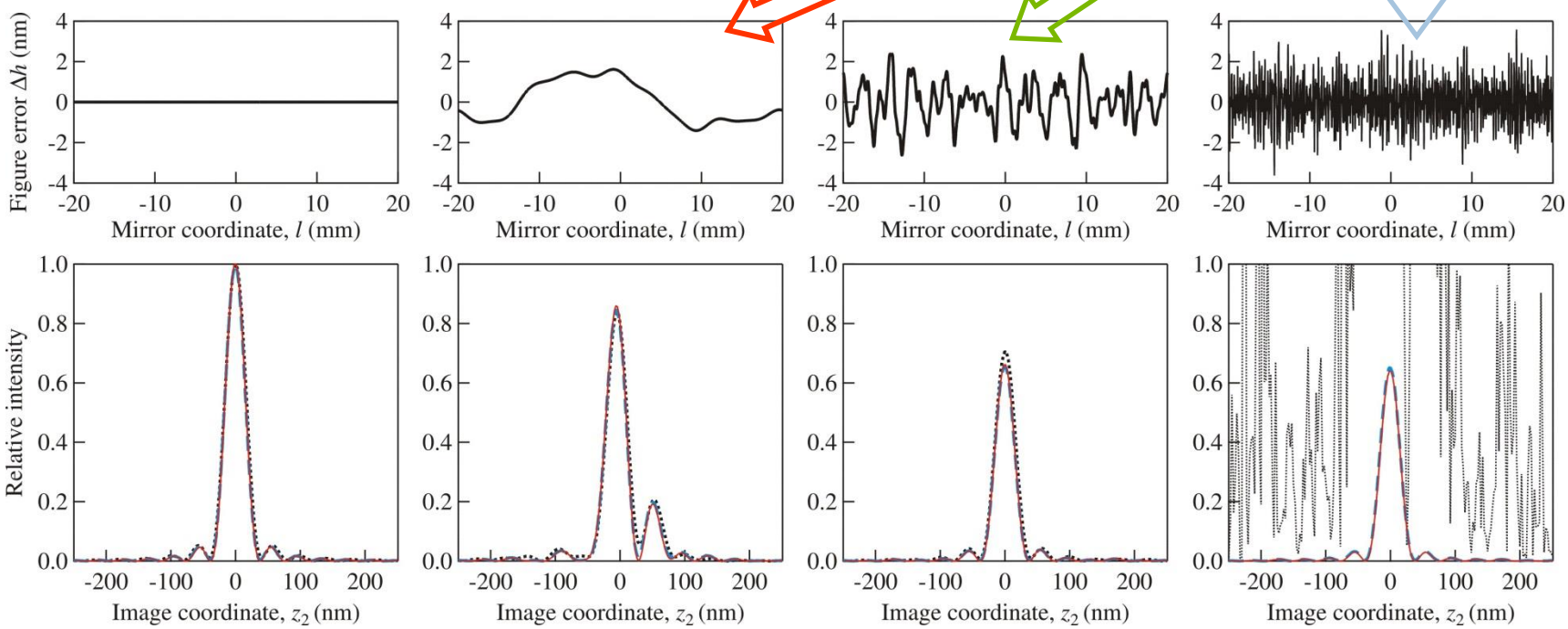
Validation of the pupil function approach

—— Fresnel-Kirchhoff diffraction integral (FKDI)

····· Stationary Phase Approximation (SPA)

— — Hybrid Method (HM)





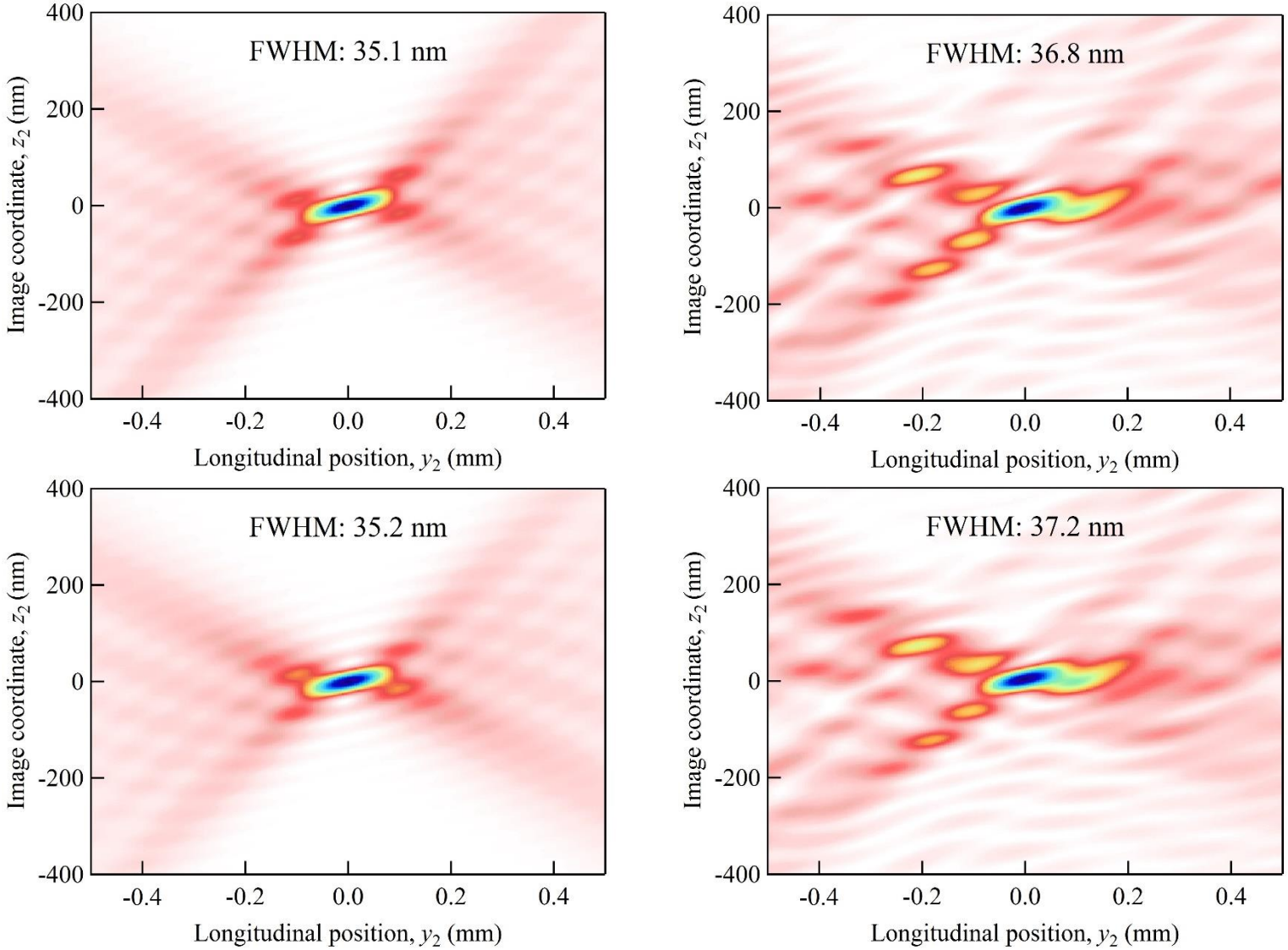
X. Shi, et al., Proc. SPIE **9209**, 920909 (2014).

Profiles near the focal plane (near-field)

Ideal mirror | SN-2

FKDI

HM



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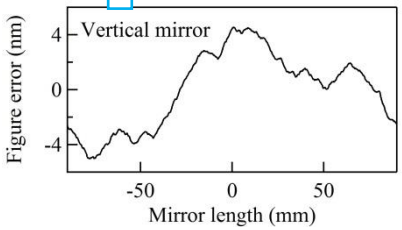

Exit pupil

Ray tracing

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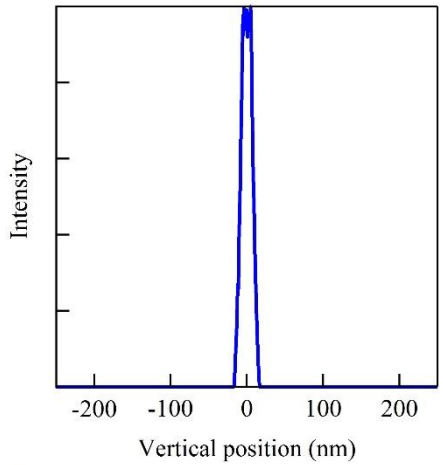
Ideal optics



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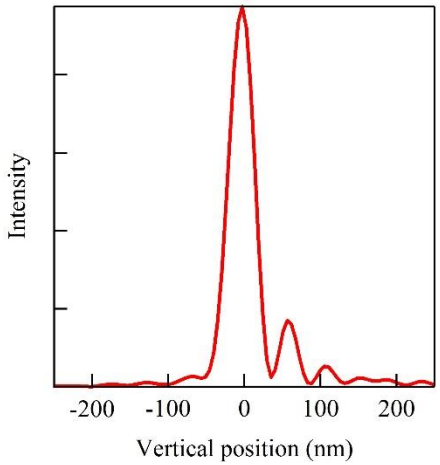

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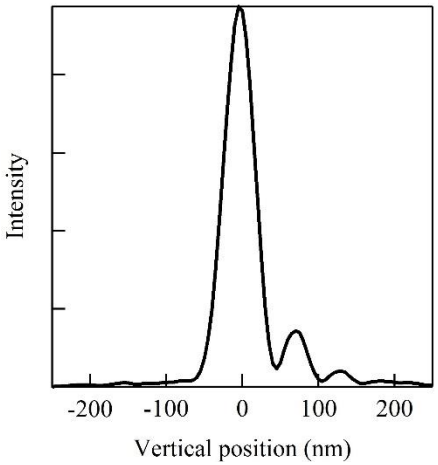
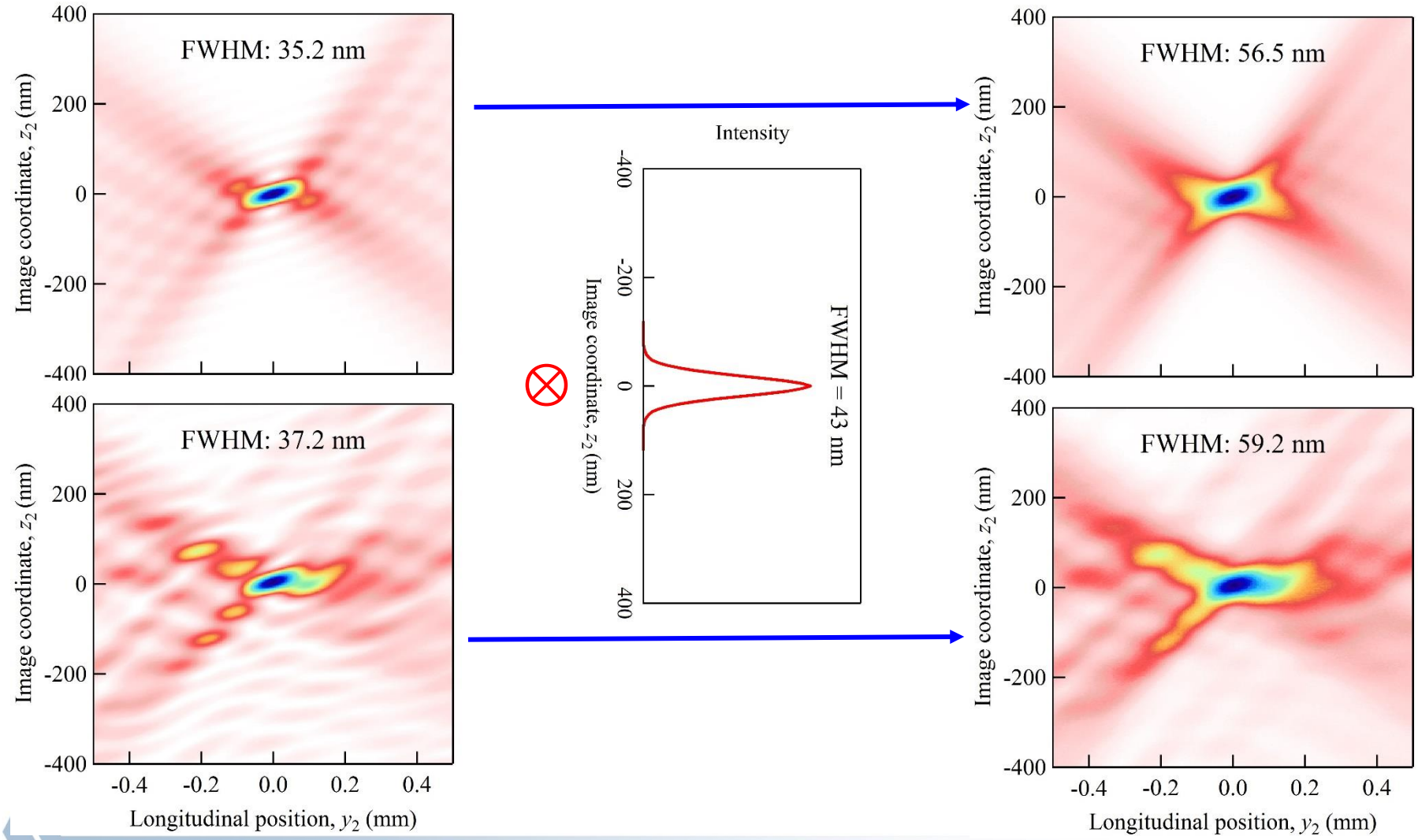
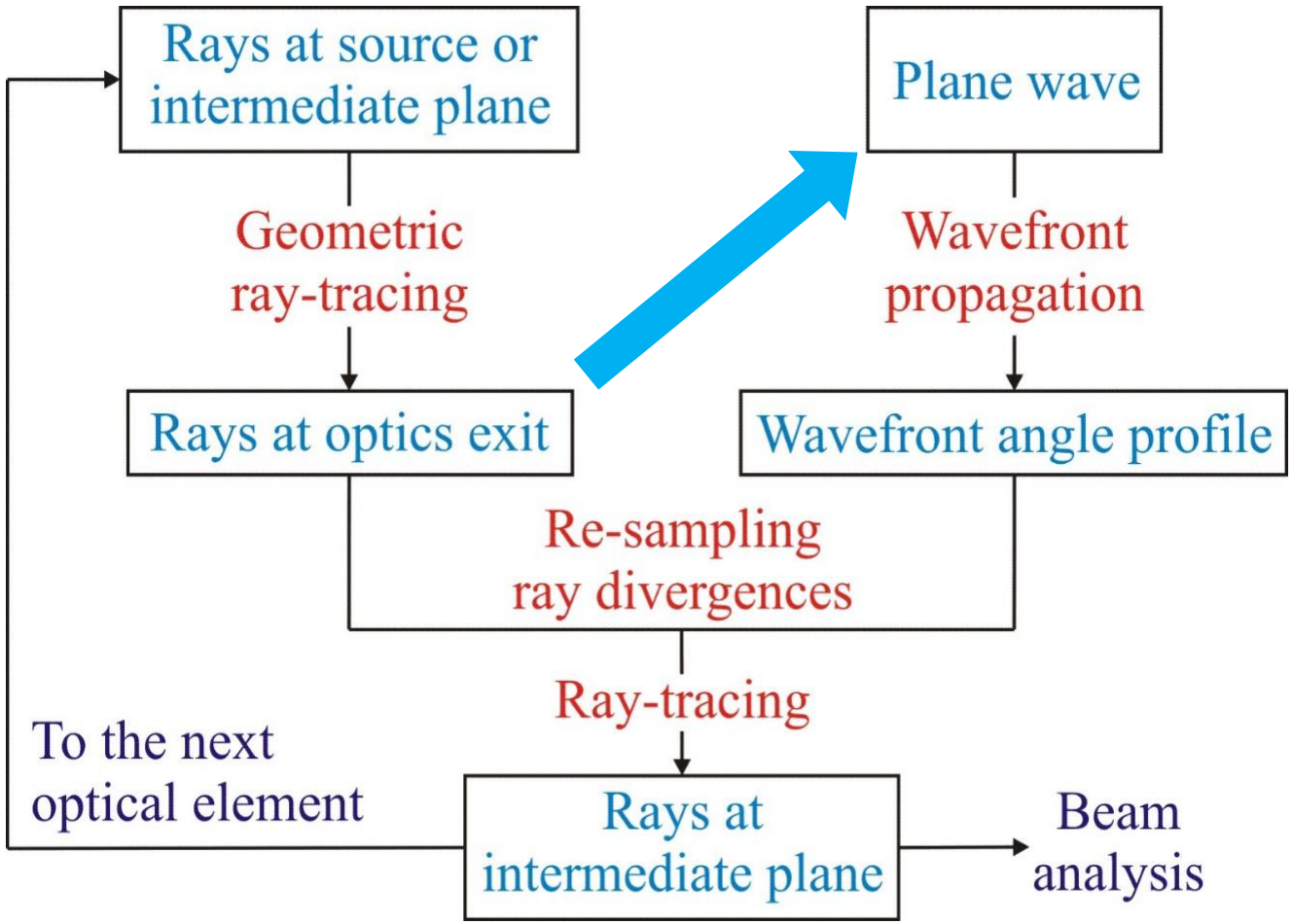


Hybrid method: partial coherent source

SN-2 mirror illuminated by an extended source which has a Gaussian size of 20 µm (rms) and a Gaussian divergence of 3 µrad (rms), respectively.



Hybrid method: Multiple optics

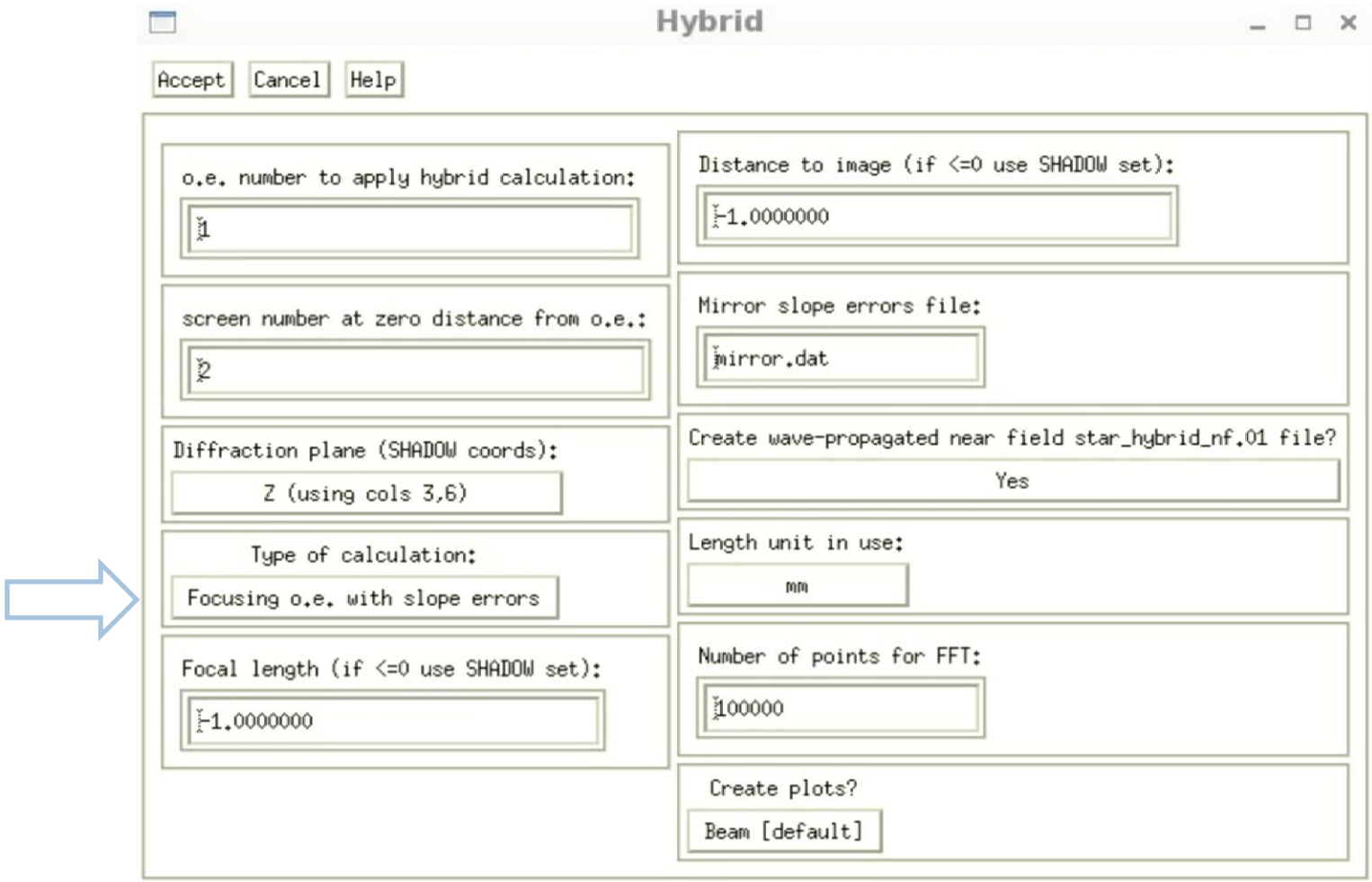


Iterative, valid in far-field approximation

X. Shi, et al., J. Synchrotron Rad. **21**, 669 (2014).

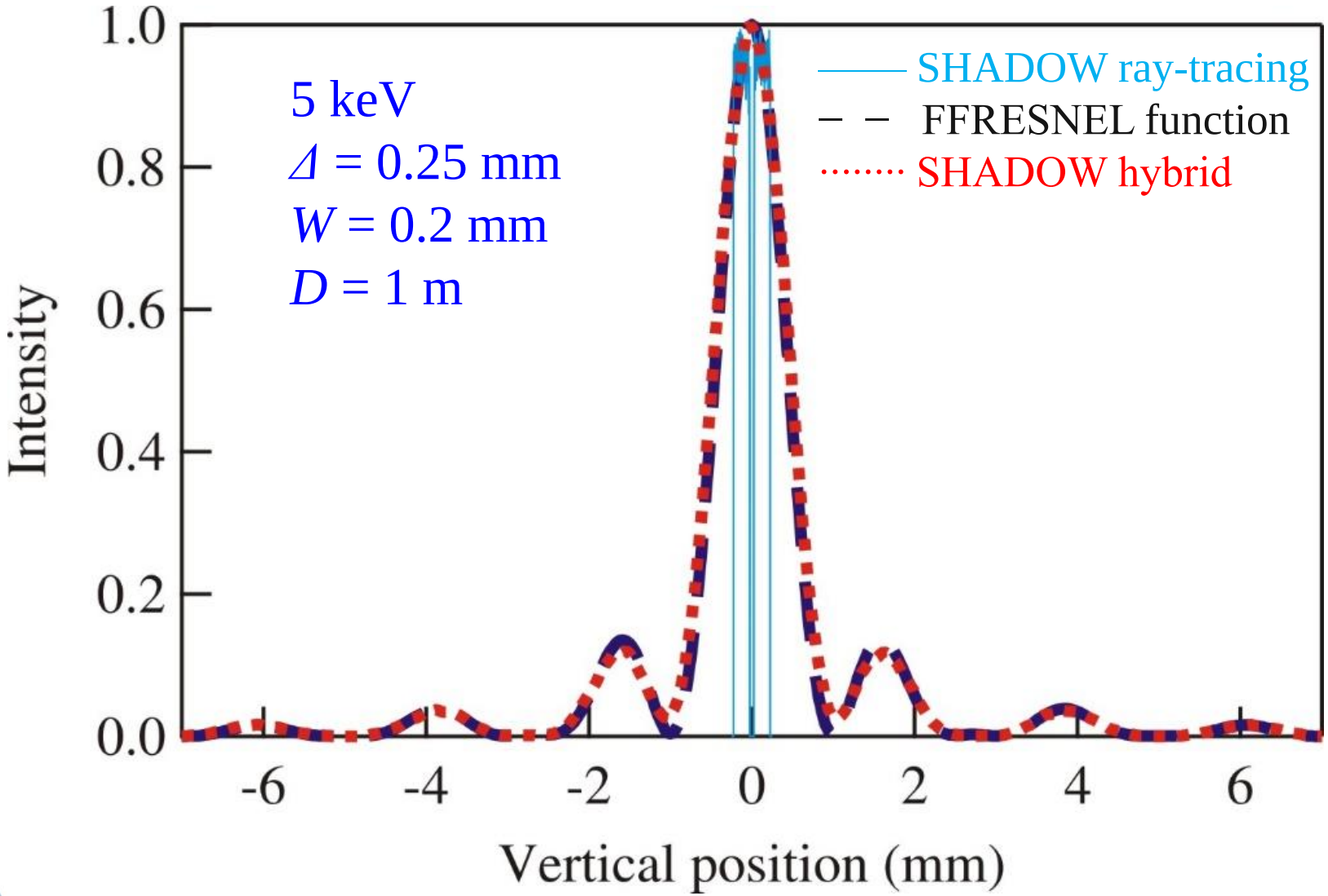
Hybrid code in XOP-SHADOWVUI

ftp.esrf.eu/pub/scisoft/xop2.3/shadowvui1.12_xxx_20140808.zip



X. Shi, et al., Proc. SPIE **9209**, 920911 (2014).

Example: double-slit interference



Mirror figure errors

Diffraction limited

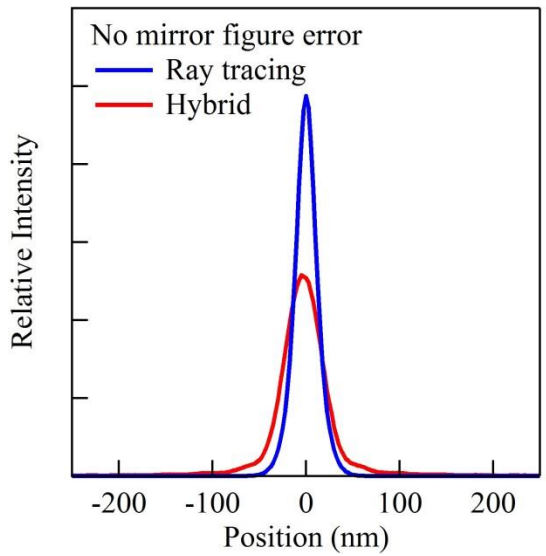
σ = 2 µm

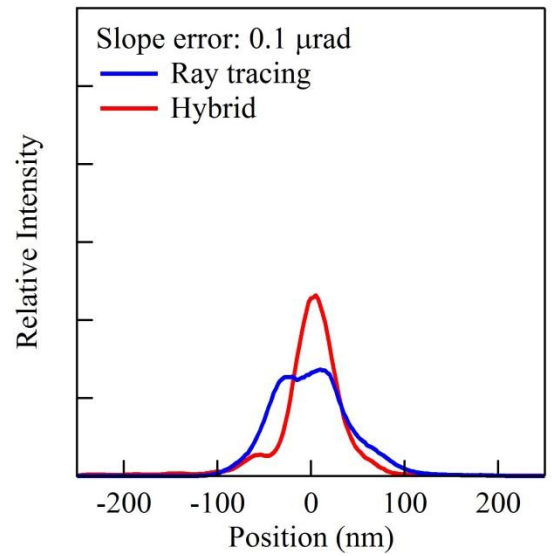
σ' = 30 µrad

p = 30 m

q = 0.2 m

l = 0.2 m





Not diffraction limited

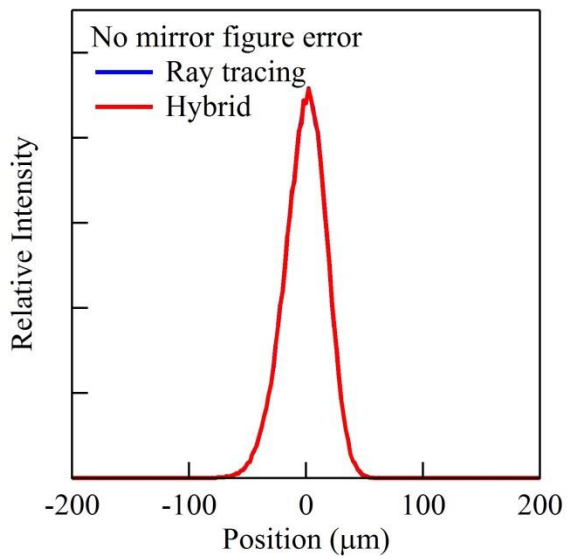
σ = 270 µm

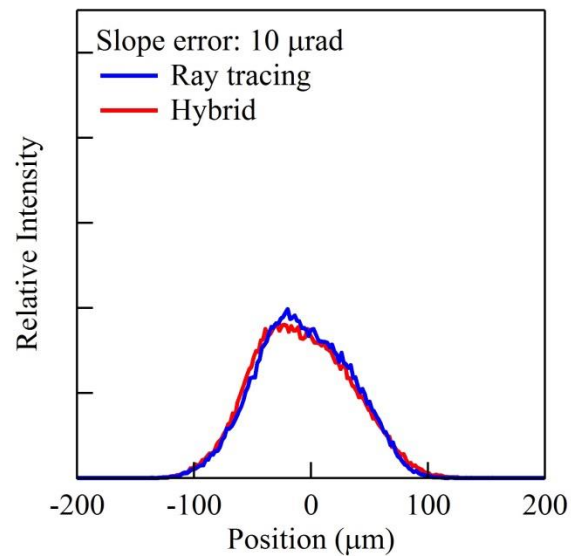
σ' = 12 µrad

p = 30 m

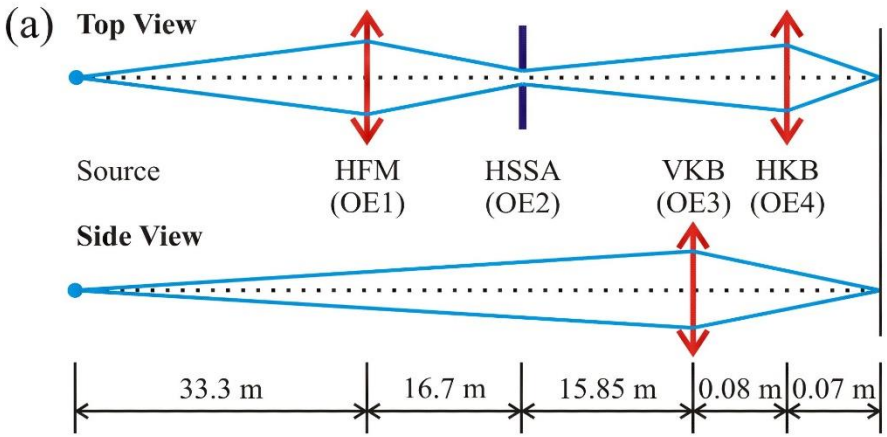
q = 2 m

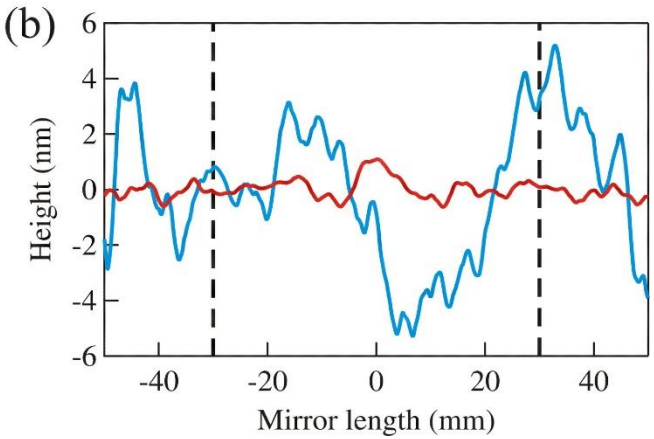
l = 1 m





SHADOWVUI hybrid code





SHADOWVUI macro

```
shadow_run, /source
shadow_run, /trace
hybrid, n_oe=1, n_screen=1, calctype=1
shadow_runtrace, previous_oe=1, star_file='star_hybrid.01‘
hybrid, n_oe=2, n_screen=1, calctype=0
shadow_runtrace, previous_oe=2, star_file='screen_hybrid.0201'
hybrid, n_oe=3, n_screen=2, calctype=2, mirrorfile='vkb.dat'
shadow_runtrace, previous_oe=3, star_file='star_hybrid.03'
hybrid, n_oe=4, n_screen=2, calctype=2, mirrorfile='hkb.dat'
```

X. Shi, et al., Proc. SPIE **9209**, 920911 (2014).

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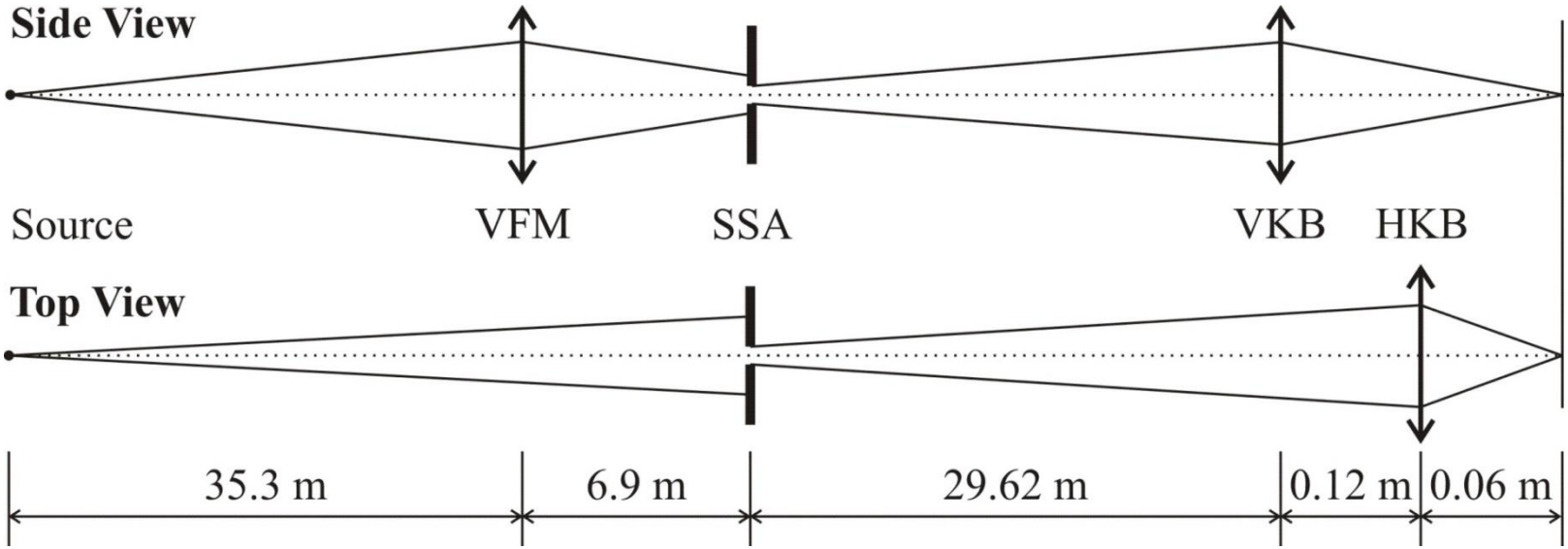
In Situ Nanoprobe beamline



Photon (10 keV)	Electron	Total
σ_r = 3.86 μm	σ_x = 274 μm	Σ_x = 274 μm
	σ_y = 10.3 μm	Σ_y = 11.0 μm
σ_ξ = 5.11 μrad	σ'_x = 11.3 μrad	Σ'_x = 12.4 μrad
	σ'_y = 3.6 μrad	Σ'_y = 6.2 μrad

Source: undulator A, 3.3 cm, 72 periods, K = 0.906, B = 0.294 T

VFM: 400 mm long, 2.5 mrad grazing angle

SSA: 11 × 4 μm^2 (h × v) → wide open

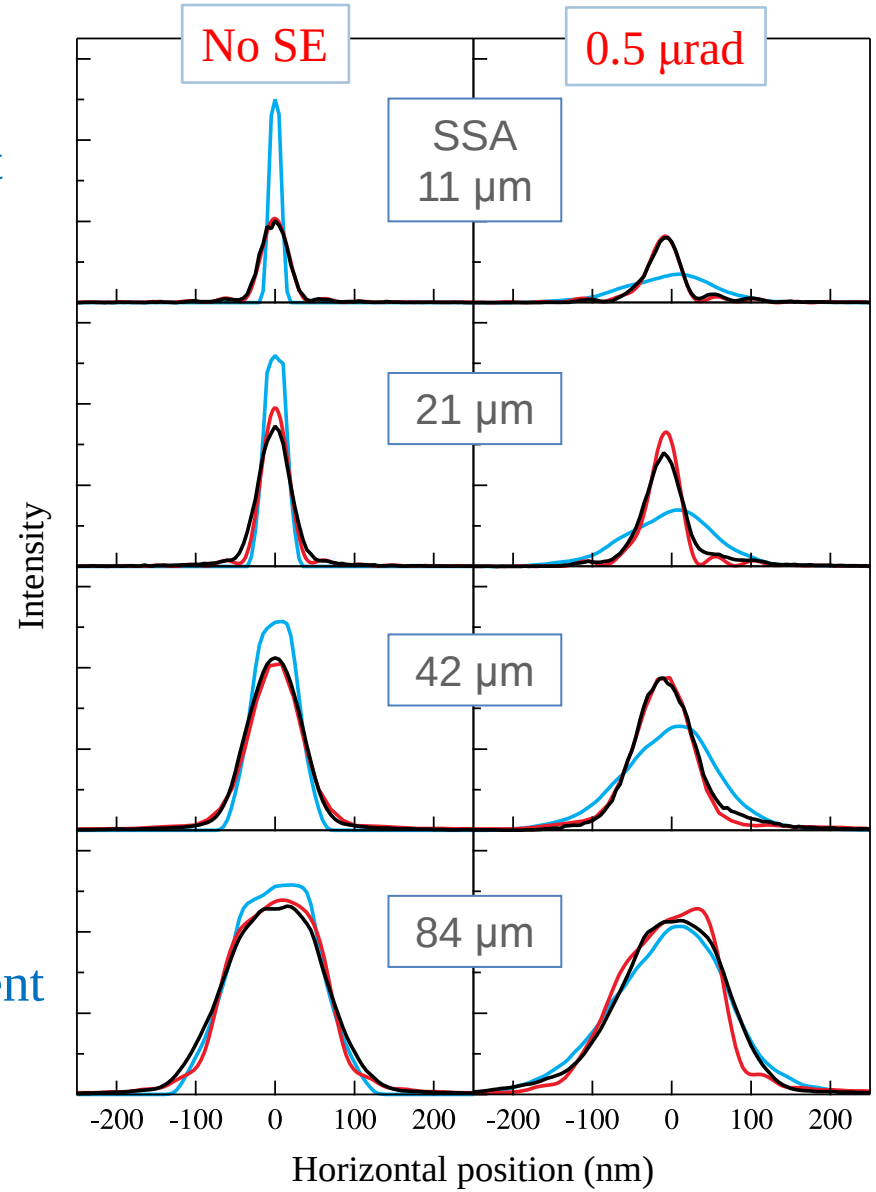
VKB: 180 mm long, 2.5 mrad grazing angle

HKB: 60 mm long, 2.5 mrad grazing angle

Comparison with SRW (multi-electron)

Full coherent

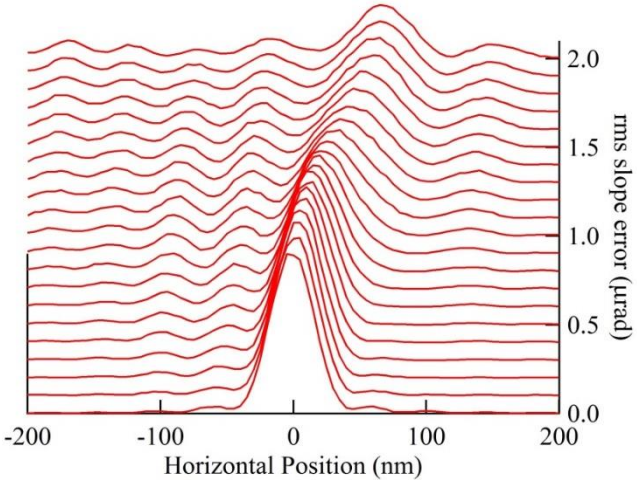
Full incoherent

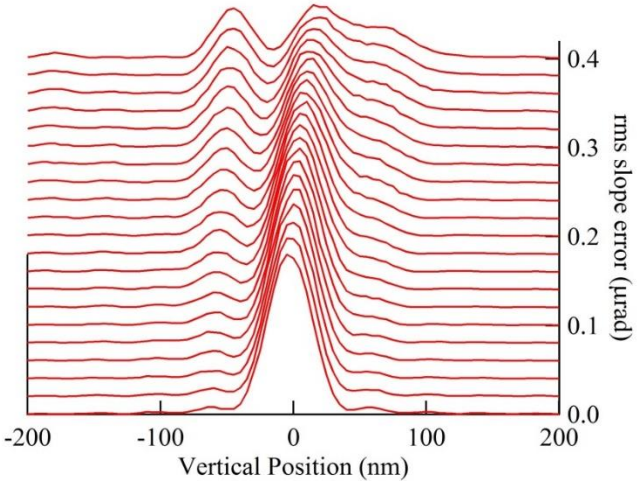


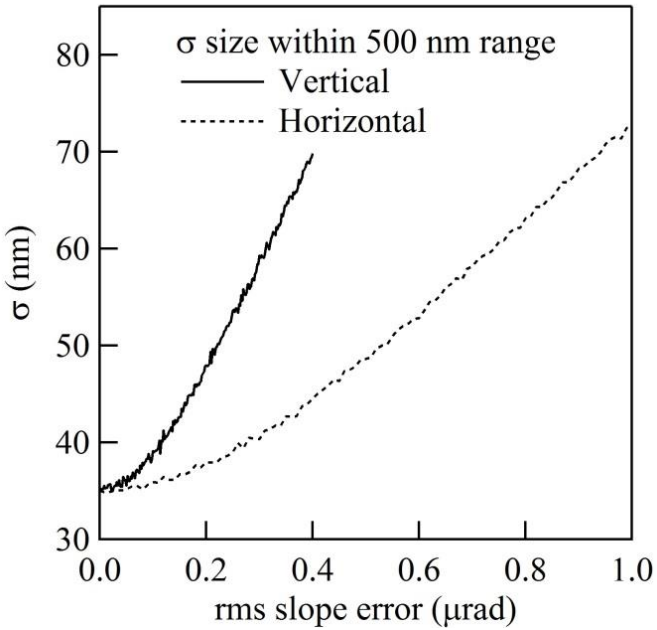
Hybrid
SHADOW
Multi-electron SRW

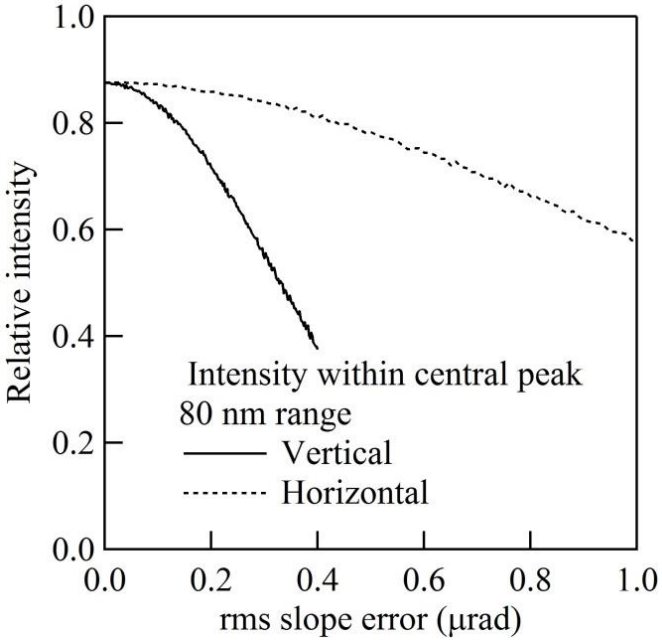
Calculation time:
SRW: 32 core × 5 hours
Hybrid: 1 core × 5 minutes

KB mirror slope error studies





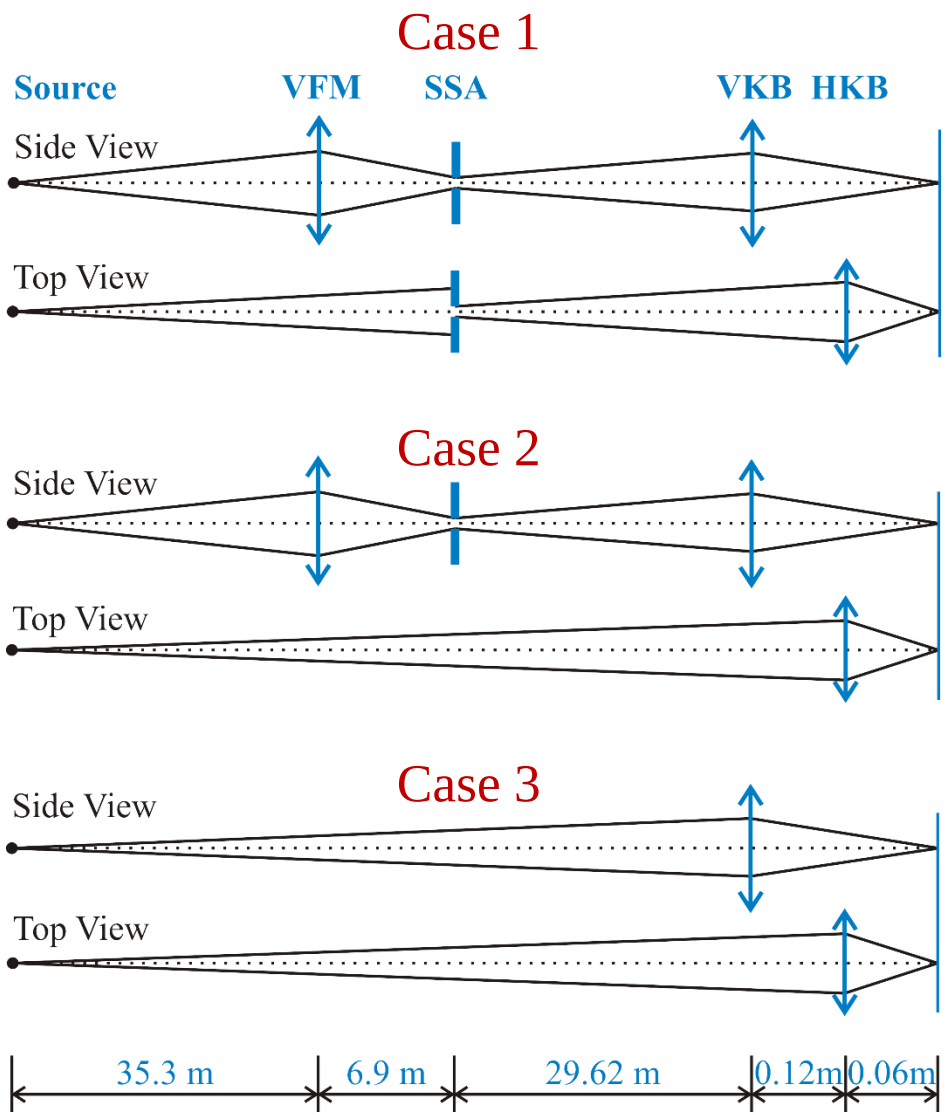




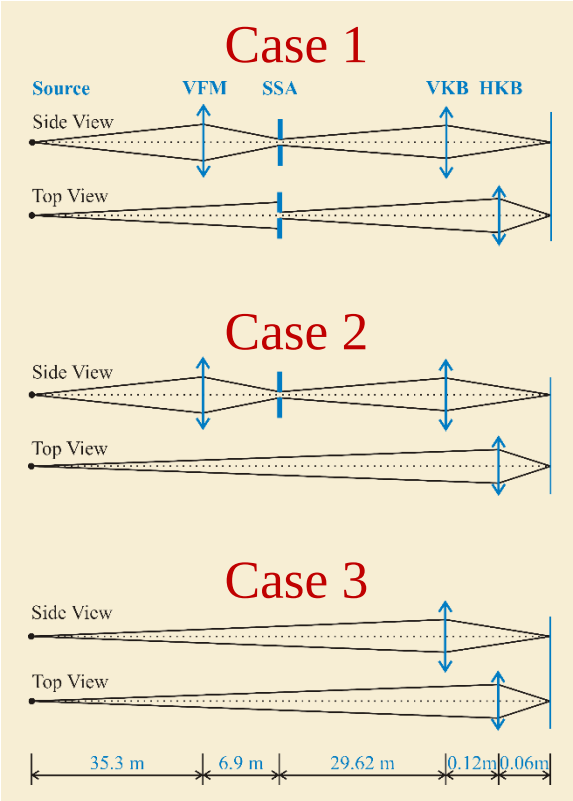
Current APS vs MBA upgrade

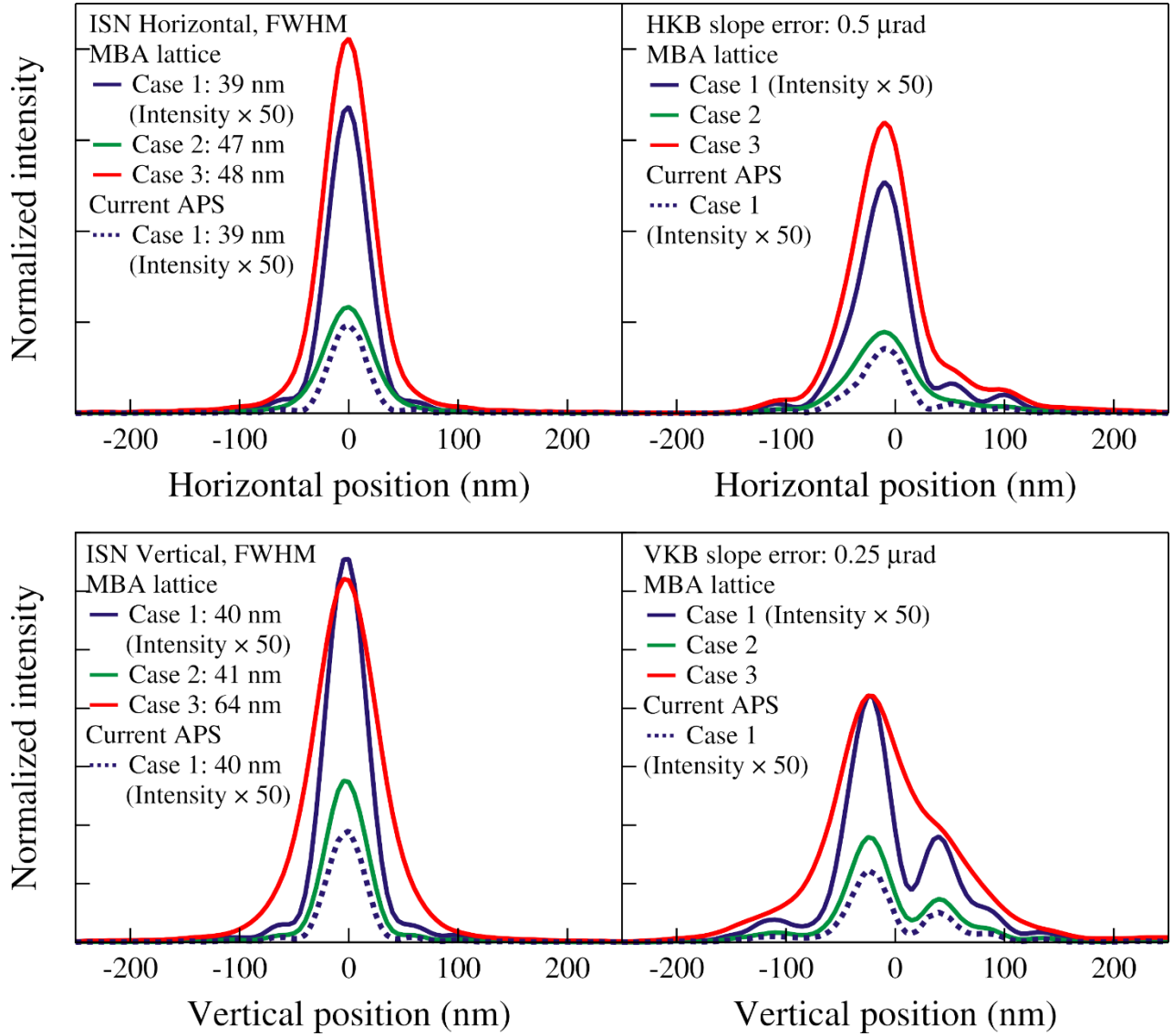
10 keV	Current APS	MBA upgrade
Σ_x (μm)	274	17.7
Σ_y (μm)	11.0	10.4
Σ'_x (μrad)	12.4	5.7
Σ'_y (μrad)	6.2	6.7

**APS MBA Accelerator Systems, March 16, 2014. $\epsilon_x = \epsilon_y = 42.9$ pm, $N_b = 162$.*



Current APS vs MBA upgrade



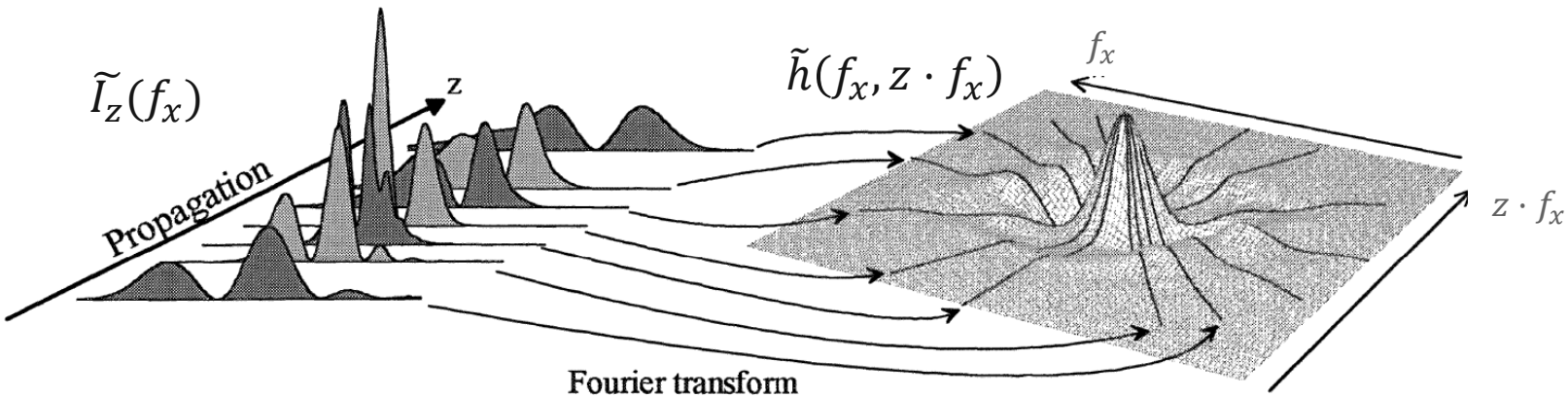


Curent & Further developments on HM

- Full 2-D simulation is needed for certain cases (toroid mirror).
- Coherence properties under investigation.
  - Wigner distribution function, $h(x,u)$, reconstruction.

T. Mey, et al., Proc. SPIE **8778**, 87780H (2013) Opt. Express **22**, 16571 (2014).

$$I_z(x) \overset{\text{FT}}{\Rightarrow} \tilde{I}_z(f_x) = \tilde{h}(f_x, z \cdot f_x) \xRightarrow{\text{2D IFT}} h(x,u) \xRightarrow{\text{1D IFT}} \Gamma(x,s)$$



B. Eppich, Proc. SPIE **4270**, 71-79 (2001).

Coherence length:

$$l_x = \text{FWHM}[\Gamma(0,s)]$$

Degree of coherence:

$$K_x = \frac{\iint h^2(x,u)dxdu}{\iint h(x,u)dxdu}$$

Summary

- ✓ The hybrid method combining ray tracing and wavefront propagation is demonstrated and benchmarked against existing codes.
- ✓ The pupil function approach used in the hybrid method can be implemented in any wavefront propagation code.
- ✓ The hybrid method can be applied to any ray-tracing code and has been implemented in SHADOWVUI.
- ✓ The hybrid method is efficient, and suitable for beamline optimization.

Acknowledgements

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Ruben Reininger

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Dean Haeffner

Chris Jacobsen

Linda Young

ESRF

Manuel Sanchez del Rio

BNL

Oleg Chubar

SOLEIL

Cameron Kewish

Thank you!