PROPAGATING PARTIAL COHERENCE — *HYBRID* AND MORE

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OUTLINE

- Beamline optics simulation at APS
- *HYBRID* method
- Non-ideal optics: simulation
- Non-ideal optics: specification
- Mutual optical intensity propagation

BEAMLINE OPTICS SIMULATION AT APS

APS upgrade project

- 8 new beamlines
  - Coherence, nano-focusing, variable focal size
  - Mirrors, CRLs, Zoom lens (a pair of dynamical focusing KB or CRL), ZPs
  - Geometry: direct focusing, secondary focusing
- Beamline enhancement for all APS beamlines
  - Do no harm
  - Replacing/refurbishing critical elements

Assess current status and readiness of beamline optics for the APS upgrade

- Beamline optics database
  - Components, positions, cooling, metrology, papers describing beamline
- Measure and simulate all beamlines
  - Spot size, flux, vibration
  - Measured 19 beamlines (28 endstations)

BEAMLINE OPTICS SIMULATION AT APS

Simulation tools for beamline design

- Levels of simulation: accuracy vs efficiency
  - Calculator estimation: source size + ideal lens
  - Analytical formula (Mathematica/Excel):
    - Gaussian source profile
    - Optics acceptance (e.g., slits, mirror aperture, CRL transmission)
    - Demagnification + diffraction formula
  - Shadow-*HYBRID* (ShadowVUI and OASYS-ShadowOui version):
    - Real source intensity profile (Shadow, Spectra)
    - More accurate optics calculation (e.g., mirror shape error, heat load)
    - Ray-tracing + wavefront propagation to deal with partial coherence.
  - Full mutual coherence function propagation:
    - SRW
    - Mutual coherence function propagation (ESRF)
    - MOI code under development at APS and SSRF
- Optics simulation combined with x-ray testing

OUTLINE

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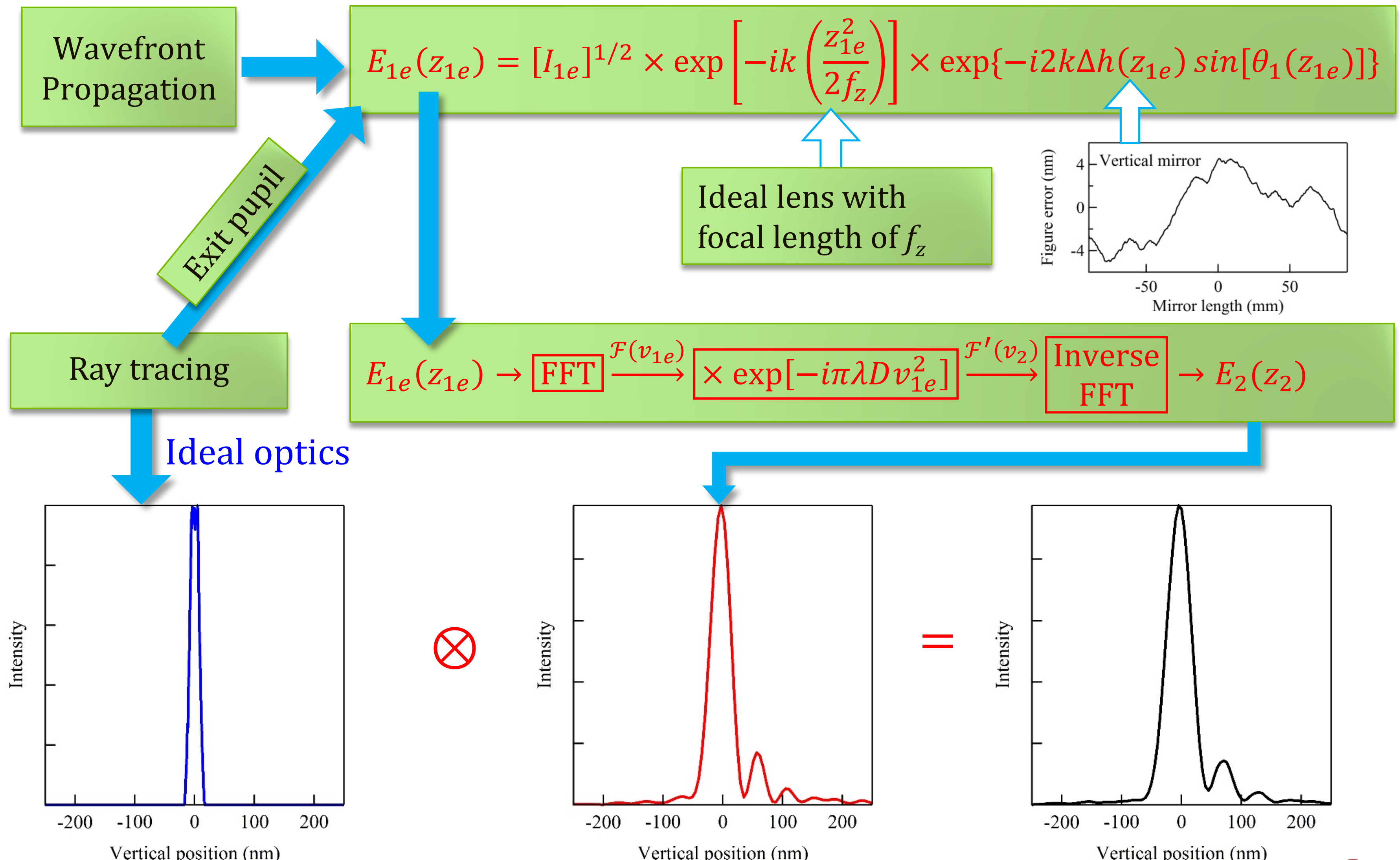
HYBRID METHOD

Motivation

- Geometrical ray tracing, e.g., SHADOW, RAY, McXtrace, …
  - 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
  - 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

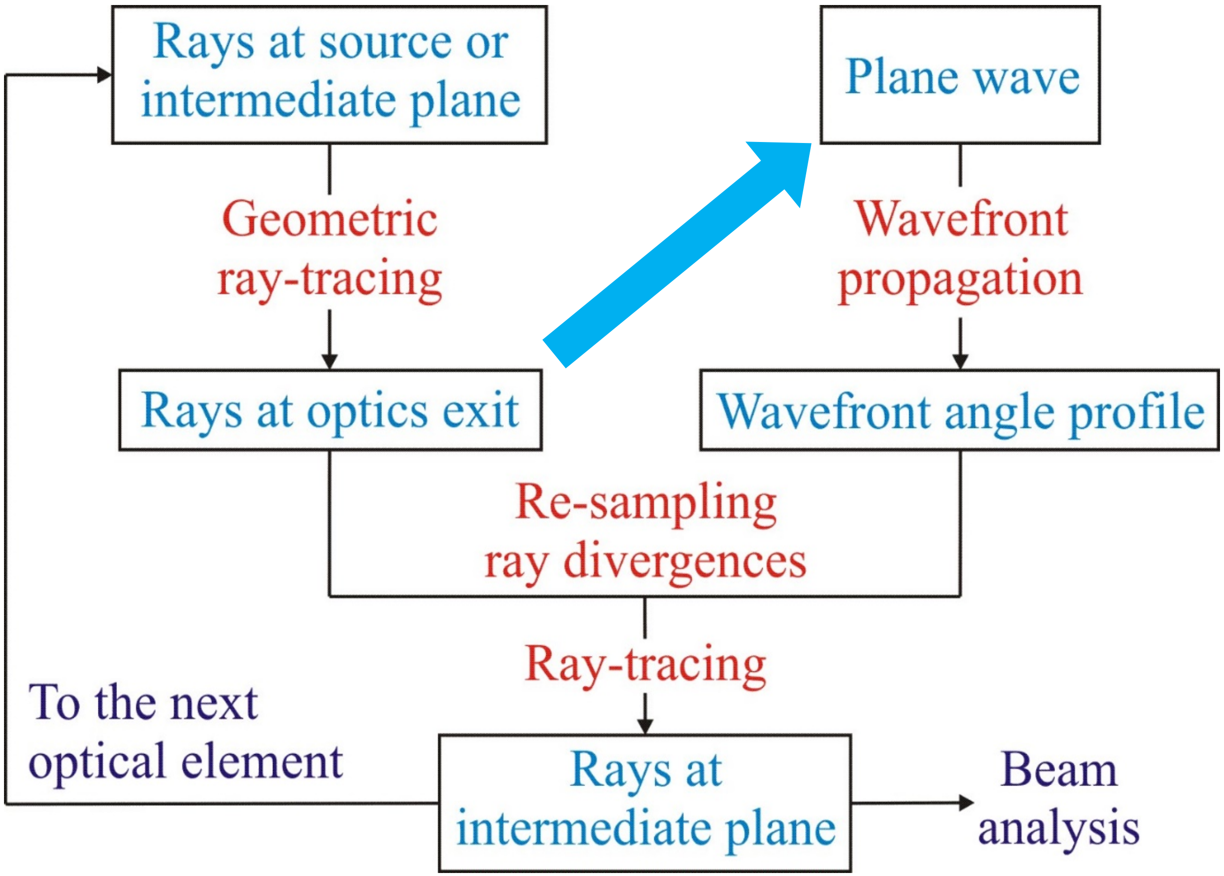
HYBRID METHOD

Basic idea — near-field mode



HYBRID METHOD

Basic idea — far-field mode

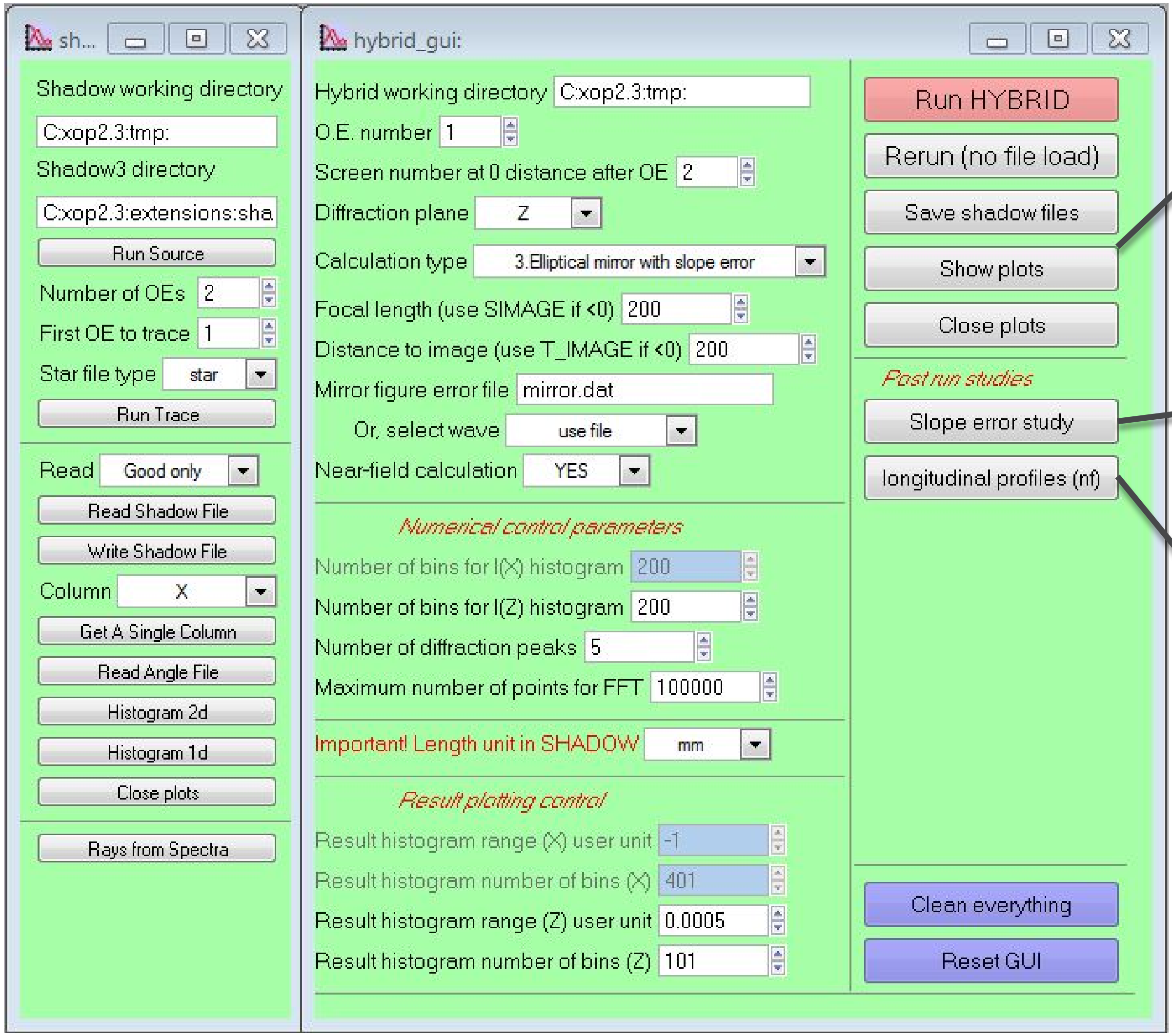


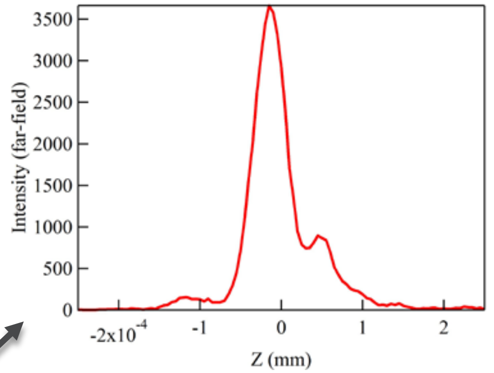
- Iterative, valid in far-field approximation

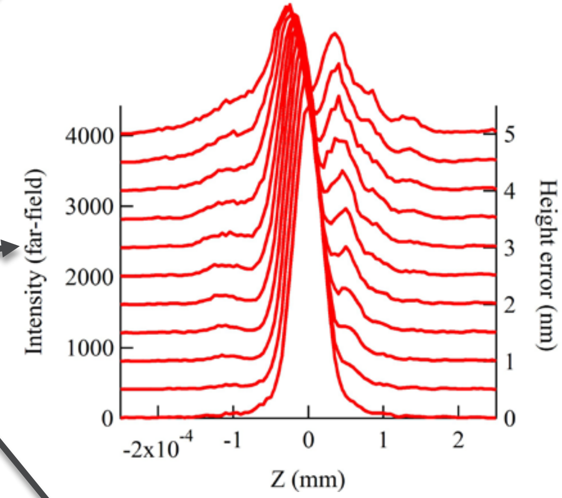
X. Shi, et al., J. Synchrotron Rad. **21**, 669 (2014).

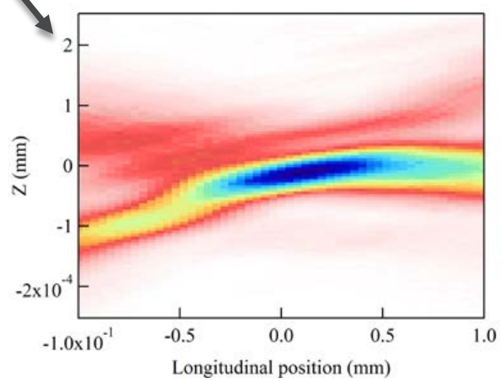
HYBRID METHOD

Distribution — Igor pro version



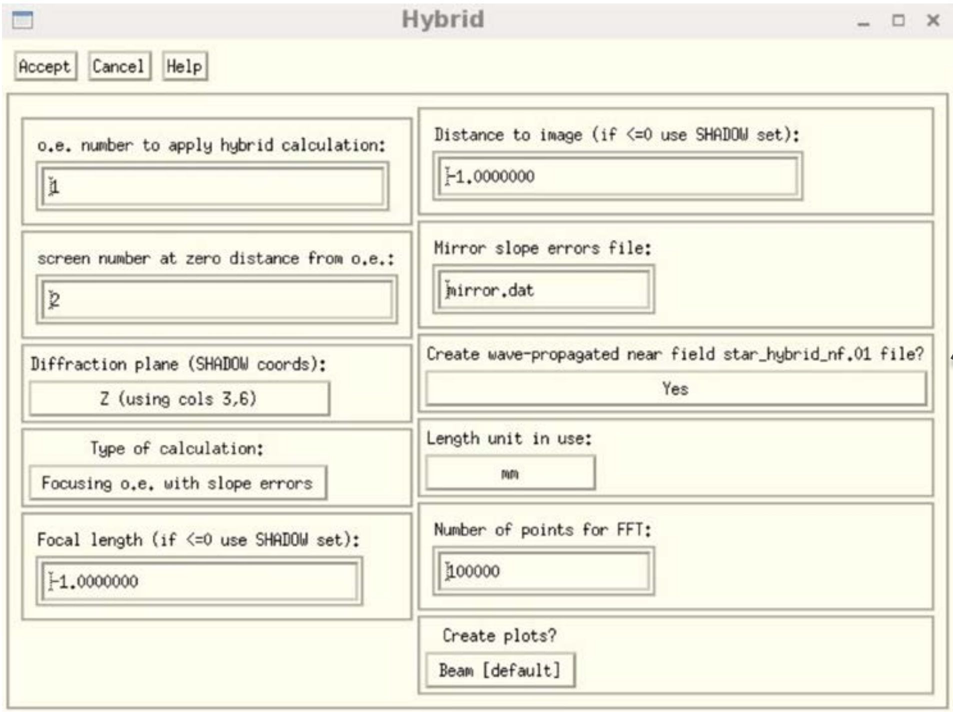


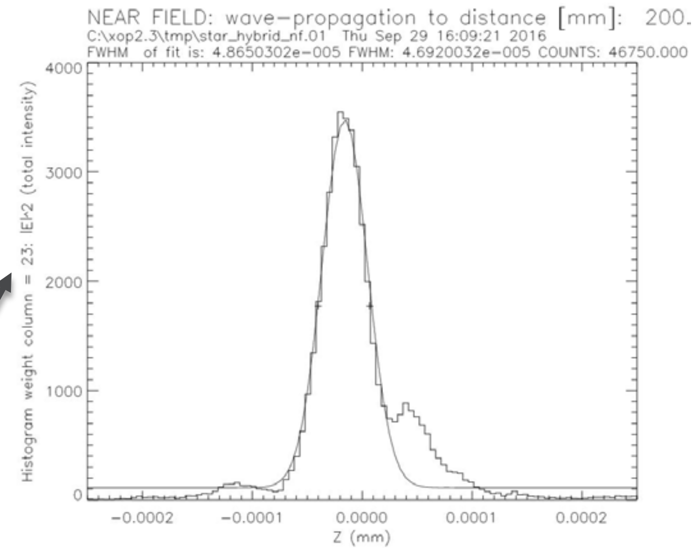


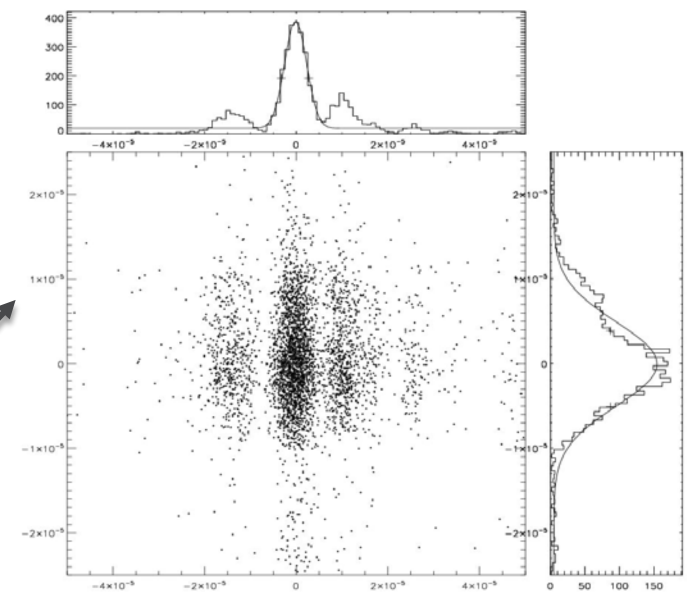


HYBRID METHOD

Distribution — ShadowVUI version







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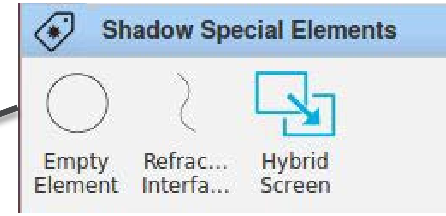
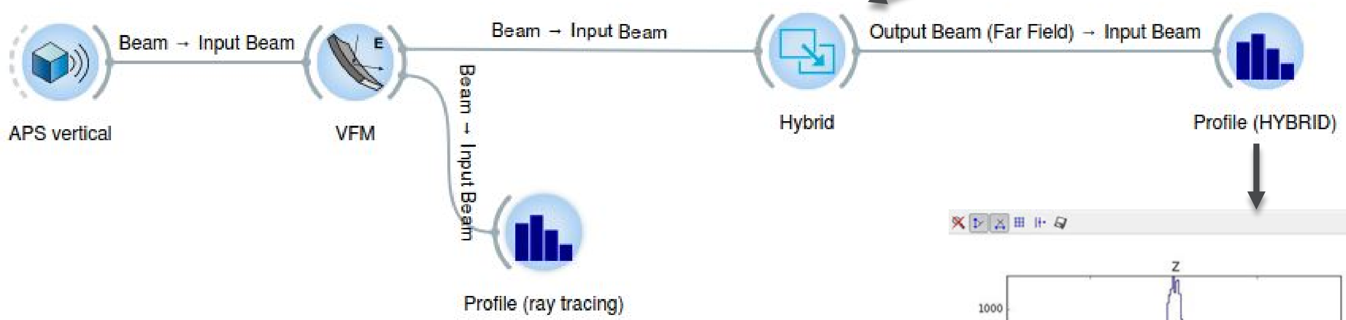
```

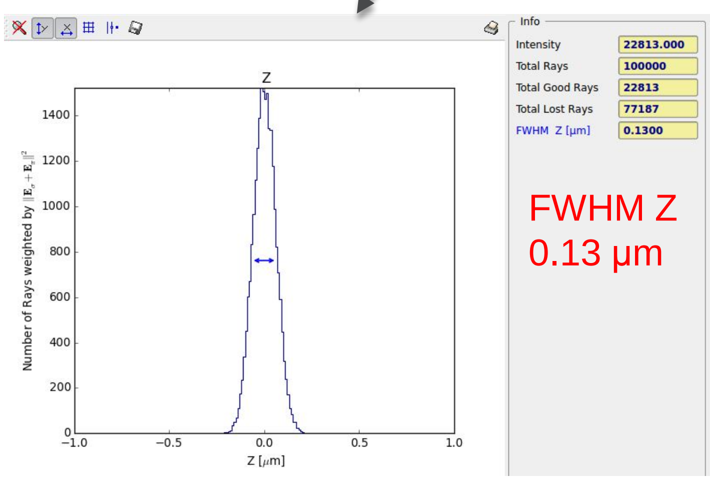
X. Shi, et al., Proc. SPIE **9209**, 920911 (2014).

HYBRID METHOD

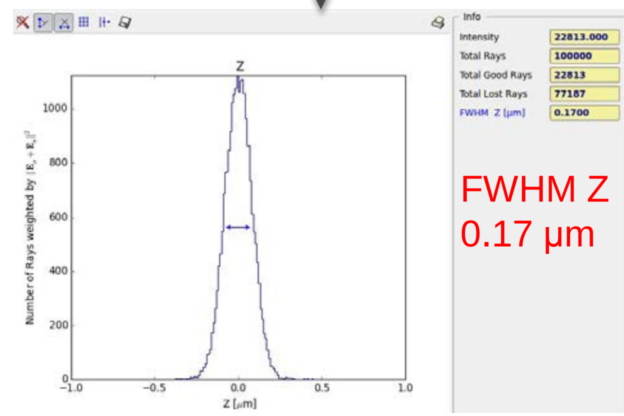
Distribution — OASYS-ShadowOui version





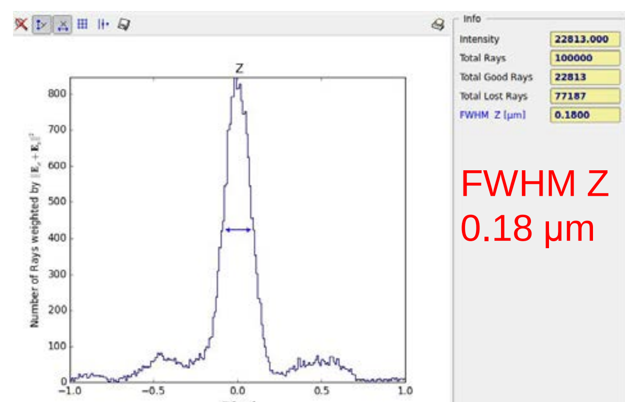


FWHM Z
0.13 μm



FWHM Z
0.17 μm

60 mm
ideal mirror



FWHM Z
0.18 μm

60 mm
mirror with
slope error

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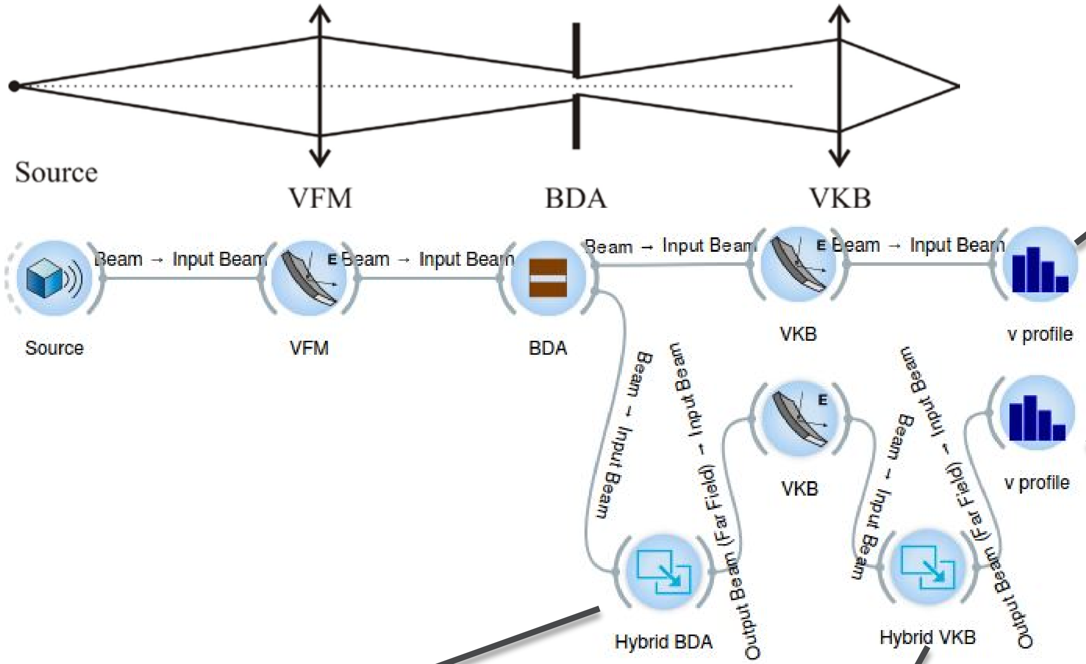
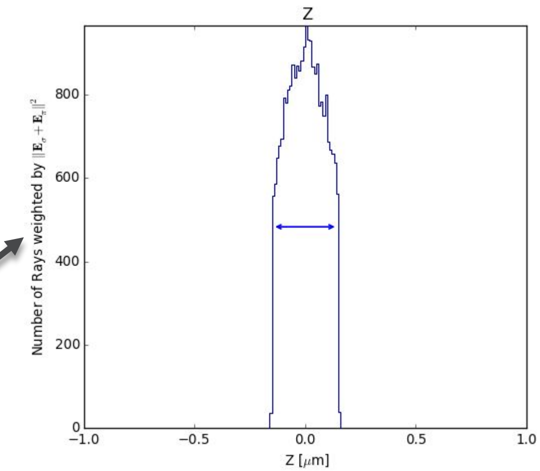
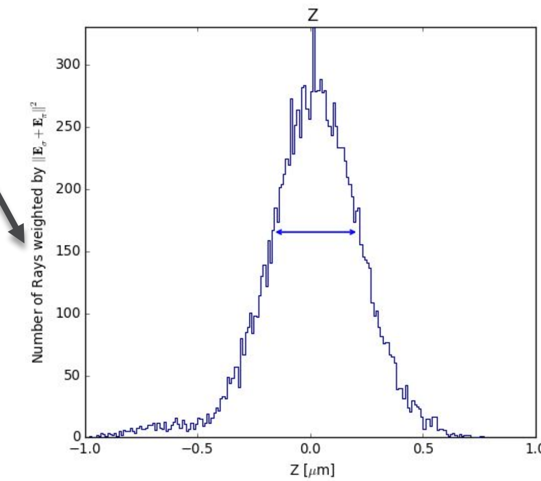
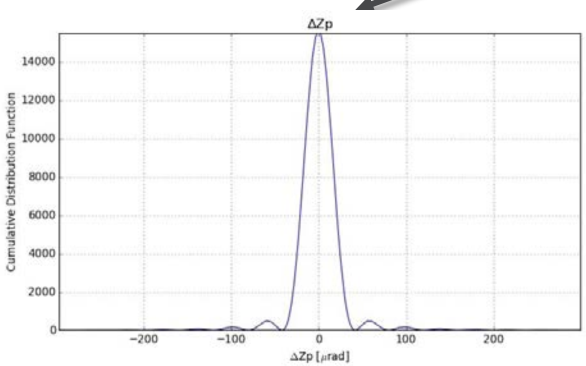
HYBRID METHOD

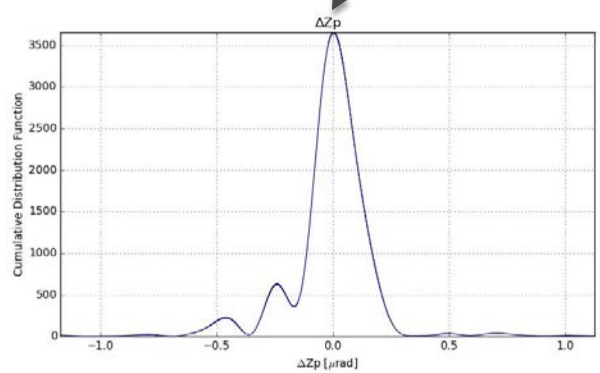
Distribution — OASYS-ShadowOui version











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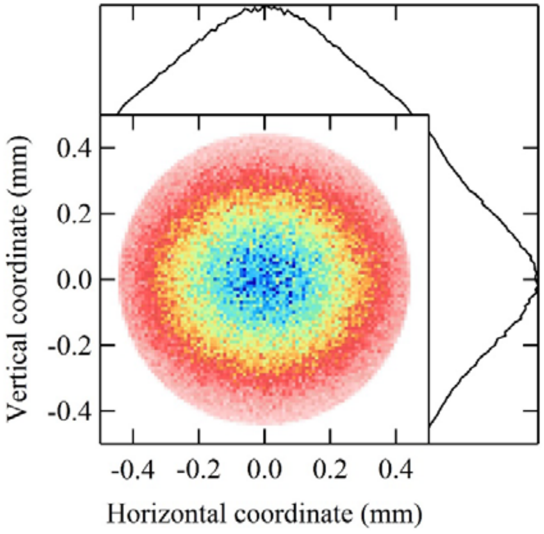
HYBRID METHOD

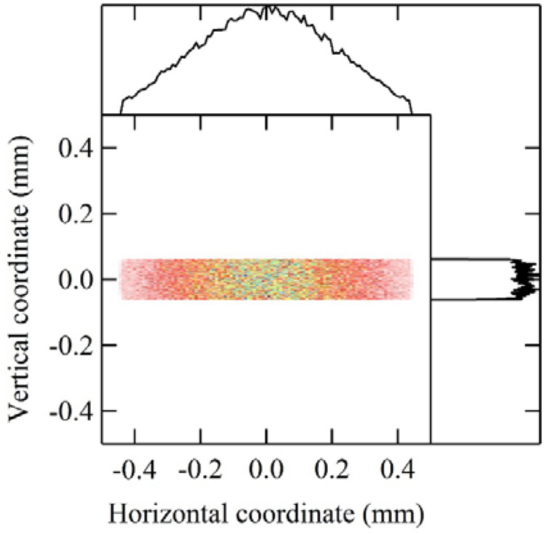
Simple aperture, CRL

- Current APS*:* E = 7350 eV undulator A, σ_x = 275 μm, σ_y = 12.6 μm
- Be parabolic lenses with R = 0.2 mm and N = 7, at 57 m from source, f = 2.26 m

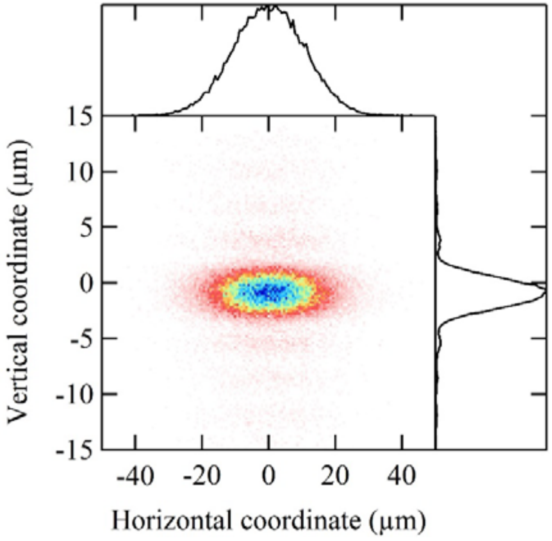
After CRL
without slit



After CRL
with 125 μm slit



Focal size at 2.35 m
FWHM: 25 μm × 3 μm



- CRL was ray traced though individual lenses and the hybrid code was applied once after the CRLs.

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NON-IDEAL OPTICS: SIMULATION

Mirror with figure errors

- Geometric opics

  σ = 270 µm

  σ' = 12 µrad

  p = 30 m

  q = 2 m

  L = 1 m

- Diffraction limited mirror

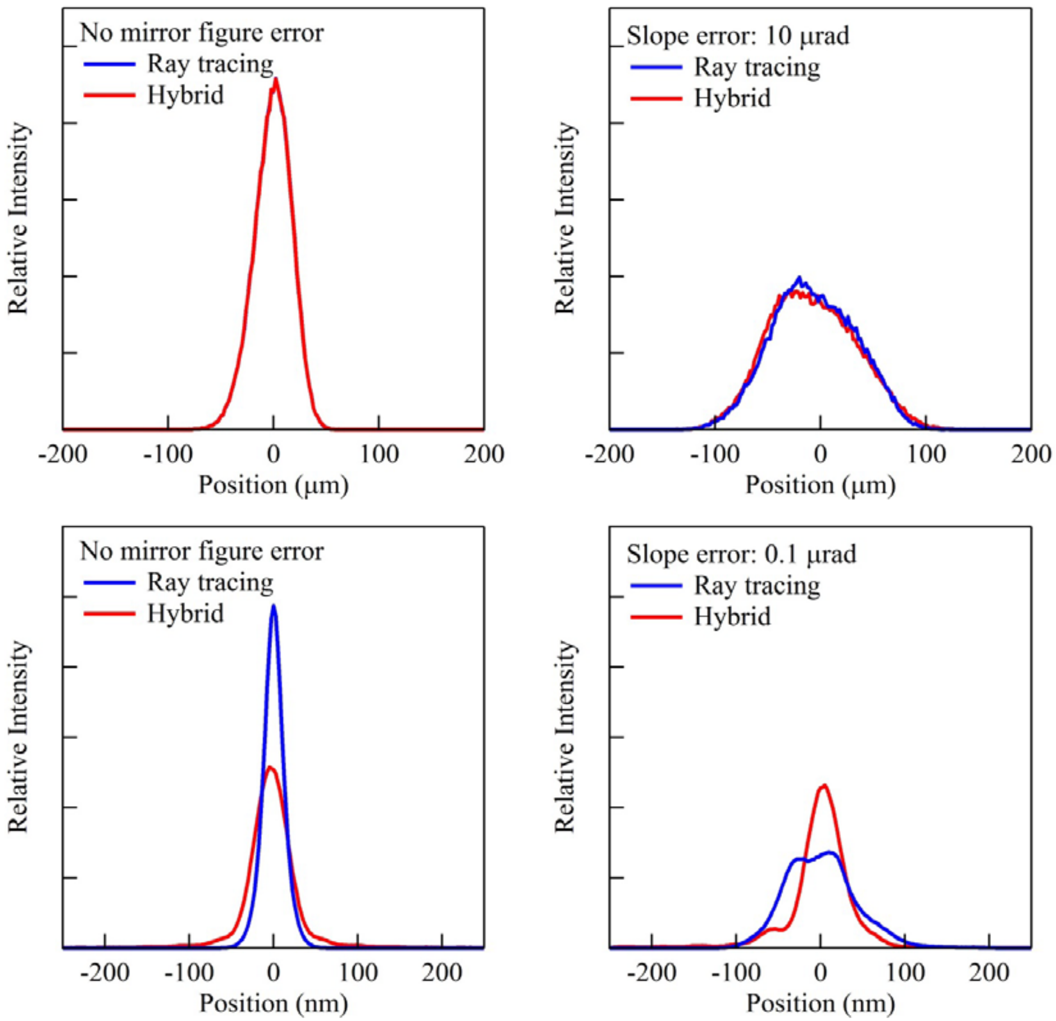
  σ = 2 µm

  σ' = 30 µrad

  p = 30 m

  q = 0.2 m

  L = 0.2 m



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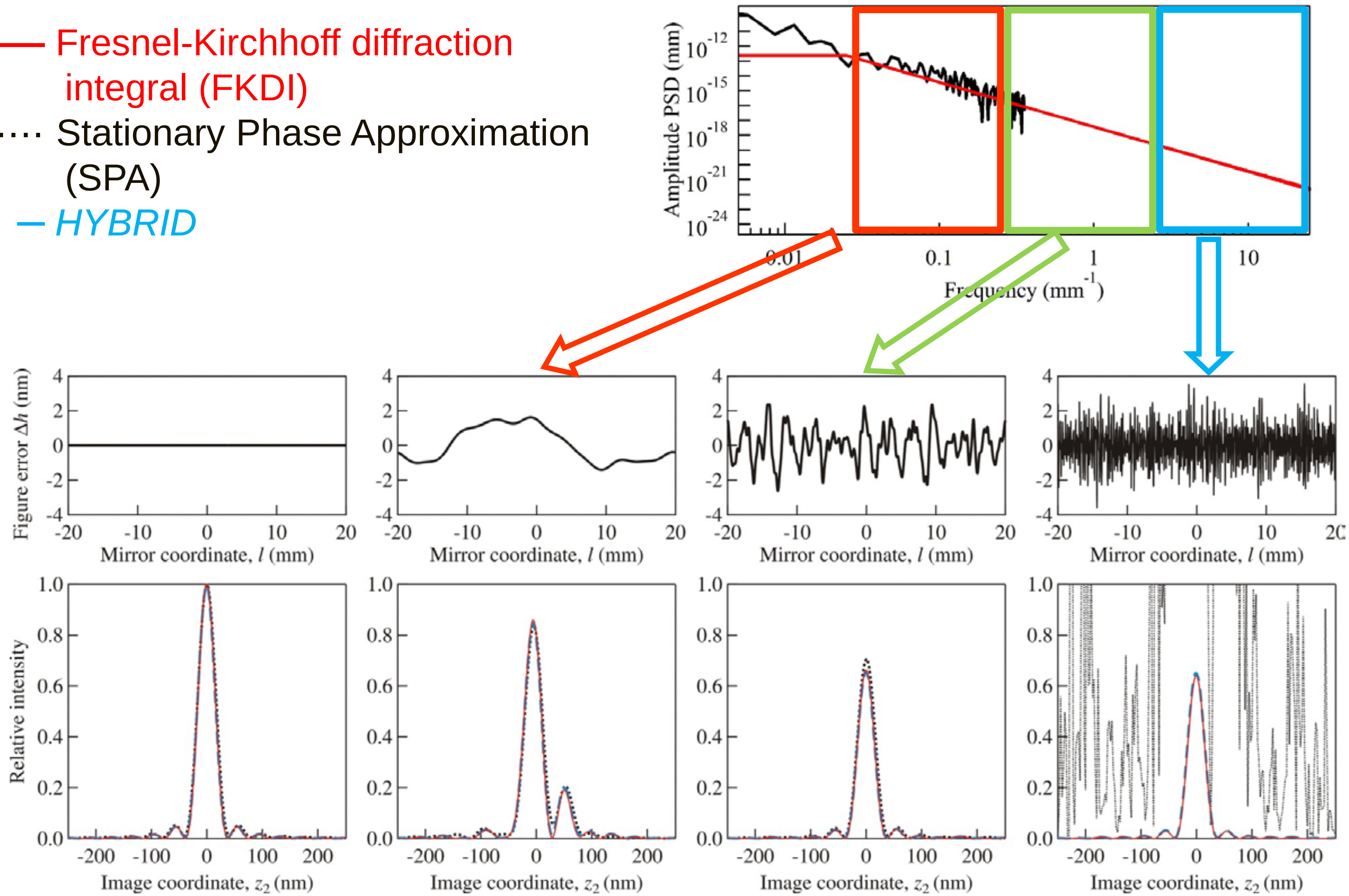
NON-IDEAL OPTICS: SIMULATION

Diffraction-limited focusing mirrors with figure errors

—— Fresnel-Kirchhoff diffraction integral (FKDI)
······ Stationary Phase Approximation (SPA)
– – *HYBRID*



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

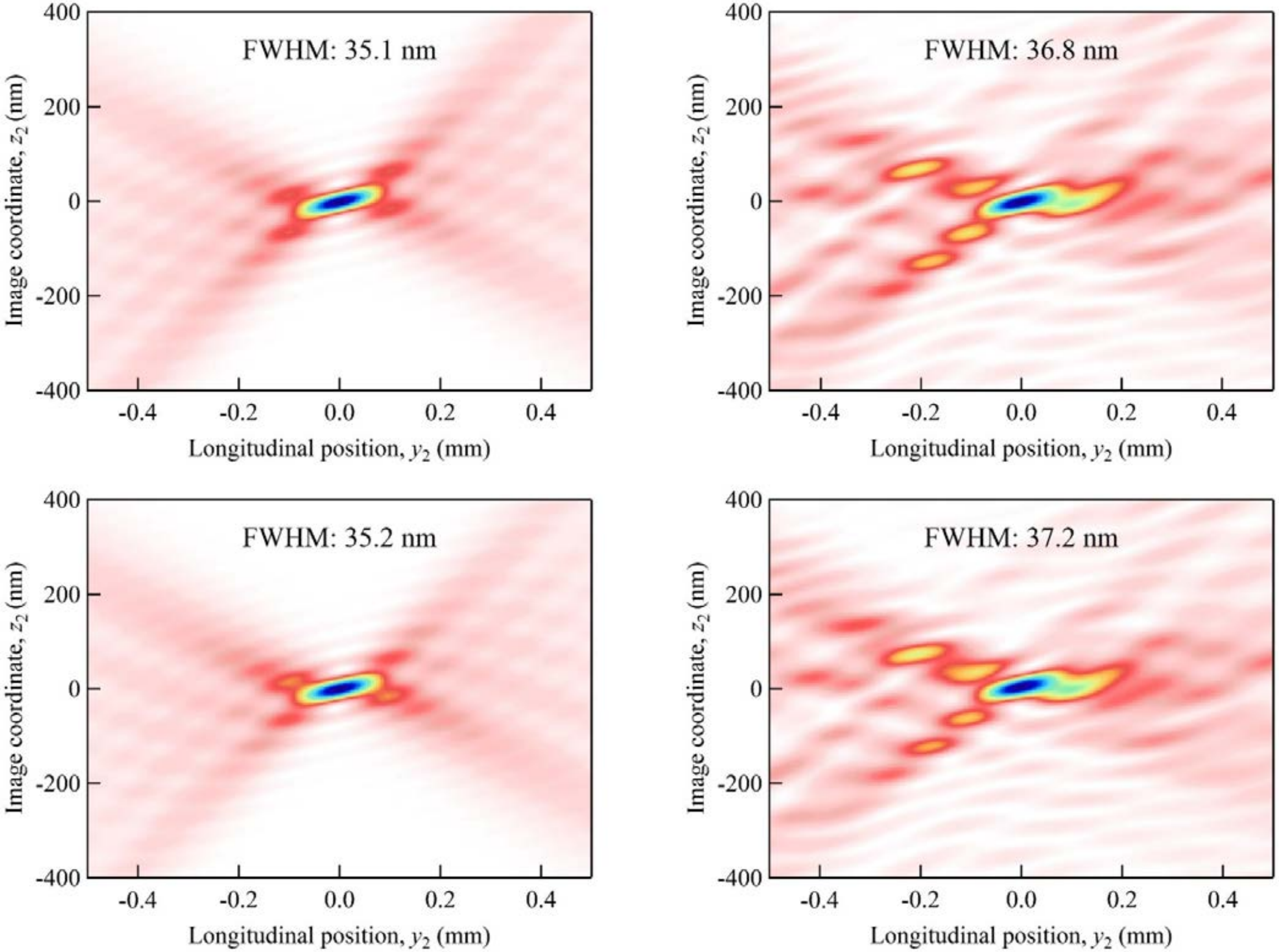
NON-IDEAL OPTICS: SIMULATION

Near-field propagation

Ideal mirror | Mirror with figure errors

FKDI

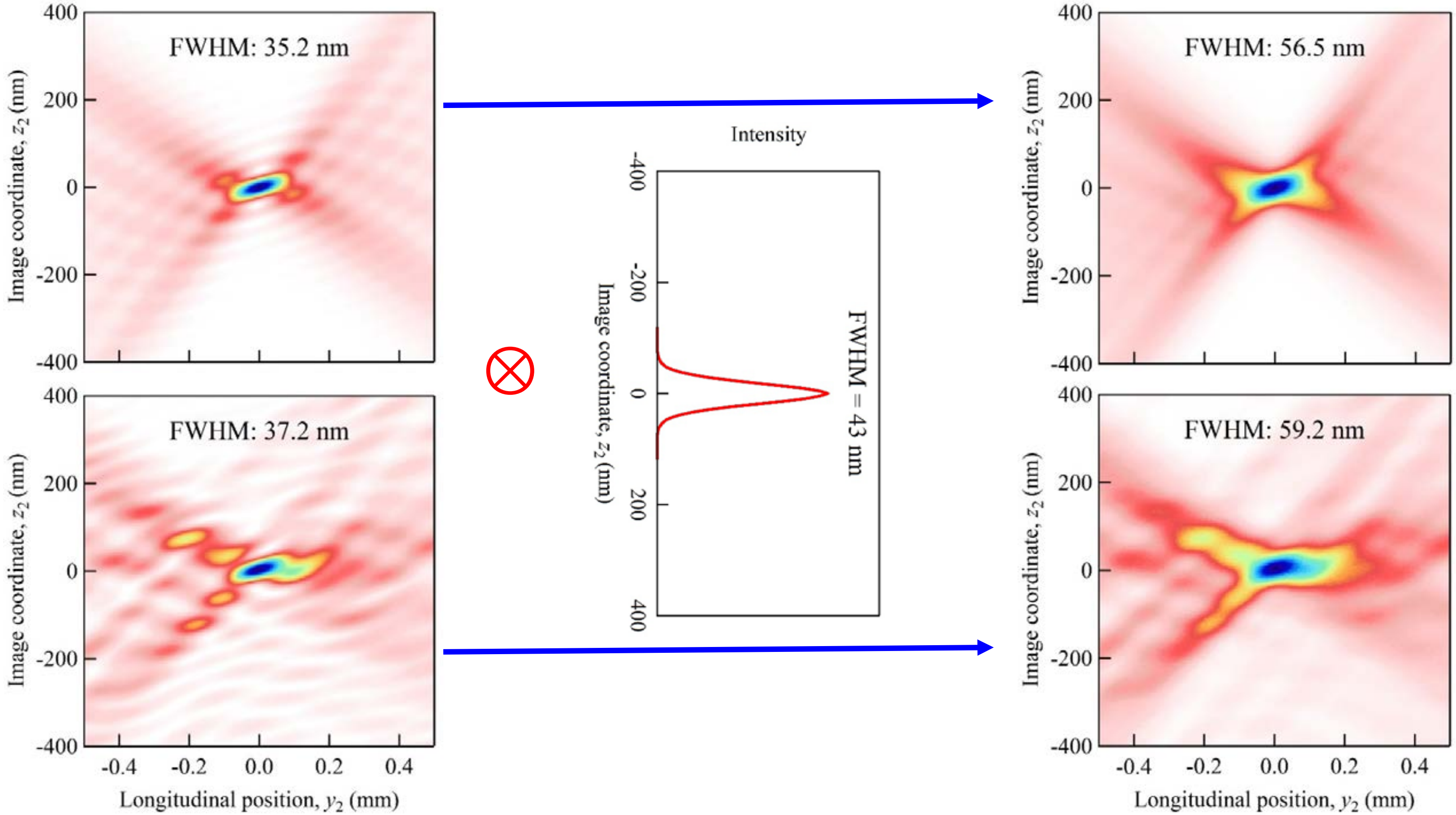
HYBRID



NON-IDEAL OPTICS: SIMULATION

Near-field propagation

- Mirror illuminated by an extended Gaussian source with the size of 20 µm (RMS) and divergence of 3 µrad (RMS).



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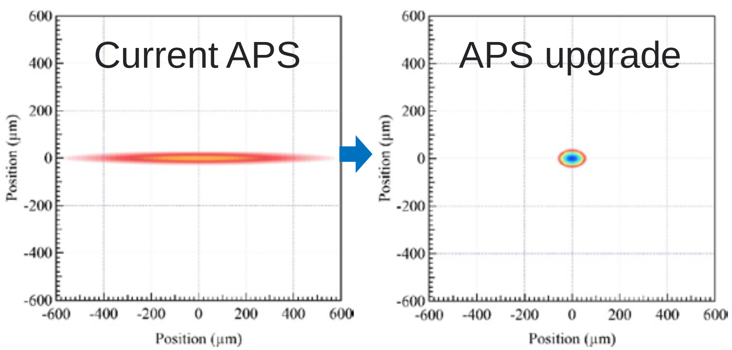
NON-IDEAL OPTICS: SPECIFICATION

Motivation and basic consideration

- New light sources and upgrades



- Require mirrors with super precise figure:

  <1 nm P-V height error

  <50 nrad RMS slope error

  and super smooth surface:

  <0.1 nm RMS roughness

- Geometrical optics approach:
  - To ensure the source are not broadened by more than 20% (the aberration contribution is less than half of the source size), the slope error of the mirror located at distance D should be

$$\sigma_{\mathrm{SE}} < \frac{\Sigma}{4D}.$$

For D = 30 m: $\sigma_{\mathrm{SE,\,H}}$<0.2 μrad, $\sigma_{\mathrm{SE,\,V}}$<0.06 μrad

- Wave optics approach:
  - Rayleigh criterion — ¼ wave P-V wavefront error
  - Maréchal criterion

$$\sigma_{\mathrm{HE}} < \frac{\lambda}{28\sin\theta}$$

At 10 keV, θ = 3 mrad: σ_{HE}<1.5nm

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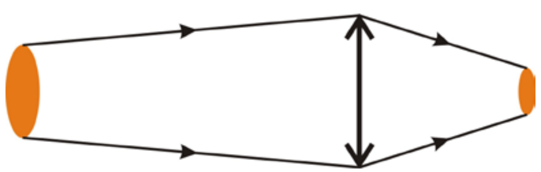
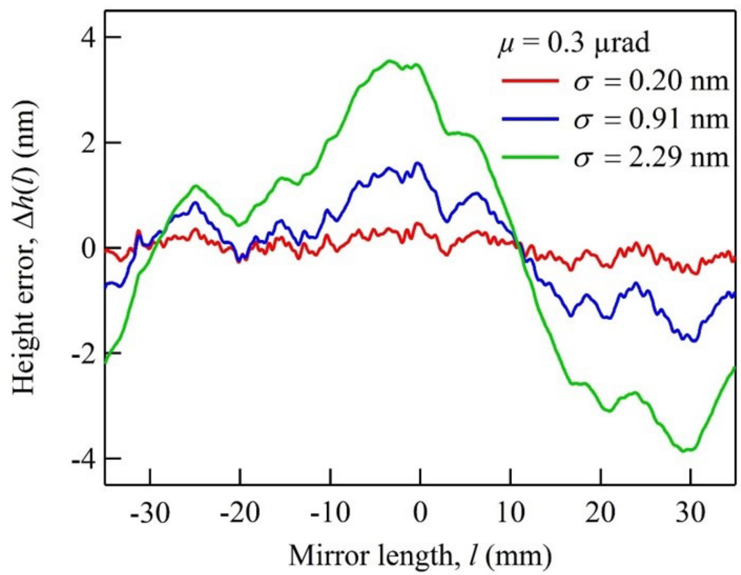
NON-IDEAL OPTICS: SPECIFICATION

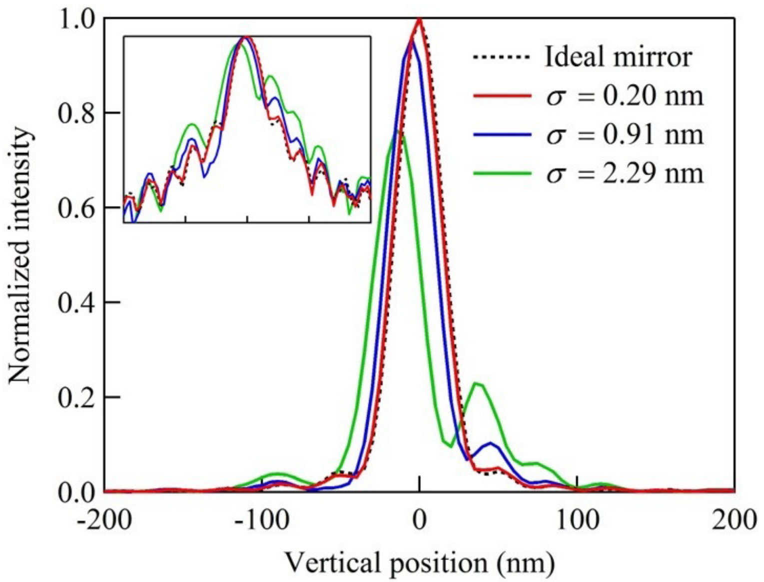
Diffraction limited focusing, 1000:1, 70 mm long mirror

$$\Delta h(l) = \sum_n \Delta h_n(l) = \sum_n b_0 n^{s_0/2} \cos\left(\frac{2\pi n}{L} l + \Psi_n\right)$$

s_0 – slope of log(PSD) vs log(f)







s_0	σ (nm)	μ (μrad)	Strehl ratio analytical	Strehl ratio from simulation	Relative RMS beam size
-1.5	0.20	0.30	1.00	1.00	1.00
-2.5	0.91	0.30	0.93	0.96	1.19
-3.5	2.29	0.30	0.54	0.76	1.91

X. Shi, et al., Proc. SPIE 9687 (2016)

NON-IDEAL OPTICS: SPECIFICATION

Diffraction limited focusing, 1000:1, 70 mm long mirror

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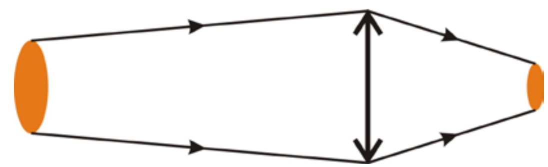
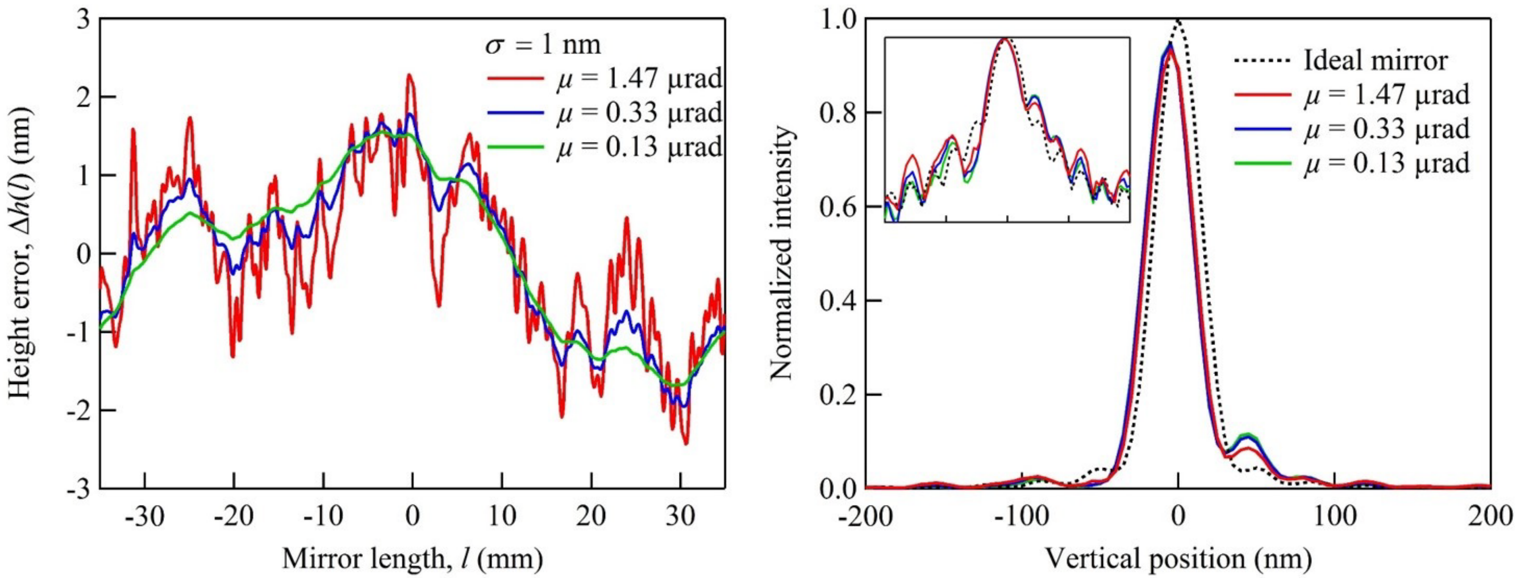


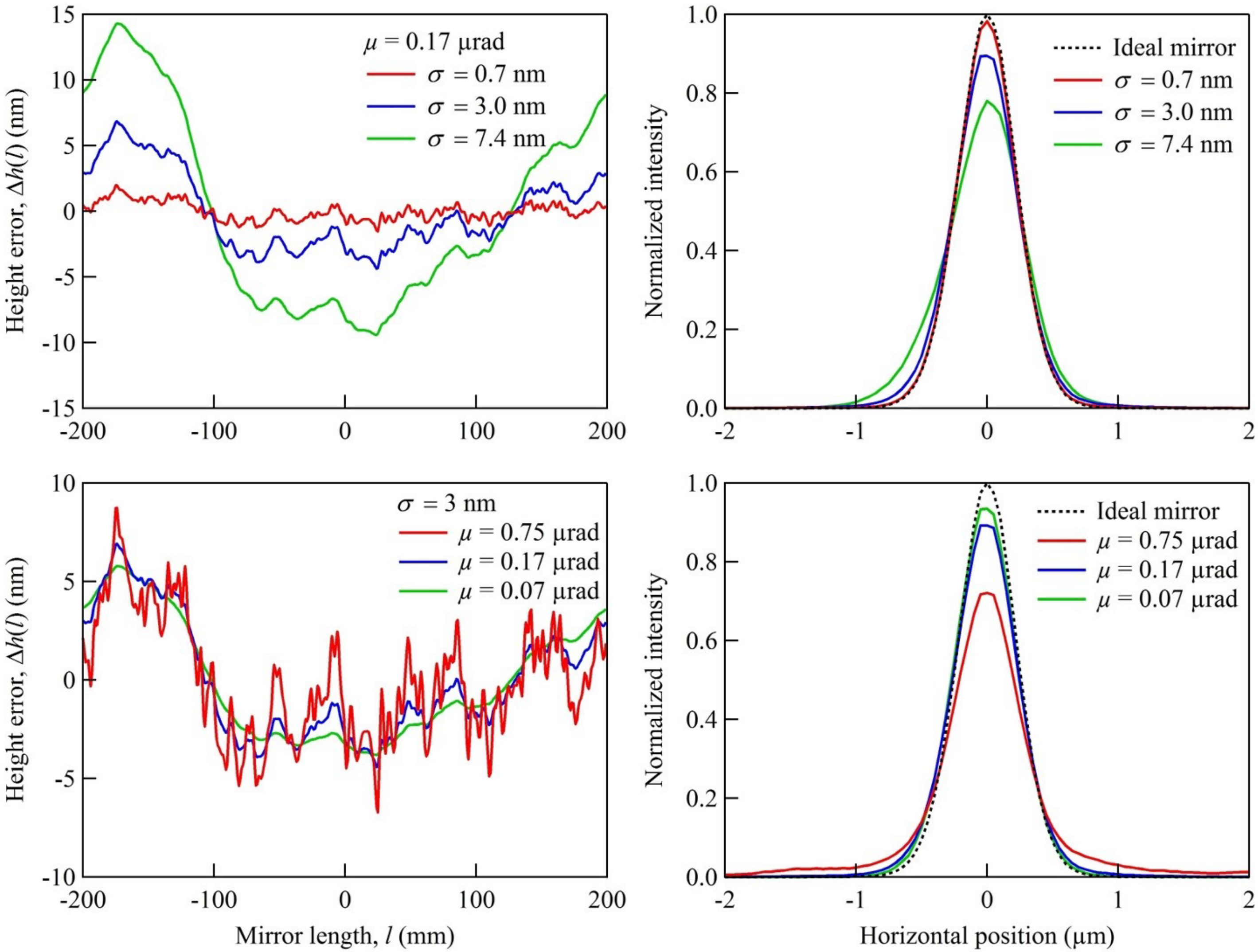


s_0	σ (nm)	μ (μrad)	Strehl ratio analytical	Strehl ratio from simulation	Relative RMS beam size
-1.5	1.0	1.47	0.91	0.93	1.17
-2.5	1.0	0.33	0.91	0.95	1.21
-3.5	1.0	0.13	0.91	0.95	1.22

X. Shi, et al., Proc. SPIE 9687 (2016)

NON-IDEAL OPTICS: SPECIFICATION

Non-diffraction limited focusing, 100:1, 400 mm long mirror



X. Shi, et al., Proc. SPIE 9687 (2016)

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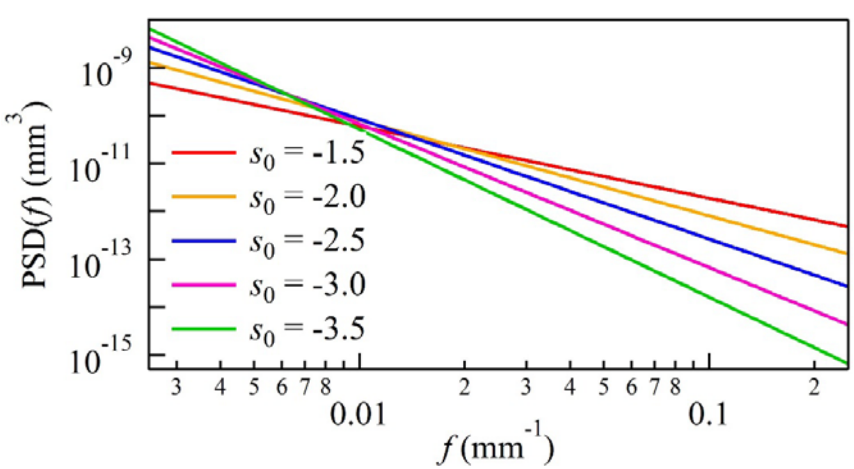
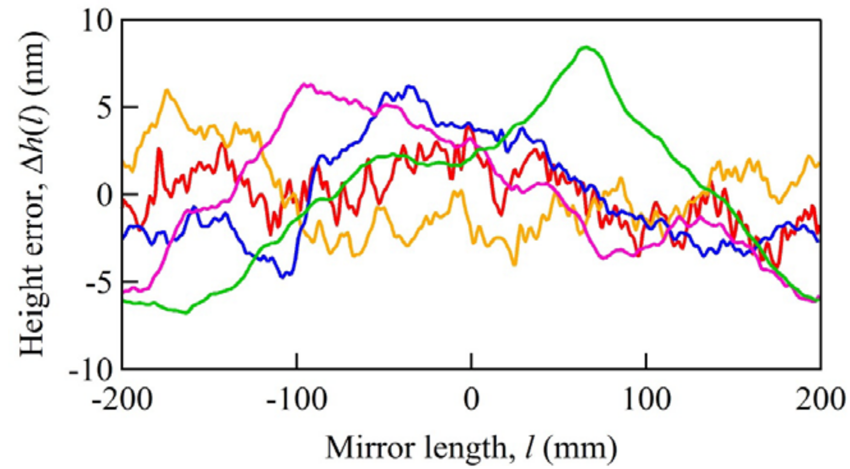
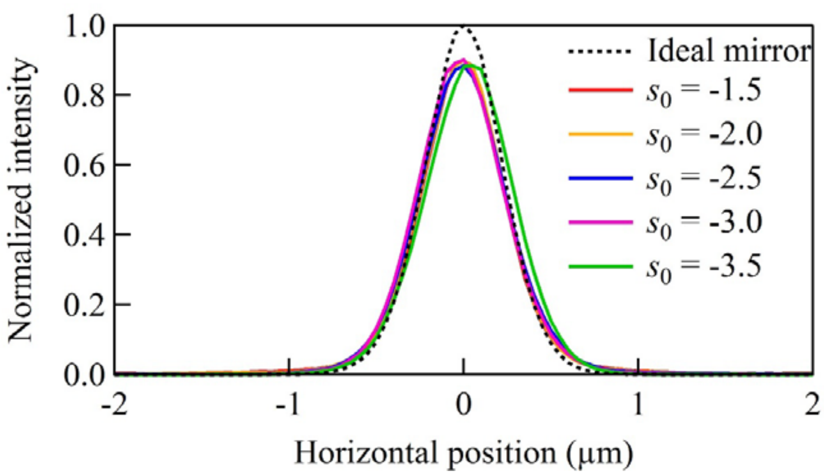
Non-diffraction limited focusing, 100:1, 400 mm long mirror





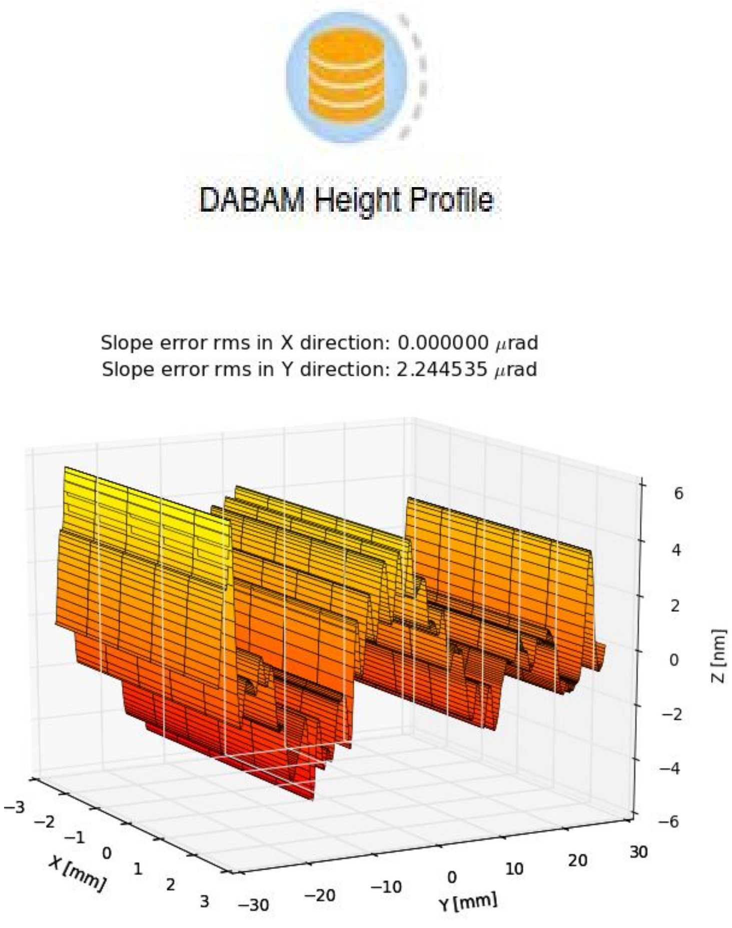


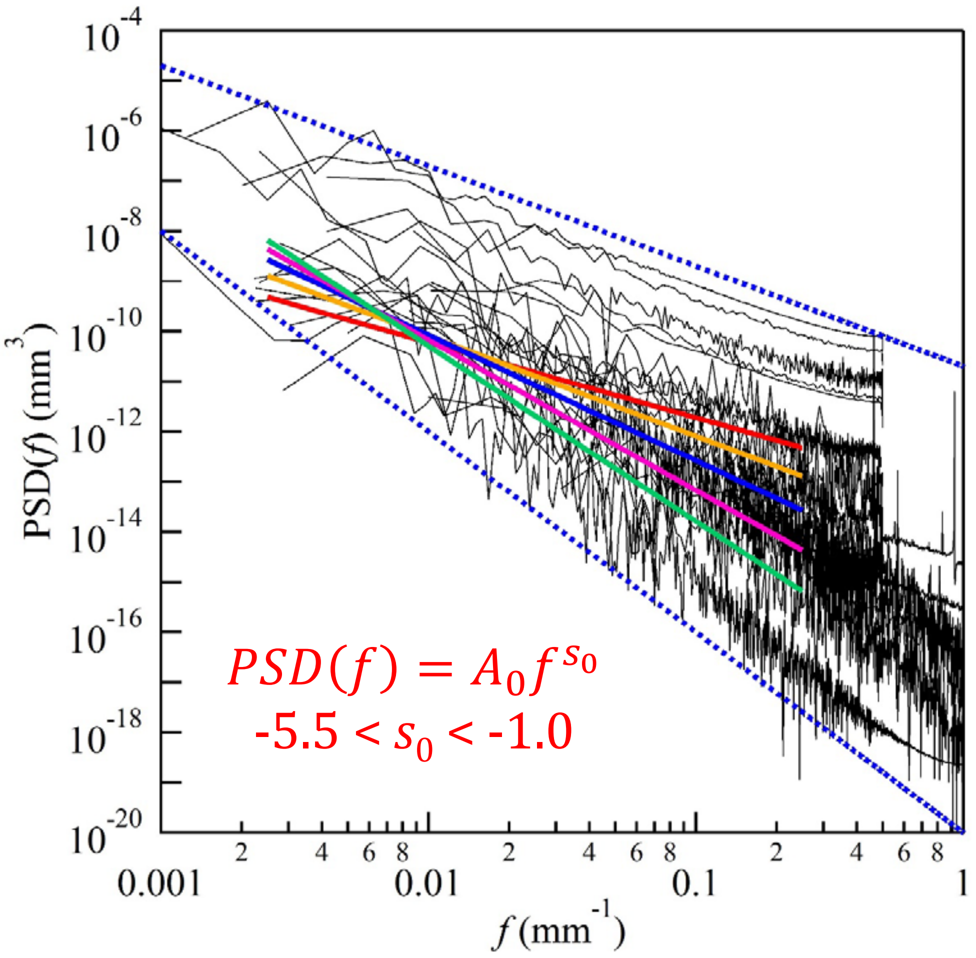
s_0	σ (nm)	μ (μrad)	Strehl ratio	Relative RMS size
-1.5	1.7	0.43	0.90	1.09
-2.0	2.3	0.27	0.90	1.10
-2.5	3.0	0.17	0.89	1.12
-3.0	3.6	0.12	0.90	1.11
-3.5	4.3	0.10	0.88	1.12

X. Shi, et al., Proc. SPIE 9687 (2016)

NON-IDEAL OPTICS: SPECIFICATION

DABAM — an open-source database of x-ray mirrors metrology





Sanchez, M. et al. J. Synchrotron Rad. (2016).

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MUTUAL OPTICAL INTENSITY PROPAGATION

Basic equations

- Collaboration with Shanghai Synchrotron Radiation Facility
- Mutual coherence function describes the correlations between two complex scalar values of the electric field

$$\Gamma_{12}(\tau) = \langle u\,(P_1, t+\tau)u^*\,(P_2, t) \rangle$$

  – In case $\tau = 0$, it becomes the mutual optical intensity (MOI)

$$\Gamma_{12}\,(0) = J(P_1, P_2) = \langle u\,(P_1, t)u^*\,(P_2, t) \rangle$$

- The four-dimensional function $J(P_1, P_2)$ describes the optical information of the wavefront, including the distribution of electric field and correlations between every two points. The propagation of MOI from wavefront *P* to wavefront *Q* is represented by equation

$$J(Q_1, Q_2) = \iint \iint J(P_1, P_2\,)\exp[-j\,\frac{2\pi}{\bar{\lambda}}\,(r_2 - r_1)]\,\frac{\chi(\theta_1)}{\bar{\lambda} r_1}\frac{\chi(\theta_2)}{\bar{\lambda} r_2}\,dS_1\,dS_2$$

- The degree of coherence between two points is defined as

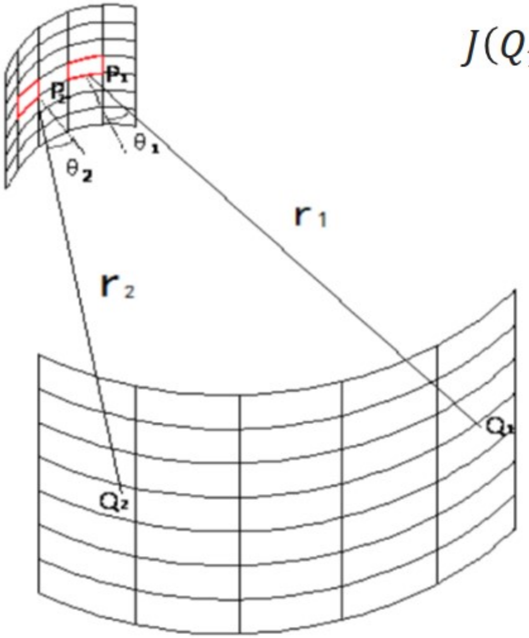
$$\gamma_{12} = \frac{|J_{12}|}{\sqrt{I_1 I_2}}$$

where I_1 and I_2 are the intensities at Q_1 and Q_2, respectively.

MUTUAL OPTICAL INTENSITY PROPAGATION

Free space propagation

- The wavefront at the source plane is separated into many elements, assumed that in every element the beam has full coherence and constant complex amplitude. It is valid as long as the dimension of the element is much smaller than the coherent length and beam spot size
- The propagation of each element is calculated with Fresnel approximations
- The MOI at the image plane after propagation can be obtained from the sum of the contributions of all elements on the source plane.



$$J(Q_1,Q_2)=\iint\iint J(P_1,P_2)\exp[-j\frac{2\pi}{\lambda}(r_2-r_1)]\frac{\chi(\theta_1)}{\lambda r_1}\frac{\chi(\theta_2)}{\lambda r_2}dS_1\,dS_2$$

discretize

$$J(Q_1,Q_2)=\sum_{kl}J(P_{ij},P_{kl})\iint e^{i\frac{2\pi}{\lambda}r_{P_{kl}Q_2}}\frac{\chi(\theta_2)}{\lambda r_{P_{kl}Q_2}}\left(\sum_{ij}\iint e^{-i\frac{2\pi}{\lambda}r_{P_{ij}Q_1}}\frac{\chi(\theta_1)}{\lambda r_{P_{ij}Q_1}}dS_{ij}\right)dS_{kl}$$

Substituted integral $I_{P_{ij}Q_1}=\iint e^{-i\frac{2\pi}{\lambda}(r_0-\frac{x_{q1}\cdot x+y_{q1}\cdot y}{r_0}+\frac{x^2+y^2}{2r_0})}\frac{\chi(\theta_1)}{\lambda r_0}dxdy$

(Fresnel integral)

Through free space: $J(Q_1,Q_2)=\sum_{kl}(I_{kl}^*\sum_{ij}J(P_{ij},P_{kl})I_{ij})$

X. Meng et al. Opt. Express 23, 29675 (2015).
X. Meng et al. Acta Optica Sinica 33, 0734001 (2013)

MUTUAL OPTICAL INTENSITY PROPAGATION

Mirror with figure errors

- The amplitude spread function of the reflecting mirror is given by

$$K(Q,P) = t(P)\exp\left[i\frac{2\pi}{\lambda}\Gamma(Q,P)\right]\delta[P - \tilde{P}(Q)]$$

  - $t(P)$ is the complex amplitude transmission function
  - $\Gamma(Q,P)$ is the optical path between the incident and exit wavefronts
  - $\tilde{P}(Q)$ is the coordinate transformation for points on the two wavefronts
- The MOI at the reflecting plane can be expressed as

$$J_r(Q_1,Q_2) = \iint\iint J_i(P_1,P_2)K(Q_1,P_1)K^*(Q_2,P_2)dS_1dS_2$$

- Use the local ray tracing to get the path length $\Gamma\left(Q,\tilde{P}(Q)\right)$, then

$$J_r(Q_1,Q_2) = J_i\left(\tilde{P}(Q_1),\tilde{P}(Q_2)\right)t\left(\tilde{P}(Q_1)\right)t^*\left(\tilde{P}(Q_2)\right)\exp\{i\frac{2\pi}{\lambda}[\Gamma\left(Q_1,\tilde{P}(Q_1)\right) - \Gamma\left(Q_2,\tilde{P}(Q_2)\right)]\}$$

X. Meng et al. Opt. Express 23, 29675 (2015).

MUTUAL OPTICAL INTENSITY PROPAGATION

Main feature

- Propagation of the MOI through the entire beamline
  - Starts with the real source (SPECTRA) MOI function or Gaussian Schell model
  - Propagates through beamline optics: free space, aperture, ideal optics, optics with figure errors.
  - Provides both the intensity and coherence information at any position of the beamline, full results can be stored and carried over.
  - Tread-off between efficiency and accuracy

MUTUAL OPTICAL INTENSITY PROPAGATION

Example

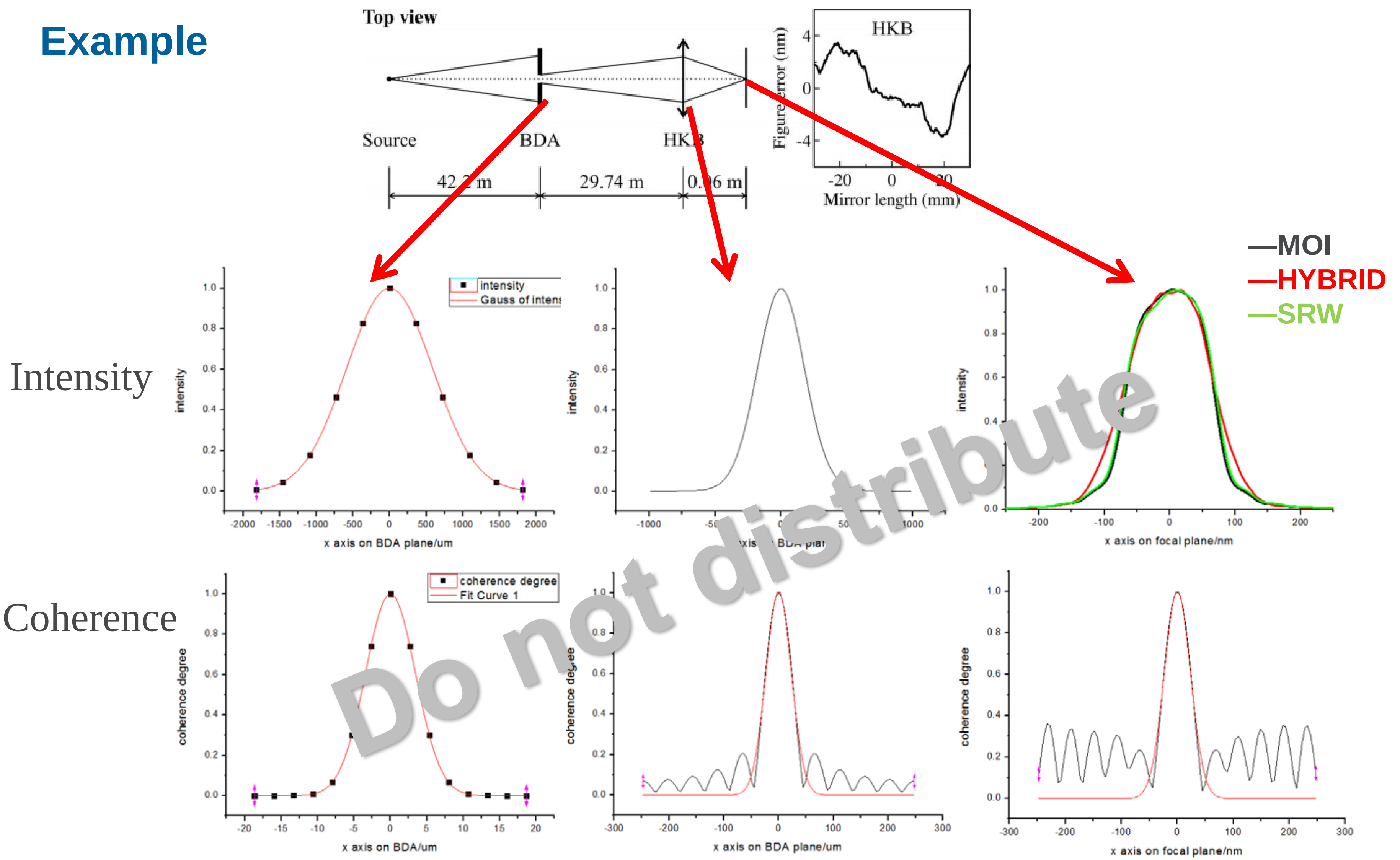


Figure courtesy of Xiangyu Meng

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