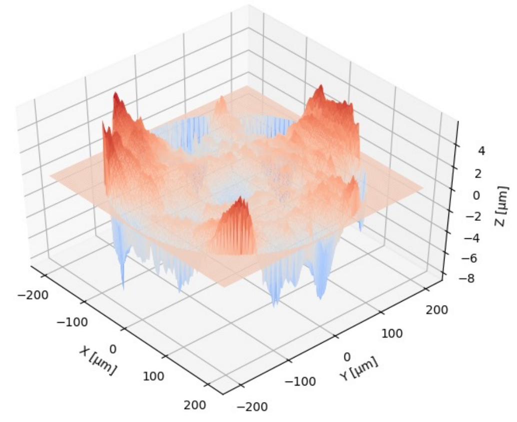
High precision X-ray measurements 2021

Optical simulation tools in the OASYS suite and their applications to x-ray optics design



Luca Rebuffi

XSD-OPT Group
Advanced Photon Source
Argonne National Laboratory

Frascati, June 9th, 2021

Outline

- Introduction to OASYS: basic features
- Basic loops, scanning loops, and thermal load calculations
- Ray-tracing and Wavefront propagation of refractive elements
- Ray-tracing of a real cylindrical mirror as generate by a bending device

Optical simulation tools in the OASYS suite and their applications to x-ray optics design

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Introduction to OASYS

Computer simulation of light sources and optical components is a mandatory step in the design and optimization of synchrotron and FEL radiation beamlines

different codes for numerical simulations are available, implementing different physical approaches

RAY-TRACING

ShadowOui

RAY

XRT

McXtrace

WAVEFRONT PROPAGATION

SRW

PHASE

WISE

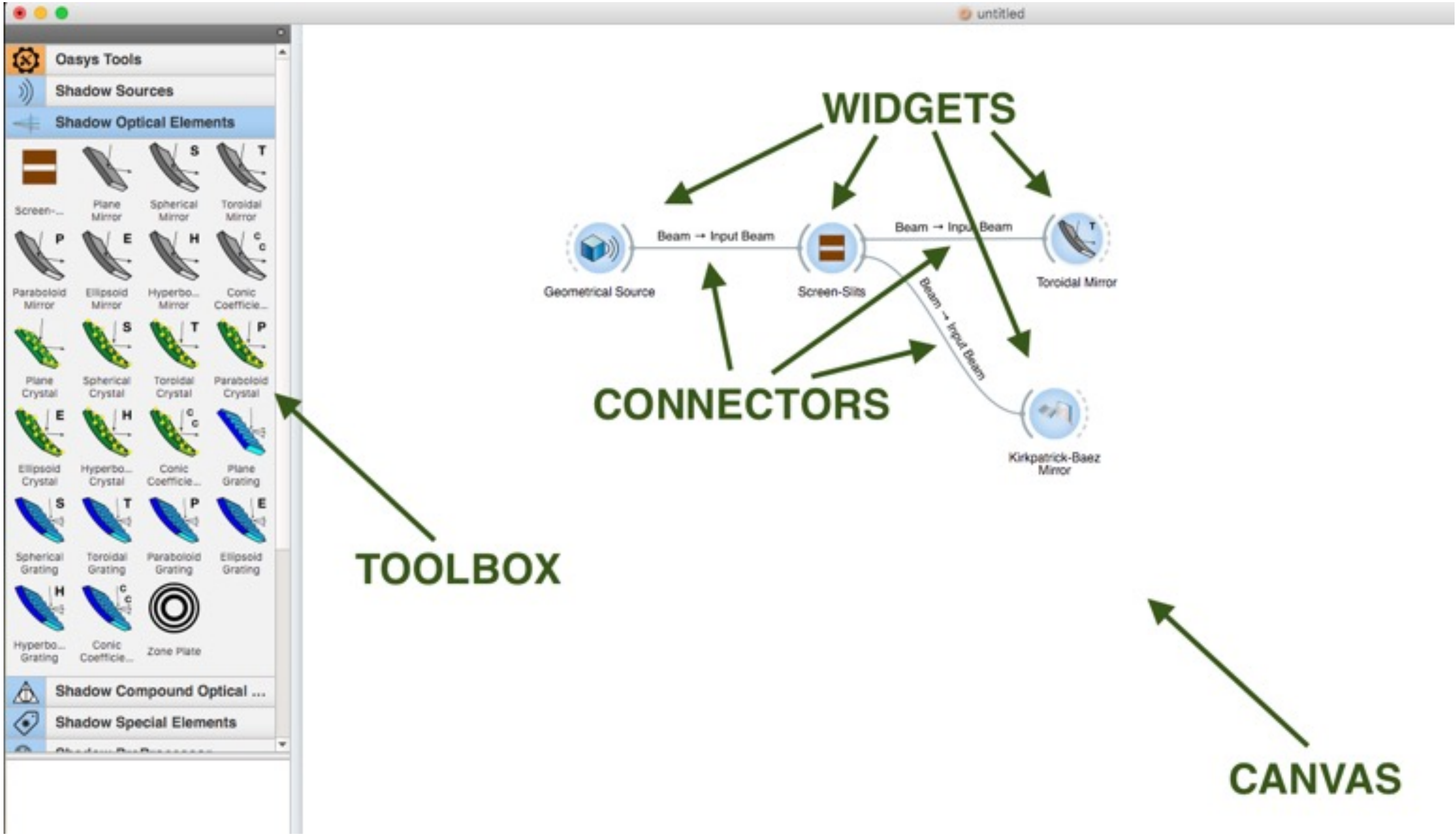
OASYS: an advanced tool for the optical design of beamlines

University of Ljubljana
Faculty of Computer and Information Science

- ✓ OASYS = OrAnge SYnchrotron Suite
- ✓ A common platform to build synchrotron-oriented User Interfaces ***that communicate***
- ✓ The upper layer of the application presented to the user

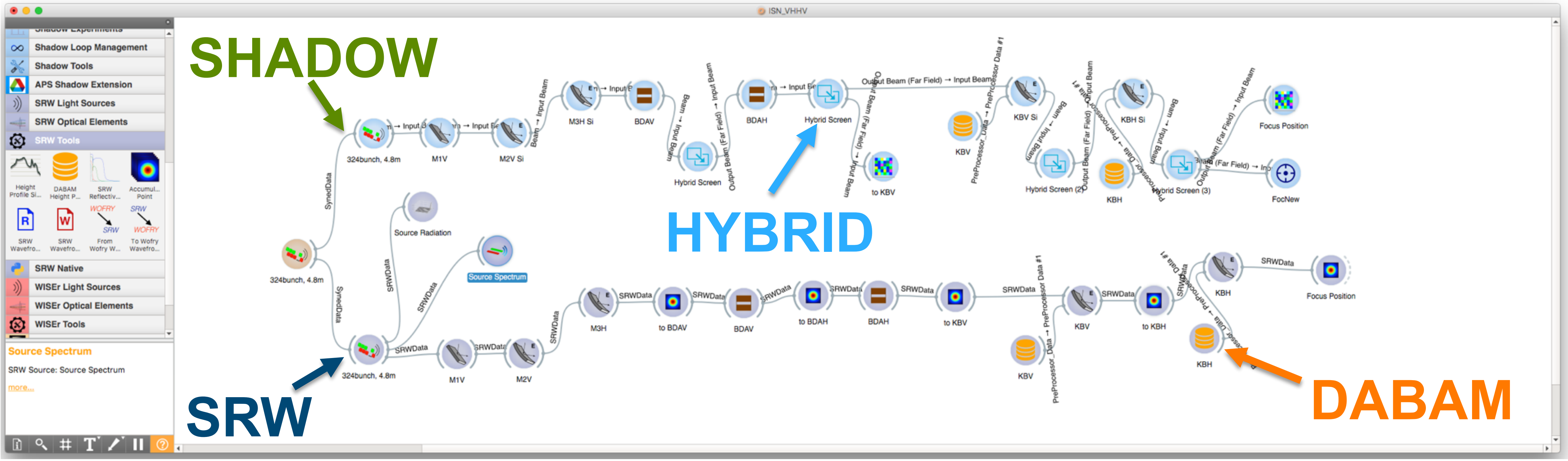
https://www.aps.anl.gov/Science/Scientific-Software/OASYS

OASYS: an advanced tool for the optical design of beamlines



OASYS: an advanced tool for the optical design of beamlines

OASYS (OrAnge SYnchrotron Suite) Multiple tools in the same environment



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

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

L. Rebuffi & M. Sanchez del Rio, J. Synchrotron Rad. 23, 1357 (2016)

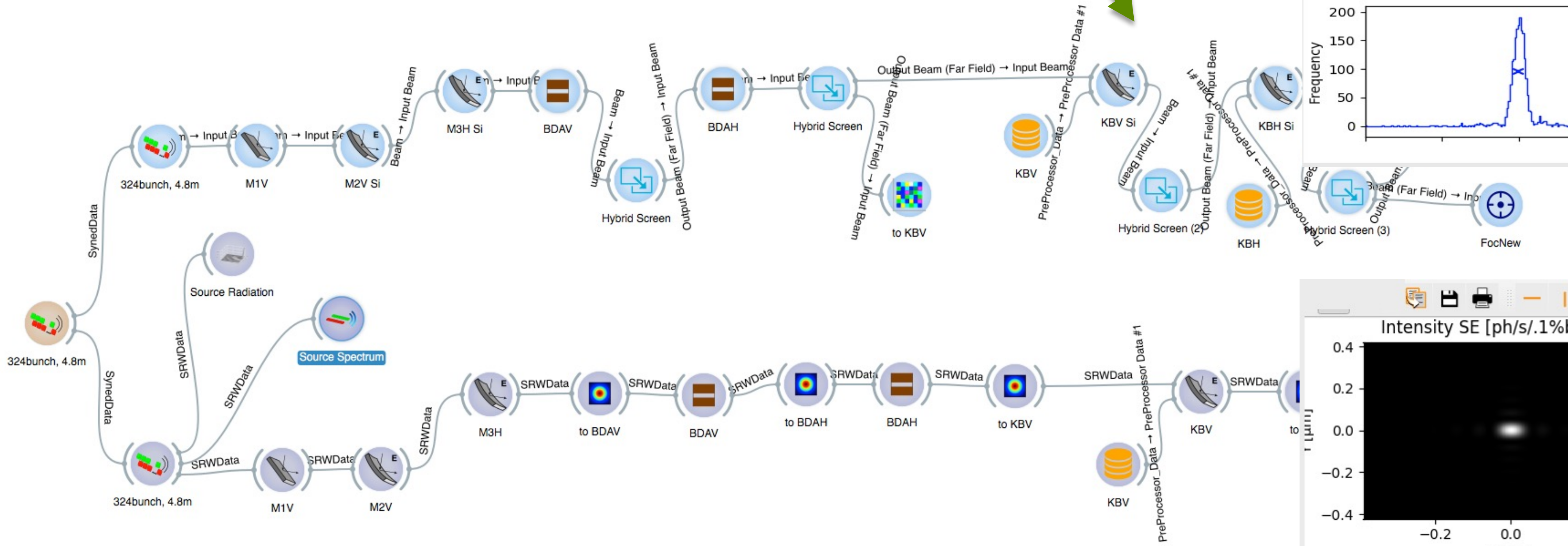
M. Sanchez del Rio et al., J. Synchrotron Rad. 23, 665 (2016)

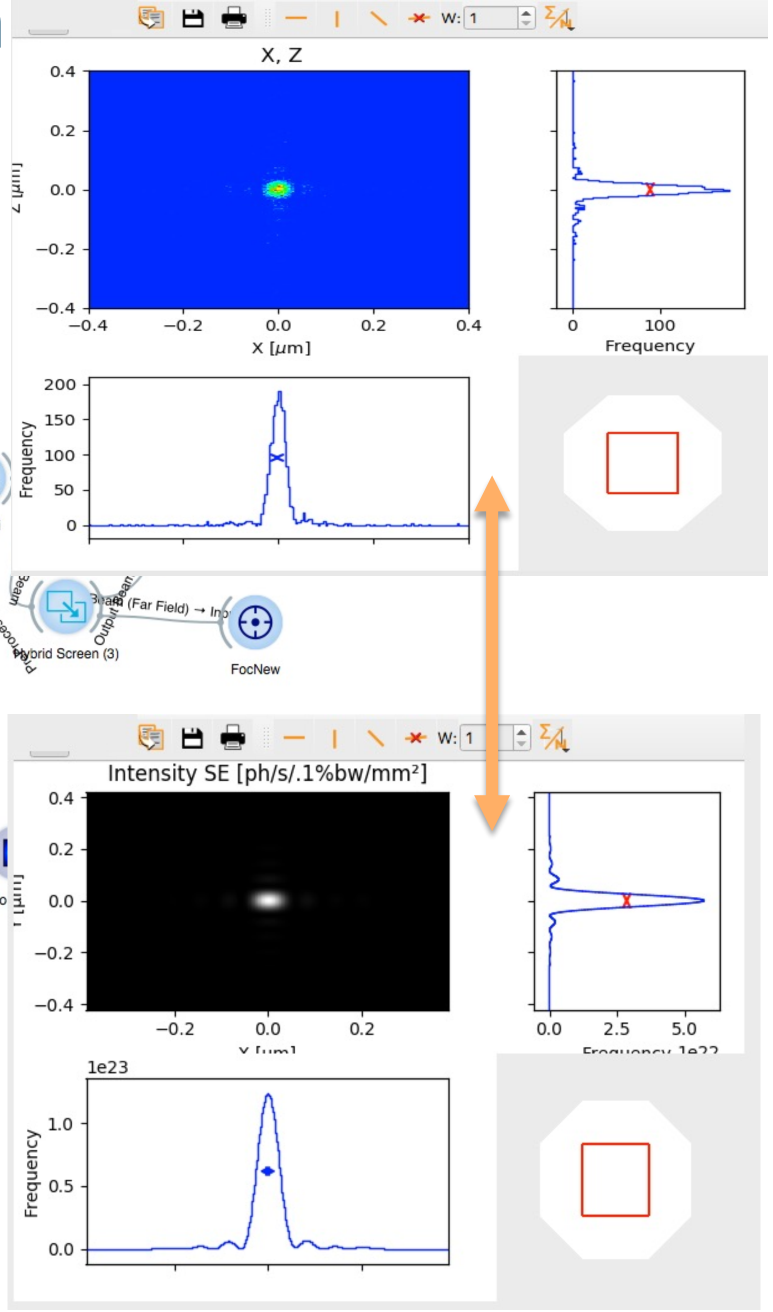
https://www.aps.anl.gov/Science/Scientific-Software/OASYS

OASYS: an advanced tool for the optical design of beamlines

OASYS (OrAnge SYnchrotron Suite)
Multiple tools in the same environment

SHADOW





SRW

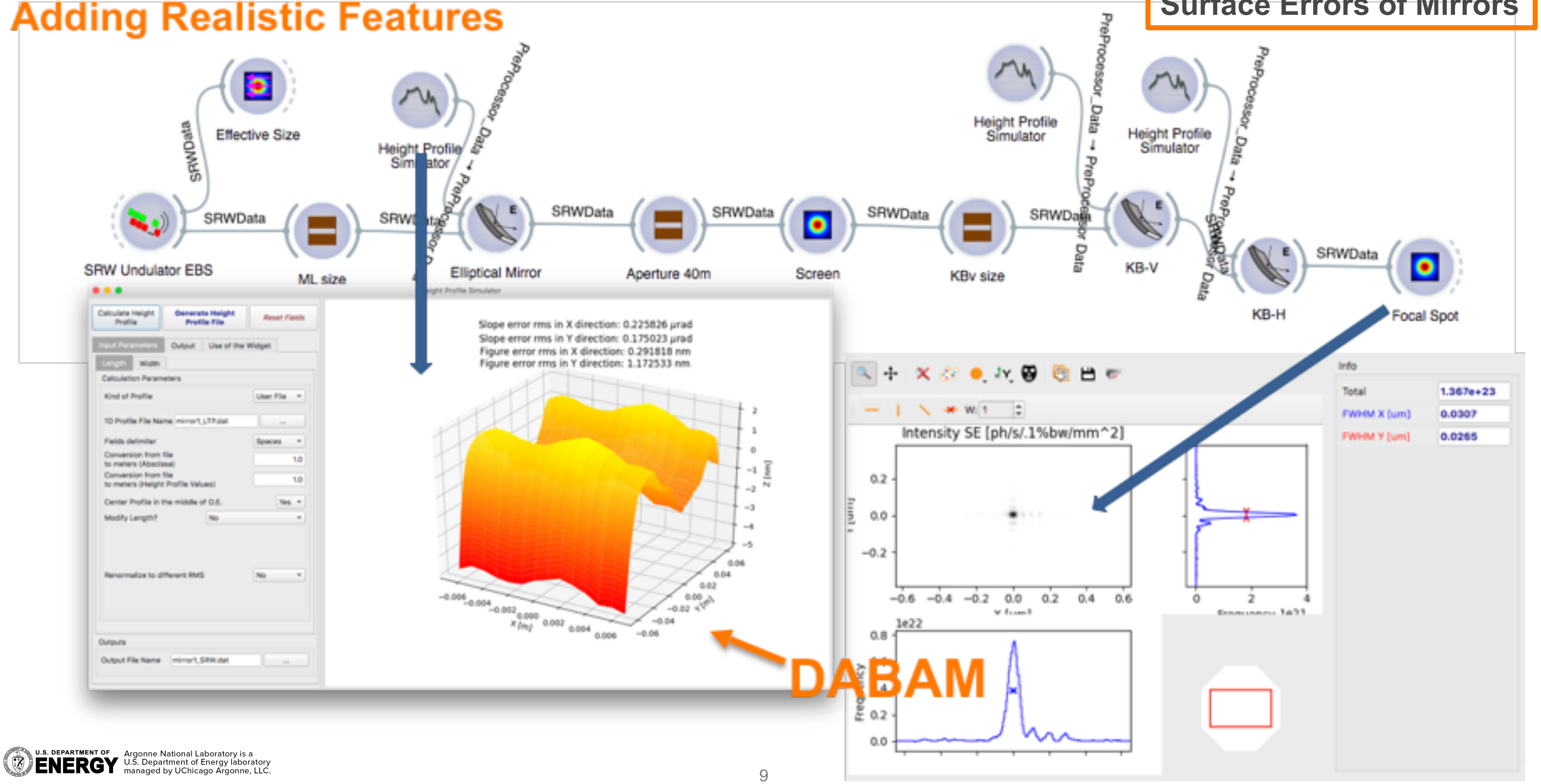
Compare and Benchmark Results

L. Rebuffi & M. Sanchez del Rio, Proc. SPIE 10388, 1038808 (2017)

OASYS: an advanced tool for the optical design of beamlines

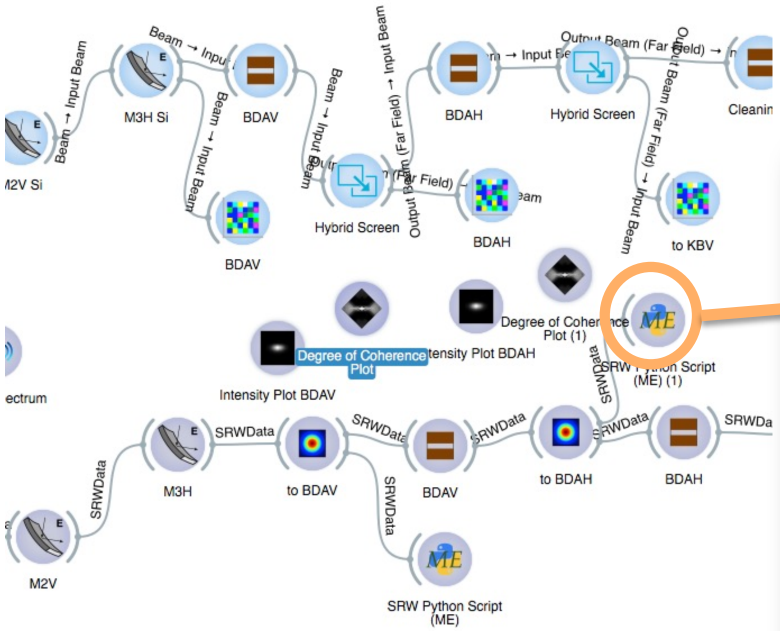
Adding Realistic Features

Surface Errors of Mirrors

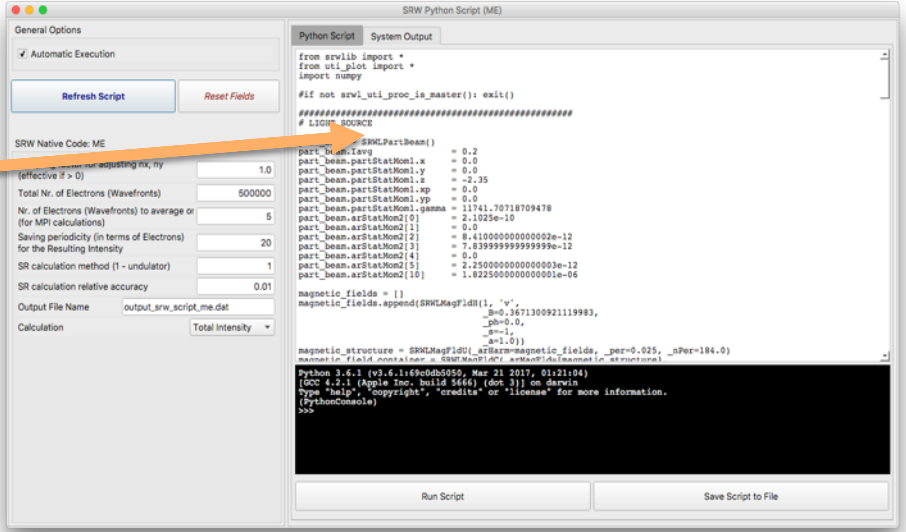


OASYS: an advanced tool for the optical design of beamlines

SRW multi-electron Simulations



Automatic generation of SRW python scripts



Accessible to super-computing

- **Optical simulation tools in the OASYS suite and their applications to x-ray optics design**
-
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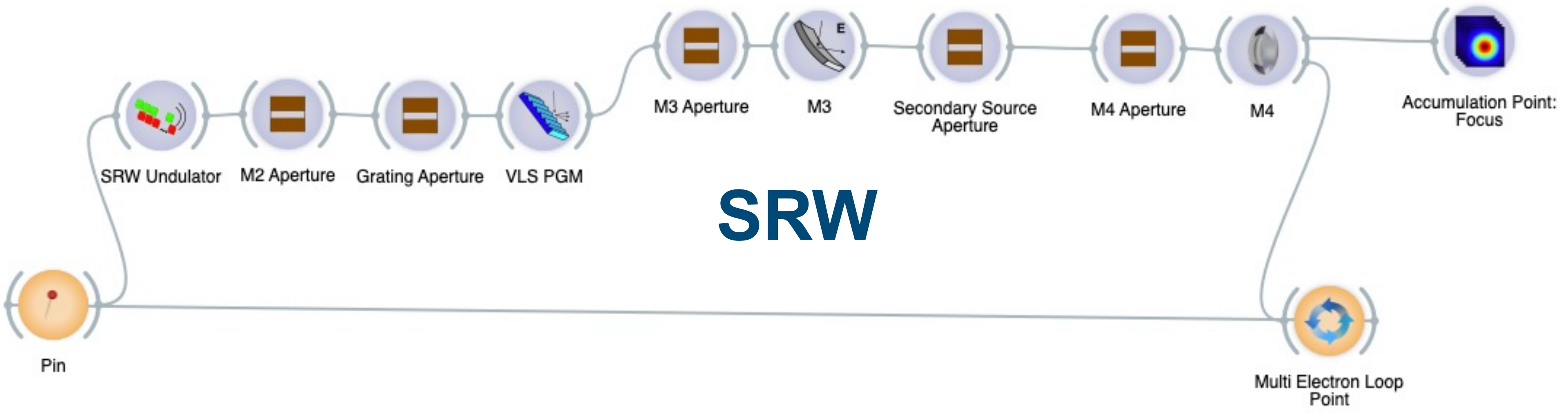
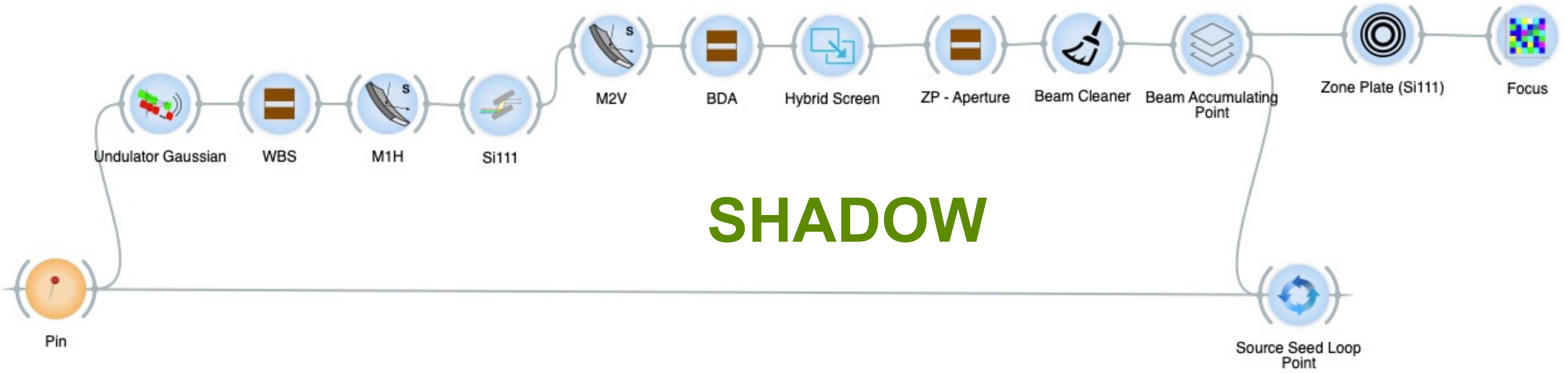
Basic Loops



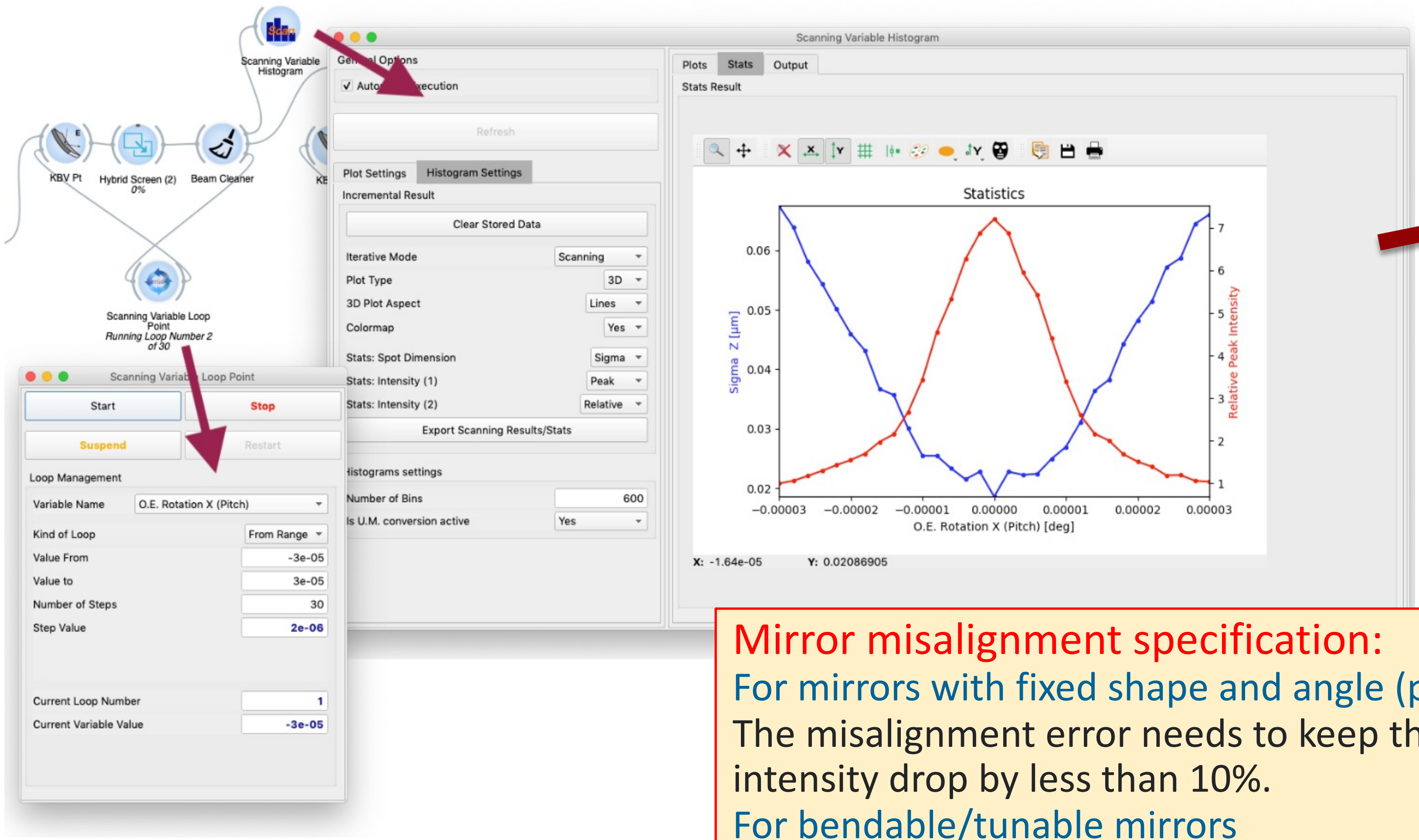
SRW
M3 Aperture
M3
Secondary Source Aperture
M4 Aperture
M4
Accumulation Point: Focus
SRW Undulator
M2 Aperture
Grating Aperture
VLS PGM
Pin
Multi Electron Loop Point

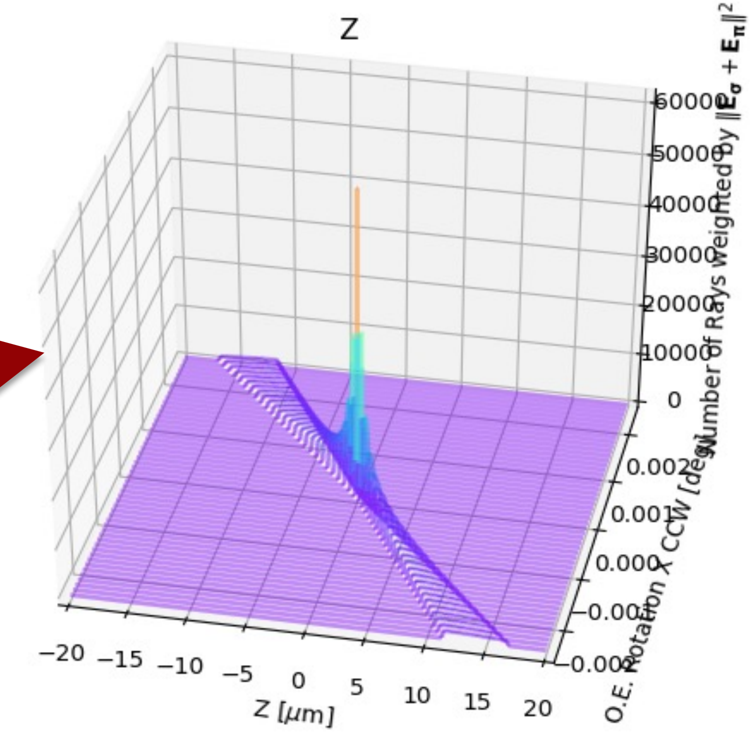


SHADOW
M2V
BDA
Hybrid Screen
ZP - Aperture
Beam Cleaner
Beam Accumulating Point
Zone Plate (Si111)
Focus
Undulator Gaussian
WBS
M1H
Si111
Pin
Source Seed Loop Point

Loops: Optics Misalignment

Study of displacement (ShadowOui + Hybrid, SRW)





Mirror misalignment specification:

For mirrors with fixed shape and angle (prealign)

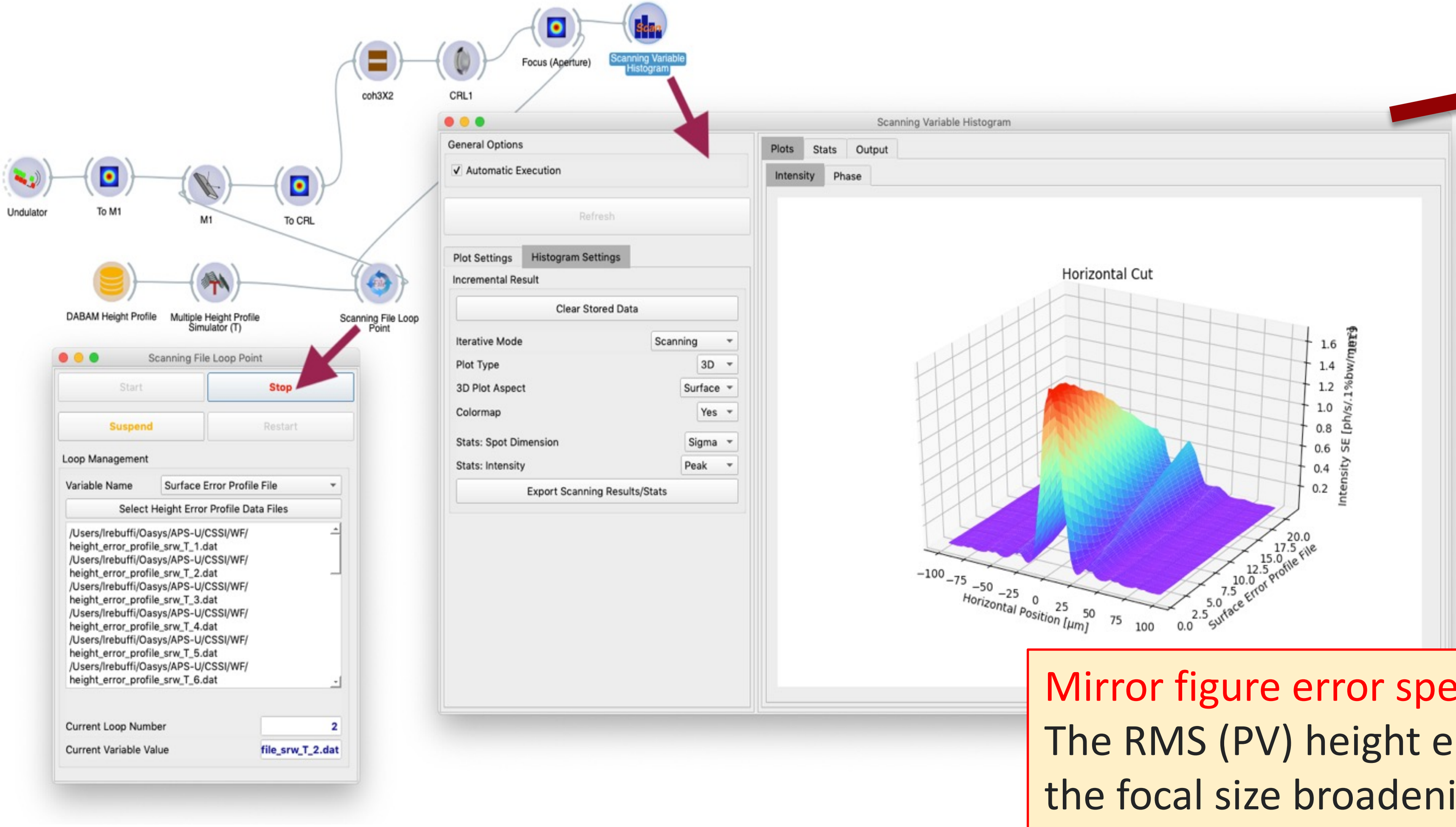
The misalignment error needs to keep the focal size broadening and the peak intensity drop by less than 10%.

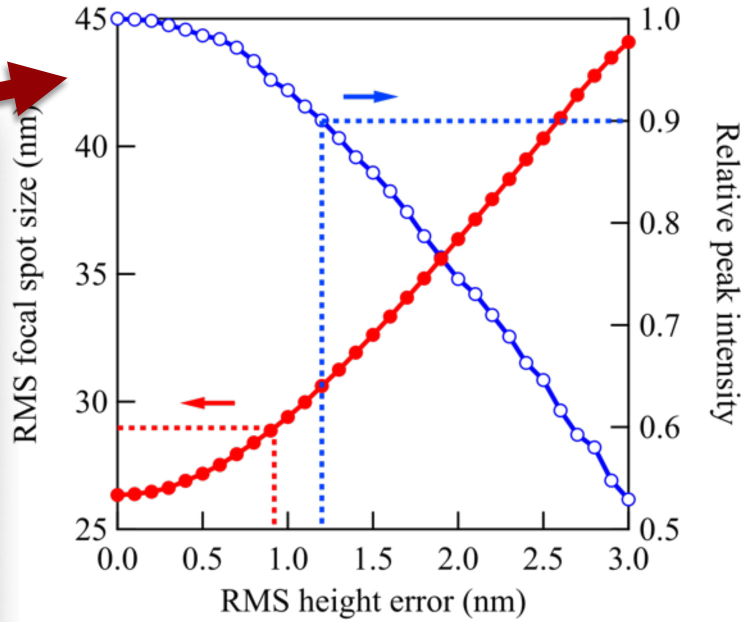
For bendable/tunable mirrors

The motor resolution needs to keep the focal spot position change by less than 10% of the FWHM spot size.

Loops: Optics Aberration - Mirror Figure Errors

Study of height error profile (ShadowOui + Hybrid, SRW)





Mirror figure error specification:
The RMS (PV) height error of the mirror to keep both the focal size broadening and the peak intensity drop by less than 10%.

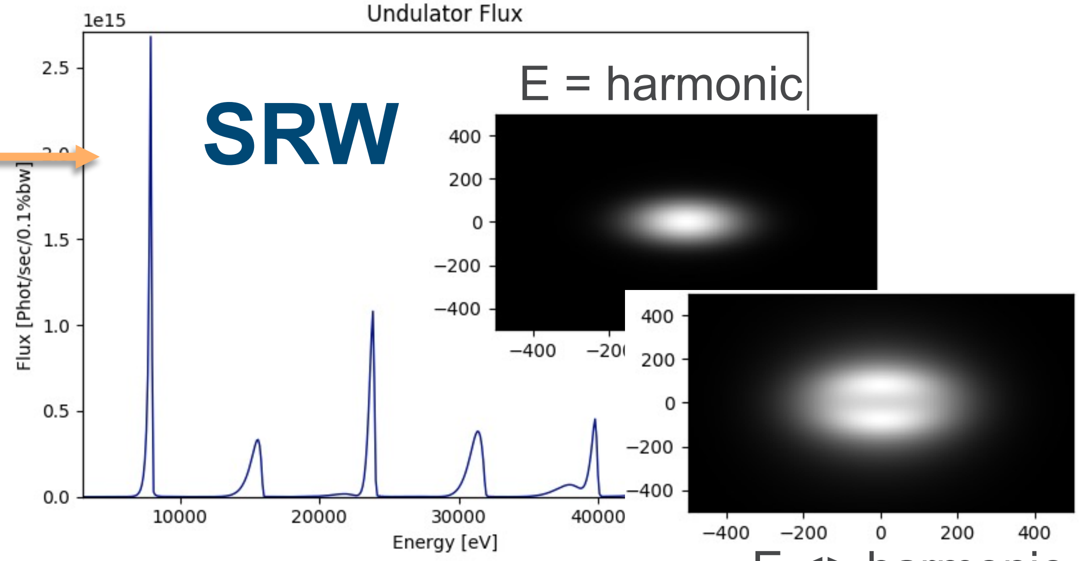
M. Sanchez, et al., *DABAM - an open-source database of x-ray mirrors metrology.* J. Synchrotron Rad. 23, 665 (2016).

Loops: Thermal Load Calculations

To evaluate heat load: Accurately calculate Power Density in any point of the beamline

- The spatial and angular distributions of the emitted radiation from an Undulator (given K values), as well as the amount of power is strongly dependent on the energy

SRW

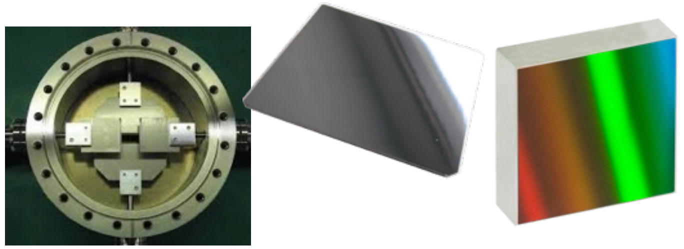


E <> harmonic

- The radiation is not only modified by the geometry of the beamline, but also by phenomena like reflection, absorption and diffraction, all strongly dependent on the energy

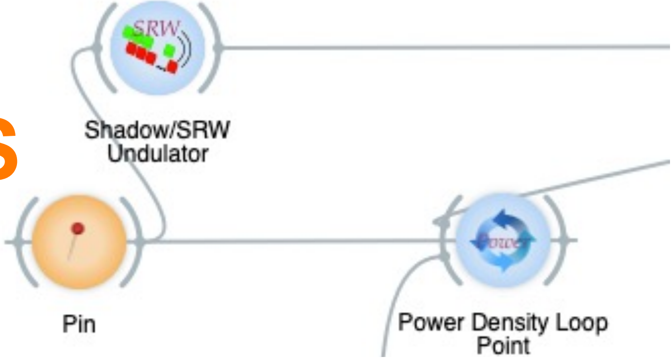
SHADOW

HYBRID



- The dependence on the energy makes the calculation iterative (cumulative) by nature

OASYS LOOPS



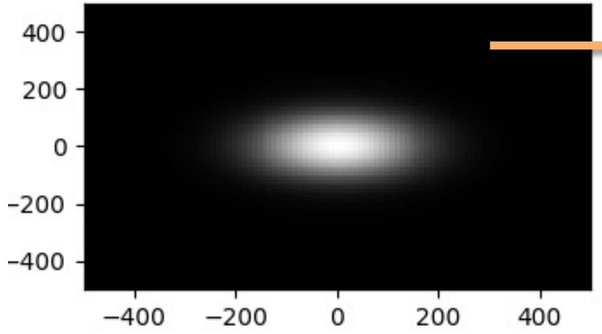
L. Rebuffi, X. Shi, R. Reininger & M. Sanchez del Rio, "*A ray-tracing algorithm for ab-initio calculation of thermal load in undulator-based synchrotron beamlines*", J. Synchrotron Rad. **27** (2020)

Loops: Thermal Load Calculations

Ray-tracing of the Undulator Radiation: (ShadowOui + SRW)

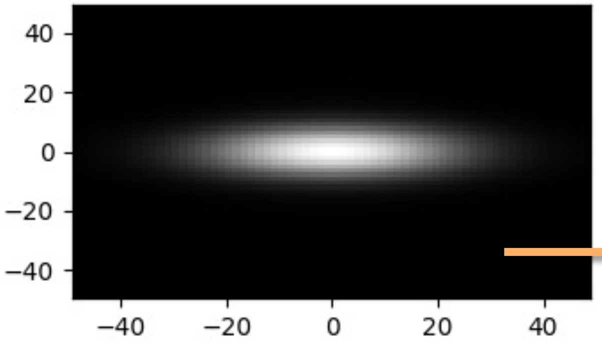
**Conceptual idea by H. Padmore (LBNL)*

SRW: radiation intensity



On a screen in front of the source

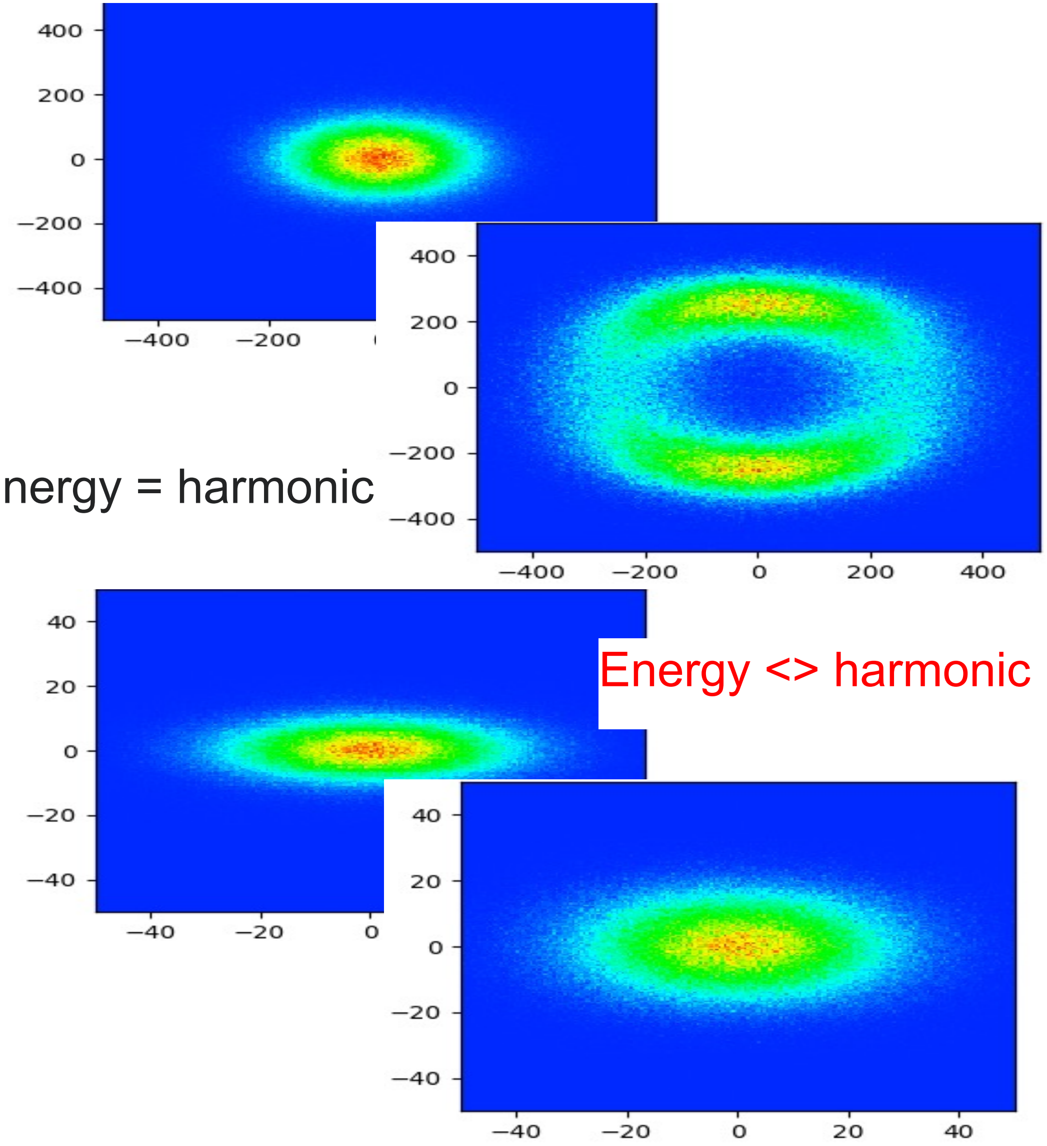
Probability distribution of directions of Shadow rays



On a screen at the center of the source

Probability distribution of positions at the center of the source of Shadow rays

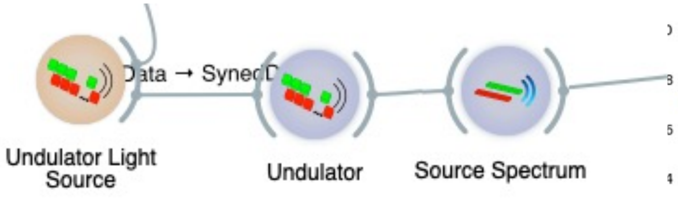
Energy = harmonic

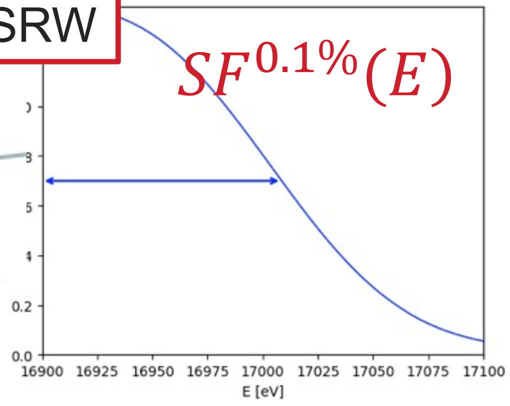


Energy <> harmonic

Power density: Combining all the tools

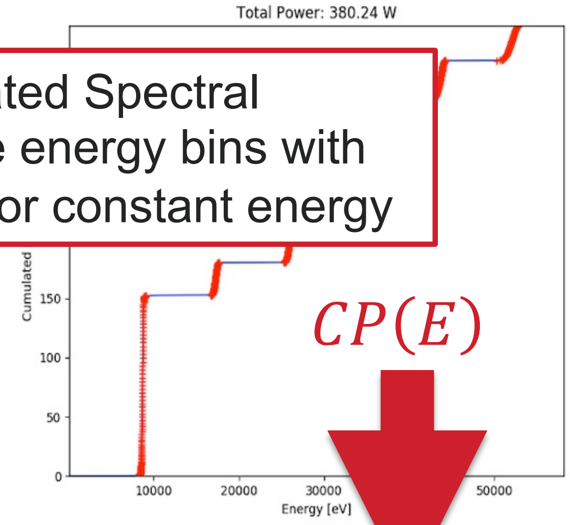
1) Spectral flux calculated by SRW





$$SF^{0.1\%}(E)$$

2) From Cumulated Spectral Power, generate energy bins with constant power or constant energy



$$CP(E)$$

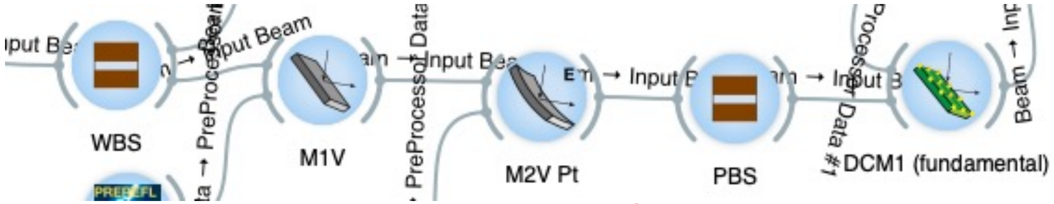
3) Loop on Energy values/bins

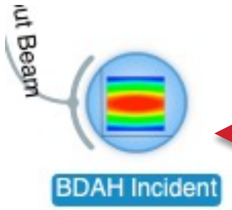
$$P^{\delta Ei}(E_i)$$

$$\delta Ei$$

$$PD(x,z) = \sum_{E_i} Histogram(x,z)\left[\frac{P^{ray,\delta Ei}(E_i)}{\delta x \cdot \delta z}\right]$$

5) ShadowOui compute the radiation transport, taking into account all physical effects





4) Generate Rays with Undulator Source

$$N_{rays}$$

$$E_{source} = E_i$$

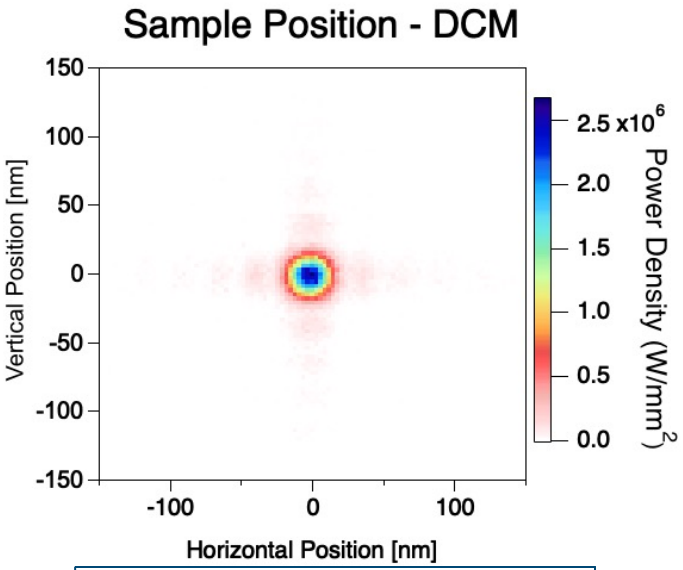
$$P^{ray,\delta Ei}(E_i) = \frac{P^{\delta Ei}(E_i)}{N_{rays}} \cdot I^{ray}$$

6) Compute and accumulate P.D.

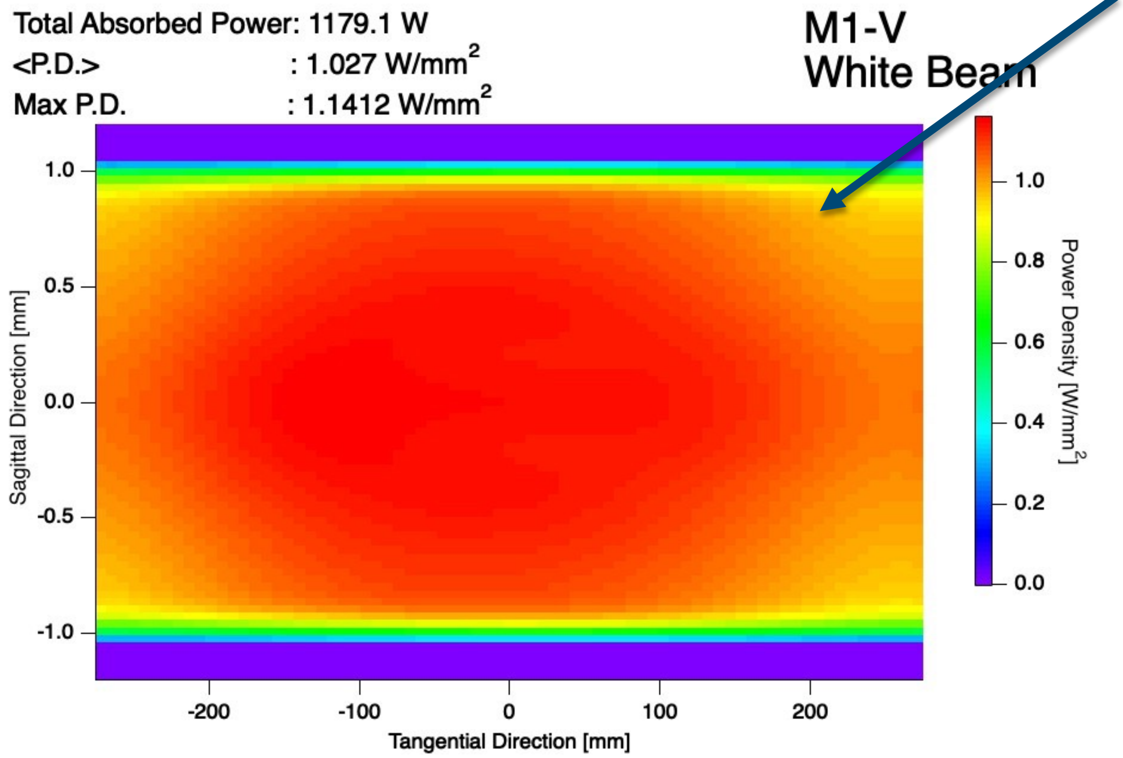
Heat Load

Power density algorithm: Final cumulative result

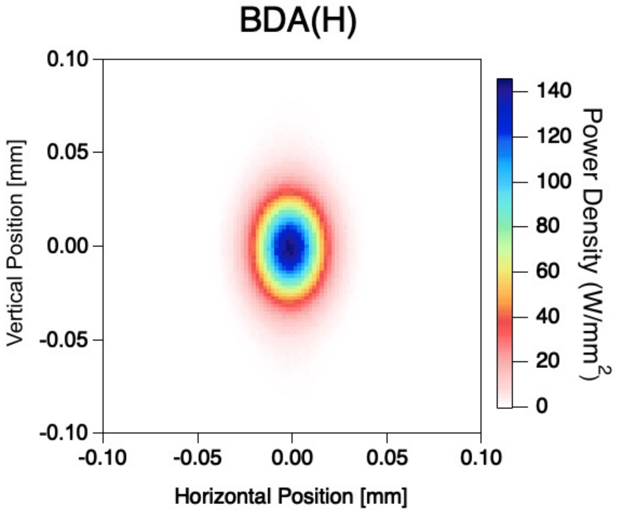
$$PD(x,z) = \sum_{E_i} Histogram(x,z)\left[\frac{P^{ray,\delta Ei}(E_i)}{\delta x \cdot \delta z}\right]$$

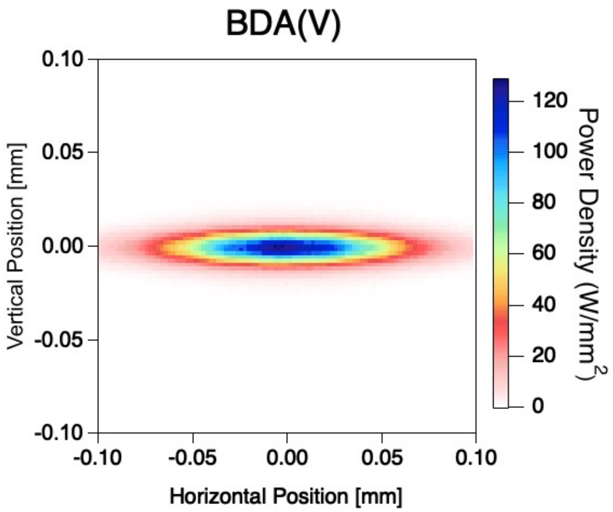


Total Power: 0.002 W



Total Power: 1180 W





Total Power: 0.2 W

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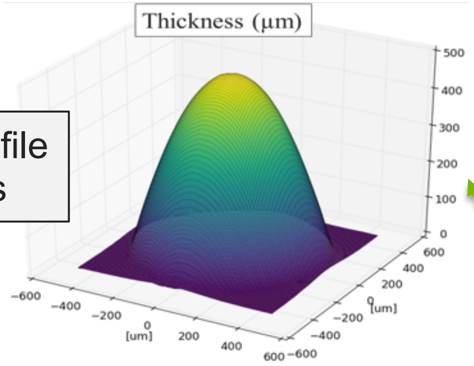
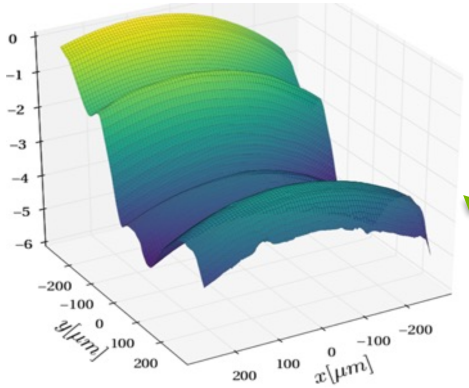
1-BM Beamline

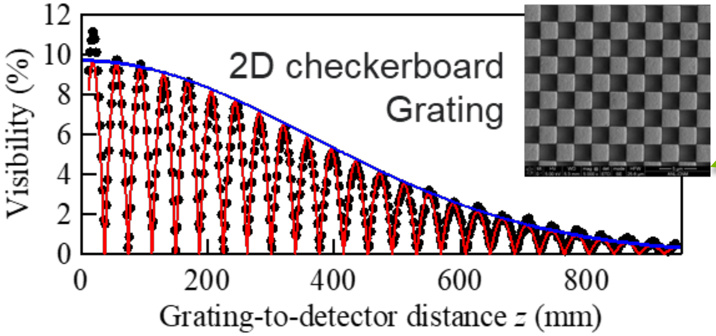
Optics characterization Tools

Thickness profile of a Be lens

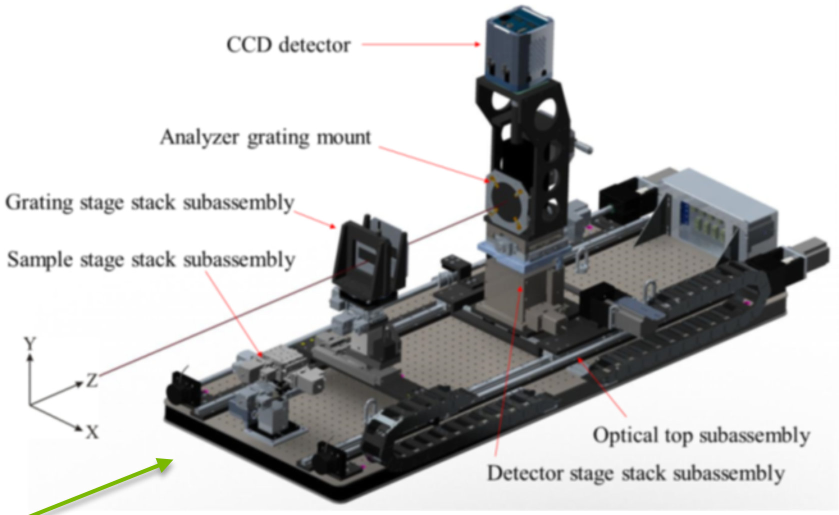


Distorted wavefront of a mirror





- **Characterization tools**
  - Techniques
    - Grating interferometry
    - Speckle tracking
  - Instruments
    - Portable Interferometer
    - Compact interferometer
  - Applications
    - At-wavelength metrology
    - Wavefront sensing
    - Coherence characterization



BES-ADR Project: Wavefront Preserving Mirrors
Eliane Lessner

Thickness Error: analysis of Talbot Images

The differential phases, or field gradients, Φ_x and Φ_y (Fig. 3c) are calculated from the phase ϕ of the Fourier transform with the following formulas

$$\Phi_x = \frac{\partial \Phi(x,y)}{\partial x} = -\frac{p_x(\phi^{01}_{\text{lens}} - \phi^{01}_{\text{ref}})}{d_T \lambda}, \quad \Phi_y = \frac{\partial \Phi(x,y)}{\partial y} = -\frac{p_y(\phi^{10}_{\text{lens}} - \phi^{10}_{\text{ref}})}{d_T \lambda}, \qquad (5)$$

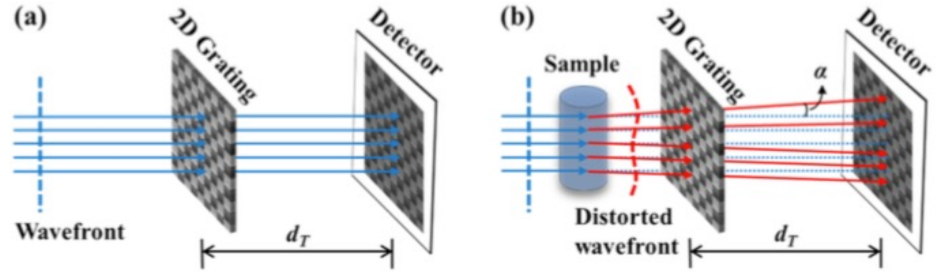
with the superscripts ^{10} and ^{01} denoting the harmonic peaks "10" and "01" in Fig. 3b, p_y and p_x are the pattern periods in y and x directions, respectively.

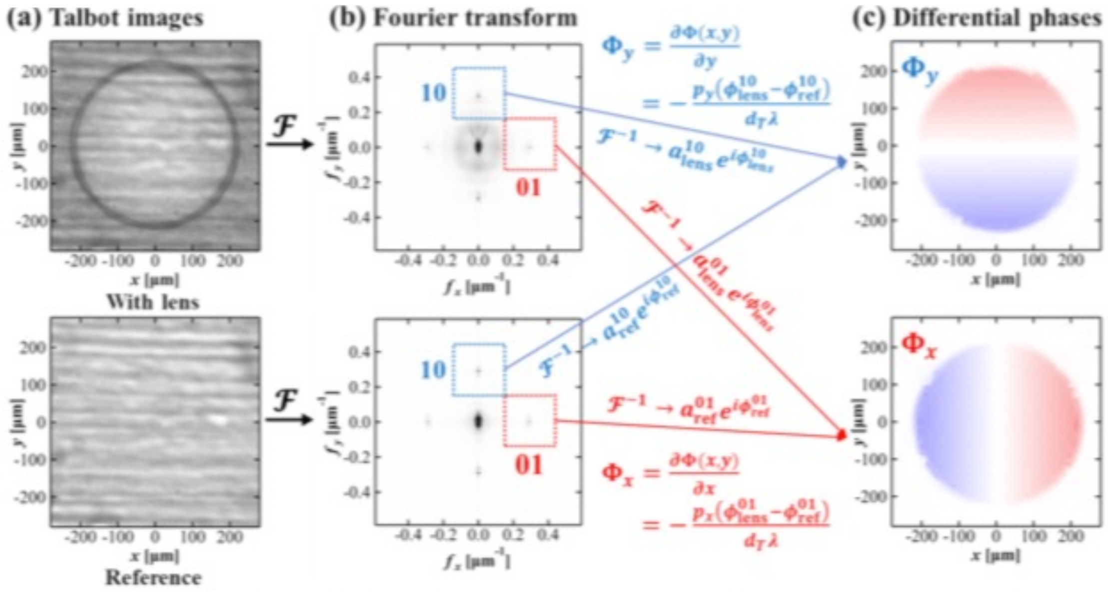
The two orthogonal differential phases are then integrated using the Frankot-Chellappa method[25] to form the phase profile,

$$\Phi(x,y) = \mathcal{F}^{-1}\left[\frac{\mathcal{F}[\Phi_x + i\Phi_y](f_x, f_y)}{2\pi i(f_x + i f_y)}\right], \qquad (6)$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ denote the Fourier and inverse Fourier transform, and (f_x, f_y) are the reciprocal coordinates of (x, y). Physically Φ is the phase shift of the wavefront introduced by passing through the lens.

$$d_{T,\theta} = \frac{(2n-1)p_\theta^2}{2\lambda},$$



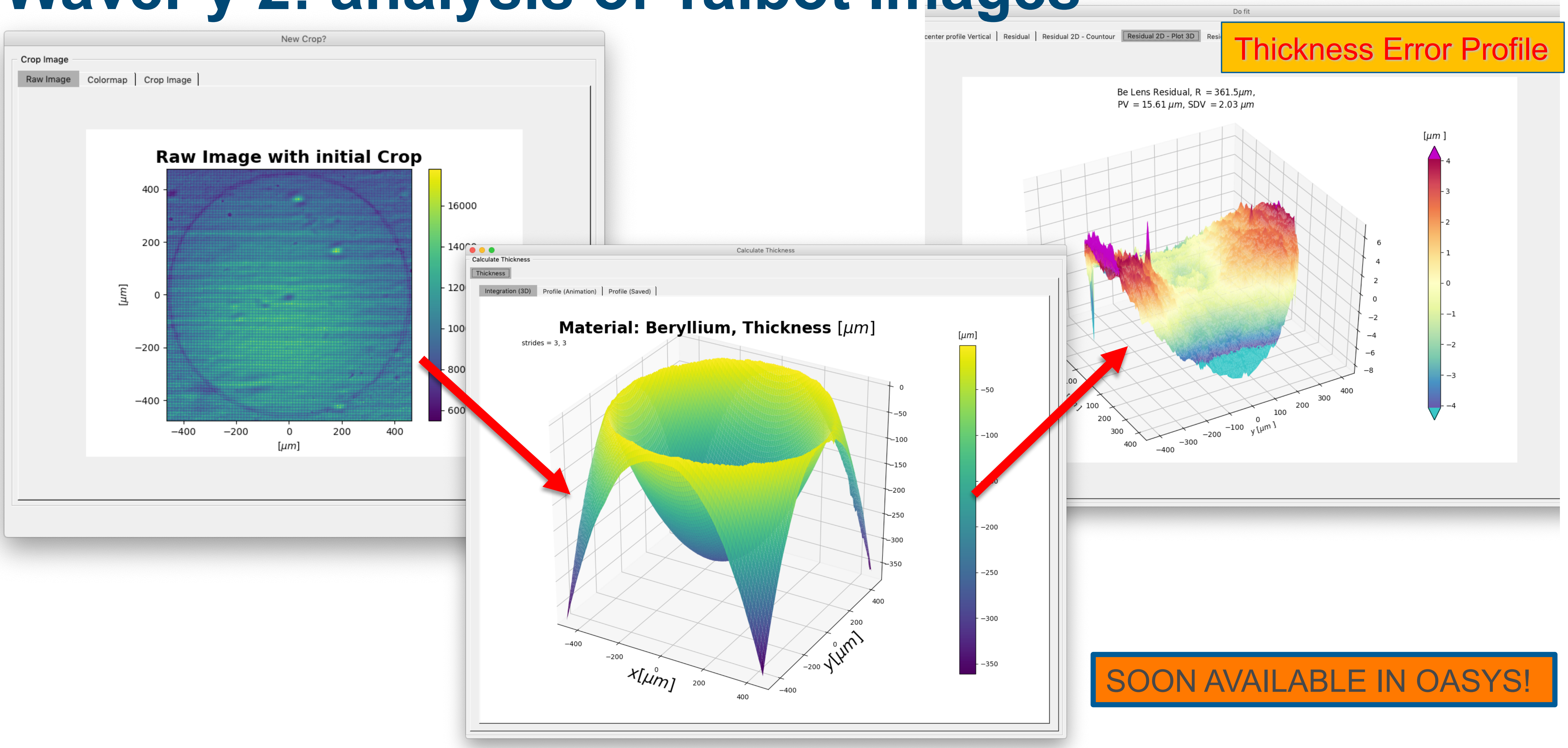


Thickness Error Profile

$$T(x,y) = -\frac{\lambda}{2\pi}\frac{\Phi(x,y)}{\delta}$$

X. Shi et al., "*High-speed characterization of refractive lenses with single-grating interferometry*", Proc. SPIE 11109, 111090K (2019)

WavePy 2: analysis of Talbot Images



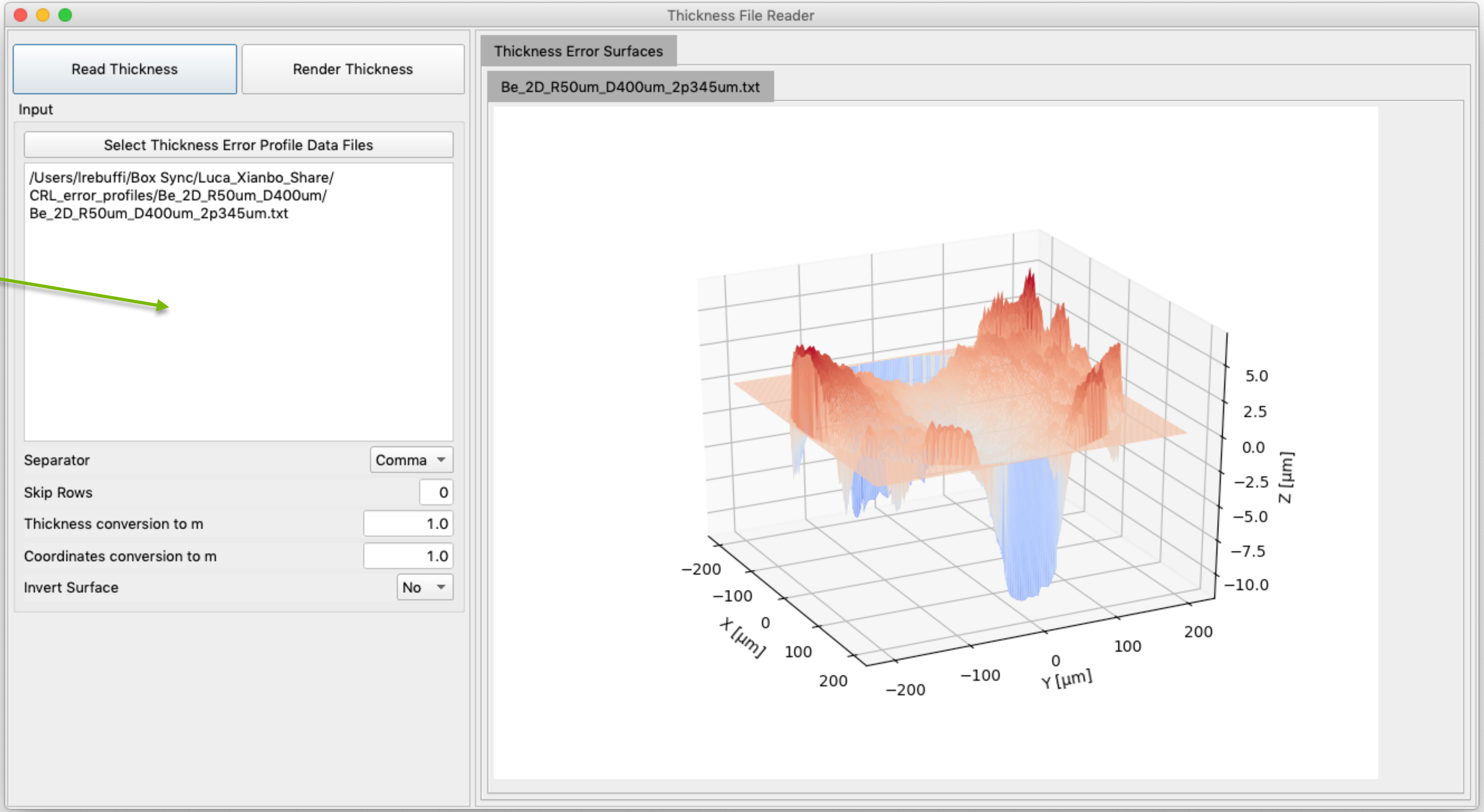
SOON AVAILABLE IN OASYS!

W. Grizolli et al., "*Wavepy - python package for x-ray grating interferometry with applications in imaging and wavefront characterization*", AIP Conference Proceedings 2054, 060017 (2019)

Thickness Error Profile

OASYS can import WavePy files

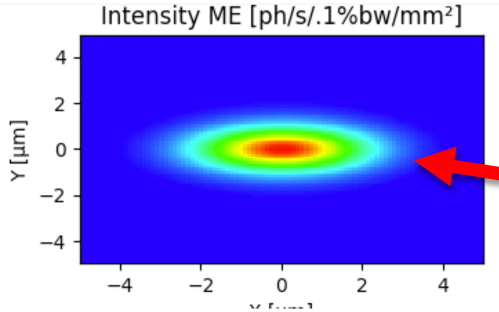
Thickness File Reader



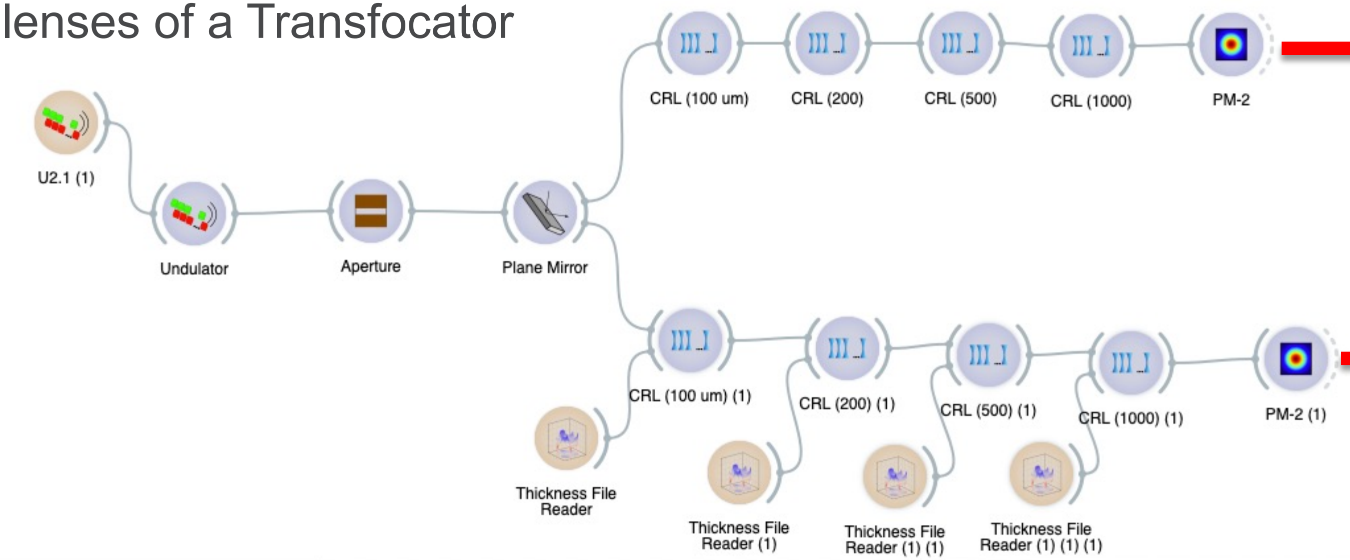
Integration in SRW: Transfocators

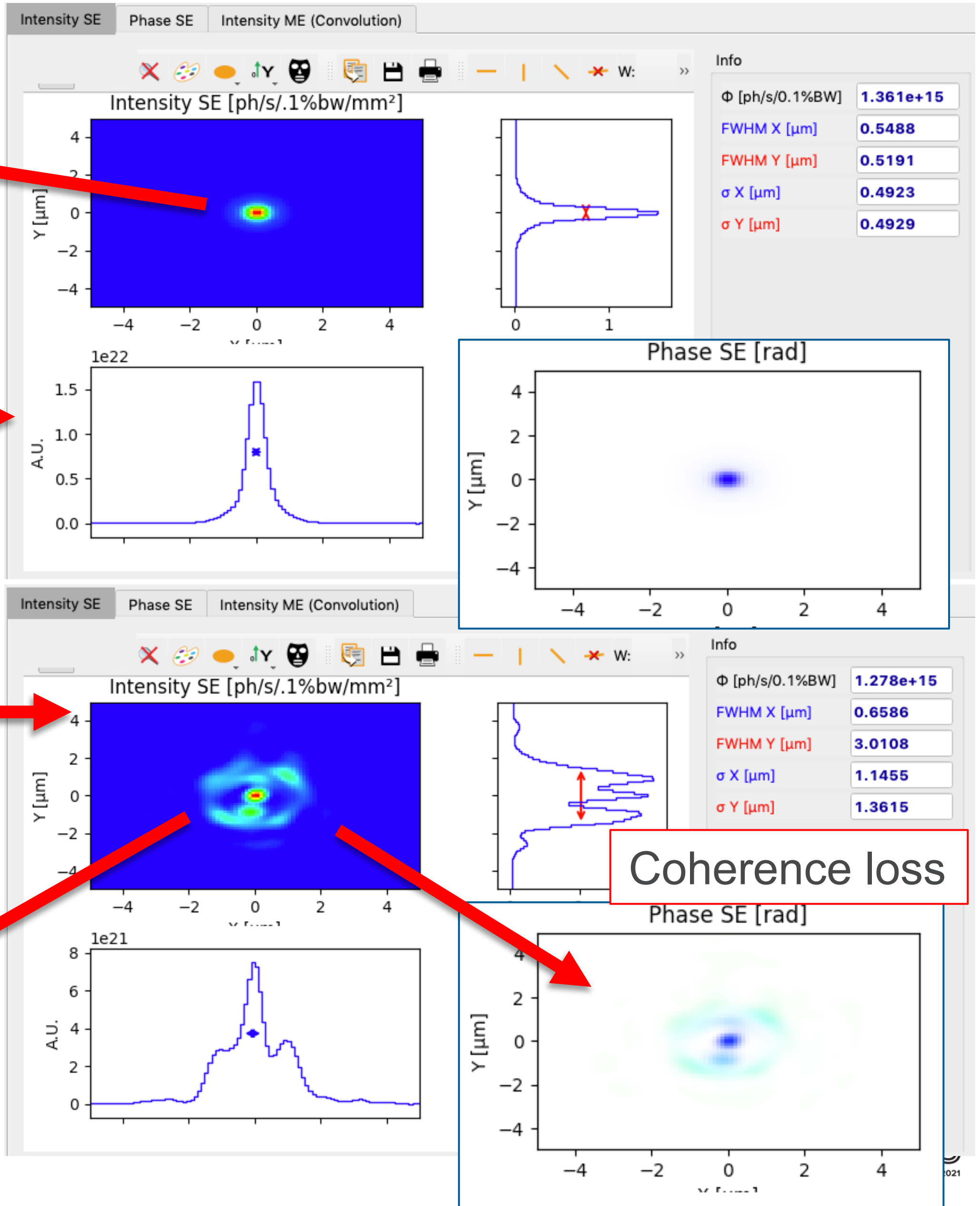
$$T(x,y,\lambda) = e^{-\frac{\Delta t(x,y)}{2 l_a(\lambda)}}$$

$$OPD(x,y,\lambda) = -\delta(\lambda)\Delta t(x,y)$$

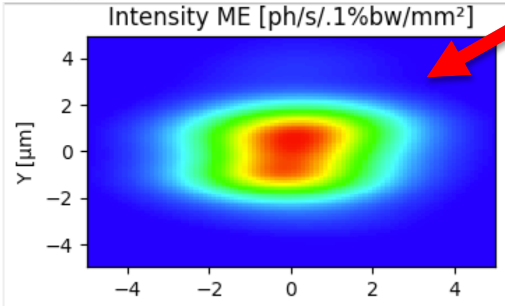


Deformation of the wavefront from the thickness errors of the lenses of a Transfocator



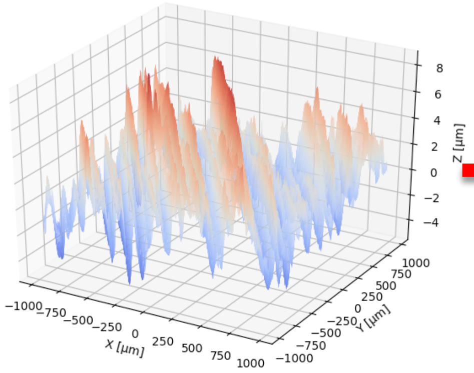


Coherence loss

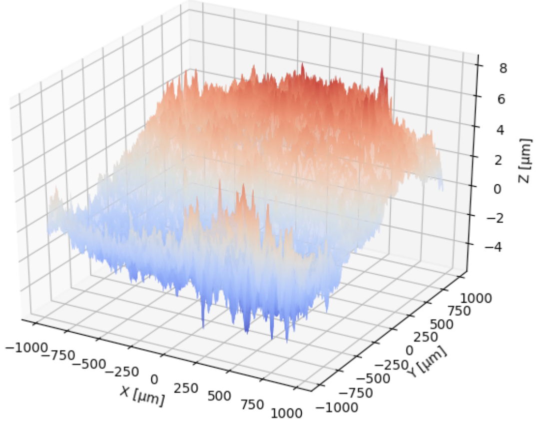


Focal spot size broadening

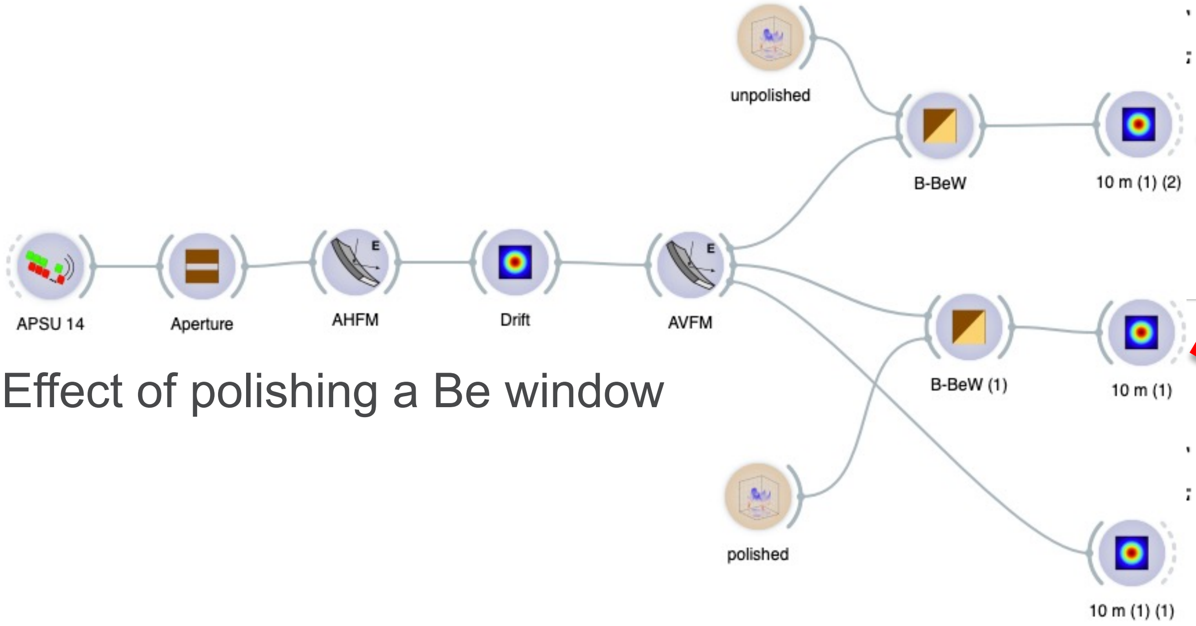
Integration in SRW: (Be) Windows



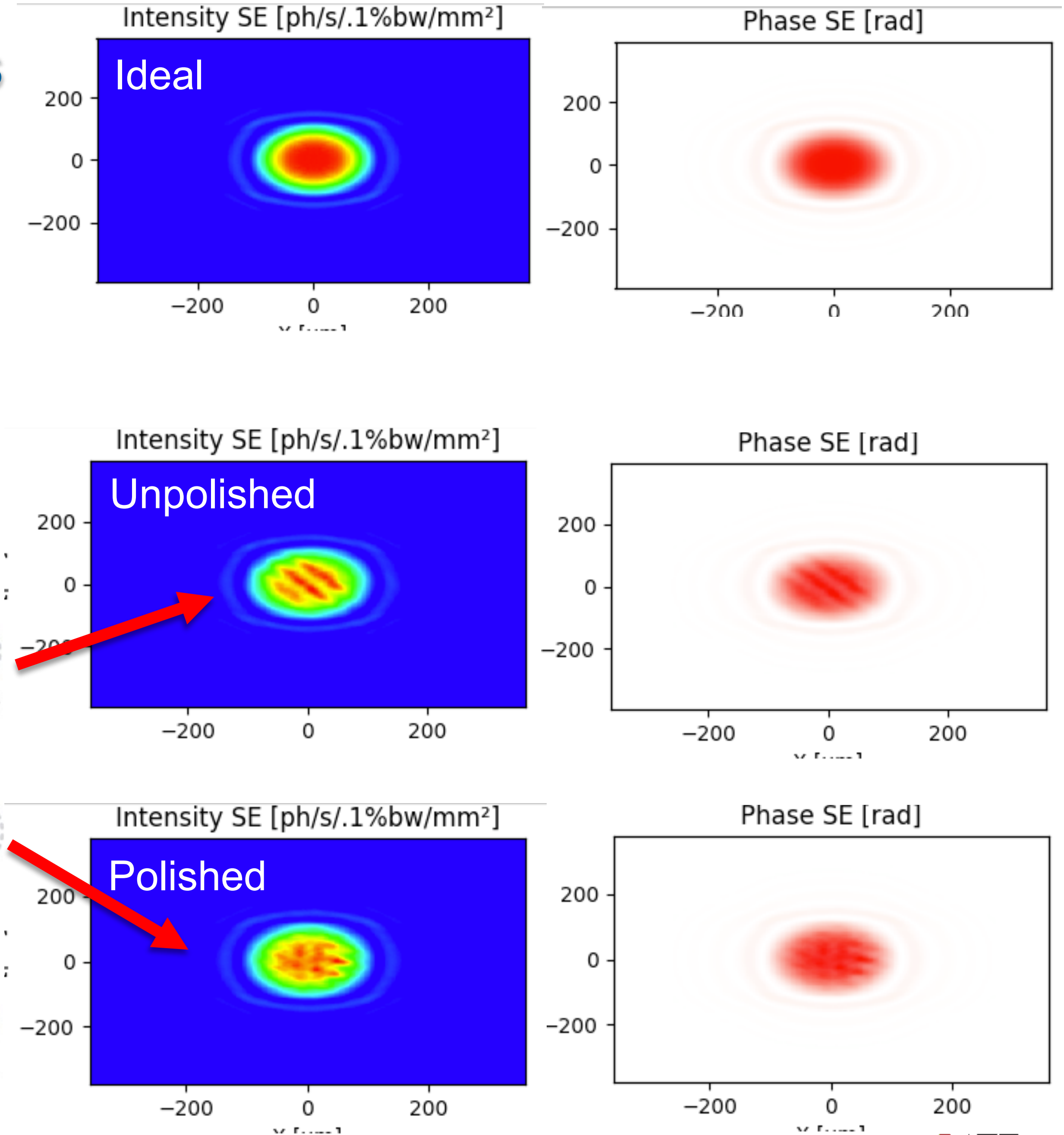
Unpolished



Polished



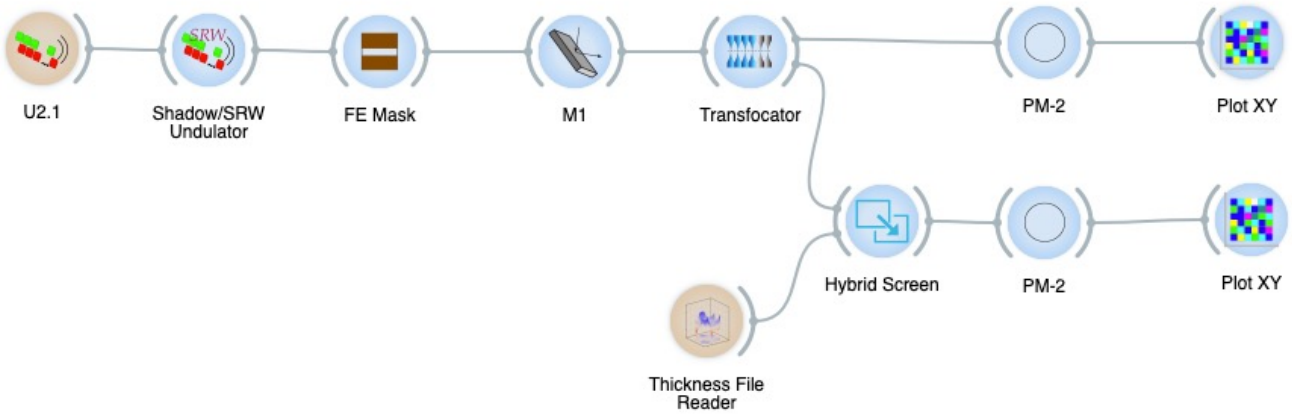
Effect of polishing a Be window

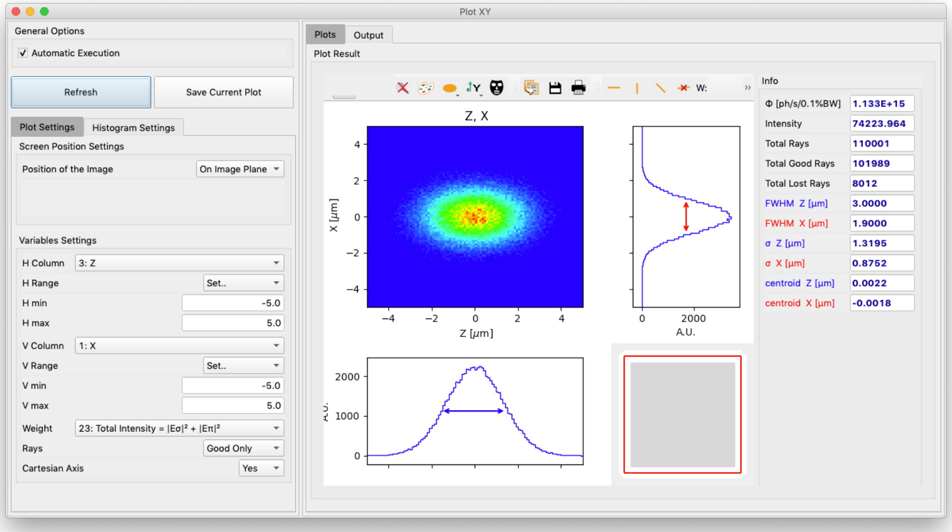


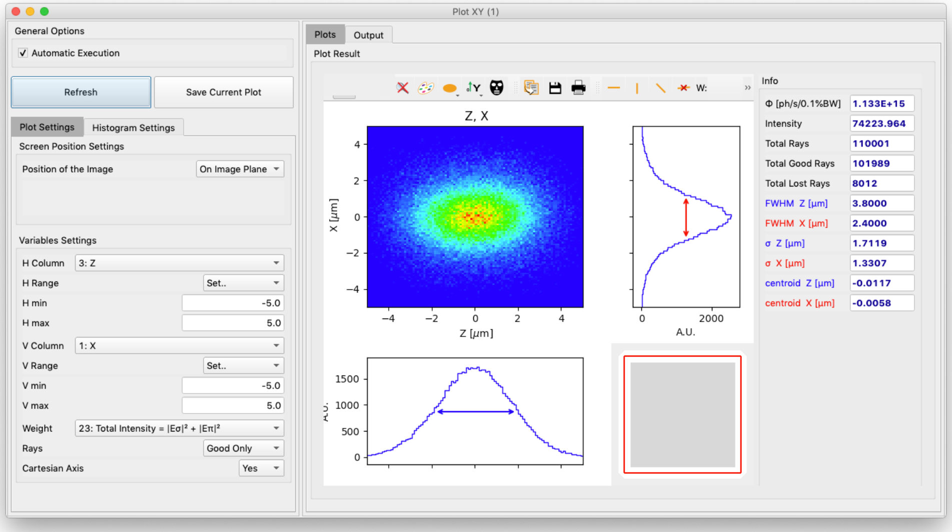
Integration in ShadowOui-Hybrid: Transfocators

$$\Delta\phi(x,y,\lambda) = -\frac{2\pi}{\lambda}\delta(\lambda)\Delta t(x,y) = \frac{2\pi}{\lambda}OPD(x,y,\lambda)$$

Deformation of the wavefront from the thickness errors of the lenses of a Transfocator







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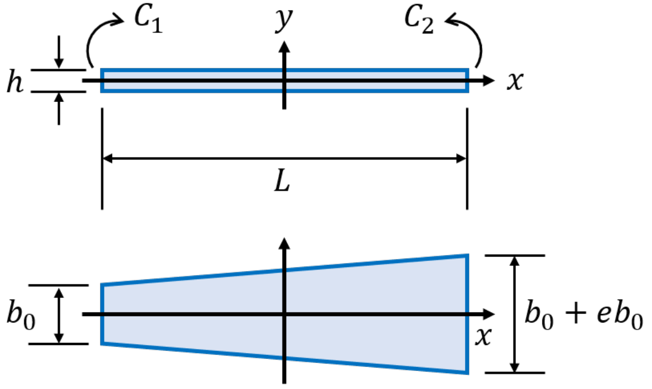
Mirror bender

- Analytical mirror bender calculation
  - M. R. Howells, et al., Opt. Eng. 39, 2748 (2000).



$$y = H\left[\left(\frac{C+Dx}{D}\right)\ln(C+Dx) - x\right] - \frac{Bx^2}{2D} + Fx + G$$

$$A = \frac{C_1+C_2}{2},\ B = \frac{C_1-C_2}{L},\ C = \frac{Eh^3}{24}(2b_0+eb_0),\ D = \frac{Eh^3eb_0}{12L},\ H = \frac{AD+BC}{D^2},$$

$$G = -\frac{H}{2}\left[\left(\frac{C-DL/2}{D}\right)\ln\left(C-\frac{DL}{2}\right) + \left(\frac{C+DL/2}{D}\right)\ln\left(C+\frac{DL}{2}\right)\right] + \frac{BL^2}{8D}$$

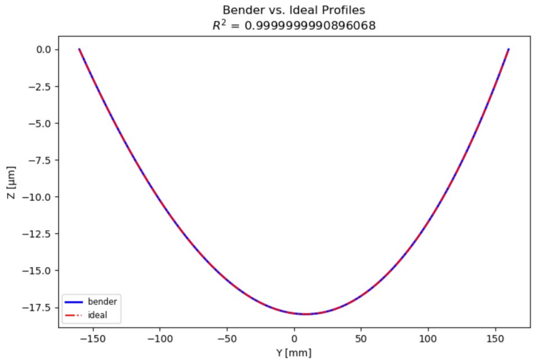
$$F = \frac{H}{L}\left[\left(\frac{C-DL/2}{D}\right)\ln\left(C-\frac{DL}{2}\right) - \left(\frac{C+\frac{DL}{2}}{D}\right)\ln\left(C+\frac{DL}{2}\right) + L\right]$$

E — Young's modulus of elasticity

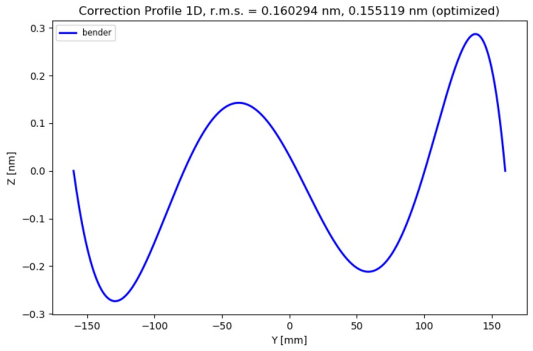
- Implementation in OASYS

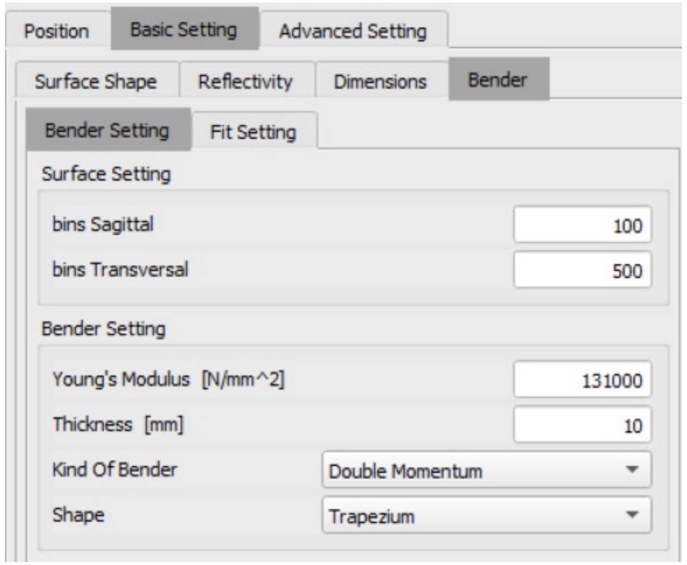
Bendable Elliptical Mirror

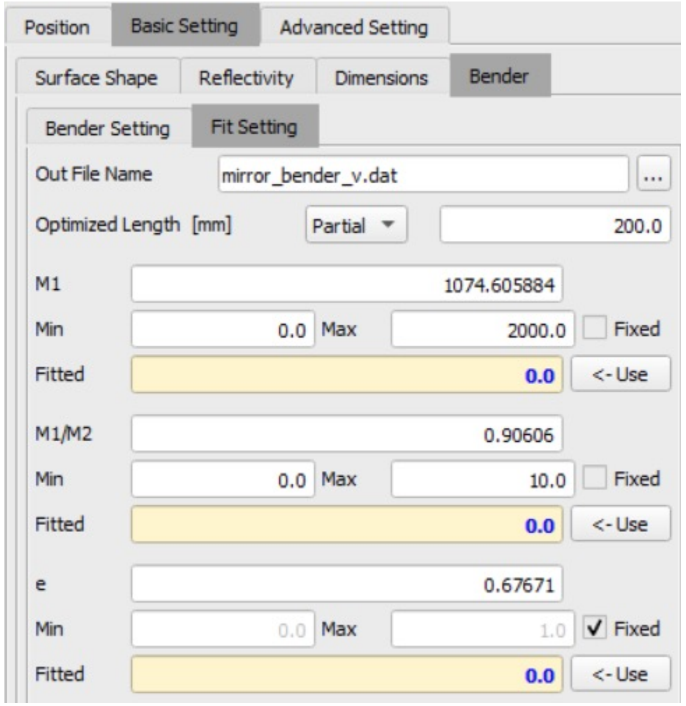
Bender vs Ideal profile



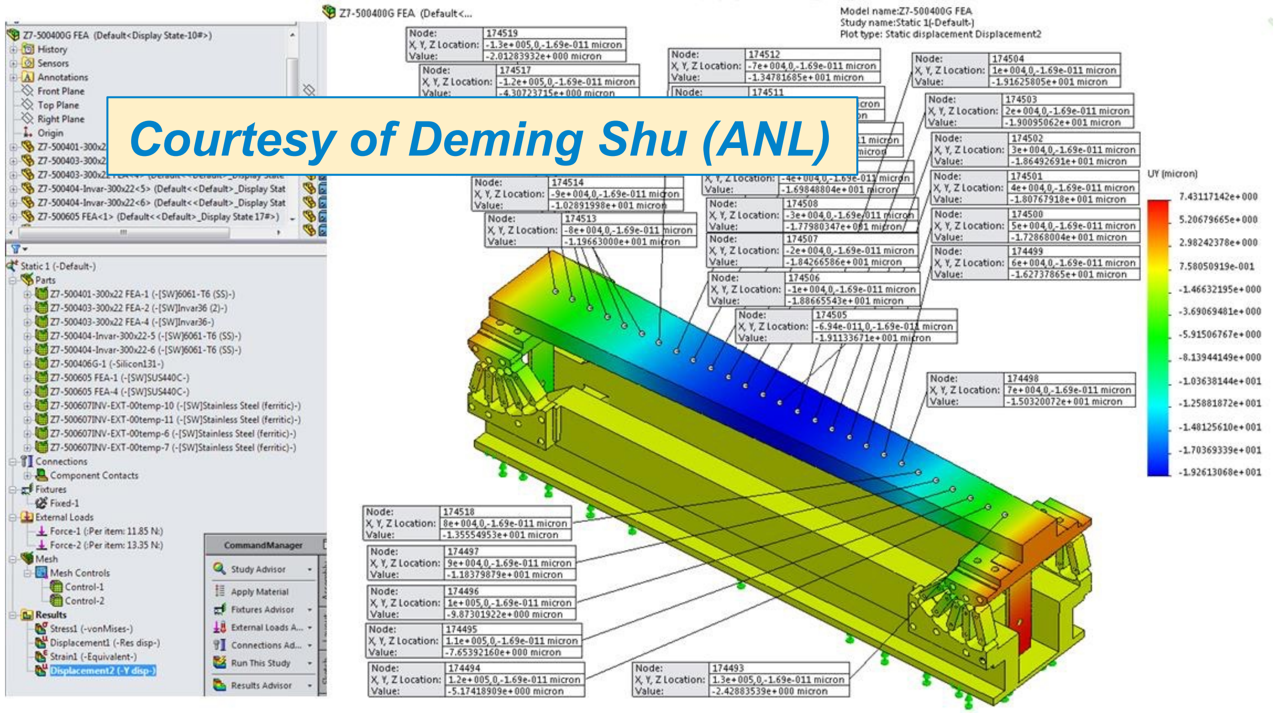
Bender error

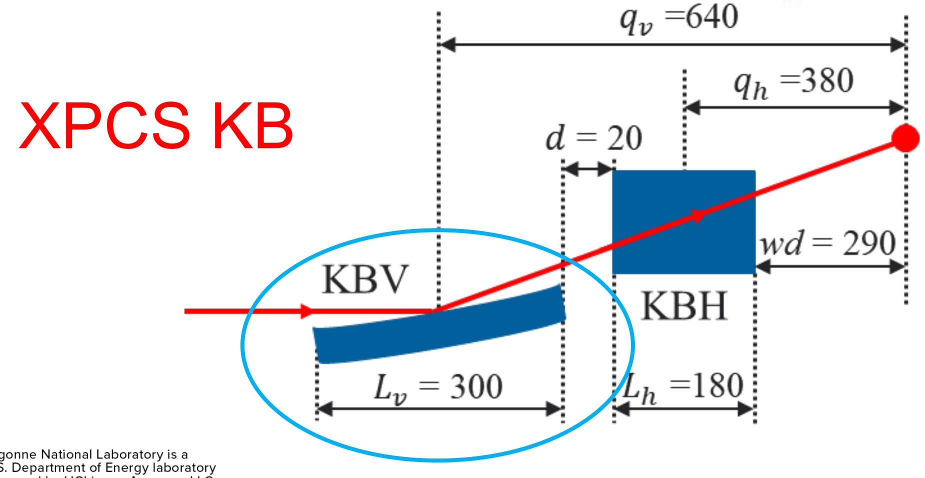


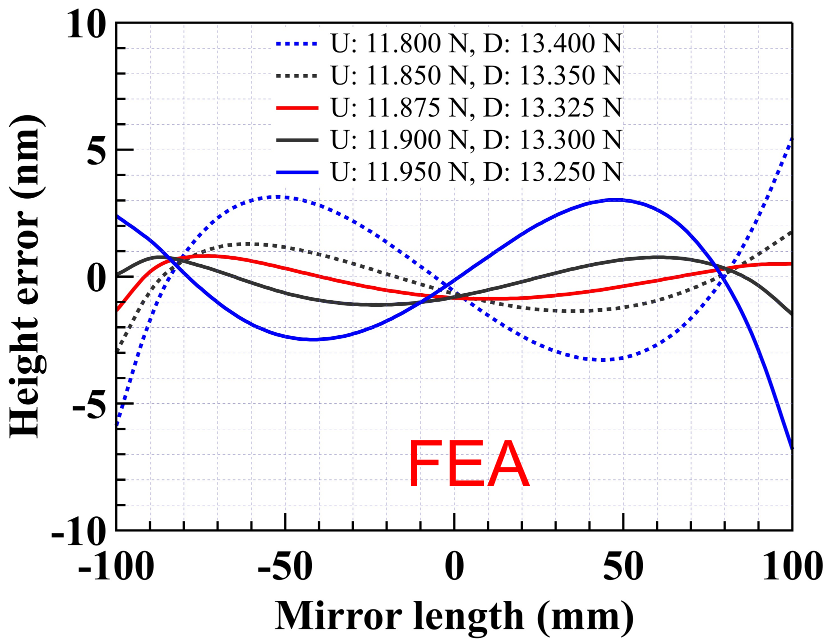


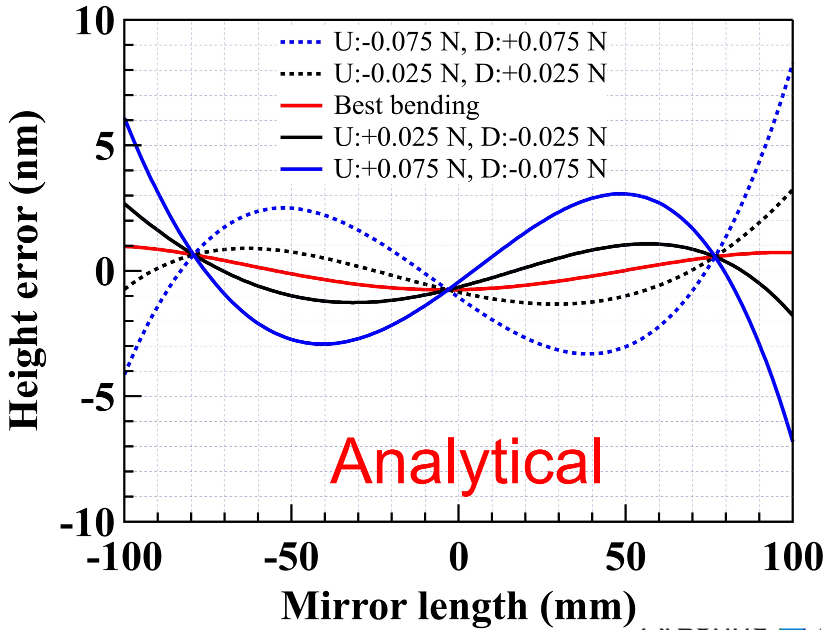


FEA analysis vs Analytical









THANK YOU!