Advances in Soft X-Ray beamlines design

- **Software for Optical Simulations WORKSHOP**
- **Trieste October 3-7, 2016**

- Ruben Reininger
- X ray Science Division / Advanced Photon Source
- Argonne National Laboratory

Outlook

- ☑ Toroidal Grating Optical Path Length
- ☑ Formulas
- ☑ Formulas
- ☑ SGM
- ☑ Vertical collimated PGM
- ☑ Follath collimated PGM — R. Follath and F. Senf, NIM A **390**, 388 (1997).
- ☑ FVLS PGM

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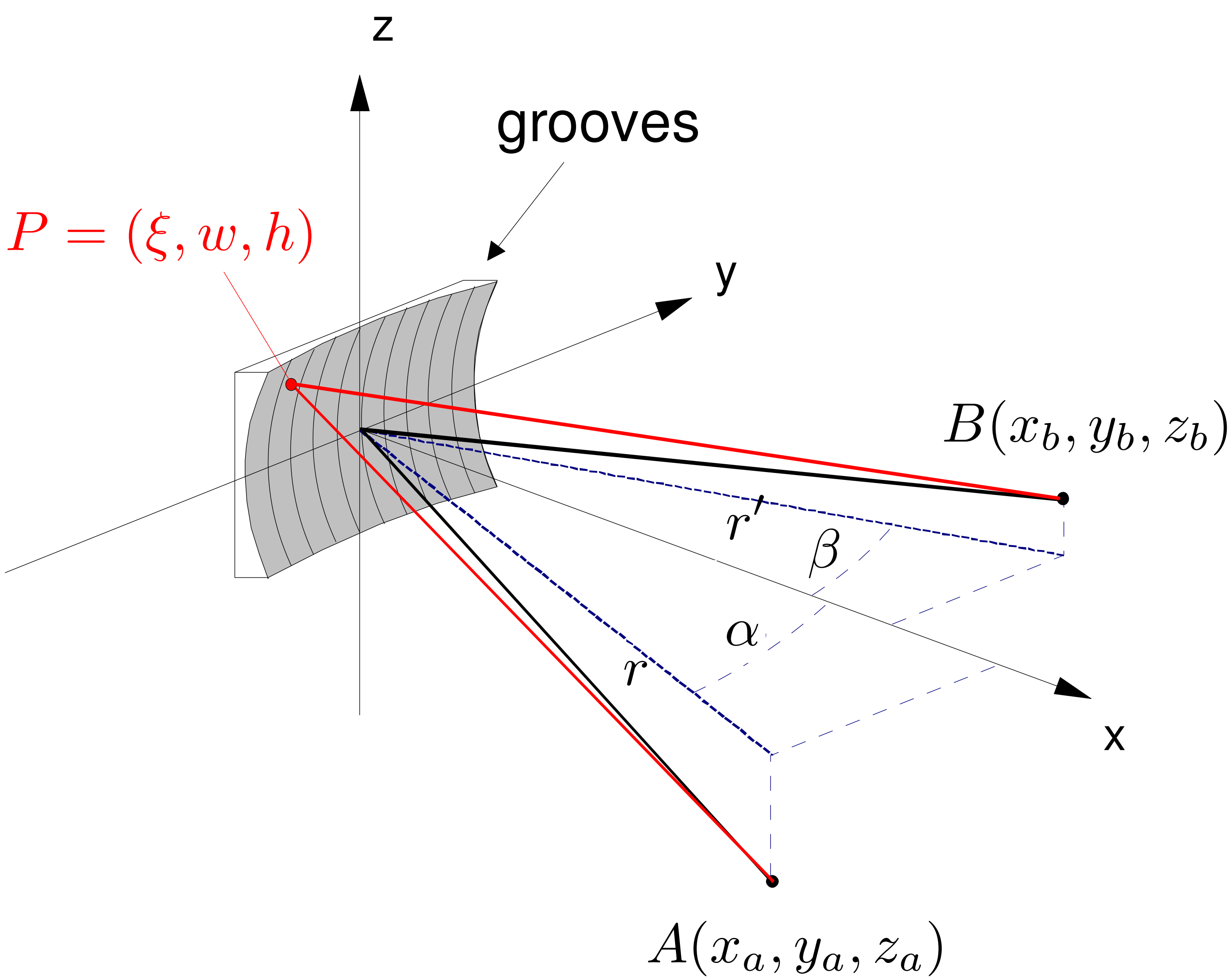
SORRY

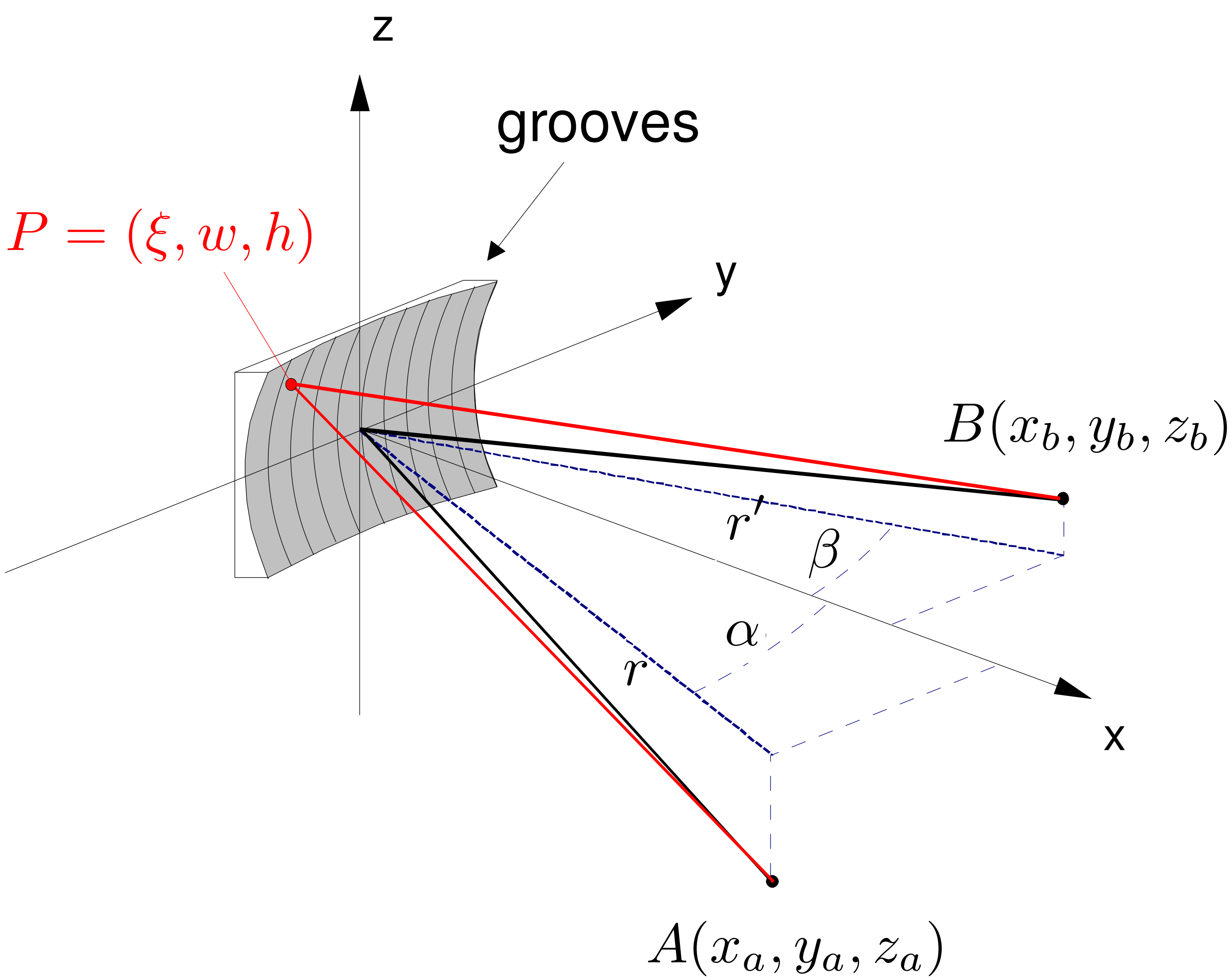
R. Follath and F. Senf, NIM A **390**, 388 (1997).

Toroidal Grating Optical Path Length



$$F = AP + PB + nm\lambda$$
$$A = (r\cos\alpha, r\sin\alpha, z_a)$$
$$B = (r'\cos\beta, r'\sin\beta, z_b)$$
$$P = (\xi, w, h)$$

Toroidal Grating Optical Path Length



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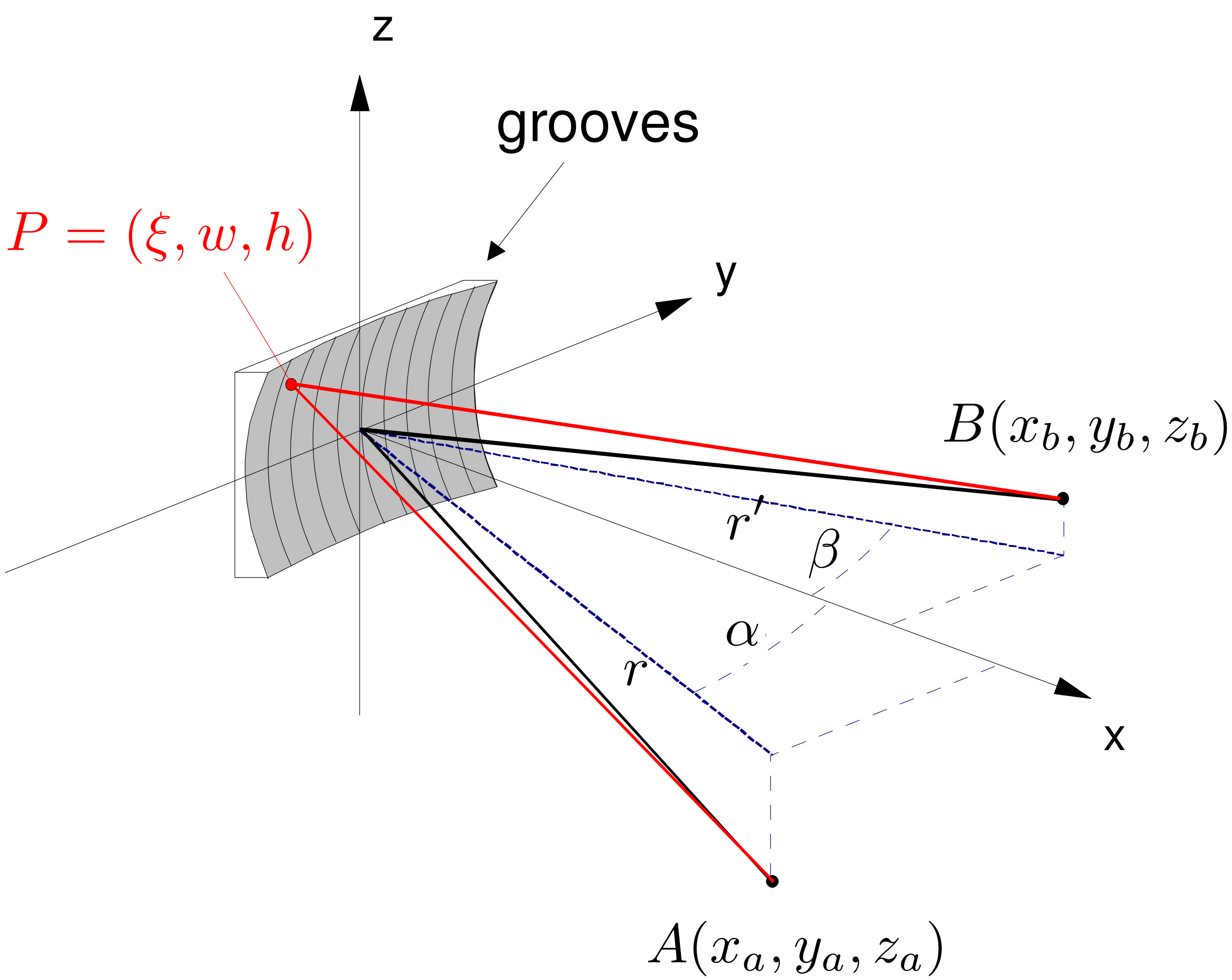
$$A = (r\cos\alpha, r\sin\alpha, z_a)$$
$$B = (r'\cos\beta, r'\sin\beta, z_b)$$
$$P = (\xi, w, h)$$
$$n = \frac{1}{d_0}(w + b_2 w^2 + b_3 w^3 + \ldots)$$
$$\xi(w, l) = \sum_i \sum_j a_{i,j} w^i l^j$$

Toroidal Grating Optical Path Length



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$$n = \frac{1}{d_0}(w + b_2 w^2 + b_3 w^3 + \ldots)$$
$$\xi(w,l) = \sum_i \sum_j a_{i,j} w^i l^j$$

$$F = F_{00} + F_{01}w + \frac{1}{2}F_{20}w^2 + \frac{1}{2}F_{02}l^2 + \frac{1}{2}F_{30}w^3 + \frac{1}{2}F_{21}w^2 l + \ldots$$

Fermat's principle: Of all possible paths, light takes the path which requires the *shortest time*.

$$\delta F = 0$$

Main terms, Toroidal Grating

$$\frac{1}{d} = k = \frac{\partial n}{\partial w} = \frac{1 + 2b_2 w + 3b_3 w^2 + ...}{d_0}$$

Groove Density

$$F_{00} = r + r'$$

$$F_{10} = m\frac{\lambda}{d_0} - (\sin\alpha + \sin\beta)$$

Grating Equation

$$F_{20} = \frac{1}{2}(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{r'} - \frac{\cos\beta}{R}) - \frac{m\lambda\, b_2}{d_0}$$

Meridional Focus

$$F_{02} = \frac{1}{r} - \frac{\cos\alpha}{\rho} + \frac{1}{r'} - \frac{\cos\beta}{\rho}$$

Sagittal Focus

$$F_{30} = \frac{1}{2}(\frac{\sin\alpha}{r}(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}) + (\beta r')) - \frac{m\lambda\, b_3}{d_0}$$

Coma

Main terms, Toroidal Grating

$$\frac{1}{d} = k = \frac{\partial n}{\partial w} = \frac{1 + 2b_2 w + 3b_3 w^2 + ...}{d_0}$$

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Coma

Sphere $\rho=R$; Plane $\rho=R=\infty$

Main terms, Toroidal Grating

$$\frac{1}{d} = k = \frac{\partial n}{\partial w} = \frac{1 + 2b_2 w + 3b_3 w^2 + \ldots}{d_0}$$

Groove Density

$$F_{00} = r + r'$$

$$F_{10} = m\frac{\lambda}{d_0} - (\sin\alpha + \sin\beta)$$

Grating Equation

$$F_{20} = \frac{1}{2}\left(\left[\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}\right] + \left[\frac{\cos^2\beta}{r'} - \frac{\cos\beta}{R}\right]\right) - \frac{m\lambda b_2}{d_0}$$

Meridional Focus

$$F_{02} = \frac{1}{r} - \frac{\cos\alpha}{\rho} + \frac{1}{r'} - \frac{\cos\beta}{\rho}$$

Sagittal Focus

$$F_{30} = \frac{1}{2}\left(\frac{\sin\alpha}{r}\left(\left[\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}\right]\right) + (\beta r')\right) - \frac{m\lambda b_3}{d_0}$$

Coma

Rowland Condition

Resolution Terms and Magnification

$$\lambda = \frac{d}{m}(\sin\alpha + sin\beta)$$

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$$\lambda = \frac{d}{m}(\sin\alpha + sin\beta)$$

$$\Delta\lambda_{so} = \frac{d}{m}\Delta\alpha\cos\alpha = \frac{d}{m}\frac{\Delta s}{r}\cos\alpha$$

Source or Entrance Slit

$$\Delta\lambda_{sl} = \frac{d}{m}\Delta\beta\cos\beta = \frac{d}{m}\frac{\Delta s'}{r'}\cos\beta$$

Exit Slit

Resolution Terms and Magnification

$$\lambda = \frac{d}{m}(\sin\alpha + sin\beta)$$

$$\Delta\lambda_{so} = \frac{d}{m}\Delta\alpha\cos\alpha = \frac{d}{m}\frac{\Delta s}{r}\cos\alpha$$

Source or Entrance Slit

$$\Delta\lambda_{sl} = \frac{d}{m}\Delta\beta\cos\beta = \frac{d}{m}\frac{\Delta s'}{r'}\cos\beta$$

Exit Slit

$$\Delta\lambda_{se} = 2.7\frac{d}{m}\sigma_{se}(\cos\alpha + \cos\beta)$$

Slope error on grating

$$\Delta\lambda_{def} = 2.7\frac{d}{m}\sigma_{le}F_{20}$$

Defocus

$$\Delta\lambda_{coma} = 2.7\frac{d}{m}\sigma_{le}^2 F_{030}$$

Coma

$$\Delta\lambda_{dif} = \frac{\lambda}{N}$$

Diffraction

Resolution Terms and Magnification

$$\lambda = \frac{d}{m}(\sin\alpha + sin\beta)$$

$$\Delta\lambda_{so} = \frac{d}{m}\Delta\alpha\cos\alpha = \frac{d}{m}\frac{\Delta s}{r}\cos\alpha$$

Source or Entrance Slit

$$\Delta\lambda_{sl} = \frac{d}{m}\Delta\beta\cos\beta = \frac{d}{m}\frac{\Delta s'}{r'}\cos\beta$$

Exit Slit

$$\Delta\lambda_{se} = 2.7\frac{d}{m}\sigma_{se}(\cos\alpha + \cos\beta)$$

Slope error on grating

$$\Delta\lambda_{def} = 2.7\frac{d}{m}\sigma_{le}F_{20}$$

Defocus

$$\Delta\lambda_{coma} = 2.7\frac{d}{m}\sigma_{le}^2 F_{030}$$

Coma

$$\Delta\lambda_{dif} = \frac{\lambda}{N}$$

Diffraction

$$\frac{\Delta s'}{\Delta s} = \frac{\cos\alpha}{\cos\beta}\frac{r'}{r} = \frac{1}{c}\frac{r'}{r}$$

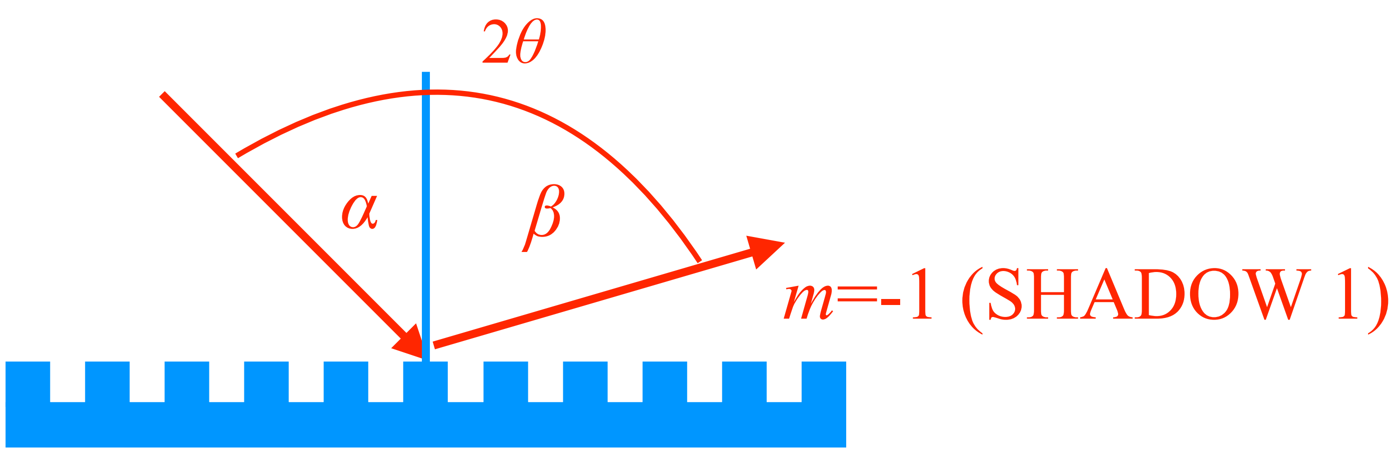
Magnification

Source: present APS, 2 m ID

Unless specified, all examples use as source

$$E = 1000\text{eV}$$
$$\Sigma_x = 280\mu\text{m}$$
$$\Sigma_z = 15\mu\text{m}$$
$$\Sigma_{x'} = 21\mu\text{rad}$$
$$\Sigma_{z'} = 18\mu\text{rad}$$

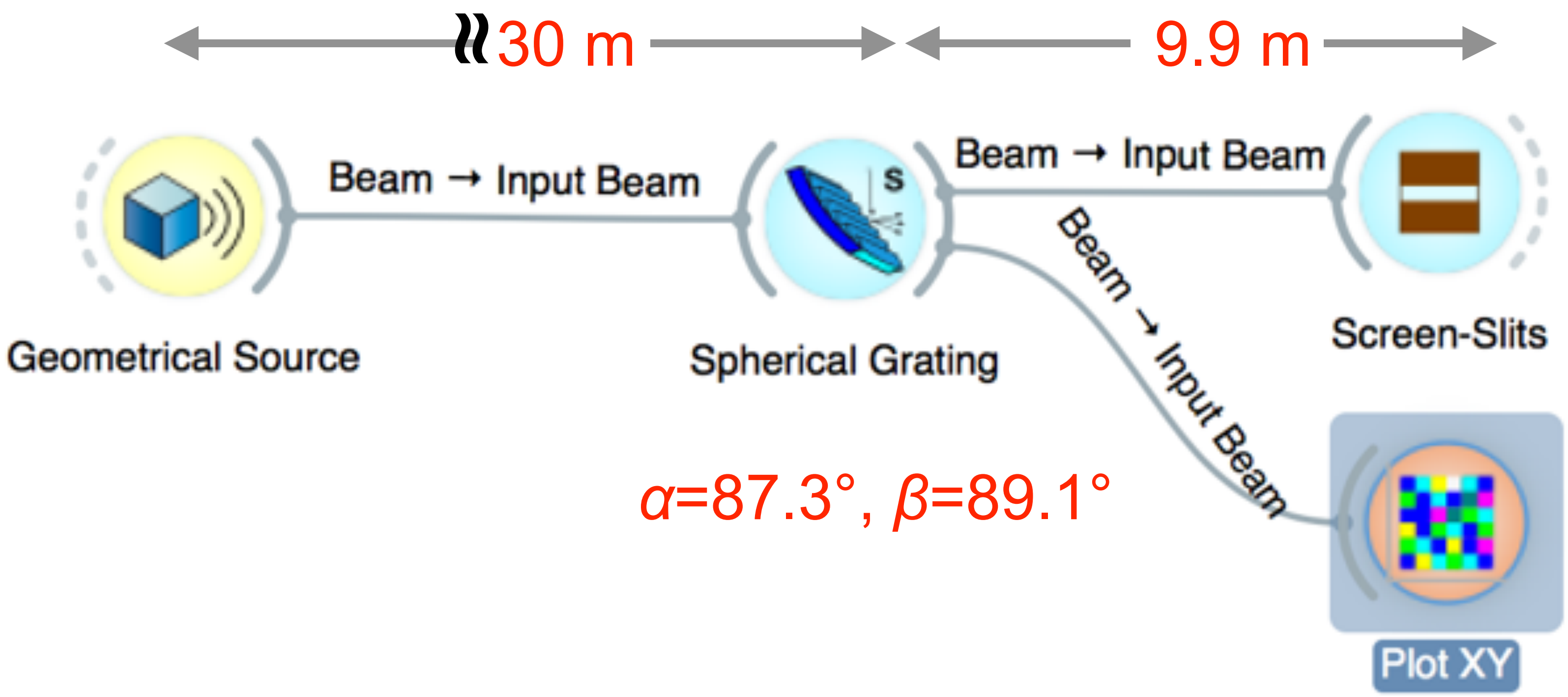
Spherical Grating Monochromator SGM



$$2\theta = \alpha - \beta$$
$$m\lambda = 2d_0 \cos\theta \sin(\theta + \beta)$$
$$\lambda_H = 2d_0 \cos^2\theta$$

$$\theta = 88.2^{\text{o}}, d_0 = 800^{-1}\text{mm}$$
$$\lambda < \lambda_H = 2.5\text{nm}, \ (500 \text{ eV})$$

Slitless SGM



$$r = 30 \text{ m}, \theta = 88.2^o,\ d_0 = 800^{-1} \text{ mm}$$

$$m = -1,\ E_0 = 1000 \text{ eV } (\lambda_0 = 1.24 \text{ nm})$$

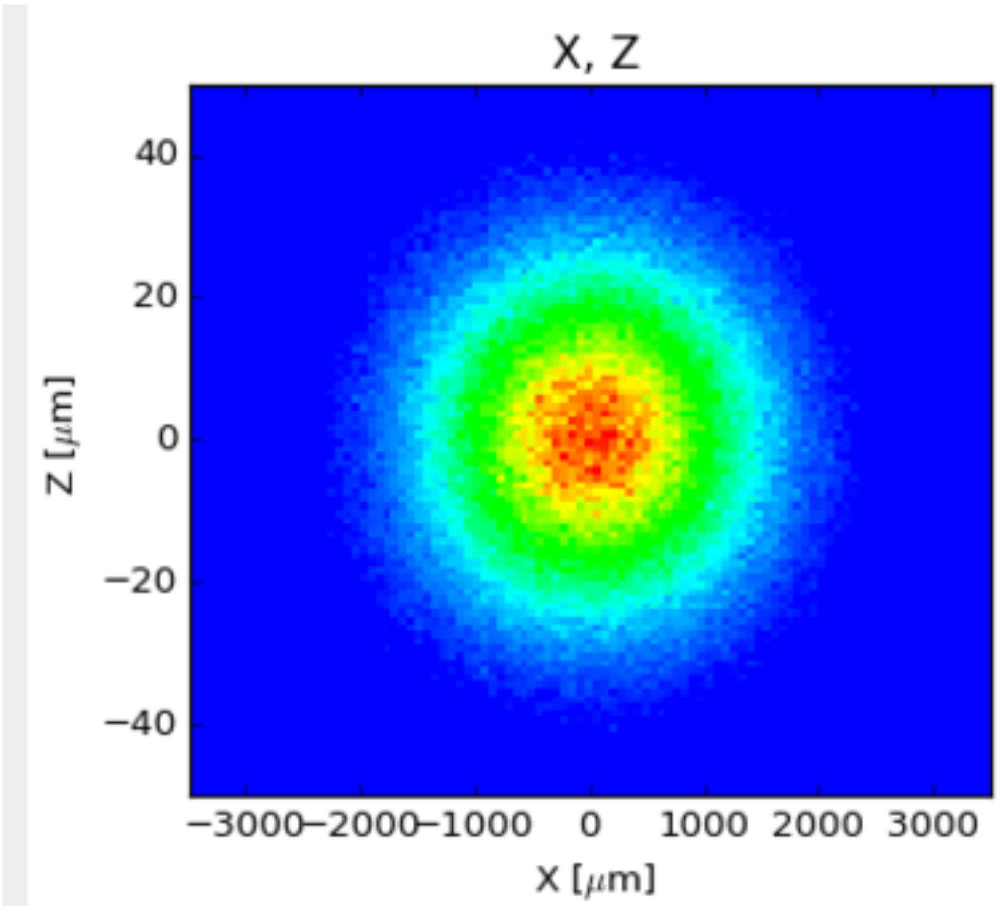
$$\text{Grating Equation } \Longrightarrow \beta_0 = -89.1^o;\ \alpha_0 = 87.3^o$$

$$\text{Rowland condition } R = \frac{r}{\cos\alpha} = \frac{r'}{\cos\beta}$$

$$\Longrightarrow R = 636 \text{ m}; r' = 9.9 \text{ m}$$

$$\frac{\cos\alpha(1000)}{\cos\beta(1000)}\frac{r'}{r} = 1$$

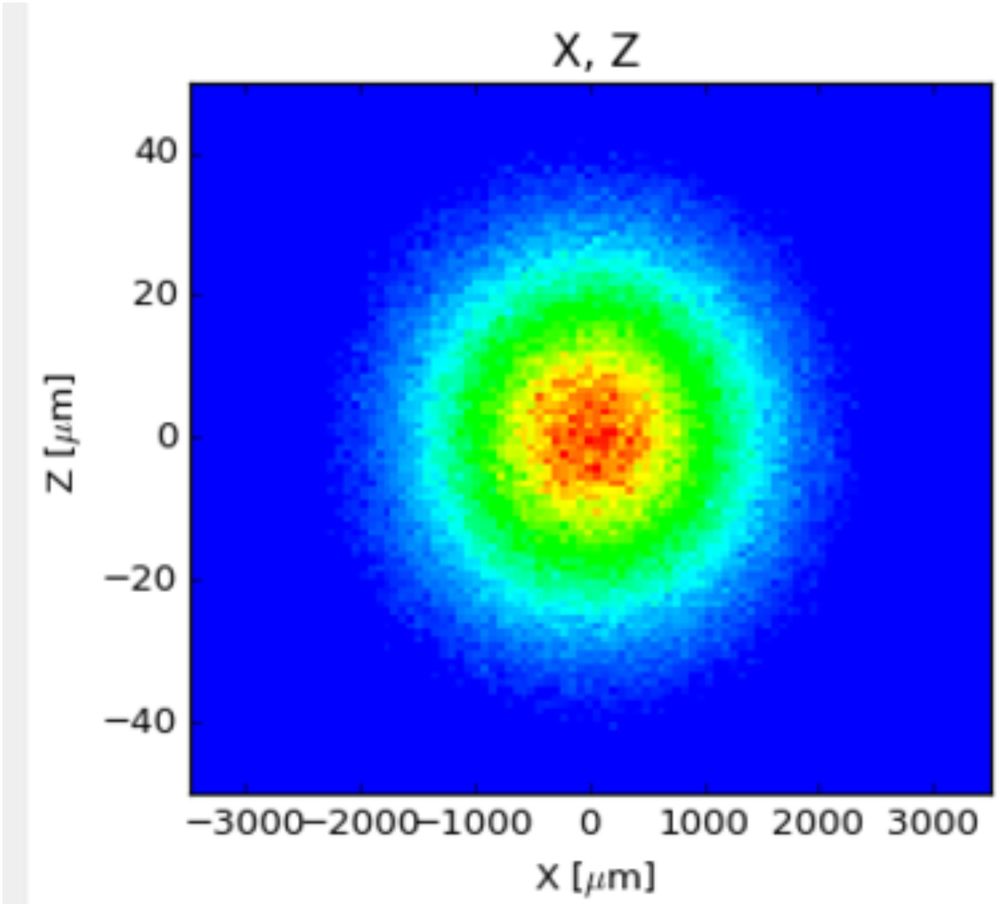
SGM Ray Tracing at 1000 eV



FWHM X [μm] 2030.0000

FWHM Z [μm] 35.0000

SGM Ray Tracing at 1000 eV

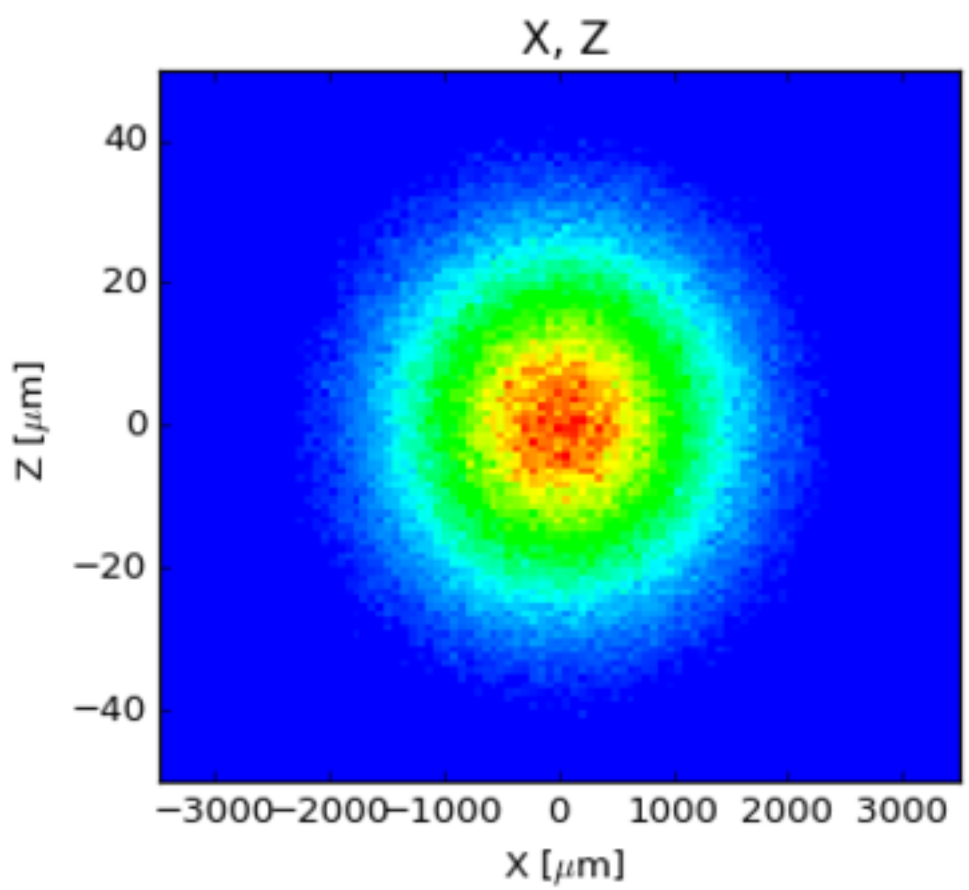


FWHM X [μm]	2030.0000
FWHM Z [μm]	35.0000

$$\Delta\lambda = \frac{d}{m}\frac{\mathrm{FWHM}}{r'}\cos\beta$$

$$RP = \frac{\lambda}{\Delta\lambda} = 18000$$

SGM Ray Tracing at 1000 eV



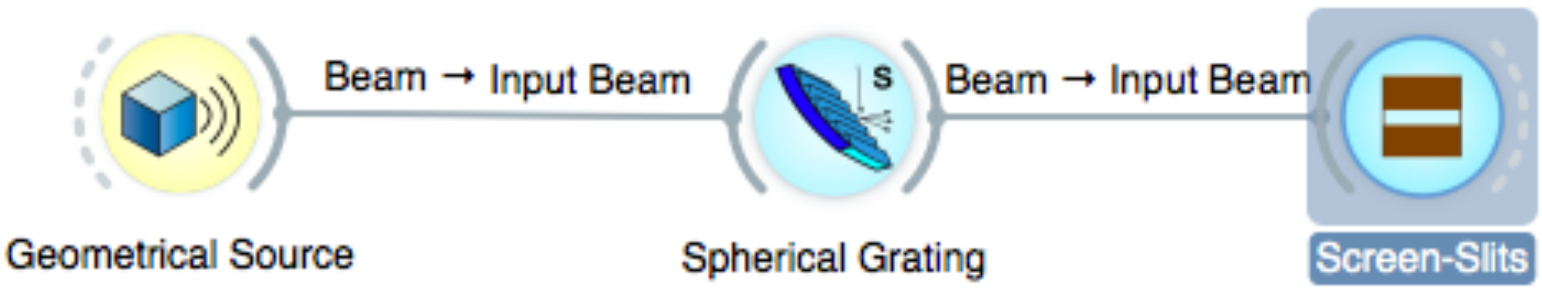
FWHM X [μm]	2030.0000 ✖
FWHM Z [μm]	35.0000 ✓

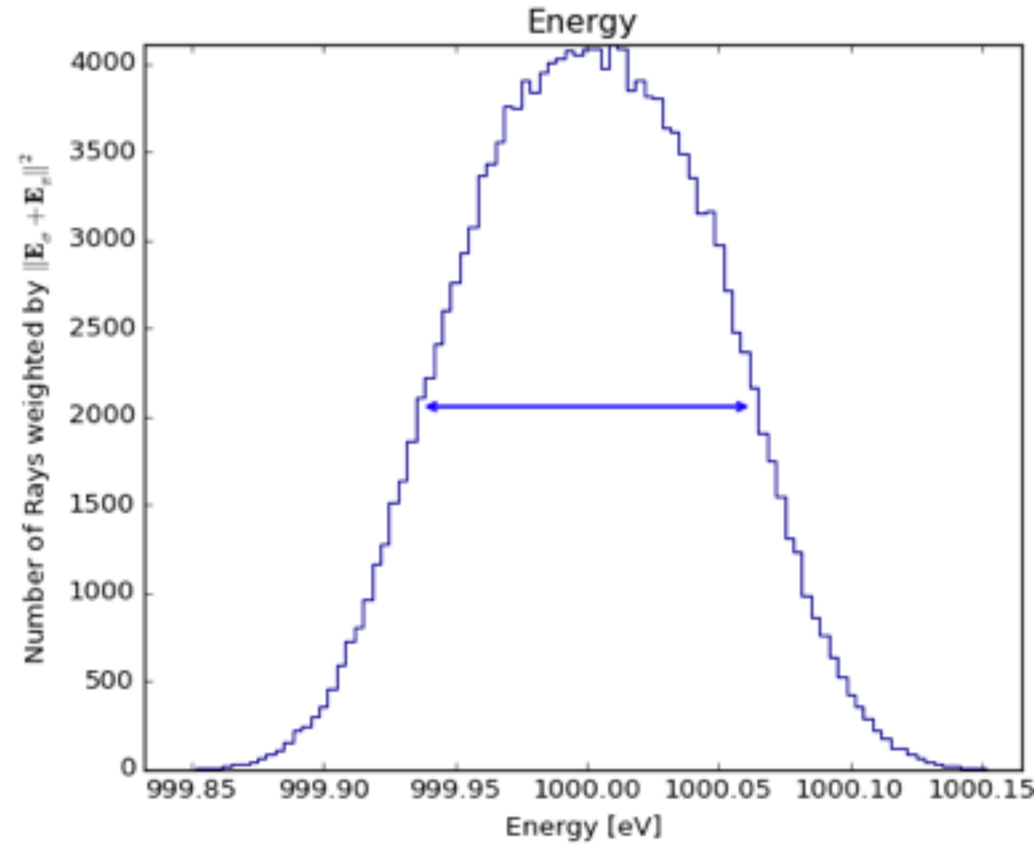
Sanity Check!

$$2.35\Sigma_z(1000)\frac{\cos\alpha(1000)}{\cos\beta(1000)}\frac{r'}{r} = 36\ \mu m$$

$$2.35\Sigma_x(1000)\frac{r'}{r} = 217\ \mu m$$

SGM Ray Tracings Resolution





Source

$999.8 < E < 1000.2$ eV

At 1000 eV

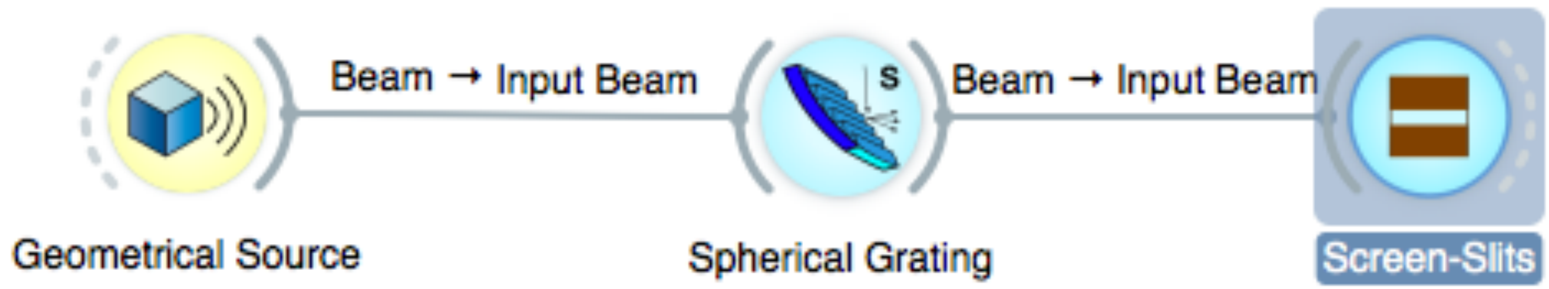
FWHM X [µm]	2030.0000
FWHM Z [µm]	35.0000

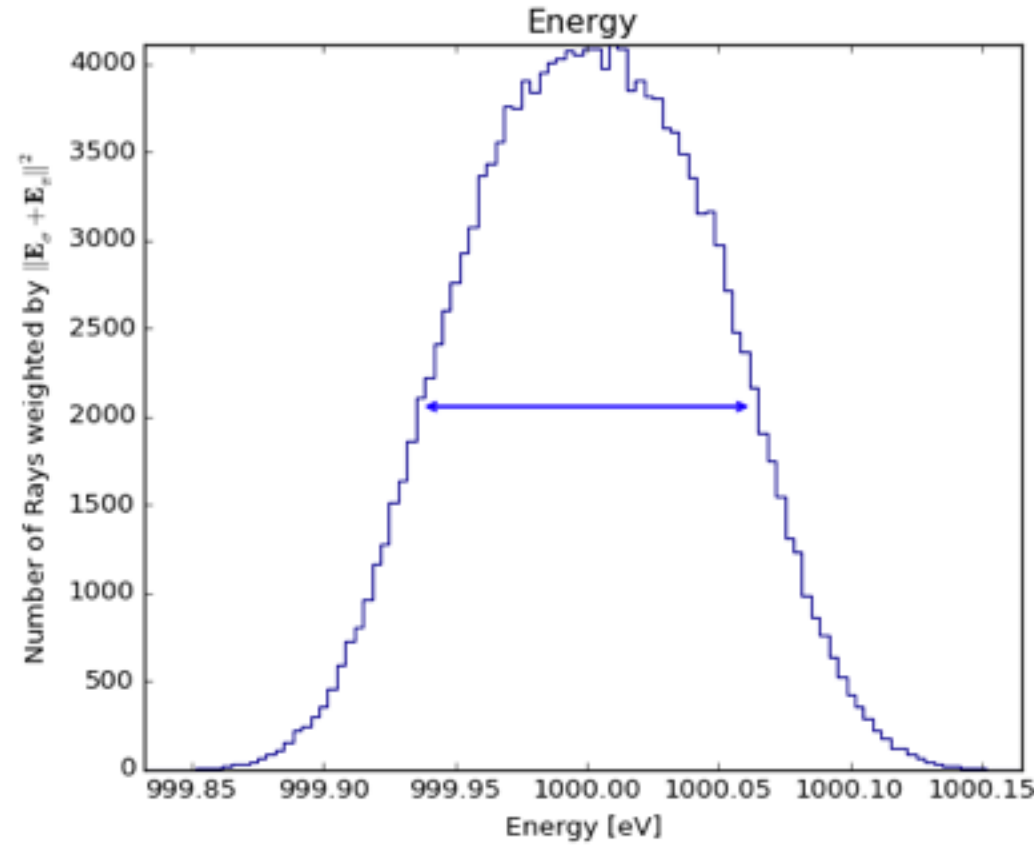
55 meV

3 µm

Intensity	5945.000
Total Rays	500000
Total Good Rays	5945
Total Lost Rays	494055
FWHM [eV]	0.0516

SGM Ray Tracings Resolution





Source

$999.8 < E < 1000.2$ eV

At 1000 eV

FWHM X [µm]	2030.0000
FWHM Z [µm]	35.0000

	3 µm	20 µm	50 µm	100 µm	200 µm
Intensity	5945.000	39850.000	98851.000	198014.000	394819.000
Total Rays	500000	500000	500000	500000	500000
Total Good Rays	5945	39850	98851	198014	394819
Total Lost Rays	494055	460150	401149	301986	105181
FWHM [eV]	0.0516	0.0575	0.0833	0.1557	0.3120

Source limited

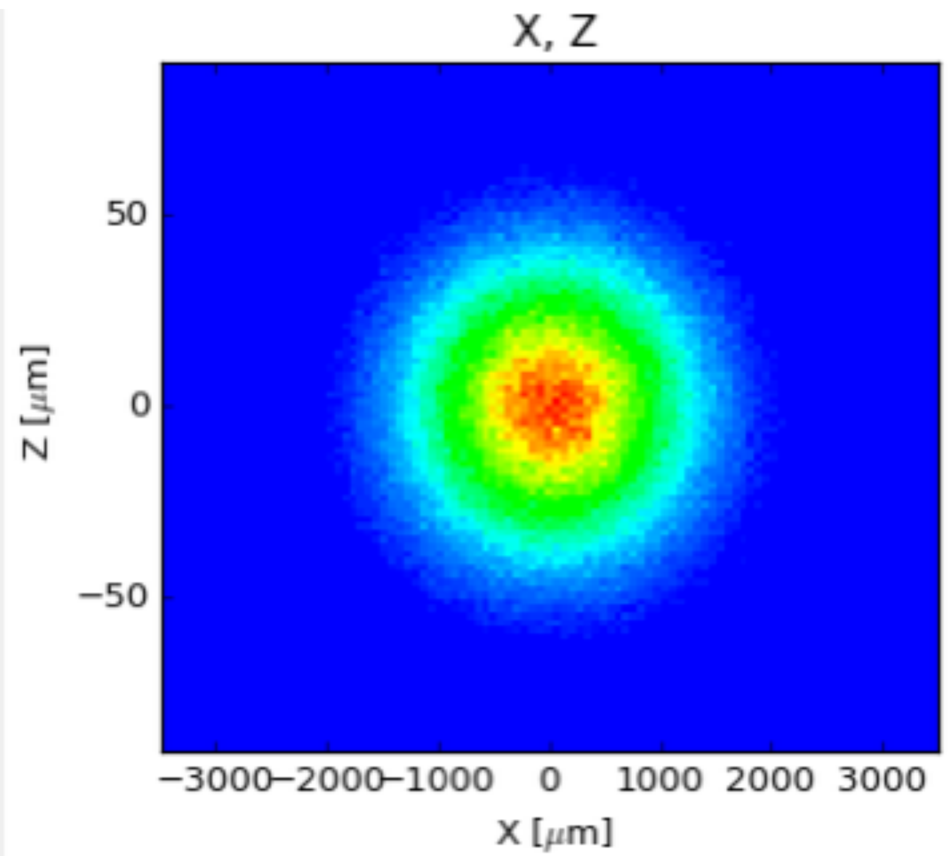
Slit limited

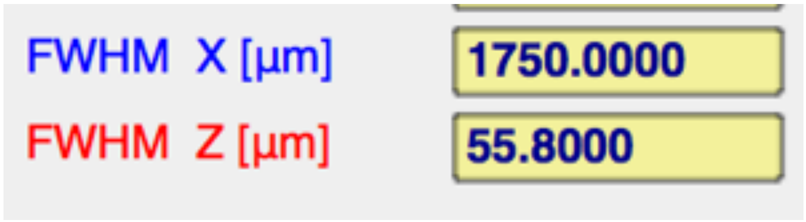
SGM Ray Tracing at 1600 eV

Source

$E = 1600\text{eV}$
$\Sigma_x = 280\mu\text{m}$
$\Sigma_z = 154\mu\text{m}$
$\Sigma_{x'} = 18\mu\text{rad}$
$\Sigma_{z'} = 14\mu\text{rad}$

$\beta = -88.77^{\text{o}}$
$\alpha = 87.63^{\text{o}}$



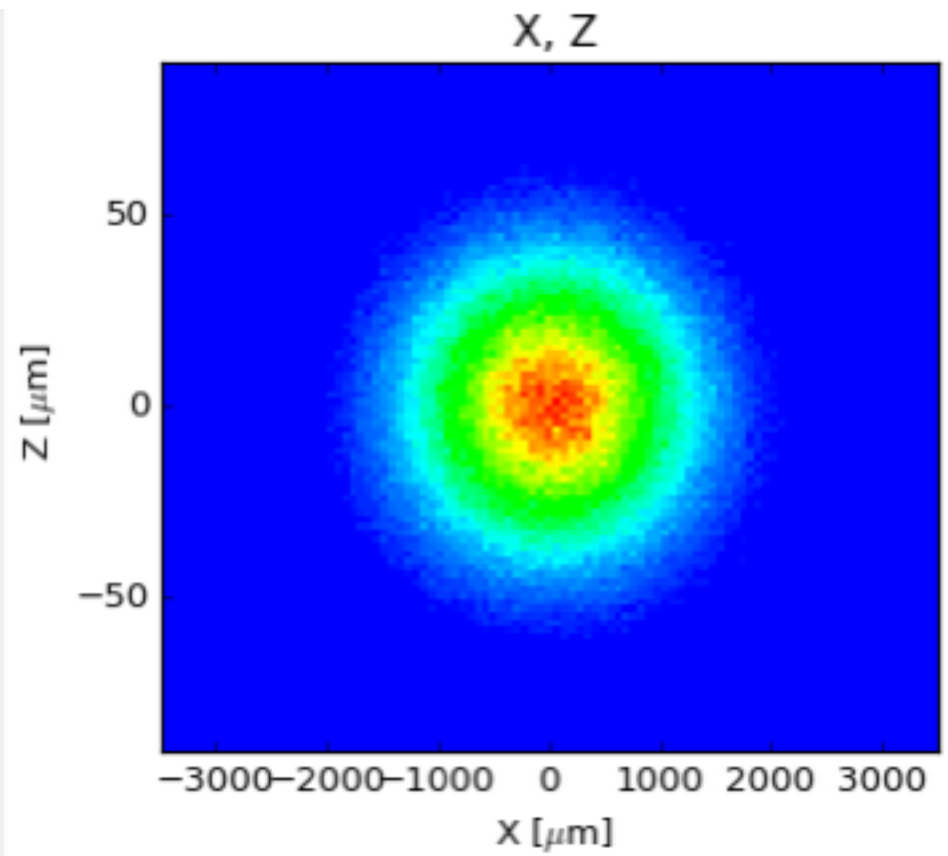


SGM Ray Tracing at 1600 eV

Source

$$E = 1600\text{eV}$$
$$\Sigma_x = 280\mu\text{m}$$
$$\Sigma_z = 154\mu\text{m}$$
$$\Sigma_{x'} = 18\mu\text{rad}$$
$$\Sigma_{z'} = 14\mu\text{rad}$$

$$\beta = -88.77^o$$
$$\alpha = 87.63^o$$



FWHM X [μm]	1750.0000
FWHM Z [μm]	55.8000 ✖

Sanity Check!

$$2.35\Sigma_z(1600)\frac{\cos\alpha(1600)}{\cos\beta(1600)}\frac{r'}{r} = 20\ \mu m$$

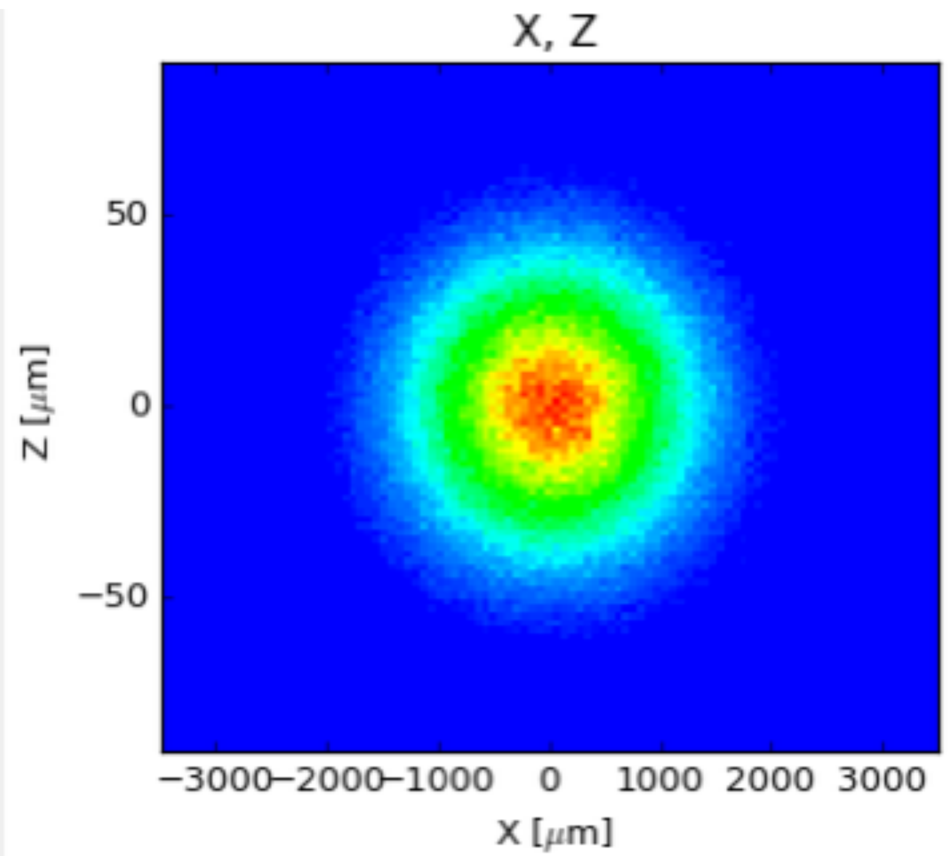
✖ Not at focus

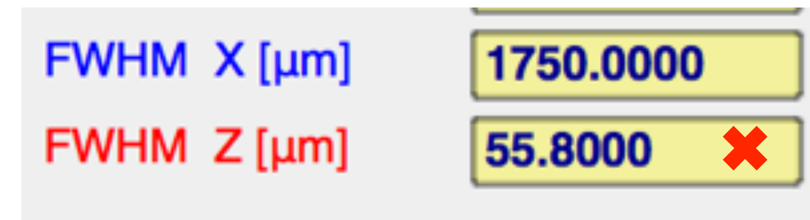
SGM Ray Tracing at 1600 eV

Source

$E = 1600\text{eV}$
$\Sigma_x = 280\mu m$
$\Sigma_z = 154\mu m$
$\Sigma_{x'} = 18\mu rad$
$\Sigma_{z'} = 14\mu rad$

$\beta = -88.77^o$
$\alpha = 87.63^o$



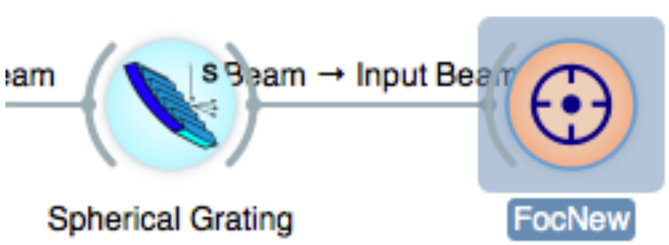


Sanity Check!

$$2.35\Sigma_z(1600)\frac{\cos\alpha(1600)}{\cos\beta(1600)}\frac{r'}{r} = 20\ \mu m$$

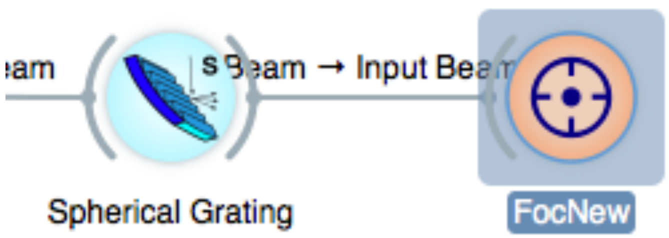
✖ Not at focus

Second Sanity Check!



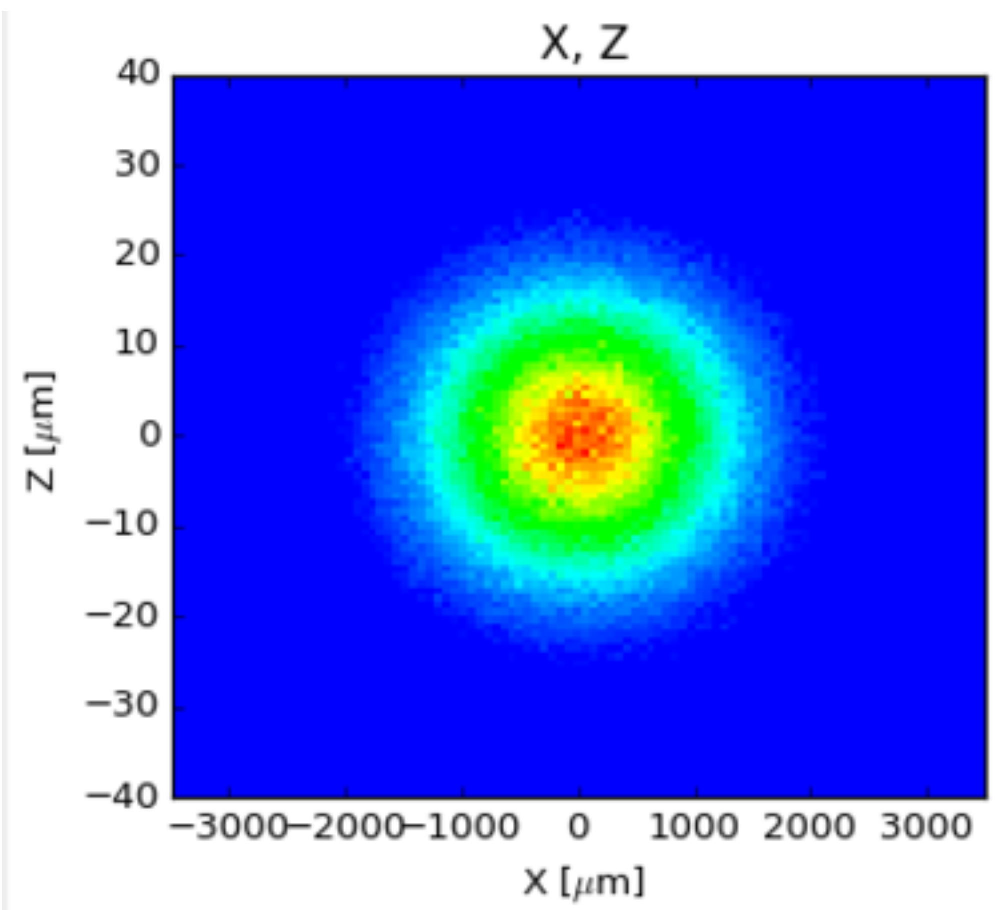
Focus along Z at : 1073.71
Waist size at best focus (rms) : 0.00967357
Waist size at origin : 0.0237598

SGM Ray Tracing at 1600 eV, slit moved



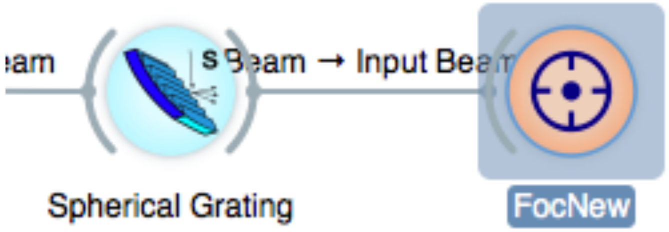
Focus along Z at : 1073.71
Waist size at best focus (rms) : 0.00967357
Waist size at origin : 0.0237598

$$F_{20}(1600\text{eV})=0 \implies r' = 11046 \text{ mm}$$



FWHM X [μm]	1890.0000
FWHM Z [μm]	21.6000

SGM Ray Tracing at 1600 eV, corrected

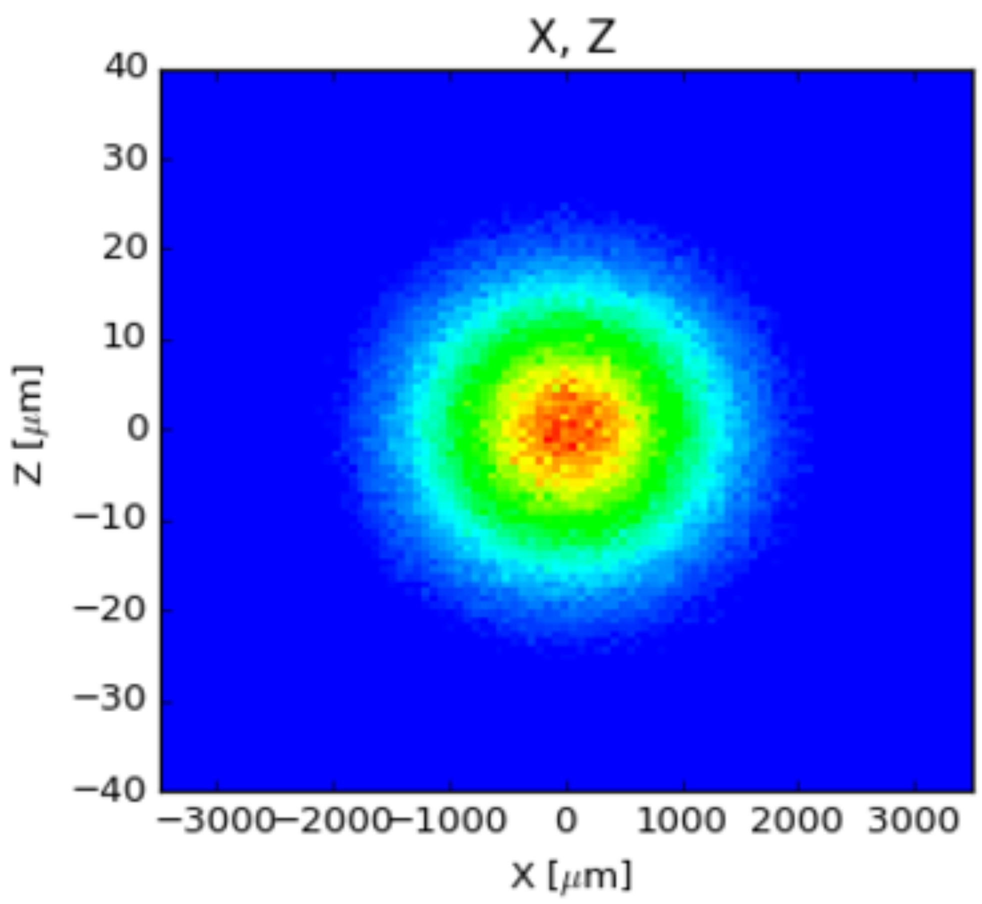


Focus along Z at : 1073.71
Waist size at best focus (rms) : 0.00967357
Waist size at origin : 0.0237598

$$F_{20}(1600\mathrm{eV})=0 \Longrightarrow r' = 11046\ \mathrm{mm}$$

Sanity Check!

$$2.35\Sigma_z(1600)\frac{\cos\alpha(1600)}{\cos\beta(1600)}\frac{r'}{r} = 22\ \mu m$$



FWHM X [μm]	1890.0000
FWHM Z [μm]	21.6000

In the SGM:
Exit slit needs to move to keep focus
(does not correct coma aberration)

Plane Grating

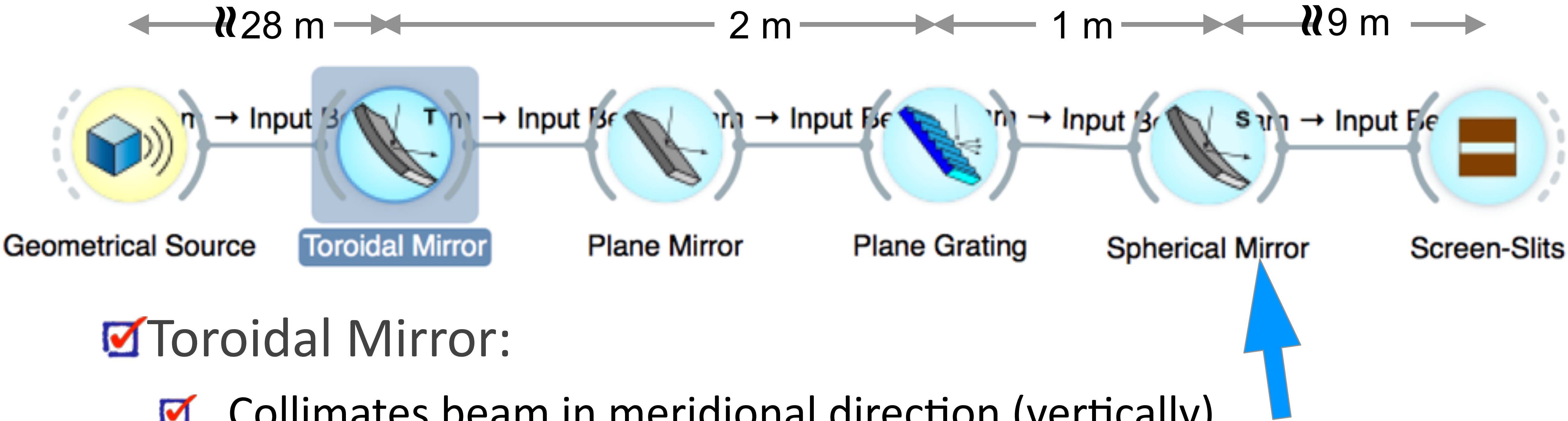
- ☑ Plane grating (without VLS) does not focus
- ☑ Focus independent of grating ➠ Fixed focal plane
- ☑ Grating magnification c^{-1} can be changed with plane mirror

$$c = \frac{\cos\beta}{\cos\alpha}$$

Grating Equation:

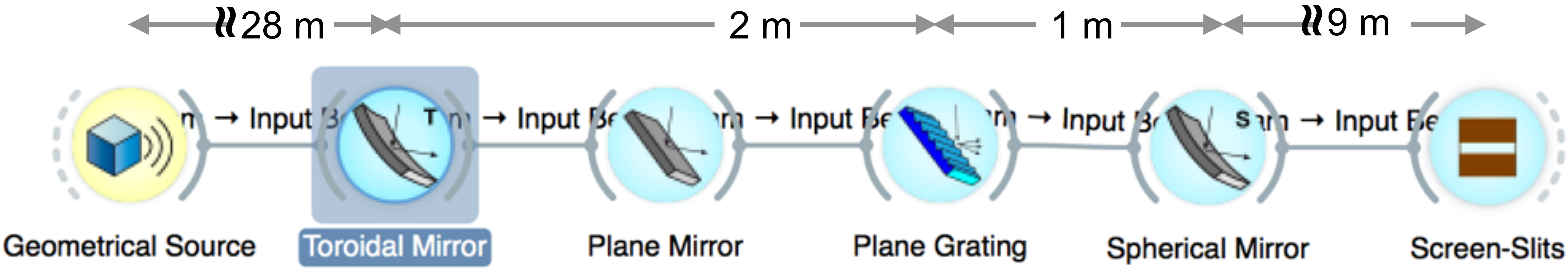
$$(\frac{m\lambda}{d} - \sin\beta)^2 = 1 - \frac{(1 - \sin^2\beta}{c^2})$$

Collimated PGM, vertical plane; c=2

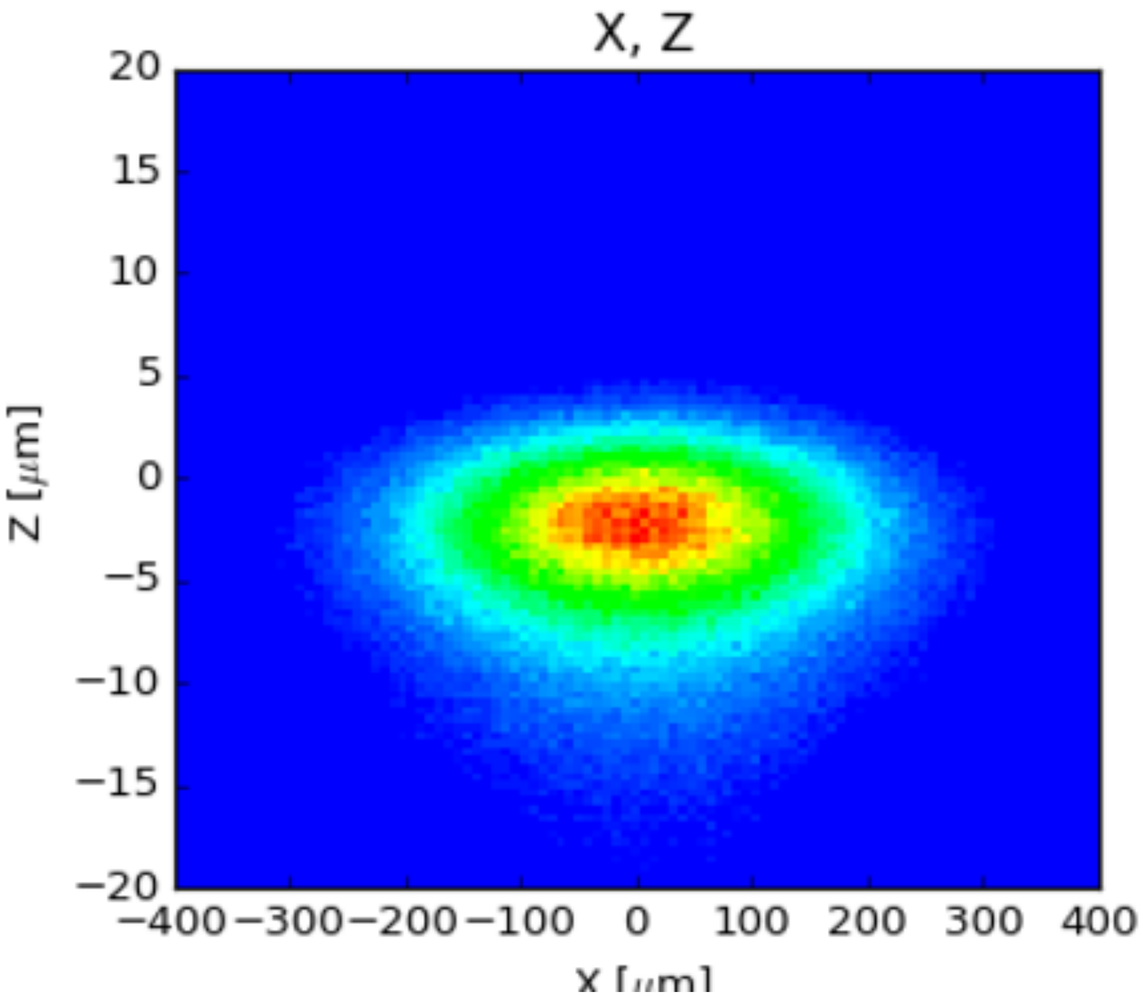


- Toroidal Mirror:
  - Collimates beam in meridional direction (vertically)
  - Focuses in sagittal direction at slit (horizontally)
- Plane Mirror + Plane grating
  - Controls grating magnification, c^{-1} and wavelength
- Cylindrical Mirror
  - Focuses the collimated beam onto the fixed exit slit
- Reflectivities in SXR not optimal due to many electronic transition in this range

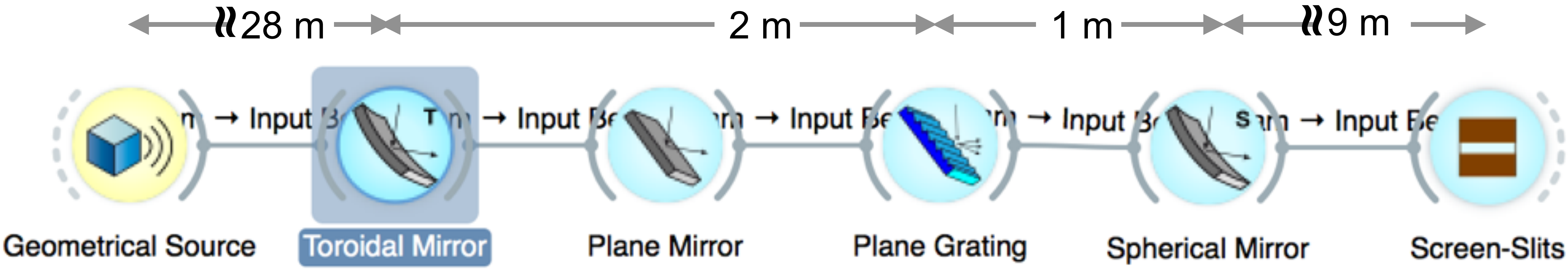
Collimated PGM, vertical plane; c=2



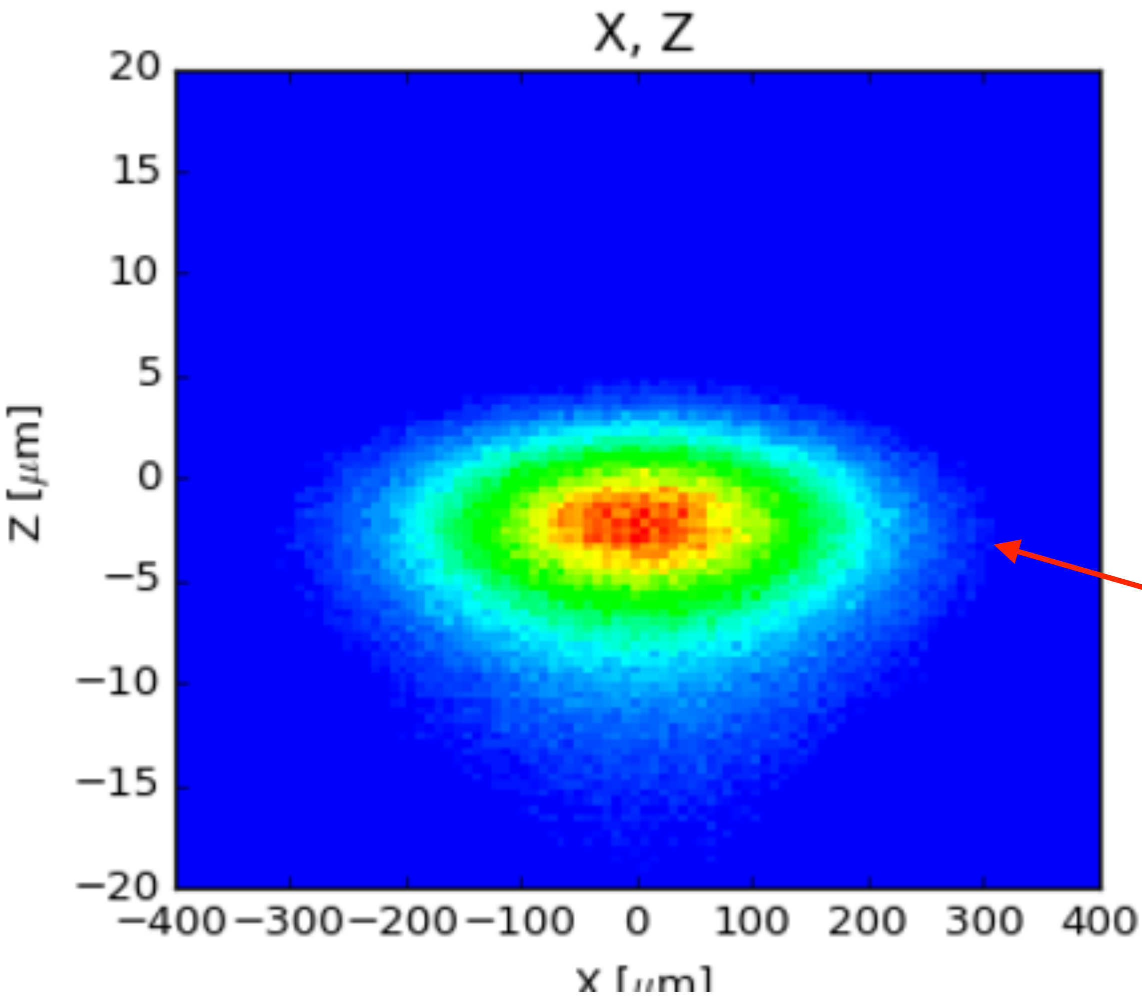
	Toroidal Mirror	Plane Mirror	Plane Grating	Spherical Mirror
	88.5° up	87.8° down	α=88.5°, β=87.1° up	88.5° down

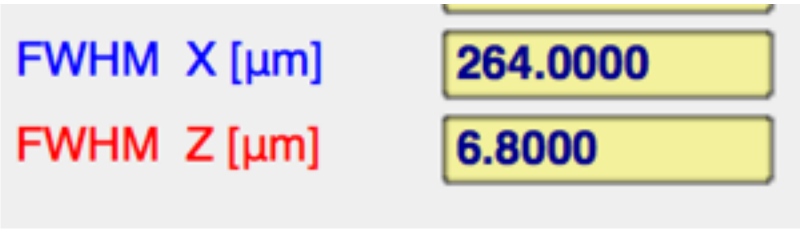


Collimated PGM, vertical plane; c=2



Toroidal Mirror	Plane Mirror	Plane Grating	Spherical Mirror
88.5° up	87.8° down	α=88.5°, β=87.1° up	88.5° down

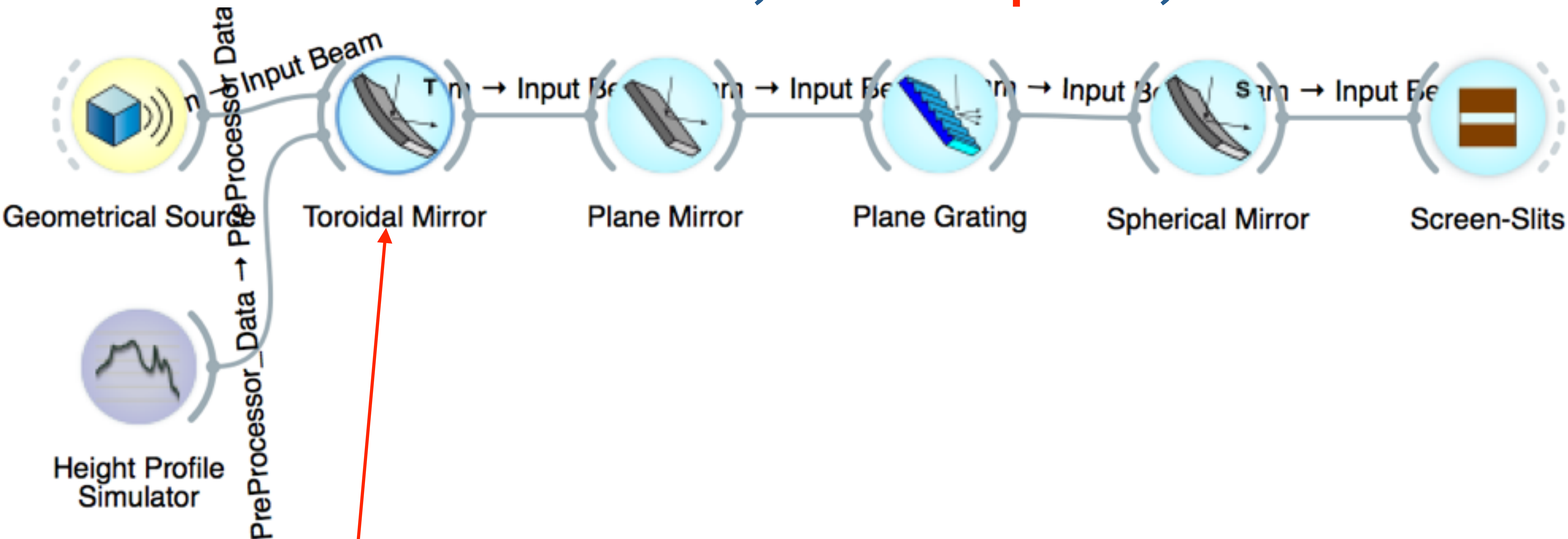


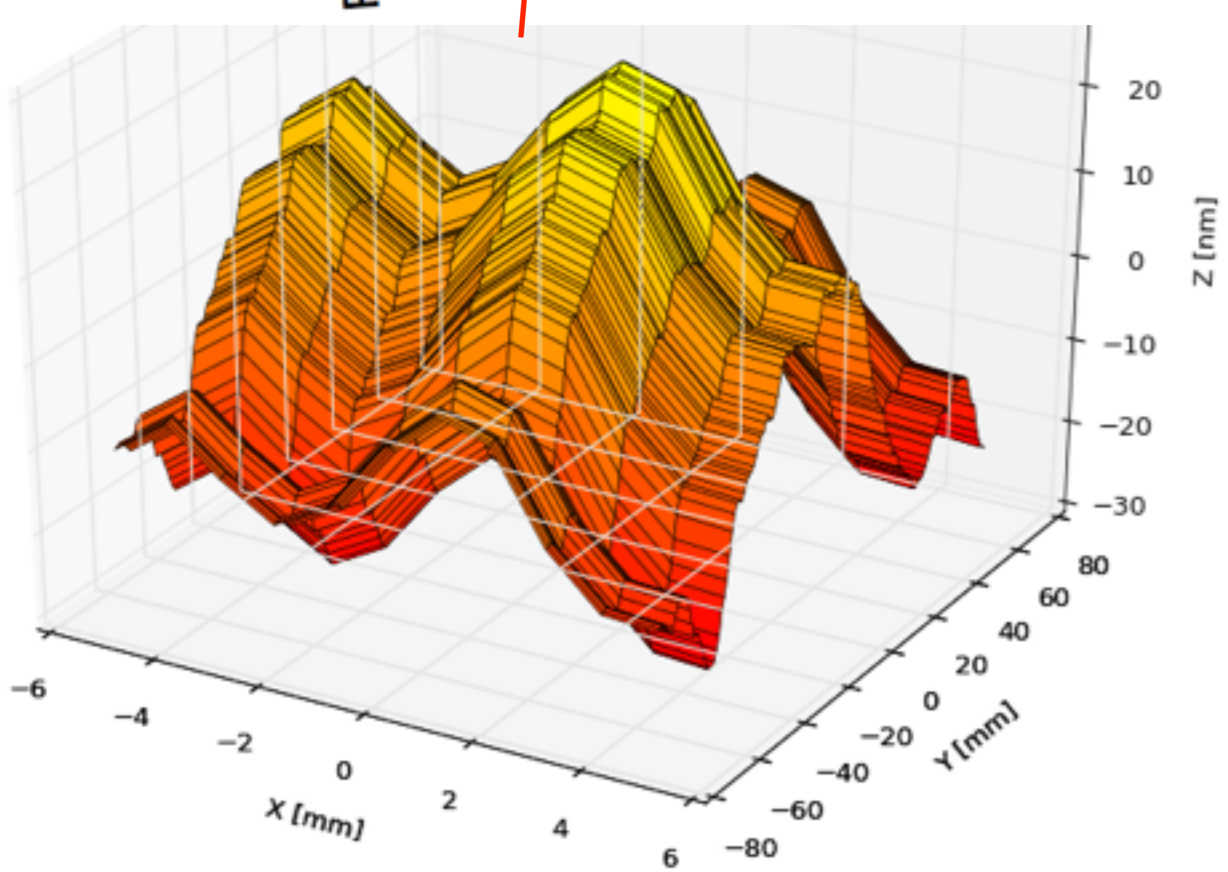


Coma

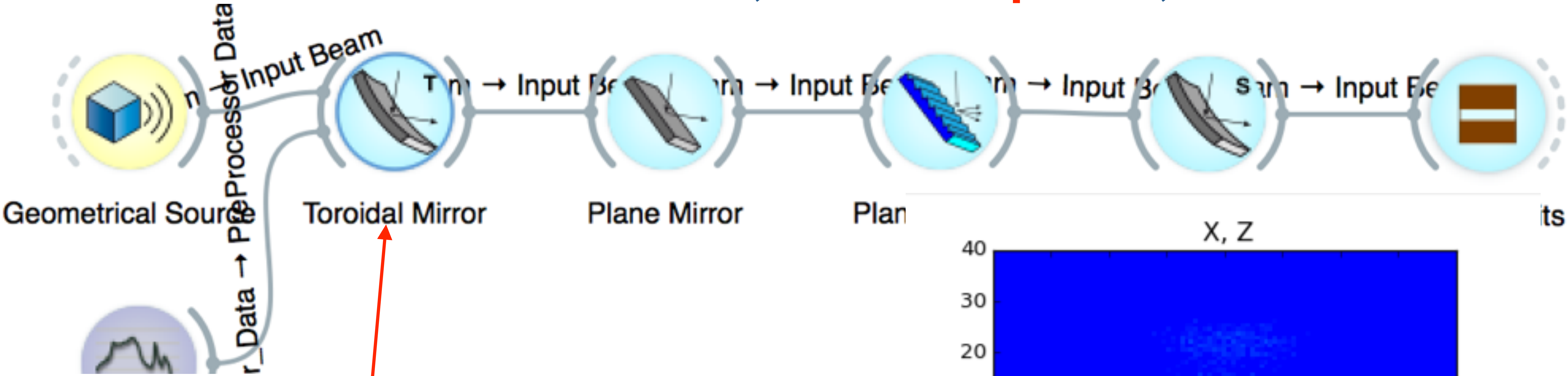
$$2.35\ \Sigma_z(1000)\frac{1}{c}\frac{dM3Ex}{dSoM1} = 5.8\ \mu m$$

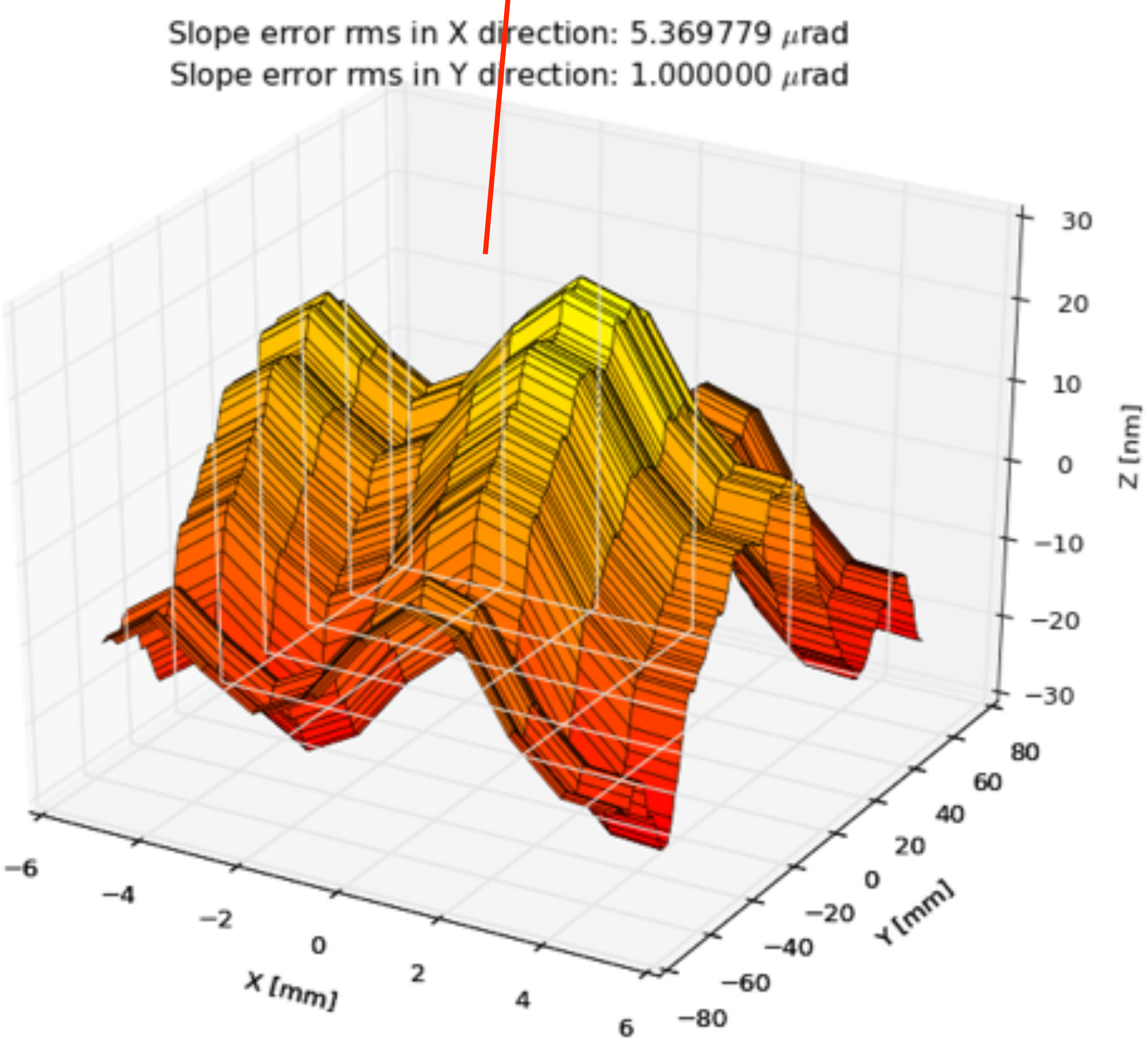
Collimated PGM, vertical plane; c=2

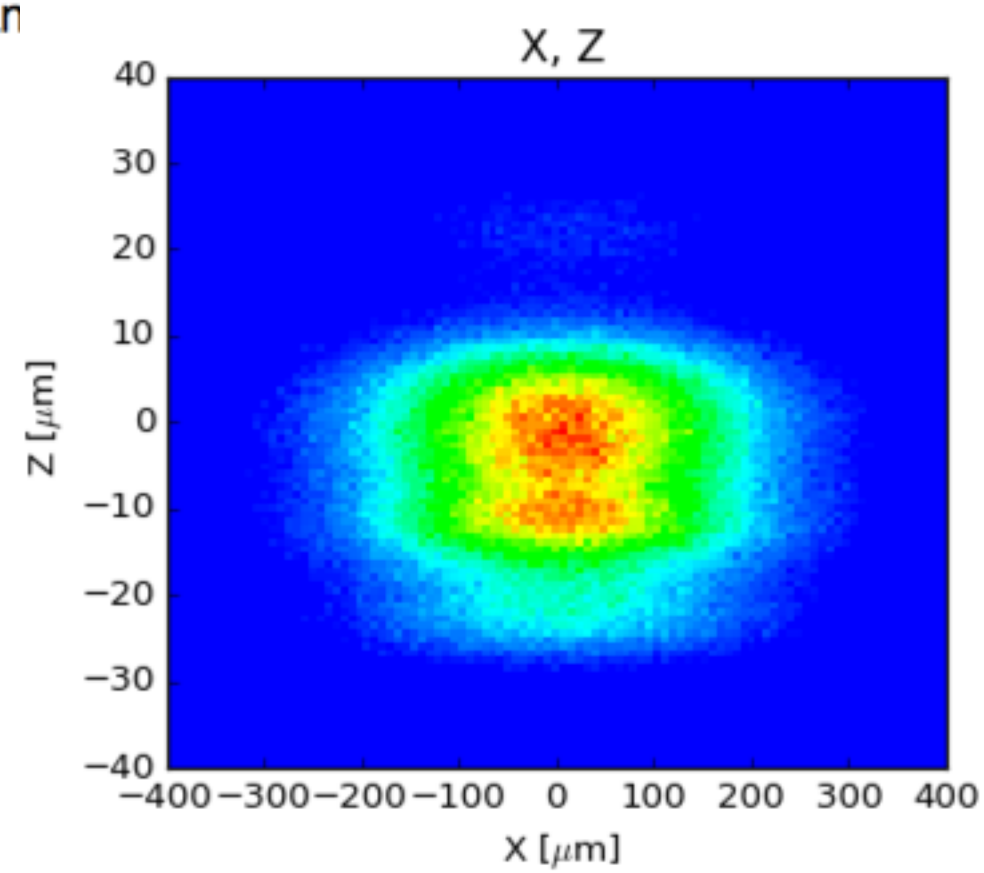




Collimated PGM, vertical plane; c=2



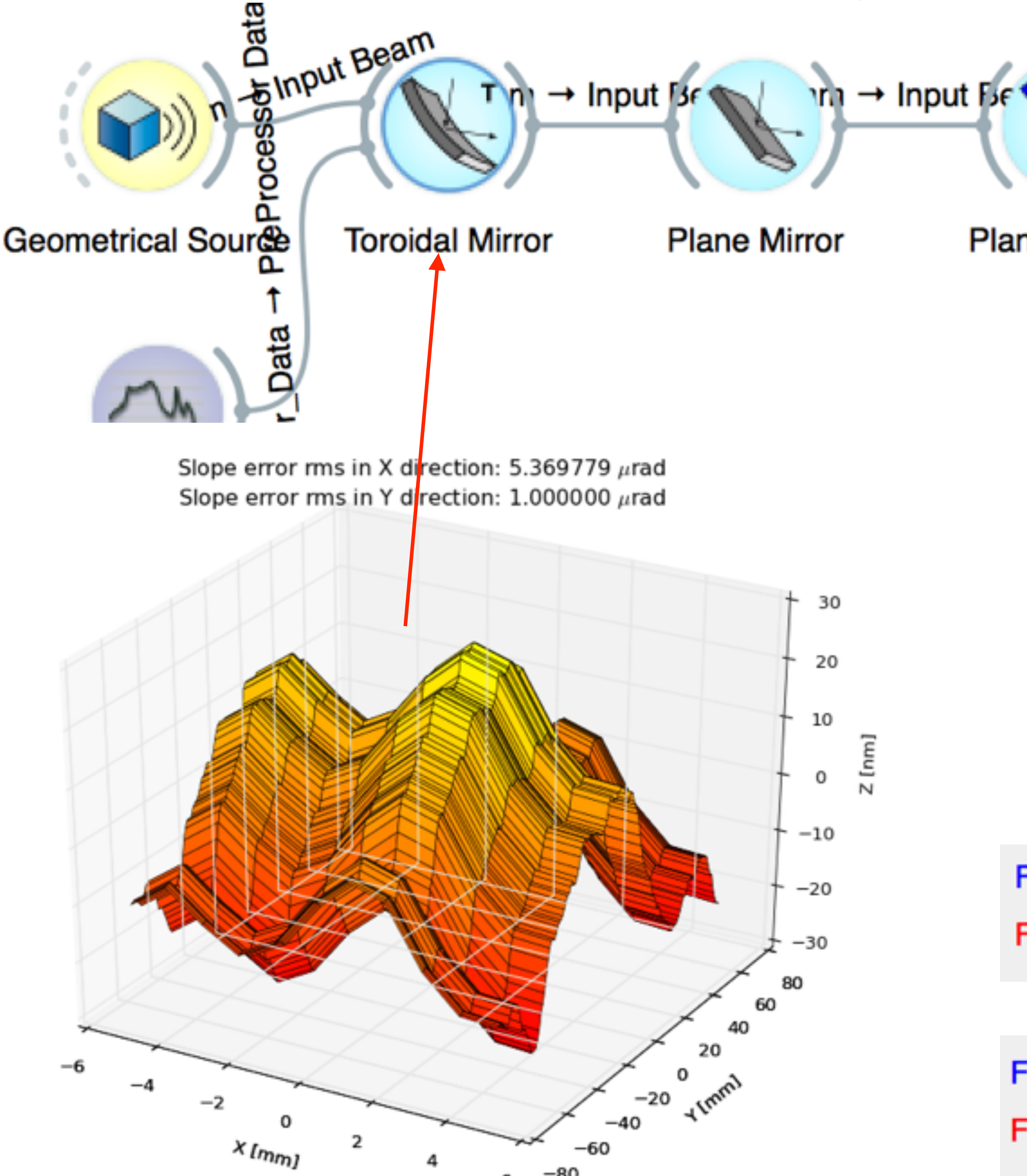


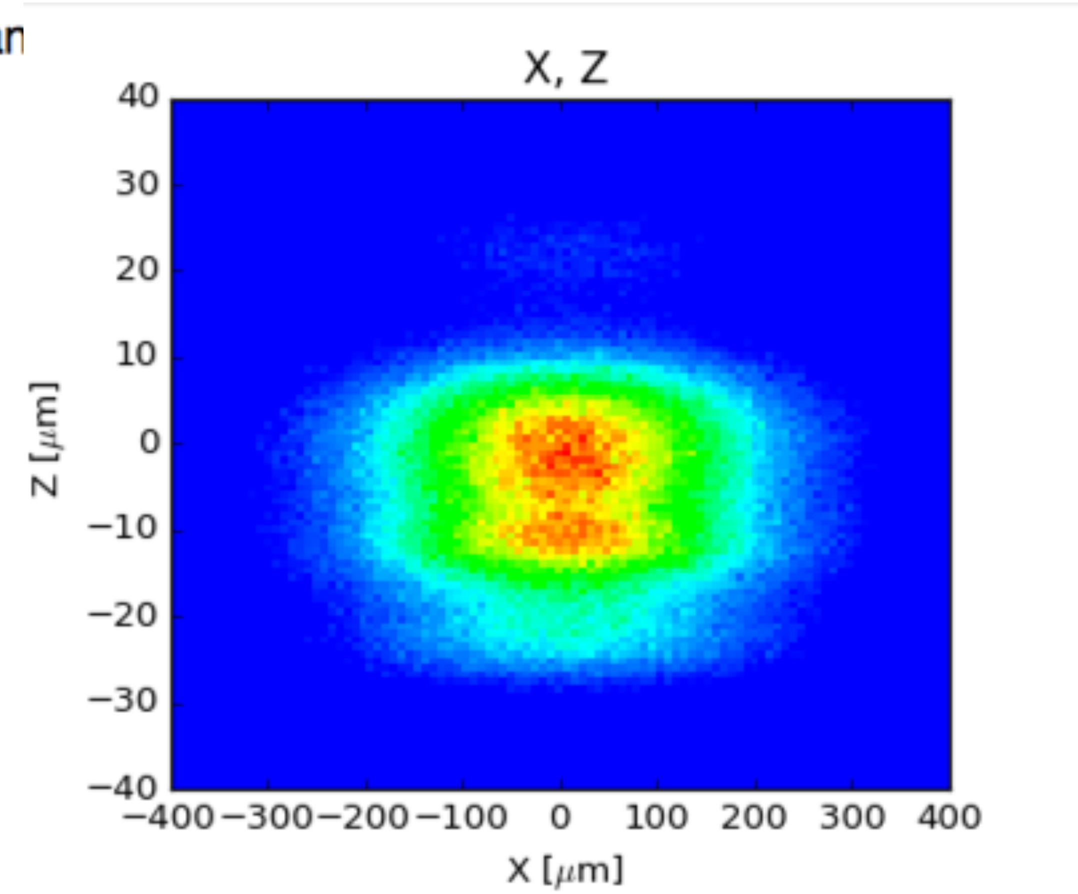


FWHM X [µm]	272.0000
FWHM Z [µm]	21.6000

With SE on Toroid

Collimated PGM, vertical plane; c=2

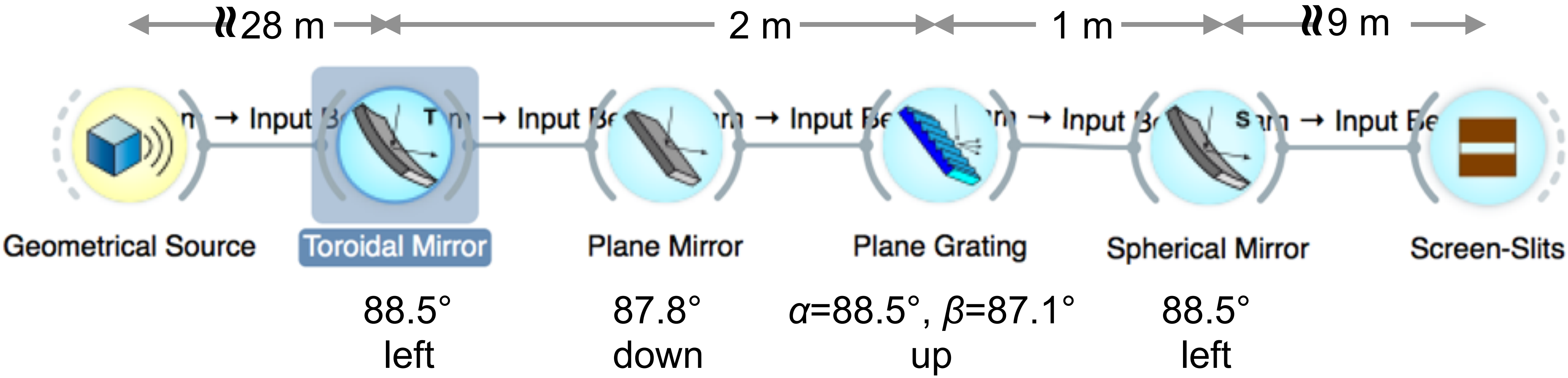




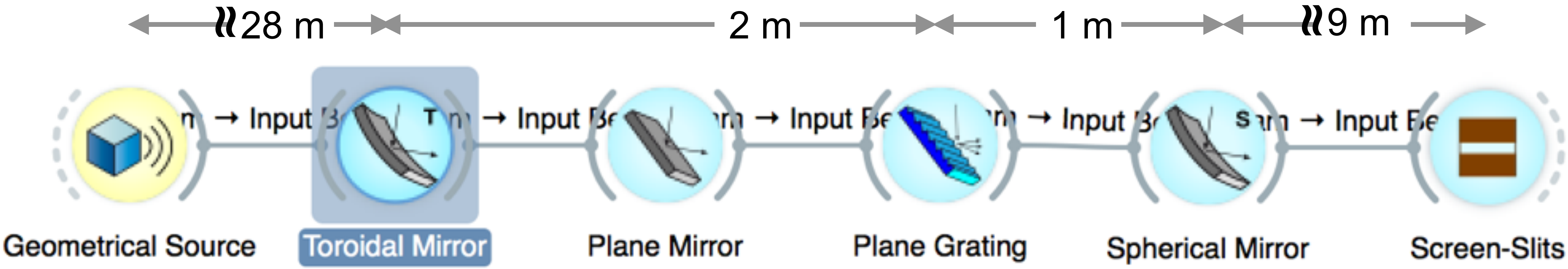
With SE on Toroid

Without SE on Toroid

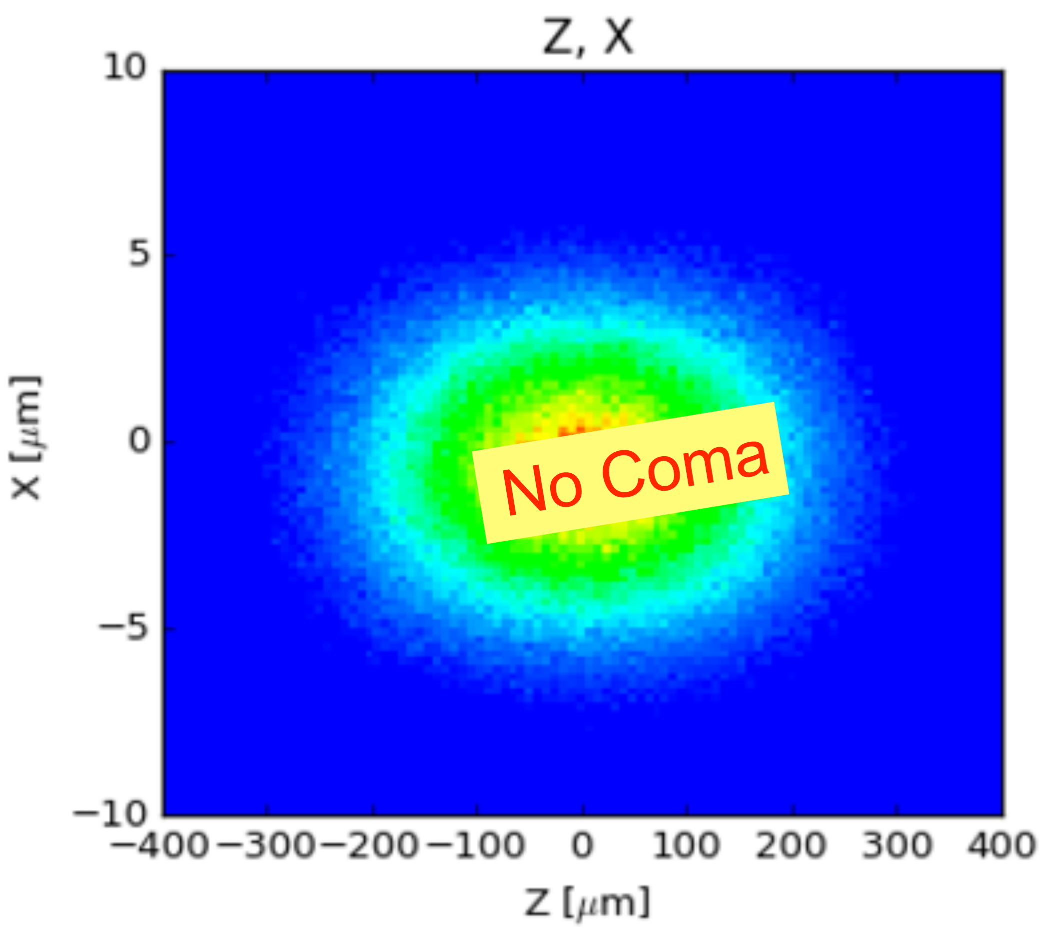
Follath Collimated PGM, TM, CM: hor plane; c=2



Follath Collimated PGM, TM, CM: hor plane; c=2



Toroidal Mirror	Plane Mirror	Plane Grating	Spherical Mirror
88.5° left	87.8° down	α=88.5°, β=87.1° up	88.5° left

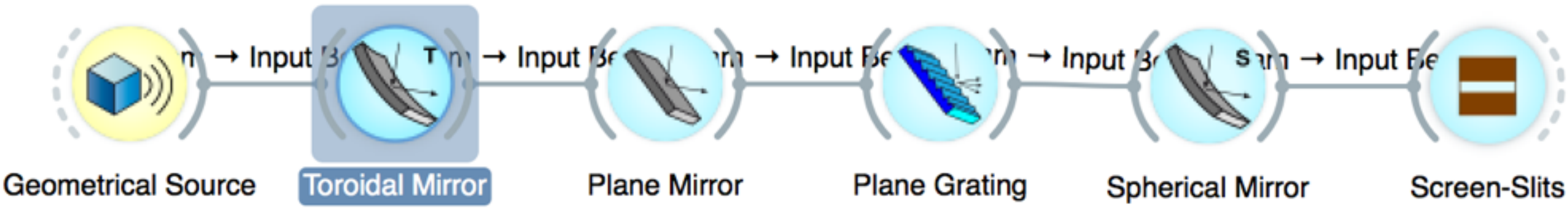


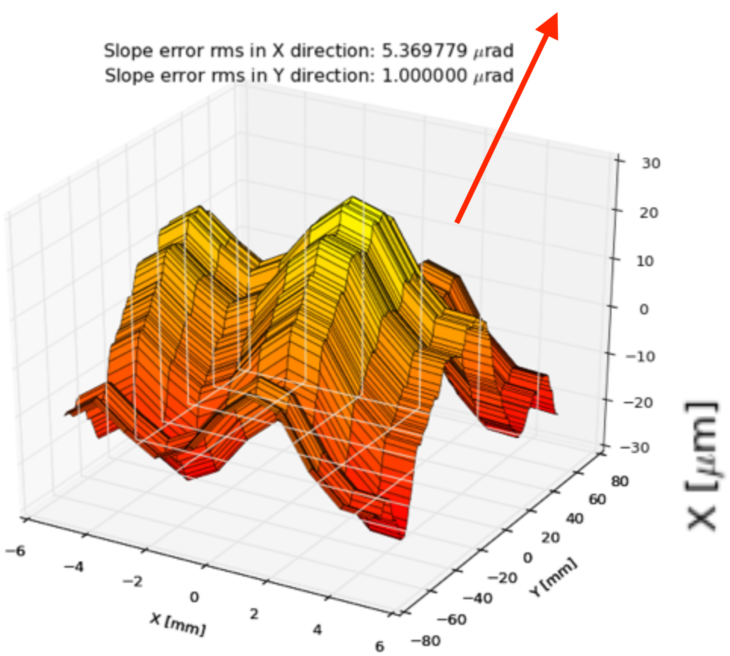
FWHM Z [μm]	272.0000
FWHM X [μm]	5.8000

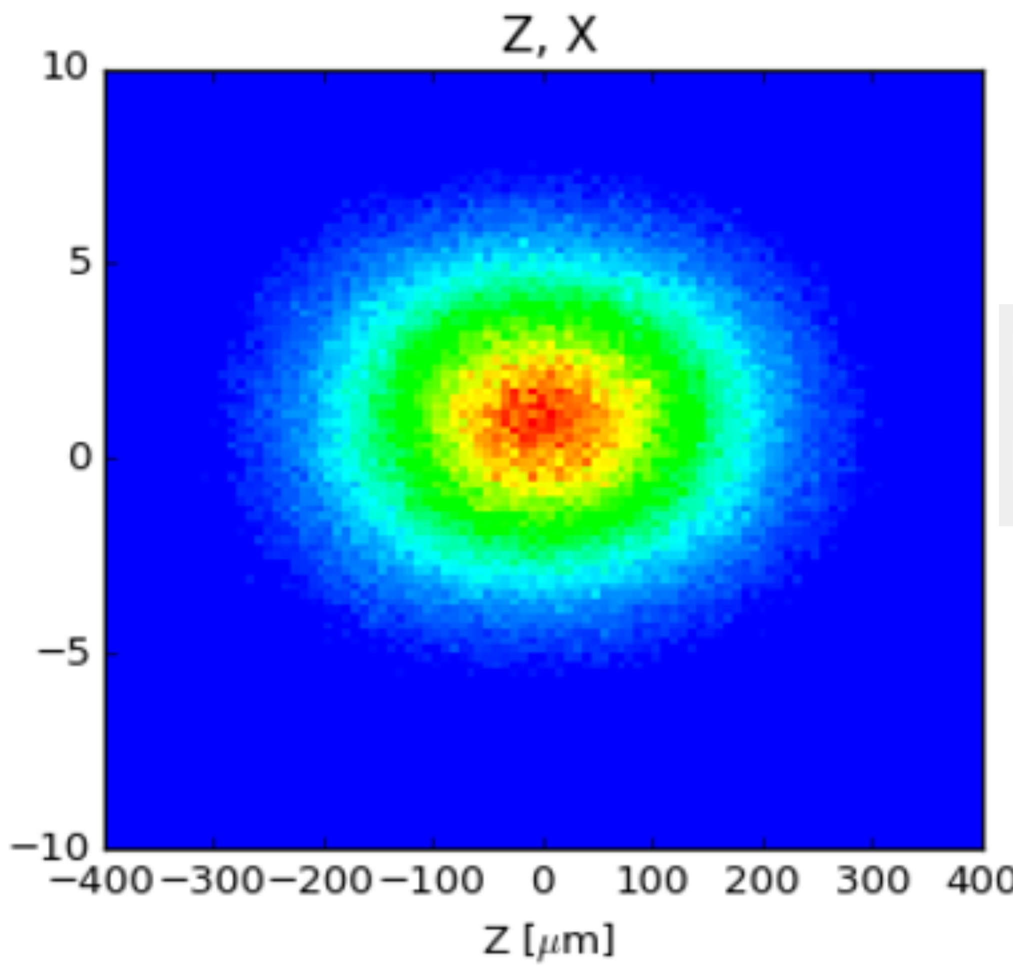
$$2.35\ \Sigma_z(1000)\frac{1}{c}\frac{dM3Ex}{dSoM1} = 5.8\ \mu m$$

Mirror rotation relative to grating
x↔z

Collimated PGM, TM, CM: horizontal plane; c=2







With SE

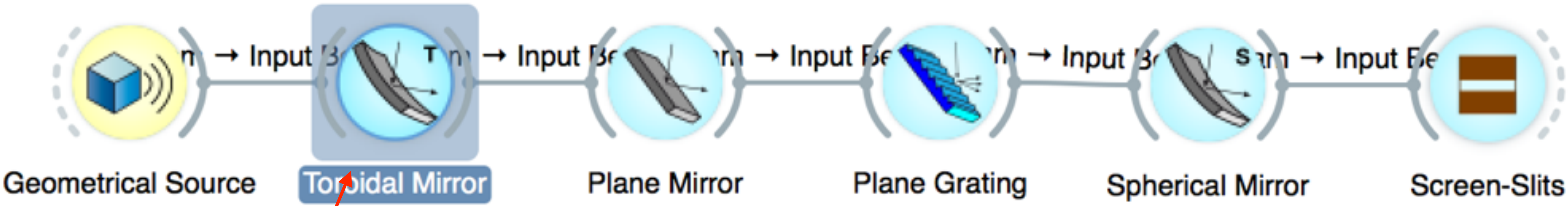
FWHM Z [μm]	272.0000
FWHM X [μm]	5.8000

Forgiveness Factor: $\times\theta_M$

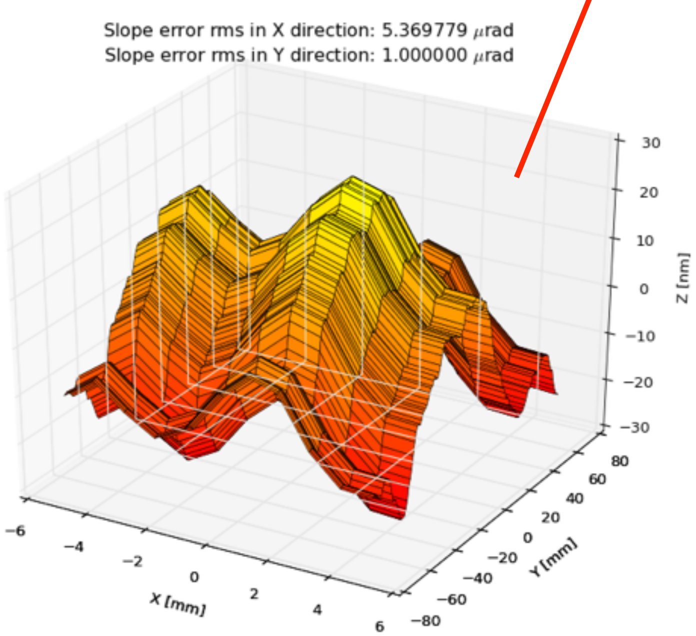
No SE

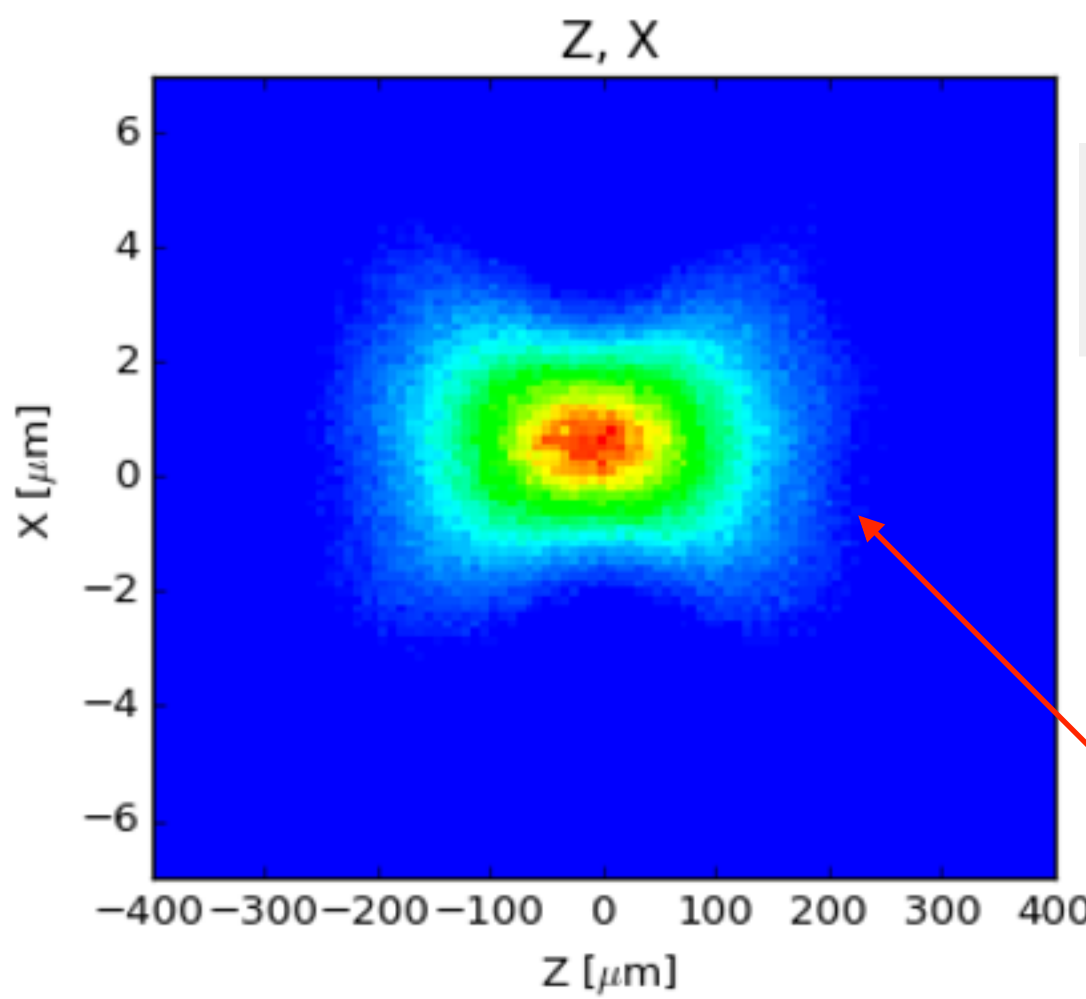
FWHM Z [μm]	264.0000
FWHM X [μm]	5.8000

Collimated PGM, TM, CM: horizontal plane; c=5



α=89.5°, β=87.4°





With slope errors

FWHM Z [μm]	264.0000
FWHM X [μm]	2.8000

Without slope errors

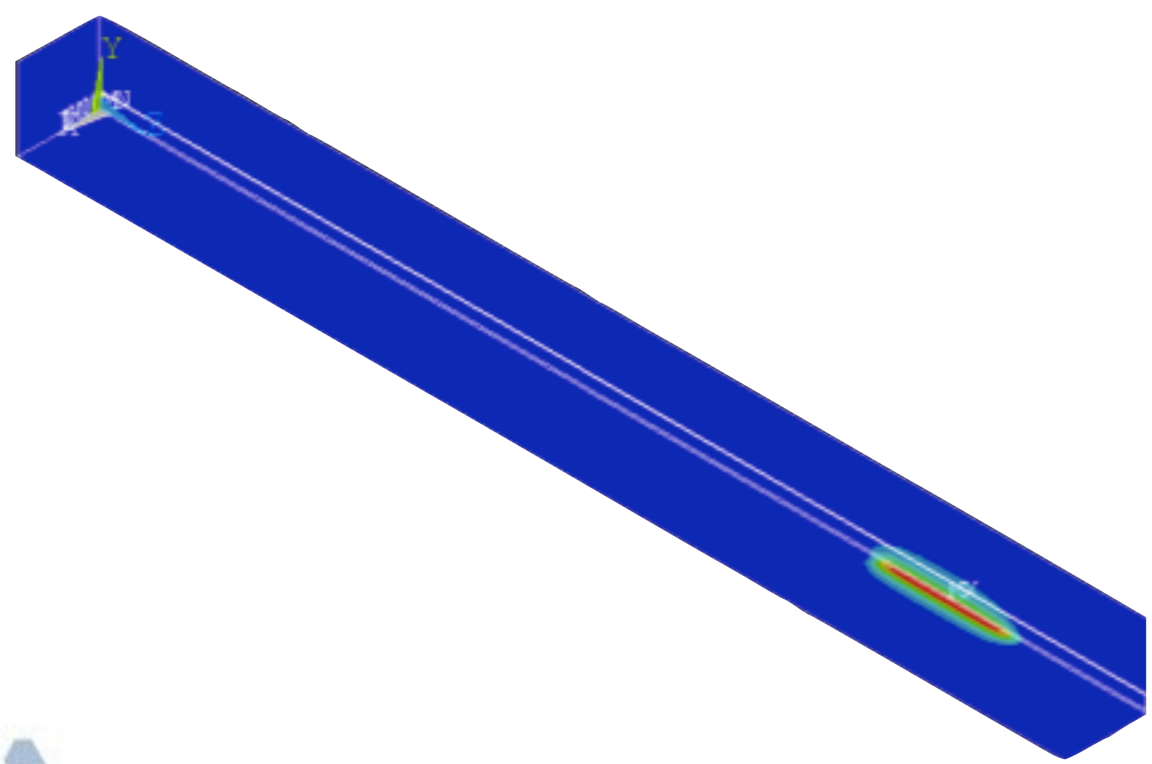
FWHM Z [μm]	272.0000
FWHM X [μm]	2.8000

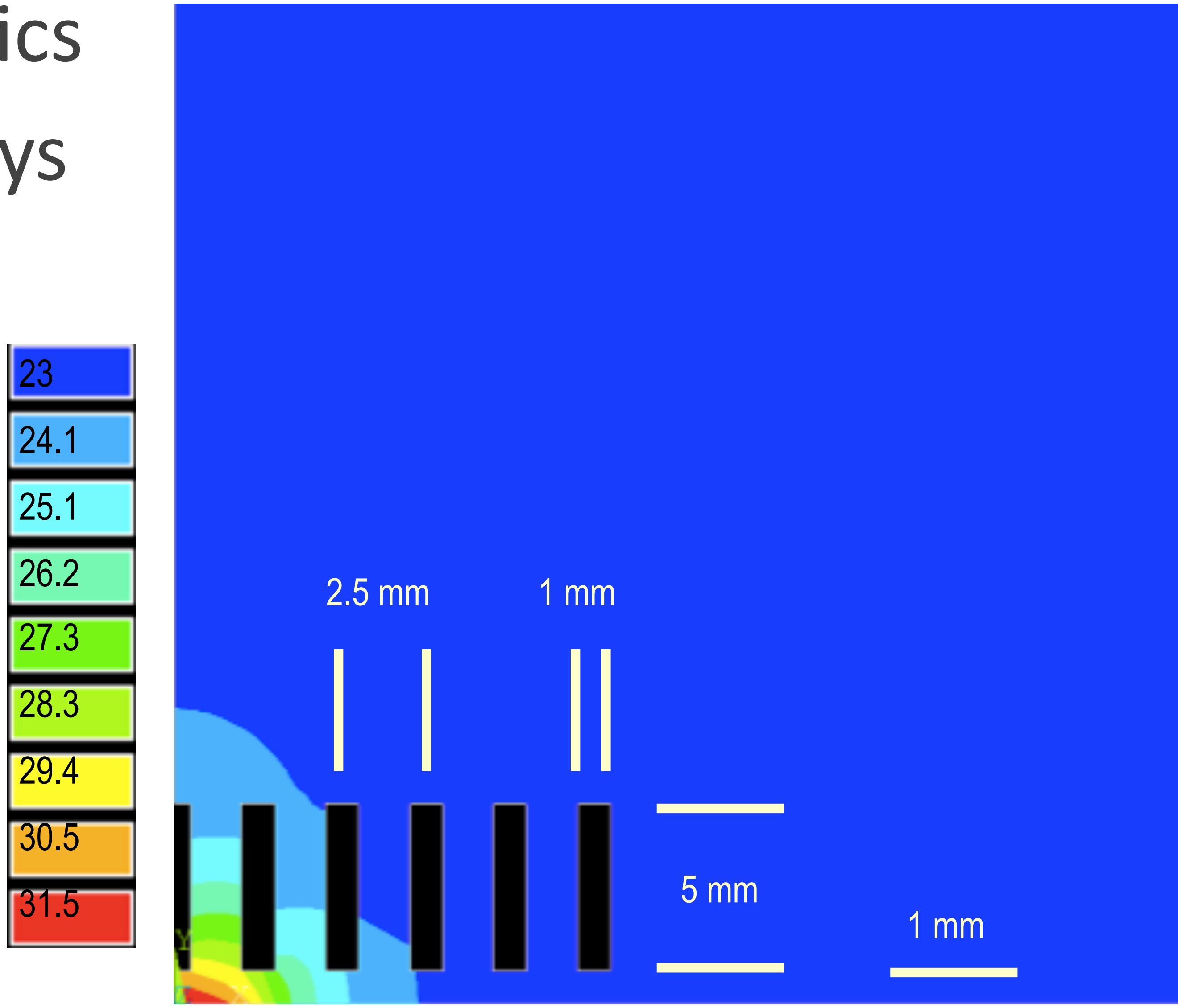
5.8/(5/2)=2.32

Astigmatic Coma

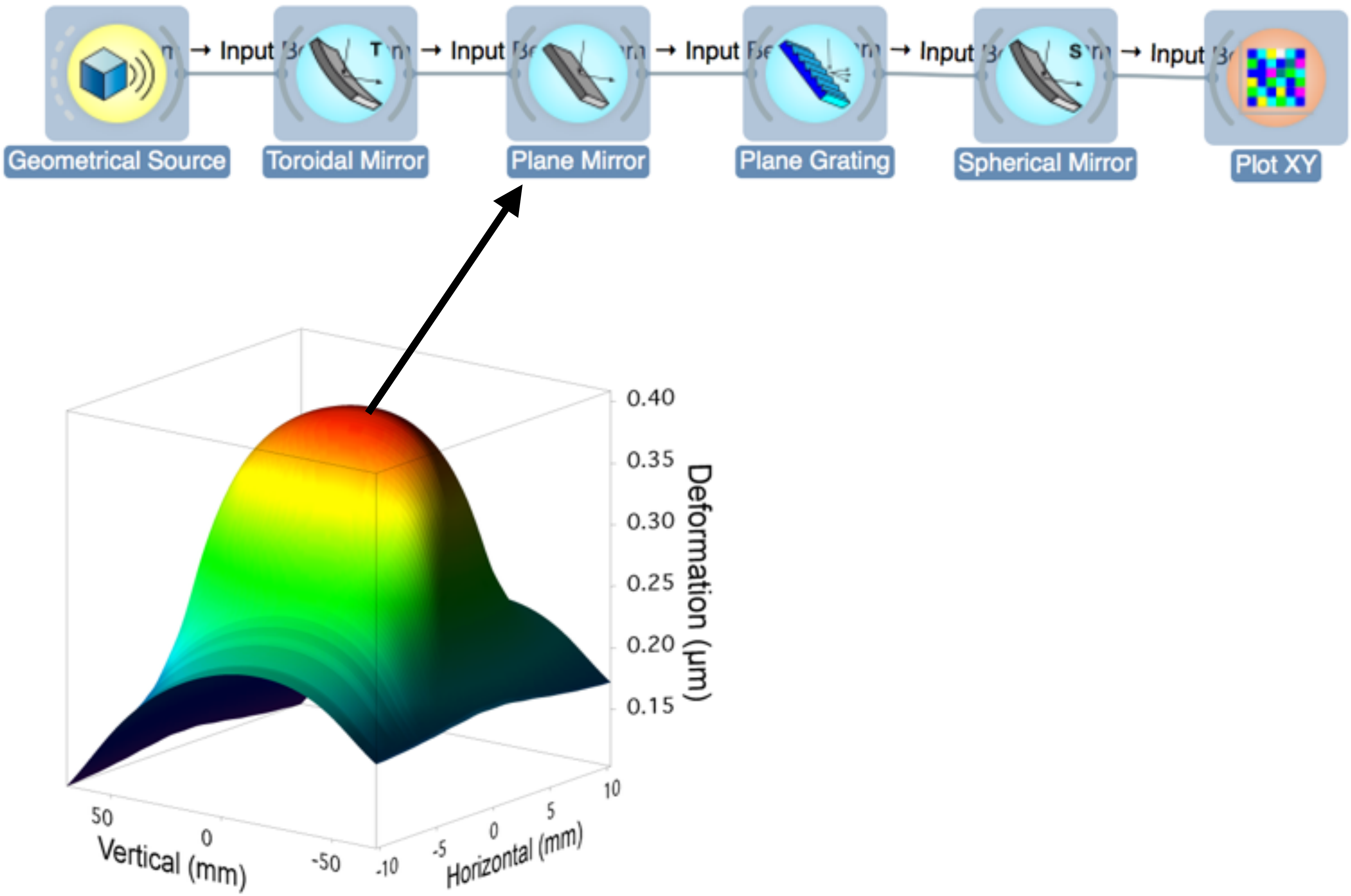
Finite Element Analysis M2

- ☑ Calculate the heat load absorbed optical elements (SRCalc, to be incorporated)
- ☑ Do finite element analysis
- ☑ Ray trace with deformed optics
- ☑ Worked at APS (XS) then Oasys



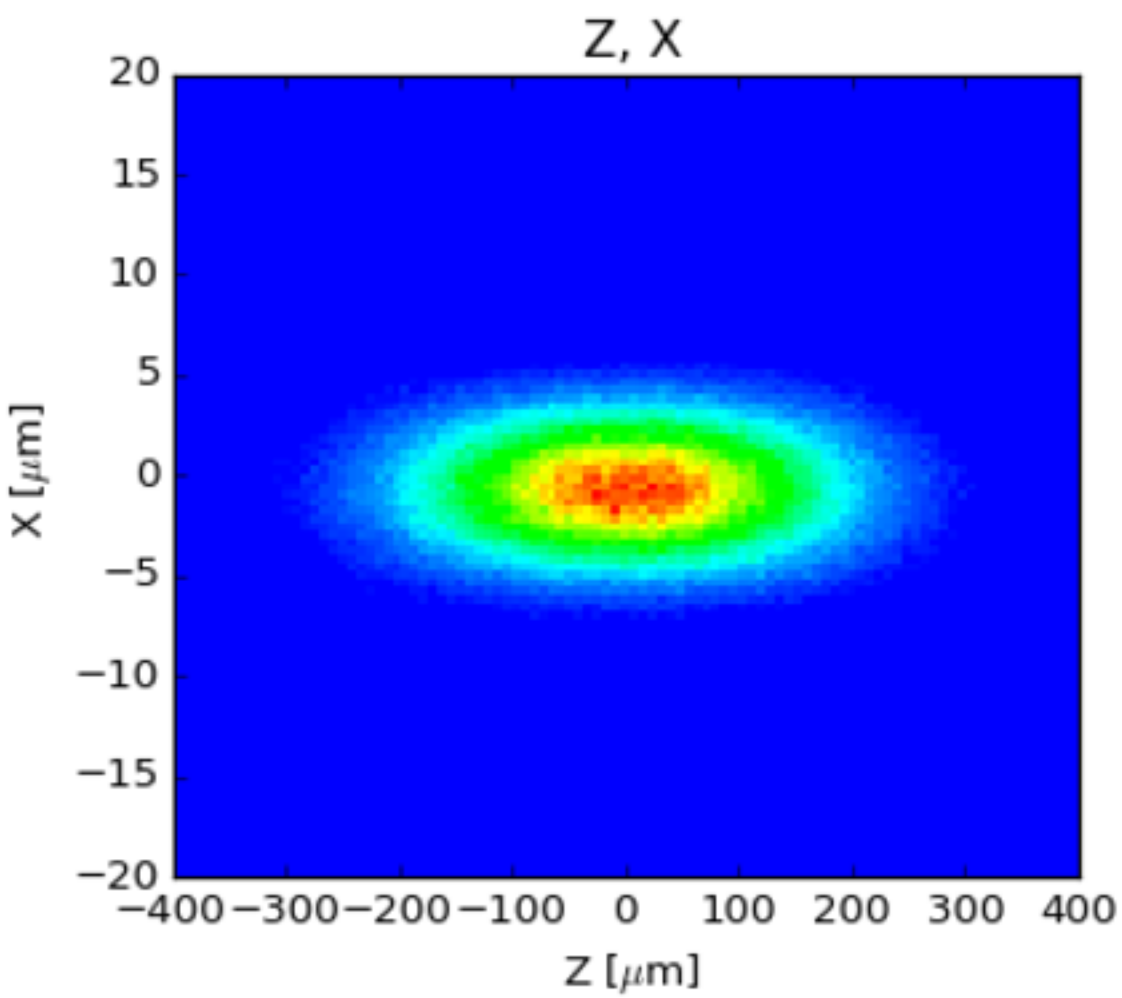


Deformation: Heat load absorbed on PM, Follath collimated PGM, c=2



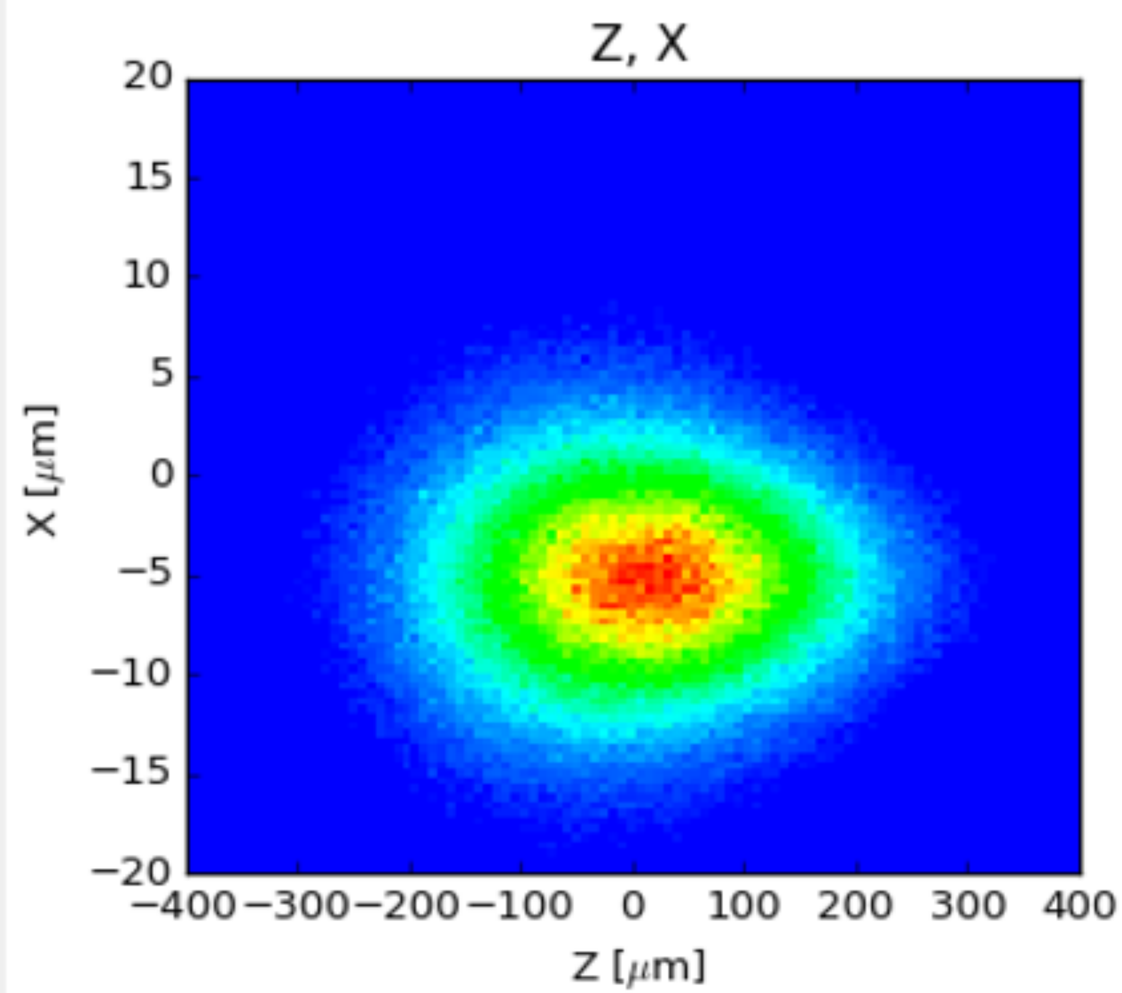
Total Absorbed Power 35 W

Follath Collimated PGM with Absorbed power, c=2



No Heat Load

FWHM Z [µm]	280.0000
FWHM X [µm]	5.6000



With Heat Load

FWHM Z [µm]	264.0000
FWHM X [µm]	10.0000

FVLSPGM

Focusing Variable Line Spacing Plane Grating Monochromator

$$k = \frac{1 + 2b_2 w + 3b_3 w^2 + ...}{d_0}$$

Choose the grating magnification c^{-1} $\quad c = \frac{\cos\beta}{\cos\alpha}$

Choose λ_0 for which $b2$ will be zero
Solve the grating equation for β_0

$$(\frac{m\lambda_0}{d} - \sin\beta_0)^2 = 1 - c^2(1 - \sin^2\beta_0)$$

get α_0 and solve for b_2

$$F_{20} = \frac{1}{2}(\frac{\cos^2\alpha_0}{r} + \frac{\cos^2\beta_0}{r'}) - \frac{m\lambda_0\ b_2}{d_0} = 0$$

same for $b3$ to zero the coma at one wavelength

$$F_{30} = \frac{1}{2}(\frac{\sin\alpha}{r}\frac{\cos^2\alpha}{r} + (\beta r')) - \frac{m\lambda\ b_3}{d_0}$$

FVLSPGM

- The defocus equation can be solved for all wavelengths by illuminating the grating at the correct angle of incidence.
  - *c* is not a free parameter.
  - R. R & A. R. B. C, NIM A 538, 760 (2005).
  - c=2 at 600 eV $\Rightarrow b2=1.44\times10^{-4}\ \text{mm}^{-1}$
  - Solving coma at one wavelength enough
  - Coma zero at 600 eV $\Rightarrow b3=1.3\times10^{-8}\ \text{mm}^{-2}$

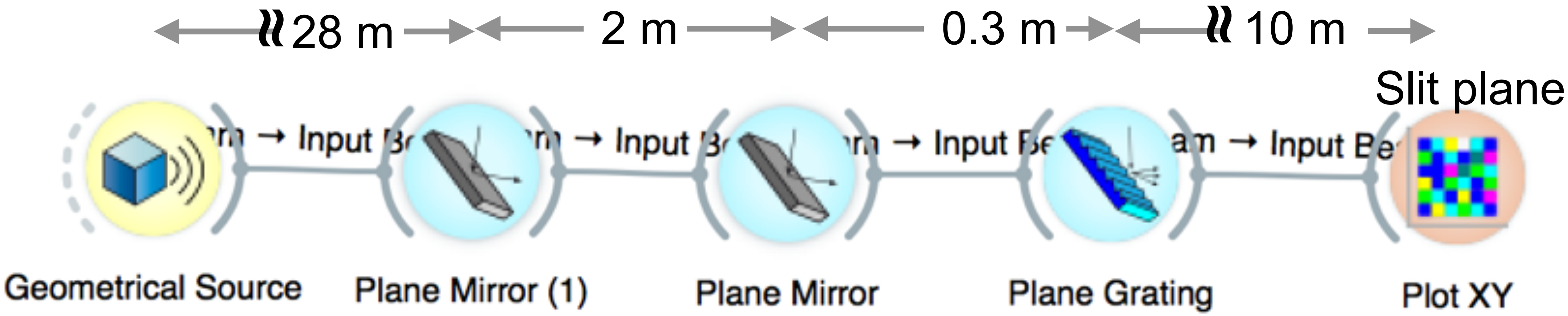
FVLSPGM

28 m — 2 m — 0.3 m — 10 m

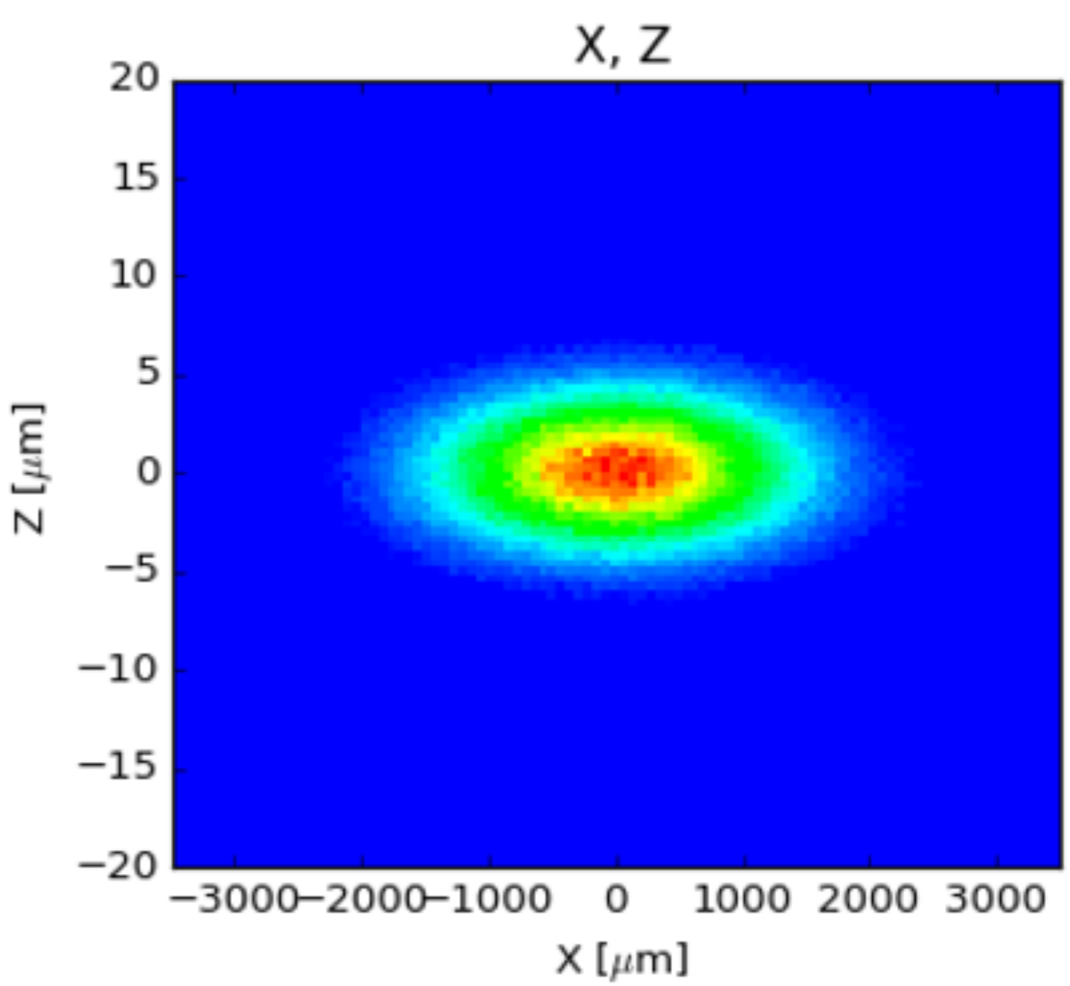
Slit plane

88.5° left	87.8° down	α=88.5°, β=87.1° up	Horizontal focus after slit

FVLSPGM



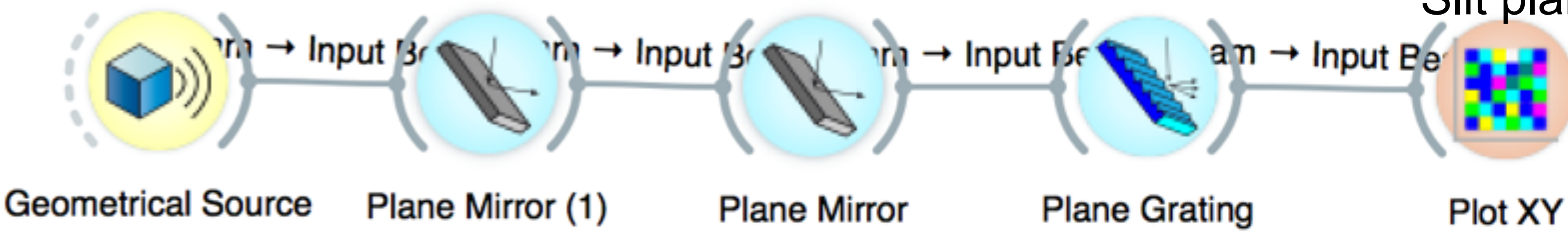
Plane Mirror (1)	Plane Mirror	Plane Grating	Plot XY
88.5° left	87.8° down	α=88.5°, β=87.1° up	Horizontal focus after slit

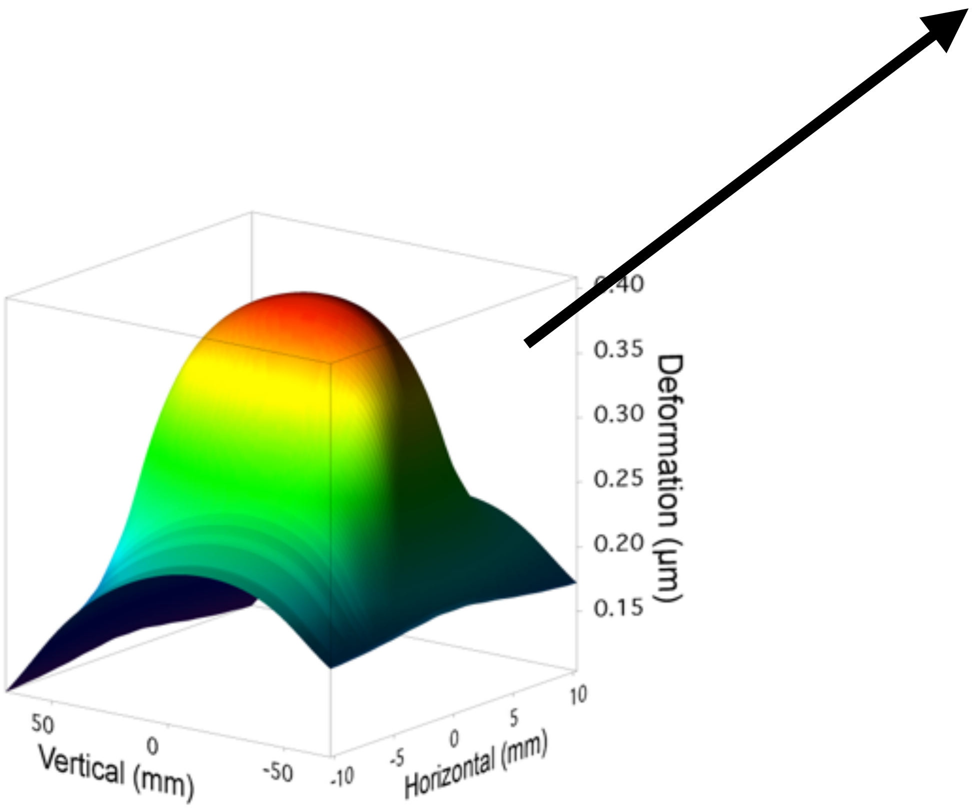


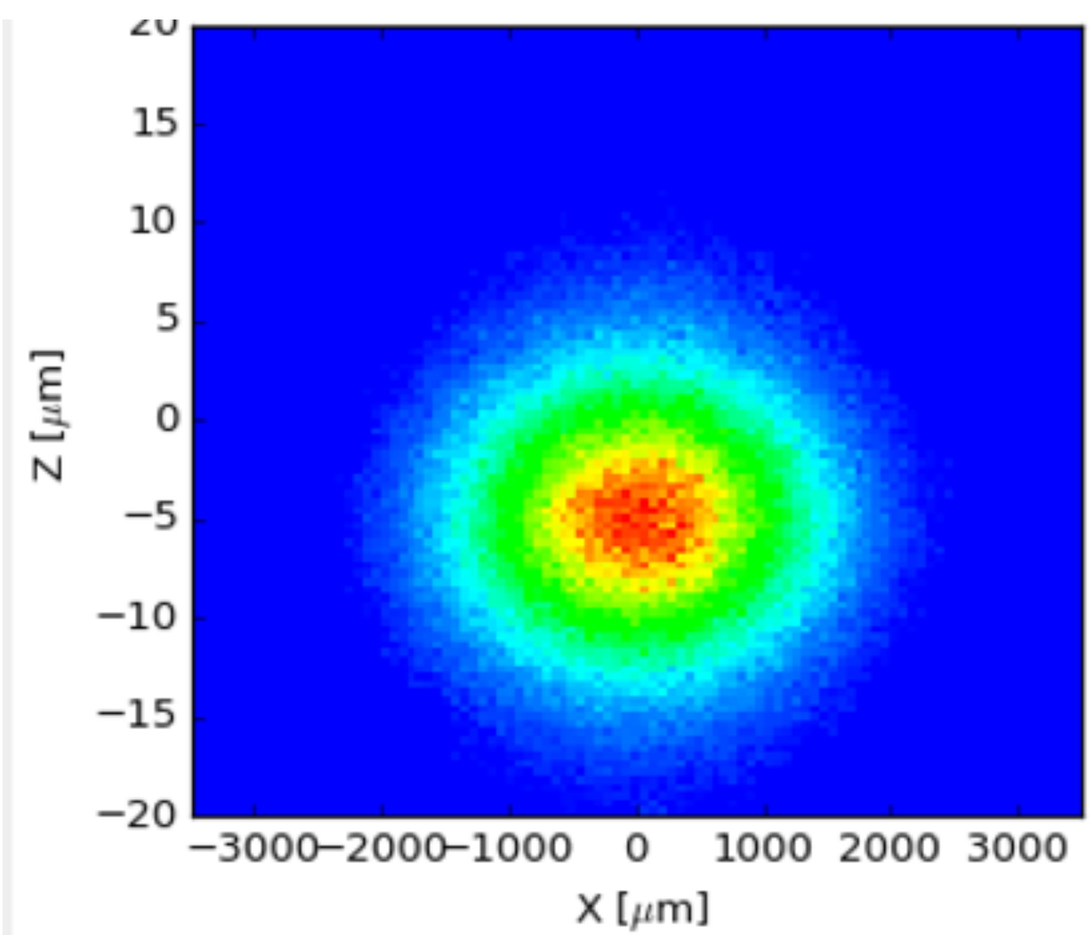
FWHM X [µm]	2030.0000
FWHM Z [µm]	5.6000

FVLSPGM with Heat Load

Slit plane







Without

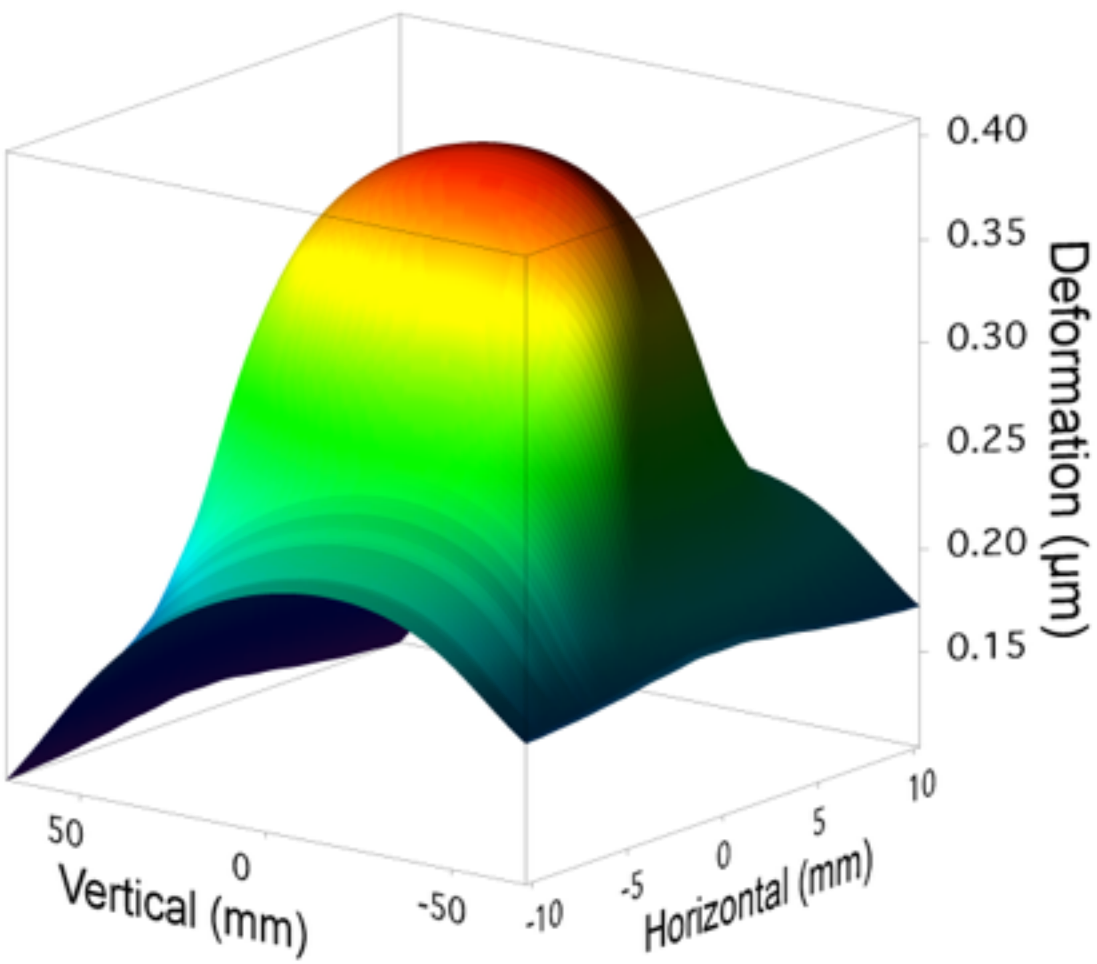
FWHM X [µm]	2030.0000
FWHM Z [µm]	5.6000

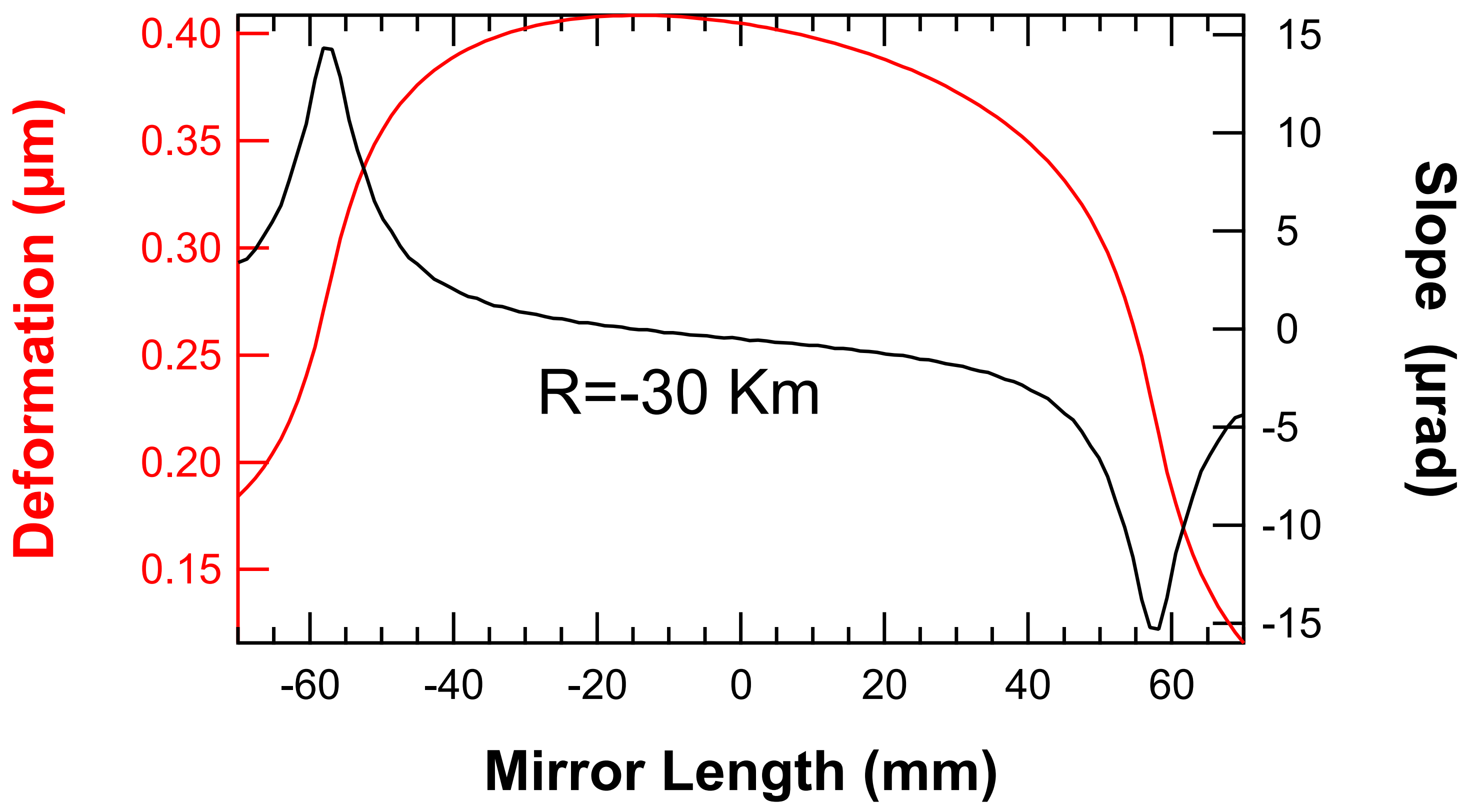
With

FWHM X [µm]	2030.0000
FWHM Z [µm]	11.2000

Deformation: Heat load absorbed on PM, c=2

Total Absorbed Power 35 W

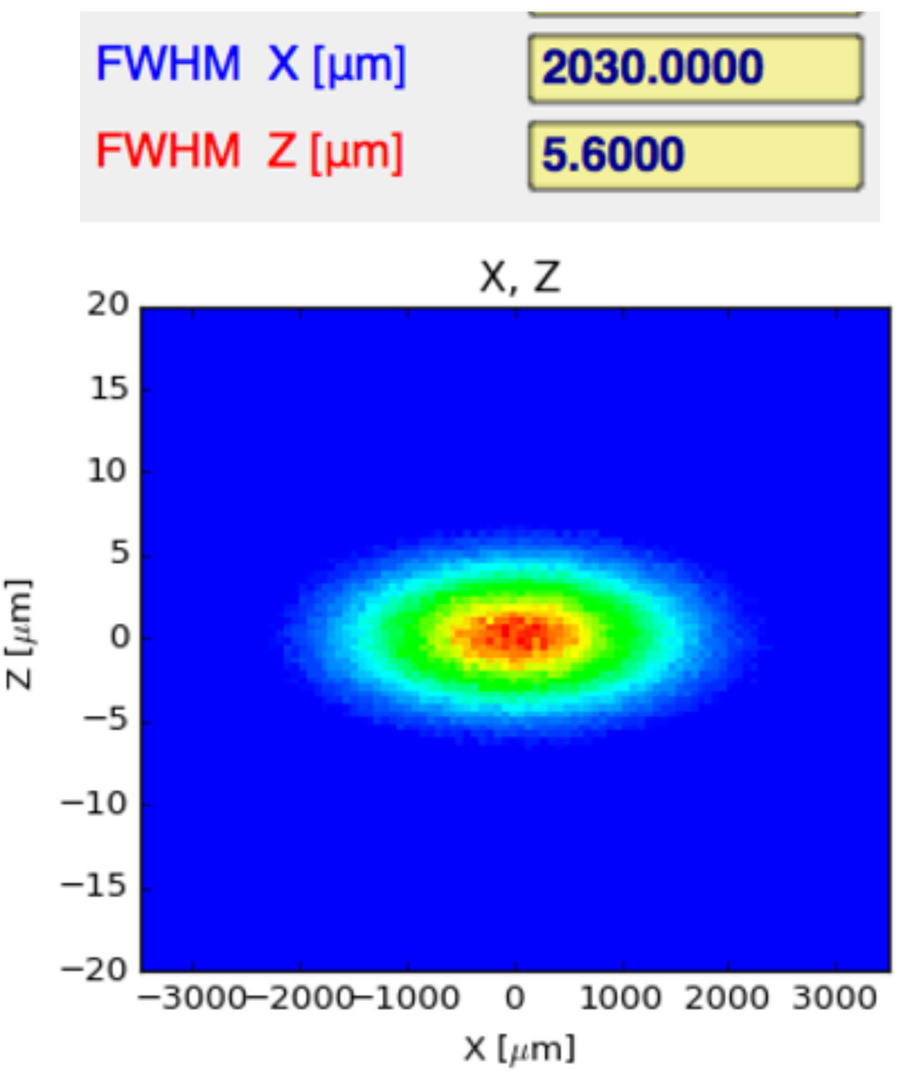




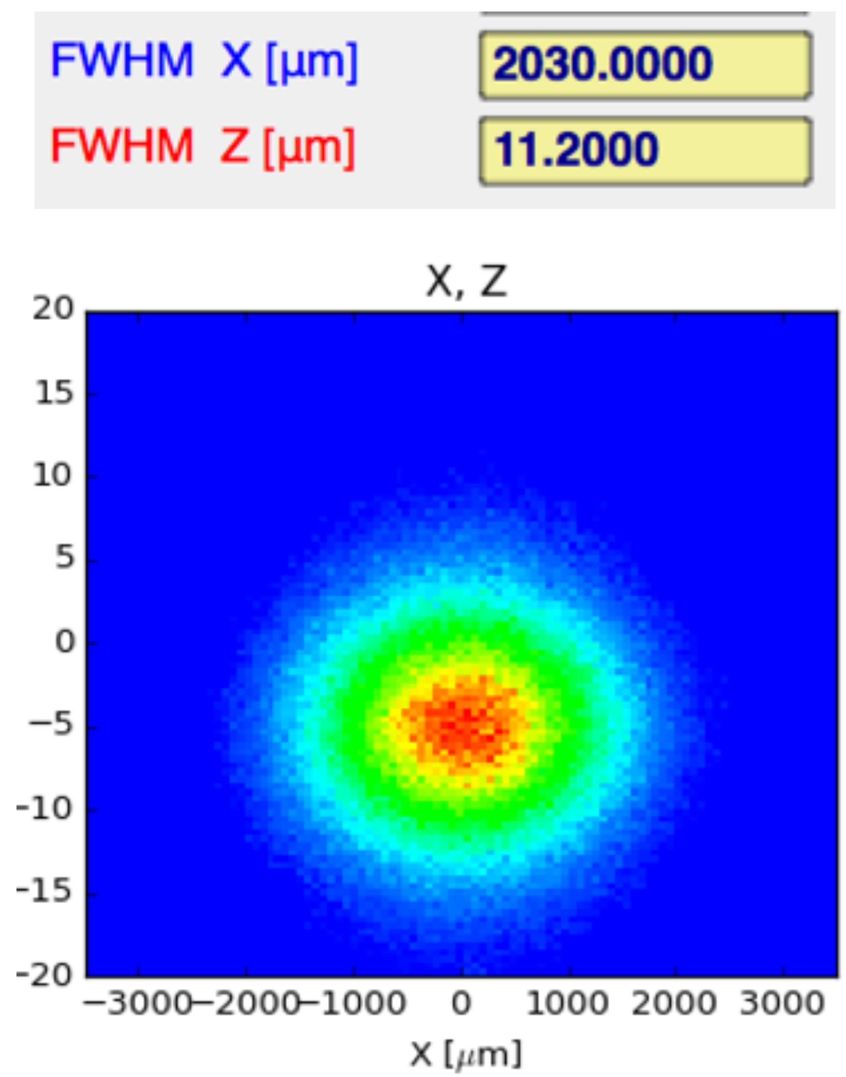
Virtual Source at 28.52 m

FVLSPGM with Heat Load and Corrected

Without



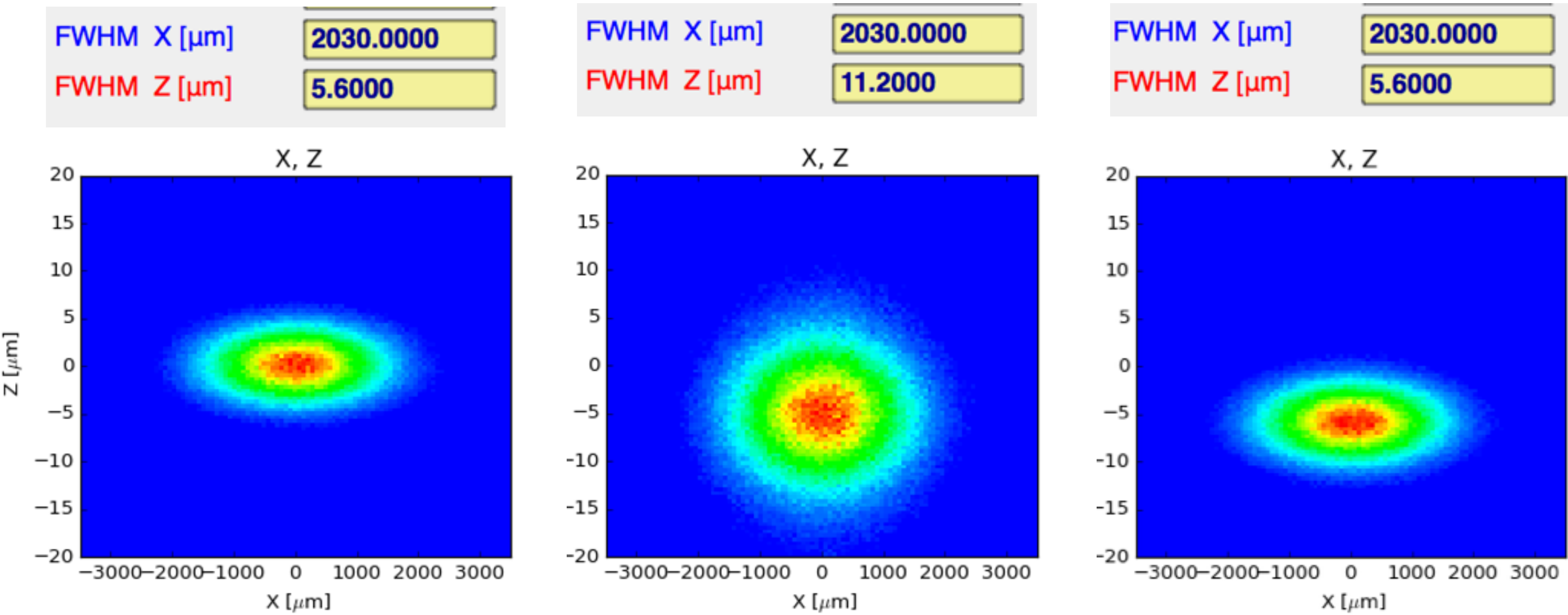
With



α=88.52843°
β=87.05389°

FVLSPGM with Heat Load and Corrected

Without | With | With Corrected



α=88.52843°
β=87.05389°

α=88.53789°
β=87.0586°

R.R, NIM A 649, 139 (2010)

Summary

- ☑ SGM requires a movable exit slit
- ☑ Collimated PGM can be used with fixed magnification or following grating efficiency
  - ☑ The slope errors in the mirrors impair the resolution in vertical PGM mirror.
  - ☑ The heat induced deformations in Follath collimated PGM impair the resolution. Could be solved by moving slit.
- ☑ Focusing VLS PGM
  - ☑ Can correct heat induced deformation
  - ☑ Cannot change the magnification

- ☑ Formulas for all monochromator types will be included in Oasys