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Title	SWORDS - SoftWare fOR Diffraction Simulation of silicon pore optics: the user manual
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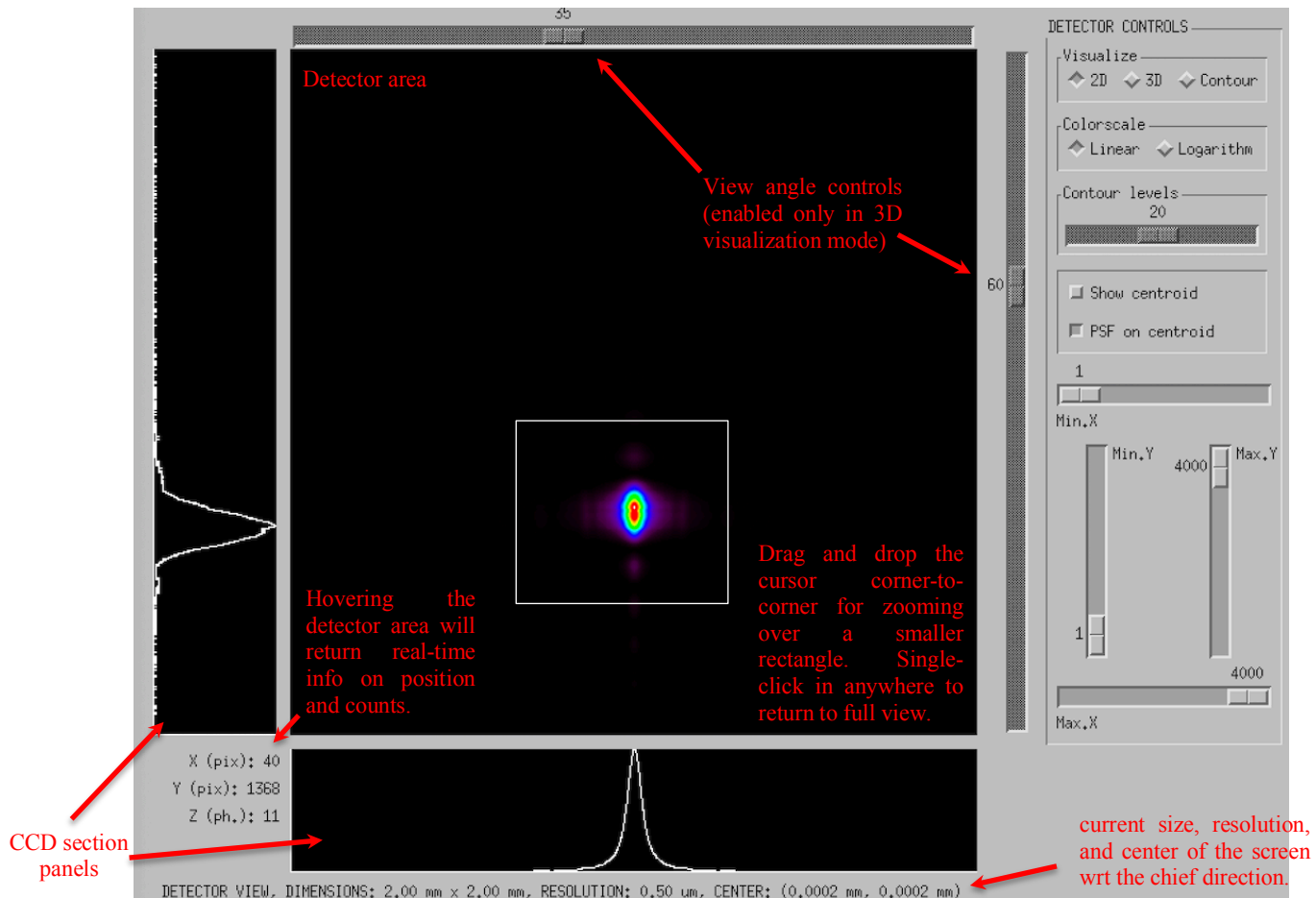


Figure 17: the right side of the GUI after the elaboration of the diffraction figure, with a 3 arcsec P-H rotation around the x-axis.

2.4. Computing and viewing the diffraction figure

2.4.1. Diffraction figure computation

When the diffraction figure computation is started, the progress can be monitored in the “Computation flow” panel. The computation goes through several steps (such as an FFT) a resampling to the actual resolution, an edge trimming from the detector area, and a convolution with the angular profile of the source, either flat-topped or gaussian. If the light source is polychromatic - as in all realistic cases - then the procedure is iterated at each wavelength considered, and the results are averaged.

If the gaussian spectrum option was selected, the average is weighted over the intensity variation throughout the gaussian line profile. The user might note that, as the wavelength is swept through the band, both resolution and size of the diffraction-limited image do change. In any case, the resolution is degraded to the actual pixel size previously selected by the user.

The diffraction pattern is displayed in the right panel of the GUI (Figure 17). Image size, resolution, center, and centroid information are displayed at any time below the detector view. The “center” is referred to the theoretical location of the focal spot on-axis and for a perfectly aligned MM, and can be subject to change, for example if either the *Track the source off-axis* or *Center focus in MM misalignments* option was previously selected (Sect. 2.2.3). Three normalization values are displayed in the bottom-right panel:

- 1) *Absolute normalization* is the ratio of the focal spot integrated on the **diffraction-limited focal plane**, inside and outside the true detector field, to the power collected in the MM aperture. In order to avoid uncanny aliasing problems, the diffraction pattern *should never become wider than the diffraction-limited detector* (this might occur, for example, due of a too large defocusing).
- 2) *Relative normalization* is the ratio of the focal spot integrated within the **detector field**, to the power collected in the MM aperture.
- 3) *Field normalization* is the normalization value within the **field of view selected**, e.g., when the focal spot is zoomed in, and can be much lower than the previous two.

The absolute and the relative normalization values should be very close to 1 if the computation was successful. A lower value of the latter means that part of the focal spot is out of the detector limits. An absolute normalization sensitively departing from 1 usually reveals an insufficient resolution of the detector used for the simulation.

```
COMPUTATION FLOW:
Computing CPF... done!
Computing OTF...
lambda (9/9) = 43,3333 Å (gaussian spectrum)
-> diffr. lim. detector size: 3,058 mm x 2,659 mm
-> diffr. lim. detector res.: 0,419 µm x 0,553 µm
-> Doing FFT...
-> ...done! Trimming to a 4766 x 3612 pixel area...
-> ...done. Shrinking to actual resolution...
...done! Convoluting with actual source profile...
...done! Fetching final image...
```

```
Absolute normalization: 0,472 (100,0%)
Relative normalization: 0,467 (98,81%)
Field normalization: 0,467 (98,81%)
Computing CPF ...
```

2.4.2. Handling the detector controls

The detector field can be visualized in 3 different modes: in 2D, 3D, and in contour plot (Figure 18), acting on the *Visualize* subpanel. The default visualization mode is a 2D intensity map in linear scale. As the cursor is moved over the viewgraph area, the x and y pixel coordinates are displayed in the lower left corner, along with the photon count value at (x, y), and the image sections along x and y are plotted in the side panels. Dragging and dropping the cursor from corner to corner, an image selection can be magnified, and updated information is reported in the lower label (Figure 17).

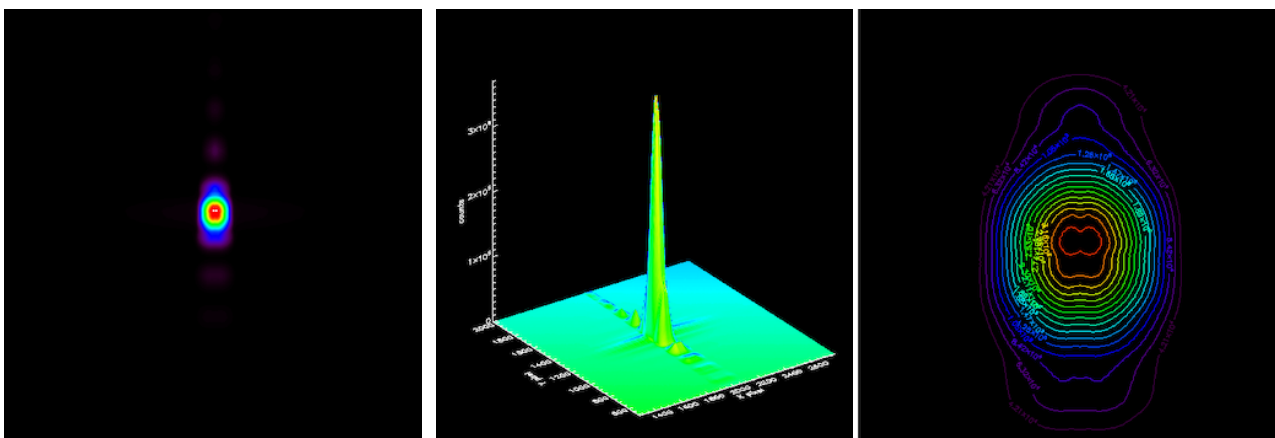




Figure 18: the three different visualization modes of the CCD field: (left) 2D, (center) 3D, and (right, magnified), contour plot mode.

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Visualization controls, on the right side, allow the user to adjust the image zoom acting on the sliders: the user can single-click anywhere on the detector to reset the zoom. Logarithmic color scale is also available. In contour mode, the number of levels in the contour plot can easily be changed using the appropriate slider. The contour plot mode works in both linear and logarithmic scale.

As the image is zoomed in or out, updated information on the coordinate centroid position, referred to the theoretical position of the ideal focus, is always displayed in the detector panel, along with the related uncertainty. The coordinates of the centroid are independent of whether the tracking options are selected or not. Finally, the detector controls in the lower panel: *Integration time*, *Quantum efficiency*, and *Noise* allow the user emulating to some extent the behavior of a real detector gain and background (Figure 19 and Figure 20, the option of keeping the focal spot centered was deselected). The background noise matrix has a gaussian distribution with rms value = $(\text{noise} \times \text{int. time})^{1/2}$. Increasing the integration time is always possible until the detector saturates (but the dynamic range can be increased selecting a 64-bit acquisition, as per Sect. 2.2.3). After changing the values, the user has to press the *Apply* button for them to take effect.

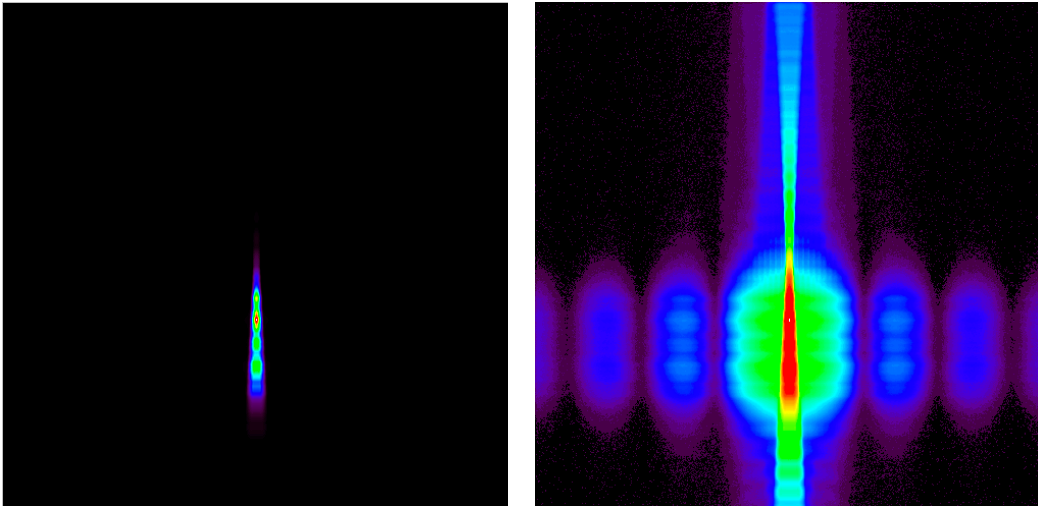


Figure 19: CCD visualization in (left) linear and (right) log color scale. The image was deliberately aberrated by misaligning the primary stack by 3 arcsec, plus a perturbation at the first harmonic, with random amplitudes between 0 and 0.1 μm and random phase shifts between 0 and 20 mm.

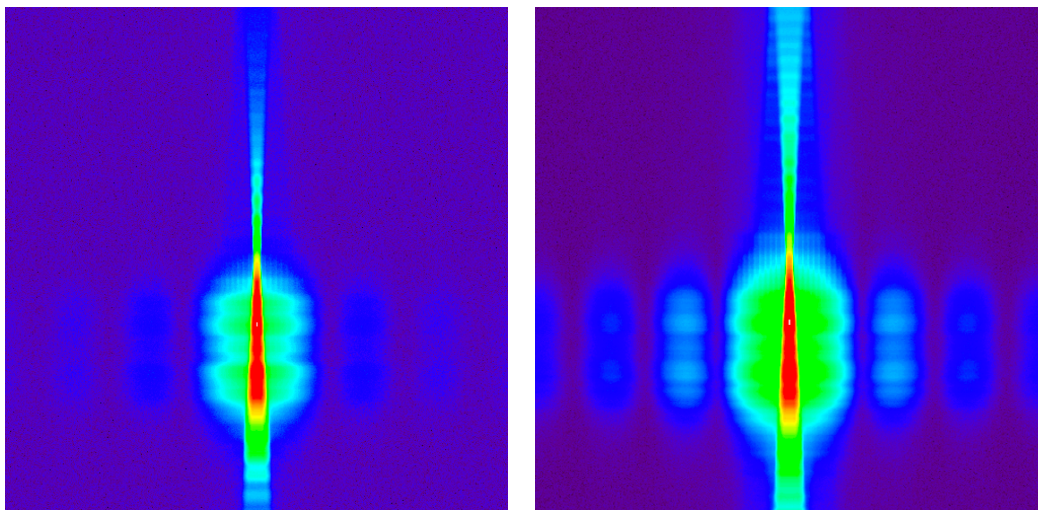




Figure 20: Left: the same image of Figure 19, right, after setting the CCD noise to 300 cts/s. Right: after increasing the integration time from 0.05 s to 5 s, the visibility of diffraction fringes is restored.

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2.4.3. More functionalities

More functionalities can be found in the upper menu. For instance, from the *Visualize* submenu:

- *Changing the color palette or the background*: the change takes effect on all the images generated from this point on, until a new palette is selected.
- *Viewing the simulation header*: selecting the *Show image header* opens a window with a summary of the simulation being carried out (Figure 21). The header is also saved to file when the image is saved in *.fits format or with the PSF in text format (Sect. 2.4.4).

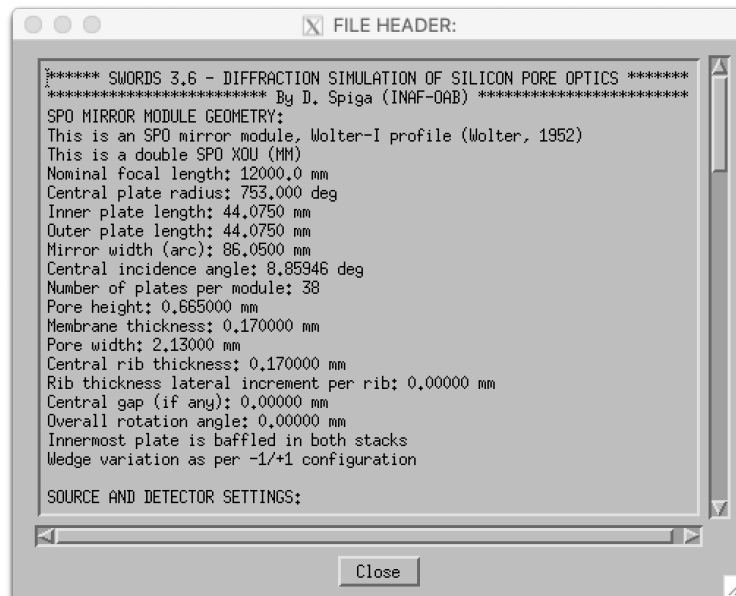
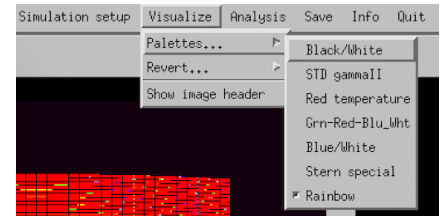
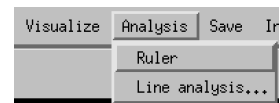


Figure 21: the header tab, summarizing the simulation configuration.

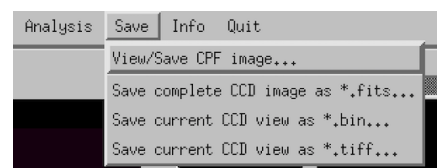
From the *Analysis* submenu:

- *Measuring a distance* enables the *Ruler* mode by pressing on the dedicated button. Dragging and dropping the cursor over the detector area returns a message with the distance between the two points (Figure 22, left). The ruler mode is disabled automatically right after closing the message window.
- *Sectioning the image*: select *Line analysis*, then drag-dropping the cursor over the detector area will return a section of the image along the selected direction, along with related information (Figure 22, right).



From the *Save* submenu:

- *Save complete CCD image as *.fits...*: this command will save the *full* detector area as a fits image, prefaced by the header shown in Figure 21.
- *Save current CCD view as *.bin...*: the detector area being visualized will be saved as binary file for easy use with IDL via the *restore* procedure. Only the currently visualized area will be saved.
- *Save current CCD view as *.tiff...*: the detector area being visualized will be saved as .tiff image. Only the currently visualized area will be saved.



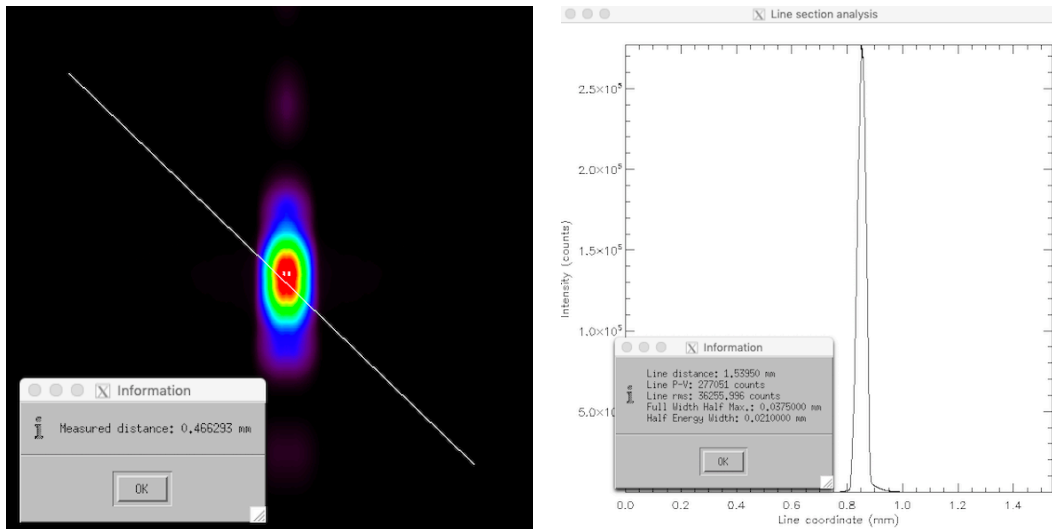


Figure 22: (left) measured distance in the image in ruler mode, and (right) line section analysis.

2.4.4. The Point Spread Function

Pressing the *Compute PSF* button under the *...DIFFRACT!!* command starts the radial integration of the image, with the center on the centroid if the *PSF on centroid* button was selected. The computation advancement can be monitored in the *Computation flow* left panel. By default, the noise is removed from the integration. When the process is complete, the PSF window is displayed as in Figure 23, and the HEW and the W90 values are reported in the same window. If the *PSF on centroid* button is de-selected, the integration starts from the center of the visualized area (Figure 24). Either the PSF or the EE function can be visualized. The PSF can be exported in text format.

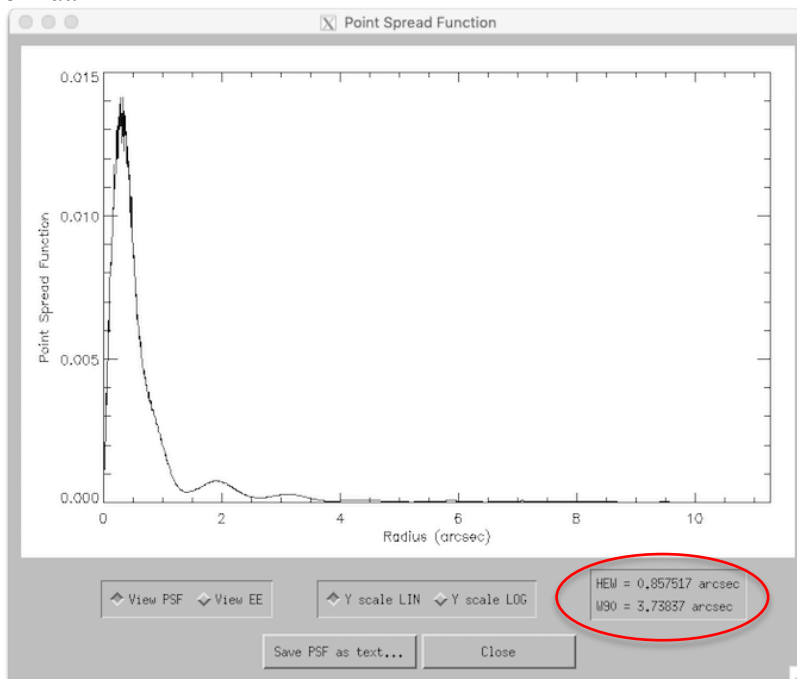
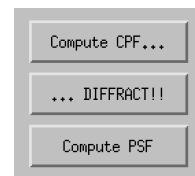


Figure 23: the Point Spread Function, centered on the centroid. The HEW and the W90 values are computed by default.

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We note that the PSF is normalized to the integral of the detector area that is currently visualized. As the integration covers the largest circle inscribed in the current view, the PSF normalization might be a smaller value, since the counts in the corners will not be included. The user can realize that by selecting the *View EE* option and reading the maximum value of the EE.

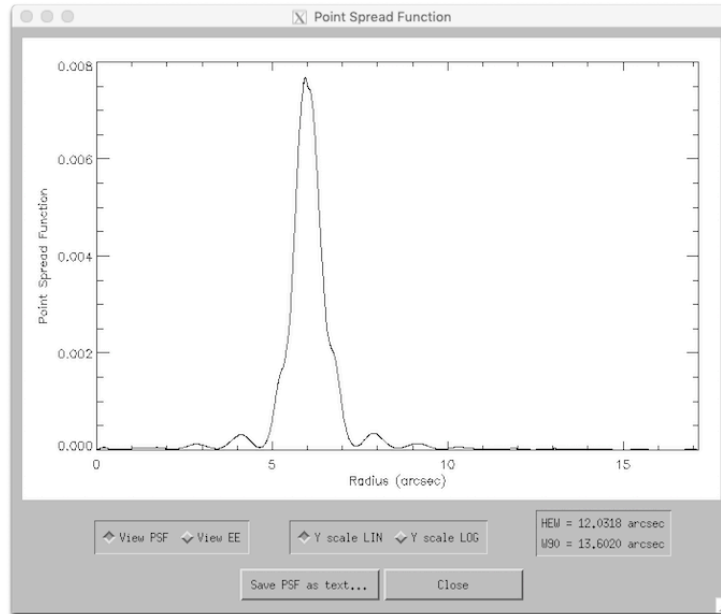


Figure 24: the Point Spread Function, centered on the detector center instead of the centroid. The PSF is clearly decentered, and the HEW and the W90 values are obviously overestimated.

3. Some examples

3.1. Perfect mirror module in X-rays e UV light

In this section, we show some examples of how to use SWORDS. We stick to the nominal parameters of the SPO MM described in Figure 2: the in-focus image in X-rays and UV light are shown in Figure 25. For comparison ease, in Figure 25 the detector is the same at the two wavelengths. In reality, it would always be recommended to scale the detector and pixel size proportionally to λ , so to visualize the full diffraction figure. In the nominal focus, the diffraction figure of the XOUs at $\lambda = 40 \text{ \AA}$, with -1/+1 wedge configuration, returns a HEW = 0.75 arcsec, and 0.69 arcsec in +1/+3 configuration. The difference accounts for the small off-axis angle of each plate (but the central one) that appears in the -1/+1. In UV light, the image is completely dominated by the aperture diffraction.

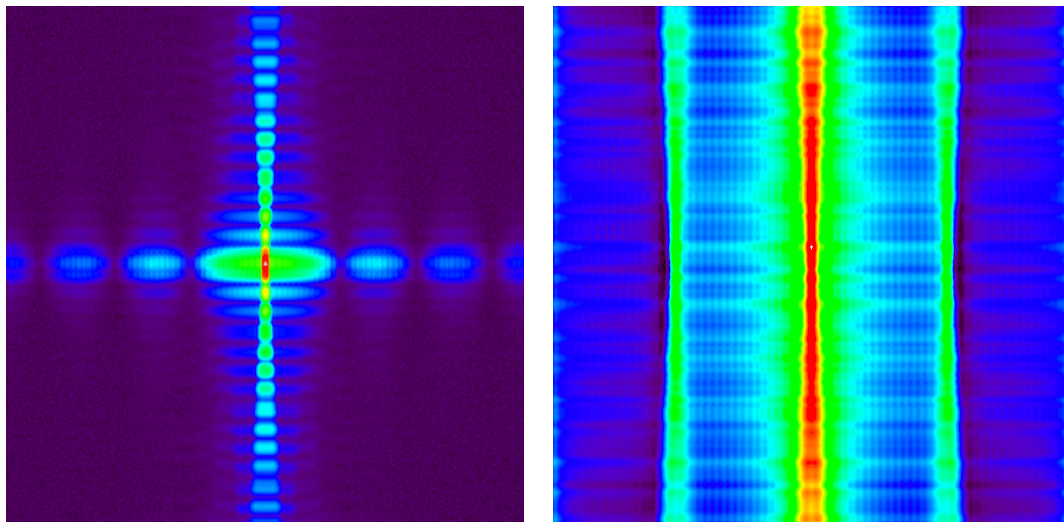


Figure 25: (left) the focal spot at $\lambda = 40 \text{ \AA}$, (right) at $\lambda = (1000 \pm 10) \text{ \AA}$. Logarithmic color scale, 2 mm field. Here aliasing effects are avoided, because the diffraction limited focal plane is much larger than the detector.

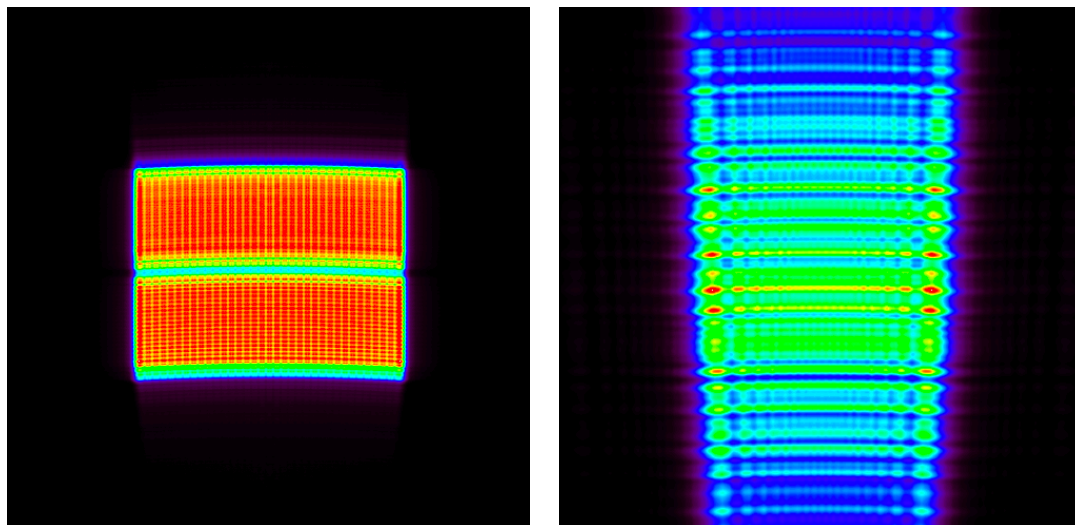


Figure 26: the two simulations of Figure 25, intra-focus by 150 mm. On the left, the double stack structure begins to be seen. The image on the right, at 1000 \AA , it is still dominated by the diffraction effects. The color scale is linear.

The simulation can be repeated also with a defocused image, caused by detector movement out-of-focus (Figure 26), or source location at a finite distance (Figure 27). The image can be *refocused* moving the detector to the best focus distance, i.e., going to the *Simulation setup* menu and pressing the button *Set best focus*, then saving the parameters and doing the CPF and the diffraction simulation again.

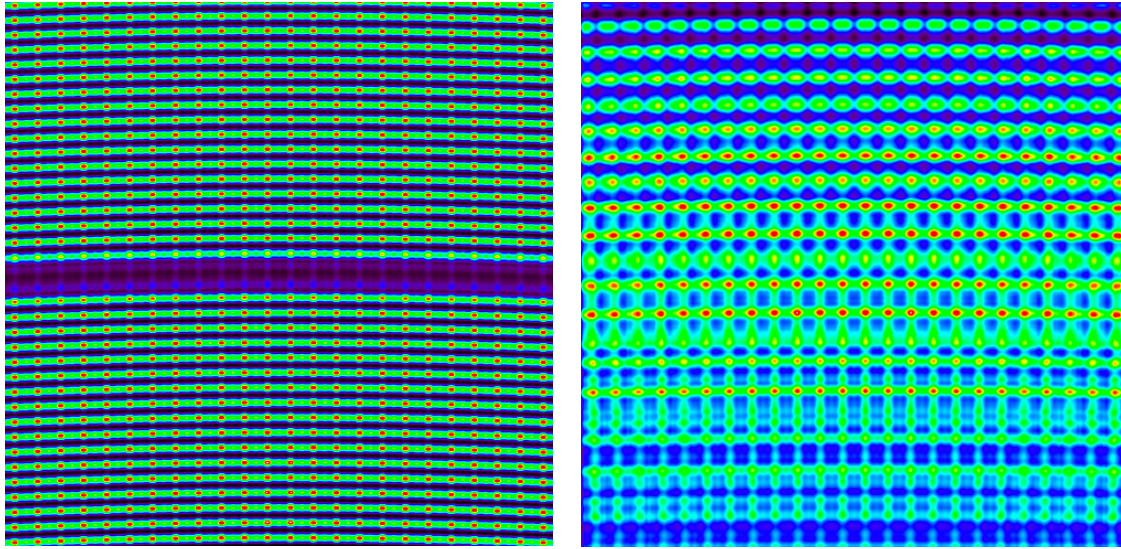


Figure 27: the two simulations of Figure 26, with the source at finite distance (500 m), and the detector intra-focus by 150 mm. Linear color scale. The same comments of Figure 26 apply.

Simulations in UV light with the source off-axis in the *x*- or the *y*-direction are displayed in Figure 28. The option *Track the source off-axis* in the *Simulation Setup* menu was selected for keeping the focal spot centered (Sect. 2.2.4); this is equivalent to tilting the MM and keeping the source and the detector still. Changes in the diffraction effects are mostly due to the enhanced obstruction of the aperture by ribs and membranes when seen off-axis (Figure 29). Simulating off-axis angles in X-rays has much less effect on the aperture diffraction, but aberrations become visible even in this case.

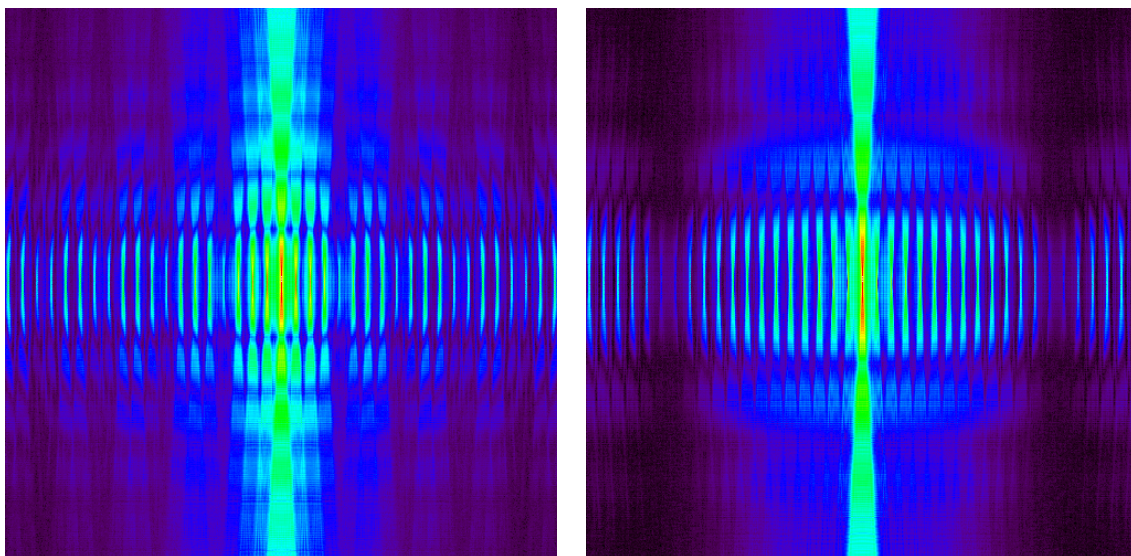


Figure 28: simulation at $\lambda = 1000 \text{ \AA}$, in a 20 mm field, with the source off-axis (left) in the *X*-direction by 15 arcmin, and (right) in the *Y*-direction by 8 arcmin. Log color scale.

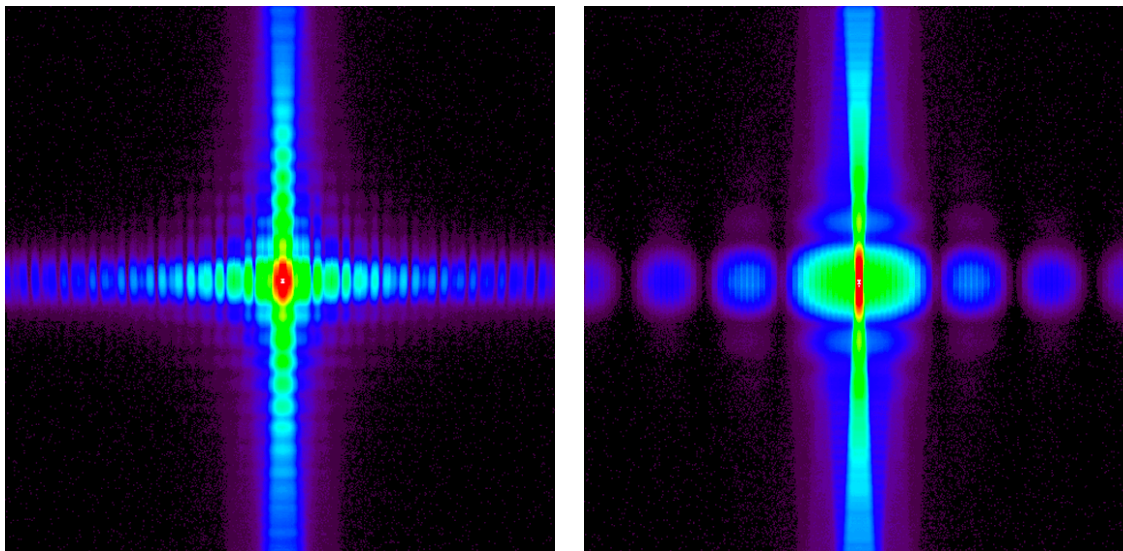


Figure 29: simulation at $\lambda = 40 \text{ \AA}$, in a 2 mm field, source off-axis (left) in the x -direction by 30 arcmin, $HEW = 1.16$ arcsec, and (right) in the y -direction by 11 arcmin ($HEW = 1.5$ arcsec). Log color scale. The source is 0.5 arcsec wide.

3.2. Removing terms from the OPD

From the release 3.7 on, removing terms from the OPD has an effect on the diffraction figure; in this way, the user can see the effect of the different contribution to the final diffraction figure. Just to provide an example, we show in Figure 30 the same simulation of Figure 29, after removing the *Wedging + 2-cone* term and after removing both *Wedging + 2-cone* and the *Defocus + offaxis* (we note that the obstruction enhancement off-axis cannot be deselected ruling the 2nd term out). It should be kept in mind that, even when the wedging is removed, the plate pairs in a MM are still kept converging to a common focus. This is necessary to avoid the computation of the image over a too wide focal plane, which would cause the elaboration time to increase beyond tolerable limits.

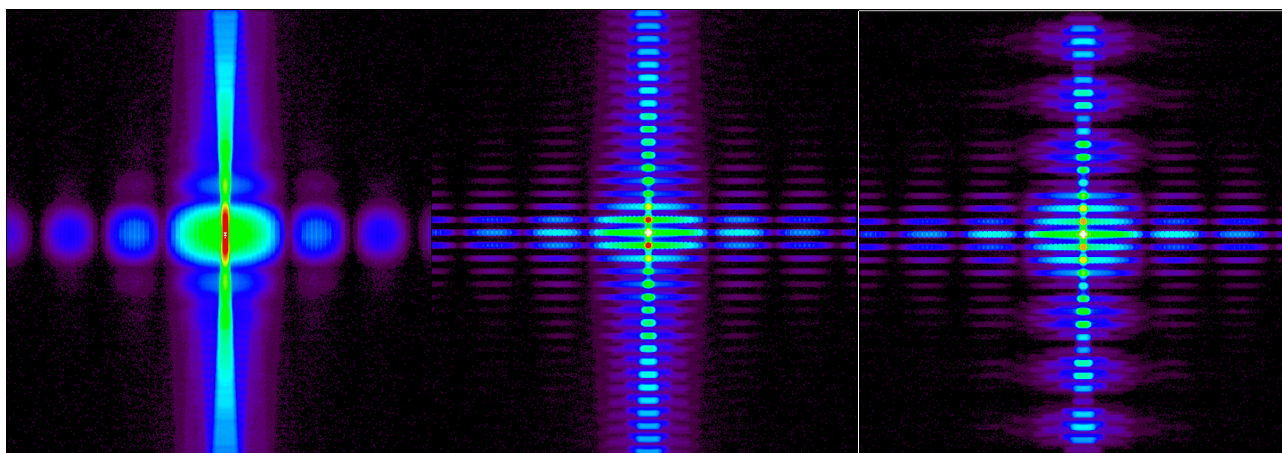


Figure 30: simulation at $\lambda = 40 \text{ \AA}$, with the source off-axis in the y -direction by 11 arcmin. (left) full OPD, (center) removing the wedging term, and (right) without the wedging and the off-axis term.

3.3. Misalignments in the primary-secondary stacks

We can now simulate imperfect mirror modules. We start from misalignments of the two segments (Sect. 2.2.2, case 1) in the x - or the y -direction. Both misalignments reduce the collecting area in the MM, as they increase the apparent thickness of either ribs or membranes, respectively. The secondary stack is always

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kept still and the primary one is roto-translated. A rotation around the x -axis (Figure 5), causing a variation of the kink angle, is simulated in Figure 31. As expected, the main effect is that focus is displaced downwards by an angle twice the angle rotation, with some aberration. The displacement would be removed if the *Center the focus in MM misalignment* option was selected (Sect. 2.2.3), but then the detector center would also be reported at a different location, i.e., at the focal spot centroid.

In contrast, a rotation of the primary stack around the y -axis returns the aberration shown in Figure 32. As expected, the centroid of the spot is still centered, but the image is aberrated vertically. If the simulation was perfectly monochromatic, the image would consist of an array of spots. Simulating a finite bandwidth causes the spots to average out, and the aberrated focus appears more uniform.

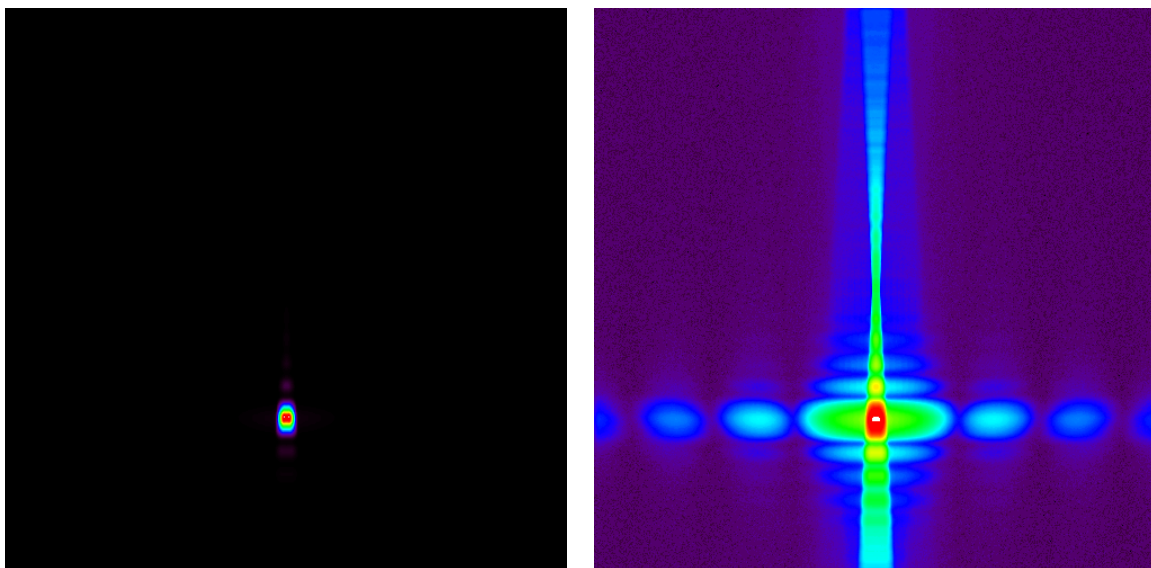


Figure 31: simulation at $\lambda = 40 \text{ \AA}$, 2 mm field, of the MM with the primary stack misaligned with respect to the secondary one. Rotation around the x -axis by 3 arcsec. (left) Linear color scale, (right) log color scale. The centroid is located at $y = -0.343 \text{ mm}$ (-5.9 arcsec). The focus centering option was not selected.

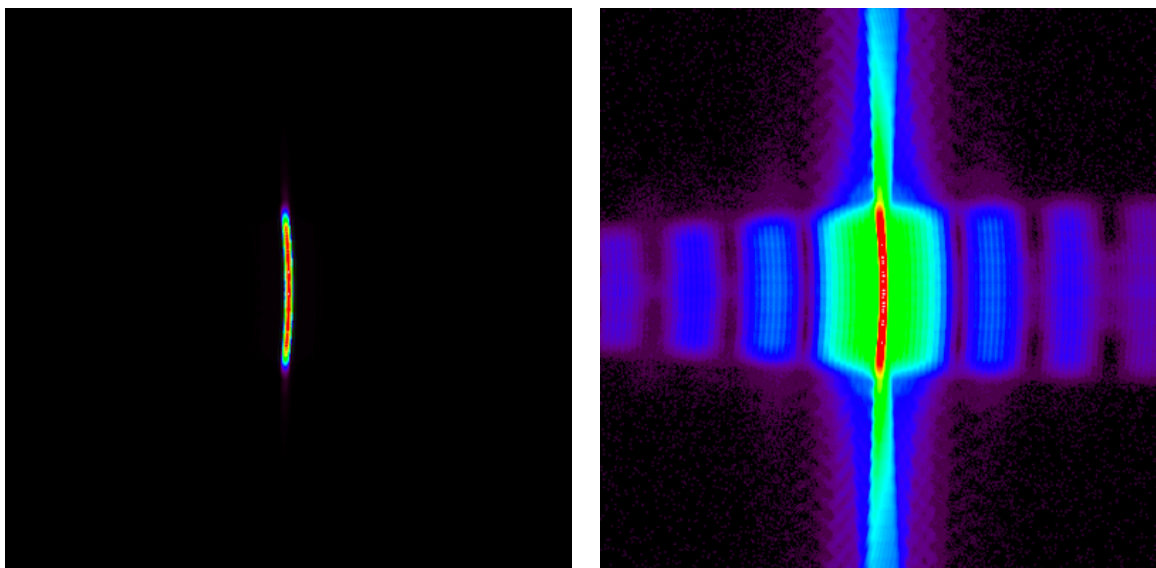


Figure 32: simulation at $\lambda = 40 \text{ \AA}$, 2 mm field, of the MM with the primary stack misaligned with respect to the secondary one. Rotation around the y -axis by 40 arcsec. (left) Linear color scale, (right) log color scale.