



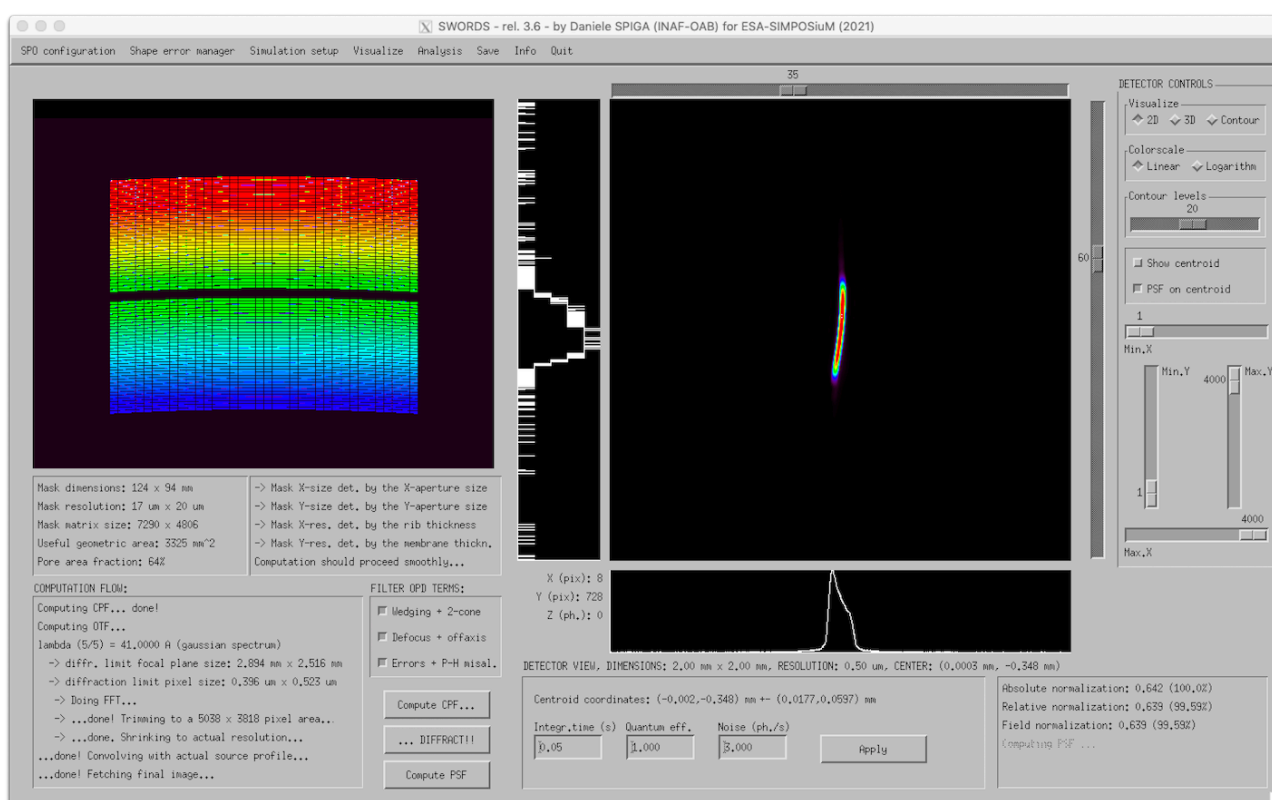
<i>Publication Year</i>	2021
<i>Acceptance in OA</i>	2023-02-01T13:14:05Z
<i>Title</i>	SWORDS - SoftWare fOR Diffraction Simulation of silicon pore optics: the user manual
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<i>Handle</i>	http://hdl.handle.net/20.500.12386/33097
<i>Volume</i>	INAF-OAB internal report 2021/06

 	SWORDS – SoftWare fOR Diffraction Simulation of silicon pore optics: the user manual				
Code: 06/2021 DOI: 10.13140/RG.2.2.22411.36647	OAB Technical Report	Issue: 3	1	Class	Page: 1 / 34

Advanced Telescope for High-Energy Astrophysics (ATHENA)

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

*Technical note by **D. Spiga** (INAF/OAB) on behalf of the **SimPOSIUM** (Silicon Pore Optics Simulation and Modelling) collaboration*



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Applicable documents

- [AD1]. "ATHENA SIMPOSiuM CCN1 SOFTWARE VALIDATION REPORT", TN5 - SOFTWARE VALIDATION REPORT (SVR)- Issue1
- [AD2] D. Spiga, "SPO diffraction simulation software for the ESA-SImPOSIUM project: the user manual," INAF/OAB internal report 04/2020

Reference documents

- [RD1]. Spiga, D., Christensen, F. E., Bavdaz, M., et al., "Simulation and modeling of silicon pore optics for the ATHENA x-ray telescope," **Proc. of SPIE**, Vol. 9905, 99055O (2016)

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- [RD2]. Spiga, D., Della Monica Ferreira, D., Shortt, B., et al., “Optical simulations for design, alignment, and performance prediction of silicon pore optics for the ATHENA x-ray telescope,” **Proc. of SPIE**, Vol. 10399, 103990H (2017)
- [RD3]. Sironi, G., Spiga, D., Della Monica Ferreira, D., et al., “Simulating the optical performances of the ATHENA x-ray telescope optics,” **Proc. of SPIE**, Vol. 10699, 103993N (2018)
- [RD4]. G. Sironi, D. Spiga, A. Moretti, G. Pareschi, G. Tagliaferri, D. Della Monica Ferreira, E. Bergbäck Knudsen, A. S. Jegers, I. Ferreira, M. Bavdaz, “Open-source simulator for ATHENA X-ray telescope optics,” **Proc. of SPIE** Vol. 11822, 118220I (2021)
- [RD5]. Raimondi, L., Spiga, D., "Mirrors for X-ray telescopes: Fresnel diffraction-based computation of point spread functions from metrology," **Astronomy & Astrophysics**, Volume 573, A22 (2015)
- [RD6]. Spiga, D., Raimondi, L., Svetina, C., et al., “X-ray beam-shaping via deformable mirrors: Analytical computation of the required mirror profile,” **Nuclear Instruments and Methods in Physics Research A** 710, 125–130 (2013)
- [RD7]. R. Willingale, R. Spaan, "Improving the angular resolution of the conical Wolter-I silicon pore optics (SPO) mirror design for the International X-ray Observatory (IXO)," *Proc. of SPIE* 7732, 773241 (2010)

Acronyms

ATHENA Advanced Telescope for High-Energy Astrophysics

CPF Complex Pupil Function

DoF Degrees of Freedom

DTU Denmark Technical University

ESA European Space Agency

EE Encircled Energy

FFT Fast Fourier Transform

GUI Graphical User Interface

HEW Half Energy Width

IDL Interactive Development Language

INAF Istituto Nazionale di Astrofisica

IP Intersection Plane

ISR Intermediate Software Review

MM Mirror Module

OAB Osservatorio Astronomico di Brera

OPD Optical Path Difference

OTF Optical Transfer Function

PSF Point Spread Function

PtV Peak to Valley

SimPOSIUM Silicon Pore Optics SimUlation and Modelling

SPO Silicon Pore Optics

SWORDS SoftWare fOR Diffraction Simulation of silicon pore optics

VM Virtual Machine

XOU X-ray Optical Unit

W90 Angular diameter including 90% of the focused rays

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1. Introduction

This brief document is a quick guide through the usage of SWORDS, a SPO diffraction simulation tool developed in the SImPOSIUM project for the ATHENA X-ray telescope [RD1-RD4] under IDL[®] environment.¹ This tool allows the user to simulate the PSF of an SPO XOu or MM using physical optics, therefore including the effects of diffraction and figure errors, following the method described in [RD1, RD2]. This program, released to ESA in the ISR of the project [AD1], is to some extent the 2D equivalent of the WISE simulation code [RD5] working in 1D for grazing incidence mirrors. The code is still been developed, but already fully functional. A previous manual for the simulation tool (release 3.0) was already issued in 2020 [AD2]. **The current manual refers to the version 3.7.2 of SWORDS.**

Some new functionalities to the program include:

- correction of numerical bugs, label reorganization, and window restyling;
- uniform curvature profile as an alternative to Wolter-I;
- gaussian line profile for non-monochromatic sources;
- gaussian-shaped sources;
- random (quasi-gaussian) phases in sinusoidal errors;
- random (quasi-gaussian) amplitudes in sinusoidal errors;
- memory cleanup during and after each routine execution;
- improved computation speed by exchanging image cropping and resampling;
- custom path selectable by the user;
- added P-H misalignment around the z-axis;
- constraint to minimum pixel size;
- maximum CCD array size limited to 4000 × 4000;
- azimuthal edge effects;
- 2D polynomial errors;
- aberrations due to finite distance and off-axis of the source;
- capability to load and use a set measured plate(s) figure error from ASCII file(s);
- inclusion/exclusion of the OPD terms into/from the computation of the diffraction figure;
- wavefront leveling for keeping the focal spot centered in the field;
- automatic best focus computation;
- *.fits output formatted to match fits standards (thanks to Arne's advices!).

Depending on the operative system and the graphical interface in use, the interface might have a different aspect and the position of the components might require some adjustment. In case, you are cordially invited to contact the author to make the necessary changes.

¹ https://www.l3harrisgeospatial.com/docs/using_idl_home.html

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2. Using SWORDS

2.1. First steps

2.1.1. Downloading and running the program

SWORDS is a GUI application, written in IDL. Release 3.7.2 is provided in two versions:

- 1) just like the previous versions, **as an IDL executable file `SWORDS_r3_7_2.sav`**; this version works on MacOS, Windows, and Linux platforms, but it requires the computer to have IDL installed because there is no IDL Virtual Machine included in it. Anyway, no IDL license is required. After installing IDL, simply double click on the file `SWORDS_r3_7_2.sav` icon to start the program. The program can also be launched from terminal, saving the `.sav` file in your home directory, then typing the following command line: `idl -vm = SWORDS_r3_7_2.sav`
- 2) from the 3.7 release on, SWORDS is also distributed **as a stand-alone application** that can be run **without having IDL installed**; no IDL license is required either. As of today, the regular operation of this self-standing version has been generated and tested **under MacOS and Windows**. A Linux version will follow shortly. The distribution comes along with an IDL VM embedded in it, using the `MAKE_RT` method.² All the necessary files are included in a package **`SWORDS_r3_7_2.zip`**, (**`SWORDS_r3_7_2_WIN.zip`** for the Windows release) which can be downloaded and unpacked in any user's directory. Then, simply double-clicking the script **`SWORDS_r3_7_2.app`** (**`SWORDS_r3_7_2_WIN.exe`** for the Windows release) will launch the IDL VM, and, upon pressing "OK", the SWORDS application.

Both versions can be downloaded from this link:

https://drive.google.com/drive/folders/1mCqIS0DCEJxqgo_VYmQNIQyNaigE5UD

Prior to running either option **under MacOS**, *make sure that you have the XQuartz graphical tool³ installed and up-to-date*. When the code is run for the first time, the GUI is visualized along with a warning message. When the "OK" button is pressed, the program writes three configuration files to the user's home directory: `SPO_MM_geometry.bin`, `SPO_MM_error_par.bin`, `SPO_MM_srcdet.bin`. These will contain the parameter values and populated with default values. The next time the program is launched, the values entered by the user will be loaded automatically, so the message should not be displayed anymore.

NOTA BENE: all the sub-windows/tabs are modal, i.e., they **mandatorily** have to be saved/closed before being allowed to return to the main interface.



² https://www.l3harrisgeospatial.com/docs/CreatingDistributionUsingMAKE_RT.html

³ <https://www.xquartz.org/>

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2.1.2. Getting familiar with the interface

If the configuration files have been correctly created, the GUI appears as in Figure 1. Most of the information contained in these panels is initially unavailable. As the computation goes by, the panels are enabled gradually.

We can recognize different elements:

- the upper menu activates the tabs that allow the user to input the parameters for the SPO MM (such as radius, focal length, wedge configuration, profile errors, source and detector distance, rib and membrane thickness, etc.);
- the viewgraphs are used to display the aperture of the SPO MM and the simulated diffraction figure;
- the *COMPUTATION FLOW* panels display the computation as it unfolds, and critical numbers obtained during the computation (such as matrix size, sampling and dimensions of the aperture pupil);
- the *FILTER OPD TERMS* button bar allows the use to select/deselect different components of the OPD, as visible in the left viewgraph, in the computation of the diffraction pattern;
- the *DETECTOR CONTROLS* panel gives the user mastery on the magnification of the simulated image and the image style (2D, 3D, contour plot, lin/log scale, etc.);
- the *DETECTOR VIEW* panel provides information on the centroid coordinates and simulates some detector settings, without the need to recalculate the diffraction pattern;
- the buttons allow the user to start the parameter elaboration and/or the PSF computation.

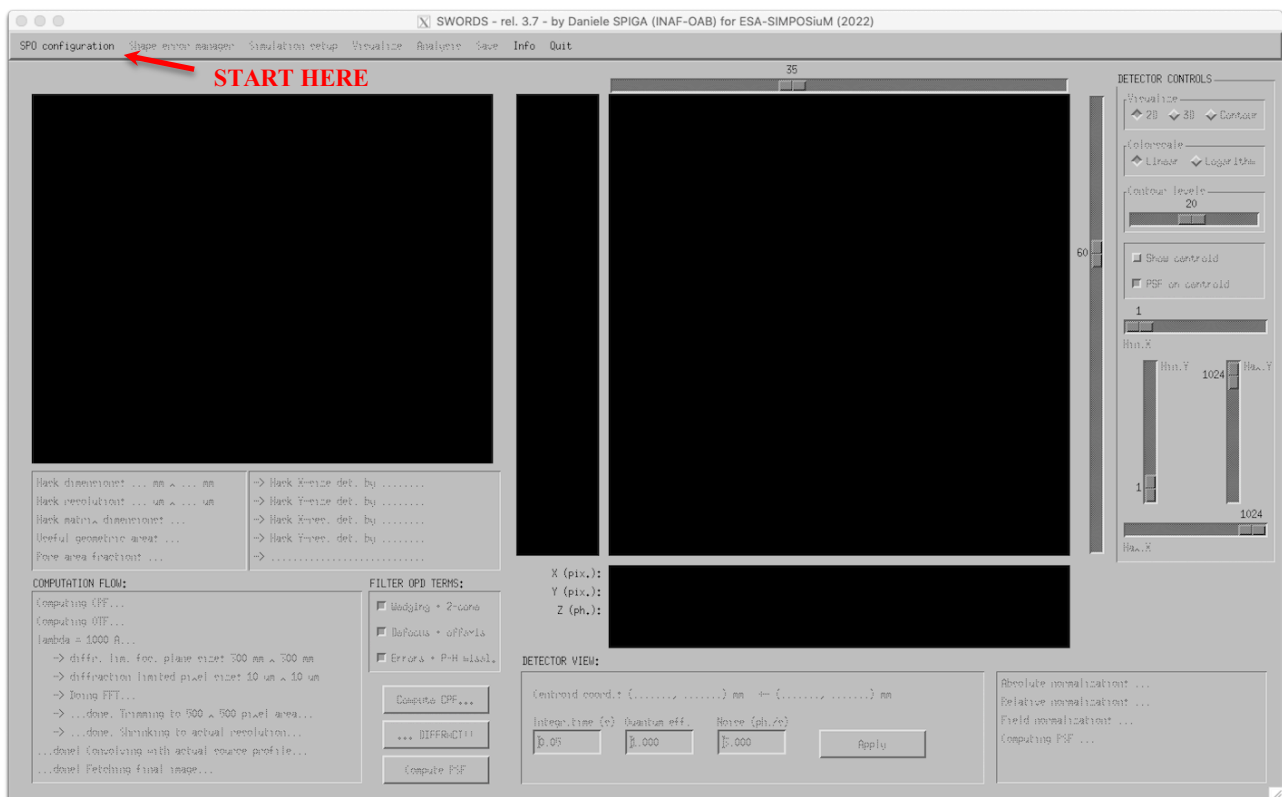


Figure 1: the SWORD 3.7 GUI at the program start. Most of the information is initially hidden.

2.2. Defining the MM setup

2.2.1. *SPO geometric parameters*

Firstly, the user selects the *SPO configuration* menu (Figure 1), and the *Single SPO MM...* submenu. Other options regarding multiple MMs are not implemented yet. After doing this, Figure 2 shows the tab that is displayed to the user. Some parameters are explained, others should be self-explanatory. Double-cone, Wolter-I, uniform curvature [RD7] longitudinal profiles can be selected, along with the option of having a single or a double stack. Other variables that can be set are: pore width, pore height, rib thickness (either constant or variable), membrane thickness, plate width and length, number of plates, central radius and focal length, overall module rotation, and wedge configuration (-1/+1, 0/+2, +1/+3). Values left blank are treated as zeroes. The user can also customize the default path where data can be loaded from or saved to.

When all the values are updated, press *Exit* to reject the changes or *Save* to write the updated values to the file *SPO_MM_geometry.bin*. In order to enable the next step, saving the values is **mandatory** the first time after starting the GUI. This approach is oriented to ensuring that the user has inspected the previously saved parameter values. Pressing *Save* then enables the next tab, the *Shape error manager* (Figure 3).

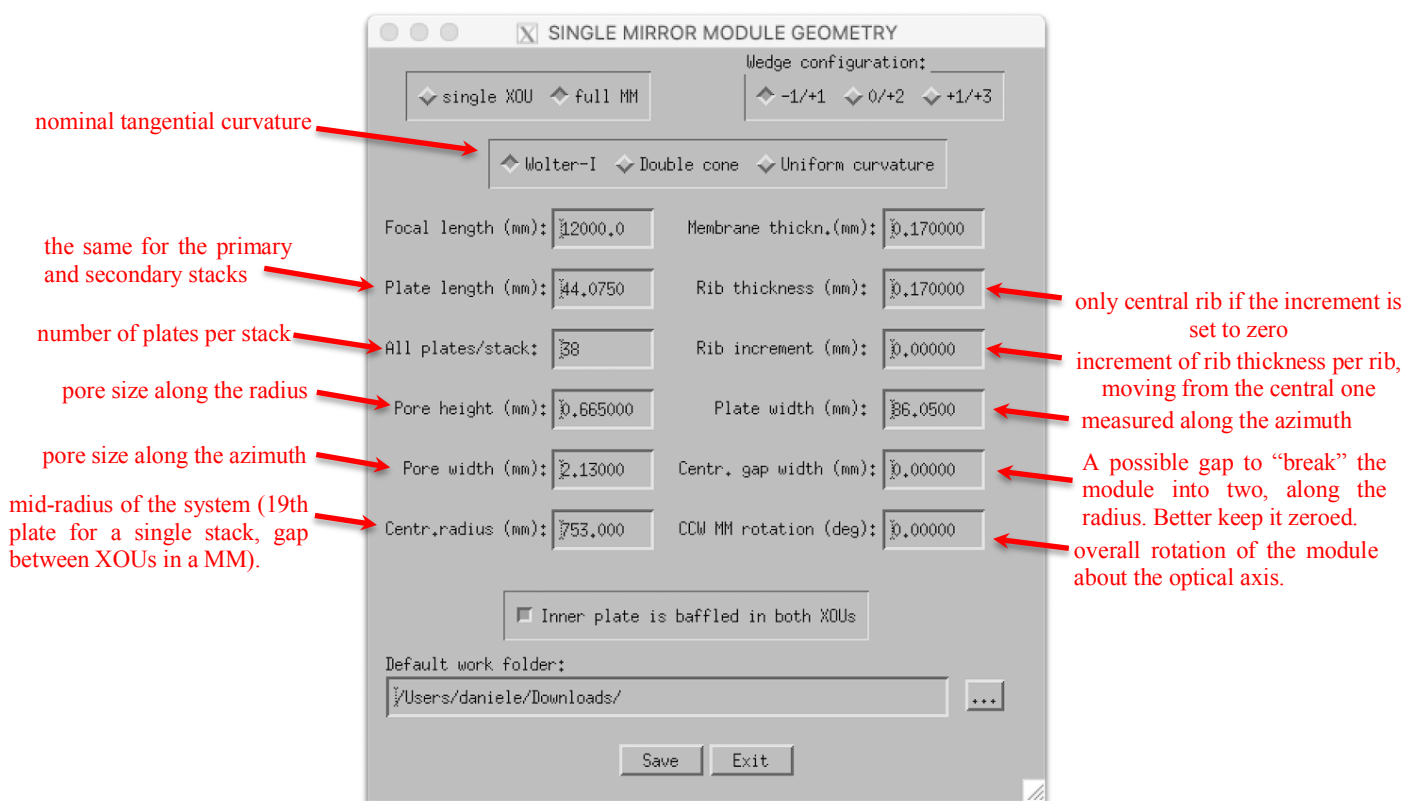


Figure 2: the input window for the single MM definition.

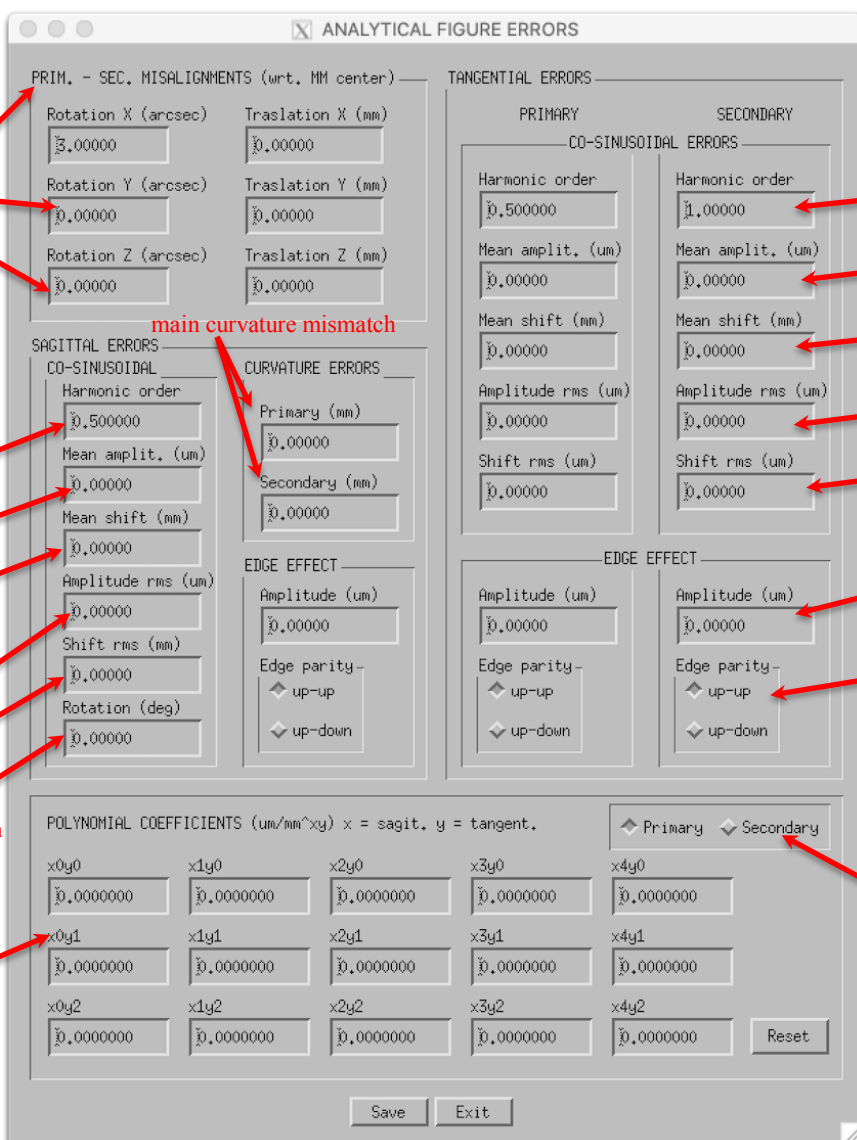


Figure 3: the Shape error manager menu is enabled after saving the geometric parameters of the MM.

2.2.2. Analytical profile errors and stack misalignments

Selecting the *Shape error manager* currently offers two options: the submenus *Analytical errors...* and *Tabulated errors...*. The first selection, the only one that is initially enabled, opens the tab in Figure 4. A variety of different shape errors are displayed, divided into 4 main sections:

- 1) *PRIM. – SEC. MISALIGNMENTS*: these are the alignment errors between the parabolic and the hyperbolic stack, 3 rotations and 3 translations. The user should refer to the reference frame in Figure 5. The rotation about z has been implemented in the current release also.
- 2) *SAGITTAL ERRORS*, errors in the azimuthal (= sagittal) shape with respect to the perfect symmetry around the optical axis. They can be of the following species:



PRIM. – SEC. MISALIGNMENTS (wrt. MM center)

- Rotation X (arcsec): 0.00000
- Rotation Y (arcsec): 0.00000
- Rotation Z (arcsec): 0.00000
- Traslation X (mm): 0.00000
- Traslation Y (mm): 0.00000
- Traslation Z (mm): 0.00000

SAGITTAL ERRORS

- CO-SINUSOIDAL**
 - Harmonic order: 0.500000
 - Mean amplit. (um): 0.00000
 - Mean shift (nm): 0.00000
 - Amplitude rms (um): 0.00000
 - Shift rms (nm): 0.00000
 - Rotation (deg): 0.00000
- CURVATURE ERRORS**
 - Primary (nm): 0.00000
 - Secondary (nm): 0.00000
- EDGE EFFECT**
 - Amplitude (um): 0.00000
 - Edge parity: up-up

TANGENTIAL ERRORS

- PRIMARY**
 - Harmonic order: 0.500000
 - Mean amplit. (um): 0.00000
 - Mean shift (nm): 0.00000
 - Amplitude rms (um): 0.00000
 - Shift rms (um): 0.00000
- SECONDARY**
 - Harmonic order: 1.00000
 - Mean amplit. (um): 0.00000
 - Mean shift (nm): 0.00000
 - Amplitude rms (um): 0.00000
 - Shift rms (um): 0.00000
- EDGE EFFECT**
 - Amplitude (um): 0.00000
 - Edge parity: up-up

POLYNOMIAL COEFFICIENTS (um/mm²xy) x = sagit. y = tangent.

x0y0	x1y0	x2y0	x3y0	x4y0
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000

Selection between primary and secondary stack for the polynomials: Primary Secondary

Buttons: Save Exit

Annotations:

- mutual misalignments of the two sections in 6 DoF (points to PRIM. – SEC. MISALIGNMENTS)
- main curvature mismatch (points to CURVATURE ERRORS)
- plate width to period of the cosine ratio (points to CO-SINUSOIDAL Harmonic order)
- 1/2 the PtV (points to CO-SINUSOIDAL Mean amplit. (um))
- shift of the cosine wrt central ribs (points to CO-SINUSOIDAL Mean shift (nm))
- quasi-gaussian random variation of the amplitude and of the shift in the stack (points to CO-SINUSOIDAL Amplitude rms (um) and Shift rms (nm))
- rotation around y-axis of the sinusoidal pattern (points to CO-SINUSOIDAL Rotation (deg))
- coefficients for a polynomial deformation in x and y, for either reflection (points to POLYNOMIAL COEFFICIENTS)
- plate length to period of the cosine ratio (points to TANGENTIAL ERRORS SECONDARY Harmonic order)
- 1/2 the PtV (points to TANGENTIAL ERRORS SECONDARY Mean amplit. (um))
- shift of the cosine wrt plate center (points to TANGENTIAL ERRORS SECONDARY Mean shift (nm))
- quasi-gaussian random variation of the amplitude and of the shift in the stack (points to TANGENTIAL ERRORS SECONDARY Amplitude rms (um) and Shift rms (um))
- amplitude of the edge flexure at plate ends (points to TANGENTIAL ERRORS EDGE EFFECT Amplitude (um))
- selection between odd and even profiles (points to TANGENTIAL ERRORS EDGE EFFECT Edge parity)
- selection between primary and secondary stack for the polynomials (points to Primary Secondary selection)

Figure 4: input parameters for modelling analytical profile errors.

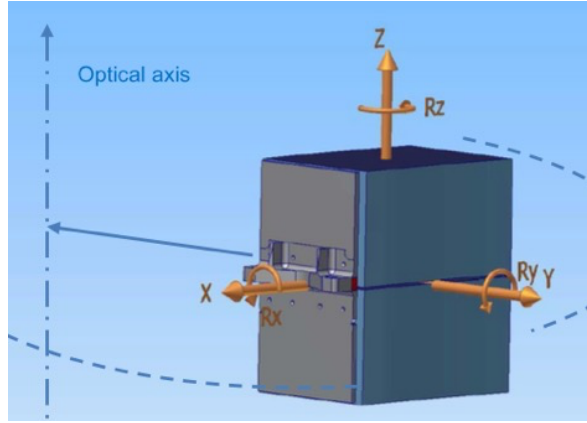


Figure 5: the standard reference frame for mirror module roto-translations (credits: Media-Lario).

- a. **CO-SINUSOIDAL ERRORS:** they are modeled as single harmonics (with the same parameters for both stacks) that can be superposed to the perfectly circular profile, with a specified period in units of the plate width. For example, a 0.5 value in the *Harmonic order* field means a period twice as large as the plate width, while a 3 input therein means a period that is 1/3 of the plate width. The *Mean amplitude* parameter denotes the average amplitude of the perturbation (1/2 the peak to valley over a full period) and it is a constant if the *Amplitude rms* is set to zero. Otherwise, the amplitude will oscillate throughout the stack around this value, in a quasi-gaussian distribution having the rms selected. We term with “quasi-gaussian” a distribution like $1/\cosh^2(x/0.6)$, which is almost identical to a gaussian with $\sigma = 1$, and allowing a CPF construction much faster than a gaussian. The *Mean shift* expresses the displacement of the cosine peak with respect to the central ribs, and it can be a constant or follow a quasi-gaussian distribution, depending on the value set in *Shift rms*. All the sinusoidal pattern can be rotated around the plate normal by the angle specified in *Rotation* (in this way one can, e.g., simulate a sinusoidal grating on the plates with a certain orientation).
- b. **CURVATURE ERRORS:** it represents a mismatch of the curvature radii, separately for the primary the “parabola” and the secondary the “hyperbola” wrt the nominal distance to the optical axis.
- c. **EDGE EFFECT:** profile error imparted to each plate of each stack, with marked deformations at the edges, in the transverse direction profile, in order to return a Lorentian PSF. The profile error has the following expression [RD4, RD5, RD6], as a function of the curvilinear coordinate of each plate, s , along the azimuth, computed from its center:

$$\epsilon_0(s) = -A \log \cos \frac{\gamma s}{W}$$

where A is the error PtV and W the width of the single plate, and γ is a constant close to π (and slightly less than π in order to avoid the edges go to infinity). The profile $\epsilon_0(s)$ is an even function (up-up), but it is also offered in an “odd” version (up-down) as follows:

$$\epsilon_1(s) = \begin{cases} +\epsilon_0(s) & \text{for } s > 0 \\ -\epsilon_0(s) & \text{for } s < 0 \end{cases}$$

which yields exactly the same HEW value, but – unlike $\epsilon_0(s)$ – it causes a displacement of the centroid.

- 3) **TANGENTIAL ERRORS,** errors in the longitudinal (= tangential) profile with respect to the nominal profile along the meridians (double cone, Wolter-I, or uniform curvature):
 - a. **CO-SINUSOIDAL ERRORS:** just like co-sinusoidal errors, but in the longitudinal direction. The origin is set at the P-H intersection plane. The selection can be different for the parabolic and the

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hyperbolic stack. Just like at point 2a), the phases and the amplitudes can be randomized as per a quasi-gaussian distribution around the mean value, acting on the same parameters.

- b. *EDGE EFFECT*: profile error imparted to each plate of each stack, in order to return a Lorentian PSF. The profile error has the following expression [RD4, RD5, RD6], as a function of the radial coordinate of each plate, r^* , computed from its center:

$$\epsilon_0(r^*) = -A \log \cos \frac{\pi r^*}{L\alpha}$$

where L is the length of the single plate, A the PtV of the profile, and α the incidence angle. The profile $\epsilon_0(r^*)$ is an even function (up-up), but it is also offered in an “odd” version (up-down) as follows:

$$\epsilon_1(r^*) = \begin{cases} +\epsilon_0(r^*) & \text{for } r^* > 0 \\ -\epsilon_0(r^*) & \text{for } r^* < 0 \end{cases}$$

which yields exactly the same HEW value, but – unlike $\epsilon_0(r^*)$ – it causes a displacement of the centroid.

- 4) *POLYNOMIAL ERRORS*: the error is computed as a 2nd-order polynomial in the tangential direction and a 4th-order polynomial in the sagittal direction, the same for all plates in the primary and in the secondary separately. The user can switch from the primary to secondary stack using the *1-ary/2-ary* buttons on the right. The coefficients can be directly input by the user to model a figure error in microns. The tangential and the sagittal coordinate are assumed to be in millimeters. The *Reset* button zeroes the coefficients for the selected reflection.

Pressing the *Save* button then writes the parameters to another configuration file (SPO_MM_error_par.bin) and closes the tab, enabling the next tab, the *Simulation Setup* (Figure 6). Saving the values is **mandatory** the first time after starting the GUI. The user is also allowed to return to the *SPO configuration* menu and update/correct the tables if needed. This action **will not require** the user to open and save the shape error manager again. The submenu *Tabulated errors...* is now enabled under the *Shape Error Manager* main menu.

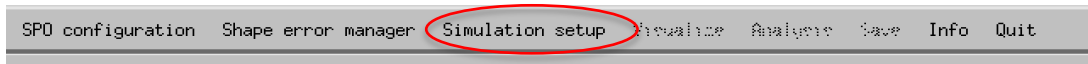


Figure 6: the Simulation setup menu is enabled after saving the shape error parameters of the MM.

2.2.3. Tabulated profile errors

Pressing *Tabulated errors...* another tab opens (Figure 7), allowing the user to upload measured surface errors and superimpose their maps to the modeled profile from the previous input. There is a separate selection for the primary stack and the secondary stack; the secondary maps will be flipped in the tangential coordinate to account for the common origin of the axial coordinates of the two segments at the IP.

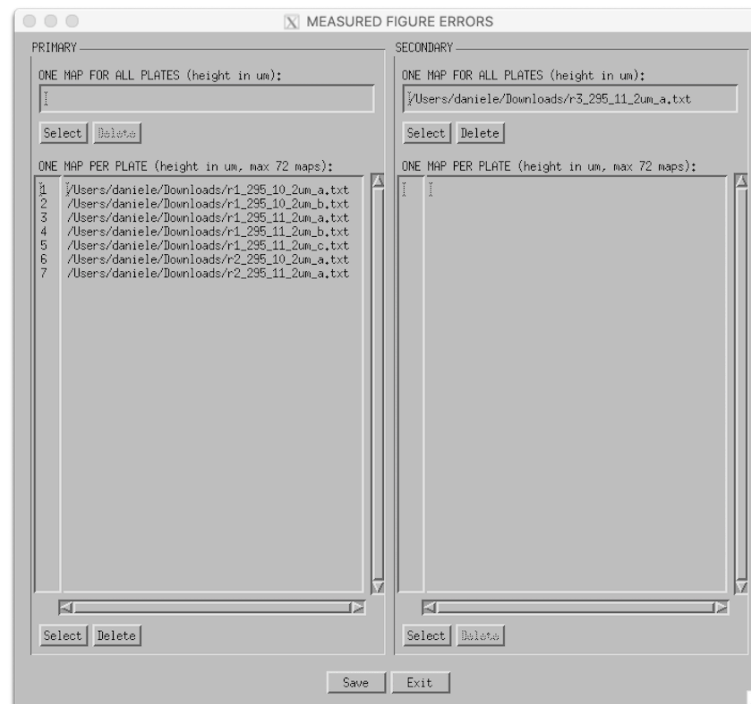


Figure 7: input parameters for including profile errors in the model.

For each stack, the user has two mutually-excluding options:

- uploading the same map to all the plates (upper panel), choosing the right file in txt format. The file has to contain an ASCII matrix, expressing the figure error with the height in microns. Any matrix size and resolution **will be ignored**: the map will rather be stretched in order to fit the plate dimensions. Pressing the button *Select* activates the file search, while pressing *Delete* will remove the file path from the memory, that will no longer be used in the computation. Selection/removal can be made for either reflection (primary and/or secondary), using the same map or different ones.
- uploading a set of ASCII maps using the lower panel, and selecting multiple text files with the same format. In this case also, the height is in microns and the maps will be stretched to fit the plate size. The selection removes any file path left in the “one map for all plates” selection. The files are numbered as the plates, from bottom to top of the double stack.

In any case, the selected files are briefly checked that the format is correct before the user can press the *Save* button and so return to the main panel.

2.2.4. Setting up the source and the detector

Selecting *Simulation setup* in the upper menu (Figure 6) opens the 3rd main tab, displayed in Figure 8. This tab includes important settings for the light source (on the left) and the detector (on the right). The light source *Wavelength*, in angströms, is referred to either a monochromatic light wavelength *or* to the central wavelength of a polychromatic light band, whose *Bandwidth* can be specified. The band is in reality made up of a number of discrete components, separated by a *Lambda step* that has to be specified by the user. The source *Distance to IP* (usually, very large), the angular *Diameter* of the source (usually very small), the source *Power* at the module entrance, and the *Off-axis* angles in *x* and *y* have to be set by the user. The option of simulating a source with *Gaussian spectrum* (the “bandwidth” field then becomes the FWHM of the gaussian) or *Gaussian shape* (the “diameter” field then becomes the FWHM), is also implemented in the current release.

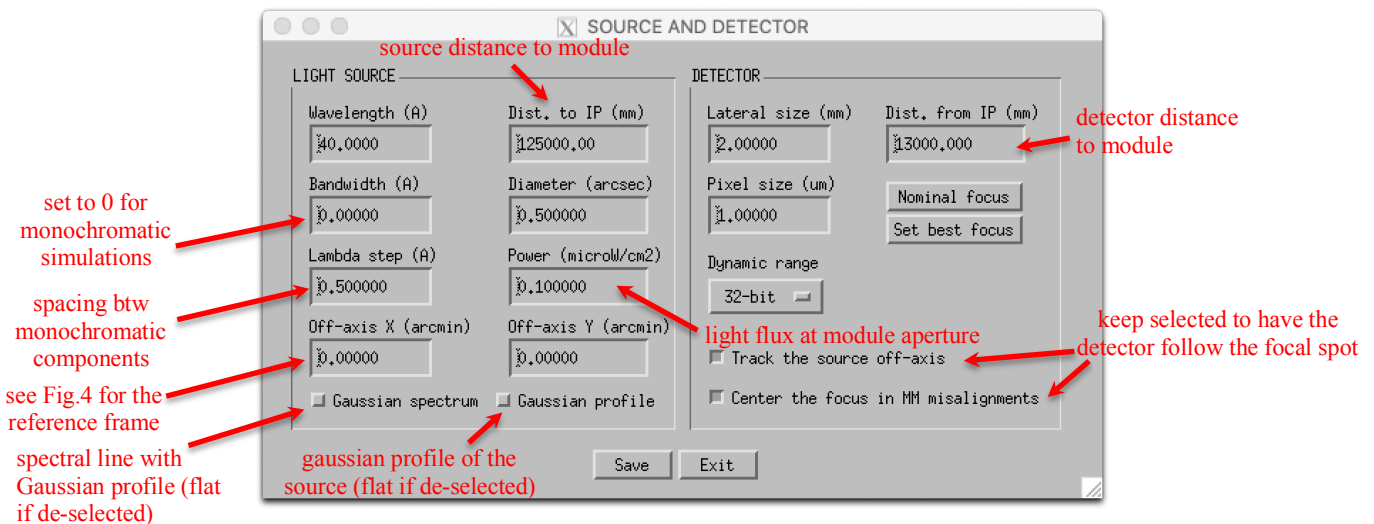
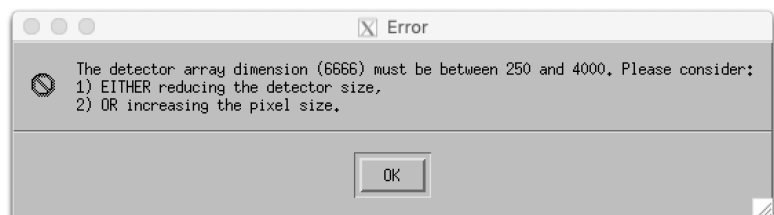
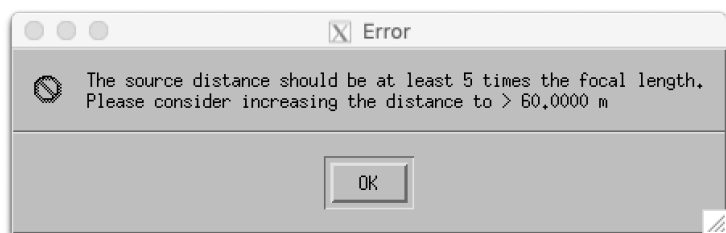


Figure 8: the simulation setup tab, including some settings for the light source and the detector.

As for the detector properties, it is always assumed to be a square area. The user can select the detector *Lateral size*, *Pixel size*, and the *Distance* from the mirror module IP, along with the *Dynamic range* (either 16-bit or 32-bit readout) and the ability to *track the source off-axis* or the focus centering when the two segments are misaligned (enabling the off-axis tracking is **recommended**). From version 3.7 on, a *Set best focus* button has been added. Pressing this button, the best focal distance is computed from the focal length and the source distance, and written in the tab (but not saved, until the user pushes the *Save* button). If the source distance is less than 5 times the focal length, an error message is raised and the user must correct either parameter before saving the data. In order to keep the computation time within acceptable limits, another error message might appear, asking the user to change some values exceeding software limits. For example:

- The detector array size has to range between 250 and 4000;
- The pixel cannot be smaller than the diffraction limit for the MM;
- The angular diameter of the source cannot exceed 150 times the pixel size;



Pressing the *Save* button then writes the parameters to the third configuration file (`SPO_MM_srcdet.bin`) and closes the tab, finally enabling the first simulation step (the *Compute CPF...* button, see Figure 9). Saving the values is **mandatory** the first time after starting the GUI. The user is also allowed to return to the *SPO configuration* and/or the *Shape error manager* menus, and update/correct the tables if needed. This action **will not require** the user to open and save the *Shape error manager* and the *Simulation setup* tabs again. However, this action will erase the CPF and the diffraction image viewgraphs.

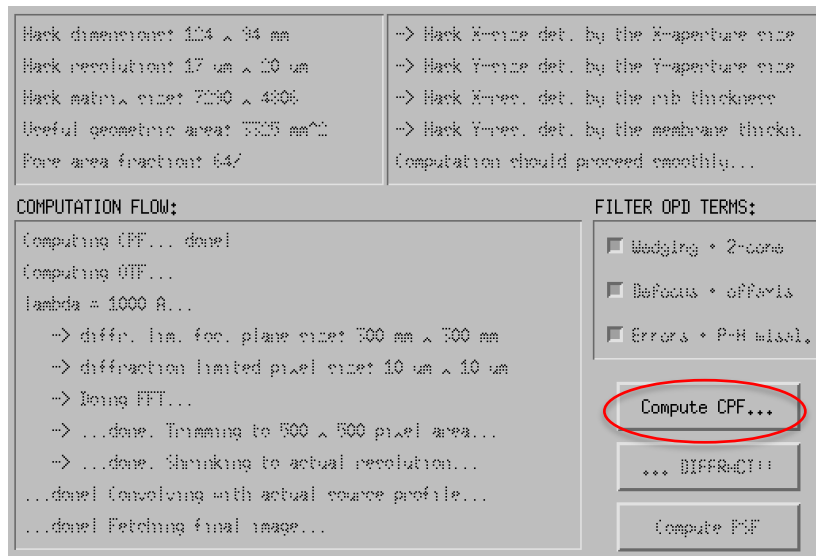


Figure 9: lower panels of the main interface after saving the simulation setup. The Compute CPF... button is now enabled.

2.3. Computing and viewing the Complex Pupil Function

2.3.1. The Complex Pupil Function

When the previous steps have been completed, the *Compute CPF...* button can be pressed. This starts the construction of the CPF, i.e., the MM structure model and the optical path difference (OPD) throughout the MM aperture. Assuming uniform illumination, the picture would represent the wavefront at the MM exit, just before the propagation to the observation plane. This is modelled as a matrix, called “mask” from this point on, where the optimal dimensions and the resolution are computed from some parameters previously entered (light wavelength, detector size, distance, resolution, rib and membrane thickness).

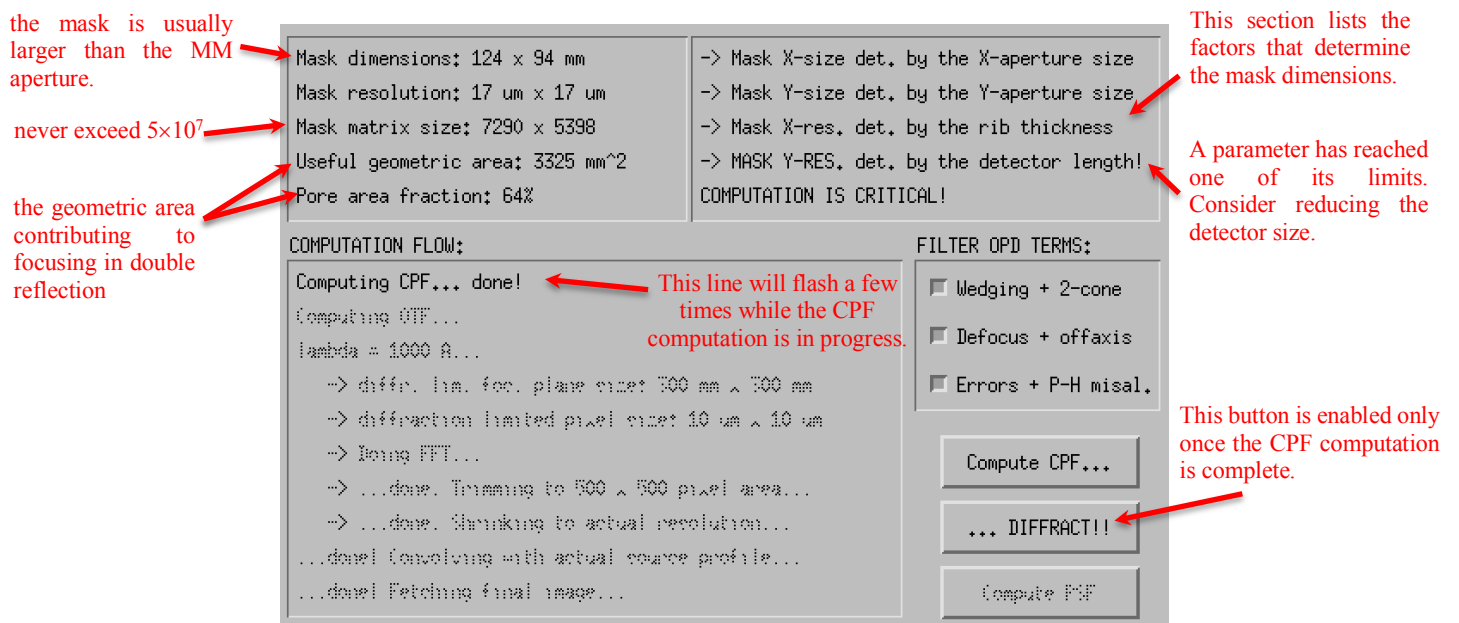
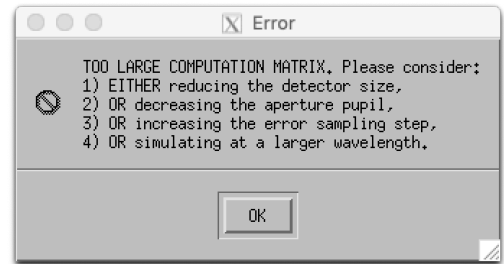


Figure 10: the left lower panel of the GUI at the end of the CPF computation.

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For example, the mask dimensions are exactly the ones needed to i) fully encapsulate the MM aperture and ii) return the desired resolution of the detector. Likewise, the mask resolution is determined by the strictest condition between iii) oversampling the rib and the membrane thickness and iv) return a diffracted image as extended as the detector area. The reasons behind these conditions are explained in detail in [RD1, RD2]. If either condition ii) or iv) is met, the matrix size is the maximum allowed value and the computation gets close to its limit. The mask properties are now displayed in the dedicated panel (see Figure 10). The right panel lists some detail on the factors impacting the mask size. When condition i) and iii) are verified, the last line will be *Computation should proceed smoothly...*, otherwise a warning message *COMPUTATION IS CRITICAL!* will appear in the same line. Anyway, **the mask size can never exceed 5×10^7 as maximum number of elements**. Otherwise, an error message is displayed, and the computation will stop. The user can subsequently follow the suggestions and so reduce the mask dimensions.



During the elaboration, the line *Computing CPF...* will flash a few times and all the controls are disabled. When the computation is complete, an image of the MM along with colors representing the OPD map is posted to the left viewgraph (Figure 11). This is a preliminary, essential step in order to compute the diffraction figure, which is basically obtained from the FFT of the CPF matrix. At last, additional elements are enabled (see Figure 10):

- the *FILTER OPD TERMS*: panel encompasses buttons that enable/disable different contributions to the OPD map (wedging+double cone, defocus+off-axis, errors and misalignments). Selecting elements automatically redisplay the requested terms.
- the *...DIFFRACT!* button is now enabled and can be pressed at any time. Before doing that, the user can return to the configuration tabs in the upper menu and correct some parameter values. If the new values are saved, however, the CPF image disappears and will have to be re-computed pressing *Compute CPF...* again, with the updated parameters.
- the *Save* button in the upper menu is now enabled, limited to the CPF visualization and saving (see next section).

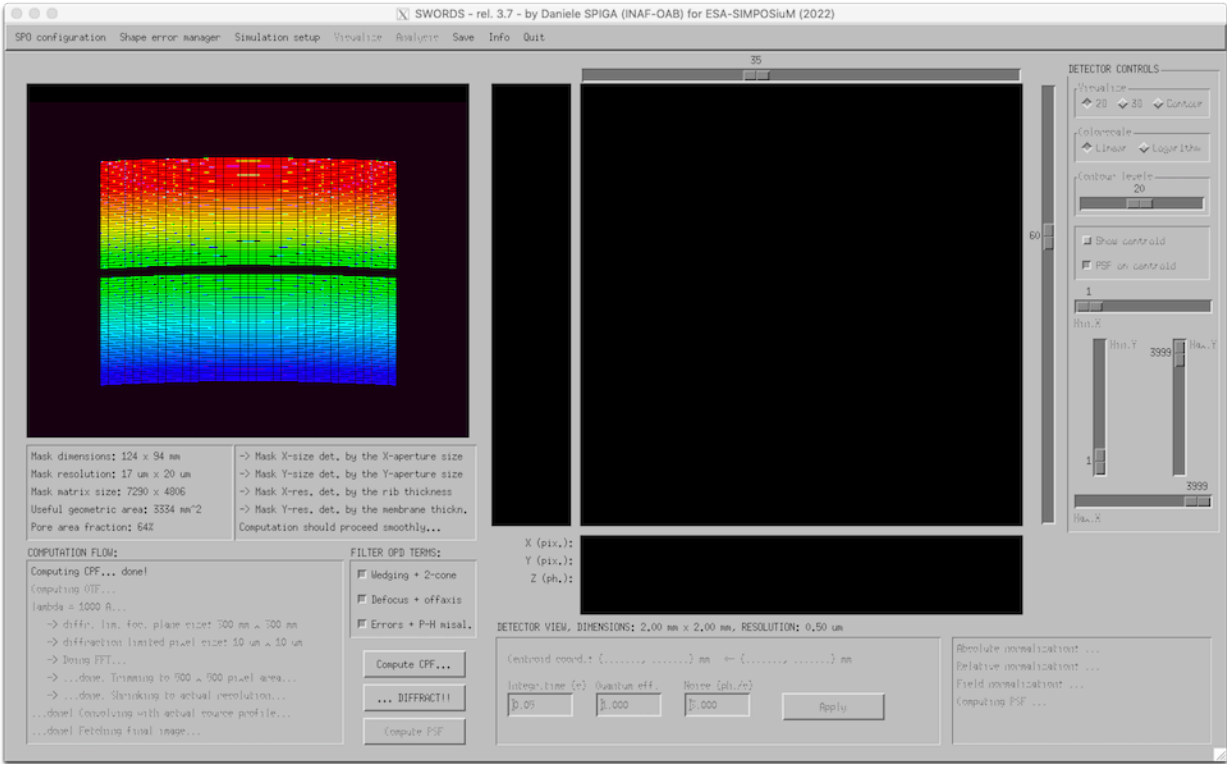


Figure 11: the main user interface after the CPF computation. More controls are available at this stage.

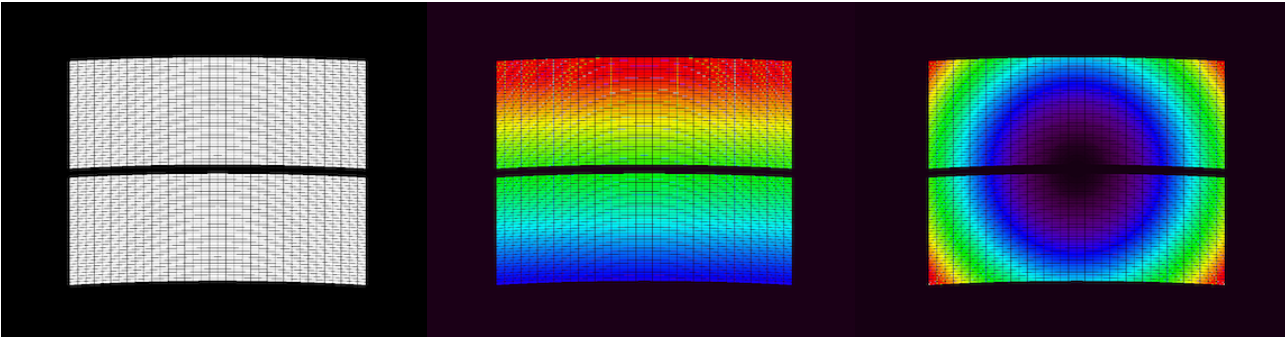


Figure 12: (left) no OPD terms selected, only the ribs and the membranes are visible. (center) the wedging+2-cone term. (right) the defocus+off-axis term.

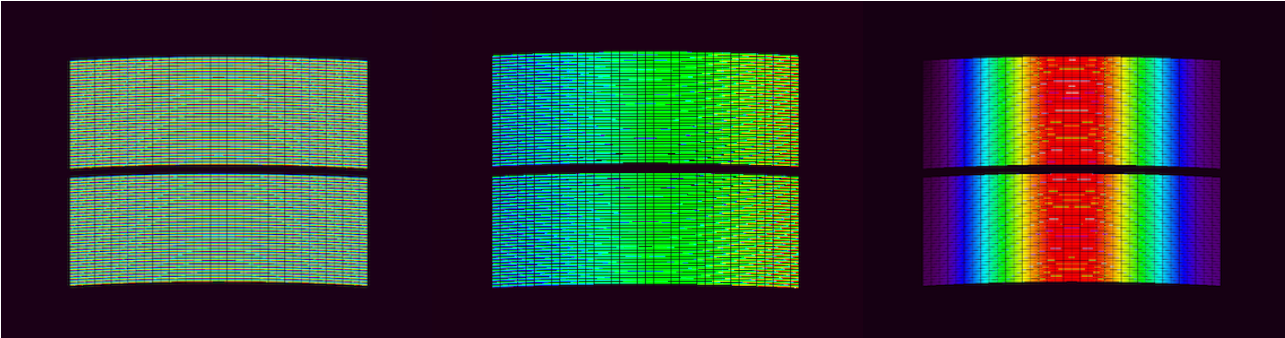


Figure 13: the errors+P-H misalign. term, in the presence of a (left) P-H rotation around x, (center) a P-H rotation around y, (right) a sinusoidal error in the sagittal direction.

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2.3.2. Exploring, viewing, and saving the CPF

After the visualization of the CPF, it becomes possible to calculate the diffraction figure pressing the ...*DIFFRACT!!* button, or repeat the CPF computation with different parameters. To better understand the factors affecting the CPF, the buttons in the *View OPD terms* can be selected or deselected. If all the terms are deselected, only the silicon structures are shown (Figure 12, left). Unlike previous versions, **only the selected terms** will be used to compute the FFT and will so contribute to the computation of the final diffraction figure. The CPF terms are saved as separate variables in an `SPO_diff_CPF.bin` file in the user's home directory.

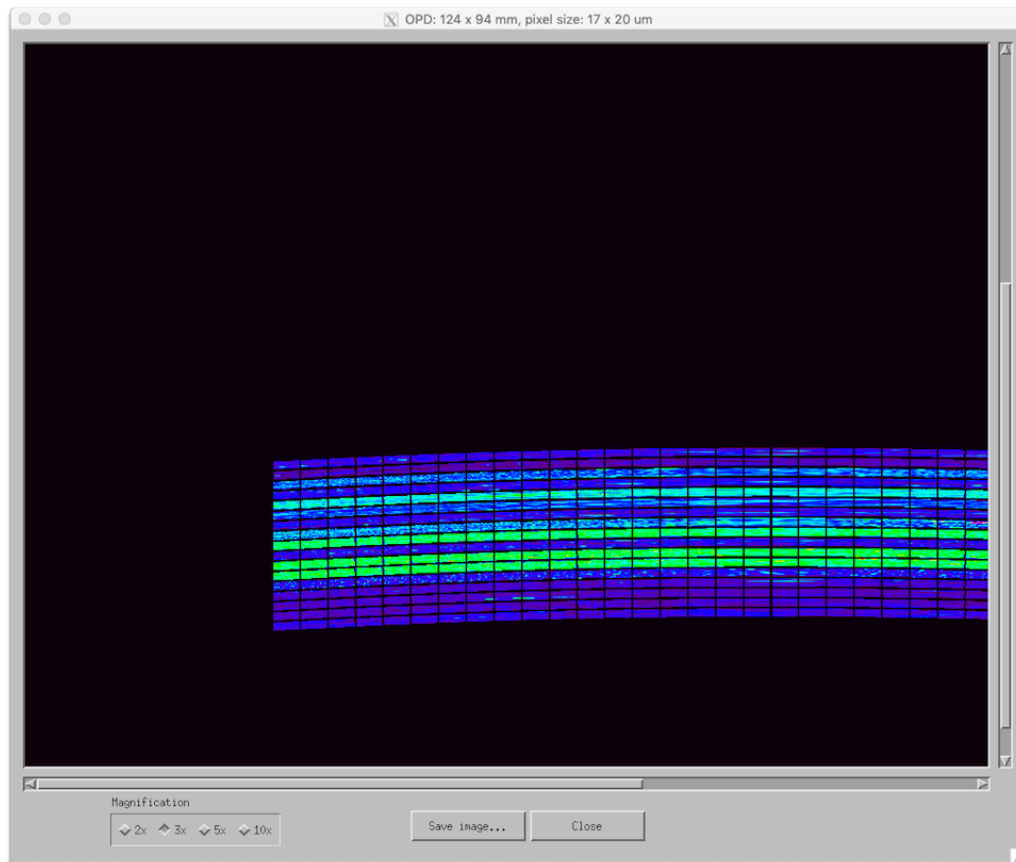


Figure 14: the OPD visualization window, in 3x magnification. 17 different error maps have been loaded and superposed to the plates from the bottom up. The wedging+double cone term has been de-selected.

- the *wedging + double cone* is usually the dominant term in the OPD map. The double cone term is clearly zero if the Wolter-I geometry was selected. The wedging term $R_n^2/2f$ is the responsible for the “rainbow” in Figure 12, center.
- the *defocus+off-axis* term includes the OPD contributions related to the finite distance of the source, the detector de-focusing, and the wavefront tilt due to off-axis setup of the source. This is shown in Figure 12, right.
- the *errors + P-H misalignments* term encompasses all the aberrations due to mirror defects and the wavefront deformations that are generated by profile errors in the tangential direction, the azimuthal direction, or by misalignments of the primary-secondary segments (see Figure 13).

Tangential errors are harder to spot in the CPF viewgraph, because the tangential direction is viewed compressed radially, while the dependence of sagittal errors is easier to inspect. Misalignments between primary and secondary stacks generate a variety of OPD maps (Figure 13, left). A better visualization of the OPD map can be achieved pressing in the upper menu *Save* → *View/Save CPF image...*, which opens another window showing a magnified view of the OPD map (Figure 14).

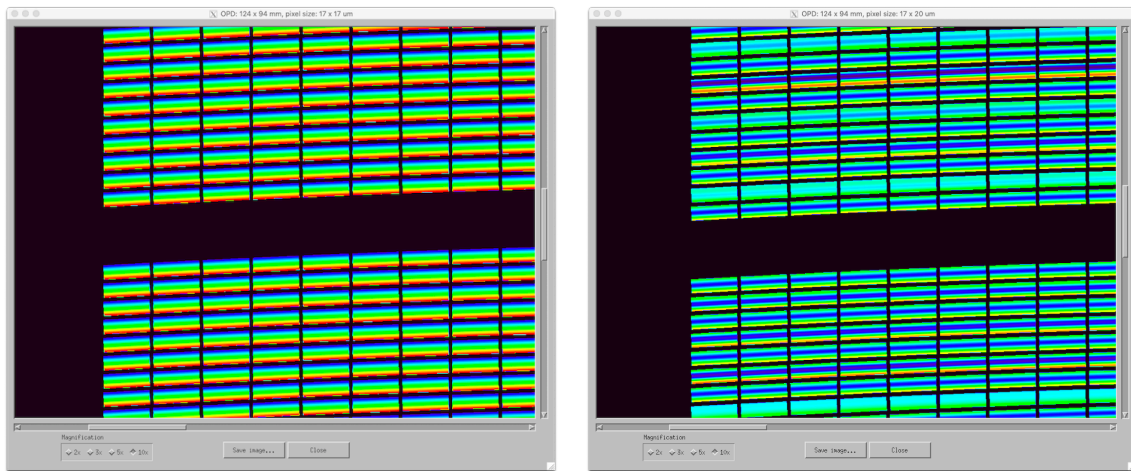
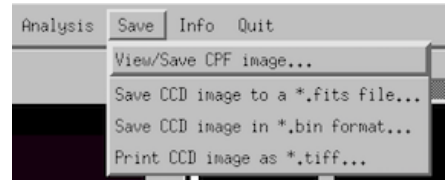


Figure 15: (left) the OPD visualization tab, in 10x magnification, for a sinusoidal error term added everywhere. (right) the same figure error, with amplitudes and phases randomized from plate to plate.

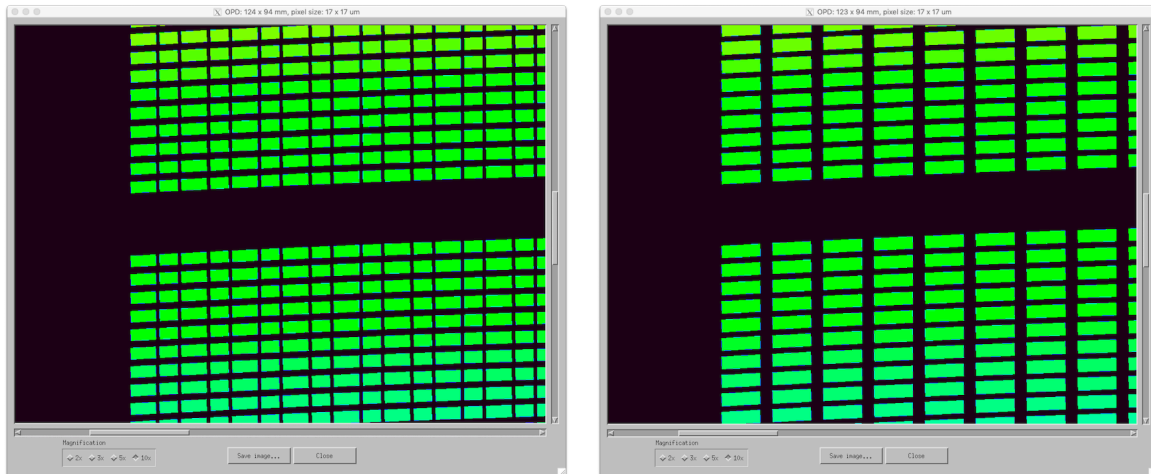


Figure 16: left: effects of a misalignment of the primary stack by -1 mm in the x direction. Ribs do not overlap anymore, with an apparent effect of “broken pores”. Right: off-axis source by 15 arcmin along x with increase of the rib vignetting.

Different magnifications can be selected to inspect the image in detail. The scrollable image shows the deformation imparted to the wavefront at the exit of each pore, for example when a tangential error is modeled (Figure 15). The image portion that is currently viewed can be saved in *.tiff format. The user can also easily inspect the effect of the misalignments of the two stacks (Figure 16, left), or the rib vignetting enhancement when the source goes off-axis (Figure 16, right).