WFSuite – User Guide

WFSuite is a graphical and command-line toolkit for **coded-mask-based X-ray wavefront sensing and phase reconstruction** at synchrotron beamlines.

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1. Installation

We suggest creating a virtual environment with virtualenv:

```
python3 -m pip install virtualenv
python3 -m venv "<path to virtual environments>/wf-suite"
source <path to virtual environments>/wf-suite /bin/activate
```

or conda:

```
conda create -y -n wf-suite python=3.1<0-3>
conda activate wf-suite
```

The program performs better with python 3.10+, and it has been tested up to python 3.13

To install it, run on a prompt of the target python environment:

```
python -m pip install wf-suite
```

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2. Global Usage and Launcher

2.1 Starting WFSuite

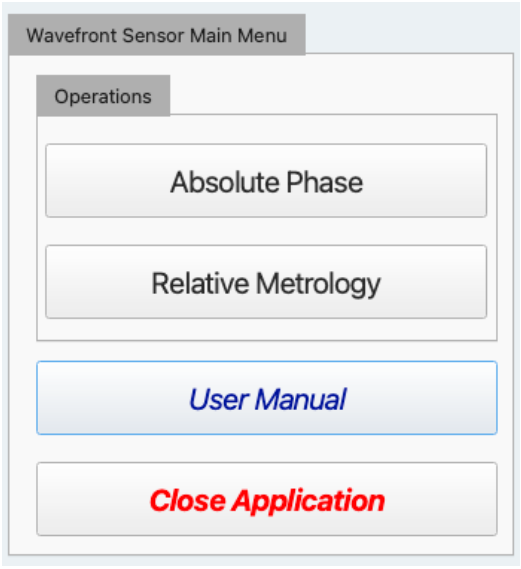
Launch the GUI launcher with:

```
python -m aps.wavefront_analysis Launcher
```

The launcher provides access to:

- Absolute Phase
- Relative Metrology
- Wavefront Sensor (automatically lunched with the GUI launcher)

All configuration is handled through the GUI and saved automatically.



2.2 Command-Line (Advanced / Batch Use)

Modules can also be launched directly:

```
python -m aps.wavefront_analysis <script_id> [options]
```

Common options:

- `--h` : show help
- `-m<N>` : logging mode
  - `0` GUI only (default)
  - `1` GUI + file
  - `2` stdout only
  - `3` stdout + file
- `-a<ACTION>` : batch-mode action (module-specific)

2.3 Configuration Persistence

- GUI settings are saved on exit.
- Configuration is stored locally as JSON (e.g. `.GUI_absolute_phase.json`).
- Settings are restored automatically on the next launch.

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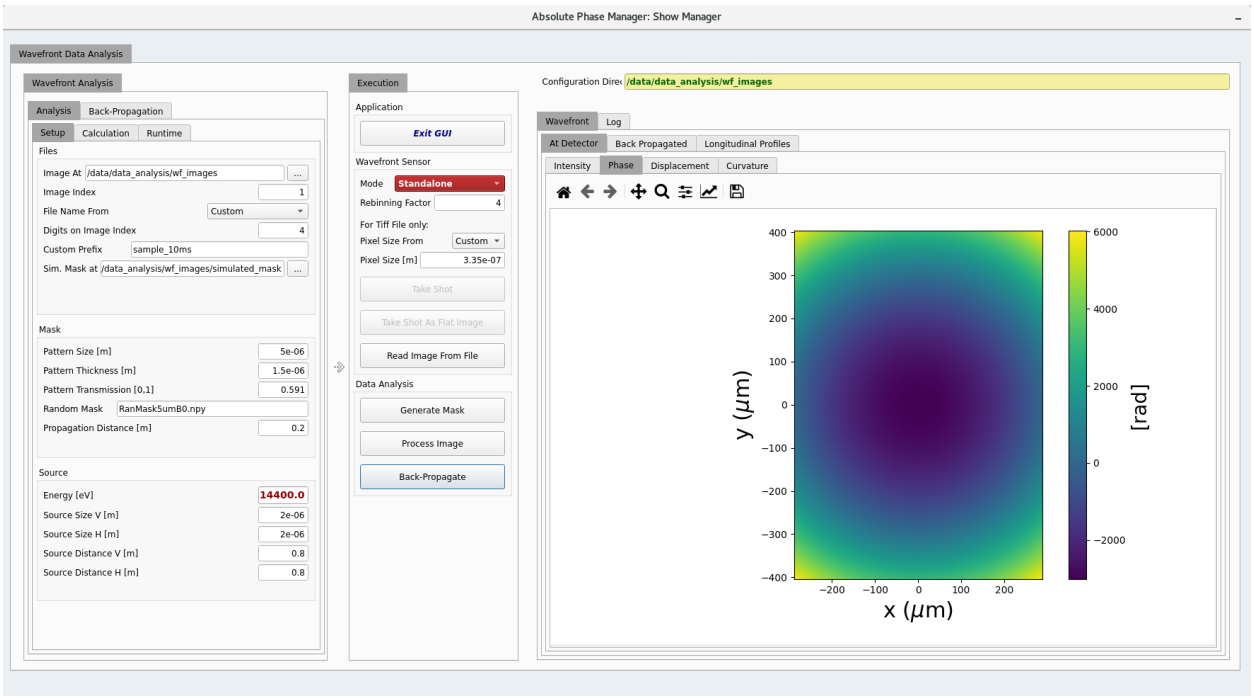
3. Absolute Phase Module

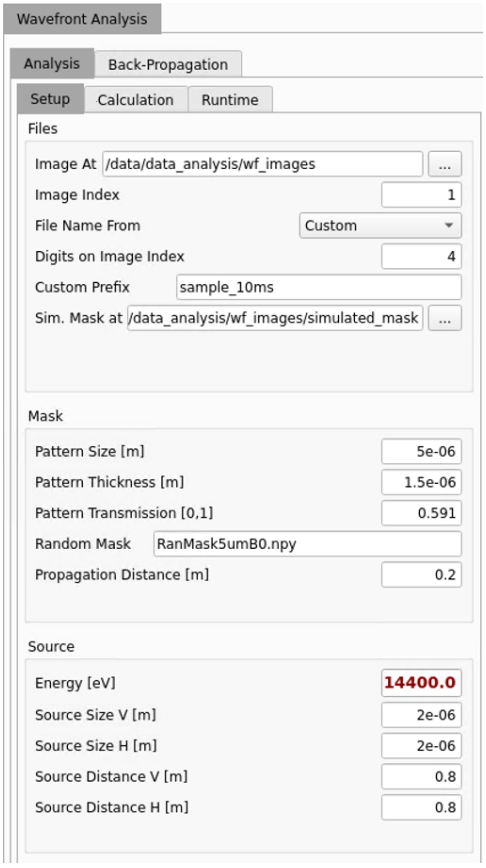
The **Absolute Phase** module reconstructs the **absolute wavefront phase** from coded-mask wavefront images.

It supports:

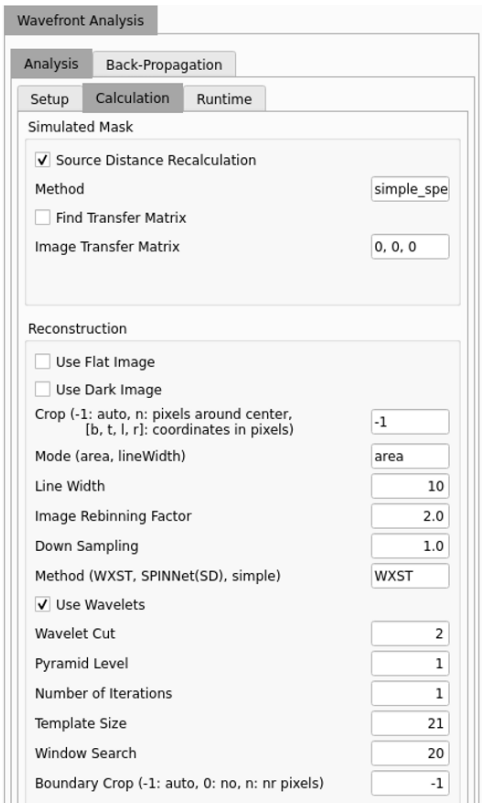
- Offline analysis from image files
- Online analysis with a wavefront sensor
- Optional wavefront back-propagation



3.1 Wavefront Analysis — Analysis Panel

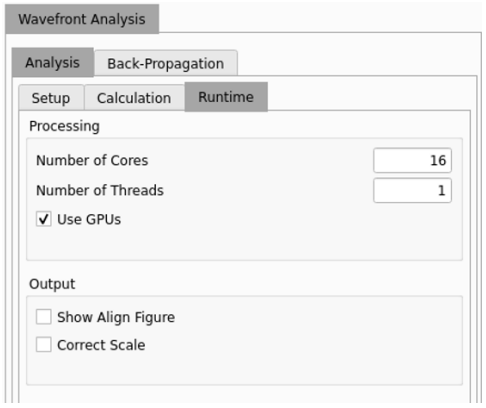


GUI element	Description
Setup — Files (Standalone mode)	
Image At	Directory containing wavefront images. Must contain valid wavefront image files (`.tif` or `.hdf5`)
Image Index	Index of the image to process. Used to construct the input image filename.
File Name From	Selects filename source. Wavefront sensor configuration (`W.S. Configuration`) or user-defined naming (`standalone`).
Digits on Image Index	Number of digits for zero-padding the image index. E.g. `4` → `0001`
Custom Prefix	Filename prefix. Only used when `File Name From` is set to `custom`
Simulated Mask At	Directory containing simulated mask files. Contain files generated after running `Generate Mask` in the Execution panel.
Setup — Mask	
Pattern Size [m]	Feature size of the coded mask.
Pattern Thickness [m]	Physical thickness of the mask. Used to calculate the phase shift introduced by the mask material.
Pattern Transmission [0,1]	Transmission of the mask material
Random Mask	Mask file used for simulation. Numpy `.npz` file containing the binary mask pattern (`0` or `1`) for the full mask area. Need to be in folder: …\absolute_phase\legacy\mask
Propagation Distance [m]	Distance from mask to detector.
Setup — Source	
Energy [eV]	X-ray photon energy.
Source Size V [m]*	Estimated vertical source size. For downstream-of-focus measurements, this corresponds to the effective focal size.
Source Size H [m]*	Horizontal source size. See above
Source Distance V [m]*	Vertical source-to-mask distance. May represent a real or virtual source.
Source Distance H [m]*	Horizontal source-to-mask distance. See above
*Note: These source sizes and distances are used for generating the simulated mask. Estimate them as accurately as possible to improve mask simulation accuracy. Larger source sizes lead to increased blurring of the mask pattern. The distances will be recalculated based on the measured image, but these values provide an important initial guess.	



GUI element	Description
Calculation — Simulated Mask	
Source Distance Recalculation	Refine source distance for simulated mask pattern generation. Usually enabled. Runs the forward simulation twice: first using the source distances defined in the **Setup – Source** panel, then recalculates the source distances based on the first result and regenerates the simulated mask.
Method	Reconstruction method: `simple_speckle` (default) or `geometric`. This step is for mask geometry identification only, not for final phase reconstruction.
Find Transfer Matrix	Recompute transfer matrix. Enable if the setup is new or has changed.
Image Transfer Matrix	Mask orientation matrix (h_flip, v_flip, transpose). Eg. `(0,0,0)`. Automatically determined if `Find Transfer Matrix` is enabled; otherwise must be provided manually.
Calculation — Reconstruction	
Use Flat Image	Flat image correction. Default unchecked. If enabled, the flat image filename must be specified in `.absolute_phase_analysis.json` under the `flat` key.
Use Dark Image	Dark image correction. Default unchecked. If enabled, the dark image filename must be specified in `.absolute_phase_analysis.json` under the `dark` key.
Crop	`-1`: automatic; `n`: crop to n pixels around the image center; `[b,t,l,r]`: manual crop using pixel coordinates.
Mode	`area` (2D reconstruction) or `centralLine` (1D reconstruction along the central line)
Line Width	Width (in pixels) used to average the central line in `centralLine` mode.
Image Rebinning Factor	Numerical rebinning at the image level (before mask simulation). Values: `1` (no rebinning), `2`, `4`, … This changes the effective output pixel size.

GUI element	Description
Down Sampling	Down sampling ratio applied at the reconstruction level (after mask simulation). Values: `1` (no downsampling), `0.5`, `0.25`, … Output pixel size is unchanged.
Use Wavelets	Enable Wavelet method. Recommended in most cases. If unchecked, no wavelet transform is applied and similarity search is performed directly on raw image data.
Wavelet Cut	Wavelet cutoff level: `0` (no cut), `1`, `2`, …. Higher values improve speed but may reduce spatial detail. For WXST, 2 is commonly used. When using large template sizes, increasing this value can significantly improve performance.
Pyramid Level	Multiscale search depth. Total levels = `Pyramid Level` + 1, processed from coarse to fine. Useful for capturing small variations on top of large background changes. Improves CPU performance; disabled in GPU mode.
Number of Iterations	Typically `1`. Increasing this value does not necessarily improve reconstruction quality and should be used with caution.
Template Size	Half-size of the template window around each pixel. The window should span several mask features. A practical guideline is ~5 mask periods across the full window.
Window Search	Correlation search window (half) size. Keep as small as possible while still capturing the maximum displacement. Inspect the displacement map: smooth interior regions and clean boundaries indicate a suitable value.
Boundary Crop	Edge cropping pixels. Removes unreliable edge regions in displacement maps; `-1` (default) auto-determines crop from search window and template size, otherwise uses a fixed pixel crop.

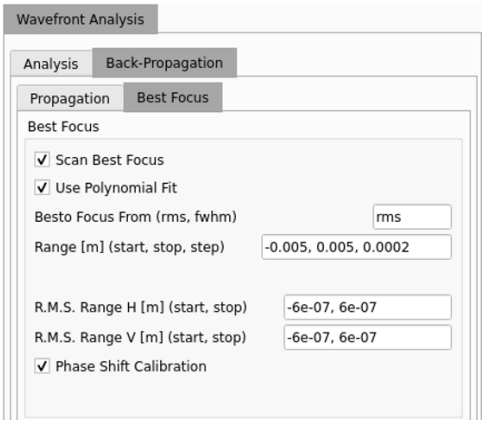


GUI element	Description
Runtime	
Number of Cores	CPU cores used for parallel processing
Number of Threads	Threads per core. Usually 1
Use GPUs	Enable GPU acceleration. Requires CUDA
Show Align Figure	Show simulated figure and raw figure comparison. Images saved no matter checked or not.
Correct Scale	Apply scale correction. Advanced use

3.2 Wavefront Analysis — Back-Propagation Panel

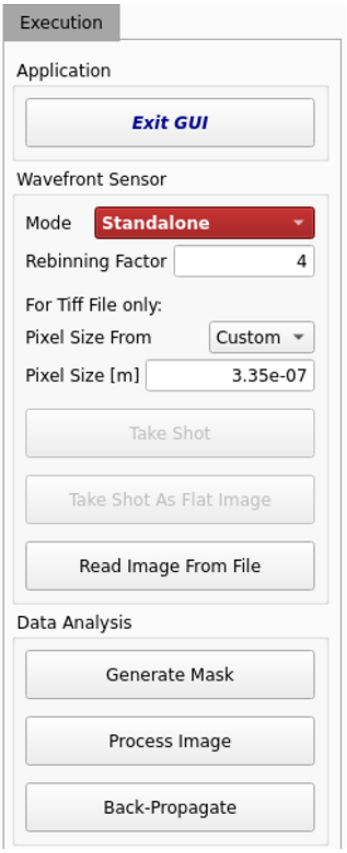
GUI element	Description
Propagation — Propagation	
Kind (1D, 2D)	Selects 1D or 2D wavefront propagation
Propagation Distance [m]	Negative values indicate back-propagation. When `Kind = 1D`, horizontal and vertical distances are specified separately.
Phase Shift H [m]	Applies a phase shift corresponding to an effective radius change (in meters). Useful for correcting astigmatism by bringing horizontal and vertical focal planes closer together.
Phase Shift V [m]	Same as horizontal phase shift, applied in the vertical direction.
Engine (WOFRY, SRW)	Selects the wavefront propagation library.
`WOFRY` options	
Magnification H	Ratio between the final-plane spatial range and the initial-plane range. Useful when propagating to a focal plane where the beam size is much smaller than the initial wavefront.
Magnification V	Same as horizontal magnification, applied in the vertical direction.
Shift Half Pixel	FFT-related parameter; normally enabled.
`SRW` options	SRW engine parameters; refer to SRW documentation.
Propagation — Image	
Wavefront Rebinning Factor	Rebinning factor applied before propagation. Default is `1`. Increase to reduce computation time at the cost of spatial resolution.

GUI element	Description
Smooth Intensity	Applies Gaussian smoothing to the intensity distribution; σ is specified in pixels.
Smooth Phase	Applies Gaussian smoothing to the phase map; σ is specified in pixels. Useful when the initial phase map is noisy.
Crop H	Horizontal crop size, in pixels
Shift H	Horizontal crop shift, in pixels
Crop V	Vertical crop size, in pixels
Shift V	Vertical crop shift, in pixels
Add shift on plots	Applies the specified shifts only to the displayed plots; does not affect calculations.



GUI element	Description
Best Focus	
Scan Best Focus	Enables an automatic focus scan along the propagation direction.
Use Polynomial Fit	Applies a polynomial fit to smooth the focus metric curve.
Best Focus From (rms, fwhm)	Metric used to determine best focus: RMS beam size or FWHM.
Range [m] (start, stop, step)	Propagation distance range and step size used for the focus scan.
R.M.S. Range H [m] (start, stop)	Horizontal region of interest used for RMS calculation.
R.M.S. Range V [m] (start, stop)	Vertical region of interest used for RMS calculation.
Phase Shift Calibration	Automatically compensates astigmatism by adjusting `Phase Shift H` and `Phase Shift V` in the **Propagation — Propagation** panel.

3.3 Execution Panel



GUI Element	Description
Execution — Wavefront Sensor	
Mode	Selects operation mode: `Standalone` (file-based) or `Connected to W.S.` (live wavefront sensor).
Rebinning Factor	Rebinning applied for visualization only. Default is `4`.
Pixel Size From	Source of detector pixel size: wavefront sensor (`W.S.`) or user defined (`Custom`)
Pixel Size [m]	Detector pixel size, used when `Pixel Size From` is set to `Custom`.
Take Shot	Acquire an image from the wavefront sensor. Available only in `Connected to W.S.` mode
Take Shot As Flat Image	Acquire a flat-field image from the wavefront sensor. Available only in `Connected to W.S.` mode; the flat image is saved with filename prefix `flat_`.
Read Image From File	Load an image from disk. Required when images are saved as `.tif` files; automatically generates a corresponding `.hdf5` file with the same base name.
Execution — Data Analysis	
Generate Mask	Generate the simulated coded mask and save it as `.npz` files.
Process Image	Perform wavefront phase reconstruction.
Back-Propagate	Perform wavefront back-propagation to the specified plane (and find the best focus).

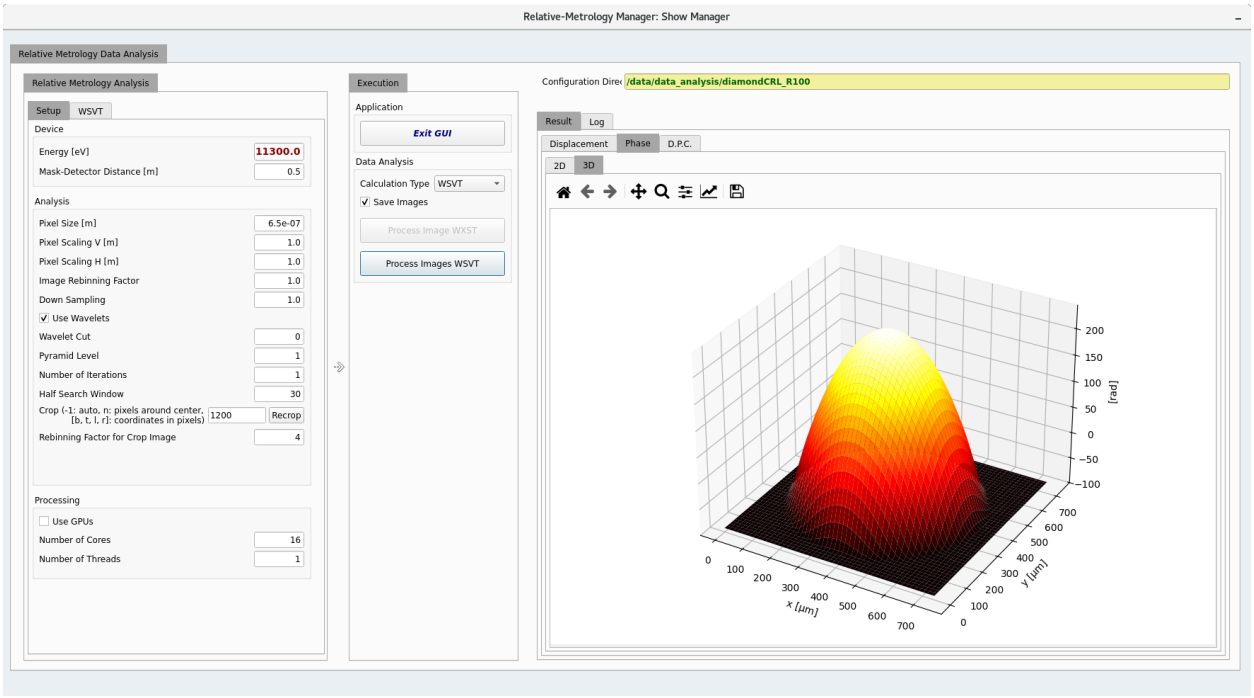
4. Relative Metrology Module

The **Relative Metrology** module reconstructs the **phase shifts induced by a sample or optical element** by comparing images acquired **with and without sample**. The speckle generator can be a coded mask or other random structures, such as sandpaper or membrane filters.

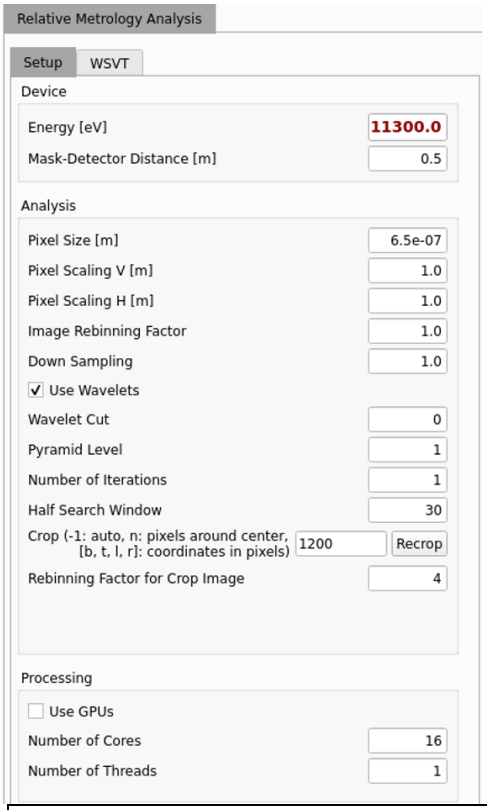
This module supports **offline analysis only**.

Two calculation types are available:

- WXST – Uses a single pair of images acquired with and without the sample.
- WSVT – Uses two sets of multiple images acquired with and without the sample. Within each set, the speckle generator is scanned transversely across multiple positions, using the same scan positions for both with-sample and without-sample measurements.

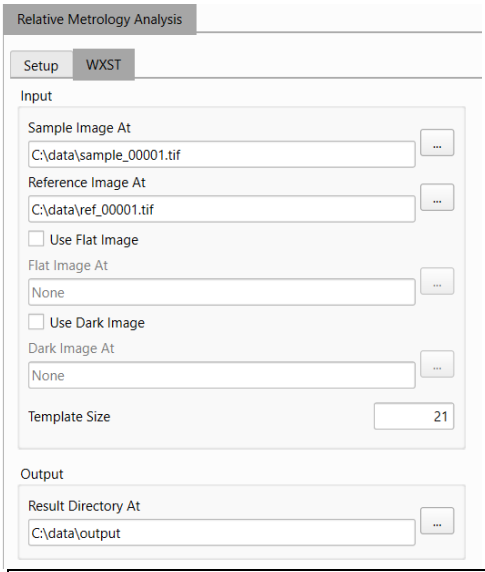


4.1 Relative Metrology Analysis Panel

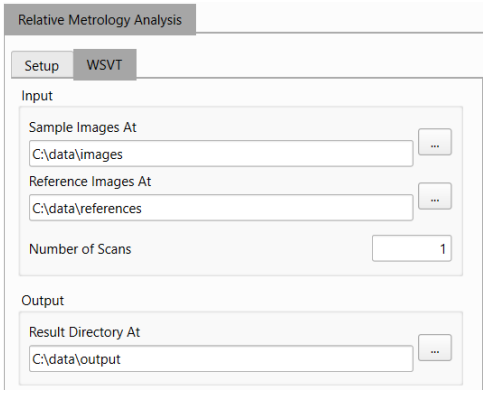


GUI Element	Description
Setup — Device	
Energy [eV]	X-ray photon energy.
Mask-Detector Distance [m]	Distance between the mask and the detector. If the sample is downstream of the mask, this corresponds to the sample–detector distance.
Setup — Analysis	
Pixel Size [m]	Image pixel size.
Pixel Scaling V [m]	Vertical pixel scaling factor, defined as $d_{source-sample}/d_{source-detector}$, where the source is the real or virtual source seen by the beam downstream of the sample.
Pixel Scaling H [m]	Save as Pixel Scaling V, applied in the horizontal direction.
Image Rebinning Factor	Numerical rebinning. Values: `1` (no rebinning), `2`, `4`, … This changes the effective output pixel size.
Down Sampling	Down sampling ratio applied at the reconstruction level. Values: `1` (no down-sampling), `0.5`, `0.25`, … Output pixel size is unchanged.
Use Wavelets	Enable Wavelet method. Recommended in most cases. If unchecked, no wavelet transform is applied and similarity search is performed directly on raw image data.
Wavelet Cut	Wavelet cutoff level: `0` (no cut), `1`, `2`, …. Higher values improve speed but may reduce spatial detail. Typical values: `2` for WXST and `0` for WSVT.
Pyramid Level	Multiscale search depth. Total levels = `Pyramid Level` + 1, processed from coarse to fine. Improves CPU performance; disabled in GPU mode.

GUI Element	Description
Number of Iterations	Number of solver iterations. Typically `1`. Increasing this value does not necessarily improve reconstruction quality and should be used with caution.
Half Search Window	Half-size of the correlation search window. Keep as small as possible while still capturing the maximum displacement. Inspect displacement maps to verify smooth interior regions and clean boundaries.
Crop	Cropping mode: `-1`: automatic; `n`: crop to n pixels around the image center; `[b,t,l,r]`: manual crop using pixel coordinates.
Rebinning Factor for Crop Image	Rebinning applied for visualization and interactive plotting only. Default is `4`.
Setup — Processing	
Use GPUs	Enable GPU acceleration. Requires CUDA.
Number of Cores	CPU cores used for parallel processing
Number of Threads	Threads per core. Usually set to `1`.

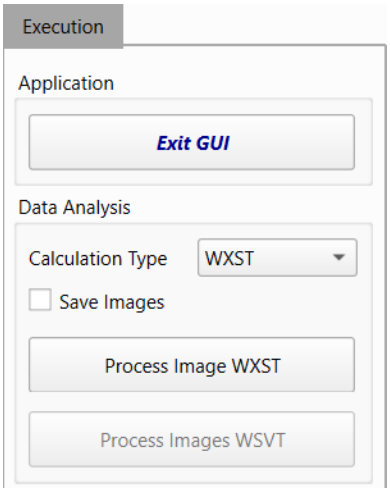


GUI Element	Description
WXST — Input	
Sample Image At	Full path to the sample image. Can be selected using the file dialog by clicking · · ·
Reference Image At	Full path to the reference image acquired without the sample.
Use Flat Image	Enable flat-field correction
Flat Image At	Full path to the flat-field image. Used only when Use Flat Image is enabled.
Use Dark Image	Enable dark-field subtraction
Dark Image At	Full path to the dark image. Used only when Use Dark Image is enabled.
Template Size	Half-window size of the correlation template window in pixels. Should span several speckle features.
WXST — Output	
Result Directory At	Directory where WXST reconstruction results are saved. Created automatically if not exist.



GUI Element	Description
WSVT — Input	
Sample Images At	Full path to the sample images. Can be selected using the file dialog by clicking · · ·
Reference Images At	Full path to the reference images acquired without the sample.
Number of Scans	Number of speckle generator scan positions. Less than or equal to the number of images in each folder.
WSVT — Output	
Result Directory At	Directory where WSVT reconstruction results are saved. Created automatically if not exist.

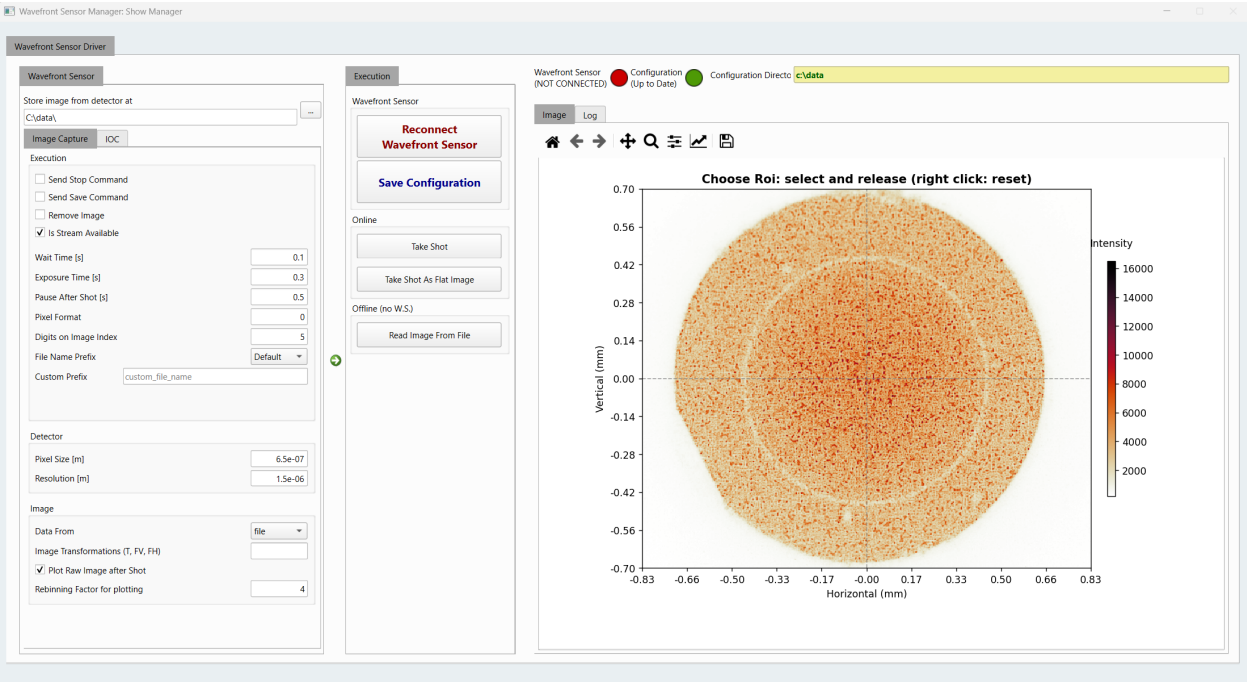
4.2 Execution Panel



GUI Element	Description
Calculation Type	Selects the relative metrology mode: `WXST` or `WSVT`
Save Images	Save reconstructed results as `.png` images when enabled.
Process Image WXST	Perform wavefront phase reconstruction using WXST.
Process Images WSVT	Perform wavefront phase reconstruction using WSVT.

5. Wavefront Sensor GUI

The **Wavefront Sensor GUI** is lunched together with the GUI Launcher. It provides a unified interface for **online image acquisition** from a connected wavefront sensor and **offline image loading** from disk. It also manages detector configuration, file naming, and basic image visualization.



This GUI is **hardware-specific**, and therefore individual input fields are not described in detail here. Users should pay particular attention to the **mode** selection in the **Execution Panel (Section 3.3)** of the **Absolute Phase Module**.

When `Connected to W.S.` is selected, **file naming** and **pixel size** may be automatically linked to the settings in the Wavefront Sensor GUI. For **offline analysis**, it is recommended to set **File Name From** and **Pixel Size From** to `Custom` in the Absolute Phase Module to avoid unintended coupling with Wavefront Sensor settings and potential confusion.