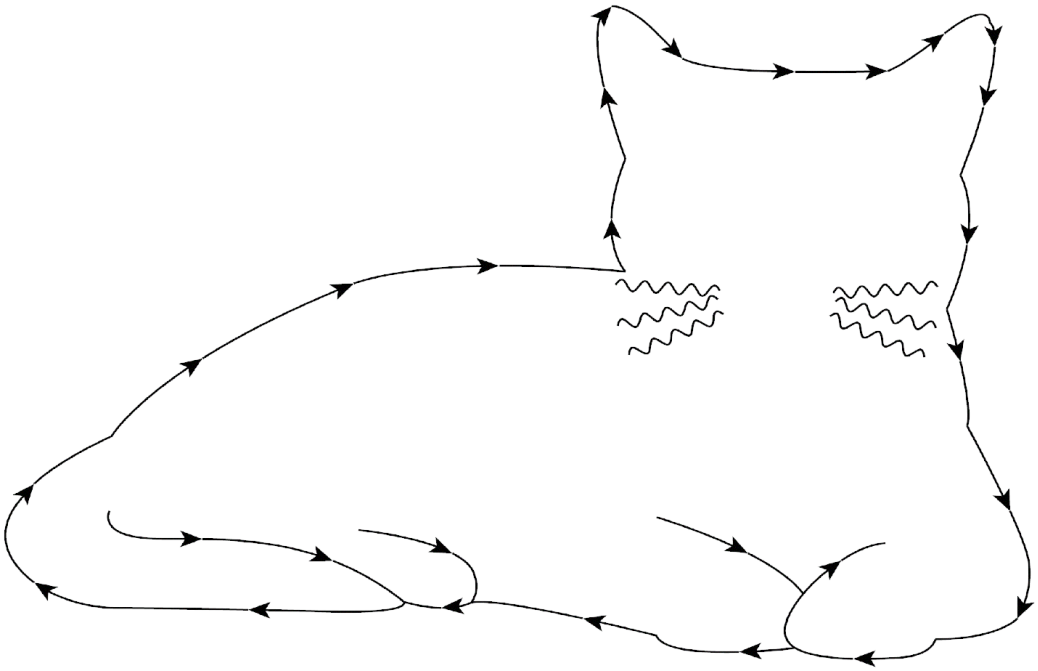

Comprehensive Analysis Toolkit for Near-field Imaging and Phase-retrieval (CATNIP) Documentation

Version 1.0

Manuel Fernando Sánchez Alarcón
Uniandes High-Energy Physics Research Group

July 8, 2025

Contents

1 Description

Comprehensive **A**nalysis **T**oolkit for **N**ear-field **I**maging and **P**hase-retrieval (**CATNIP**) is a software tool for rapidly generating simulated datasets based on wave-optics simulations, intended for testing multimodal retrieval algorithms in X-ray near-field imaging. It is developed and maintained by the High-Energy Physics Research Group at Universidad de los Andes (Uniandes). The frontend and backend are implemented in Python, and the graphical interface runs within the **CATNIP** virtual environment, whose installation is described later in this manual.

The simulations rely on the projection approximation, valid for thin samples, with future versions expected to include the multi-slice approach [1]. **CATNIP** supports simulations for edge illumination (EI) [2], single-grating-based imaging (SGBI) [3], speckle-based imaging (SBI) [4], and propagation-based imaging (PBI) [5]. It can generate data for both 2D multimodal retrieval and computed tomography (CT) reconstruction. It also includes implementations of state-of-the-art algorithms such as unified modulated pattern analysis (UMPA) [6] and low coherence system (LCS) [7].

2 Prerequisites

To run **CATNIP**, you must have **Python** version `3.12.2` or higher installed on your system. You can verify your Python version by running the following command in your terminal:

```
python --version
```

If your system does not meet this requirement, please install the appropriate version from the official Python website: https://www.python.org/downloads/.

3 Installation Instructions

Follow the steps below to install all necessary components to run **CATNIP**.

1. **Clone the GitHub repository:**

```
git clone https://github.com/Spoksonat/CATNIP.git
```

2. **Create the CATNIP virtual environment:**

```
python3 -m venv CATNIP_env
```

3. **Activate the CATNIP virtual environment:**

   - On Linux/Mac:

```
    source CATNIP_env/bin/activate

```

   - On Windows:

```
    CATNIP_env\Scripts\activate

```

     or

```
    CATNIP_env\Scripts\activate.bat

```

4. **Install the required dependencies:**

```
pip install -r CATNIP/requirements.txt
```

5. **Verify the installed packages:**

```
pip list
```

6. **Deactivate virtual environment:**

```
deactivate
```

Note: If your default Python version is older than `3.12.2`, and you have installed a compatible version separately, replace the command `python3` with the full path to the correct Python binary, e.g., `/path/to/python3.12`. To locate the path, you can use:

```
which python3.12
```

Common installation paths include:

- `/usr/local/bin/python3.12` (Linux/macOS)
- `~/.pyenv/versions/3.12.2/bin/python` (Linux/macOS with pyenv)
- `C:\Users\YourUser\AppData\Local\Programs\Python\Python312\python.exe` (Windows)

4 Execution

To launch the **CATNIP** graphical interface, follow these steps:

1. **Activate the CATNIP virtual environment:**
   - On Linux/macOS:

```
source CATNIP_env/bin/activate
```

   - On Windows:

```
CATNIP_env\Scripts\activate
```

     or

```
CATNIP_env\Scripts\activate.bat
```

2. **Navigate to the CATNIP main directory:**

```
cd CATNIP
```

3. **Run the main file:**

```
python main.py
```

5 Simulation Description

CATNIP adopts the wave-optics simulation approach described in [1] and [8], but treats the sample and the grating as a single slice under the projection approximation. For completeness, a detailed overview of the simulation algorithm is provided below for a monochromatic beam of energy E.

5.1 Generation of Initial Wavefront

The initial wavefield $\psi_0^E(x, y)$—immediately outside the source—is defined in Python as a 2D array of ones, where (x, y) are the transverse coordinates in planes orthogonal to the propagation axis (z-axis), and E denotes the energy of the monochromatic beam.

If EI, SBI, or SGBI is selected, the wavefield is first propagated to the grating or sandpaper plane using:

$$\psi_{BG}^{E}(x,y) = P_{\zeta_{S-G}}\{\psi_{0}^{E}(x,y)\}, \tag{1}$$

where $\psi_{BG}^{E}(x,y)$ is the wavefield just before the grating or sandpaper, ζ_{S-G} is the source-to-grating distance, and P_{ζ} is the propagation operator over a distance ζ:

$$P_{\zeta}\{\psi(x,y)\} = \mathcal{F}^{-1}\{\mathcal{F}\{\psi(x,y)\}H(k_x,k_y,\zeta)\}, \tag{2}$$

with $\mathcal{F}$ denoting the Fourier transform and $H(k_x,k_y,\zeta)$ the Fresnel propagator in Fourier space:

$$H(k_x,k_y,\zeta) = \exp\left(i\zeta\sqrt{k^2-k_x^2-k_y^2}\right), \tag{3}$$

where k_x and k_y are the spatial frequencies along x and y, and k is the wavenumber [8].

If PBI is selected, the wavefield is instead propagated to the front surface of the sample using:

$$\psi_{BS\text{-}PBI}^{E}(x,y) = P_{\zeta_{S\text{-}FS}}\{\psi_{0}^{E}(x,y)\}, \tag{4}$$

where $\zeta_{S\text{-}FS}$ is the distance from the source to the front surface of the sample.

5.2 Interaction with Grating or Sandpaper (only for EI, SGBI, and SBI)

The interaction between the wavefield and the grating is modeled as:

$$\psi_{IG}^{E}(x,y) = T_G(x,y)\psi_{BG}^{E}(x,y), \tag{5}$$

where $\psi_{IG}^{E}(x,y)$ is the wavefield after interaction and $T_G(x,y)$ is the transmission function of the grating. For EI or SGBI:

$$T_G(x,y) = \exp(-ik\delta_G(E)t_G(x,y))\exp\left(-\frac{\mu_G(E)}{2}t_G(x,y)\right), \tag{6}$$

with $\delta_G(E)$ the refractive index decrement, $\mu_G(E)$ the attenuation coefficient, and $t_G(x,y)$ the grating thickness map.

For SBI:

$$T_G(x,y) = \exp\left(-ik\sum_{n=S,P}\delta_n(E)t_n(x,y)\right)\exp\left(-\frac{1}{2}\sum_{n=S,P}\mu_n(E)t_n(x,y)\right), \quad (7)$$

with $\delta_n(E)$ and $\mu_n(E)$ the refractive index decrement and attenuation coefficient of the sandpaper grains ($n = S$) and paper ($n = P$), and $t_n(x,y)$ their respective thickness maps.

After this interaction, the wavefield is propagated to the sample's front surface:

$$\psi^E_{BS}(x,y) = S_{1\to M_S}\left\{P_{\zeta_{G\text{-}FS}}\left\{\psi^E_{IG}(x,y)\right\}\right\}, \quad (8)$$

where:

$$\zeta_{G\text{-}FS} = z_{G\text{-}FS}\frac{1}{M_S}, \quad M_S = \begin{cases}\frac{z_{S\text{-}FS}}{\zeta_{S-G}} & \text{cone-beam}\\ 1 & \text{parallel-beam}\end{cases}, \quad (9)$$

$z_{G\text{-}FS}$ is the grating-to-sample-front distance, and the operator $S_{M_1\to M_2}$ scales coordinates:

$$S_{M_1\to M_2}\left\{\psi\left(\frac{x}{M_1},\frac{y}{M_1}\right)\right\} = \psi\left(\frac{x}{M_2},\frac{y}{M_2}\right). \quad (10)$$

Note: Propagation inside the grating is neglected in the present model, which assumes the grating can be treated as a thin phase and/or absorption mask. This approximation is valid when the thickness of the grating is small relative to the distance between the grating center and the front surface of the sample. Under this assumption, the phase shift and attenuation introduced by the grating are accounted for via a multiplicative transmission function, while diffraction effects occurring within the grating itself are ignored.

5.3 Interaction with Sample

For EI, SBI, and SGBI:

$$\psi^E_{IS}(x,y) = T_S(x,y)\psi^E_{BS}(x,y), \quad (11)$$

and for PBI:

$$\psi^E_{IS}(x,y) = T_S(x,y)\psi^E_{BS\text{-}PBI}(x,y), \quad (12)$$

where:

$$T_S(x,y) = \exp\left(-ik\sum_{n=1}^{N_m}\delta_n(E)t_n(x,y)\right)\exp\left(-\frac{1}{2}\sum_{n=1}^{N_m}\mu_n(E)t_n(x,y)\right), \qquad (13)$$

$\delta_n(E)$ and $\mu_n(E)$ are respectively the refractive index decrement and the attenuation coefficient of the n-th material in the sample, both evaluated at energy E. The function $t_n(x,y)$ represents the thickness map of the n-th material at the transverse coordinates (x,y).

Depending on the sample geometry, the value of N_m and the definition of $t_n(x,y)$ changes:

- **Mammo Phantom**: In this case, the phantom is composed of three main parts ($N_m = 3$): the background, the slab of wax and the microcalcifications embedded in the slab. The thickness map $t_1(x,y)$ is the thickness map of the microcalcifications, the thickness map $t_2(x,y)$ is the thickness map of the background, and the thickness map $t_3(x,y)$ is the thickness map of the slab.
- **Block**: In this case, the phantom is composed of two main parts ($N_m = 2$): the background and a centered block of material. The thickness map $t_1(x,y)$ is the thickness map of the block, and the thickness map $t_2(x,y)$ is the thickness map of the background.
- **Angio tube**: In this case, the phantom is composed of three main parts ($N_m = 3$): the background, a centered tube (hollow cylinder) and the filling of the tube. The thickness map $t_1(x,y)$ is the thickness map of the filling of the tube, the thickness map $t_2(x,y)$ is the thickness map of the background, and the thickness map $t_3(x,y)$ is the thickness map of the tube.
- **Sphere**: In this case, the phantom is composed of two main parts ($N_m = 2$): the background and a centered sphere. The thickness map $t_1(x,y)$ is the thickness map of the sphere, and the thickness map $t_2(x,y)$ is the thickness map of the background.
- **Fibre**: In this case, the phantom is composed of two main parts ($N_m = 2$): the background and the fibre. The thickness map $t_1(x,y)$ is the thickness map of a centered fibre inclined 45 degrees, and the thickness map $t_2(x,y)$ is the thickness map of the background.

- **Wedge**: In this case, the phantom is composed of two main parts (N_m = 2): the background and a centered wedge of material. The thickness map $t_1(x,y)$ is the thickness map of the wedge, and the thickness map $t_2(x,y)$ is the thickness map of the background.

Note: Propagation inside the sample is neglected under the projection approximation. This is valid when the sample thickness is small compared to the propagation distance to the detector. In this framework, the sample is treated as a thin, semi-transparent object whose effect on the wavefield is described by a complex transmission function.

5.4 Propagation to Detector

When EI, SBI, or SGBI is selected:

$$\psi_D^E(x,y) = S_{M_S \to M_D}\left\{P_{\zeta_{BS\text{-}D}}\left\{\psi_{IS}^E(x,y)\right\}\right\}, \tag{14}$$

where:

$$\zeta_{BS\text{-}D} = z_{BS\text{-}D}\frac{M_S}{M_D}, \quad M_D = \begin{cases} \frac{z_{S\text{-}D}}{z_{S\text{-}BS}} & \text{cone-beam} \\ 1 & \text{parallel-beam} \end{cases}, \tag{15}$$

z_{BS-D} is the distance from the back of the sample to the detector, z_{S-BS} is the distance between the source and the back of the sample, and z_{S-D} is the source-to-detector distance.

For PBI:

$$\zeta_{BS\text{-}D} = z_{BS\text{-}D}\frac{1}{M_D}. \tag{16}$$

When no sample is considered in the optical path, i.e. to obtain reference images:

For EI, SBI, SGBI:

$$\psi_D^E(x,y) = S_{1 \to M'_D}\left\{P_{\zeta_{G\text{-}D}}\left\{\psi_{IG}^E(x,y)\right\}\right\}, \quad \zeta_{G\text{-}D} = z_{G\text{-}D}\frac{1}{M'_D}, \quad M'_D = \frac{z_{S\text{-}D}}{\zeta_{S-G}}, \tag{17}$$

where z_{G-D} is the grating-to-detector distance

For PBI:

$$\psi_D^E(x,y) = P_{z_{S\text{-}D}}\left\{\psi_0^E(x,y)\right\}. \tag{18}$$

5.5 Image Formation and Detector Effects

The detector image is:

$$I_D^E(x,y) = \left|\psi_D^E(x,y)\right|^2. \tag{19}$$

To simulate detector noise, Poisson statistics are applied to $I_D^E(x,y)$, using a mean photon number per pixel specified by the user via the `Num.events per pixel` parameter (see subsubsection 6.1.2 for details).

After adding noise, the image is convolved with a Gaussian kernel to incorporate the system point spread function (PSF), characterized by [4]:

$$PSF_{sys} = \sqrt{\left(\frac{PSF_{det}}{M}\right)^2 + \left(\frac{M-1}{M}\right)^2 D^2}, \tag{20}$$

where PSF_{det} is the detector intrinsic PSF, D is the focal spot size, and M is the magnification factor:

$$M = \begin{cases} 1 & \text{parallel-beam or PBI reference} \\ M_D & \text{cone-beam with sample} \\ M'_D & \text{cone-beam reference image} \end{cases}$$

6 General Structure and Use

After executing the command:

```
python main.py
```

the main window of **CATNIP** opens, as shown in Figure 1. This menu contains three buttons: **2D Simulation** and **CT Simulation**, which enable PBI, SBI, SGBI, and EI simulations for generating 2D and tomographic multimodal data; and **Multimodal Retrieval**, which provides access to a menu with three different phase and dark-field retrieval methods. Each of these options is described below.

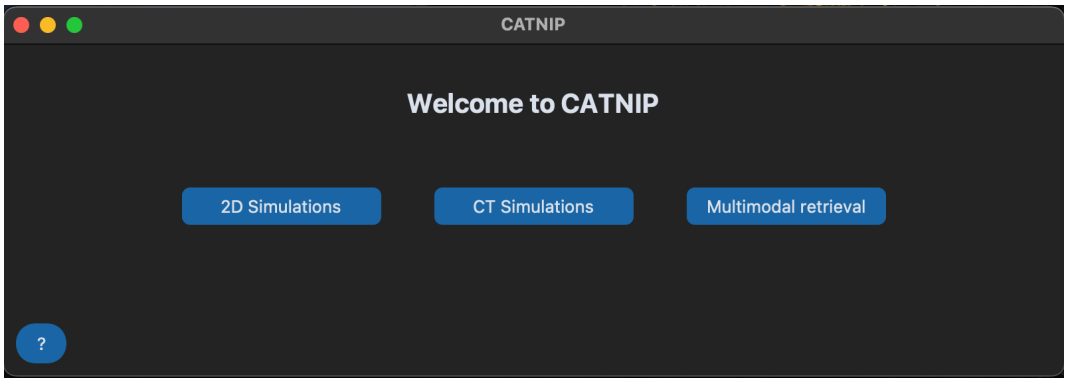

Figure 1: Main menu of **CATNIP**.

6.1 2D Simulation and CT Simulation

The **2D Simulation** and **CT Simulation** buttons lead to a technique selection menu, as shown in Figure 2, where the user can choose the desired simulation mode. The available techniques include PBI, SBI, SGBI, and EI.

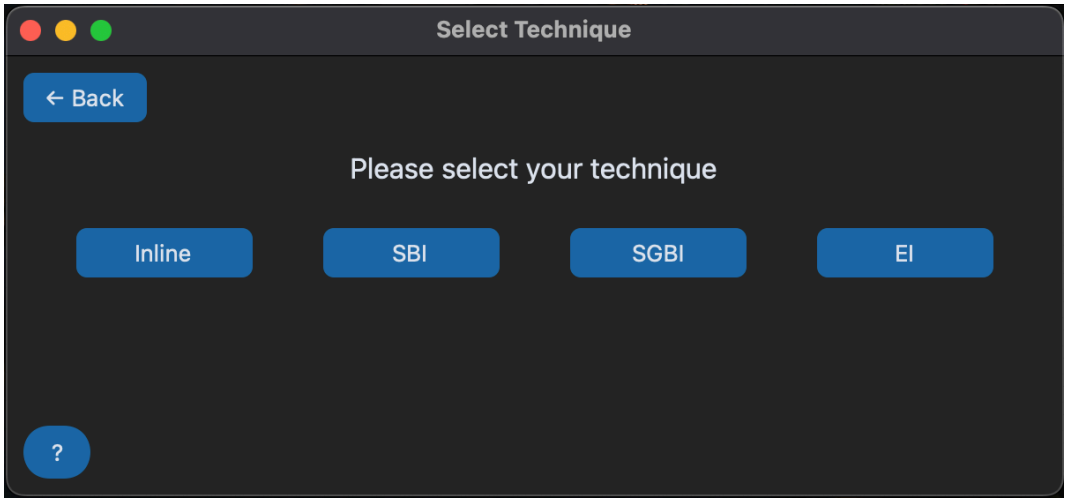

Figure 2: Technique selection menu of **CATNIP**.

Selecting any of the techniques opens a new window, as shown in Figure 3, which contains two tabs: **Parameters** and **Run Simulations**.

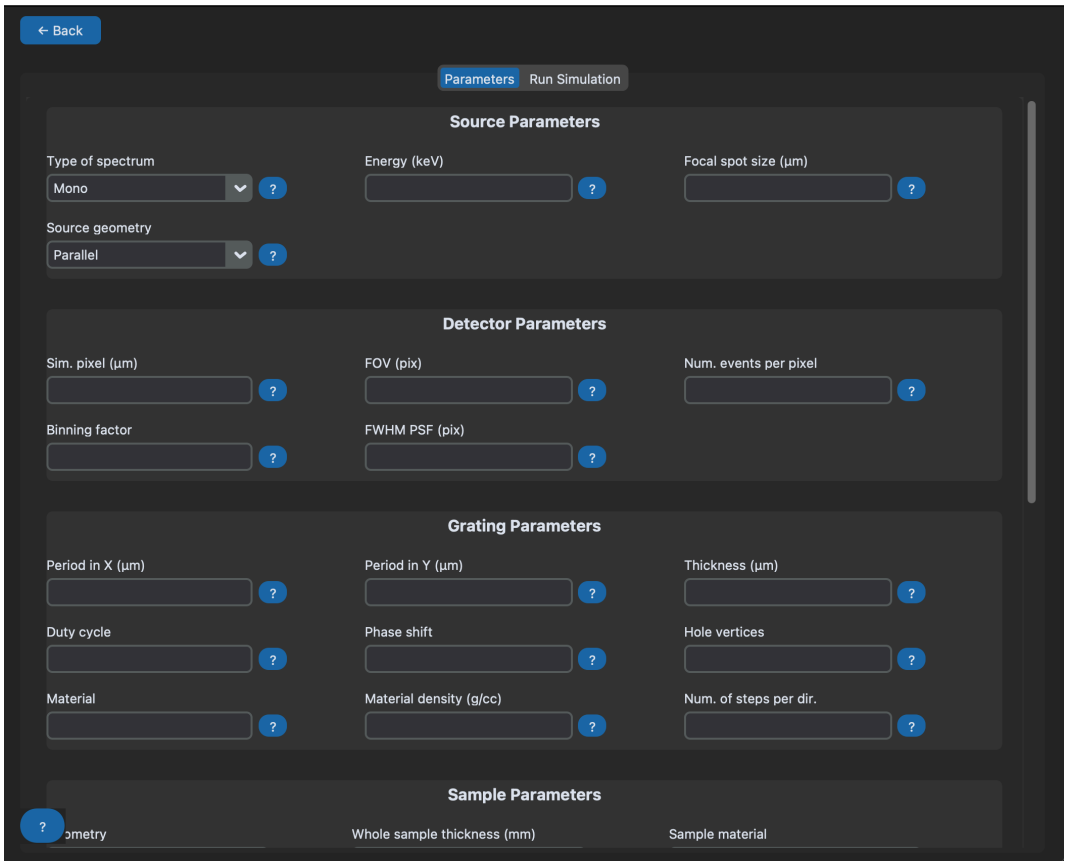

Figure 3: Simulation configuration menu of **CATNIP**.

The **Parameters** tab includes all necessary settings to configure a simulation for the selected technique. These cover both geometric and physical properties of the optical components, and are organized into the following sections:

6.1.1 Source Parameters

The source parameters are shown in Figure 4 and include:

- **Type of spectrum**: Specifies whether the simulation uses a monochromatic or polychromatic X-ray spectrum.
- **Energy/Spectrum file**: If a monochromatic spectrum is selected, the beam energy must be specified. If a polychromatic spectrum is selected, a button next to the `Spectrum file` label will appear, allowing the user to import a text file containing the spectral data. This file must

contain two columns: the first with energies in keV, and the second with corresponding spectral values (e.g., number of photons, flux, or intensity). An additional button is also shown to plot the imported spectrum.

- **Focal spot size**: Defines the focal spot size of the X-ray source in micrometers. This value is used to calculate the system's full width at half maximum (FWHM) according to [4].
- **Source geometry**: Specifies the beam geometry as either `Parallel` or `Cone`. When `Cone` is selected, the simulation applies Fresnel scaling to account for magnification effects, following the approach described by Shanblatt et al. [8].

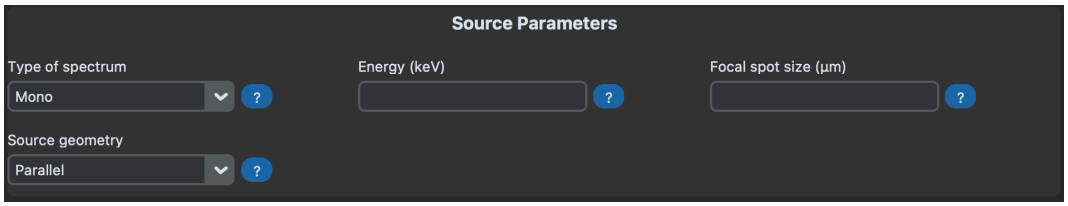

Figure 4: Source parameters (2D and CT Simulations).

6.1.2 Detector Parameters

The detector parameters are shown in Figure 4 and include:

- **Sim. pixel**: Defines the detector pixel size in micrometers.
- **FOV**: Specifies the detector's field of view (FOV) in pixels, given as a tuple. For example, a 100 $\times$ 100 detector should be entered as `(100, 100)`.
- **Num. events per pixel**: Sets the mean number of detected photons per pixel. This value is used to introduce Poisson noise in the simulation.
- **Binning factor**: Adjusts the simulation resolution. When set to a value greater than 1, the pixel size is divided by this value, and the FOV is scaled up proportionally. After simulation, the detector images are downsampled (binned) by the same factor.
- **FWHM PSF**: Specifies the FWHM of the detector's PSF, in pixels. This value is used to compute the system's FWHM following the method described in [4].

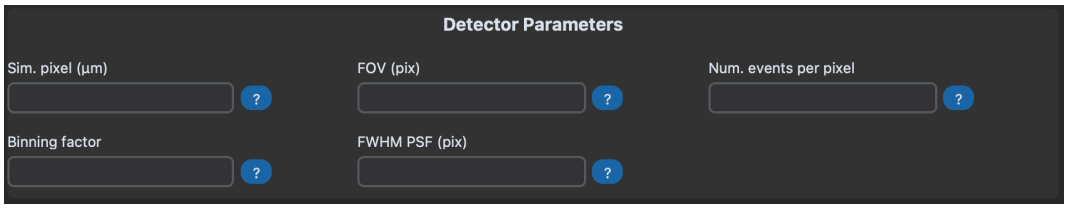

Figure 5: Detector parameters (2D and CT Simulations).

6.1.3 Grating/Sandpaper Parameters (only for EI, SGBI, and SBI)

When EI, SGBI, or SBI is selected as the simulation technique, a section like the one shown in Figure 4 appears in the `Parameters` tab. The displayed parameters vary depending on the selected technique.

For EI, the following parameters are shown:

- **Period**: Grating period along the horizontal axis, in micrometers.
- **Fringe width**: Width of the grating material fringes, in micrometers.
- **Grating thickness**: Thickness of the grating along the beam propagation direction (z axis), in micrometers.
- **Material**: Chemical formula of the grating material (e.g., `Au`, `Al2O3`).
- **Material density**: Density of the grating material, in g/cm^3.
- **Number of steps**: Number of discrete steps used to scan the sample across one grating period along the horizontal axis. Each step corresponds to a shift of p/N, where p is the grating period and N is the number of steps.

For SGBI, the following parameters are shown:

- **Period in X**: Horizontal period of the grating hole pattern, in micrometers.
- **Period in Y**: Vertical period of the grating hole pattern, in micrometers.
- **Thickness**: Grating thickness along the beam propagation direction (z axis), in micrometers.
- **Duty cycle**: Ratio given in multiples of π, used to compute the hole radius as $r = p_x \times DC$, where p_x is the horizontal period and DC is the duty cycle.

- **Phase shift**: Phase shift induced by the grating material. If set to `Auto`, it is computed from the grating material, thickness, and source energy.
- **Hole vertices**: Number of vertices used to define the shape of each hole in the grating pattern. This value must be at least 3.
- **Material**: Chemical formula of the grating material (e.g., `Si`, `Al2O3`).
- **Material density**: Density of the grating material, in g/cm^3.
- **Num. of steps per dir.**: Number of discrete steps along each axis used to scan the sample across one grating period. Each step shifts the grating by p_x/N in the horizontal and p_y/N in the vertical direction, where p_x and p_y are the respective periods and N is the number of steps per direction. The total number of steps is therefore N^2.

For SBI, the following parameters are shown:

- **Grain size**: Diameter of the sandpaper grains, assumed to be spherical, in micrometers.
- **Paper thickness**: Thickness of the paper supporting the grains, in micrometers.
- **Grain material**: Chemical formula of the grain material (e.g., `SiC`, `TiC`).
- **Grain material density**: Density of the grain material, in g/cm^3.
- **Paper material**: Chemical formula of the paper material (e.g., `C6H10O5`).
- **Paper material density**: Density of the paper material, in g/cm^3.
- **Number of sandpapers**: Number of sandpapers used in the setup. They are assumed to be stacked with zero spacing along the propagation axis.
- **Number of steps**: Number of discrete steps used to scan the sample across the sandpaper plane.
- **Step size**: Step length along the scanning direction, in micrometers.
- **Number of grains**: Total number of grains in the sandpaper.

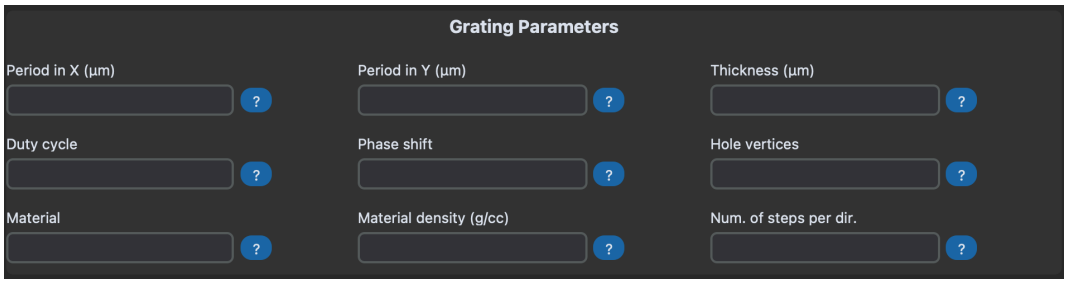

Figure 6: Grating/Sandpaper parameters (2D and CT Simulations).

6.1.4 Sample Parameters

The sample parameters are shown in Figure 7 and include:

- **Geometry**: Defines the sample type. For 2D simulations, the options are: `Mammo Phantom`, `block`, `angio tube`, `sphere`, `fibre`, and `wedge`. For CT simulations, the options are: `Mammo Phantom`, `block`, `angio tube`, `sphere`, and `fibre`.
- **Whole sample thickness**: Thickness of the material containing all sample components, in millimeters.
- **Sample material**: Chemical formula of the innermost element (e.g., `Al2O3`). If `Geometry = Mammo Phantom`, this is assumed to be the material of the microcalcifications. If `Geometry = angio tube`, it corresponds to the material inside the tube.
- **Sample material density**: Density of the innermost element, in g/cm^3.
- **Background material**: Chemical formula of the outermost material (e.g., `C5H8O2`).
- **Background material density**: Density of the background material, in g/cm^3.
- **Specific parameters**: Depending on the selected geometry, additional parameters appear:
  - If `Geometry = Mammo Phantom`:
    - **Sample 2 material**: Chemical formula of the material containing the microcalcifications (e.g., `CH4`).
    - **Sample 2 material density**: Density of this material, in g/cm^3.

    * **Diameter uC**: Diameter of each microcalcification, in micrometers.
    * **Radius pentagon**: Radius of the pentagon where the five microcalcifications are arranged.
    * **Thickness wax**: Thickness of the material embedding the microcalcifications, in millimeters.
- If `Geometry = block`:
    * **Block thickness**: Thickness of the block embedded in the background, in millimeters.
- If `Geometry = angio tube`:
    * **Sample 2 material**: Chemical formula of the tube material (e.g., `C5H8O2`).
    * **Sample 2 material density**: Density of the tube material, in g/cm^3.
    * **External diameter**: Outer diameter of the tube, in millimeters.
    * **Internal diameter**: Inner diameter of the tube, in millimeters.
- If `Geometry = sphere`:
    * **Sphere diameter**: Diameter of the sphere, in millimeters.
- If `Geometry = fibre`:
    * **Fibre diameter**: Diameter of the fibre, in millimeters.
- If `Geometry = wedge`:
    * **Wedge diameter**: Maximum thickness of the wedge, in millimeters.

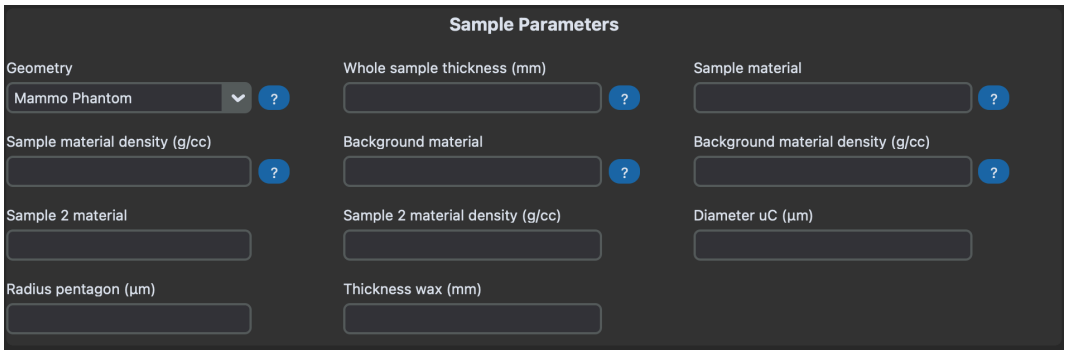

Figure 7: Sample parameters (2D and CT Simulations).

6.1.5 Dark-Field Parameters (only for EI, SGBI, and SBI)

The dark-field parameters are shown in Figure 8 and include:

- **RMS scattering angle in X**: Maximum expected scattering angle in the horizontal axis in the detector plane, in microradians.
- **RMS scattering angle in Y**: Maximum expected scattering angle in the vertical axis in the detector plane, in microradians.

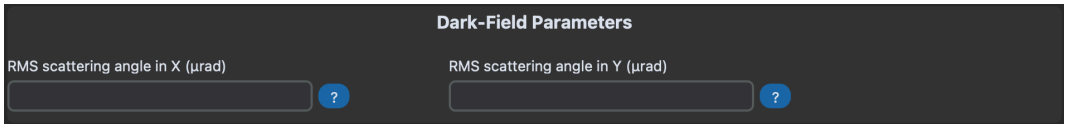

Figure 8: Dark-field parameters (2D and CT Simulations).

6.1.6 Setup Geometrical Parameters

When EI, SGBI, PBI, or SBI is selected as the simulation technique, a section like the one shown in Figure 9 appears in the `Parameters` tab. The displayed fields depend on the selected technique.

For PBI, the following parameters are shown:

- **Source-Detector distance**: Distance between the source and the detector, in meters.
- **Source-Sample distance**: Distance between the source and the center of the sample, in meters.

For EI, the following parameters are shown:

- **Source-Detector distance**: Distance between the source and the detector, in meters.
- **Grating-Sample distance**: Distance between the grating and the center of the sample, in meters.
- **Shift grating in prop. axis**: Shift of the grating along the propagation axis, in centimeters. Used to align the grating pattern with the detector and minimize Moiré effects in the single-mask EI configuration.
- **Shift grating lateral axis**: Shift of the grating along the horizontal axis within the grating plane, in micrometers. Also used for alignment and Moiré suppression in the single-mask EI setup.

Note: The grating-to-detector distance—and hence the source-to-grating distance—is internally computed so that the magnified grating period at the detector matches twice the simulated detector pixel size, as required by the single-mask EI technique.

For SGBI and SBI, the following parameters are shown:

- **Source-Detector distance**: Distance between the source and the detector, in meters.
- **Source-Grating distance**: Distance between the source and the grating or sandpaper, in meters.
- **Grating-Sample distance**: Distance between the grating or sandpaper and the center of the sample, in meters.

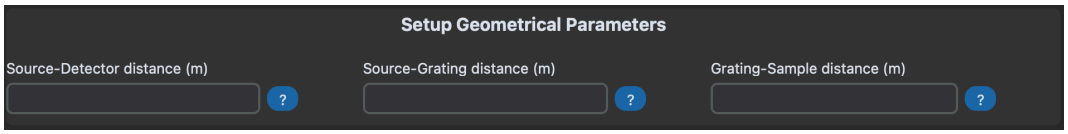

Figure 9: Geometrical parameters (2D and CT Simulations).

6.1.7 CT Parameters

The CT parameters are shown in Figure 10 and include:

- **Initial angle**: Starting angle of the CT scan, in degrees.
- **Final angle**: Final angle of the CT scan, in degrees.

- **Number of projections**: Number of 2D X-ray projections used to build the sinograms from the intensity values detected along each detector row.

Note: The rotation axis is assumed to be vertical and centered on the sample along the propagation axis.

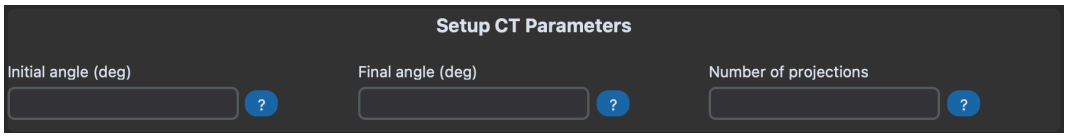

Figure 10: CT parameters (2D and CT Simulations).

6.1.8 Bottom section of the parameters tab

At the bottom of the `Parameters` tab, a set of four to five buttons is displayed, depending on the selected simulation technique, as shown in Figure 11. The first four buttons are common to all techniques:

- **Load Parameters**: Loads a previously saved parameter set, allowing reuse without manual re-entry.
- **Save Parameters**: Saves the current parameters to an `.npy` file.
- **Update Parameters**: Applies any recent changes made to the parameter fields.
- **Show Setup**: Displays a schematic of the X-ray setup with the positions of the optical elements along the propagation axis, in meters.

A fifth button appears only for EI, SGBI, and SBI, allowing the user to visualize a reference image—i.e., a detector image from a simulation without a sample—revealing the pattern produced by the grating or sandpaper. In the case of EI, it also shows a histogram comparing odd and even detector columns to assess grating alignment (the histograms should match).

Note: The reference image is generated using a monochromatic beam at 21 keV.

Figure 11: Bottom section of the parameters tab.

The **Run Simulation** tab includes a read-only console and two to four buttons at the bottom of the window, as shown in Figure 12. These buttons allow the user to run the simulation locally (**Run Simulation**), run it on a server (**Run Simulation on Server**), and open the window for multimodal retrieval using methods suited to the selected technique.

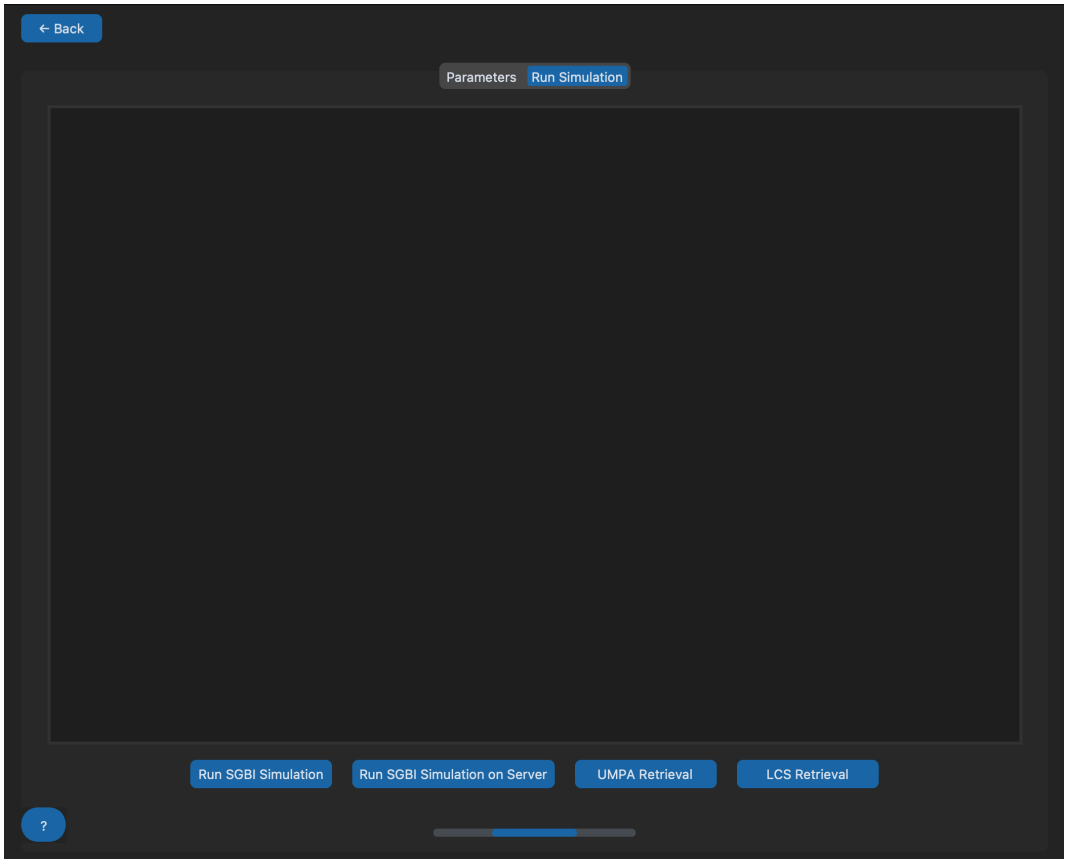

Figure 12: **Run Simulation** tab for the SGBI technique.

When **Run Simulation** is pressed, the user is prompted to choose a location to save the simulation results. These results consist of two `.npy` arrays: one containing the detector images without the sample (reference images), and the other containing the images with the sample (sample images).

Upon pressing **Run Simulation on Server**, the user is redirected to the window shown in Figure 13. In this window, the username, server address, and password for the server account must be provided. Once this information is entered, Python (via the `Paramiko` library) uploads a copy of

the `remote_simulations` folder (located within the **CATNIP** directory) to `/home/username/` on the server, renaming it `remote_project`. If required libraries are missing on the server, they are automatically installed. The resulting `.npy` files generated by the simulation are saved in the `temp` folder within the `remote_project` directory.

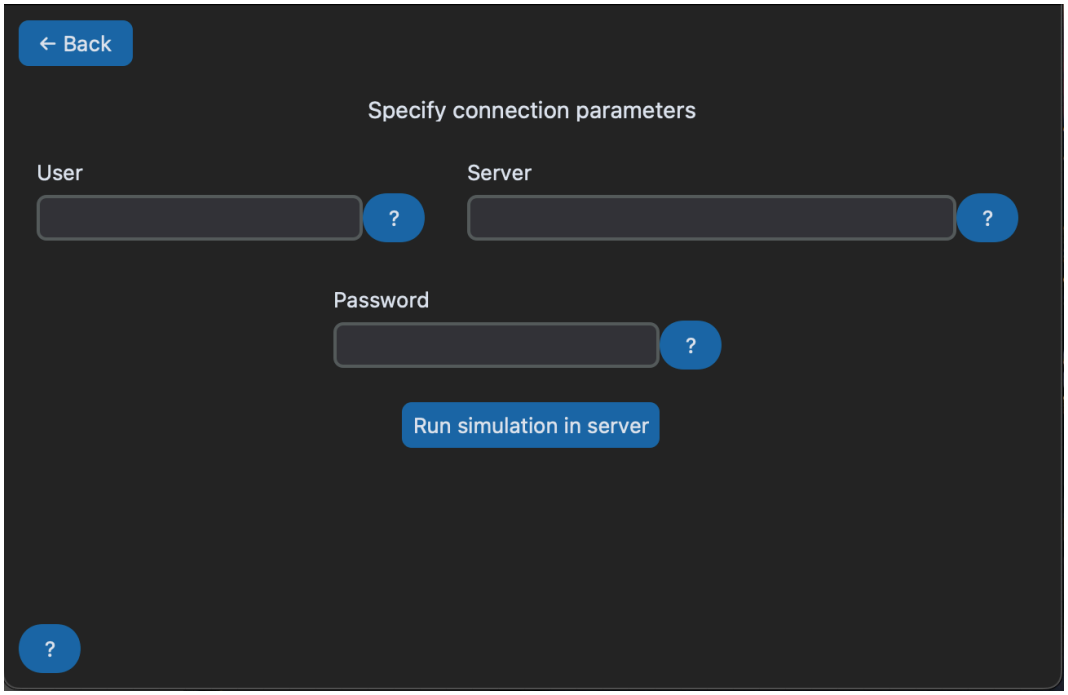

Figure 13: **Run Simulation on Server** window.

6.2 Multimodal retrieval

When the **Multimodal retrieval** button is pressed in the main menu of **CATNIP**, the window shown in Figure 14 appears.

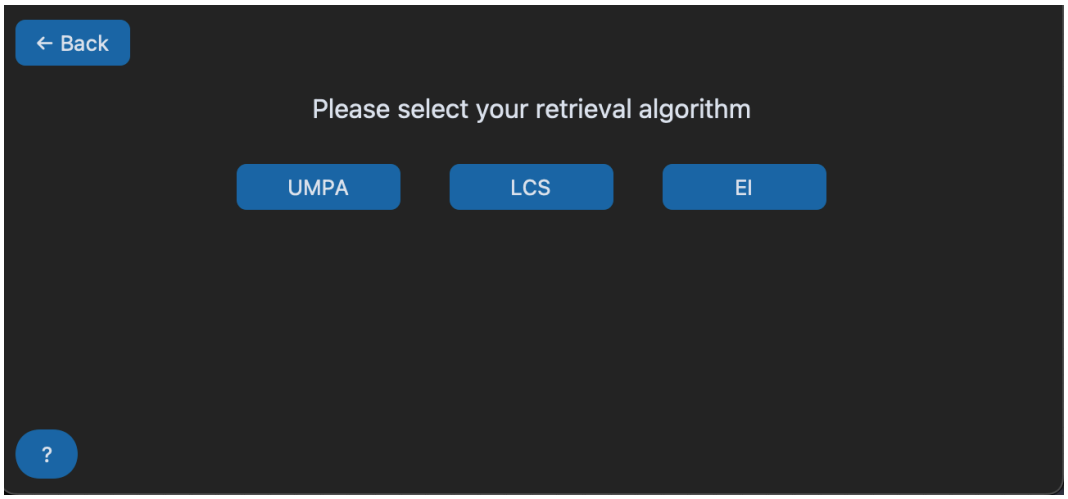

Figure 14: **Multimodal retrieval** menu.

This menu offers three multimodal retrieval algorithms: UMPA, using the implementation by Pierre Thibault available on GitHub[1]; an in-house implementation of LCS; and a phase-retrieval method for single-mask EI, based on the algorithm developed by Jurado [9].

Pressing the **UMPA**, **LCS**, or **EI** button opens a corresponding retrieval window, as shown in Figures 15, 16, and 17. Each interface includes a set of fields:

- **Analysis Window Index (UMPA only)**: Sets the size of the analysis window used in the retrieval algorithm.
- **Max. Speckle Shift (UMPA only)**: Sets the maximum speckle shift, as discussed in [6].
- **Find Dark Field image? (UMPA only)**: Enables or disables retrieval of the dark-field signal.
- **Binning (EI only)**: Allows binning of reference and sample images by the specified factor.
- **Correct Damaged Pixels**: If enabled, replaces dead pixels with the mean of their neighboring values.
- **Save results as NPY**: Specifies whether to save the retrieved multimodal images to an `.npy` file.

[1] https://github.com/pierrethibault/UMPA/tree/master

At the bottom of each window, a button lets the user load simulation or experimental data and immediately apply the selected retrieval algorithm. After execution, the retrieved multimodal images are displayed in a new window.

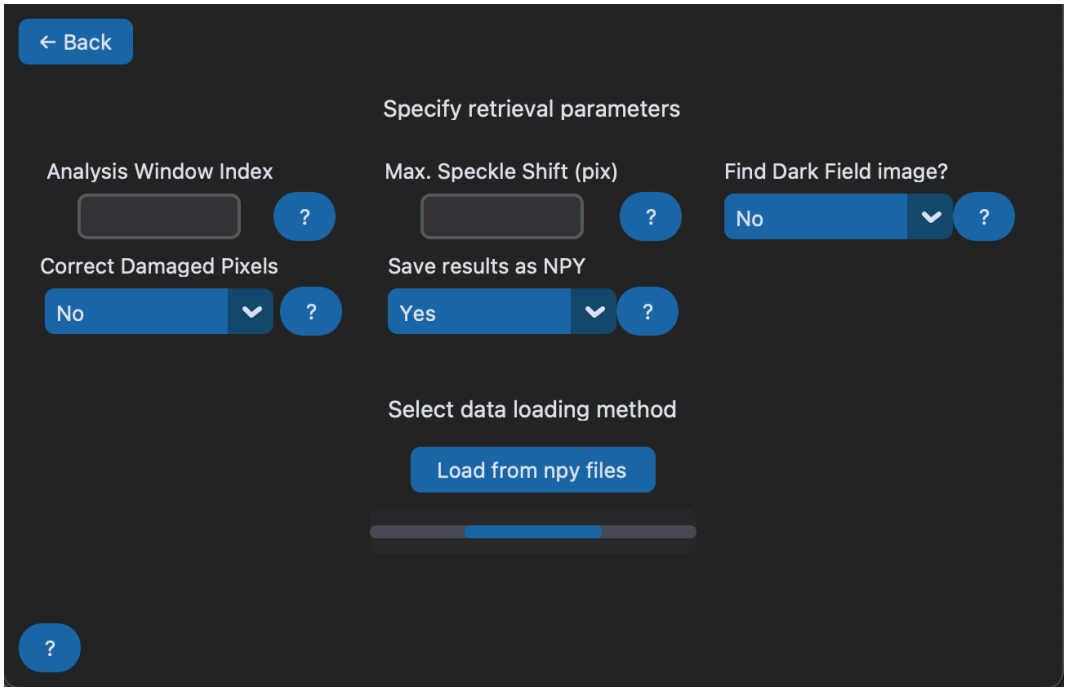

Figure 15: **UMPA** menu.

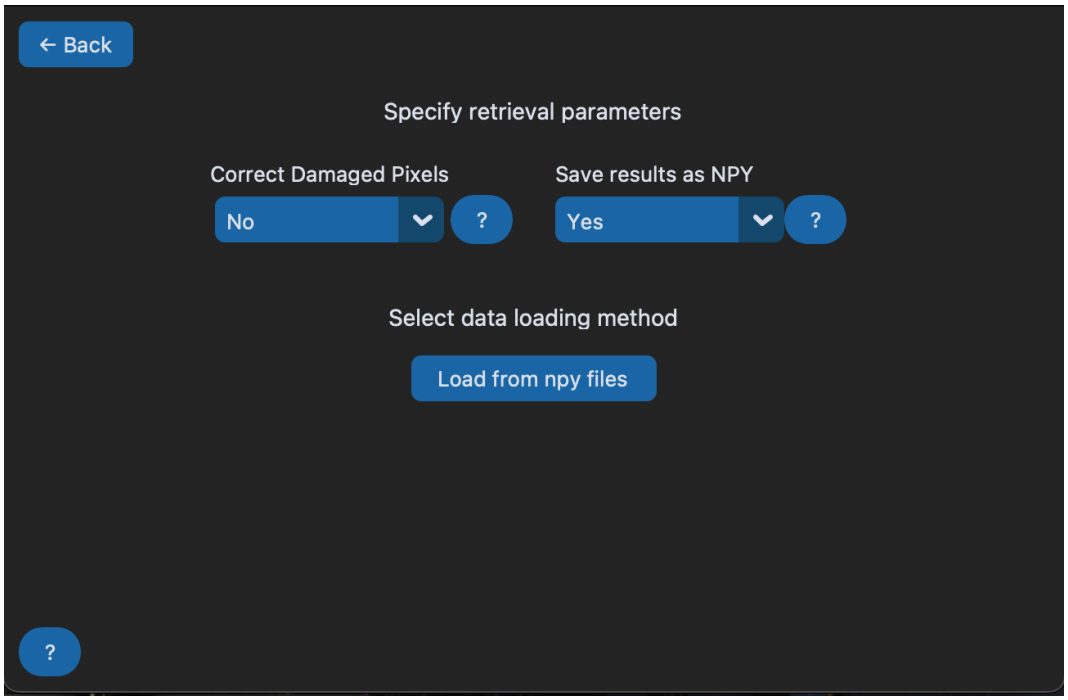

Figure 16: **LCS** menu.

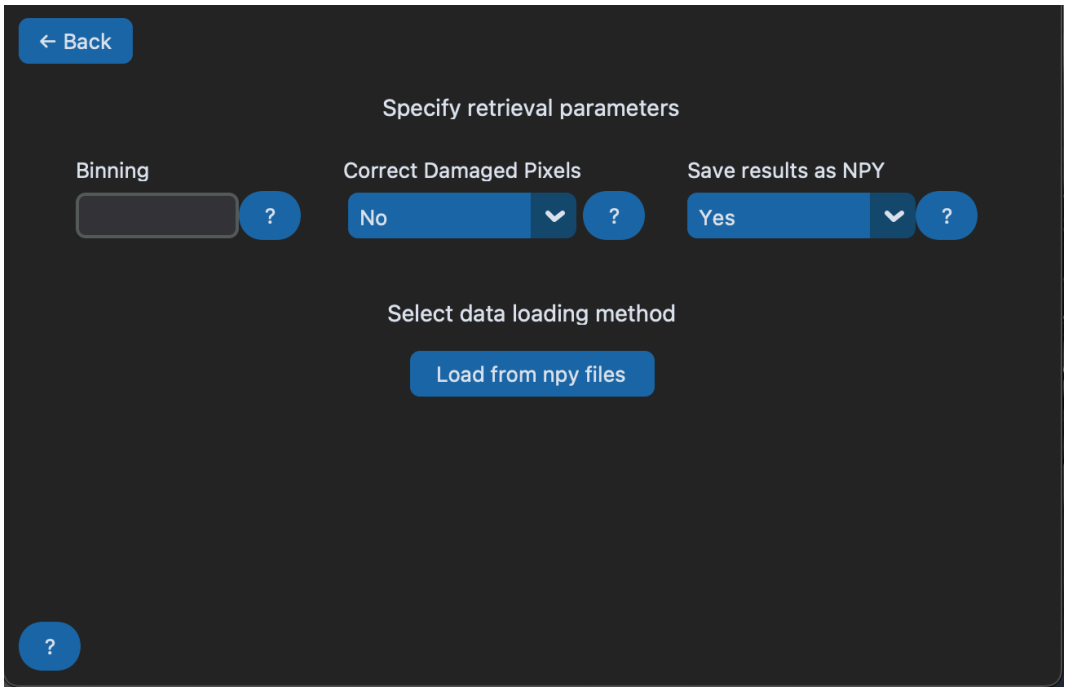

Figure 17: **EI** retrieval menu.

7 List of Acronyms

EI edge illumination

CT computed tomography

SBI speckle-based imaging

PBI propagation-based imaging

SGBI single-grating-based imaging

UMPA unified modulated pattern analysis

LCS low coherence system

FWHM full width at half maximum

FOV field of view

PSF point spread function

8 Contact Information

For any questions or suggestions, please contact:

- **Main Developer**:
  Manuel Fernando Sánchez Alarcón (mf.sanchez17@uniandes.edu.co)

References

[1] Kenan Li, Michael Wojcik, and Chris Jacobsen. “Multislice does it all; calculating the performance of nanofocusing X-ray optics”. In: *Opt. Express* 25.3 (Feb. 2017), pp. 1831–1846. DOI: 10.1364/OE.25.001831. URL: https://opg.optica.org/oe/abstract.cfm?URI=oe-25-3-1831.

[2] Alessandro Olivo. “Edge-illumination x-ray phase-contrast imaging”. In: *Journal of Physics: Condensed Matter* 33.36 (July 2021), p. 363002. DOI: 10.1088/1361-648X/ac0e6e. URL: https://dx.doi.org/10.1088/1361-648X/ac0e6e.

[3] A. Hipp et al. “Single-grating interferometer for high-resolution phase-contrast imaging at synchrotron radiation sources”. In: *Developments in X-Ray Tomography X*. Ed. by Stuart R. Stock, Bert Müller, and Ge Wang. Vol. 9967. International Society for Optics and Photonics. SPIE, 2016, p. 996718. DOI: 10.1117/12.2237582. URL: https://doi.org/10.1117/12.2237582.

[4] Vittorio Di Trapani et al. “Speckle-based imaging (SBI) applications with spectral photon counting detectors at the newly established OPTIMATO (OPTimal IMAging and TOmography) laboratory”. In: *Journal of Instrumentation* 19.01 (Jan. 2024), p. C01018. DOI: 10.1088/1748-0221/19/01/C01018. URL: https://dx.doi.org/10.1088/1748-0221/19/01/C01018.

[5] Regine Gradl et al. “Propagation-based Phase-Contrast X-ray Imaging at a Compact Light Source”. In: *Scientific Reports* 7 (July 2017), p. 4908. DOI: 10.1038/s41598-017-04739-w.

[6] Fabio De Marco et al. “High-speed processing of X-ray wavefront marking data with the Unified Modulated Pattern Analysis (UMPA) model”. In: *Opt. Express* 31.1 (Jan. 2023), pp. 635–650. DOI: 10.1364/OE.474794. URL: https://opg.optica.org/oe/abstract.cfm?URI=oe-31-1-635.

[7] Laurène Quénot et al. “Implicit tracking approach for X-ray phase-contrast imaging with a random mask and a conventional system”. In: *Optica* 8.11 (Nov. 2021), pp. 1412–1415. DOI: 10.1364/OPTICA.434954. URL: https://opg.optica.org/optica/abstract.cfm?URI=optica-8-11-1412.

[8] Elisabeth R. Shanblatt et al. “Forward model for propagation-based x-ray phase contrast imaging in parallel- and cone-beam geometry”. In: *Opt.*

Express 27.4 (Feb. 2019), pp. 4504–4521. DOI: 10.1364/OE.27.004504. URL: https://opg.optica.org/oe/abstract.cfm?URI=oe-27-4-4504.

[9] Gibran David Jurado. “Multimodal X-ray edge illumination imaging for medical applications with polychromatic sources”. MA thesis. Universidad de los Andes, 2024. URL: https://hdl.handle.net/1992/73943.