About ConeX

ConeX is a program for the angular calibration of flat 2D detectors in the context of scattering by isotropic samples, notably of X-rays. The purpose of the software is to average the 2D images recorded by the detector into 1D scattering patterns.

The analysis is based on a modeling of the shape of iso-angle scattering lines by conical sections -or conics: ellipses, parabolae, hyperbolae- hence the name of the software.

The typical use of ConeX comprises 3 consecutive steps: (i) the determination of the 3D position of the detector starting from the scattering patterns of calibration samples; (ii) the creation of an averaging procedure which specifies the desired resolution, the region of interest of the detector, etc. and (iii) the data processing itself.

The present manual guides the user step by step through a practical example. More thorough explanations can be found in our paper

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ConeX, a program for angular calibration and averaging of 2D powder scattering patterns

which you are kindly asked to refer to when using ConeX for your research.

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An Example

In this example, a 2D CCD detector was used to measure wide-angle X-ray scattering patterns at X-ray energy of 12 keV. The scattering patterns of two calibrants were measured, namely high-density polyethylene and silver behenate. Both patterns were saved as files HDPE.tif and AgBh.tif. We use both calibrants to estimate the position of the detector, from which we convert the 2D images into 1D scattering patterns.

Step 1: Determination of the 3D position of the detector

When you execute ConeX1.exe, the following window appears.

![Window for ConeX1.exe](image)

Go to the window “Create a New Angle Calibration” and follow the instructions to open the file HDPE.tif. The following window appears

![Window for angle calibration](image)

Use the sliders to adjust the contrast

Select the calibrant “HDPE” and set the energy to 12 keV

These are the 4 lines we are going to use for the calibration.

when the calibrant and energy are set, the scattering angles are updated, based on the known spacings.
Once you have selected a particular line that you want to use for the calibration, you can simply add points to it by selecting them manually on the image. This is done in 2 steps. A rough position is first selected on the grey-tone pattern, and a detailed area appears automatically on which the point position has to be chosen as accurately as possible.

Click the left mouse button to add a point, and click the right button to stop adding points. All points of a given line have to be added at once. If you select a line that has already some points, this will erase them. Incidentally, this provides you with a way of correcting any spurious point that you may want to remove.

Note that the shape of the lines carries information about the position of the detector. You should therefore also include points that close to the limit of the detector so that the shapes of the lines are well captured.
At the end of the process, when you have added points to all of the 4 lines of HDPE in that particular angular range, the window should look like this.

Click then “Add Calibration Sample” and open the “AgBh.tif” file. Silver behenate is more commonly used to calibrate detectors in small-angle scattering configuration, but some higher order \([0 0 l]\) lines are also visible at wide angles.

We know by trial and error that the first three lines seen on the right of the detector are those that are expected at 5.1°, 6.1° and 7.1° at 12 keV.

After proceeding like with the HDPE calibrant, the window looks like this.
If you want to use yet another calibration image, you can do that by clicking again on “Add Calibration Sample”. There is no limit to the number of calibrants that can be used.

As a rule of thumb, the better the calibration points cover the detector area, the more accurate the determination of the detector position will be.

If the calibration sample is not HDPE or AgBh, you should choose “Other” instead of “HDPE” or “AgBh”. In this case, you proceed as described previously, but you have to calculate by yourself the scattering angles (in degrees) and type them the empty white area right to the colored check boxes.

Once you have added all points to all the scattering lines of all the calibration samples you want to use, just press “Done”. 

You can select “Other”…

… and enter yourself the angle (in degrees) of the scattering lines you want to use for the calibration.
Once you have pressed “Done” in the “Calibration Data” window, the following window appears, in which all the points you have selected are plotted. This is the window where the detector position will be estimated.

To initiate the calculation, click in the central panel where you think the center of all these arcs are. This is just a starting point for an optimization; it doesn’t have to be accurate: it just has to be on the correct side of scattering line with the smallest angle.

Once the optimization is finished the theoretical lines appear. Depending on the speed of your computer, this may take a few seconds.

This shows the 3D position of the detector with respect to the scattering cones.

These are the theoretical lines (conics) corresponding to the calibration angles.

These sliders enable you to assign a different weight to each line for the fit.

These are the values of the optimized parameters. You can change them manually to start the fit again.
If the solution of the optimization is not satisfactory, you can change manually the fitted parameters. The theoretical conics and the 3D view in the upper left corner will be modified accordingly to help you find visually a suitable set of parameters. You can then do the optimization again, starting from these values, by clicking on the “Fit” button.

You may want to force the detector to be vertical and put manually the $\beta$ value to 90°. To get a better agreement with the theoretical lines, you then have to change also the values of X and Y to $X = 1000$ and $Y = 2500$. This leads you to the following situation.

![Image of detector position with modified parameters]

Changed manually the values to $\beta = 90$, $X = 1000$, and $Y = 2500$.

To optimize the fit starting from these new values, press “Fit”. In this particular case, you will see that this brings you back to the original configuration, which corresponds to the actual position of the detector!

![Image of detector position with optimized fit]

When you fit, starting from these new values, this brings you back to the actual position of the detector.
For the optimization, you can also adjust the statistical weight of each line by using the sliders on the right side of the window. This is sometimes helpful when trying to troubleshoot a failed optimization.

For instance, if you want to know what the calibration would look like with only the HDPE calibrant, move all sliders of AgBh to the left, and then press the “Fit” button.

![Image of software interface showing sliders and a graph]

All sliders of AgBh were moved to their leftmost position, and the fit was done on HDPE alone.

Of course, by doing this the AgBh lines are not well described anymore by the calibration.

You can play around with the sliders, trying e.g. to calibrate the detector with only two lines: the 5° line of AgBh and the 24° line of HDPE, etc., etc. etc.

Once you are satisfied with the optimization click “Keep values”. You will be asked to give a name to the file in which the optimized parameters are saved. The extension of the file is “.pos”, which stands for position.
Step 2: Creation of an averaging procedure

Once a pos file exists, you can use it to create an averaging procedure. Creating an averaging procedure means to specify the region of the detector to use, as well as the required angular accuracy.

For that purpose, go to the main window of ConeX and select the appropriate menu.

![Diagram of ConeX software interface](image)

You are then asked to open a pos file, and a “typical file to be processed”. Suppose we are interested in polyethylene and open the HDPE.tif file.

The following window appears, in which the chosen “typical file” is overlapped with a grid of lines taken every degree. The latter are the conics calculated based on the pos file.

![Averaging Procedure window](image)

Select here the minimum and maximum angle to consider, as well as the total number of points wanted in the 1D pattern.

The two red lines are the minimum and maximum angles to consider.

You should also select a Region of Interest in the detector, and possibly Blind Regions.
Typically, not all parts of the detector are usable. In this particular case for instance, the corners of the detector should be removed before the averaging. You may also want to restrict the averaging to areas of the detector where the grid follows nicely the shape of the scattering lines.

You therefore have to select a region of interest (ROI). When clicking the button on the right side, a window appears in which you are asked to select manually a polygonal area by simply clicking with the mouse. You finish the procedure by double-clicking inside the polygonal area.

The blind regions, i.e. regions possibly inside the ROI that have to be excluded, are selected in the same way.

There is just one ROI, but there can be as many blind regions as necessary. They can be reset at any stage: by default the ROI is the entire detector and there are no blind regions.
At the end, the window should look like this.

By creating the averaging procedure, a mapping is made between any pixel in the detector’s ROI and the scattering angles. The solid angle corresponding to any group of pixels is also calculated based on the pos file.

All relevant information for further data processing is stored in a file with extension .avg.

You can create several avg files corresponding to a single pos file. This may be necessary, for instance, when different types of samples are measured with the same detector at the same position.

Note that the number of points in the 1D pattern does not have to be too large. In this particular case, 300 points is 20 points per degree, which is more than enough.
Step 3: Data Processing

When you start ConeX, before being able to process data, you need to load an averaging procedure. This is done by going to the leftmost menu of the main window, and by loading an .avg file.

Once this is done, the “Processing” menu becomes active, and you can go to the “Angular Averaging” menu.
You can load either a single file or multiple files by holding ctrl down (or shift + ctrl) while selecting the files.

The following window appears.

For the purpose of the present demo, just load the two files HDPE.tif and AgBh.tif. The following window appears.

By default, the dark image is supposed to be 0 everywhere and the detector response is 1 everywhere. Files with the measured dark image and detector response can be loaded. The “Reset Dark & Response” button puts these values back to 0 and 1.
The “Convert All” button converts all the loaded files into 1D scattering patterns. The patterns are saved in a text file with (i) the first column being the scattering angles $2\theta$ in degrees, and (ii) the subsequent columns being the calculated 1D patterns, in the order in which they appear in the upper-right popupmenu (that is the order in which they were opened).

A preview jpeg file is also created.

**File conversion from BSL/OTOKO format to Tiff**

ConeX 1.0 accepts only tiff as an input format. There is a menu in the main window for converting BSL SAXS data into tiff images.

The input file should be the BSL header file (the name of which has the structure *000.*) The tiff files corresponding to all frames are created in the same directory as the BSL file, as well as a single text file that contains the calibration data stored in the file *002.*. At the DUBBLE beamline, the first three columns in this file correspond to the total detector intensity and to signals from the first and second ionization chambers.