temDM STEMcor advanced version

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Use this manual in combination with the guide for the temDM STEMcor basic version. The present manual considers only the issues NOT COVERED in the previous manual.

CONTENTS

1 INSTALLATION

Installation of the advanced version is not more difficult than that for the basic one.

You should place the **temDM STEMcor.gtk** plugin into a PlugIns folder of DigitalMicrograph. There are typically several such folders. As for the basic version, the script **find plugins folders.s** included in the distribution package can help you to localize the desired folders. Open **find plugins folders.s** in DigitalMicrograph and run it by pressing execute or by pressing ENTER with holding the CNTR key. As the advanced version of **temDM STEMcor** is of restricted access, you are recommended to install it in the user-specific folder available only for you in a given PC. This should be in the first line of the folders list displayed by the **find plugins folders.s**script. Read the folder path and drop **temDM STEMcor.gtk** there. If you cannot localize the user-specific plugins folder, then use any available plugins folder.

Some folders can be hidden in Windows. If you do not see all folders, make them visible in the Windows explorer:

Windows 7: Organize tab - Folders and search options - View tab - click show hidden files, folders and drivers checkbox.

Window 10: View tab - click hidden items checkbox.

IMPORTANT: if you have already installed the basic version of **temDM STEMcor***, you should OVER-WRITE it with the plugin of the advanced version (the plugins have the same names). This is also applicable for updating the version.* All versions of temDM STEMcor have the same name to avoid confusion with loading ambiguous commands. If you have several versions, it is recommended to keep plugins in individual folders with meaningful names like

```
temDM STEMcor GMS2 advanced version 1
XX.
```

During the first start of the advanced version, the program will request you to input your individual installation code. You have to do it only once for a given PC.

- Input your installation code in the prompt string. Confirm with OK.

After successful installation, choose STEMcor in the temDM menu of DigitalMicrograph. Your **STEM-**

cor tool should look like:
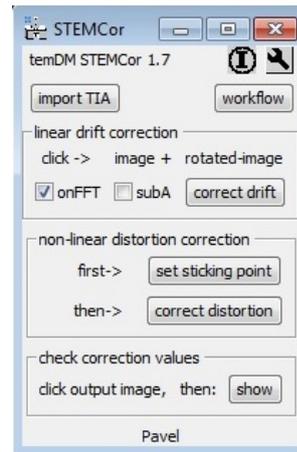
You are probably already familiar with the upper box in this tool. That is the correction for linear drift incorporated in the basic version of the **temDM STEM-cor** plugin. This is unchanged in the advanced version. A new feature is a box below with the correction for non-linear distortions.

2 WHY NON-LINEAR CORRECTION IS NEEDED ?

The assumption of a linear drift distorting STEM images is the only first order approximation. In reality, there is a lot of sources for the non-linear distortions like sudden shaking the sample, inaccuracy or instability of the scan generator and so on. These non-linearities show up clearly with increasing the magnification. In particular, atomic resolution STEM images virtually always require a non-linear correction. The figures below demonstrate examples of the unacceptable distortions - a sudden vertical jump (left image) or a horizontal jump (right image) between the subsequent scanned rows.

Such distortions can be however removed when analyzing a couple of images - one with the original orientation and another one with 90°-rotated scanning orientation; both images must (at least partially) cover the same area in the sample. The reconstruction can be performed after, for instance C. Ophus et al. Ultramicroscopy 162 (2016) 1, who assumed that there is no distortion within any given scanning row but distortions show up as the X,Y-shifts of the rows relative their "true" positions. If we change the direction of fast scanning, the scanning columns will be rigid while probably X,Y-shifted relative each other as shown in the figure.

fast scan direction →   slow scan direction →

slow scan direction ↓   fast scan direction ↓
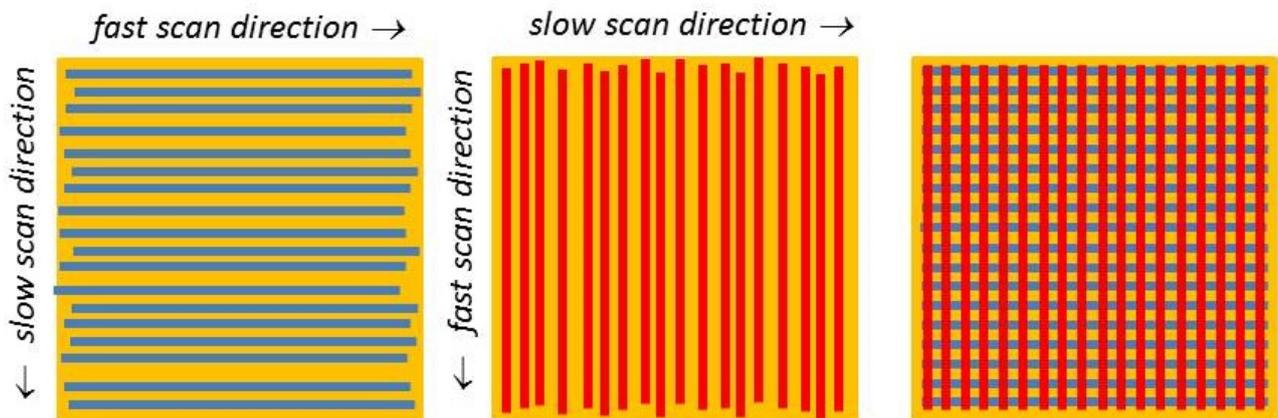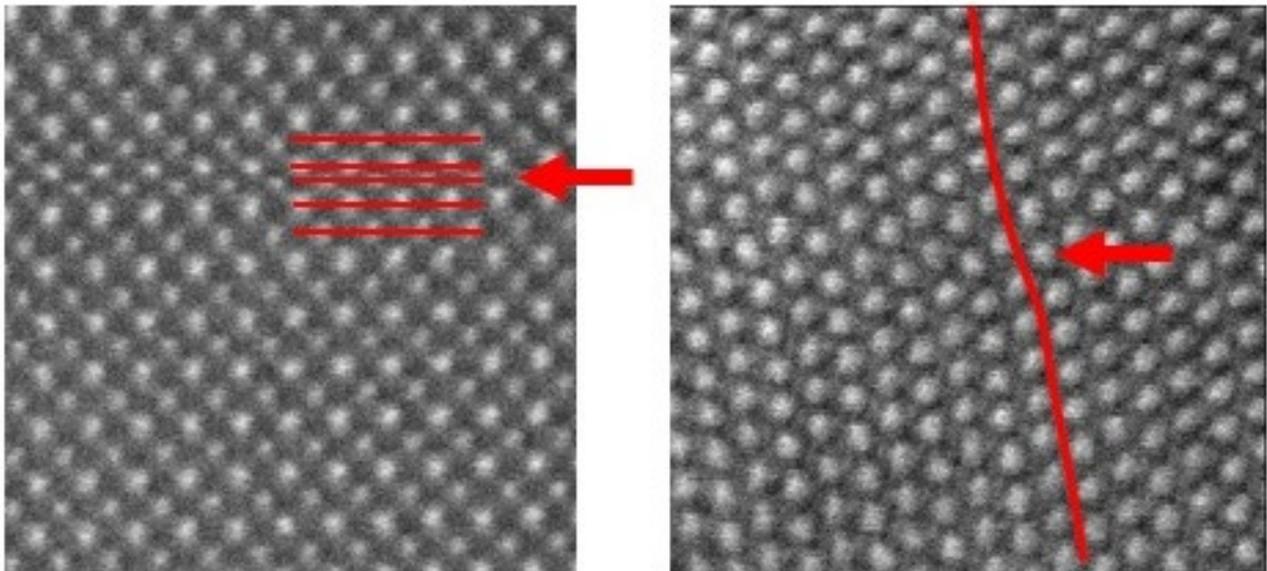
To reconstruct an undistorted image, all these shifts must be retrieved. This is a complicated but doable task. Just overlap the *original* and *rotated* images and shuffle the rows in the former and the columns in the latter until two images show the best agreement.

The **temDM STEMcor** plugin follows conceptually the approach of Colin Ophus et al. although technically uses a rather different algorithm.

## 3 PREPARE IMAGES BEFORE CORRECTION FOR NON-LINEAR DISTORTIONS

Your couple of images (*original* and *rotated* orientations) should be first corrected for the linear drift - this is pre-requirement for more advanced actions. As soon as you obtained the couple of *linearly corrected* images you can start the non-linear correction. It is an order of magnitude more complicated treatment than linear correction, thus the system needs some minimal guideline from you. Namely, you should identify one point that you think is same in the *original* and *rotated* images.
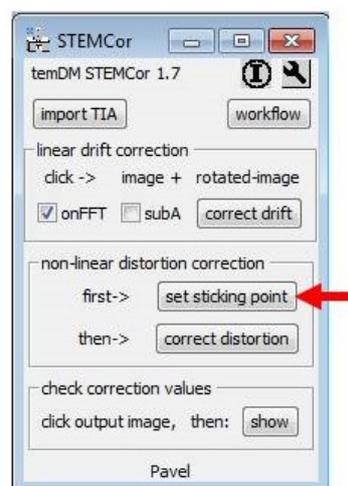

- Having the linearly corrected *original* and *rotated* images in front press the set sticking point button in the "non-linear distortion correction" box.

- You see a panel consisting of two images. The left one is your *original* image while the right one is your second image *rotated back* such as the orientation of both images is now identical.

- There are two colored markers - red in the left image and green in the right one. They are supposed to point at the position assumed to be same in both images. But initially it is never same because of the STEM distortions. First drag the red marker to the recognizable place in the left image. Then drag the green marker to the place you suppose to be same in the right image.

- In the floating dialog window, press Confirm.
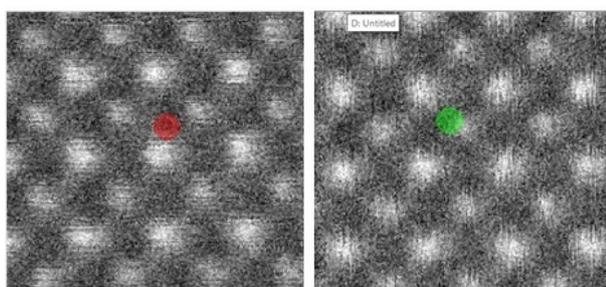
drag the markers such as they point to the identical atomic column
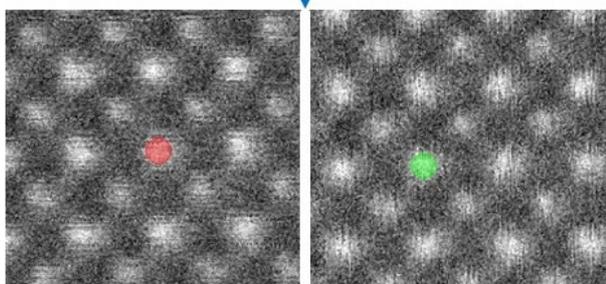
Why this is needed ? The non-linear correction is mostly applied to the atomic resolution STEM images. The lattice is often composed of two or more sublattices (like in the exampe below), which are hard to distinguish by an algorithm. The script might easily confuse the sublattices while human eye has a greater chance to make it correctly. Such supervision helps a lot to the program and it would not take much time from you, just few seconds.

Do not afraid to confuse the original and rotated images (for linear correction, it was mandatory needed to click first the original and then the rotated image, remember?). Now the images are internally tagged, so even if you click in the wrong order, the script knows who is who.

Setting the sticking point is user-friendly. You can zoom the left image to see better the place of interest. The right image will be zoomed synchronously. Start always with positioning the red marker because the green marker will move accordingly. When you are sure with landing the red marker, go to the movement of the green one. The red marker will stay unchanged - the synchronization works only in one direction.

Sometimes, it is not easy to find the exact correspondence between two images. The well recognizable features might be at the periphery of the image while the sticking point should be rather placed in the central part. Just count carefully the number of unit cells from your sticking point to some unique marker in both images.
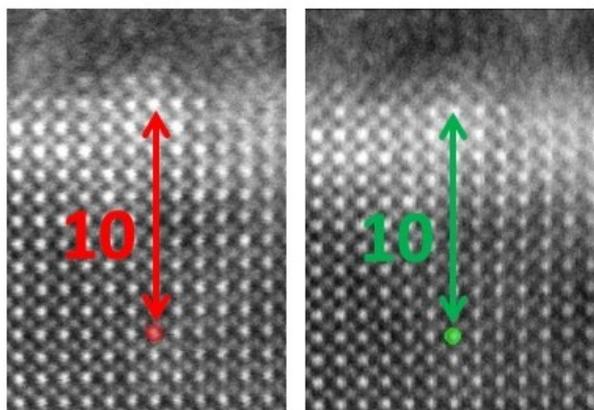
It is not necessary to position markers very precisely. The script will refine the exact position anyway. Just ensure that the required atomic column is within the red (green) marker and press Confirm.

Now, everything is prepared for automatic alignment (everywhere, not just at the sticking point you set!) of your *original* and *rotated* images.

4   CORRECTION FOR NON-LINEAR DISTORTIONS

The further correction is pretty easy.

- Having the linearly corrected *original* and *rotated* images in front press the correct distortion button in the "non-linear distortion correction" box. Wait a bit

After the fitting procedure is finished, two new images appear - they are non-linearly corrected images in the *original* and *rotated* orientation. Red rectangular ROIs in both images indicate the calculated area of
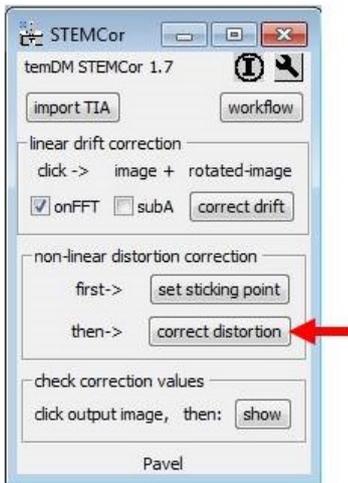
their overlap.
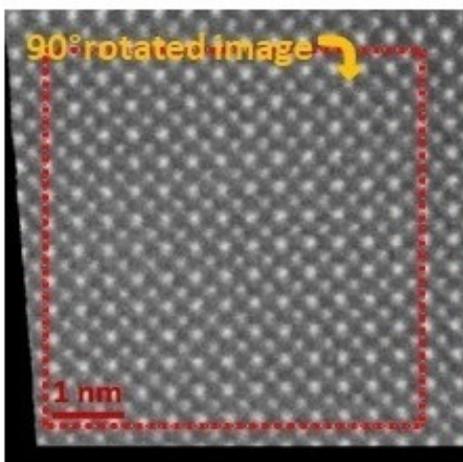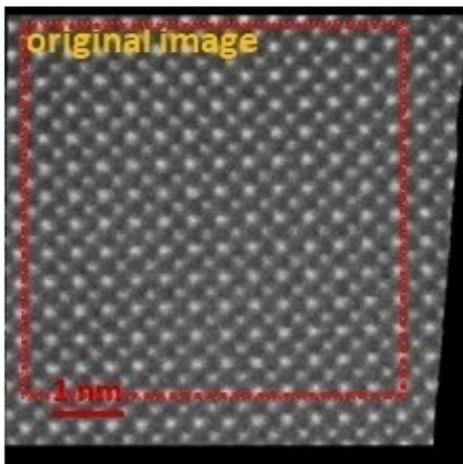
Additionally, a new image, which is combined from the *original* and *rotated* images by simple summation within of their areas of overlap appears. This image will be slightly smaller in size comparing to the both input images as the overlap area is smaller than the original scan size. The combined image is calculated in the *original* orientation, not in the 90°-rotated one.

The algorithm was not specifically aimed to remove
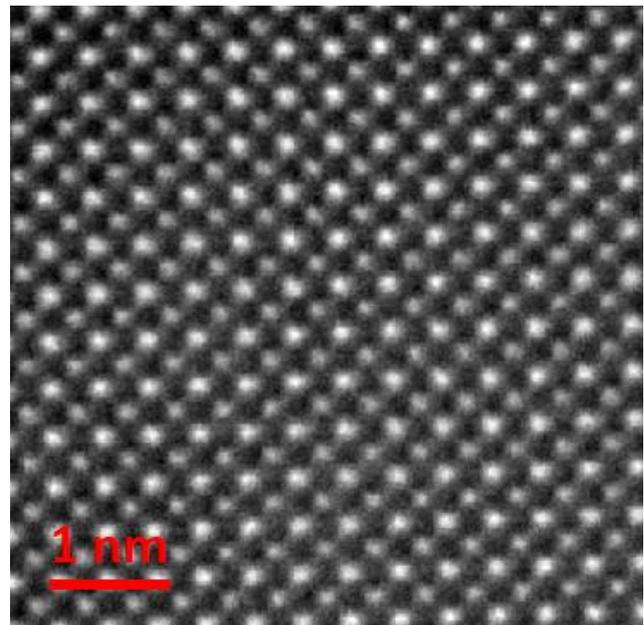
so-called STEM jitters (jagged shapes of atomic columns). However you can notice that the jitters are significantly suppressed after the non-linear corrections. That is because the random shifts among rows are minimized, while the sporadic jumps within the rows are still present. The applied strategy results in the most reliable positioning of the atomic columns although their shapes might show some negligible jags. We however consider this as a rather cosmetic issue.
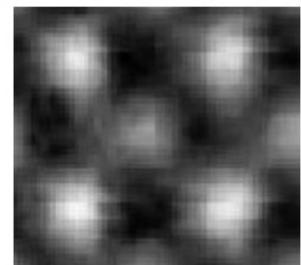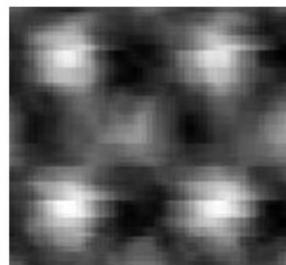
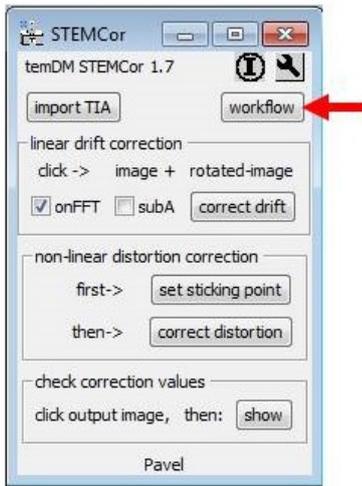linearly corrected   non-linearly corrected

5 WORKFLOW

You might wish to make all treatments (linear + non-linear correction) as a continuous workflow.

- Just click the "workflow" button.

The linearly corrected images are not delivered, you will only see them when prompted to set the sticking point.

This is probably the most convenient way to work. However, if you feel some issues, please turn to the
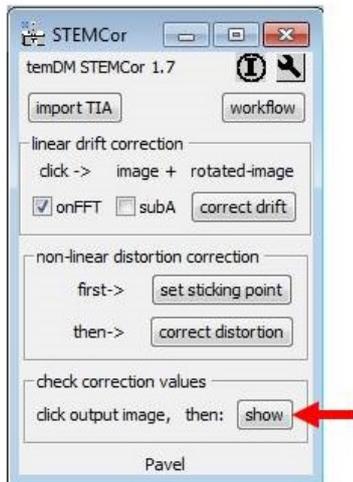
step-by-step treatment (first linear correction, then sticking point and finally - non-linear correction).
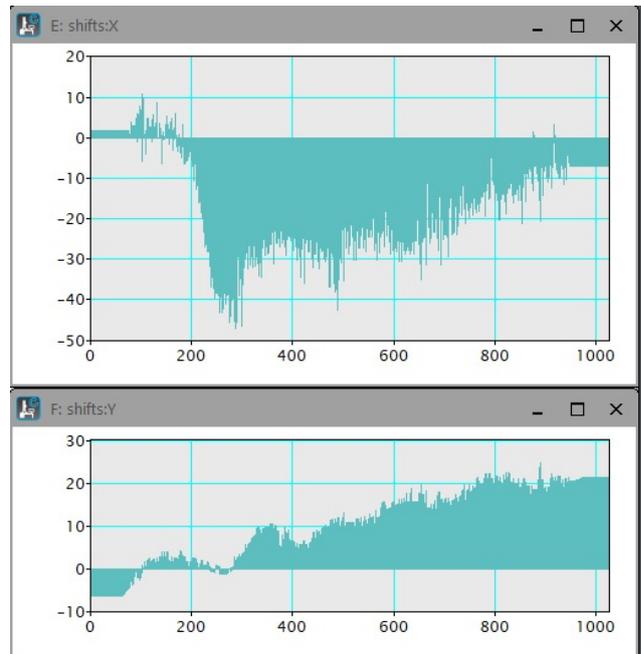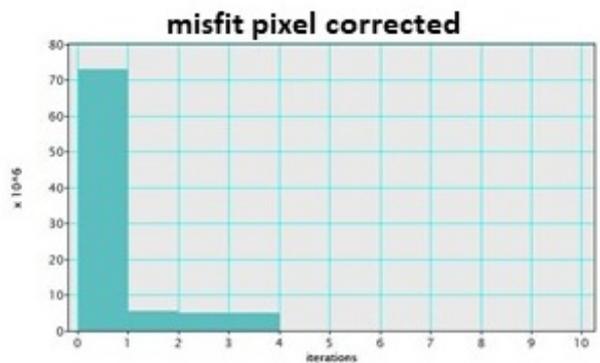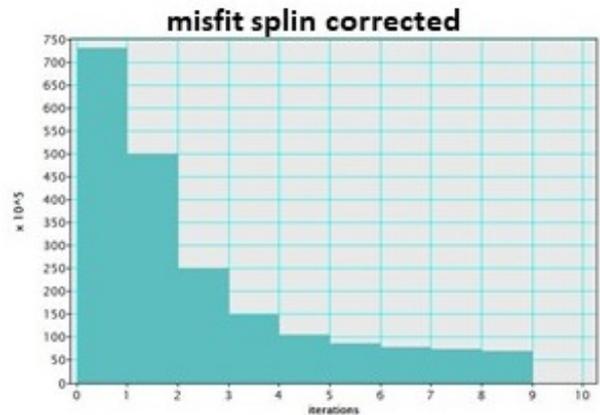
6 CHECK CORRECTION VALUES

Finally you might be curious how much correction was applied to the images.

- Having the non-linearly corrected *original* image in front press the show button in the "check correction values" box. Two plots will appear indicating the applied shifts (in pixels) for each row in the X- and Y-directions.

    Do not be surprised that the shifts are flattened at the edges. There is no images overlap there thus the shifts are assumed to be constant and equal to the nearest available shift in the overlapped area. Similarly, the shifts applied to the columns in the *rotated* image can be extracted when having it in front.

   Another kind of information is stored in the *combined* image.

- Having the *combined* image in front press the show button in the "check correction values" box. The graphs showing convergence of iterations will appear.

    The criterion of convergence in this case is the squared difference between the *original* and *rotated* images at each iteration. The fitting is executed in two stages: first, the shifts are smoothed with a cubic spline (spline correction) ; second, the shifts of individual rows are

varied independently (pixel correction). Correspondingly, two convergence graphs for the first and second stages are displayed.

7 SETTINGS

Click a spanner icon to assess the settings. The upper part of the appearing page is the setting for the linear correction that was described in the manual for the basic version. The setting relevant for non-linear correction start with the caption advanced:.
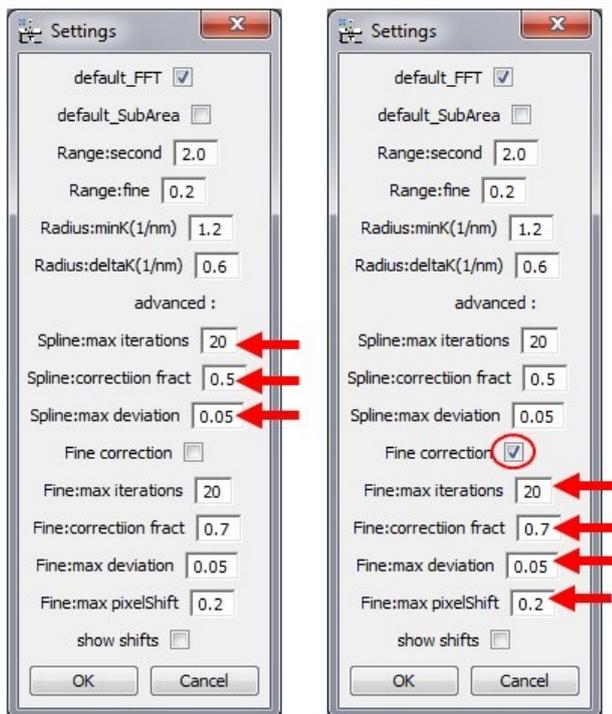
Spline:max iterations defines the maximal number of iteration for the first stage of fitting (shifts smoothed with a cubic spline).

Spline:correction fract defines the value of correction applied after each iteration. It is expressed as a fraction of the measured deviation. This value must be always less than unity, otherwise the convergence might be unstable.

Spline:max deviation defines the halting criterion for iterations. Namely, when the relative difference between two subsequent iterations becomes less than this value, the iterations stop.

The next group of settings is relevant for the second, finer stage of fitting (when pixels are fitted independently). You can enable or disable this stage in the checkbox Fine correction. The advantage of fine fitting is apparently more accurate results. The disadvantage is the noticeably longer execution time. It is your choice to enable or disable this option. The meaning of the fitting parameters is analogous to those for the first fitting stage.

Fine:max iterations defines the maximal number of iteration for the fine stage of fitting (pixels are shifted independently).

Fine:correction fract defines the value of correction applied after each iteration. It is expressed as a fraction of the measured deviation. This value must be always less than unity, otherwise the convergence might be unstable.

Fine:max deviation defines the halting criterion for iterations. Namely, when the relative difference between two subsequent iterations becomes less than this value, the iterations stop.

Fine:max pixelShift limits the shift of rows or columns during the optimization. This is expressed in the fraction of maximal shift applied in the previous (smooth) fitting step. This value should be kept small (ultimatively less tahn 1) otherwise the program might fall into the false optimum.
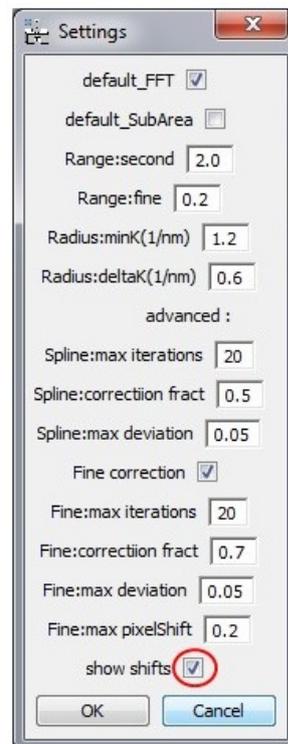
show shifts You might prefer to see the values of the applied shifts every time after the fitting is finished. Then activate this option.