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Jitterbug for DigitalMicrograph

Scan-noise and Drift Compensation Plug-in



Jitterbug Manual 3.6

HREM Research Inc.

Preface

This user manual describes how to install and operate the *Jitterbug* scan-noise and drift compensation plug-in (version 3.x) for Digital Micrograph.

The software is based on the full-length manuscript by Dr Lewys Jones and Prof Peter D. Nellist:

Lewys Jones and Peter D. Nellist. "Identifying and Correcting Scan Noise and Drift in the Scanning Transmission Electron Microscope". *Microscopy and Microanalysis* (2013) **19**, p.1050-1060.

As this tool applies post-processing steps to experimental data, users should state explicitly when such steps have been applied by citing the above paper such as:

"image scan-noise and drift was compensated using the Jitterbug software described in [1]".

Contact

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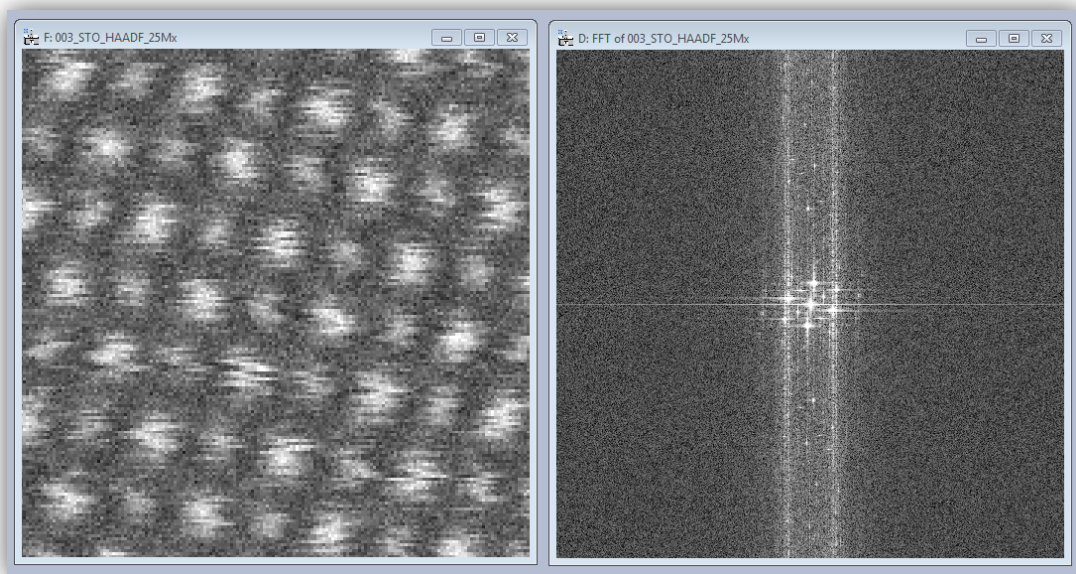
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When to use this Plug-in

The *Jitterbug* plug-in for Digital Micrograph is designed to correct some of the most common image distortions encountered during atomic-resolution imaging in the scanning transmission electron microscope (STEM) including scan-noise and image drift.

Scan-noise will often appear in images as 'sliced' or 'torn' atomic features and is also often observed in Fourier transforms as white vertical bands streaking from low order spots (see below). Alternatively, image drift can be observed as a deviation of known lattice plane angles (expected to be 90° in the example below) or distortion of known lattice plane spacing.



If your data includes these types of distortion then it may be possible to recover some or all of the lost performance caused by scan-noise. Of course if the image is very heavily degraded it will not be possible to compensate this entirely. Equally this plug-in cannot create resolution that did not exist prior to the incorporation of scan-noise. For further information and some related reading please see the reference given on page 2.

Installation

Software Requirements

The following is a list of the software requirements necessary to run the Jitterbug plug-in:

- DigitalMicrograph (GATAN™)
- USB Key Driver
- HREM Mouse Tool Plug-in (Free-ware downloadable from www.hremresearch.com)
- IPU Plug-in (Free-ware downloadable from www.hremresearch.com)
- Matlab MCR (Matlab Compiler Runtime)

Software Installation

Installing USB Key Driver

The user key driver should be installed by following the instructions given by the key driver installer. The key driver installer can be found on our web site.

Installing Jitterbug Plug-in

The plug-in can be installed by drag-and-drop copy to the folder “PlugIns” (The PlugIns folder should exist under a normal installation of the DigitalMicrograph.)

When the DigitalMicrograph is launched after placing the plug-ins into the PlugIns folder, Jitterbug menu commands will appear under “Jitterbug” menu.

Installing Mouse Tools

All the files relating Mouse tool plug-in can be installed by drag-and-drop copy to the folder “PlugIns.” (The PlugIns folder should exist under a normal installation of the DigitalMicrograph.)

When the DigitalMicrograph is launched after placing the plug-ins into the PlugIns folder, the Mouse tool will appear as an addition to the standard tools.

Installing IPU Plug-in

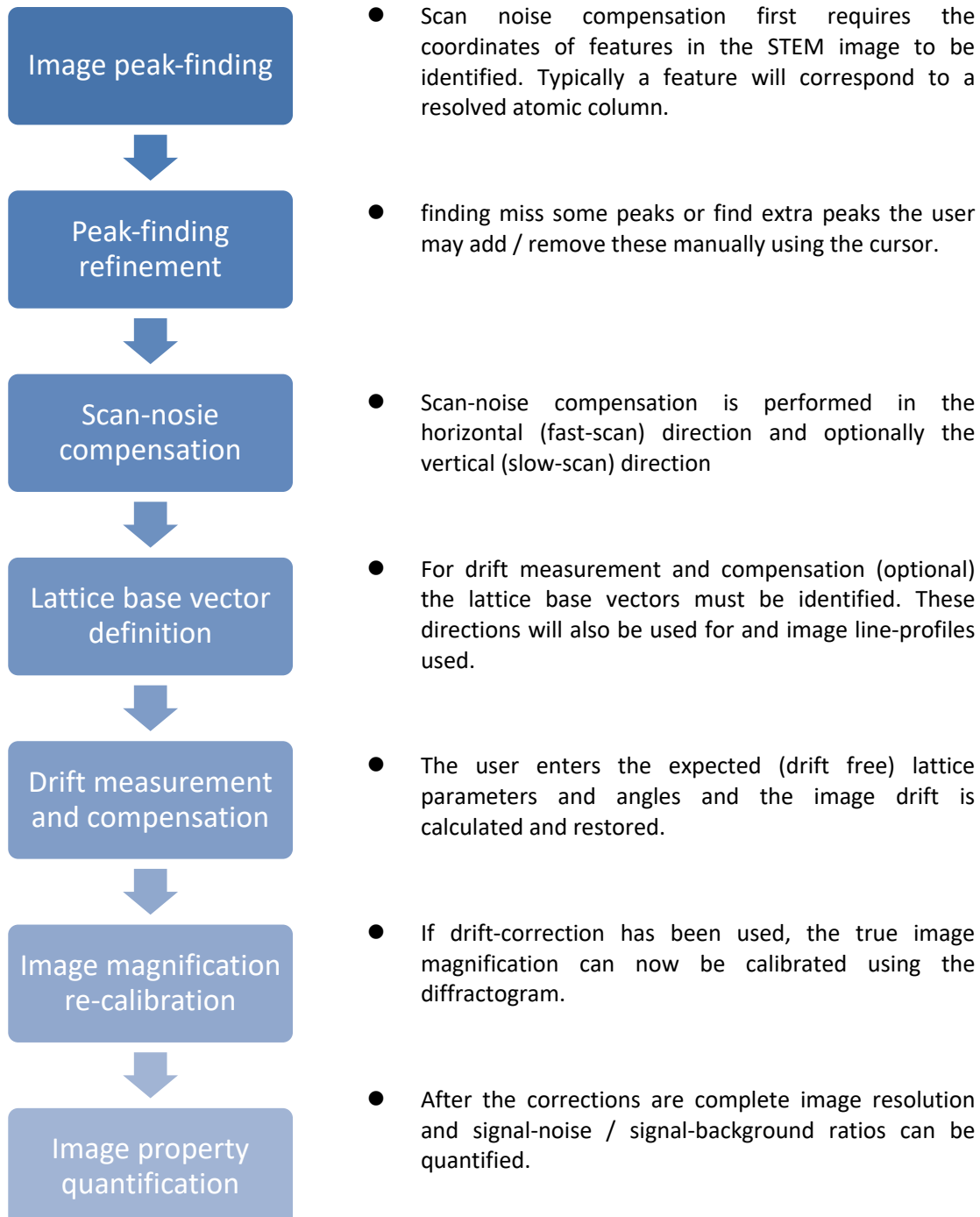
Jitterbug uses some functions based on the Intel’ MKL (Math Kernel Library) provided by the IPU plug-in. All the files relating the IPU plug-in can be installed by drag-and-drop copy. Please consult the ReadMe file that comes with the IPU plug-in.

Installing Matlab MCR

The Matlab MCR should be installed by following the instructions given by the installer. The Matlab MCR that is compatible with the Jitterbug can be found on our web site.

Typical Workflow

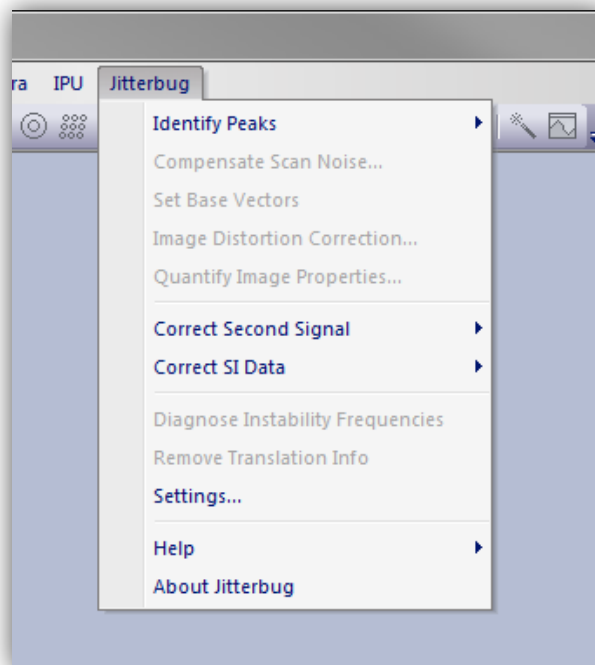
Many of the tools included in this plug-in can be used independently as required. Where tools depend upon using one or more features together this will be described in the sections that follow. A typical user workflow for the correction of image scan-noise and drift is shown below:



The following examples will use the supplied example image to demonstrate the various steps.

Plug-in Menu

The figure below shows the default menu for the Jitterbug plug-in:



In the menu, items that are currently unavailable are shown in grey. As you move through the workflow, further options become available as needed.

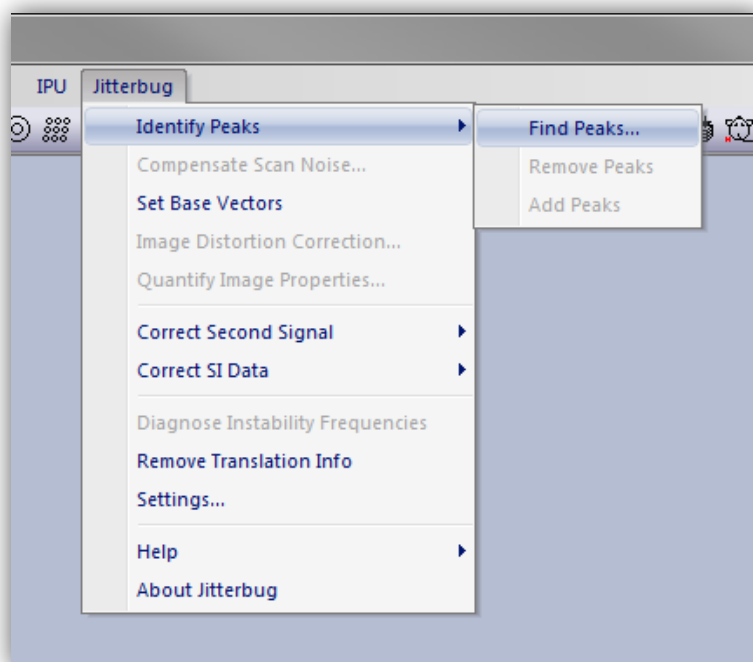
Supported File Types

To begin, the user should have the file open within the Digital Micrograph workspace. To open a file either open it from your computer or from within DM by going to File > Open.

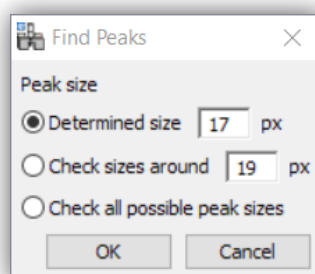
The plug-in supports all image formats supported by DM, however, it is essential that the images to be processed have received no image compression (such as JPEGs) and have had no pixel resampling (either up-sampling or down-sampling).

Peak Finding

Scan-noise compensation requires the peak positions of features to have been identified. This is done using the menu: Jitterbug > Identify Peaks:



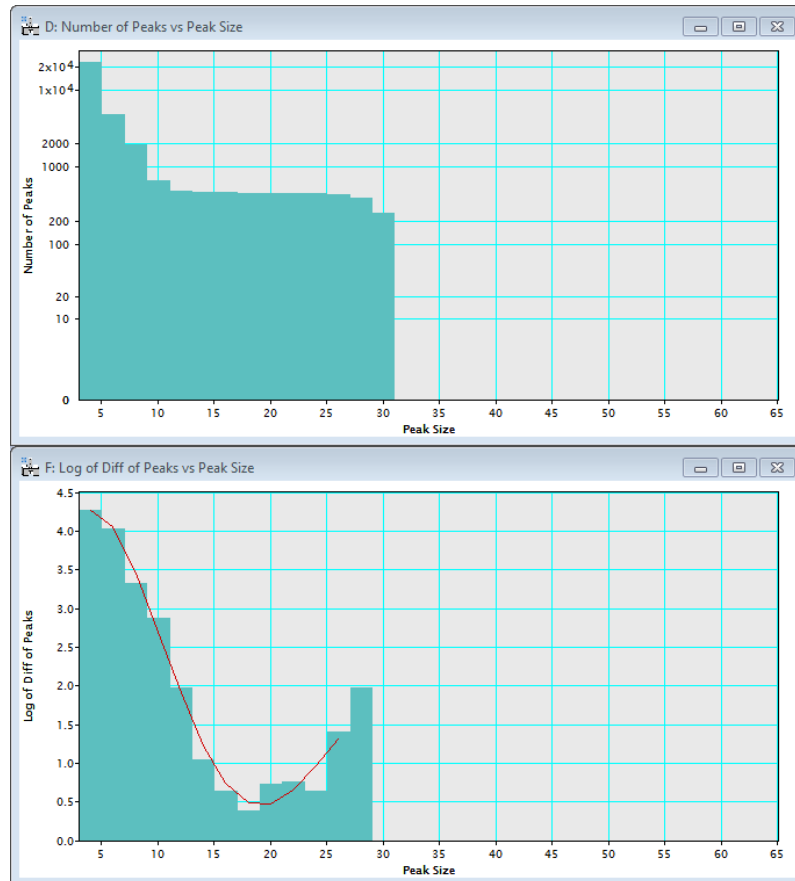
Three options are presented for the peak-finding, manual target-separation, approximate peak-separation search, or fully automatic. If the exact separation between atomic features is known (in units of pixels) then this can be input in the dialogue box and the software will search for features at this separation from one another. If the separation is *approximately* known but not precisely, then the estimate can be entered and the software will search around this range. If nothing is known, then a full search can be performed, but this may be slow for very large images. There is no requirement for the features to be in a regular array nor for any template to be specified. If time-series data is selected, then peak-finding will be performed on the stack-average.



For the example image supplied the separation of features is approximately 19 pixels. Alternatively the option of "Check all possible peak sizes" can be used. In this mode all possible target-separations will be evaluated and the plug-in will try to automatically select the best

value. This option is slower and should generally be avoided for images larger than 512x512 px. (The next release will give a possibility to select a search area, if the image size is larger than 512x512 px.)

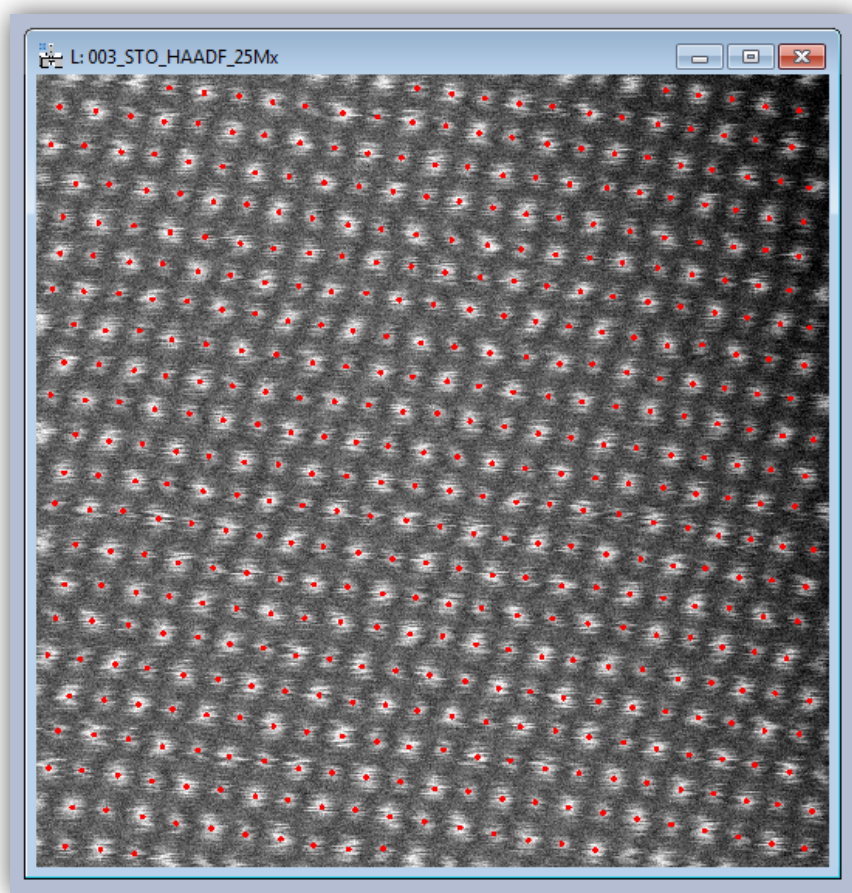
If 'Search full range' is selected, then during the peak-distance optimization stage an additional data output will be displayed:



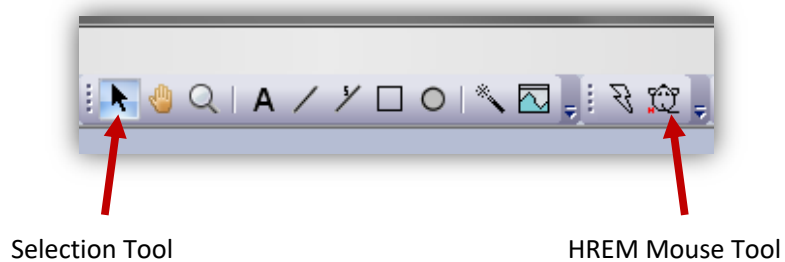
These figures show (top) the absolute number of possible candidate peaks found for different search settings, and (bottom) the fitting used to determine the best plateau in the peak-number data. This point indicates the most robust size parameter and hence is the best choice for the automated optimization step. The value from the optimization is then taken for the automated peak-finding.

If for some reason the automated optimization is not able to produce an acceptable result (such as very noisy data) then the user may use these figures to choose a reasonable manual estimate.

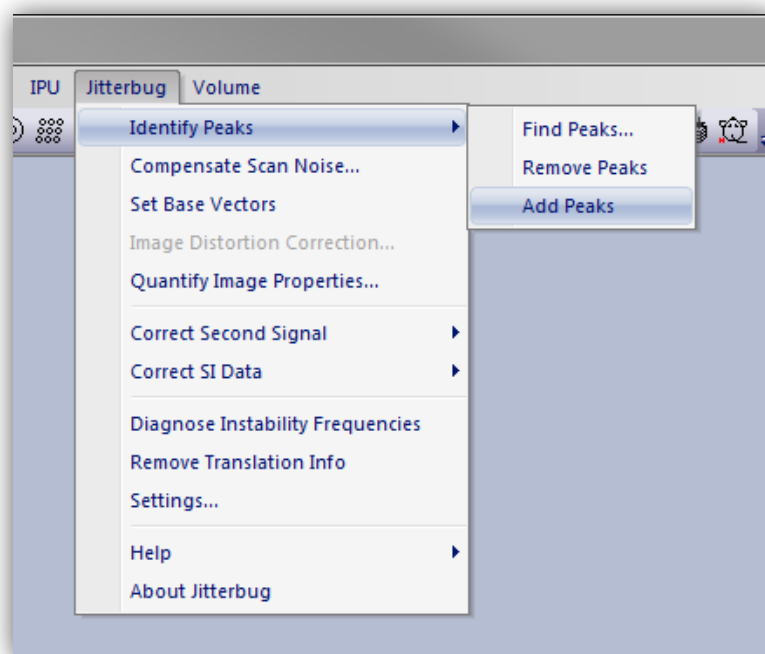
After the peak finding is complete a new image will open with the results indicated by red dots:



Here all features have been identified successfully, however the user can also add or remove points manually. Adding or removing points is done using the HREM Mouse cursor:



To add additional peaks simply click one or more points on the image. These will appear as numbered squares around the point clicked. When finished add the peak manually using the Jitterbug menu:

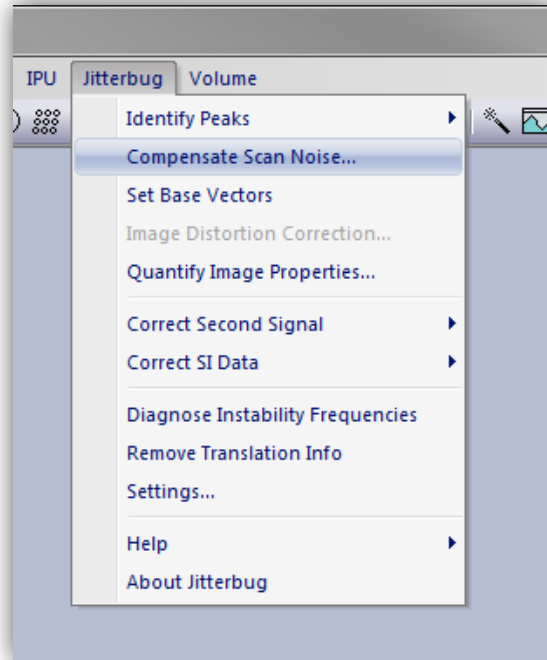


To remove peaks, use the same Mouse tool and click nearby the feature(s) to be removed. Again select the “Remove Peaks” option from the menu and the feature closest to the position clicked will be removed.

The process of adding or removing peaks can be repeated as many times as needed until the desired result is achieved.

Scan-noise Compensation

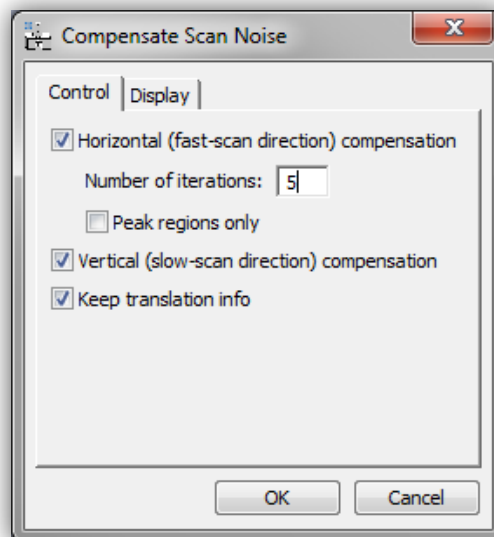
Once feature positions are identified the menu option to “Compensate Scan Noise...” will be available:



The dialogue box for scan-noise compensation options will then open.

Horizontal (Fast-scan Direction) Compensation

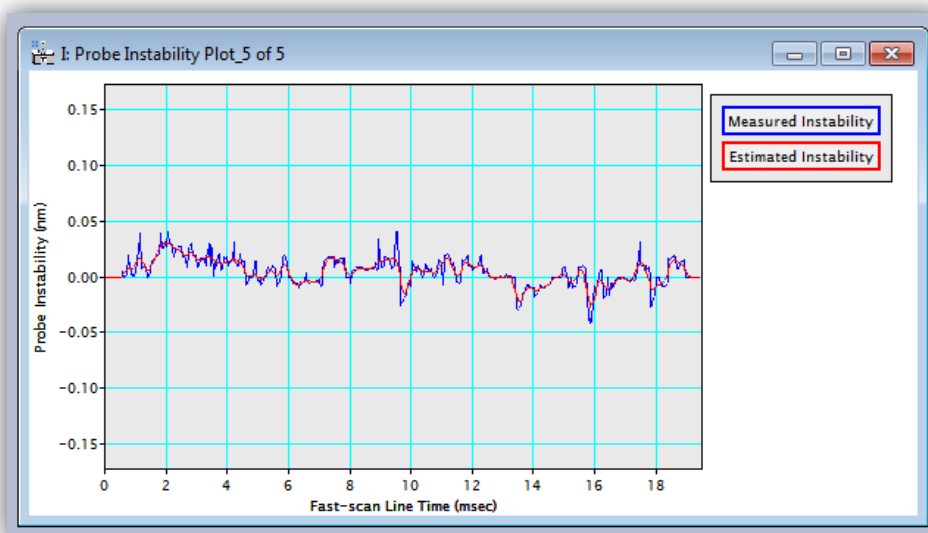
In this plug-in scan-noise compensation is achieved through comparison of image data with neighboring rows. Of course in the original data these rows too may be themselves distorted and so the restoration is performed iteratively. By default horizontal scan-noise compensation is on.



For larger images (bigger than 512x512px) it is recommended to use no more than five iterations. Restoration performance improves only slightly beyond two iterations.

If you intend to go onwards to correct a second image signal or a spectrum-image volume, you should select “Keep translation info”. This will store all the data to enable identical pixel shifts to be applied a second time. If you do not need this you can un-check this box to slightly reduce computer memory usage.

During the correction of horizontal scan noise the diagnosed probe offset plot will be displayed. If the image magnification has been calibrated this will be shown in units of nanometers, otherwise pixels.



This distortion offset profile will be updated as each scan-line is processed and with each iteration during the restoration. The figure will remain after compensation is complete showing the final scan-line of the final iteration (5 in the above example). After the compensation is complete you may close this figure if you wish as it is not needed by any of the onward processing steps.

Vertical (Slow-scan Direction) Compensation

In the “Compensate Scan Noise” dialogue box, compensation of vertical scan-noise may be selected as an option. In general this option should be left on (box checked) but there are certain circumstances where this option should not be used.

This feature will attempt to locally re-order parts of the scan lines in the slow-scan direction by sorting rows based on their intensity. Where atomic features are only just resolved (such as a very close dumbbells), and the nearest neighbor is along a near vertical direction, it may not be possible to correctly identify this vertical scan-noise and the option should be un-checked.

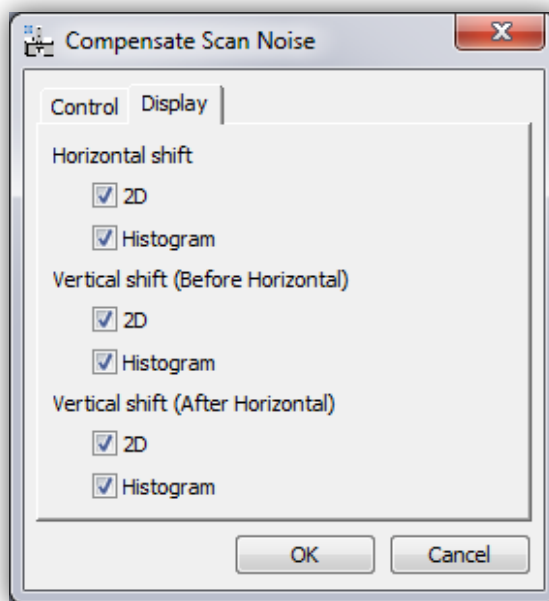
Fast Mode for Sparse Images

For images where the field of view is not filled with sample (such as nano-particles or samples with an edge) it may not be necessary to scan-noise compensate the whole image. In regions which do not contain atomic resolution information (and hence are not identified by the peak-finding) no benefit will be observed upon this correction. In this situation a ‘fast mode’ may be used which will aim to reduce the number of calculations made where possible to speed up the restoration. To use this mode select the option “Peak regions only”.

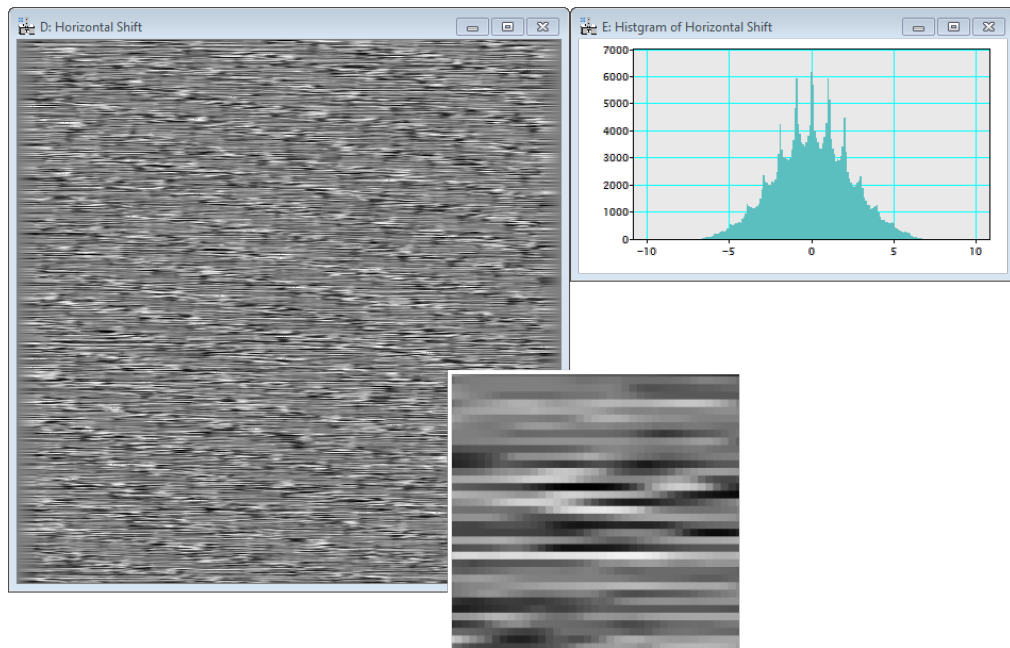
After scan-compensation is complete the restored image will be returned in a new window with a title that reflects this result.

Compensate Scan Noise – Display Options

The second tab of the ‘Compensate Scan Noise’ dialogue gives users the choice to generate extra diagnostic data about the applied corrections. By default these are not needed but may be useful for power users or debugging.



Horizontal shifts that are diagnosed can be displayed as an image plot and also as a histogram. The user may find it interesting to observe the ‘fast-scan’ direction streaking of the diagnosed horizontal shifts. Users may for example take line profiles of this shift plot to observe the distortions.



Similar figures can be displayed for the vertical (row-sorting) operation. As this is performed at the start and end of the correction process, both a 'before' and 'after' version are displayed.

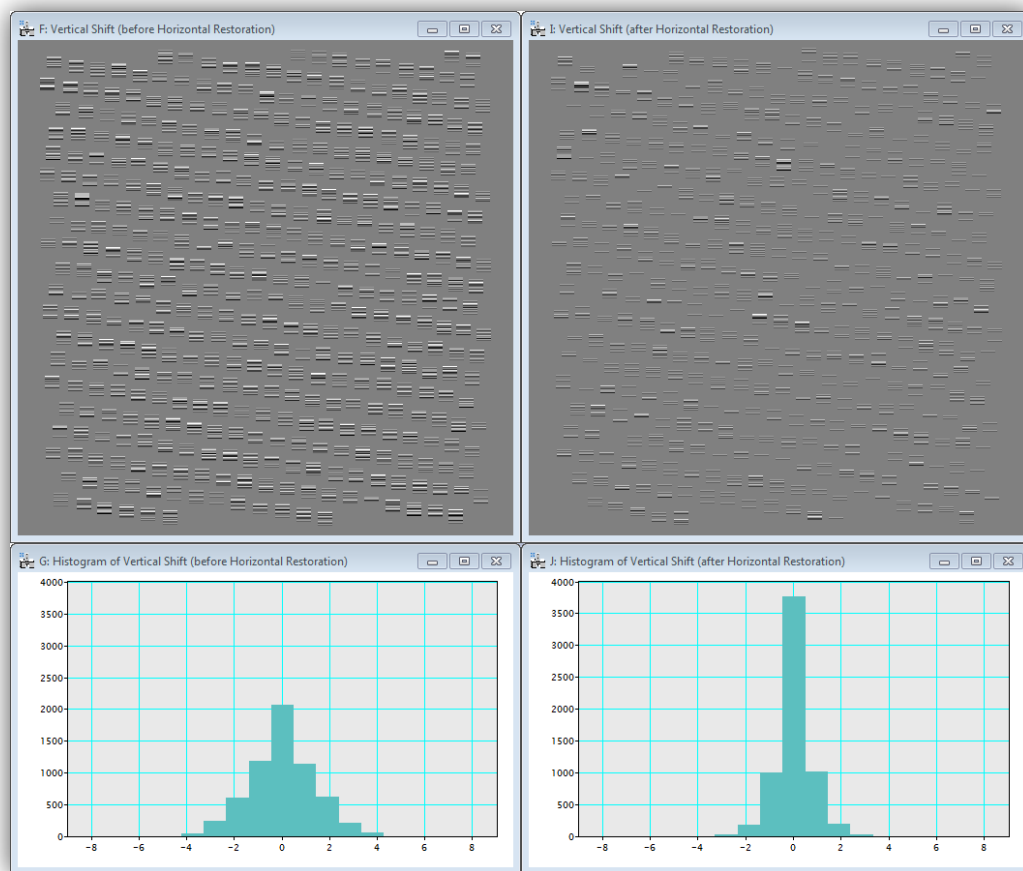
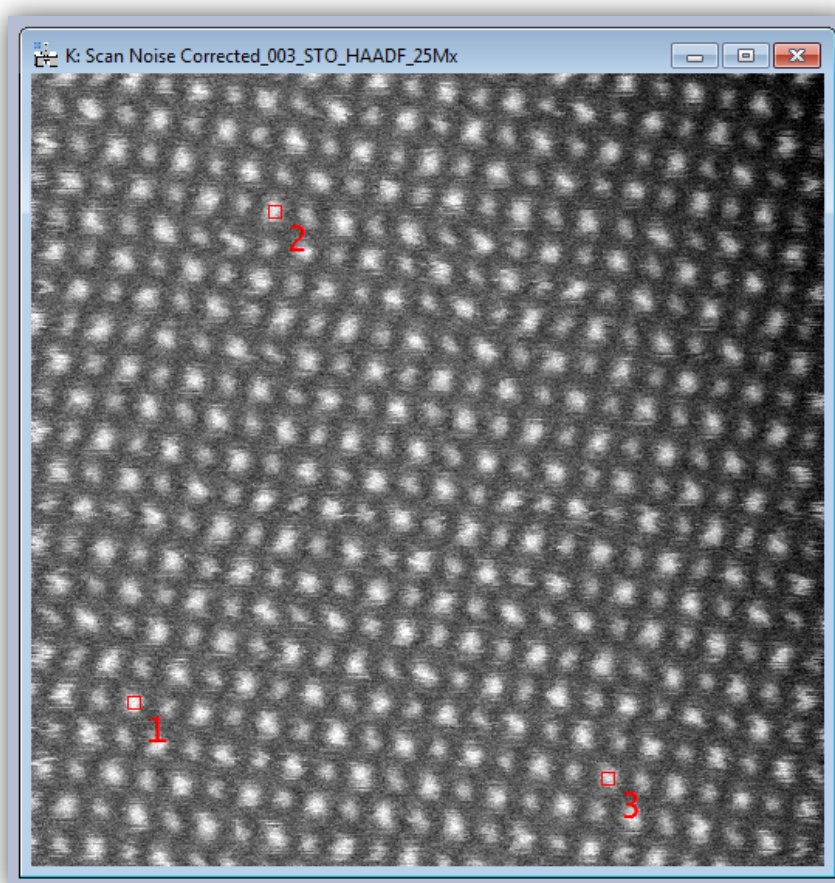


Image Drift Correction

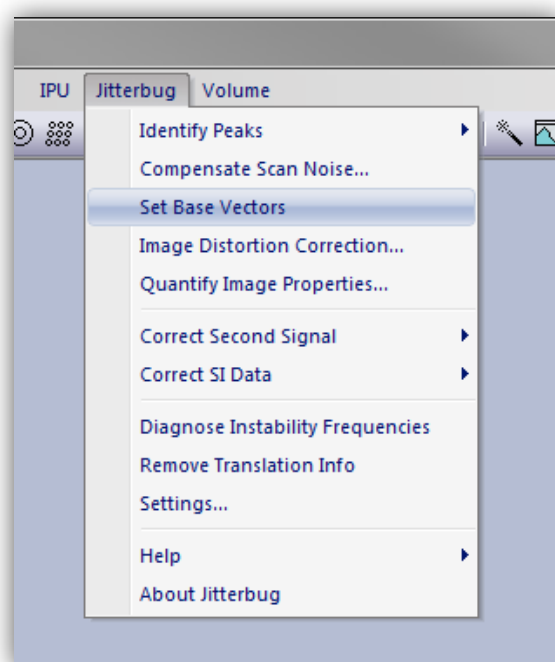
In practice image / stage / sample drift may be present. These drifts appear as a single overall drift vector and may be present in any arbitrary direction; because of this no specific scan-rotation need be prescribed when recording image data to use with this plug-in.

Setting of Base Vectors

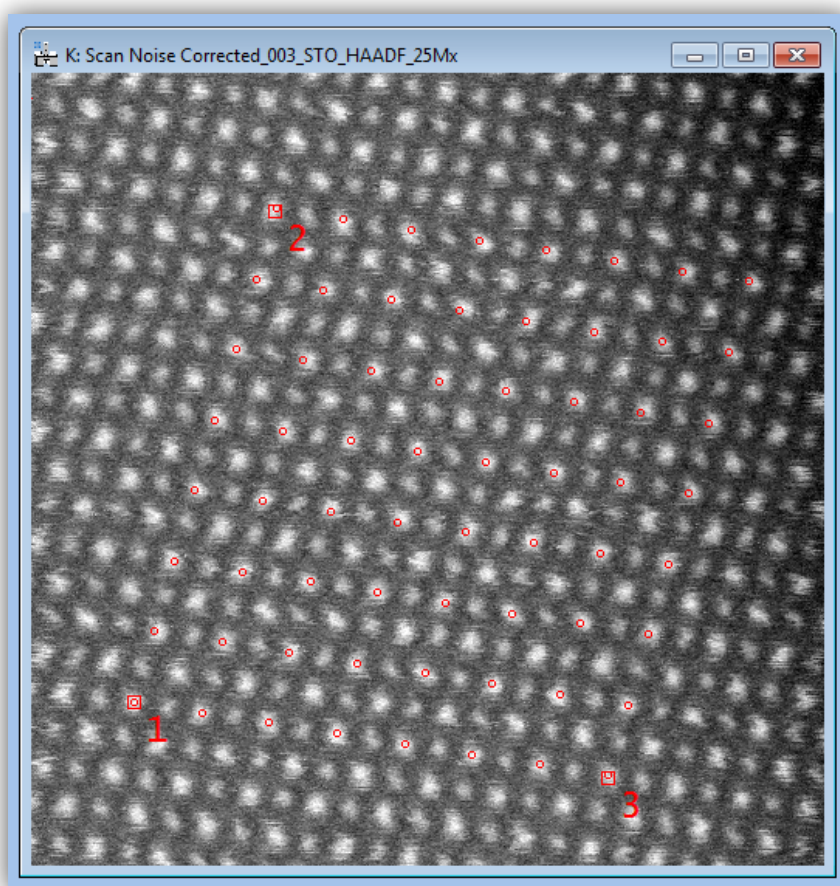
To diagnose any variation from the expected crystal structure a pair of base vectors must first be defined. This is done using the HREM Mouse tool. The process for this is to first click on an atomic column that is to be used as the origin and then to click two points that define the ends of the two basis vectors.



The points will be indicated by red squares and labeled 1,2 and 3. If you make an error and / or wish to change the selection, simply remove the points (using Cntr+A / Cmnd+A and backspace / delete) and identify new ones. After you are happy with the designation then select "Set Base Vectors" from the Jitterbug menu.



This will generate an array of points (see below) to highlight repeat units of the identified crystallography. Again the user should verify the result here is acceptable and if not repeat the selection of the base vectors.

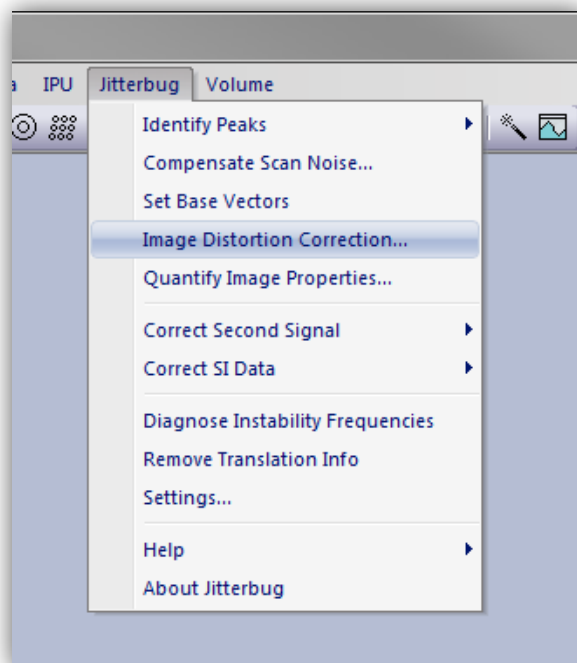


In general selecting base vectors that are larger will lead to a more precise measurement of the properties of this repeat unit.

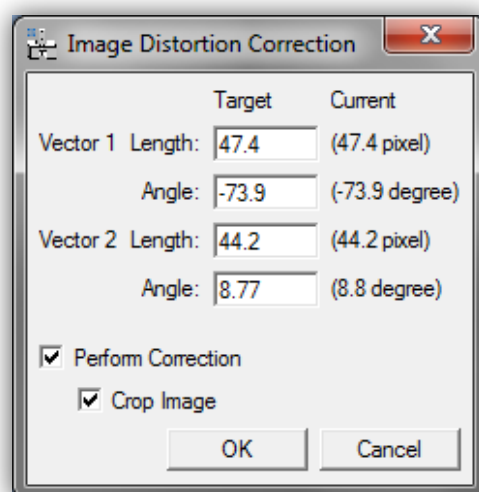
If the image used contains more than one crystal (e.g. a grain boundary) then either region may be used and should yield the same result. If the sample contains a defect or some irregular structure then the above process should be performed on the bulk region in the image.

Description of Expected Geometry

After the base vectors have been defined as above the user may now correct for the image drift. This is done from the Jitterbug menu selecting “Image Distortion Correction”:

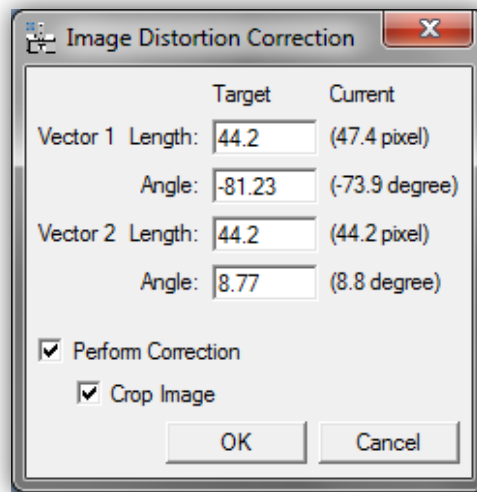


This will open the “Image Distortion Correction” dialog window which will show both the current and target lengths and angles of the repeat unit identified by the base vectors:



In this example data (strontium titanate [100] projection) the repeat unit should be square, that is the two base vectors should be identical lengths and separated by 90°. The dialog window shows the lengths to be different by around 7% and the angle between them to be only 83°. To

correct this you may modify either the first or second vector's properties or some mixture of both. For this example vector 1 will be modified to match vector 2:



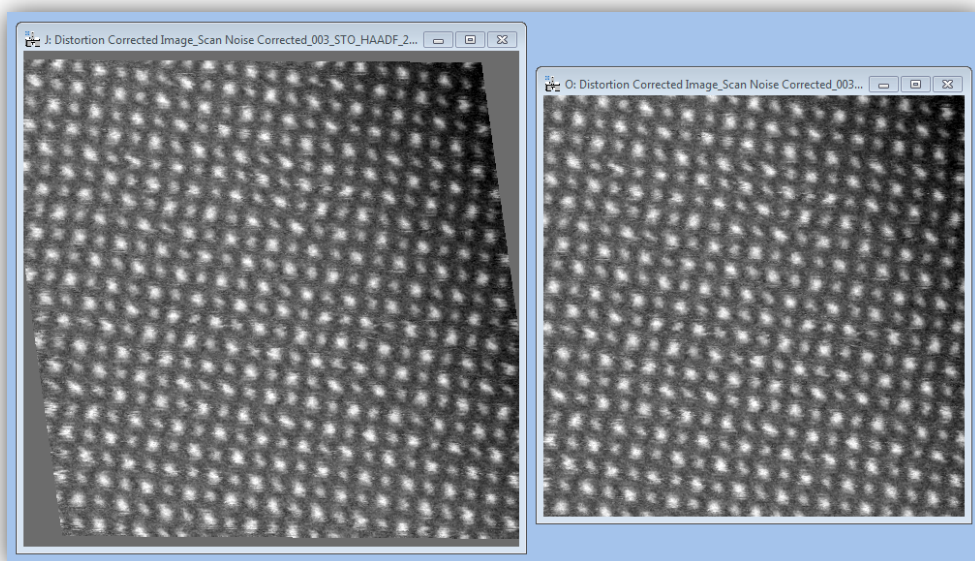
Two final options are presented for the user to choose: whether to perform correction and whether to crop the image. The default mode is for both to be on (checked).

The distortion correction feature can be used to only measure the drift without correcting it. This may be used for example to compare the raw and restored image results. The second option is whether to crop the image after the correction transform.

The vectors used here could have been identified in the opposite sense (separated by 97°) and would have yielded the same results.

Image Cropping

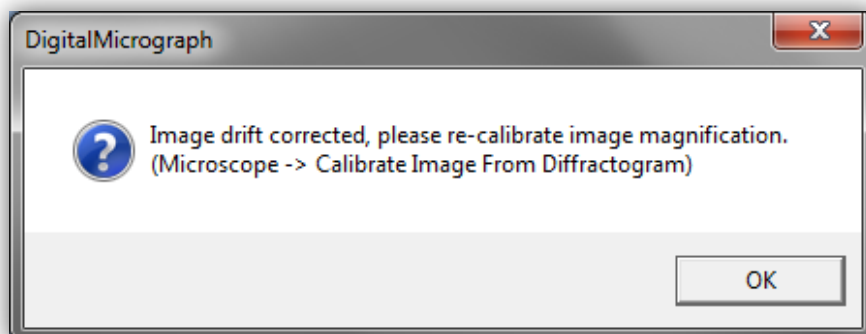
In general after drift correction the true scanned area will be slightly off-square (usually a rotated parallelogram). If the user is interested in the shape of this image then cropping may be disabled. For general use though this option should be left on and the plug-in will return the largest possible square image suitable for further analysis. A comparison of these two results for this is shown below:



In both images the same correction was applied but as expected with cropping a slightly smaller field of view is returned.

Magnification Re-calibration

After drift correction an important warning message will be displayed:

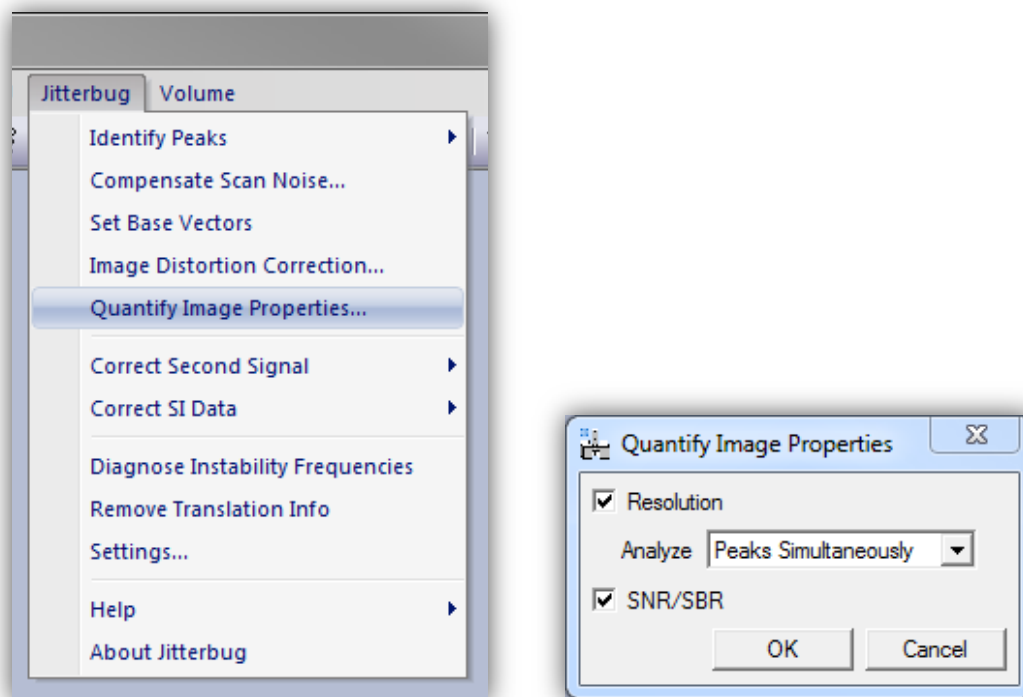


As a result of the previously asymmetric magnification (around 7% difference in vector lengths) the magnification of the new image must now be re-calibrated. If this stage is ignored then any measurements or scale-bars applied to the data may yield an error of a similar magnitude.

To calibrate the image magnification the spacing of a family of lattice planes must be known and applied using the Digital Micrograph menu option "Microscope > Calibrate Image From Diffractogram". The difference between the original distorted data and the drift corrected result can be seen if the image tags are inspected (right click on image > ImageDisplay...).

Image Property Quantification

The *Jitterbug* plug-in contains tools to quantify the image properties before and after processing to determine the level of improvement delivered. All these tools are accessed from the main menu under: Jitterbug > Quantify Image Properties. Selecting this will open a dialogue box from which you can choose the details to quantify:



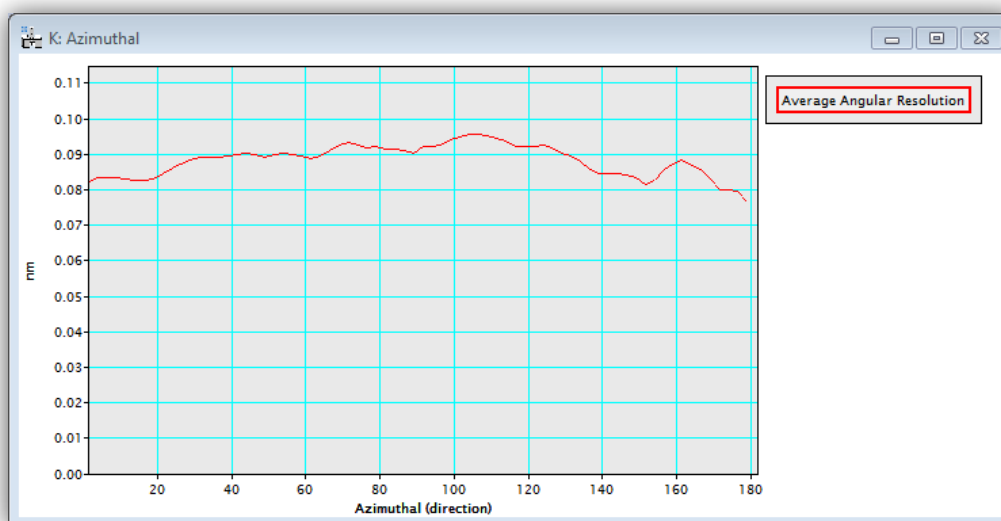
Resolution (Peak width)

The image resolution is determined by the fitting of one-dimensional Gaussian profiles to a large number of peaks (atomic-columns) in a large number of directions (0.5° steps). The positions of these peaks are taken from all across the field of view to give the fairest estimate possible. Because of this resolution quantification can only proceed after peak positions have been identified, if not this option will be 'greyed out' in the menu. In the 'Quantify Image Properties' dialogue box (shown above-right) three options are available for the resolution analysis as described below:

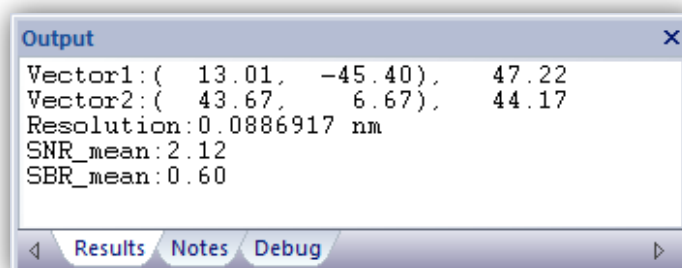
Method	Approach	Useful for...
"Averaged Peak"	A single averaged peak is first computed and then quantified.	Useful when a fast estimate is needed (as only a single fitting is performed). Useful when the image SNR is extremely low and the fitting of each individual peak may not be trusted
"Peaks Simultaneously"	All peaks are analysed simultaneously as a function of azimuth.	Most useful general setting for standard computers and image qualities.

“Peaks Separately”	Each peak is analysed sequentially.	Useful for computers with little memory but will be slower.
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The results of the second and third methods should be the same. A typical output is shown below:



If the image has its magnification calibrated then this display will be in units of nanometers, otherwise pixels. In addition to this output the numerical results will be printed to the “Output Window”:

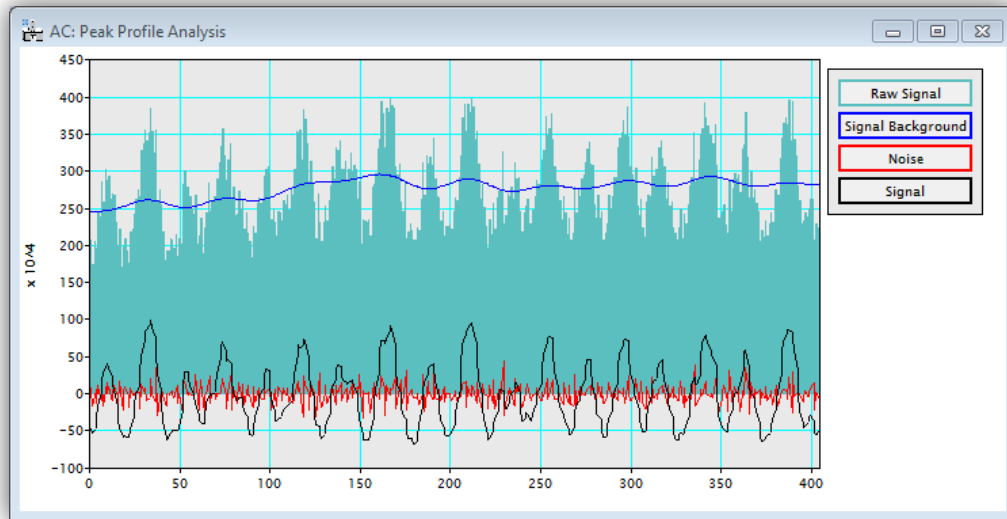


Signal-noise Ratio & Signal-background Ratio (SNR/SBR)

The image SNR/SBR is calculated using many 1D line profiles through the data as described in the academic manuscript. The positions and directions of these line profiles are defined based on the based vectors set in the image (see above section on drift correction). If appropriate base vectors are not set then the option to quantify SNR/SBR will be ‘greyed out’ in the “Quantify Image Properties” dialogue box. The directions used will be along both of the set base vectors

and also along directions bisecting these two (a total of four directions). The number of line profiles in each direction is set in the settings dialogue (see below).

During the analysis a green line running through the specified directions will indicate where the line-profiles are being taken from. With each line-profile a figure will show the analysis:



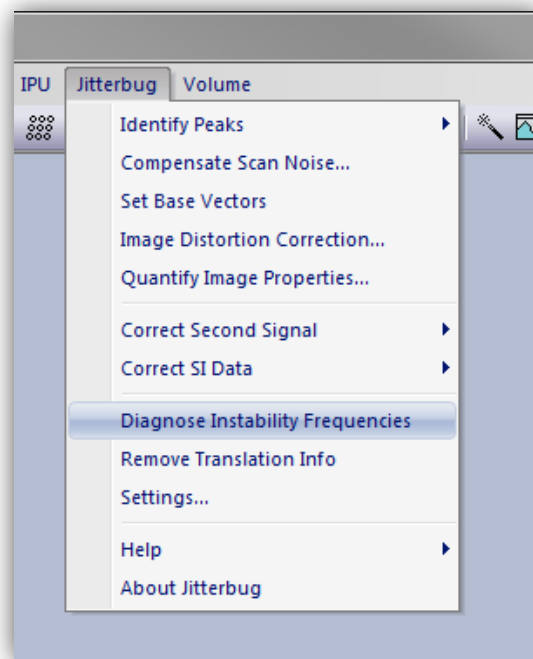
The units here represent image counts and all numerical ratios for SNR and SBR are expressed without units. Again these are also printed to the Output Window.

Scan-noise Spectral Analysis

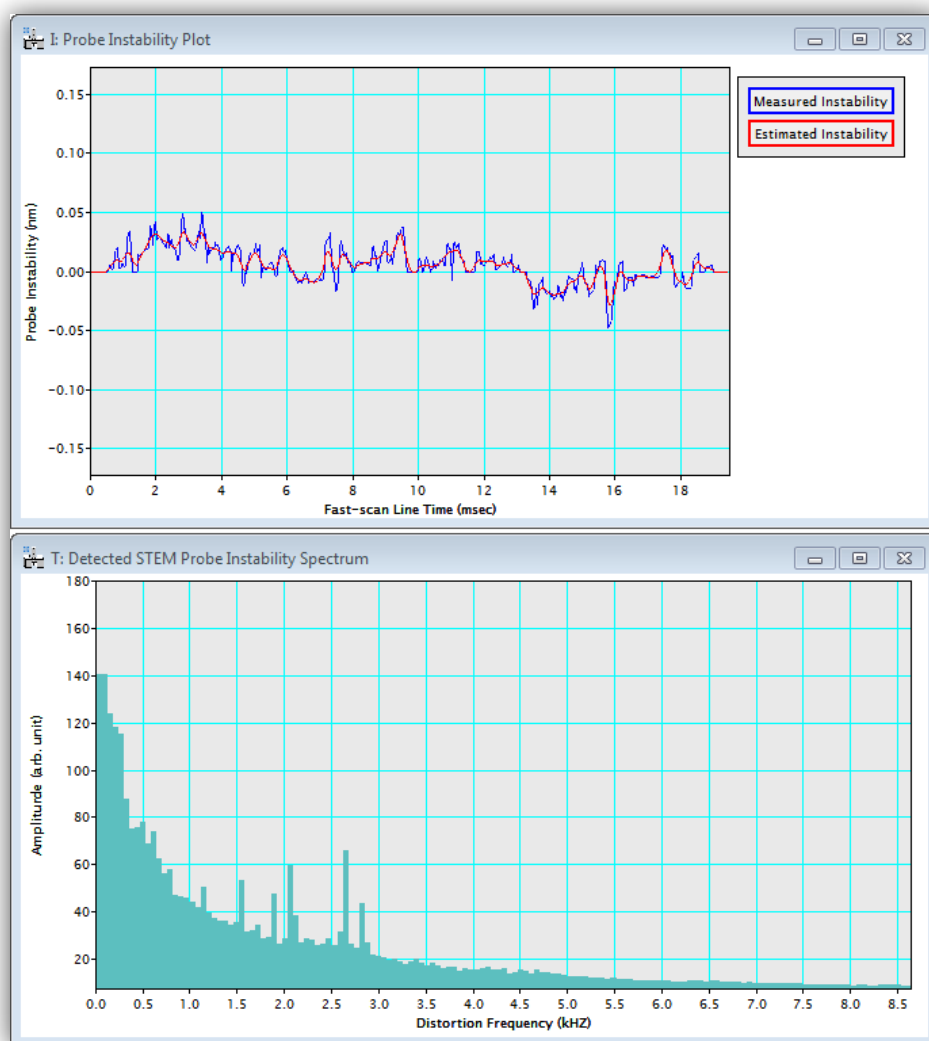
The *Jitterbug* plug-in can also be used to estimate the dominant distortions present in the EM suite.

NOTE: this data should be used as a guide to EM suite diagnosis only and does not replace a full suite analysis consolation.

To use this function the image must already have its peak features identified, otherwise this option will be 'greyed out'. From the main Jitterbug menu, select "***Diagnose Instability Frequencies***".



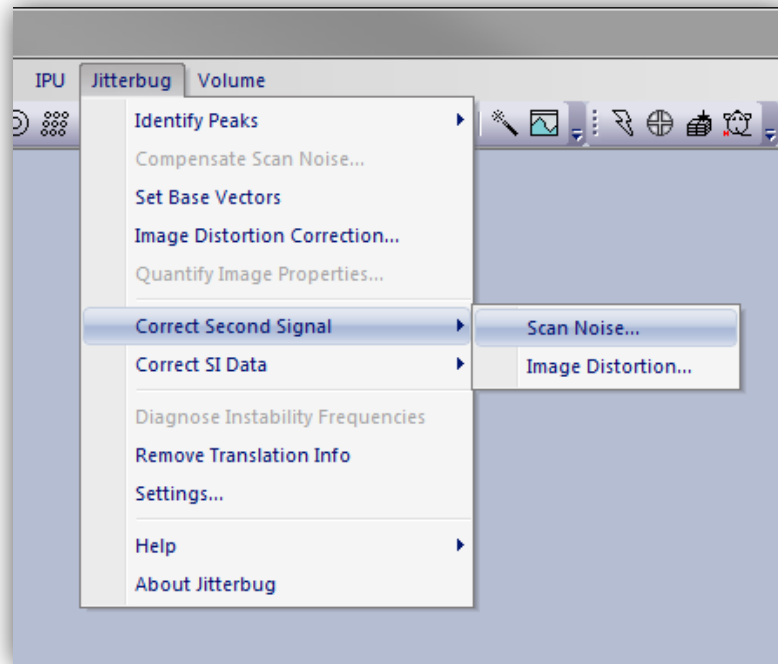
Once running two windows will be displayed; the first represents the 'distortion oscilloscope' and shows the analysis being performed in real-time. The second window shows the average distortion spectrum calculated so far. This will improve as the image rows are analysed and the spectrum built up. An example is shown below where the dominant distortions are visible around the 2kHz range typical of many sample holder resonant frequencies.



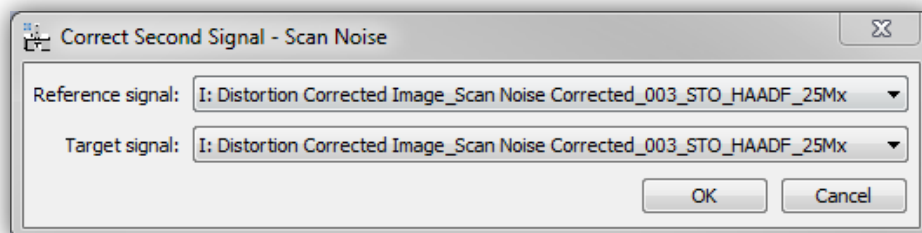
The units on the distortion spectrum are relative and are not intended to indicate an absolute measurement. The frequency scale will be accurately calibrated if the pixel dwell-time has been correctly specified in the settings dialogue (see below). This can often be found in the image 'tags' (right click on image, select "ImageDisplay").

Processing a Second Image or a Spectrum Image

If you have a second image channel such as ADF and also ABF, or an image plus a spectrum-image, recorded simultaneously, then it is possible to use the diagnosis from one signal to correct the other. To perform this, select the relevant choice from the menu:



After this is displayed you will need to select the “Reference signal” which has the translation info stored, and the “Target signal” that you want to reapply the shifts to:



After correcting scan-noise on the second signal / spectrum, you can subsequently follow the same procedure to correct image distortion.

Remember the images / SI must be precisely simultaneous with the same pixilation for this mode.

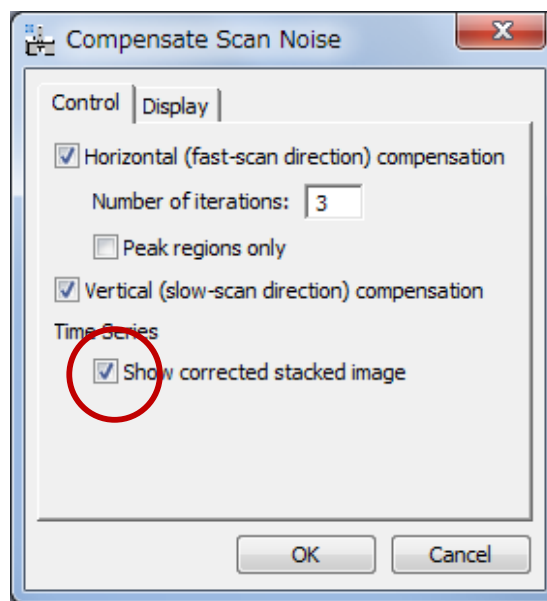
Processing Time-series Data

Processing of time-series (multi-frame) data is supported in *Jitterbug* from version 2.0 onwards. There are some extra options and settings for this and they are described in this section.

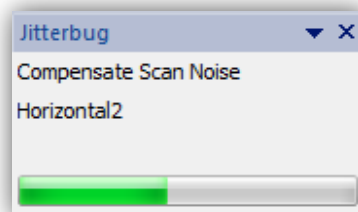
First the raw data must be realigned before processing to remove offsets from stage drift.,

If the front image is a time series, the average through the stack is automatically creates and used to give precise peak-positions during peak-finding.

When correcting vertical or horizontal scan-noise, this is done within each slice of the data, using the mean of the data as the reference. By default the average image will be shown after scan-noise correction. The corrected individual frames can be shown by selecting "Show corrected stacked image" in the 'Correct Scan-noise options:

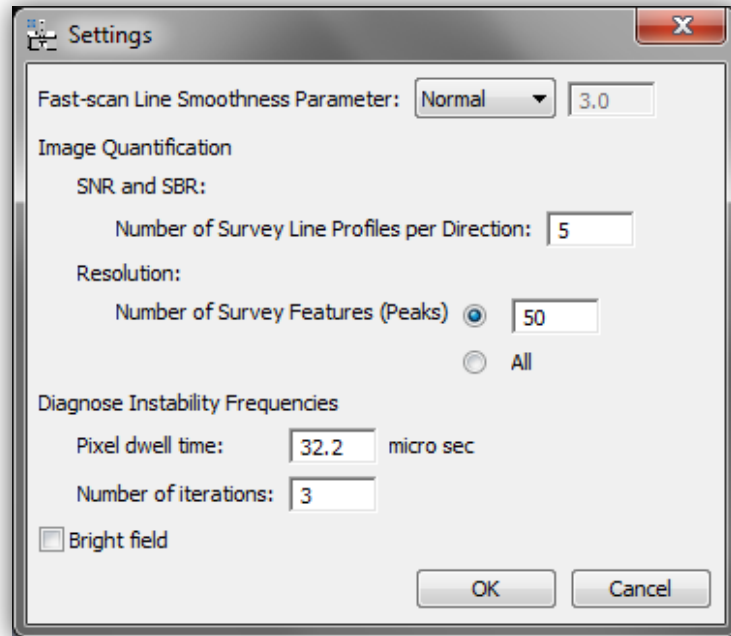


The time needed for this scales linearly with the number of images and may take several minutes. To monitor the progress an additional window will display when processing multi-frame data:



Advanced Options (the Settings Menu)

Several of the features above can be tailored by adjusting the options in the *Jitterbug* settings menu: Jitterbug > Settings. Options are saved when the menu is closed.



Fast-scan Line Smoothness Parameter

Introduced in Jitterbug version 2.0, the user has more choice over the smoothing used on the measured scan-noise offsets. Weak smoothing will only remove the most extreme outlier measurements, while stringer smoothing reduces these further and should be used for the lowest SNR raw data. The user can also enter a custom number; in most cases the 'Normal' smoothing strength is sufficient.

Image Quantification Options

Here options relating the image quantification can be set including the number of repeat line-profiles per direction, as well as the total number of features to use in resolution analysis. The pixel-dwell time should be input here to calibrate any distortion spectrum analysis as well as the number of scan-noise correction iterations to make before outputting the frequency spectrum.

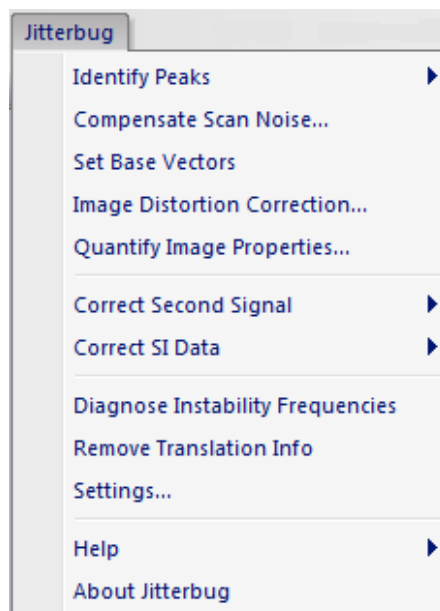
Bright Field Option

Here bright-field mode can be selected and 'peaks' will be defined as dark features rather than bright.

Quick Reference Guide

The Main Menu

Jitterbug is controlled from a single main menu within DigitalMicrograph.



The commands in the Jitterbug menu are described below.

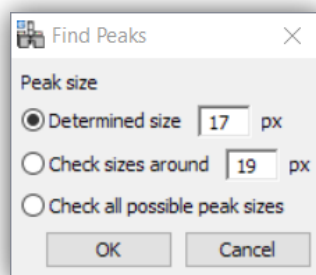
Command	Description
Identify Peaks (see sub menus)	Identifies image intensity peaks (atomic columns) automatically, and then allows Remove/Add peaks manually using the HREM mouse.
Compensate Scan Noise...	Runs horizontal/vertical scan noise restoration
Set Base Vectors	It allows defining manually the base vectors on an image.
Image Distortion Correction...	Runs Drift Restoration using the Base vector information
Quantify Image Properties...	Image properties (resolution, SNR and SBR) will be evaluated.
Correct Second Signal (see sub menus)	Used to copy diagnosed scan-noise from one image to another e.g. from ADF to ABF.
Correct SI Data (see sub menus)	Used to copy diagnosed scan-noise from one image to a spectral volume e.g. from ADF to EELS SI.
Diagnose Instability Frequencies	Shows noise frequency profile.
Remove Translation Info	Removes saved scan-noise diagnosis metadata to reduce file size for saving.
Settings...	Some parameters will be altered here.

Identify Peaks SubMenu

Component	Description
Find Peaks...	Identifies image intensity peaks (atomic columns) automatically
Remove Peaks	Removes peaks manually selected by using the HREM mouse. (Launch this command after placing the mouse selections.)
Add Peaks	Adds peaks manually selected by using the HREM mouse. (Launch this command after placing the mouse selections.)

Identify Peaks Dialog

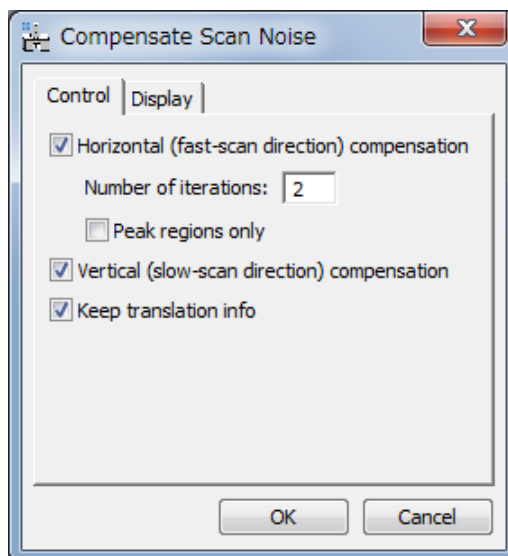
The components of the dialog are described below.

Dialog

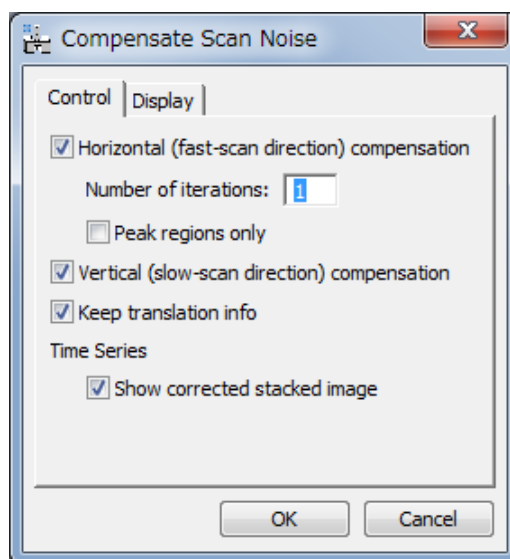
Component	Description
Peak size	<p>There are three options for peak-separation: using a pre-determined peak size, the peak size searched around a specified size, or the peak size searched fully automatic.</p> <p>If there is a small Rectangular ROI around a single peak, its size will be shown in the box as the Determined peak size.</p> <p>If there is a large Rectangular ROI, the peak size search will be done within the ROI, which will speed up the peak size search.</p>

Compensate Scan Noise Dialog

Control Tab



For a normal 2D image

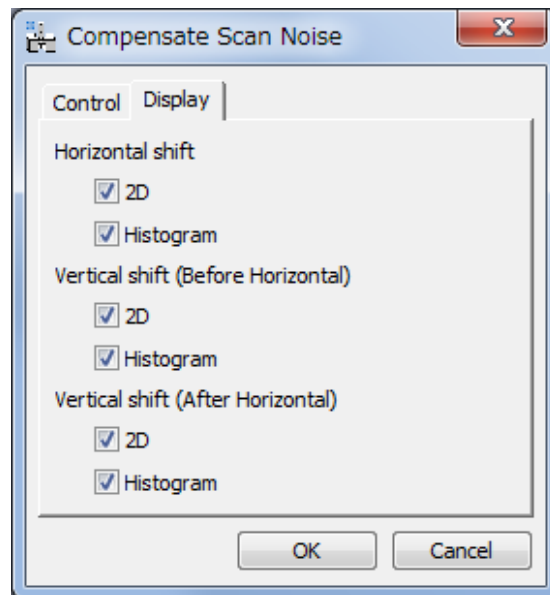


For a Time Series (3D image)

Component	Description
Horizontal (fast-scan direction) compensation	If checked, restoration along horizontal direction will be done.
Number of iterations	Specifies a number of iterations of horizontal restoration.
Peak regions only	Switches between whole pixels (area) or the pixels within each peak area.
Vertical (slow-scan direction) compensation	If checked, restoration along vertical direction will be done.

Keep translation info	If checked, scan-noise diagnosis is stored to be used for correction of a second image or for SI data.
Time Series: Show corrected stacked image	If checked, a corrected individual frames will be shown as a stacked image, as well as the averaged image after scan noise correction.

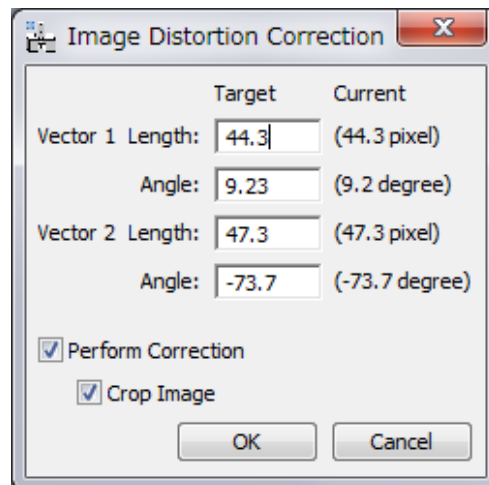
Display Tab



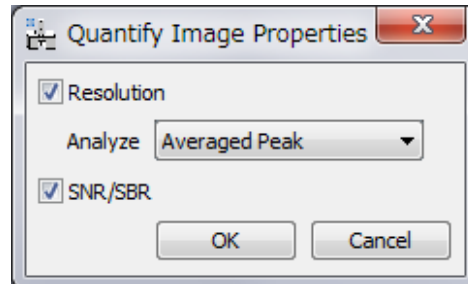
Component	Description
Horizontal shift	
2D	If checked, a 2D map of horizontal shift at each pixel will be displayed in a separate window.
Histogram	If checked, a histogram of horizontal shifts will be displayed in a separate window.
Vertical shift (Before Horizontal)	
2D	If checked, a 2D map of vertical shift (before horizontal compensation) at each pixel will be displayed in a separate window.
Histogram	If checked, a histogram of vertical shifts (before horizontal compensation) will be displayed in a separate window.
Vertical shift (After Horizontal)	
2D	If checked, a 2D map of vertical shift (after horizontal compensation) at each pixel will be displayed in a separate window.
Histogram	If checked, a histogram of vertical shifts (after horizontal compensation) will be displayed in a separate window.

Image Distortion Correction Dialog

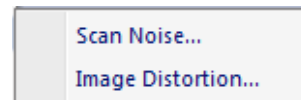
Dialog



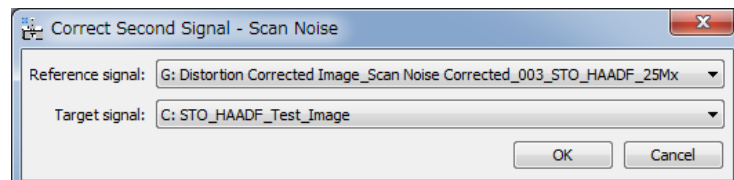
Component	Description
Vector 1	
Length	Length of the vector 1. Measured value (current value) is shown in the parenthesis. You can specify the Target value.
Angle	Angle of the vector 1. Measured value (current value) is shown in the parenthesis. You can specify the Target value.
Vector 2: same as Vector 1	
Perform Correction	If checked, information necessary to correct distortion is estimated, and an image corrected for distortion will be created. If not checked, estimated distortion information is output in the Results window.
Crop Image	If checked, a rectangular part is extracted from the distortion corrected image.

Quantify Image Properties Dialog**Dialog**

Component	Description
Resolution	If checked, resolution (peak size) will be estimated for various directions.
Analyze	Averaged Peak: Averaged peak profile is analyzed. Peaks Simultaneously: Each peak is simultaneously analyzed for each direction. Peaks Separately: Each peak is analyzed separately for each direction.
SNR/SBR	If checked, SNR (signal-to-noise ratio) and SBR (signal-to-background ratio) will be estimated.

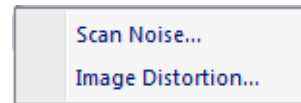
Correct Second Signal SubMenu

Component	Description
Scan Noise...	Used to copy the scan-noise correction from the reference signal image to a target signal image.
Image Distortion...	Used to copy the image-distortion correction from the reference signal image to a target signal image.

Scan Noise Dialog Image Distortion Dialog**Dialog**

Component	Description
Reference signal	Select the image with the stored scan-noise diagnosis.
Target signal	Select the new image to be corrected.

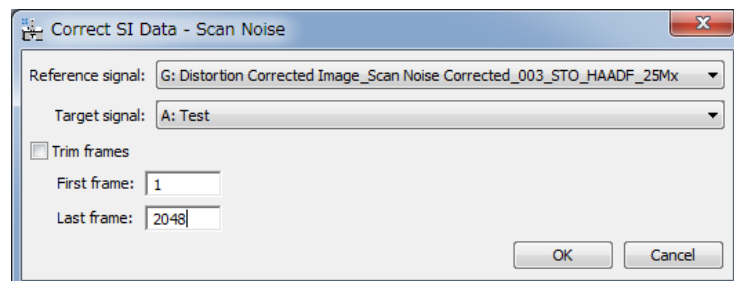
Correct SI Data SubMenu



Component	Description
Scan Noise...	Used to copy the scan-noise correction from the reference signal image to a target SI image.
Image Distortion...	Used to copy the image-distortion correction from the reference signal image to a target SI image.

Scan Noise Dialog Image Distortion Dialog

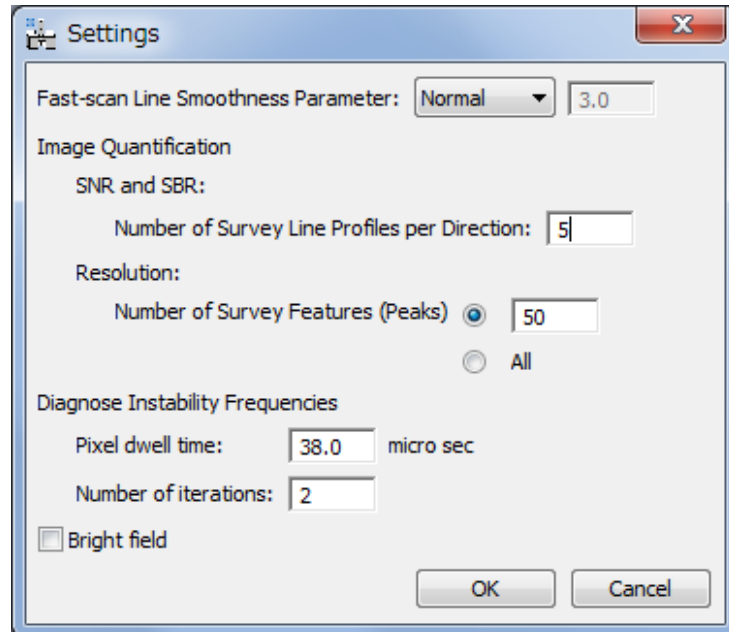
Dialog



Component	Description
Reference signal	Select the image with the stored scan-noise diagnosis.
Target signal	Select the spectrum image to be corrected.
Trim frames	If checked, will extract and correct only a subset of the energy channels. Can be useful to reduce processing time if only one part of the spectrum is wanted.
First frame	The first channel to use when trimming.
Last frame	The last channel to use when trimming.

Settings Dialog

Dialog



Component	Description
Fast-scan Line Smoothness Parameter	This parameter will control the smoothness of an estimate of the horizontal (fast-scan) noise offsets. In most cases the 'Normal' smoothing strength is sufficient, while the user can enter a custom number.
Image Quantification	
SNR and SBR:	
Number of Survey Line Profiles per Direction:	Number of line profile with the high peak density to be analyzed. Four (4) directions (two base-vectors, and their sum and difference directions) will be surveyed.
Resolution:	
Number of Survey Features (Peaks)	Number of peaks used to estimate resolution (peak width)
Diagnose Instability Frequencies	
Pixel dwell time	The pixel dwell time will be used to calculate the highest frequency.
Number of iterations	Instability frequencies will be estimated after the specified cycles of horizontal restoration.
Bright field	If checked, a bright field image can be analyzed.