Designing Robust Procedures for Rigid and Non-rigid Registration of STEM Image Data

Lewys Jones*, Hao Yang, Peter D. Nellist
Department of Materials, University of Oxford

Background

In the scanning transmission electron microscope (STEM), there are many applications where recording a series of sequential images can be valuable. These can include frame-averaging to improve signal-noise ratios (SNR), focal-series for optical-sectioning experiments or aberration studies, time-series to study dynamic processes like beam-damage, or camera-length series to study the effects of strain. However, STEM data is recorded serially and acquisition times can be tens of seconds long. Now the operator has to not only worry about stage / sample drift but also low frequency distortions that can perturb the image locally. Often the first stage in any quantitative image interpretation is to correct for these drifts and distortions using so-called rigid and non-rigid registrations respectively.

Here we describe an improved automated software called ***'Smart Align'*** that performs this registration, customised for the challenges unique to STEM data. Specifically we address the challenges of registering images which contain a large proportion of crystalline material and / or local features of interest such as dislocations or edges or other defects.

'Crystal-hop' Free Rigid Registration

Unwanted 'crystal-hops' in the rigid-registration can be avoided using the software's new 'learning mode' where the image offsets are found iteratively. This uses a normalised correlation function[1,2] multiplied by a weighting function which is determined from previous registration results:

$$NCF(i_{n-1}, i_n) = (W \otimes G) \circ F^{-1}\left(\frac{F(i_{n-1}) \circ F(i_n)^*}{|F(i_{n-1}) \circ F(i_n)^*|^{\alpha}}\right)$$

where G is a Gaussian blurring and W is given by the results of a previous iteration:

$$W = \frac{1}{N-1} \cdot \int_2^N NCF(i_{n-1}, i_n)\, dn$$

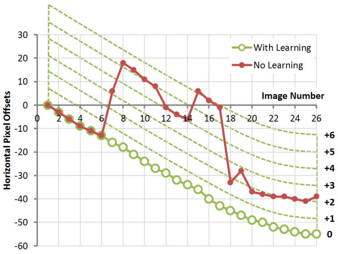

Figure 1. Plot of the x-component of the diagnosed image offsets, simply taking the MCF maxima (closed circles) compared with the 'learning mode' (open circles).

Artefact-free Non-rigid Registration

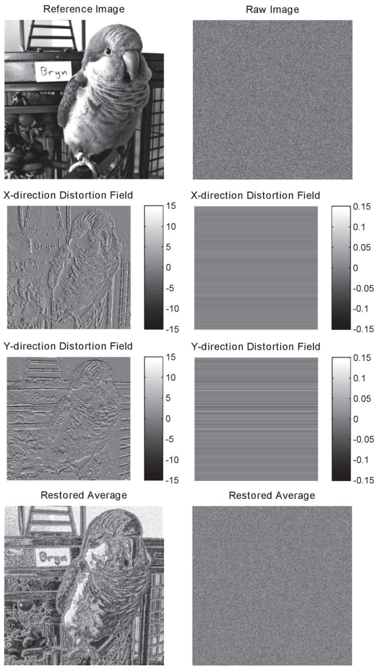

Figure 2. Example non-rigid registration artefact-introduction test results. Top row shows the reference image and an example of one of the pure-noise images to be registered. Middle rows show the x- and y-direction distortion maps determined by the non-rigid registration code with (left) unconstrained movement and (right) fast-scan row locking. Bottom row shows the result of averaging the 250 registered frames. Note, the colour scale is 100x smaller on the constrained distortion maps.

In general non-rigid registration can be done by either defining specific control points to be morphed onto one another or by a 'first order gradient descent' method where the differences between images is used to directly infer the direction of local motion[3]. In the former case manual input is usually needed to define the control points, whereas the gradient descent method is well suited to automation and is what is discussed here. However, this method was not designed for use with serial acquired data as in the STEM.

Here four enhancements are discussed tailored to be specifically useful for the registration of serial acquired STEM data; these are:

- fast-scan row locking (optional),
- restoration of parallel signals (e.g. ABF),
- convergence detection, and
- distortion frequency analysis.

'Fast-scan row-locking' allows for regions of regular crystal to guide the transformation field, while preserving edges, defects, and local strains (Figure 3). This also has a powerful effect at preventing artefact introduction (Figure 2).

Parallel signals in the STEM all arise from the same probe-sample interaction. In the software a high SNR signal such as the ADF can be used to register other data-sets that were acquired in parallel who themselves have insufficient SNR for reliable registration.

The gradient-descent method for non-rigid registration runs iteratively, and specifying a fixed number of iterations risks either poor convergence (too few) or wasted time (too many). Using a convergence detection metric the software self-optimises the iteration performance.

Lastly, by taking the Fourier transform in the slow-scan direction of the transformation-fields (Figure 3) a diagnostic is produced of the instability frequency in the EM suite.

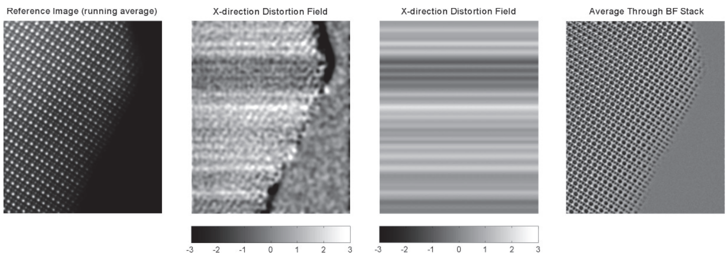

Figure 3. Demonstration of the 'row-locking' and secondary signal principles. The first panel shows the reference image used to register the dark-field time-series. Next, a typical x-direction distortion map from an un-constrained non-rigid registration. Third, the x-direction result with row-locking engaged. For both maps the scale indicates the shift in units of pixels. Far right, the simultaneously acquired bright-field data registered as a secondary signal using the offsets diagnosed from the DF data.

Improved PCA Performance

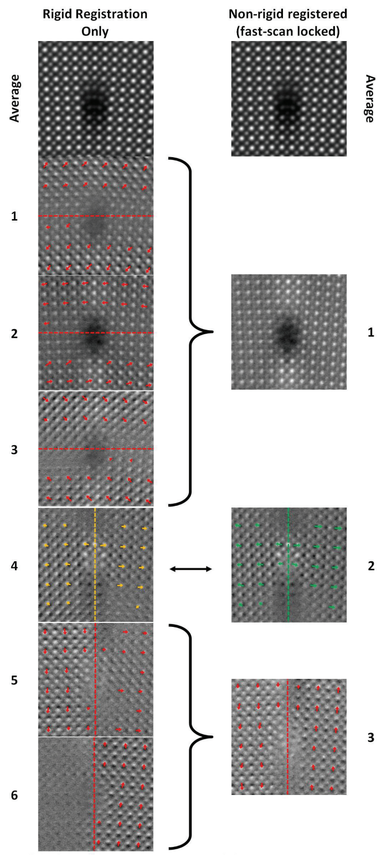

Figure 4. Comparison of the first six principal components of the rigid-registered data-set versus the first three components of the non-rigid registered data-set. Arrowhead annotations indicate the feature-shift polarity seen in the components. Image width is 4.5 nm in all cases.

Non-rigid registration operates across multiple frames and in this sense contains the redundant information necessary to separate genuine sample structure from the effects of scan-distortion and sample-drift. Using many images of a nominally identical structure, such as the low-angle grain-boundary dislocation cores (Fig. 4), the data can be decomposed to extract correlations using, for example, principal component analysis (PCA). However, accurate PCA requires data free from any other geometric-distortion; in this case STEM scan-distortions.

Figure 4 shows the first six components from a data set that was rigid registered only (realigned but with no distortion correction) and the corresponding components from data registered using the new ***'Smart Align'*** software.

In all of the first three components from the rigid-only set we see a band through the centre of diffuse grey, above and below this we see two distinctly different behaviours in the feature polarity (STEM image feature-shift). The first and third components exhibit a shearing type behaviour inclined at 45° from the horizontal and 90° from one another; the second again shows a similar shearing type behaviour but now roughly parallel to the fast-scan (horizontal) direction.

The next comparable components are the 4th rigid-only and the 2nd non-rigid; here we see a component that describes the correlation between an increased occupancy of the terminating half-plane with an outward displacement of the adjacent planes. This is consistent with elastic theory and offers a useful route to studying this occupancy versus strain relationship.

Lastly the fifth and sixth components of the rigid-only data-set and the third component of the non-rigid are closely comparable. In this component we see the effect of the previously mentioned left- or right-handedness of the staggered dislocations.

Conclusions

Crystal periodicity can make atomic resolution STEM image-series challenging to register due to so-called 'crystal-hops', while low frequency scanning-distortions in the STEM in the range 0.5-5 Hz can cause image features to be shifted or skewed or lead to additional misleading components to be observed in PCA studies. Here a new rigid registration method with a 'learning mode' and a new 'fast-scan row-locking' non-rigid registration method was introduced. These enhancements eliminate some of the previous issues surrounding STEM time series and are available in the ***'Smart Align'*** software free of charge for academic use.

References

1) Heel, M. van, Schatz, M., & Orlova, E. (1992). Correlation functions revisited. *Ultramicroscopy*, **46**, 307–316.
2) Kuglin, C. D., & Hines, D. C. (1975). *Proc. Int. Conf. on Cybernetics and Society*, 163–165.
3) Cachier, P., Pennec, X., & Ayache, N. (1999). Fast Non Rigid Matching by Gradient Descent, 1-25.

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* lewys.jones@materials.ox.ac.uk Copies of this poster, the software described and the associated manuscript are available online at: **www.lewysjones.com**