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PyfastSPM: A Python package to convert 1D FastSPM data streams into publication quality movies



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ABSTRACT

Since the invention of scanning probe microscopy, researchers have desired to use this technique to monitor sub-second surface dynamics with atomic spatial resolution. A recently presented add-on electronics module enables the speed-up of existing, conventional scanning probe microscopes without any modification of the actual instrument. The resulting one-dimensional (1D) data stream, recorded while the tip oscillates in a sinusoidal motion, has to be reconstructed into a layered rectangular matrix in order to visualize the movie. The Python-based `pyfastspm` package performs this conversion, while also correcting for sample tilt, noise frequencies, piezo creep, and thermal drift. Quick automatic conversion even of considerable batches of data is achieved by efficient algorithms that bundle time-expensive steps, such as interpolation based on Delaunay triangulation.

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Code metadata

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Permanent link to code/repository used for this code version	https://doi.org/10.5281/zenodo.6824215
Legal Code License	MIT, Apache-2.0
Code versioning system used	git
Software code languages, tools, and services used	Python 3, FFmpeg
Compilation requirements, operating environments & dependencies	http://fastspm.gitlab.io/pyfastspm
If available Link to developer documentation/manual	http://fastspm.gitlab.io/pyfastspm
Support email for questions	carlo.dri@gmail.com

1. Motivation and significance

On the sub-second timescale, a multitude of surface dynamics occur that can be revealed particularly well by video-rate scanning probe microscopies (SPM) – from equilibrium molecular diffusion [1,2] to film growth [3], from cluster isomerization [4]

to potential-dependent electrochemical surface processes [5,6]. Time-resolved SPM techniques can reveal particular dynamics at the atomic scale that would otherwise be overlooked [3].

In SPM, a point-like sensor (tip) typically moves stepwise across a sample and records local information on a square spatial grid. Scanning tunnelling microscopy (STM), for example, provides information on local electronic states that contribute to the tunneling current flowing between the tip and the sample, thus convolving topographic and chemical signatures. The tunneling current is typically kept constant by a feedback loop that regulates the vertical tip position, which is in fact the measured

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quantity. Stepwise motion and feedback make the measurement inherently slow.

While several successful, yet experimentally demanding and expensive implementations of fast SPM setups allow for imaging under full feedback conditions [6,7], most experimental groups face the challenge of accelerating their existing, slow setups to access fast surface dynamics. This speed-up can be realized with the previously reported FAST (fast acquisition of SPM time series) module by simply inserting an electronics add-on module that performs a synchronized fast scanning and tunneling current acquisition [8]. Briefly, this module controls a sinusoidal motion of the tip at a given frequency in the fast scan direction and a triangular motion in the orthogonal slow scan direction, while recording the current signal at a constant rate (i.e. pixel frequency), thus creating a 1D data stream of tunneling current values. This approach comes at the price, however, of quasi-constant height imaging, where the acquired signal is measured as a current instead of a topography, because the feedback is not sufficiently fast to follow the surface and even reduced to avoid excitation of higher resonance frequencies. The feedback is thus used only to control the average tip position. Data points are recorded continuously by binning over constant-duration time steps. Obtainable pixel frequencies can reach up to 1 MHz [3], by using adequate fast preamplifiers (e.g. FEMTO DLPA-200: 10^8 gain, high speed with 200 kHz bandwidth). Hence, lateral positions corresponding to each bin have to be determined retrospectively during data evaluation, by means of adequate interpolation, which is the central topic of this paper. The continuous sinusoidal oscillation, that replaces the typical triangular tip motion, leads to a higher pixel density at the left and right edges of the final movie images compared to the center. Similar to recent spiral movement approaches [9–12], a dedicated image reconstruction software is required to create movies and image frames that reveal the dynamics of interest for further data analysis.

Here, we present a Python-based software package, called `pyfastspm`, which is openly accessible and easy to use for a non-dedicated user. It converts 1D SPM data streams, such as those recorded by the FAST module, into 2D MPEG4 movies, optionally in batch automation. Specifically, the software corrects for several aspects relating to the tip movement across the surface, as well as for additional interfering signals:

1. *Background frequencies.* Residual sample tilt, which occurs mainly in the fast x -direction, can be removed by filtering out x and y scanning frequencies and their overtones in the original 1D data time series via FFT. In this process, additional background noise, e.g. of electronic or mechanical origin, can be eliminated as well.
2. *Tip path.* Common movie formats require the pixels to be placed on square grids. Thus, the complex tip path has to be taken into account correctly while transforming the acquired 1D SPM data stream into a 3D stack consisting of 2D movie frames. This correction occurs on the basis of an estimated tip path that takes into account (a) the sinusoidal tip motion in the fast x -direction, including phase shifts between tip motion and data acquisition; (b) the triangular tip motion in the slow y -direction; and (c) possible creep distortions due to acceleration delays at the tip turnaround points between frames. It is performed based on a Delaunay transformation [13], with parameters that can be automatically extracted from the FastSPM data stream. As a result, every single measured pixel can be included in the movie (from forward and backward, up and down motion), allowing a doubling of both, the temporal and spatial movie resolution.

3. *Lateral drift.* At the atomic scale, lateral image shifts are often encountered due to thermal drift. The `pyfastspm` package determines and corrects for the lateral drift path by evaluating image correlations between entire movie frames at variable temporal delays, after the above corrections have been made. Averaging over frames of a drift-corrected movie can lead to superior spatial resolution of structures underlying highly mobile, streaky surface dynamics [14].

In the following, we will describe these steps in more detail, in the sequence in which they are called in a typical movie reconstruction and conversion pipeline. `pyfastspm` unleashes the full potential of SPM when it comes to exploring surface dynamics studies [2–4,14] and gives the experimentalist the freedom to focus on the scientific questions at hand. In the following, we give STM examples in which the acquired signal is tunneling current, but `pyfastspm` is generally applicable for any kind of local probe microscopy.

2. Software description

`pyfastspm` is a standalone Python package, but also comes with a Jupyter notebook that includes standard input parameters and default values for easy conversion.

2.1. Software architecture

Central to the package is the `FastMovie` class that loads the acquired 1D SPM data stream $I(t)$ from a Hierarchical Data Format HDF5 file. Fig. 1 shows the general workflow, including all transformations to the final 3D stack of 2D frames, $I(x, y, t)$, that can be exported as a movie. The first step, *assign frame*, sections the data stream into the respective frames. The second main step removes the distortion from the measured sine-shaped tip path by *interpolating* onto a square grid. These are the minimum steps required to write the data into a movie file. Further optional correction steps (upper row in the Figure) can be included to remove measurement artifacts: *FFT filter* removes background frequencies in the time domain, *determine creep* identifies additional distortions at the tip turnaround point in the y -direction and *correct drift* shifts frames with respect to each other according to their lateral drift.

2.2. Software functionalities

FFT filter. This function applies low-, high- and band-pass filters of selectable frequencies and widths to the FFT-transformed 1D data stream. Furthermore, the convolution with a Gaussian of selectable width can be applied to eliminate noise in the fast x -direction. Back transformation results in background-corrected and smoothed data that typically do not require further filtering in the spatial domain.

Assign frame. A complete period of the tip movement results in an *image* that is composed of an up ‘u’ and down ‘d’ *frame* pair (slow y -movement), each composed of forward and backward lines (fast x -movement). This conversion step distributes the data points into frames.

To account for the overall delay between the physical tip position and consequently the acquired data in the forward and backward lines, a phase shift in the fast x -direction needs to be applied, as illustrated in Fig. 2(a). This phase shift is calculated automatically by correlating the current signal of sequential forward and backward lines or defined manually by the user. A well-corrected phase allows the combination of forward ‘f’ and backward ‘b’ parts of the frames into a single, interlaced ‘i’

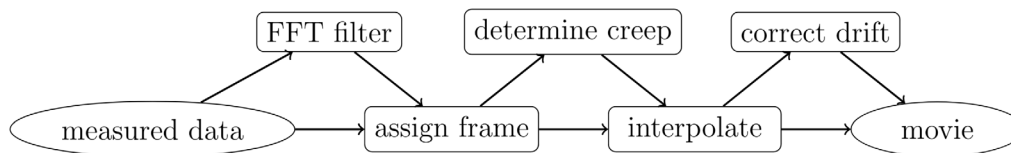


Fig. 1. The workflow sequence of PyfastSPM functionalities, including the two main transformation steps *assign frame* and *interpolate* as well as optional corrections, to create a movie from the measured 1D data stream.

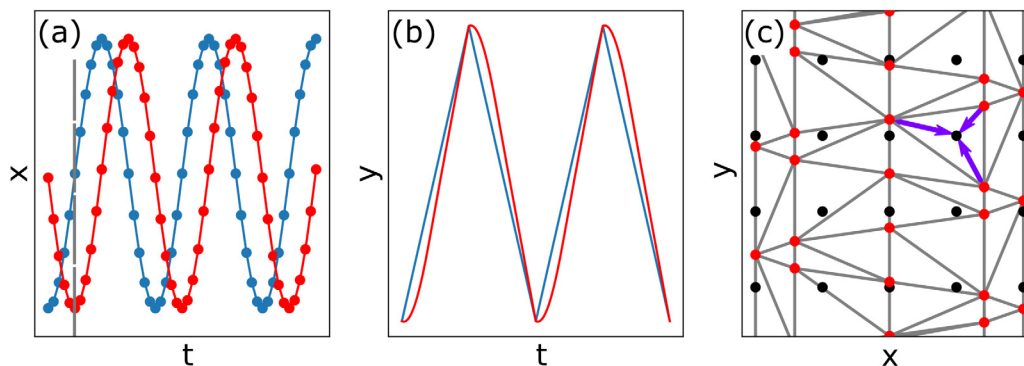


Fig. 2. Tip path in (a) x - and (b) y -directions as a function of time (solid lines). The nominal tip path is indicated in blue, the actual one in red. The deviations stem from a delayed piezo response and creep, respectively. Dots in (a) mark measurement positions along x . Note that the image reconstruction always starts at an x -turnaround point (gray dashed line). (c) The deduced x/y tip positions, indicated by the red dots, are then mapped onto a square grid, marked in black. The Delaunay triangulation is indicated by the gray lines. The resulting barycentric coordinates used for interpolation are exemplified by the purple arrows. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

frame. The resulting movie mode that contains the full acquired data is called ‘udi’, but also movies with partial data sets can be generated, e.g. ‘uf’, ‘udb’, etc. An ‘i’ frame contains twice the data points of a ‘f’ or a ‘b’ frame. A ‘ud’ movie contains twice the frames of a ‘u’ or a ‘d’ movie.

Determine creep. While the sinusoidal fast x -direction has a smooth turnaround to allow the piezo to perfectly follow the intended motion, the sharp turnaround in the slow y -direction leads to a significant piezo delay (creep). Other approaches avoid such creep problems in the experiment by suppressing high frequency Fourier components [15], while here we add an optional post-measurement correction to `pyfastspm`. The piezo creep leads to a distorted movement in y that is illustrated in red in Fig. 2(b), resulting in a compression at the bottom of the up frame and at the top of the down frame. In a single frame, this is often barely perceptible, but in ‘ud’ movies, it results in a flickering (see left side of the Supporting Movie).

Here, creep is corrected for by distorting sequential up and down frames in y until they match. This distortion is calculated on a selected line of pixels in y -direction by fitting the y -positions with a B-spline as a computationally cheap curve fitting approach. In order to account for possible differences between microscopes, three functions have been implemented in `pyfastspm` to map the y -positions, a Bézier function, a sine function that merges into a linear function, and a square root correction to a linear function (as described by Choi and coworkers [16]). The Bézier fit is less constrained and thus maps the creep well and relatively quickly, but it can fail in the absence of pronounced features. Here, the more constrained sine and square root options yield a more stable fit; in our experience, the sine function yields the best results for batch conversions (see Supporting Movie). Finally, the user has the option to manually input known creep parameters, e.g. those obtained from measurements under equal scan conditions. Custom creep functions can easily be added by the user.

Interpolate. This function removes the distortion induced by the sinusoidal tip trajectory. To this purpose, the sinusoidal movement is reconstructed and overlaid by a square grid. Hereby, the x -phase shift obtained in the *assign frame* and, optionally, the creep parameters obtained in the *determine creep* step are taken into account. The values associated with this fully described tip path are then used to interpolate onto a square grid. The Delaunay triangulation, described in Fig. 2(c), serves as a basis for the high quality interpolation [17]: the determined tip positions are divided into sets of three points that do not include further points within their circumcircles. The value of any point on the square grid is then calculated by a weighted sum of the three points surrounding it (normalized barycentric coordinates, see purple arrows in Fig. 2(c)). Importantly, this approach combines all corrections (except the drift) into a single interpolation step. Since the tip path is the same for all images, a significant acceleration of 4 orders of magnitude (in the limit of long movies) over readily available packages is achieved by performing the Delaunay triangulation only for a single image and then using it for the full 3D stack. This computation is performed in a matrix multiplication formalism, using sparse matrices to hold the barycentric interpolation coordinates for all images within a movie. Other interpolation methods exist and have been successfully implemented, which are particularly useful for alternative scanning patterns, e.g. spirals [9].

Correct drift. The drift trajectory is calculated by a sliding FFT-based cross correlation (implemented with `scipy`) of frame pairs taken at a chosen time separation [18]. In a first step, the frames are enlarged in the x - and y -dimensions to an appropriate power of 2 number of pixels. The time separation needs to be selected such that significant drift is detected between the compared frames, without losing track of drift details on shorter time scales. Drift values for the last frames for which no calculation is possible are linearly extrapolated from preceding ones. A median filter of variable width smoothes drift noise without removing abrupt changes in drift velocity. Additionally, an optional boxcar filter

can be applied. The drift path is saved as a text file which can be adjusted manually and subsequently reloaded.

In the resulting movie, the drift is accounted for only by shifting entire frames by integer pixels since thermal drift within a single frame is typically minimal in fast acquired STM movies and the number of pixels can be increased accordingly. Two correction modes can be chosen for the drift corrected movie: It can be cropped down to the 'greatest common' area of all drifting frames, or, alternatively, the complete frames can be embedded into an enlarged array by zero padding ('full').

Export. The final corrected movie is exported into an MPEG4 file or single frames into common image file formats or the Gwyddion native data format, .gwy, for further analysis [19]. Frame range, color map, contrast and frame rate can be adjusted and, optionally, frame numbers overlaid as text. It should be noted that the contrast is evaluated globally by a histogram, spanning over the entire frame range in an exported movie, allowing for quantitative comparisons of contrast (i.e. apparent heights) in different frames of the same movie. In addition, the user has the option to save the converted movie in a pickle file format to be reimported for further analysis, to store the acquisition and export parameters as a meta file, and to output a log that describes the sequence of the applied conversion processes.

2.3. Sample code snippets analysis

The movie conversion essentially consists of a few key steps which are summarized below. The respective steps in the workflow of Fig. 1 are indicated as code comments. The *interpolate* step is divided into the construction of the Delaunay-based interpolation matrices and the actual interpolation. Having all parameters (see Supporting Information for an example of input parameters), these commands are sufficient to perform the complete movie conversion.

```
import pyfastspm as pf

ft = pf.FastMovie(file_name)
ft.reshape_to_movie() # assign frame
pf.filter_movie(ft.filterparam) # FFT filter
creep = pf.Creep(ft, creep_mode='sin') # determine creep
grid = creep.fit_creep()
matrix_up, matrix_down = pf.interpolate(
    ft,
    grid,
    give_grid=True,
) # interpolate
pf.interpolate(ft, grid, matrix_up, matrix_down)
drift = pf.Drift(ft) # correct drift
ft.data, drift_path = drift.correct(drift_type)
ft.export_movie
```

3. Illustrative example

Fig. 3 shows the effect of the main conversion steps on a sample movie where the dynamic closing of holes is observed on a reduced magnetite $\text{Fe}_3\text{O}_4(001)$ surface under an oxygen atmosphere at elevated temperatures. As described in detail in the figure caption, starting from the full image on the left, single movie frames on the right can be obtained, where every pixel is included without introducing flickering or distortions. The high quality of the image conversion is best observed in the Supporting Movie that displays the dynamics of a five-fold accelerated movie, comparing side-by-side the uncorrected (left) and corrected (right) data. The parameters used for this movie conversion are also included in the Supporting Information.

Once individual frames have been ideally reconstructed, thermal drift effects can be removed. As described above, the frames

are simply shifted with respect to each other. This is done in a separate step that acts on the reconstructed 3D stack, illustrated in Fig. 4. The two alternative export modes, either cropping the 'greatest common' or exporting the 'full' area, are indicated in the figure. As the example shows, the drift correction algorithm is robust enough to cope not only with linear drift but also with discontinuities (here, for example around frame 400).

The full conversion and writing of this example movie file of 1044 frames can be performed fully automatically in a couple of minutes on a standard laptop (e.g. by using the example notebook available as part of the package), thus providing an easy and quick data analysis pathway. In our experience, for a given acquisition parameter set recorded with the same microscope, the conversion parameters remain largely constant. They can be optimized sequentially, for each individual step and do not influence each other significantly.

4. Impact

pyfastspm provides a highly convenient and efficient tool for the non-specialized user to convert fast SPM data into publication quality movies. The software package thus paves the way for investigating surface dynamics that have typically only been accessible to a few specialized groups. In the four years of PyfastSPM development alone, the authors have demonstrated its power in three distinct examples of surface dynamics studies:

- *Imaging of short-lived intermediate species*, critical especially for the investigation of detailed mechanisms, e.g. in catalysis and thin film growth [3].
- *Access to diffusion paths and statistics* beyond simple residence times, e.g. hopping of small metal clusters in pores of a 2D film revealing support symmetries [4]. The improved image stability opens the possibility to quantitatively evaluate hopping processes with atomic resolution over large time intervals [2].
- *Recovery of atomic resolution* underneath highly mobile species which dominate the contrast in single SPM images (streaks), i.e. by averaging many drift-corrected frames [14]. Here, PyfastSPM provides a new modality for SPM imaging under extreme conditions (e.g. elevated temperatures, in gas atmospheres or at solid/liquid interfaces).

While all these features have already been feasible in principle, the FAST module [8] and open source pyfastspm software package allow for a smooth switch between standard and time resolved SPM imaging, and a nearly perfect movie visualization close to real time. We expect that this will encourage users in the wider SPM community to routinely investigate surface dynamics, as was the experience in the daily practice of our own groups.

At the time of writing this article, the software package is in routine use in groups that are part of the European Nanoscience Foundries and Fine Analysis (NFFA) project. Further requests have already been received, from users that use the commercially available FAST module [20]; the software package, however, is available open source. With appropriate minor modifications of the data import, pyfastspm empowers every SPM user to build publication ready movies from fast SPM data.

5. Conclusions

In conclusion, we have presented a freely available new open-source software module for easy and complete conversion of 1D fast SPM data streams into optimally corrected movie frames with the additional option of drift compensation. Specifically, these corrections concern noise reduction, background removal, phase shifts in the fast scanning direction, piezo creep distortions and

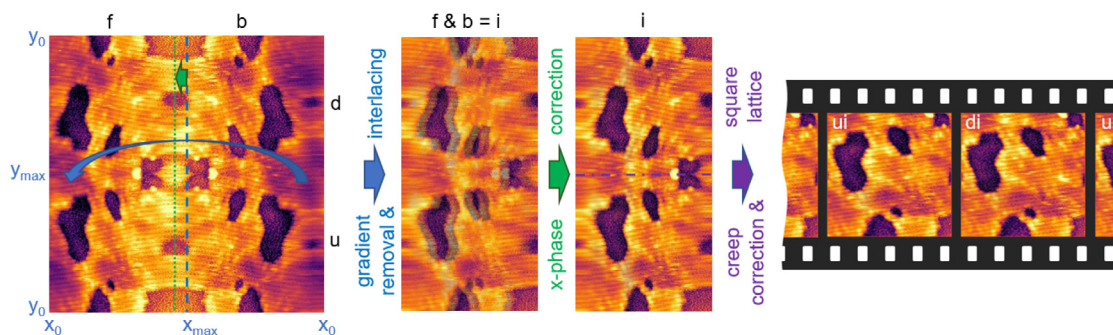


Fig. 3. Effect of the conversion steps on an experimental example, a reduced $\text{Fe}_3\text{O}_4(001)$ surface observed at 657 K under 5×10^{-7} mbar oxygen under which holes successively close, imaged at 4.0 nA, 0.5 V and with an image size of $18 \text{ nm} \times 18 \text{ nm}$. The approximately horizontal lines represent the Fe rows of the surface structure of $\text{Fe}_3\text{O}_4(001)$. Movie frequencies: 4 fps resp. 2 images/s, fast scanning frequency (x-direction) 785 Hz, acquisition rate (pixel frequency) 307 kHz. The left-most image contains the full information of one full scan cycle, including forward (f), backward (b), up (u) and down (d) motion. The tip moves in lines from left to right (fast x-direction), from bottom upwards and down again (slow y-direction). Each horizontal line in the shown image contains thus the forward and backward scan sequence, while the temporal succession from bottom upwards represents the various y-positions, first the upward, then the downward movement. The symmetry axes of this representation reveal the x- and y-phase shifts. In a first step, FFT filtering removes the residual sample tilt gradient (typically strongest in the x-direction). To fold the f and b signals correctly onto each other into an interlaced (i) image, the correct x-phase shift (and thus the frame assignment of the pixels) has to be applied in a second step. Finally, the creep and sinusoidal distortions are removed, and the pixels interpolated onto a square lattice. The resulting two u and d frames can both contribute to a movie.

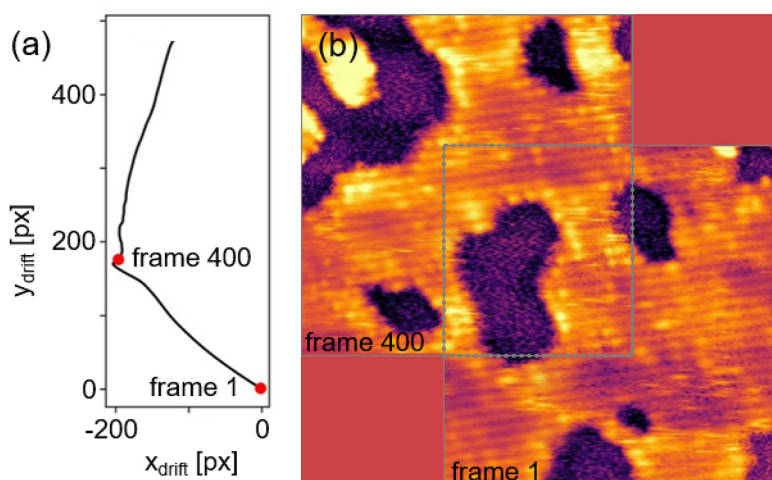


Fig. 4. (a) Drift path of the movie shown in Fig. 3 as calculated by a sliding cross correlation of frame pairs taken at a chosen time separation (here 20 s; the drift for the last 19 s is thus extrapolated). (b) Illustration of the two possible export options on the example of two drift corrected frames. Either the full explored range is retained by padding with background pixels (all shown data) or the field of view is cropped to the greatest common area of all frames (gray dashed box).

removal of sinusoidal tip movement distortions. The result is a stable movie obtained without loss of any pixel information, which opens the way for the non-specialized user to routinely evaluate fast SPM data in a quantitative manner, down to the atomic scale. Examples were given for the investigation of elusive intermediate species, of fast diffusion dynamics, and of a new mode of image reconstruction by averaging under highly dynamic, extreme imaging conditions.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.softx.2022.101269>. Experimental details of the Supporting Movie as well as the parameters used for movie conversion are given in the supplementary material. Additional link to our work can be found at: <https://doi.org/10.5281/zenodo.7371526>.

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