**Report Title:** Essential Image Processing for Magnetic-Resonance Force Microscopy

**Abstract:**
Report developed under STTR contract DAAD19-02-C-0093 for topic ARMY02-T010.

This report covers work performed on two-dimensional and three-dimensional reconstruction of magnetic images derived from synthetic data sets of a model magnetic-resonance force microscope. Specifically, Pixon LLC has employed it’s proprietary Pixon-method image reconstruction algorithm in order to perform the reconstructions. We find that the algorithm yields excellent results, in particular as regards image accuracy, resolution, and suppression of noise. A specific and robust regimen for performing the reconstructions within the Pixon-method paradigm has been developed. The regimen is robust against varying signal-to-noise ratio and varying tip-to-sample separation in the MRFM instrument model. Moreover, a data-capture scanning strategy has been discovered that optimizes performance of the reconstruction (resolution and sensitivity) while simultaneously minimizing the data acquisition time. These results should make straightforward the application of the algorithm in a real-world instrument. The results also favor adaptation of Pixon-method image reconstruction techniques to three-dimensional imaging with conventional magnetic-force microscopes.

**Subject Terms:**
STTR Report, image reconstruction, image restoration, Pixon method, magnetic-resonance force microscopy
Overview


Work Performed

(1) Development of a preliminary mathematical model of an MRFM transducer.

(2) Generation of 3D synthetic data with which to perform deconvolutions of the MRFM instrumental response.

(3) Performance of reconstructions using Wiener filtering, maximum likelihood, and Pixon methods in 3D.

(4) Development of software to perform 1D reconstructions by Landweber iterative method.


(6) Completed comparisons of reconstructions using conventional sampling and the new methods developed for 2D reconstructions. Began systematic investigations of two-dimensional MRFM image reconstruction.

(7) Generated synthetic data with which to perform deconvolutions of the MRFM instrumental response.

(8) Completed exhaustive investigation of Pixon-method 2D reconstruction techniques including 1-step bootstrap and annealing procedures.

(9) Investigated reconstruction fidelity as a function of signal-to-noise ratio in 2D.

(10) Investigated reconstruction fidelity as a function of sampling density for constant data acquisition time in 2D.

(11) Re-examined trade off between signal-to-noise ratio and sampling density for two-dimensional MRFM image reconstruction.

(12) Created new data sampling functions that implement a new scan strategy for 2D data capture and subsequent reconstruction.

(13) Carried out initial explorations of atomic-scale resolution in 2D.

(14) Generalized 2D reconstruction techniques to three dimensions.

(15) Developed final sampling and reconstruction techniques that prove robust across varying signal-to-noise ratio and varying spatial resolutions.

(16) Investigated reconstruction fidelity as a function of signal-to-noise ratio at spatial resolutions of 50 nm, 10 nm, and 1 nm.

Milestones Reached

(1) Demonstrated for the first time successful 3D reconstructions of MRFM data.

(2) Pixon reconstructions exhibited superior performance with respect to low-level signal recovery, suppression of artifacts, and spatial resolution relative to Wiener filtering and maximum-likelihood
reconstructions. Computation times were short.

(3) Preliminary comparison of Pixon and Landweber methods on a 1D (non MRFM) deconvolution problem showed high speed but poor performance for an unregularized Landweber reconstruction. Specifically, the Landweber method exhibited an over interpretation of the data (statistically unjustified high resolution) and significant noise.

(4) Officially documented MRFM instrument model via a Mathematica script.

(5) Established “scale annealing” as the initial preferred technique for executing Pixon method reconstructions.

(6) Demonstrated that an optimal sampling density exists for a given scan geometry. This validates a key premise of the original proposal that software simulations of MRFM image reconstructions would have a major impact on the instrumentation design and implementation.

(7) Revised previous assessment that optimal scan densities exist for given scan geometry. Only a weak dependence on sampling density is observed when a fixed image grid is used independent of the sampling density. This allows for more honest direct comparisons.

(8) Although “scale annealing” is the preferred technique for executing Pixon method reconstructions, the single-step bootstrap method yields excellent results as well.

(9) Atomic-scale resolution should be achievable with probe-to-sample separations of ~500 nm provided this separation yields sufficient SNR (~ 5 per sample).

(10) Major discovery: An optimal scan geometry exists that minimizes data acquisition time, eliminates cross-coupling of the vertical and horizontal resolution, yields higher resolution than previous scan methods, and reduces reconstruction compute time. The strategy is to scan the sample region twice (for 2D, it’s 3 times in 3D) using different sections of the MRFM point-response function. Each section is chosen to yield information along a single orthogonal axis in the sample.

(11) Established “triple sampling” as the preferred technique for 2D data acquisition. This approach maximizes sensitivity and spatial resolution while maintaining minimal vulnerability to reconstruction ambiguity and minimum data acquisition time.

(12) Scale annealing discovered not to prove as robust as initially believed, especially with triple sampling technique of data acquisition. A new technique involving an initial image estimation method designated “uniform-minimal-Pixon non-negative least squares” was developed and tested. The technique’s performance is excellent: In conjunction with triple sampling, it yields consistent results across varying signal-to-noise ratios and varying spatial resolutions while maintaining strong immunity to spurious signals.

(13) Established instrumental parameters and data requirements for achieving reconstructions with resolutions of 50 nm, 10 nm, and 1 nm in 2D.

(14) Successfully translated 2D techniques to three dimensions.

(15) Established instrumental parameters and data requirements for achieving reconstructions with resolutions of 50 nm, 10 nm, and 1 nm in 3D.

Items Received or Shipped

None.
Conclusions

(1) The Pixon minimum-complexity image reconstruction method has proven successful for reconstruction of MRFM imaging data in both two and three dimensions.

(2) The method yields superior noise suppression and sensitivity to weak signals.

(3) A specific implementation of the Pixon method has been developed that is robust against varying signal-to-noise ratio and varying tip-to-sample separation. This development makes straightforward the adaptation of this reconstruction implementation to a real-world instrument.

(4) Atomec-scale resolution is achieved in 2 and 3 dimensions at a tip-to-sample separation of 500 nm.

(5) Although a specific MRFM instrument model has been used for this study, the conclusions presented here will hold for other MRFM models.

(6) An especially important technique for scanning of the MRFM probe has been discovered: By selective interrogation of the magnetic sample with the MRFM probe (implemented in this study as multiple point-response functions), significant improvements in sensitivity and resolution are obtained.

(7) Compared with alternative techniques for reconstruction of MRFM data, the Pixon method yields improvements in sensitivity of at least a factor of 10. Further study is needed to more fully quantify the performance advantages.

(8) Pixon-method reconstruction will prove especially valuable at the low signal-to-noise ratios inherent in MRFM.
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REPORT TITLE: Systematic Investigation of 3D MRFM Image Reconstruction with the Pixon Method, Part I I

is forwarded for your information.

SUBMITTED FOR PUBLICATION TO (applicable only if report is manuscript):

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