Mitigating Tip-Induced Artifacts in AFM Images Using Autoencoder-Based Solutions

Hackathon 17/12/2024

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Motivation

Accurate imaging is critical in nanoscale characterization techniques, such as Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM), where structural and topographical details are analyzed at an atomic or molecular level. However, the quality of these images is often compromised by tip-induced artifacts caused by blunt, imperfect, or contaminated probe tips. These artifacts distort the features of the sample, resulting in unreliable data interpretation, which can impact critical applications in fields such as materials science, nanotechnology, and biological imaging.

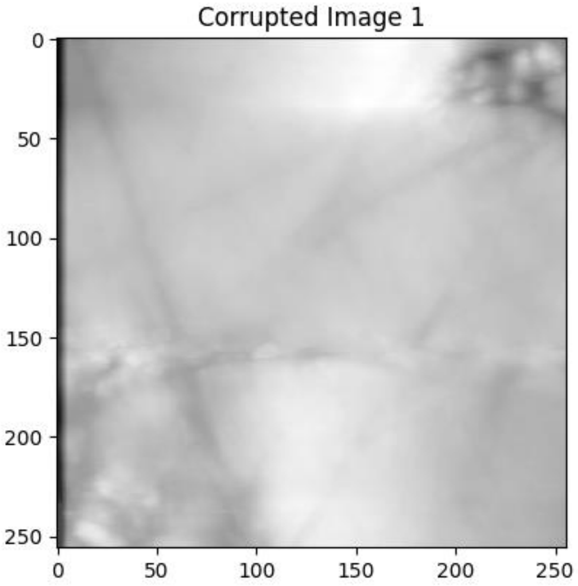
The motivation behind this project based on the need to automatically detect and mitigate these tip-induced artifacts to ensure more reliable and accurate imaging. Traditional methods, such as Gwyddion's tip estimation and surface reconstruction tools, are often limited by manual intervention, computational inefficiency, or incomplete removal of artifacts. Additionally, advancements in deep learning techniques—particularly autoencoder-based approaches—present an opportunity to address these limitations by leveraging data-driven methods to restore images and reduce distortions effectively.

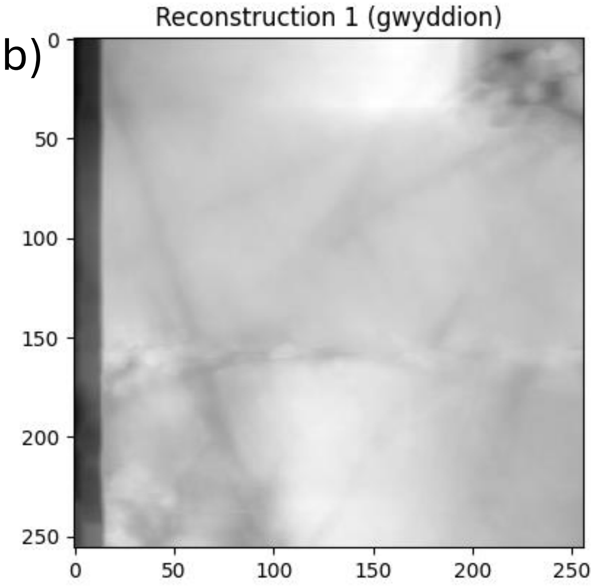
The project goals

- **Improve image reliability:** By mitigating artifacts, we enable better interpretation of nanoscale structures, which is crucial for high-stakes research and industrial applications.

- **Explore deep learning in AFM/STM:** It highlights the feasibility of using machine learning to automate artifact correction, a step toward more robust and scalable solutions.

- **Lay groundwork for future applications:** While focusing on blunt tip artifacts, the methodology can be expanded to address other challenges, such as double-tip effects or transferability to other microscopy techniques.

(a)


(b)


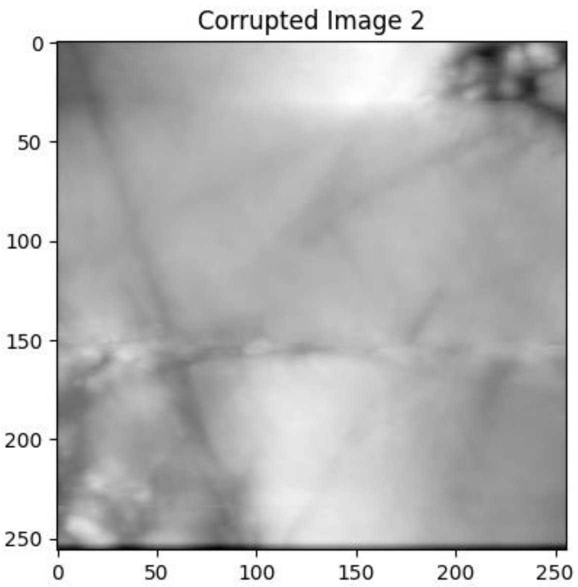
(c)

(d)

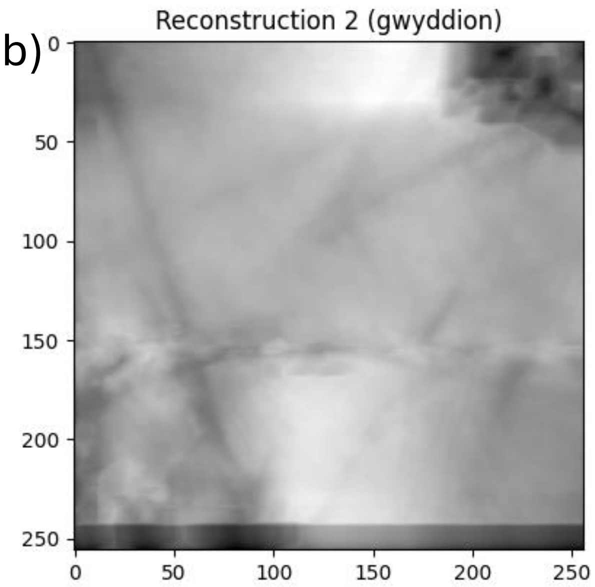
(a) Is the corrupted image. It was made with a tip radius of 0.0580 and tip centre of [0.4837, 0.2528]. (b) This image reconstruction was made using gwyddion. (c) Image recontruction done using model 1. (d) Tip reconstruction done using model 2.

Method	PSNR score	VIF score
Original corrupted image	16.9	0.086
Gwyddion	16.5	0.086
Model 1	15.2	0.107
Model 2	4.04	0.008

(a)



(b)

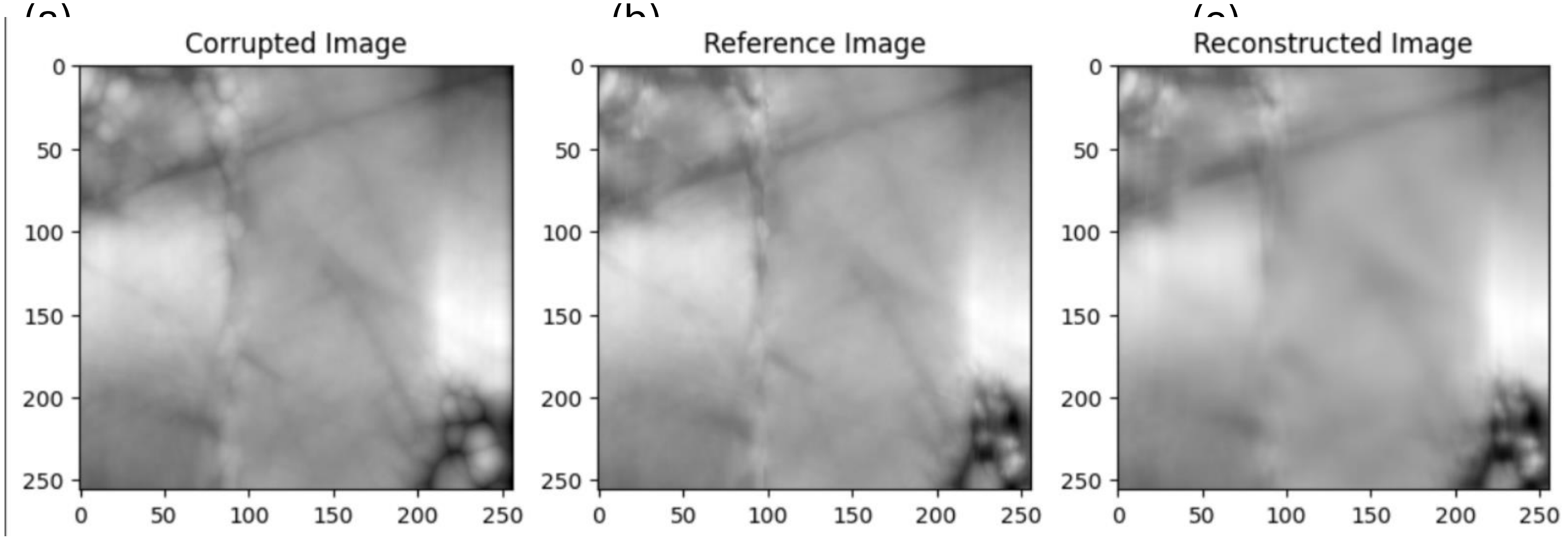


(c)

(d)

(a) Is the corrupted image. It was made with a tip radius of 0.0750 and tip centre of [0.3292, 0.4286]. (b) This image reconstruction was made using gwyddion. (c) Image recontruction done using model 1. (d) Tip reconstruction done using model 2.

Method	PSNR score	VIF score
Original corrupted image	24.8	0.069
Gwyddion	22.1	0.063
Model 1	15.2	0.057
Model 2	4.04	0.008



(a) Is the corrupted image. It was made with a tip radius of 0.0800 and tip centre of [0.3998, 0.4218]. (b) This was the reference image for the given corrupted image (c) Image reconstruction done using model 3.

Model 3	Val Lose after 75 epochs	SSIM
	0.026	0.9534

Hackathon submission (17/12/2024) for tip deconvolution.

In this hackathon submission, we focus on mitigating tip-induced artifacts in AFM images, particularly those arising from blunt or imperfectly shaped tips. The dataset consists of a single AFM scan of unspecified lateral dimensions, from which we generate synthetic training examples by convolving the original image with a Gaussian kernel. The Gaussian's standard deviation (tip radius) and center coordinates are randomly sampled from a uniform distribution in [0.2, 0.8), enabling controlled generation of blunt tip artifacts. Although we intended to model double-tip artifacts as well, time constraints precluded this addition.

We acknowledge that using a single image for training may lead to substantial overfitting, and thus any derived metrics should be interpreted with caution. Nonetheless, our primary objective was to explore the feasibility of autoencoder-based solutions. Drawing on established literature, we tested various architectures and loss functions, notably combining MAE and SSIM metrics. As a comparative baseline, we employed Gwyddion's tip estimation, surface reconstruction methods and also SSIM on select images and contrasted these with our trained models' outputs.

Additionally, we extended the same methodology to an experimental STM dataset, artificially introducing blunt tip defects as a preliminary proof of concept for transferability to other scanning probe or electron microscopy techniques. While initial STM results appear promising, further research is necessary to address specific artifacts associated with STM tip geometries and to rigorously evaluate the approach's generalizability.

Model summaries

We do not give the full architecture here, that can be seen from the code, just a rough overview of the differences.

Model 1: Similar to Unet but no skip connections. Was trained for 70 epochs and with a lr=0.0001. Notably, the ground truth for this model was the difference between the corrupted image and the uncorrupted image i.e. it was trying to predict the “noise”. Loss was MAE combined with SSIM.

Model 2: Autoencoder with 33k parameters. It was trained for 1000 epochs on the dataset of 1200 STM images (128x128 px) with normalization. Loss was MAE.

Model 3: Autoencoder with 6.7 million parameters and skip connections. It was trained for 75 epochs on the dataset of 100 STM images (256 x256 px) with normalization. Loss was MAE combined with SSIM as well as a custom gradient loss to help reduce blur in reconstructed image and add more detail. Ideally, this model should be run for more epochs but due to time constraints was limited to only 75 epochs. The reconstructed image shows promise for getting rid of blunt tip affect but is blurry in regions lacking much detail. Further hyperparameter tuning, lower learning rate and optimized loss function weights(more SSIM and gradient loss) could possibly help gain clearer reconstruction image.