Data driven identification of tip-sample interaction in atomic force microscopy

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Summary. Dynamic AFM is transitioning from a high-resolution imaging tool to a nanomechanical probe that can perform precise quantification of matter in fields as varied as microbiology, molecular metrology, and material science. To date, this has been achieved by estimating the nanoscale forces that exist between the probe and the sample, using empirical models that are merely approximations of the true probe-sample interaction physics. Here, we go beyond such approximations by making use of the recent advances in data-science and machine learning to distil nonlinear governing equations of dynamic AFM, and thus predict tip-sample forces directly from experimental raw deflection data. Our data-driven algorithm obtains physics-based models from experiments and is able to estimate time-resolved nanoscale interactions with sub-microsecond resolution.

Introduction

Dynamic atomic force microscopy (AFM) has become an indispensable tool for resolving mechanical, chemical and biological properties of samples at nanoscale. The precise quantification of materials at the nanoscale is achieved with accurate estimation of the tip-sample interaction force. However, dynamic AFM in contrast to its name does not measure directly the interaction force while imaging in any of its modalities. Instead, the interaction force is often reconstructed indirectly by combining different information channels like the frequency, amplitude and phase of the oscillating cantilever, while modulating the height of the probe above the sample surface [4]. The existing reconstruction techniques in dynamic AFM posses several drawbacks such as inability to resolve instantaneous tip-sample force, requiring a priori knowledge on the transfer function of the cantilever or large number of harmonics, which makes them cumbersome and inefficient to study the fast processes encountered in biological and chemical systems [3]. Thus a generalized approach for dynamic AFM that allows direct access to time-resolved surface forces irrespective of the chosen probe-sample configuration is currently missing.

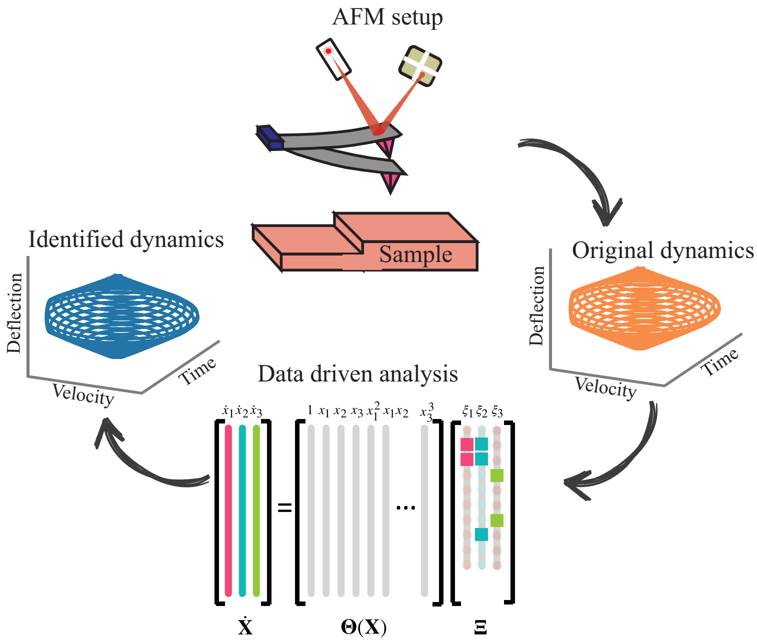

Figure 1: Schematic of the identification process. The data (orange trajectories) from the AFM setup is used as input to the sparse identification algorithm. The algorithm determines the governing model of the system and predicts the corresponding dynamics as shown by the blue phase space trajectories.

In this regard, here we demonstrate that data-driven identification applied to dynamic AFM experiments can provide physically interpretable models and simultaneously estimate the time-resolved interaction forces. We make use of the recent advances in sparse identification [1] and machine learning [2] techniques to identify the governing equations directly from the experimental measurements. In contrast to existing methods, the data-driven approach has no inherent assumptions on the type of interactions or mathematical models but relies solely on the measurements and thus can be generalized to any cantilever-sample configuration. Furthermore, based on the identified governing equations, our method also quantifies the tip-sample force with a sub-microsecond resolution. We showcase this experimentally by using the data-driven algorithm on the temporal data obtained from a silicon cantilever interacting with a two-component polymeric sample made up of Polystyrene (PS) and Low-Density-Polyethylene (LDPE). The results and insights obtained from the identification procedure are in excellent agreement with the expected tip-sample interaction mechanism in polymers. In particular, we showcase the variation in contact duration, peak loading forces in stiff and compliant materials as well as highlight the ability of the technique to probe transient surface forces and capture the hysteresis phenomenon. A schematic of such an identification is shown in Fig. 1.

Methods and Results

In order to characterize the tip-sample force in experimental scenario, we first begin by training the algorithm on several standard AFM models such as Derjaguin-Muller-Toporov (DMT), Johnson, Kendall and Roberts (JKR) and Lennard-Jones (LJ) among others. This step allows us to expand the library of functions which is used to reconstruct the tip-sample nonlinearities from polynomials, trigonometric terms to specific nonlinear functions that are capable of describing the nano-scale forces encountered in dynamic AFM. We present in Fig.2 the identification results on synthetic data obtained from DMT model. Here, Fig.2(a) shows the identified dynamics (Orange) and the original dynamics (blue) of the system in a 2D phase-space portrait. Whereas, Fig.2(b) shows the identified versus the original co-efficients of the dynamical system governed by DMT tip-sample interaction force. The difference in the identified co-efficients is attributed to the noise added to the synthetic data to mimic the experimental conditions. By utilizing the co-efficients of the identified system, the tip-sample force is re-constructed with sub-microsecond resolution.

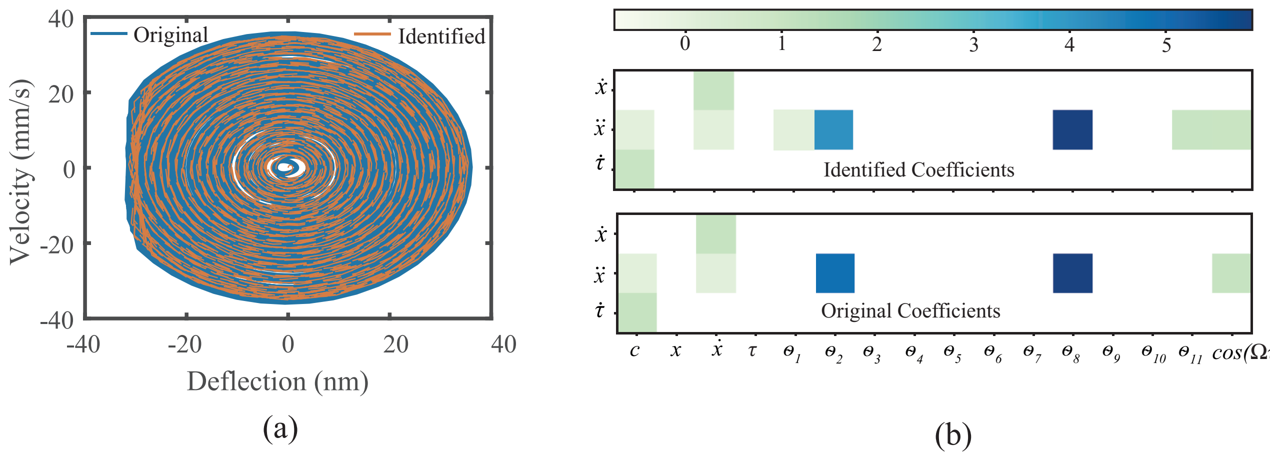

Figure 2: Identification of DMT model dynamics. (a) Identified (orange) trajectories from data driven analysis superimposed on the original trajectories (blue) obtained from simulations. (b) Map showing the strength of identified versus the original coefficient values used in the simulations.

Conclusion

We report here a novel approach at identifying the governing equations of motion and the associated tip-sample force in dynamic AFM using machine learning and data science techniques. The data driven algorithm based on sparse identification is trained on standard AFM models and a condensed library of functions capable of identifying experimental tip-sample interaction mechanics is determined. To highlight the capability of the technique, numerical simulations with noise corrupted synthetic data and experiments on polymer materials are performed. The analysis of the results show that the technique is able to obtain the dynamical trajectory of the underlying system without any prior assumption on the nature of tip-sample interaction. The method thus opens a completely new window into using machine learning algorithms in AFM nano-characterization with real-time data as well in developing novel feedback architectures and high-speed imaging.

References

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