Control of Atomic Force Microscopy Tip

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I. & II. Problem Statement

The project I am working on is the Atomic Force Microscope. Atomic force microscopes are used for imaging, nano manipulation etc. There are two main modes of the AFM, one is the contact mode and the other is the tapping mode. The system uses a cantilever beam and a tip that is in contact with the surface or has a vibration being passed through it via a piezoelectric which results in an oscillatory motion of the cantilever (this is called the tapping mode). The tapping mode AFM is the most common form and will be studied in this project. Tapping mode basically means, the cantilever is vibrated with an oscillatory motion and a fixed frequency. The control is actuated by a piezo element that controls the vertical position of the cantilever base or in other words there is a feedback control in the Z direction. The following is a model of the system:

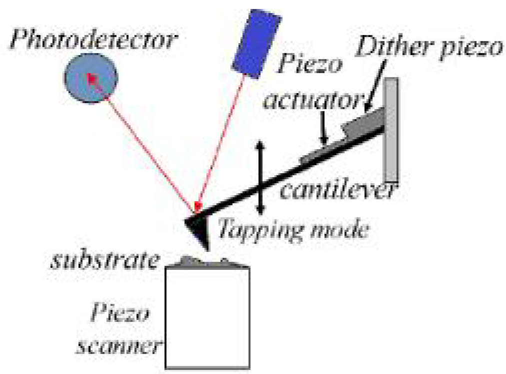

Figure 1: AFM Model

<u>Problem to solve and Approach:</u>
The distance between the tip and the sample is kept constant by the system using a pre-defined point, but the relative z motion of the tip and sample distance changes as topographical changes are encountered by the tip on the sample. The feedback signal from this tip and sample distance is then used to create the trajectory of the AFM. The trajectory of the AFM is the images that are created by the AFM. The purpose for this project is to control the oscillations of the micro-cantilever i.e. the displacement of the cantilever in the z direction. Most of the papers regarding control of AFM attempt to control these oscillations via different methods. The control in the X and Y direction has already been achieved to a great degree and is not really studied. However for the sake of simplicity, only the study in z direction is done like the papers cited.
First the observability, controllability and stability of the system will be check. If all are satisfied, then Optimal Linear Control using the LQR/ State dependent Riccati Equation method will be attempted to be used for the control system. Comparing them and with the desired oscillation waves of the velocities and the displacement of the oscillations we will see if the solution is found or not. A flat topographical terrain and a square wave topographical terrain will be used.

III. System Modeling

According to the paper [2], the mathematical models governing the dynamics of (AFM) cantilevers, generally, have one of two simplifications: assuming that the cantilever bends as if a static point load is being applied at the cantilevers free end and using the corresponding static stiffness to derive a single degree of freedom point-mass model of discretizing the classical beam equation based on its eigeenmodes leading to either single or multiple degrees of freedom models [2]. According to the paper, Chaos Control of atomic Force Microscope System using Nonlinear Model Predictive

Control[3], The cantilever system in an interaction with a surface or material (called as a substrate) can be modeled as the following:

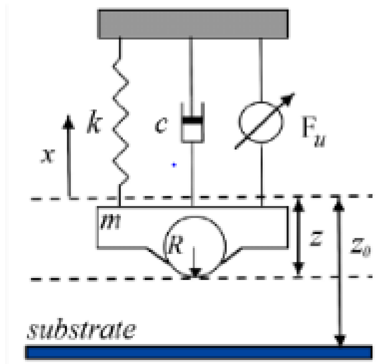

Figure 2: Model of the Cantilever in Tapping Mode

The Cantilever system is modeled as a single spring-mass low damping system when the cantilever is put through the vibration. There is a spring constant k and equivalent mass m. The cantilever tip sample is taken as a sphere of radius R and mass. Using the Lagrange method, the equation of motion for the tip in an interaction with the substrate is found as follows:
Using the Lagrangian , L= T V + P

$$L = T - V + P$$
$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 + \frac{1}{2}c\dot{x}^2$$
$$\frac{d}{dt}(\frac{dL}{d\dot{q}i}) - \frac{dL}{dqi} + \frac{dP}{d\dot{q}i}$$

$\frac{dL}{d\dot{q}i} = m\dot{x}$ and $\frac{d}{dt}(\frac{dL}{d\dot{q}i}) = m\ddot{x}$

$\frac{dL}{d\dot{q}i} = -kx$ and $\frac{dP}{d\dot{q}i} = c\ddot{x}$

Putting it all together we get the following equations of motion:

$$m\ddot{x} + c\dot{x} + kx = Forces$$

The forces in play are the exitation of the cantilever $F_1 cos(\omega t)$ and the tip and sample interaction force which is given in the form of a Leonard Jones potential as follows:

$$F_{LJ} = \frac{H_1 R}{180(z_0 + x)^8} + \frac{H_2 R}{6(z_0 + x)^2}$$

Where H1 and H2 are constants that can be found from a commercial AFM website and R is the radius of the tip. The control F_u is applied by the dither piezo actuator, only in the z direction, or in other words the direction of the displacement. The sensors in the system are the photodiodes, which measure the displacement of the problem via the laser rays that are deflected of the tip. So the final equation of motion for the cantilever looks like the following:

$$m\ddot{x}+c\dot{x}+kx=\varphi cos(\omega t)+F_{LJ}+F_u$$

The following relationships can be use just like they are used in the paper, Chaos Control of Atomic Force Microscope System Using Nonlinear Model Predictive Control [3].

$$T=\omega t,\ z_s=\tfrac{3}{2}\sqrt[3]{\tfrac{H_2R}{3k}},\ y=\tfrac{x}{z_s},\ \dot{y}=\tfrac{\dot{x_s}}{z_s},\ \omega=\sqrt{\tfrac{k}{m}},\ a=\tfrac{z_0}{z_s}$$

$$b=\tfrac{c}{mw},\ h=\tfrac{H_1R}{180m\omega^2z_s^9},\ d=\tfrac{H_2R}{6m\omega^2z_s^3},\ u=\tfrac{F_u}{m\omega^2z_s}$$

Thus, the equation of motion now can be written as the following:

$$\ddot{y}+b\dot{y}+y+\frac{d}{(a+y)^2}-\frac{h}{(a+y)^8}-fcos(T)=u$$

In order to get the final equations of motion, the following is done:

$$x_1=y$$

$$x_2=\dot{y}$$

Therefore, the following are the equations of motions:

$$x_1=x_2$$

$$x_2=-bx_2-x_1-\frac{d}{(a+x_1)^2}+\frac{h}{(a+x_1)^8}-fcos(T)+u$$

Discretizing the equations of motion, will give the following:

$$x_1(k+1)=x_1(k)+x_2(k)\Delta T$$

$$x_2(k+1)=X_2(k)+[-bx_2-x_1-\frac{d}{(a+x_1)^2}+\frac{h}{(a+x_1)^8}-fcos(T)+u]\Delta T$$

The following table summarizes the parameter properties that were taken from the VEECO commercial AFM, used in the paper Chaos Control of Atomic Force Microscope System Using Nonlinear Model Predictive Control [3].

Linearization of the system around a nominal desired trajectory:

A nonlinear system can be linearized around a desired trajectory. Suppose there is a trajectory of the form $\dot{X_D}=f(X_d,u_d)$. Then $e=X-X_D$ and $\delta u=u-u_d$ which gives us $\dot{e}=f(X_d+e,u_d+\delta u)-f(X_d,u_d)$. If we take the Taylor series expansion about X_d, then we get $\dot{e}=f(X_d,u_d)$ + $(\frac{\partial f}{\partial X} around(X_d,u_d))e$ + $(\frac{\partial f}{\partial u} around(X_d,u_d))$ - $f(X_d,u_d)+H.O.T$. After ignoring the higher order terms, we get $\dot{e}=A_de+B_d\delta u$, where A_d and B_d are the matrices with partial derivatives.

For the problem in hand, suppose we have a desired trajectory $x_d=\begin{bmatrix}x_{d1}\\x_{d2}\end{bmatrix}$, then the following can be said:

$$\begin{bmatrix}e_1\\e_2\end{bmatrix}=\begin{bmatrix}x_1-x_{d1}\\x_2-x_{d2}\end{bmatrix}\text{ and }\delta u=u-u_d$$

Table 1 Properties and dimensions of the cantilever [10].

descriptions	symbol	value
length	L_1	$449\,\mu m$
thickness	t_1	$1.7\,\mu m$
width	w_1	$46\,\mu m$
Tip radius	R	$150nm$
Material density	ρ	$2330\ kgm^{-3}$
Static stiffness	k	$0.11\ Nm^{-1}$
Elastic modulus	E	$176\ GPa$
1st resonance	f_1	$11.804\ kHz$
Q factor (air)	Q	100
Hamaker(rep.)	H_1	$1.3596\times10^{-70}\,Jm^{6}$
Hamaker(att.)	H_2	$1.865\times10^{-19}\,J$

Figure 3: Properties taken from the paper [3]

Taking the derivative of e, we have the following A_d and B_d matrices:

$$A_d = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(x_d,u_d)}$$

$$B_d = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} \\ \frac{\partial f_2}{\partial u_1} \end{bmatrix}$$

The linearized matrices around a desired trajectory for the equations of motion of atomic force microscope probe are as follows:

$$A_d = \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_{d1})^3} - \frac{8h}{(a+x_{d1})^9} & -b \end{bmatrix}$$

$$B_d = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Therefore, the linearized state space representation is as follows:

$$\dot{e} = \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_d)^3} - \frac{8h}{(a+x_d)^9} & -b \end{bmatrix} \begin{bmatrix} e1 \\ e2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \delta u$$

Only the displacement measurements are found. Thus, $h(x,u) = x_1$ and $y = h(x,u)$. Taking the Jacobean matrix around the desired trajectory we get the following C matrix and the measurement representation:

$$C_d = \begin{bmatrix} 1 & 0 \end{bmatrix}$$
$$\Delta y = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \dot{e_1} \\ \dot{e_2} \end{bmatrix}$$

IV System Anaylsis

The system is a non-linear system. The system in equations can be written as follows:

$$\begin{bmatrix} \dot{x_1} \\ \dot{x_2} \end{bmatrix} = \begin{bmatrix} x_2 \\ -bx_2 - x_1 - \frac{d}{(a+x_1)^2} + \frac{h}{(a+x_1)^8} + fcos(T) \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u$$

<u>Controllability</u>

Computing the controllability matrix using the linearized A and B matrices, we get the following for the linear controllability matrix:

$$M_a = \begin{bmatrix} B & AB \end{bmatrix} = \begin{bmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_d)^3} - \frac{8h}{(a+x_d)^9} & -b \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{bmatrix}$$
$$M_a = \begin{bmatrix} 0 & 1 \\ 1 & -b \end{bmatrix}$$

The linear controllability matrix, M_a, has a full rank of 2 therefore it is controllable around the desired nominal trajectory.

However, if we want to check controllability of the original nonlinear system. We do so using Lie derivatives. Using notes from [4], lie derivatives must be taken to see if we get other directions and if the number of directions were the same as the number of states then we can say the system is controllable although this is not always true as nonlinear systems are difficult to work with. Lets say

$$f = \begin{bmatrix} x_2 \\ -bx_2 - x_1 - \frac{d}{(a+x_1)^2} + \frac{h}{(a+x_1)^8} + fcos(T) \end{bmatrix}$$

$$g = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Then,

$$adj_f^0 g(x) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$adj_f^1 g(x) = \begin{bmatrix} f, g \end{bmatrix}(x) = \frac{\partial g}{\partial x} f(x) - \frac{\partial f}{\partial x} g(x)$$
$$\frac{\partial g}{\partial x} = 0$$
$$\frac{\partial f}{\partial x} = \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_1)^3} - \frac{8h}{(a+x_1)^9} & -b \end{bmatrix}$$

Therefore,

$$adj_f^1 g(x) = [f,g](x) = 0 - \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_1)^3} - \frac{8h}{(a+x_1)^9} & -b \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ b \end{bmatrix}$$

The next ad-joint is as follows:

$$adj_f^2 g(x) = [f,[f,g]](x) = \frac{\partial [f,g]}{\partial x} f(x) - \frac{\partial f}{\partial x} [f,g](x)$$

$$\frac{\partial [f,g]}{\partial x} = 0$$

$$\frac{\partial f}{\partial x} = \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_1)^3} - \frac{8h}{(a+x_1)^9} & -b \end{bmatrix}$$

Therefore,

$$adj_f^2 g(x) = [f,[f,g]](x) = 0 - \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_1)^3} - \frac{8h}{(a+x_1)^9} & -b \end{bmatrix} \begin{bmatrix} 0 \\ b \end{bmatrix} = \begin{bmatrix} -b \\ b^2 \end{bmatrix}$$

Two different directions were found. System is controllable.

$$M_{fg} = \begin{bmatrix} 0 & 0 & -b \\ 1 & b & b^2 \end{bmatrix}$$

<u>Observability</u>

We also want to see if given the measurements, can we estimate the states. The observability matrix of the linearized system can be given as follows:

$$Obs(C,A) = \begin{bmatrix} C \\ CA \end{bmatrix}$$

$$Obs(C,A) = \begin{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \\ \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 + \frac{2d}{(a+x_1)^3} - \frac{8h}{(a+x_1)^9} & -b \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The observability matrix for the linearized system has a full rank of 2 therefore it should be observable.
However, checking the observability for the original non-linear system. We again take lie derivatives.
$h(x) = \begin{bmatrix} x_1 \\ 0 \end{bmatrix}$ and $f(x) = \begin{bmatrix} x_2 \\ -bx_2 - x_1 - \frac{d}{(a+x_1)^2} + \frac{h}{(a+x_1)^8} + fcos(T) \end{bmatrix}$

Therefore, $L_f^0 h^T = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $L_f^1 h^T = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Thus, the observability matrix for the original non-linear system is as follows:

$$O(f,h) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The observability matrix has a full rank therefore it should be observable. However, if the observability matrix of nonlinear systems is not computed properly then maybe the system is not observable for this problem.

Stability of Unactuated System

We want to see how the system is performing without any control input. The following are the cantilever displacement and velocity without control and the phase plot of the system. The common initial conditions x=[0.6,0] as used in Chaos Control of Atomic Force Microscope System Using Nonlinear Model Predictive Control [3]were used.

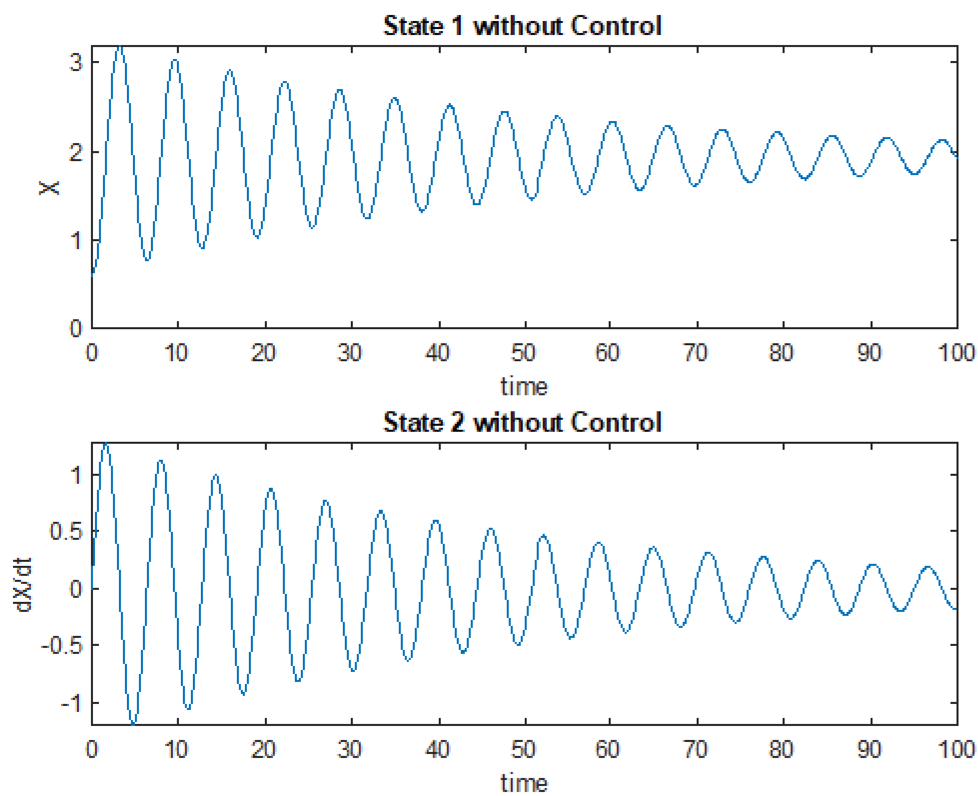

Figure 4: States of the system without control

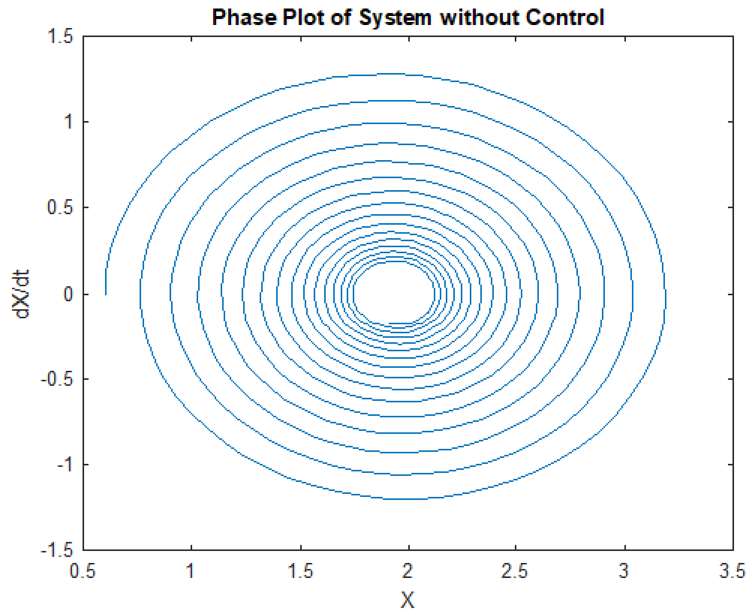

Figure 5: Phase Plot of the system

After changing the parameters slightly, you get the phase plot:

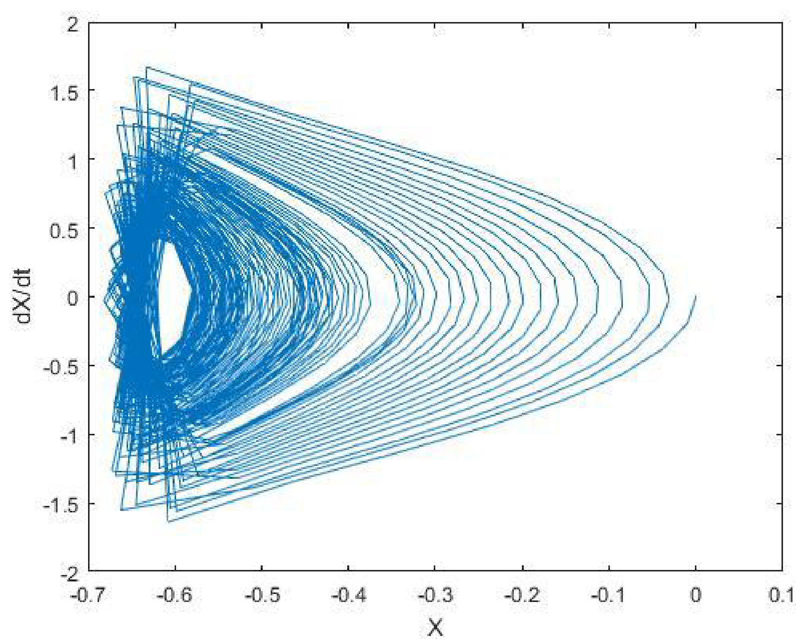

Figure 6: Phase Plot Chaotic

Lyapunov Method for Nonlinear Stability Analysis:

The equation before being non-dimensionalized is

$$m\ddot{x}+c\dot{x}+kx-\varphi cos(\omega t)-F_{LJ}=0$$

We can say that the sum of external forces is F_{all} for now and that the system is represented as follows:

$$m\ddot{x}+c\dot{x}+kx=F_{all}$$

Now, we can solve for the equation at the equilibrium which is at the origin. Lets say $\widetilde{x}$ is the equilibrium condition [1]. Thus, the following happens:

$$m(0)+c(0)+k\widetilde{x}=F$$

$$\widetilde{x}=\frac{F}{k}$$

Let's say $r=x-\widetilde{x}$. Therefore,

$$m\ddot{r}+c\dot{r}+kr+k(\frac{F}{k})=F$$

$$m\ddot{r}+c\dot{r}+kr=0$$

$$m\ddot{r}=-c\dot{r}-kr$$

Energy functions are the best candidates for Lyapunov functions therefore, we define the Lyapunov fuction for this system as the following:

$$V(r,\dot{r})=\frac{1}{2}m\dot{r}^2+\frac{1}{2}kr^2$$

When you consider the above mentioned function, it can never be negative. Also,the lyapunov function will be 0 only when the input is 0 , which is the equilibrium pt i.e. $r=0$ and $\dot{r}=0$. [1]

$$V(r,\dot{r})=\frac{d}{dt}(\frac{1}{2}m\dot{r}^2+\frac{1}{2}kr^2)$$

$$V(r,\dot{r})=m\dot{r}\ddot{r}+k\dot{r}\ddot{r}$$

Substituting into the derivative of the lyapunov, we get

$$V(r,\dot{r})=\dot{r}(-c\dot{r}-ky+ky)$$

$$V(r,\dot{r})=\dot{r}(-c\dot{r})$$

Thus, we can say the system is stable as the derivative of the Lyapunov function is always negative and can never be positive. It can only be less than or equal to 0.

Controller Synthesis

The controller scheme applied is optimal linear control using LQR to the linearized system. Recall, our linearized system looks like the following

$$\dot{e}=\begin{bmatrix}0 & 1\\ -1+\frac{2d}{(a+x_d)^3}-\frac{8h}{(a+x_d)^9} & -b\end{bmatrix}\begin{bmatrix}e_1\\ e_2\end{bmatrix}+\begin{bmatrix}0\\ 1\end{bmatrix}\delta u$$

With, $\delta u=u-u_d$

The goal is to go from any initial state to the final state, $e(\infty)=0$. The cost function to minimize is the following:

$$J(\delta u)=\int_0^{\infty}(e^TQe+(\delta u)^TR\delta u)dt$$

Therefore, the control $\delta u = -K_{opt}e$, where $K_{opt} = R^{-1}B^TP$. The P matrix is found by solving the Ricatti algebraic equation:

$$PA + A^TP - PBR^-1B^TP + Q = 0$$

Optimal control depends on Q and R matrices. The goal is to have the norm of Q to be much greater than the norm of R in order to penalize the trajectory error costs more, so that the controller drives the errors quickly, therefore the following Q and R matrix were chosen:

$$Q = \begin{bmatrix} 250 & 0 \\ 0 & 20 \end{bmatrix}$$

$$R = \begin{bmatrix} 0.1 \end{bmatrix}$$

The Q and R values were tuned to get the best results. However the Q and R matrices were eventually used from [2], as they provided the best results.

The desired trajectory is $x_d = (.6)sin(\omega t)$, and with the A_d and B_d matrices, we find the P and K_opt using the MATLAB LQR function:

$$P = \begin{bmatrix} 86.4829 & 4.9580 \\ 4.9580 & 1.7256 \end{bmatrix}$$

$$K_{opt} = \begin{bmatrix} 49.5803 & 17.2563 \end{bmatrix}$$

To check if the optimal gain matrix is good, the eigenvalues of $A_d - B_dK_{opt}$ were calculated and were found to be the following:

$$Eigenvalues = \begin{bmatrix} -3.6693 \\ -13.6270 \end{bmatrix}$$

They are both negative so the optimal gain matrix is good for the control. The parameters for the controller are the Q and R weighing factors. The excitation frequency is also a big parameter coming into play. The optimal gain matrix found from K_{opt} is the parameter that is finally applied on the system as the control. Next we perform a Lyapunov stability analysis to check the stability of the controller.

Recall after linearization our system looks:

$$\dot{e} = (A(X_d, u_d) - B(X_d)K)e + \Delta e$$

Where $\delta u = -Ke$ and Δe is the higher order terms or the linearization error. Therefore, setting up a Lyapunov function as the following:

$$L = \frac{1}{2}e^Te$$

Taking the derivative of the function we get the following:

$$\dot{L} = e^T((A(X_d, u_d) - B(x_d)K)e + \Delta e)$$

Therefore, saying that in the neighborhood $\in$ of X_d, $\Delta e < \gamma$

$$\dot{L} \leq lambdamin * e^Te + e^T\Delta e \leq -lambdamin|e|^2 + |e|^2|\Delta e| \leq -lambdamin|e|^2(1 - \frac{\gamma}{lambdamin})$$

Thus the gain K should be chosen such that the eignevalues of A-BK should satisfy $(1 - \frac{\gamma}{lambdamin}) \geq 0$

V Observer Synthesis

An observer can be used with the system. The system satisfies non-linear observability as mentioned before so it should be observable. It also satisfied linear observability for the linearized system around the desired trajectory. However, if the observability matrix wasnt computed properly then maybe system does loose observability and an observer cant be applied.

<u>Kalman Filter Implementation</u>

Extended Kalman filter was implemented. Assume that the uncertainty is only in parameter a. The discretized equations of motion are as follows with uncertainties in the parameter a.

$$x_1(k+1) = x_1(k) + x_2(k)\Delta T$$

$$x_2(k+1) = x_2(k) + [-bx_2(k) - x_1(k) - \frac{d}{((a+w_a)+x_1(k))^2} + \frac{h}{((a+w_a)+x_1(k))^8} - fcos(T) + u]\Delta T$$

The A and B matrices are the following:

$$A_{discrete} = \begin{bmatrix} 1 & \Delta T \\ (-1 + \frac{2d}{(a+x_d)^3} - \frac{8h}{(a+x_d)^9})\Delta T & -b(\Delta T) \end{bmatrix}$$

$$B_{discrete} = \begin{bmatrix} 0 \\ \Delta T \end{bmatrix}$$

Separating the noise and the state, we get the following:

$$\begin{bmatrix} x_1(k+1) \\ x_2(k+1) \end{bmatrix} = \begin{bmatrix} 1 & \Delta T \\ (-1 + \frac{2d}{(a+x_d)^3} - \frac{8h}{(a+x_d)^9})\Delta T & -b(\Delta T) \end{bmatrix} + \begin{bmatrix} 0 \\ \Delta T \end{bmatrix} \begin{bmatrix} 0 \\ w_a \end{bmatrix}$$

The extended kalman filter implemented had assumed R sensor noise of 10^{-4} and Q process noise of 10^{-2}. The sensor noises were varied too see any changes. However, it is possible the extended Kalman filter wasnt implemented properly.

VI Simulation Experiments

When running the simulation with a desired trajectory of $x_d = .6sin(\omega t)$, with the substrate being a flat surface we have the following results:

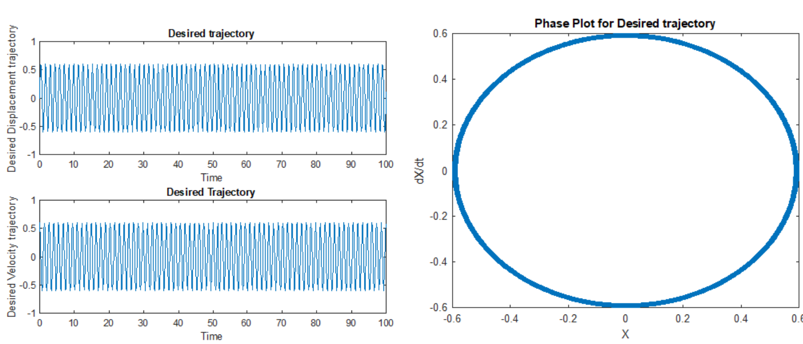

Figure 7: Desired Trajectory

Here in figure 8, we see that the states with control and desired states match each other perfectly except in the beginning which is why it is hard to see the values of x with control.

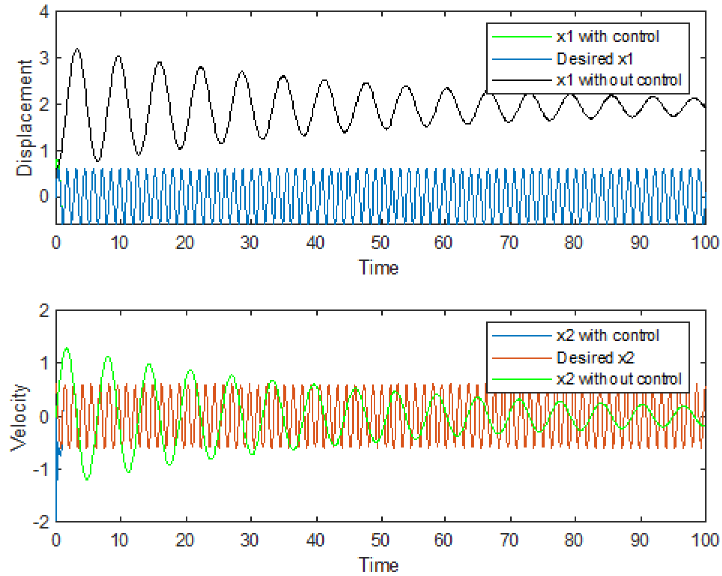

Figure 8: Comparison of final results

In figure 9, I show a close up where it is from time 0 to 10 seconds.

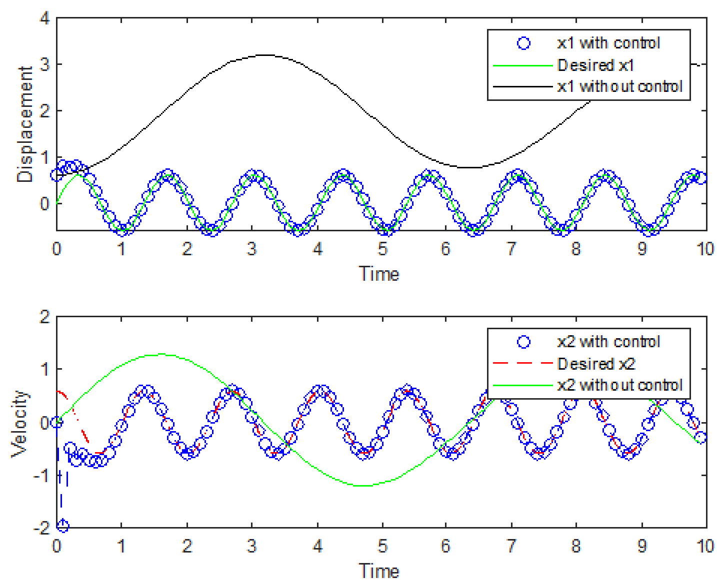

Figure 9: Comparison of final results from t=0:10

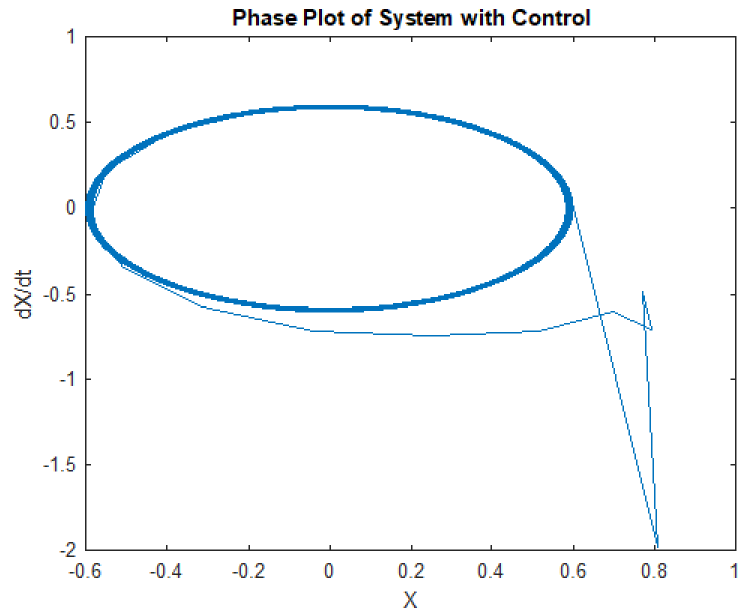

Figure 10: Phase Plot after Control

Now lets add an example where we change the topography we oscillate about:

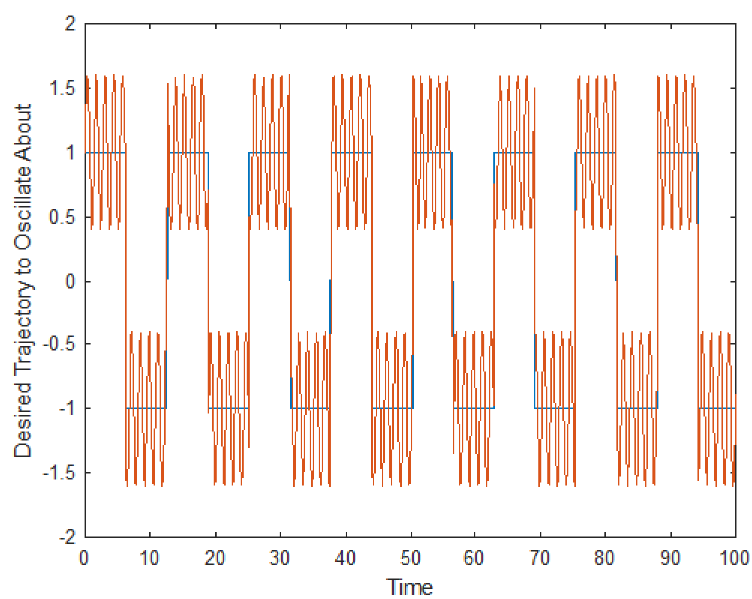

Figure 11: Square Wave

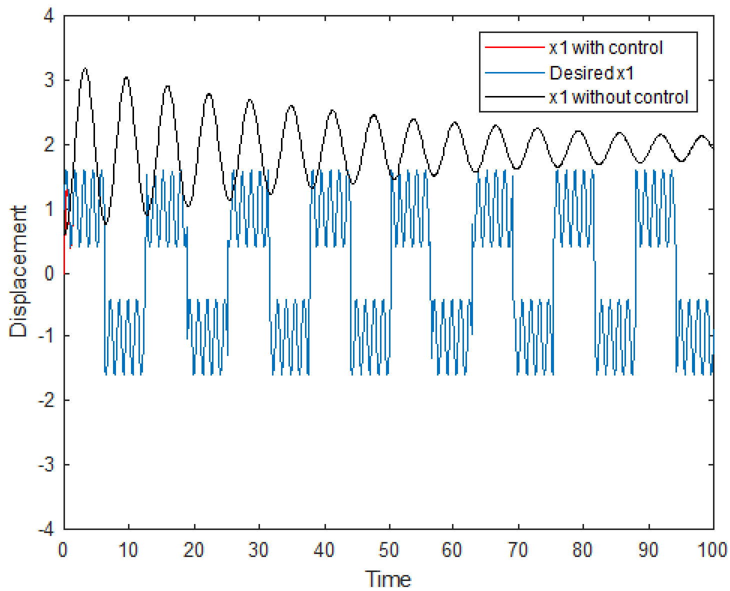

Figure 12: Control about Square wave

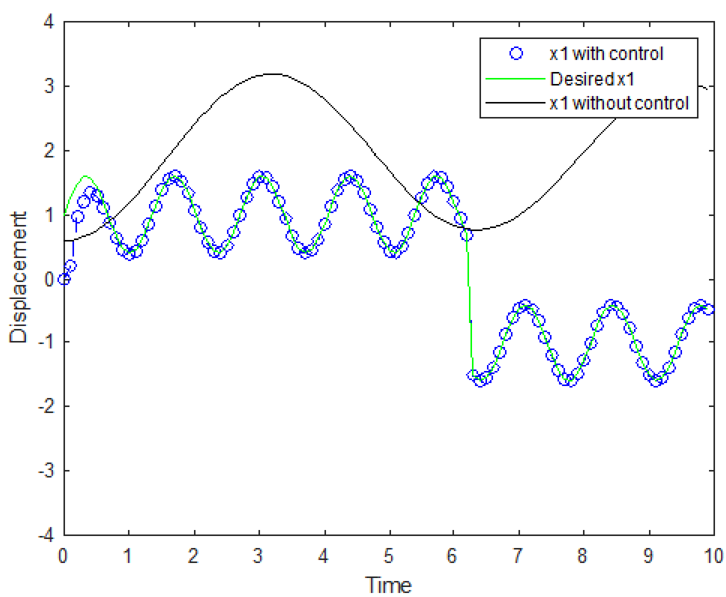

Figure 13: Closer Image of Control about Square wave

In fig 14., we have included the value of measurement noise stated $R = .1$ with some randomness and it did create fluctuations about the desired states.

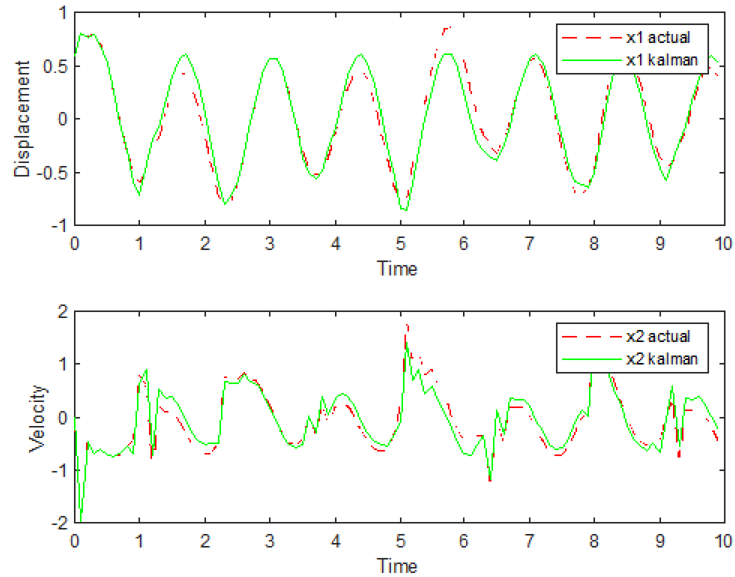

Figure 14: Kalman Filter with minimal measurement noise

Here we see that if we added disturbance to the states it creates a dramatic change due to the system dynamics being chaotic.

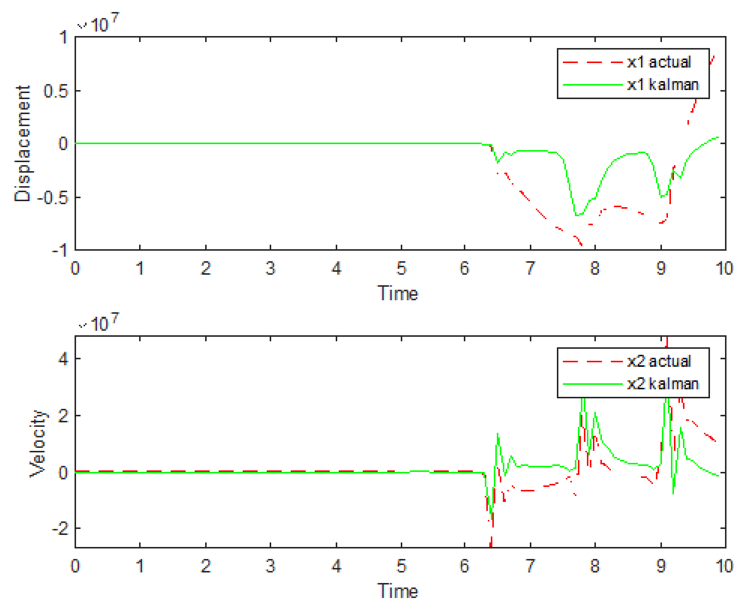

Figure 15: Kalman filter with system noise added to parameter a

VII Conclusion

I was able to control the AFM microscope to oscillate about the desired trajectory and surface using the LQG control. It is shown that this dynamic system is very unstable due to the values of frequency or parameter changes. The limitations of this paper is that there are other possible control algorithms used that make use of the nonlinear systems instead of linearizing them, but it was shown that the system is controllable and observable as non linear systems. I would like to change different parameters or initial conditions to further explore what is the limit of the LQG control.

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