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Topography and Force Estimation in Atomic Force Microscopy by State and Parameter Estimation

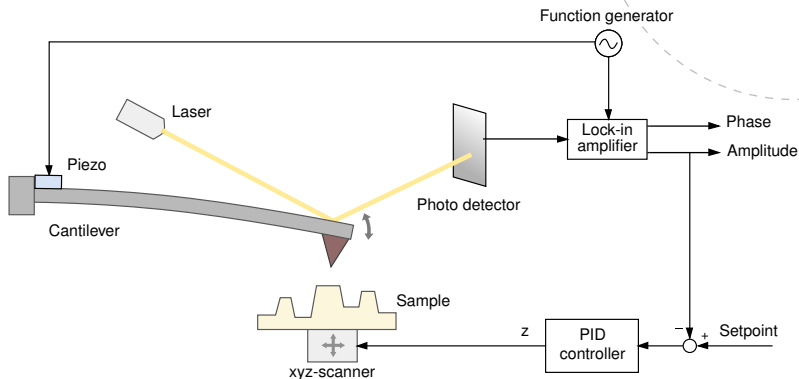
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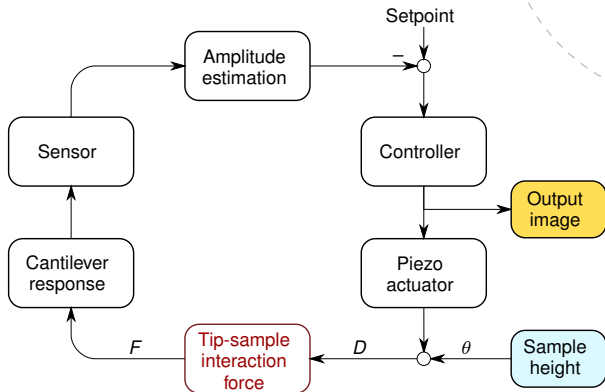
ACC Chicago, July 1–3, 2015

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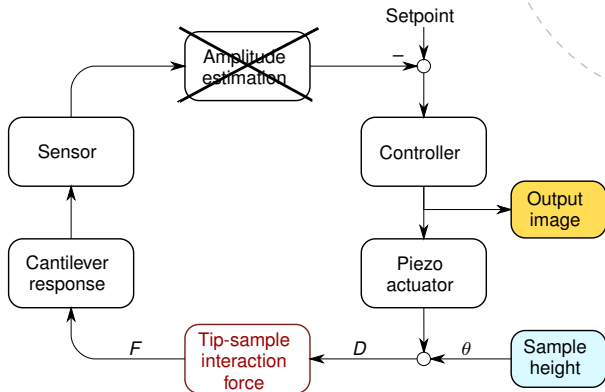
Introduction – AFM AM Loop



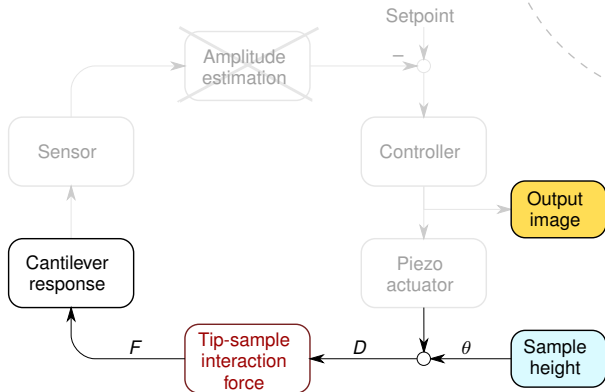
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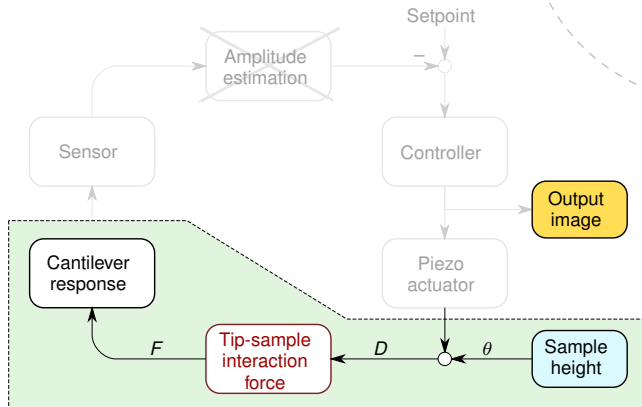
Introduction – AFM AM Loop



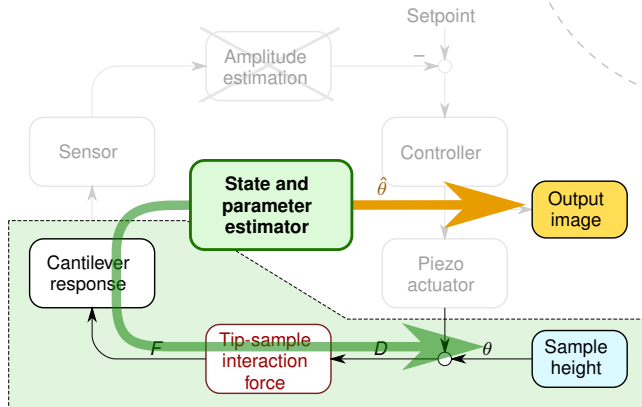
Introduction – AFM AM Loop



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Introduction – AFM AM Loop



Introduction

- We will employ observers to directly estimate the topography
 - By considering the cantilever dynamics and interaction force
- Two observers were designed for the same purpose:
 - A nonlinear observer with well-defined exponential stability results.
 - An extended Kalman Filter for comparison.

Outline

Introduction

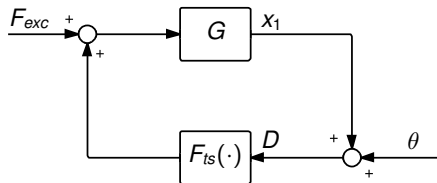
System Modeling

Observer Design

Simulation Results

Conclusion and Further Work

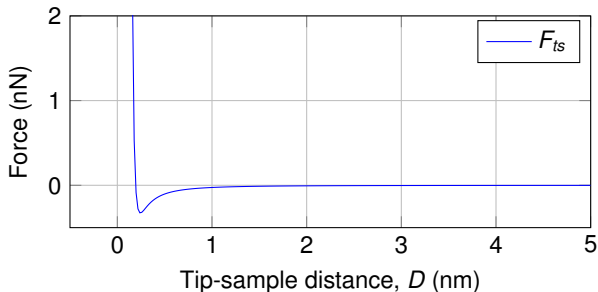
System Modeling



- G : Cantilever model from applied force, to tip deflection.
 - Second order harmonic oscillator.
- F_{ts} : Tip-sample interaction force: Modeled by Lennard-Jones potential.

System Modeling – Lennard-Jones potential

$$F_{ts}(D) = k_1 \left[\frac{\sigma^2}{D^2} - \frac{1}{30} \frac{\sigma^8}{D^8} \right] \quad (1)$$



System Modeling – State-space form

System can be expressed as an extended state-space model suitable for the state- and parameter estimator.

$$\begin{bmatrix} \dot{x} \\ \dot{\phi} \end{bmatrix} = \begin{bmatrix} A & E \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ \phi \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix} u + \begin{bmatrix} 0 \\ 1 \end{bmatrix} d \quad (2)$$

$$A = \begin{bmatrix} 0 & 1 \\ -\omega_0^2 & -2\zeta\omega_0 \end{bmatrix}, B = E = \begin{bmatrix} 0 \\ 1 \\ m \end{bmatrix}, C = [1 \ 0] \quad (3)$$

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where

- the state $x \triangleq (x_1, x_2)^T$ represent the cantilever deflection and the deflection velocity
- the Lennard-Jones force F_{ls} has been introduced as a state ϕ
- d is the time-derivative of ϕ
- and the input u is the driving force of the cantilever.

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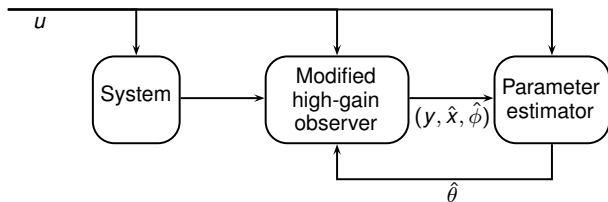
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Nonlinear Observer

Based on Håvard F. Grip's article: *"Estimation of States and Parameters for linear systems with nonlinearly parameterized perturbations"* (2011).



Structure of the state- and parameter estimator. From (Grip et al., 2011).

Nonlinear Observer – Modified High-Gain Observer

Observes the state $(\hat{x}, \hat{\phi})$ as if the parameter estimate $\hat{\theta}$ is perfectly known.

$$\begin{aligned}\dot{\hat{x}} &= A\hat{x} + Bu + E\hat{\phi} + K_x(\varepsilon)(y - C\hat{x}) \\ \dot{z} &= -\frac{\partial g}{\partial \theta}\hat{\theta} - \frac{\partial g}{\partial x}K_x(\varepsilon)(y - C\hat{x}) + K_\phi(\varepsilon)(y - C\hat{x}) \\ \hat{\phi} &= g(\hat{x}_1, \hat{\theta}) + z\end{aligned}\tag{4}$$

- Need to determine $K_x(\varepsilon)$, $K_\phi(\varepsilon)$ such that the error dynamics of the observer are input-to-state stable.

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Result

$$K_x(\varepsilon) = \begin{bmatrix} 4.0\varepsilon^{-1} \\ 5.04\varepsilon^{-2} \end{bmatrix} \quad (5)$$

$$K_\phi(\varepsilon) = 4.0\omega_0^2\varepsilon^{-1} + 10.08\zeta\omega_0\varepsilon^{-2} + 2.08\varepsilon^{-3} \quad (6)$$

Nonlinear Observer – Parameter Estimator

Need to find an update law

$$\dot{\hat{\theta}} = u_{\theta}(\nu, \hat{x}, \hat{\phi}, \hat{\theta}) \quad (7)$$

such that the origin of the error dynamics

$$\dot{\tilde{\theta}} = -u_{\theta}(\nu, \hat{x}, \hat{\phi}, \theta - \tilde{\theta}) \quad (8)$$

is uniformly exponentially stable whenever $\hat{x} = x$ and $\hat{\phi} = \phi$.

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Assumption 6

There exist a differentiable function $V_u : \mathbb{R}_{\geq 0} \times (\Theta - \Theta) \rightarrow \mathbb{R}_{\geq 0}$ and positive constants a_1, \dots, a_4 such that for all $(t, \tilde{\theta}) \in \mathbb{R}_{\geq 0} \times (\Theta - \Theta)$,

$$\begin{aligned} a_1 \|\tilde{\theta}\|^2 &\leq V_u(t, \tilde{\theta}) \leq a_2 \|\tilde{\theta}\|^2 \\ \frac{\partial V_u}{\partial t}(t, \tilde{\theta}) - \frac{\partial V_u}{\partial \tilde{\theta}}(t, \tilde{\theta}) u_{\theta}(\nu, x, \phi, \theta - \tilde{\theta}) &\leq -a_3 \|\tilde{\theta}\| \\ \left\| \frac{\partial V_u}{\partial \tilde{\theta}}(t, \tilde{\theta}) \right\| &\leq a_4 \|\tilde{\theta}\| \end{aligned}$$

Furthermore, the update law (7) ensures that if $\hat{\theta}(0) \in \Theta$, then for all $t \geq 0$, $\hat{\theta} \in \Theta$.

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is uniformly exponentially stable whenever $\hat{x} = x$ and $\hat{\phi} = \phi$.

Assumption 6 satisfied by the following update law:

$$u_{\theta}(\nu, \hat{x}, \hat{\phi}, \hat{\theta}) = \text{Proj} \left(\Gamma M(\nu, \hat{x}, \hat{\theta})(\hat{\phi} - g(\nu, \hat{x}, \hat{\theta})) \right) \quad (9)$$

$$M = \frac{1}{2} M_{\max} \left[\tanh(M_{\text{rate}}(\hat{D} - D_M)) + 1 \right] \quad (10)$$

Nonlinear Observer – Assumptions

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- Bounded topography, well defined input signal and time-derivative
- Operation in noncontact mode – allows the force profile to be represented by a monotonic function
- Known Lennard-Jones parameters
 - Parameters appear linearly in Lennard-Jones function \Rightarrow Method can easily be extended to simultaneously determine these.

Nonlinear Observer – Stability Theorem

Theorem 1 (Abbreviated)

If all assumptions are satisfied and $\hat{\theta}(0) \in \Theta$, there exists $0 < \varepsilon^* \leq 1$ such that for all $0 < \varepsilon \leq \varepsilon^*$, the origin of the error dynamics of the observer and parameter estimator is exponentially stable.

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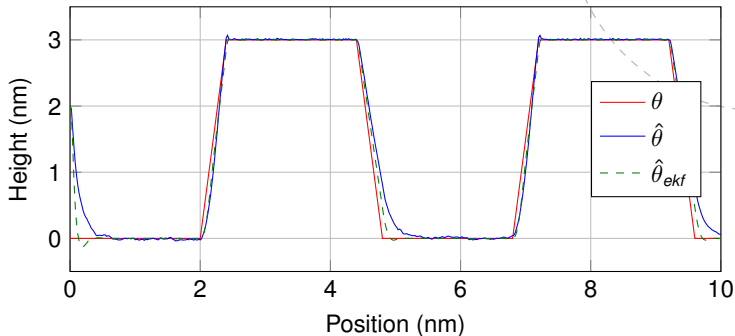
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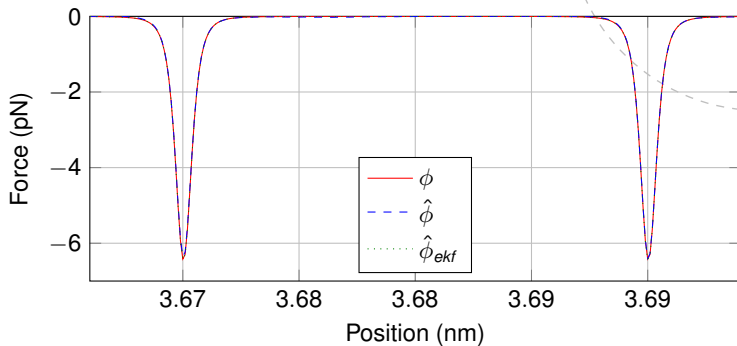
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Simulation Results



Topography estimate with output noise.

Simulation Results



Estimated interaction force ϕ with noise.

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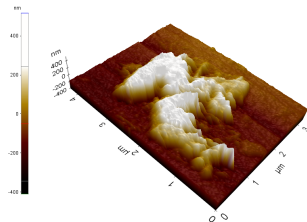
Conclusion and Further Work

Conclusion

- New dynamic mode imaging method.
- Cantilever dynamics and interaction force "inverted" to estimate topography.
- Avoids bandwidth-limiting amplitude estimation.
- Exponentially stable observer.

Further Work

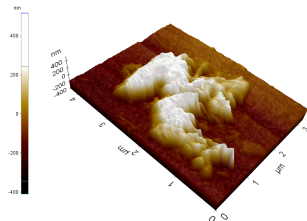
- Experimental results.
- Include estimation of Lennard-Jones parameters.
- Use observer in feedback loop for control.
- Proper analysis of closed-loop bandwidth.



Further Work

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Questions?



References

- Håvard Fjær Grip, Ali Saberi, and Tor A Johansen. Estimation of states and parameters for linear systems with nonlinearly parameterized perturbations. *Systems & Control Letters*, 60(9):771–777, 2011.
- Michael R P Ragazzon, J Tommy Gravdahl, Kristin Y Pettersen, and Arnfinn A Eielsen. Topography and Force Imaging in Atomic Force Microscopy by State and Parameter Estimation. In *American Control Conference, 2015*, 2015.