Mechanisms & Control of Friction at the Atomic Scale

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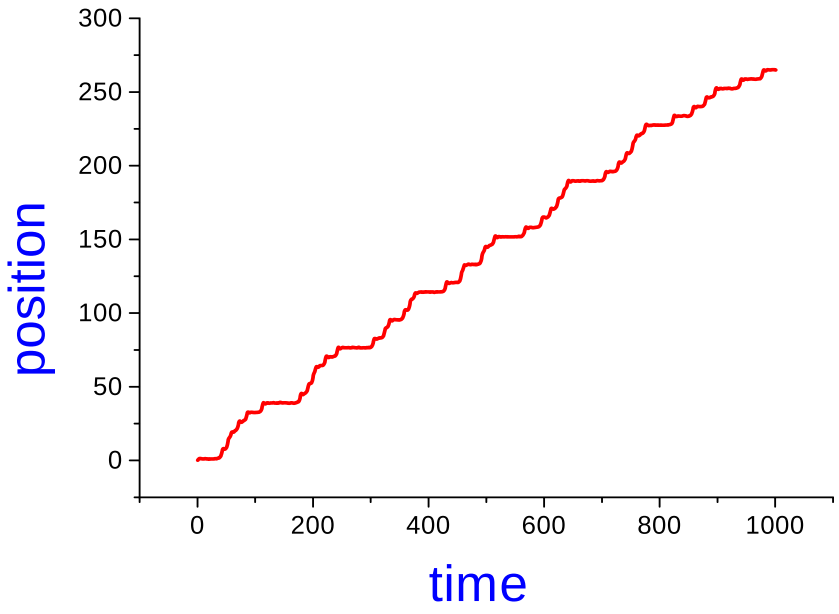
Content

- Introduction
- Friction Models
- Dynamics of Atomic Chains
- Effects of Disorder
- Friction Control – Terminal Attractors
- Effects of Surface Oscillations on Friction
- Summary

Stick-Slip Dynamics

- Has been observed from the nano - to macro scales - from the atomic scale to earthquakes.

Both periodic and chaotic stick-slip dynamics have been observed



Friction Models

$$m\ddot{x}_n + \gamma \dot{x}_n = -\partial U / \partial x_n - \partial V / \partial x_n + f_n + \eta_n$$

$$m\ddot{x} = -k(x - vt) - F_0$$

$$F_0 = \theta + \beta x$$

$$\dot{\theta} = (\theta - \theta_{\min})(\theta_{\max} - \theta)/\tau - \alpha(\theta - \theta_{\min})\dot{x}$$

Carlson and Batista, PRE **53**, 4153 (1996)

$$m\ddot{x} = k(vt - x) - F_0$$

$$F_0 = F_b + \Delta F_0(1 - \exp(-\phi/\tau)) + \gamma\dot{x}$$

$$\dot{\phi} = 1 - \dot{x}\phi/D$$

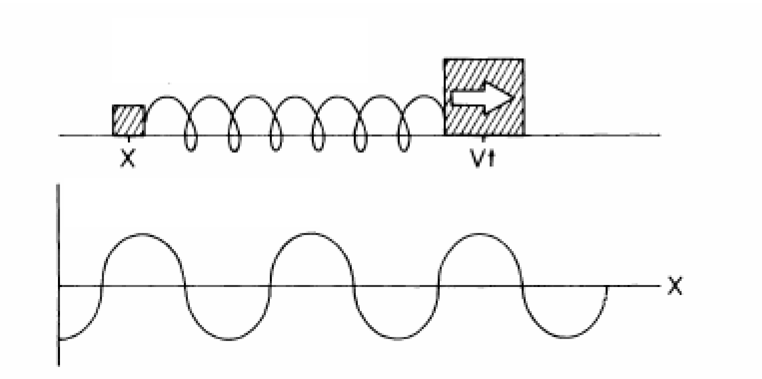
Persson, PRB **55**, 8004 (1997)

Friction is ruled by robust dynamics

Good qualitative agreement between variety of models and types of interaction potentials used for a model choice of parameters may be even more important than the choice of a model !!!

Initial conditions !

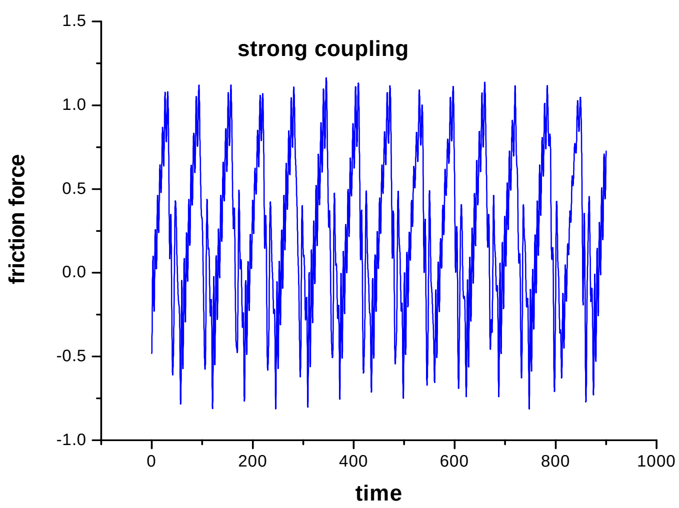
Modeling the AFM Motion

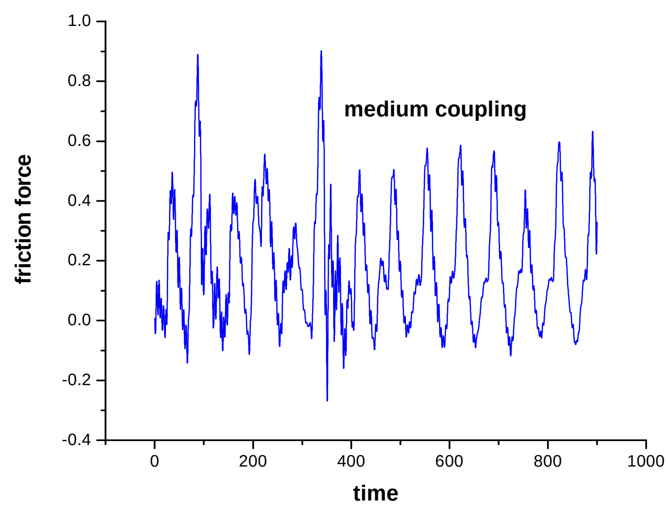


$$\ddot{x} + \gamma \dot{x} + \sin x = K(vt - x)$$

J. S. Helman, W. Baltensperger, and J. A. Holst, Phys. Rev. B 49, 3831 (1994)

$$\ddot{x}_n + \gamma \dot{x}_n + \sin x_n = K(vt - x_{cm}) + F_{\text{int}}(x_{n+1}, x_n) + F_{\text{int}}(x_{n-1}, x_n)$$

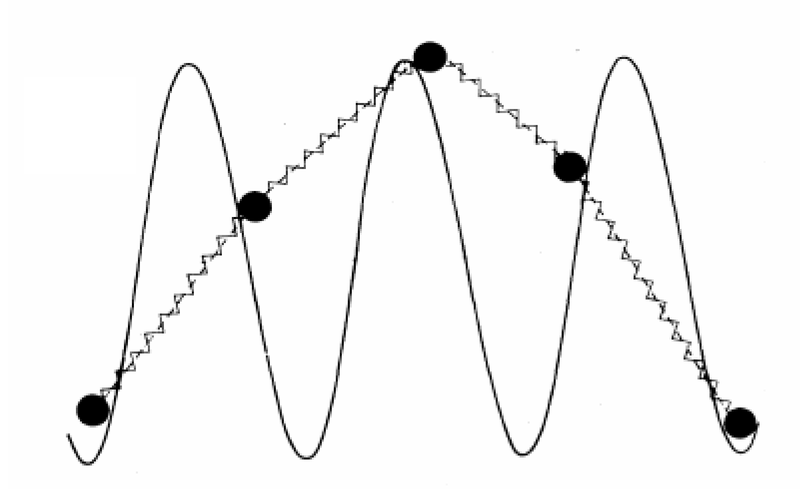




Frenkel-Kontorova Model - QCM Experiment

$$m\ddot{x}_n + \gamma \dot{x}_n = -\partial U / \partial x_n - \partial V / \partial x_n + f_n + F_n$$

m - the mass of the sliding particle
γ - the dissipation coefficient
U - the interaction potential between the particles
V - the surface potential (surface – particle interaction)
f - the external driving force
F - the thermal noise

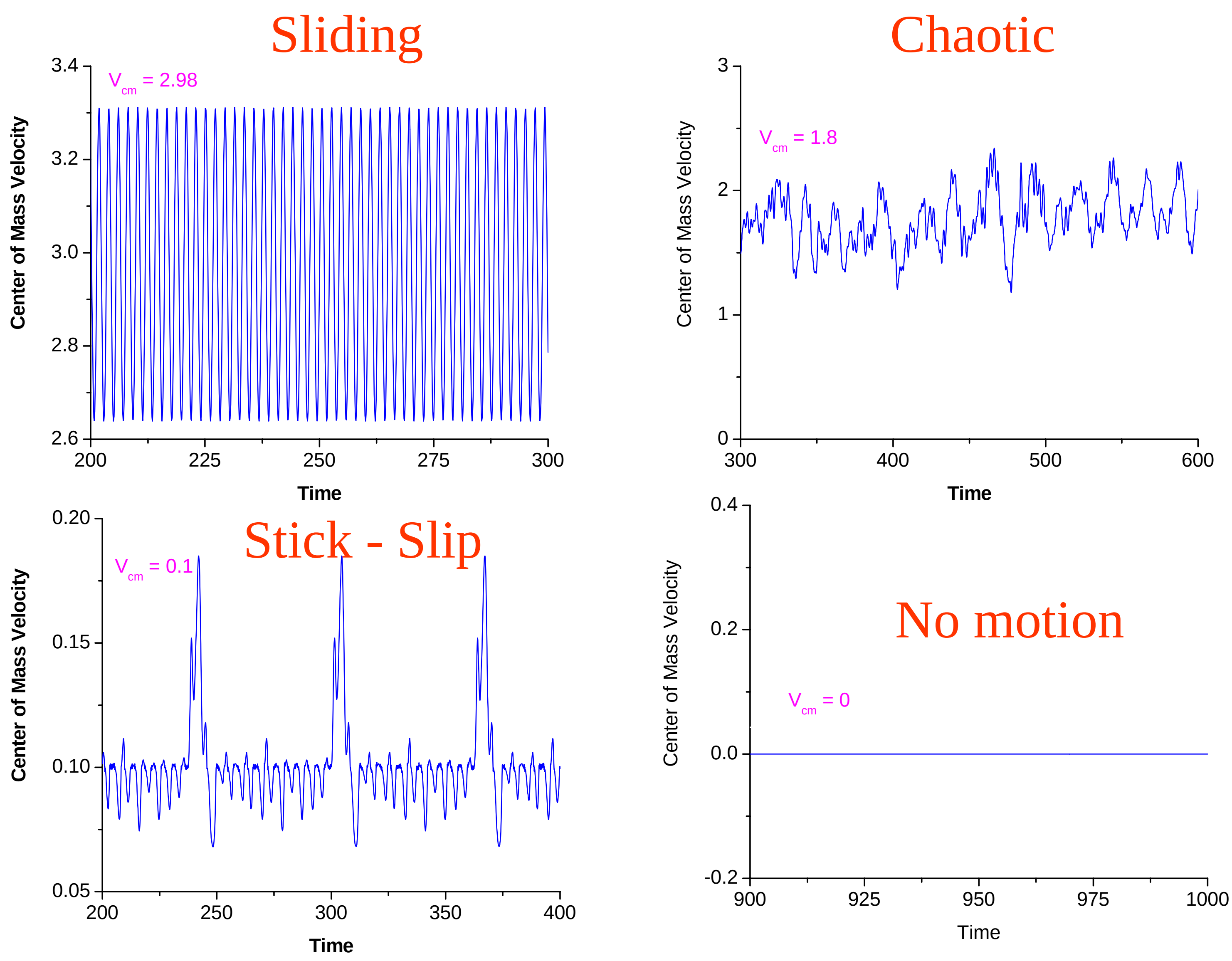


$$< F(t)F(t') >= 2\gamma k T \delta(t - t')$$

Dimensionless units, sinusoidal potential, F=0

$$\ddot{x}_n + \gamma x_n + \sin x_n = f + \kappa(x_{n+1} - 2x_n + x_{n-1})$$

$\kappa \propto$ inter-atomic interaction/atom-substrate interaction potentials



Sliding
Center of Mass Velocity
V_{cm} = 2.98
3.4
3.2
3.0
2.8
2.6
200
225
250
275
300
Time
Chaotic
Center of Mass Velocity
V_{cm} = 1.8
3
2
1
0
300
400
500
600
Time
Stick - Slip
Center of Mass Velocity
V_{cm} = 0.1
0.20
0.15
0.10
0.05
200
250
300
350
400
Time
No motion
Center of Mass Velocity
V_{cm} = 0
0.4
0.2
0.0
-0.2
900
925
950
975
1000
Time

Values of the Sliding Velocities for Small Forcing

Only particular values of velocities
of the "uncontrolled motion" can be observed:

$v = f/\gamma$ - free sliding

$v = v_{chaotic} = 1.8$ (just a single value
for given parameter set)

$v = kv_0$ here $$v_0 = \frac{2\pi}{mN\gamma}\left(\frac{\pi - \cos^{-1} f}{\pi}\right)^{1/2}(\kappa - \kappa_c)^{1/2}$$

N is the number of particles
and k is an integer

Y. Braiman, F. Family, and H. G. E. Hentschel, Phys. Rev. E 53, R3005 (1996)

Dynamics of Propagating Arrays

We separate the center of mass motion of array from spatiotemporalfluctuations (which only dissipate energy)

$$x_n(t) = x(t) + \delta x_n(t)$$

where $< \delta x_n(t) > = 0$ by construction

Keeping fluctuations small, the center of mass obeys

$$\ddot{x} + \gamma \dot{x} + \sin(x)[1 - < \delta x_n^2 > / 2] = f$$

The spatiotemporal fluctuations obey

$$\delta \ddot{x}_n + \gamma \; \delta \dot{x}_n + C \cos(x) \; \delta x_n = \kappa(\; \delta x_{n+1} - 2 \; \delta x_n + \; \delta x_{n-1})$$

Resonant Parametric Forcing

We make the Fourier decomposition

$$\delta x_n(t) = \sum_m \delta x_m(t) e^{2\pi i m n / N}$$

and equations of motion for the modes

$$\delta \ddot{x}_m + \gamma \; \delta \dot{x}_m + [\Omega_m^2 + C \cos(x)] \delta x_m = 0$$

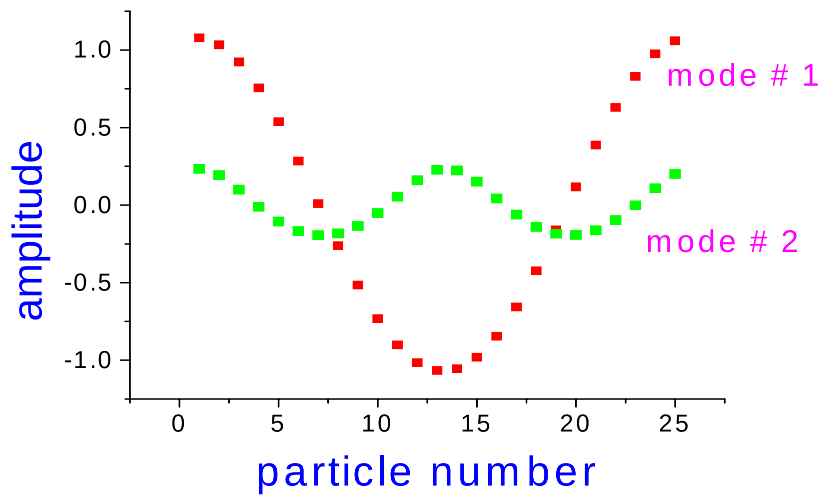
where $$\Omega_m = 2\sqrt{\kappa} \sin(\pi m / N)$$

Shows parametric forcing when $\Omega_m = \omega / 2$

Spatial Coherence and Mode Selection

If we look for a solution for the ***m***'th mode of the form

$$\delta x_m = b_m \sin(\omega t / 2 + \beta_m)$$



we then find:

Only one mode can exist at a time.

There are N such solutions. Each is spatially coherent with a different center of mass velocity and different amplitude fluctuations.

As the spatial fluctuations b_m increase, phase synchronization decreases, and so the average center of mass velocity decreases.

Velocity of the Center of Mass

If we look for a solution for the ***m***'th mode of the form

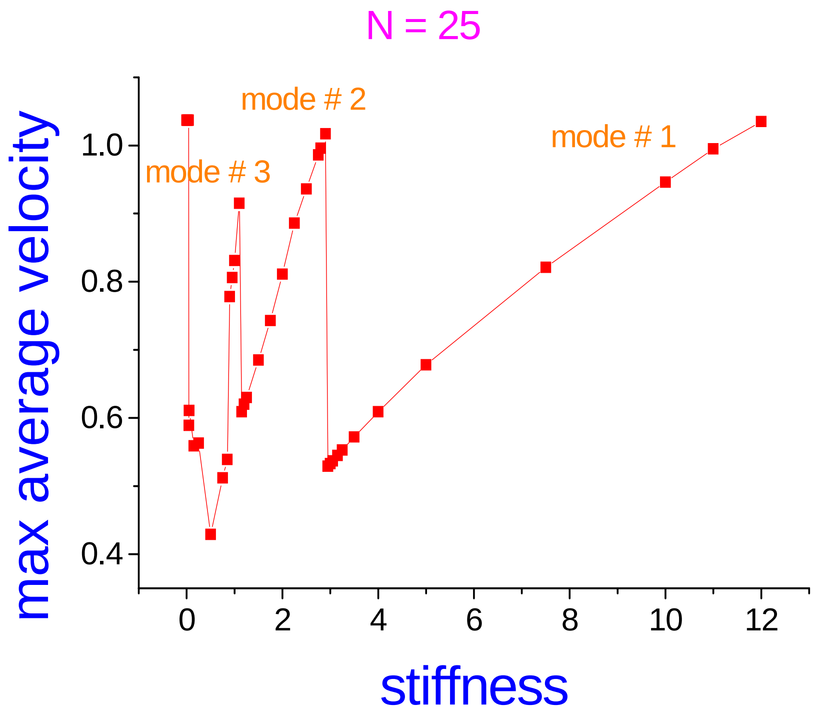
$$\delta x_m = b_m \sin(\omega t / 2 + \beta_m)$$

and the center of mass motion is described by

$$x = x_0 + \omega t + B \sin(\omega t)$$

then the velocity of the center of mass is

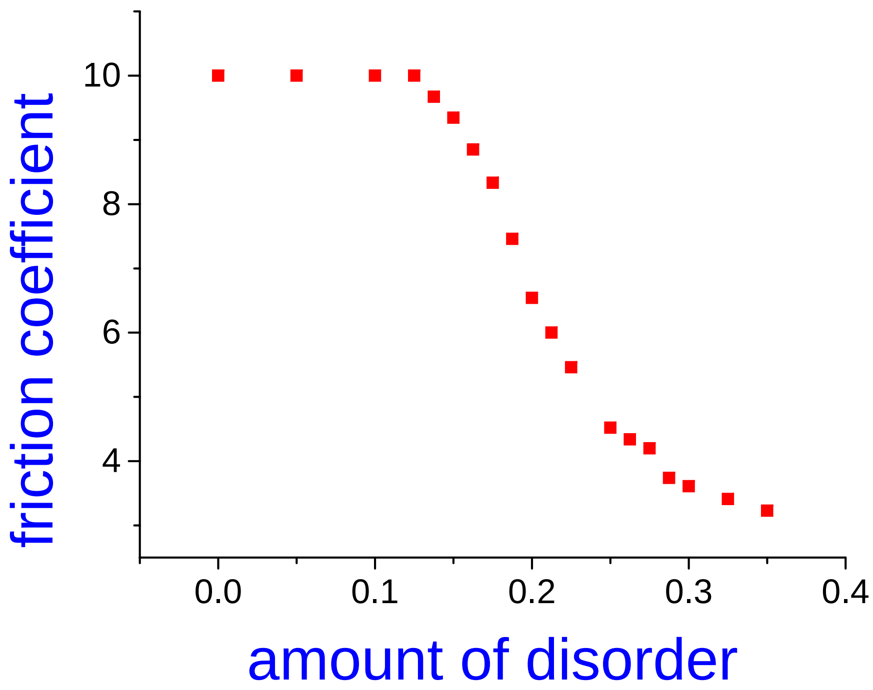
$$v_m = (f / \gamma)/[(1 + B^2/2) + b_m^2/8]$$



H. G. E. Hentschel, F. Family, and Y. Braiman, PRL 83, 104 (1999)

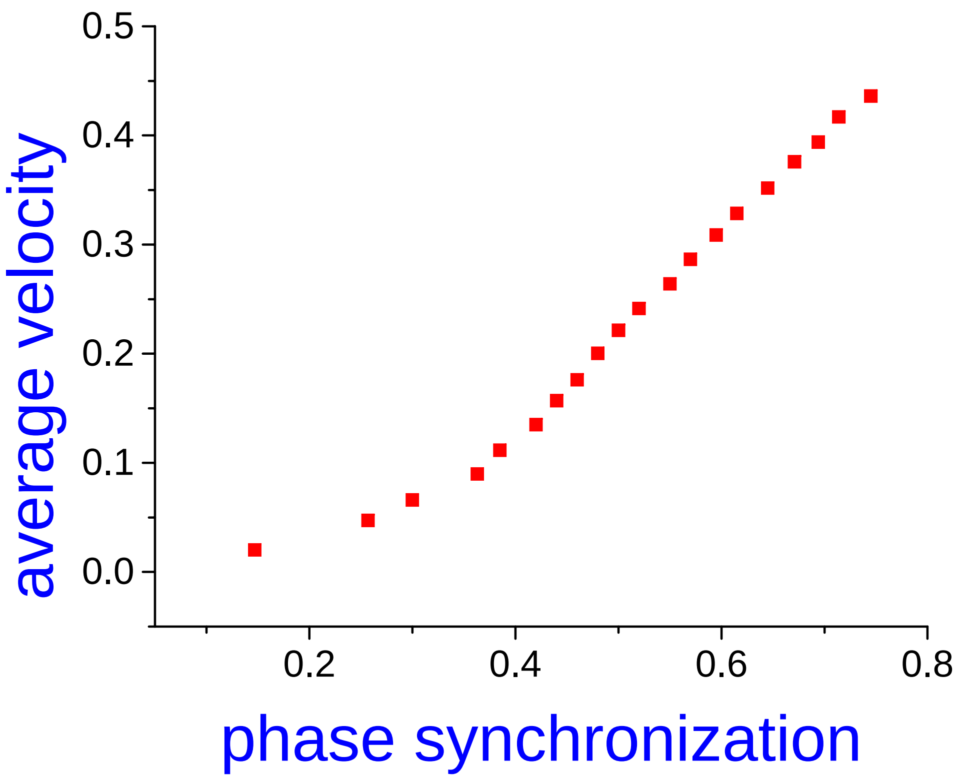
Sliding on Disordered Substrate

Friction coefficient can be significantly reduced
(by orders of magnitude) when sliding on irregular surfaces



Y. Braiman, F. Family, H. G. E. Hentschel,
C. Mak, and J. Krim, PRE 59, R4737 (1999)

Key Issue ⇒ Phase Synchronization

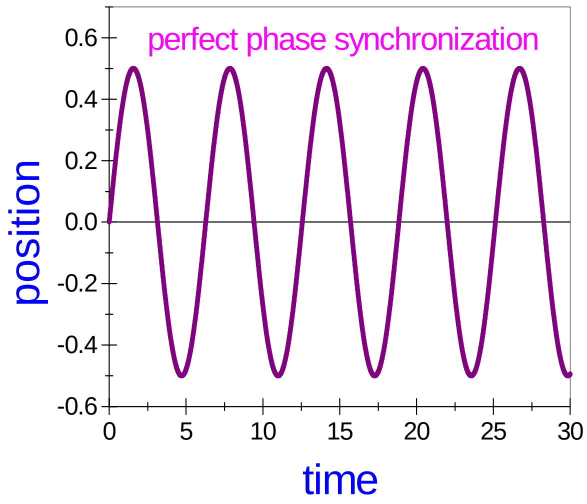


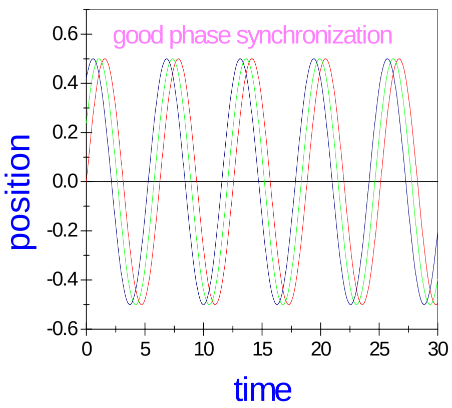
The better the array is phase synchronized - the faster it moves !

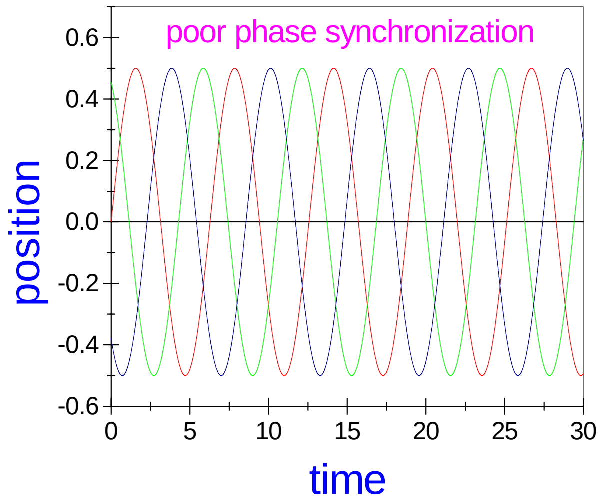
Phase Synchronization

We define phase synchronization as the inverse of the fluctuations σ from the center of mass motion

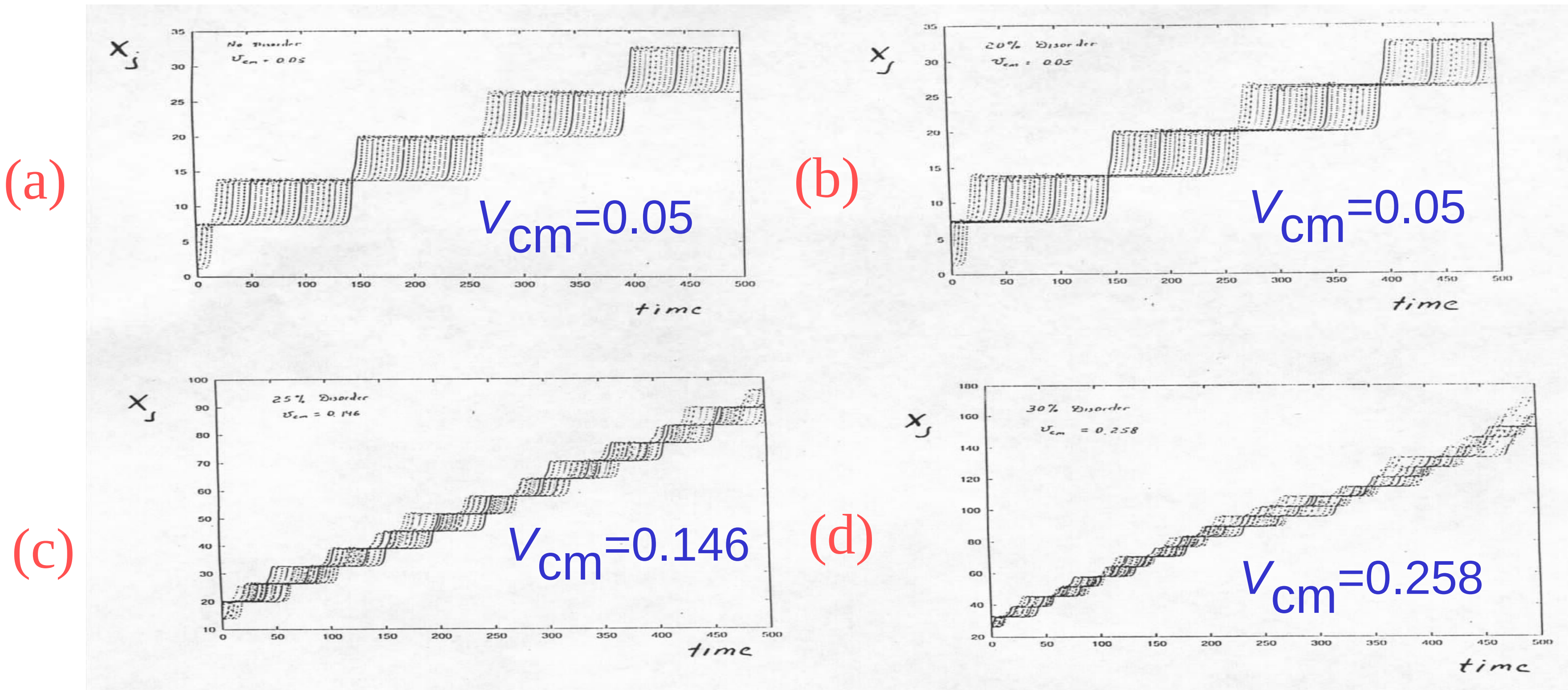
$$\sigma = \lim_{T\to\infty} \frac{1}{T}\int_0^T \frac{\sqrt{\sum_j^N (x_j - x_{av})^2}}{x_{av}}$$





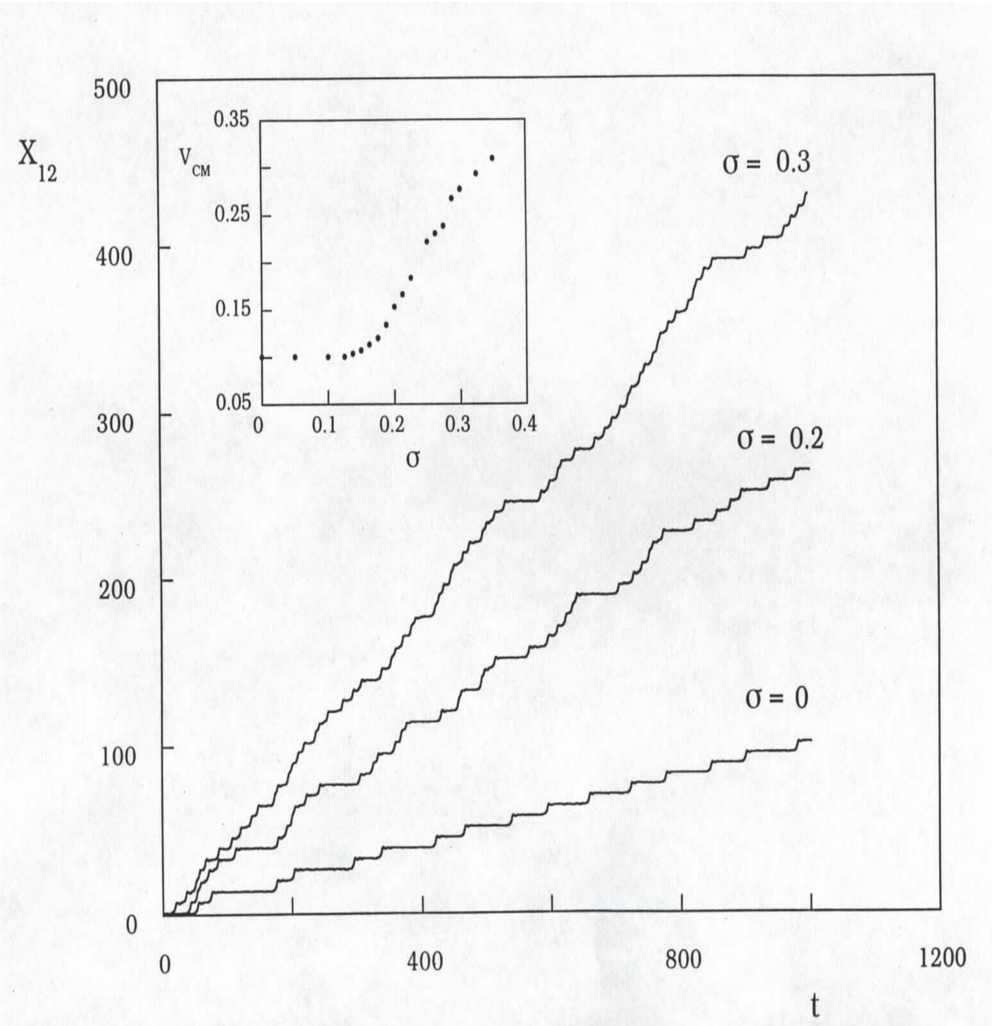


Disorder - Enhanced Synchronization



Time series of positions of all the particles in N=25 particle array for:
(a) the identical array; (b) 20% of disorder;
(c) 25 % of disorder; (d) 30 % of disorder

Sliding is Faster on Disordered Surfaces



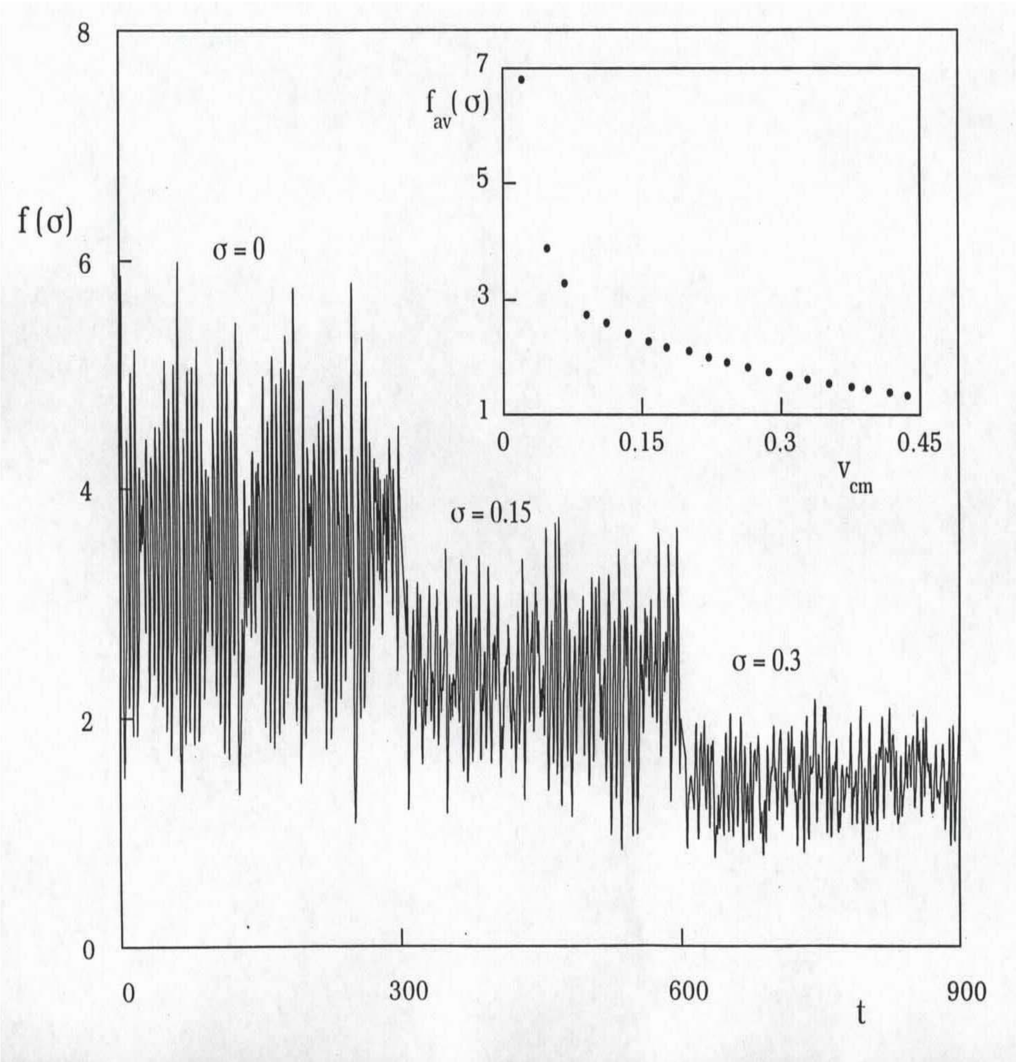
The position of a particle #12 in array as a function of time.

The bottom curve corresponds to the identical array.
The middle curve corresponds to to the arrays with 20% of disorder,
The top curve corresponds to the array with 30% of disorder.

The inset shows the average velocity of the center of mass as a function of the amount of disorder

Y. Braiman, F. Family, H. G. E. Hentschel, C. Mak, and J. Krim, PRE 59, R4737 (1999)

Sliding is Faster for a Better Synchronized Array

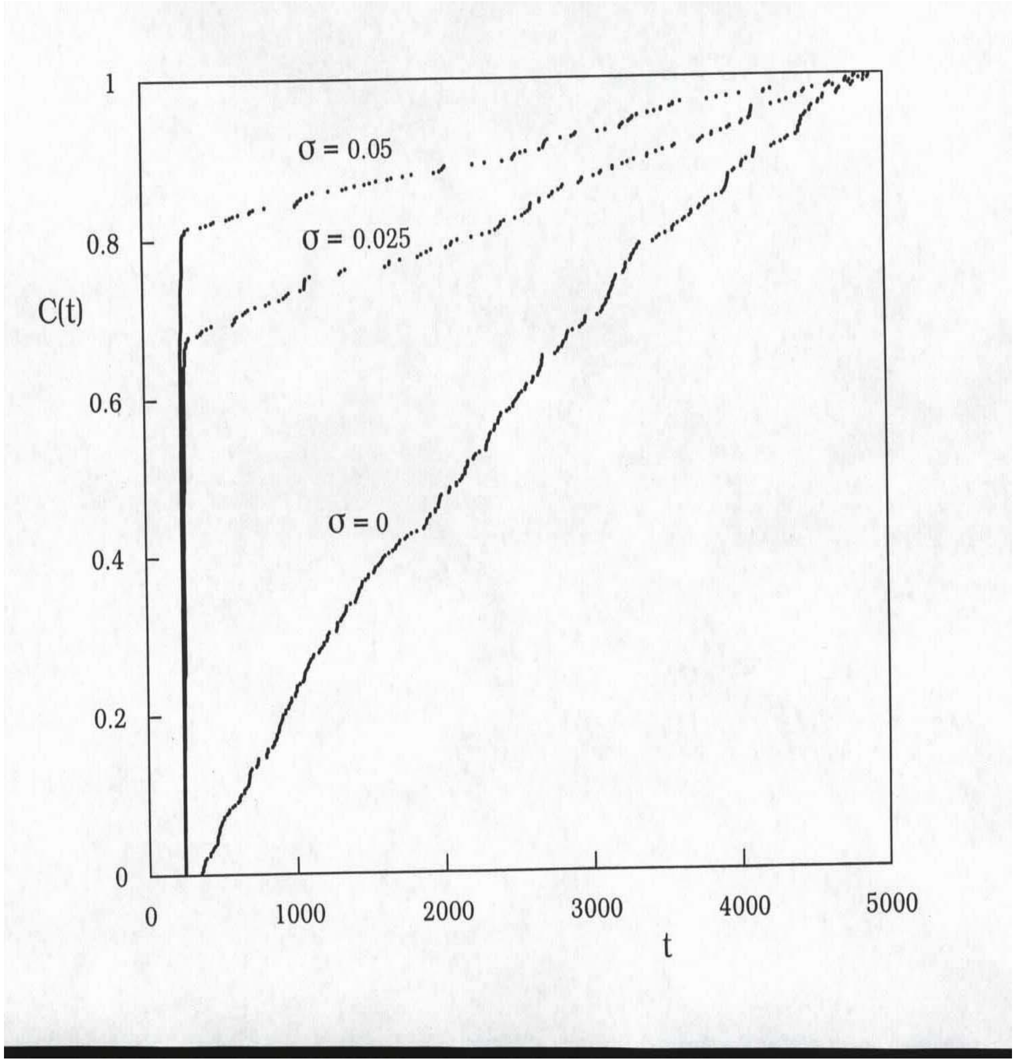


Time series of the fluctuations from the center of mass f(σ) for different amounts of disorder.

The left-hand part of the plot corresponds to the identical array.
The middle part corresponds to σ=15%.
The right-hand part corresponds to σ=30%.
The inset shows the average fluctuations from the center of mass as the function of the velocity of the center of mass.

Y. Braiman, F. Family, H. G. E. Hentschel, C. Mak, and J. Krim, PRE 59, R4737 (1999)

Disorder Induced Depinning



Cumulative slip time distribution for the array.

The bottom curve corresponds to the identical array.

The middle curve corresponds to σ = 2.5%.

The top curve corresponds to σ = 5%.

Y. Braiman, F. Family, H. G. E. Hentschel, C. Mak, and J. Krim, PRE 59, R4737 (1999)

Friction Control - Motivation

- Velocity/friction force control *during sliding*
- Ability to reach desired targeted behavior
- Achieve fast transient times
- The applied control is limited in strength
- Requires only limited accessibility
- Uses global variables

Friction can be manipulated by applying small perturbations to accessible elements and parameters of the sliding system.

- Using a surface force apparatus, modified for measuring friction forces while simultaneously inducing normal (out-of-plane) vibrations between two boundary-lubricated sliding surfaces, load- and frequency-dependent transitions between a number of "dynamical friction" states have been observed [1].
- Extensive grand-canonical molecular dynamics simulations [2] revealed the nature of the dynamical states of confined sheared molecular films, their structural mechanisms, and the molecular scale mechanisms underlying transitions between them.
- Methods to control friction in systems under shear that enable to eliminate chaotic stick-slip motion were proposed in [3]. Significant changes in frictional responses were observed in the two-plate model [4] by modulating the normal response to lateral motion [5].
- The surface roughness and the thermal noise are expected to play a significant role in deciding control strategies at the micro and the nano-scale [6].

1. M. Heuberger, C. Drummond, and J. Israelachvili, J. Phys. Chem. B 102, 5038 (1998).
2. J. P. Gao, W. D. Luedtke, and U. Landman, J. Phys. Chem. B, 102, 5033 (1998).
3. M. G. Rozman, M. Urbakh, and J. Klafter, Phys. Rev. E 57, 7340 (1998).
4. M. G. Rozman, M. Urbakh, and J. Klafter, Phys. Rev. Lett., 77, 683 (1996), and Phys. Rev. E 54, 6485 (1996).
5. V. Zaloj, M. Urbakh, and J. Klafter, Phys. Rev. Lett., 82, 4823 (1999).
6. Y. Braiman, F. Family, H. G. E. Hentschel, C. Mak, and J. Krim, Phys. Rev. E, 59, R4737 (1999).

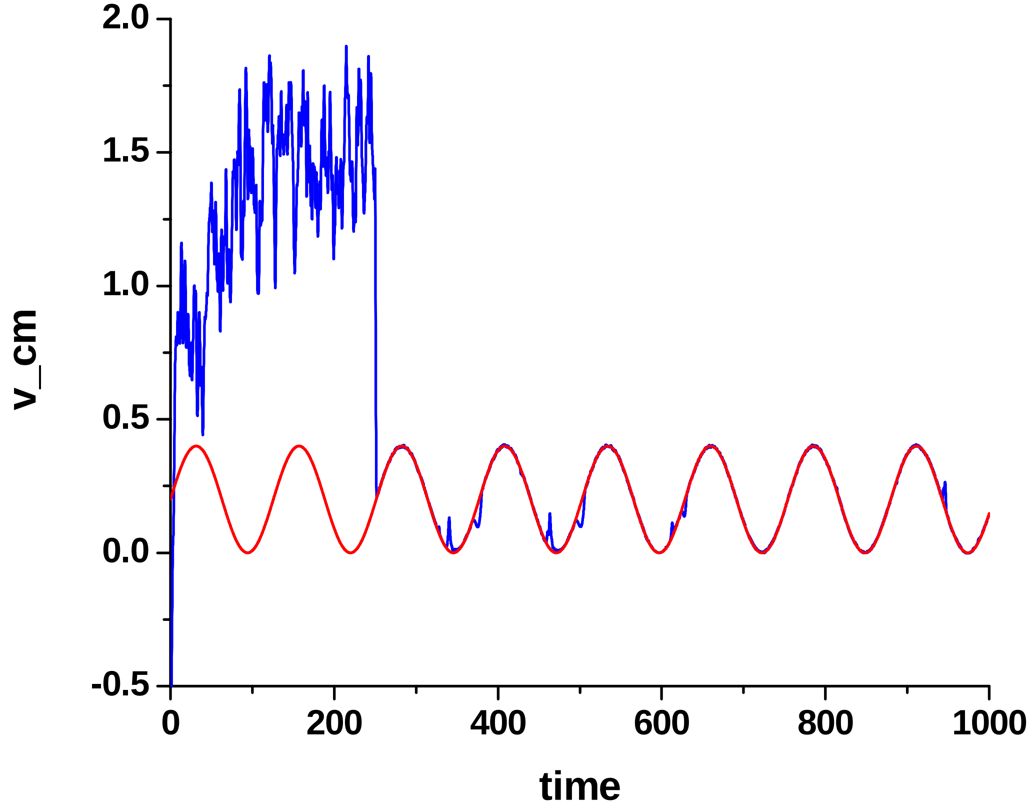
- **Experimentally, friction can be manipulated by applying in-plane and out-of-plane surface vibrations. This is realized, for example, by the use of a quartz piezo-element that oscillates the surface of frictional contact. The frequency of such an oscillation may vary from few Hz to MHz, and, perhaps to GHz limit using micro/nano cantilevers**

- **Our experiments demonstrate that already very slow (in the range of 100 Hz) vibrations can significantly alter the frictional behavior of the sliding system. This evidence strongly indicates the existence of a much slower time scale that governs the dynamics of the frictional system.**

- **From the algorithmic standpoint, friction can be controlled by applying small perturbations to accessible elements and parameters of the sliding system. Here, the challenge is to design control strategies that require only minimal accessibility.**

- **Both feedback and non-feedback means of control have been considered and speed, accessibility, and predictability considerations are those that prevail in choosing the optimal best strategy.**

Friction Control



Time series of the center of mass velocity (in dimensionless units). The red line shows the target velocity function, $v(t) = 0.2 + 0.2 \sin(0.05\ t)$, and the blue line shows the center of mass velocity. The control is applied every time step, starting at $t = 250$. The parameters are: $N = 15$, $\gamma = 0.1$, $f = 0.3$, $\kappa = 0.26$, $\alpha = 1$, $b = 0$, and $\zeta = 7$.

Non-Lipschitzian Dynamics

Lipschitz condition: **the derivatives of the right-hand side of the dynamical equations with respect to the state variables is bounded**

Consider: $\dot{\phi}(t) = -\phi^{1/7}$

At the equilibrium point, $\phi = 0$, ***Lipschitz condition is violated, since*** $\partial\dot{\phi} / \partial\phi = -(1/7)\phi^{-6/7}$ **tends to** $-\infty$ **as** ϕ **tends to zero.**

Thus the equilibrium point $\phi = 0$ **is an attractor with "infinite" attraction power (terminal attractor).**

Non-Lipschitzian Control of Friction for AFM and SFM-type experiments

Attractor: $C_1(t) = \alpha(f(t)_{target} - f_m)^\beta$

Repeller:

$$C_2(t) = \rho(f_{av} - f_m)^\beta \times \mathrm{sgn}[(f_{av} - f_m)(f_m - f(t)_{target})] \times H[r - |f(t)_{target} - f_{av}|]$$

$$H(z) = 1 \; for \;\; z > 0, \;\; \text{and} \;\; H(z) = 0 \; for \;\; z < 0$$

$\beta = 1/(2n+1), \; n = 1, 2, 3, \ldots$

Control: $C(t) = C_1(t) - C_2(t)$

Non-Lipschitzian Control of Friction for QCM-type of experiment

Attractor: $f_1(t) = \alpha(v(t)_{target} - v_{cm})^{\beta}$

Repeller:

$$f_2(t) = \rho(v_{av} - v_{cm})^{\beta} \times \mathrm{sgn}[(v_{av} - v_{cm})(v_{cm} - v_{target})] \times H[r - |v_{target} - v_{av}|]$$

$$H(z) = 1 \; for \; z > 0, \text{ and } H(z) = 0 \; for \; z < 0$$

$$\beta = 1/(2n+1), \; n = 1, 2, 3, \ldots$$

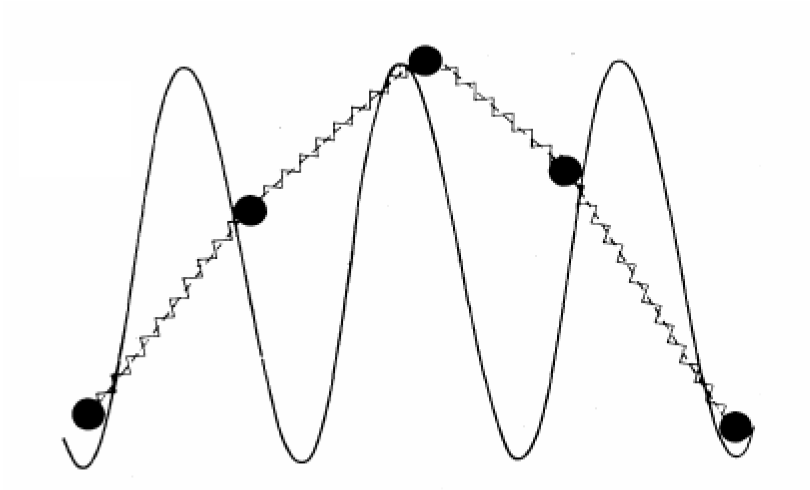
Control: $f_c(t) = f_1(t) - f_2(t)$

Y. Braiman, J. Barhen, & V. Protopopescu, Physical Review Letters 90, 094301 (2003).

Friction Control - a Model

$$m\ddot{x}_n + \gamma \dot{x}_n = -\partial U / \partial x_n - \partial V / \partial x_n + f_n + F_n + Control$$

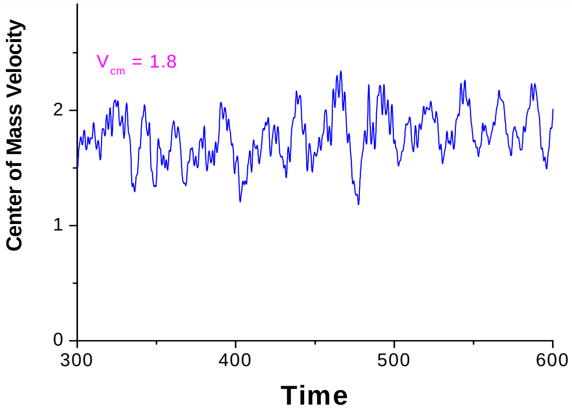
x_j is the position of the particle j
m is the mass of the sliding particle
γ is the dissipation coefficient
U is the interaction potential
V is the surface potential
f is the external driving force
η is the thermal noise (temperature effect)



Control:

$$C(t) = \alpha \left(v(t)_{target} - v_{cm} \right)^{\beta}$$

$$\beta = 1/(2n+1), \; n = 1, 2, 3, \ldots$$

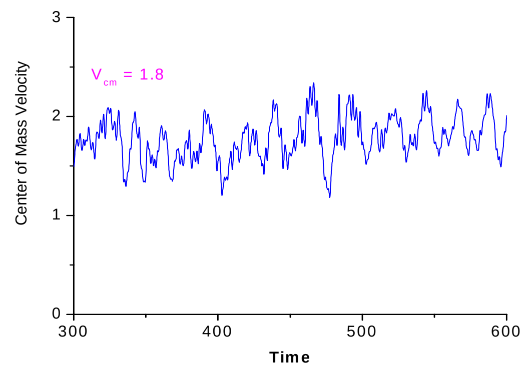


Y. Braiman, J. Barhen, & V. Protopopescu, Physical Review Letters 90, 094301 (2003).

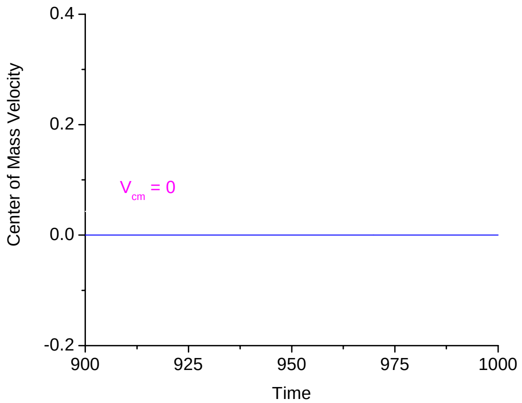
The Model

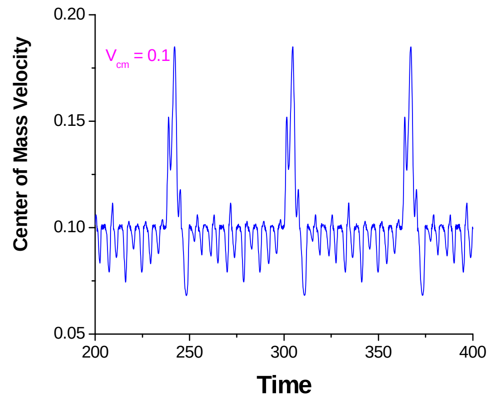
Driven Frenkel-Kontorova Model

$$\ddot{x}_n + \gamma \dot{x}_n + \sin x_n = f + \kappa (x_{n+1} - 2x_n + x_{n-1}) + Control$$



x_j - position of the particle j
γ - single particle dissipation
f - external forcing
κ - the ratio of the interparticle to substrate interactions





Demonstration of Friction Control

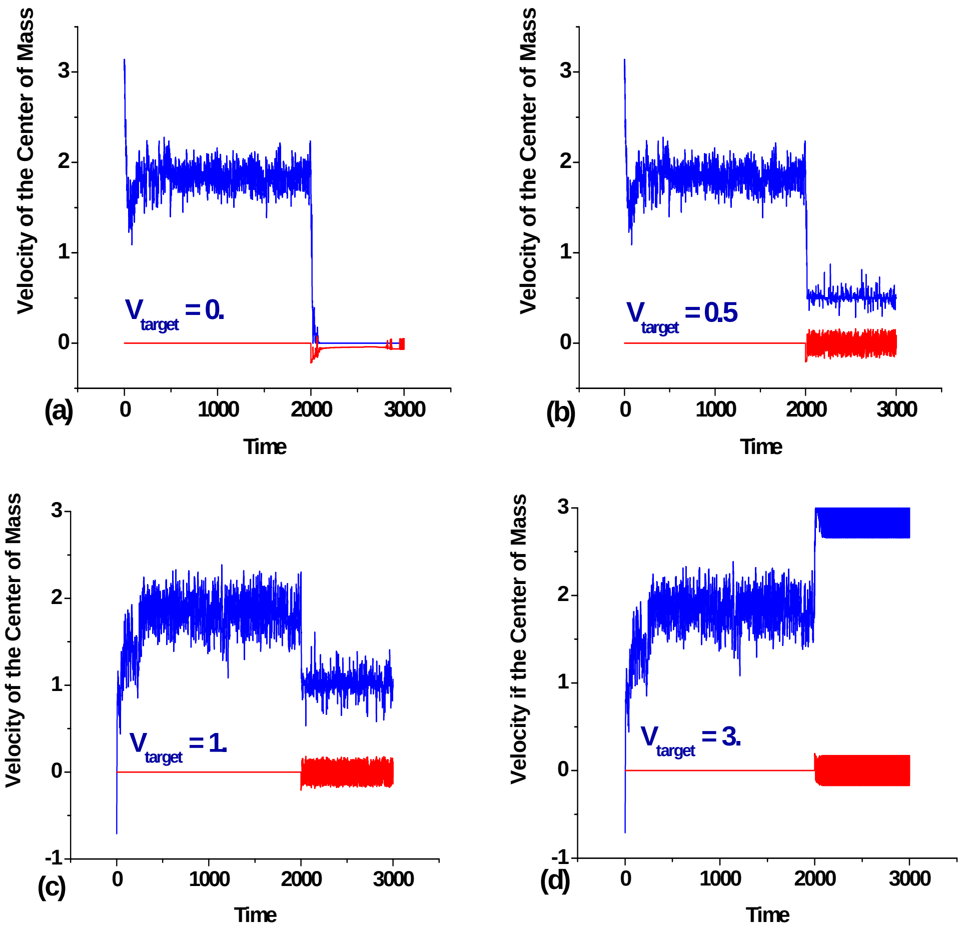


Figure: Performance of control algorithm for four values of the center of mass velocity (0, 0.5, 1.0, and 3.0) for a 15 - particle array. **Control was initiated at *t=2000***. Blue lines show time series of the center of mass velocities, while red lines show the control. In all cases, the desired behavior was rapidly achieved. All the units are dimensionless and initial conditions were chosen randomly.

1. New algorithm developed

- –fast and efficient
- –enables to induce any arbitrarily chosen behavior compatible with the system's dynamics.

2. Methodology is based on two original concepts:

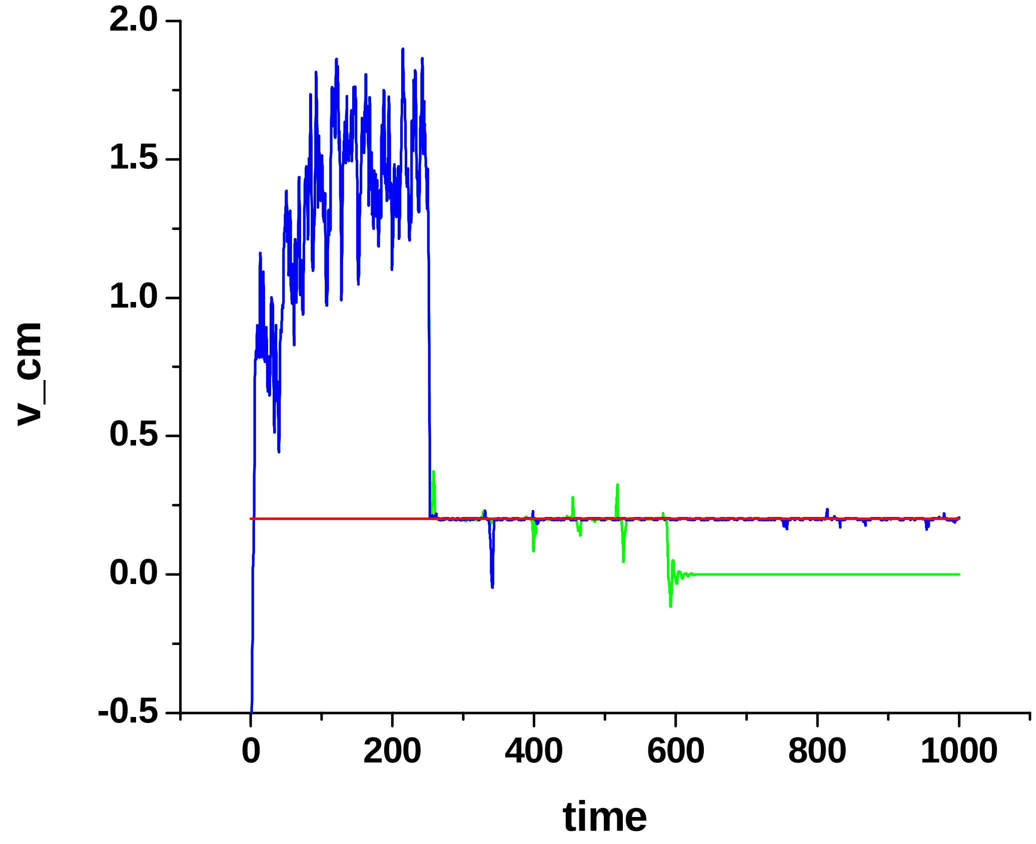
- – non-Lipschitzian dynamics
- – global behavior targeting

3. Quickly reaches targeted behavior.

Y. Braiman, J. Barhen, & V. Protopopescu,

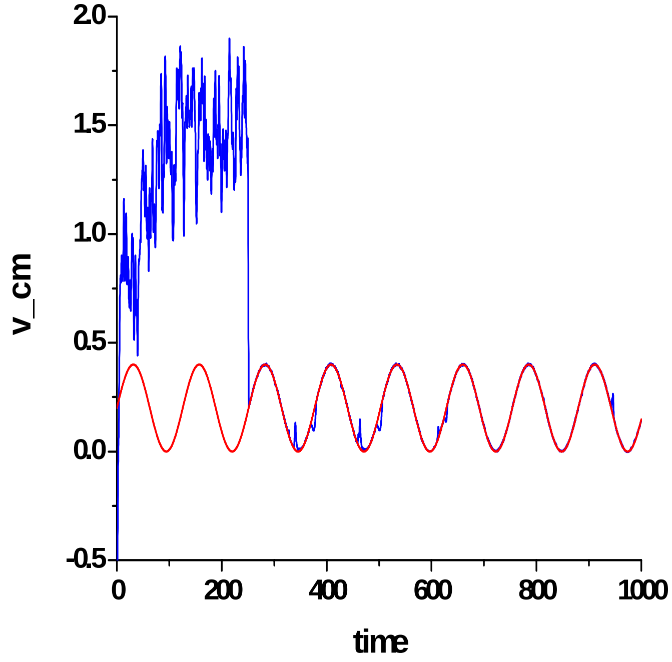
Physical Review Letters 90, 094301 (2003).

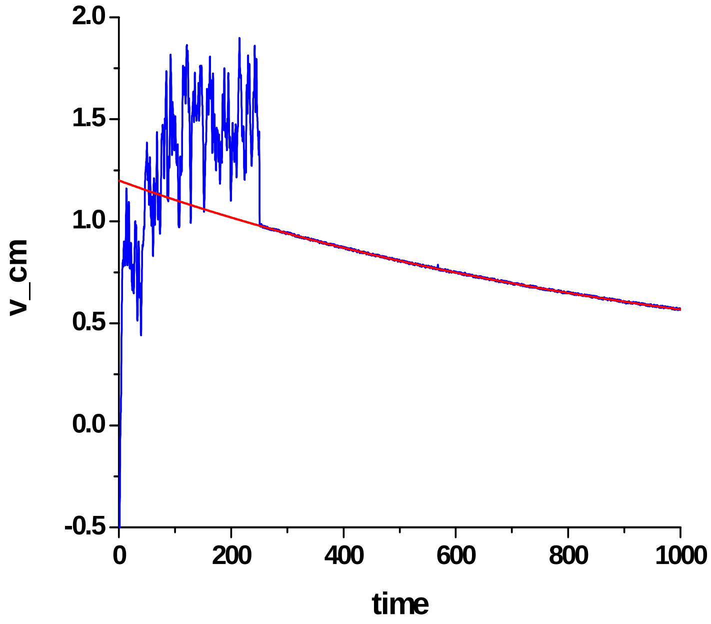
Effect of the Repeller



V. Protopopescu & J. Barhen, Chaos 14, 400 (2004).

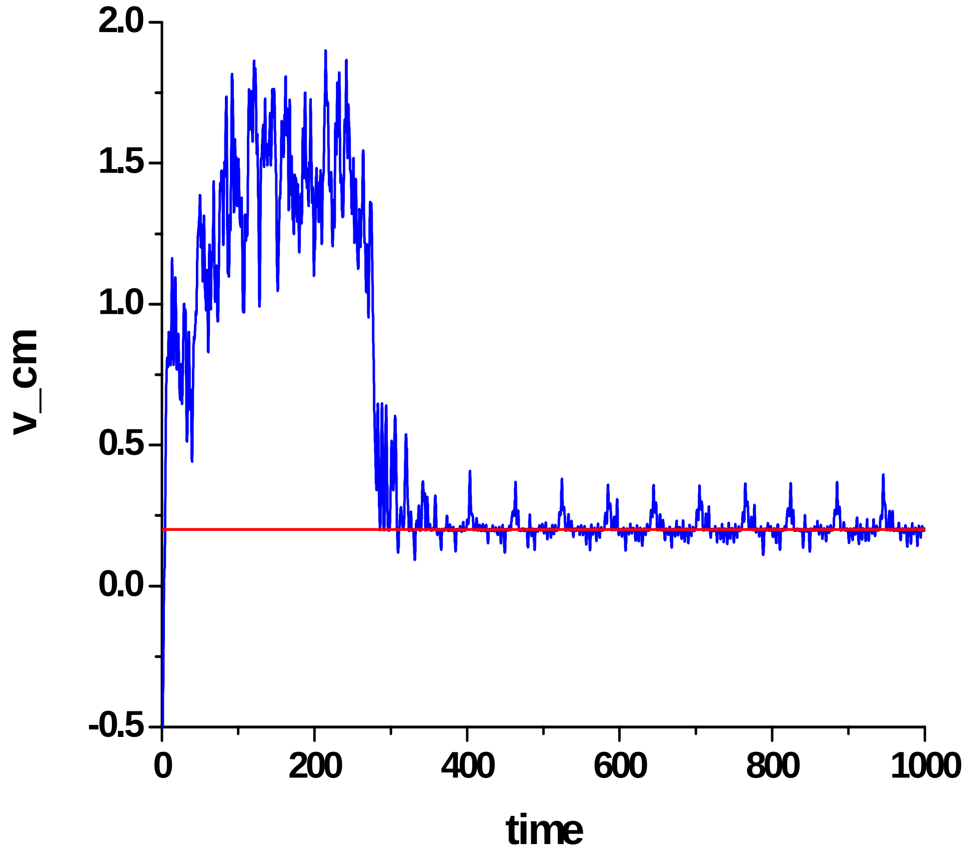
Control Towards Desired Functional Behavior



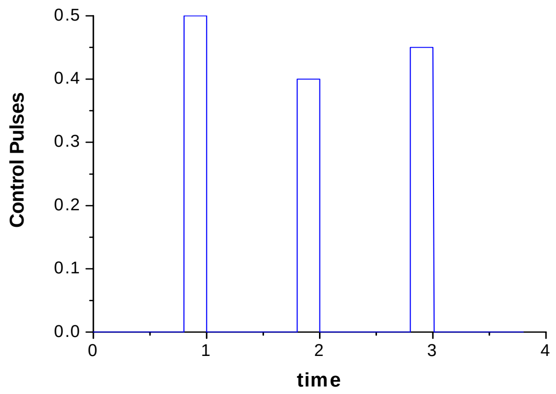


V. Protopopescu & J. Barhen, Chaos 14, 400 (2004).

Pulsed Control

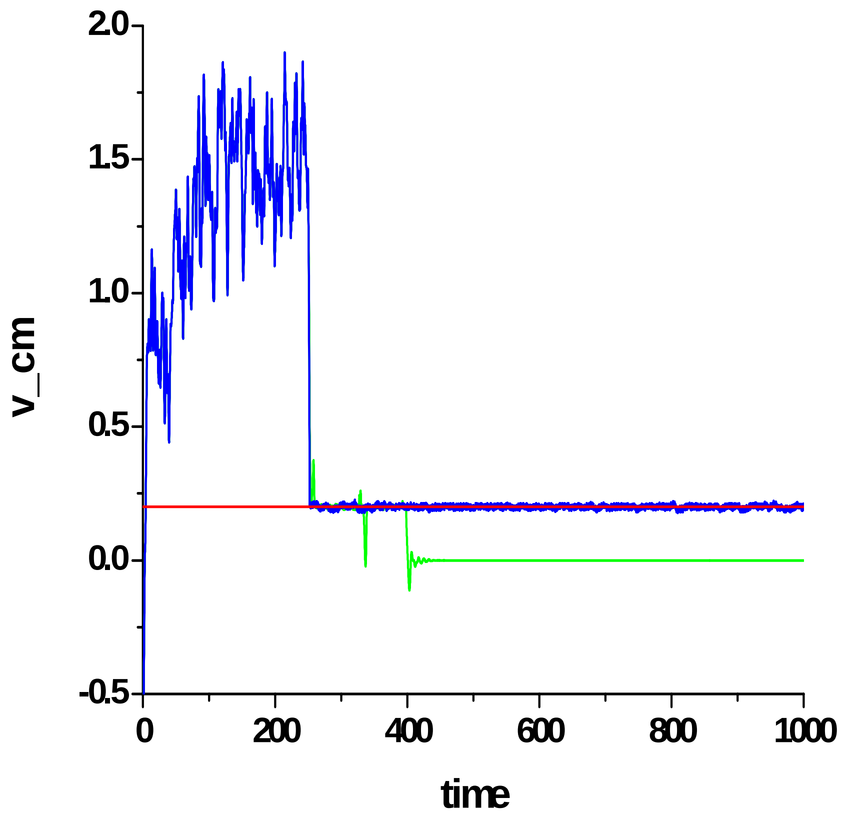


Pulsed Control Schematic

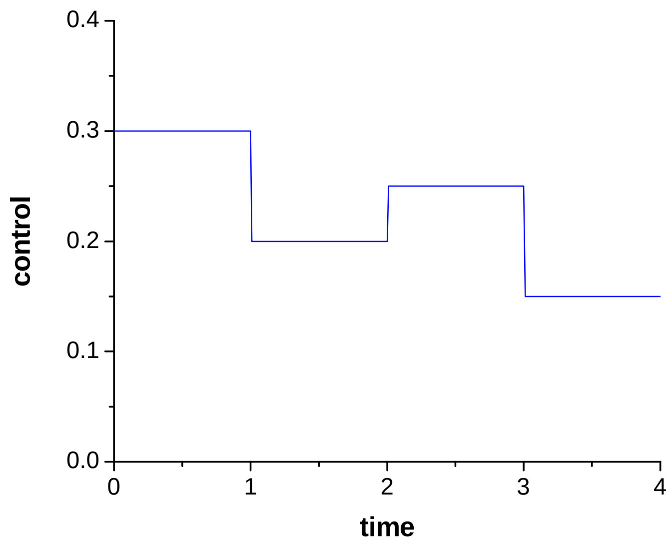


V. Protopopescu & J. Barhen, Chaos 14, 400 (2004).

Step-Like Control

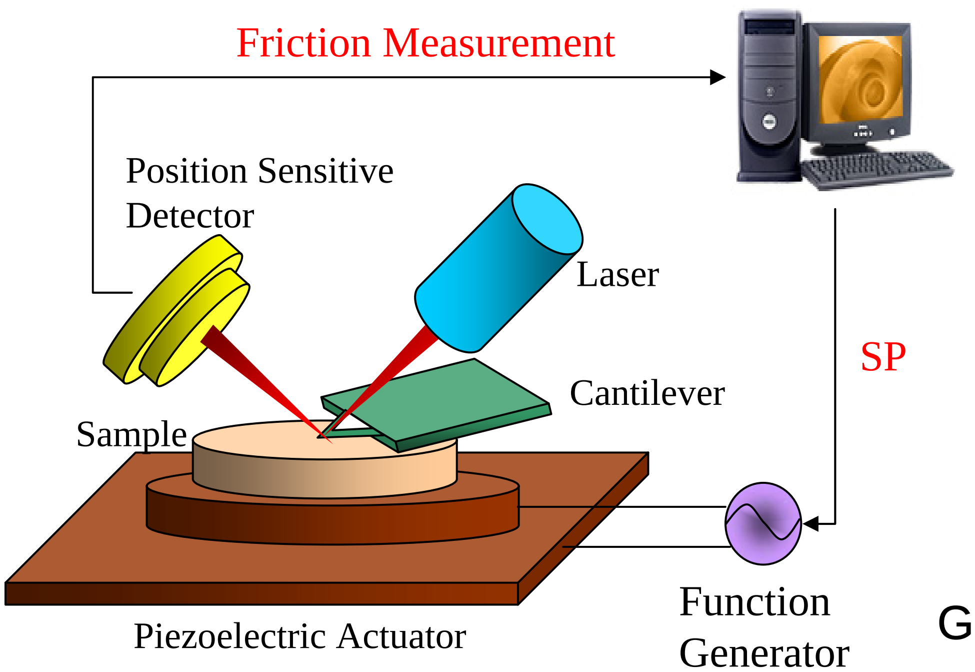


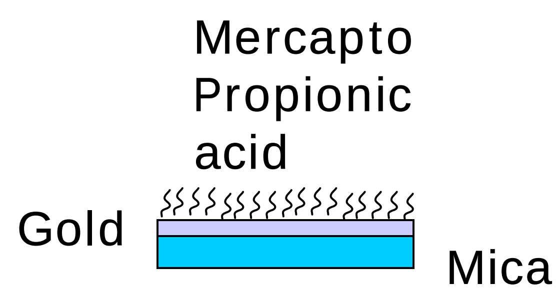
Step-Like Control Schematic



V. Protopopescu & J. Barhen, Chaos 14, 400 (2004).

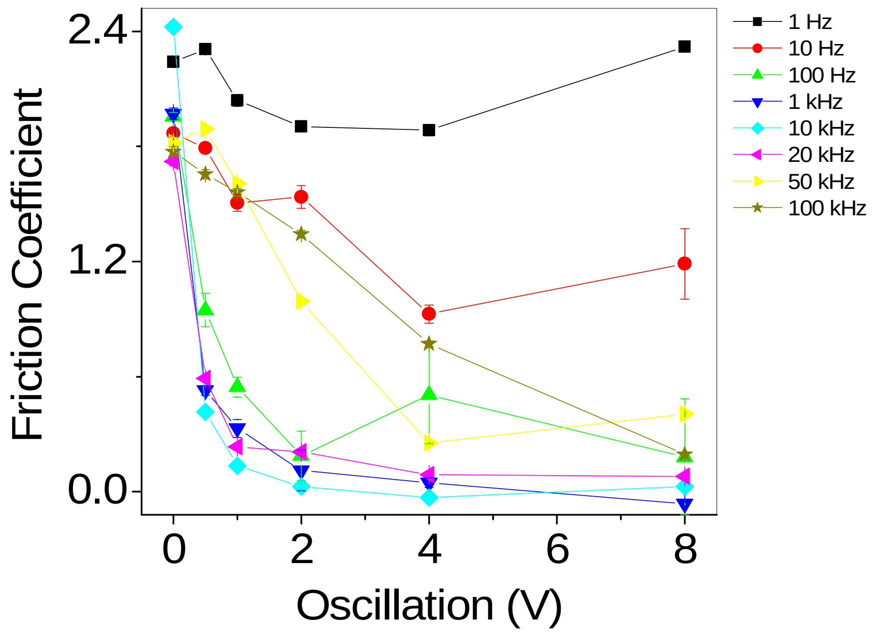
Surface Normal Oscillations
Experimental Setup



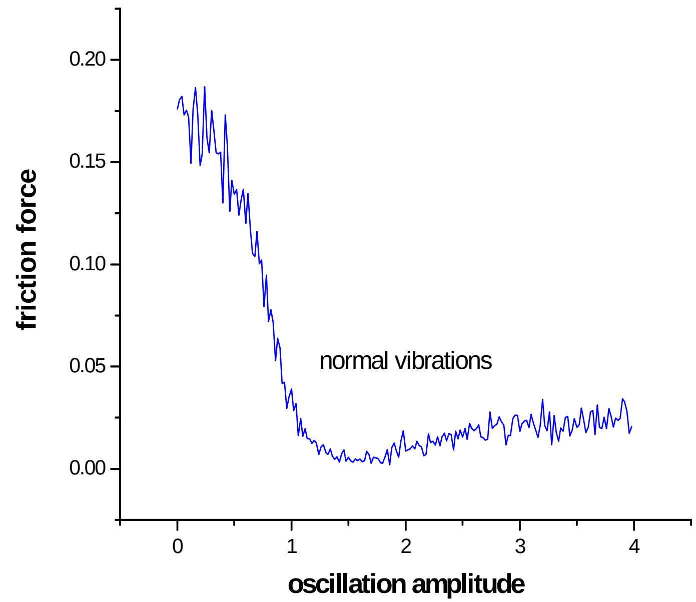


Dependence on Oscillation Amplitude

Experimental



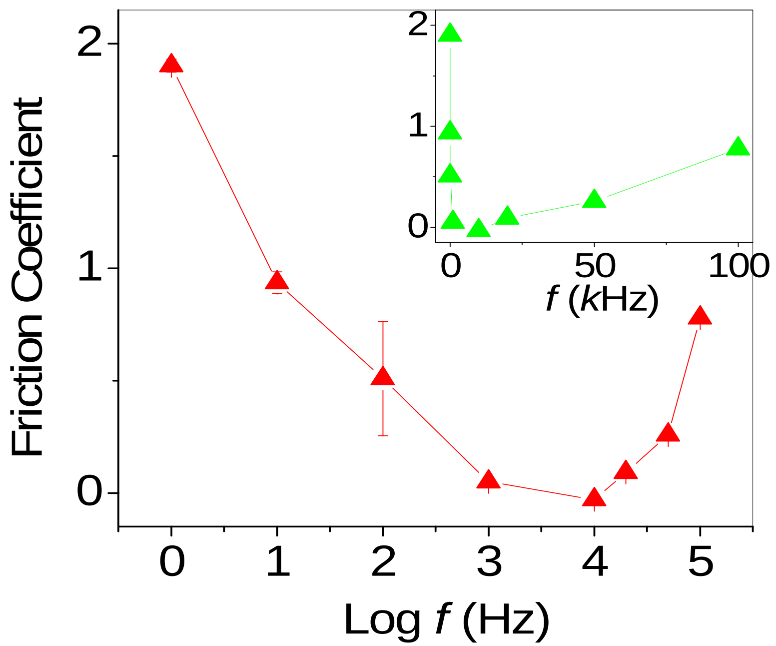
Numerical Simulations



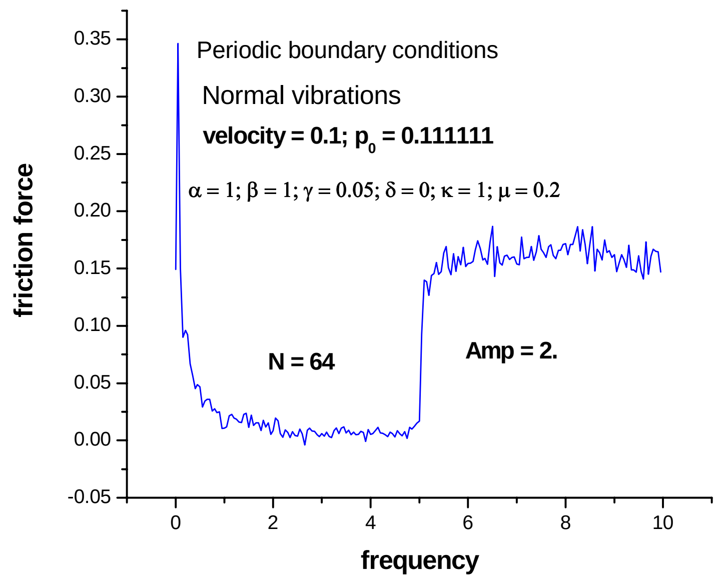
S. Jeon, T. G. Thundat, and Y. Braiman, submitted to Applied Physics Letters

Dependence on the Frequency of Oscillations

Experimental

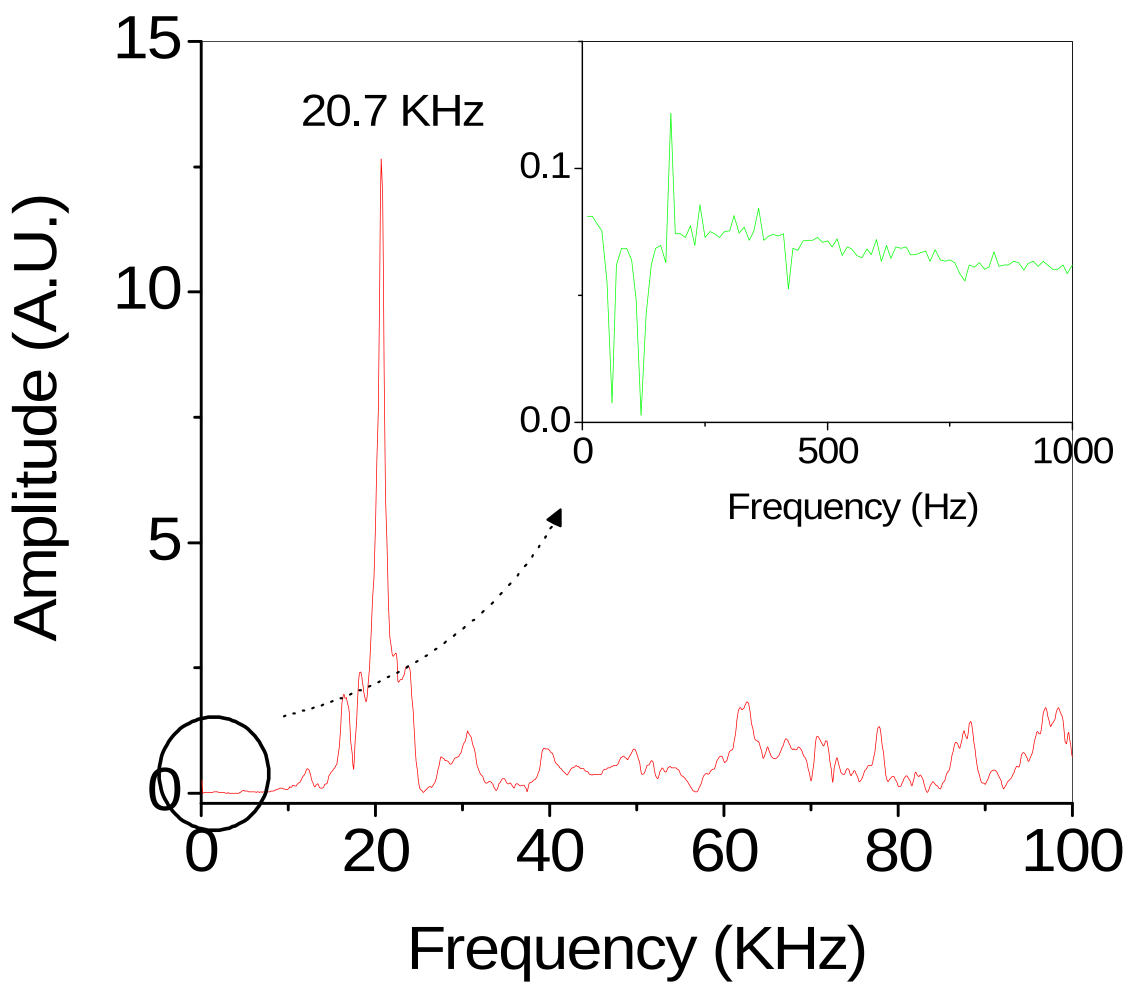


Numerical Simulation

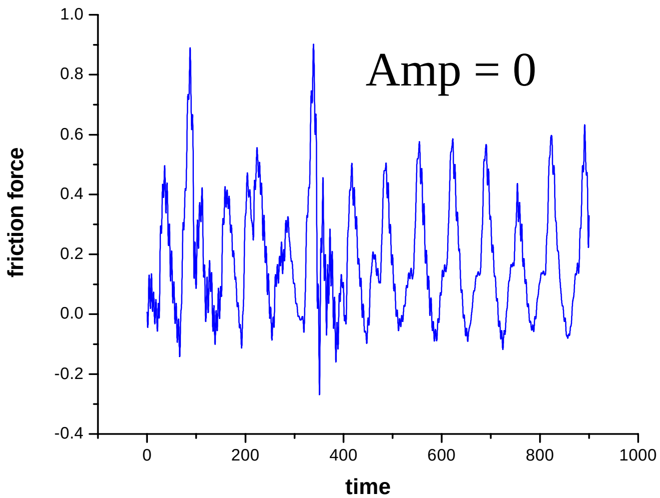


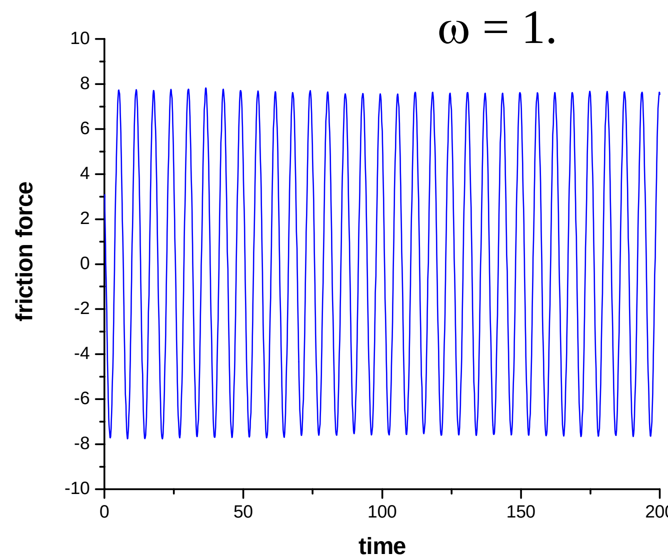
S. Jeon, T. G. Thundat, and Y. Braiman, submitted to Applied Physics Letters

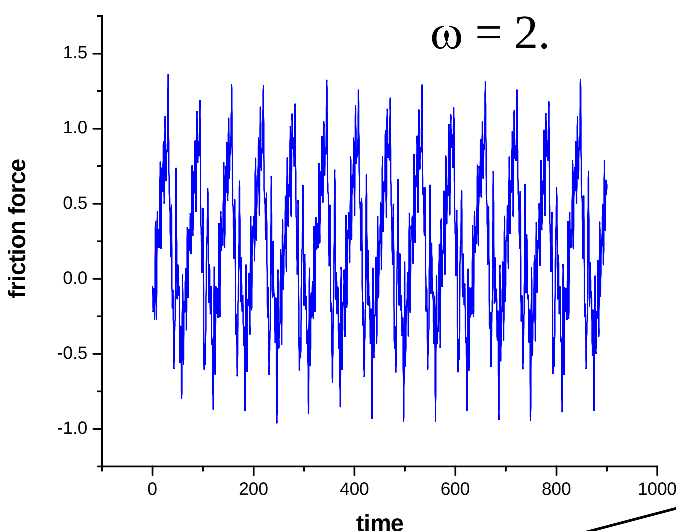
Resonance Response

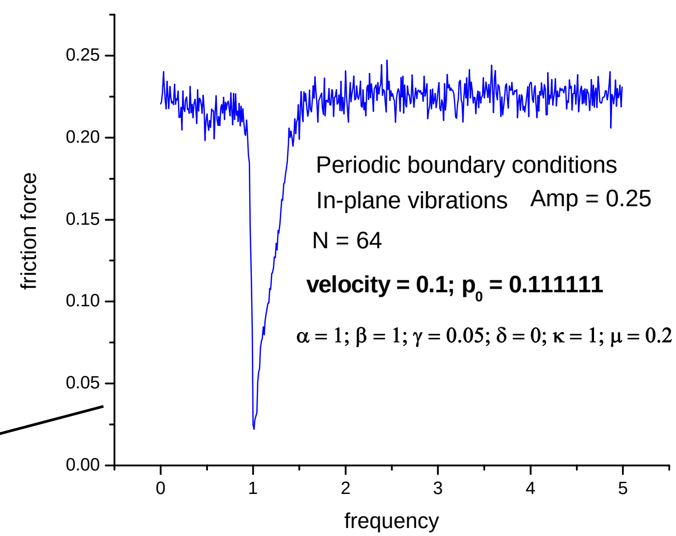


Lateral Oscillations









Experimental observation in - E. Riedo, E. Gnecco, R. Bennewitz, E. Meyer, and H. Brune, PRL **91**, 084502 (2003).

Summary

- Nanoscale arrays can exhibit a variety of modes of motion with different degrees of spatial coherence which affects frictional properties of the array

- Spatiotemporal fluctuations in small discrete nonlinear arrays affect the dynamics of the center of mass. Here we presented numerical evidence indicating that phase synchronization is related to the frictional properties of such sliding atomic scale objects.

- We discussed mechanisms and implementation of how the resulting atomic scale friction can be tuned with noise, quenched disorder, and surface vibrations.

Summary

We derived the properties of a general control algorithm for quantities describing global features of nonlinear extended mechanical systems. The control algorithm is based on the concepts of non-Lipschitzian dynamics and global targeting. We showed that:

- **(i)** **Certain average quantities of the controlled system can be driven – exactly or approximately – towards desired targets which become linearly stable attractors for the system's dynamics;**
- **(ii)** **The basins of attraction of these targets are reached in very short times; and**
- **(iii)** **While within reasonably broad ranges, the time-scales of the control and of the intrinsic dynamics may be quite different, this disparity does not affect significantly the overall efficiency of the proposed scheme, up to natural fluctuations.**