Friction at the Atomic Scale: Dynamics and Control

Y. Braiman and V. Protopopescu

Center for Engineering Science Advanced Research

Computer Science and Mathematics Division

Oak Ridge National Laboratory

Warning: This document contains information proprietary to the Oak Ridge National Laboratory, operated by UT-Battelle LLC, for the Department of Energy under contract DE-AC05-00OR22725. Unauthorized use of any portion thereof subject the violators to prosecution under the law.

Collaborations

F. Family - Emory University

H. G. E. Hentschel - Emory University

J. Krim - NC State University

Robustness of Friction Mechanisms

Friction is ruled by robust dynamics

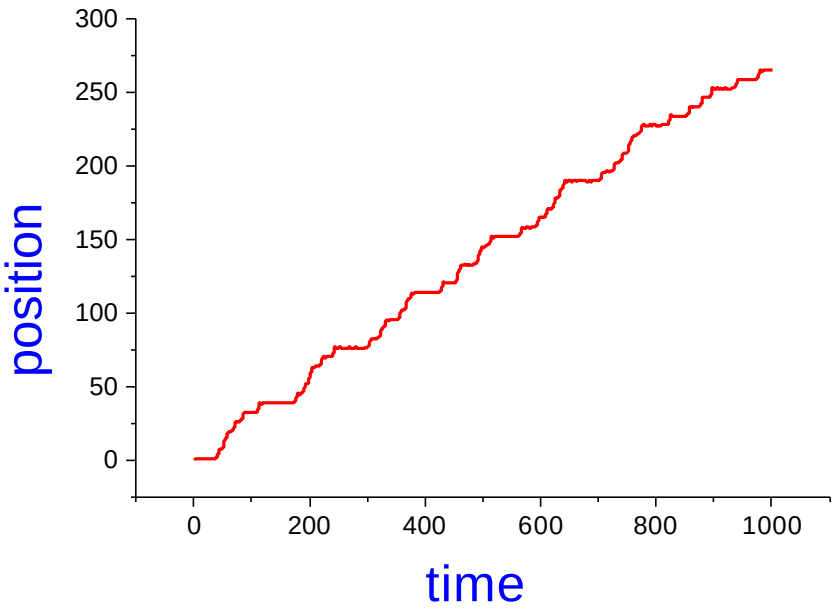
good qualitative agreement between variety of models and types of interaction potentials used for a model

- choice of parameters may be even more important than the choice of a model !!!
- Initial conditions !

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



Different Regimes of Motion

- Single - particle dynamics

Very limited correlation between particles in array

High temperature (high noise)
Large external forcing
Small coupling

- Collective dynamics

Propagation of well defined moving structures

Small-medium forcing
Large-intermediate coupling
Reasonable noise/disorder

Understanding collective dynamics is the key issue for controlling and manipulating nano-motion.
It has not been studied before in regard to nano-motion.
We have suggested a link from collective motion to friction.
Some of the predictions based on our approach have already been successfully tested experimentally.

Different Regimes of Motion

- Single - particle dynamics

Very limited correlation between particles in array

High temperature
(high noise)
Large external forcing
Small coupling

- Collective dynamics

Propagation of well defined moving structures

Small-medium forcing
Large-intermediate coupling
Reasonable noise/disorder

Collective Dynamics

Understanding collective dynamics is the key issue

It has not been studied before in regard to friction

There exist a link from collective motion to friction

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

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

M. Porto, M. Urbakh, and J. Klafter, Europhysics Lett. **50**, 326 (2000).

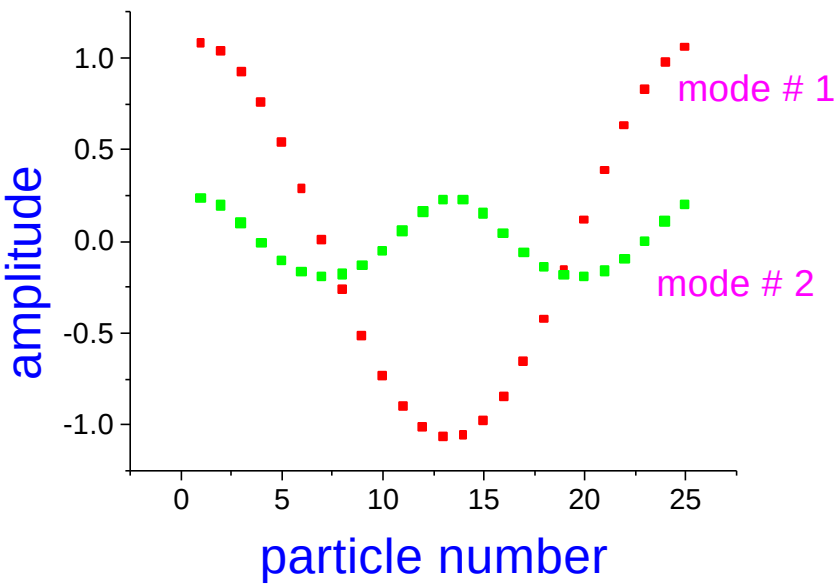
M. Porto, M. Urbakh, and J. Klafter, J. Phys. Chem. B **104**, 3791 (2000).

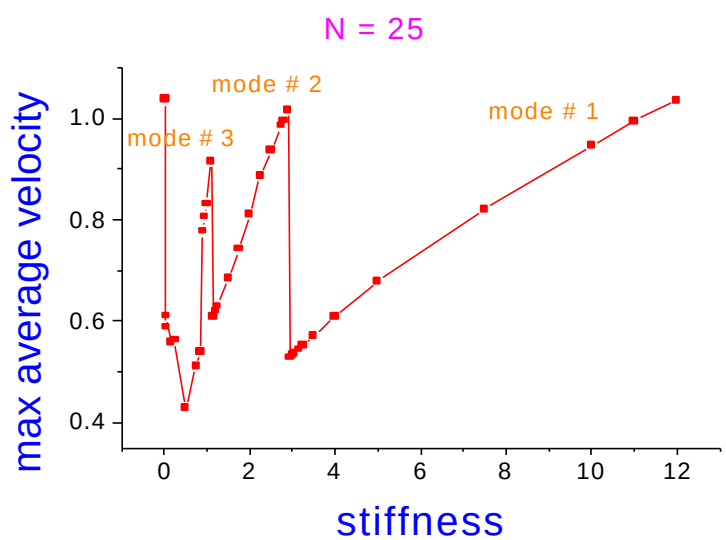
Locking of the Temporal and Spatial Dynamics (Modes)

Small size and confinement

The outcome Þ Propagation modes

Each mode is characterized by different frictional behavior





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

Nonlinear Friction Selection

- Simulations using F-K model show that for intermediate to high values of the coupling and small applied force

  a series of quantized transitions in the maximum propagation velocity occur.

- It is possible to scale the position at which these maximum velocity jumps occur using the size ***N*** of the array and the coupling ***k.***

- At low enough values of the coupling a transition back to synchronous motion occurs independent of system size ***N.***

$$k_m(N) \sim (N/m)^2$$

Friction Models

$$m\ddot{x}_j + g\,\dot{x}_j = -\partial U/\partial x_j - \partial V/\partial x_j + f_j + h_j$$

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

$$F_0 = q + b\,x$$

$$\dot{q} = (q - q_{\min})(q_{\max} - q)/t - a\,(q - q_{\min})\dot{x}$$

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

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

$$F_0 = F_b + \Delta F_0(1 - \exp(-f/t)) + g\,\dot{x}$$

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

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 !

Theoretical Modeling

- Phenomenological models
- F-K-Tomlinson model

$$m\ddot{X}_j + g\,\dot{X}_j = -\partial U / \partial X_j - \partial V / \partial X_j + f_j + h_j$$

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

Dynamics of Propagating Arrays

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

$$X_n(t) = X(t) + dX_n(t)$$

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

Keeping fluctuations small, the center of mass obeys

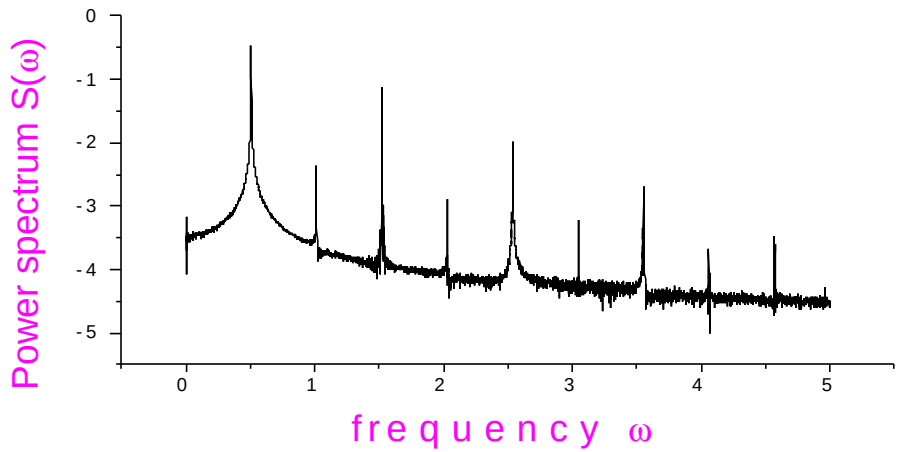
$$\boxed{\ddot{X} + g\dot{X} + \sin(X)[1 - < dX_n^2 > / 2] = f}$$

The spatiotemporal fluctuations obey

$$\boxed{d\ddot{X}_n + g\, d\dot{X}_n + C\cos(X)\, dX_n = k\,(dX_{n+1} - 2\,dX_n + dX_{n-1})}$$

Assumptions

We assume that the main mechanism for the energy transfer from the center of mass motion to the spatiotemporal fluctuations in the array is due to a subharmonic parametric resonance.



We have made a self-consistent approximation by replacing nonlinear terms by a quasilinear term.

$$C = \sqrt{1/[1 + 2 < \overline{dX_n^2} >]}$$

Resonant Parametric Forcing

We make the Fourier decomposition

$$dX_n(t) = \sum_m dX_m(t) e^{2pimn/N}$$

and equations of motion for the modes

$$d\ddot{X}_m + g\, d\dot{X}_m + [\Omega_m^2 + C\cos(X)]dX_m = 0$$

where $\Omega_m = 2\sqrt{k}\sin(pm/N)$

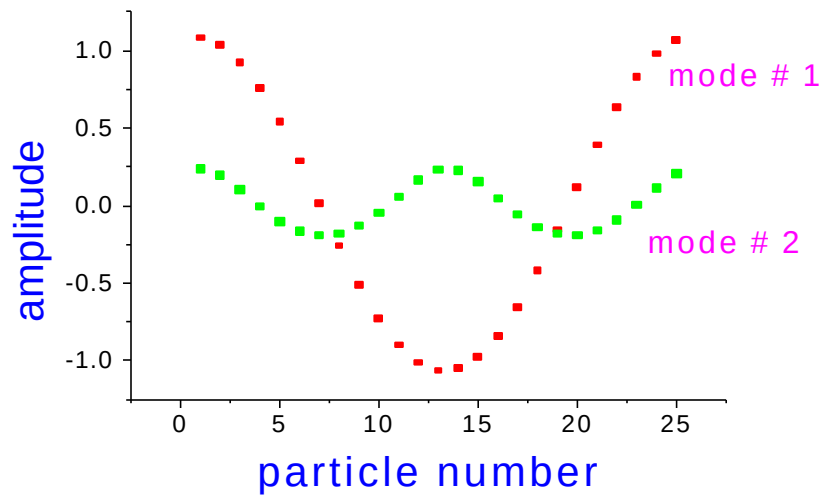
Shows parametric forcing when $\Omega_m = w/2$

Spatial Coherence and Mode Selection

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

$$dX_m = b_m \sin(wt/2 + b_m)$$

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

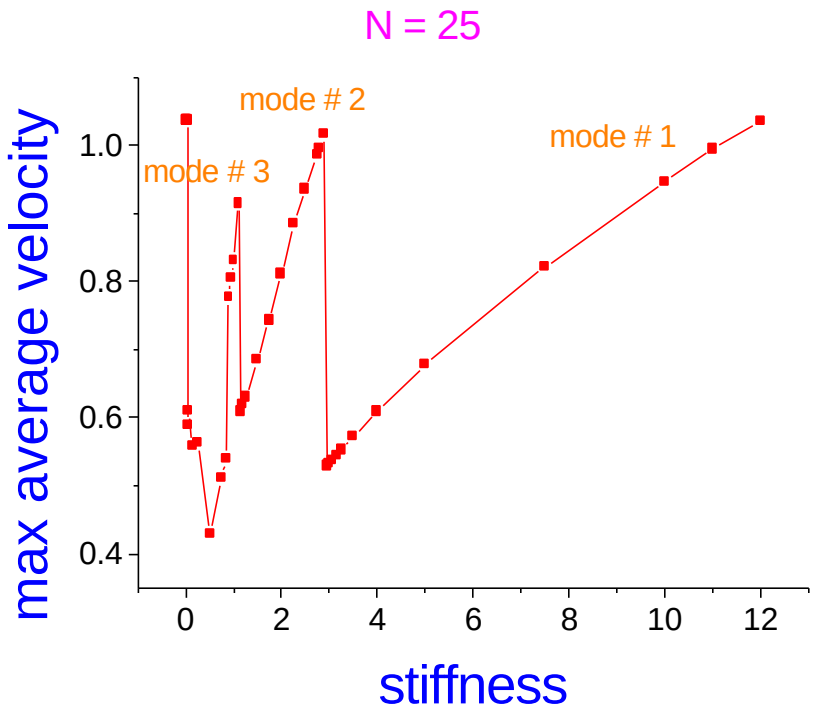
$$dX_m = b_m \sin(wt/2 + b_m)$$

and the center of mass motion is described by

$$X = X_0 + wt + B\sin(wt)$$

then the velocity of the center of mass is

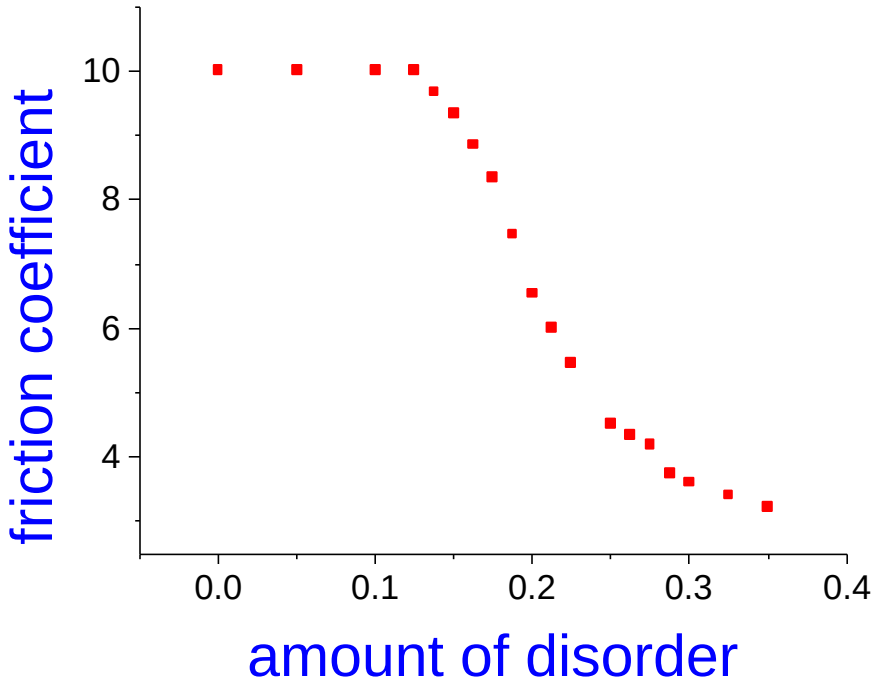
$$v_m = (f/g)/[(1+B^2/2)+b_m^2/8]$$



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

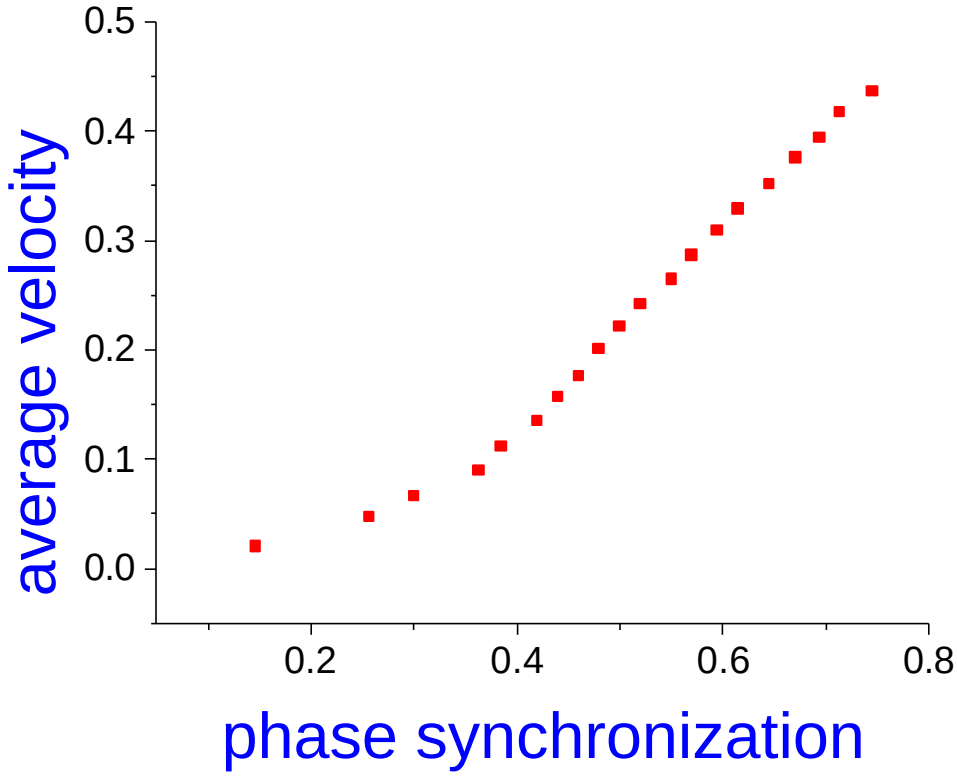
Sliding on Disordered Substrate

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 Þ Phase Synchronization

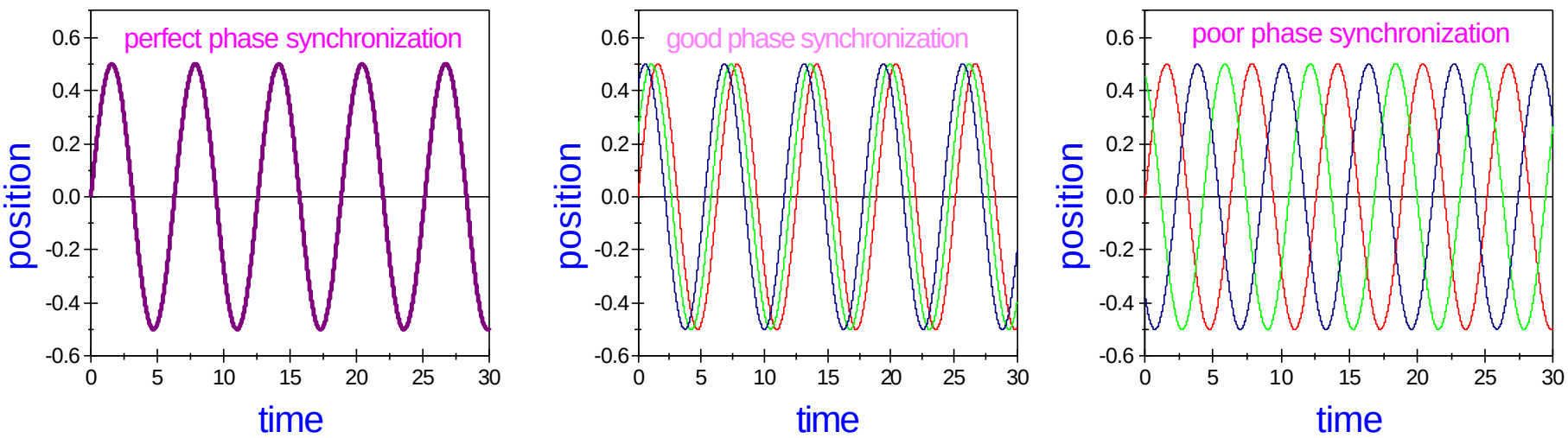


The better the array is phase synchronized - the faster it moves !

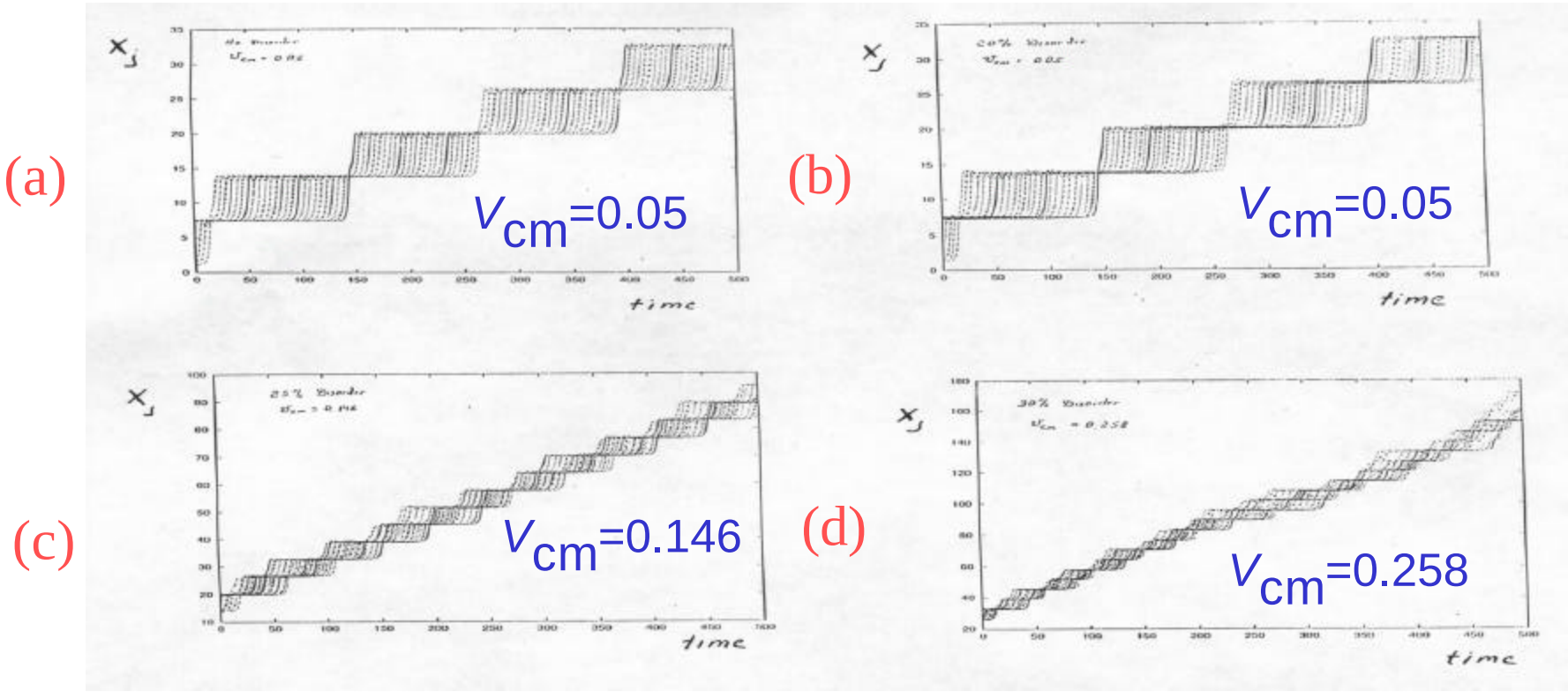
Phase Synchronization

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

$$s = \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{\sqrt{\sum_j^N (X_j - X_{av})^2}}{X_{av}}$$

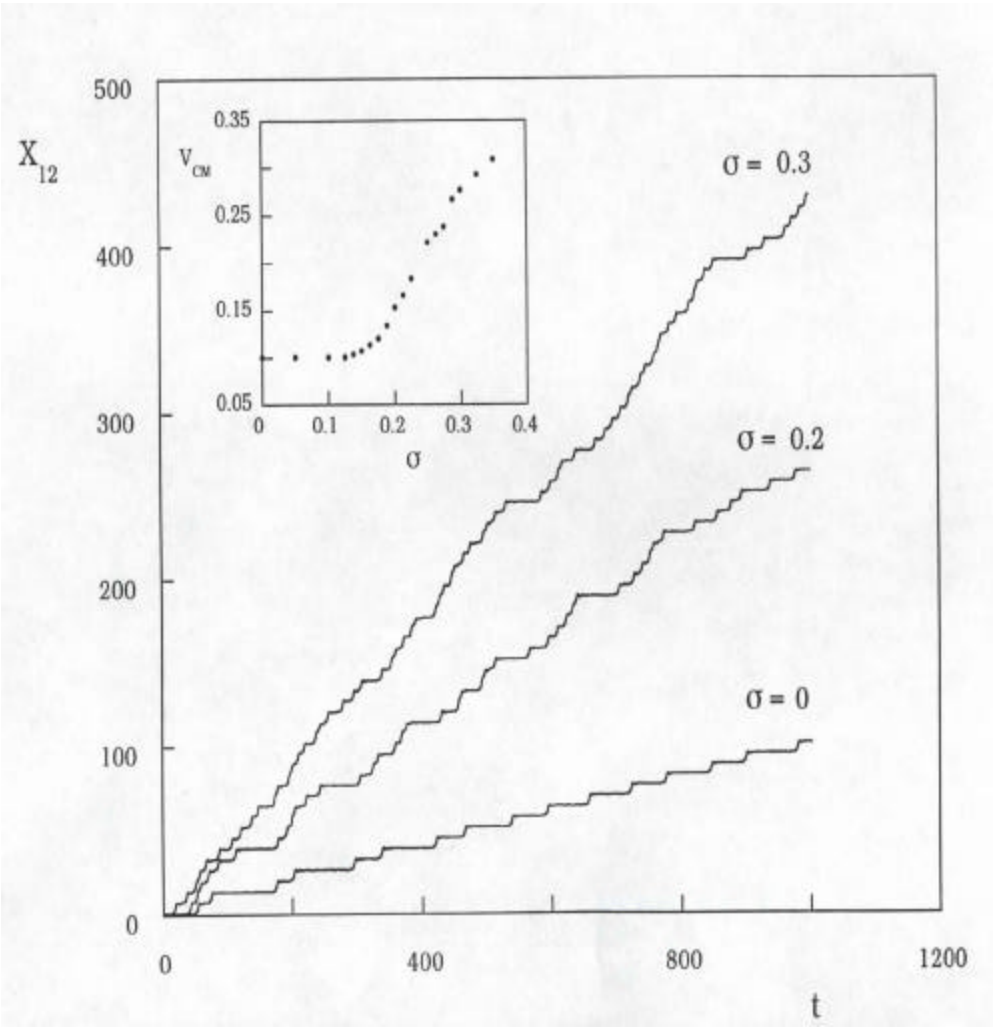


Disorder - Enhanced Synchronization



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



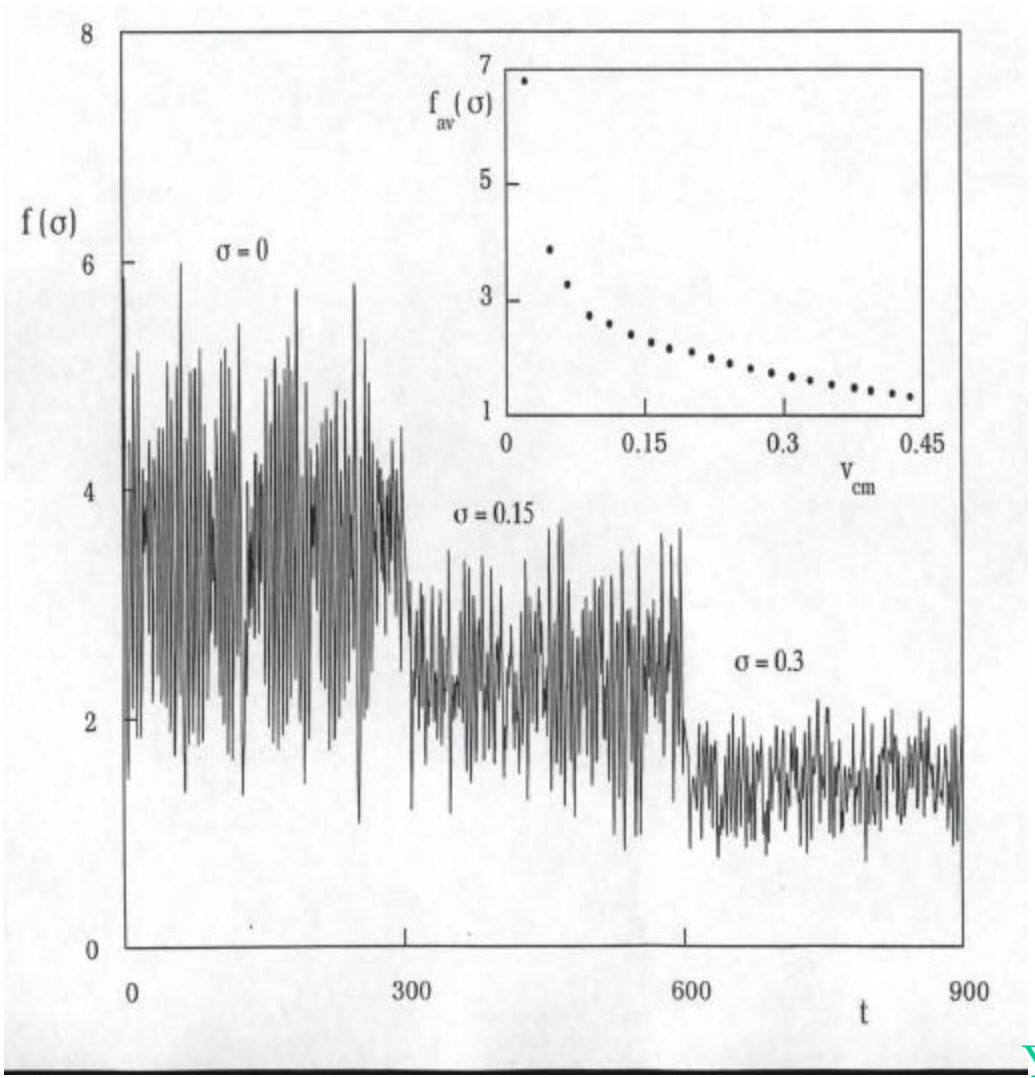
The position of a particle #12 in array as a function of time.

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

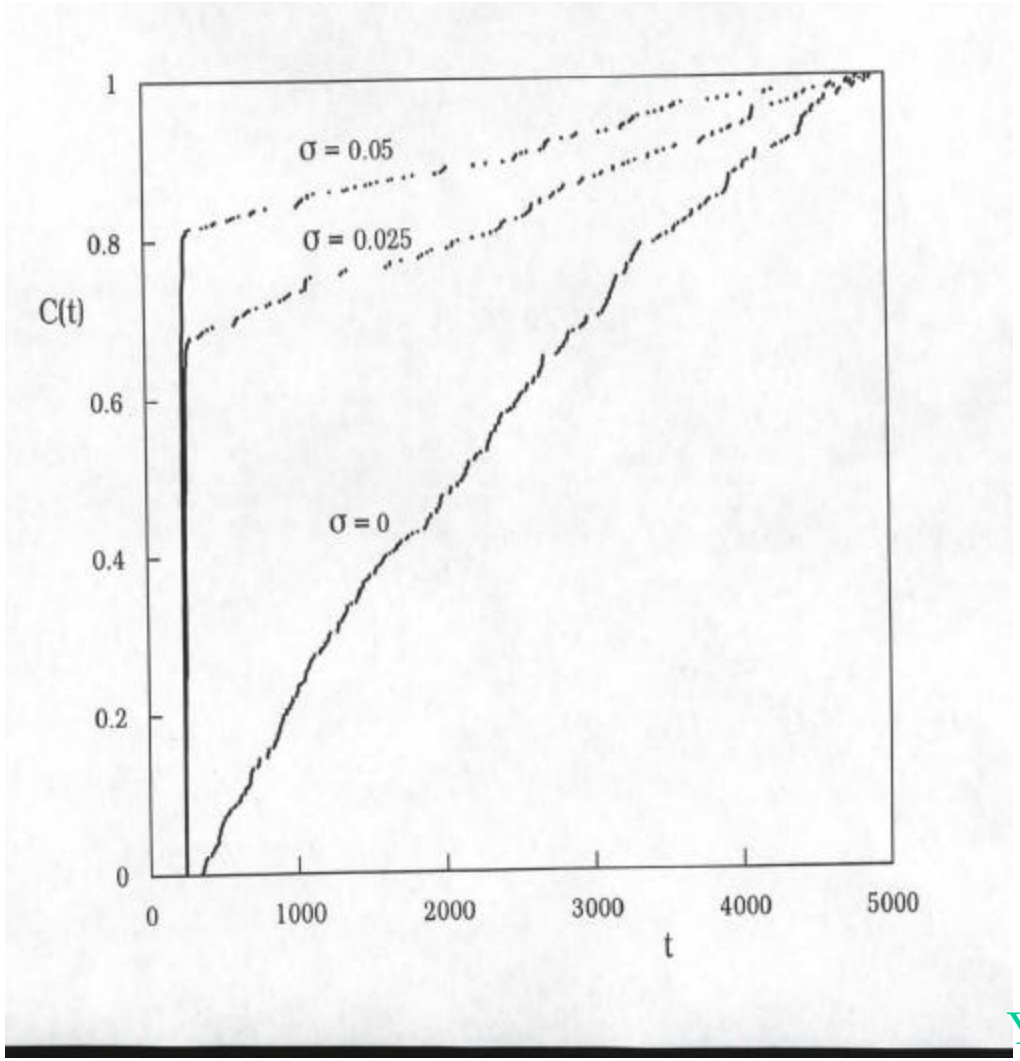


Time series of the fluctuations from the center of mass f(σ) for different amounts of disorder.

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.

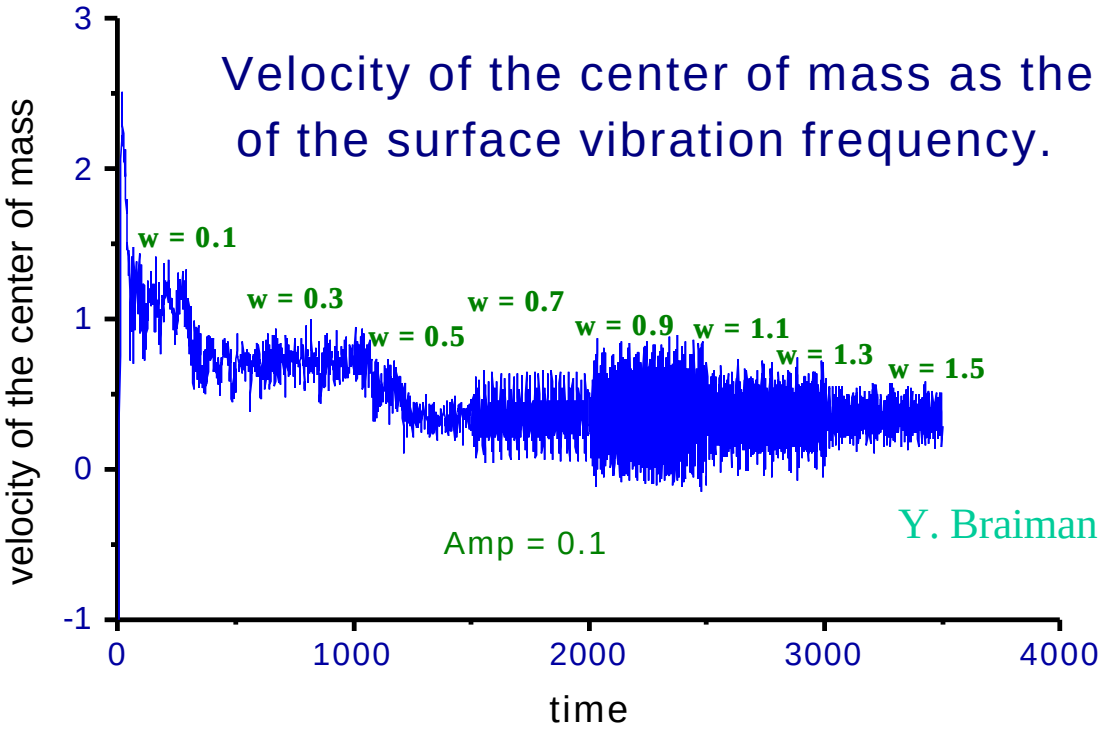
The bottom curve corresponds to the identical array.

The middle curve corresponds to $\sigma = 2.5\%$.

The top curve corresponds to $\sigma = 5\%$.

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

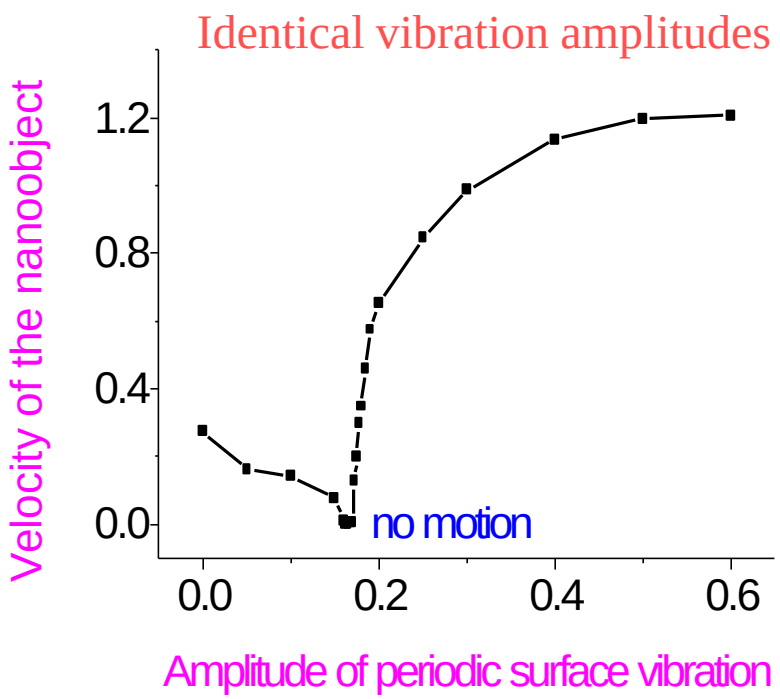
Friction Control by Surface Vibrations

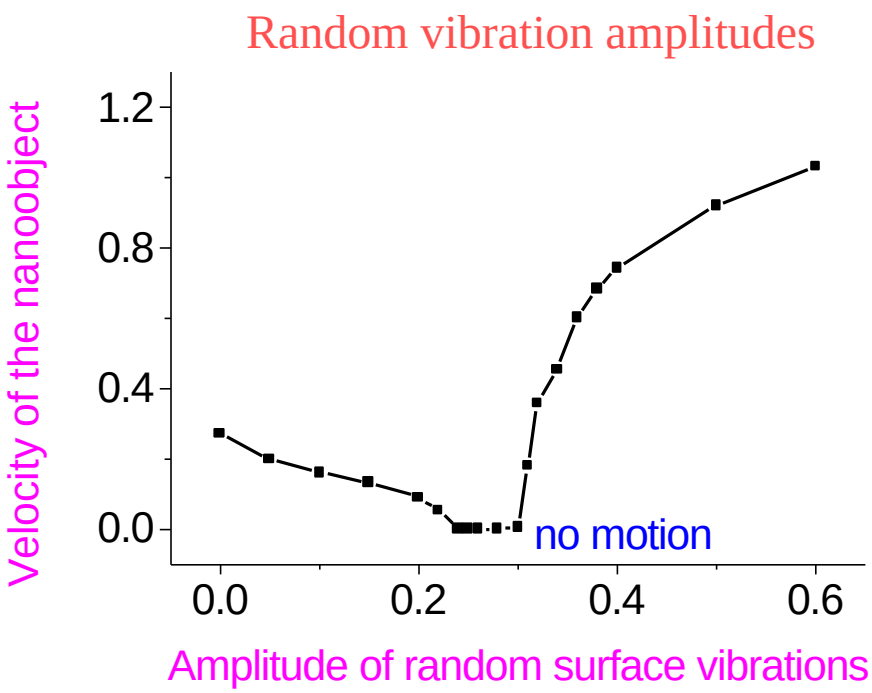


Y. Braiman and V. Protopopescu, (in preparation)

M. Heuberger, C. Drummond, and J. Israelachvili, J. Chem. Phys. B **102**, 5038 (1998);
J. Gao, W. D. Luedtke, and u. Landman, J. Phys. Chem. B **102**, 5033 (1998);
M. G. Rozman, M. Urbakh, and J. Klafter, Phys. Rev. E **57**, 7340 (1998);
F.-J. Elmer, Phys. Rev. E **57**, R4903 (1998).

Theoretical Demonstration of the Effect of Surface Vibrations

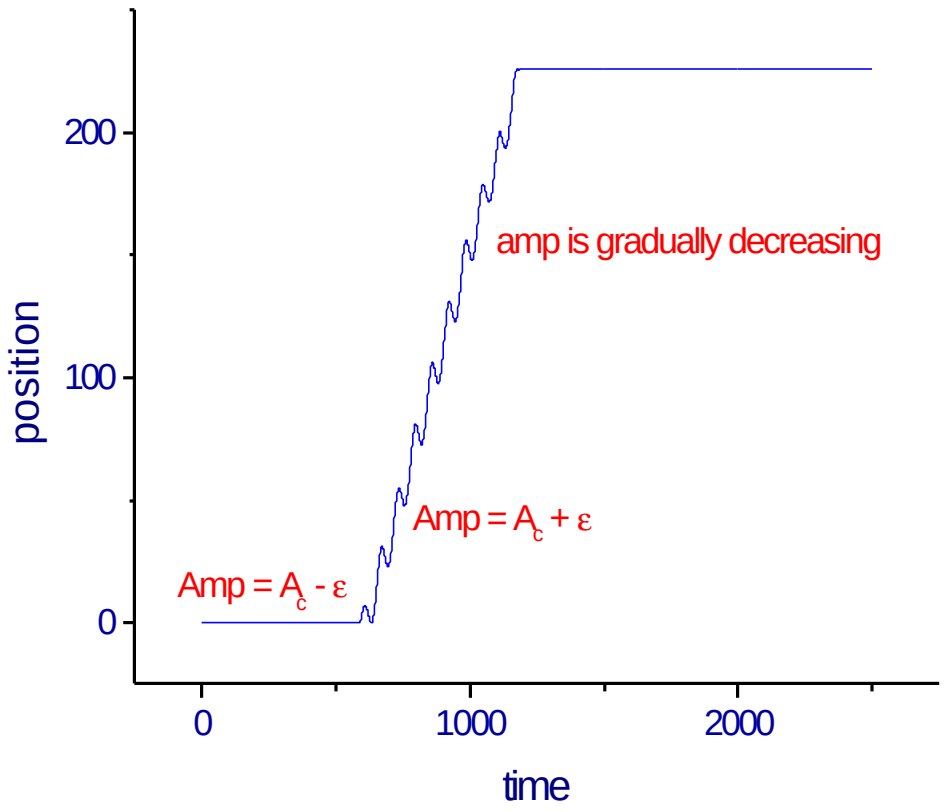


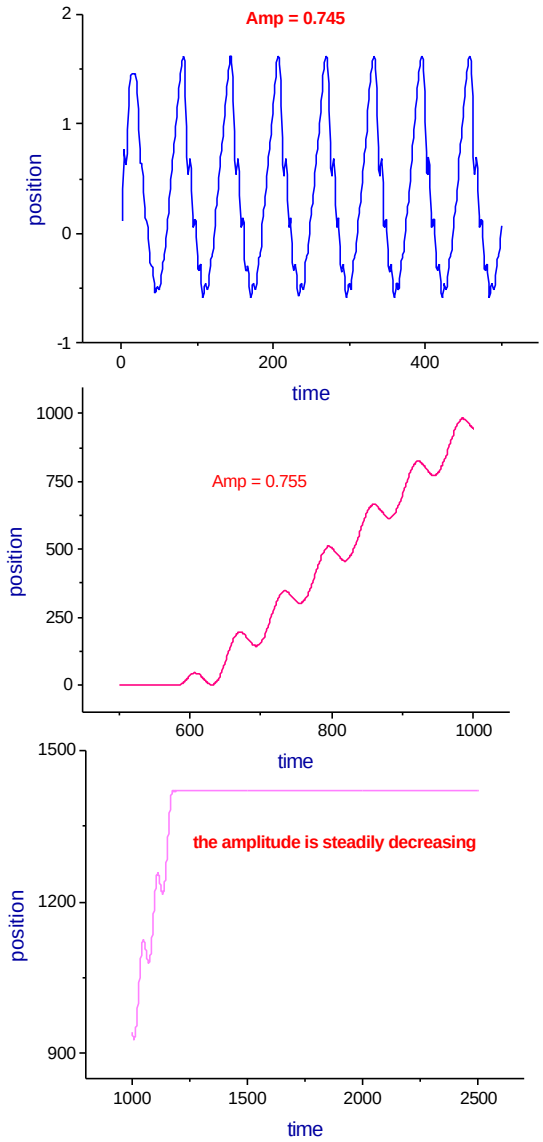


Velocity is controlled by the amplitude of surface vibrations.

Y. Braiman and V. Protopopescu, (in preparation)

Transition to Sliding Behavior





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.

Publications

- Friction

J. Chem. Phys. B **104**, 3984 (2000)
Phys. Rev. Lett. **83**, 104 (1999)
Phys. Rev. E **59**, R4737 (1999)
Phys. Rev. E **58**, R4057 (1998)
Phys. Rev. B **55**, 5491 (1997)
Phys. Rev. E **53**, R3005 (1996)
in the Proceedings of "Friction, Arching & Contact Dynamics" World Scientific (1996)

- Dynamics

Phys. Rev. Lett. **66**, 2545 (1991)
Phys. Lett. A **206**, 54 (1995)
Nature **378**, 465 (1995)