Control of Friction at the Nanoscale

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We propose a new algorithm to control frictional dynamics of a small array of particles towards preassigned values of the average sliding velocity. The control is based on the concepts of non-Lipschitzian dynamics and terminal attractor. Extensive numerical simulations illustrate the robustness, efficiency, and convenience of the algorithm.

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Despite the great progress made during the past half century, many issues in fundamental tribology (such as the origin of friction and the failure of lubrication) have remained unsolved. Moreover, the current reliable knowledge related to friction and lubrication is mainly applicable to macroscopic systems and machinery and, most likely, will be only of limited use for microsystems and nanosystems [1]. Better understanding of the intimate mechanisms of friction, lubrication, and other interfacial phenomena at the atomic and molecular scales is expected to provide the required tools to control friction, reduce unnecessary wear, and predict mechanical faults and failure of lubrication in microelectromechanical systems and nanodevices [2].

The ability to control and manipulate friction during sliding is extremely important for a large variety of technological applications. Friction can be manipulated by applying small perturbations to accessible elements and parameters of the sliding system [3–9]. Recently, Heuberger *et al.* [3] (experimental) and Gao *et al.* [4] (molecular dynamics simulation) showed that friction in thin-film boundary lubricated junctions can be reduced by coupling the small amplitude (of the order of 1 Å) directional mechanical oscillations of the confining boundaries to the molecular degree of freedom of the sheared interfacial lubricating fluid. Methods to control friction in systems under shear which enable one to eliminate chaotic stick-slip motion were proposed by Rozman *et al.* [5]. Significant changes in frictional responses were observed in the two-plate model [6] by modulating the normal response to lateral motion [7]. In addition, the surface roughness and the thermal noise are expected to play a significant role in deciding control strategies at the microscale and the nanoscale [8,9].

In this Letter, we address some fundamental issues related to targeting and control of friction in nanoscale driven nonlinear particle arrays, by proposing a global feedback control scheme, based on the properties of terminal attractors [10,11]. This type of control has been successfully implemented in first order systems such as neural networks [10,11] but has not been applied to second order systems. This scheme presents several advantages. First, the presence of a terminal attractor in the control term provides robustness and ensures a very fast approach to target. Second, the global control turns out to be more efficient and easier to implement.

As shown in the following, terminal dynamics has several general consequential properties, namely, (i) large dissipative forces in the vicinity of the targeted points, (ii) finite convergence times to targets, and (iii) smooth transitions between various regimes, in particular, static and kinetic friction. In some sense, one may think of the non-Lipschitzian terminal attractor as a very strong concentrator of energy towards its basin of attraction. Indeed, in that region, the control term dominates the dynamics resulting in finite (and usually rather short) convergence times [11]. We illustrate the proposed control strategy on a phenomenological model of friction [6,12–14]. Despite their relative simplicity, phenomenological models of friction at the atomic level show a fair agreement with many experimental results using either surface force apparatus [6,15,16] or quartz crystal microbalance [8,17].

The basic equations for the driven dynamics of a one dimensional particle array of N identical particles moving on a surface are given by a set of coupled nonlinear equations of the form [13]

$$m\ddot{x}_n + \gamma\dot{x}_n = -\partial U/\partial x_n - \partial V/\partial x_n + f_n + \eta(t), \qquad n = 1, \ldots, N, \quad (1)$$

where x_n is the coordinate of the nth particle, m is its mass, γ is the linear friction coefficient representing the single particle energy exchange with the substrate, f_n is the applied external force, and $\eta(t)$ is Gaussian noise. The particles in the array are subjected to a periodic potential, $U(x_n + a) = U(x_n)$, and interact with each other via a pairwise potential $V(x_n - x_m)$, $n, m = 1, 2, \ldots, N$. System (1) provides a general framework of modeling friction although the amount of details and complexity varies in different studies from simplified 1D models [13,18,19] through 2D and 3D models [14,20,21] to a full set of molecular dynamics simulations [22,23].

To better present our ideas, we make the following simplifications, namely, (i) the substrate potential is assumed to have a simple periodic form, (ii) there is a zero misfit length between the array and the substrate, (iii) the same force f is applied to each particle, and (iv) the interparticle coupling is linear. The coupling with the substrate is, however, strongly nonlinear. For this case, using the dimensionless phase variables $\phi_n = 2\pi x_n/a$, the equation of motion reduces to the dynamic Frenkel-Kontorova model [15]

$$\ddot{\phi}_n + \gamma\dot{\phi}_n + \sin(\phi_n) = f + \kappa(\phi_{n+1} - 2\phi_n + \phi_{n-1}). \tag{2}$$

Extensive numerical simulations have been performed on arrays of different sizes ($3 < N < 256$) in order to verify size effects are not critical for the proposed control. The numerical and graphical results are presented for a typical nanoarray of $N = 15$ particles. Without control, Eq. (2) exhibits four different regimes: (i) rest (no motion), (ii) periodic sliding, (iii) periodic stick-slip, and (iv) chaotic stick-slip. Different motion types are obtained by changing only the initial conditions of the particle's positions and velocities, but not the system's parameters. The average velocity of the center of mass for the "natural" (i.e., uncontrolled) motion, may take only a limited range of values, namely, (i) $v = 0$ for rest (no sliding), (ii) $v = f/\gamma$ for periodic sliding motion, and (iii) $v = nv_0$, where n is an integer, $v_0 = \frac{2\pi}{nN\gamma}\sqrt{\frac{\pi-\cos^{-1}f}{\pi}}(\kappa - \kappa_c)^{1/2}$, for periodic stick-slip motion [13]. In the range of parameters under consideration, we observed only one single value of the average velocity of the center of mass for chaotic stick-slip.

When applying the control to the nanoarray, our objectives are to (i) reach any targeted value of the *average sliding velocity* using only small values of the control and (ii) significantly reduce the transient time needed to reach the desired behavior. To that effect, we propose a global feedback control algorithm that uses the concept of "terminal attractor" [10,11] which is usually associated to non-Lipschitzian dynamics. The equations of motion in the presence of the control term $C(t)$ read

$$\ddot{\phi}_n + \gamma\dot{\phi}_n + \sin(\phi_n) = f + \kappa(\phi_{n+1} - 2\phi_n + \phi_{n-1}) + C(t), \tag{3}$$

where

$$C(t) = \alpha(v_{\text{target}} - v_{\text{cm}})^{\xi} \tag{4}$$

is the non-Lipschitzian control term based on the concept of terminal attractor [10,11]. In Eq. (4), $v_{\text{cm}} = (1/N)\sum_{n=1}^{N}\dot{\phi}_n$ is the average (center of mass) velocity, and v_{target} is the targeted velocity for the center of mass, $\xi = 1/(2n+1)$, and $n = 1, 2, 3\ldots$. In this Letter we present results for $\xi = 1/7$, but the algorithm is performing equally well for other values. We note that the control requires only the knowledge of the average velocity of the array, which is an experimentally available quantity and is applied identically and concomitantly to all the particles in the array upon which it acts as a uniform force proportional to $(v_{\text{target}} - v_{\text{cm}})^{\xi}$.

We note that most dynamical systems satisfy the Lipschitz condition, namely, the derivatives of the right-hand side of the dynamical equations with respect to the state variables are bounded. The terminal attractor dynamics that we are utilizing violates it by design. As a result, trajectories reach the terminal attractor in finite time [10]. To illustrate this phenomenon, consider a simple example of a terminal attractor, namely, the equation $\dot{\phi} = -\phi^{1/7}$. At the equilibrium point, $\phi = 0$, the Lipschitz condition is violated, since $\partial\dot{\phi}/\partial\phi = -(1/7)\phi^{-6/7}$ tends to minus infinity as ϕ tends to zero. Thus the equilibrium point $\phi = 0$ is an attractor with "infinite" local stability.

This is precisely the effect realized with the control term $C(t)$. Indeed

$$\frac{dC}{dv_{\text{cm}}} = -(1/7)\alpha(v_{\text{target}} - v_{\text{cm}})^{-6/7}; \tag{5}$$

i.e., $dC/dv_{\text{cm}} \to -\infty$ as $v_{\text{cm}} \to v_{\text{target}}$.

The "infinite attraction power" of the "terminal" (non-Lipschitzian) attractor endows the proposed algorithm with excellent efficiency and robustness, as illustrated in Fig. 1 for four values of the target velocity, namely, $v_{\text{target}} = 0$, 0.5, 1, and 3. Red lines indicate the time series of the control [Eq. (4)], while the blue lines show the time series of the velocity of the center of mass. In all cases, we reached the (arbitrarily chosen) target values for rather small values of the control and very short transient times.

To assess the performance of the proposed algorithm for more "realistic" interaction potentials, we replaced the linear interaction in Eq. (3) by the Morse interaction:

$$F_j = \frac{\gamma}{\beta}\{\exp[-\beta(\phi_{j+1} - \phi_j)] - \exp[-2\beta(\phi_{j+1} - \phi_j)]\} - \frac{\gamma}{\beta}\{\exp[-\beta(\phi_j - \phi_{j-1})] - \exp[-2\beta(\phi_j - \phi_{j-1})]\}.$$

While our simulations indicate that the control algorithm remains robust and efficient, more studies are needed to fully generalize this conclusion. As already mentioned, we also performed preliminary simulations for arrays as large as $N = 256$. The outcome is comparable to the results reported here, which suggests that the proposed control is efficient in systems larger than atomic size.

We performed extensive testing of the proposed algorithm [Eqs. (3) and (4)] by choosing numerous values of the target velocity. Figure 2 illustrates the performance of the algorithm for different values of the target velocities as a function of the parameter α [see Eq. (3)]. We have chosen a random set of initial conditions for each value of

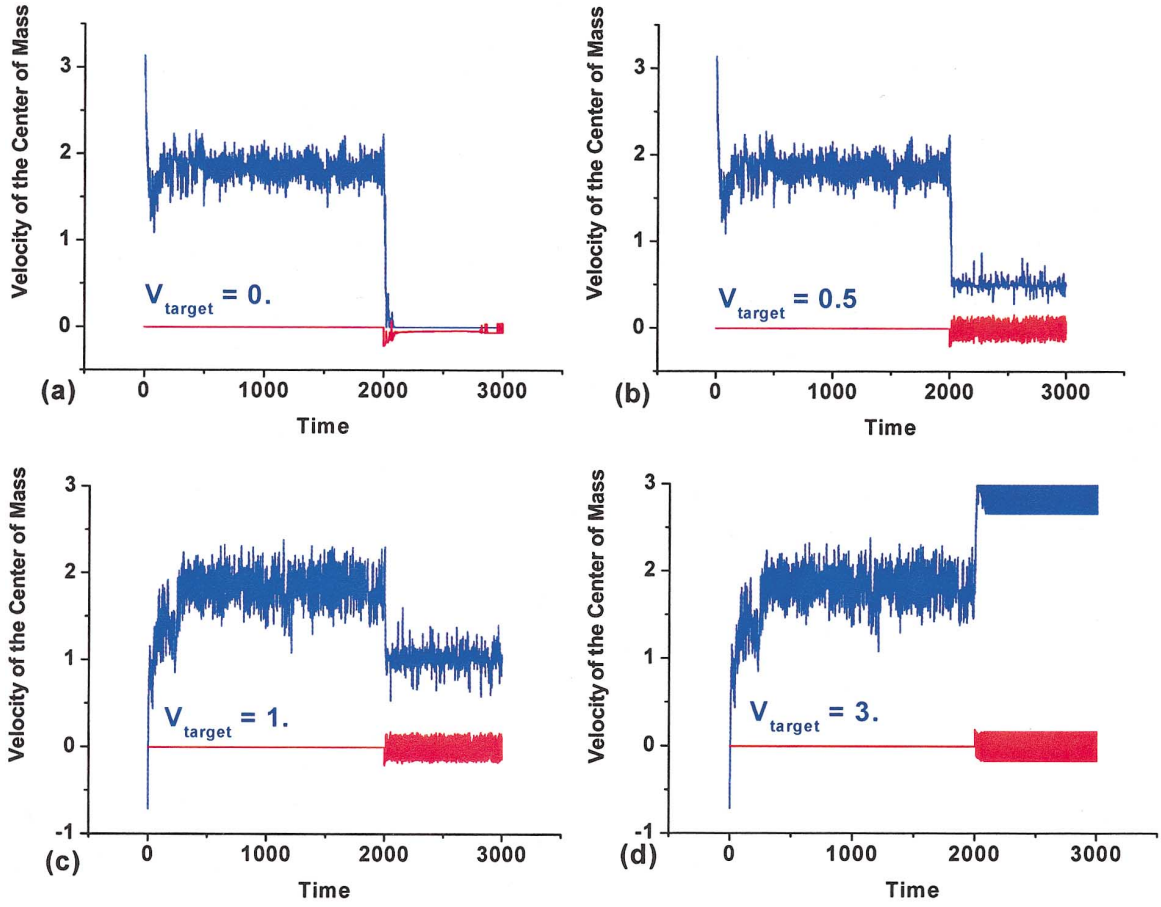

FIG. 1 (color). Performance of the control algorithm. We picked four values of the average velocities: $v = 0$, 0.5, 1.0, and 3.0 for $N = 15$ particle array. Control was initiated at $t = 2000$. The blue lines show the time series of the center of mass velocities while red lines show the control. In all cases, the desired behavior was achieved. The parameters are $f = 0.3$, $\gamma = 0.1$, $\kappa = 0.26$, and $\xi = 1/7$. All the units are dimensionless and initial conditions are chosen randomly.

α. Indeed, for some values of v_{cm} the convergence to the target value is straightforward (see upper and middle curves). For other values of v_{target}, the dependence of the center of mass velocity, v_{cm} on α is irregular. These are the cases where the targeted values of the average velocities are in close proximity with those values without control (i.e., the desired behavior is in the vicinity of self-attractors of the uncontrolled array). Thus we modified the control as follows:

$$C(t) = \alpha(v_{\mathrm{target}} - v_{\mathrm{cm}})^{\xi} - \rho(v_{\mathrm{av}} - v_{\mathrm{cm}})^{\xi} \times \mathrm{sgn}[(v_{\mathrm{av}} - v_{\mathrm{cm}})(v_{\mathrm{cm}} - v_{\mathrm{target}})] \times H[r - |v_{\mathrm{target}} - v_{\mathrm{av}}|]. \quad (6)$$

The second term in Eq. (6) represents a repelling from a possible natural attractor of system (2) that would deflect the trajectory towards the target velocity and away from natural attractors. In general, the natural attractors are not known analytically and/or *a priori*. Their presence is indicated only by the behavior of the system and accounted for by v_{av}, which is the "running" (time dependent) average velocity and represents the moving run-time average of v_{cm}. $H(.)$ denotes the Heaviside function, defined as $H(z) = 1$ for $z > 0$, and $H(z) = 0$ for $z < 0$. The role of this function is to activate the terminal repeller only within a neighborhood of radius r from the natural attractor. The coefficients α and ρ are positive numbers that represent the weights of the non-Lipschitzian attractor and repeller, respectively.

We applied the algorithm [Eq. (4)] to target the value of $v = 0.1$ (see the bottom curve in Fig. 2). Here, we are close to the static solution (stable fixed point) $v = 0$. Therefore, for some values of the control amplitude α, the outcome average velocity is $v = 0$ (instead of the desired velocity $v = 0.1$). The triangles in Fig. 2 show the center of mass velocity as a function of α but using control defined in Eq. (6). This control will repel away from the fixed point $v = 0$; therefore, we observe much better performance of the proposed control.

We discuss briefly the applicability of the proposed algorithm [based on terminal (non-Lipschitzian) dynamics] for control of friction. While in this Letter we do not suggest a specific implementation of the proposed control, we do provide a solid demonstration of a proof of principle that is relevant for both quartz microbalance

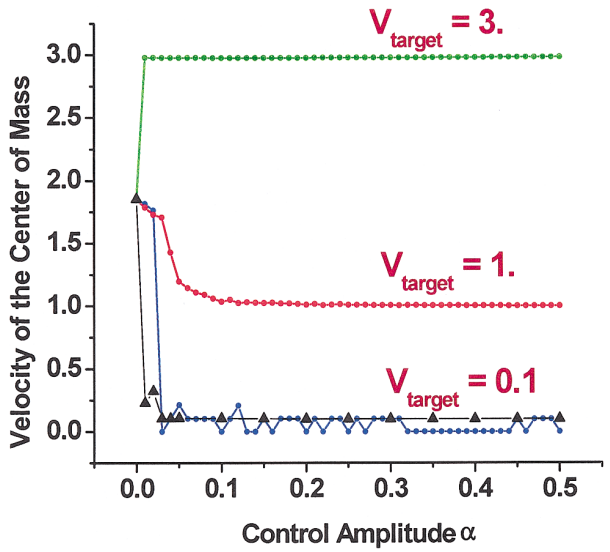

FIG. 2 (color). The center of mass velocity as a function of the maximum control amplitude α. We have chosen three values of the target velocity, namely, 0.1 (blue), 1.0 (red), and 3.0 (green). The triangles show the velocity of center of mass for control defined by Eq. (6). All the parameters are the same as in Fig. 1 and initial conditions were chosen randomly.

and surface force-type experiments. In the former, the control term is a force, while in the latter it is a velocity. For other applications, the physical realization of the control term may be a different physical quantity. The speed requirement may limit the current applicability of the proposed algorithm only to fast controls such as optical, or usage of micro/nano cantilevers [24]. However, implementation of the proposed algorithm at slower time scales is possible. Indeed, numerical simulations show that one can apply the control at much slower rates, while still maintaining the average value of the velocity close to the target. Not surprisingly, the "price" of such relaxed requirements is a longer time needed to reach the target and larger fluctuations from the averaged value.

In summary, we proposed a new type of algorithm to control friction of the sliding nanoarrays. This control is based on the concept of terminal attractor and is global in that (i) it requires only the knowledge of the velocity of the center of mass and (ii) is applied globally to the whole array. We demonstrated the efficiency and robustness of the control by reaching a broad spectrum of target velocities—both close to or far from natural attractors—in very short transient times.

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