Molecular dynamics simulation of synchronization in driven particles

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Abstract

We study synchronization of interacting particles confined to a narrow channel driven by an externally applied force. With numerical simulations, we control the particle interactions, external force and particle environment in order to mimick experimental studies of driven colloidal particles confined by light-fields. We use molecular dynamics simulations to model the particle dynamics, using overdamped equations of motion suitable for a viscous suspension of microscopic particles. We study particle synchronization under a variety of conditions, including static and dynamic patterns formed on periodic and quasiperiod substrates, kink propagation on these surfaces, and the limits of applied force that cause the particles to transition to chaotic behavior. We demonstrate the transition from trapped to sliding dynamics in quasiperiodic landscapes differs from that of a periodic landscape by [TBD], and that kinks of high density propagate [more/less ?] when [what?]. We include sample code and exercises for students that include opportunties to reproduce our results and propose new numerical experiments. With only a few particles in two-dimensions, the simulation runs quickly, making this an appropriate model for undergraduates to explore.

I. INTRODUCTION

Numerical simulations of confined, driven particles can be used to model a diverse variety of physical phenomena. Particles which interact over long distances include colloids, magnetic beads, superconducting vortices, dusty plasmas, electron gases. [more detail and references] Particles which interact over short distances include bubble arrays/emulsions [more systems and references].

Particles in confined geometries behave differently than free particles. Stabilized charged particles form patterns due to the interplay of the confining environment and particle interactions. Narrow channels studies are useful to provide insights of how particles move through systems such as wires and fluid microchannels. Biological systems such as neuron axons and capillaries can also be studied with these models [more detail and references]. Many such systems execute local oscillations about stable points [elaborate]. An applied external force increases the diversity of behaviors, and can cause particles to flow in a variety of non-linear complex behaviors including synchronized, aperiod, or chaotic dynamical patterns. The presence of a modulating surface can modify these patterns in a variety of ways, changing the onset of dynamical flows, and the overall flow patterns.

Colloidal particles trapped in light fields have proven a particularly useful medium for studying these behaviors.The relatively large size of the colloids and ease in control has lead to a rich array of experimental results. Such studies are considered model systems for experimental systems relatively hard to access and visualize, such as cold atoms or electron gases.

Synchronization has been studied for over three centuries, and is observed in different forms from Huygens pendulum clocks to the rhythmic beats of the flapping wings in a flock of birds. Controlling synchronization phenomena in weakly coupled oscillators can be achieved with an external driving force that causes the syncing of natural oscillation frequencies, dynamic phase locking[1]. [useful and interesting because?]

Disordered chaotic dynamics are also possible, where irregular, unpredictable time evolution of nonlinear systems and occurs in mechanical oscillators[?] .

In the following paper we describe our molecular dynamics model in Section II, including various particle interactions and confining environments. In Section III B we demonstrate how uniform environments and applied forces and create synchronized flow patterns. We

present these results using standard tools of non-linear oscillators such phase diagrams. We modify the environment and applied forces and show aperiodic, or nearly periodic flow behaviors in Section IV. Finally we explore the transition to chaos in in Section V.

II. MOLECULAR DYNAMICS MODEL

We use a classical two-dimensional model for studying particle dynamics. Particles are confined in a two-dimensional (2D) simulation of area $A = L \times L$ where $L = 36.5$. An individual particle has position $\vec{r}_i = x_i\hat{i} + y_i\hat{j}$. We use periodic boundary conditions such that a particle leaving the edges of the system is mapped back to a position within the simulation by the rules $x_i + L = x_i$ and $y_i + L = y_i$.

Particles are subject to external driving forces $F_{Drive}(t)$ that change as a function of time. We create several model light fields, creating a landscape of potential minima and maxima that modify the local force on a particle as a function of position $\vec{F}_{landscape,i} = \vec{F}_{landscape}(\vec{r}_i)$ These landscape potential are static, with fixed minima and maxima that are periodic or quasi-periodic, as described in Sec. III.

We model particle interactions with the Yukawa potential $\vec{F}_{ij} = \nabla V_{ij}(r_{ij})$,

$$V_{ij}(r_{ij}) = \frac{E_0}{r_{ij}} e^{-\kappa r_{ij}}, \tag{1}$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$. This is a screened Coulomb potential $E_0 = 2$ scales strength of repulsion where $E_0 = kq_1q_2$. [CHECK scaling/units] $\kappa = 1/R_0$ is the screening parameter, that screening accounts for the lengthscale at which many particle interactions and local environment that reduces the interaction range of individual particles. We fix R_0 to be unity in our simulation units.

Particle dynamics are modeled with an overdamped equation of motion integrated with the Verlet method. A single particle has the equation of motion

$$\eta\vec{v}_i = \vec{F}_{landscape,i} + \sum_{i \neq j}^{N} \vec{F}_{ij} + \vec{F}_{Drive}(t). \tag{2}$$

where $\eta = 1$. Since $\vec{a}$ is zero, the Verlet method simplifies to the Euler method $\vec{r}_i(t + \Delta t) = \vec{v}_i(t)\Delta t + \vec{r}_i(t)$.

The driving force $\vec{F}_{Drive}(t) = [F_{DC} + F_{AC}\sin(\omega t)]\hat{y}$, where frequency is defined as $\omega = 2\pi f$. We modify f and observe the change in dynamics. The landscape is a sine function that

is position dependent and calculate the landscape force on the particle directly from its location. The driving force does add energy into the system, and some of it is lost. The damping comes from the viscous fluid providing a nonconservative force.

Overdamped dynamics is a common assumption in models of colloid particles. This is an assumption that the suspending fluid is highly viscous and exerts a damping force on the particles equivalent to a linear drag force $F_{drag} = -\eta v$ and the acceleration of the particle is zero. The equation of motion we include makes both assumptions and is rearranged to reflect that. The equation of motion is not integrated for the velocity, instead it provides a direct calculation of the velocity.

In this model the Verlet method is equivalent to the Euler method. Euler's method is then used to calculate the position. Most undergraduate students learn the Euler method in Computational Physics and Differential Equations, but don't encounter the Verlet method. It is a nice opportunity to teach an extension of a method they know.

III. RESULTS

A. Single particle system

We used our model to generate a system, Fig. 1a), where the particle hops between troughs in the energy landscape. In the attached movie, Figure1.mp4, we apply a constant F_{AC} with frequency f then slowly increase F_{DC} to achieve a variety of modes. A mode is a periodic pattern of hops with a constant average particle velocity, $\bar{v}_y$ over a range of driving forces F_{DC}. In the velocity-force plot in Fig. 1b) $\bar{v}_y$ is increasing non-uniformly, with steps, indicating mode locking. A related experiment[1] revealed the microscopic dynamics of mode locking by driving colloids across a periodic landscape generated by optical tweezers.

B. Synchronization in multi-particle systems

We simulated a twenty particle system confined to a narrow channel, as shown in Fig. 2a). The interparticle forces of neighboring particles cause the system to form a buckled chain when the system is annealed. When a single particle is driven, the neighboring particles act

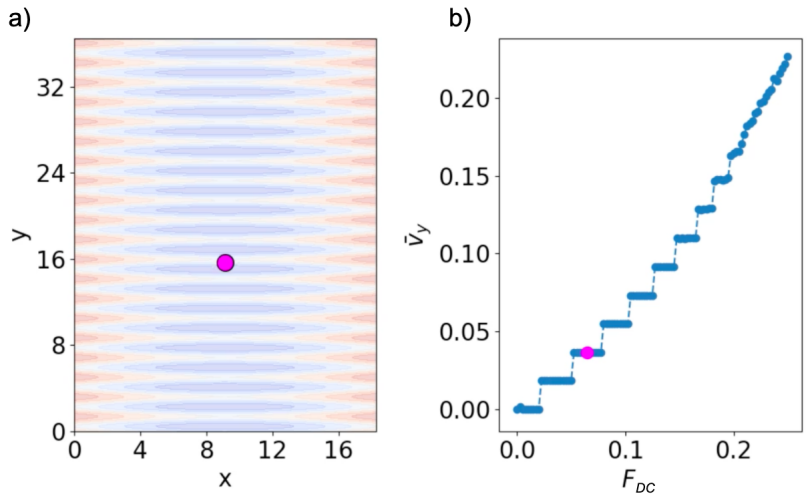

FIG. 1: **(a)** The particle is driven with a constant F_{AC} and f through a periodic potential landscape where blue are minima and red are maxima in the potential. **(b)** An average particle velocity in the y-direction $\bar{v}_y$ as a function of the driving force F_{DC}. In the animation the magenta dot represents the $\bar{v}_y$ at which the particle in Fig. 1a) is moving.

similarly to a periodic landscape to impede its motion. A driven particle can exhibit mode locking with a well-chosen AC drive and frequency. In the attached movie, Figure2.mp4, we show the complex dynamics of mode locking, where the driven particle leap-frogs past the other particles.

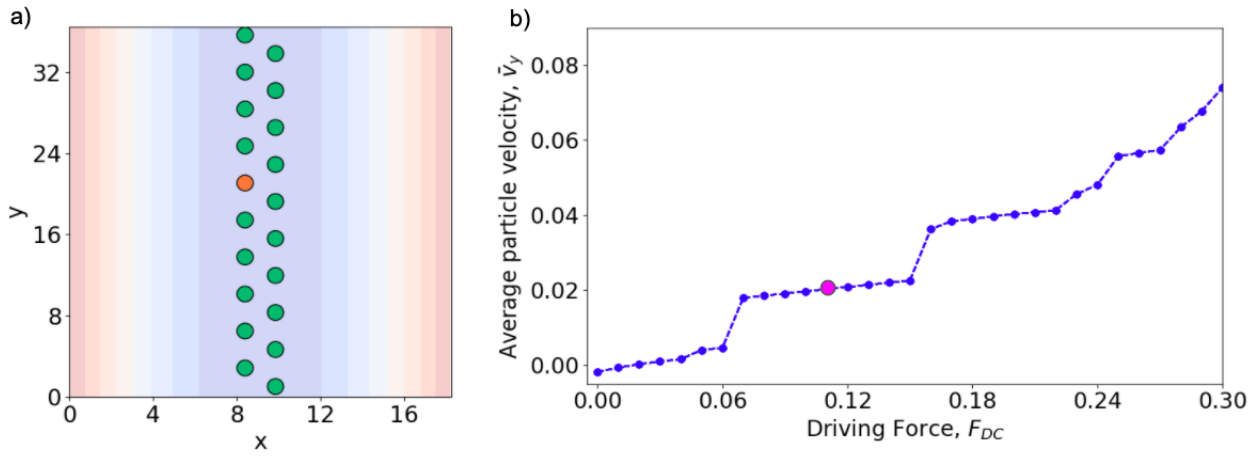

FIG. 2: **(a)** The orange particle is driven with a constant F_{AC} and f through 19 particles, colored green, confined by a quasi one-dimensional channel. The landscape is colored as in Fig. 1. **(b)** $\bar{v}_y$ versus F_{DC}, where $\bar{v}_y$ is the average particle velocity of the driven particle in the y-direction.

C. Kinked system

IV. QUASIPERIODIC SUBSTRATE

V. CHAOTIC DYNAMICS

VI. ASSOCIATED PROBLEMS

VII. CONCLUSION

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