Molecular dynamics simulation of synchronization in driven particles

Tiare Guerrero* and Danielle McDermott†

Department of Physics, Pacific University, Forest Grove, OR 97116

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Abstract

We study synchronization of interacting particles confined to a narrow channel driven by an externally applied force. Using 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. The molecular dynamics simulations model the particle dynamics using overdamped equations of motion suitable for a viscous suspension of microscopic particles. We observe 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 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 of particle velocity vs. position. 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 the dynamics of N interacting particles. Particles are confined in a two-dimensional (2D) simulation of area $A = L \times L$ where $L = 36.5$. An individual particle i has position $\vec{r}_i = x_i\hat{x} + y_i\hat{y}$. Particles are subject to 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 an external time-dependent driving force $\vec{F}_D(t)$ applied parallel to the y-direction. We model this force as

$$\vec{F}_D(t) = [F_{DC} + F_{AC}\sin(\omega t)]\hat{y}, \tag{1}$$

with modifiable parameters including a constant component F_{DC}, and a time dependent component with amplitude F_{AC} and frequency $\omega = 2\pi f$. The frequency is scaled in time units, where [finish]. We demonstrate how a single particle (Sec. III A) and many particles move (Sec. **??**) in response to this applied force in a variety of light fields. In Sec. **??** we set F_{DC} to zero and track the motion of a high density area of a particle chain (i.e. kink dynamics).

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 $\vec{F}_{l,i} = \vec{F}_l(\vec{r}_i)$. The landscape potential $V(\vec{r})$ are static, generating a conservative force $\vec{F}_l = -\nabla V_l(\vec{r})$ with fixed minima and maxima that are periodic or quasi-periodic, as described in Sec. III. In every simulation, we confine the particles to a quasi-one-dimensional geometry using

$$V_{q1D} = V_0 \cos(\pi x/L) \tag{2}$$

.

One example of a periodic light field is where

$$V_l = V_0 \cos(N_p \pi y/L) \tag{3}$$

where N_p are the number of troughs in the landscape, and V_0 is an adjustable parameter to set the depth of the troughs.

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

$$V_{ij}(r_{ij}) = \frac{E_0}{r_{ij}} e^{-\kappa r_{ij}}, \tag{4}$$

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 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.

We model the particle dynamics with an overdamped equation of motion integrated with the Verlet method. Here the suspending fluid is highly viscous and exerts a damping force on the particles equivalent to a linear drag force. The damping comes from a viscous fluid model providing a nonconservative force, modeled as a linear friction $F_{drag} = -\eta\vec{v}_i$ sufficient so that the acceleration of the particle is zero. [This model is encountered in Ch. 2 of Taylor's Classical Mechanics....]

A single particle has the equation of motion

$$\eta\vec{v}_i = \vec{F}_{l,i} + \sum_{i\neq j}^{N} \vec{F}_{ij} + \vec{F}_D(t). \tag{5}$$

where $\eta = 1$. The equation of motion provides a direct calculation of the velocity of an individual particle from its location. Since we model the acceleration $\vec{a}$ as zero, the Verlet method simplifies to the Euler method, which is used to calculate the position.

$$\vec{r}_i(t + \Delta t) = \vec{v}_i(t)\Delta t + \vec{r}_i(t). \tag{6}$$

III. RESULTS

A. Single particle system

We place a single particle in a periodic light field is

$$V_l = V_{0x} \cos(\pi x/L) + V_{0y} \cos(N_p \pi y/L) \tag{7}$$

where $N_p = 20$ are the number of troughs in the landscape, and $V_{0x} = 2$ and $V_{0x} = 2$.

We used our model to generate a system, Fig. 1(a), 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.

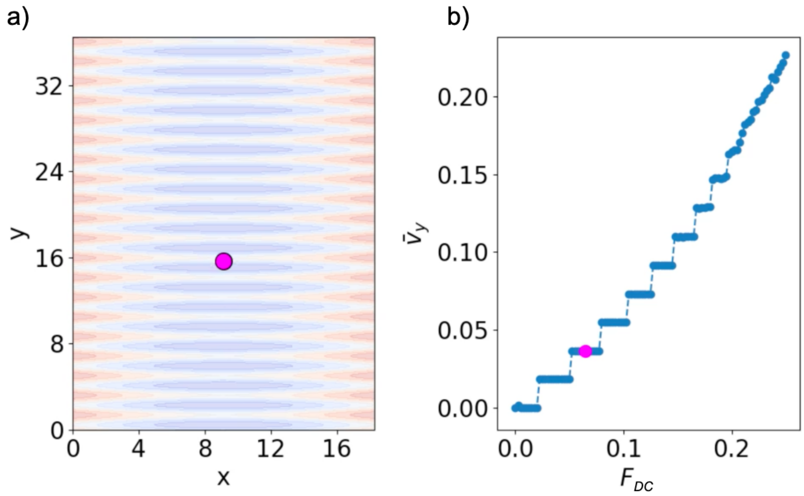

FIG. 1: **(a)** The particle is driven with a constant F_{AC} and f through a periodic potential landscape where blue are minima and red are maxima in the potential. **(b)** An average particle velocity in the y-direction $\bar{v}_y$ as a function of the driving force F_{DC}. In the animation the magenta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

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 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.

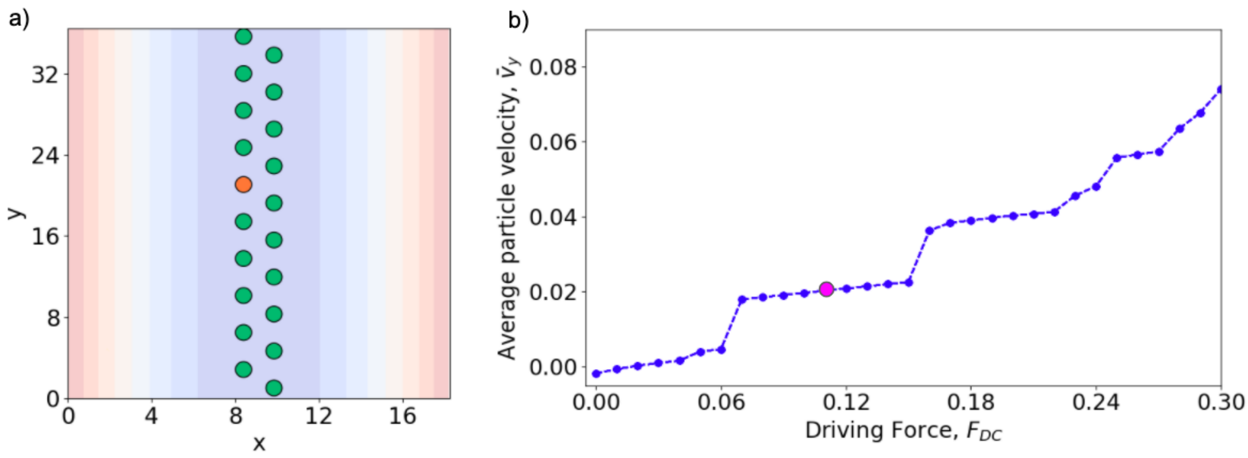

FIG. 2: **(a)** The orange particle is driven with a constant F_{AC} and f through 19 particles, colored green, confined by a quasi one-dimensional channel. The landscape is colored as in Fig. 1. **(b)** $\bar{v}_y$ versus F_{DC}, where $\bar{v}_y$ is the average particle velocity of the driven particle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

C. Kinked system

We confine N particles to $N-1$ troughs to create a local high density region. $F_{DC}/F_{AC} = 1$ [CHECK!]

IV. QUASIPERIODIC SUBSTRATE

V. CHAOTIC DYNAMICS

VI. ASSOCIATED PROBLEMS

VII. CONCLUSION

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* Electronic address: guer9330@pacificu.edu

† Electronic address: mcdermott@pacific.edu

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