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 external applied force. Using numerical simulations we control the particle interactions, external force and confining environment in order to mimick experimental studies of driven colloidal particles confined by light-fields. The molecular dynamics simulations use overdamped equations of motion suitable for a viscous suspension of microscopic particles to model the dynamics. We observe particle synchronization under a variety of conditions, including static and dynamic patterns formed on periodic and quasiperiod substrates and the propagation of high density regions of particles, or kinks. 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 also explore the limits of applied force that cause the dynamics to transition to chaotic behavior. We include sample code and exercises for students with 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

Synchronization is a universal phenomena that can be modeled with numerical studies of confined, driven particles. Examples of synchronization occur in many naturally oscillating systems, from Huygens 1665 observation of in-phase oscillation of pendulum clocks[?] , to fireflies signaling in time with a pulsed light emitting diode, to coordinated flapping of birds wings, to simultaneous neuronal firing in cardiac muscle and brain tissue.

Dynamical mode locking is a controlled synchronization phenomena in which an external driving force causes weakly coupled oscillators to come into phase. Mode locking is often observed in quantum electronic devices such as Josephson junctions and phase-locked current loops. Instead of ohmic current-voltage (I-V) relationships, such devices exhibit stepped regions such as Shapiro steps [explain].

Recent experiments of colloidal particles confined in optical traps subject to external driving forces have been used to examine the microscopic dynamics of mode-locking[1]. Colloidal particles trapped in light fields are a particularly useful medium for studying complex dynamical behaviors. The relatively large size of the colloids (micrometers) makes colloids easy to control and image, and the interaction forces between colloids can be modified by tuning the chemistry of the suspending fluid or surface ligands of the colloidal particles[?] . This ease in control of colloids has lead to a rich array of experimental results considered models for experimental systems relatively hard to access and visualize, such as cold atoms or electron gases.

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 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]. 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.

The dynamics of particles subject to an applied external force apply to many physical systems. For instance the flow of charges in a conductor, or cells responding to a chemical gradient. The external force increases the diversity of dynamical behaviors, and can cause particles to flow in a variety of non-linear complex patterns that may be synchronized. Disordered chaotic dynamics are also possible, where irregular, unpredictable time evolution of nonlinear systems and occurs in mechanical oscillators[?] .

Numerical modeling of colloids can provide mechanistic insight that can be difficult to achieve in experimental conditions where Brownian motion and other sources of noise dominate. [elaborate]

In this work, we perform numerical simulations of confined, driven particles to model a variety of physical phenomena. In the following paper we describe our molecular dynamics model in Section II. We include code to simulate and visualize the dynamics in this section and supplementary material. In Section III we summarize our results, including synchronized motion of a single confined particle driven across a periodic landscape in Section III A and multiple interacting particles in Section III B, including stationary propagation of high density kinks in Sec. III C. We present these results using standard tools of non-linear oscillators such phase diagrams of velocity versus position. In Section IV, we show how an aperiodic landscape modifies the particle dynamics. Finally we explore the transition to chaotic dynamics in Section V and conclude in Section VII. In each section we suggest exercises for interested students, as summarized in Section VI.

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 $L = 36.5a_0$ where a_0 is a dimensionless unit of length. 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 $x_i + L = x_i$ and $y_i + L = y_i$. The units of the simulated variables are in Table I.

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

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

TABLE I: Simulation units defined in the code.

Quantity	Unit
length	a_0
energy	$E_0 = q^2 Z^{*2}/4\pi\epsilon\epsilon_0 a_0$
dimensionless interaction strength	q
effective colloidal charge	Z^*
solvent dielectic constant	$\epsilon\epsilon_0$
force	E_0/a_0
viscosity/damping constant	η
time	η/E_0
velocity	$E_0/\eta a_0$

where particle i and j are distance $r_{ij} = |\vec{r}_i - \vec{r}_j|$ apart. This screened Coulomb potential is scaled in terms of energy unit E_0 defined in Table I. $\kappa = 1/R_0$ is the screening parameter that describes the lengthscale at which particles interact. We fix R_0 to be a_0. In experiments charge screening is observed due to ions in the suspending fluid and the charges of surrounding particles which reduces the interaction range of individual particles. Because the particles interact over short ranges, the numerical models can be run efficiency using a neighbor list algorithm determined using a cell method. [explain!]

Particles are subject an external time-dependent driving force $\vec{F}_D(t)$ applied parallel to the y-direction. We model this force as

$$\vec{F}_D(t) = [F_{DC} + F_{AC}\sin(\omega t)]\hat{y}, \tag{2}$$

with modifiable parameters including a constant component F_{DC}, and a time dependent component with amplitude F_{AC} and frequency $\omega = 2\pi f$.

We use several model enviroments to confine the particles, assuming the confining force arises from a potential function $\vec{F}_l(\vec{r}) = -\nabla V_l(\vec{r})$. The landscape potential $V(\vec{r})$ are static with fixed minima and maxima that are periodic or quasi-periodic, as described in Sec. III. In multi-particle simulations, we confine the particles along the $x-$direction using a periodic function

$$V_{q1D}(x) = V_0 \cos(\pi x/L) \tag{3}$$

. This channel potential keeps the particles interacting at short range confined primarily to motion along the y-direction but allows for some lateral motion of particles. This is sometimes referred to as a quasi-one-dimensional geometry.

The simulation is controlled by a $for()$ loop which runs from an initial to maximum $time$ integer. Each integer timestep represents a simulation time of $\Delta t = 0.001$. At each timestep we evaluate the net force on each particle as a function of its position $\vec{r}_i(t)$ and then integrate the equation of motion to move particles to an updated position $\vec{r}_i(t + \Delta t)$. The integration is simple because we model the particle dynamics with an overdamped equation of motion. The damping comes from a viscous fluid model providing a nonconservative force, modeled as a linear friction $\vec{F}_{drag} = -\eta\vec{v}_i$ sufficient so that the acceleration of the particle is zero. Such a model is appropriate when the particles are small and the viscosity is high [finish... reference...] This model should be familiar to readers modeling Milliken's oil drops in a standard classical mechanics text[?] .

A particle has the equation of motion

$$\eta\vec{v}_i = \vec{F}_{l,i} + \sum_{i \neq j}^{N} \vec{F}_{ij} + \vec{F}_D(t). \tag{4}$$

where $\eta = 1$. The equation of motion provides a direct calculation of the velocity of an individual particle from its location in the simulation with respect to other particles j. Since the acceleration as zero, the Verlet method simplifies to the Euler method, which is used to calculate the position at subsequent time steps.

$$\vec{r}_i(t + \Delta t) = \vec{v}_i(t)\Delta t + \vec{r}_i(t). \tag{5}$$

III. RESULTS

We demonstrate how a single particle (Sec. III A) and many particles move (Sec. III B) in response to this applied force in a variety of environments. In Sec. III C we set F_{DC} to zero and track the motion of a high density area of a particle chain (i.e. kink dynamics).

A. Single particle system

We drive a single particle across a periodic landscape along the y-direction

$$V_l(y) = V_{0y} \cos\left(N_p \pi y / L\right) \tag{6}$$

with $N_p = 20$ troughs in the landscape. This is illustrated in Fig. 2(a) where the red (blue) regions show local maxima (minima). The code for generating a two dimensional colored plot of the potential landscape is calculated by evaluating the analytic function in Eq. 7 for a grid of values (x_n, y_n). The numerical implementation of the landscape is calculated with

$$F_y(y) = F_{0y} \sin\left(N_p \pi y / L\right) \tag{7}$$

where $F_{0y} = 0.1$. We drive the particle with $F_{AC} = 0.2$, $F_{DC} = 0.01$, and $f = 0.01$ cycles per time unit. When the superposition of F_{AC} and F_{DC} is large enough to overcome the barrier height of the landscape troughs, the particle hops between troughs in the energy landscape. In Fig. 1 we show the relationship between the applied force and particle position. In Fig. 1(a) we plot the applied driving force as a function of time and in Fig. 1(b) we show the position of the particle as a function of time. The initial position is near $y = 0$ and the initial driving force is minimum $F_D(t = 0) = F_{DC}$. Over the time period $T/2 = 50$ the particle moves in the positive y-direction while $F_D(t) > 0$ through three substrate troughs, reaching a maximum of $y/\lambda = 3$. When $F_D(t) < 0$ the particle moves in the negative y-direction reaching a minimum position of $y/\lambda = 1$ over the period $T = 1/f = 100$. The average velocity $\bar{v}_y$ is the average displacement $\Delta y = y(t_0 + T) - y(t_0)$ over the period of the driving force. In Fig. 1 the displacement is a single wavelength of the substrate $y(t_0+T)-y(t_0) = \lambda$. Thus the average velocity is $\bar{v}_y = \lambda f$, where $T = 1/f$.

The hopping pattern of the driven particle is periodic, and could be achieved over a range of F_{DC}. We explore the ranges of periodic hopping patterns by increasing F_{DC} as a function of time, as shown in Fig. 2. We apply an external applied force, with a constant F_{AC} with frequency $\omega = 2\pi f$ then slowly increase F_{DC} at a rate of $\Delta F_{DC} = 0.001$ every $\Delta t = 4000$ integer timesteps or 40 time units. By modifying F_{DC} we achieve a variety of oscillation 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}. We illustrate mode-locking in the velocity-force plot in Fig. 2(b). Here $\bar{v}_y$ is increasing in non-uniform steps, with a quantized height of $\bar{v}_y = n\lambda f$, where n is an integer, $\lambda = S_Y/N_p = 36.5/20 = 1.825$ is the spatial period, or wavelength of the landscape, and $f = 0.01$ cycles per time unit.

Our simulations reproduce results presented in Juniper *et al.*[1] which demonstrated mode locking in experiments of driven colloids on a optical periodic landscape.

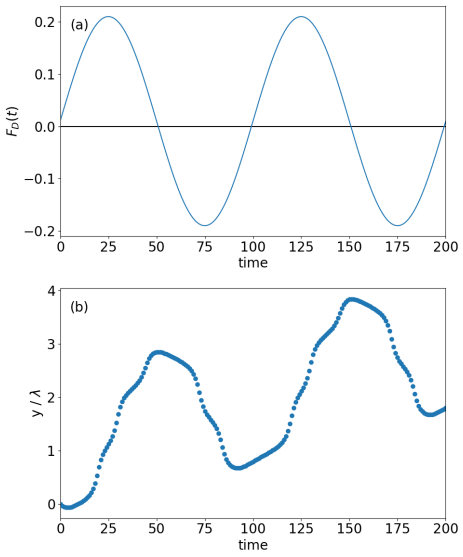

FIG. 1: The position as a function of time of a single driven particle normalized by the period of the substrate λ.

We illustrate the hopping pattern in Fig. 2(b) and show the dynamics in supplementary materials[2].

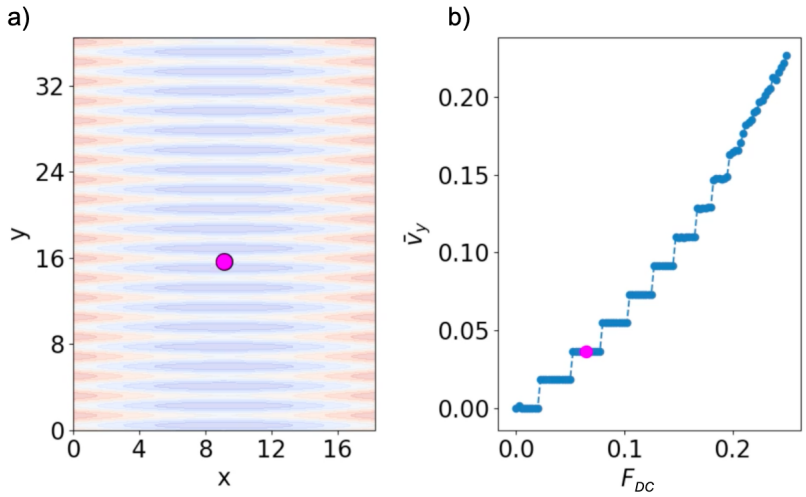

FIG. 2: **(a)** The particle is driven with a constant amplitude F_{AC} and frequency ω through a periodic spatial potential landscape. The landscape is represented with a colormap where blue are minima and red are maxima in the potential. **(b)** An average particle velocity in the y-direction $\bar{v}_y$ as a function of a constant driving force F_{DC}. In the animation available in Ref.[2] the magenta dot represents the average velocity of the particle $\bar{v}_y$ at which the particle in Fig. 1(a) is moving.

B. Synchronization in multi-particle systems

We simulated a twenty particle system confined to a narrow channel, as shown in Fig. 2a). We create the confining channel with a sinusoidal function with a single period.

$$V_l(x) = V_{0x} \cos(\pi x/L) \tag{8}$$

where the trough heights is larger V_{0x}, and the associated force

$$\vec{F} = -\nabla V(x) = -\frac{dV}{dx}\hat{x} = -\frac{V_{0x}\pi}{L} \sin(\pi x/L)\hat{x} \tag{9}$$

restores particles to the center of a long narrow region of the simulation. The landscape is illustrated in Fig. 3(a) where red regions are high potential and blue regions are low potential.

The initial configuration of the system is shown in Fig. 3(a). We annealed the system into a ground-state configuration by raising the system to a high temperature T, and slowly lowering the temperature in steps of $dT = -0.01$ until the particles form a buckled chain in the low region of the channel due to the competition between particle repulsion and channel confinement. The interparticle forces between neighboring particles cause the system to form a buckled chain. The molecular dynamics of simulated annealing is described in Ref. **??**, and presented simulations begin with particle configurations that result from the annealing process, as listed in Appendix [ref] and available in supplementary material.

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.

C. Kinked system

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

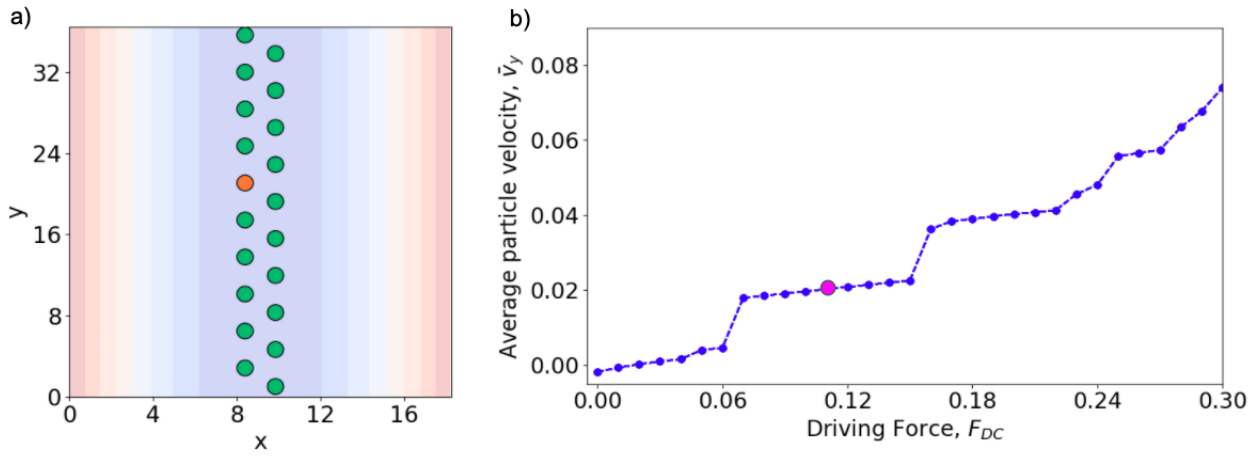

FIG. 3: **(a)** A single particle (colored orange - mark in some manner for non-color views) is driven with a constant amplitude F_{AC} and frequency ω through 19 neighboring particles (colored green - mark differently) confined by a quasi one-dimensional channel. The landscape is colored as in Fig. **??**(a). **(b)** Average $\bar{v}_y$ versus F_{DC}, where $\bar{v}_y$ is the average particle velocity of the driven particle in the y-direction.

IV. QUASIPERIODIC SUBSTRATE

V. CHAOTIC DYNAMICS

VI. ASSOCIATED PROBLEMS

VII. CONCLUSION

VIII. SUPPLEMENTARY MATERIALS

A. Gridded Contour Plot of landscape

```
############################################################
#ADD CONTOUR PLOT
############################################################
def add_contour(ax,L,N,corrugated = True):
    '''
    Hardwired to color in the quasi1D potential to contain
```

```
the particles in a trough.
Can also add the washboard/corrugated substrate.

Required Arguments

Optional Arguments:

corrugated (default = True)
Adds the washboard in the y-direction.
Hardwired for a single parameter set.
'''

a_p = L/N

#assuming Tiare's trough system, so we won't want to cover the entire range
X = np.arange(0, L/2.0, 0.1)
Y = np.arange(0, L, 0.1)
X, Y = np.meshgrid(X, Y)

Z_mag = 2.0 # set by what "looks good"
Z = Z_mag*np.sin(2*np.pi*X/L)
if corrugated == True:
    Z += np.sin(2*np.pi*(Y+1.75)/a_p)

cmap=cm.coolwarm_r

#alphs is the degree of transparency, again, set by what looks good.
cset = ax.contourf(X, Y, Z, cmap=cmap,alpha=0.25)

#ax1.set_xlim(15,20)
#ax1.set_ylim(15,20)
```

```
    #ax1.set_xlabel(r"$X$")
    #ax1.set_ylabel(r"$y$",rotation='horizontal',ha='right')

    #ax1.set_xticks([])
    #ax1.set_yticks([])
    return
```

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[1] M. P. N. Juniper, A. V. Straube, R. Besseling, D. G. A. L. Aarts, and R. P. A. Dullens, Microscopic dynamics of synchronization in driven colloids. Nat. Commun. 6, 7187 (2015).

[2] See Figure1.mp4 in appropriate