Non-equilibrium dynamics as polymer conformations

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1 Introduction

2 Smarticles

We conducted our experiments with a collection of small simple robots called "Smarticles" (smart active particles) (fig. 1). Each one is comprised of three connected links, with the two hinges being controlled by a programmable micro-controller via stepper motors. When the Smarticle is sitting on its base, the arms do not touch the ground, and so an individual smarticle cannot move. A

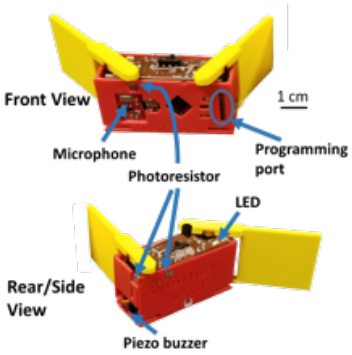


Figure 1: *[label base]* single smarticle with various sensors labelled

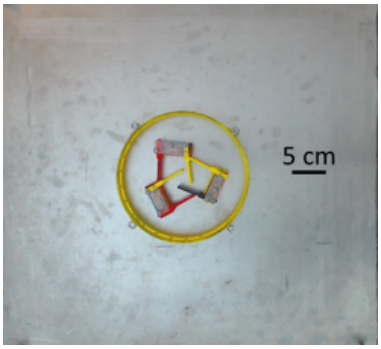


Figure 2: View from above. Regular state testing setup. The whole setup placed on an aluminum plate leveled to $< 0.1°$. The ring is 19.2 cm in diameter, and is glued to the plate below such that it cannot move or deform. The smarticles perform a square gait locked in phase with each other.

group of them, on the other hand, can achieve complex motion by pushing off each other. Here we will focus on the regime where their arms are executing a periodic motion pattern, which we call "gait," with no feedback from the environment (note that the gait timing is kept by the controller, and hence the cycle's phase is not affected by forces on the arms). Such gaits can be represented (uniquely up to rate) as closed loops in the two-dimensional conformation space (the two hinge angles) of the Smarticle (fig. 1). In the first part of the paper, we will have all Smarticles execute a synchronized "square" gait (fig. 1). *[Include all the technical details of realization and construction of Smarticles and synchronization in an appendix?]*

We place three Smarticles on a flat aluminium plate, inside a glued-down plastic ring (fig. 2). By moving their arms, the robots can push off each other, while the ring prevents them from decoupling – thus forming an optimal play-ground to look for dynamical emergence. To get data, we use Optitrack *[details]* to track the full time-evolution of the 2D coordinates and body-angle (x, y, θ) of each robot at 120 frames per second (we do not track the arm positions).

For experiment prototyping and better sampling statistics, we have also built a simulation of this setup, described in Appendix B, and benchmarked it against experiments. Both experimental and simulation data are then fed through a pre-processing pipe-line, which mods out the rotation and permutation symmetries of the 3-Smarticle setup, thus reducing the effective configuration space substantially (Appendix A).

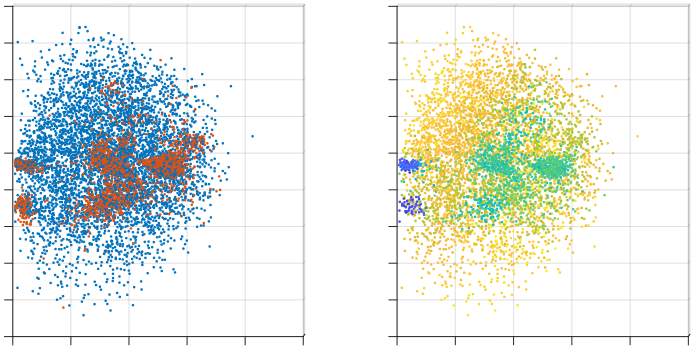


Figure 3: Stroboscopic, 3D projection resolving clusters, of some function of the 9D space (see A), ordered v null, color by delta over one period

3 Regularization

When all the Smarticles are executing a phase-synchronized square gait, the triplet typically organizes into one of several periodic dynamical patterns (a sort of collective organized dance) *[videos in supplement]*. Figure 3 gives some illustration of the fine-tuning. Such self-organization is perplexing, and its interpretation depends on the perspective we take – that of dynamical systems theory, or thermodynamics.

From the context of dynamical systems, perhaps it is not surprising that the dynamics of a time-periodic system are governed by several limit-cycle attractors. On the other hand, not all periodic systems relax to such attractors – even here we can make slight changes to our setup, such as changing relative gait phases, or making Smarticles inertial *[figures for this here?]*, so as to make the system behave chaotically. Furthermore, this system cannot really be seen as deterministic, as we know that it is strongly affected by the stochasticity coming from the hard-boundary interactions between non-smooth shapes, and highly surface-sensitive effects of sliding friction.

From the perspective of equilibrium thermodynamics, where entropy and disorder tend to a maximum, this sort of self-organization may seem extremely surprising. Of course, this system is far from equilibrium, and so entropy need not grow. Indeed, for a Brownian particle diffusing in a compact domain of inhomogeneous temperature $T(\vec{x})$ (and no other forces), we know that the steady-state probability distribution will be $p_{s.s.} \propto 1/T(\vec{x})$ – which is far from the maximum-entropy uniform distribution. We want to use this example to motivate our explanation of the fine-tuning we observe.

While we could try to go into a mechanistic explanation for the self-organization in our setup, it would likely be very specific to the parameters and choices used here and would not generalize well to other configurations of Smarticles, or to other active matter systems. Instead, we want to give a less fundamental, but more generalizable explanation. We note that for most initial configurations of the three Smarticles in a ring, after one period of arm motion they go to a new configuration. For some specific configurations, however, they stay in the same place – and these are precisely the periodic limit-cycle attractors we see in any long trajectory (fig. 3). This may at first seem tautological: at long times the system tends to be found in places from where it does not leave. The rest of the paper will be explaining why this is both, highly non-trivial in a precise mathematical sense, and also profound for understanding real-world strongly-driven systems *[references to sections]*.

[not synchronization]

A Identifying dynamical phases from data

Once we have the tracked coordinates of the smarticles, we want to map the data into a "collective behavior space" – something that can usefully inform us about the dynamical patterns of motion, especially those relevant for slow time-scales. This behavior space will typically be very high-dimensional, and to work with it we try to either cluster the data into different discrete behaviors (or dynamical phases), or perform a dimensionality-reduction to embed the data in a 2 or 3 dimensional space we can visualize (and could subsequently cluster if desired). In either case, what we care about is not the location of points in behavior space (which would be arbitrary anyway), but only about the distances between them – i.e., some measures of similarity of different behaviors.

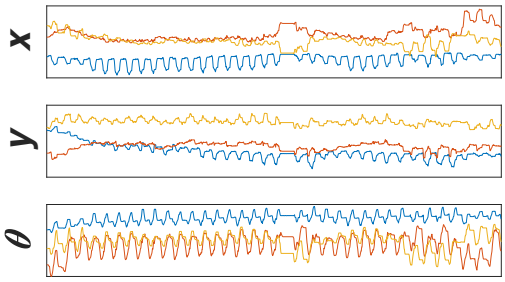
The raw data from particle tracking gives position and orientation time-traces $(x_i(t), y_i(t), \theta_i(t))$ for each smarticle (fig. 4a), and contains lots of information that is irrelevant for the questions we care about. The first challenge in dealing with this is to chose a set of macroscopic observables of interest (such as collective angular velocity, or average pressure on the walls perhaps). We can then study the well-posed question of how much the different pieces of measured data affect these observables. In principle, understanding this would allow us to define a distance metric on our data space that we could then use for clustering or dimensionality reduction. There are some pieces of data which we know, from first principles, to be entirely irrelevant – corresponding to symmetries in the system. In the simplest setup, these are global rotation symmetry, and smarticle permutation symmetry. Thus, two configurations that differ only by a permutation of smarticles should be considered to have distance =0. While these exact symmetries show us which data is entirely irrelevant, the biggest challenge is in identifying the relative importance of the remaining data for our questions.

Doing this exactly is an insurmountable feat, and so we must resort to reasonable approximations. While constructing such approximations is in general a rich and interesting problem, here we simply use a reasonable heuristic based on some physical intuitions.

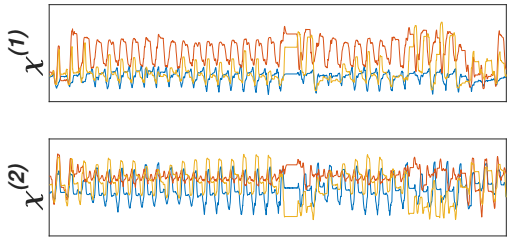
A.1 Modding out symmetries

We begin by constructing functions of the raw data that are invariant under the symmetries we mentioned, but still sensitive to the information we may care about. The two symmetries are global rotations and permutation. To take care of the first, we find the coordinates of the c.o.m. $\vec{X} = \frac{1}{3}\sum_i \vec{x}_i$ (note: permutation invariant) in the reference frame of each smarticle: $\vec{\chi}_i \equiv \mathcal{R}(\theta_i)\cdot(\vec{X} - \vec{x}_i)$, where $\mathcal{R}(\theta_i)$ is the rotation matrix for i-th smarticle (fig 4b). Note that this is not a perfect choice: it is entirely invariant under c.o.m. translations (which is relevant, but we assume it to be small for a confined system), and smarticle orientation matters more the further it is from c.o.m. (so we must assume that their distance to c.o.m. stays relatively constant). We can often get away with such imperfect choices because we have so much overloaded data for the questions.

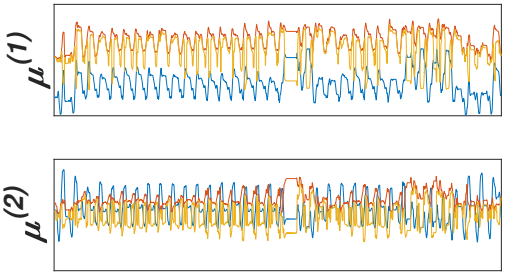
Next, the permutation-invariant functions we choose are just the first three moments of the distribution of the three $\{\chi_i\}$ at any fixed time. In order for these functions to have relatively similar sensitivity to changes in raw data, it helps to ensure that they have the same units – by raising them to the appropriate fractional powers. I.e., $\mu_1 = \frac{1}{3}\sum_i \chi_i$, $\mu_2 = \sqrt{\frac{1}{3}\sum_i (\chi_i - \mu_1)^2}$, $\mu_3 = \sqrt[3]{\frac{1}{3}\sum_i (\chi_i - \mu_1)^3}$ (fig. 4c). Note also that up to 3, these are the same as the cumulants – which may be a better alternative for more smarticles.



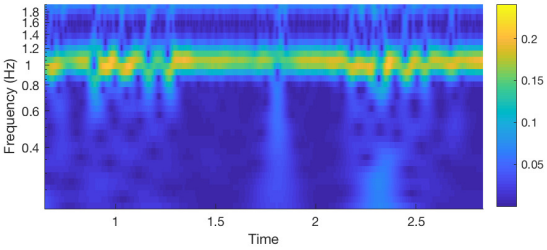
(a) Smarticle coordinates and angles as tracked from experiments



(b) Rotationally invariant observables: c.o.m. coordinate as seen in the reference frame of each smarticle



(c) Permutation invariant observables: first 3 moments of the distributions in 4b



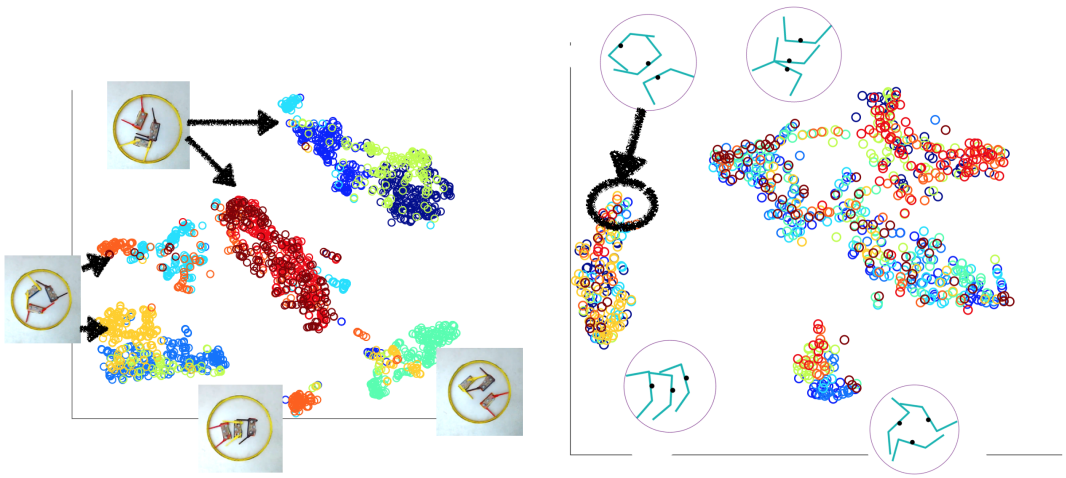
(d) Wavelet transform of one of the curves in 4c. We choose the values along the bright line for our feature vector.

Figure 4: Data processing steps

A.2 Capturing dynamics

Now we can proceed to dealing with the fact that behaviors we are looking for are dynamic states, and thus depend on multiple time-points. We thus want to construct some feature vector that captures the dynamics. The simplest idea of simply stacking μ_i at different time-points on top of each other is not obviously wrong, but will give a feature vector that is very sensitive to the noise. Instead, the dynamical features we are looking for are better captured by Fourier modes. Further, since the dynamical phase can change on the time-scale of a few arm oscillations, we don't want to transform the entire time-series, but instead consider a continuous wavelet transform of the data (fig. 4d). This beautifully separates out behaviors on different time-scales, and we can choose our feature vector based on the time-scale(s) we most care about. The simplest choice here is to take the time-scale corresponding to one gait-period – since most of the activity happens there. Again, this is throwing away lots of data, but since at the end we just care about some low-dimensional behavior space, we are still left with more than enough (including other time-scales had little effect).

This way our feature vector consists of 6 complex numbers (3 moments for each dimension of the 2D χ vector). We do care about relative phase of oscillation in the wavelet transform – to keep this in the most unbiased way, we simply take the 36 possible differences between the 6 complex numbers, and then take their absolute value. While this makes the feature vector unnecessarily long, this is fine since we only care about the relative distances between these, and duplicate vector components will simply sum up.



(a) Experiment (b) Simulation

Figure 5: Dimensionally reduced data. Insets show what sort of behavior each cluster corresponds to. Note that the cluster positions in the two plots are unrelated as the 2D embedding was done separately on two data sets. Color indicates different trials of the same experiment – confirming that the behaviors are reproducible.

A.3 Dimensional reduction and clustering

Now that we have our feature vector, we can dimensionally reduce or cluster the data. The former is, in a sense, a "smoother," less dramatic operation, and thus turns out to produce more accurate results. We can understand this by realizing that in either case, the goal is to preserve pair-wise distances as best as possible, and this is much easier to accomplish if you allow points to be placed anywhere in the $\mathbb{R}^2$ plane, rather than in one of 5 discrete states. Curiously, clustering even works better when performed on dimensionally reduced, rather than original data. The other advantage of dimensionally reducing first is that this gives us more information about how the data is distributed, without imposing the assumption that it is well-clustered.

We use Matlab's built-in t-Distributed Stochastic Neighbor Embedding (tSNE) algorithm, which basically tries to embed the data in a 2D space preserving all the pair-wise distances as much as possible (fig. 5a). It has the effect of largely preserving, or even highlighting, clusters in the original data, but also allows visualizing transitions between them and other hierarchical structure in the data. Note that the two pairs of clusters corresponding to the same pictures are chiral complements (the other two clusters correspond to non-chiral states). In section **??** below we will cluster this data and study the slow transition statistics between different dynamical phases.

B Simulation

For easier exploration of hypothesis space of this system, we have constructed a numerical simulation with the following algorithm. We approximate smarticles by three-segment lines (insets in fig. 5b). At each time-step, the algorithm moves the arms slightly according to the chosen gait, and then iteratively cycles through smarticle pairs in random order, checking for collisions, and moving one in each pair slightly according to the net interaction force. If there are multiple points of contact for a given pair, the move is a translation in the direction of the total force, otherwise, it is a

rotation about a pivot point chosen so as to balance the forces and torques. Choosing which in the pair moves is random, weighted by their relative friction coefficients (as motivated by difficulty of predicting static friction). Note that since a move can create new collisions with other smarticles, it is important to take small steps and iterate. The algorithm continues looping through pairs until all collisions are resolved, then proceeding to the next time-step. While this describes the core of the algorithm, there are a number of bells and whistles necessary to improve its stability and reliability:

- If two arms are near-parallel when they approach each other, they can pass through each other between ticks without ever intersecting. To prevent this, along with collision detection, we must explicitly test for this in each pair. We then store the order of the arms for a few ticks into the future to prevent them passing through each other in any of those times.

- In case a smarticle with small friction gets trapped between two others, it might rattle back and forth on each iteration of collision-resolution, with no net effect. To prevent this, we temporarily (until next tick) increase its friction each time a smarticle moves.

- In experiment, when resolving collision is too hard, the motor simply does not move (jams up). To allow for that possibility in simulation, we add an exit condition from the collision-resolving loop for when any one smarticle's temporary friction becomes very large - as this serves as a proxy for how much force a motor must provide. We then move the most colliding arm back to its last time-step, and try collision-resolving again. If everything resolves, that arm will then have a chance to catch up to where it needed to be over the following ticks.

- The resulting simulation turns out to be too clean, and so dynamical phases much more stable than in experiments. Since we want to study transition statistics, we must find ways to destabilize them. There are a number of places we can add noise: slight fluctuations of smarticles' positions and angles at each tick, or on each move, randomly varying gait amplitude, varying arm velocity, etc.

- The ring boundary is implemented similar to other smarticles, and collisions with it are resolved in the same loop. Alternatively, we can implement weakly confining potential to keep smarticles together in a more smooth way.

Even with all these additions, many differences remain between simulation and experiment: smarticles have non-zero thickness in experiments, friction forces between smarticles are often important on collisions, there are relief features on smarticle body not present in simulation that can get caught, and others. The consequence in this system is that while qualitative features can be recovered in the simulation, we don't generally expect quantitative agreement. We guess that these differences may become less important for ensembles with more smarticles – as universal collective properties start to dominate. We also guess that analytical predictive power of least-rattling, or other similar techniques, could be more applicable in that regime.

References