Dissipation Learning in Active Matter

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INTRODUCTION

Active matter is, broadly, a subcategory of condensed matter systems distingushed primarily by energy input homogenously distributed across all constituents (agents) of the system, which in turn set their own self-propelled motion across a medium. The agents therefore have *direct* access to energy, and use it to autonomously propel and direct themselves (with different models and situations allowing for various degrees of freedom) [1]. The study of active matter is generally grounded in (but not limited to) observed behaviour of biological agents, as they are the primary (though not only) examples of active matter in nature.

The evident motivation in studying active matter is that it helps understand biological behaviours, and therefore the world of living organisms, where energy is constantly dissipated in order to perform various biological functions. Macroscopically, the construction of theoretical models can help explain, and to a limited degree predict, the behaviour of animals (such as locusts) undergoing collectively-emergent swarming behaviours (where each animal can be treated as its own autonomous agent, sharing the same generally stable 'rules' of altering speed and orientation while interacting with each other and the environment)[2].

This biological emulation through physical models is not limited to what can be termed 'simple' behaviour; human behaviour can be partially mapped and understood within physically-indexed accounts of autonomous choices within (overtly or suggestively) constrained collective action. Interesting examples are swarming behaviours identified in traffic, crowd disasters and concerts[3]. Note however that physical models are sometimes challenged in literature due to potential oversimplifications, insofar as, for instance, cognitive heuristics (the autonomous individual behaviour of a human) under duress might deal holistically, rather than individually, with other human agents[4]. The issue is that most active matter systems only form individual relationships between agents, and do not account for the way an agent interacts with the group as a whole - the resulting individual behaviour is merely a summation of the agent's response to each other agent around it. There are psychological arguments that this is not the case, and that instead humans might under duress conceptualise crowds as a collective, and take actions in relation to the collective itself. This objection rests on the assumption that this holistic heuristic does not *emerge* from individual relations, of course (in which case mapping relationships strictly between individuals is unproblematic).

These insights lead to the exploration of various models. For flocks of birds, individual cogntive heuristics tend to suffice - self-propelled particles with adaptive movement patterns based on neighbours can accurately reproduce some migrational patterns [5]. Microscopically, active matter models offer insight into understanding how hierarchically-organised emergence happens within cell tissues, and how it may be leveraged by medicine[6]. Bacteria lends a great example for exploring the intertwining of phenomena to be emulated by active matter. Some strains (such as *Bacillus subtilis*) can be modelled using both direct physical interaction (between individuals) and long-distance biochemical signalling (within the collective), with complexity and clustering developing in response to harsh external conditions [7]. The latter interaction is called quorum sensing, the adaptation of the individual to local population density; this has developed into its own active matter branch of individual-to-collective behaviour [8]. Using such models, it is possible to recover the aforementioned human holistic cognitive heuristics [9].

Outside of biology, active matter research serves to emulate, or otherwise learn from, naturally-occurring behaviours in order to analyse a potentially more general thermodynamic framework. Due to the necessarily dissipative use of energy within self-organised agents, and their internally-induced behaviour, active matter is not described by the statistical mechanics of equilibrium states. The question then arises whether, through quantitative computation and qualitative modelling/theorising, the thermodynamic laws of equilibria can be modified and generalised to non-equilibrium states. Exploring how these generalisations would hold as departure from equilibrium through various means is increased is then paramount[10]. These generalisations would, ideally, collapse into the known statistical thermodynamics states within the equilibrium limit. These insights, in turn, would facilitate the creation of synthetic active matter, whose potential, although speculatory, ranges from the biomedical application of nanomachine targeted drug delivery possibilities to the location-mapping application of nanoscopic/microscopic enivronmental sensing[11].

The feature in active matter of converting stored and homogenously available energy, such as chemical potential, into mechanical work is also of great importance to the field: understanding how this can work and how to facilitate, among other things, long-term energy access across the active matter substance is a key pursuit of nanotechnology[12]. Statistical and computational models can lend insight into individual and collective dynamics, and in turn give way to new experimental designs of nano/micromechanical systems.

ACTIVE MATTER MODELS

A few active matter models are briefly presented in this section, each introducing a specific behavioural phe-

nomenon. First, Active Brownian Particles (ABPs) are self-propelled particles (SPPs) interacting strictly through (soft or hard) repulsive collisions and affected by friction within the medium[13]. This model emerges from classical Brownian motion, the latter constituting a stochastic, but passive, system of collisions; unlike active matter systems, Brownian motion has no active supply of energy to the particles, and particles are placed within an energy equilibrium with their surrounding medium, expressed by a fluctuation-dissipation theorem[14]. By contrast, this theorem does not apply to ABPs, since the latter exhibit an autonomous force. The most frequent models have the acting force on and subsequent velocity of the particle be constant, such that terminal velocity is instantly exhibited, although recently there have been generalised extensions which account for deviations from stationary velocity[14].

Second, (AOUPs and MODEL B)

PERSISTENT EXCLUSION PROCESS

A method of emulating particle behaviour are *lattice models*: these suppress the pseudo-infinite location possibilities (only limited by floating point operators) to an established positional grid. This grid is discrete, and as a result represents a limitation of the position degree of freedom, in the interests of better tracking interactive behaviour.

There are two important principles that can be applied to lattice models: the zero range process (ZRP) and the simple exclusion interaction (SEI). The former is concerned with movement - an integer number of particles can occupy a site, and each particle can 'hop' to a neighbouring site at a rate that usually scales in some way with the amount of particles present in the site it is leaving[15]. The latter, on the other hand, is concerned with prohibiting movement - it broadly forbids a particle from occupying a lattice site that is already occupied[16].

Taking the above principles and applying a run-and-tumble behavioural pattern to the particles - wherein they have a certain speed distribution and a 'tumbling rate' which can periodically cause them to change orientation - we obtain the **persistence exclusion process** (PEP). It is essentially a single-occupancy, multi-particle lattice structure with autonomous orientation changing and proppulsion that operates without velocity-altering collision: a particle maintains its speed and orientation upon contact, but it does not move or push the particle it is facing towards. There are a few alterable properties: the density ρ of the system alongside the lattice size N (the latter naturally influencing the former), as well as the tumbling probability P_{tumble}, which influences departure from equilibrium[17].

The main background results of this experiment were achieved by Soto and Golestanian, in their one and two-dimensional application of PEP. They showed clustering behaviour occurring under three processes: cluster formation through particle collision, cluster growth by absorbing new particles at boundaries, and cluster reduction through 'evaporation' at boundaries, as particles tumble outwards and away from the structure[17]. Quantitative analysis of cluster size distributions and persistence length-dependent cluster formation alongside statistical analysis of overlap functions and stopping times was also thoroughly done[17].

CURRENT PROGRESS

The current goal of this project has been to experiment with and modify in-house PEP code in order to contrast and compare with the Soto and Golestanian analysis mentioned above. The in-house code is a hybrid Python-C two-dimensional application of persistent exclusion process as outlined in the above section. As it stands, the tumbling rate P_{tumble} and density ρ have been tuned to experiment with how the system distribution qualitatively changes. A quantitative display can be seen in Figure 1, which presents a 3x5 grid variation of density and tumbling rate, with the lattice site number kept constant (128x128). It is at this point useful to define the following relation between density ρ, total site number N_{total} and total particle number N_p:

$$N_p = \rho N_{total} = \rho N_x N_y$$

where N_x and N_y are the number of lattice sites along the horizontal and vertical directions, respectively. Density is thus defined through lattice square units.

Some qualitative analysis can be derived from Figure 1. At low densities, no meaningful clustering occurs irrespective of P_{tumble}, as there are not enough particles occupying the sites: $N_p \ll N_{total}$. At very high densities (where $N_p < N_{total}$ still), clusters are not meaningfully separated from each other - this is the range of percolation. For intermediate densities, clustering occurs with a sufficiently small P_{tumble}, and in fact the cluster sizes scale inversely-proportional with the tumbling rate. Too high a P_{tumble} will not allow clustering to form, as there is not enough time for outer particles to confine inner particles before direction is changed as the emerging cluster is dissipated. In Soto and Golestanian's terms[17], the clusters require a certain tumbling rate (dependent on the total system density) in order to form, and once formed, in order to statistically balance out the cluster evaporation with cluster growth.

Having obtained snapshots (as well as animations) of PEP simulations, basic cluster analysis could then be conducted. Such a process is shown in Figure 2, for $\rho = 0.3$ and $P_{tumble} = 0.157$, still keeping N_{total} as 128x128. The snapshot is already sorted using a colour map by orientation (with the background being set to black), and its colour map is converted to colour particles by the cluster they belong to - these clusters are delimited by the adjacency of vertical or horizontal neighbours. The obtained separated clusters are then mapped in a histogram against their size, fitted logarithmically in base 2. They seem to somewhat match the results

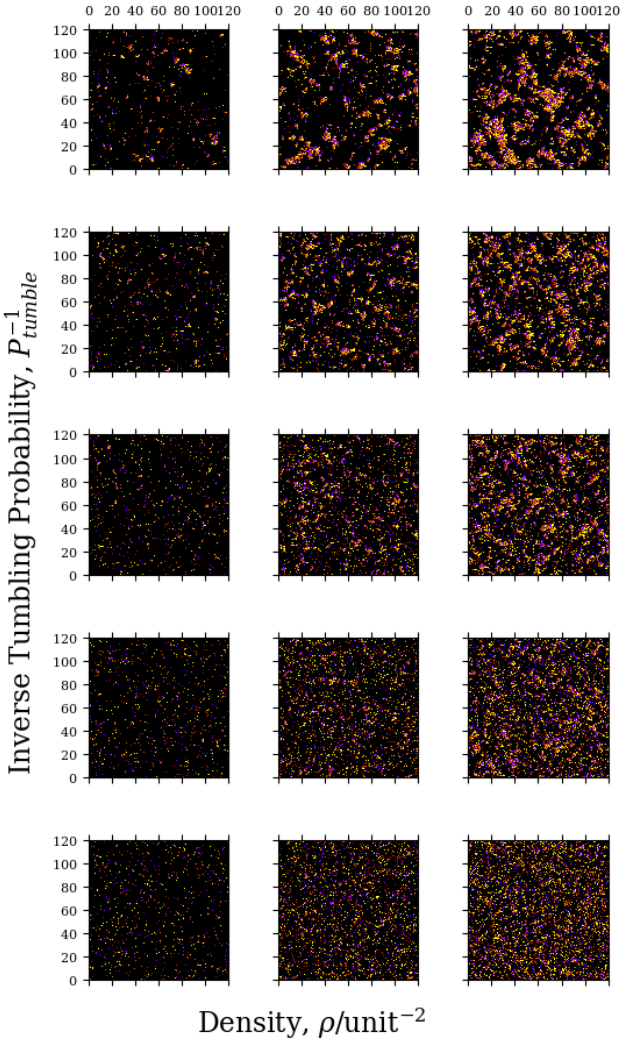

FIG. 1. Grid plot of 2D persistent exclusion process snapshots taken at the same time with varying densities (increasing from left to right) and tumbling probabilities (increasing downwards). Particle colours represent orientation.

in Soto and Golestanian's paper[17], though more analysis is required.

We can also chart how the mean total orientation of the system varies with time.

DISCUSSION AND PLANS

There is significant improvement to be done. We have recently discovered that the tumbling rate has an equal probability of tumbling into any of the four directions - effectively, there is a 25% chance for the particle to 'tumble forward', effectively not changing orientation. The probability is therefore slightly skewed, and ought to be revised.

MORE DISCUSSION

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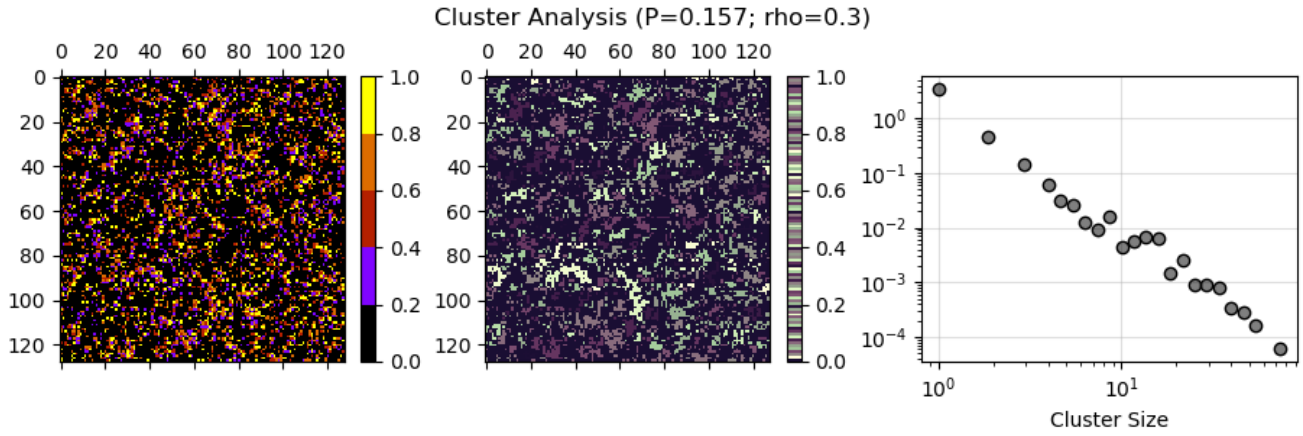

FIG. 2. Three graphs showing cluster analysis method. Graph on the left displays the PEP particles coloured by orientation, as shown by adjacent colour map; graph in the middle colour-codes particles based on clusters they belong to, emphasised by adjacent colour map; graph on the left displays a log fit (base 2) of cluster sizes.