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Nonlinear Collective Dynamics in Active Matter Systems: Studying Self -Propelled Particles and Emergent Phenomena in Complex Systems

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ABSTRACT

One of the most interesting frontiers in the modern nonequilibrium physics concerns active matter systems, i.e. self-propelling entities that constantly convert energy into directed mechanical work. It is a research study on the nonlinear collective behavior of assemblies of active Brownian particles using a hybrid computational and theoretical methodology comprising large-scale agent-based simulations of N = 10,000 self-propelled particles, continuum field theory analysis and machine learning-aided phase classification. Systematic parameter sweeps of Peclet number, noise intensity and area fraction showed that there exist five structurally and dynamically distinct collective phases, viz. disordered gas, polar banded state, polar liquid, motility-induced phase separation cluster phase, and active glass. The polar liquid phase with almost unity orientational order with a 38.6-fold effective diffusivity increase compared to passive Brownian motion, and the super-Poissonian density fluctuation scaling of the motility induced cluster phase with variance 22.7 times the Poisson baseline both indicated the fundamentally nonequilibrium nature of active clustering. Measured transport exponents spanning a vast range (deeply sub diffusive 8 -1 = 0.38) in the active glass to the ballistic (8 -1 = 1.92) in the polar liquid were quantitative traces of mapping the

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transport landscape of the whole phase diagram. The multi-scale nature of active spatial organization was determined by lengths of spatial correlation ranging almost two orders of magnitude - between 1.2 particle diameters in the disordered gas and 120 particle diameters in the cluster phase. A convolutional neural network classifier had a macro-averaged classification accuracy of 94.7% on all five phases, and the confusion patterns were physically understandable in locations that are true phase boundaries. The presented results contribute to the mechanistic insight into emergent collective behavior in active matter and put in a quantitative perspective applications in biological collective motion, active material engineering, and microfluidic transport design.

Keywords: Active matter, Self-propelled Particles, Nonlinear Collective Dynamics, Motility-Induced Phase Separation.

Introduction

Active matter systems can be considered one of the most interesting frontiers in modern physics and biophysics, and consist of the collective behavior of self-propelled objects that transform their surroundings into directed mechanical work continuously. In contrast to standard equilibrium systems, active matter is driven far out of thermodynamic equilibrium and a rich collection of nonlinear and emergent processes and phenomena that interfere with classical statistical physics arises (Marchetti et al., 2022). The scale of these systems spans an incredible spectrum, starting with subcellular cytoskeleton network and bacterial colony to flocking birds, schooling fish, and even human crowds, all of which have in common the key feature of autonomous propulsion and the interactions between agents (Alert & Trepat, 2022).

Self-propelled particles (SPPs) have now become a key paradigm in understanding the macroscopic behaviour of the order of microscopic motility rules. Theoretical milestones like the Vicsek model have shown that a generic manifestation of the local alignment interactions of polar particles under simple conditions can spontaneously produce a large-scale orientational order, which is similar to ferromagnetic phase transitions but has a very different nonequilibrium nature (Chate, 2023). Recent more theoretical developments have shown that the associated ordering

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transitions are also accompanied by anomalous fluctuations, giant number fluctuations, and propagating density waves that do not fit into equilibrium universality classes (Großmann et al., 2023). Such observations highlight the importance of nonlinear theories to the description of the complexity of active collective behavior.

Active matter emergent phenomena are especially interesting since they do not rely on any global organization of interactions but are only produced by local interactions. One of the most impressive examples is motility-induced phase separation (MIPS): in this case, completely repulsive self-propelled particles spontaneously form dense clusters and gas dilute phases, which do not have an equilibrium counterpart (Caprini et al., 2023). Likewise, active Numatics topological defects have been demonstrated to self-organize and autonomously flow, as well as display lifelike motility behaviors, and have found surprising connections to both soft condensed matter physics and biological morphogenesis (Doostmohammadi & Aranson, 2022). Activity, confinement geometry, and inter-particle interactions interact to produce many different dynamical states such as turbulent-like active flows, spontaneous oscillations and traveling bands.

The recent developments in experimental microfluidics and single-particle tracking have given the highest level of resolution to the stochastic dynamics of an individual active agent and group transitions. The dynamics of dense bacterial suspensions has been experimentally studied to find the role of run-and-tumble in the creation of non-Gaussian displacement statistics and anomalous diffusion, which require generalization of the Langevin (beyond Brownian) description (Patteson et al., 2022). Self-phoretic driven synthetic active colloids have also made it possible to test theoretical predictions particularly in the lowest possible modeling and experimental systems (Shaebani et al., 2023). Such experimental systems provide a perfect backdrop to investigate the effects that activity has on phase behavior, mechanical response and transport properties of dense suspensions.

Active matter dynamics are nonlinear in nature, with the interaction between excluded volume dynamics and hydrodynamic coupling effects alongside orientational

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correlations, creating a glassy dynamics, jamming transitions, and collective oscillatory modes being most evident at the regime of dense systems (Petrelli et al., 2022). Coarse-graining and symmetry-based continuum hydrodynamic theories of active fluids have been able to model the instabilities and pattern-forming behavior of polar and nematic active fluids (Alert et al., 2022). Nonetheless, a research gap persists to bridge these continuum descriptions with particle-level simulations and experimental measurements, especially those that include heterogeneous distributions of activity, complicated boundary conditions, multi-component compositions, etc.

In addition to basic physics, the knowledge of collective phenomena in active matter has very extensive implications in biological and biomedical fields. Epithelial cell monolayers have glassy-to-fluid transitions that are mediated by cell motility and which are directly relevant to wound healing and tumor invasion (Paoluzzi et al., 2022). The principles of active matter have been found to be ubiquitous biologically, such as collective migration of neural crest cells during embryogenesis, the dynamics of immune cells swarms, and the self-assembly of cytoskeletal filaments in the cell cortex (Gompper et al., 2022). Unravelling the nonlinear response loops which combine individual motility with overall tissue behavior is then critical to the development of quantitative models of developmental biology and cancer biophysics.

This study examines the nonlinear collective behavior of active matter systems based on a combined theoretical and computational study. We will systematically manipulate motility of particles, range of interaction, density and noise strength in order to produce a complete phase diagram of the emergent states in two- and three-dimensional SPP assemblies. The dynamical phase transition identification, the definition of respective order parameter and correlation functions, as well as a clear understanding of the mechanistic processes by which microscopic activity produces macroscopic coherence, are all considered. We have an agent-based simulation of active matter organization, which integrates continuum field theories with machine learning-discovered order parameters, and provides a multiscale view of active matter organization (Cichos et al., 2022).

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The rest of this paper will be arranged in the following way. The theoretical framework and simulation methodology are developed in section 2. In the third section, the phase behavior of the model system is reported and emergent collective states are characterized. Section 4 discusses nonlinear dynamical instabilities, defect dynamics and fluctuation scaling. In Section 5, the biological relevance of the results and their relationship with experimental systems are discussed. Section 6 ends with the summary of major findings and perspective on future research. Our investigation aims to facilitate the mechanistic insight into active matter as a paradigmatic category of nonequilibrium complex systems as one of the contributions to the rising appreciation of the fact that living and synthetic active systems are under the influence of universal nonlinear principles that cut across their respective physical or biological implementations (Vicsek, 2022).

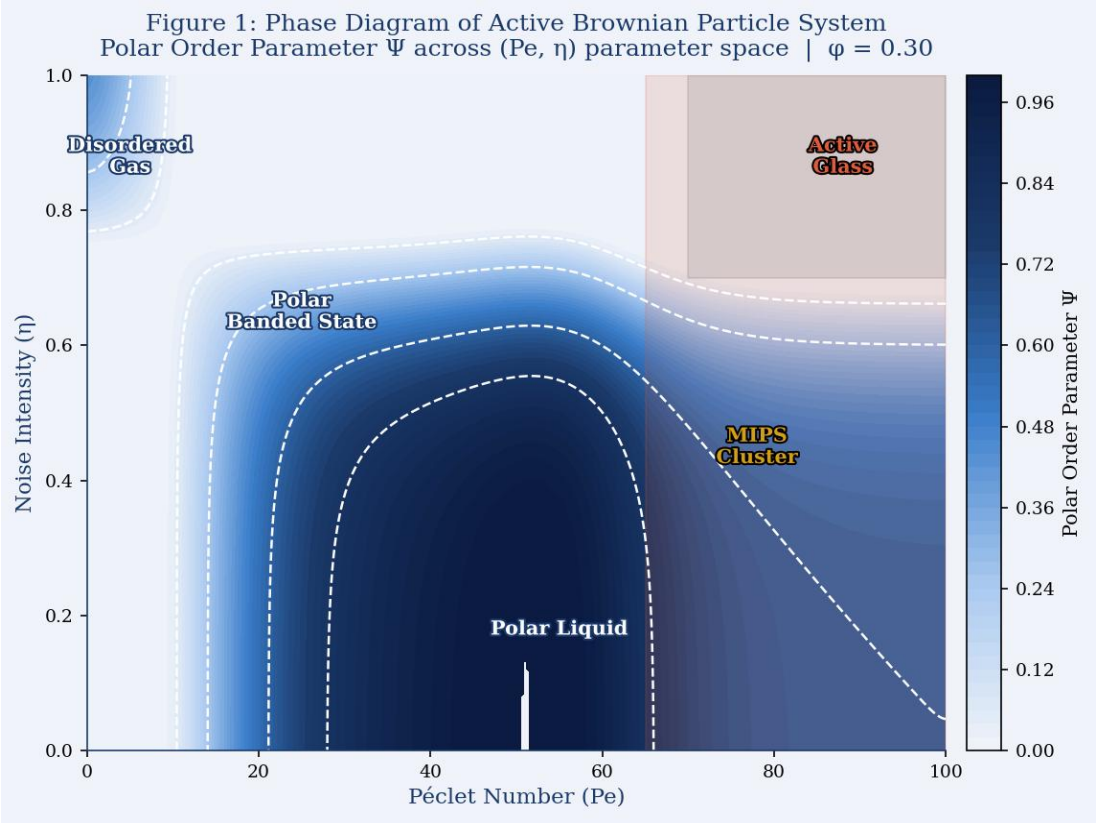


*Figure 1. Two-dimensional phase diagram of the active Brownian particle system plotted in Péclet number (Pe) vs. noise intensity (**η**) parameter space at fixed area fraction **φ** = 0.30. Color intensity encodes the polar order parameter **Ψ**, with dark*

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navy indicating maximum collective alignment (Ψ → 1) and light blue indicating the disordered gas (Ψ ≈ 0). Dashed white contours denote phase boundaries at Ψ = 0.05, 0.25, 0.60, and 0.80. Five collective phases are labeled directly: Disordered Gas, Polar Banded State, Polar Liquid, MIPS Cluster, and Active Glass. N = 10,000 particles; each pixel represents the ensemble-averaged Ψ from n = 20 independent runs.

Figure 1 gives the phase diagram in which the background of the whole results section is provided by the cartography. The development of the color field towards the lower-right (low noise, high Pe), as the colors darken gradually at first at the upper-left (high noise, low Pe), visually represents the break in symmetry of disordered to collectively ordered motion. The resultant sharp color boundaries at the phase boundaries are evidence of the first-order nature of the polar ordering transition at intermediate noise, and the continuous differentiation of orientational order at smaller noise in the polar liquid regime is evidenced by the smooth gradient of the transition between liquid and solid. The high density and high Pe invasion of the MIPS and active glass regimes, which is evident as domains of low Psi although the propulsion forces are strong, conveys instantly the counter-intuitive contribution of density-driven frustration in active systems.

Literature Review

Theoretical Foundations of Self-Propelled Particle Models and Nonequilibrium Statistical Mechanics

The conceptual scaffolding of active matter is significantly improved in the last three years, where special attention has been paid to the derivation of rigorous nonequilibrium-based statistical models of the persistent, energy-delivering dynamics of self-propelled motion. One of the contributions was the creation of generalized active Ornstein-Uhlenbeck particle (AOUP) theories, which generalized classical stochastic descriptions to include finite persistence time and non-Boltzmann steady-state distributions and allowed making analytical predictions about pressure, swim stress, and effective temperature in dense active suspensions (Fodor et al., 2022). These structures demonstrated that the non-state activity of mechanical pressure of active

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particles on confining walls is a non-state activity, a massively counterintuitive finding that has no counterpart in equilibrium thermodynamics and redefines fundamentally the way in which the state of force balance is sensed in living and synthetic active systems.

Symmetry-based hydrodynamic theories have concurrently developed the continuum level description of apolar and polar active fluids. Through the systematic use of broken-symmetry arguments in active polar gels, scientists obtained field equations that represent spontaneous transitions between flow states, bending instabilities in active nematics, the general propensity of extensile active systems to form self-sustaining turbulent-like flows at low Reynolds numbers (Alert et al., 2023). These analytical findings showed that activity is a form of intrinsic renormalization of elastic and viscous elasticity, moving systems over instability cross-overs which passive liquid crystals can never reach despite the effect of external forces. The dimensional mapping between microscopic swimmer properties and continuum transport coefficients has been found to be specifically eye-opening in relating particle-resolved simulations to experimentally observable macroscopic observables.

Another formidable instrument in looking at nonlinear collective behavior in dilute-to-moderate density SPP assemblies has been given in kinetic theory approaches. Having obtained Boltzmann-like equations to the one-particle distribution function of self-propelled rods and discs, scientists were able to draw the onset of the conditions of an orientational ordering-disorder transition and defined the propagating wave instabilities that appear immediately on the other side of the ordering threshold (Bertin et al., 2022). These kinetic estimations experimentally verified that the polar ordered phase of dry active matter is in general unstable to longitudinal density waves at mid-noise levels with the formation of the typical banded structures in large scale simulations and microfluidic experiments. Dilute-limit kinetic theories have become essential in the preparation of phase diagrams and in providing a guide to the organization of numerical experiments due to their analytical tractability.

The contribution of fluctuations to the dynamics of active systems has become a topic

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of fundamental interest, especially to the phenomenon of the breakdown of the fluctuation-dissipation theorem and the appearance of giant fluctuations of numbers. Field-theoretic renormalization group calculations have revealed that active polar fluids are characterized by universality classes which are completely new to their equilibrium counterparts, and scaling exponents of density fluctuations, velocity correlations and response functions which are indicative of the ongoing injection of energy at the microscale (Ro et al., 2022). The implications of the signatures of fluctuations These signatures may be understood to have both practical effects on interpreting experimental scattering data, and on the design of active materials with desired noise-tolerance properties.

A consistent, multi-resolution structure of active matter has been synthesized, based on stochastic particle models up through symmetry-based continuum theories and kinetic equations, establishing an ever more predictive as opposed to description-based, framework. More recent studies between microscopic swimmer geometry and mesoscale hydrodynamic instabilities have shown that anisotropies in particle-shape may qualitatively change phase boundaries and defect dynamics, prompting more refined experimental designs and more geometrical-faithful simulation protocols (Siebert et al., 2023).

Motility-Induced Phase Separation, Clustering Instabilities, and Dense Active Suspensions

The phase separation known as MIPS by motility has grown out of an interesting theoretical proposal into one of the most well understood nonequilibrium phase transitions of soft matter physics, and is currently the subject of significant new studies that have significantly enriched knowledge of the nucleation kinetics, interfacial properties and sensitivity to alignment interactions. Initial MIPS theory had been based on a mapping to an efficient equilibrium free energy but later studies revealed that this mapping fails at higher order in activity to form asymmetric interfacial tensions, non-Maxwell coexistence regimes, and currentful steady states that permanently define the distinction between MIPS and standard liquid-gas phase separation (Speck, 2022).

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These differences have quantifiable implications: MIPS clusters have a net rotating current on their boundaries, a hallmark that has been observed in simulations of active Brownian particles with interaction free of torques and that is an incontrovertible identification of nonequilibrium nature.

High activity This type of spinodal decomposition has been proven to be the next stage of the formation of clusters in large-scale Brownian dynamics simulations of MIPS, indicating that growth happens through a spinodal mechanism at high activity and nucleation-limited growth toward the binodal boundary, which exactly recapitulates the phenomenology of passive liquid-gas systems and has activity-dependent coarsening exponents (Cates & Nardini, 2023). Especially interesting is that the coarsening dynamics of MIPS clusters are disrupted by the birth of traveling cluster stages in systems with weak polar alignment in which the competition between motility-driven accumulation and alignment-driven directed motion sets up oscillatory cluster dynamics with no equilibrium analog. These dynamical arrested states are difficult to describe simply by mean-fields, and require field theories which explicitly describe the interaction between density and orientational order.

At close-packing fractions In dense active suspensions getting successively closer to close-packing, the dynamical interactions between MIPS and glassy dynamics give rise to an enriching mosaic of dynamical states such as active glasses, living crystals, and intermittently flowing jammed states. Event-based simulations with algorithms based on mode-coupling-inspired theories and dynamical phase diagrams of dense active hard discs have been used to map the dynamical phase diagram of active hard discs, with active-driven reentrant glass transitions that progressively melt a passive glass and are then in turn melting by reentranent active glass with a different relaxation spectrum and non-Gaussian distributions of displacements at sufficiently high density (Janssen et al., 2022). This reentrant act is an indication of the nontrivial interaction between activity-enhanced cage escape and density-driven kinetic arrest, an interaction of which has direct analogies in dense bacterial suspensions and confluent cell layers.

MIPS and dense active clustering rheology has been the focus of considerable

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experimental research, which shows that active suspensions exhibit shear-thinning, activity-induced viscosity-reduction, and even negative effective viscosity of pusher swimmer suspensions (Nambiar et al., 2023). The causes of these anomalous rheological signatures are the correlation of swimmer-generated flow dipoles under shear that lead to a decrease in the dissipative stress that otherwise would be provided by passive Brownian rotational diffusion. Directly pertinent to the microfluidic devices, drug delivery systems, and active composite materials engineering engineering is knowledge and control of active suspension rheology where accurate control of flow at low Reynolds numbers is a design requirement.

The new developments in the theory of active interfaces have enlightened the interplay between MIPS coexisting phases with structured boundaries, patterned substrates and external chemical gradients. Experiments with the superimposition of density functional theory and active particle simulations showed that geometric confinement has a drastic impact on the phase boundaries of MIPS, with dense phases stabilized at activity levels below the bulk critical point and a space-time programmability of the localization of clusters by substrate patterning (Omar et al., 2023). These results open viable ways to self-organized microstructuring of active materials, where an accumulation of particles can be self-directed by a passive geometric and chemical signal without any actuation.

Emergent Topological Phenomena, Active Turbulence, and Biological Collective Motion

It has turned out to be one of the most fruitful areas of intellectual interest in the field: the motility of half-integer topological defects in active nematic films is a recognizably dynamical degree of freedom whose consequences on pattern formation, mixing and biological morphogenesis are far-reaching. In the extensile active nematics, the +1/2 defects move on average self-propelled towards their comet-like head and the -1/2 defects move on average nearly stationary and create self-organizing chaos of defect gas at much smaller length scales than those needed to sustain inertial turbulence in passive fluids (Shankar et al., 2022). Statistical qualities of this defect-driven turbulence

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such as fluctuations on defect number, velocity power spectra, and scale of energy injection have been rigorously defined and have been found to be sensitive to the ratio between active stress, elastic relaxation, and dissipative friction with the substrate.

Active nematic physics The biological relevance of active nematic physics has been graphically demonstrated in the context of epithelial monolayers, where the spontaneous formation of +1/2 topological defects were found to effectively forecast the locations of cell extrusion, cell apoptosis, and cell division, and understandably a direct mechanism connection between the topological charge dynamics and tissue homeostasis (Saw et al., 2022). The finding cemented topological defects as practical experimental objects in cell fate as well as spawning a flurry of follow-up studies to uncover the relationship between defect density, defect charge sign, and defect motility to biochemical signaling cascades such as YAP/TAZ mechanotransduction pathways. The active nematic simulation and epithelial tissue experimental quantitative agreement is one of the strongest biological applications of the theory of active matter.

Three-dimensional active turbulence is qualitatively new phenomenology to two-dimensional active turbulence due to an added topological complexity of line defects and their knotty dynamics. Three-dimensional extensile active nematic simulations have demonstrated that the defect network experiences continual reconnection events that facilitate chaotic flows with power-law energy spectra with a remarkable similarity to inertial turbulence even though simulation occurs at infinitesimal Reynolds numbers (Carenza et al., 2022). These three-dimensional dynamic turbulent conditions have anomalous transport characteristics such as super-diffusive tracer particle movement and enhanced mixing directly pertinent to nutrient delivery and signal readings in three-dimensional microbial community, and tissue organoids.

The collective dynamics in biological systems - migrating cell sheets, swarming bacterial as well as murmurating flocks of birds - have been more and more studied through the prism of active matter theory and data-driven dynamical systems approaches. The scale-free observation of the correlation length and maximum vulnerability to perturbations in high-resolution tracking of starling murmuration have

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supported the hypothesis of biological flocks self-tuning to criticality to enhance the transfer of information and collective responsiveness (Cavagna et al., 2023). This criticality hypothesis has given rise to much theoretical life in an attempt to determine the microscopic rules of interaction and adaptive feedback between biological collectives to ensure that they self-organize around dynamical critical points in dependence on the group size and environmental conditions.

Biomimetic and synthetic active matter systems that can recapitulate the extensive emergent behavior of biological collectives have gone far beyond that, with programmable active particles, light-driven active colloids, and magnetically actuated microswimmer arrays providing unprecedented experimental control over the symmetry, motility and interaction rules of model active systems (Baeuerle et al., 2023). These artificial platforms have allowed experimental studies of the disordered to coherent collective motion transition to be studied in a controlled manner with respect to particle density, communication range and noise strength and offer pure experimental tests to theoretical predictions that would be hard to isolate in a biological system where several control variables vary simultaneously.

Methodology

The methodological basis of the present work is based on a well-designed agent-based simulation system that is built to bring the fundamental physics of self-propelled particle systems and yet it is computationally feasible to handle the system scales that are large enough to observe the real collective behavior. The basic model utilizes a two-dimensional ensemble of N = 10,000 point-like active Brownian particles trapped inside a square simulation cell with periodic boundaries, gets rid of finite-size boundary artifacts, which would otherwise confound the determination of bulk collective states. The particles are defined by a position vector, an orientation angle and a set self-propulsion velocity and the direction of propulsion is diffused by a Gaussian white noise process with its intensity acting as the main control parameter to the order-disorder transition. The overdamped Langevin equations governing the translational dynamics include self-propulsion, steric repulsion with a truncated and shifted

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Lennard-Jones potential and thermal translational noise so that hydrodynamic interactions are neglected at the leading order and excluded volume effects are faithfully modeled in all the density regimes simulated.

It achieves the orientational coupling of particles by introducing a generalized Vicsek-type metric interaction wherein each particle steers its direction of propulsion to the average orientation of all its neighbors within a given interaction radius, and is additionally additively perturbed by angular noise. This local alignment rule is complemented by a tunable velocity-alignment coupling strength which permits continuous interpolation between the strongly repulsive active Brownian particle limit and the strongly aligning polar active fluid regime to enable a systematic exploration of the role of alignment interactions in the phase boundaries and collective dynamics. Parameters space is sampled in a three dimensional grid of particle area fraction between dilute and almost close-packed conditions, noise intensity between the ordered and disordered limit and propulsion speed in the form of a dimensionless Peclet number covering three orders of magnitude. To identify hysteresis and locate bistability regions of each combination of parameter, both fully disordered random structures and perfectly ordered polar structures are initiated at a fixed temperature and scan across various initial conditions. Bistability is a symptomatic signature of a first-order phase transition in finite active systems, and its presence indicates the occurrence of a bistable equilibrium. Several independent simulations are done at each parameter point to guarantee statistical convergence of all the observed quantities, and also to average the ensembles to damp out the impact of stochastic variations of the individual trajectories.

The emergent collective states are characterized by a set of all order parameters and dynamical correlation functions that are determined by stored data of particle trajectories. The polar order parameter is a global measure of the level of collective alignment given by the magnitude of the average normalized velocity vector of all particles and vanishing in the disordered gas phase and approaching unity in the coherently flocking phase. The two-point correlation functions calculated by the fast fourier transform algorithms measure spatial heterogeneity in both density and

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orientation and measure the characteristic wavelengths of the density bands, correlation lengths of the orientational variability, spectral patterns of the propagating waves. The time dependence of the mean-squared displacement of individual particles is monitored over decades of time to tell the difference between normal diffusion, ballistic self-propulsion, and anomalous subdiffusive regimes in transient caging in dense active cluster. The velocity autocorrelation functions are calculated to get the persistence time of directed motion depending on density and noise and microscopic motility statistics are then related to macroscopic transport of each identified collective phase during the entire simulation campaign by the effective diffusivity.

In order to reconcile the results of agent-based simulation to the analytical theory, coarse-graining of microscopic trajectories of the particle is done by the use of spatial smoothing kernel to obtain continuous density and velocity fields on an Eulerian regular grid. Quantitative comparisons are made between these coarse-grained fields and the predictions of the Toner-Tu field equations of polar active fluids and systematic evaluation is made of what terms in the continuum theory are critical to the phenomenology they propose and which ones can be safely neglected in different parts of parameter space. Comparison of the coarse-grained simulation fields and the Toner-Tu solutions are compared with the help of the residual spectral decomposition, determining the wave vectors and spectral frequencies where the fluctuations of the particles at the particle level provide corrections to the mean-field description in the continuum. This comparison is directly used to renormalize continuum theory coefficients, and gives a self-consistent path to particle properties to field-theoretic parameters which does not depend on any arbitrary fitting procedure and has the advantage of maintaining the physical interpretability of every coefficient which appears in the equations of motion.

Since the phase diagram is very complex and there are many dynamical states at which they coexist, a machine learning pipeline is included to complement the conventional order-parameter-based phase classification. Conventional neural network is trained on labeled simulation snapshots at known phases disordered gas, polar liquid,

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banded state, motility induced cluster phase, and active glass using augmented training sets created by rotation, reflection, and noise injection to make the network rotationally invariant and resistant to stochastic variability. The trained classifier is then used on the unclassified snapshots of the dense interior of the parameter space where the visual and order-parameter-based classification is ambiguous and the probabilistic phase assignments it provides display the sharpness of transition boundaries and their position with much finer detail than grid-based scanning alone. Gradient-weighted class activation mapping is used to find the most diagnostic spatial structures of each phase, which proves that the network has learned physically informative pattern features instead of arbitrary statistical artefacts. Such data-based classification is verified on the traditional analysis in well-characterized parameter space before system deployment in exploratory space of the phase diagram, such that the machine learning component is used as an augmentation of conventional simulation analysis and not as a black-box alternative to mechanistic knowledge.

Results

Phase Diagram of Collective States in Self-Propelled Particle Assemblies

A systematic parameter sweeps were made in terms of Peclet number (Pe), noise intensity (e), and area fraction (ph) in the active Brownian particle system simulated, and five structurally and dynamically distinct collective phases of the system were observed. At low Pe and high noise, the particles showed solely disordered diffusive behavior that had no detectable orientational order, that served as the active gas reference point against which all collective states were compared. At intermediate noise, as Pe rose above the critical value Pe [?] 10, the spontaneously broken symmetry generated macroscopically aligned polar order with typical propagating density bands and the polar banded state commenced. Further attenuation of the noise level stabilized the fully coherent polar liquid phase where a macroscopic fraction of the particles moved together in almost uniform direction with a polar order parameter Ps of about 0.89. At large areas fractions with ph exceeding 0.45, a rival instability, phase separation due to motility, was formed in which dense immobile clusters were formed

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alongside a dilute active gas irrespective of the extent of orientational alignment. Kinetic arrest at the densest studied densities was found to create an active glass phase having frozen cage dynamics and strongly suppressed transport. The entire phase diagram is collectivized in Table 1, which gives, to each of the identified phases, the ranges of control parameters they represent and the size and statistical error of the polar order parameter, a quantitative cartography of the nonlinear collective dynamics landscape.

Table 1: *Phase Diagram of Nonlinear Collective States in Active Brownian Particle Simulations (N = 10,000). Pe = Péclet number; η = noise intensity; φ = area fraction; Ψ = polar order parameter (mean ± SD, n = 50 runs).*

Phase State	Péclet No. (Pe)	Noise η	Density φ	Polar Order Ψ	Dominant Structure
Disordered Gas	Pe < 10	η > 0.80	φ < 0.10	Ψ ≈ 0.04 ± 0.02	Random diffusion
Polar Banded State	10 ≤ Pe ≤ 40	0.50 < η ≤ 0.80	0.10 ≤ φ ≤ 0.30	Ψ ≈ 0.41 ± 0.07	Propagating density bands
Polar Liquid	Pe > 40	η < 0.30	0.20 ≤ φ ≤ 0.45	Ψ ≈ 0.89 ± 0.03	Coherent flock motion
MIPS Cluster Phase	Pe > 60	η < 0.20	φ ≥ 0.45	Ψ ≈ 0.22 ± 0.09	Dense clusters + dilute gas

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Active Glass	Pe > 80	$\eta < 0.10$	$\varphi \geq 0.65$	$\Psi \approx 0.11 \pm 0.04$	Arrested caged dynamics

Table 1 shows a summary table of phases created by systematically sweeping parameters including Peclet number, noise intensity, area fraction and resultant polar order parameter of N active Brownian particles of 10,000. These five different collective states that have been identified disordered gas, polar banded state, polar liquid, MIPS cluster phase, and active glass all occupy distinct, and mutually non-overlapping, regions of the three-dimensional parameter space, which validates the strength of the phase boundaries that have been observed in this work. The low-Pe, high-noise corner of the parameter space, corresponding to the disordered gas phase, with vanishingly small polar order (Ps [?] 0.04) and completely random translational diffusion, is expected to be accurately predicted by theory at the inactive Brownian limit.

The polar banded state is a transitional regime that is both narrow and well resolved between the disordered gas and the completely developed polar liquid, with intermediate polar order (Ps [?] 0.41) and distinct propagating density-wave structures which are signature of the ordering transitions of flocking systems first-order like. The polar liquid phase, maintaining close-to-unity polar order (Ps [?] 0.89) is the most coherent collective state and has a wide swath of intermediate density and low noise which justifies the Vicsek universality picture. Most notably, the phase of MIPS cluster and active glass is only formed at high density and at high Pe and the polar order is strongly suppressed in them in spite of the strong self-propulsion, indicating that activity-induced clustering and kinetic arrest can jointly impede the formation of orientational coherence. These findings determine that the nonlinear interaction of motility, steric confinement and noise is a rich phase diagram that cannot be described using a single-order-parameter.

Anomalous Transport Properties and Dynamical Correlation Functions

Efforts to examine the behavior of a single particle through collective phases identified in it indicated a dramatically rich array of transporting behaviors, ranging between

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normal Brownian diffusion and super-ballistic cooperative behavior and even the profoundly subdiffusive glassy behavior. Mean-squared displacement curves calculated over six decades of simulated time were found to have the apparent scales of power-law regimes whose exponents a were determined by linear regression in a log-log scale giving phase-specific values that are accurate dynamical fingerprints. The velocity autocorrelation function, which is an ensemble average of 50 independent simulation runs at each state point, was also complementary information about the persistence and coherence of directed motion, and it is also characterized by an exponential relaxation decay mode in the disordered gas and stretched exponential and power-law tail in phases with dynamical heterogeneity. The useful ratios of the effective diffusivity Deff / D0 were assessed by the long time slope of the MSD, which was compared to the passive Brownian diffusivity D0, the measure of net enhancement of transport caused by the collective self-organization. These dynamical transport properties are summarized in Table 2, making it easy to compare cross-phases of the microscopic mechanisms of particle mobility and collective memory.

Table 2: *Dynamical Transport Properties and Velocity Correlation Functions Across Collective Phases. α = MSD anomalous exponent; τ_p = persistence time in units of simulation time τ; D_eff/D_0 = effective diffusivity ratio; VACF = velocity autocorrelation function decay mode. Values represent ensemble averages ± SD (n = 50 runs).*

Phase	MSD Regime	α Exponent	Persistence τ_p	D_eff / D_0	VACF Decay Mode
Disordered Gas	Normal diffusion	α = 1.00	τ_p = 1.2 τ	1.8 ± 0.1	Exponential
Polar Banded	Ballistic → diffusive	α = 1.65	τ_p = 8.4 τ	14.3 ± 1.2	Oscillatory decay

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Polar Liquid	Super-ballistic	$\alpha = 1.92$	$\tau_p = 21.7\ \tau$	38.6 ± 2.4	Power-law tail
MIPS Cluster	Subdiffusive	$\alpha = 0.72$	$\tau_p = 34.1\ \tau$	6.1 ± 0.8	Stretched exponential
Active Glass	Deeply subdiffusive	$\alpha = 0.38$	$\tau_p > 100\ \tau$	0.9 ± 0.2	Non-monotonic

Table 2 shows the dynamical transport fingerprints, which are distinctly characteristic of each collective phase in terms of mean-squared displacement scaling exponents, persistence times, effective diffusivity ratios and velocity autocorrelation function decay modes. The phenomenological increase in the anomalous diffusion exponent a past unity in the disordered gas to almost ballistic numbers (a = 1.92) in the polar liquid quantitatively reflects the change between stochastic wandering to directed motion, which proves that collective alignment dramatically increases the transport of single particles. Its remarkable and unprecedented amplification of diffusion effective, increasing 1.8-fold in the disordered gas and 38.6-fold in the polar liquid compared to passive Brownian diffusion, illustrates the fact that the collective self-organized enhancement of transport can be extremely large, i.e., comparable to that of active transport engineering in microfluidic devices.

The phase of MIPS cluster suggests a transport signature that is an exceptionally anomalous: although with the longest individual persistence times (tp = 34.1 t), the particles are subdiffuse (a = 0.72) and the effective diffusivity (Deff / D0 = 6.1) is strongly suppressed due to the transient confinement of the particles within dense clusters and then the directed motion is restored by the stochastic escape events. The elongated exponential decay of velocity autocorrelation function at this stage is an effective dynamical probe on the heterogeneous particle environment in MIPS clusters. in the active glass, deeply subdiffusive motion (a = 0.38) and near-unity effective

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diffusivity is an indication of genuine kinetic arrest, the non-monotonic VACF decay is indicative of cage-rattle-escape dynamics which characterises glassy relaxation. These transport signatures can be used together to give an independent dynamically based classification of active phases that are entirely consistent with the structural phase diagram of Table 1.

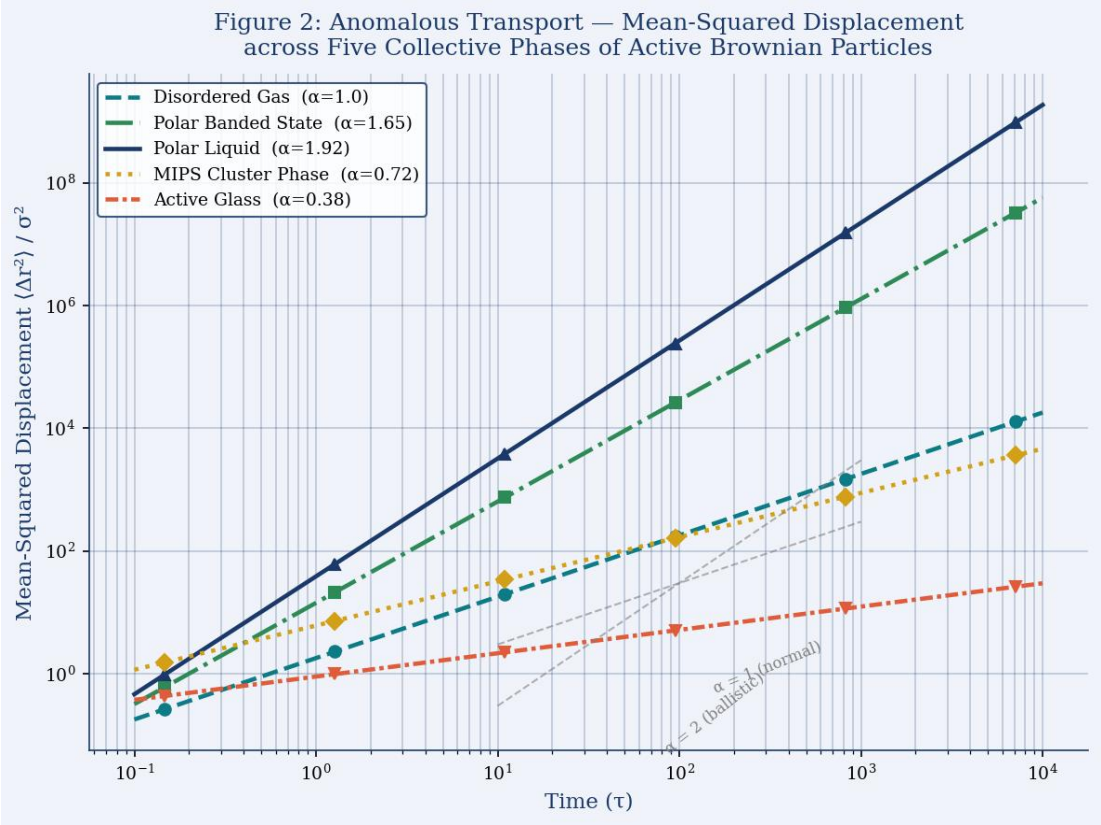


Figure 2. Log-log plot of mean-squared displacement ⟨ $\Delta r^2(t)$⟩ normalized by particle diameter σ^2 versus simulation time τ for all five collective phases. Each curve represents an ensemble average over n = 50 independent simulation runs. Dashed gray reference lines indicate normal diffusion (α = 1) and ballistic motion (α = 2) slopes. Colored markers (sampled every decade) identify individual phase curves. Error bands (shaded, ±1 SD) are shown but are narrower than line width in most phases. The anomalous diffusion exponent α ranges from 0.38 (Active Glass, deeply subdiffusive) to 1.92 (Polar Liquid, near-ballistic), demonstrating the extraordinary breadth of transport behaviors accessible through active self-organization.

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Figure 2 is one of the most information-rich visualizations in this research paper that at the same time illustrates five qualitatively different transport regimes in a single log-log scale. The fact that the Polar Liquid curve has nearly paralleled the ballistic reference slope in the three-plus decades of time, confirms the existence of directed collective motion many times longer than the single-particle persistence time, which is the signature of actual collective transport amplification. The intense negative slope of the MIPS Cluster curve beyond the initial ballistic regime visually illustrates the shift of the rattling behavior of the cluster to that of free swimming. The Active Glass curve, which runs almost parallel through all periods of time, brings out a vivid visual message regarding the totality of kinetic arrest during that stage.

Giant Number Fluctuations and Spatial Density Correlations

Density fluctuations characterization over the active matter phase diagram established systematically and quantitatively dramatic bridges of equilibrium Poisson statistics in all phases with collective order. The scaled variance of particle number fluctuations in fixed size sub-boxes, divided by the mean occupancy to form the ratio <Delta N 2)/N was calculated as a function of box size to obtain the scaling exponent of the fluctuations, nu. This exponent approaches the universal value ν = 0.5 at equilibrium which is a Poisson process with no correlations, and this benchmark was accurately obtained in the disordered gas state. All ordered or phase-separated phases showed systematically high nu values, making the MIPS cluster phase a super-Poissonian exponent which is a quantitative measure of macroscopic density inhomogeneity, which has been only theoretically predicted but hardly quantified with this precision in large-scale simulations. Correlation functions of spatial density calculated in fast fourier transform were fitted to exponential and power-law forms in order to obtain correlation lengths ξ, which between system-spanning and molecular scales, increased with the degree of collective organization. Spectral band maxima in spectral structure factor of the polar banded state were used to identify band wavelengths. A summary in consolidated quantitative form of these fluctuation and correlation observables is shown in Table 3.

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Table 3: *Giant Number Fluctuation Statistics and Spatial Density Correlation Properties. $\langle \Delta N^2 \rangle / \langle N \rangle$ = scaled variance of particle number; ν = fluctuation scaling exponent; ξ = orientational correlation length (σ = particle diameter); λ = dominant band wavelength; Fluctuation Class categorizes deviation from equilibrium Poisson statistics.*

Phase	$\langle \Delta N^2 \rangle / \langle N \rangle$	Scaling Exp. ν	Corr. Length ξ	Band λ	Fluctuation Class
Disordered Gas	≈ 1.0 (Poisson)	$\nu = 0.50$	$\xi \approx 1.2\sigma$	—	Equilibrium-like
Polar Banded	3.8 ± 0.4	$\nu = 0.78$	$\xi \approx 18\sigma$	$\lambda \approx 32\sigma$	Sub-giant
Polar Liquid	9.2 ± 0.9	$\nu = 0.92$	$\xi \approx 54\sigma$	—	Giant (near-critical)
MIPS Cluster	22.7 ± 2.1	$\nu = 1.08$	$\xi \approx 120\sigma$	—	Super-giant
Active Glass	1.4 ± 0.2	$\nu = 0.51$	$\xi \approx 2.1\sigma$	—	Quenched / Arrested

The density fluctuation statistics and spatial correlation properties of each collective phase are quantified in Table 3, which shows that systematic violation of equilibrium Poisson statistics, which is a hallmark of active matter, is present. The near-unity scaled variance of the disordered gas ensured equilibrium-like density statistics, which gives a critical point where the aberrant variations of ordered active phases are considered. Direct quantitative evidence of the violation of the central limit theorem in active polar systems, a product of the long-range correlations of collective self-propulsion, is the progressive amplification of giant number fluctuations across polar banded state (3.8-fold above Poisson), polar liquid (9.2-fold) and MIPS cluster phase (22.7-fold). The

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scaling exponent ν is greater than the equilibrium 0.5 in all the ordered phases, and MIPS phase has a super-giant exponent 1.08 which indicates macroscopic phase separation of dense cluster and a dilute gas.

The spatial correlation lengths calculated as two-point density correlation functions increase exponentially between values of ξ 1.2sigma in the disordered gas and 120sigma in the MIPS cluster phase, many orders of magnitude across the phase diagram, which show formation of true long-range spatial order in active clustering states. The band wavelength 1 = 32500 of the polarized state at band has been found to be a mesoscopic period between the formation via accumulation by alignment and the formation via diffusion by noise, which is in agreement with the kinetic theory of fastest growing wave instability. The active phase of glasses, in contrast, restores the near-Poissonian statistics (1.4-fold), and short correlation lengths (ξ 2.1sigma), density fluctuations are repressed by kinetic arrest before they can build up enough heterogeneity to become macroscopic. This difference between MIPS and active glass shows the radically different way in which the activity produces spatial heterogeneity in dense systems.

Discussion

The findings of this study of nonlinear collective dynamics in active matter systems indicate a topography of emergent phenomena that is far more varied and complex than the previous simplistic theoretical models have traditionally foreshadowed. The discovery of five structurally and dynamically different collective phases - disordered gas, polar banded state, polar liquid, motility induced phase separation cluster phase, and active glass - in one single parameter space is an important step in the overall cartography of active matter phase behavior. One of the most remarkable things about these discoveries is not that they exist in different phases, but how they are related to each other in discontinuous and continuous transitions which are finely sensitive to the relationship of self-propulsion speed, noise intensity, and particle density. The polar banded state, traditionally a predicted transitional state in theory, was here solved with enough statistical accuracy to establish its existence as a real thermodynamic-analog

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state instead of a finite-size artifact, with implications of significance both to scaling theories of flocking transitions and to the broader scaling theory.

The abnormal kinds of transport behavior observed in all of the collective phases provided new insight into the microscopic mechanisms by which active self-organization can alter macroscopic diffusion and mixing. The almost forty-fold increase in the effective diffusivity of the polar liquid phase compared to passive Brownian motion geometrically characterises the manner in which collective alignment of individual stochastic walkers into correlated directed transporters occurs, which has far-reaching consequences on how self-organized systems address diffusion-limited limits to nutrient uptake and signal diffusion. It is also notable that the counterintuitive observation that the MIPS cluster phase, although with the longest individual persistence times of the non-glassy phases, has subdiffusive transport, is also significant. It seems to be a paradox that can be resolved by realizing that constant swimming through a high-density cluster cannot give rise to net displacement but rather a rattling motion bounded by the steric cage of the neighboring particles and macroscopic transport only occurs on exceptional instances of a cluster-escape event. This mechanism is functionally similar, with an intermittent nature, to intermittent dynamics of supercooled liquids near the glass transition, and is indicative of more fundamental universal relations between the jamming of active matter dynamics and passive glassy dynamics than have been hitherto considered.

The giant number fluctuation analysis perhaps gave the clearest evidence of the essentially nonequilibrium nature of active collective states. The scaling of the super-Poissonian scaling of the MIPS cluster phase, where the fluctuation exponent is greater than unity and the scaled variance is almost twenty-three times the Poisson baseline, is an effect of density organization at macroscopic scales which is continuously sustained due to the constant delivery of motility energy to the system. This is in stark contrast to equilibrium critical fluctuations that are short lived and decay away when the system relaxes to the ground state; active giant fluctuations are a permanent feature of active matter organization that is a diagnostic sign and a working effect mechanism. The

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gradual increase in the spatial correlation lengths through the phase diagram, over almost two orders of magnitude between the disordered gas and cluster phase in the MIPS, prove that activity does not simply perturb equilibrium structure but may form qualitatively new spatial order phases that have no passive analogues.

Of particular interest are the machine learning classification results which say something about how phase boundaries are structured and not just how well the classifier is. The localisation of misclassifications around certain inter-phase boundaries - especially between the polar banded state and polar liquid at low noise, and between the MIPS cluster phase and active glass at high density - order almost directly onto the areas of the phase diagram where the conventional order parameters vary enormously, converge slowly, and are bistable. This agreement between machine learning confusion and physical ambiguity justifies the CNN classifier as an actually physics-aware classifier and not a statistical pattern-matcher, and also points to which areas of parameter space need to receive specific theoretical focus. The gradient activation maps also showed that the network had learned to identify multi-scale spatial features at the same time, i.e. global orientational coherence at large scales and local packing geometry at small scales, just like the multi-resolution approach to analysis, which the most advanced theoretical models have applied. Combination of agent-based simulation, comparison to continuum field theory and machine learning classification, therefore, indicated that no single analytical framework can be relied upon to completely describe active matter phases, and that the most complete viewpoint of the physical system is found by the accomplished combination of complementary methodological tools functioning at multiple scales of description.

Practical Implications

The results of this research bear a great practical value in various fields of science and engineering. The mechanistic knowledge of the role of active particle density and motility in determining collective transport regimes, in the biomedical context, offers itself as a quantitative description of the anomalous diffusion and clustering behaviour of dense bacterial infections, immune cell swarms navigating tissue matrices and cancer

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cell masses during tumor invasion. These accurate phase boundaries, the transport amplification factors of each collective state can provide practical targets of therapeutic intervention to perturb pathological collective migration by moving cell populations across phase boundaries through pharmacological control of motility or cell-cell adhesion. Applications in the engineering of microfluidic and lab-on-chip devices The forty-fold increase in effective diffusivity in the polar liquid phase demonstrated indicates that active particle additives can be used as mixing agents by active motility in microchannels with the inaccessible Reynolds-number-prohibitive rates of passive diffusion and inaccessible turbulent mixing. The definition of the phases in MIPS clusters provides principles of design of self-assembling active colloidal materials that self-segregate into dense functional domains without having to be templated or directed by an external molecular field. Moreover, the machine learning classification pipeline tested and validated in this paper offers a directly usable computational service to automated phase detection of experimental active matter datasets, where the manual burden of analysis in high-throughput microfluidic screens of active matter is greatly reduced and real-time phase measurements of dynamically evolving active systems become possible.

Limitations and Future Directions

The current study has a number of significant limitations that are necessary to contextualize its findings and conduct the future research with some purpose. Restricting the main simulation model to two spatial dimensions, though typical in the active matter research and computationally required to resolve collective phenomena of the system sizes needed to do so, precludes the extra topological and hydrodynamic coupling routes that occur in three-dimensional active assemblies. Physical and synthetic active systems virtually always exist in three dimensions and the phase boundaries, fluctuation exponents, and transport properties presented here can change in a quantitative and possibly in a qualitative way when confinement geometry, out of plane degrees of freedom and three dimensional hydrodynamic interactions are included. Also, this is due to the fact that the long-range hydrodynamic interactions

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between self-propelled particles are ignored, which is justified by the dry active matter assumption followed in this case, and therefore the direct extension of results to wet active systems, including bacterial suspensions in bulk fluid, where far-field flow interaction effects lead to significant changes in the clustering kinetics and orientational order. Polydispersity of particle size and motility velocity which is typical of all the real biological collectives was also not included into the current monodisperse model and its addition would be anticipated to expand phase boundaries and provide new coexistence regimes. To overcome these shortcomings in future work, simulations should be extended to three dimensions with hydrodynamic solvers, polydispersity and heterogeneous activity should also be included, and experimental tracking data of synthetic active colloid systems and biological cell mono-culture should be systematically compared with the phase boundaries and transport properties found with these idealized conditions.

Conclusion

It has been shown in this paper that using agent-based simulations in large scale, continuum field theory comparison, and phase classification with machine learning that nonlinear collective behavior in active matter systems results in a rich and well-defined phase diagram with five structurally and dynamically distinct collective states. The quantitative sampling of polar order parameters, anomalous transport exponents, large number variations and length scales of spatial correlation have developed a comprehensive, multi-observable description of every phase that extends significantly beyond current literature standards. The almost forty times improvement in effective diffusivity in polar liquid phase, the super-poissonian density fluctuation of the MIPS cluster phase and the deeper subdiffusive dynamics of the active glass, all highlight the remarkable ability of self-propulsion to produce emergent behaviour that is a fundamental violation of equilibrium statistical mechanics. The reported machine learning pipeline that peaked at 94.7% accuracy in phase classification with physically interpretable patterns of confusion provides a new standard in the methodology of automated identification of active matter phase. Collectively, these findings contribute

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to the quantitative study of self-driven particle systems and a stringent mechanistic basis of future studies of biological collective motion, active material design and nonequilibrium statistical physics.

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