

# STEADY STATE PHENOMENA IN SOFT MATTER, ACTIVE AND BIOLOGICAL SYSTEMS

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# **Approaching the Steady State: A Focus on Extremes**

# Mustansir Barma (TIFR-Hyderabad)

# Abstract of the Oral Presentation

An important general question in statistical physics concerns the nature of steady states, and the way they are approached. In this talk, we focus on what we can learn about both these aspects from the behaviour of extremes. In particular, we study systems which exhibit fluctuation-dominated phase ordering and separately, aggregation-fragmentation dynamics, and find that certain long-held tenets do not necessarily hold.

#### **Collapse Dynamics of Flexible Active Polymer**

Namita Jain, Snigdha Thakur (IISER Bhopal)

#### Abstract of the Oral Presentation

The active matter systems feature the perpetual conversion of chemical energy or other forms of energy into mechanical motion that drives the system out-of-equilibrium. In the biological context, the active matter system spans all the length scales of living organisms, from bacterial colonies, sperm cells, self-organising bio-polymers such as microtubules and actin to the school of fish, the flock of birds, human crowds etc., which ranges from microscopic length scale to macroscopic. There are many applications such as transportation of materials, targeted drug delivery, flagellar motion shown by cilia and flagella, collective behaviour, pattern formation during motion etc., where self-propulsion is essential. Microtubule filaments are an important active polymer where the motor protein (kinesin) make use of chemical energy derived from the hydrolysis of adenosine triphosphate (ATP) to induce the conformational changes, which then leads to its motion on microtubule. These examples help us to gain an understanding about the modeling of active matter (or self-propulsion) systems. In this work, we are interested in studying one particular branch of such active systems, that is the active polymer which exhibits various interesting dynamics like self-propulsion, swelling, shrinkage, loop formation, spontaneous oscillation, spiral formations, enhanced diffusion etc [1, 2, 3].

In our study, we investigate the structural and dynamical properties of a chemically active flexible polymer chain immersed in a solvent bath by using hybrid simulation techniques in a three-dimensional space [4]. The source of activity on the polymer is the self-generating, nonequilibrium solvent gradient caused by the chemical reaction at different sites on the polymer. The chemical gradient then leads to the generation of the local tangential force along the filament. Here we present the effect of activity on the configurational dynamics of a flexible chain emphasizing globulelike transformation at the higher activity. Particular attention is paid to how the radius of gyration (Rg) changes with the activity. We find that the polymer undergoes a coil-to-globule-like transition with increasing active force. Decreasing the Flory scaling exponent of Rg, the correlation of the end-to-end vector and radial

distribution of the monomers around the filament quantifies this transition. We also analyze the motion of a polymer and its center of mass in terms of time-averaged mean-squared displacement (MSD). The superdiffusive motion of the active flexible polymer reverts to random walk at a long time scale with an enhanced diffusion, where the scaling of the diffusion coefficient is the same as the Zimm model.

# References

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#### Non-equilibrium phases in systems of active Brownian particles

#### Raghunath Chellakot (IIT Bombay)

#### Abstract of the Oral Presentation

Active Brownian particles are known to form motility-induced dense phases at sufficiently large activity and density. Such dense phases are characterised by a high degree of structural order. We show that the dense phase is destabilised at large motilities to form porous, disordered clusters if the inter-particle interaction is soft. We also show that this transition exhibits all the characteristics of a standard percolation transition in 2D. This `soft limit' can be achieved either by increasing the particle motility or by increasing the interaction softness. Introducing heterogeneity in the system by including soft and hard particles, we also obtain a percolated cluster of hard particles inside the dense phase containing both hard and soft particles. With these additional new phases, the phase diagram of repulsive active particles is revealed to be richer than we previously conceived.

# Topology driven organization of ring polymers: Relevance to bacterial chromosomes

#### Debarshi Mitra (IISER Pune)

#### Abstract of the Oral Presentation

The mechanism of chromosome segregation and organization in the bacterial cell cycle of E. coli is one of the least understood aspects in its life cycle. The E.coli chromosome is often modeled as a bead spring ring polymer. We introduce cross-links in the DNA-ringpolymer, resulting in the formation of loops within each replicating bacterial chromosome. We use simulations to show that the chosen polymer-topology ensures its self-organization along the cell long-axis, such that various chromosomal loci get spatially localized as seen *in-vivo*. The localization of loci arises due to entropic repulsion between polymer loops within each daughter DNA confined in a cylinder. The cellular addresses of the loci in our model are in fair agreement with those seen in experiments as given in Biophys. J., 110, 2597 (2016). We also show that the adoption of such modified polymer architectures by the daughter DNAs leads to an enhanced propensity of their spatial segregation. Secondly, we match other experimentally reported results, including observation of the cohesion time and the ter-transition. Additionally, the contact map generated from our simulations reproduces the macro-domain like organization as seen in the experimentally obtained Hi-C map. Lastly, we have also proposed a plausible reconciliation of the 'Train Track' and the 'Replication Factory' models which provide conflicting descriptions of the spatial organization of the replication forks. Thus, we reconcile observations from complementary experimental techniques probing bacterial chromosome organization.

# Correlating microscopic viscoelasticity and structure of an aging colloidal gel via optical tweezer-based active microrheology and cryogenic scanning electron microscopy

Ranjini Bandyopadhyay (RRI, Bengaluru)

Abstract of the Oral Presentation

<u>TBA</u>

# Stories that randomness tells: how the analysis of fluctuations of single optically trapped colloidal microparticles reveal the physics of nonequilibrium steady states

#### Ayan Banerjee (IISER Kolkata)

#### Abstract of the Oral Presentation

The trajectories of Brownian particles - in the absence of directed forces - are random, dominated by fluctuations. The study of the fluctuations of the particles reveals information about the environment, as well as the nature of the forces acting on the particles. Especially in optical traps, the fluctuations of the trapped particle(s) are quantified to measure the trap stiffness, as well for interesting microrheological measurements. Recently, there has been a spate of excitement in developing non-equilibrium steady state (NESS) systems, and extracting some of the rich physics that lies embedded in such systems using optical traps. In this talk, we shall describe our work in confining single colloidal particles in optical traps and creating various NESS conditions by driving the mean position of the trap by a Gaussian white noise, or by subjecting a particle to a hydrodynamical flow field. We shall then describe our studies using the recently developed short-time inference scheme derived from the Thermodynamic Uncertainty Principle on time-integrated observables such as the entropic current in order to find the entropy production of the system – a very 'quantitative' measure of non-equilibrium. We shall then show, that for any finite-time measurement in a nonequilibrium steady state, rather counter-intuitively, fluctuations below the average are more probable, with this discrepancy being higher when the system is further away from equilibrium. Interestingly, there is even an optimal time when time-integrated current fluctuations mostly lie below the average, which we deduce theoretically and validate by experiments. Finally, we shall very briefly describe our recent work on the work fluctuation theorem in viscoelastic systems, where we find that viscoelasticity leads to the reduction of negative work fluctuations with stronger violation of the work fluctuation theorem. The main goal of this talk, however, will be to describe the experimental strategies we use in our lab at IISER Kolkata to probe NESS, that may be useful to researchers attempting to unravel stories still hidden in NESS systems.

# Current fluctuations in models of interacting self-propelled particles : microscopic approach

Tanmoy Chakraborty (SNBNCBS, Kolkata)

Abstract of the Oral Presentation

We calculate the fluctuation of the time-integrated or cumulative bond current Q(X,T) up to time T in a prototypical one-dimensional model, having variable-range hopping, which mimics passive diffusion and the ballistic motion of hard-core active, or self-propelled, particles with a persistence length. We have developed a closure scheme that enables us to precisely determine the fluctuation using density-current and density-density correlations. Our analysis captures the short-time (T<<L2) sub-diffusive growth ~  $\sqrt{T}$  as well as the linear or diffusive growth of the fluctuation at longer times T>>L2. Although the system violates detailed balance at the microscopic level, we have recovered an equilibrium-like Green-Kubo relationship linking the current fluctuation with the linear response function or the conductivity. Remarkably, in the limit of infinite persistence length, tuning the density causes the steady-state fluctuation to diverge, revealing the dynamical origin of the previously observed condensation transition of the system [1].

# References

[1]. Hydrodynamics, superfluidity, and giant number fluctuations in a model of self-propelled particles, Tanmoy Chakraborty, Subhadip Chakraborti, Arghya Das, and Punyabrata Pradhan, PHYSICAL REVIEW E 101, 052611 (2020).

# XY model on a substrate: Density fluctuations and phase ordering

# Astik Haldar (SINP, Kolkata)

#### Abstract of the Oral Presentation

The generic long wavelength properties of an active XY model on a substrate, consisting of collection of nearly phase-ordered active XY spins in contact with a diffusing, conserved species, as a representative system of active spinners with a conservation law. The scaling of both phase and density fluctuations in the stable phase-ordered states is nonuniversal. This theory for active spinners, provides a minimal framework for wide-ranging systems, e.g., active superflu- ids on substrates, synchronization of oscillators, active carpets of cilia and bacterial flagella, active membranes and sandblasting.

#### Transient-linking activity in subnuclear media and spatiotemporal organization

Rakesh Das (NUS, Singapore)

#### Abstract of the Oral Presentation

Spatiotemporal organization of the chromatin and various subnuclear condensates (SNCs) in the subnuclear media (SNM) inside a typical eukaryotic cell nucleus plays a critical role in genome regulation. In general, the SNM is full of various type of enzymes which perturb the media in a variety of mechanistic ways. Here, we investigate the role of transient-linking activity (TLA), like that of Topoisomerase-II topological constraint-resolving enzyme (chromatin's active protein). in spatiotemporal organization of chromatin and discuss the underlying mechanism. We an out-of-equilibrium polymer physics model mimicking construct Topoisomerase-II's mechanistic scheme of action. Using computer simulations, we show that TLA phase separates the chromatin into euchromatin and heterochromatin regions with robust characteristic organization features— the euchromatin regions are organized like walls and the euchromatic segments lie along the wall-plane. We show that an equilibrium version of this model can capture the essence of the phase separation but fails to explain the emergence of such characteristic features. The existence of these characteristic features, even with a non-localized choice of the linking sites, highlights the importance of the mechanistic schemes like TLA of Topoisomerase-II and analogous enzymes in chromatin organization [1]. Following this understanding, we focus on the spatiotemporal coordination among the chromatin and SNCs. Using a similar model setting, we show that TLA-induced fluctuation in the chromatic environment enhances the dynamics of an inclusion (mimicking a SNC) immersed in the SNM.

#### References

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# Work fluctuations and entropy production of a trapped Brownian Particle in an "active-like" viscoelastic bath

**Biswajit Das** (IISER Kolkata)

Abstract of the Oral Presentation

Fluctuations are inevitable in mesoscopic systems and they can lead to large variability in measurements of different thermodynamical parameters. Often, such systems encounter viscoelastic environments (e.g., intra-cellular environments) where the nature of these fluctuations becomes more intriguing due to the inherent memory in the surroundings. Here, we experimentally and theoretically study the work fluctuations of an optically trapped micro-particle in a viscoelastic bath [1], driven by an external Ornstein-Uhlenbeck (OU) noise. The noise is chosen such that it mimics the force in an active bath [2] and therefore can be easily extended to several biological processes involving active viscoelastic backgrounds. We find excellent agreements of experimentally determined work probability density functions for various forcing amplitudes to the corresponding theoretical predictions. This provides a clear insight into the work fluctuation theorem (WFT) and the regime where it deviates. We find that the deviation in a viscoelastic medium happens for comparatively lower forcing amplitude than that in a viscous medium. This is because of the viscoelastic medium's time-dependent friction coefficient, which leads to higher mean work done by the external noise relative to that in a viscous bath. We have also estimated a bound to the entropy production rate of the system [3,4], indicating the better directionality of a process in a viscoelastic medium

# References

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[2] C. Maggi, M. Paoluzzi, N. Pellicciotta, A. Lepore, L. Angelani, and R. Di Leonardo, Generalized energy equipartition in harmonic oscillators driven by active baths, Physical Review Letters 113, 238303 (2014).

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### Analytic approaches for microscopic models of active matter

# Abhishek Dhar (ICTS-TIFR, Bengaluru)

### Abstract of the Oral Presentation

The talk will give an overview of some of our recent results on various exact and analytic approaches for models of active matter, including both single particle and many particle systems.

# Current reversal in polar flock at order-disorder interface

# Shradha Mishra (IIT BHU)

#### Abstract of the Oral Presentation

We studied a system of polar self-propelled particles (SPPs) on a thin rectangular channel designed into three regions of order-disorder-order. The division of the three regions is made on the basis of the noise SPPs experience in the respective regions. The noise in the two wide region is chosen lower than the critical noise of order-disorder transition and noise in the middle region or interface is higher than the critical noise. This makes the geometry of the system analogous to the Josephson Junction (JJ) in solid state physics. Keeping all other parameters fixed, we study the properties of the moving SPPs in the bulk as well as along the interface for different widths of the junction. On increasing interface width, system shows a order-to-disorder transition from coherent moving SPPs in the whole system to the interrupted current for large interface width. Surprisingly, inside the interface we observed the current reversal for intermediate widths of the interface. Such current reversal is due to the strong randomness present inside the interface that makes the wall of the interface reflecting. Hence Our study gives new interesting collective properties of SPPs at the interface which can be useful to design devices like switches using active agents.

# A semiflexible polymer in a gliding assay : morphological and dynamical properties

#### Abhishek Chaudhuri (IISER Mohali)

# Abstract of the Oral Presentation

We consider an explicit model of a semiflexible filament moving in two dimensions on a gliding assay of motor proteins, which attach to and detach from filament segments stochastically, with a detachment rate that depends on the local load experienced. Attached motor proteins move along the filament to one of its ends with a velocity that varies nonlinearly with the motor protein extension. The resultant force on the filament drives it out of equilibrium. We will discuss morphological and dynamical properties of the filament that undergoes a first order transition from an open chain to spiral conformation and shows a reentrant behavior in both the active extension and the turnover, defined as the ratio of attachment–detachment rates. **Rajesh Ganapathy (JNCASR, Bengaluru)** 

<u>TBA</u>

#### Is a dense bacterial suspension turbulent?

Samriddhi S Ray (ICTS-TIFR, Bengaluru)

Abstract of the Oral Presentation

Active turbulence --- the spatio-temporally complex motion of a dense suspension of microorganisms such as bacteria --- has gathered great traction recently as an intriguing class of emergent, complex flows, occurring in several living systems at the mesoscale, whose understanding lies at the interface of non-equilibrium physics and biology. However, are these low Reynolds number living flows really turbulent or just chaotic with structural, or even superficial, similarities with high Reynolds number (classical) inanimate turbulence? This is a vital question as the fingerprints of classical turbulence —-- universality, intermittency and chaos —-- makes it unique amongst the many different driven-dissipative systems. In this talk we address these questions with a focus on the issues of (approximate) scale-invariance, intermittency and maximally chaotic states and how they lead to anomalous diffusion in bacterial suspensions. In particular, we show the existence of a critical level of activity beyond which the physics of bacterial flows become universal, accompanied by maximally chaotic states which allow for efficient, Levy-walk mediated foraging strategies.

#### Hydrodynamics of microswimmers with deformable flagella in shear flow

Derek Cyrus Gomes (IISER Tirupati)

#### Abstract of the Oral Presentation

In dense suspensions of flagellated microswimmers the detailed near-field hydrodynamics is strongly cou- pled to the motion of the constituent particles. Consequently, theoretical understanding of such systems pose utmost challenges. While dilute suspensions have been studied and analyzed widely, dense suspensions are poorly understood. Experimentally however, they have been shown to exhibit several nontrivial and striking properties. Therefore, these systems urgently require theoretical analysis in order to understand as well as harness the wealth of the novel physical phenomena they exhibit. Here, we present our approach that suitably captures the effects of crowded environments by modeling a deformable flagellar bundle for the microswim- mer and include appropriately detailed hydrodynamics. We will discuss our findings on the nonlinear behavior and asymmetric dynamics of single swimmers in quiescent and shear flows and show how such phenomena are a consequence of the unique interplay among activity, flexibility and hydrodynamics. We will also present our preliminary results from our analysis on the interactions among the microswimmers and report interesting collision states which are not captured by previously used minimal models.

#### Nonexistence of motility induced phase separation transition in one dimension

# **Indranil Mukherjee** (IISER Kolkata)

# Abstract of the Oral Presentation

We introduce and study a model of hardcore particles obeying run-and-tumble dynamics on a one-dimensional lattice, where particles run in either +ve or -ve x-direction with an effective speed v and tumble (change their direction of motion) with a constant rate  $\omega$  when assisted by another particle from right. We show that the coarse-grained dynamics of the system can be mapped to a beads-in-urn model called misanthrope process where particles are identified as urns and vacancies as beads that hop to a neighbouring urn situated in the direction opposite to the current. The hop rate is same as the magnitude of the particle current; we calculate it analytically for a two-particle system and show that it does not satisfy the criteria required for a phase separation transition. Nonexistence of phase separation in this model, where tumbling dynamics is rather restricted, necessarily imply that motility induced phase separation transition can not occur in other models in one dimension with unconditional tumbling.

# Origin of two distinct stress relaxation regimes in shear jammed dense suspensions

Sachidananda Barik, and Sayantan Majumdar (RRI, Bengaluru)

# Abstract of the Oral Presentation

Many dense particulate suspensions show a stress-induced transformation from a liquid-like state to a solid-like shear jammed (SJ) state. However, the underlying particle-scale dynamics leading to such a striking, reversible transition of the bulk remains unknown. Here, we study the transient stress relaxation behaviour of SJ states formed by a well-characterized dense suspension under a step strain perturbation. We observe a strongly non-exponential relaxation that develops a sharp discontinuous stress drop at a short time for high enough peak-stress values. High-resolution boundary imaging and normal stress measurements confirm that such stress discontinuity originates from the localized plastic events, whereas, the system spanning dilation controls the slower relaxation process. We also find an intriguing correlation between the nature of transient relaxation and the steady state shear jamming phase diagram obtained from the Wyart-Cates Model.

# **Reference:**

[1] Origin of two distinct stress relaxation regimes in shear jammed dense suspensions; Sachidananda Barik, and Sayantan Majumdar, Phys. Rev. Lett. 128 (25), 258002 (2022).

# Active Dynamics of Linear Chains and Rings in Porous Media

Ligesh Theeyancheri, Subhasish Chaki, Tapomoy Bhattacharjee, and <u>Rajarshi</u> <u>Chakrabarti (</u>IIT Bombay)

# Abstract of the Oral Presentation

In order to elucidate the navigation strategy adapted by deformable active agents in porous media [1, 2], we computationally investigate the dynamics of active linear chains and rings [3]. In porous media, linear chains migrate faster than the rings. Flexible linear chains and rings undergo activity-induced swelling. In contrast, linear semiflexible chains swell. Rings, if semiflexible, shrink, get trapped, and escape only at higher activity. This demonstrates how activity and topology interplay and control the structure and dynamics of linear chains and rings in porous media.

References

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#### Accuracy in readout of glutamate concentrations by neuronal cells.

# Swoyam Srirupa Biswal (IIT Goa)

#### Abstract of the Oral Presentation

Glutamate and glycine are important neurotransmitters in the brain. An action potential propagating in the terminal of a presynatic neuron causes the release of glutamate and glycine in the synapse by vesicles fusing with the cell membrane, which then activate various receptors on the cell membrane of the post synaptic neuron. Entry of Ca2+ through the activated NMDA receptors leads to a host of cellular processes of which long term potentiation is of crucial importance because it is widely considered to be one of the major mechanisms behind learning and memory. By analysing the readout of glutamate concentration by the post synaptic neurons during Ca2+ signaling, we find that the average receptor density in hippocampal neurons has evolved to allow for accurate measurement of the glutamate concentration in the synaptic cleft.

# Liquid-state properties and jamming dynamics of persistent athermal active matter

#### Suman Dutta (ICTS-TIFR, Bengaluru)

#### Abstract of the Oral Presentation

Models of dense athermal active matter offer unique scope to investigate the role of non-thermal fluctuations in dynamic arrest. In this work, we consider a two dimensional binary mixture of Lennard-Jones particles with random, persistent active forces. We focus on the liquid state properties of such systems, using large scale molecular simulations and investigate how a dense active liquid obtained at large values of the active force approaches a force-balanced jammed state when the active force is removed or reduced to small values. We show that the jamming proceeds via a three-stage relaxation process whose timescale grows with the magnitude of the active force and the system size. We relate the dependence on the system size to a length-scale extracted from velocity correlations of the initial liquid state that increases with system size.

### Polygenic adaptation dynamics in a large, finite population

#### Kavita Jain (JNCASR, Bengaluru)

#### Abstract of the Oral Presentation

Although many phenotypic traits are determined by a large number of genetic variants, how a polygenic trait adapts in response to a change in the environment is not completely understood. I will describe our recent results on the adaptation dynamics of a large but finite population evolving under stabilizing selection. It is known that in an infinitely large population, selective sweeps at a major locus are prevented and adaptation proceeds exclusively via subtle changes in the allele frequency; in contrast, we find that the chance of sweeps is substantially enhanced in a finite population and therefore polygenic adaptation can occur via small to moderate changes in the allele frequencies at many loci as well as large shifts in the allele frequencies at a few loci.

# Nonequilibrium thermodynamics of Reaction Network: Pattern, Instabilities and Chimera of chemical waves

Premashis Kumar and Gautam Gangopadhyay (SNBNCBS, Kolkata)

# Abstract of the Oral Presentation

A diverse class of reaction-diffusion systems are considered for elucidating nonlinear dynamical features of arbitrary open chemical reaction systems. For example, entropic features and energetics of Turing-Hopf interaction are shown to be controlled through chemostatic openness of the system with cross diffusion. In this presentation we shall discuss on the nonequilibrium thermodynamics of open chemical reaction networks especially to understand pattern, dynamical instabilities and chimeras appeared in the chemical waves. The emergence of the chimera state as the counterintuitive spatial coexistence of synchronous and asynchronous regimes is addressed here in a continuum chemical oscillator system by a relevant complex Ginzburg-Landau equation.

# Effect of receptor clustering on E.coli chemotaxis: Sensing versus adaptation

# **Shobhan Dev Mondal** (SNBNCBS, Kolkata)

# Abstract of the Oral Presentation

The cooperative behaviour of receptor dimers forming densely packed clusters is recently found to be a significant source of fluctuation in E. coli chemotaxis pathway. Highly dense large clusters can sense the nutrient concentration more efficiently, which enhances the chemotactic performance. But large clusters increase the fluctuation also, which causes adaptation module to respond strongly. Therefore, a competition develops be- tween sensing and adaptation. At very large cluster size adaptation wins the competition resulting decrease in the sensitivity of Hence chemotactic efficiency deteriorates resulting in a chemoreceptors. performance peak[1]. To explore the sensing versus adaptation competition further we have observed the methylation dynamics of chemoreceptors during a run[2]. Change of the methylation level in a run depends sensitively on strength of concentration gradient and direction of cell movement. In weak gradient for both uphill and downhill runs, after initial demethylation we see late time methylation and range of this methylation-demethylation gets amplified as cluster size increases. In strong gradient uphill runs also show similar behaviour in methylation dynamics whereas the downhill runs show highly non-trivial dependence of methylation level on cluster size due to sens- ing and adaptation interplay[2]. In another study we see faster switching rate of receptor activity enhances chemotactic performance. Variation of activity for small and large value of switching rate is significantly different in downhill runs and this asymmetry causes the enhancement[3].

# References

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[2] Effect of receptor cooperativity on methylation dynamics in bacterial chemotaxis with weak and strong gradient, by Shobhan Dev Mandal and Sakuntala Chatterjee, Phys. Rev. E 105, 014411(2022).

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#### **Coarse-grained model of protein with structural informations**

#### Abhik Ghosh Moulick (SNBNCBS, Kolkata)

#### Abstract of the Oral Presentation

Information on protein dihedral angle give insight to the function of protein. Typically dihedral angle information extracted from the all atom description of the protein. We treat each atom including solvent explicitly and interactions between atoms are described based on validated force-field. The major drawback is that the all atom approach is computationally very expensive. Often, Various cellular phenomena involve ample number of bio-molecules ranging from water, small and medium-size oligomers and co-polymers (peptides, proteins, RNA, etc) to huge co-polymers, such as DNA. For instance, obtaining all atom description in the process of membraneless organelles via liquid-liquid phase separation is computationally difficult. Lowering the representation from all explicit atoms to coarse grained (CG) model show new possibility to study systems involving large numbers of bio-molecules. The main drawback of CG model is these kind of analysis does not provide any structural information in terms of protein dihedral angle. Motivated by this, we build a coarse-grained model of protein with structural information. We represent an amino acid as a bead. They are connected by spring representing the backbone. Each bead is assigned with a couple of orientation degrees of freedom representing the backbone dihedral angles. The energy cost of these degrees of freedom is obtained from the joint distribution of the fluctuations of the backbone dihedral in fully atomic simulations. We perform Monte-Carlo (MC) simulation on CG model of protein in canonical (NVT) ensemble utilizing metropolis algorithm. Using monte carlo simulations on such a model, we reproduce the protein structure comparable to the crystal structure and with all atom descriptions. This can pave the way for the CG model of protein with structural information and may be useful to study phenomena involving many protein molecules, like protein aggregations.

Dipak Sinha (IACS Kolkata)

<u>TBA</u>

#### Role of spatial organization of chromatin in dynamics of transcription factors.

# **Shuvadip Dutta** (IIT Bombay)

#### Abstract of the Oral Presentation

Proteins search for target sites on the DNA backbone, in order to complete essential biological processes. The landscape of this DNA polymer is fluctuating, and characterised by collapsed domains called TADs with large numbers of intersegmental contacts. Search processes and exit times on such highly connected and fluctuating domains thus regulate timescales of biological events. Using a minimal model, we investigate the exit times from a one-dimensional network with additional intersegmental contacts. We show that exit times show a non-monotonic dependence on the number of the intersegmental contacts, suggesting an optimal compaction of polymer domains for which exit times are minimum. We show our results continue to hold true for more realistic polymer models. Further, we show the relevance of our results using chromatin network structures generated from experimental data. Our results give an insight into how chromatin self-organizes into multiple domains affects search and exit times of DNA-binding proteins.

#### Current fluctuations in interacting and non-interacting active particle systems

#### Kabir Ramola (TIFR Hyderabad)

#### Abstract of the Oral Presentation

We study the fluctuations of the integrated density current across the origin up to time T in one dimensional systems of non-interacting as well as interacting active particles. For non-interacting particles, we focus on the case of zero diffusion and study the differences between annealed and guenched initial conditions. We show that for the case of particles initiated with an initial bias in the positive direction, the fluctuations of the current at short times display a surprising difference: Tversus  $T^2$  behaviours respectively, with a  $T^{1/2}$  behaviour emerging at large times. For the interacting case, we explore a lattice model of active particles with hard-core interactions that is amenable to an exact description within a fluctuating hydrodynamics framework. For the case of uniform initial profiles, we show that the second cumulant of the integrated current displays three regimes: an initial  $T^{1/2}$ rise with a coefficient given by the symmetric simple exclusion process, a cross-over regime where the effects of activity increase the fluctuations, and a large time  $T^{1/2}$  behavior. In the limit of zero diffusion for the interacting system, we show that the fluctuations once again exhibit a  $T^2$  behavior at short times. Finally, we show that the results for non-interacting active particles are recovered for low densities.

# Steady state structure formation by thermoresponsive particles in presence of temperature difference

Rahul Karmakar (SNBNCBS, Kolkata)

Abstract of the Oral Presentation

Structure formation in non-equilibrium steady state conditions is poorly understood. Nonequilibrium steady state can be achieved in a system by maintaining temperature gradient. Recent experiments show that the inter-particle interaction in metallic nanoparticles with ligand capping is sensitive to temperature. The zeta potential of the nano particles is reduced in the cold region. The nanoparticles form aggregates in cold region of the system in presence of temperature difference. We study here systems with temperature sensitive interaction. We study the system using Brownian dynamics(BD) simulations. We find that the clusters in the cold region with long-ranged order grow with the Avrami like crystal growth kinetics. Physically, the long-ranged order in cold region form due to increase in density and slow diffusion.

Experiments further report on thermoresponsive particles, PNIPAAM, a cross-linked micro-gel particles, are reported to increase in size due to absorption of water with decrease in temperature. These thermo-responsive particles are experimentally reported to form aggregates in cold region of the system in presence of temperature gradient. Here we study particles with temperature sensitive diameter, using Molecular dynamics simulation with Langevin thermostat. We find long-ranged structural order using bond order parameters in both cold and hot region of the system beyond a certain diameter ratio of the cold and hot particles. The intriguing phenomenon of ordering in the hot region is due to increase in packing and order of magnitude increase of overall steady state pressure. Our model illustrates a simple case where high temperature crystallization can be studied in the laboratory and provide insight to mechanism of formation of long-ranged order in extreme condition in steady state.

#### Concentration-driven instability in inertial polar active suspensions

#### Purnima Jain (TIFR-Hyderabad)

#### Abstract of the Oral Presentation

Active Polar Fluids consist of head-tail asymmetric self-propelled particles (SPPs) suspended in a fluid medium. They show spectacular collective behavior across a broad range of length scales, for example, bacterial suspensions at the microscopic level to fish schools in an ocean. In the Stokesian regime, where viscosity dominates over inertia, the flocking state is unstable to small perturbations. This instability leads to complex spatiotemporal flows also known as Active Turbulence. Recent works have shown that inertia can stabilize the ordered state and drives a flocking transition from defect turbulence to noisy but aligned states. However, these results are limited to the regime where concentration relaxes quickly and is not considered a hydrodynamic variable of the system. We show that when concentration fluctuations are taken into account, a hitherto unseen instability of the ordered state arises. This instability occurs from the interplay of inertia, the self-propulsion speed of SPPs, and concentration fluctuations. Using high-resolution direct numerical simulations we show that it leads to new kinds of non-equilibrium steady states which are absent in the concentration-free limit.

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#### Hydrodynamics of flagellated microswimmers in confined fluids

#### Ambareesh Shrivastav (IISER Tirupati)

Abstract of the Poster Presentation

Microswimmers have become an important topic of research in soft matter physics. Understanding their individual dynamics and the study of their interactions among each other and with the substrate, involve challenging physics. Confinements introduce modifications to the hydrodynamic flows and interactions, resulting in rich phenomenology and many surprising and puzzling collective behaviors. This ongoing work aims to investigate the effect of plane surfaces on the self-propulsion and interactions of flagellated microswimmers, such as bacteria, swimming near a substrate or in thin films. Using a minimal model of flagellated bacteria, we derive the flow fields around the swimmer near a substrate, considering simultaneous reflections of the flows off the cell-surface and the substrate to a good approximation. We demonstrate that the extended nature of the flagella leads to crucial hydrodynamic interactions which strongly influences the overall cell dynamics near the substrate. Detailed investigations of the cell-wall interactions and the hydrodynamic interaction between different swimmers under confinement are on-going. Our results are important to understand living and confined active matter, as well as, biological processes, such as the formation of bacterial biofilms.

# Molecular dynamics investigation of the dynamics of water, Hyaluron and lipids at the Hyaluron-DPPC interface

# Anirban Paul (SNBNCBS, Kolkata)

#### Abstract of the Poster Presentation

Hyaluronic acid (HA) is a long, highly hydrophilic polyanion that is overexpressed in cells and body fluids during pathogenic situations. Previous studies have shown that water molecules mediate the interaction between HA and lipid molecules[1]. Although HA is known to provide orientational ordering and restricted dynamics to its proximal water molecules[2], no theoretical study of HA's significance in water dynamics near lipid vesicles has been reported. We take DPPC bilayer and HA of different sizes and concentrations in our all-atom molecular dynamics simulation. Our findings suggest that at the HA-DPPC bilayer interface, HA can restrict the translational and rotational diffusion of water. When HA concentration is changed in the system, the effect becomes more noticeable. However, the effect is minor for the range of HA sizes we consider in our study.

# References

[1] Paul Smith, Robert M Ziolek, Elena Gazzarrini, Dylan M Owen, and Christian D Lorenz. On the interaction of hyaluronic acid with synovial fluid lipid membranes. Physical Chemistry Chemical Physics, 21(19):9845–9857, 2019

[2] Johannes Hunger, Anja Bernecker, Huib J Bakker, Mischa Bonn, and Ralf P Richter. Hydration dynamics of hyaluronan and dextran. Biophysical journal, 103(1):L10–L12, 2012

#### Dynamics in an unconserved junction model

# Ankita Gupta (IIT Ropar)

#### Abstract of the Poster Presentation

Over decades, there has been a great deal of interest in stochastic transport phenomena of various complex systems such as intracellular transport of cargo vesicles and vehicular flow, both theoretically and physically. Particles either self-driven or driven by some external field traveling stochastically along a one or multi-dimensional lattice have been utilized to model various transport processes, both natural as well as man-made. In order to analyze the propelled dynamics of these driven diffusive systems, Totally Asymmetric Simple Exclusion Process (TASEP) is widely used as the most prominent paradigm of the driven models to examine several stationary system features.

To mimic the complex transport-like collective phenomena in a man-made or natural system, we study an open network junction model of totally asymmetric simple exclusion process with bulk particle attachment and detachment. The stationary system properties such as particle density, phase transitions, and phase diagrams are derived theoretically utilizing the mean field approach. The steady-state phases have been categorized into various sub-classes based upon the phase transitions occurring across the junction. It is found that the number of steady-state phases depends on the number of incoming and outgoing segments at the junction. Further, an increase in the particle non-conserving rates significantly affects the topology of the phase diagram, and the number of stationary phases changes in a non-monotonic way. For both the case of equal and unequal incoming and outgoing segments, the critical values of non-conserving rates at which the topology of the phase diagram changes are identified. The theoretical results are validated using extensive Monte Carlo simulations.

#### Active rods in a temperature gradient

#### Anweshika Pattanayak (IISER Mohali)

Abstract of the Poster Presentation

Thermophoresis or thermodiffusion can be defined as the drift motion of a particle, immersed in a fluid, under the influence of temperature gradient. The phenomenological thermophoretic velocity of a point particle is taken to be proportional to the gradient of temperature. Unlike spherical point particles, rod-like polymers have two components of thermophoretic velocity, one parallel to the temperature gradient and another perpendicular to the temperature gradient.Due to its anisotropy, rod-like polymers can rotate and arrange themselves into nematic state beyond a certain density. The effect of self-propulsion velocity is also well-known as it gives rise to a steady polarized state. In this work, we have taken a collection of self-propelled active rods in some external temperature gradient. We look at the effect of the thermophoretic force on the steady liquid crystalline state.

# Effect of relative time-scale on steady state measure of a coupled driven system

# Chandradip Khamrai (SNBNCBS, Kolkata)

# Abstract of the Poster Presentation

We study a coupled driven diffusive system [1] with two species of particles advected by a fluctuating potential energy landscape. As a result of two-way coupling between the landscape and the particles, the system shows an interesting phase diagram as the coupling parameters are varied. In the disordered phase, the landscape and the particles show no long-ranged order. However, the steady state does not satisfy the product measure in general as there are short-ranged correlations present in the system whose exact form

is not known. From simulations we have observed that these local short-ranged correlations change systematically with a relative time scale introduced in the dynamics. There is a critical time scale for which the product measure holds. By using the concept of bunchwise balance and irreducible sequence introduced in [2] we can prove the product measure exactly and explain the qualitative change in the short range correlations as the relative time-scale differs from the critical value. The recently developed formalism of nonlinear fluctuating hydrodynamics (NLFH) [3] is being extensively used to study coupled driven systems with multiple conserved quantities. In principle, this formalism requires the knowledge of the exact expression of locally conserved current in terms of local density of the conserved components. Within this formalism we have been able to obtain an exact expression [4] for the critical time-scale at which product measure holds.

# References

[1] Large compact clusters and fast dynamics in coupled nonequilibrium systems by Shauri Chakraborty, Sukla Pal, Sakuntala Chatterjee and Mustansir Barma, Phys Rev E Rapid Comm 93, 050102(R) (2016).

[2] Light and heavy particles on a fluctuating surface: Bunchwis balance, irreducible sequences, and local density-height correlations by Samvit Mahapatra, Kabir Ramola, and Mustansir Barma, Physical Review Research, 2(4):043279, 2020.

[3] Fibonacci family of dynamical universality classes by Vladislav Popkov, Andreas Schadschneider, Johannes Schmidt, and Gunter M Sch ü tz, Proceedings of the National Academy of Sciences, 112(41):12645–12650, 2015.

[4] Effect of relative time-scale on steady state measure of a coupled driven system by Chandradip Khamrai and Sakuntala Chatterjee, (manuscript in preparation).

#### Matrix Product Ansatz in 2D

#### Chandraniva Guha Ray (IISER Kolkata)

Abstract of the Poster Presentation

Non-equilibrium systems are ubiquitous in nature, but solutions to higher dimensional lattice-based systems have not been studied analytically in great detail. On the other hand, the matrix product ansatz (MPA) formalism has been considerably successful in describing the exact solutions of one dimensional out-of-equilibrium systems. In this poster, I will use a non-trivial ansatz for 2-dimensional (2D) lattice-based models. I will use our ansatz to arrive at the exact steady state weight of a 2D nonequilibrium lattice gas dynamics which destroys consecutive \$0\$'s. The critical exponents for the system will be analyzed and compared with numerical simulations. Our methodology is a natural, yet non-trivial extension of the MPA formalism, and serves as a novel approach to tackle 2D lattice-based systems which are far out-of-equilibrium.

#### **Optimum transport with periodic drive and short-ranged interaction.**

#### Deepsikha Das (SNBNCBS, Kolkata)

#### Abstract of the Poster Presentation

We study a model of hardcore particles with nearest neighbour interaction moving on a one dimensional ring lattice in presence of a time-periodic external potential generated by periodic movement of a defect in the lattice. Using numerical simulations and mean-field calculations we have derived the conditions for optimal transport, i.e. maximum possible particle current in the system and find that the presence of nearest neighbour interaction considerably affects the current. We observe that a repulsive interaction generally enhances the current, while attractive interaction suppresses it. We show that a moving defect always induces current in the direction opposite to that of the defect movement, while bulk diffusion causes a current in the same direction of the defect movement. Interplay between the periodicity of the external drive and particle diffusion, causes net current to reverse its direction on variation of particle density, defect velocity and interaction strength. For small particle density, current becomes maximum when the repulsion is strongest. However, for large particle density, when the system is overcrowded, very strong repulsion blocks certain transitions and reduces the current. In this case, optimum transport is obtained when the interaction is strongly repulsive but not assuming its highest possible strength.

#### Interaction of NaCl with anionic membranes : Effect of cholesterol

Kalyan Kumar Banerjee (Jadavpur University)

Abstract of the Poster Presentation

Biological membranes are complex and regulated by various proteins, cholesterol and bio-active molecules. Structure and function of biological membranes are difficult to study in vivo. Therefore it is often useful to study model membrane to get insights into the structure and functions of biomembranes. Cholesterol in a bio-membrane plays a significant role in many cellular event and is known to regulate the functional activity of protein and ion channel. In this study we have investigated the effect of cholesterol on the ion-membrane interaction. We prepare large unilamellar vesicles, composed of anionic lipid DOPG and zwitterionic lipid DOPC for different cholesterol concentration. Electrostatics of anionic membranes containing cholesterol in the presence of NaCl has systematically been investigated using dynamic light scattering and zeta potential. Negative zeta potential decreases with increasing ion concentration for all cholesterol concentrations. However, zeta potential itself decreases with increasing cholesterol content even in the absence of monovalent ions. Electrostatic behaviour of the membrane is determined from well-known Gouy Chapmann model. Negative surface charge density of the membrane decreases with increasing cholesterol content. Binding constant, estimated from the electrostatic double layer theory, is found to increase significantly in the presence of cholesterol. Comparison of electrostatic parameters of the membrane in the presence and absence of cholesterol suggests that cholesterol significantly alter the electrostatic behaviour of the membrane.

#### Collapse dynamics of chemically flexible active polymer

#### Namita Jain (IISER BHOPAL)

#### Abstract of the Poster Presentation

In our study, we investigate the structural and dynamical properties of chemically active flexible polymer chain immersed in a solvent bath, by using hybrid molecular dynamics (MD) and multiparticle collision dynamics (MPCD) simulations technique, in a three dimensional space. The activity is introduced in the system by generating non-equilibrium solvent gradient due to the chemical reaction at the catalytic (C) and the distinct choice of energy parameter on the non-catalytic (N) monomers, that leads to the generation of local active force on each set of C-N pair, which is tangent to the filament. Here we present the effect of activity on the configuration dynamics of a flexible chain. Particular attention is paid to how the radius of gyration ( $R_g$ ) changes with the activity. We find that the polymer undergoes coil-to globulelike transition with increasing activity (Pe). This transition can be quantified by decreasing the flory scaling exponent of R\_g, correlation of end-to-end vector C(t), and radial distribution g(r) of the monomers around the filament.

# Nonequilibrium steady states in a resource-constrained exclusion process with site-wise dynamic defects.

#### Nikhil Bhatia (IIT Ropar)

#### Abstract of the Poster Presentation

This study investigates a TASEP where the inhomogeneities on the lattice appear in the form of defects that stochastically bind and unbind the lattice. The effect of constrained resources on the stationary properties of the system has been comprehended in the form of the filling factor. The influence of defects at the boundary sites is considered, due to which the entry rate of particles is affected. Utilizing different mean-field approximations, we characterize the stationary state properties of the system and investigate the evolution of the phase diagram with respect to the filling factor and obstruction factor.

# Passive Star polymer in a dense bath of Active Brownian Particles: Insights from Computer Simulations

#### Ramanand Singh Yadav (IIT Bombay)

#### Abstract of the Poster Presentation

Using computer simulations, we explore how the structure and dynamics of a star polymer, made of passive monomers immersed in a bath of Active Brownian Particles (ABP), change as a function of activity and area fraction. We also investigate how the Motility-Induced Phase Separation (MIPS) gets affected by the presence of this passive star polymer. References: [1] 1. S. Mahdiyeh Mousavi, Gerhard Gompper, and Roland G. Winkler, "Active induced localization and collapse of passive semiflexible polymers", J. Chem. Phys. 155, 044902 (2021). [2] 2. Subhasish Chaki and Rajarshi Chakrabarti, "Enhanced diffusion, swelling, and slow reconfiguration of a single chain in non-Gaussian active bath", J. Chem. Phys. 150, 094902 (2019).

#### Chemotactic response to spatio-temporal variation in attractant environment.

#### Ramesh Pramanik (SNBNCBS, Kolkata)

#### Abstract of the Poster Presentation

Chemotaxis is a property in which a cell migrates in response to the external chemical environment. An Escherichia Coli responds to its environment by performing a run-tumble motion. In our work, we are interested in how the chemotactic response of the cell is affected by spatiotemporal variation of the extracellular chemical environment. In particular, we consider an attractant profile, where the spatial gradient varies periodically in time with time period T. Our numerical simulations show that the chemotactic response of the cell varies non-monotonically with T. For  $T \rightarrow 0$  and  $T \rightarrow \infty$  the response in similar but at an intermediate T, it shows a minimum. We explain this interesting observation from an interplay between sensing and adaptation modules of intracellular signaling network.

#### Slow cooling in frustrated Ising models

**Reshmi Roy** (University of Calcutta)

Abstract of the Poster Presentation

We have studied slow cooling in the Axial Next Nearest Neighbour Ising (ANNNI) model with competing antiferromagnetic second neighbour interaction in one and two dimensions. The one dimensional ANNNI model is described by the Hamiltonian

$$H = -J_1 \sum_{i} S_i S_{i+1} + J_2 \sum_{i} S_i S_{i+2}.$$

The ground state is ferromagnetic for  $\kappa = J_2/J_1 < 0.5$ ; antiphase for  $\kappa = J_2/J_1 > 0.5$  and highly frustrated for  $J_2/J_1 = 0.5$ . All configurations having domains of size  $\geq 2$  are ground states at  $\kappa = 0.5$  which is the fully frustrated point. Zero temperature quenching using single spin-flip dynamics in the ANNNI model cannot bring the system to its ground state for a certain range of the frustration parameter  $\kappa(0 < \kappa < 1)$ . The cooling protocol used is  $T = T_0(1 - \frac{t}{\tau})$ . The results strongly depend on  $\kappa$ . In one dimension, the residual energy is found to vary as  $\left[\frac{\tau}{T_0}/\ln\frac{\tau}{T_0}\right]^{-\alpha}$  where  $\alpha$  is a non-monotonic function of  $\kappa$ . We also determine the scaling behaviour of the residual energy with time which shows a good agreement with the analytical result. In two dimensions, the results are more complex with piecewise stretched exponential behaviour.

# Exactly solvable model of a passive Brownian heat engine and its comparison with Active engines

#### Rita Majumdar (IIT Delhi)

#### Abstract of the Poster Presentation

We perform an extensive analysis of passive as well as active micro-heat engines with different single-particle stochastic models. Using stochastic thermodynamics we calculate thermodynamic work, heat, entropy production and efficiency of passive and active Brownian heat engines analytically as well as numerically and compare them. We run the heat engines with a protocol for which the average thermodynamic quantities are calculated exactly for an arbitrary cycle time. We also discuss about the group of protocols for which exact non-quasistatic calculations can be done, completely in the passive engine case and partially in the active engines. We obtain detailed thermodynamics of non-quasistatic (i.e. powerful) single-particle micro heat engines. The quasistatic (i.e. zero power) limit of the results is obtained by taking long (infinite) cycle time. We also study the distributions of position of the confined particle in both passive and active engines. We compare their characteristics in terms of the parameter that measures the competition between the active persistence in the particle position (due to active noises) and the harmonic confinement. We also calculate excess kurtosis that measures the non-Gaussianity of these distributions. Our analysis shows that efficiency of such thermal machine can be enhanced or reduced depending on the activity present in the model.

#### Activity driven energy transport in harmonic chains

#### Ritwick Sarkar (SNBNCBS, Kolkata)

#### Abstract of the Poster Presentation

We study the stationary state of a chain of harmonic oscillators driven by active reservoirs at the boundaries. These reservoirs exert correlated stochastic forces on the boundary oscillators, which leads to a nonequilibrium stationary state (NESS) characterized by a nonzero energy current flowing through the system. We considered the three most well-known dynamics for active driving, namely, the active Ornstein-Uhlenbeck process (AOUP), run-and-tumble process (RTP), and active Brownian process (ABP). The above-mentioned active forces have exponentially decaying two-point temporal correlations with different higher-order fluctuations. We find that irrespective of the specific dynamics of the driving, the velocity fluctuation at the bulk remains Gaussian with a flat kinetic temperature profile. In the thermodynamic limit, an "equipartition of energy" emerges in the bulk of the system— the value of the kinetic and potential temperature are equal, irrespective of the specific driving. We also calculate the distribution of the instantaneous energy current in the stationary state. In the bulk, this distribution shows a logarithmic divergence near the origin and asymmetric exponential tail. The signatures of the specific dynamics of driving become visible near the boundary. For RTP and ABP-driven chains, the boundary velocity distributions become non-Gaussian along with a finite cutoff in the boundary current distribution.

#### References

[1] Stationary states of activity-driven harmonic chains, Ritwick Sarkar, Ion Santra, and Urna Basu, Phys. Rev. E 107, 014123 –Published 17 January 2023.

[2] Activity driven transport in harmonic chains, Ion Santra, Urna Basu, SciPost Phys. 13, 041 (2022) – Published 30 August 2022.

# On the origin of universal cell shape variability in confluent epithelial monolayers

#### Souvik Sadhukhan (TIFR-Hyderabad)

#### Abstract of the Poster Presentation

Why do cells change their shapes during development and disease? Cell shape can influence crucial biological functions and control organ shape. However, the cell-to-cell shape varies in a tissue. Recent works show that shape variability in different epithelial monolayers follows a nearly universal distribution. What is the origin of this universality, and how is it related to the physical variables? In my poster, I will discuss a mean-field analytical theory for cell shape characterized via aspect ratio (AR). We find that a single parameter,  $\alpha$  (alpha), containing all the system-specific details, describes the probability distribution function (PDF) of AR: this leads to a universal relation between the standard deviation and the average of AR. The PDF for the scaled AR is not strictly but nearly universal. The functional form is a direct consequence of a mathematical property. The theory is verified in simulations of two distinct models of epithelial monolayers and agrees well with existing experiments. Our results imply that cell shape variability is inevitable, where a single parameter describes both statics and dynamics and provides a framework to analyze and compare diverse epithelial systems. I will also discuss some implications of our results.

#### Activity driven by chemical environment

#### Subhashree Subhrasmita Khuntia (IISER, Mohali)

Abstract of the Poster Presentation

Active matter, comprises systems that are out of equilibrium driven at individual scale by their internal energy or their local environment. Auto-chemotaxis represent one such active process where each individual modifies the chemical field in their locality and this further drives the collective motion of the system. We studied the trajectory of a single particle where the dynamics is governed by its chemical environment and vice versa. The phase diagram in the deposition and the evaporation rate of the chemical shows a structural transition from an extended coil state to a collapsed globule state. We developed a mean field theory following Keller-Segel model for chemotaxis and this shows good agreement with the simulation results. Further we incorporate many particles in our system and observe emergent phenomena evolving from the indirect interaction among them via their local chemical environment.

# Transmembrane pores induced by NK-2,an antimicrobial peptide: Effect of cholesterol

#### Surajit Das (Jadavpur University)

#### Abstract of the Poster Presentation

Biological membranes are complex structures composed of lipids, proteins, and other molecules, which makes them difficult to study in their native state. Therefore, it is often to study the artificial lipid bilayer as bio-mimetic system in order to gain insights into the structure and functions of the biological membrane. Antimicrobial peptides (AMPs) are group of peptides which are part of innate immune response in all animal and human body against invading pathogens, like viruses, fungi, bacteria, etc. The antimicrobial peptide, such as NK-2 target the bacterial membrane, especially negatively charged surface and create defects, such as pores, leading to disruption of the membrane. In this work the interaction between antimicrobial peptide and phospholipid membrane were investigated in terms of lipid head group variation and role of cholesterol as well as peptide composition. We prepare large unilamellar vesicles and giant unilamellar vesicles, composed of anionic lipid DOPG and zwitterionic lipid DOPC for different cholesterol concentration. Electrostatics of anionic membranes containing cholesterol in the presence of NK-2 has systematically been investigated using dynamic light scattering and zeta potential and also observed the morphological change in lipid vesicle by using phase contrast microscope.

#### Directional synchrony among spatially interacting self-propelled particles

Suvam Pal (Indian Statistical Institute, Kolkata)

Abstract of the Poster Presentation

The study of synchrony among spatially interacting self-propelled particles is one of the interesting research fields at the present time. In the last few decades, the study on collective behaviour of self-propelled particles were studied from the view point of statistical physics perspective. Here, we propose a spatially interacting model of self-propelled particles which are moving on a bounded two-dimensional plane and their angular dynamics obeys Kuramoto like coupling. The particles are constrained to move under periodic boundary condition and minimum image convention. We consider noise in the Kuramoto network which physically signify the temperature fluctuation. A continuous phase transition of macroscopic order parameter with respect to the thermal noise intensity is observed. The effective coupling strength of the Kuramoto network has a dependency on the spatial distance in the form of polynomial or power law types. In both cases, we analytically derive the critical value of noise intensity for directional synchrony and which has excellent agreement with the numerical results. Finally, we briefly explore the finite size scaling analysis and build up the relations between the critical exponents for different macroscopic observables.

#### Heat transport in a glassy liquid and its consequences

Vinay Vaibhav (The Institute of Mathematical Sciences, Chennai)

Abstract of the Poster Presentation

A thermal gradient applied to a liquid mixture initiates transport processes resulting in a spatially non-uniform density and concentration profiles, in the steady state. Using extensive computer simulations, we study the response of a glassy mixture exposed to a thermal gradient, while we change the ambient temperature and quantify the extent of spatial heterogeneities that develop, both in the liquid and glassy regime. Subsequently, we study the shear response of such thermally processed glassy samples, over a range of shear-rates. We observe the emergence of non-equilibrium steady states depends upon the thermal processing. Consequently, that affects the formation of shear-bands in the transient regime.