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**Carine Beatrici** (FIOCRUZ, Brazil) / **Hugues Chaté** (CEA – Saclay, France) / **Ronald Dickman** (DF-UFMG, Brazil)

## Invited Talks

### **Francesco Ginelli**

University of Aberdeen, UK

#### *Giant number fluctuations and structure in a flocking epithelium*

Epithelial cells cultured in a monolayer are very motile in isolation but reach a near-jammed state when mitotic division increases their number above a critical threshold. It was recently shown that a monolayer can be reawakened by over-expression of a single protein, RAB5A. This reawakening leads to large-scale collective migratory patterns, displaying long-range polar order.

We find that the flocking monolayer is characterized by a fluidization at the single cell level and by non-equilibrium anomalous number fluctuations at a larger length scale. Also with the help of numerical simulations, we trace back the origin of these fluctuations to the self-propelled active nature of the constituents and to the existence of a local alignment mechanism, leading to the spontaneous breaking of the orientational symmetry.

### **Igor Aranson**

Penn State University, USA

#### *Topological defects in a living nematic capture swimming bacteria*

Active matter exemplified by suspensions of motile bacteria or synthetic self-propelled particles exhibits a remarkable propensity to self-organization and collective motion. The local input of energy and simple particle interactions often lead to complex emergent behavior manifested by formation of macroscopic vortices and coherent structures with long-range order. A realization of an active system has been conceived by combining swimming bacteria and a nematic liquid crystal [1]. Here, by coupling the well-established and validated model of nematic liquid crystals with the bacterial dynamics we developed a computational model describing intricate properties of such a living nematic.

We take advantage of the fact that descriptions for both constituents, suspending a liquid crystal and the suspended bacteria in isotropic liquids, are well established and validated by experiments and simulations. In faithful agreement with the experiment, the model reproduces the onset of periodic undulation of the nematic director and consequent proliferation of topological defects with the increase in bacterial concentration. It yields testable prediction on the accumulation of bacteria in the cores of  $+1/2$  topological defects and depletion of bacteria in the cores of  $-1/2$  defects. Our new experiment on motile bacteria suspended in a free-standing liquid crystalline film fully confirmed this prediction [2].

[1] S. Zhou, A. Sokolov, O. D. Lavrentovich, and I. S. Aranson, Living Liquid Crystals, Proc. Natl. Acad. Sci. U.S.A. 111, 1265 (2014).

[2] M. M. Genkin, A. Sokolov, O. D. Lavrentovich, and I. S. Aranson, Topological Defects in a Living Nematic Ensnare Swimming Bacteria, Phys. Rev. X 7, 011029 (2017)



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**José S. Andrade Jr.**

Universidade Federal do Ceará,  
Fortaleza, Ceará, Brazil

*Keep-Left Behavior Induced by Asymmetrically Profiled Walls*

We show, computationally and analytically, that asymmetrically shaped walls can organize the flow of pedestrians driven in opposite directions through a corridor. Precisely, a two-lane ordered state emerges in which people always walk on the left-hand side (or right-hand side), controlled by the system's parameters. This effect depends on features of the channel geometry, such as the asymmetry of the profile and the channel width, as well as on the density and the drift velocity of pedestrians, and the intensity of noise. We investigate in detail the influence of these parameters on the flow and discover a crossover between ordered and disordered states. Our results show that an ordered state only appears within a limited range of drift velocities. Moreover, increasing noise may suppress such flow organization, but the flow is always sustained. Besides pedestrian flow, this new phenomenon has other potential applications in microfluidics systems.

**Masaki Sano**

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*Rosette and Comet: Possible Roles of Topological Defects in Biological Active Matter*

Self-motility is an important character of living matter. Ranging from filamentous bacteria to mobile cells, ensembles of self-propelled particles generate highly non-trivial collective behaviors. In such dynamical collective behaviors, order and disorder can be well characterized by using polar or nematic order parameters and the concept of topological defects. Recently, we found nematic order in the culture of neural stem cells (NSC) in which cells are elongated and align without head-tail polarity. Cells persistently move along the elongated axes, but change their directions of motion probabilistically. Domains of nematic order are interspersed by  $+1/2$  and  $-1/2$  topological defects. We found that cells are not differentiated and accumulate at  $+1/2$  defect (comet type structure) while escape from  $-1/2$  defects. These phenomena of accumulation and escape were described by a generic mechanism by the interplay between active force and anisotropic frictions of the cells [1]. Similar mechanism was found in the tissue culture of epithelial cells in which cell density controlled by extrusion and death at  $+1/2$  defects [2]. Other type of topological defect is known as rosette structure appearing in ESC derived neuroectodermal culture or neural tube like structures. In rosette structures, NSCs are polarized due to localization of cell adhesive molecules and form  $+1$  topological defect. Rosette has been also observed in neurosphere cultured in weakly adhesive environment. In the talk, I will discuss on the possible roles of topological defects in biological active matter.



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## References

- [1] K. Kawaguchi, R. Kageyama, and M. Sano, “Topological defects control collective dynamics in neural progenitor cell cultures”, Nature 544 (2017) in press.
- [2] T.B. Saw et al., “Topological defects in epithelia govern cell death and extrusion”, Nature 544, 212–216 (2017).

## Ramin Golestanian

University of Oxford, UK

### *Enhanced diffusion of catalytically active enzymes*

In the last few years a number of groups have reported measuring enhanced diffusion of enzymes by about 10-20 percent - when they are catalytically active - with a diffusion coefficient that follows the Michaelis-Menten curve of the catalysis itself. I will present the story of how various attempts failed to unravel the (dominant) governing mechanism behind this phenomenon, and present a mechanism that seems to be able to capture all the features of the observations reported so far.

## Silke Henkes

University of Aberdeen, UK

### *Dynamical patterns in active nematics on a sphere*

Using agent-based simulations of self-propelled particles subject to short-range repulsion and nematic alignment we explore the dynamical phases of a dense active material confined to the surface of a sphere. We map the dynamical phase diagram as a function of curvature, alignment strength and activity and reproduce phases seen in recent experiments on active microtubules moving on the surfaces of vesicles. At low driving, we recover the equilibrium nematic ground state with four  $+1/2$  defects. As the driving is increased, geodesic forces drive the transition to a band of polar matter wrapping around an equator, with large bald spots corresponding to two  $+1$  defects at the poles. Finally, bands fold onto themselves, followed by the system moving into a turbulent state marked by active proliferation of pairs of topological defects. We highlight the role of nematic persistence length and time for pattern formation in these confined systems with finite curvature.

## Xiaqing Shi

Center for soft condensed matter physics and interdisciplinary research, Soochow University

### *From MIPS to Vicsek: A comprehensive phase diagram for self-propelled rods*



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Self-propelled rods interacting by volume exclusion is one of the simplest active matter systems. Despite years of effort, no comprehensive picture of their phase diagram is available. Furthermore, results on explicit rods are so far largely disconnected from those obtained on the relatively better understood cases of motility induced phase separation (MIPS) of (usually) isotropic active particles, and from our current knowledge of Vicsek-style aligning point particles. In this talk, I will present a complete phase diagram of a generic model of self-propelled rods and show how it is connected to both MIPS and Vicsek worlds.

**Hugues Chaté**<sup>1,2</sup>

<sup>1</sup> Service de Physique de l'Etat Condensé, CEA, CNRS, Université Paris-Saclay,

<sup>2</sup> Beijing Computational Science Research Center, Beijing, China

*Weak synchronization and large-scale collective oscillation in dense bacterial suspensions*

Collective oscillatory behavior is ubiquitous in nature and it plays a vital role in many biological processes, including embryogenesis, organ development, and pace-making in neuron networks or in cardiac tissues. Elucidating the mechanisms that give rise to collective oscillations is essential to the understanding of biological self-organization. In this talk, I report the discovery of striking very large-scale collective oscillations in a quasi- two- dimensional dense suspensions of swimming E coli bacteria. This system was studied before but the phenomenon we observed was overlooked due to its elusive nature: individual trajectories and movies do not show the weak synchronization of cell trajectories. But passive particles floating on the surface or mesoscale averaging of the cell's velocities reveal regular oscillatory behavior organized over centimeter scales. I will then present a self-propelled particle model which demonstrates that this spectacular phenomenon can arise without long-range interactions. These findings expand our knowledge of biological self-organization as well as reveal a new type of long-range order in active matter systems.

**Short Talks**



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**Ronald Dickman and M.L.L. Iannini**

Departamento de Física and

National Institute of Science and Technology for Complex Systems,

Universidade Federal de Minas Gerais

*Traffic model with an absorbing-state phase transition*

We consider a modified Nagel-Schreckenberg (NS) model in which drivers do not decelerate if their speed is smaller than the headway (number of empty sites to the car ahead). (In the original NS model, such a reduction in speed occurs with probability  $p$ , independent of the headway, as long as the current speed is greater than zero.) In the modified model the free-flow state (with all vehicles traveling at the maximum speed,  $v_{max}$ ) is *absorbing* for densities  $\rho$  smaller than a critical value  $\rho_c = 1/(v_{max} + 2)$ . The phase diagram in the  $\rho - p$  plane is reentrant: for densities in the range  $\rho_{c, <} < \rho < \rho_c$ , both small and large values of  $p$  favor free flow, while for intermediate values, a nonzero fraction of vehicles have speeds  $< v_{max}$ . In addition to representing a more realistic description of driving behavior, this change leads to a better understanding of the phase transition in the original model. Our results suggest an unexpected connection between traffic models and stochastic sandpiles.

**Carine P. Beatrici**,<sup>1,2</sup> Rita M. C. de Almeida,<sup>1,3</sup> and Leonardo G. Brunnet<sup>1</sup>

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<sup>3</sup> Instituto Nacional de Ciência e Tecnologia - Sistemas Complexos

*Mean cluster approach and Active Matter Simulations indicate cell sorting time scales are determined by collective dynamics*

Cell migration is essential to cell segregation, playing a central role in tissue formation, wound healing, and tumor evolution. Considering random mixtures of two cell types, it is still not clear which cell characteristics define clustering time scales. The mass of diffusing clusters merging with one another is expected to grow as  $t^{d/d+2}$  when the diffusion constant scales with the inverse of the cluster mass. Cell segregation experiments deviate from that behavior. Explanations for that could arise from specific microscopic mechanisms or from collective effects, typical of active matter. Here we consider a power law connecting diffusion constant and cluster mass to propose an analytic approach to model cell segregation where we explicitly take in to account



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finite size corrections. The results are compared with active matter model simulations and experiments available in the literature. To investigate the role played by different mechanisms we considered different hypotheses describing cell-cell interaction: differential adhesion hypothesis (DAH) and different velocities hypothesis (DVH). We find that the simulations yield normal diffusion for long time intervals. Analytic and simulation results show that i) cluster evolution clearly tends to a scaling regime, disrupted only at finite size limits; ii) cluster diffusion is greatly enhanced by cell collective behavior, such that for high enough tendency to follow the neighbors, cluster diffusion may become independent of cluster size; iii) the scaling exponent for cluster growth depends only on the mass-diffusion relation, not on the detailed local segregation mechanism. These results apply for active matter systems in general and, in particular, the mechanisms found underlying the increase in cell sorting speed certainly have deep implications in biological evolution as a selection mechanism.

**Carine P. Beatrici**<sup>1,2</sup> and Hugues Chaté<sup>3,4</sup>

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<sup>4</sup> Beijing Computational Science Research Center, Beijing, China

### *Active Clock Model*

We study a Vicsek-style active clock model in two space dimensions: constant speed point particles locally align their velocities onto a discrete set of  $q$  equi-spaced angles. This model interpolates between the active Ising model (AIM) studied by Solon & Tailleur ( $q=2$ ) and the classic Vicsek model (VM) ( $q=\infty$ ). In both limits, the ordered, collectively moving phase is known to exhibit very different properties: whereas the transition to collective motion is best described as a phase-separation scenario in both models, in the VM the coexistence phase consists of a smectic arrangement of traveling bands (micro-phase separation), while in the AIM normal phase separation occurs. Moreover, the ordered liquid phase of the VM is characterized by the long-range correlations and anomalous (“giant”) number fluctuations predicted by Toner and Tu, while the AIM has short-range correlations and normal fluctuations. Microphase separation and giant number fluctuations thus seem linked together. Our clock model aims at understanding better the connection between these two properties.



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We will present and discuss the results obtained so far: up to  $q=6$ , we find normal phase separation, while multi-band solutions are seen for  $q>6$ . Number fluctuations are normal for  $q=4,5,6$ , but only after a crossover scale that increases with  $q$ . For  $q>6$ , we are currently unable to decide whether number fluctuations are anomalous at all scales or whether this crossover scale is larger than the scales explored so far numerically.

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### *Diffusion on surfaces: from theory to experiments and back*

Diffusion is ubiquitous. It permeates physics, chemistry, biology, even sociology and economics. In physics, it has been associated to famous names like Maxwell, Einstein and Boltzmann, among others. Over the past decade, great theoretical attention has been given to the possibility, as in general relativity, that the curvature of the environment could change a particle diffusing behavior [1,2]. For instance, it was found that the root mean square displacement, which behaves linearly with time for the classical diffusion phenomena in flat space, may have nonlinear corrections if the diffusion occurs on a curved surface [1]. Very recently, these theoretical predictions were put to test experimentally for nanoparticles diffusing on a *spherically* curved oil/water interface by Zhong et al. [3]. However, for some small radii of the spherical water-oil interface, where the theoretical predictions for diffusion on curved surfaces would manifest, an unexpected behavior was observed for the root mean square displacement that requires further theoretical investigation. In this work, we argue that thermal fluctuations allow the spherical particles to diffuse in the interface's normal direction, so that we have three-dimensional diffusion within the annular space between two concentric spheres with radii  $r$  and  $r + \varepsilon$ , respectively, where  $\varepsilon$  is of the same order of magnitude of the diameter of the diffusing particle. Moreover, the compatibility between the measured and the predicted diffusion coefficient is achieved when we estimate the *projected* geodesic displacement on the spherical droplet. Without this, the standard result for three-dimensional diffusion emerges. By doing so, we successfully explain theoretically the recent unexpected experimental results found by Zhong et al. [3] Since purely two-dimensional surfaces are practically unachievable in classical experiments, this behavior may emerge in a large class of experiments performed in quasi two-dimensional curved systems, i.e., surfaces with thickness.

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[2] N. Ogawa, *Curvature-dependent diffusion flow on a surface with thickness*, Phys. Rev. E **81**, 061113 (2010).



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[3] Y. Zhong, L. Zhao, P. Tyrlik, and G. Wang, *Investigating Diffusing on Highly Curved Water-Oil Interface Using Three-Dimensional Single Particle Tracking*, J. Phys. Chem C 121 (14) 8023 (2017)

**Tiago Venzel Rosenbach** and Ronald Dickman

Departamento de Física

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*Migration of MDCK cells in culture: A quantitative characterization*

The study of active matter has attracted great interest in the present time. In particular, the so-called "living active" matter has been widely studied because of the patterns and/or interactions that are responsible for guiding and coordinating various processes, such as wound healing, tumor formation and aggregation of bacteria/cells, among others. All these efforts are aimed at understanding such emerging and self-organized phenomena that can be used in the prevention and combat of various pathologies, in the development of new materials or processes of energy production and transport of matter. The present research project aimed to quantitatively characterize the collective migration of in vitro MDCK cells. It was divided into two work fronts: the first consisted of producing and studying samples of MDCK cells cultured at various densities. The second work front was to simulate some theoretical models, such as that proposed by Vicsek et al. and some of its variations, to understand part of the results obtained experimentally. From this work was possible to show that MDCK cells in culture can exhibit an anomalous motility, leading to a diffusion regime that undergoes subdiffusive and superdiffusive stages and that in some cases, inter changed between them more than once. Furthermore, we can observe that in some densities the cell velocities only correlate to small distances, since they tend to form agglomerates with few cells, mostly two cells. From simple models it was possible to obtain some results similar to the experimental ones. For example, q-Weibull speed distributions, with velocity correlations only between close neighbors were generated.

**Paulo Casagrande Godolphim** and Leonardo Gregory Brunnet

Instituto de Física – UFRGS

*Cell propagation modes in non-periodic boundary conditions wound healing simulation*

Efficient wound healing is an evolutive advantage acquired over millions and millions of years of mutations and natural selection. This mechanism is important not only for its obvious biological role, but also for the knowledge that its study can offer about tissue growing, collective cell migration and the cell-to-cell feedback process, tumor growth, dynamics and transport of information in systems far from equilibrium and also as a story teller of the evolutive past of living beings. The wound healing assay - which usually consists in creating a model wound by the removal of cells rows from a monolayer and analyzing the subsequent cellular movement - is largely used to study cicatrization in in vitro and in vivo experiments. As consequence





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of recent advance in computing science together with the emergence of physical and mathematical models applied to biological dynamics, there has been a forthcoming possibility of studying this subject through in silico simulations. Besides introducing a new approach to already known problems, this numerical simulations allow significant savings of time and resources. Two of the most applied numerical models to characterize collective movement are: the Potts model - similar to Monte Carlo model - and the Self Propelled Particles (SPP) model - where complex collective behaviour is verified only within simple local interactions. Hence in this work we used a SPP model in which the particles were subjected to different geometrical constraints to approach a recent theme and not yet fully understood: how different boundary conditions can affect collective cell migration movements? Our motivation came from Vedula's work from 2011 where in a wound healing experiment was shown that sheets of migrating cells, confined to different geometries, present different emergent behaviour modes and that the cell-to-cell interaction has a fundamental role on the cohesion of these migration behaviours. Therefore we developed a program with aperiodic contour conditions of the rigid wall type to reproduce an in silico version of Vedula's experiment. For that we stocked cells in a reservoir and then released them in tracks with different widths. As a result we found that not just the track width, but also the shape of the reservoir can define the emergence of different migration patterns, as to those found experimentally in vitro. This detail was not mentioned in the experimental result, but resulted to be important in the simulations. Hence we concluded that the shape and size of the reservoir are fundamental aspects to be analyzed in future experiments of this nature.

**Cássio Kirch** , Carolina Brito, Carine Beatrici and Leonardo Gregory Brunnet

Instituto de Física – UFRGS

### *Extended Active Matter Cell Model*

Biological phenomena like cell segregation and wound healing involve cell movement inside tissues. Unlike granular media cell tissue presents no empty spaces of the size of a cell. Under these conditions a cell has to change its form to be able to change its position in a tissue. Up to now active matter models for cells have used single particle models to simulate, for example, cell sorting dynamics with success, but they are unable to differentiate the roles of cell adhesion and cell cortex tension in such a process. We propose an active matter model where a central particle connected to other surrounding particles represent a single tissue cell. In this work we explore the possible physical states of a set of such cells when interacting with each other by means of simple short range forces.